Supporting information

An interrupted Heyns rearrangement approach to regioselective synthesis of acylindoles

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Contents

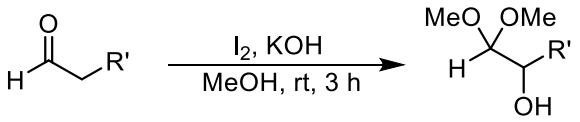
1. General Comments:

All reactions were carried out under atmospheric pressure using reaction tubes. Column chromatography was performed using Rankem Silica gel (100-200 mesh) and the solvent system used unless otherwise specified, was ethyl acetate-hexane with various percentage of polarity depending on the nature of the substrate. All chemicals and acids were purchased from either AVRA chemicals or Spectrochem and used as received. *α*-Amino carbonyl derivatives **2** were synthesized employing the literature procedure.[1]

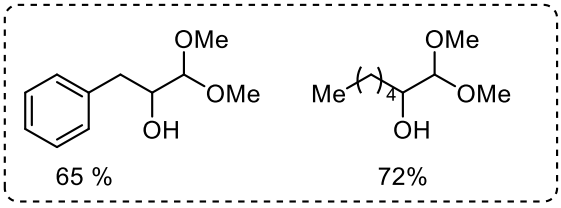
NMR data were recorded on a Bruker (400 MHz and 500 MHz) spectrometer. ^{1}H and ^{13}C NMR spectra were referenced to signals of deutero solvents and residual protiated solvents, respectively. Infrared spectra were recorded on a Thermo Nicolet iS10 FT and Jasco ATR-IR spectrometer. HRMS were recorded by electrospray ionization (ESI) method on a Q-TOF Micro with lock spray source. The crystal data was collected and integrated using a BrukerAxs kappa apex2 CCD diffractometer, with graphite monochromated Mo-Kα radiation.

3. Synthesis of *α*-hydroxy dimethoxy acetal:

Approach 1:

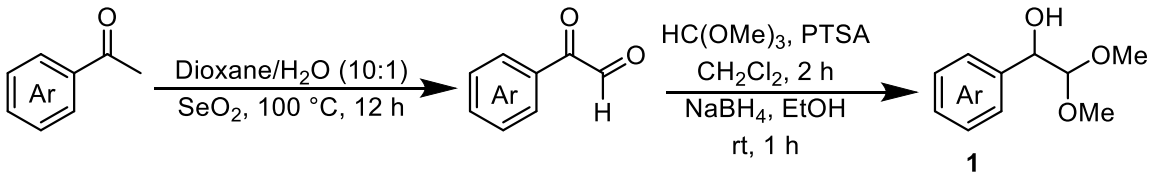


A solution of KOH (2.0 g, 35.82 mmol, 2.4 equiv) in 15 mL of MeOH was cooled to 0-5 ℃. Then, the corresponding ketone (14.92 mmol, 1 equiv) was added dropwise. The reaction mixture was stirred for 10 minutes, then I_2 (4.1 g, 16.41 mmol, 1.1 equiv) in MeOH (10 mL) was slowly added to the reaction mixture and stirred for 3 h at the same temperature. After completion of the reaction, it was quenched with saturated solution of $Na_2S_2O_3$ and extracted with EtOAc. The combined organic layer was dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude product was suitable for further use or can be purified by column chromatography. Below derivatives were synthesized using this approach in one step from aliphatic aldehydes. *α*-Hydroxy dimethoxy acetal derivatives **1** were also synthesized from the corresponding phenyl acetaldehydes in one step. [3]



Approach 2: [4–6]

Few of the *α*-hydroxy dimethoxy acetal derivatives were synthesized by following this alternative approach from acetophenone derivatives.



In an oven-dried 50 mL round bottom flask equipped with a reflux condenser, SeO_2 (2 g, 18.33 mmol, 1.1 equiv) was added followed by 10 mL of Dioxane/H_2O (10:1) was introduced. After refluxing the reaction mixture for 15 min at 100 ºC, the reaction mixture was cooled down to 50 ºC then the corresponding acetophenone derivative (16.66 mmol, 1 equiv) was added dropwise. Subsequently, the temperature was increased to 100 ºC and the stirring was continued at the same temperature for 12 h. Then the reaction mixture was cooled down to

room temperature and filtered through a silica-gel bed. The filtrate was dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was used for subsequent step without any further purification.

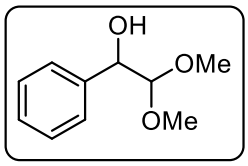
The resultant aryl glyoxal monohydrate (16.64 mmol, 1 equiv) was taken in a 100 mL round bottom flask and dissolved in 30 mL of DCM followed by PTSA (950 mg, 4.99 mmol, 0.3 equiv) and trimethylorthoformate (5.3 g, 49.92 mmol, 3 equiv) were added to the solution dropwise at room temperature. The stirring was continued at the same temperature for 2 h. After the reaction was complete, as indicated by TLC, stirring was stopped and was washed with water. The organic layer was then concentrated under reduced pressure to give *α,α*-dimethoxy methyl aryl ketone. The crude product was then subjected to the next step without further purification.

α,α-dimethoxymethyl aryl ketone (16.50 mmol, 1 equiv) was taken in a 100 mL round bottom flask and 30 mL of EtOH was added. The solution was cooled to 0 ºC and $NaBH_4$ (1.25 g, 33 mmol, 2 equiv) was added portion wise. The reaction was then allowed to warm to room temperature and stirring was continued for 1 h. After the completion of reaction, as indicated by TLC ($KMnO_4$ was used for product confirmation), it was quenched with the addition of saturated solution of NH_4Cl. The reaction mixture was extracted with DCM and then the organic layer was collected and dried over Na_2SO_4. The solvent was removed under reduced pressure and the crude residue was then further purified by column chromatography over silica-gel to afford the expected products in good over three steps.

3.1: Properties of synthesized compounds 1:

2,2-Dimethoxy-1-phenylethan-1-ol (1a)

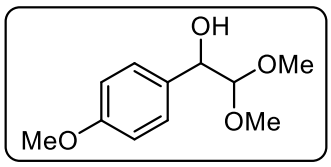
Yield: 64% (1.94 g); viscous liquid; R_f=0.3 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3445, 2899, 2831,



1452, 1194, 1061, 972, 755, 699. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.40 (d, J = 8.0 Hz, 2H), 7.34 (t, J = 7.6 Hz, 2H), 7.29 (d, J = 7.2 Hz, 1H), 4.60 (d, J = 6.4 Hz, 1H), 4.28 (d, J = 6.4 Hz, 1H), 3.45 (s, 3H), 3.40 (s, 1H), 3.24 (s, 3H).$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 139.5, 128.2, 127.9, 127.1, 107.6, 74.0, 55.9, 54.9.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{10}H_{14}O_3$+Na: 205.0841; found: 205.0831.

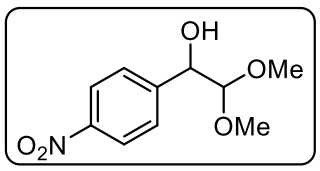
2,2-Dimethoxy-1-(4-methoxyphenyl)ethan-1-ol (1b)

Yield: 66% (2.33 g); viscous liquid; R_f= 0.2 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3461, 2943, 2832, 1609, 1510, 1245, 1028, 830, 755. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.32 (d, J = 8.6 Hz, 2H), 6.88 (d, J = 8.6 Hz, 2H), 4.55 (d, J = 6.4 Hz, 1H), 4.26 (d, J = 6.6 Hz, 1H), 3.79 (s, 3H), 3.46 (s, 3H), 3.25 (s, 3H), 2.74 (s, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 159.3, 131.6, 128.3, 113.7, 107.8, 73.6, 55.9, 55.2, 54.9.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{11}H_{16}O_4$+Na: 235.0946; found: 235.0938.



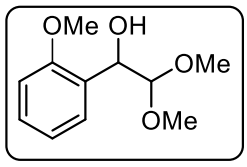
2,2-Dimethoxy-1-(4-nitrophenyl)ethan-1-ol (1c)

Yield: 50% (1.89 g); Solid; m.p. 65- 67 °C; R_f=0.2 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3422, 2943, 1602, 1518, 1343, 1073, 856, 754, 711. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.21 (d, J = 8.0 Hz, 2H), 7.61 (d, J = 8.0 Hz, 2H), 4.73 (d, J = 6.3 Hz, 1H), 4.25 (d, J = 6.3 Hz, 1H), 3.49 (s, 3H), 3.32 (s, 3H), 2.84 (s, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 147.7, 146.8, 128.0, 123.4, 107.2, 73.2, 56.5, 55.1.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{10}H_{13}NO_5$+Na: 250.0691; found: 239.0684.



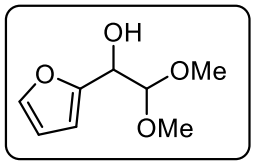
2,2-Dimethoxy-1-(2-methoxyphenyl)ethan-1-ol (1d)

Yield: 75% (2.64 g); viscous liquid; R_f=0.2 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3475, 2941, 1240, 1057, 974, 754. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.39 (d, J = 7.4 Hz, 1H), 7.28- 7.24 (m, 1H), 6.97 (t, J = 7.4 Hz, 1H), 6.88 (d, J = 8.2 Hz, 1H), 5.00 (s, 1H), 4.52 (d, J = 5.2 Hz, 1H), 3.84 (s, 3H), 3.40 (s, 3H), 3.32 (s, 3H), 2.94 (s, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 156.9, 128.9, 128.3, 127.9, 120.8, 110.6, 105.9, 70.0, 55.5, 55.2, 55.0.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{11}H_{16}O_4$+Na: 235.0946; found: 235.0947.



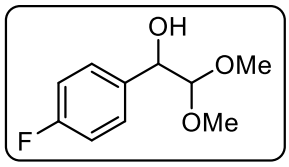
1-(Furan-2-yl)-2,2-dimethoxyethan-1-ol (1e):

Yield: 62% (1.77 g); viscous liquid; R_f=0.3 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3441, 2940, 2833, 1126, 1064, 970, 745. ^1H NMR (500 MHz, $CDCl_3$, 24 °C): δ 7.39 (d, J = 0.9 Hz, 1H), 6.35-6.34 (m, 2H), 4.65 (d, J = 6.3 Hz, 1H), 4.56 (dd, J = 6.3, 1.5 Hz, 1H), 3.47 (d, J = 1.8 Hz, 3H), 3.33 (d, J = 1.8 Hz, 3H), 2.74 (d, J = 1.2 Hz, 1H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, 24 °C): δ



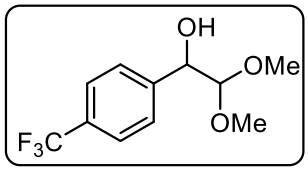
152.5,142.4, 110.4, 108.3, 105.2, 68.0, 55.5, 55.1.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_8H_{12}O_4$+Na: 195.0633; found: 195.0629.

1-(4-Fluorophenyl)-2,2-dimethoxyethan-1-ol(1f):



Yield: 52% (1.73 g); viscous liquid; R_f=0.3 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3453, 2941, 1509, 1221, 1065, 973, 835, 754. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.39- 7.35 (m, 2H), 7.02 (t, J = 8.7 Hz, 2H), 4.57 (d, J = 6.3 Hz, 1H), 4.22 (d, J = 6.5 Hz, 1H), 3.45 (s, 3H), 3.25 (s, 3H), 2.86 (s, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 163.7, 161.3, 135.3, 135.2, 128.8, 128.7, 115.2, 115.0, 107.7, 73.4, 56.1, 55.0.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{10}H_{13}FO_3$+Na: 223.0746; found: 223.0739.

2,2-Dimethoxy-1-(4-(trifluoromethyl)phenyl)ethan-1-ol (1g):

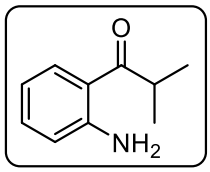


Yield: 65% (2.70 g); viscous liquid; R_f= 0.3 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3452, 2944, 1322, 1117, 1059, 974, 839, 756. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.60 (d, J = 8.2 Hz, 2H), 7.54 (d, J = 8.0 Hz, 2H), 4.67 (d, J = 6.2 Hz, 1H), 4.25 (d, J = 6.3 Hz, 1H), 3.47 (s, 3H), 3.29 (s, 3H), 2.91 (s, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 143.5, 127.5, 125.22, 125.18, 125.14, 125.11, 107.4, 73.4, 56.3, 55.0.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{11}H_{13}F_3O_3$+Na: 273.0714; found: 273.0704.

4: Properties of synthesized compounds 2:

1-(2-Aminophenyl)-2-methylpropan-1-one (2b):

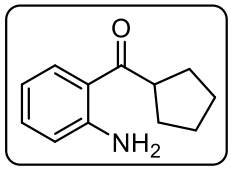
Yield: 85% (0.35 g); viscous liquid; R_f= 0.5 in 5% EtOAc; IR (ν_{max}, cm^{-1}): 3463, 3341, 2971,



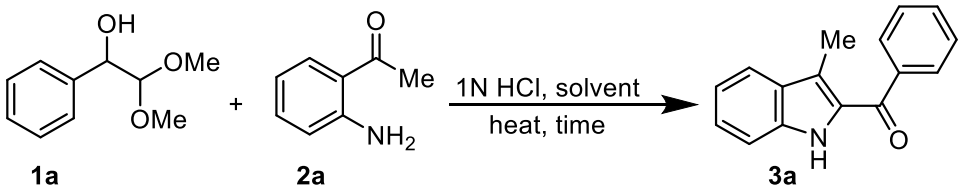
1640, 1578, 1217, 1153, 970, 748. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.76 (d, J = 8.1 Hz, 1H), 7.26-7.23 (m, 1H), 6.66- 6.63 (m, 2H), 6.27 (s,1.6 H), 3.59 (m, 1H), 1.20 (d, J = 6.7 Hz, 6H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 207.1, 151.0, 134.1, 131.1, 117.6, 117.0, 115.8, 35.3, 19.7.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{10}H_{13}NO$+Na: 186.0895; found: 186.0884.

(2-Aminophenyl)(cyclopentyl)methanone(2d):

Yield: 14% (68 mg); viscous liquid; R_f= 0.5 in 5% EtOAc; IR (ν_{max}, cm^{-1}): 3465, 3341, 2949, 1639, 1571, 1213, 1156, 748. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.77 (d, J = 8.1 Hz, 1H), 7.23 (t, J = 7.5Hz, 1H), 6.65- 6.62 (m, 2H), 6.27 (s, 2H), 3.74-3.66 (m, 1H), 1.92- 1.87 (m, 4H), 1.75- 1.60 (m, 4H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 205.5, 150.7, 133.9, 131.4, 117.8, 117.4, 115.7, 46.7, 30.4, 26.3.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{12}H_{15}NO$+Na: 212.1051; found: 212.1045.



Optimization: Synthesis of 3a from 1a and 2a

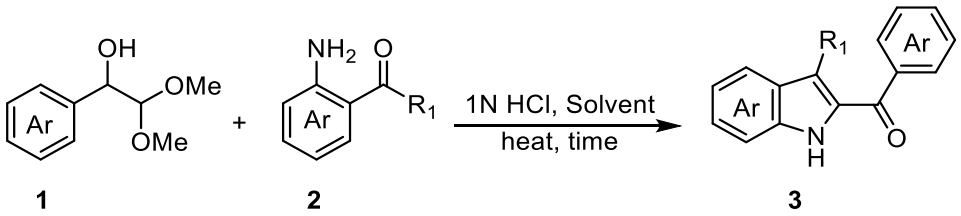


Entry	Acids (equiv)	Temp (°C)	Solvent	Yield (%)
1	-	rt	EtOH	-
2	AcOH (1)	rt	EtOH	-
3	PTSA (1)	rt	EtOH	-
4	1N HCl (2)	rt	EtOH	34
5	1N HCl (2)	60	EtOH	50
6	1N HCl (2)	80	EtOH	83
7	1N HCl (2)	90	EtOH	84
8	1N HCl (2)	90	Dioxane	90
9	1N HCl (2)	90	CH_3CN	87
10	**1N HCl** (2)	**100**	**Dioxane**	**94**
11	1N HCl (2)	120	Dioxane	93
12	Conc. HCl (2)	120	Toluene	65
13[a]	Conc. HCl (2)	120	Toluene	76
14[b]	Conc. HCl (2)	120	Toluene	79
15[c]	Conc. HCl (2)	120	Toluene	74
16	Conc. HCl (2)	90	Toluene	29

17	Conc. HCl (2)	130	DMF	57
18	H_2SO_4 (2)	80	EtOH	35
19	PTSA (1)	80	EtOH	60
20	Conc. HCl (2)	70	MeOH	36
21	1N HCl (2)	90	H_2O	66

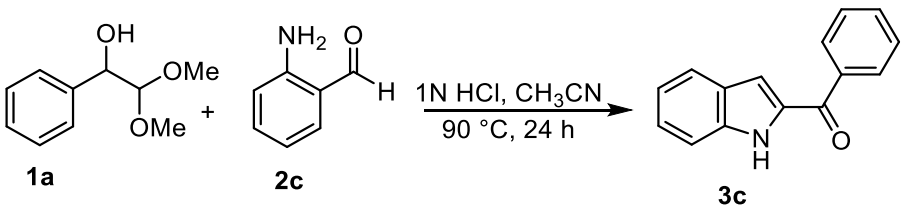
Reaction conditions: **1a** (0.23 mmol, 1 equiv), **2a** (0.23 mmol, 1 equiv), acid (equiv), solvent (3 mL for 0.23 mmol), temp, 18 h. Additive: [a] $BF_3.Et_2O$ (0.5 equiv), [b] $FeCl_3$ (0.5 equiv), [c] $ZnCl_2$ (0.5 equiv).

5. General procedure for synthesis of 2-acyl indole derivatives 3



In an oven dried 20 mL reaction tube, compound **1** (0.23 mmol, 1 equiv), and α-aminocarbonyl derivative **2** (0.23 mmol, 1 equiv) were taken in dioxane solvent (3 mL) and 0.5 mL of 1N HCl (2 equiv) was added. The reaction tube was sealed and kept in a pre-heated oil bath at 100 ºC and stirred at the same temperature for 18 h. After consumption of starting material as indicated by TLC, reaction mixture was cooled down to room temperature and extracted with DCM. The organic layer was dried over Na_2SO_4 and evaporated in rotary evaporator. The crude product was then further purified by column chromatography using ethyl acetate: hexane (1:9) as an eluting solvent to afford the 2-acylindole **3** in good to excellent yields.

5.1. Synthesis of compound 3c

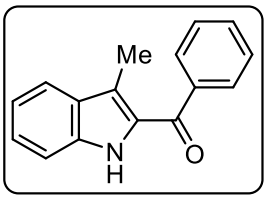


In an oven dried reaction tube, compound **2c** (50 mg, 0.41 mmol, 1 equiv) was taken in 3 mL of acetonitrile and **1a** (76 mg, 0.41 mmol, 1 equiv) was added. To the reaction mixture, 0.5 mL of 1N HCl (2 equiv) was added and the reaction tube was sealed and kept in a pre-heated oil bath at 90 ºC and was stirred for 24 h at the same temperature. After the reaction was completed, as indicated by TLC, it was cooled down to room temperature and extracted with DCM. The organic layer was then dried over Na_2SO_4 and evaporated under reduced pressure. The crude residue was then purified by column chromatography to afford the product **3c** in 72% (65 mg) yield.

5.2. Properties of synthesized 2-acyl indoles:

(3-Methyl-1H-indol-2-yl)(phenyl)methanone (3a):

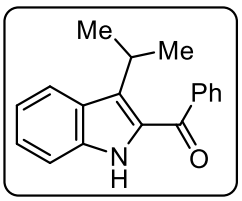
Yield: 87% (47 mg); White solid; m.p. 105-107 ºC; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}):



3311, 3054, 1607, 1435, 1266, 945, 742, 690. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.84 (s, 1H), 7.77 (d, J = 7.1 Hz, 2H), 7.68 (d, J = 8.2 Hz, 1H), 7.59 (t, J = 7.1 Hz, 1H), 7.51 (t, J = 7.6 Hz, 2H), 7.41-7.35 (m, 2H), 7.16 (t, J = 7.2 Hz, 1H), 2.27 (s, 3H).^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.5, 139.5, 136.7, 132.0, 131.7, 129.0, 128.9, 128.5, 126.6, 121.3, 120.6, 120.2, 112.0, 11.3.; HRMS (ESI/Q-TOF) m/z: [M + Na] $^+$ Calcd for $C_{16}H_{13}NO$+Na: 258.0895; found: 258.0877.

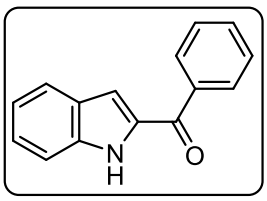
(3-Isopropyl-1H-indol-2-yl)(phenyl)methanone (3b):

Yield: 84% (51 mg); Solid; m.p. 75-77 ºC; R_f= 0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3335, 2969,



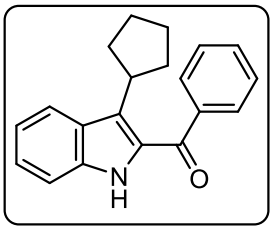
1618, 1524, 1322, 1256, 734, 702. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.91 (s, 1H), 7.92 (d, J = 8.8 Hz, 1H), 7.81 (d, J = 7.1 Hz, 2H), 7.60 (t, J = 7.1 Hz, 1H), 7.51 (t, J = 7.2 Hz, 2H), 7.41 (d, J = 8.2 Hz, 1H), 7.33 (t, J = 7.7 Hz, 1H), 7.13 (t, J = 8.0 Hz, 1H), 3.27 (m, 1H), 1.41 (d, J = 7.1 Hz, 6H).^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.9, 139.7, 137.3, 132.3, 131.0, 130.3, 128.9, 128.4, 126.5, 125.8, 123.5, 119.8, 112.4, 26.3, 23.0.; HRMS (ESI/Q-TOF) m/z: [M + Na] $^+$ Calcd for $C_{18}H_{17}NO$+Na: 286.1208; found: 286.1193

(1H-Indol-2-yl)(phenyl)methanone (3c):

Yield: 72% (65 mg); White Solid; m.p. 130-132 ºC; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 

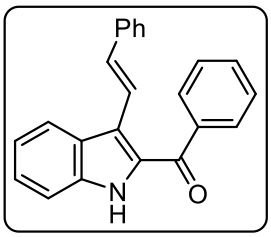
3313, 2920, 1619, 1516, 1261, 735, 684. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.47 (s, 1H), 8.00 (d, J = 7.8 Hz, 2H), 7.72 (d, J = 8.0 Hz, 1H), 7.63 (t, J = 7.5 Hz, 1H), 7.56- 7.48 (m, 3H), 7.38 (t, J = 7.8 Hz, 1H), 7.19-7.15 (m, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 187.3, 138.1, 137.6, 134.4, 132.4, 129.3, 128.6, 127.8, 126.6, 123.3, 121.1, 112.9, 112.3.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{11}NO$+Na: 244.0738; found: 244.0725.

(3-Cyclopentyl-1H-indol-2-yl)(phenyl)methanone (3d):

Yield: 86% (57 mg); Solid; Melting point; 105-107 ºC; R_f= 0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 

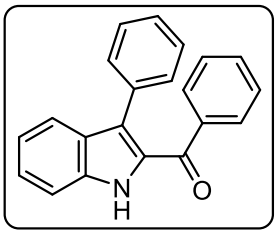
3330, 2950, 2868, 1613, 1523, 1324, 1252, 733, 695. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.72 (s, 1H), 7.80 (d, J = 7.8 Hz, 3H), 7.59 (t, J = 7.2 Hz, 1H), 7.50 (t, J = 7.7 Hz, 2H), 7.41 (d, J = 8.1 Hz, 1 H), 7.33 (t, J = 8.1 Hz, 1H), 7.10 (t, J = 7.9 Hz, 1H), 3.24-3.15 (m, 1 H), 2.08-1.99 (m, 2H), 1.91- 1.89 (m, 4H), 1.56-1.54 (m, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.9, 139.7, 137.3, 132.3, 131.4, 129.1, 128.8, 128.4,126.4, 125.9, 123.0, 119.8, 112.4, 37.5, 33.7, 26.8.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{19}NO$+Na: 312.1364; found: 312.1352.

(E)-Phenyl(3-styryl-1H-indol-2-yl)methanone (3e):

Yield: 71% (52 mg); Solid; m.p. 150-152 ºC; R_f=0.45 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3313, 

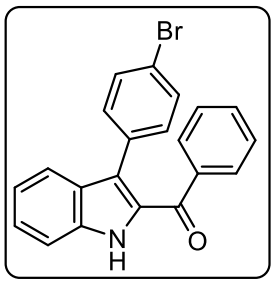
3056, 1611, 1501, 1330, 1252, 736, 695. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.22 (s, 1H), 8.11 (d, J = 8.3 Hz, 1H), 7.83 (d, J = 7.0 Hz, 2H), 7.60 (t, J = 7.5 Hz, 1H), 7.51- 7.38 (m, 4H), 7.28-7.24 (m, 3H), 7.22-7.08 (m, 5H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 188.9, 139.3, 137.7, 137.2, 132.3, 132.0, 131.2, 129.5, 128.7, 128.6, 127.6, 126.8, 126.2, 123.0, 121.9, 121.5, 112.4.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{23}H_{17}NO$+Na: 346.1208; found: 346.1188.

Phenyl(3-phenyl-1H-indol-2-yl)methanone (3f):

Yield: 96% (65 mg); Solid; m.p. 170-172 ºC; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3312, 

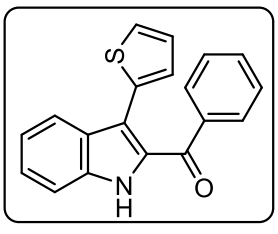
3057, 1610, 1333, 1262, 743, 685. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.33 (s, 1H), 7.65 (d, J = 8.3 Hz, 1H), 7.46 – 7.42 (m, 3H), 7.33 (t, J = 7.7 Hz, 1H), 7.20-7.16 (m, 1H), 7.12- 7.09 (m, 3H), 7.05- 7.04 (m, 3H), 6.99 (t, J = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.6, 137.5, 136.4, 133.7, 131.7, 130.8, 129.5, 127.9, 127.6, 127.5, 126.8, 126.6, 125.3, 122.1, 121.1, 112.0.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{15}NO$+Na: 320.1051; found: 320.1032

(3-(4-Bromophenyl)-1H-indol-2-yl)(phenyl)methanone (3g):

Yield: 96% (83 mg); Solid; m.p. 150-152 ºC; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3335, 

2927, 1630, 805, 729, 696. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.39 (s, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.52 (d, J = 6.8 Hz, 3H), 7.43 (t, J = 7.2 Hz, 1H), 7.35 (t, J = 7.6 Hz, 1H), 7.27 (d, J = 2.9 Hz, 1H), 7.21 (t, J = 7.2 Hz, 1H), 7.13 (t, J = 7.8 Hz, 2H). 7.06 (d, J = 8.2 Hz, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.4, 137.5, 136.4, 132.8, 132.4, 132.0, 131.2, 131.0, 129.5, 127.8, 127.5, 126.8, 123.9, 121.8, 121.5, 121.1, 112.2.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{14}BrNO$+H:376.0337; found: 376.0309

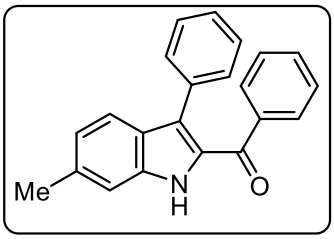
Phenyl(3-(thiophen-2-yl)-1H-indol-2-yl)methanone (3h):

Yield: 81% (57 mg); Solid; m.p. 135- 137 ºC; R_f= 0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3293, 

3054, 1617, 1323, 1250, 1000, 730, 655. ^{1}H NMR (500 MHz, $CDCl_3$, 24 °C): δ 9.57 (s, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.73-7.71 (m, 2H), 7.57 (dd, J = 8.3, 0.8 Hz, 1H), 7.48 (td, J = 8.2, 0.9 Hz, 1H), 7.44-7.40 (m, 1H), 7.32-7.24 (m, 4H), 6.87-6.85 (m, 1H), 6.83 (dd, J = 3.4, 1.1 Hz, 1H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 24 °C): δ 189.4, 137.7, 136.3, 134.6, 132.0, 131.6, 129.3, 128.9, 128.0, 127.8, 127.1, 126.8, 126.5, 122.3, 121.5, 117.2, 112.1; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{13}NOS$+Na: 326.0616; found: 326.0598.

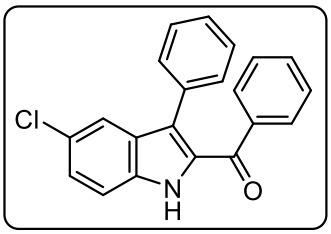
(6-Methyl-3-phenyl-1H-indol-2-yl)(phenyl)methanone (3i):

Yield: 84% (60 mg); Solid; m.p. 160-162 ºC; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3308, 2923, 1607, 1258, 734, 688. ^1H NMR (500 MHz, $CDCl_3$, 24 °C): δ 9.37 (s, 1H), 7.60 (d, J = 8.2 Hz, 1H), 7.52 (dd, J = 8.1, 1.1 Hz, 2H), 7.28 (s, 1H), 7.26-7.23 (m, 1H), 7.19-7.17 (m, 2H), 7.13-7.11 (m, 3H), 7.06 (t, J = 8.0 Hz, 2H), 7.02 (d, J = 8.0 Hz, 1H), 2.51 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, 24 °C): δ 189.5, 137.8, 137.1,137.0, 134.0, 131.6, 130.9, 130.6, 129.5, 127.9, 127.6, 126.8, 125.8, 125.7, 123.4, 121.9, 111.6, 22.1.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{17}NO$+H: 312.1388; found 312.1374.



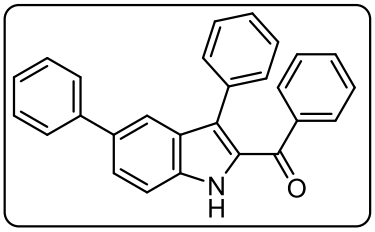
(5-Chloro-3-phenyl-1H-indol-2-yl)(phenyl)methanone (3j):

Yield: 93% (71 mg); Solid; m.p. 150-152 ºC; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3305, 2922, 1625, 1255, 798, 732, 692. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.47 (s, 1H), 7.68 (s, 1H), 7.51 (d, J = 7.6 Hz, 2H), 7.44 (d, J = 8.8 Hz, 1H), 7.35 (dd, J = 8.8, 1.9 Hz, 1H), 7.27(d, J = 7.7 Hz, 1H), 7.16-7.12 (m, 5H), 7.07 (t, J = 7.5 Hz, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.5, 137.2, 134.7, 133.2, 132.0, 131.9, 130.8, 129.6, 128.7, 128.2, 127.7, 127.2, 127.1, 127.0, 124.7, 121.4, 113.3.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{14}ClNO$+H: 332.0842; found 332.0822.



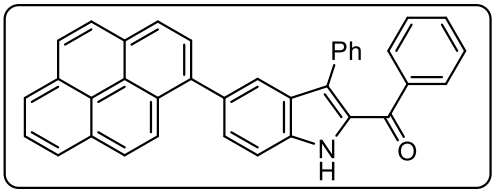
(3,5-Diphenyl-1H-indol-2-yl)(phenyl)methanone (3k):

Yield: 85% (73 mg); Solid; m.p. 180-182 ºC; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3308, 3017, 1709, 1357, 1223, 743, 695. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.56 (s, 1H), 7.91 (s, 1H), 7.68 (d, J = 8.6 Hz, 1H), 7.62-7.54 (m, 5H), 7.43 (t, J = 7.4 Hz, 2H), 7.34- 7.27 (m, 2H), 7.26-7.22 (m, 2H), 7.15- 7.14 (m, 3H), 7.08 (t, J = 7.4 Hz, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.6, 141.9, 137.6, 136.0, 134.9, 133.7, 131.8, 131.6, 131.0, 129.6, 128.8, 128.2, 128.1, 127.6, 127.4, 127.0, 126.8, 126.7, 125.7, 120.3, 112.4.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{27}H_{19}NO$+H: 374.1545; found 374.1525.



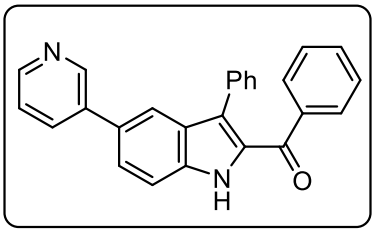
Phenyl(3-phenyl-5-(pyren-1-yl)-1H-indol-2-yl)methanone (3l):

Yield: 96% (110 mg); Solid; m.p. 235- 237 ºC; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3318, 3046, 1617, 1265, 753, 697. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.46 (s, 1H), 8.19- 8.14 (m, 4H), 8.08 (s, 2H), 8.01 (d, J = 8.1 Hz, 3H), 7.96 (s, 1H), 7.69 (s, 2H), 7.57 (d, J = 7.2 Hz, 2H), 7.29- 7.23 (m, 3H), 7.10-7.07 (m, 5H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.6, 138.3, 137.5, 135.8, 134.5, 133.6, 131.9, 131.6, 131.1, 131.0, 130.5, 129.8, 129.6, 128.8, 128.1, 127.7, 127.5, 127.4, 127.0, 126.1, 125.6, 125.5, 125.2, 125.1, 125.0, 124.8, 124.6, 123.7, 111.8.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{37}H_{23}NO$+Na:520.1677; found 520.1643.



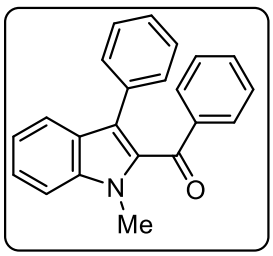
Phenyl(3-phenyl-5-(pyridin-3-yl)-1H-indol-2-yl)methanone (3m):

Yield: 80% (69 mg); Solid; m.p. 210- 212 ºC; R_f=0.2 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3056, 2926, 1700, 1628, 1267, 744, 701. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.69 (s, 1H), 8.87 (s, 1H), 8.56 (s, 1H), 7.89 (d, J = 7.7 Hz, 2H), 7.63 (s, 2H), 7.54 (d, J = 7.7 Hz, 2H), 7.35 (d, J = 3.8 Hz, 1H), 7.25-7.21 (m, 3H), 7.15 (s, 3H), 7.08 (t, J = 6.5 Hz, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.6, 148.4, 147.9, 137.4, 136.2, 134.6, 133.5, 131.9, 131.8, 131.2, 130.9, 129.6, 128.4, 128.3, 128.2, 127.7, 127.1, 126.2, 125.5, 123.6, 120.7, 112.9.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{26}H_{18}N_2O$+H:375.1497; found 375.1491.



(1-Methyl-3-phenyl-1H-indol-2-yl)(phenyl)methanone(3n):

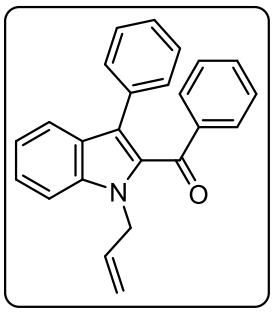
Yield: 87% (63 mg); viscous liquid; R_f=0.7 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3056, 2941, 1634, 1251, 950, 730, 694. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.78 (d, J = 8.1 Hz, 1H), 7.70-7.67 (m, 2H), 7.50-7.42 (m, 2H), 7.31-7.20 (m, 4H), 7.14 (t, J = 7.3 Hz, 4H), 7.08-7.05 (m, 1H), 3.97 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 190.7, 138.7, 138.2, 134.0, 133.0, 132.6, 130.5, 130.2, 128.1, 127.9, 126.6, 125.9, 125.3, 123.6, 121.5,



121.0, 110.3, 31.7; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{17}NO$+H: 312.1388; found 312.1371.

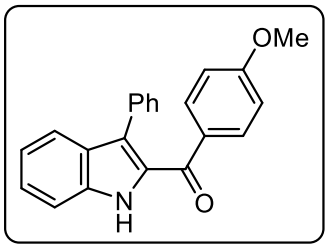
(1-Allyl-3-phenyl-1H-indol-2-yl)(phenyl)methanone (3o):

Yield: 51% (40 mg); viscous liquid; R_f=0.7 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3058, 2924, 1635, 1259, 934, 730, 699. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.78 (d, J = 8.1 Hz, 1H), 7.65 (d, J = 7.3 Hz, 2H), 7.48 (d, J = 8.4 Hz, 1H), 7.41 (t, J = 7.0 Hz, 1H), 7.29-7.20 (m, 4H), 7.14-7.09 (m, 4H), 7.05 (t, J = 7.2 Hz, 1H). 6.06-5.97 (m, 1H), 5.12-5.02 (m, 4H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 190.8, 138.2, 138.1, 134.0, 133.9, 132.6, 130.5, 130.2, 128.1, 127.8, 126.6, 126.1, 125.4, 124.2, 121.6, 121.2, 116.8, 110.7, 46.9; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{19}NO$+H:338.1545; found 338.1522.



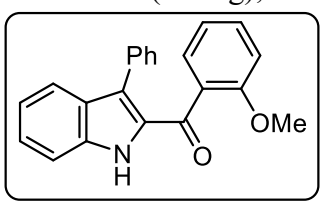
(4-Methoxyphenyl)(3-phenyl-1H-indol-2-yl)methanone (3p):

Yield: 97% (73 mg); Solid; m.p. 130-132 ºC; R_f=0.3 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3308, 3056, 1596, 1250, 1161, 734, 703. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.40 (s, 1H), 7.75 (d, J = 8.1 H z, 1H), 7.56 (d, J = 8.8 Hz, 2H), 7.51 (d, J = 8.6 Hz, 1H), 7.39 (t, J = 7.9 Hz, 1 H), 7.24 (d, J = 7.9, 2H), 7.20-7.14 (m, 4 H), 6.57 (d, J = 8.7 Hz, 2 H), 3.73 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 188.3, 162.7, 136.3, 134.1, 132.1, 131.2, 131.0, 130.1, 128.1, 127.7, 126.8, 126.2, 124.4, 122.0, 121.1, 113.0, 112.0, 55.4.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{17}NO_2$+H:328.1338; found 328.1324.



(2-Methoxyphenyl)(3-phenyl-1H-indol-2-yl)methanone (3q):

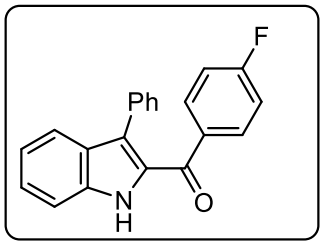
Yield: 88% (66 mg); Solid; m.p. 125-127 ºC; R_f=0.3 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3319, 3058, 1610, 1250, 1025, 744, 701. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.30 (s, 1H), 7.59 (d, J = 8.2 Hz, 1H), 7.47 (d, J = 8.2 Hz, 1H), 7.38 (t, J = 7.7 Hz, 1H), 7.21 (d, J = 7.8 Hz, 1H), 7.14-7.07 (m, 7H), 6.73 (t, J = 7.5 Hz, 1H), 6.43 (d, J = 8.5 Hz, 1H), 3.51 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 188.4, 156.9, 136.3, 133.2, 131.9, 131.8,



130.5, 129.6, 128.9, 128.3, 127.3, 126.8, 126.7, 126.0, 122.4, 120.9, 120.0, 112.0, 110.3, 55.2.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{17}NO_2$+H:328.1338 found 328.1324.

(4-Fluorophenyl)(3-phenyl-1H-indol-2-yl)methanone (3r):

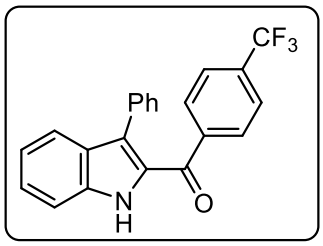
Yield: 96% (70 mg); Solid; m.p. 140-142 ºC; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3320,



2925, 1598, 1230, 1152, 841, 741, 704. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.75 (s, 1H), 7.74 (d, J = 8.1 Hz, 1H), 7.58- 7.52 (m, 3H), 7.42 (t, J = 7.8 Hz, 1H), 7.21-7.18 (m, 6H), 6.75 (t, J = 8.4 Hz, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 188.3, 166.1, 163.6, 136.6, 133.8, 133.7, 132.2, 132.1, 131.0, 130.8, 128.1, 127.6, 127.1, 126.7, 125.5, 122.2, 121.3, 114.8, 114.6, 112.2.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{14}FNO$+H: 316.1138 found 316.1121.

(3-Phenyl-1H-indol-2-yl)(4-(trifluoromethyl)phenyl)methanone (3s):

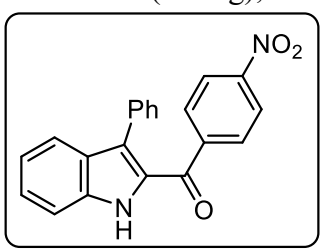
Yield: 84% (71 mg); Solid; m.p. 190-192 ºC; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3323,



1737, 1614, 1324, 1119, 1066, 751. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.41 (s, 1H), 7.66 (d, J = 8.2 Hz, 1H), 7.51- 7.46 (m, 3H), 7.39 (t, J = 8.2 Hz, 1H), 7.25 (d, J = 7.9 Hz, 2H), 7.15 (t, J = 7.4 Hz, 1H), 7.07 (s, 5H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 188.4, 140.9, 136.7, 133.3, 130.9, 130.6, 129.5, 128.1, 127.7, 127.3, 126.6, 124.6, 124.59, 124.56, 124.52, 122.4, 121.5, 112.2; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{14}F_3NO$+H: 366.1106 found 366.1086.

(4-Nitrophenyl)(3-phenyl-1H-indol-2-yl)methanone (3t):

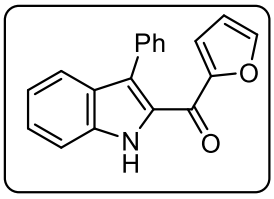
Yield: 84% (66 mg); Solid; m.p. 195-197 ºC; R_f=0.4 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3332,



1719, 1519, 1345, 1222, 783, 732. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.34 (s, 1H), 7.88 (d, J = 8.7 Hz, 2H), 7.70 (d, J = 8.2 Hz, 1H), 7.59 (d, J = 8.9 Hz, 2H), 7.52 (d, J = 8.2 Hz, 1H), 7.45 (t, J = 8.2 Hz, 1H), 7.20 (t, J = 8.0 Hz, 1H), 7.16- 7.09 (m, 5H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 187.5, 149.0, 143.2, 136.9, 133.1, 131.0, 130.4, 130.2, 128.2, 127.7, 127.66, 127.62, 126.9, 122.7, 122.5, 121.6, 112.2.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{14}N_2O_3$+Na: 365.0902 found 365.0882.

Furan-2-yl(3-phenyl-1H-indol-2-yl)methanone (3u):

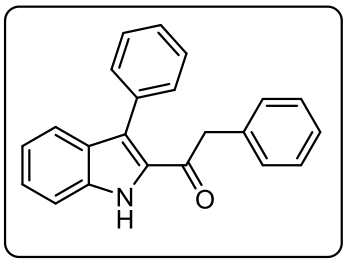
Yield: 85% (56 mg); Solid; m.p. 160-162 ºC; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3315,



2924, 1590, 1454, 1267, 754, 693. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.33 (s, 1H), 7.64 (d, J = 8.1 Hz, 1H), 7.40 (d, J = 8.2 Hz, 1H), 7.35-7.33 (m, 2H), 7.31-7.25 (m, 3H), 7.23-7.16 (m, 2H), 7.09 (t, J = 7.6 Hz, 1H), 6.74 (d, J = 3.5 Hz, 1H), 6.21 (dd, J = 3.5, 1.3 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 174.7, 151.9, 146.2, 136.4, 134.5, 130.5, 130.3, 128.4, 127.7, 127.2, 126.5, 124.8, 122.1, 121.3, 119.9, 112.1, 112.0.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{19}H_{13}NO_2$+H: 288.1025 found 288.1013.

2-Phenyl-1-(3-phenyl-1H-indol-2-yl)ethan-1-one (3v):

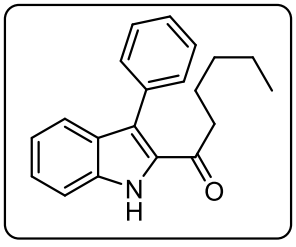
Yield: 88% (63 mg); Solid; m.p. 155-160 ºC; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3443,



3056, 1647, 1265, 740, 462. ^{1}H NMR (500 MHz, $CDCl_3$, 24 °C): δ 9.38 (s, 1H), 7.53-7.43 (m, 6H), 7.37–7.32 (m, 2H), 7.22-7.15 (m, 3H), 7.11-7.08 (m, 1H), 6.96-6.95 (m, 2H), 3.84 (s, 2H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 24 °C): δ 191.6, 135.9, 134.4, 134.2, 131.5, 130.8, 129.3, 128.9, 128.6, 128.3, 128.0, 126.7, 126.6, 124.6, 122.1, 120.9, 111.8, 46.1.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{17}NO$+H: 312.1388 found 312.1387.

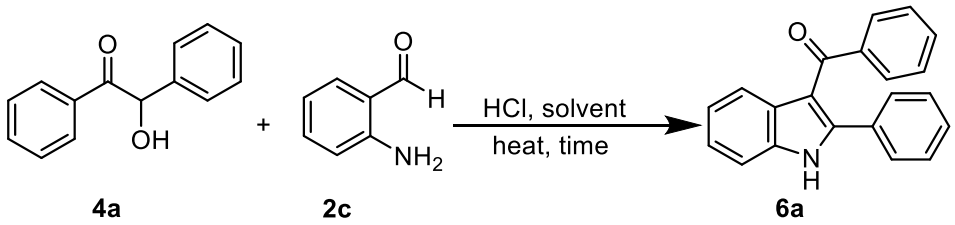
1-(3-Phenyl-1H-indol-2-yl)hexan-1-one (3w):

Yield: 89% (56 mg); Solid; m.p. 60-65 ºC; R_f=0.6 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3439, 2929,



1643, 1487, 1265. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.44 (s, 1H), 7.49-7.42 (m, 7H), 7.35 (t, J = 8.4 Hz, 1H), 7.10 (t, J = 7.2 Hz, 1H), 2.46 (t, J = 7.3 Hz, 2H), 1.57-1.50 (m, 2H), 1.17- 1.03 (m, 4H), 0.79 (t, J = 7.2 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 194.8, 135.6, 134.4, 131.8, 130.5, 128.9, 128.4, 127.9, 126.4, 124.1, 122.1, 120.7, 111.8, 40.0, 31.3, 24.5, 22.3, 13.9.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{21}NO$+H: 292.1701 found 292.1710.

6. Optimization: Synthesis of 3-Acylindole 6a



4a **2c** **6a**

Entry	Acid (equiv)	Temp (°C)	Solvent	Yield (%)
1	PTSA (0.5)	100	Dioxane	36
2	MSA (0.5)	100	Dioxane	22
3	TFA (0.5)	100	Dioxane	29
4	H_2SO_4 (0.5)	100	CH_3CN	15
5	Conc.HCl (2)	100	CH_3CN	40
6	Conc.HCl (2)	80	THF	44
7	1N HCl (2)	100	Dioxane	32
8	1N HCl (2)	100	EtOH	20
9	Conc.HCl (2)	100	Dioxane	55
10	Conc.HCl (2)	120	Dioxane	65
11	Conc.HCl (2)	100	EtOH	20

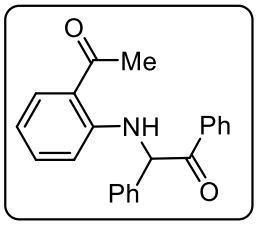
Reaction conditions: **4a** (0.23 mmol, 1 equiv), **2c** (0.23 mmol, 1 equiv), Conc. HCl (11.5 M, 0.5 mmol, 2 equiv), Dioxane (3 mL for 0.23 mmol), 120 ºC, 24 h.

General procedure for synthesis of 3-acyl indoles 6:

In a 20 mL reaction tube, benzoin **4a** (0.23 mmol, 1 equiv) and 2-aminobenzaldehyde **2c** (28 mg, 0.23 mmol, 1 equiv) was taken in 3 mL of dioxane. Conc. HCl (11.5 M, 20 mg, 0.5 mmol, 2 equiv) was added to the reaction mixture and the tube was sealed and kept in a pre-heated oil bath at 120 ºC and was then stirred for 24 h. After the completion of reaction, as indicated by TLC, it was cooled down to room temperature and extracted with DCM. The organic layer was then dried over Na_2SO_4 and evaporated under reduced pressure. The crude product was then further purified by silica gel chromatography using ethyl acetate:hexane as an eluent to afford 3-acylindole **6** in good yield.

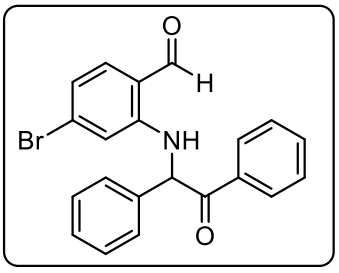
2-((2-Acetylphenyl)amino)-1,2-diphenylethan-1-one (5):

Yield: 87% (168 mg); Solid; m.p. 105-110 ºC; R_f=0.6 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3456, 3288, 1683, 1639, 1570, 1510, 1452, 1246, 1169, 964, 753, 698. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 10.21 (d, J = 6.0 Hz, 1H), 8.01 (d, J = 7.5 Hz, 2H), 7.75 (d, J = 7.7 Hz, 1H), 7.49 - 7.47 (m, 3H), 7.40 (t, J = 7.5 Hz, 2H), 7.28-7.19 (m, 4H), 6.63-6.57 (m, 2H), 6.10 (d, J = 6.2 Hz, 1 H), 2.58 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 200.7, 195.7, 148.8, 137.1, 135.0, 134.8, 133.4, 132.8, 129.1, 128.9, 128.6, 128.2, 128.1, 118.6, 115.0, 112.5, 62.4, 28.0.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{19}NO_2$: 330.1494 found 330.1507.



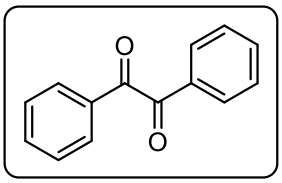
4-bromo-2-((2-oxo-1,2-diphenylethyl)amino)benzaldehyde (5'):

Yield: 39% (36 mg); Yellow solid; m.p. 160-165 ºC; R_f = 0.6 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 1671, 1592, 1208, 870, 754. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.85-9.80 (m, 2H), 8.02 (d, J = 8.2 Hz, 2H), 7.53 (t, J = 7.5 Hz, 1H), 7.48-7.41 (m, 4H), 7.33-7.29 (m, 3H), 7.25-7.21 (m, 1H), 6.83-6.81 (m, 2H), 6.06 (d, 6.2 Hz, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 194.7, 193.0, 148.8, 137.9, 136.2, 134.4, 133.7, 131.1, 129.3, 128.9, 128.7, 128.5, 128.1, 119.1, 118.3, 114.6, 61.9.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{16}BrNO_2$+H: 394.0443 found 394.0452.



Benzil:

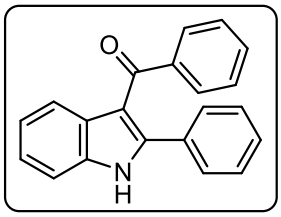
Yield: 20% (20 mg); Liquid; R_f = 0.8 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3063, 2924, 1672, 1589, 1210, 874, 715.; ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.97 (d, J = 7.9 Hz, 2H), 7.65 (t, J = 7.5 Hz, 1H), 7.5 (t, J = 7.7 Hz, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 194.6, 134.9, 133.0, 129.9, 129.0.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{14}H_{10}O_2$+H: 211.0759 found 211.0758.



6.1. Properties of synthesized 3-acyl indoles:

Phenyl(2-phenyl-1H-indol-3-yl)methanone (6a):

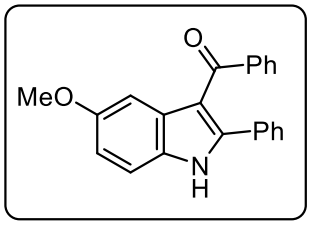
Yield: 65% (45 mg); Solid; m.p. 190-192 ºC; R_f = 0.5 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3289,



2992, 1765, 1245, 1067, 978, 752, 696. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.68 (s, 1H), 7.94 (d, J = 7.8 Hz, 1H), 7.64 (d, J = 7.5 Hz, 2H), 7.45-7.15 (m, 11H) $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 193.3, 143.7, 139.7, 135.5, 131.8, 131.6, 129.7, 129.3, 128.9, 128.7, 128.5, 127.8, 123.7, 122.3, 121.8, 113.9, 111.1.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{15}NO$+H: 298.1232 found 298.1251.

(5-Methoxy-2-phenyl-1H-indol-3-yl)(phenyl)methanone (6b):

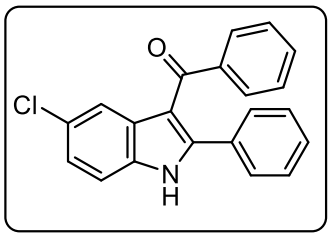
Yield: 51% (39 mg); Solid; m.p. 160-165 ºC; R_f =0.4 in 20 % EtOAc; IR (ν_{max}, cm^{-1}): 3435,



1624, 1457, 1421, 1269, 1211, 696. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.57 (s, 1H), 7.59 (d, J = 7.8 Hz, 2H), 7.55 (s, 1H), 7.34-7.25 (m, 4H), 7.18-7.11 (m, 5H), 6.94 (d, J = 9.1 Hz, 1H), 3.83 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 193.3, 156.0, 144.3, 139.7, 131.8, 131.3, 130.4, 129.6, 129.5, 129.2, 128.6, 128.3, 127.6, 114.3, 113.6, 111.8, 102.9, 55.7.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{17}NO_2$+H: 328.1338 found 328.1337.

(5-Chloro-2-phenyl-1H-indol-3-yl)(phenyl)methanone (6c):

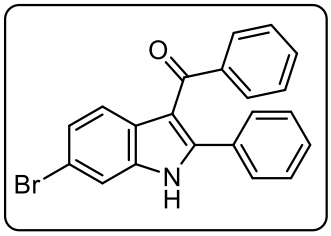
Yield: 42% (32 mg); Solid; m.p. 250-255 ºC; R_f =0.6 in 20 % EtOAc; IR (ν_{max}, cm^{-1}): 3338,



2946, 2832, 1662, 1452, 1024, 651. ^{1}H NMR (400 MHz, DMSO-d_6, 24 °C): δ 12.42 (s, 1H), 7.78 (s, 1H), 7.54-7.48 (m, 3H), 7.37-7.33 (m, 3H), 7.28-7.17 (m, 6H). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6, 24 °C): δ 192.3, 146.1, 139.9, 134.8, 131.9, 131.5, 130.0, 129.7, 129.4, 129.2, 128.5, 128.2, 126.5, 123.4, 120.1, 113.9, 112.1.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{14}ClNO$+H: 332.0842 found 332.0853.

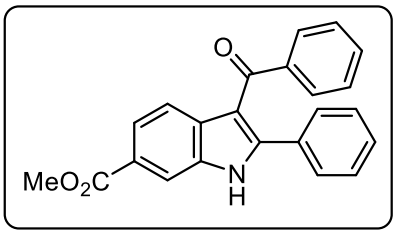
(5-Bromo-2-phenyl-1H-indol-3-yl)(phenyl)methanone (6d):

Yield: 35% (31 mg); Solid; m.p. 255-260 ºC; R_f=0.5 in 20 % EtOAc; IR (ν_{max}, cm^{-1}): 3358, 2944, 2832, 1661, 1451, 1113, 1025, 646. ^1H NMR (400 MHz, DMSO-d_6, 24 °C): δ 12.37 (s, 1H), 7.69-7.67 (m, 2H), 7.51 (d, J = 7.7 Hz, 2H), 7.38-7.35 (m, 3H), 7.32-7.18 (m, 6H). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6, 24 °C): δ 192.4, 145.2, 139.8, 137.1, 132.0, 131.5, 129.9, 129.5, 129.2, 128.5, 128.3, 127.6, 124.8, 122.7, 115.7, 114.8, 112.5.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{14}BrNO$+H: 376.0337 found 376.0346.



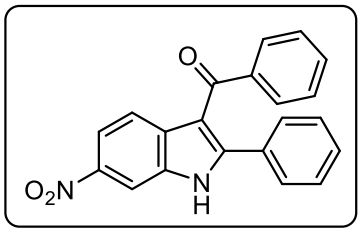
Methyl 3-benzoyl-2-phenyl-1H-indole-6-carboxylate (6e):

Yield: 48% (40 mg); Solid; m.p. 165-170 ºC; R_f=0.6 in 20 % EtOAc; IR (ν_{max}, cm^{-1}): 3430, 2075, 1633, 1016, 766, 502. ^1H NMR (400 MHz, DMSO-d_6, 24 °C): δ 12.57 (s, 1H), 8.14 (s, 1H), 7.84-7.76 (m, 2H), 7.53 (d, J = 7.6 Hz, 2H), 7.42-7.36 (m, 3H), 7.28-7.19 (m, 5H). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6, 24 °C): δ 192.4, 167.2, 147.3, 139.7, 135.6, 132.2, 132.1, 131.4, 130.0, 129.5, 129.4, 128.6, 128.3, 124.2, 122.4, 120.8, 114.0, 112.8, 52.4.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{23}H_{17}NO_3$+H: 356.1287 found 356.1288.



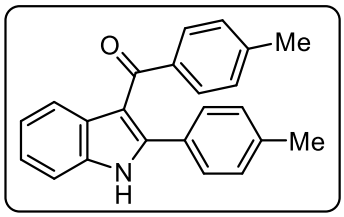
(6-Nitro-2-phenyl-1H-indol-3-yl)(phenyl)methanone (6f):

Yield: 46% (37 mg); Solid; m.p. 245-250 ºC; R_f=0.4 in 20 % EtOAc; IR (ν_{max}, cm^{-1}): 3446, 1631, 1510, 1334, 725, 693. ^1H NMR (400 MHz, DMSO-d_6, 24 °C): δ 8.37 (s, 1H), 8.05 (d, J = 9.0 Hz, 1H), 7.87 (d, J = 8.9 Hz, 1H), 7.55 (d, J = 7.9 Hz, 2H), 7.44-7.38 (m, 3H), 7.33-7.21 (m, 5H). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6, 24 °C): δ 192.2, 149.2, 143.3, 139.3, 134.9, 133.4, 132.4, 130.9, 130.0, 129.8, 129.6, 128.7, 128.4, 121.2, 116.9, 113.1, 108.7.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{14}N_2O_3$+H: 343.1083 found 343.1096.



p-Tolyl(2-(p-tolyl)-1H-indol-3-yl)methanone (6g)

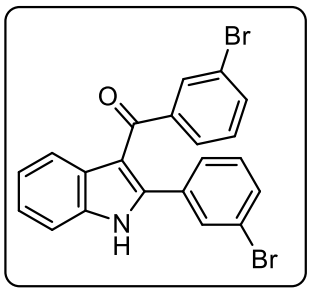
Yield: 56% (42 mg); Solid; m.p. 185-187 ºC; R_f=0.5 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3342,



2989, 1763, 1376, 1241, 1053. ^{1}H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.78 (s, 1H), 7.72 (d, J = 8.3 Hz, 1H), 7.55 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz,1H), 7.21-7.17 (m, 3H), 7.12 (t, J = 7.2 Hz, 1H), 6.98- 6.93 (m, 4H), 2.26 (s, 3H), 2.22 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 24 °C): δ 193.2, 143.4, 142.3, 138.8, 137.2, 135.5, 130.0, 129.2, 129.1, 129.0, 128.8, 128.6, 123.3, 121.9, 121.6, 113.7, 111.1, 21.6, 21.3.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{23}H_{19}NO$+H: 326.1545 found 326.1558.

(3-bromophenyl)(2-(3-bromophenyl)-1H-indol-3-yl)methanone (6h):

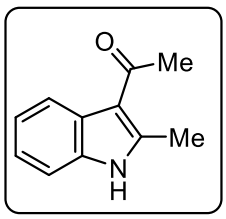
Yield: 70% (73 mg); Solid; m.p. 190-195 ºC; R_f=0.6 in 20 % EtOAc; IR (ν_{max}, cm^{-1}): 3363,



2945, 2832, 1661, 1448, 1029, 702. ^{1}H NMR (400 MHz, DMSO-d_6, 24 °C): δ 12.41 (s, 1H), 7.92 (d, J = 7.7 Hz, 1H), 7.55-7.52 (m, 4H), 7.46 (d, J = 7.4 Hz, 2H), 7.35-7.27 (m, 2H), 7.24-7.15 (m, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C): δ 190.6, 143.8, 142.3, 136.3, 134.1, 134.0, 132.6, 132.0, 131.8, 130.4, 129.2, 128.2, 128.1, 123.9, 122.4, 121.7, 121.6, 121.3, 112.7, 112.5.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{13}Br_2NO$+H: 453.9442 found 453.9450.

1-(2-Methyl-1H-indol-3-yl)ethan-1-one (6i)

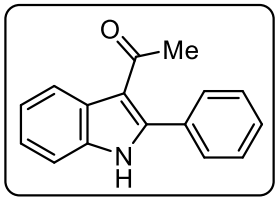
Yield: 50% (20 mg); Solid; m.p.185- 187 ºC; R_f=0.5 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3630,



2988, 1764, 1712, 1374, 1237, 1044. ^{1}H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.50 (s, 1H), 8.01 (d, J = 8.0 Hz, 1H), 7.33 (d, J = 7.8 Hz, 1H), 7.26-7.19 (m, 2H), 2.76 (s, 3H), 2.66 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 24 °C): δ 194.7, 143.6, 134.6, 127.1, 122.5, 122.2, 121.0, 114.9, 110.9, 31.3, 15.5.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{11}H_{11}NO$+H: 174.0919 found 174.0923.

1-(2-Phenyl-1H-indol-3-yl)ethan-1-one (6j)

Yield: 62% (35 mg); Solid; m.p. 210-202 ºC; R_f=0.5 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 2989,

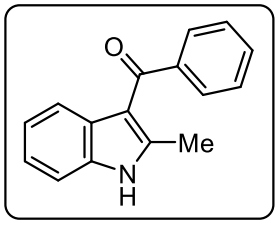


1762, 1375, 1240, 1050. ^{1}H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.67 (s, 1H), 8.48-8.46 (m, 1H), 7.67- 7.65 (m, 2H), 7.61- 7.59 (m, 3H), 7.49-7.47 (m, 1H), 7.42- 7.37 (m, 2H), 2.28 (s, 3H). ^{13}C{^{1}H} NMR

(125 MHz, $CDCl_3$, 24 °C): δ 195.4, 144.3, 135.2, 132.9, 129.9, 129.8, 128.8, 127.5, 123.8, 122.8, 122.7, 115.9, 110.8, 30.4.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{13}NO$+H: 236.1075 found 236.1085.

(2-Methyl-1H-indol-3-yl)(phenyl)methanone (6j')

Yield: 25% (14 mg); Solid; m.p. 175 -178 ºC; R_f=0.3 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 2990, 1763, 1377, 1242, 1058. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.04 (s, 1H), 7.75 (d, J = 7.1 Hz, 2H), 7.54 (t, J = 7.4 Hz, 1H), 7.47-7.39 (m, 3H), 7.29 (d, J = 7.8 Hz, 1H), 7.14 (t, J = 8.2 Hz, 1H), 7.06 (t, J = 7.8 Hz, 1H), 2.50 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 193.5, 143.9, 141.4, 134.8, 131.6, 128.9, 128.4, 127.7, 122.5, 121.6, 121.0, 114.0, 110.8, 14.6; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{13}NO$+H: 236.1075 found 236.1166.

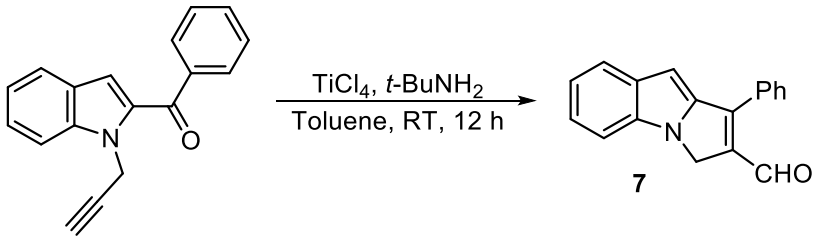


7. Synthetic application:

7.1. Gram scale synthesis

In an oven dried reaction tube compound, **1a** (0.92 g, 5.07 mmol, 1 equiv) and 2-amino benzophenone (1 g, 5.07 mmol, 1 equiv) was taken in 10 mL of dioxane. 5 mL of 1 N HCl was added to the reaction mixture and the reaction mixture was sealed and kept in a pre-heated oil bath at 100 ºC and stirred for 18 h at the same temperature. After completion of reaction, as indicated by TLC, it was cooled down to room temperature and the reaction mixture was extracted with DCM. The solvent was dried over Na_2SO_4 and evaporated under reduced pressure. The crude was further purified by column chromatography to afford the product **3f** in 94% yield (1.54 g).

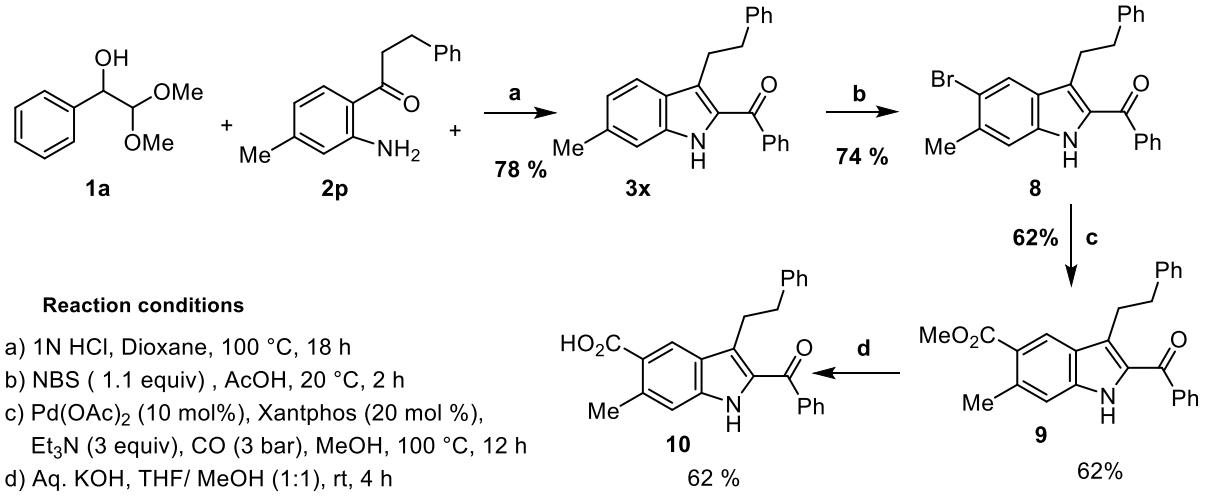
7.5. Synthesis of 1-Phenyl-3H-pyrrolo[1,2-a]indole-2-carbaldehyde (7)[9]



In an oven dried Schlenk tube, a solution of *N*-alkylated product (95 mg, 0.37 mmol, 1 equiv) was taken in 3 mL of dry toluene under nitrogen atmosphere and *t*-$BuNH_2$ (1.4 mL, 3.30 mmol,

9 equiv) was added. When the starting materials were completely dissolved, $TiCl_4$ (0.1 mL,0.55 mmol, 1.5 equiv) was dissolved in 2 mL of dry toluene and was added dropwise to the reaction mixture. The reaction mixture was stirred at room temperature until starting material was completely consumed, as indicated by TLC. The reaction mixture was then quenched with saturated solution of $NaHCO_3$ and extracted with EtOAc. The organic layer was then dried over Na_2SO_4 and the solvent was evaporated at reduced pressure. The crude product was then purified by column chromatography using ethyl acetate:hexane as an eluent to afford the product **10** in 66 % (62 mg) yield as yellow solid. m.p. 150-152 ºC R_f=0.5 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 2989, 1762, 1375, 1239, 1048. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.95 (s, 1H), 7.73 (s, 2H), 7.67 (d, J = 7.97, 1H), 7.57 (s, 3H), 7.40 (d, J= 7.97, 1H), 7.30- 7.25 (m, 1H), 7.13 (t, J = 7.5 Hz, 1H), 6.73 (s, 1H), 4.97 (s, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 187.1, 150.1, 145.5, 137.3, 134.9, 132.4, 130.6, 129.5, 129. 2, 123.9, 122.7, 120.4, 109.9, 98.6, 48.5.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{18}H_{13}NO$+H:260.1075 found 260.1066.

7.6. Synthesis of anti-tumor agent: 10



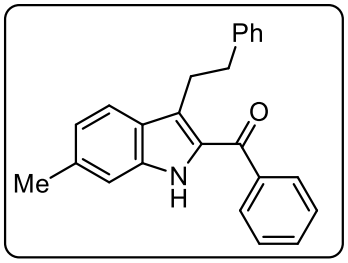
Step-b: 3x was synthesized employing the general procedure mentioned earlier. **3x** (50 mg, 0.15 mmol, 1 equiv) was taken in 3 mL of glacial acetic acid and the reaction mixture was kept at 20 ºC. N-Bromosuccinimide (29 mg, 0.16 mmol, 1.1 equiv) was added portion wise and the reaction mixture was stirred for 2 h. After the completion of reaction, as indicated by TLC, the reaction mixture was extracted with DCM and the organic layer was dried with Na_2SO_4 and was evaporated under reduced pressure. The crude was then purified by silica gel chromatography to afford the corresponding brominated product **8** in 74% (45 mg) yield.

Step-c: The brominated product **8** (0.21 mmol, 1 equiv) was taken in dry MeOH (3 mL). Pd $(OAc)_2$ (10 mol %), Xantphos (20 mol%), and 3 equiv of Et_3N were added and pressurized 3 bar with CO. The reaction was continued for 12 h at 100 ºC. After the completion of reaction, as indicated by TLC, the reaction was cooled down to room temperature and extracted with DCM. The organic layer was then dried with Na_2SO_4 and was evaporated under reduced pressure. The crude reaction mixture was then purified by column chromatography to afford the corresponding ester **9** in 62% yield.

Step-d: The ester **9** (75 mg, 0.19 mmol, 1 equiv) was dissolved in 2 mL of THF/MeOH (1:1). 2 mL of saturated aq. KOH was added and stirred at room temperature for 4 h. After the completion of reaction, the reaction mixture was extracted with DCM and the water layer was collected separately. The water layer was then acidified with 1N HCl and extracted with EtOAc. The organic layer was dried over Na_2SO_4. Evaporation of solvent followed by purification of crude product using column chromatography gave the desired product **10** as a white solid in 62% (45 mg) yield.

(6-Methyl-3-phenethyl-1H-indol-2-yl)(phenyl)methanone (3x):

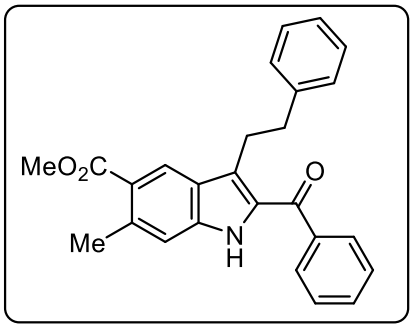
Yield: 56% (43 mg); Yellow Solid; m.p. 120-125 ºC; R_f=0.6 in 15% EtOAc; IR (ν_{max}, cm^{-1}):



3447, 3055, 1624, 1265, 744. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.69 (s, 1H), 7.70 (d, J = 7.5 Hz, 2H), 7.60 (d, J = 7.5 Hz, 2H), 7.50 (t, J = 7.5 Hz, 2H), 7.19-7.14 (m, 4 H), 7.00 (d, J = 7.9 Hz, 1 H), 6.89 (d, J = 7.1 Hz, 2H), 3.30 (t, J = 8.8 Hz, 2H), 2.78 (t, J = 7.6 Hz, 2H), 2.49 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.1, 141.6, 139.6, 137.1, 136.9, 131.7, 130.9, 128.5, 128.4, 128.3, 128.2, 126.0, 125.9, 124.9, 122.6, 120.9, 111.6, 37.5, 27.6, 22.1; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{21}NO$+H: 340.1701 found 340.1708.

Methyl 2-benzoyl-6-methyl-3-phenethyl-1H-indole-5-carboxylate (9):

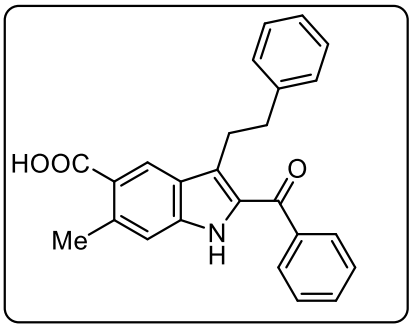
Yield: 62% (25 mg); White Solid; 105-110 ºC; m.p. R_f =0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}):



3434, 1716, 1627, 1264, 1062, 741, 702. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.01 (s, 1H), 8.37 (s, 1H), 7.69 (d, J = 7.5 Hz, 2H), 7.61 (t, J = 7.2 Hz, 1H), 7.50 (d, J = 7.4 Hz, 2H), 7.22 (s, 1H), 7.19-7.12 (m, 3 H), 6.87 (d, J = 7.1 Hz, 2H), 3.93 (s, 3H), 3.06 (t, J = 7.2 Hz, 2H), 2.79 (t, J = 7.4 Hz, 2H), 2.72 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.1, 168.3, 141.2, 139.1, 138.5, 138.3, 132.2, 132.1, 128.6, 128.5, 128.3, 128.2, 126.0, 125.9, 125.7, 125.6, 122.8, 113.9, 51.8, 37.5, 27.3, 22.9.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{26}H_{23}NO_3$+H: 398.1756 found 398.1763.

2-Benzoyl-6-methyl-3-phenethyl-1H-indole-5-carboxylic acid (10):

Yield: 63% (45 mg); White Solid; m.p. 210-215 ºC*;* R_f =0.2 in 20 % EtOAc; IR (ν_{max}, cm^{-1}):



3438, 3212, 1695, 1627, 1571, 1441, 1211, 789, 748, 693. ^{1}H NMR (400 MHz, DMSO-d_6, 24 °C): δ 11.6 (s, 1H), 8.33 (s, 1H), 7.70-7.65 (m, 3H), 7.56 (t, J = 7.2 Hz, 2H), 7.31 (s, 1H), 7.17 (t, J = 6.8 Hz, 1H), 7.10 (t, J = 6.6 Hz, 1H), 6.94 (d, J = 7.2 Hz, 2H), 3.01 (t, J = 8.0 Hz, 2H), 2.75 (t, J = 8.0 Hz, 2H), 2.64 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C): δ 189.0, 169.5, 141.6, 139.5, 139.0, 132.7, 132.6, 129.0, 128.6, 128.5, 126.3, 125.4, 124.5, 114.7, 37.4, 27.2, 23.0.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{25}H_{21}NO_3$+H: 384.1600 found 398.384.1607.

8. References

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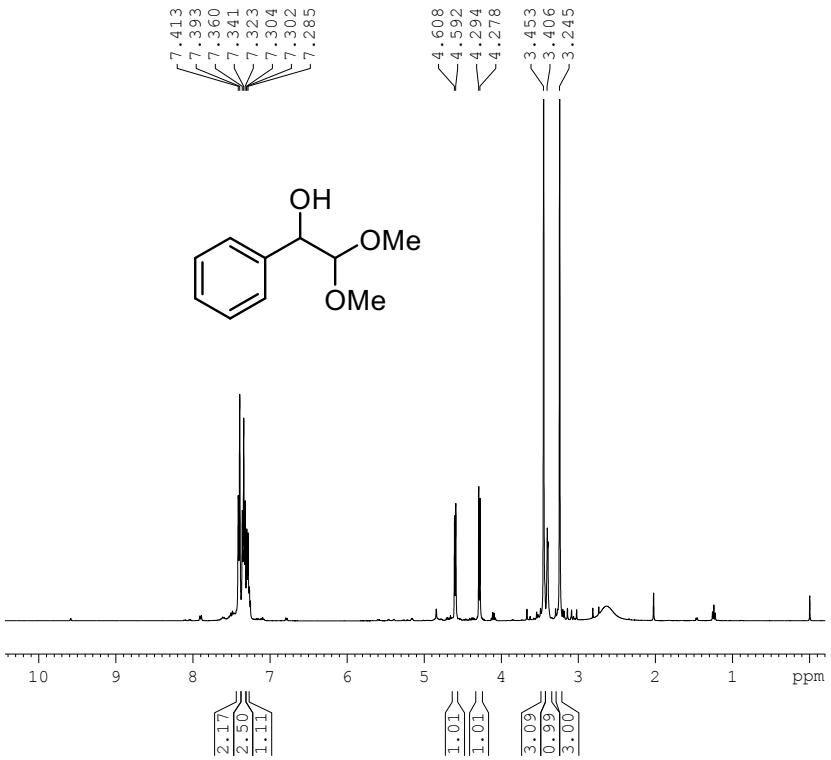
9. Spectral data

2,2-dimethoxy-1-phenylethan-1-ol:1a

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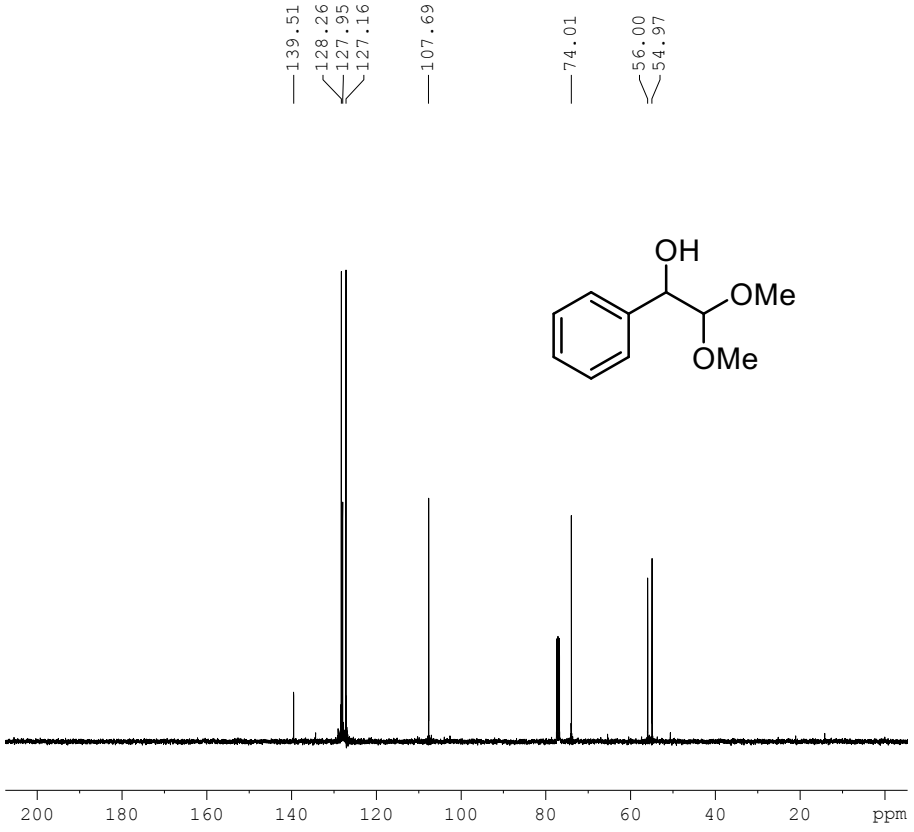
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **1a**

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PLW12          0.29166999 W
PLW13          0.14670999 W

F2 - Processing paramete
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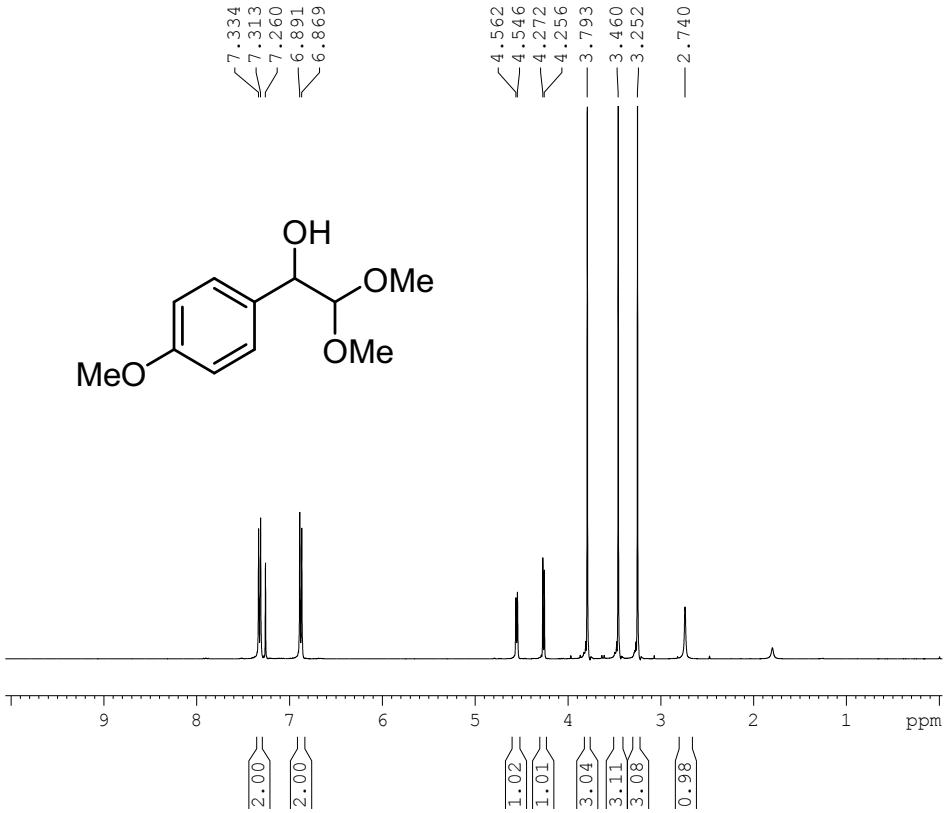
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **1a**

2,2-dimethoxy-1-(4-methoxyphenyl)ethan-1-ol: 1b

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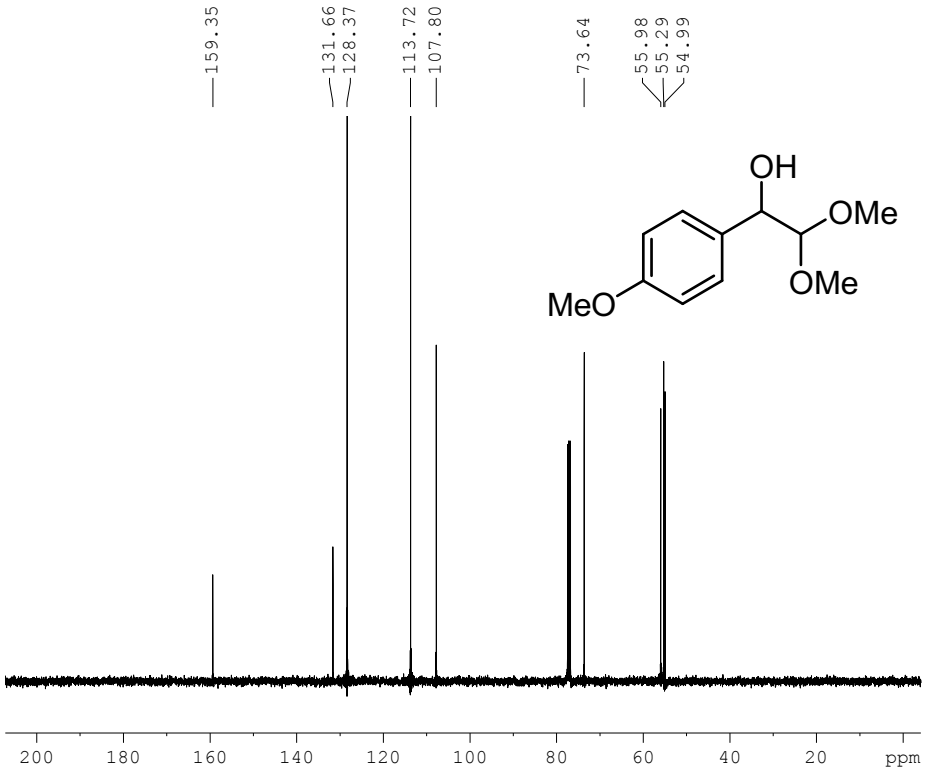
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **1b**

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D11         0.03000000 sec
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F2 - Processing parameters
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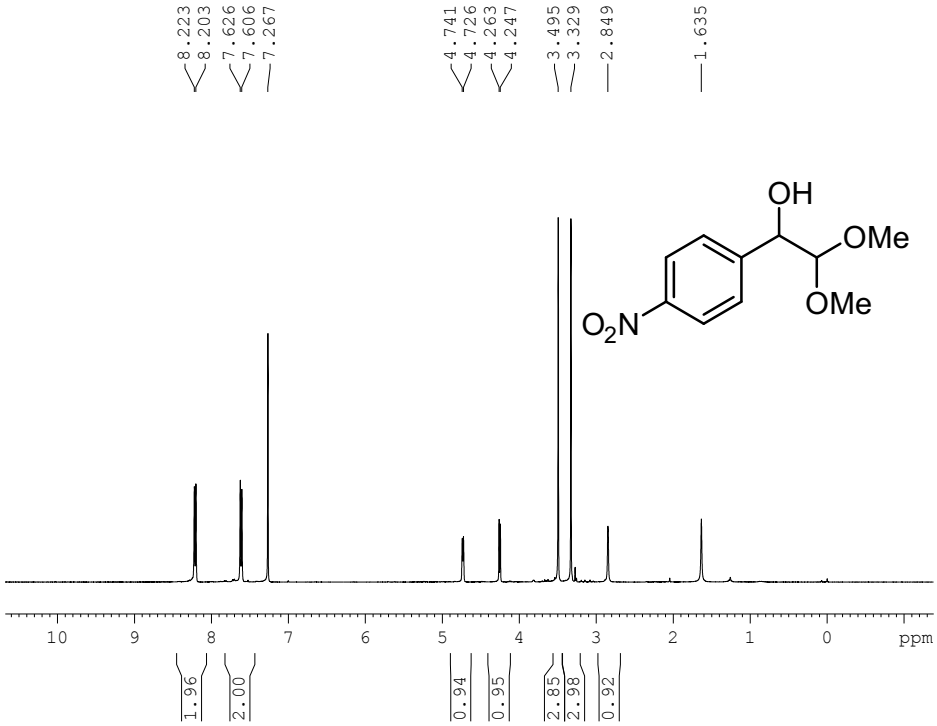
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **1b**

2,2-dimethoxy-1-(4-nitrophenyl)ethan-1-ol: 1c

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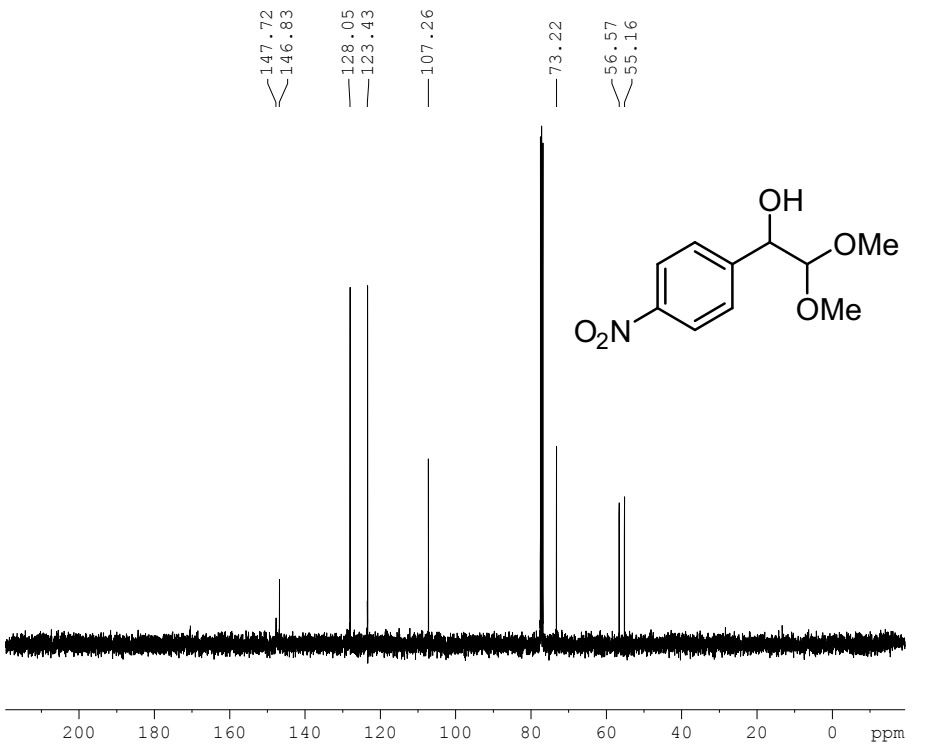
TD0
SFO1         400.132000
NUC1                  1
P1                15.0
PLW1         10.5000000

F2 - Processing parame
SI                 6553
SF           400.130006
WDW                   E
SSB
LB                  0.3
GB
PC                  1.0
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **1c**



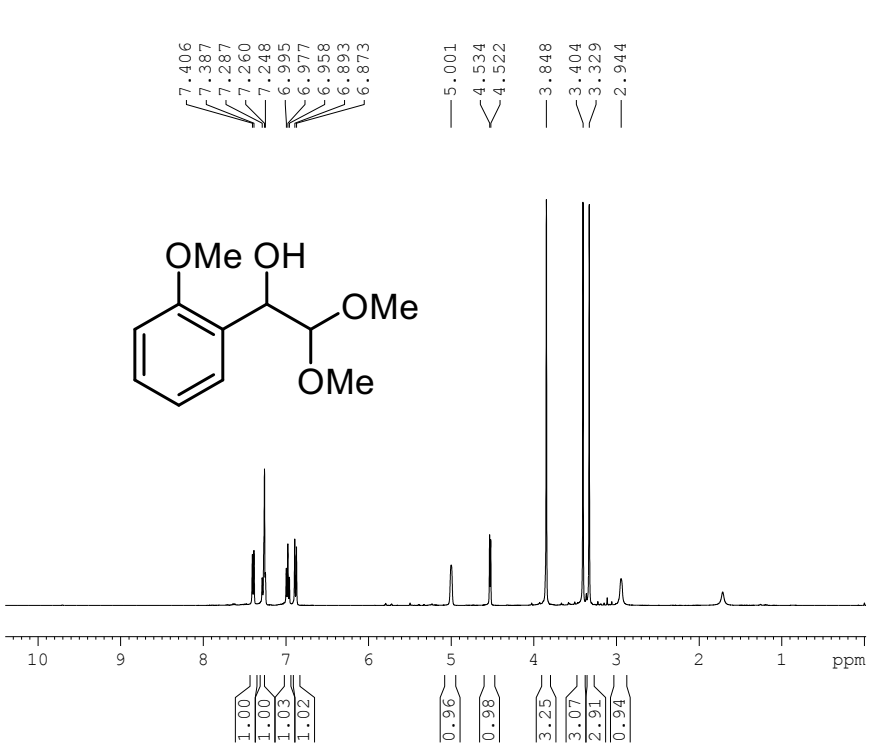

```
Current Data Parameters
NAME                  925
EXPNO                 249
PROCNO                  1

F2 - Acquisition Paramet
Date_           20210811
Time                3.39
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            24038.461
FIDRES          2.906706
AQ              0.3440320
RG                200.34
DW                20.800
DE                 6.50
TE                296.5
D1            1.00000000
D11           0.03000000
TD0                    1
SFO1         100.6228289
NUC1                 13C
P1                10.00
PLW1         47.00000000
SFO2         400.1316005
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00
PLW2         10.50000000
PLW12         0.29166999
PLW13         0.14670999

F2 - Processing paramete
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **1c**

2,2-dimethoxy-1-(2-methoxyphenyl)ethan-1-ol: 1d

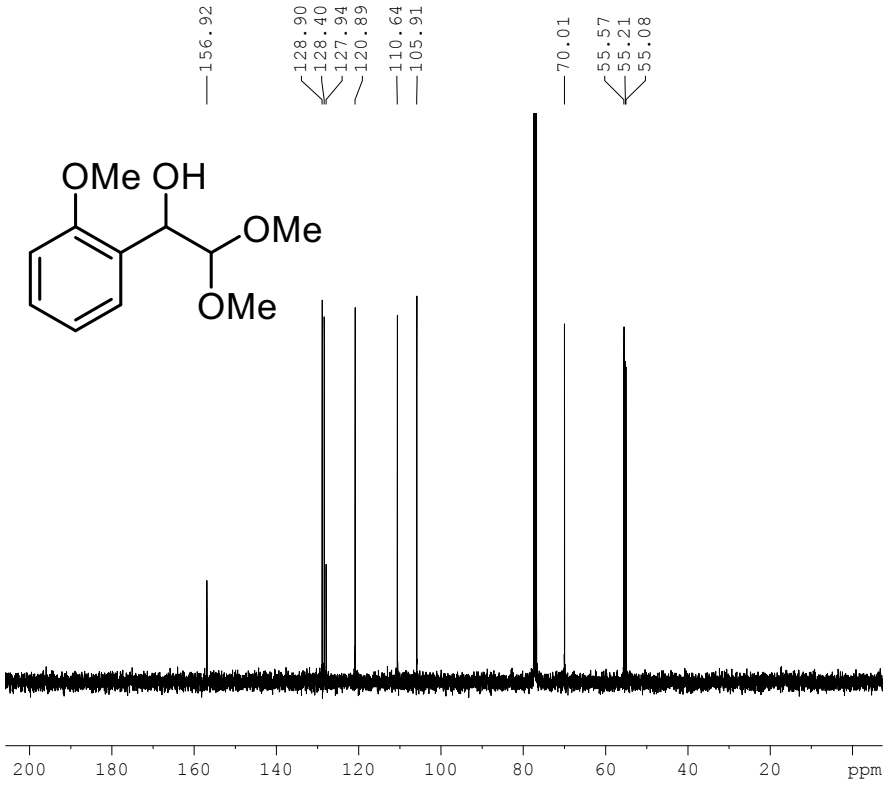



```
Current Data Parameters
NAME                  929
EXPNO                 326
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210814
Time                0.58 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                124.58
DW                62.400 usec
DE                 6.50 usec
TE                297.9 K
D1           0.50000000 sec
TD0                    1
SFO1        400.1320007 MHz
NUC1                  1H
P1                15.00 usec
PLW1         10.50000000 W

F2 - Processing parameters
SI                 65536
SF          400.1300097 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **1d**



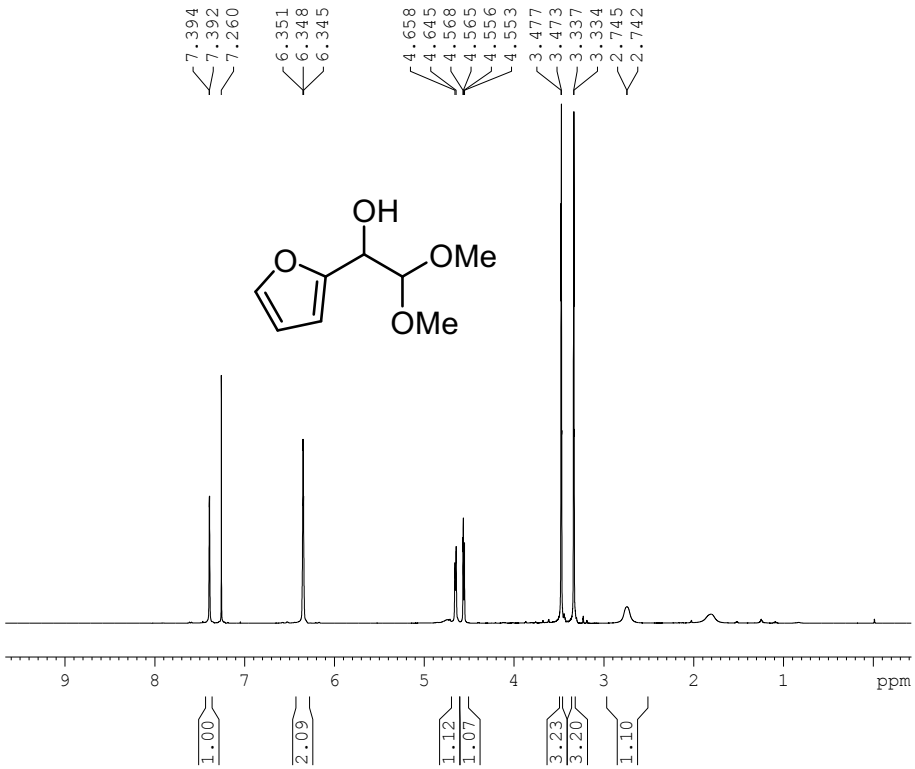

```
Current Data Parameters
NAME                  929
EXPNO                 327
PROCNO                  1

F2 - Acquisition Parameter
Date_            20210814
Time                1.05 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            24038.461 Hz
FIDRES          2.906706 Hz
AQ              0.3440320 se
RG                200.34
DW                20.800 us
DE                 6.50 us
TE                297.7 K
D1           1.00000000 se
D11          0.03000000 se
TD0                    1
SFO1        100.6228289 MH
NUC1                 13C
P1                10.00 us
PLW1         47.00000000 W
SFO2        400.1316005 MH
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             90.00 us
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W

F2 - Processing parameters
SI                 32768
SF          100.6127600 MH
WDW                   EM
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **1d**

1-(furan-2-yl)-2,2-dimethoxyethan-1-ol:1e



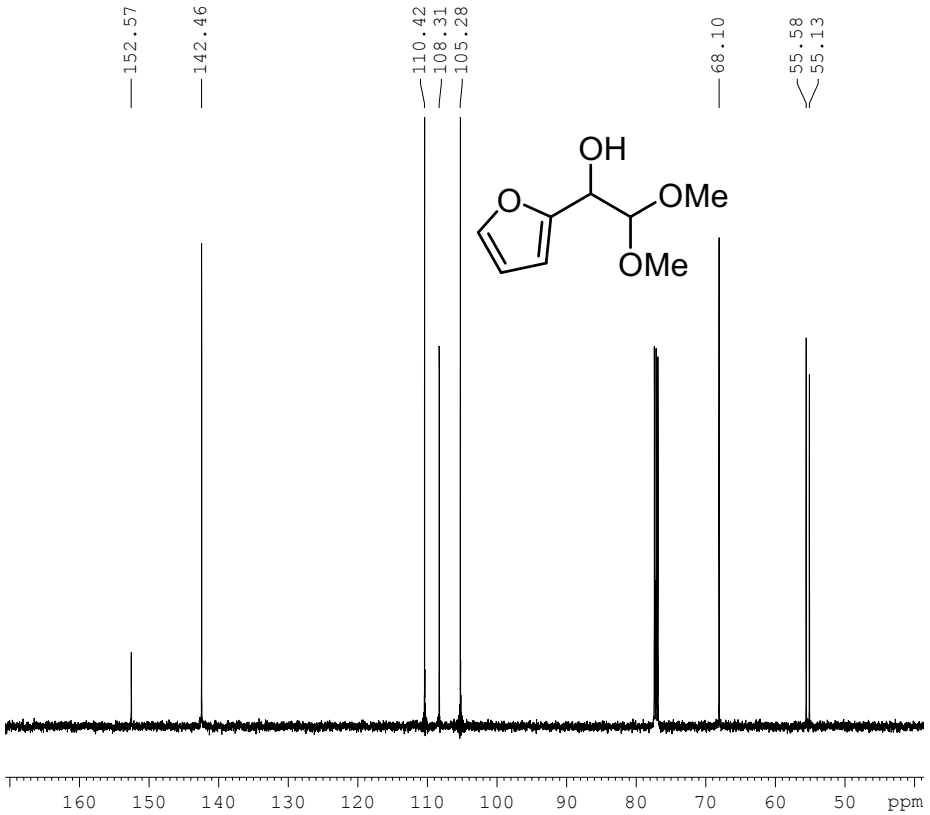

```
Current Data Parameters
NAME                  M529
EXPNO                   10
PROCNO                   1

F2 - Acquisition Paramete
Date_            20221109
Time                19.24
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      2
SWH             10000.000 H
FIDRES          0.305176 H
AQ              1.6384000 s
RG                     64
DW                50.000 u
DE                 6.50 u
TE                300.6 K
D1             0.50000000 s
TD0                     1

======== CHANNEL f1 =====
SFO1         500.1525008 M
NUC1                  1H
P1                11.75 u
PLW1         15.30000019 W

F2 - Processing parameter
SI                    65536
SF            500.1500119 M
WDW                     EM
SSB                      0
LB                  0.30 H
GB                       0
PC                    1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **1e**




```
Current Data Parameters
NAME                  M529
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_            20221109
Time                19.37
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                  20480
SOLVENT             CDCl3
NS                    512
DS                      4
SWH            29761.904 Hz
FIDRES          1.453218 Hz
AQ             0.3440640 sec
RG                 202.34
DW                16.800 usec
DE                 6.50 usec
TE                 301.2 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                     1

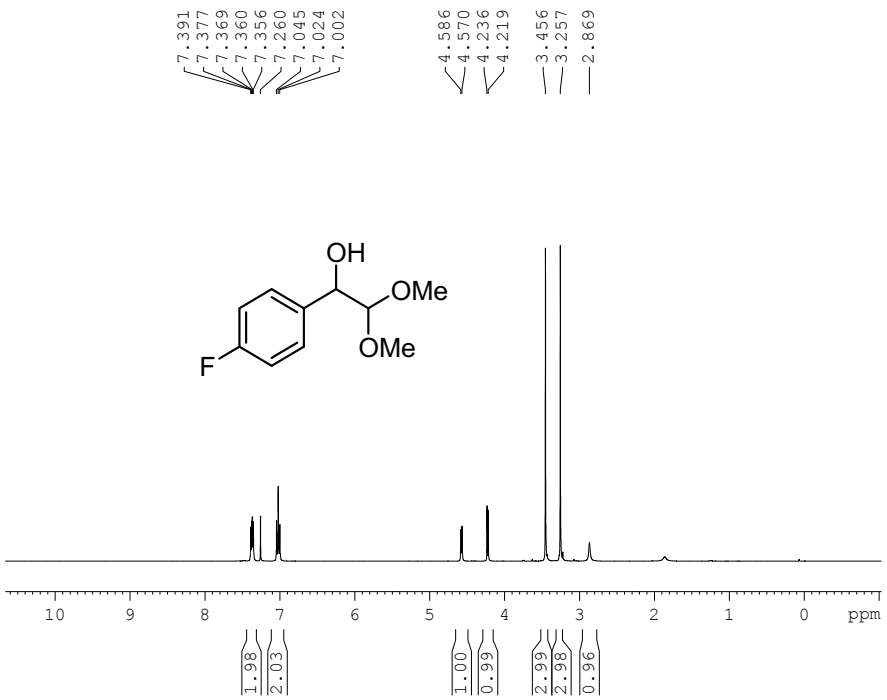
======== CHANNEL f1 ========
SFO1         125.7753932 MHz
NUC1                  13C
P1                10.20 usec
PLW1        103.00000000 W

======== CHANNEL f2 ========
SFO2         500.1520006 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         15.30000019 W
PLW12         0.39658999 W
PLW13         0.19948000 W

F2 - Processing parameters
SI                    32768
SF           125.7628069 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    1.40
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **1e**

1-(4-fluorophenyl)-2,2-dimethoxyethan-1-ol: 1f

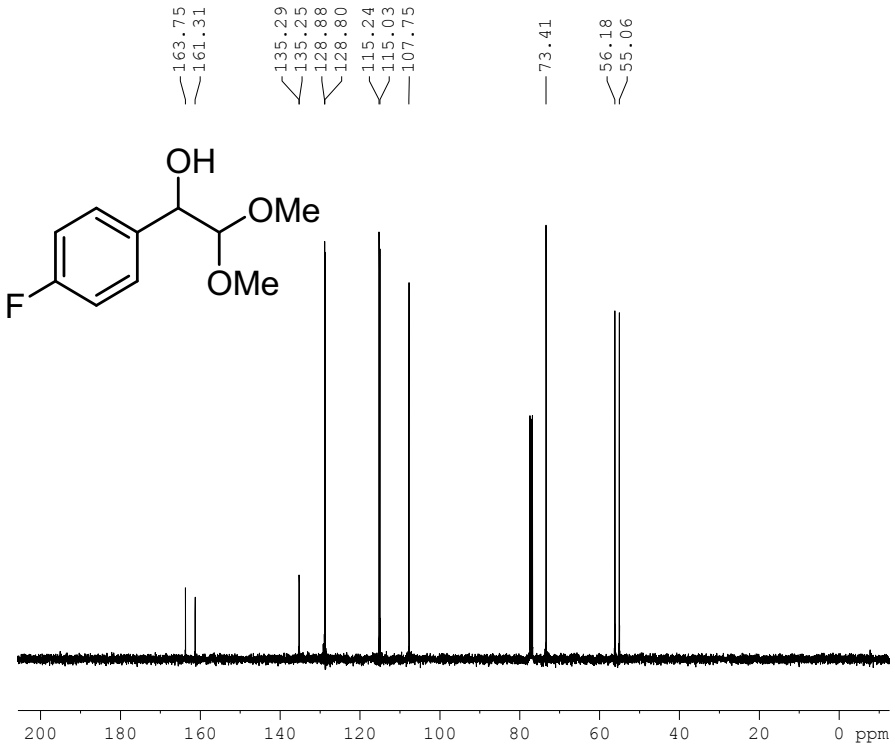



```
Current Data Parameters
NAME                  M559
EXPNO                  350
PROCNO                   1

F2 - Acquisition Parameters
Date_            20221126
Time               15.02 h
INSTRUM             spect
PROBHD    Z129392_0001 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                  88.51
DW                  62.400 usec
DE                   6.50 usec
TE                  297.7 K
D1              0.50000000 sec
TD0                     1
SFO1           400.1320007 MHz
NUC1                   1H
P1                  15.00 usec
PLW1           10.50000000 W

F2 - Processing parameters
SI                  65536
SF             400.1300095 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **1f**



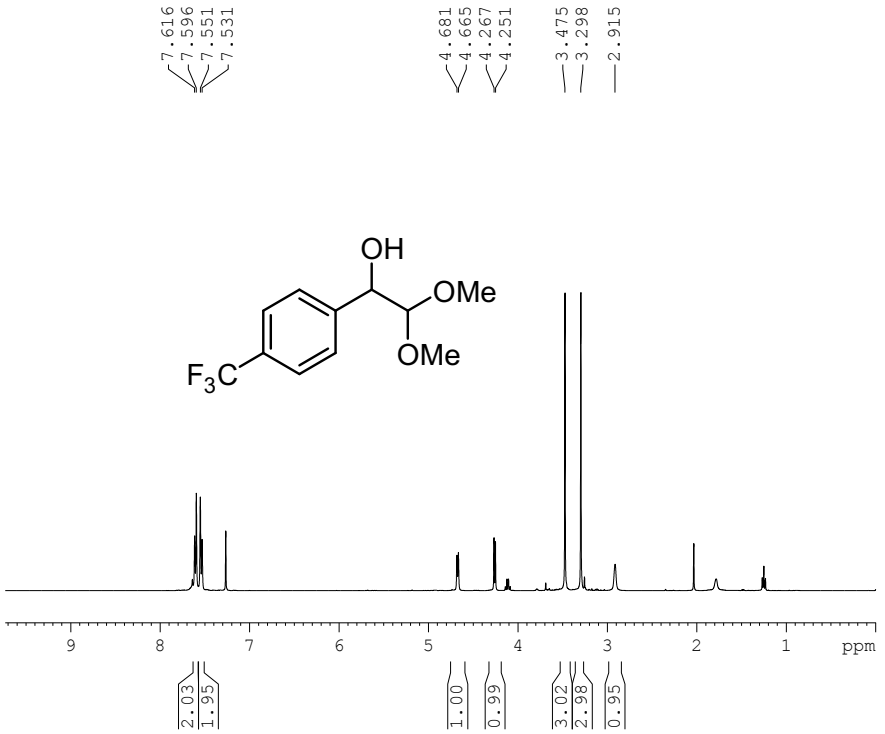

```
Current Data Parameters
NAME                  M559
EXPNO                  351
PROCNO                   1

F2 - Acquisition Paramete
Date_            20221126
Time               15.09 h
INSTRUM             spect
PROBHD    Z129392_0001 (
PULPROG           zgpg30
TD                  16540
SOLVENT             CDCl3
NS                    256
DS                      4
SWH             24038.461 H
FIDRES           2.906706 H
AQ               0.3440320 s
RG                  200.34
DW                  20.800 u
DE                   6.50 u
TE                  298.2 K
D1              1.00000000 s
D11             0.03000000 s
TD0                     1
SFO1           100.6228289 M
NUC1                  13C
P1                  10.00 u
PLW1           47.00000000 W
SFO2           400.1316005 M
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 u
PLW2           10.50000000 W
PLW12           0.29166999 W
PLW13           0.14670999 W

F2 - Processing parameter
SI                  32768
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **1f**

2,2-dimethoxy-1-(4-(trifluoromethyl)phenyl)ethan-1-ol: 1g

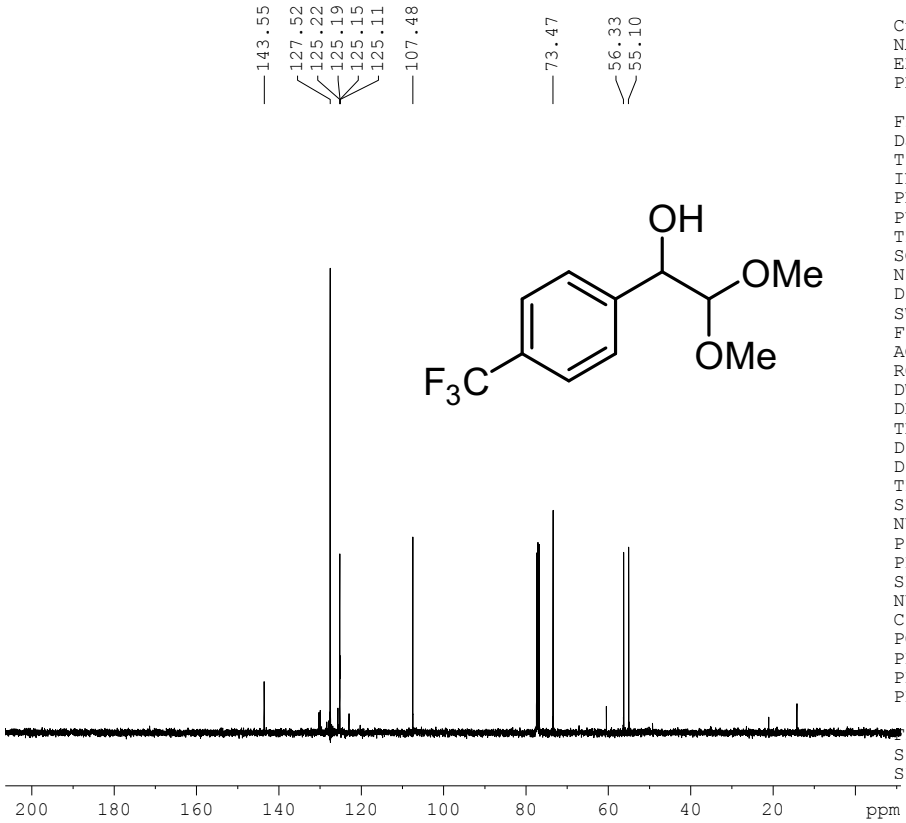



```
Current Data Parameters
NAME                  M657
EXPNO                  313
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230113
Time                  2.36 h
INSTRUM              spect
PROBHD   Z129392_0001 (
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8012.820 Hz
FIDRES               0.244532 Hz
AQ                4.0894465 sec
RG                   95.73
DW                   62.400 usec
DE                    6.50 usec
TE                   297.6 K
D1              0.50000000 sec
TD0                      1
SFO1           400.1320007 MHz
NUC1                    1H
P1                   15.00 usec
PLW1           10.50000000 W

F2 - Processing parameters
SI                   65536
SF             400.1300069 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **1g**



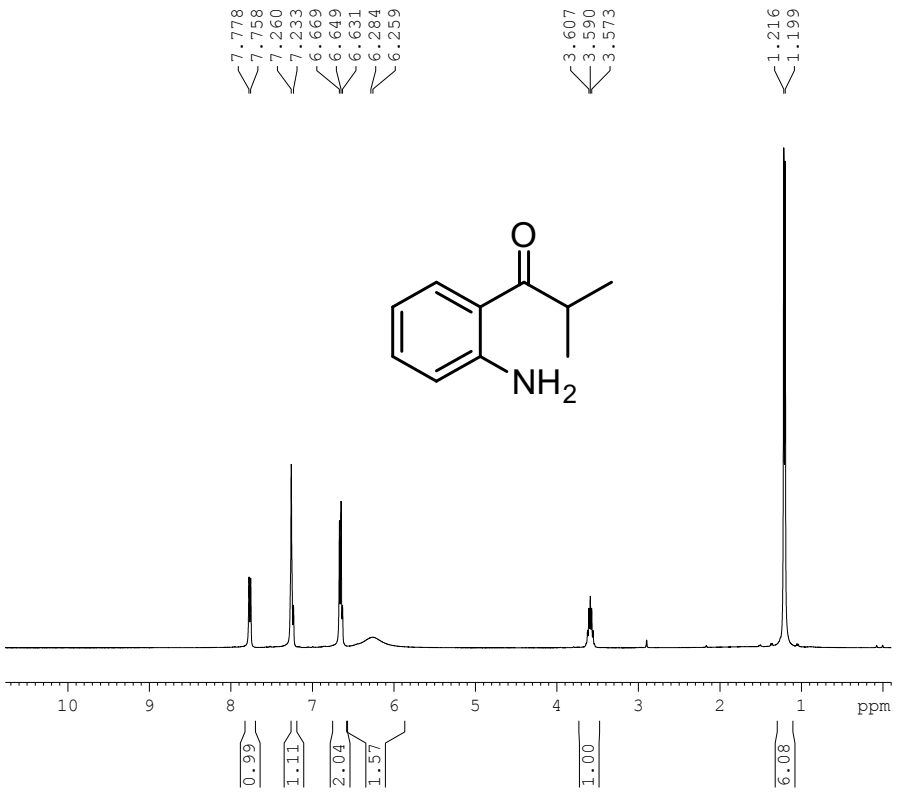

```
Current Data Parameters
NAME                  M657
EXPNO                  314
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230113
Time                  2.42 h
INSTRUM              spect
PROBHD   Z129392_0001 (
PULPROG             zgpg30
TD                   16540
SOLVENT              CDCl3
NS                     256
DS                       4
SWH              24038.461 Hz
FIDRES               2.906706 Hz
AQ                0.3440320 sec
RG                   200.34
DW                   20.800 usec
DE                    6.50 usec
TE                   297.9 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1           100.6228289 MHz
NUC1                   13C
P1                   10.00 usec
PLW1           47.00000000 W
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2          waltz16
PCPD2                90.00 usec
PLW2           10.50000000 W
PLW12           0.29166999 W
PLW13           0.14670999 W

F2 - Processing parameters
SI                   32768
SF             100.6127581 MHz
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **1g**

1-(2-aminophenyl)-2-methylpropan-1-one: 2b

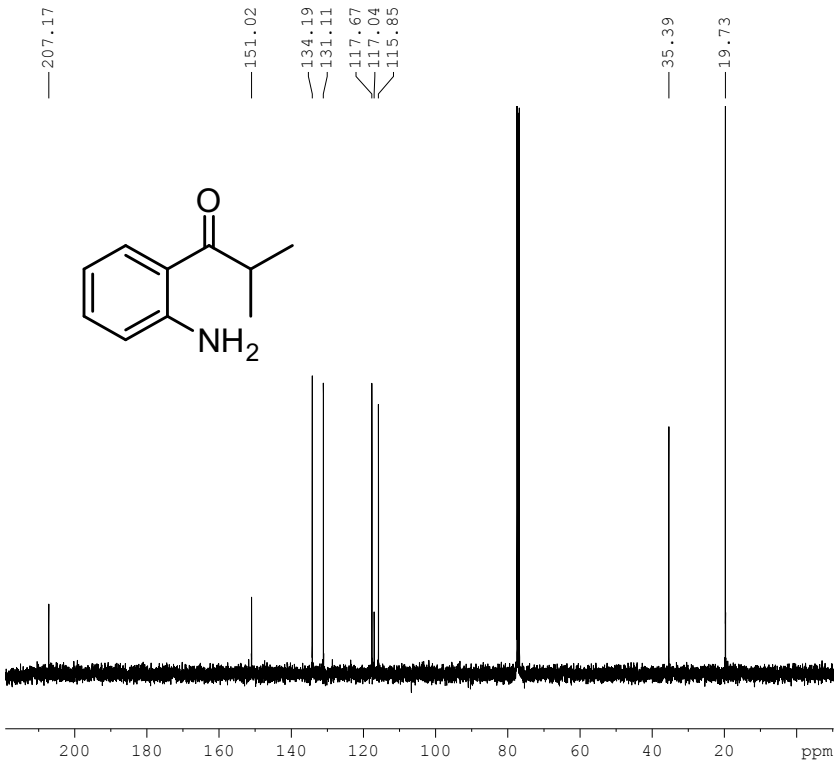



```
Current Data Parameters
NAME                  947
EXPNO                 654
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210827
Time               22.10 h
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ             4.0894465 sec
RG                 138.85
DW                 62.400 usec
DE                  6.50 usec
TE                 300.9 K
D1             0.50000000 sec
TD0                     1
SFO1          400.1320007 MHz
NUC1                   1H
P1                 15.00 usec
PLW1          10.50000000 W

F2 - Processing parameters
SI                  65536
SF            400.1300082 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **2b**



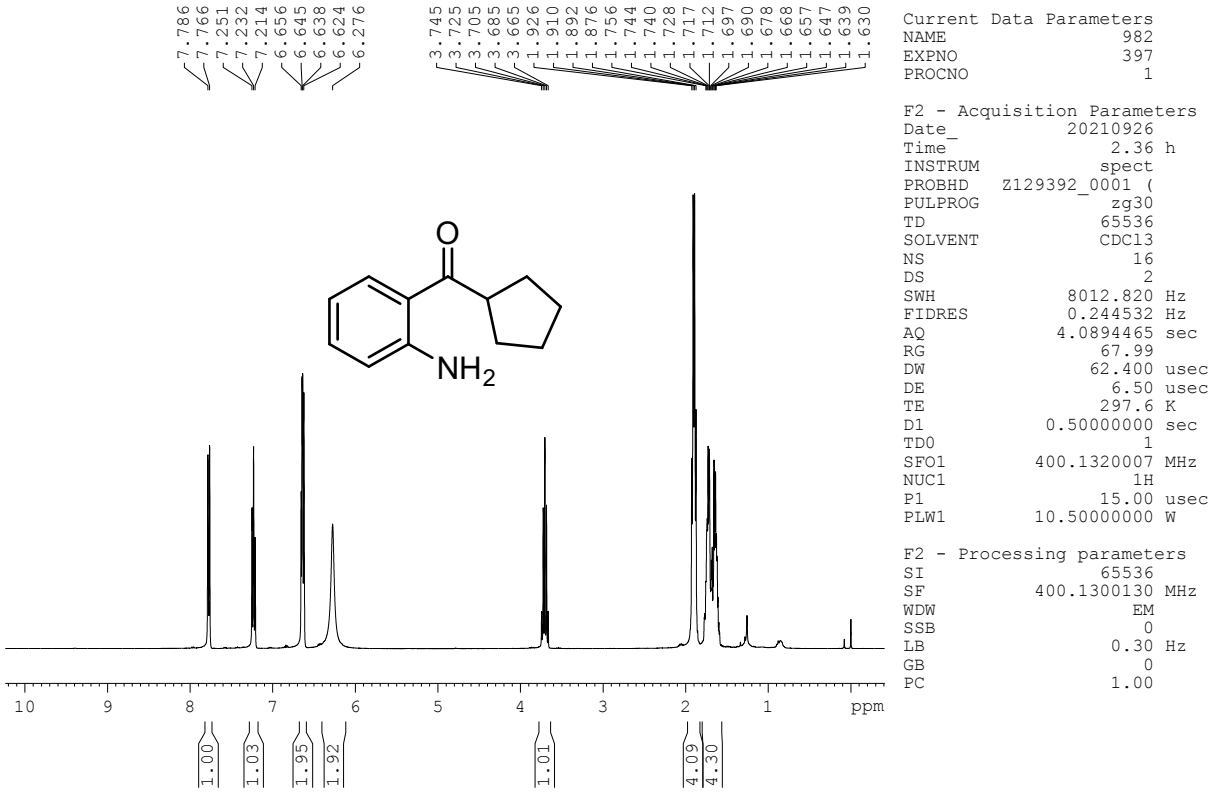

```
Current Data Parameters
NAME                  947
EXPNO                 655
PROCNO                  1

F2 - Acquisition Paramete
Date_            20210827
Time               22.16 h
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                  16540
SOLVENT             CDCl3
NS                    256
DS                      4
SWH           24038.461 H
FIDRES         2.906706 H
AQ             0.3440320 s
RG                 200.34
DW                 20.800 u
DE                  6.50 u
TE                 300.8 K
D1             1.00000000 s
D11            0.03000000 s
TD0                     1
SFO1          100.6228289 M
NUC1                  13C
P1                 10.00 u
PLW1          47.00000000 W
SFO2          400.1316005 M
NUC2                   1H
CPDPRG[2         waltz16
PCPD2              90.00 u
PLW2          10.50000000 W
PLW12          0.29166999 W
PLW13          0.14670999 W

F2 - Processing parameter
SI                  32768
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **2b**

(2-aminophenyl)(cyclopentyl)methanone: 2d

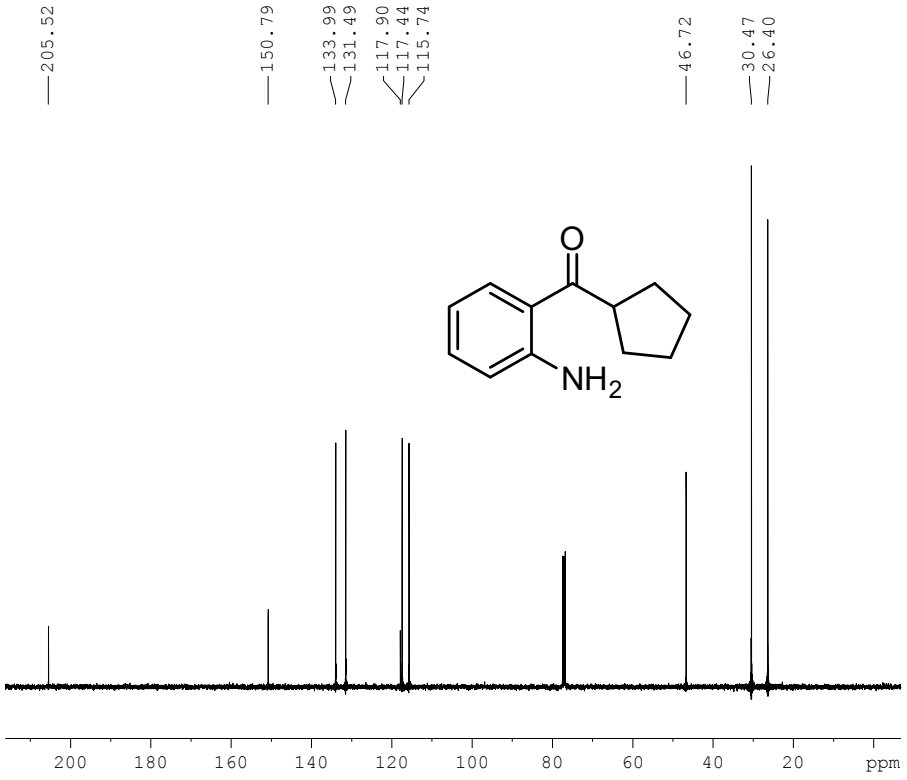


Current Data Parameters
NAME 982
EXPNO 397
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210926
Time 2.36 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 67.99
DW 62.400 usec
DE 6.50 usec
TE 297.6 K
D1 0.50000000 sec
TD0 1
SFO1 400.1320007 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.50000000 W

F2 - Processing parameters
SI 65536
SF 400.1300130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **2d**



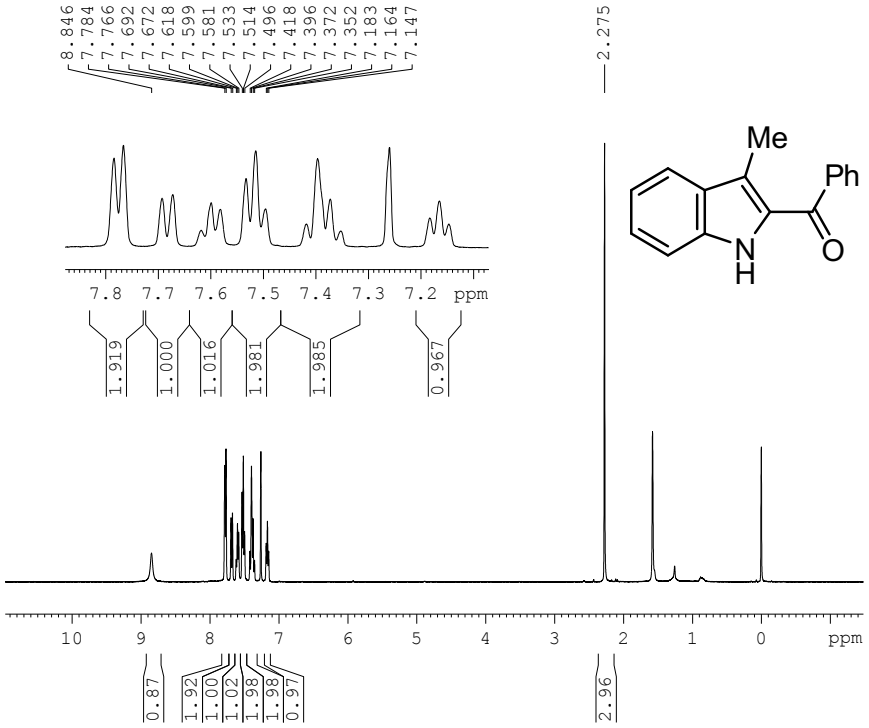
Current Data Parameters
NAME 982
EXPNO 398
PROCNO 1

F2 - Acquisition Parameter
Date_ 20210926
Time 2.43 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 H
FIDRES 2.906706 H
AQ 0.3440320 s
RG 200.34
DW 20.800 u
DE 6.50 u
TE 298.3 K
D1 1.00000000 s
D11 0.03000000 s
TD0 1
SFO1 100.6228289 M
NUC1 13C
P1 10.00 u
PLW1 47.00000000 W
SFO2 400.1316005 M
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 u
PLW2 10.50000000 W
PLW12 0.29166999 W
PLW13 0.14670999 W

F2 - Processing parameter
SI 32768

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **2d**

(3-methyl-1H-indol-2-yl)(phenyl)methanone: 3a



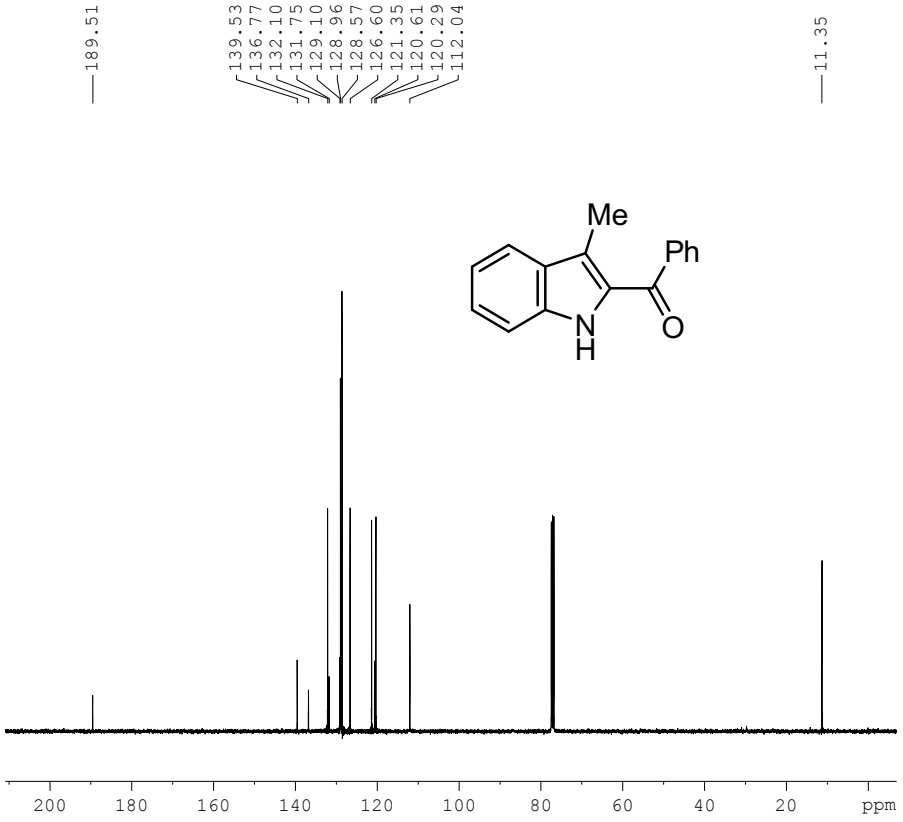

```
Current Data Parameters
NAME                 771(3)
EXPNO                   108
PROCNO                    1

F2 - Acquisition Parameters
Date_             20210108
Time                14.33
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                   200.34
DW                   62.400 usec
DE                    6.50 usec
TE                   297.0 K
D1              0.50000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          400.1320007 MHz
NUC1                     1H
P1                    15.70 usec
PLW1           7.75000000 W

F2 - Processing parameters
SI                    65536
SF            400.1300097 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3a**




```
Current Data Parameters
NAME                 771(3)
EXPNO                   687
PROCNO                    1

F2 - Acquisition Paramet
Date_             20210201
Time                 1.16
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  16540
SOLVENT             CDCl3
NS                   2000
DS                      4
SWH              24038.461
FIDRES            1.453353
AQ                0.3440320
RG                   200.34
DW                   20.800
DE                    6.50
TE                   297.6
D1              1.00000000
D11             0.03000000
TD0                       1

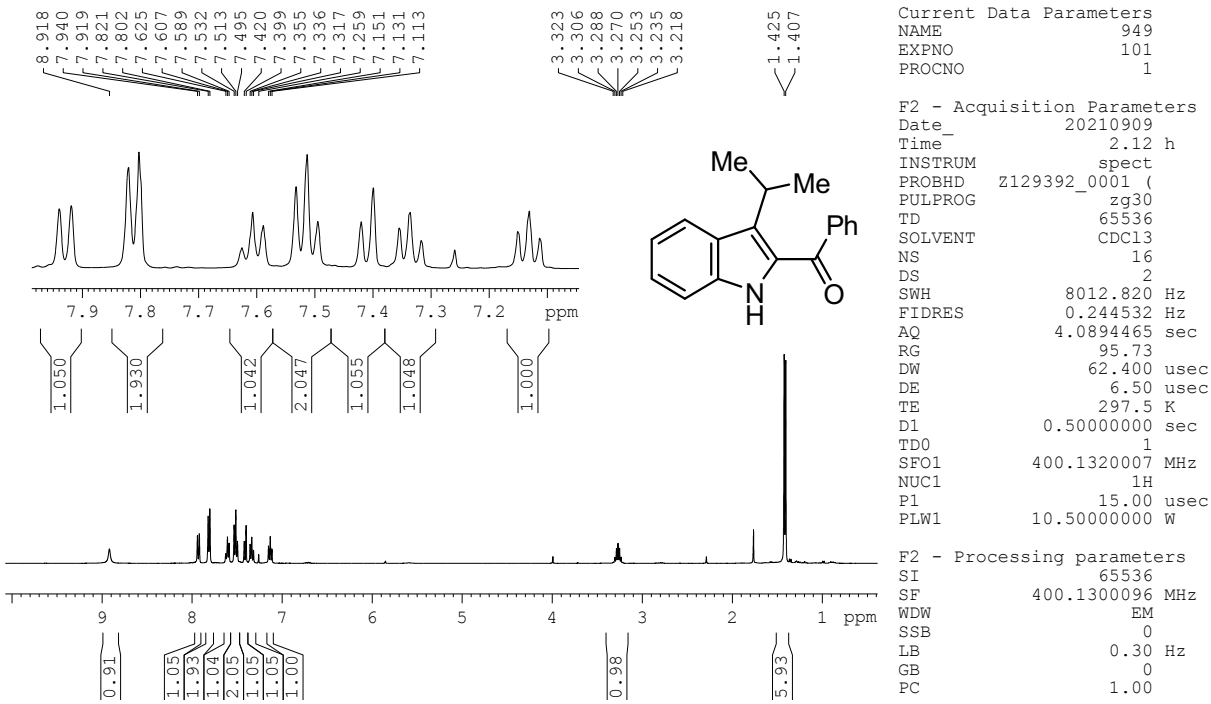
======== CHANNEL f1 ====
SFO1          100.6228289
NUC1                    13C
P1                    9.25
PLW1          47.00000000

======== CHANNEL f2 ====
SFO2          400.1316005
NUC2                     1H
CPDPRG[2          waltz16
PCPD2                90.00
PLW2           7.75000000
PLW12          0.23583999
PLW13          0.11863000

F2 - Processing paramete
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3a**

(3-isopropyl-1H-indol-2-yl)(phenyl)methanone: 3b

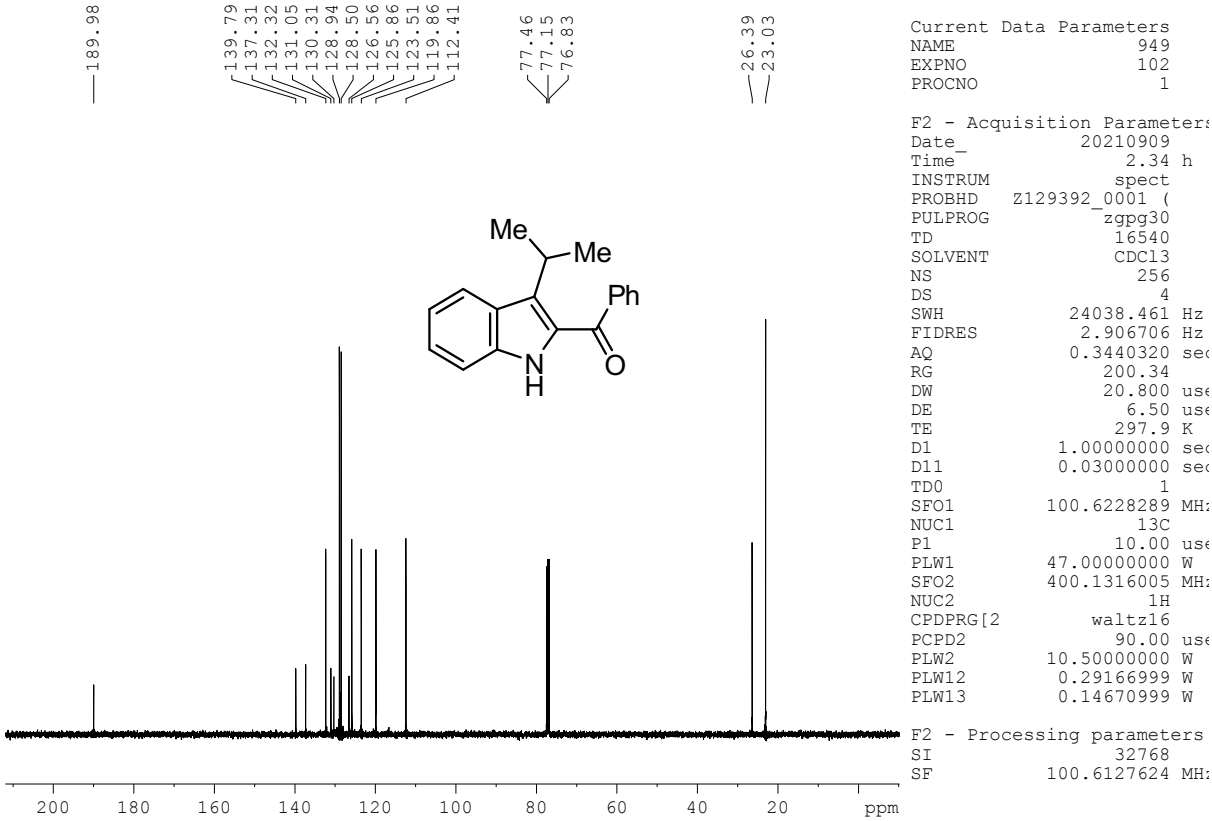



```
Current Data Parameters
NAME                  949
EXPNO                 101
PROCNO                  1

F2 - Acquisition Parameters
Date_           20210909
Time                2.12 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                  95.73
DW                62.400 usec
DE                 6.50 usec
TE                297.5 K
D1             0.50000000 sec
TD0                    1
SFO1          400.1320007 MHz
NUC1                  1H
P1                 15.00 usec
PLW1          10.50000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300096 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3b**



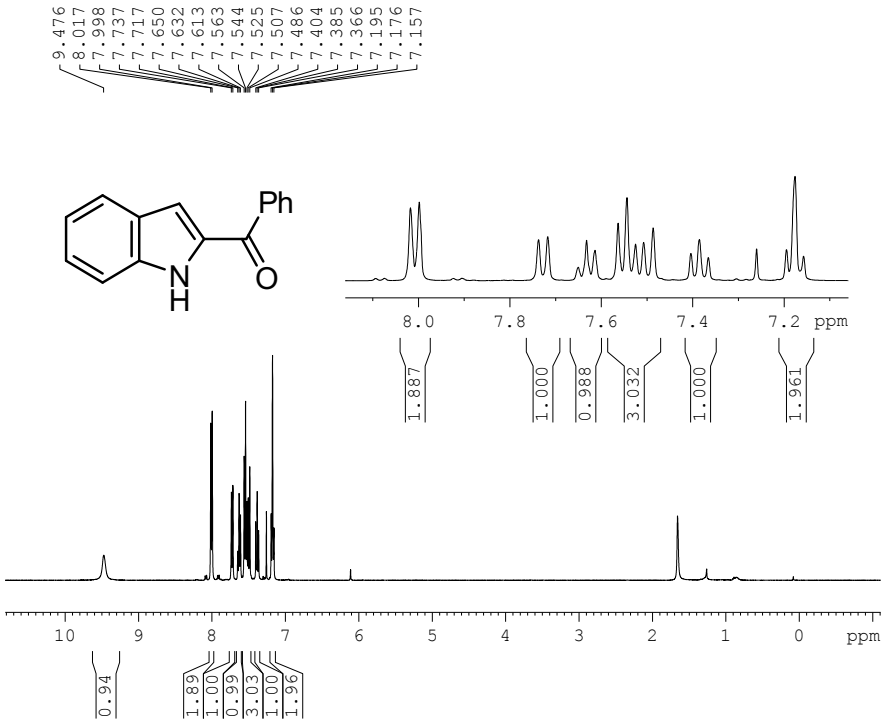

```
Current Data Parameters
NAME                  949
EXPNO                 102
PROCNO                  1

F2 - Acquisition Parameters
Date_           20210909
Time                2.34 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                   256
DS                     4
SWH             24038.461 Hz
FIDRES           2.906706 Hz
AQ               0.3440320 sec
RG                 200.34
DW                20.800 usec
DE                 6.50 usec
TE                297.9 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6228289 MHz
NUC1                 13C
P1                 10.00 usec
PLW1          47.00000000 W
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          10.50000000 W
PLW12          0.29166999 W
PLW13          0.14670999 W

F2 - Processing parameters
SI                 32768
SF            100.6127624 MHz
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3b**

(1H-indol-2-yl)(phenyl)methanone: 3c



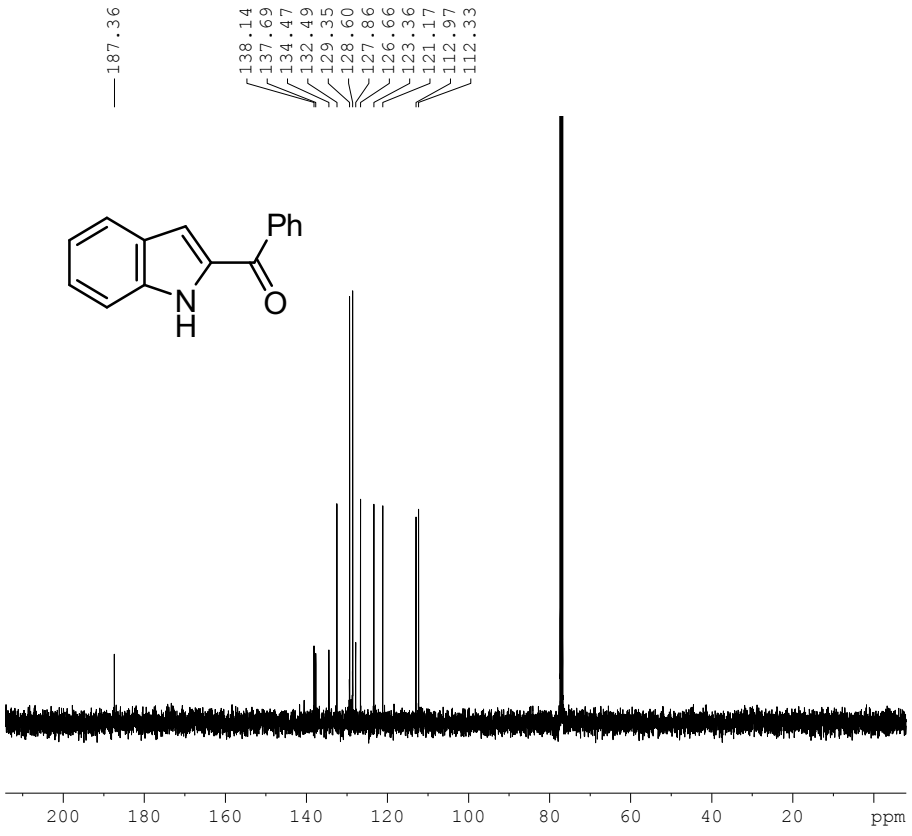

```
Current Data Parameters
NAME                  833(B)
EXPNO                    254
PROCNO                     1

F2 - Acquisition Parameters
Date_              20210316
Time                   1.35
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                   200.34
DW                   62.400 usec
DE                    6.50 usec
TE                   298.9 K
D1              0.50000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           400.1320007 MHz
NUC1                     1H
P1                    15.00 usec
PLW1           10.50000000 W

F2 - Processing parameters
SI                    65536
SF               400.1300095 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3c**




```
Current Data Parameters
NAME                  833(B)
EXPNO                    669
PROCNO                     1

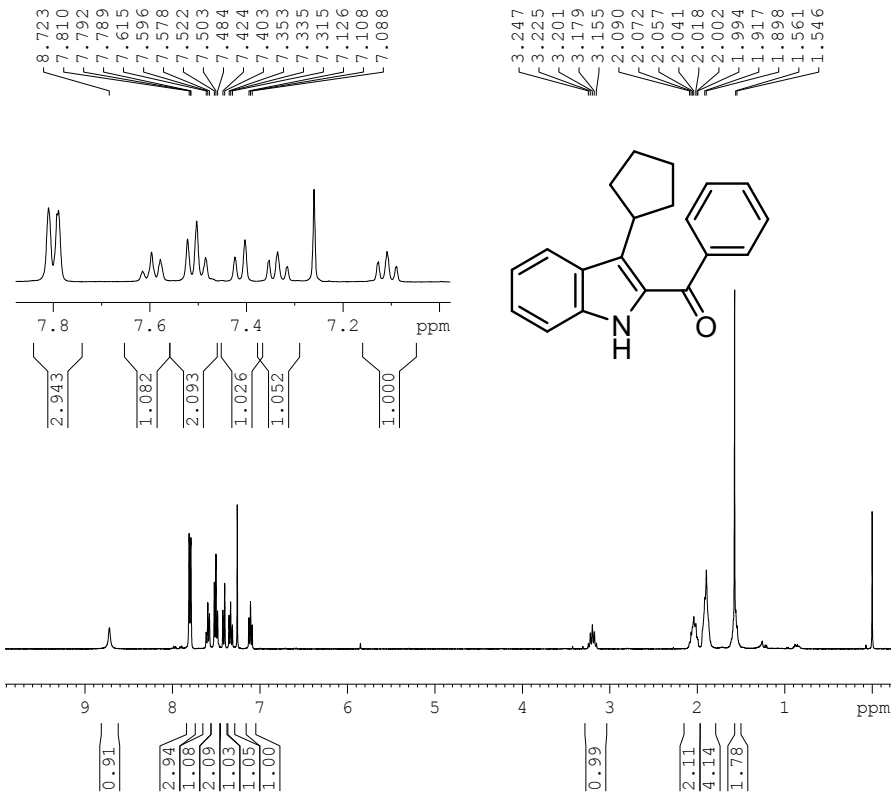
F2 - Acquisition Paramete
Date_              20210131
Time                  22.11
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG               zgpg30
TD                    16540
SOLVENT               CDCl3
NS                      256
DS                        4
SWH               24038.461 H
FIDRES             1.453353 H
AQ                0.3440320 s
RG                   200.34
DW                   20.800 u
DE                    6.50 u
TE                   297.5 K
D1              1.00000000 s
D11             0.03000000 s
TD0                        1

======== CHANNEL f1 =====
SFO1           100.6228289 M
NUC1                    13C
P1                    9.25 u
PLW1           47.00000000 W

======== CHANNEL f2 =====
SFO2           400.1316005 M
NUC2                     1H
CPDPRG[2            waltz16
PCPD2                 90.00 u
PLW2            7.75000000 W
PLW12           0.23583999 W
PLW13           0.11863000 W
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3c**

(3-cyclopentyl-1H-indol-2-yl)(phenyl)methanone: 3d

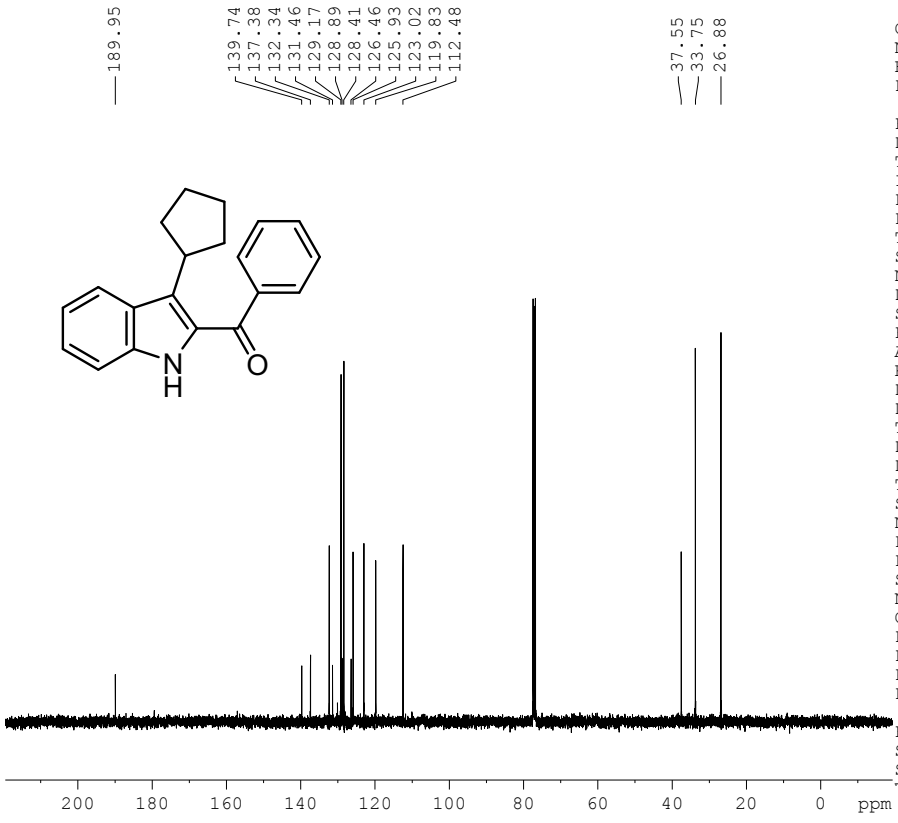



```
Current Data Parameters
NAME                  983
EXPNO                 457
PROCNO                  1

F2 - Acquisition Parameters
Date_           20211001
Time               5.59 h
INSTRUM           spect
PROBHD   Z129392_0001 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                200.34
DW                62.400 usec
DE                 6.50 usec
TE                297.9 K
D1            0.50000000 sec
TD0                  1
SFO1         400.1320007 MHz
NUC1                1H
P1                15.00 usec
PLW1         10.50000000 W

F2 - Processing parameters
SI                65536
SF           400.1300098 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3d**



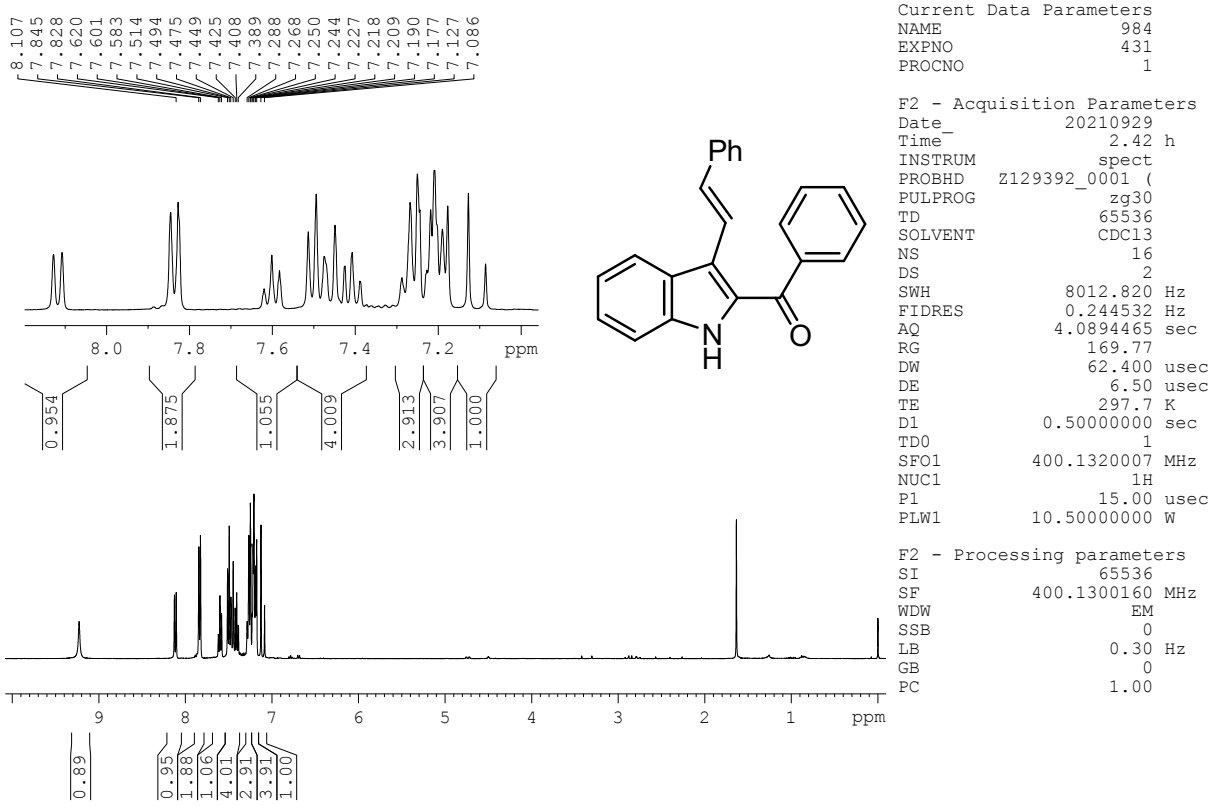

```
Current Data Parameters
NAME                  983
EXPNO                 441
PROCNO                  1

F2 - Acquisition Parameters
Date_           20210930
Time               0.49 h
INSTRUM           spect
PROBHD   Z129392_0001 (
PULPROG         zgpg30
TD               16540
SOLVENT          CDCl3
NS                 256
DS                   4
SWH           24038.461 Hz
FIDRES         2.906706 Hz
AQ             0.3440320 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE                297.8 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                  1
SFO1         100.6228289 MHz
NUC1                13C
P1                10.00 usec
PLW1         47.00000000 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W

F2 - Processing parameters
SI                32768
SF           100.6127592 MHz
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3d**

(E)-phenyl(3-styryl-1H-indol-2-yl)methanone: 3e

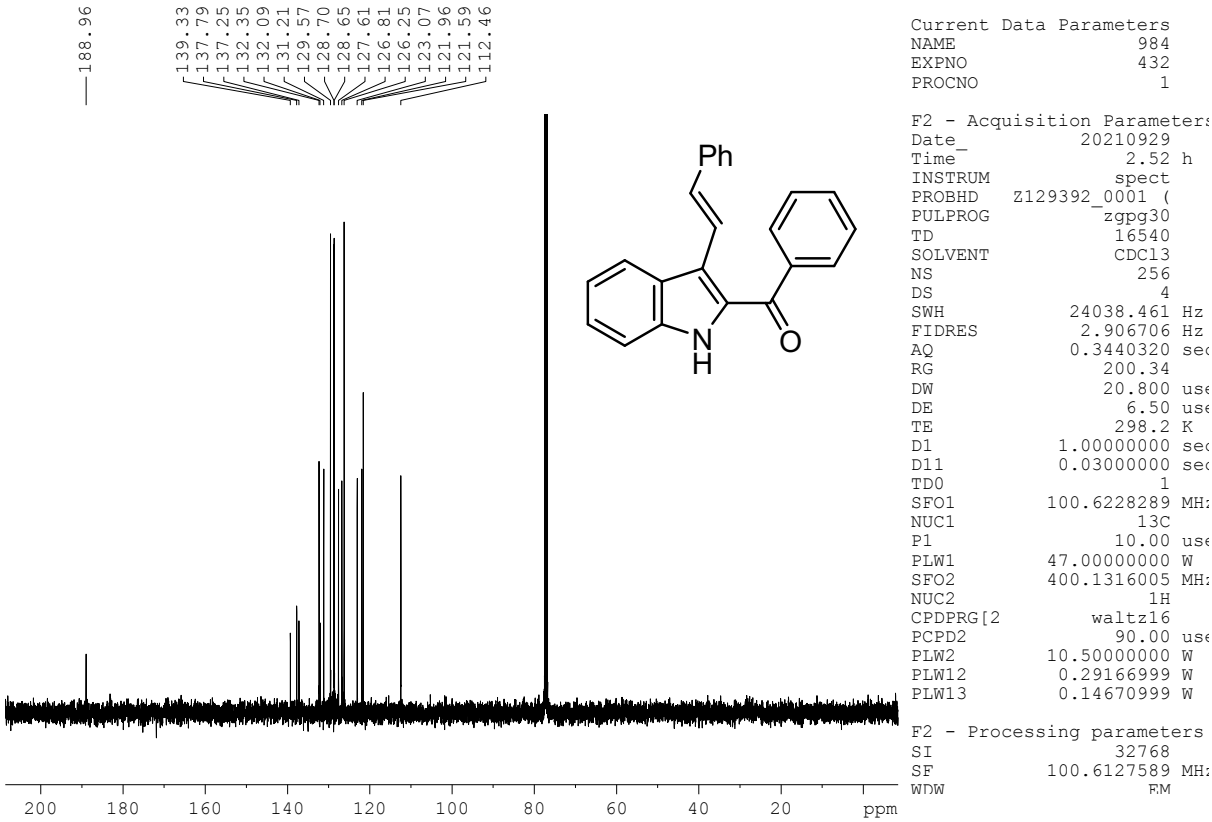



```
Current Data Parameters
NAME                  984
EXPNO                 431
PROCNO                  1

F2 - Acquisition Parameters
Date_           20210929
Time               2.42 h
INSTRUM           spect
PROBHD   Z129392_0001 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                169.77
DW                62.400 usec
DE                 6.50 usec
TE                297.7 K
D1            0.50000000 sec
TD0                   1
SFO1         400.1320007 MHz
NUC1                 1H
P1                15.00 usec
PLW1         10.50000000 W

F2 - Processing parameters
SI                65536
SF           400.1300160 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3e**



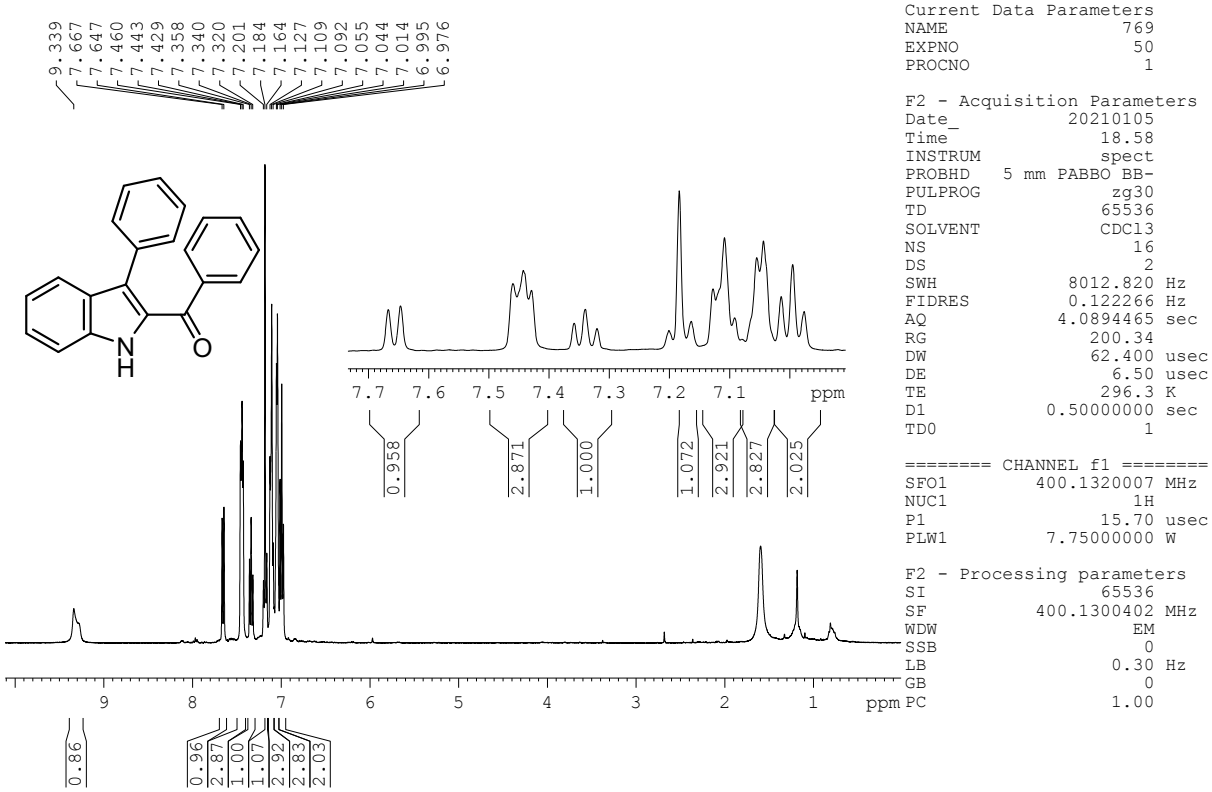

```
Current Data Parameters
NAME                  984
EXPNO                 432
PROCNO                  1

F2 - Acquisition Parameters
Date_           20210929
Time               2.52 h
INSTRUM           spect
PROBHD   Z129392_0001 (
PULPROG          zgpg30
TD                16540
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24038.461 Hz
FIDRES         2.906706 Hz
AQ             0.3440320 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE                298.2 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6228289 MHz
NUC1                 13C
P1                10.00 usec
PLW1         47.00000000 W
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W

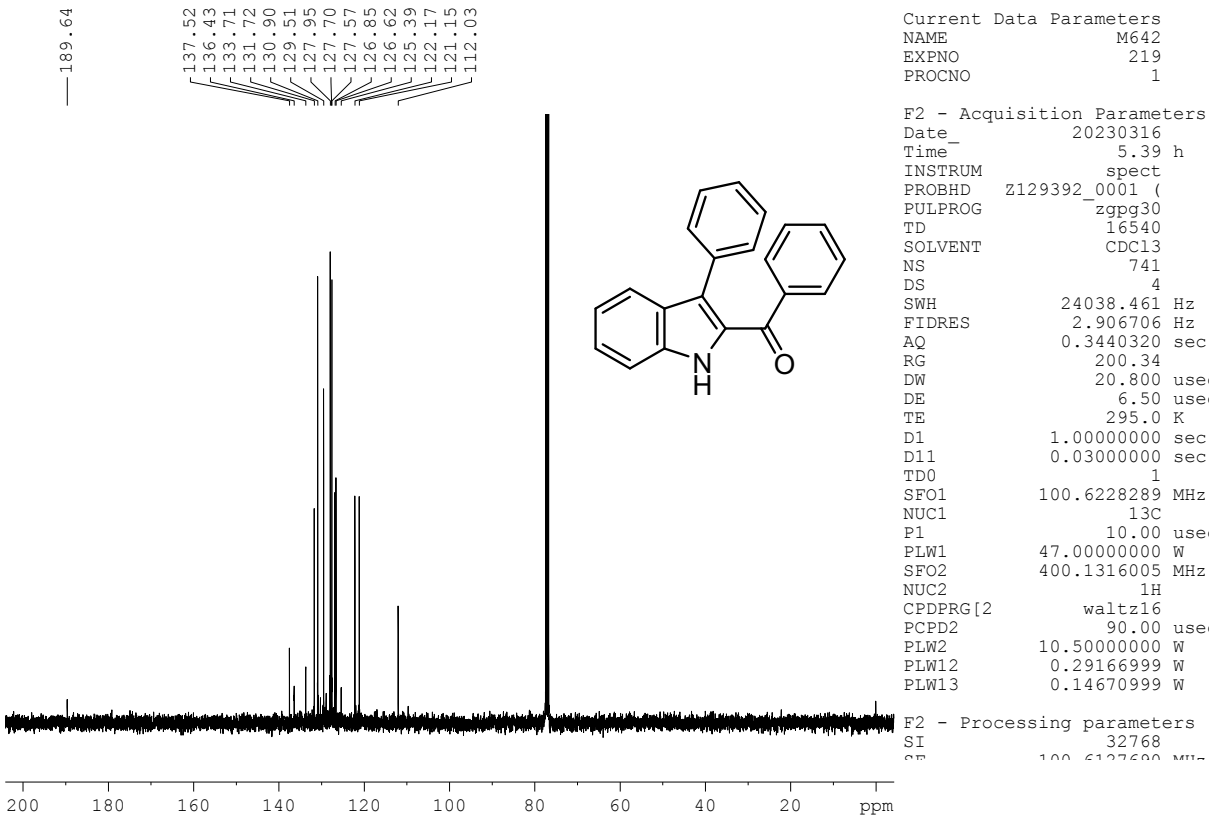
F2 - Processing parameters
SI                32768
SF           100.6127589 MHz
WDW                  EM
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3e**

phenyl(3-phenyl-1H-indol-2-yl)methanone: 3f

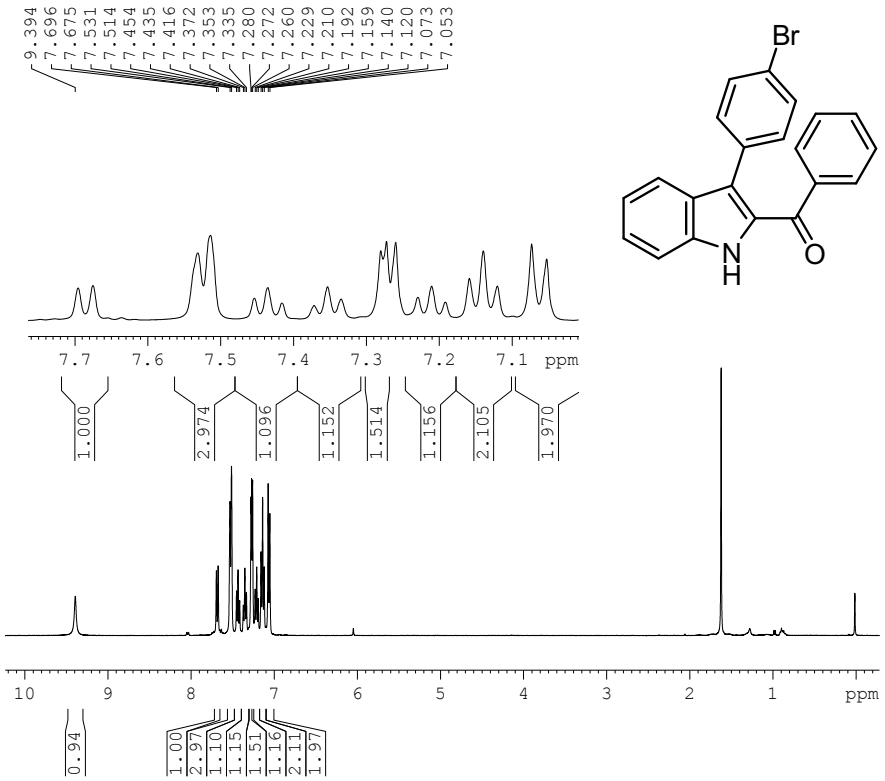


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3f**



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3f**

(3-(4-bromophenyl)-1H-indol-2-yl)(phenyl)methanone: 3g

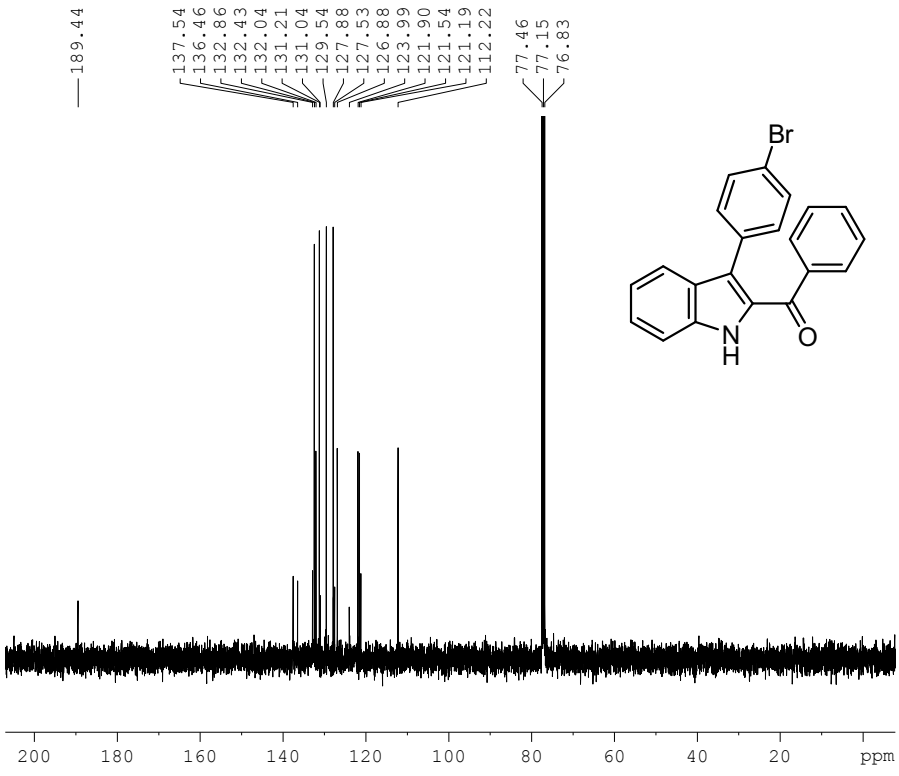



```
Current Data Parameters
NAME                  958
EXPNO                 177
PROCNO                  1

F2 - Acquisition Parameters
Date_           20210912
Time               1.52 h
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                200.34
DW                62.400 usec
DE                 6.50 usec
TE                297.6 K
D1             0.50000000 sec
TD0                    1
SFO1         400.1320007 MHz
NUC1                  1H
P1                15.00 usec
PLW1         10.50000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300046 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3g**

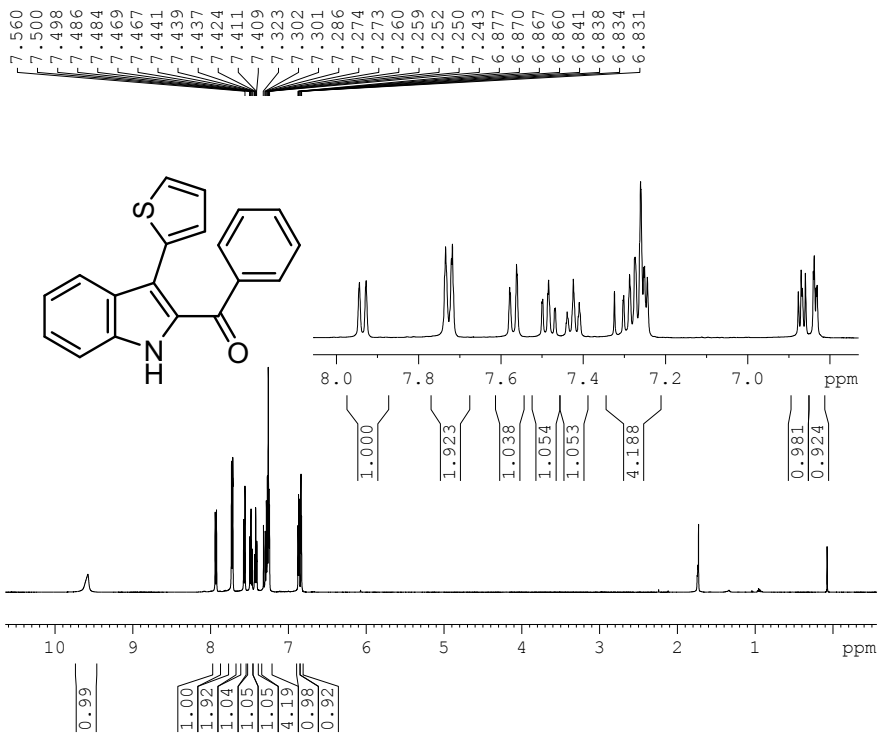



```
Current Data Parameters
NAME                  958
EXPNO                 178
PROCNO                  1

F2 - Acquisition Parameter
Date_           20210912
Time               22.05 h
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                   500
DS                     4
SWH            24038.461 Hz
FIDRES          2.906706 Hz
AQ              0.3440320 se
RG                200.34
DW                20.800 us
DE                 6.50 us
TE                298.0 K
D1             1.00000000 se
D11            0.03000000 se
TD0                    1
SFO1         100.6228289 MH
NUC1                  13C
P1                10.00 us
PLW1         47.00000000 W
SFO2         400.1316005 MH
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 us
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3g**

phenyl(3-(thiophen-2-yl)-1H-indol-2-yl)methanone: 3h



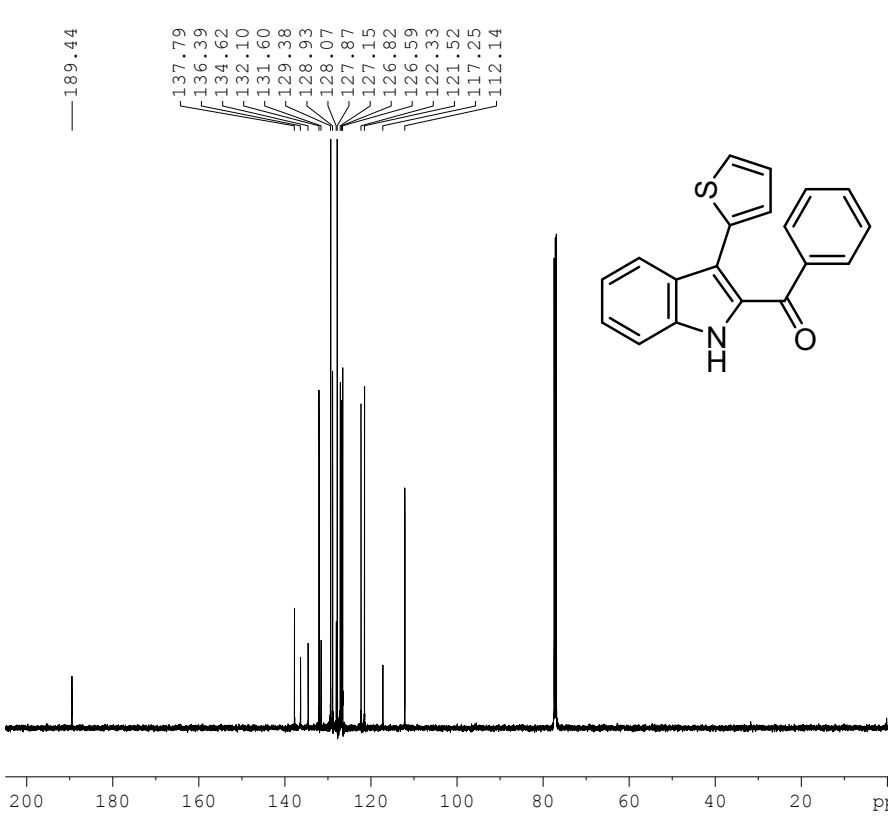

```
Current Data Parameters
NAME                   971
EXPNO                   69
PROCNO                   1

F2 - Acquisition Parameters
Date_           20210923
Time                0.54
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     2
SWH            10000.000 Hz
FIDRES          0.305176 Hz
AQ             1.6384000 sec
RG                114.76
DW                50.000 usec
DE                 6.50 usec
TE                298.4 K
D1             0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1525008 MHz
NUC1                   1H
P1                 11.75 usec
PLW1         15.30000019 W

F2 - Processing parameters
SI                 65536
SF           500.1499805 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3h**




```
Current Data Parameters
NAME                   971
EXPNO                   70
PROCNO                   1

F2 - Acquisition Parameters
Date_           20210923
Time                1.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 20480
SOLVENT            CDCl3
NS                  2000
DS                     4
SWH            29761.904 Hz
FIDRES          1.453218 Hz
AQ             0.3440640 sec
RG                202.34
DW                16.800 usec
DE                 6.50 usec
TE                299.2 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1

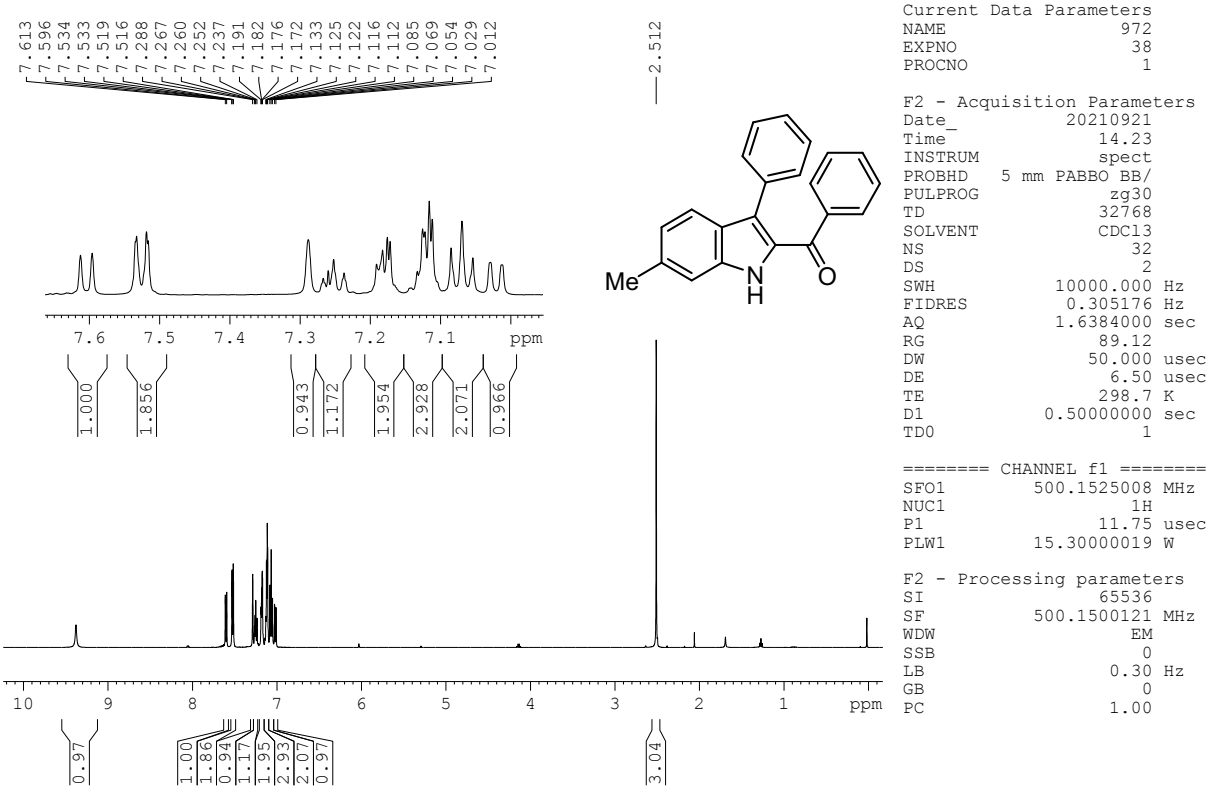
======== CHANNEL f1 ========
SFO1         125.7753932 MHz
NUC1                   13C
P1                 10.20 usec
PLW1        103.00000000 W

======== CHANNEL f2 ========
SFO2         500.1520006 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2         15.30000019 W
PLW12         0.39658999 W
PLW13         0.19948000 W

F2 - Processing parameters
SI                 32768
SF           125.7628053 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3h**

(6-methyl-3-phenyl-1H-indol-2-yl)(phenyl)methanone: 3i



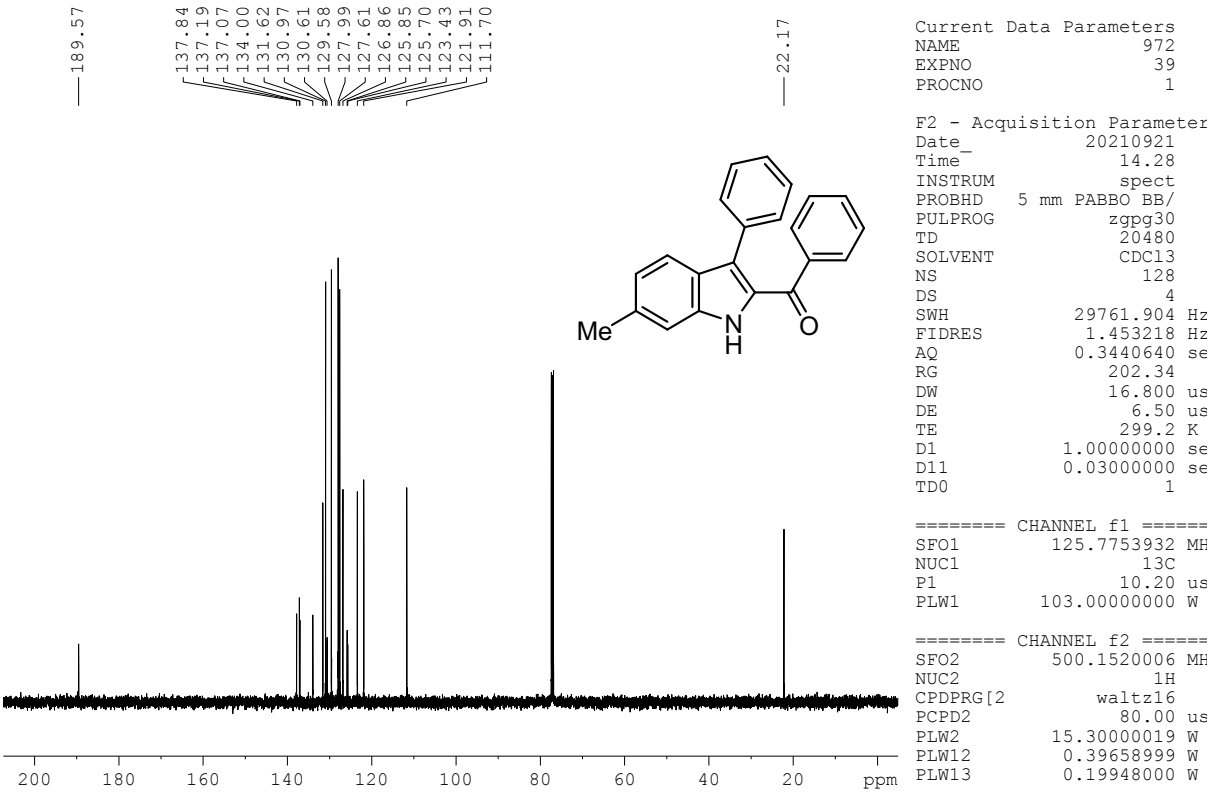

```
Current Data Parameters
NAME                  972
EXPNO                  38
PROCNO                  1

F2 - Acquisition Parameters
Date_           20210921
Time               14.23
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ            1.6384000 sec
RG                 89.12
DW               50.000 usec
DE                6.50 usec
TE                298.7 K
D1           0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        500.1525008 MHz
NUC1                   1H
P1                 11.75 usec
PLW1        15.30000019 W

F2 - Processing parameters
SI                 65536
SF          500.1500121 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3i**




```
Current Data Parameters
NAME                  972
EXPNO                  39
PROCNO                  1

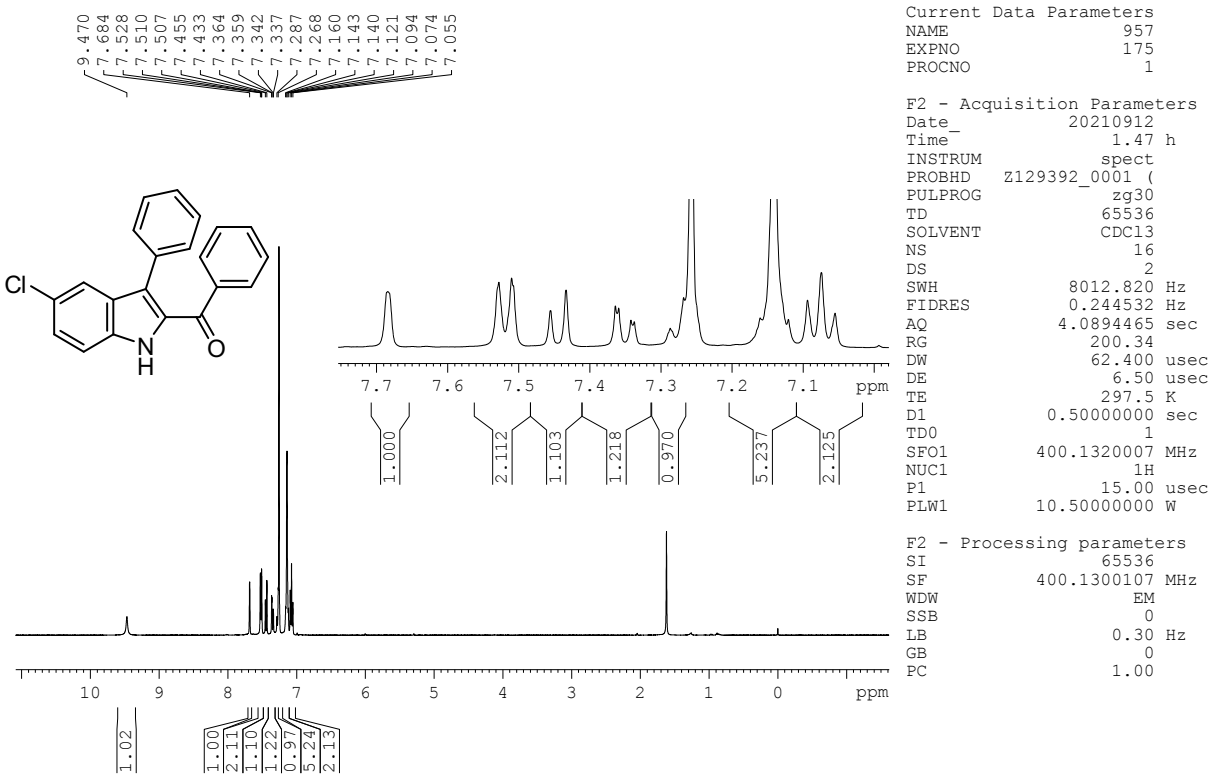
F2 - Acquisition Parameter
Date_           20210921
Time               14.28
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 20480
SOLVENT            CDCl3
NS                   128
DS                     4
SWH           29761.904 Hz
FIDRES         1.453218 Hz
AQ            0.3440640 se
RG                202.34
DW                16.800 us
DE                 6.50 us
TE                299.2 K
D1           1.00000000 se
D11          0.03000000 se
TD0                    1

======== CHANNEL f1 ======
SFO1        125.7753932 MH
NUC1                  13C
P1                10.20 us
PLW1        103.00000000 W

======== CHANNEL f2 ======
SFO2        500.1520006 MH
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              80.00 us
PLW2        15.30000019 W
PLW12        0.39658999 W
PLW13        0.19948000 W
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3i**

(5-chloro-3-phenyl-1H-indol-2-yl)(phenyl)methanone: 3j

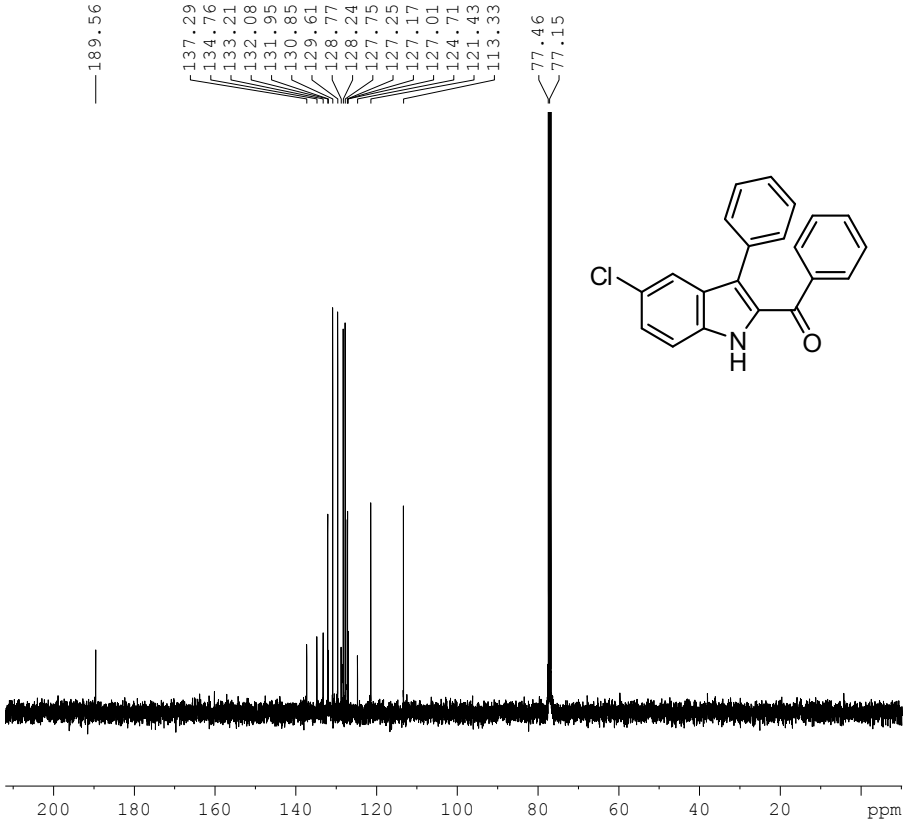



```
Current Data Parameters
NAME                  957
EXPNO                 175
PROCNO                  1

F2 - Acquisition Parameters
Date_           20210912
Time                1.47 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                 200.34
DW                 62.400 usec
DE                  6.50 usec
TE                 297.5 K
D1              0.50000000 sec
TD0                    1
SFO1           400.1320007 MHz
NUC1                  1H
P1                 15.00 usec
PLW1           10.50000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300107 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3j**



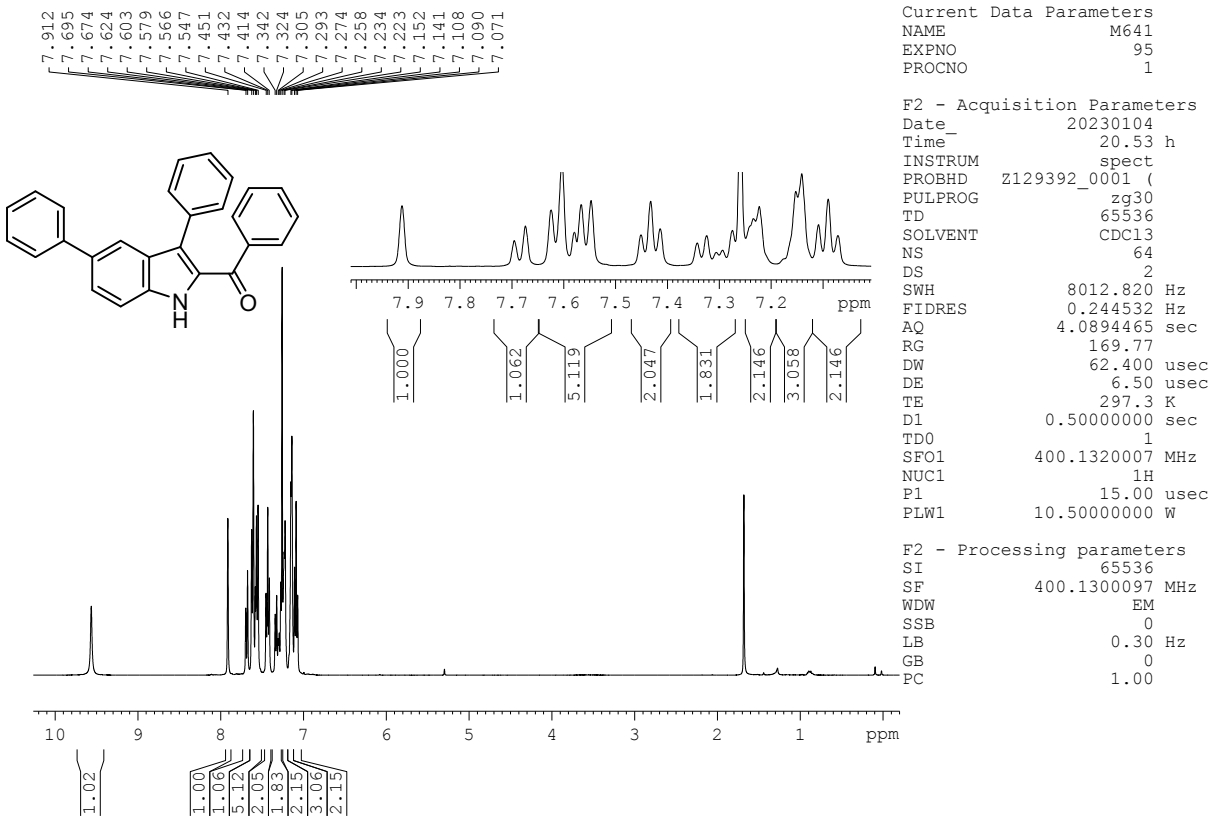

```
Current Data Parameters
NAME                  957
EXPNO                 176
PROCNO                  1

F2 - Acquisition Paramet
Date_           20210912
Time               21.50
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                   500
DS                     4
SWH             24038.461
FIDRES           2.906706
AQ               0.3440320
RG                 200.34
DW                 20.800
DE                  6.50
TE                 297.6
D1              1.00000000
D11             0.03000000
TD0                    1
SFO1           100.6228289
NUC1                  13C
P1                 10.00
PLW1           47.00000000
SFO2           400.1316005
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00
PLW2           10.50000000
PLW12           0.29166999
PLW13           0.14670999

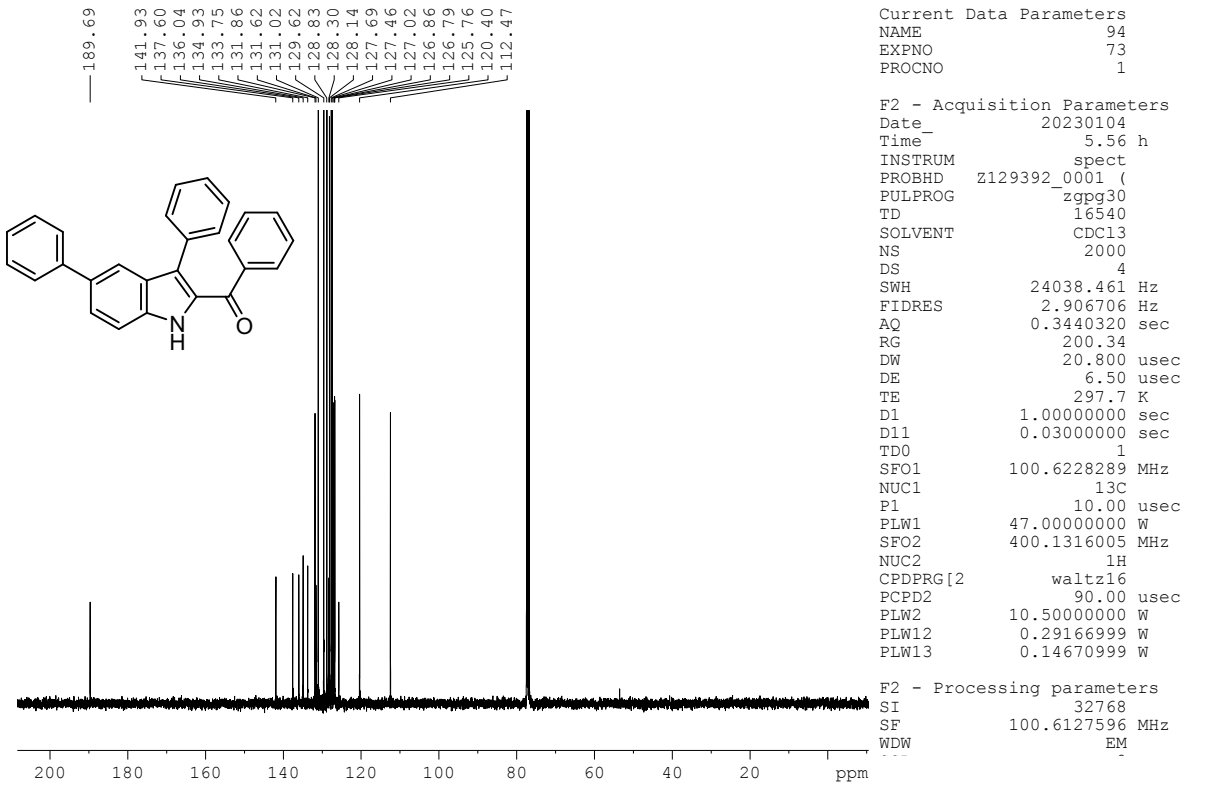
F2 - Processing paramete
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3j**

(3,5-diphenyl-1H-indol-2-yl)(phenyl)methanone: 3k

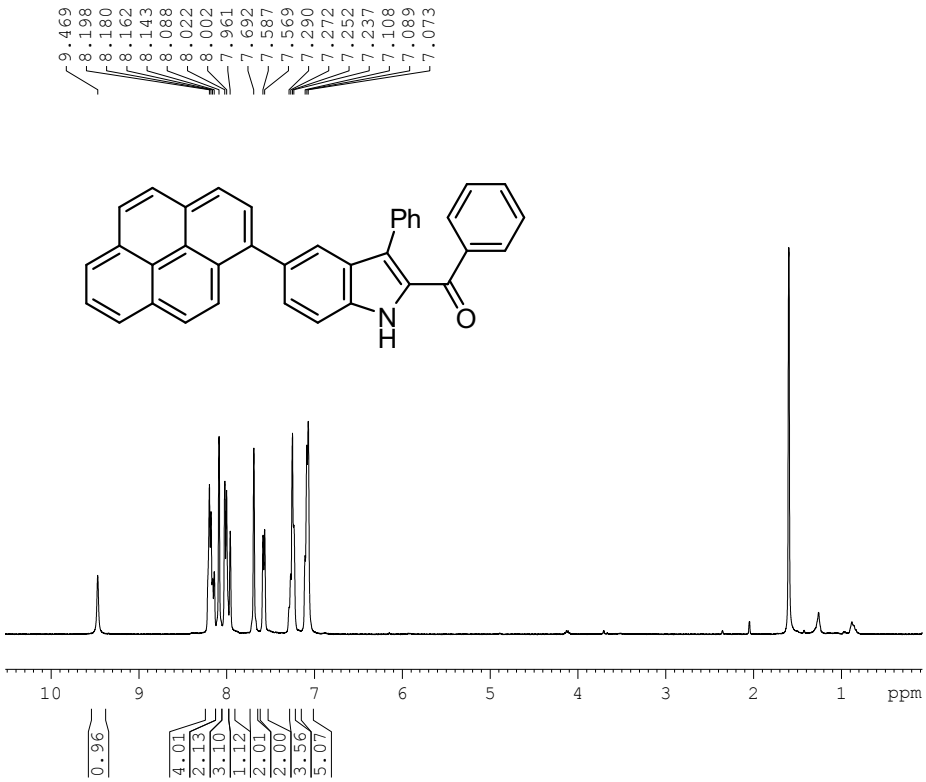


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3k**



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3k**

phenyl(3-phenyl-5-(pyren-1-yl)-1H-indol-2-yl)methanone: 3l

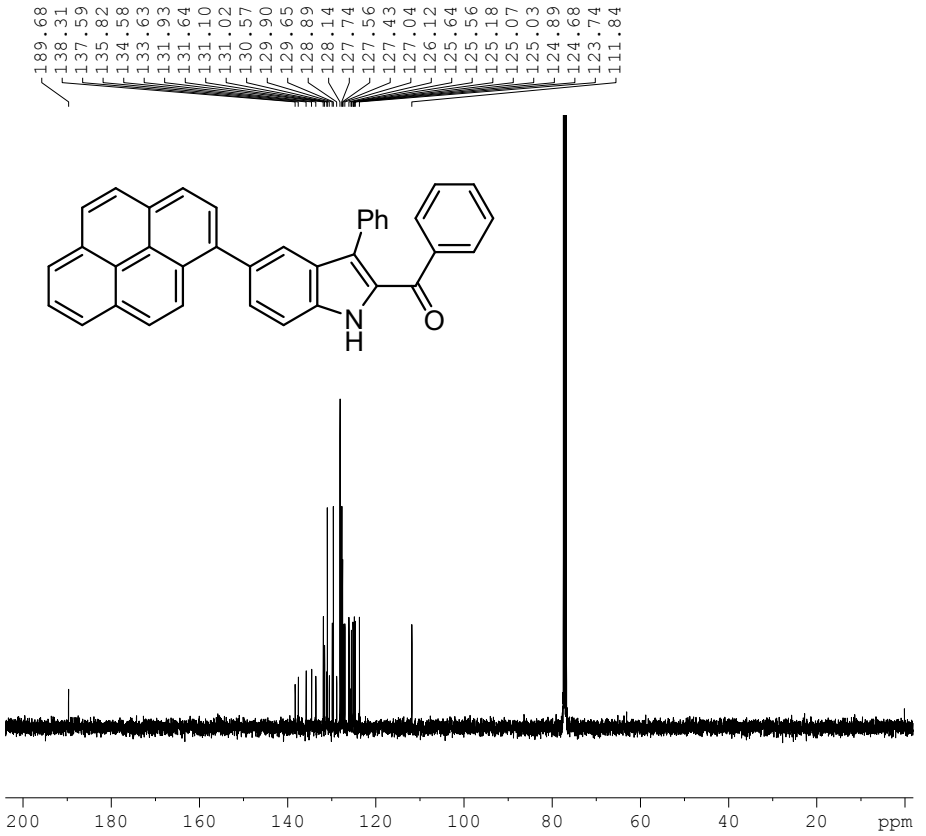


Current Data Parameters
NAME JAN 2023 (604-7
EXPNO 768
PROCNO 1

F2 - Acquisition Paramet
Date_ 20230130
Time 17.17
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820
FIDRES 0.244532
AQ 4.0894465
RG 200.34
DW 62.400
DE 6.50
TE 294.4
D1 0.50000000
TD0 1
SFO1 400.1320007
NUC1 1H
P1 15.00
PLW1 10.50000000

F2 - Processing paramete
SI 65536
SF 400.1300114
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3l**



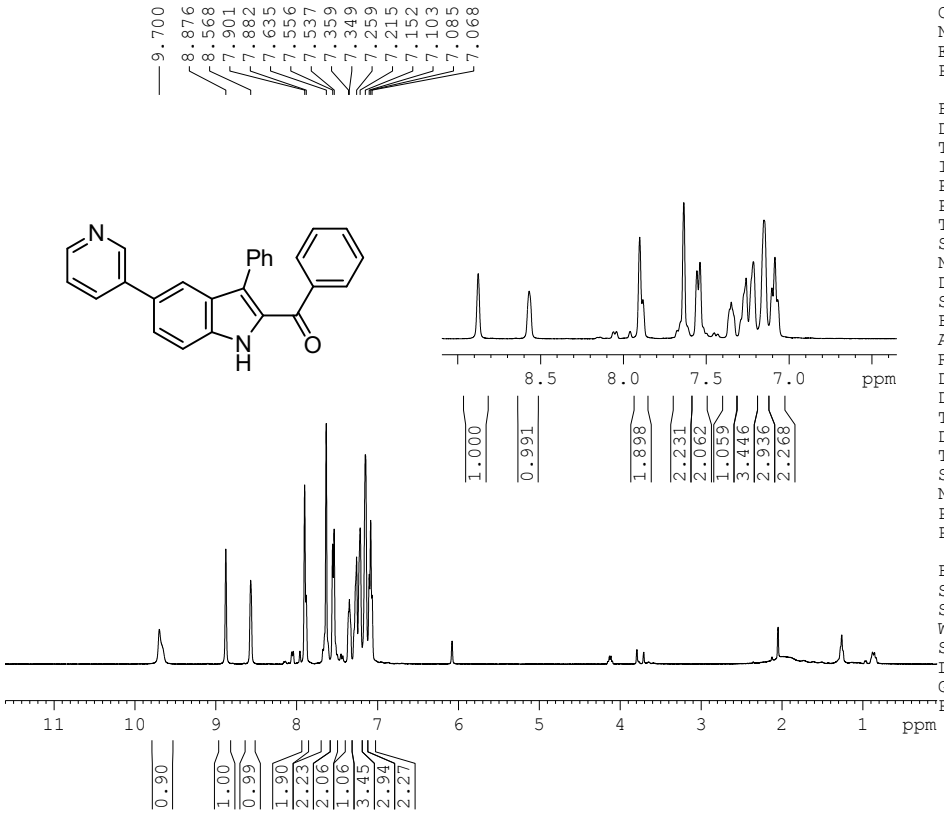
Current Data Parameters
NAME JAN 2023 (604-
EXPNO 780
PROCNO 1

F2 - Acquisition Paramet
Date_ 20230131
Time 2.03
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 2000
DS 4
SWH 24038.461
FIDRES 2.906706
AQ 0.3440320
RG 200.34
DW 20.800
DE 6.50
TE 295.2
D1 1.00000000
D11 0.03000000
TD0 1
SFO1 100.6228289
NUC1 13C
P1 10.00
PLW1 47.00000000
SFO2 400.1316005
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00
PLW2 10.50000000
PLW12 0.29166999
PLW13 0.14670999

F2 - Processing paramete
SI 32768
SF 100.6127577
WDW EM

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3l**

phenyl(3-phenyl-5-(pyridin-3-yl)-1H-indol-2-yl)methanone : 3m

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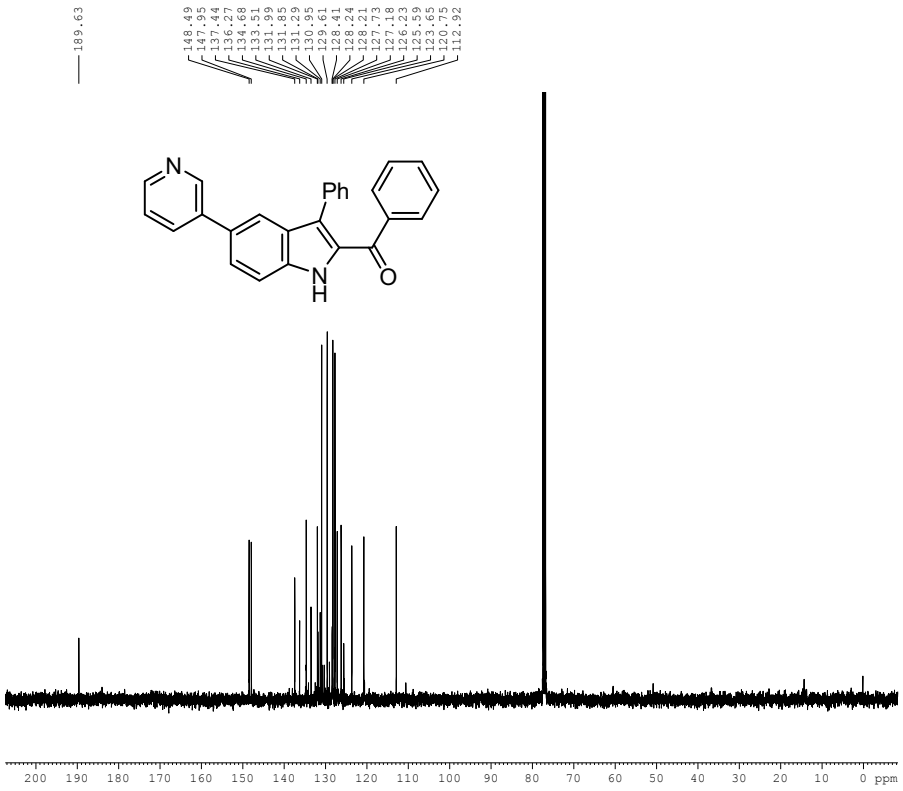
Current Data Parameters
NAME              M690(R)
EXPNO                 285
PROCNO                  1

F2 - Acquisition Paramet
Date_            20230206
Time                18.29
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              8012.820
FIDRES           0.244532
AQ               4.0894465
RG                200.34
DW                62.400
DE                  6.50
TE                295.0
D1             0.50000000
TD0                    1
SFO1          400.1320007
NUC1                  1H
P1                 15.00
PLW1          10.50000000

F2 - Processing paramete
SI                 65536
SF            400.1300091
WDW                   EM
SSB                    0
LB                  0.30
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3m**



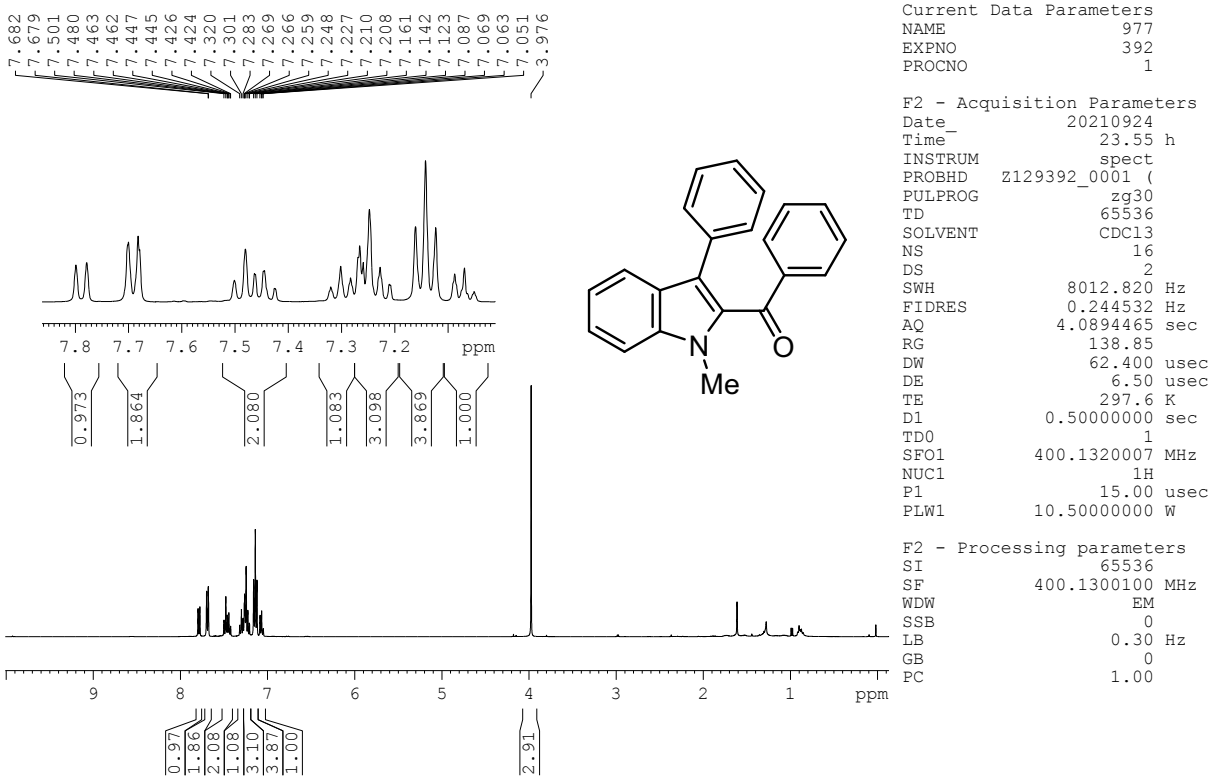

```
Current Data Parameters
NAME              M690(R)
EXPNO                 349
PROCNO                  1

F2 - Acquisition Paramete
Date_            20230208
Time                3.21 h
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                  1500
DS                     4
SWH           24038.461 H
FIDRES         2.906706 H
AQ             0.3440320 s
RG                200.34
DW                20.800 u
DE                 6.50 u
TE                296.1 K
D1           1.00000000 s
D11          0.03000000 s
TD0                    1
SFO1         100.6228289 M
NUC1                 13C
P1                10.00 u
PLW1         47.00000000 W
SFO2         400.1316005 M
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             90.00 u
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W

F2 - Processing parameter
SI                 32768
SF           100.6127585 M
WDW                   EM
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3m**

(1-methyl-3-phenyl-1H-indol-2-yl)(phenyl)methanone: 3n

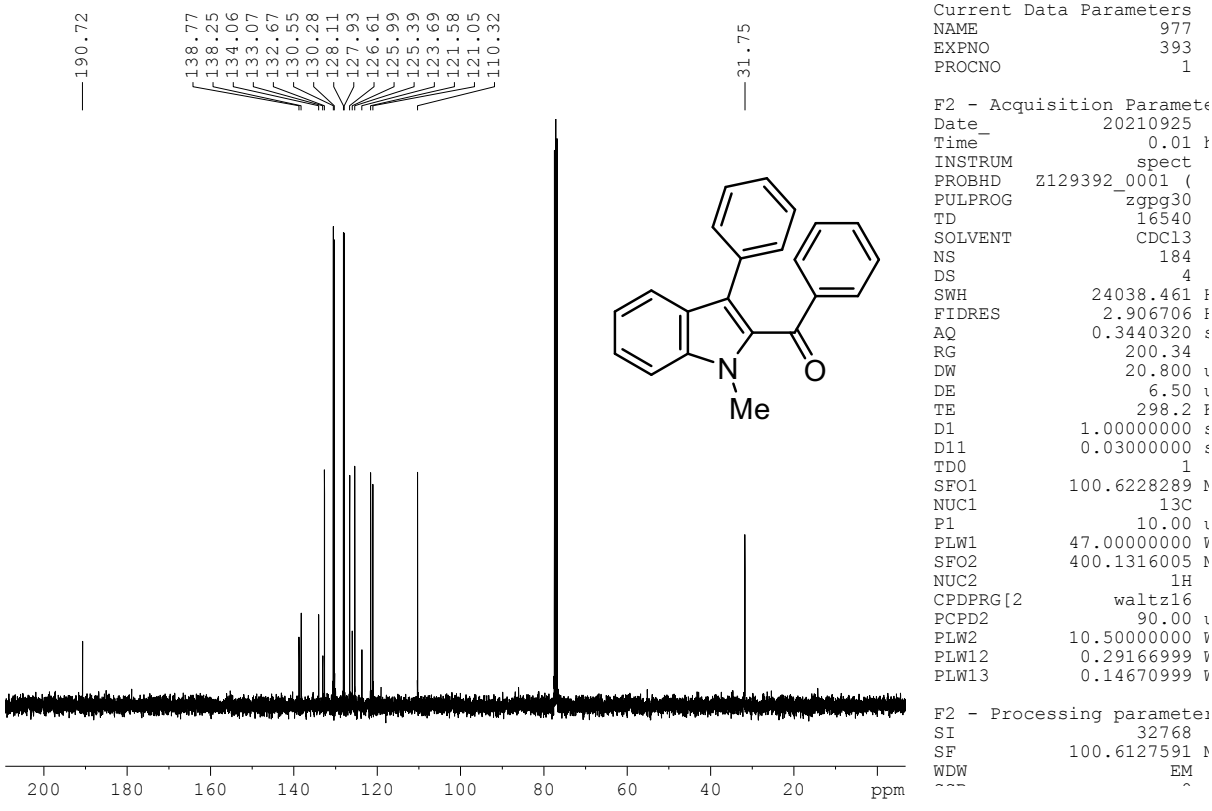


Current Data Parameters
NAME 977
EXPNO 392
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210924
Time 23.55 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 138.85
DW 62.400 usec
DE 6.50 usec
TE 297.6 K
D1 0.50000000 sec
TD0 1
SFO1 400.1320007 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.50000000 W

F2 - Processing parameters
SI 65536
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3n**



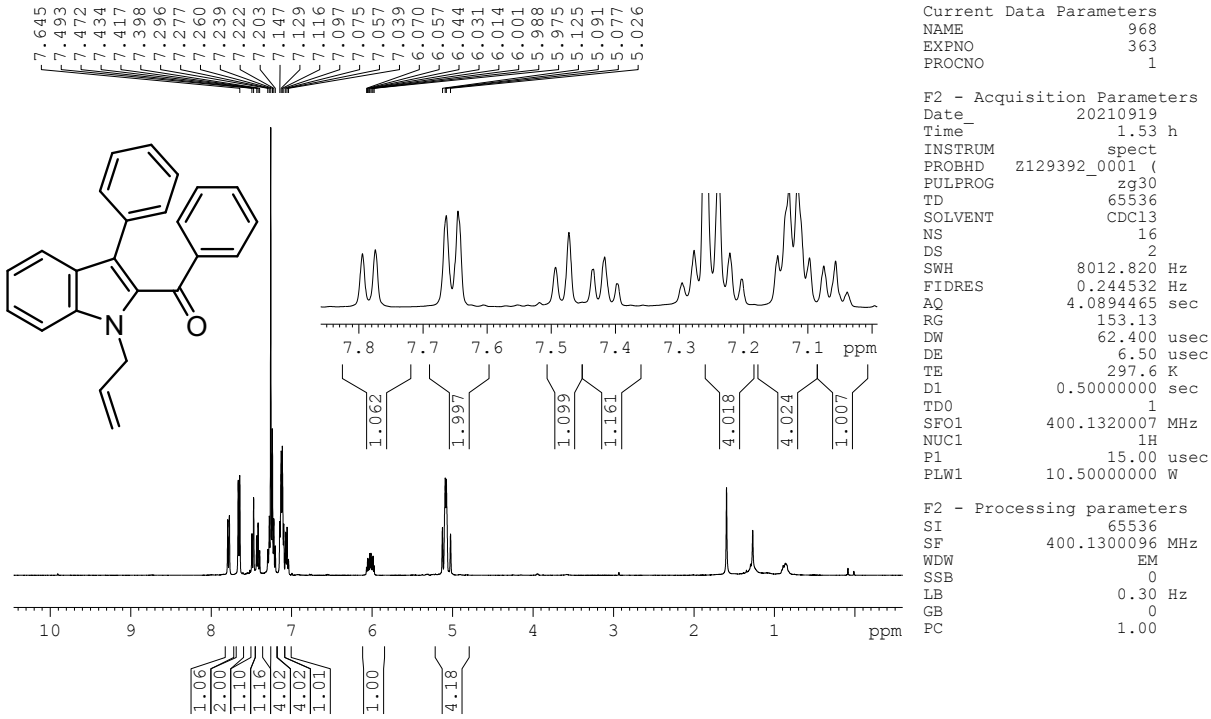
Current Data Parameters
NAME 977
EXPNO 393
PROCNO 1

F2 - Acquisition Parameter
Date_ 20210925
Time 0.01 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 184
DS 4
SWH 24038.461 H
FIDRES 2.906706 H
AQ 0.3440320 s
RG 200.34
DW 20.800 u
DE 6.50 u
TE 298.2 K
D1 1.00000000 s
D11 0.03000000 s
TD0 1
SFO1 100.6228289 M
NUC1 13C
P1 10.00 u
PLW1 47.00000000 W
SFO2 400.1316005 M
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 u
PLW2 10.50000000 W
PLW12 0.29166999 W
PLW13 0.14670999 W

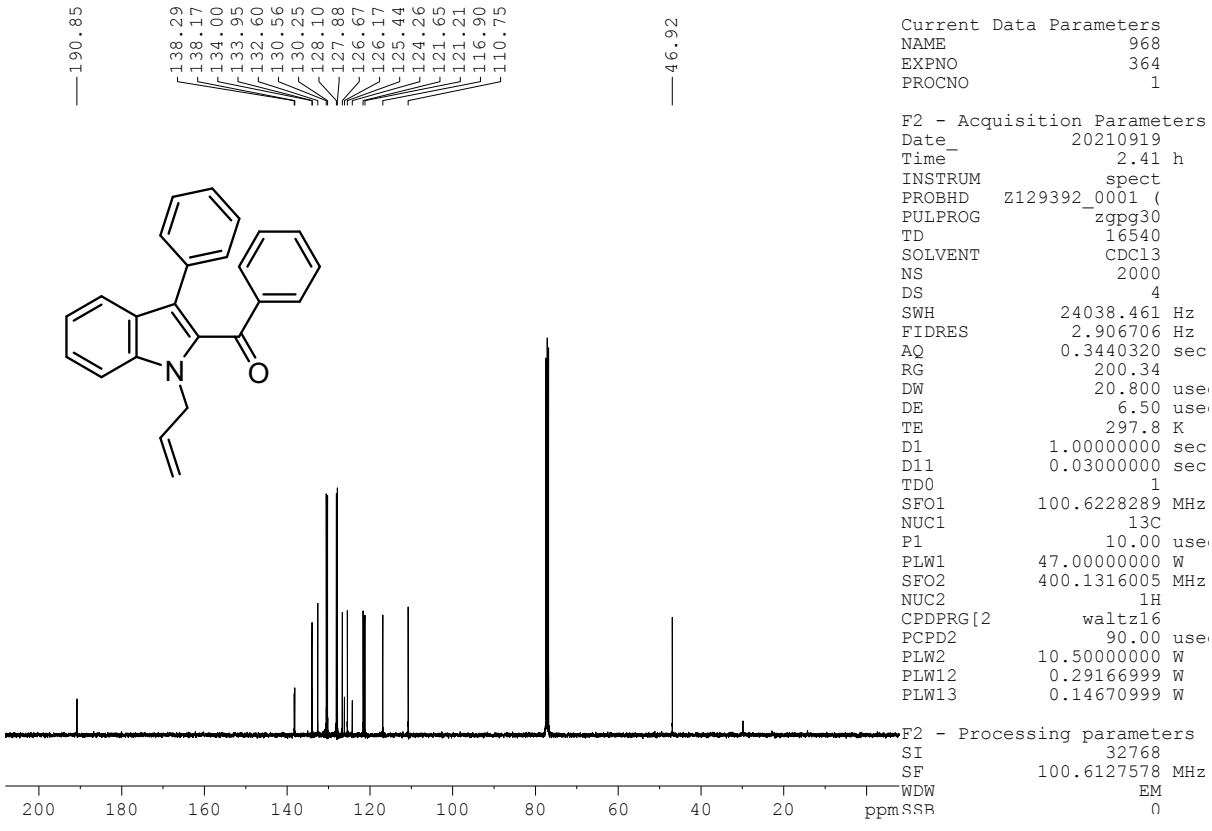
F2 - Processing parameter
SI 32768
SF 100.6127591 M
WDW EM

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3n**

(1-allyl-3-phenyl-1H-indol-2-yl)(phenyl)methanone: 3o

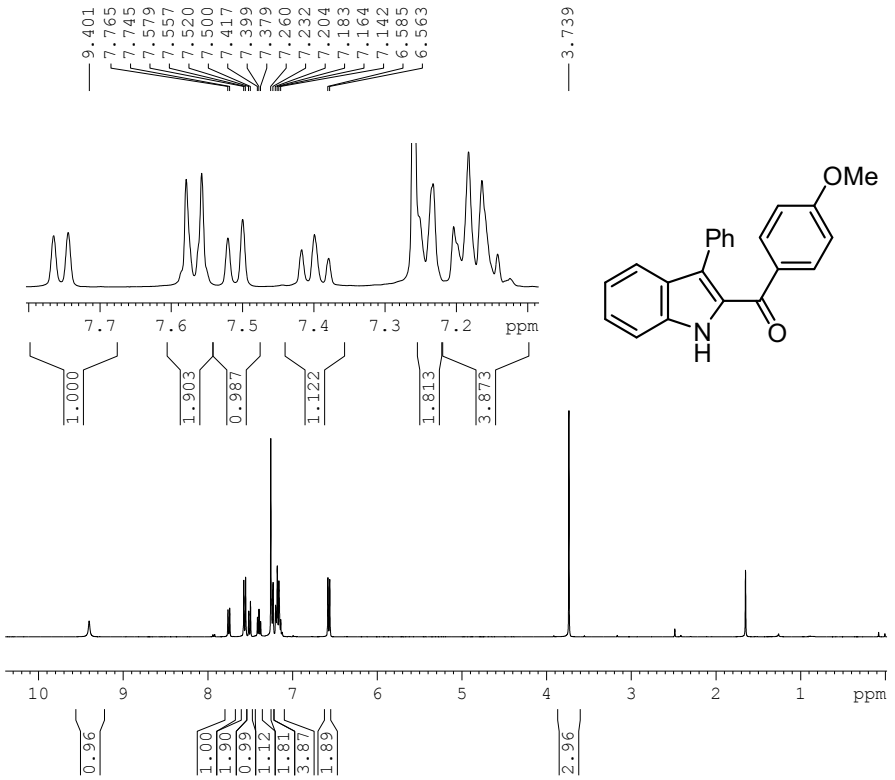


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3o**



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3o**

(4-methoxyphenyl)(3-phenyl-1H-indol-2-yl)methanone: 3p

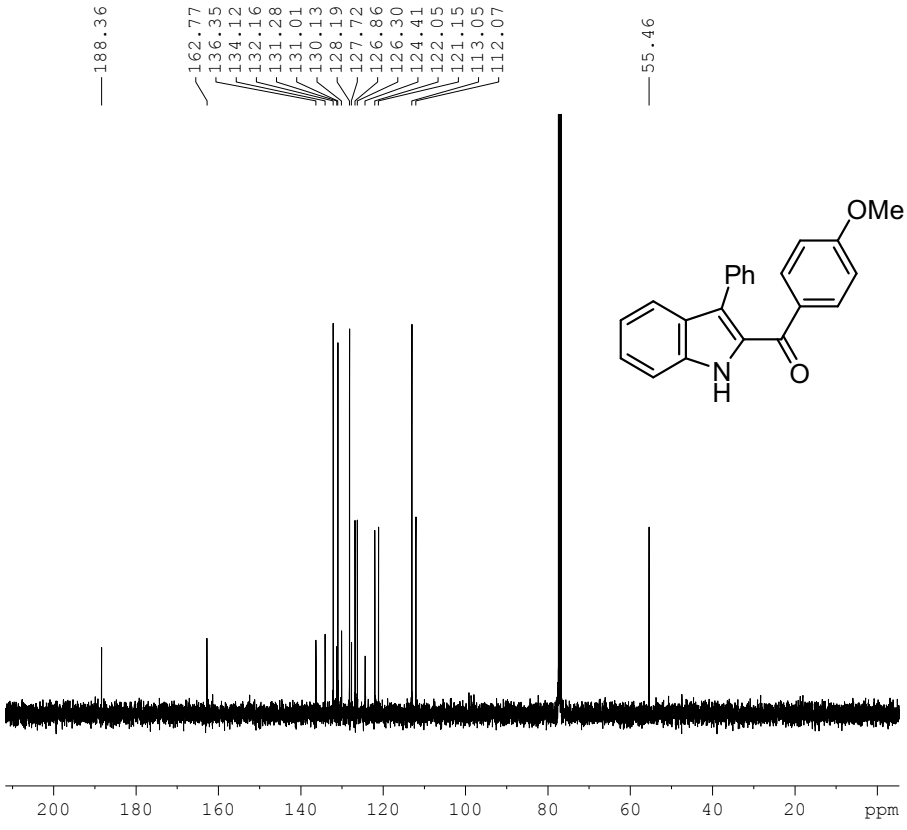



```
Current Data Parameters
NAME                 922(B)
EXPNO                   173
PROCNO                    1

F2 - Acquisition Parameters
Date_              20210807
Time                 18.08 h
INSTRUM                spect
PROBHD   Z129392_0001 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES            0.244532 Hz
AQ                4.0894465 sec
RG                   200.34
DW                   62.400 usec
DE                    6.50 usec
TE                   297.0 K
D1              0.50000000 sec
TD0                       1
SFO1           400.1320007 MHz
NUC1                    1H
P1                   15.00 usec
PLW1           10.50000000 W

F2 - Processing parameters
SI                    65536
SF             400.1300096 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3p**



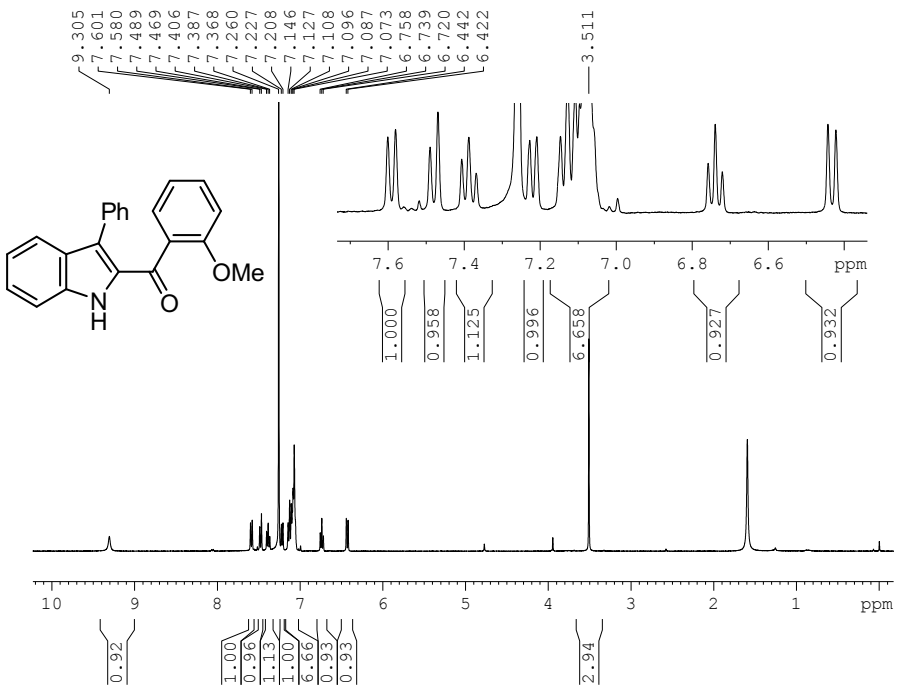

```
Current Data Parameters
NAME                 922(B)
EXPNO                   174
PROCNO                    1

F2 - Acquisition Paramet
Date_              20210807
Time                 18.15
INSTRUM                spect
PROBHD   Z129392_0001 (
PULPROG              zgpg30
TD                    16540
SOLVENT               CDCl3
NS                      256
DS                        4
SWH               24038.461
FIDRES             2.906706
AQ                0.3440320
RG                   200.34
DW                   20.800
DE                    6.50
TE                   297.4
D1              1.00000000
D11             0.03000000
TD0                       1
SFO1           100.6228289
NUC1                    13C
P1                   10.00
PLW1           47.00000000
SFO2           400.1316005
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                90.00
PLW2           10.50000000
PLW12           0.29166999
PLW13           0.14670999

F2 - Processing paramete
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3p**

(2-methoxyphenyl)(3-phenyl-1H-indol-2-yl)methanone: 3q

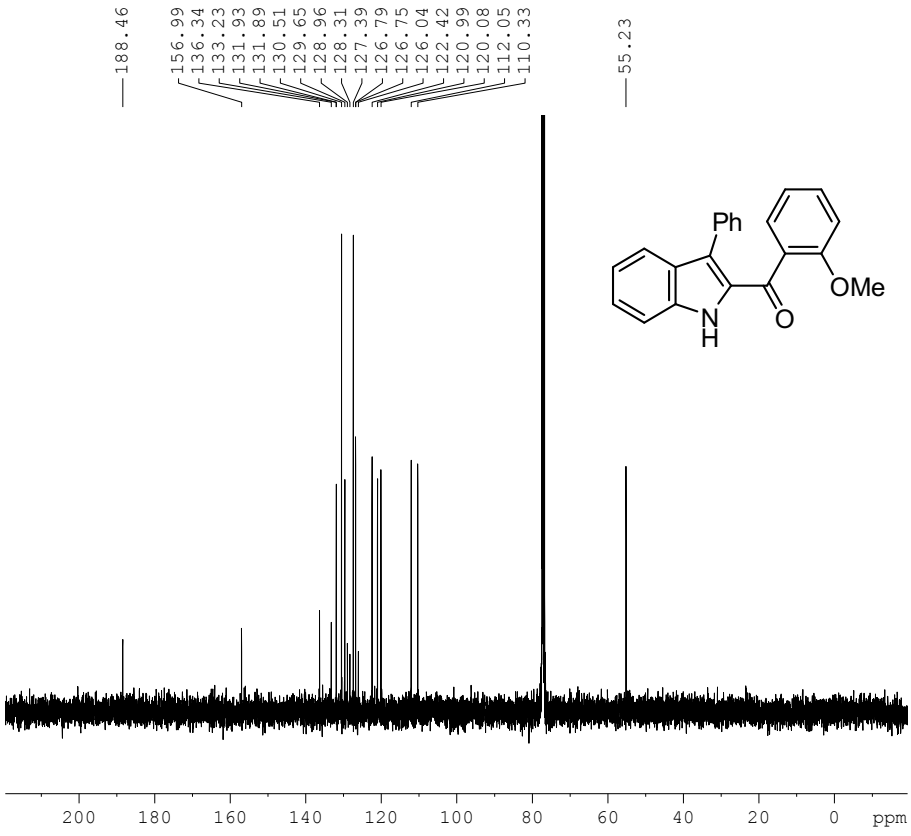



```
Current Data Parameters
NAME                  935
EXPNO                 354
PROCNO                  1

F2 - Acquisition Parameters
Date_           20210816
Time                2.51 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                 200.34
DW                 62.400 usec
DE                  6.50 usec
TE                 296.7 K
D1              0.50000000 sec
TD0                    1
SFO1          400.1320007 MHz
NUC1                  1H
P1                 15.00 usec
PLW1          10.50000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300099 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3q**



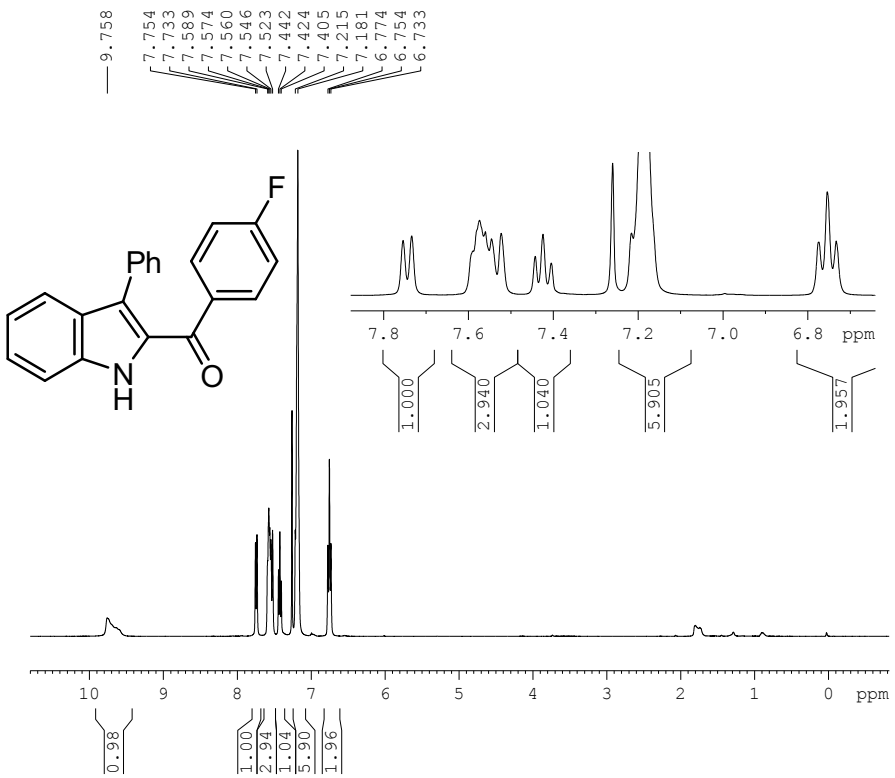

```
Current Data Parameters
NAME                  935
EXPNO                 355
PROCNO                  1

F2 - Acquisition Paramet
Date_           20210816
Time                4.05
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                  3000
DS                     4
SWH             24038.461
FIDRES           2.906706
AQ               0.3440320
RG                 200.34
DW                 20.800
DE                  6.50
TE                 297.1
D1              1.00000000
D11             0.03000000
TD0                    1
SFO1          100.6228289
NUC1                  13C
P1                 10.00
PLW1          47.00000000
SFO2          400.1316005
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              90.00
PLW2          10.50000000
PLW12          0.29166999
PLW13          0.14670999

F2 - Processing paramete
SI                 32768
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3q**

(4-fluorophenyl)(3-phenyl-1H-indol-2-yl)methanone: 3r

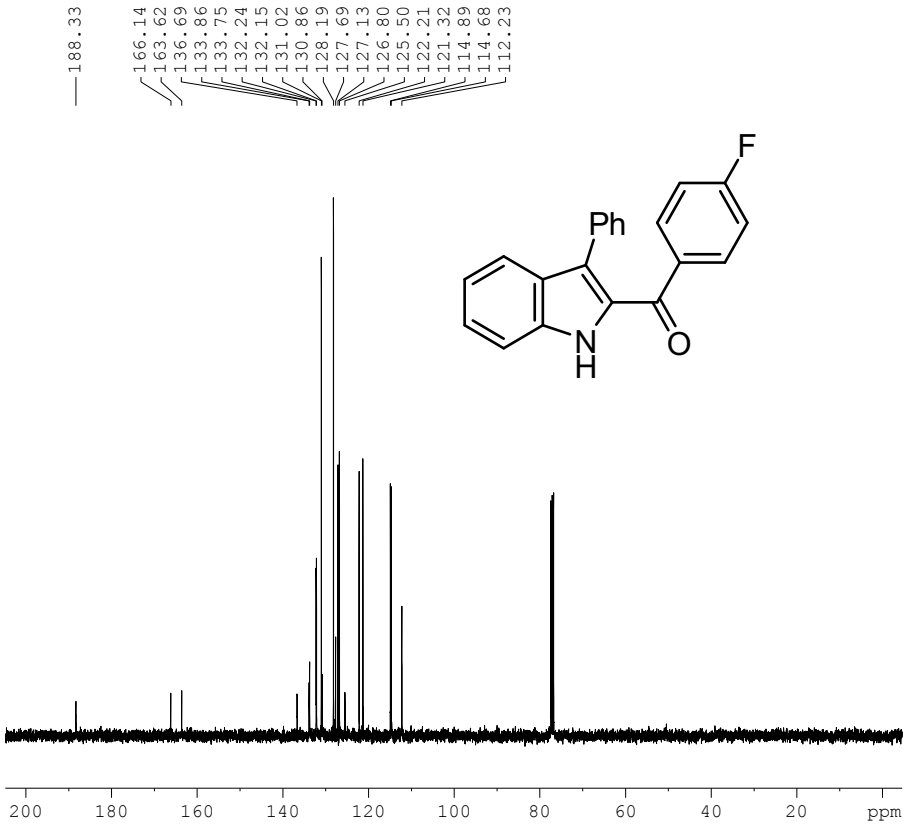



```
Current Data Parameters
NAME                  M649
EXPNO                  143
PROCNO                   1

F2 - Acquisition Parameters
Date_            20230105
Time                22.19 h
INSTRUM             spect
PROBHD    Z129392_0001 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                  138.85
DW                  62.400 usec
DE                    6.50 usec
TE                   297.1 K
D1             0.50000000 sec
TD0                     1
SFO1          400.1320007 MHz
NUC1                   1H
P1                  15.00 usec
PLW1          10.50000000 W

F2 - Processing parameters
SI                  65536
SF            400.1300094 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3r**



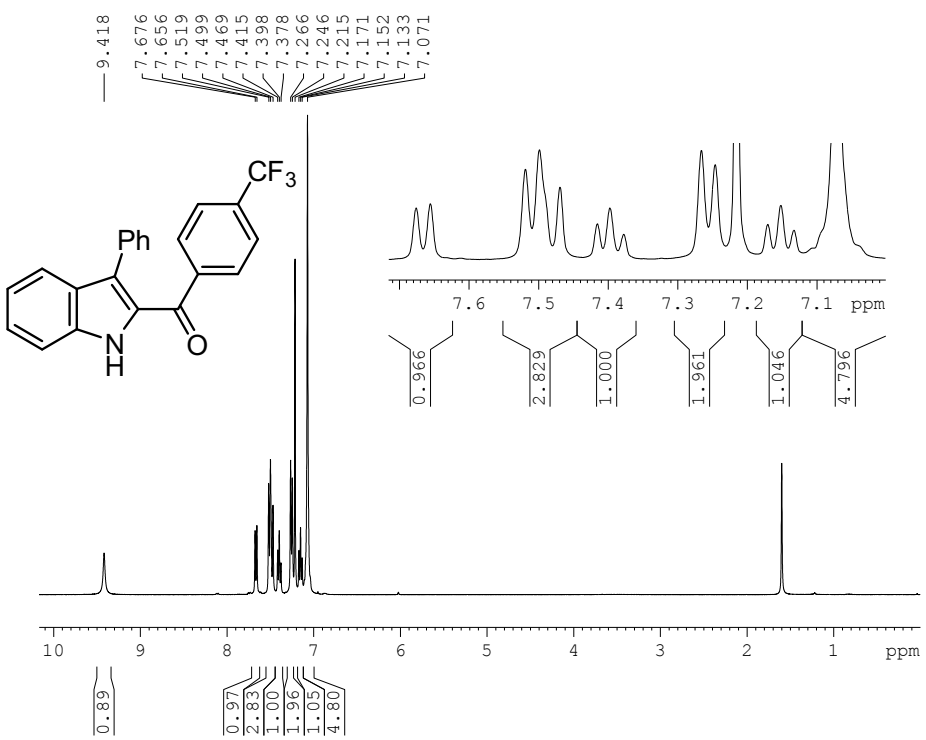

```
Current Data Parameters
NAME                  M649
EXPNO                  144
PROCNO                   1

F2 - Acquisition Paramete
Date_            20230105
Time                22.26 h
INSTRUM             spect
PROBHD    Z129392_0001 (
PULPROG           zgpg30
TD                  16540
SOLVENT             CDCl3
NS                    256
DS                      4
SWH             24038.461 H
FIDRES           2.906706 H
AQ               0.3440320 s
RG                  200.34
DW                  20.800 u
DE                    6.50 u
TE                   297.3 K
D1             1.00000000 s
D11            0.03000000 s
TD0                     1
SFO1          100.6228289 M
NUC1                  13C
P1                  10.00 u
PLW1          47.00000000 W
SFO2          400.1316005 M
NUC2                   1H
CPDPRG[2         waltz16
PCPD2               90.00 u
PLW2          10.50000000 W
PLW12          0.29166999 W
PLW13          0.14670999 W

F2 - Processing parameter
SI                  32768
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3r**

(3-phenyl-1H-indol-2-yl)(4-(trifluoromethyl)phenyl)methanone: 3s

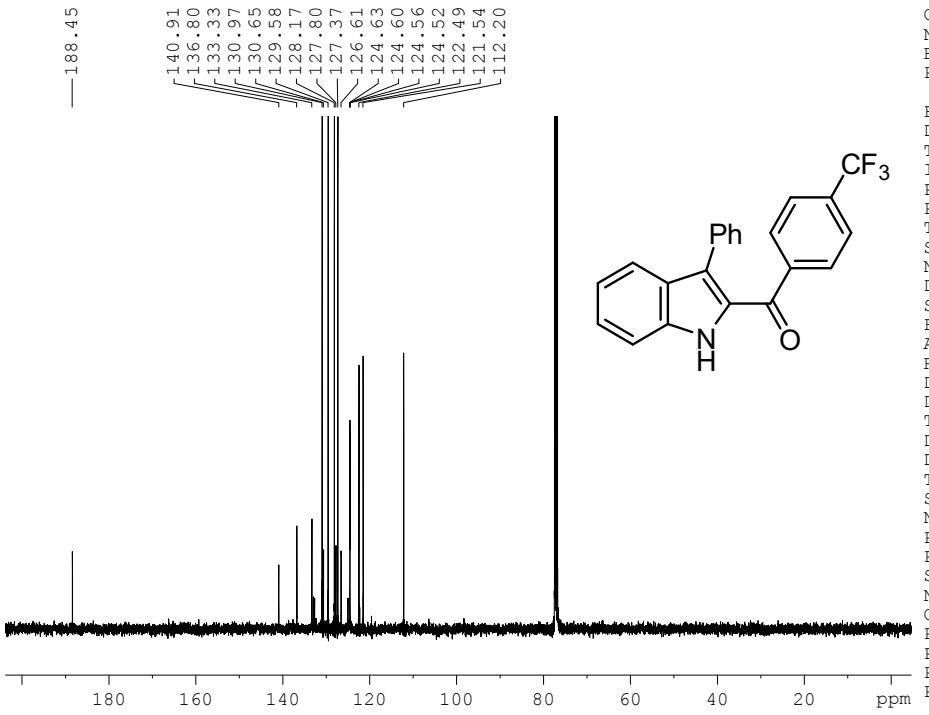



```
Current Data Parameters
NAME                  M664
EXPNO                  339
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230114
Time                  0.11 h
INSTRUM              spect
PROBHD   Z129392_0001 (
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8012.820 Hz
FIDRES               0.244532 Hz
AQ                4.0894465 sec
RG                   200.34
DW                   62.400 usec
DE                    6.50 usec
TE                   297.4 K
D1                0.50000000 sec
TD0                      1
SFO1           400.1320007 MHz
NUC1                    1H
P1                   15.00 usec
PLW1           10.50000000 W

F2 - Processing parameters
SI                   65536
SF             400.1300274 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3s**

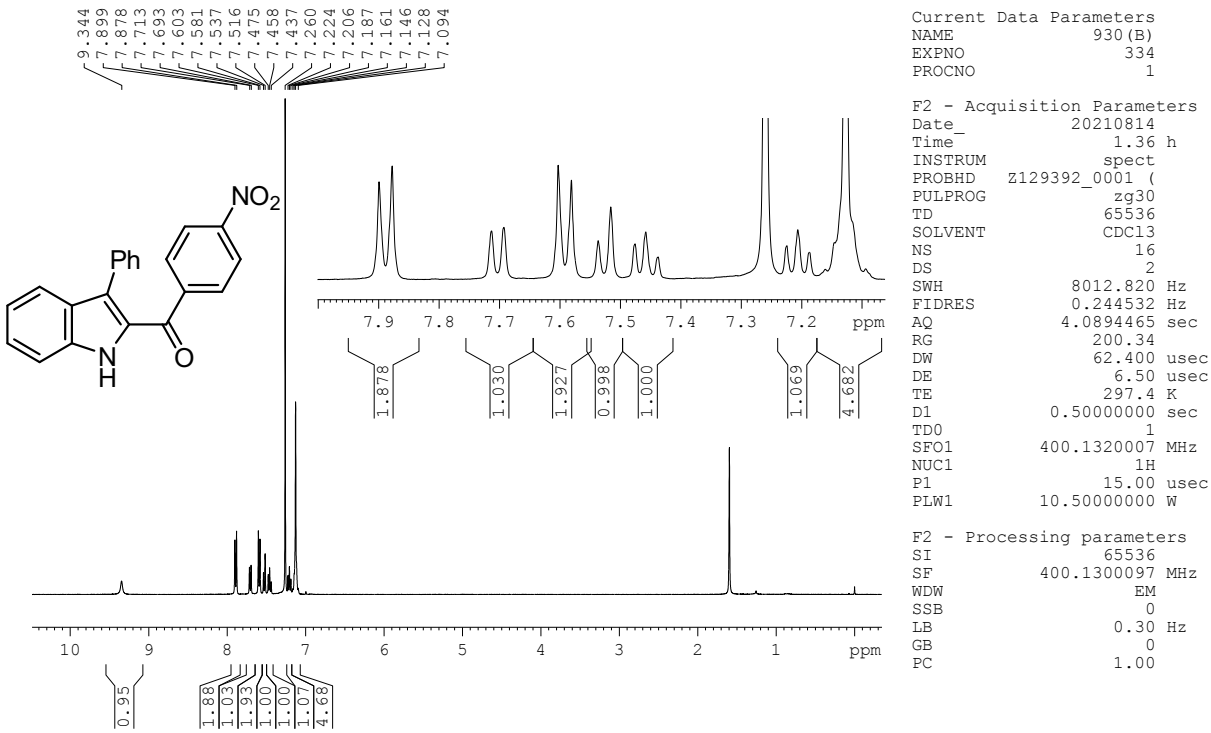



```
Current Data Parameters
NAME                  M664
EXPNO                  348
PROCNO                   1

F2 - Acquisition Parameter
Date_              20230114
Time                  1.36 h
INSTRUM              spect
PROBHD   Z129392_0001 (
PULPROG             zgpg30
TD                   16540
SOLVENT              CDCl3
NS                    2000
DS                       4
SWH              24038.461 Hz
FIDRES               2.906706 Hz
AQ                0.3440320 se
RG                   200.34
DW                   20.800 us
DE                    6.50 us
TE                   297.9 K
D1                1.00000000 se
D11               0.03000000 se
TD0                      1
SFO1           100.6228289 MH
NUC1                   13C
P1                   10.00 us
PLW1           47.00000000 W
SFO2           400.1316005 MH
NUC2                    1H
CPDPRG[2          waltz16
PCPD2                90.00 us
PLW2           10.50000000 W
PLW12           0.29166999 W
PLW13           0.14670999 W
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3s**

(4-nitrophenyl)(3-phenyl-1H-indol-2-yl)methanone: 3t

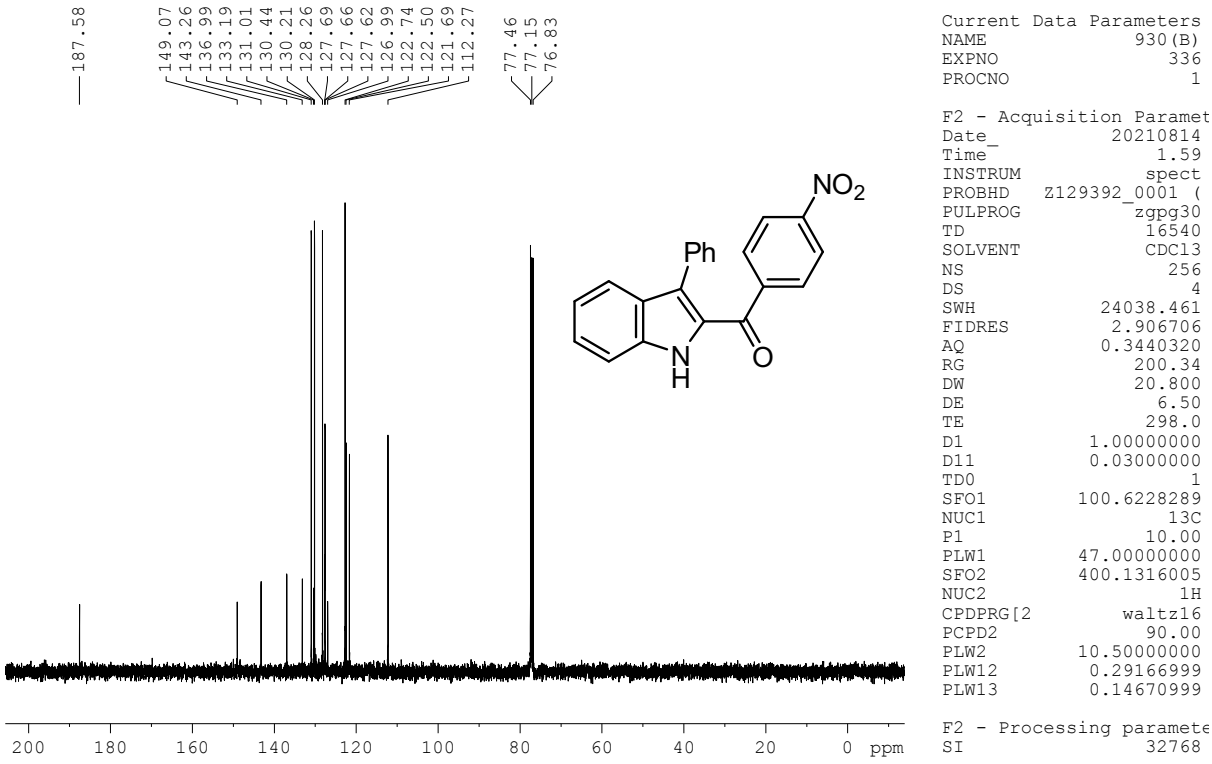



```
Current Data Parameters
NAME                  930(B)
EXPNO                    334
PROCNO                     1

F2 - Acquisition Parameters
Date_              20210814
Time                   1.36 h
INSTRUM               spect
PROBHD    Z129392_0001 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES             0.244532 Hz
AQ                 4.0894465 sec
RG                    200.34
DW                    62.400 usec
DE                     6.50 usec
TE                    297.4 K
D1              0.50000000 sec
TD0                        1
SFO1           400.1320007 MHz
NUC1                      1H
P1                    15.00 usec
PLW1           10.50000000 W

F2 - Processing parameters
SI                    65536
SF             400.1300097 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3t**



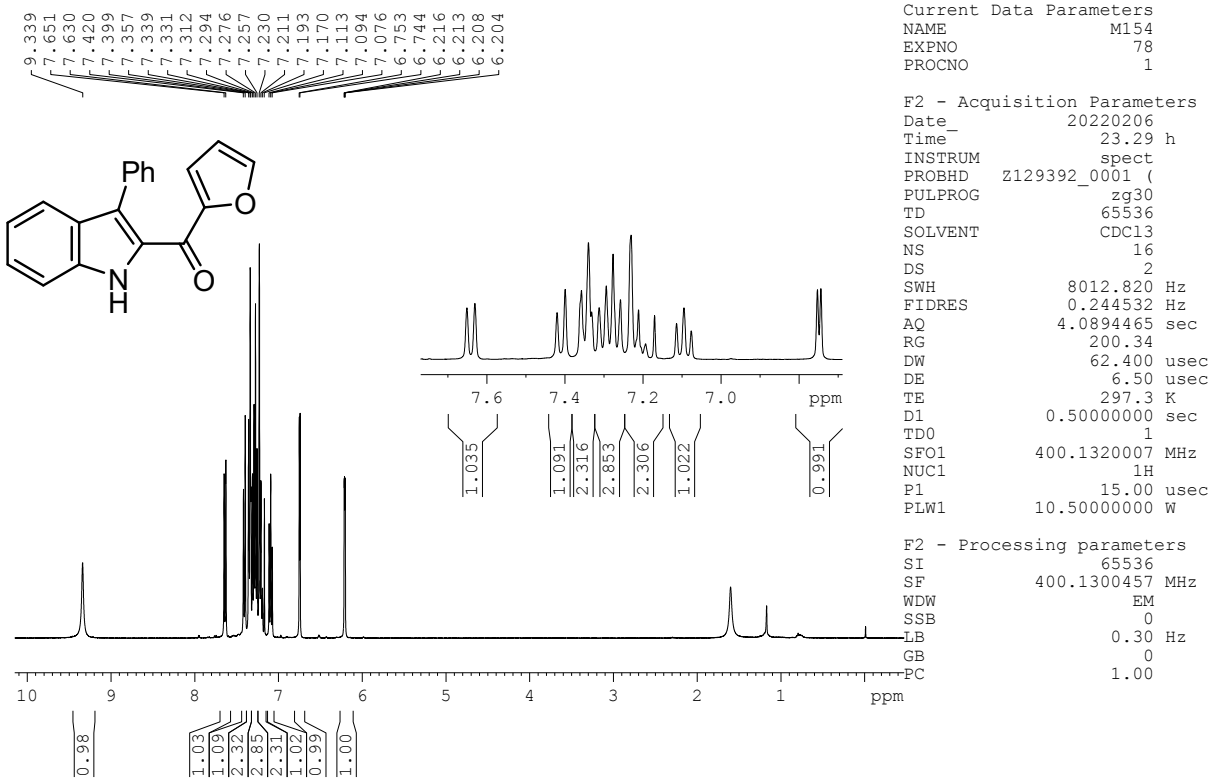

```
Current Data Parameters
NAME                  930(B)
EXPNO                    336
PROCNO                     1

F2 - Acquisition Paramet
Date_              20210814
Time                   1.59
INSTRUM               spect
PROBHD    Z129392_0001 (
PULPROG              zgpg30
TD                    16540
SOLVENT               CDCl3
NS                      256
DS                        4
SWH               24038.461
FIDRES             2.906706
AQ                 0.3440320
RG                    200.34
DW                    20.800
DE                     6.50
TE                    298.0
D1              1.00000000
D11             0.03000000
TD0                        1
SFO1           100.6228289
NUC1                     13C
P1                    10.00
PLW1           47.00000000
SFO2           400.1316005
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                 90.00
PLW2           10.50000000
PLW12           0.29166999
PLW13           0.14670999

F2 - Processing paramete
SI                    32768
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3t**

furan-2-yl(3-phenyl-1H-indol-2-yl)methanone: 3u

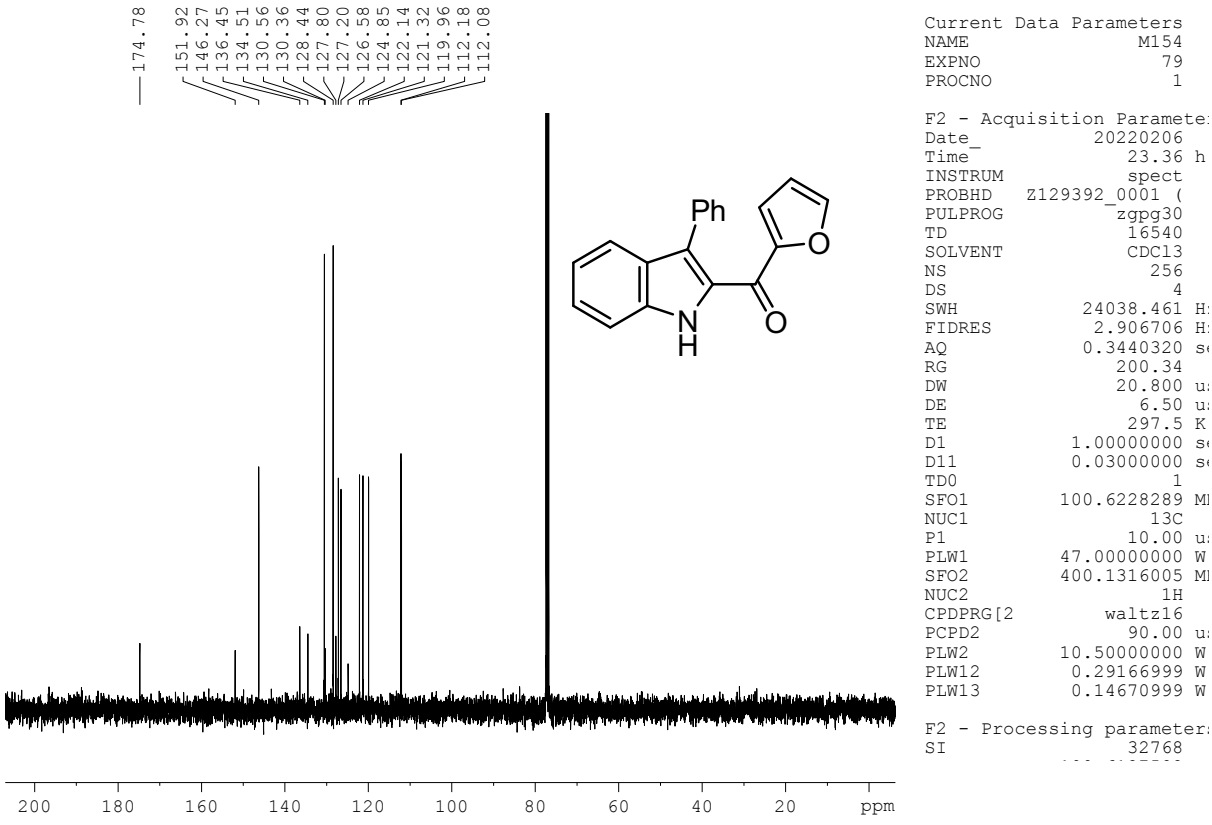



```
Current Data Parameters
NAME                  M154
EXPNO                   78
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220206
Time                 23.29 h
INSTRUM              spect
PROBHD     Z129392_0001 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES            0.244532 Hz
AQ                4.0894465 sec
RG                   200.34
DW                   62.400 usec
DE                    6.50 usec
TE                   297.3 K
D1                0.50000000 sec
TD0                       1
SFO1           400.1320007 MHz
NUC1                     1H
P1                   15.00 usec
PLW1           10.50000000 W

F2 - Processing parameters
SI                    65536
SF             400.1300457 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3u**



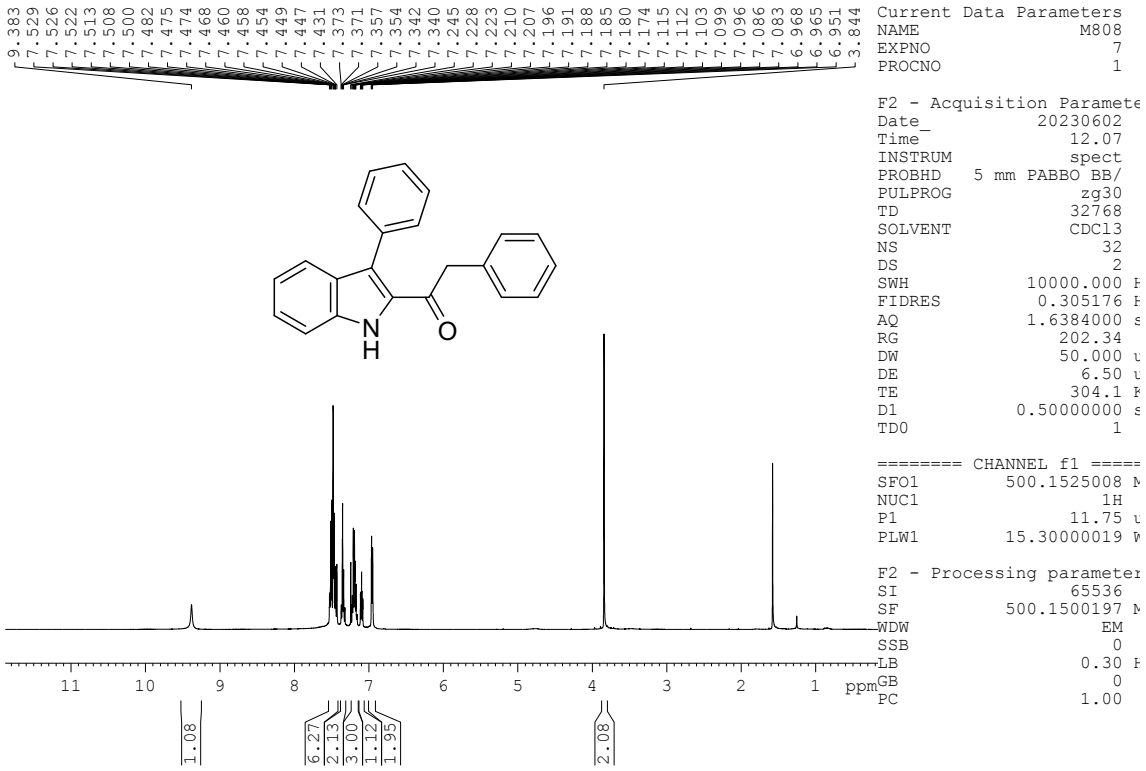

```
Current Data Parameters
NAME                  M154
EXPNO                   79
PROCNO                   1

F2 - Acquisition Parameter
Date_              20220206
Time                 23.36 h
INSTRUM              spect
PROBHD     Z129392_0001 (
PULPROG           zgpg30
TD                    16540
SOLVENT               CDCl3
NS                      256
DS                        4
SWH               24038.461 H
FIDRES             2.906706 H
AQ                0.3440320 s
RG                   200.34
DW                   20.800 u
DE                    6.50 u
TE                   297.5 K
D1                1.00000000 s
D11               0.03000000 s
TD0                       1
SFO1           100.6228289 M
NUC1                    13C
P1                   10.00 u
PLW1           47.00000000 W
SFO2           400.1316005 M
NUC2                     1H
CPDPRG[2          waltz16
PCPD2                90.00 u
PLW2           10.50000000 W
PLW12           0.29166999 W
PLW13           0.14670999 W

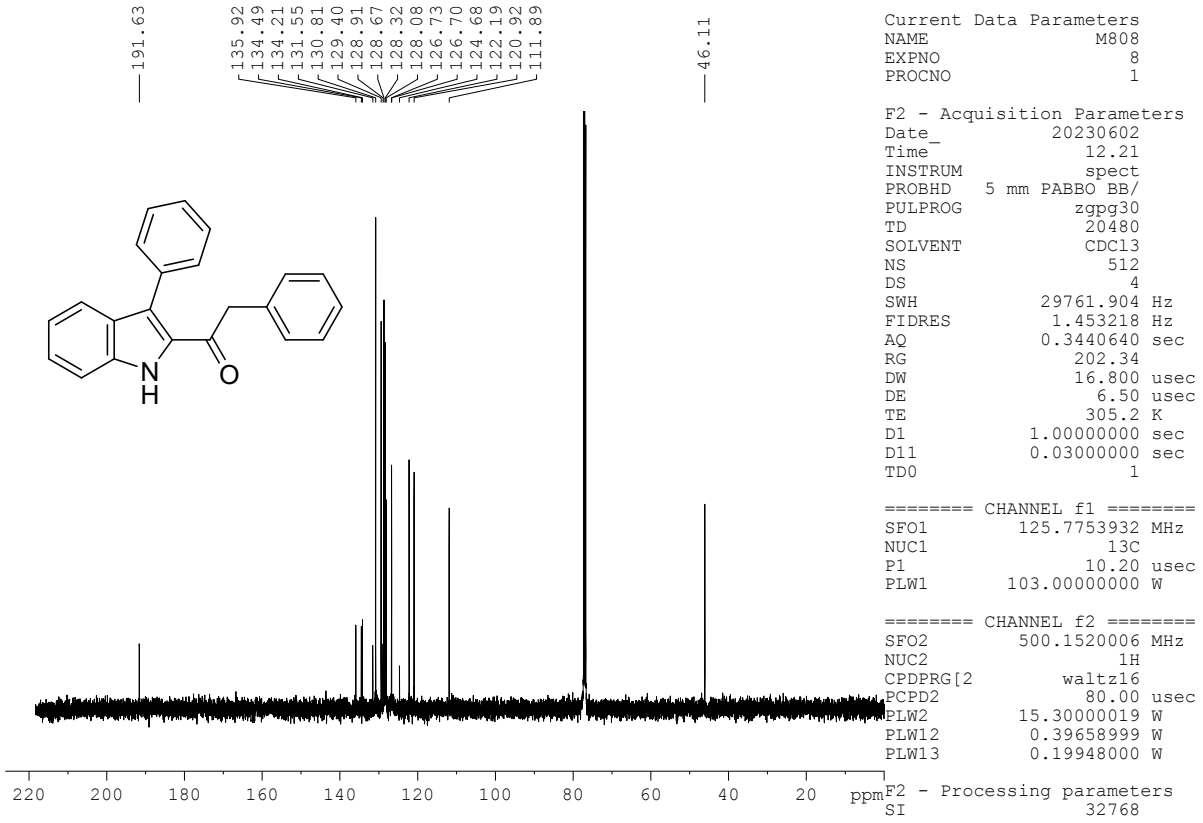
F2 - Processing parameter
SI                    32768
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3u**

2-phenyl-1-(3-phenyl-1H-indol-2-yl)ethan-1-one:3v

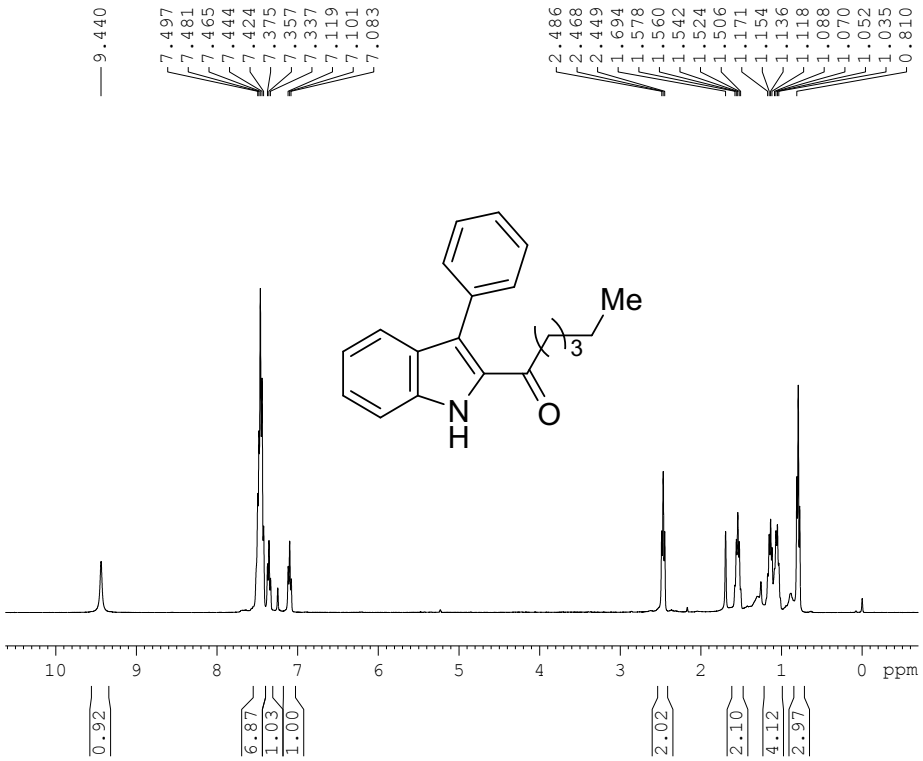


^{1}H NMR (500 MHz, $CDCl_3$, 24 °C) of the compound **3v**



^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 24 °C) of the compound **3v**

1-(3-phenyl-1H-indol-2-yl)hexan-1-one: 3w

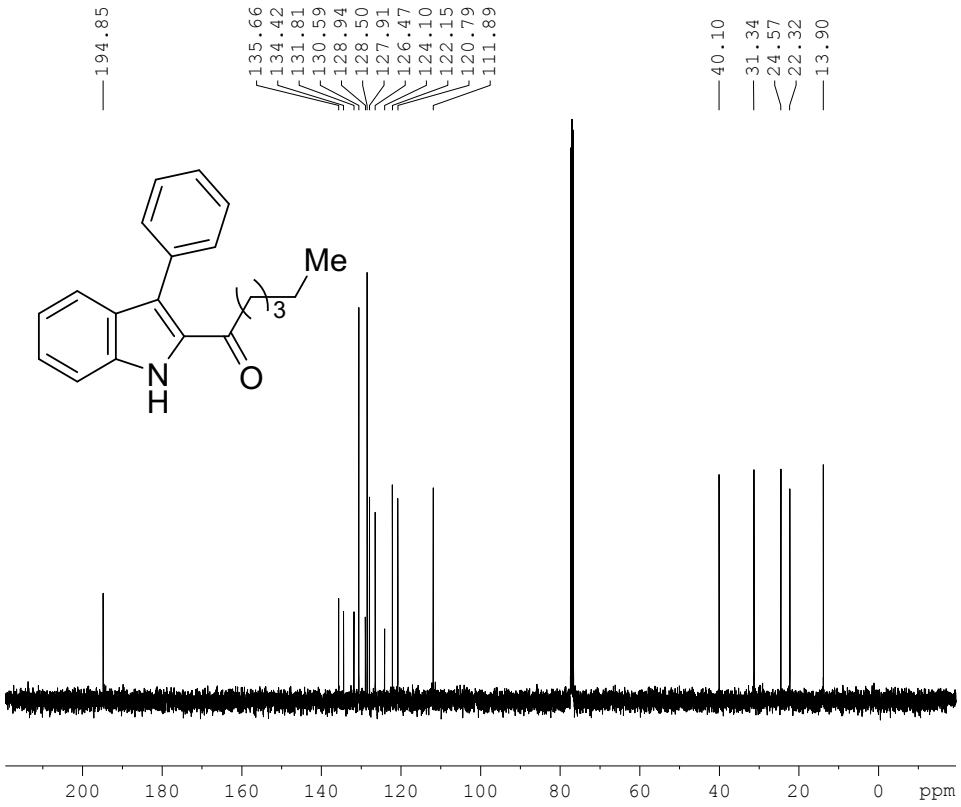



```
Current Data Parameters
NAME                  M812
EXPNO                   47
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230605
Time              10.41 h
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ             4.0894465 sec
RG                138.85
DW                62.400 usec
DE                16.92 usec
TE                294.8 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P0                 5.00 usec
P1                15.00 usec
PLW1         10.50000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300141 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3w**



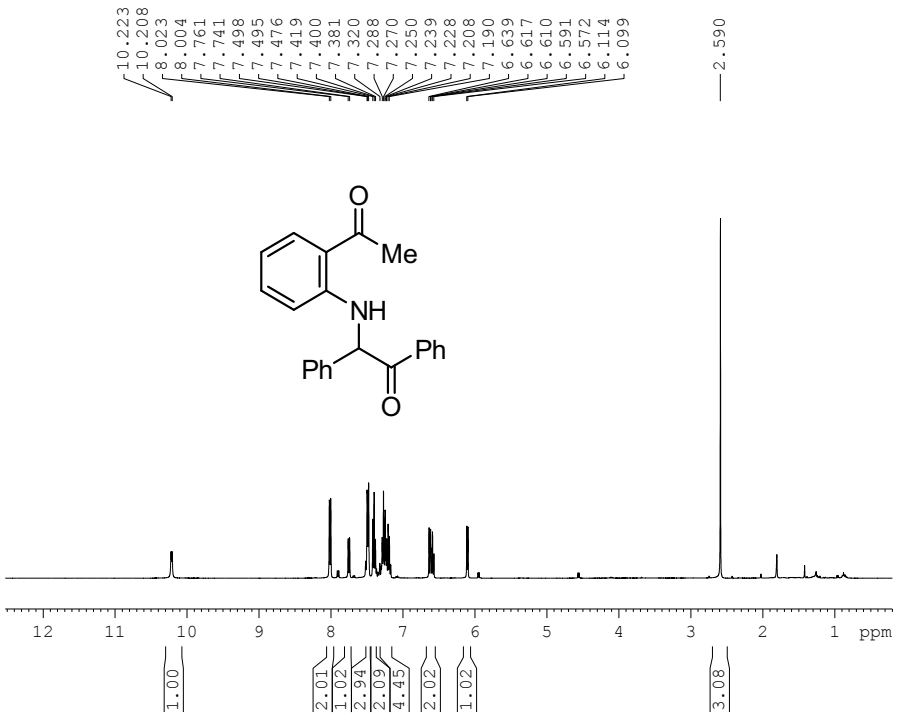

```
Current Data Parameters
NAME                  M812
EXPNO                   48
PROCNO                   1

F2 - Acquisition Paramet
Date_           20230605
Time              10.46
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    79
DS                     4
SWH            24038.461
FIDRES          0.733596
AQ             1.3631488
RG                200.34
DW                20.800
DE                 6.50
TE                295.2
D1             2.00000000
D11            0.03000000
TD0                    1
SFO1         100.6228298
NUC1                 13C
P0                  3.33
P1                 10.00
PLW1         47.00000000
SFO2         400.1316005
NUC2                  1H
CPDPRG[2          waltz65
PCPD2              90.00
PLW2         10.50000000
PLW12         0.29166999
PLW13         0.14670999

F2 - Processing paramete
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3w**

2-((2-acetylphenyl)amino)-1,2-diphenylethan-1-one: 5

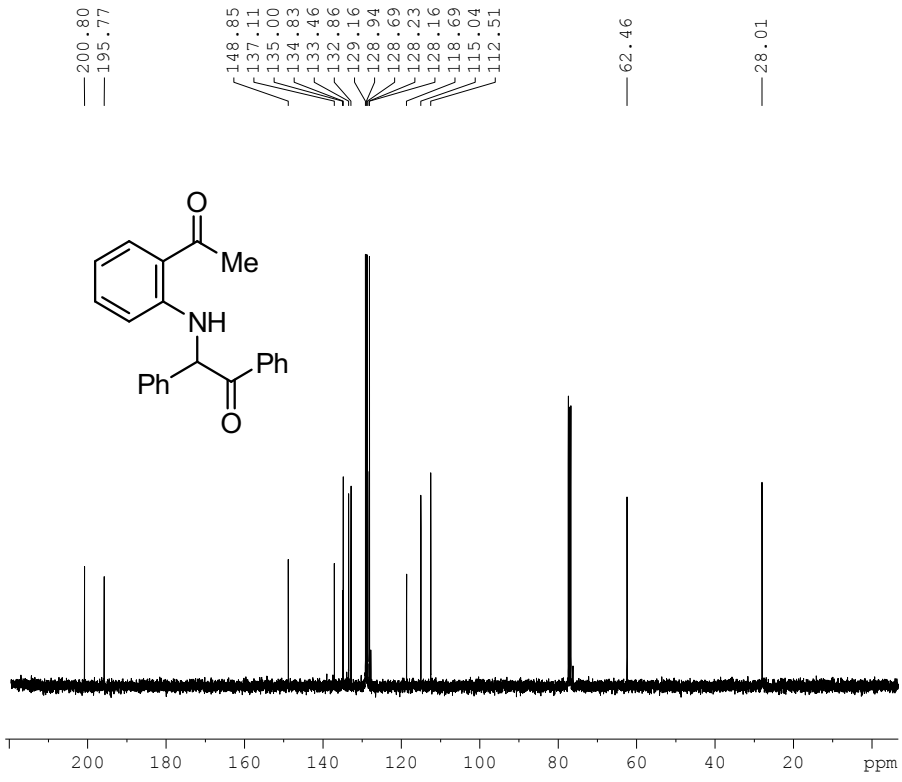



```
Current Data Parameters
NAME      M944(A) AND (B)
EXPNO                364
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230721
Time              22.49 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    10
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                 88.51
DW                62.400 usec
DE                16.92 usec
TE                406.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P0                  5.00 usec
P1                 15.00 usec
PLW1          10.50000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300177 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **5**



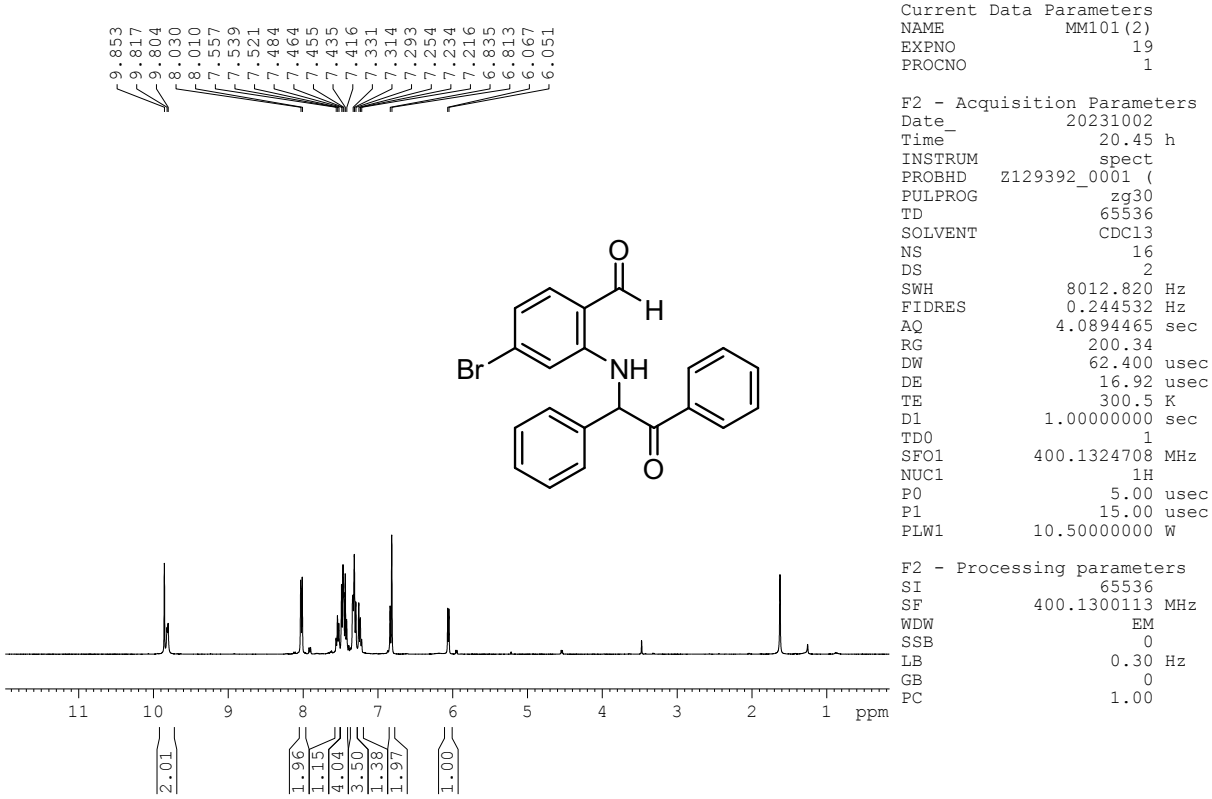

```
Current Data Parameters
NAME      M944(A) AND (B)
EXPNO                365
PROCNO                 1

F2 - Acquisition Parameter
Date_           20230721
Time              22.52 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    48
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 se
RG                200.34
DW                20.800 us
DE                 6.50 us
TE                395.1 K
D1             2.00000000 se
D11            0.03000000 se
TD0                    1
SFO1         100.6228298 MH
NUC1                  13C
P0                 3.33 us
P1                10.00 us
PLW1          47.00000000 W
SFO2         400.1316005 MH
NUC2                  1H
CPDPRG[2          waltz65
PCPD2              90.00 us
PLW2          10.50000000 W
PLW12          0.29166999 W
PLW13          0.14670999 W

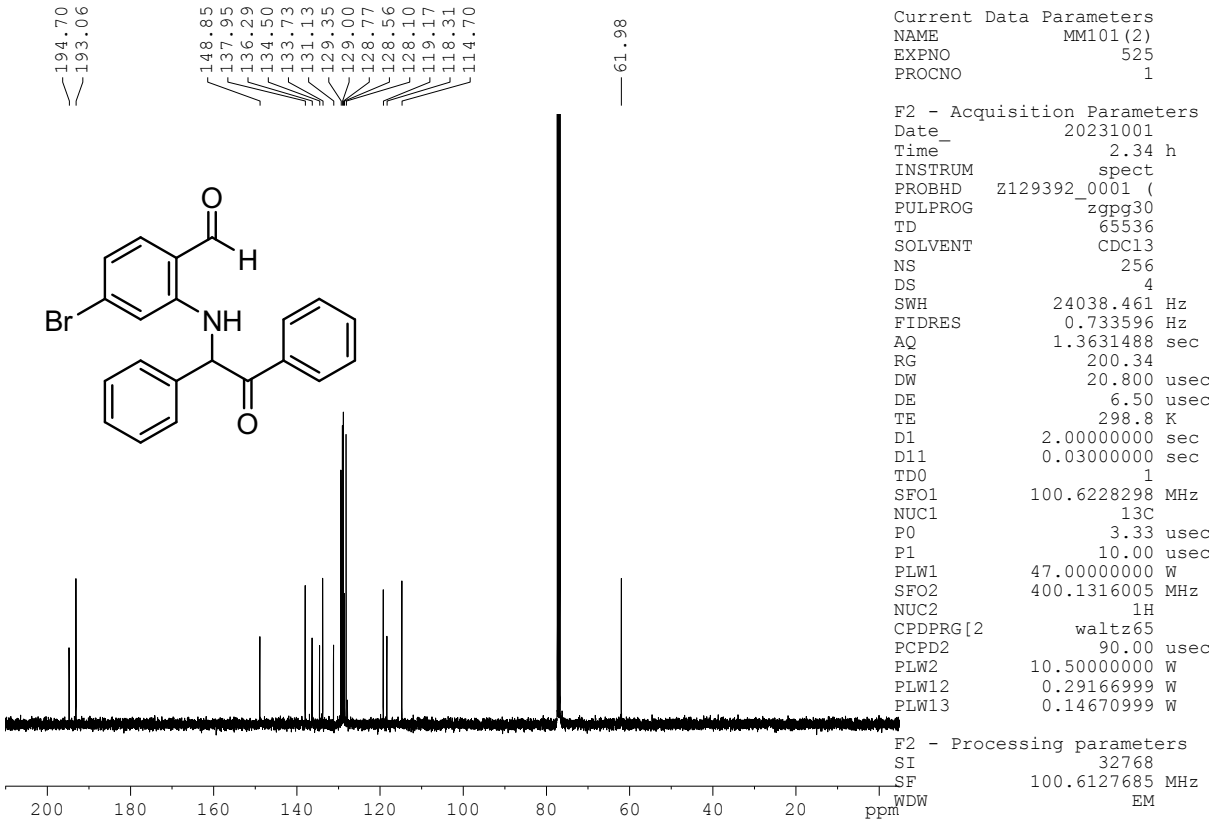
F2 - Processing parameters
SI                 32768
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **5**

4-bromo-2-((2-oxo-1,2-diphenylethyl)amino)benzaldehyde: 5’



^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of **5’**



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of **5’**

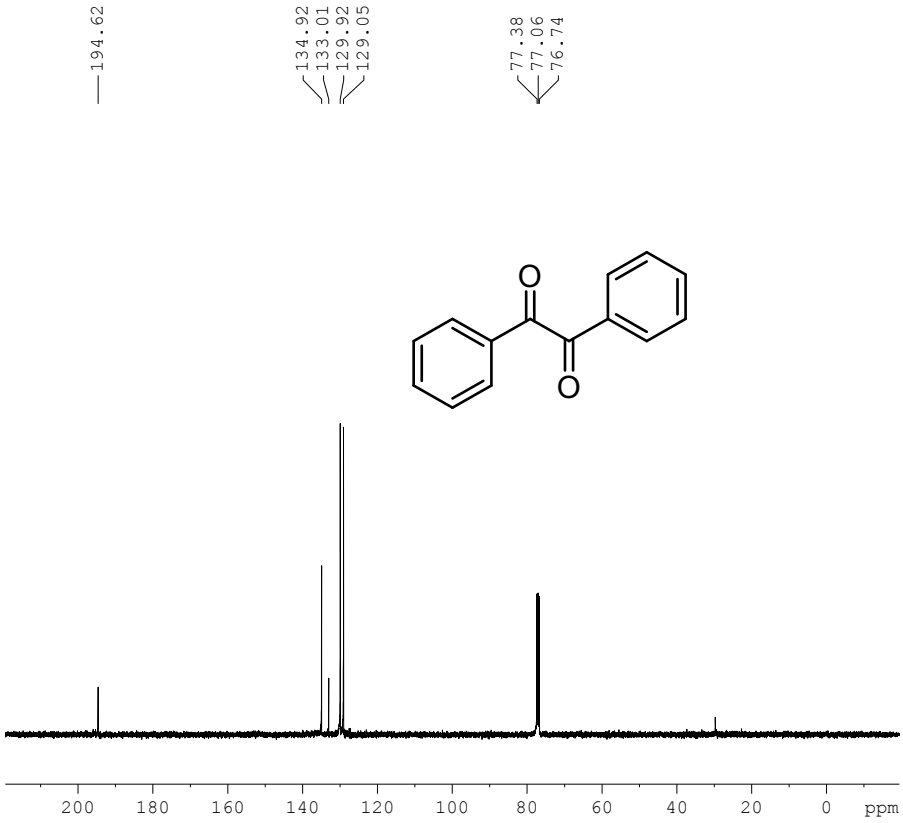
Benzil


```
Current Data Parameters
NAME            MM100(1)
EXPNO                 18
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231002
Time              20.40 h
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     5
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                153.13
DW                62.400 usec
DE                16.92 usec
TE                300.6 K
D1             1.00000000 sec
TD0                    1
SFO1          400.1324708 MHz
NUC1                  1H
P0                  5.00 usec
P1                 15.00 usec
PLW1          10.50000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300110 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of **Benzil**



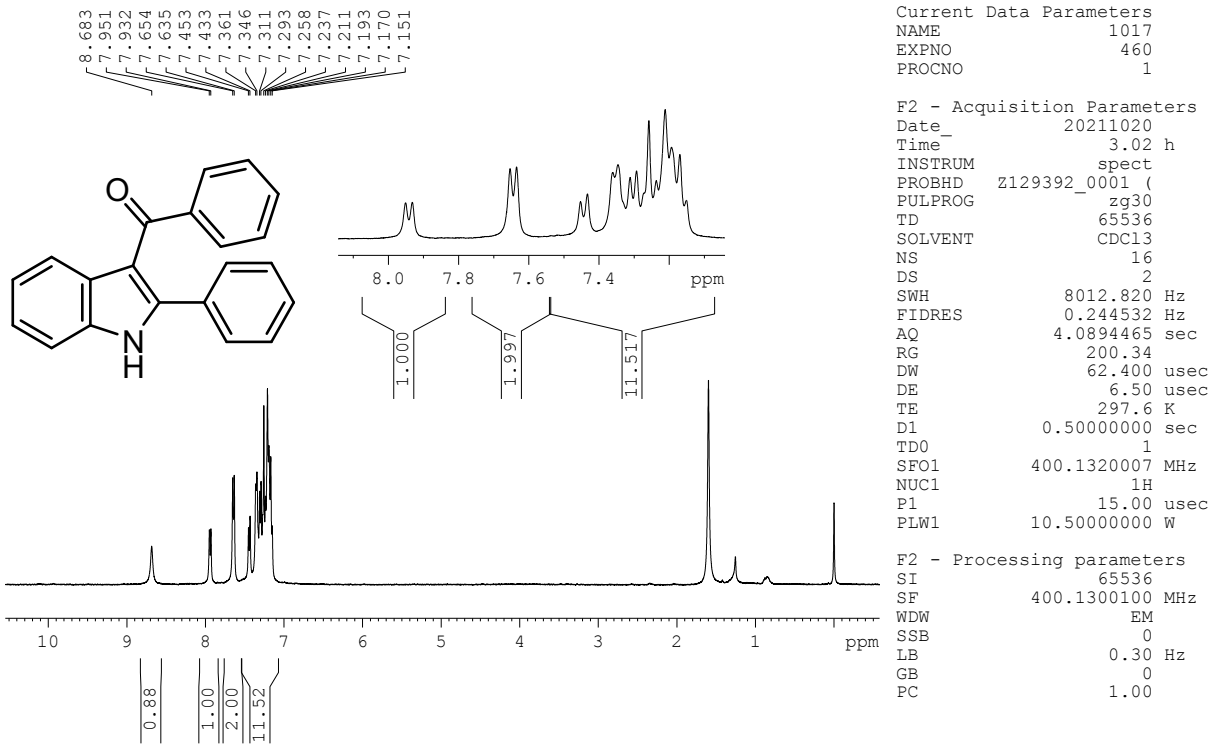

```
Current Data Parameters
NAME            MM100(1)
EXPNO                519
PROCNO                 1

F2 - Acquisition Parameter
Date_           20230930
Time              13.59 h
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            24038.461 H
FIDRES          0.733596 H
AQ              1.3631488 s
RG                200.34
DW                20.800 u
DE                 6.50 u
TE                299.0 K
D1             2.00000000 s
D11            0.03000000 s
TD0                    1
SFO1          100.6228298 M
NUC1                 13C
P0                 3.33 u
P1                10.00 u
PLW1          47.00000000 W
SFO2          400.1316005 M
NUC2                  1H
CPDPRG[2         waltz65
PCPD2              90.00 u
PLW2          10.50000000 W
PLW12          0.29166999 W
PLW13          0.14670999 W

F2 - Processing parameter
SI                 32768
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of **Benzil**

phenyl(2-phenyl-1H-indol-3-yl)methanone: 6a

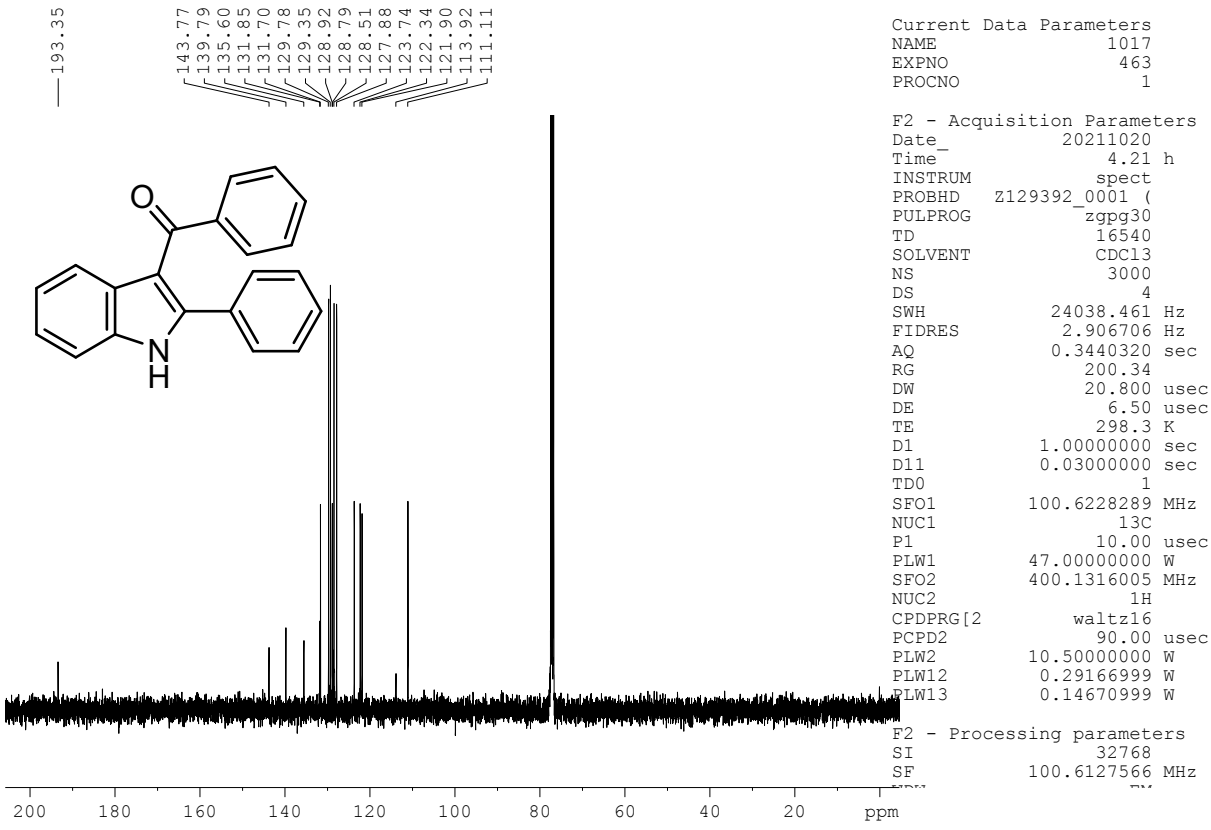



```
Current Data Parameters
NAME                  1017
EXPNO                  460
PROCNO                   1

F2 - Acquisition Parameters
Date_           20211020
Time                3.02 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES              0.244532 Hz
AQ               4.0894465 sec
RG                  200.34
DW                  62.400 usec
DE                    6.50 usec
TE                   297.6 K
D1              0.50000000 sec
TD0                    1
SFO1           400.1320007 MHz
NUC1                  1H
P1                  15.00 usec
PLW1           10.50000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300100 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **6a**



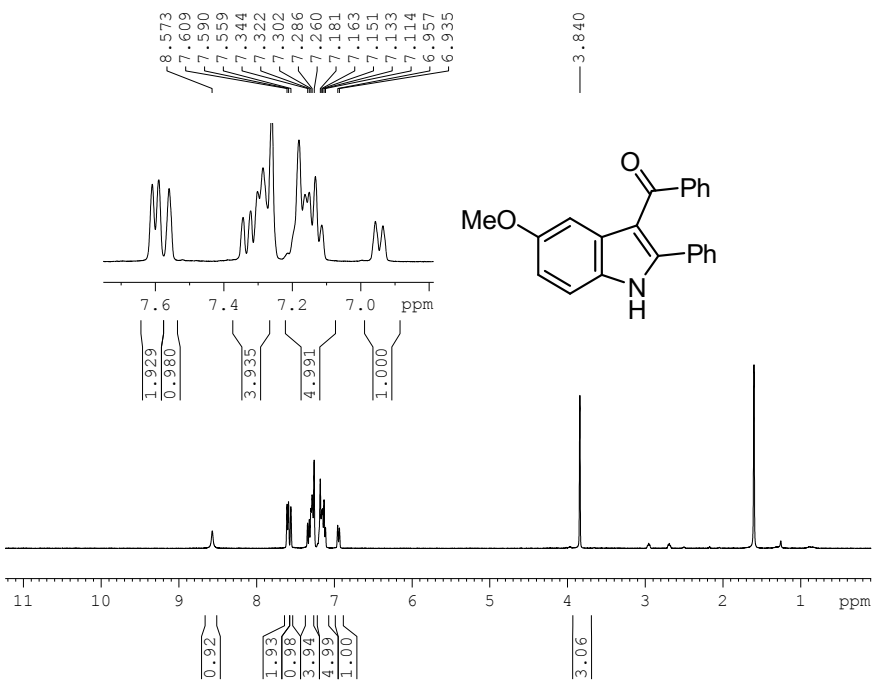

```
Current Data Parameters
NAME                  1017
EXPNO                  463
PROCNO                   1

F2 - Acquisition Parameters
Date_           20211020
Time                4.21 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                  3000
DS                     4
SWH             24038.461 Hz
FIDRES              2.906706 Hz
AQ               0.3440320 sec
RG                  200.34
DW                  20.800 usec
DE                    6.50 usec
TE                   298.3 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                    1
SFO1           100.6228289 MHz
NUC1                  13C
P1                  10.00 usec
PLW1           47.00000000 W
SFO2           400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2           10.50000000 W
PLW12           0.29166999 W
PLW13           0.14670999 W

F2 - Processing parameters
SI                 32768
SF           100.6127566 MHz
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **6a**

(5-methoxy-2-phenyl-1H-indol-3-yl)(phenyl)methanone: 6b

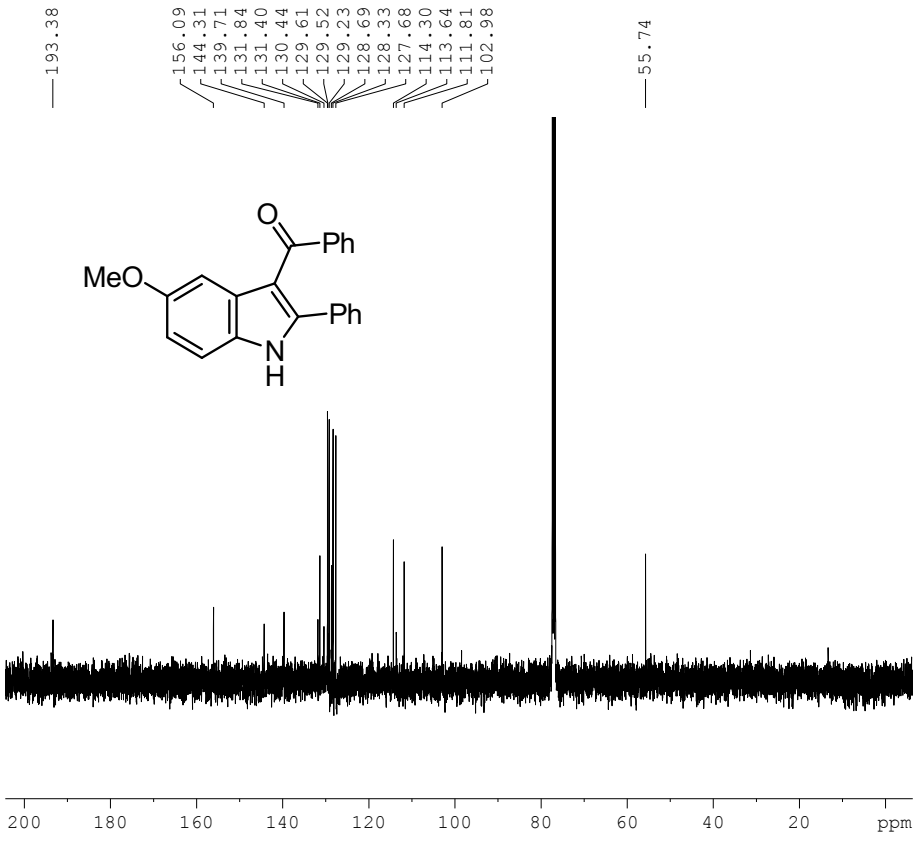



```
Current Data Parameters
NAME                  M765
EXPNO                  300
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230617
Time                0.15 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                 200.34
DW                 62.400 usec
DE                 16.92 usec
TE                 295.1 K
D1              1.00000000 sec
TD0                    1
SFO1          400.1324708 MHz
NUC1                  1H
P0                  5.00 usec
P1                 15.00 usec
PLW1          10.50000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300091 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **6b**



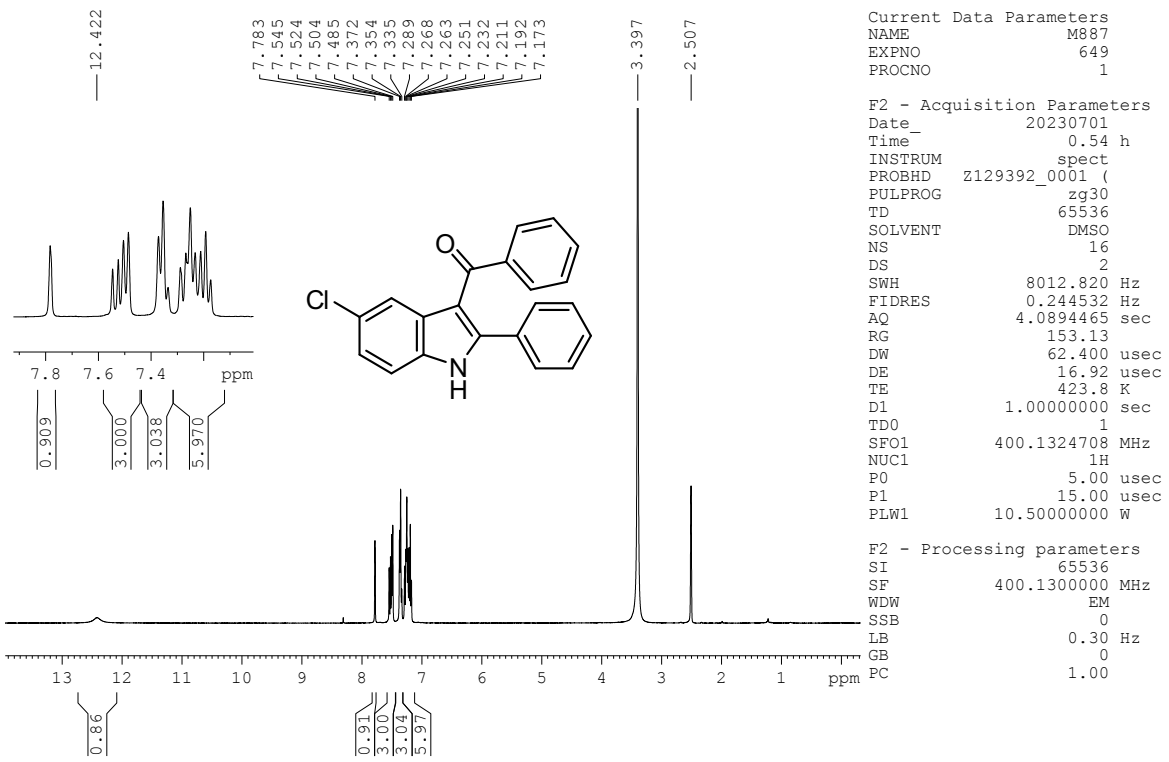

```
Current Data Parameters
NAME                  M765
EXPNO                  309
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230617
Time                3.10 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               1.3631488 sec
RG                 200.34
DW                 20.800 usec
DE                  6.50 usec
TE                 295.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1
SFO1          100.6228298 MHz
NUC1                  13C
P0                  3.33 usec
P1                 10.00 usec
PLW1          47.00000000 W
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz65
PCPD2              90.00 usec
PLW2          10.50000000 W
PLW12          0.29166999 W
PLW13          0.14670999 W

F2 - Processing parameters
SI                 32768
SF            100.6127685 MHz
WDW                   EM
SSB                    0
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **6b**

(5-chloro-2-phenyl-1H-indol-3-yl)(phenyl)methanone: 6c

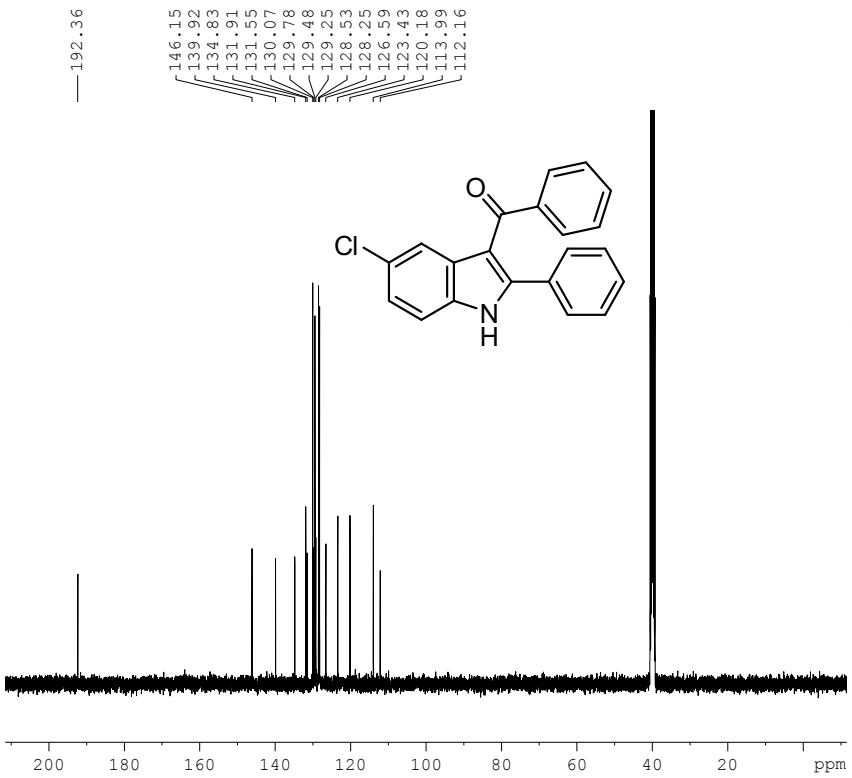


Current Data Parameters
NAME M887
EXPNO 649
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230701
Time 0.54 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 153.13
DW 62.400 usec
DE 16.92 usec
TE 423.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 10.50000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H NMR (400 MHz, DMSO-d_6, 24 °C) of the compound **6c**



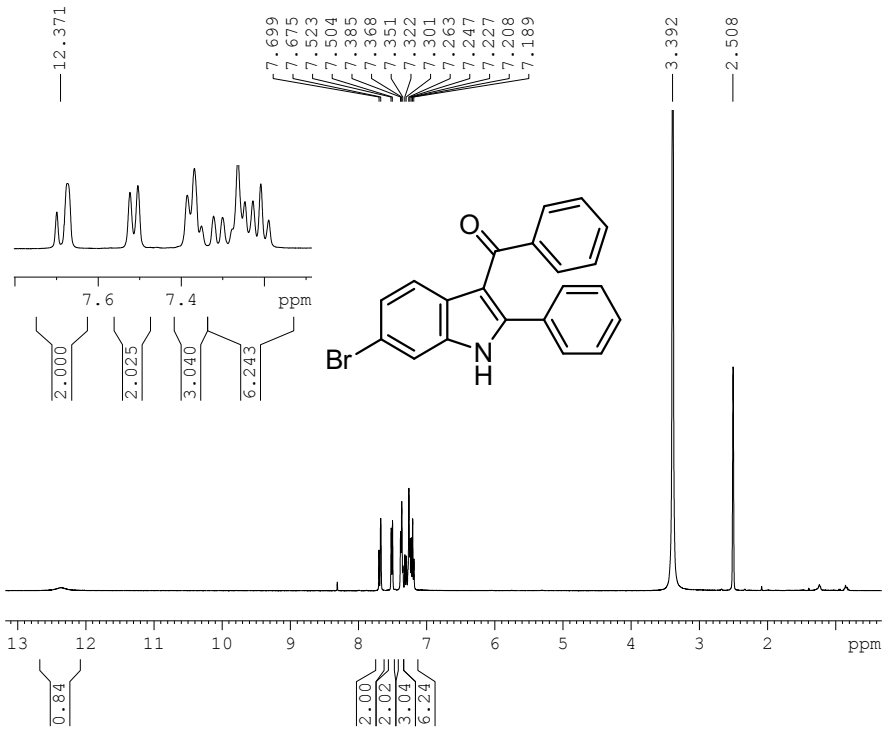
Current Data Parameters
NAME M887
EXPNO 655
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230701
Time 4.18 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 452.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 47.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 10.50000000 W
PLW12 0.29166999 W
PLW13 0.14670999 W

F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM

^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C) of the compound **6c**

(5-bromo-2-phenyl-1H-indol-3-yl)(phenyl)methanone: 6d

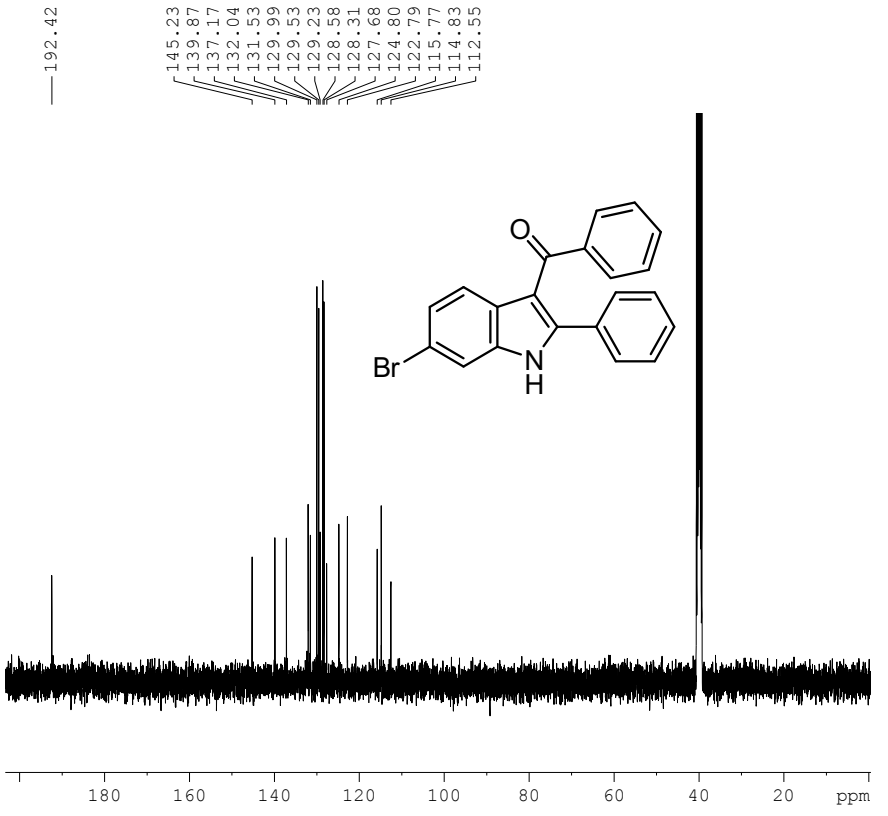



```
Current Data Parameters
NAME                  M886
EXPNO                  656
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230701
Time                4.22 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ             4.0894465 sec
RG                169.77
DW                62.400 usec
DE                16.92 usec
TE                443.9 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P0                  5.00 usec
P1                 15.00 usec
PLW1         10.50000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, DMSO-d_6, 24 °C) of the compound **6d**



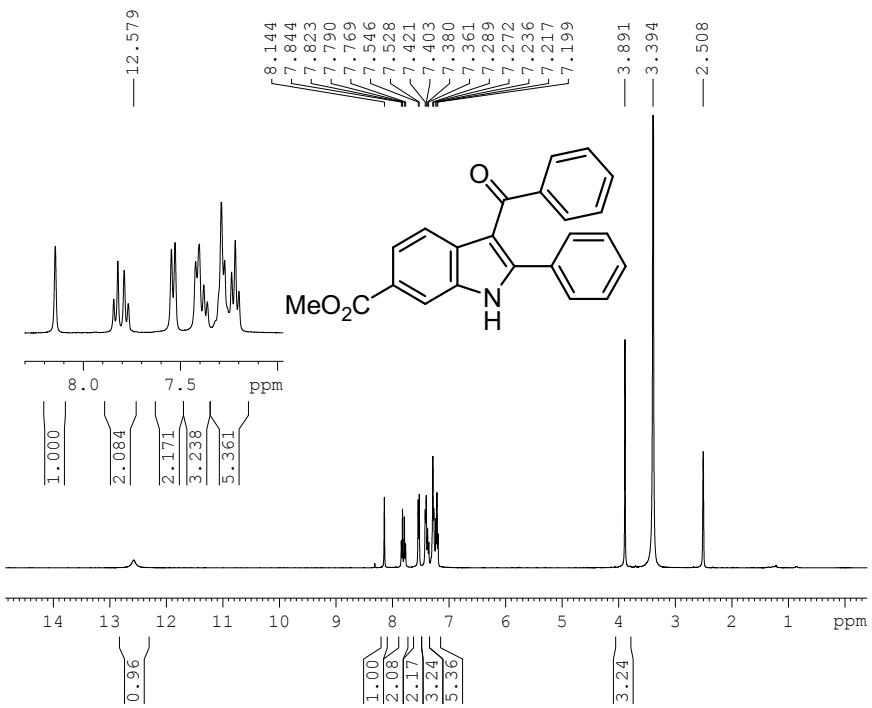

```
Current Data Parameters
NAME                  M886
EXPNO                  653
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230701
Time                5.21 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  1024
DS                     4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ             1.3631488 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE                479.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         100.6228298 MHz
NUC1                 13C
P0                  3.33 usec
P1                 10.00 usec
PLW1         47.00000000 W
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz65
PCPD2              90.00 usec
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W

F2 - Processing parameters
SI                 32768
SF           100.6127685 MHz
WDW                   EM
```

^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C) of the compound **6d**

methyl 3-benzoyl-2-phenyl-1H-indole-6-carboxylate: 6e

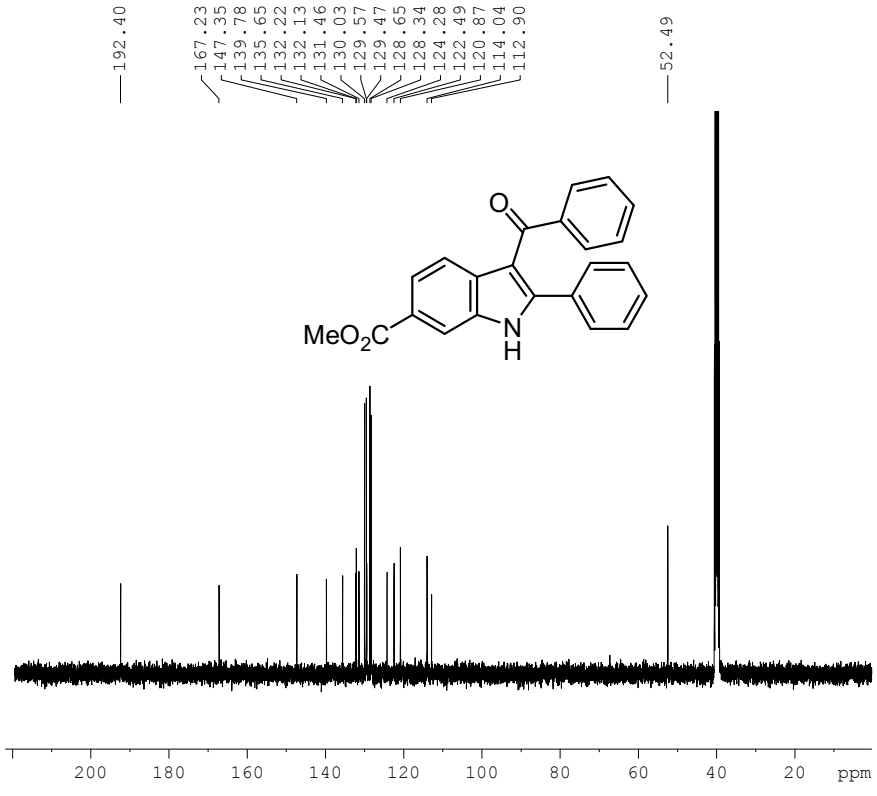



```
Current Data Parameters
NAME                  M889
EXPNO                   13
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230702
Time                  3.18 h
INSTRUM              spect
PROBHD   Z129392_0001 (
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES             0.244532 Hz
AQ                 4.0894465 sec
RG                    138.85
DW                    62.400 usec
DE                    16.92 usec
TE                    489.0 K
D1              1.00000000 sec
TD0                       1
SFO1           400.1324708 MHz
NUC1                     1H
P0                    5.00 usec
P1                   15.00 usec
PLW1           10.50000000 W

F2 - Processing parameters
SI                    65536
SF             400.1300000 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```

^{1}H NMR (400 MHz, DMSO-d_6, 24 °C) of the compound **6e**

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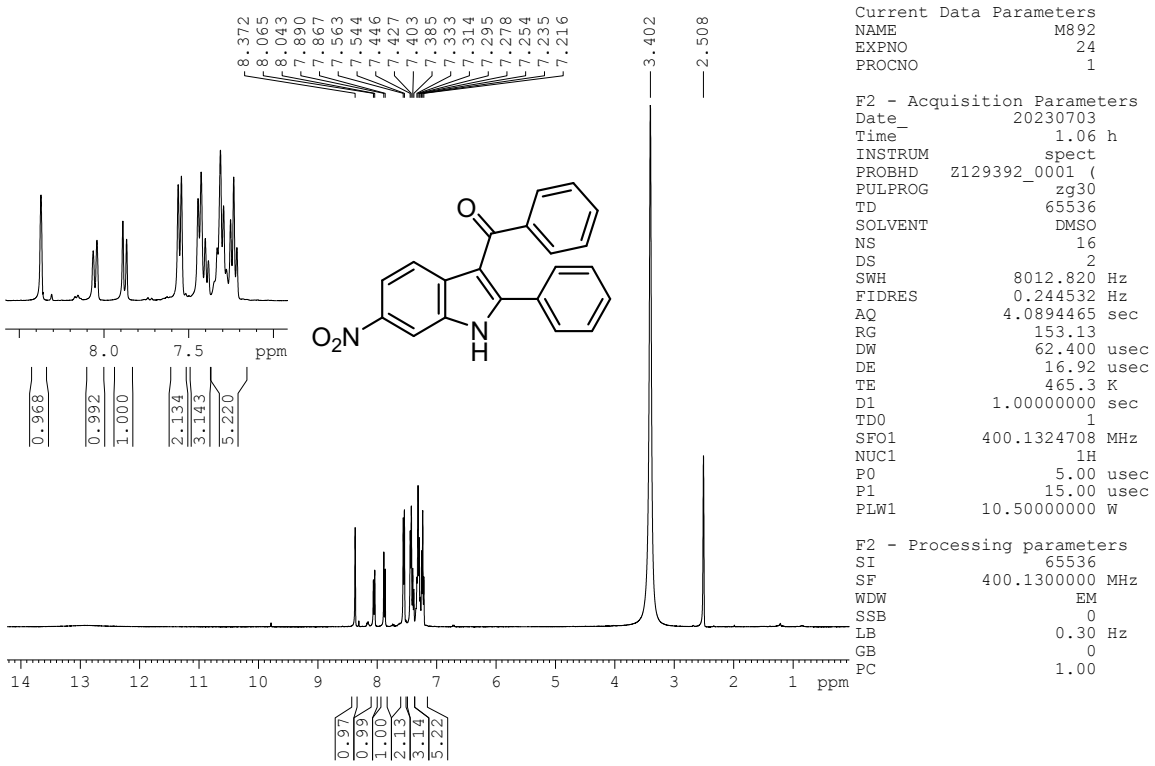
Current Data Parameters
NAME                  M889
EXPNO                   14
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230702
Time                  4.21 h
INSTRUM              spect
PROBHD   Z129392_0001 (
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                      512
DS                        4
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                 1.3631488 sec
RG                    200.34
DW                    20.800 usec
DE                     6.50 usec
TE                    464.7 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1
SFO1           100.6228298 MHz
NUC1                    13C
P0                    3.33 usec
P1                   10.00 usec
PLW1           47.00000000 W
SFO2           400.1316005 MHz
NUC2                     1H
CPDPRG[2            waltz65
PCPD2                90.00 usec
PLW2           10.50000000 W
PLW12           0.29166999 W
PLW13           0.14670999 W

F2 - Processing parameters
SI                    32768
SF             100.6127685 MHz
WDW                      EM
```

^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C) of the compound **6e**

(6-nitro-2-phenyl-1H-indol-3-yl)(phenyl)methanone: 6f

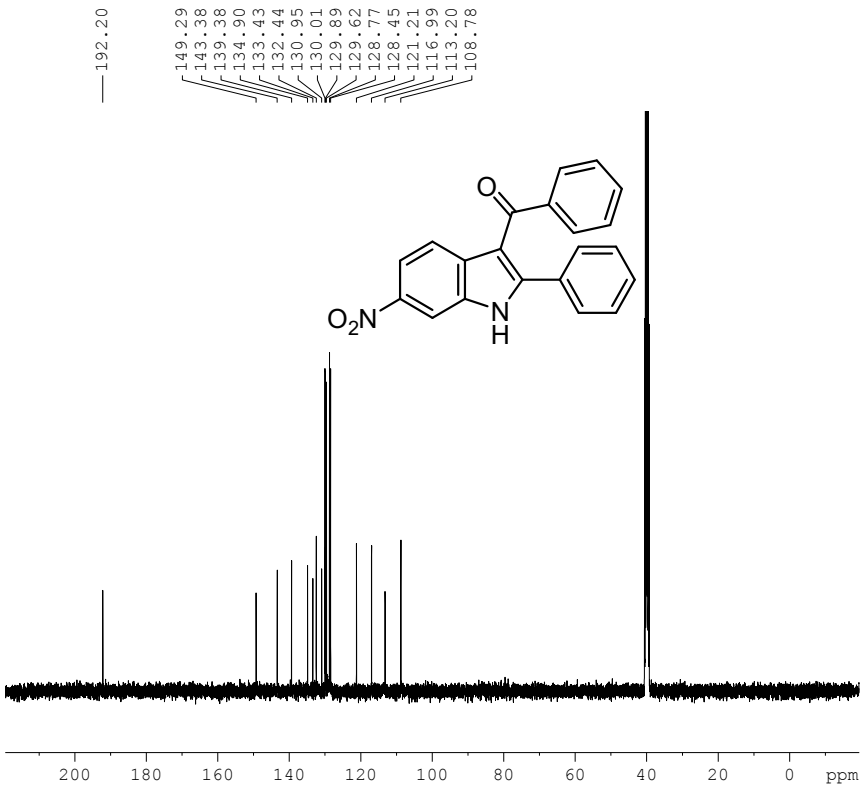


Current Data Parameters
NAME M892
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230703
Time 1.06 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 153.13
DW 62.400 usec
DE 16.92 usec
TE 465.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 10.50000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H NMR (400 MHz, DMSO-d_6, 24 °C) of the compound **6f**



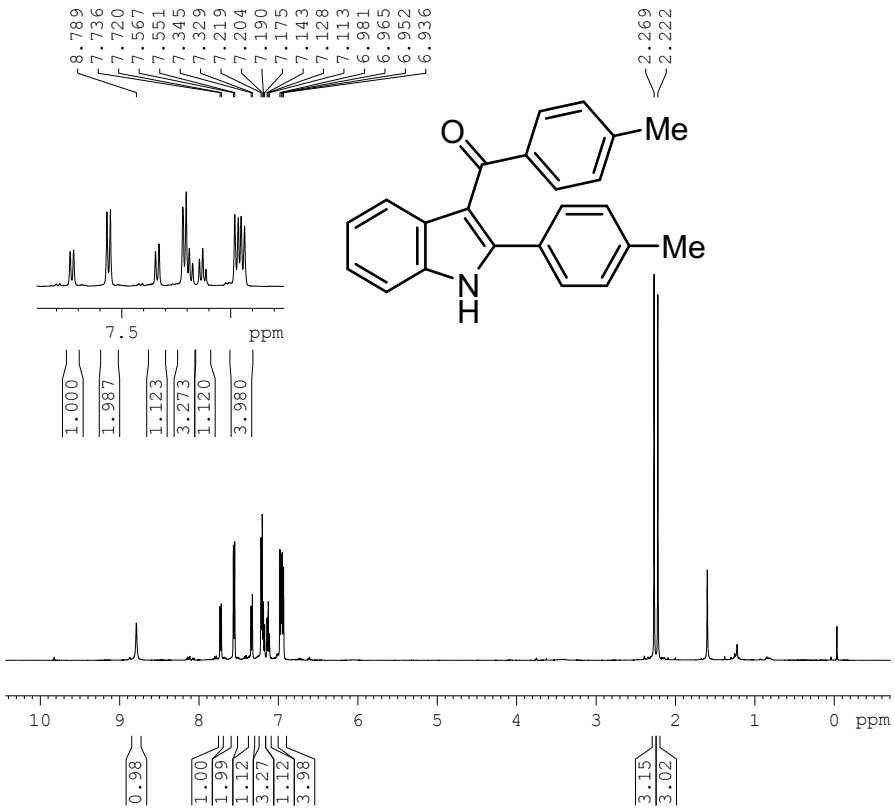
Current Data Parameters
NAME M892
EXPNO 25
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230703
Time 4.12 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 200.34
DW 20.800 use
DE 6.50 use
TE 408.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 use
P1 10.00 use
PLW1 47.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 use
PLW2 10.50000000 W
PLW12 0.29166999 W
PLW13 0.14670999 W

F2 - Processing parameters
SI 32768

^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C) of the compound **6f**

p-tolyl(2-(p-tolyl)-1H-indol-3-yl)methanone: 6g



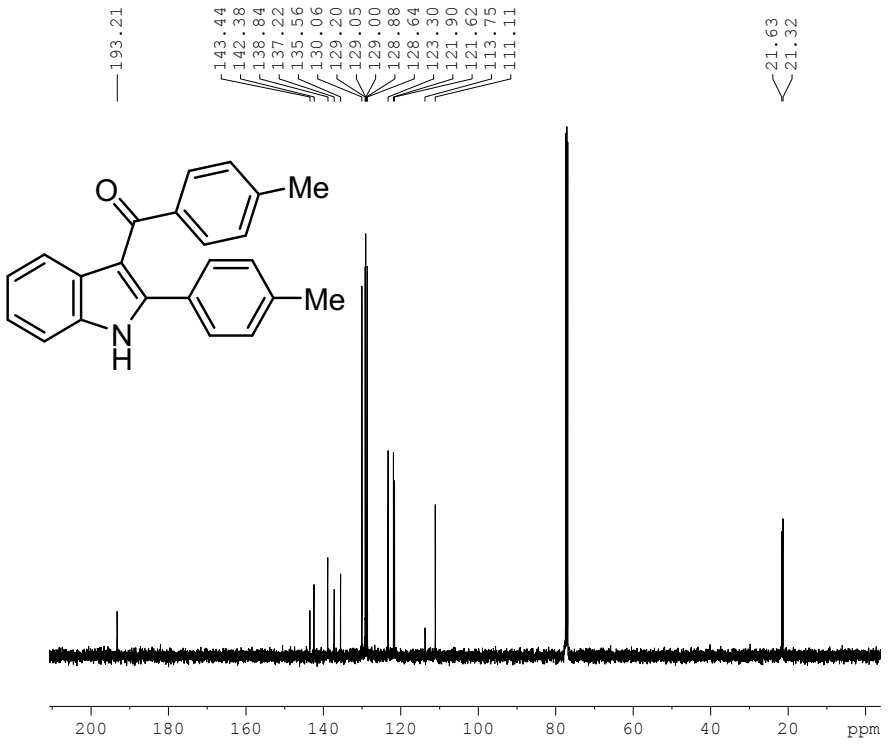

```
Current Data Parameters
NAME                  M732
EXPNO                  170
PROCNO                   1

F2 - Acquisition Parameter
Date_              20230328
Time                 11.36
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      2
SWH             10000.000 Hz
FIDRES              0.305176 Hz
AQ                1.6384000 se
RG                   124.08
DW                   50.000 us
DE                    6.50 us
TE                   302.9 K
D1              0.50000000 se
TD0                      1

======== CHANNEL f1 ======
SFO1          500.1525008 MH
NUC1                    1H
P1                  11.75 us
PLW1          15.30000019 W

F2 - Processing parameters
SI                    65536
SF            500.1500336 MH
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C) of the compound **6g**




```
Current Data Parameters
NAME                  M732
EXPNO                  171
PROCNO                   1

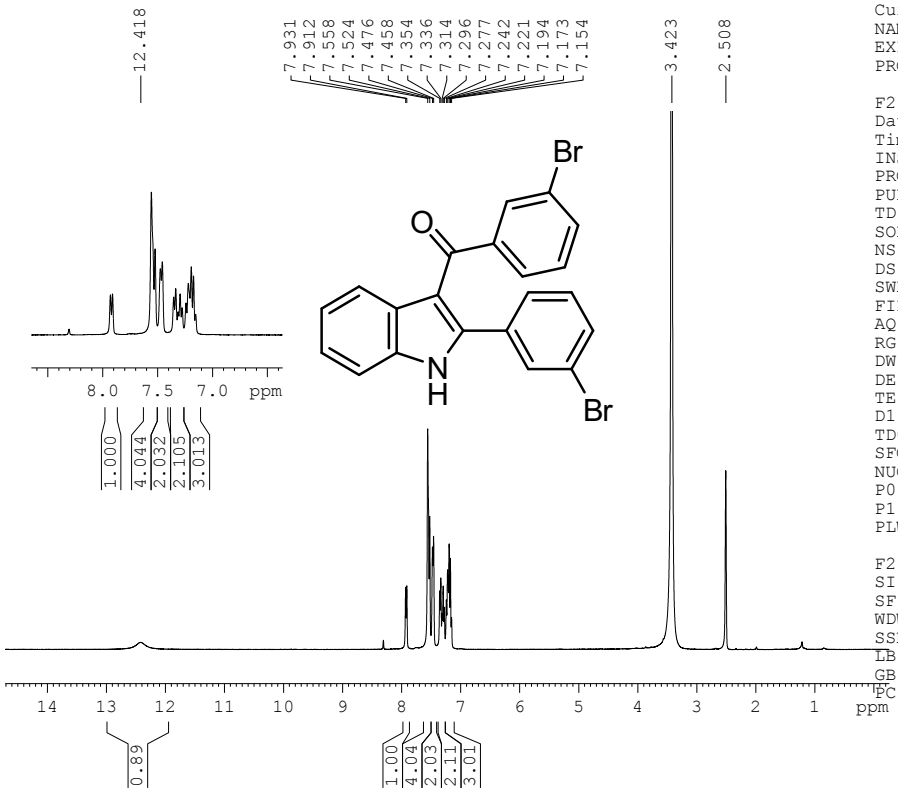
F2 - Acquisition Parameters
Date_              20230328
Time                 11.49
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   20480
SOLVENT             CDCl3
NS                     512
DS                       4
SWH            29761.904 Hz
FIDRES             1.453218 Hz
AQ              0.3440640 sec
RG                   202.34
DW                 16.800 usec
DE                    6.50 usec
TE                   303.7 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          125.7753932 MHz
NUC1                    13C
P1                  10.20 usec
PLW1         103.00000000 W

======== CHANNEL f2 ========
SFO2          500.1520006 MHz
NUC2                    1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2          15.30000019 W
PLW12          0.39658999 W
PLW13          0.19948000 W
```

^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 24 °C) of the compound **6g**

(3-bromophenyl)(2-(3-bromophenyl)-1H-indol-3-yl)methanone: 6h

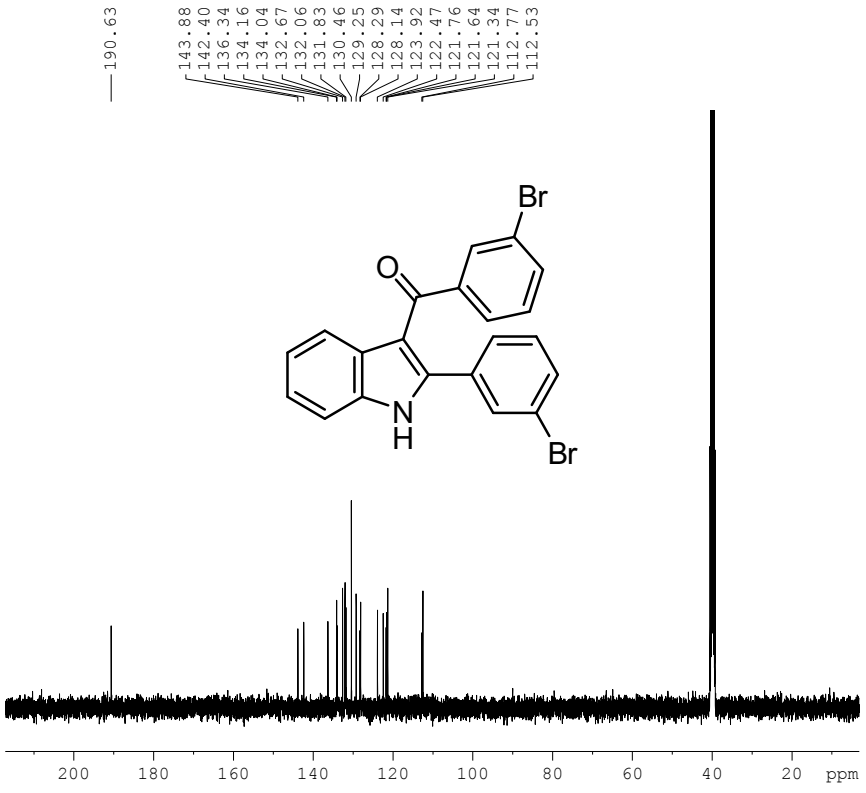



```
Current Data Parameters
NAME                  M865
EXPNO                  502
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230624
Time                 23.27 h
INSTRUM              spect
PROBHD   Z129392_0001 (
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                      16
DS                       2
SWH               8012.820 Hz
FIDRES            0.244532 Hz
AQ                4.0894465 sec
RG                   124.58
DW                   62.400 usec
DE                   16.92 usec
TE                   295.6 K
D1             1.00000000 sec
TD0                      1
SFO1           400.1324708 MHz
NUC1                    1H
P0                    5.00 usec
P1                   15.00 usec
PLW1           10.50000000 W

F2 - Processing parameters
SI                   65536
SF           400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

^{1}H NMR (400 MHz, DMSO-d_6, 24 °C) of the compound **6h**



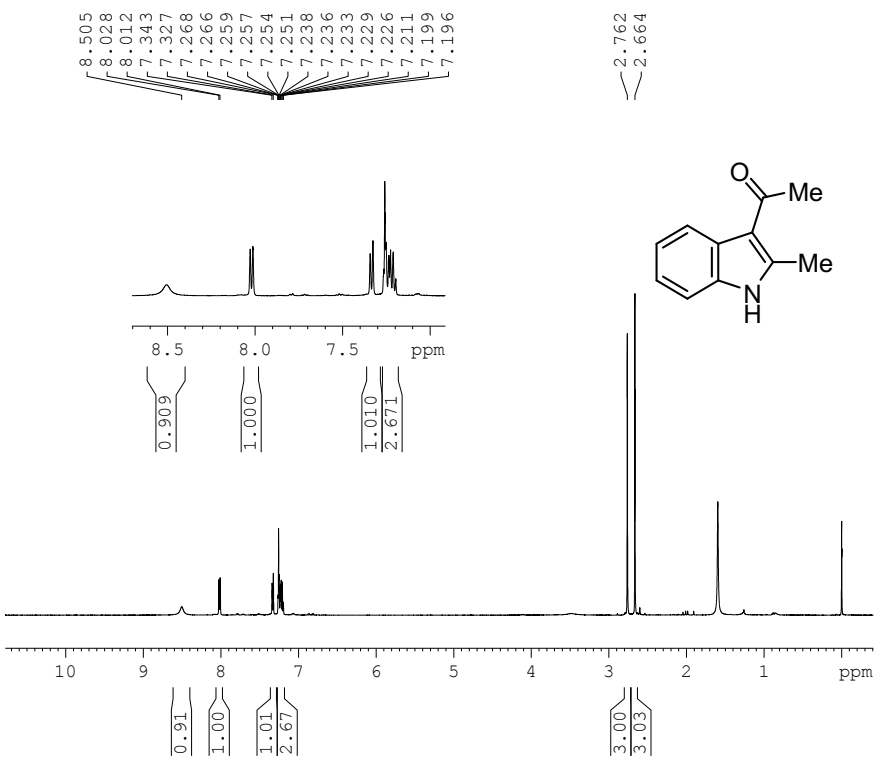

```
Current Data Parameters
NAME                  M865
EXPNO                  503
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230624
Time                 23.42 h
INSTRUM              spect
PROBHD   Z129392_0001 (
PULPROG            zgpg30
TD                  65536
SOLVENT              DMSO
NS                     256
DS                       4
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ                1.3631488 sec
RG                   200.34
DW                   20.800 usec
DE                    6.50 usec
TE                   296.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1
SFO1           100.6228298 MHz
NUC1                   13C
P0                    3.33 usec
P1                   10.00 usec
PLW1           47.00000000 W
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2            waltz65
PCPD2                90.00 usec
PLW2           10.50000000 W
PLW12           0.29166999 W
PLW13           0.14670999 W

F2 - Processing parameters
SI                   32768
SF           100.6127685 MHz
WDW                     EM
```

^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C) of the compound **6h**

1-(2-methyl-1H-indol-3-yl)ethan-1-one: 6i



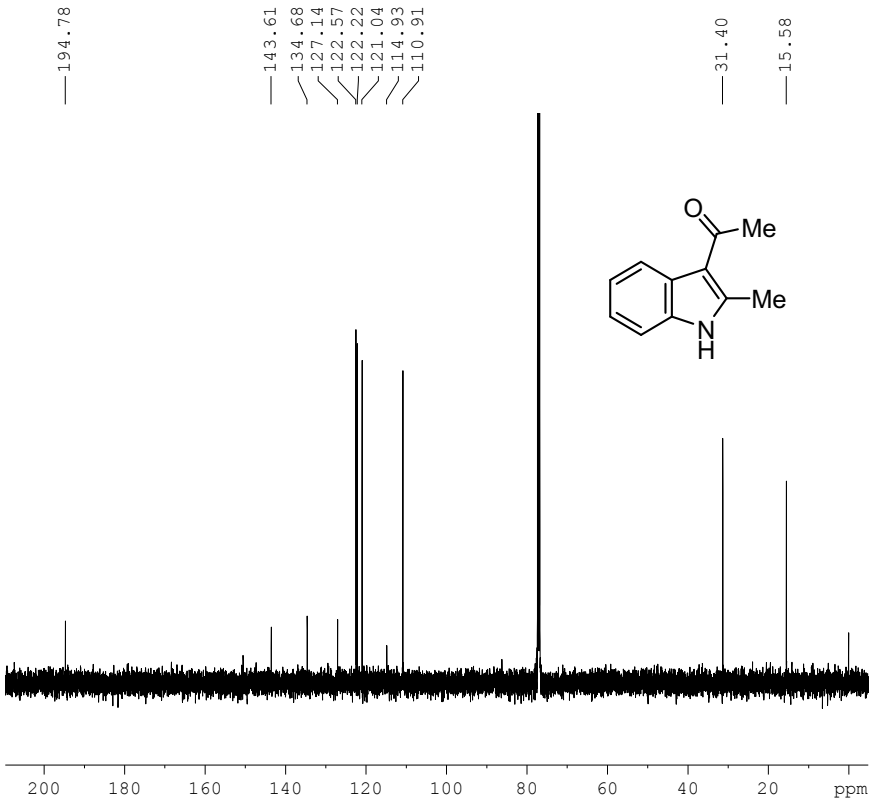

```
Current Data Parameters
NAME                  M735
EXPNO                   35
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230405
Time               22.33
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     2
SWH            10000.000 Hz
FIDRES             0.305176 Hz
AQ              1.6384000 sec
RG                202.34
DW                 50.000 usec
DE                   6.50 usec
TE                 305.3 K
D1              0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.1525008 MHz
NUC1                  1H
P1                 11.75 usec
PLW1          15.30000019 W

F2 - Processing parameters
SI                 65536
SF            500.1500115 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C) of the compound **6i**




```
Current Data Parameters
NAME                  M735
EXPNO                   36
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230405
Time               23.22
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 20480
SOLVENT            CDCl3
NS                  2000
DS                     4
SWH            29761.904 Hz
FIDRES             1.453218 Hz
AQ              0.3440640 sec
RG                202.34
DW                 16.800 usec
DE                   6.50 usec
TE                 306.3 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                    1

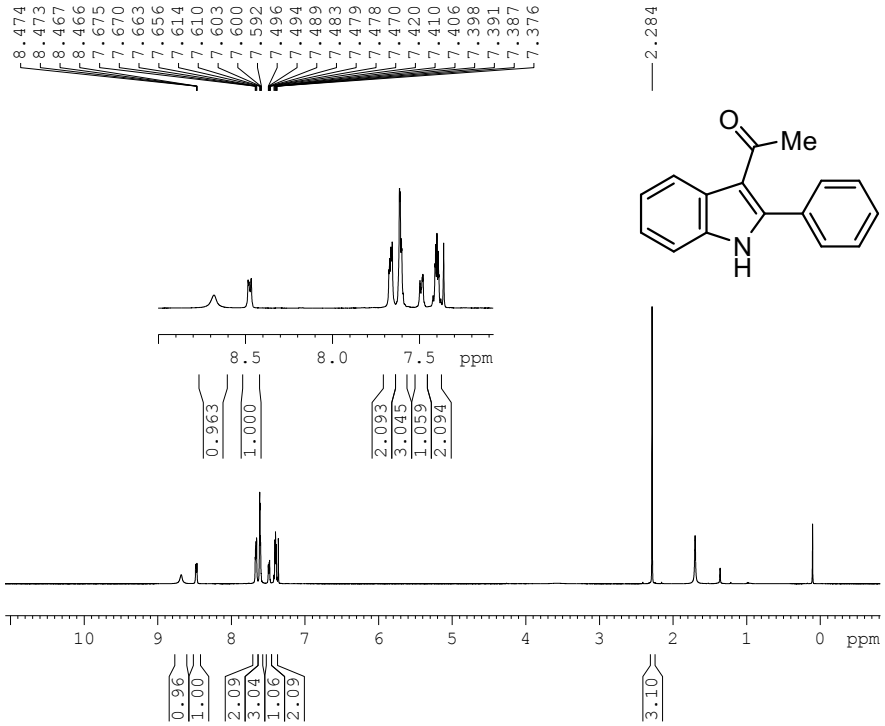
======== CHANNEL f1 ========
SFO1          125.7753932 MHz
NUC1                  13C
P1                 10.20 usec
PLW1        103.00000000 W

======== CHANNEL f2 ========
SFO2          500.1520006 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          15.30000019 W
PLW12          0.39658999 W
PLW13          0.19948000 W

F2 - Processing parameters
SI                 32768
```

^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 24 °C) of the compound **6i**

1-(2-phenyl-1H-indol-3-yl)ethan-1-one: 6j



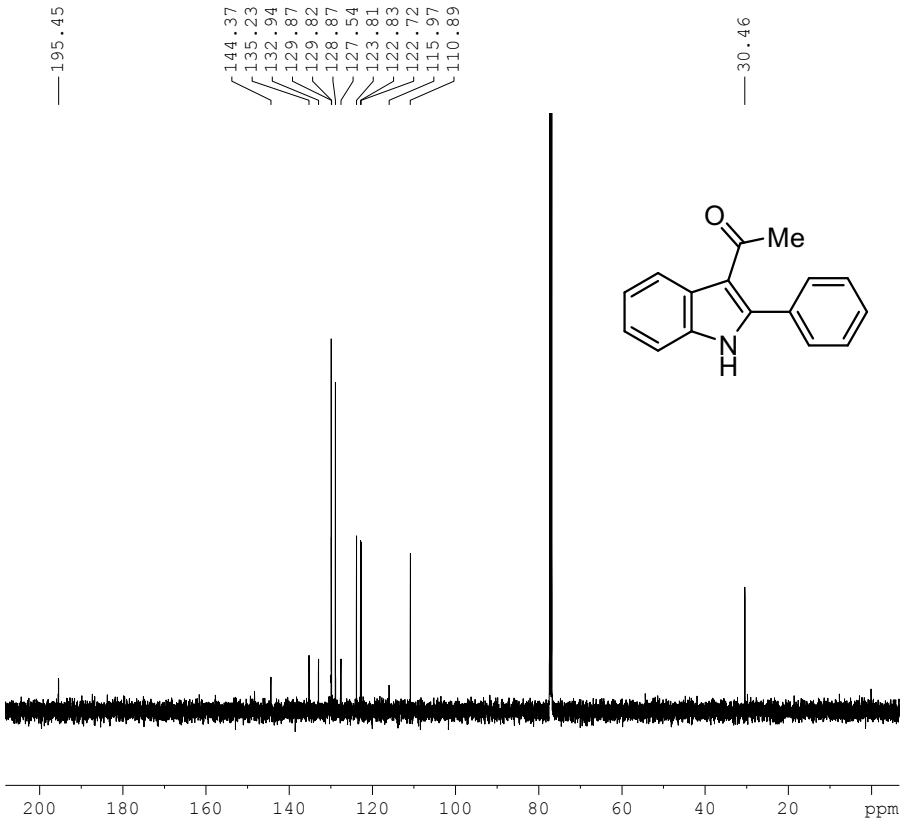

```
Current Data Parameters
NAME                  M736
EXPNO                  193
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230331
Time                  9.41
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      32
DS                       2
SWH              10000.000 Hz
FIDRES           0.305176 Hz
AQ               1.6384000 sec
RG                  202.34
DW                  50.000 usec
DE                    6.50 usec
TE                   303.2 K
D1              0.50000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           500.1525008 MHz
NUC1                     1H
P1                   11.75 usec
PLW1           15.30000019 W

F2 - Processing parameters
SI                    65536
SF             500.1499619 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C) of the compound **6j**




```
Current Data Parameters
NAME                  M736
EXPNO                  194
PROCNO                   1

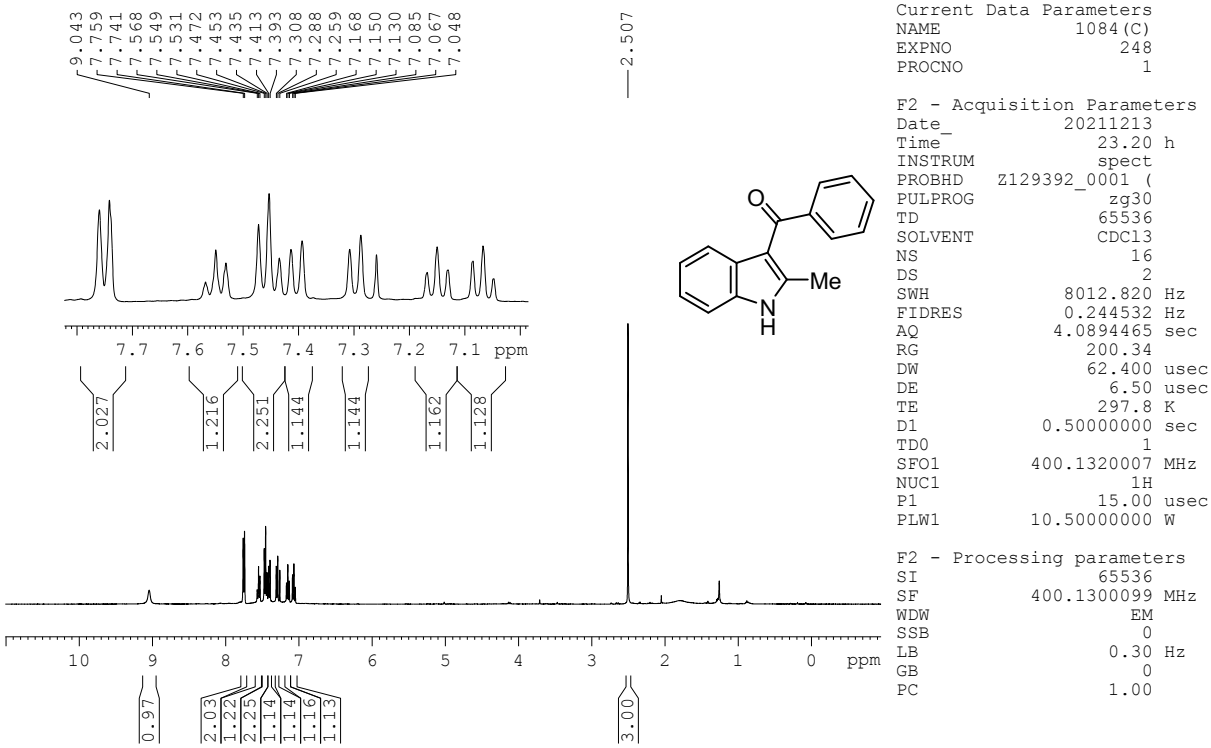
F2 - Acquisition Paramete
Date_              20230331
Time                  9.55
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                   20480
SOLVENT              CDCl3
NS                     512
DS                       4
SWH              29761.904 H
FIDRES            1.453218 H
AQ               0.3440640 s
RG                  202.34
DW                  16.800 u
DE                    6.50 u
TE                   304.2 K
D1              1.00000000 s
D11             0.03000000 s
TD0                      1

======== CHANNEL f1 =====
SFO1           125.7753932 M
NUC1                    13C
P1                   10.20 u
PLW1          103.00000000 W

======== CHANNEL f2 =====
SFO2           500.1520006 M
NUC2                     1H
CPDPRG[2            waltz16
PCPD2                80.00 u
PLW2           15.30000019 W
PLW12           0.39658999 W
PLW13           0.19948000 W
```

^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 24 °C) of the compound **6j**

(2-methyl-1H-indol-3-yl)(phenyl)methanone: 6j'

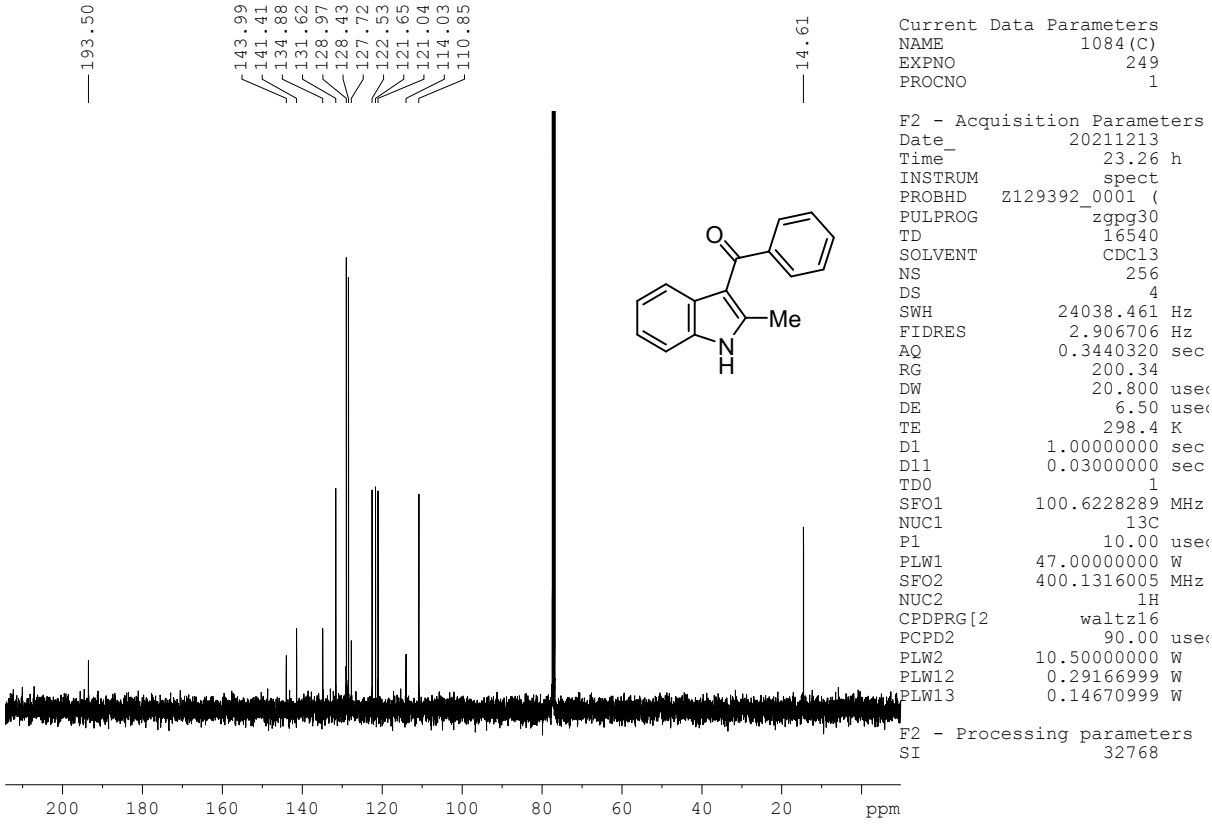


Current Data Parameters
NAME 1084(C)
EXPNO 248
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211213
Time 23.20 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 297.8 K
D1 0.50000000 sec
TD0 1
SFO1 400.1320007 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.50000000 W

F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **6j'**



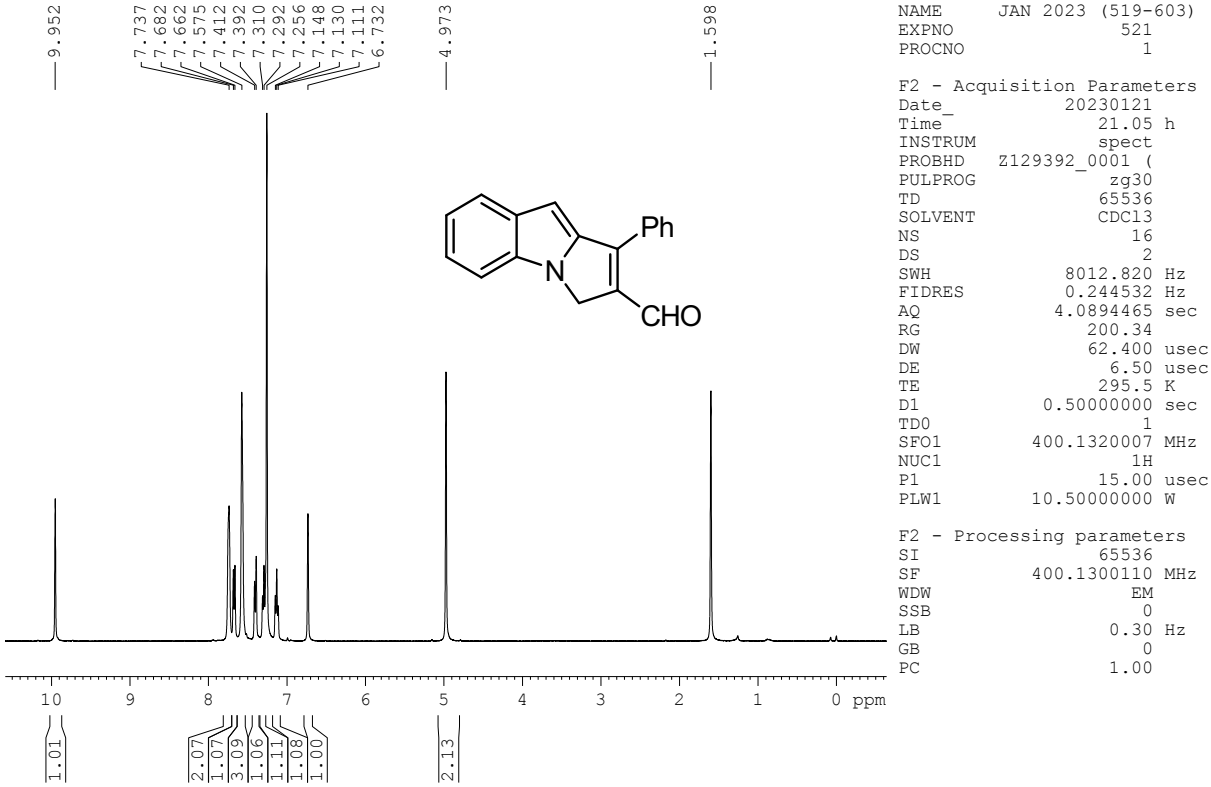
Current Data Parameters
NAME 1084(C)
EXPNO 249
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211213
Time 23.26 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 2.906706 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228289 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.50000000 W
PLW12 0.29166999 W
PLW13 0.14670999 W

F2 - Processing parameters
SI 32768

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **6j**

1-phenyl-3H-pyrrolo[1,2-a]indole-2-carbaldehyde 7

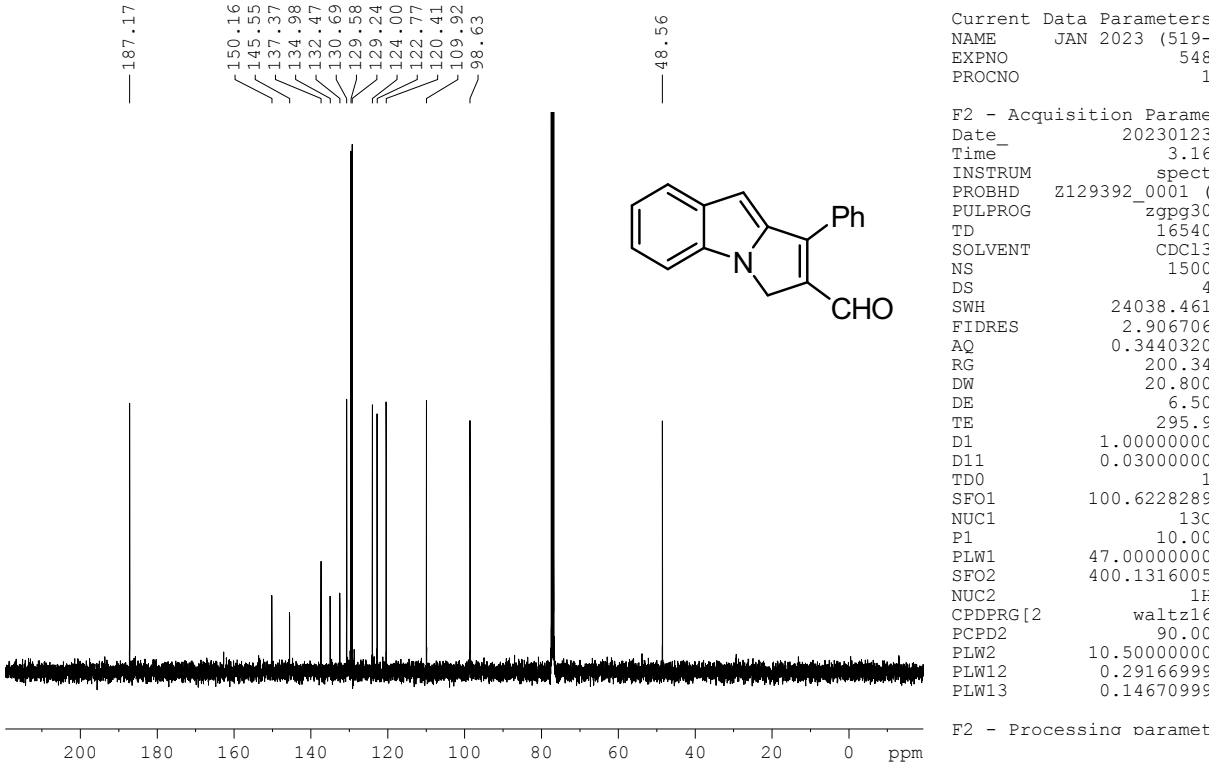



```
Current Data Parameters
NAME      JAN 2023 (519-603)
EXPNO                  521
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230121
Time              21.05 h
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.244532 Hz
AQ              4.0894465 sec
RG                200.34
DW                62.400 usec
DE                 6.50 usec
TE                295.5 K
D1             0.50000000 sec
TD0                    1
SFO1          400.1320007 MHz
NUC1                  1H
P1                 15.00 usec
PLW1          10.50000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300110 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **7**



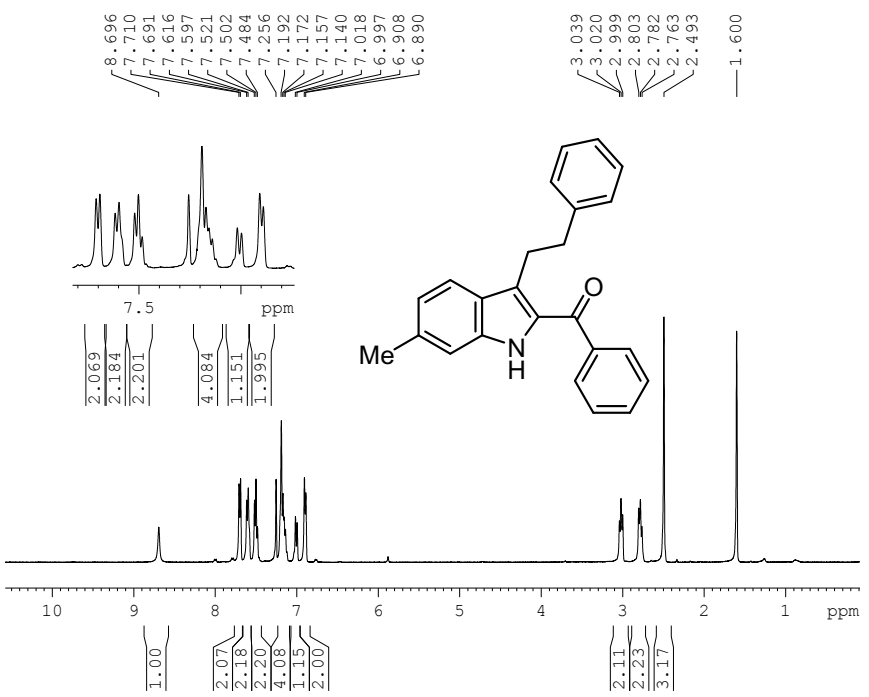

```
Current Data Parameters
NAME      JAN 2023 (519-
EXPNO                548
PROCNO                 1

F2 - Acquisition Parame
Date_           20230123
Time                3.16
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG          zgpg30
TD                16540
SOLVENT            CDCl3
NS                 1500
DS                    4
SWH            24038.461
FIDRES          2.906706
AQ              0.3440320
RG                200.34
DW                20.800
DE                 6.50
TE                295.9
D1             1.00000000
D11            0.03000000
TD0                    1
SFO1          100.6228289
NUC1                  13C
P1                 10.00
PLW1          47.00000000
SFO2          400.1316005
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00
PLW2          10.50000000
PLW12          0.29166999
PLW13          0.14670999

F2 - Processing paramet
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **7**

(6-methyl-3-phenethyl-1H-indol-2-yl)(phenyl)methanone: 3x

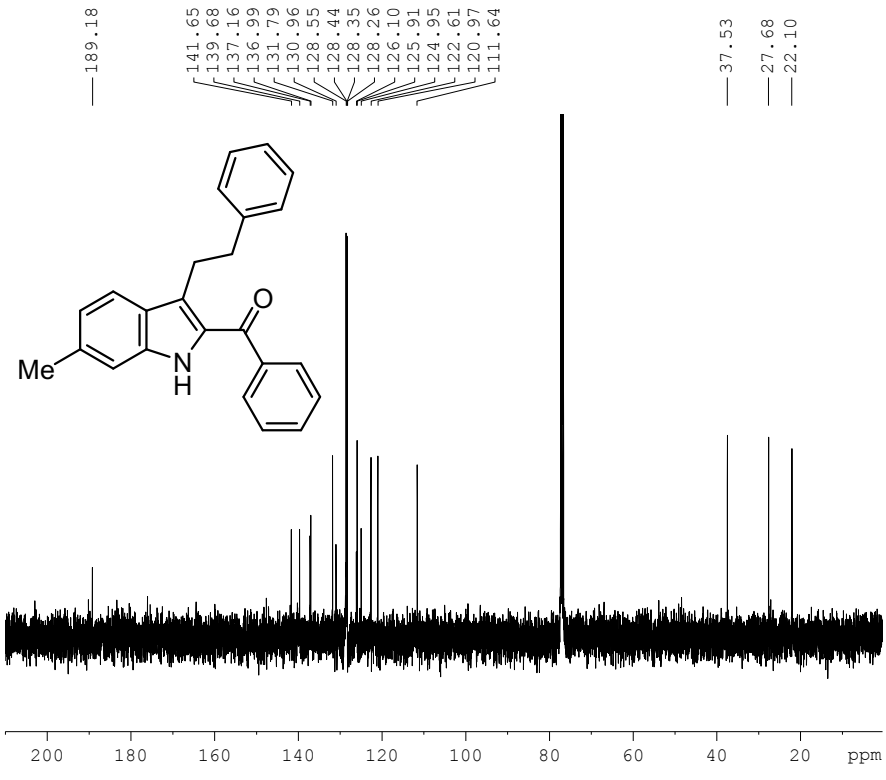


Current Data Parameters
NAME M864
EXPNO 495
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230624
Time 21.05 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 16.92 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 10.50000000 W

F2 - Processing parameters
SI 65536
SF 400.1300114 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3x**



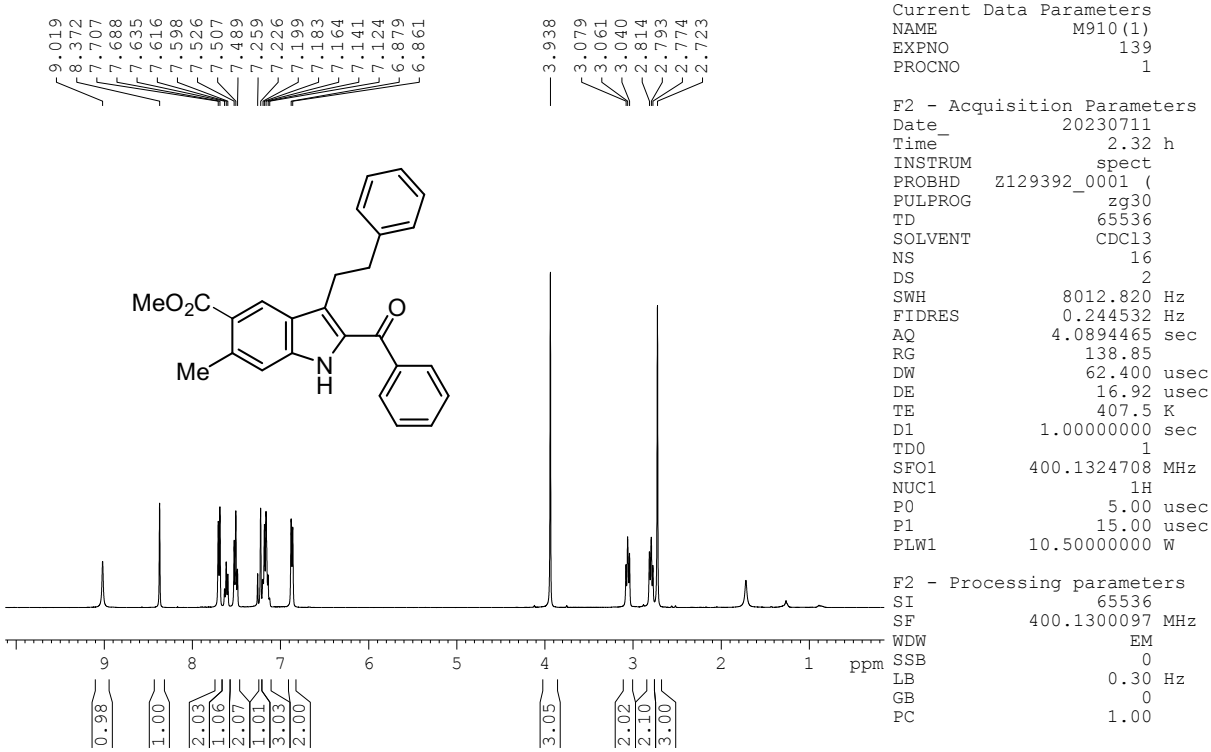
Current Data Parameters
NAME M864
EXPNO 496
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230624
Time 21.20 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 47.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 10.50000000 W
PLW12 0.29166999 W
PLW13 0.14670999 W

F2 - Processing parameters
SI 32768

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3x**

methyl 2-benzoyl-6-methyl-3-phenethyl-1H-indole-5-carboxylate: 9

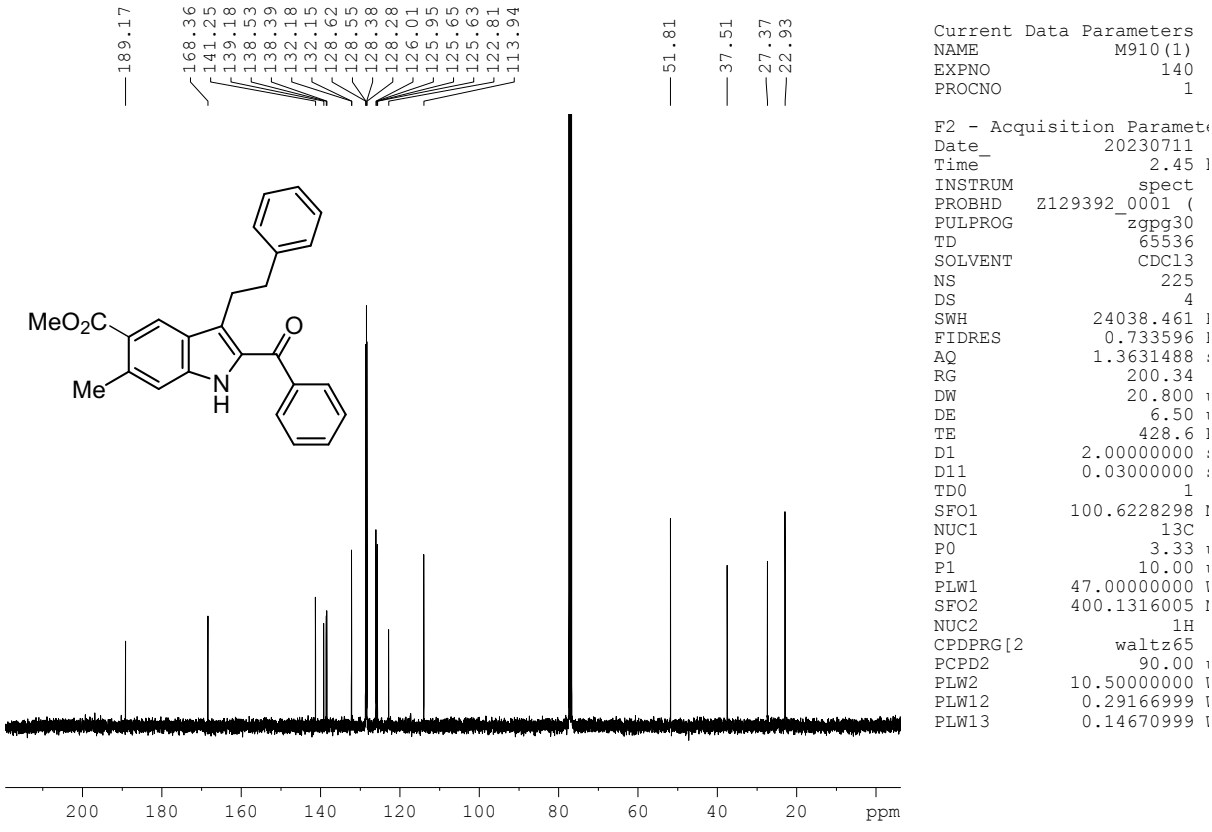


Current Data Parameters
NAME M910(1)
EXPNO 139
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230711
Time 2.32 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 138.85
DW 62.400 usec
DE 16.92 usec
TE 407.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 10.50000000 W

F2 - Processing parameters
SI 65536
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **9**



Current Data Parameters
NAME M910(1)
EXPNO 140
PROCNO 1

F2 - Acquisition Paramet
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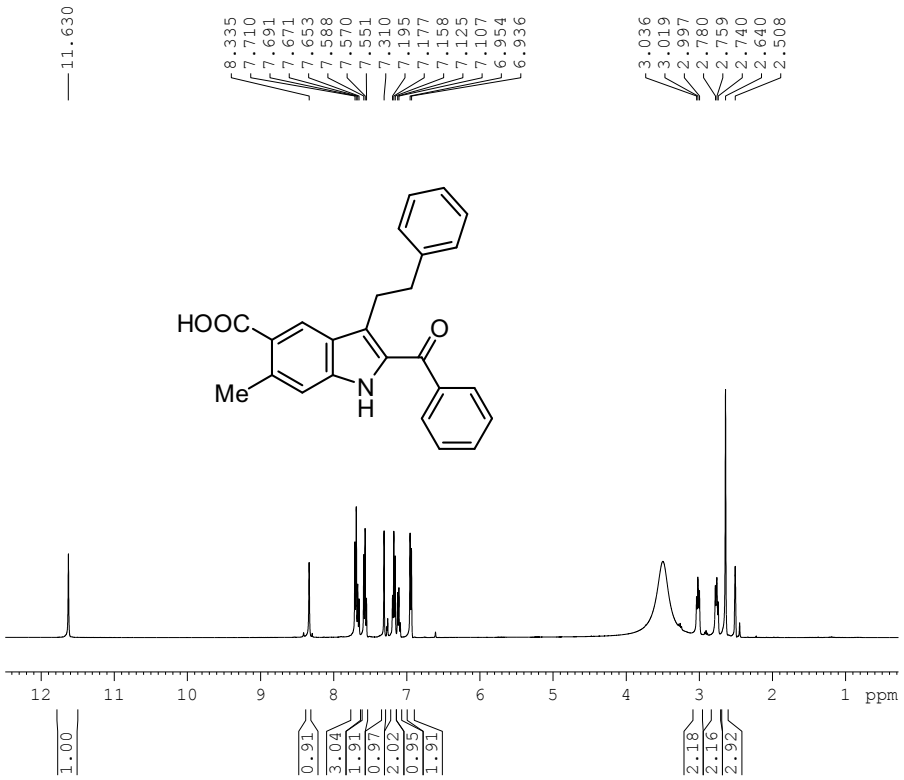
Time 2.45
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 225
DS 4
SWH 24038.461
FIDRES 0.733596
AQ 1.3631488
RG 200.34
DW 20.800
DE 6.50
TE 428.6
D1 2.00000000
D11 0.03000000
TD0 1
SFO1 100.6228298
NUC1 13C
P0 3.33
P1 10.00
PLW1 47.00000000
SFO2 400.1316005
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00
PLW2 10.50000000
PLW12 0.29166999
PLW13 0.14670999

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **9**

2-benzoyl-6-methyl-3-phenethyl-1H-indole-5-carboxylic acid: 10

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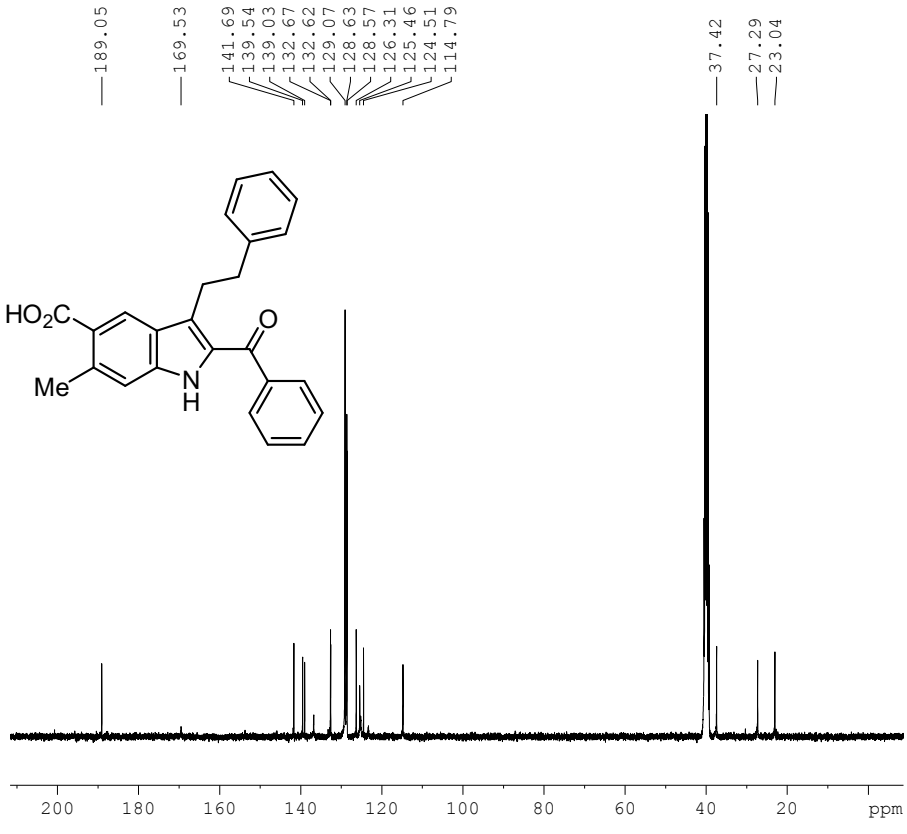
Current Data Parameters
NAME                  14
EXPNO                498
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230731
Time              11.55 h
INSTRUM           spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                 79.8
DW                62.400 usec
DE                16.92 usec
TE                297.7 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P0                 5.00 usec
P1                15.00 usec
PLW1         10.50000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, DMSO-d_6, 24 °C) of the compound **10**

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Current Data Parameters
NAME                 M933
EXPNO                 463
PROCNO                  1

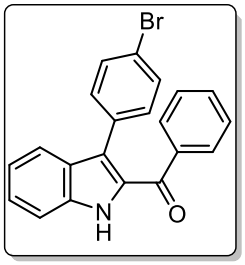
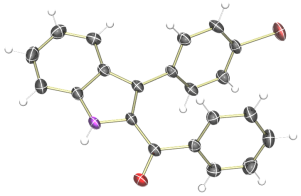
F2 - Acquisition Parameters
Date_           20230728
Time               3.26 h
INSTRUM           spect
PROBHD   Z129392_0001 (
PULPROG          zgpg30
TD                 65536
SOLVENT             DMSO
NS                  2500
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                200.34
DW                20.800 use
DE                 6.50 use
TE                297.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         100.6228298 MHz
NUC1                  13C
P0                 3.33 use
P1                10.00 use
PLW1         47.00000000 W
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz65
PCPD2             90.00 use
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W

F2 - Processing parameters
SI                 32768
SF           100.6127685 MHz
```

^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C) of the compound **10**

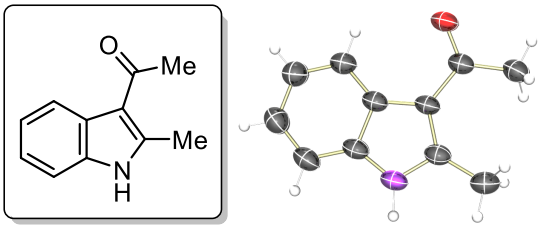
10. XRD data of 3g, 6i, and 6j

a. Single crystal XRD data of 3g:

DATA	3g
Molecular Structure (ORTEP Structure)	 
Formula	$C_{21}H_{14}BrNO$
Formula weight	376.24
Color	Brownish white
Temperature/K	296(2)
Radiation	Mo Kα
Wavelength/Å	0.71073
Crystal system	Triclinic
Space group	P -1
a (Å)	8.6408(5)
b (Å)	9.9341(5)
c (Å)	10.3685(5)
α (°)	98.203(2)
β (°)	101.166(2)
γ (°)	103.107(2)
Volume (Å^3)	834.05(8)
Z	2
Density (g/mL)	1.498

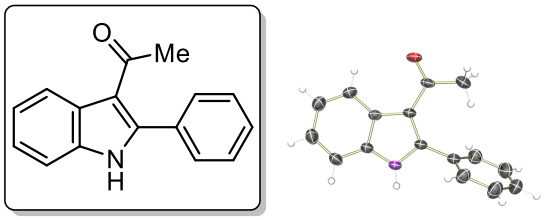
μ (1/mm)	2.470
F (000)	380
θ(min, max)	2.49 to 26.21
No. of unique reflns	12302
No. of parameters	222
R_obs, wR_2_obs	0.0302, 0.0727
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (eÅ^{-3})	0.0390, 0.0769
GooF	1.040

b. Single crystal XRD data of 6i:

DATA	**6i**
Molecular Structure (ORTEP Structure)	
Formula	$C_{11}H_{11}NO$
Formula weight	173.21
Color	Yellowish white
Temperature/K	296(2)
Radiation	Mo Kα
Wavelength/Å	1.54178
Crystal system	monoclinic
Space group	C 2/c
a (Å)	13.5293(7)
b (Å)	7.3263(3)
c (Å)	19.0986(9)
α (°)	90

β (°)	99.741(3)
γ (°)	90
Volume (Å^3)	1865.75(15)
Z	8
Density (g/mL)	1.233
μ (1/mm)	0.632
F (000)	736
θ(min, max)	4.70 to 71.47
No. of unique reflns	13865
No. of parameters	124
R_obs, wR_2_obs	0.0568, 0.1576
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (eÅ^{-3})	0.0693, 0.1763
GooF	1.065

c. Single crystal XRD data of 6j:

DATA	**6j**
Molecular Structure (ORTEP Structure)	
Formula	$C_{16}H_{13}NO$
Formula weight	235.27
Color	Yellowish white
Temperature/K	296(2)
Radiation	Mo Kα
Wavelength/Å	0.71073
Crystal system	triclinic

Space group	P -1
a (Å)	7.4062(4)
b (Å)	7.8098(5)
c (Å)	10.9025(6)
α (°)	101.137(2)
β (°)	93.235(2)
γ (°)	96.394(2)
Volume (Å^3)	612.92(6)
Z	2
Density (g/mL)	1.275
μ (1/mm)	0.080
F (000)	248
θ(min, max)	3.242 to 33.143
No. of unique reflns	39332
No. of parameters	166
R_obs, wR_2_obs	0.0575, 0.1773
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (eÅ^{-3})	0.0832, 0.2091
GooF	1.013