Supporting information

α-Hydroxydimethylacetal/ketal as *α*-hydroxycarbonyl equivalent in interrupted Heyns/Amadori rearrangement: Regioselective synthesis of substituted C2 and C3-acylindoles

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1. General Comments:

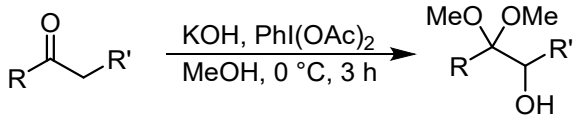
All reactions were carried out under atmospheric pressure using reaction tubes. Column chromatography was performed using Rankem Silica gel (100-200 mesh) and the solvent system used unless otherwise specified, was ethyl acetate-hexane with various percentage of polarity depending on the nature of the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

2. Analytical Methods:

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.

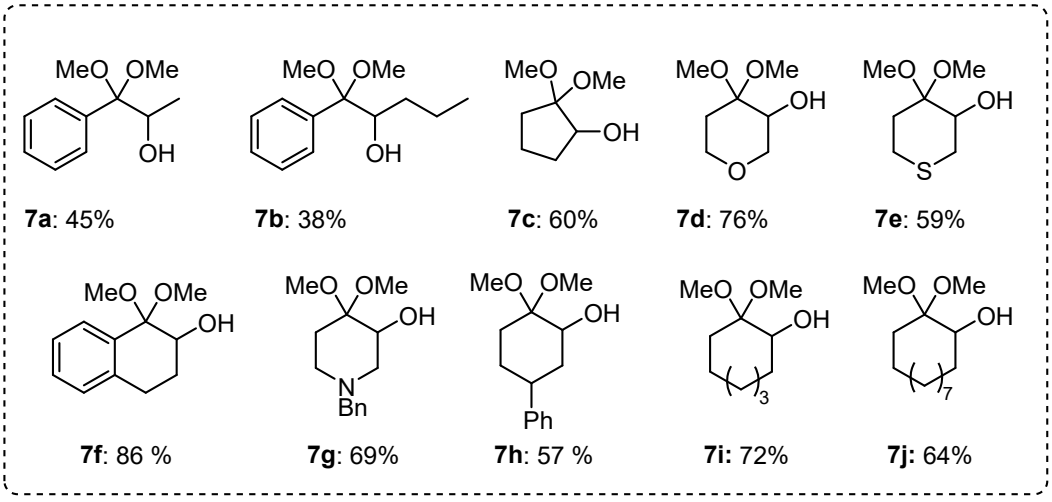
3. Synthesis of *α*-hydroxydimethylacetal/ketal:

Approach 1:

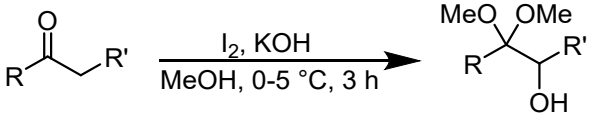


To a round bottom flask KOH (862 mg, 15.4 mmol, 4.5 equiv) was added in 10 mL of MeOH at 0 ℃. After 5 minutes the corresponding ketone (3.4 mmol, 1 equiv) is added dropwise. The mixture was stirred for 10 minutes then $PhI(OAc)_2$ (1.32 g, 4.1 mmol, 1.2 equiv) is added portion wise to the solution at 0 ℃. After stirring the reaction mixture for 3 h at the same temperature, it was quenched with water and extracted with EtOAc. The organic layer was then dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure. The obtained crude product was then purified by silica gel chromatography using ethylaceate:hexane as an eluent to afford the product in good yield. [2]

Below derivatives were synthesized using this approach in one step from the ketone derivatives.

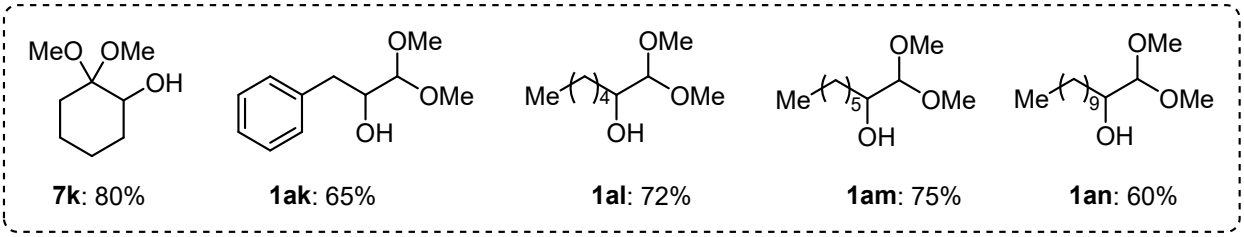


Approach 2:



A solution of KOH (711 mg, 12.7 mmol, 2.5 equiv) in 10 mL of MeOH was cooled to 0-5 ℃. Then, the corresponding carbonyl derivative (0.5 g, 5.1 mmol, 1 equiv) was added dropwise. The reaction mixture was stirred for 10 minutes, then I_2 (1.42 g, 5.61 mmol, 1.1 equiv) dissolved in MeOH (5 mL) was slowly added to the reaction mixture and stirred for 3 h at the

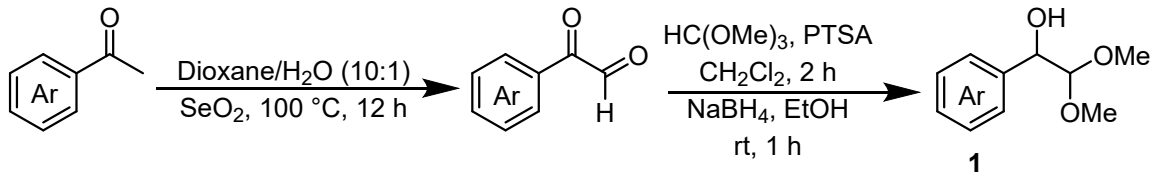
same temperature. After completion of the reaction, it was quenched with saturated solution of $Na_2S_2O_3$ and extracted with EtOAc. The combined organic layer was dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude product was suitable for further use or can be purified by column chromatography. Below derivatives were synthesized using this approach in one step from aliphatic aldehydes and ketone derivatives.[3]



7k: 80% **1ak**: 65% **1al**: 72% **1am**: 75% **1an**: 60%

Approach 3: [4–6]

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



1

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 °C, the reaction mixture was cooled down to 50 °C then the corresponding acetophenone derivative (16.66 mmol, 1 equiv) was added dropwise. Subsequently, the temperature was increased to 100 °C 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.

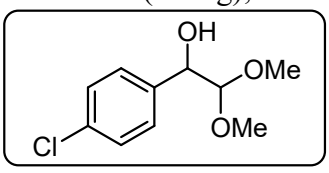
α,α-dimethoxymethyl aryl ketone (16.50 mmol, 1 equiv) was taken in a 100 mL round bottom flask and 30 mL of EtOH was added. The solution was cooled to 0 °C and $NaBH_4$ (1.25 g, 33 mmol, 2 equiv) was added portion wise. The reaction was then allowed to warm to room temperature and stirring was continued 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 *α*-hydroxydimetylacetals in good yield over three steps.

Properties and spectral data of **1a, 1z, 1aa, 1ac, 1af, 1ag, 1ai**, **2c** and **2f** were reported in our earlier communication.[7]

3.1: Properties of synthesized compounds 1:

1-(4-chlorophenyl)-2,2-dimethoxyethan-1-ol (1ad)

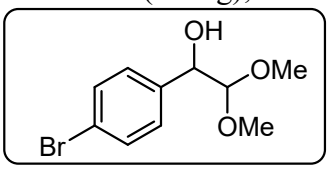
Yield: 69% (2.48 g); viscous liquid; R_f= 0.3 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3453, 2941, 2832,



1487, 1071, 973, 827, 754. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): *δ* 7.25- 7.18 (m, 4H), 4.47 (d, *J* = 6.3 Hz, 1H), 4.12 (d, *J* = 6.3 Hz, 1H), 3.35 (s, 3H), 3.16 (s, 3H), 3.01 (s, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): *δ* 138.0, 133.4, 128.4, 128.2, 107.4, 73.2, 56.1, 54.9.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{10}H_{13}ClO_3$+Na: 239.0451; found: 239.0444.

1-(4-bromophenyl)-2,2-dimethoxyethan-1-ol (1ae):

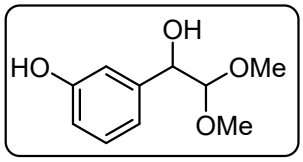
Yield: 63% (2.73 g); viscous liquid; R_f= 0.3 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3445, 2940, 1120,



1085, 972, 825. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): *δ* 7.38 (d, *J* = 8.4 Hz, 2H), 7.20 (d, *J* = 8.6 Hz, 2H), 4.48 (d, *J* = 6.3 Hz, 1H), 4.14 (d, *J* = 6.3 Hz, 1H), 3.37 (s, 3H), 3.19 (s, 3H), 2.86 (s, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): *δ* 138.5, 131.3, 128.8, 121.8, 107.5, 73.3, 56.2, 55.0.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{10}H_{13}BrO_3$+Na: 282.9946; found: 282.9939.

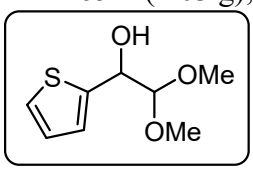
3-(1-hydroxy-2,2-dimethoxyethyl)phenol (1ah):

Yield: 58% (1.91 g); viscous liquid; R_f= 0.2 in 30% EtOAc; IR (ν_{max}, cm^{-1}): 3379, 1596, 1455, 1265, 1122, 1058, 970, 758, 697. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.18 (t, J = 7.6 Hz, 1H), 6.90 (s, 2H), 6.75 (d, J = 7.9 Hz, 1H), 4.56 (d, J = 6.1 Hz, 1H), 4.28 (d, J = 6.1 Hz, 1H), 3.44 (s, 3H), 3.26 (s, 1H), 2.11 (s, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 156.0, 140.9, 129.6, 119.3, 115.3, 114.0, 107.5, 73.9, 56.1, 55.2.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{10}H_{14}O_4$+Na: 221.0790; found: 221.0785.



2,2-dimethoxy-1-(thiophen-2-yl)ethan-1-ol (1aj)

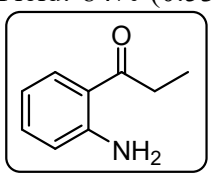
Yield: 65% (2.03 g); viscous liquid; R_f= 0.3 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3441, 2939, 2832, 1123, 1062, 970, 755, 701. ^1H NMR (500 MHz, $CDCl_3$, 24 °C): δ 7.27 (d, J = 5.0 Hz, 1H), 7.07 (d, J = 2.8 Hz, 1H), 6.99-6.97 (m, 1H), 4.88 (d, J = 6.0 Hz, 1H), 4.35 (d, J = 6.1 Hz, 1H), 3.49 (s, 3H), 3.37 (s, 3H), 2.86 (s, 1H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, 24 °C): δ 142.6, 126.6, 125.5, 125.3, 107.2, 70.5, 56.1, 55.3.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_8H_{12}O_3S$+Na: 211.0405; found: 211.0398.



4: Properties of synthesized compounds 2:

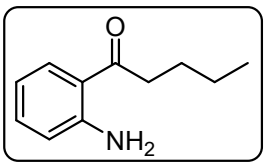
1-(2-aminophenyl)propan-1-one (2b):

Yield: 84% (0.53 g); Solid; m.p. 45- 47 °C; R_f= 0.5 in 95:5 hexane/EtOAc; IR (ν_{max}, cm^{-1}): 3463, 3343, 2978, 1643, 1581, 1214, 945, 751. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.74 (d, J = 7.5 Hz, 1H), 7.26-7.23 (m, 1H), 6.65- 6.62 (m, 2H), 6.20 (s, 1.6 H), 2.97 (q, J = 7.3 Hz, 2H), 1.20 (t, J = 7.3 Hz, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 203.4, 150.3, 134.1, 131.1, 117.9, 117.4, 115.8, 32.4, 8.8.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_9H_{11}NO$+Na: 172.0738; found: 172.0734.



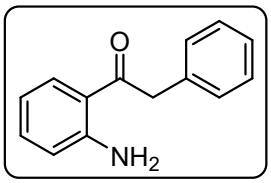
1-(2-aminophenyl)pentan-1-one(2d):

Yield: 88% (0.65 g); viscous liquid; R_f = 0.5 in 95:5 hexane/EtOAc; IR (ν_{max}, cm^{-1}): 3464, 3342, 2954, 1641, 1251, 1204, 964, 750. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.74 (d, J = 8.3 Hz, 1H), 7.25-7.23 (m, 1H), 6.65- 6.62 (m, 2H), 6.20 (s, 1.7 H), 2.92 (t, J = 7.6 Hz, 2H), 1.73- 1.66 (m, 2H), 1.43-1.38 (m, 2H), 0.95 (t, J = 7.3 Hz, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 203.3, 150.4, 134.2, 131.3, 118.1, 117.4, 115.8, 39.1, 27.2, 22.6, 14.0.; HRMS (ESI/Q-TOF) m/z: [M + Na]$^+$ Calcd for $C_{11}H_{15}NO$+Na: 200.1051; found: 200.1044.

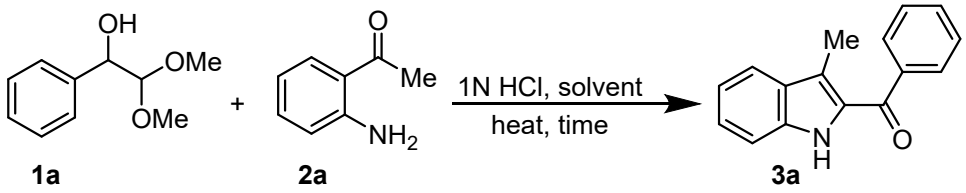


1-(2-aminophenyl)-2-phenylethan-1-one(2g):

Yield: 63% (0.56 g); White solid; m.p. 80-82 °C; R_f= 0.5 in 95:5 hexane/EtOAc; IR (ν_{max}, cm^{-1}): 3467, 3341, 3032, 1611, 1578, 1325, 1206, 978, 747. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.83 (d, J = 8.4 Hz, 1H), 7.32 (t, J = 7.0 Hz, 2H), 7.25- 7.23 (m, 4H), 6.64-6.61 (m, 2H), 4.25 (s, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 200.0, 150.9, 135.4, 134.5, 131.6, 129.5, 128.7, 126.8, 117.6, 117.5, 115.9, 46.2.; HRMS (ESI/Q-TOF) m/z: [M + Na]$^+$ Calcd for $C_{14}H_{13}NO$+Na: 234.0895; found: 234.0890.



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

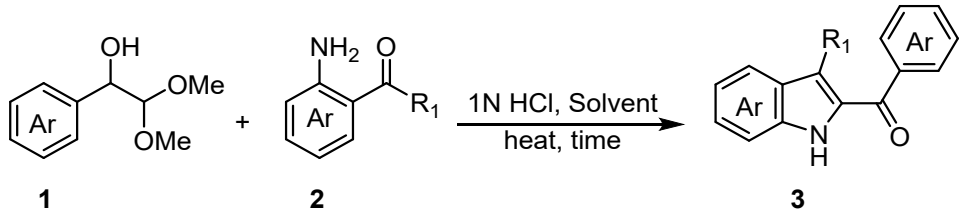


Entry	Acids (equiv)	Temp (°C)	Solvent	Yield (%)[a]
1	-	rt	EtOH	-
2	AcOH (1)	rt	EtOH	-
3	PTSA (1)	rt	EtOH	-
4	1N HCl (2)	rt	EtOH	34
5	$ZnCl_2$ (0.5)	rt	EtOH	-
6	$Sc(OTf)_3$ (0.5)	rt	EtOH	-
7	1N HCl (2)	60	EtOH	50
8	1N HCl (2)	80	EtOH	83
9	1N HCl (2)	90	EtOH	84

10	1N HCl (2)	90	Dioxane	90
11	1N HCl (2)	90	CH_3CN	87
12	**1N HCl** (2)	**100**	**Dioxane**	**94**
13	1N HCl (2)	120	Dioxane	93
14	Conc. HCl (2)	90	Toluene	28[b]
15	PTSA (1)	80	EtOH	60
16	1N HCl (2)	90	H_2O	66

Reaction conditions: **1a** (0.23 mmol, 1 equiv), **2a** (0.23 mmol, 1 equiv), acid (0.5-2 equiv), solvent (3 mL for 0.23 mmol), temp, 18 h. [a] All are isolated yields. [b] formation of heyns adduct **I** was observed in 40% yield.

5. General procedure for synthesis of 2-acylindole derivatives 3

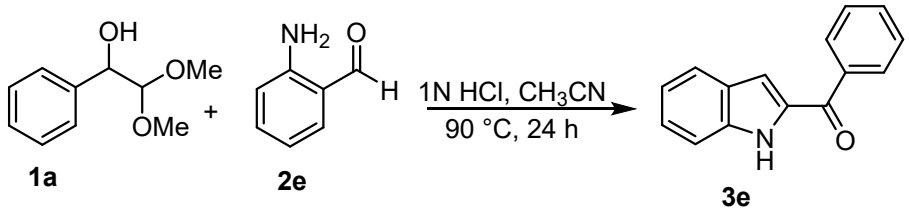


1 **2** **3**

In an oven dried 20 mL reaction tube, compound **1** (0.23 mmol, 1 equiv), and *o*-acylaniline 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 °C 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.

Properties and spectral data of **3a, 3c, 3e, 3f, 3h, 3i, 3j, 3k, 3l, 3m, 3p, 3r, 3t, 3u, 3w, 3z, 3aa, 3ac, 3af, 3ag, 3ai, 3ak, 3al and 5** were reported in our earlier communication.[7]

5.1. Synthesis of compound 3e

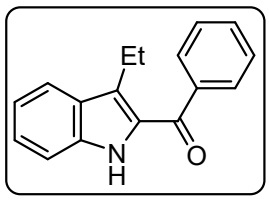


In an oven dried reaction tube, compound **2e** (50 mg, 0.41 mmol, 1 equiv) was taken in 3 mL of acetonitrile and **1a** (76 mg, 0.41 mmol, 1 equiv) was added. To the reaction mixture, 0.5 mL of 1N HCl (2 equiv) was added and the reaction tube was sealed and kept in a pre-heated oil bath at 90 °C and 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 **3e** in 72% (65 mg) yield.

5.2. Properties of synthesized 2-acylindoles:

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

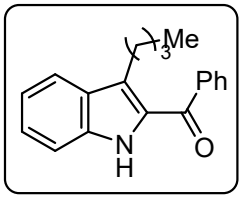
Yield: 81% (46 mg); Solid; m.p. 75-77 °C; R_f= 0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3327, 2970,



1611, 1526, 1256, 735, 693. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.86 (s, 1H), 7.78 (d, J = 7.4 Hz, 2H), 7.73 (d, J = 8.2 Hz, 1H), 7.60 (t, J = 7.4 Hz, 1H), 7.51 (t, J = 7.6 Hz, 2H), 7.41-7.34 (m, 2H), 7.15 (t, J = 7.8 Hz, 1H), 2.78 (q, J = 7.7 Hz, 2H), 1.18 (t, J = 7.7 Hz, 3H).^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.5, 139.7, 136.8, 132.0, 130.8, 128.6, 128.5, 128.1, 127.5, 126.4, 121.6, 120.3, 112.1, 18.6, 15.7.; HRMS (ESI/Q-TOF) m/z: [M + Na] $^+$ Calcd for $C_{17}H_{15}NO$+Na: 272.1051; found: 272.1036.

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

Yield: 95% (61 mg); Solid; m.p. 75-77 °C; R_f= 0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3333, 2954,

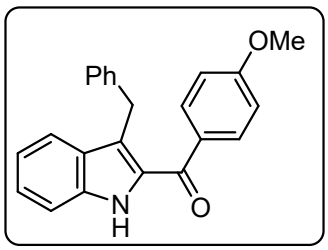


1614, 1525, 1329, 1254, 732, 695. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.82 (s, 1H), 7.77 (d, J = 7.3 Hz, 2H), 7.71 (d, J = 8.2 Hz, 1H), 7.59 (t, J = 7.3 Hz, 1H), 7.50 (t, J = 7.3 Hz, 2H), 7.40-7.33 (m, 2H), 7.15 (t, J = 7.1 Hz, 1H), 2.74 (t, J = 8.4 Hz, 2H), 1.57-1.49 (m, 2H), 1.22-1.13 (m, 2H),

0.77 (t, J = 7.2 Hz, 3H).$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.6, 139.7, 136.7, 131.9, 131.2, 128.6, 128.5, 128.4, 126.4, 126.2, 121.7, 120.2, 112.0, 33.5, 25.0, 22.8, 13.8.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{19}NO$+Na: 300.1364; found: 300.1348.

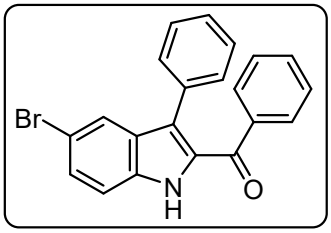
(3-benzyl-1H-indol-2-yl)(4-methoxyphenyl)methanone (3g):

Yield: 74% (58 mg); Solid; m.p. 110-112 °C; R_f = 0.4 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3322, 3057, 1600, 1253, 1170, 1024, 734. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.11 (s, 1H), 7.78 (d, J = 8.8 Hz, 2H), 7.54 (d, J = 8.0 Hz, 1H), 7.42 (d, J = 8.5 Hz, 1H), 7.35-7.31 (m, 1H), 7.20 (t, J = 7.4 Hz, 2H), 7.14 (d, J = 7.1 Hz, 1H), 7.11- 7.08 (m, 3H), 6.89 (d, J = 8.5 Hz, 2H), 4.24 (s, 2H), 3.85 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 188.2, 163.1, 140.8, 136.6, 132.2, 131.7, 131.5, 128.6, 128.4, 128.3, 126.0, 125.9, 121.8, 121. 7, 120.5, 113.8, 112.0, 55.5, 31.3.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{23}H_{19}NO_2$+Na: 364.1313; found: 364.1299.



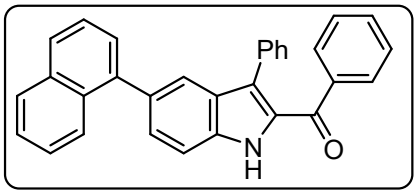
(5-bromo-3-phenyl-1H-indol-2-yl)(phenyl)methanone (3n):

Yield: 74% (64 mg); Solid; m.p. 175- 177 °C; R_f = 0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3313, 3059, 1620, 1258, 740, 696. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.49 (s, 1H), 7.84 (s, 1H), 7.52 (d, J = 7.8 Hz, 2H), 7.48 (d, J = 8.7 Hz, 1H), 7.40 (d, J = 8.8 Hz, 1H), 7.28- 7.26 (m, 1H), 7.14 (s, 5H), 7.07 (t, J = 7.6 Hz, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.5, 137.2, 135.0, 133.1, 132.0, 131.7, 130.8, 129.6, 129.4, 128.2, 127.7, 127.2, 124.5, 114.4, 113.7.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{14}BrNO$+H: 376.0337; found 376.0315.



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

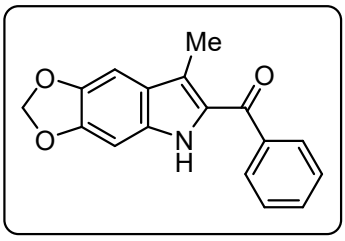
Yield: 92% (89 mg); Solid; m.p. 185-187 °C; R_f =0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3325, 3054, 1621, 1258, 789, 741, 696. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.45 (s, 1H), 7.90 (d, J = 7.6 Hz, 2H), 7.84 (d, J = 12 Hz, 2H), 7.61 (d, J = 8.3 Hz, 1H), 7.56 (d, J = 7.3 Hz, 3H), 7.52- 7.39 (m, 4H), 7.28-7.24 (m, 1H), 7.20 (s, 2H),



7.09- 7.07 (m, 5H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.7, 140.7, 137.6, 135.8, 134.1, 133.8, 133.6, 132.1, 131.8, 131.5. 131.0, 129.6, 129.4, 128.3, 128.1, 127.9, 127.7, 127.5, 127.3, 126.9, 126.3 126.1, 125.8, 125.6, 125.4, 123.1, 111.7.; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{31}H_{21}NO+Na$:446.1521; found 446.1497.

(7-methyl-5H-[1,3]dioxolo[4,5-f]indol-6-yl)(phenyl)methanone (3s):

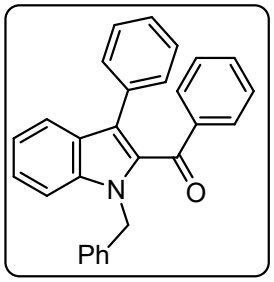
Yield: 84% (54 mg); Yellow Solid; m.p. 170-175 °C; R_f= 0.6 in 15% EtOAc; IR (ν_{max}, cm^{-1}):



3447, 3055, 1597, 1264, 744. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.97 (s, 1H), 7.72 (d, J = 7.5 Hz, 2H), 7.56 (t, J = 7.2 Hz, 1H), 7.48 (t, J = 7.2 Hz, 2H), 6.94 (s, 1H), 6.79 (s, 1H), 5.97 (s, 2H), 2.15 (s, 1H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 188.1, 148.9, 143.9, 139.7, 133.0, 131.6, 131.2, 128.6, 128.4, 123.4, 121.1, 101.1, 98.4, 91.7, 11.4.

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

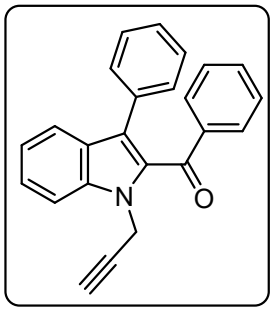
Yield: 31% (28 mg); viscous liquid; R_f=0.7 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3057, 2923, 1635,



1450, 1342, 1255, 938, 729, 697. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.80 (d, J = 7.9 Hz, 1H), 7.58 (d, J = 7.2 Hz, 2H), 7.47 (d, J = 8.2 Hz, 1H), 7.38 (t, J = 7.4 Hz, 1H), 7.28-7.20 (m, 6H), 7.18-7.11 (m, 5H), 7.09-7.05 (m, 3H). 5.70 (s, 2H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 190.9, 138.5, 138.1, 138.0, 133.8, 132.7, 132.5, 130.5, 130.1, 128.6, 128.0, 127.7, 127.4, 126.7, 126.6, 126.2, 125.5, 124.5, 121.6, 121.3, 110.9, 47.9; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{28}H_{21}NO+H$:388.1701; found 388.1678.

phenyl(3-phenyl-1-(prop-2-yn-1-yl)-1H-indol-2-yl)methanone(3x):

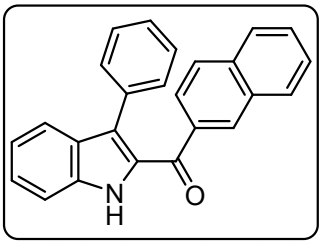
Yield: 28% (22 mg); viscous liquid; R_f=0.7 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3290, 3058, 2921,



1625, 1246, 926, 732, 695, 640. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.76 (d, J = 8.2 Hz, 1H), 7.66 (d, J = 7.3 Hz, 2H), 7.59 (d, J = 8.4 Hz, 1H), 7.47 (t, J = 7.5Hz, 1H), 7.29-7.21 (m, 5H), 7.13-7.03 (m, 4H), 5.27 (d, J = 2.4 Hz, 2H), 2.23 (t, J = 2.4 Hz, 1H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 190.6, 138.2, 138.1, 133.6, 132.6, 132.1, 130.6, 130.2, 128.1, 127.8, 126.8, 126.5, 125.9, 125.5, 121.9, 121.6, 110.5, 78.8, 72.6, 34.0.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{17}NO+H$: 336.1388; found 336.1363.

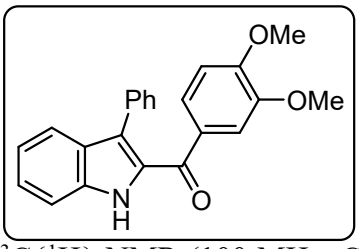
naphthalen-2-yl(3-phenyl-1H-indol-2-yl)methanone (3y):

Yield: 96% (77 mg); Solid; m.p. 140-142 °C; R_f = 0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3316, 3055, 1605, 1328, 1266, 742, 700. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.48 (s, 1H), 7.97 (s, 1H), 7.67- 7.59 (m, 3H), 7.52- 7.44 (m, 3H), 7.38-7.28 (m, 3H),7.15- 7.11 (m, 3H), 6.90- 6.88 (m, 2H), 6.81- 6.79 (m, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.4, 136.5, 134.8, 134.5, 133.9, 132.0, 131.9, 131.2, 130.8, 129.1, 128.0, 127.9, 127.8, 127.6, 127.5, 126.8, 126.6, 126.2, 125.4, 125.2, 122.2, 121.2, 112.1.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{25}H_{17}NO$+H:348.1388 found 348.1378.



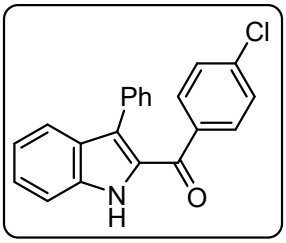
(2,3-dimethoxyphenyl)(3-phenyl-1H-indol-2-yl)methanone (3ab):

Yield: 55% (45 mg); Solid; m.p. 210- 212 °C; R_f = 0.2 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3262, 1711, 1266, 1147, 1019, 750, 701. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.28 (s, 1H), 7.78 (d, J = 8.2 Hz, 1H), 7.50 (d, J = 8.2 Hz, 1H), 7.40 (t, J = 8.0 Hz, 1H), 7.28-7.26 (m, 3H), 7.21-7.13 (m, 5H), 6.56 (d, J = 8.3 Hz, 1H), 3.82 (s, 3H), 3.67 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 188.2, 152.5, 148.2, 136.3, 134.1, 131.1, 130.9, 130.2, 128.2, 127.6, 127.0, 126.3, 124.6, 124.1, 122.0, 121.2, 112.3, 112.0, 109.9, 56.0, 55.8.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{23}H_{19}NO_3$+H: 358.1443 found 358.1428.



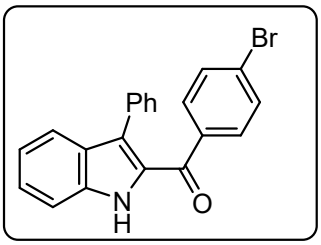
(4-chlorophenyl)(3-phenyl-1H-indol-2-yl)methanone (3ad):

Yield: 91% (69 mg); Solid; m.p. 150-152 °C; R_f = 0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3590, 3003, 1710, 1360, 1220. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.40 (s, 1H), 7.72 (d, J = 8.1 H z, 1H), 7.51(d, J = 8.4 Hz, 1H), 7.45-7.40 (m, 3H), 7.20-7.18 (m, 6H), 7.03 (d, J = 8.1, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 188.3, 138.0, 136.6, 136.0, 133.6, 131.0, 130.9, 130.7, 128.2, 127.9, 127.7, 127.2, 126.9, 125.7, 122.3, 121.4, 112.1.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{14}ClNO$+H: 332.0842; found 332.0830.



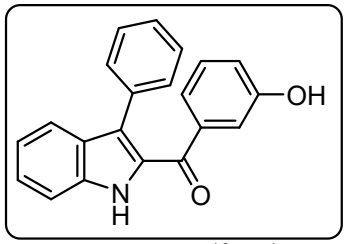
(4-bromophenyl)(3-phenyl-1H-indol-2-yl)methanone (3ae)

Yield: 98% (85 mg); Solid; m.p. 165- 167 °C; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3328, 3057, 1612, 1333, 1262, 750, 702. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.53 (s, 1H), 7.72 (d, J = 8.2 Hz, 1H), 7.51 (d, J = 8.4 Hz, 1H), 7.44-7.36 (m, 3H), 7.20-7.17 (m, 8H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 188.5, 136.6, 136.4, 133.5, 131.1, 131.0, 130.8, 130.7, 128.2, 127.7, 127.1, 126.9, 126.6, 125.8, 122.3, 121.4, 112.2.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{14}BrNO$+H: 376.0337 found 376.0318.



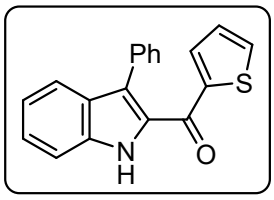
(3-hydroxyphenyl)(3-phenyl-1H-indol-2-yl)methanone (3ah):

Yield: 97% (70 mg); Solid; m.p. 175-177 °C; R_f= 0.2 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3326, 1704, 1587, 1276, 754, 700. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.21 (s, 1H), 7.68 (d, J = 8.2 Hz, 1H), 7.46 (d, J = 8.2 Hz, 1H), 7.38 (t, J = 6.9 Hz, 1H), 7.17-7.13 (m, 6H), 7.02 (d, J = 6.6 Hz, 1H), 6.97 (s, 1H), 6.88 (t, J = 7.5 Hz, 1H), 6.72 (d, J = 7.9 Hz, 1 H), 5.06 (s, 1 H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.1, 155.2, 138.9, 136.4, 133.9, 130.8, 129.0, 128.1, 127.8, 127.1, 126.8, 125.6, 122.4, 122.3, 121.3, 119.1, 116.1, 112.0.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{15}NO_2$+H: 314.1181 found 314.1170.



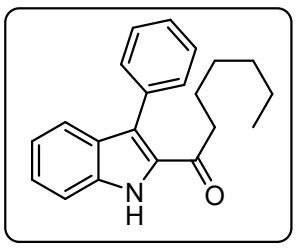
(3-phenyl-1H-indol-2-yl)(thiophen-2-yl)methanone (3aj):

Yield: 96% (66 mg); Solid; m.p. 195-197 °C; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3321, 2926, 1574, 1410, 1262, 750, 694. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.19 (s, 1H), 7.69 (d, J = 8.2 H z, 1H), 7.43 (d, J = 8.4 Hz, 1H), 7.39 (dd, J = 5.0, 0.9 Hz, 1H), 7.35-7.31 (m, 3H), 7.23- 7.10 (m, 5H), 7.06 (dd, J = 3.8, 0.9 Hz, 1H), 6.61 (dd, J = 4.8, 3.9 Hz, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 180.8, 142.5, 136.3, 135.0, 134.2, 133.3, 131.0, 130.8, 128.5, 127.7, 127.4, 127.2, 126.4, 123.9, 122.0, 121.3, 112.0.; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{19}H_{13}NOS$+H: 304.0796 found 304.0796.



1-(3-Phenyl-1H-indol-2-yl)heptan-1-one (3am):

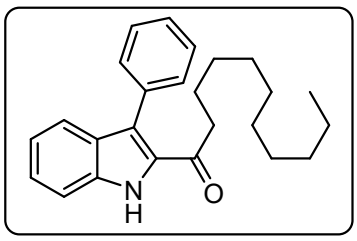
Yield: 82% (56 mg); Solid; m.p. 65-70 °C; R_f= 0.6 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3441, 3331, 3055, 2929, 1643, 1426, 1265, 741. ^1H NMR (400 MHz, $CDCl_3$, 24



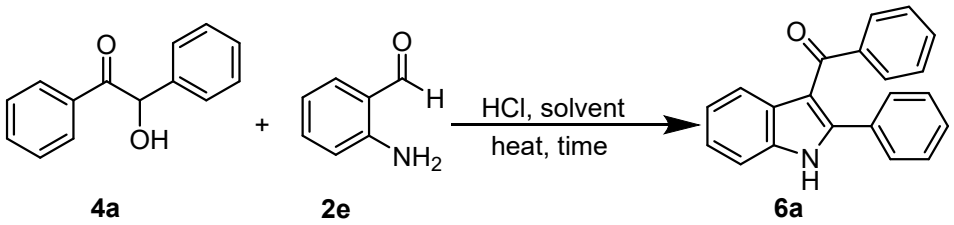
°C): δ 9.51 (s, 1H), 7.49-7.42 (m, 7H), 7.35 (t, J = 7.8 Hz, 1H), 7.09 (t, J = 7.2 Hz, 1H), 2.47 (t, J = 7.7 Hz, 2H), 1.55-1.52 (m, 2H), 1.20-1.16 (m, 2H), 1.08 (s, 4H), 0.81 (t, J = 7.1 Hz, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 194.8, 135.7, 134.4, 131.8, 130.6, 128.9, 128.5, 127.9, 126.4, 124.1, 122.1, 120.7, 111.9, 40.1, 31.4, 28.8, 24.8, 22.4, 14.0.

1-(3-phenyl-1H-indol-2-yl)undecan-1-one (3an):

Yield: 85% (71 mg); Solid; m.p. 40-45 °C; R_f=0.6 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3442, 3328, 3056, 2927, 2855, 1643, 1265, 745. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.59 (s, 1H), 7.42-7.33 (m, 7H), 7.26 (t, J = 7.9 Hz, 1H), 7.00 (t, J = 7.5 Hz, 1H), 2.39 (t, J = 7.6 Hz, 2H), 1.48-1.44 (m, 2H), 1.17 - 1.09 (m, 11H), 1.00 (s, 3H), 0.78 (t, J = 6.9 Hz, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 194.9, 135.7, 134.5, 131.8, 130.6, 128.9, 128.5, 127.9, 126.4, 124.1, 122.1, 120.7, 112.0, 40.1, 31.9, 29.5, 29.4, 29.3, 29.2, 29.1, 24.9, 22.7, 14.1.



6. Optimization: Synthesis of 3-acylindole 6a



4a **2e** **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), **2e** (0.23 mmol, 1 equiv), Conc. HCl (11.5 N, 0.5 mmol, 2 equiv), Dioxane (3 mL for 0.23 mmol), 120 °C, 24 h.

General procedure for synthesis of 3-acylindoles 6:

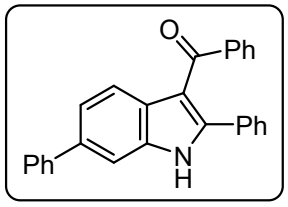
In a 20 mL reaction tube, benzoin derivative **4** or dimethylketal derivative **7** (0.23 mmol, 1 equiv) and 2-aminobenzaldehyde derivative **2** (28 mg, 0.23 mmol, 1 equiv) were taken in 3 mL of dioxane. Conc. HCl (11.5 N, 20 mg, 0.5 mmol, 2 equiv) was added to the reaction mixture and the tube was sealed and kept in a pre-heated oil bath at 120 °C 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 EtOAc. 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 Ethylacetate:hexane as an eluent to afford 3-acylindole derivatives **6** in good yield.

Properties and spectral data of **6a, 6c, 6e, 6f, 6j, 6k, 6l, 6n, 6o, 6p, 6p' and II** were reported in our earlier communication.[7]

6.1. Properties of synthesized 3-acylindoles:

(2,6-diphenyl-1H-indol-3-yl)(phenyl)methanone (6b):

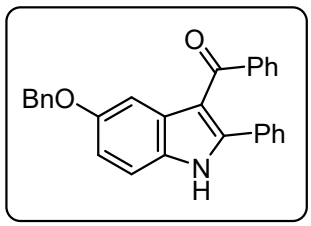
Yield: 61% (52 mg); white solid; m.p. 175-180 °C; R_f = 0.3 in 15% EtOAc; IR (ν_{max}, cm^{-1}):



3236, 3057, 1600, 1452, 1412, 1268, 906, 755. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.31 (s, 1H), 7.91 (d, J = 8.2 Hz, 1H), 7.63 (d, J = 7.6 Hz, 2H), 7.59-7.56 (m, 3H), 7.44-7.39 (m, 3H), 7.32-7.27 (m, 4H), 7.17-7.06 (m, 5H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 193.6, 144.6, 141.6, 139.6, 136.9, 136.2, 131.7, 131.5, 129.7, 129.2, 128.8, 128.7, 128.3, 127.9, 127.8, 127.3, 126.9, 121.9, 121.7, 113.4, 109.6.

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

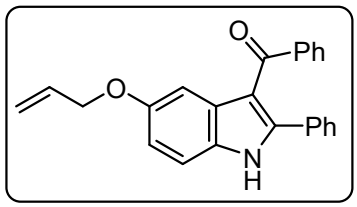
Yield: 43% (40 mg); brown solid; m.p.160-165 °C; R_f=0.2 in 10 % EtOAc; IR (ν_{max}, cm^{-1}):



3238, 3008, 1600, 1455, 1268, 757.; ^{1}H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.68 (s, 1H), 7.53-7.51 (m, 3H), 7.37-7.35 (m, 2H), 7.30-7.24 (m, 4H), 7.22-7.20 (m, 3H), 7.10-7.04 (m, 5H), 7.92(dd, J = 8.8, 2.4 Hz, 1H), 4.99 (s, 2H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 24 °C): δ 193.2, 155.2, 144.3, 139.7, 137.4, 131.8, 131.3, 130.6, 129.5, 129.2, 128.6, 128.4, 128.2, 127.8, 127.7, 127.6, 114.8, 113.6, 111.8, 104.5, 70.6.

(5-(allyloxy)-2-phenyl-1H-indol-3-yl)(phenyl)methanone (6g) :

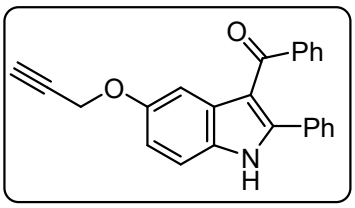
Yield: 45% (37 mg); brown solid; m.p. 165-170 °C; R_f= 0.2 in 10 % EtOAc; IR (ν_{max}, cm^{-1}):



3262, 3009, 1600, 1455, 1269, 753. ^{1}H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.64 (s, 1H), 7.52-7.51 (m, 2H), 7.46 (d, J = 2.4 Hz, 1H), 7.25-7.20 (m, 4H), 7.10-7.04 (m, 5H), 6.88 (dd, J = 8.7, 2.5 Hz, 1H), 6.03-5.96 (m, 1H), 5.33 (dd, J = 17.2, 1.6 Hz, 1H), 5.18 (dd, J = 10.5, 1.4 Hz, 1H), 4.48-4.47 (m, 2H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 24 °C): δ 193.2, 155.0, 144.3, 139.7, 133.6, 131.8, 131.3, 130.6, 129.5, 129.4, 129.2, 128.6, 128.2, 127.6, 117.4, 114.7, 113.6, 111.7, 104.5, 69.4.

phenyl(2-phenyl-5-(prop-2-yn-1-yloxy)-1H-indol-3-yl)methanone (6h):

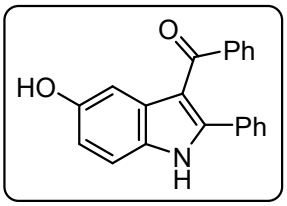
Yield: 38% (31 mg); brown solid; m.p.155-160 °C; R_f = 0.2 in 10 % EtOAc; IR (ν_{max}, cm^{-1}):



3291, 3057, 1617, 1455, 1268, 755.; ^{1}H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.70 (s, 1H), 7.60-7.58 (m, 3H), 7.32 (d, J = 8.6 Hz, 1H), 7.29-7.25 (m, 3H), 7.18-7.11 (m, 5H), 6.99 (dd, J = 8.7, 2.4 Hz, 1H), 4.69 (d, J = 2.3 Hz, 2H), 2.48 (t, J = 2.3 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 193.3, 153.9, 144.6, 139.6, 133.6, 131.6, 131.4, 131.0, 129.6, 129.3, 129.2, 128.7, 128.3, 127.7, 114.7, 113.6, 111.9, 104.8, 78.8, 75.3, 56.5.

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

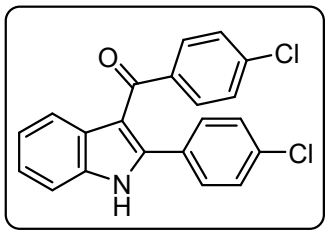
Yield: 29% (21 mg); light green solid; m.p. 230-235 °C; R_f = 0.2 in 30 % EtOAc; IR (ν_{max}, cm^{-1}):



3008, 1456, 1269, 753. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 11.96 (s, 1H), 9.02 (s, 1H), 7.48 (d, J = 7.4 Hz, 2H), 7.32-7.21 (m, 4H), 7.21-7.16 (m, 6H), 6.75 (d, J = 8.5 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 192.5, 153.2, 144.9, 140.5, 132.3, 131.5, 130.5, 129.9, 129.7, 129.4, 128.6, 128.3, 128.1, 113.4, 112.7, 112.1, 105.3.

(4-chlorophenyl)(2-(4-chlorophenyl)-1H-indol-3-yl)methanone (6m)

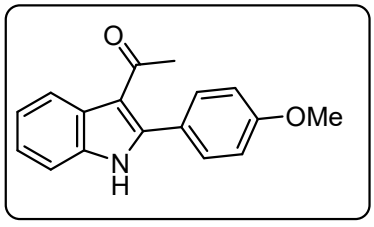
Yield: 57% (48 mg); Solid; m.p. 245-250 °C; R_f =0.6 in 20 % EtOAc; IR (ν_{max}, cm^{-1}): 3596,



3053, 2777, 1590, 1433, 1088, 780. ^{1}H NMR (400 MHz, DMSO-d_6, 24 °C): δ 12.34 (s, 1H), 7.77 (d, J = 7.9 Hz, 1H), 7.53-7.49 (m, 3H), 7.40-7.25 (m, 7H), 7.18 (t, J = 7.4 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C): δ 191.1, 143.6, 138.9, 136.6, 136.3, 133.9, 131.8, 131.3, 130.7, 128.5, 128.3, 123.6, 122.1, 121.1, 112.7, 112.4.

1-(2-(4-methoxyphenyl)-1H-indol-3-yl)ethan-1-one (6q):

Yield: 53% (32 mg); Solid; m.p. 205-207 °C; R_f = 0.4 in 20 % EtOAc; IR (ν_{max}, cm^{-1}): 2989,

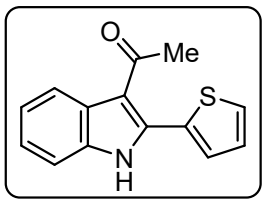


1763, 1376, 1241, 1054. ^{1}H NMR (400 MHz, DMSO-d_6, 24 °C): δ 11.9 (s, 1H), 8.18 (d, J = 7.0 Hz, 1H), 7.57 (d, J = 8.0 Hz, 2H), 7.41 (d, J = 7.5 Hz, 1H), 7.23-7.16 (m, 2H), 7.11 (d, J = 7.8 Hz, 2H), 3.85 (s, 3H), 2.09 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C): δ 194.1, 160.5, 145.4, 135.7, 131.8, 127.5, 125.1, 123.1, 122.1,

121.9,114.4, 114.3, 111.9, 55.7, 30.5.; HRMS (ESI/Q-TOF) m/z: [M + H] $^{+}$ Calcd for $C_{17}H_{15}NO_2$+H: 266.1181 found 266.1193.

1-(2-(thiophen-2-yl)-1H-indol-3-yl)ethan-1-one (6r)

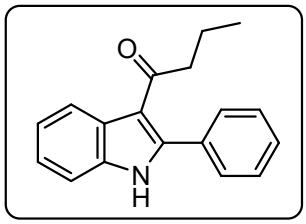
Yield: 51% (29 mg); Solid; m.p. 155- 157 °C; R_f= 0.4 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3291,



1763, 1242, 1061, 744. ^{1}H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.65 (s, 1H), 7.61- 7.58 (m, 2H), 7.25 (d, J = 8.4 Hz, 1H), 7.12 (t, J = 7.1 Hz, 1H), 7.07- 7.03 (m, 2H), 2.53 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 24 °C): δ 184.5, 146.2, 142.1, 134.8, 133.3, 132.6, 127.5, 127.3, 122.5, 121.4, 120.8, 114.3, 110.8, 14.1; HRMS (ESI/Q-TOF) m/z: [M + H] $^{+}$ Calcd for $C_{14}H_{11}NOS$+H: 242.0640 found 242.0652.

1-(2-phenyl-1H-indol-3-yl)butan-1-one (6s):

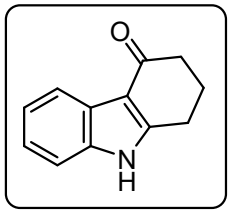
Yield: 48% (30 mg); Solid; m.p. 150-155 °C; R_f= 0.5 in 20 % EtOAc; IR (ν_{max}, cm^{-1}): 3607,



3098, 2844, 2523, 1655, 1413, 1112, 1003, 750. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.62 (s, 1H), 8.32-8.31 (m, 1H), 7.55-7.53 (m, 2H), 7.49-7.46 (m, 3H), 7.38-7.36 (m, 1H), 7.28-7.26 (m, 2H), 2.45 (t, J = 7.5 Hz, 2H), 1.62-1.55 (m, 2H), 0.75 (t, J = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 198.4, 143.4, 135.1, 132.9, 129.6, 129.5, 128.6, 127.4, 123.5, 122.5, 122.4, 115.5, 110.7, 43.9, 18.3, 13.7.

1,2,3,9-tetrahydro-4H-carbazol-4-one (6t):

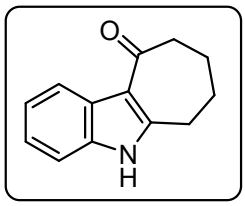
Yield: 88% (38 mg); Solid; m.p. 210-215 °C; R_f= 0.3 in 40 % EtOAc; IR (ν_{max}, cm^{-1}): 3646,



3101, 2838, 2128, 1670, 1468, 1021, 511.^{1}H NMR (400 MHz, DMSO-d_6, 24 °C): δ 11.85 (s, 1H), 7.95 (d, J = 7.1 Hz, 1H), 7.39 (d, J = 7.3 Hz, 1H), 7.18- 7.11 (m, 2H), 2.96 (t, J = 5.9 Hz, 2H), 2.42 (t, J = 6.2 Hz, 2H), 2.14-2.10 (m, 2H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C): δ 193.3, 152.7, 136.3, 124.9, 122.8, 121.9, 120.6, 112.2, 111.9, 38.2, 23.8, 23.1.

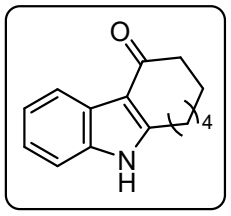
6,7,8,9-tetrahydrocyclohepta[b]indol-10(5H)-one (6u):

Yield: 93% (43 mg), Solid; m.p. 210-215 °C; R_f = 0.3 in 40 % EtOAc; IR (ν_{max}, cm^{-1}): 3420, 2939, 2085, 1622, 1455, 1016, 747, 410. ^1H NMR (400 MHz, DMSO-d_6, 24 °C): δ 11.75 (s, 1H), 8.15 (d, J = 6.9 Hz, 1H), 7.35 (d, J = 6.9 Hz, 1H), 7.12 (s, 2H), 3.10 (d, J = 4.7 Hz, 2H), 2.66-2.65 (m, 2H), 1.91-1.83 (m, 4H). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6, 24 °C): δ 197.0, 149.6, 135.5, 127.7, 122.6, 121.7, 121.3, 114.2, 111.4, 43.1, 27.5, 24.7, 22.2.



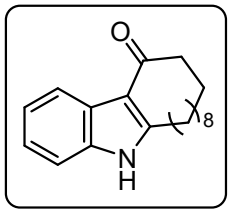
6,7,8,9,10,11-hexahydrocyclonona[b]indol-12(5H)-one (6v):

Yield: 48% (25 mg); Solid; m.p. 255-260 °C; R_f = 0.3 in 40 % EtOAc; IR (ν_{max}, cm^{-1}): 3631, 3060, 2855, 2731, 1629, 1271, 1071, 956, 429. ^1H NMR (400 MHz, DMSO-d_6, 24 °C): δ 11.73 (s, 1H), 8.21 (d, J = 7.3 Hz, 1H), 7.34 (d, J = 7.2 Hz, 1H), 7.15- 7.08 (m, 2H), 3.21 (s, 2H), 2.78 (d, J = 7.7 Hz, 1H), 1.73- 1.68 (m, 4H), 1.51- 1.45 (m, 4H). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6, 24 °C): δ 198.6, 147.5, 135.1, 127.8, 122.6, 121.9, 121.7, 115.8, 111.3, 31.0, 29.2, 27.0, 26.1, 25.7.



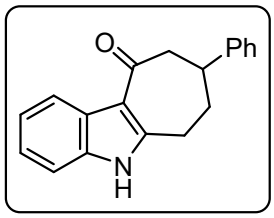
6,7,8,9,10,11,12,13,14,15-decahydrocyclotrideca[b]indol-16(5H)-one (6w):

Yield: 35% (23 mg); Solid; m.p. 190-195 °C; R_f = 0.3 in 40 % EtOAc; IR (ν_{max}, cm^{-1}): 3635, 3062, 2862, 2709, 1611, 1329, 1168, 1068, 927. ^1H NMR (400 MHz, DMSO-d_6, 24 °C): δ 11.84 (s, 1H), 7.79 (d, J = 3.6 Hz, 1H), 7.37 (d, J = 4.1 Hz, 1H), 7.14-7.12 (m, 2H), 3.18 (s, 2H), 2.88 (s, 2H), 1.74- 1.72 (m, 4H), 1.33-1.31(m, 2H), 1.18 (s, 6H), 1.04- 0.96 (m, 4H). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6, 24 °C): δ 198.5, 148.2, 135.3, 126.3, 121.9, 121.4, 120.6, 113.9, 111.9, 43.0, 27.2, 26.6, 26.1, 25.98, 25.93, 25.7, 25.1, 24.8, 23.4.



8-phenyl-6,7,8,9-tetrahydrocyclohepta[b]indol-10(5H)-one (6x):

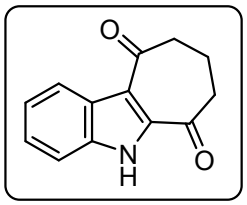
Yield: 56% (36 mg); Solid; m.p. 210-215 °C; R_f = 0.3 in 40 % EtOAc; IR (ν_{max}, cm^{-1}): 3631, 3060, 2862, 2736, 1597, 1074, 939, 429. ^1H NMR (400 MHz, DMSO-d_6, 24 °C): δ 11.84 (s, 1H), 8.18 (d, J = 6.9 Hz, 1H), 7.38 (d, J = 7.0 Hz, 1H), 7.32- 7.12 (m, 7H), 3.37- 3.10 (m, 3H), 2.80 (d, J = 12.9 Hz, 1H), 2.28- 1.97 (m, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6, 24 °C):



δ 196.8, 195.2, 149.8, 148.0, 147.6, 147.4, 135.6, 135.5, 129.0, 128.9, 127.69, 127.64, 127.2, 127.1, 126.7, 126.5, 122.8, 121.9, 121.4, 114.1, 111.5, 50.7, 42.2, 34.6, 33.8, 31.1, 26.8.

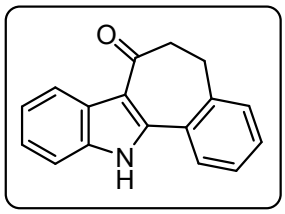
8,9-dihydrocyclohepta[b]indole-6,10(5H,7H)-dione (6y):

Yield: 41% (20 mg); Solid; m.p. 180-185 °C; R_f = 0.1 in 10 % EtOAc; IR (ν_{max}, cm^{-1}): 3923, 3812, 3307, 1650, 1508, 1422, 11240, 757. ^{1}H NMR (500 MHz, DMSO-d_6, 24 °C): δ 12.41 (s, 1H), 8.38 (d, J = 8.2 Hz, 1H), 7.55 (d, J = 8.2 Hz, 1H), 7.37 (t, J = 7.6 Hz, 1H), 7.26 (t, J = 7.2 Hz, 1H), 2.98 (t, J = 5.7 Hz, 2H), 2.91 (t, J = 5.7 Hz, 2H), 2.10-2.05 (m, 2H). ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6, 24 °C): δ 197.5, 194.1, 136.7, 136.2, 126.9, 126.6, 124.3, 123.6, 116.3, 113.4, 44.3, 42.9, 19.3.



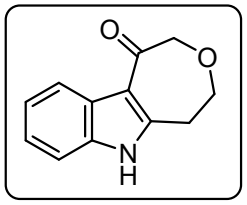
5,12-dihydrobenzo[6,7]cyclohepta[1,2-b]indol-7(6H)-one (6z):

Yield: 40% (23 mg); Solid; m.p. 215-220 °C; R_f = 0.3 in 40 % EtOAc; IR (ν_{max}, cm^{-1}): 3656, 3102, 2129, 1689, 1603, 991, 753. ^{1}H NMR (400 MHz, DMSO-d_6, 24 °C): δ 11.98 (s, 1H), 8.41 (d, J = 5.3 Hz, 1H), 7.90 (d, J = 7.6 Hz, 1H), 7.46 (t, J = 7.1 Hz, 1H), 7.39 (t, J = 8.6 Hz, 3H), 7.20- 7.18 (m, 2H), 3.20 (s, 4H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C): δ 187.0, 150.6, 140.2, 139.4, 135.7, 131.6, 129.97, 129.95, 128.4, 127.2, 123.1, 122.2, 114.0, 111.7, 33.7, 28.1.



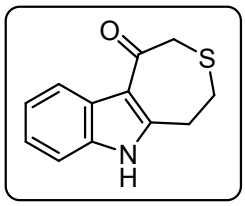
5,6-dihydro-2H-oxepino[4,5-b]indol-1(4H)-one (6aa):

Yield: 56% (26 mg) Solid; m.p. 255-260 °C; R_f = 0.3 in 40 % EtOAc; IR (ν_{max}, cm^{-1}): 3600, 3053, 2865, 2719, 1627, 1071, 954. ^{1}H NMR (400 MHz, DMSO-d_6, 24 °C): δ 11.9 (s, 0.7 H), 11.8 (s, 0.2 H), 8.24 (d, J = 7.2 Hz, 1H), 7.37 (d, J = 6.9 Hz, 1H), 7.20-7.13 (m, 2H), 5.09 (s, 0.5 H), 4.36 (s, 1.5 H), 4.11-4.08 (m, 1.5H), 4.03-4.01 (m, 0.5H), 3.34-3.32 (m, 1.5H), 2.87-2.84 (m, 0.5 H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C): δ 196.5, 195.0, 147.9, 147.4, 136.2, 135.9, 127.7, 127.5, 123.3, 123.2, 122.2, 122.1, 121.8, 121.7, 112.8, 111.7, 111.4, 78.9, 68.6, 68.1, 66.4, 46.3, 32.1.



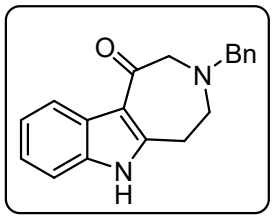
5,6-dihydro-2H-thiepino[4,5-b]indol-1(4H)-one (6ab):

Yield: 34% (17 mg); Solid; m.p. 250-255 °C; R_f= 0.3 in 40 % EtOAc; IR (ν_{max}, cm^{-1}): 3628, 3105, 2729, 2254, 2129, 1632, 987, 765. ^1H NMR (400 MHz, DMSO-d_6, 24 °C): δ 12.00 (s, 1H), 8.15 (d, J = 7.6 Hz, 1H), 7.42 (d, J = 7.3 Hz, 1H), 7.21-7.14 (m, 2H), 3.53 (s, 2H), 3.44-3.39 (m, 2H), 3.04 (t, J = 6.1 Hz, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6, 24 °C): δ 192.7, 148.0, 135.4, 127.6, 123.0, 122.0, 121.2, 113.6, 111.8, 37.6, 28.3, 27.4.



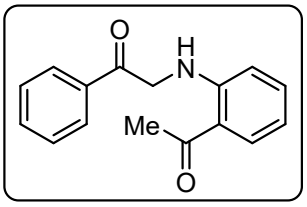
3-benzyl-3,4,5,6-tetrahydroazepino[4,5-b]indol-1(2H)-one (6ac):

Yield: 25% (17 mg); Solid; m.p. 250-255 °C; R_f=0.3 in 40 % EtOAc; IR (ν_{max}, cm^{-1}): 3647, 3073, 2853, 2727, 2129, 1627, 1269, 983, 829. ^1H NMR (400 MHz, DMSO-d_6, 24 °C): δ 11.82 (s, 1H), 8.22 (d, J = 7.4 Hz, 1H), 7.37- 7.33 (m, 5 H), 7.27 (s, 1H), 7.18- 7.11 (m, 2H), 3.83 (s, 2H), 3.61 (s, 2H), 3.22-3.18 (m, 4H). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6, 24 °C): δ 196.8, 148.1, 139.3, 136.1, 128.9, 128.7, 127.8, 127.5, 123.0, 121.9, 121.7, 113.8, 111.3, 67.2, 58.5, 51.0, 29.4.



2-((2-acetylphenyl)amino)-1-phenylethan-1-one (I):

Yield: 64% (88 mg); White solid; m.p. 100-105 °C; R_f= 0.2 in 10% EtOAc; IR (ν_{max}, cm^{-1}): 3306, 3070, 1694, 1640, 1514, 1241, 750.; ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 9.64 (s, 1H), 8.03 (d, J = 7.5 Hz, 2H), 7.80 (d, J = 7.8 Hz, 1H) 7.61 (t, J = 6.9 Hz, 1H), 7.51 (t, J = 7.2 Hz, 2H), 7.38 (t, J = 7.9 Hz, 1H), 6.66 (t, J = 8.1 Hz, 2H), 4.71 (s, 2H), 2.62 (s, 3H).$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 200.7, 193.8, 149.6, 134.9, 133.7, 132.8, 128.8, 127.8, 118.5, 114.8, 111.9, 49.6, 27.9.



7. Synthetic application:

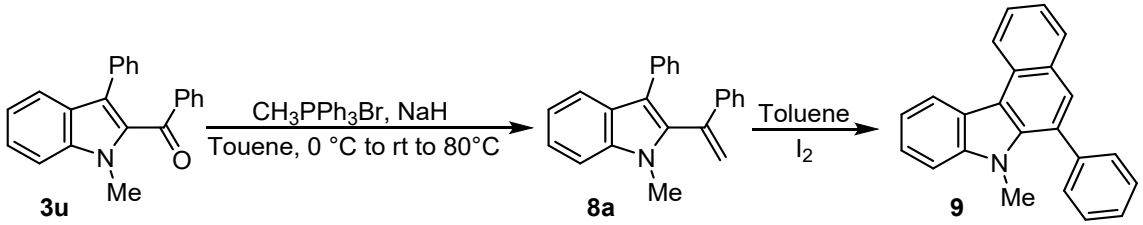
Synthesis, properties and spectral data of **14** was reported in our earlier communication.[7]

7.1. Gram scale synthesis

In an oven dried reaction tube **1a** (0.92 g, 5.07 mmol, 1 equiv) and 2-amino benzophenone **2i** (1 g, 5.07 mmol, 1 equiv) were 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 °C 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 **3i** in 94% yield (1.54 g).

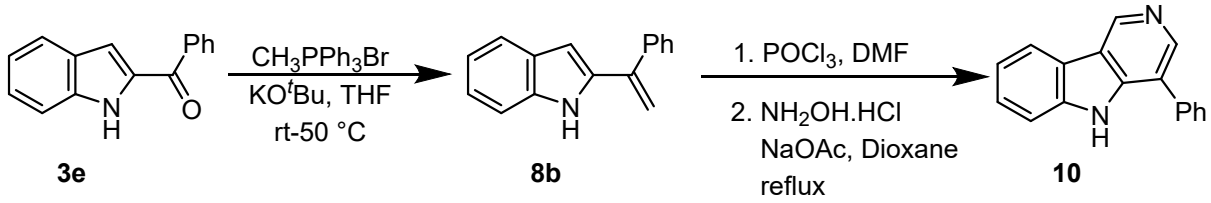
7.2. 7-methyl-6-phenyl-7H-benzo[c]carbazole (9) [8]



In a 50 mL round bottom flask equipped with a reflux condenser, CH_3PPh_3Br (861 mg, 2.4 mmol, 2.5 equiv.) was taken under nitrogen atmosphere. Then, dry toluene (4 mL) was added under nitrogen and the resulting mixture was cooled down to 0 °C. To the stirring solution, NaH (2.4 mmol, 2.5 equiv., 60% dispersion in mineral oil) was added portion wise at the same temperature. The reaction mixture was allowed to warm to rt, and stirred at the same temperature for 45 min. The solution of **3u** (300 mg, 0.9 mmol, 1 equiv) in 4 mL of toluene was added slowly to the stirring solution and then heated at 80 °C for 2 h. After the completion of reaction, as indicated by TLC, reaction mixture was cooled down to room temperature and quenched with saturated solution of NH_4Cl. The reaction mixture was extracted with DCM, washed with water, and the organic layer was collected and evaporated under reduced pressure. The crude product was then further purified by column chromatography using ethyl acetate:hexane as an eluent to afford the 2-alkenylindole **8a** in 86% (251 mg) yield as viscous liquid. R_f = 0.6 in 10% EtOAc; IR (ν_{max}, cm^{-1}): 3350, 2924, 1763, 1246, 1063, 745, 701. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.82 (d, J = 8.1 Hz, 1H), 7.53 (d, J = 7.2 Hz, 2H), 7.40 - 7.33 (m, 9H), 7.25-7.16 (m, 2H), 6.00 (s, 1H), 5.37 (s, 1H), 3.48 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 139.7, 139.4, 137.1, 135.4, 129.5, 128.8, 128.3, 128.2, 127.0, 126.4, 125.8, 122.2, 120.7, 120.0, 119.4, 116.4, 109.4, 30.7; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{23}H_{19}N$+H: 310.1596 found 310.1597.

2-Alkenylindole **8a** (47 mg, 0.15 mmol, 1 equiv) was taken in a 20 mL reaction tube and dry toluene (10 mL) was added. I_2 (0.015 mmol, 0.1 equiv) was added to the reaction mixture and was stirred for 3 days under 254 nm light at room temperature. After the completion of reaction, the reaction mixture was extracted with DCM and the organic layer was dried with Na_2SO_4 and evaporated under reduced pressure. The crude was then purified through silica gel chromatography using ethyl acetate:hexane as an eluent to afford the product **9** in 65% (30 mg) yield as white solid. m.p. 105-110 °C; R_f = 0.6 in 10% EtOAc; IR (ν_{max}, cm^{-1}): 3436, 2925, 1591, 1473, 1306, 1084, 1034, 745. ^1H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.86 (d, J = 8.7 Hz, 1H), 8.65 (d, J = 7.7 Hz, 1H), 7.97 (d, J = 8.1 Hz, 1H), 7.71-7.69 (m, 2H), 7.57- 7.55 (m, 2H), 7.51- 7.46 (m, 6H), 7.42-7.39 (m, 1H), 3.46 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, 24 °C): δ 141.2, 140.5, 136.8, 129.8, 129.3, 129.0, 128.9, 128.5, 128.1, 127.8, 127.5, 126.7, 124.2, 123.4, 123.2, 122.9, 122.0, 120.0, 116.0, 109.4, 33.1.

7.3. Synthesis of 4-phenyl-5H-pyrido[4,3-b]indole (10):

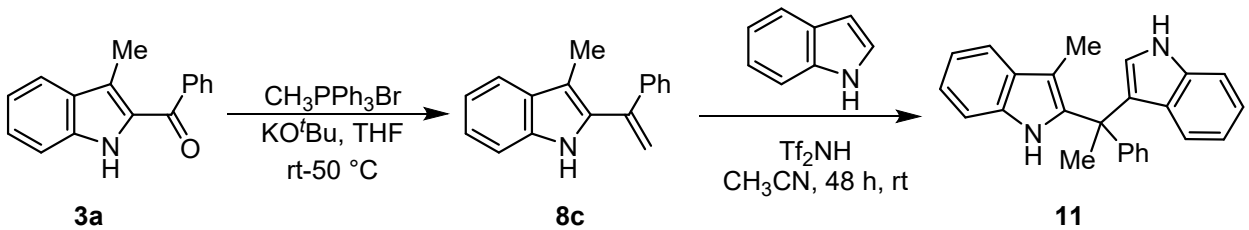


KO^{t}Bu (608 mg, 5.42 mmol, 3 equiv) was taken in 10 mL of dry THF in a 50 mL two neck round bottom flask under nitrogen atmosphere. $MePPh_3Br$ (1.93 g, 5.42 mmol, 3 equiv) was added to the reaction mixture at room temperature. After stirring the mixture for 15 min compound **3e** (400 mg, 1.80 mmol, 1 equiv) dissolved in 5 mL of dry THF was added dropwise to the reaction mixture. Then the mixture was heated to 50 °C. The reaction mixture was then stirred for overnight. After the completion of reaction, the reaction was quenched with water and extracted with DCM. The organic layer was then dried over Na_2SO_4 and evaporated under reduced pressure. The crude product was then purified by column chromatography over hexane/ethylacetate (10:1) as an eluent to afford the corresponding olefin derivative **8b** in 53% (208 mg) yield as brown solid; m.p. 60-65 °C; R_f = 0.5 in 10% EtOAc; IR ((ν_{max}, cm^{-1}): 3412, 3053, 2886, 1448, 1307, 904, 740, 699.; 1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.03 (s, 1H), 7.48 (d, J = 5.6 Hz, 1H), 7.39 (s, 2H), 7.31 (s, 3H), 7.23 (d, J = 7.8 Hz, 1H), 7.10 (s, 1H), 7.00 (s, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 141.6, 140.0, 137.8, 136.4, 128.6, 128.5, 128.4, 128.3, 122.7, 120.8, 120.1, 112.8, 110.8, 103.3.

2 mL of DMF was taken in a 25 mL round bottom flask. $POCl_3$ (0.1 mL, 0.91 mmol, 2 equiv) was added dropwise to the reaction mixture at 0 ℃ under inert atmosphere. After 15 min olefin compound **8b** (100 mg, 0.45 mmol, 1 equiv) was dissolved in 2 mL of DMF and was added dropwise to the reaction mixture at 0 ℃. The reaction mixture was gradually allowed to warm to room temperature and stirred for 45 min. Ice water 10 mL was added to the reaction mixture followed by 2 mL of 1N NaOH. The reaction mixture was then extracted with ethyl acetate and washed with water. The organic layer was then dried over Na_2SO_4 and evaporated in rotavapor. The crude product was then purified by column chromatography over hexane/EtOAc (10:2) to afford the formylated product as brown solid.

The formylated product (22 mg, 0.08 mmol, 1 equiv) was taken in a 20 mL reaction tube. $NH_2OH.HCl$ (13 mg, 0.17 mmol, 2 equiv), NaOAc (14 mg, 0.17 mmol, 2 equiv) was added to the reaction tube followed by 4 mL of Dioxane. The reaction tube was then refluxed for 24 h. After the completion of reaction as indicated by TLC it was cooled down to room temperature and extracted with EtOAc and washed with water. The organic layer was then dried over Na_2SO_4 and evaporated under reduced pressure. The crude product was then purified by column chromatography over hexane/EtOAc (10:2) as eluent to afford the desired product **10** in 91% (20 mg) yield as brown solid. ; m.p. 240-245 °C; R_f = 0.2 in 20% EtOAc; IR (ν_{max}, cm^{-1}): 3008, 2986, 1598, 1269, 754, ^1H NMR (400 MHz, DMSO-d_6, 24 °C): δ 11.69 (s, 1H), 9.35 (s, 1H), 8.47 (s, 1H), 8.27 (d, J = 7.7 Hz, 1H), 7.76 (d, J = 7.0 Hz, 2H), 7.61-7.60 (m, 3H), 7.52- 7.46 (m, 2H), 7.29 (t, J = 7.3 Hz, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6, 24 °C): δ 143.5, 141.7, 141.0, 140.2, 135.5, 129.2, 128.5, 127.9, 126.7, 120.7, 120.6, 120.2, 111.9.

7.4. Synthesis of 2-(1-(1H-indol-3-yl)-1-phenylethyl)-3-methyl-1H-indole (11):

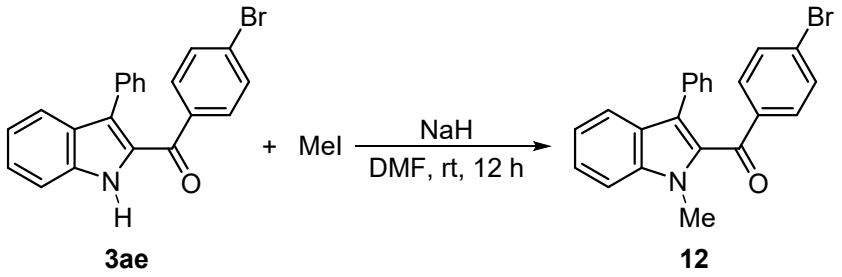


KO^{t}Bu (651 mg, 5.82 mmol, 3 equiv) was taken in a 50 mL two neck round bottom flask and 10 mL of dry THF was added to it under nitrogen atmosphere. $MePPh_3Br$ (2.07 g, 5.82 mmol,

3 equiv) was added to the reaction mixture at RT. After stirring the mixture for 15 min compound **3a** (456 mg, 1.94 mmol, 1 equiv) dissolved in 5 mL of dry THF was added dropwise to the reaction mixture. Then the reaction mixture was heated to 50 °C. The reaction mixture was then stirred for overnight. After the completion of reaction, the reaction was quenched with water and extracted with DCM. The organic layer was then dried over Na_2SO_4 and evaporated under reduced pressure. The crude product was then purified by column chromatography over hexane/ethylacetate (10:1) as an eluent to afford the corresponding olefin derivative **8c** in 44% (200 mg) yield.; Yellow solid; m.p. 55-60 °C; R_f= 0.6 in 10% EtOAc; IR (ν_{max}, cm^{-1}): 3412, 3054, 1452, 1325, 904, 749, 700.; ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.67 (s, 1H), 7.48 (d, J = 7.1 Hz, 1H), 7.26 (s, 5H) 7.16-7.03 (m, 3H), 5.56 (s, 1H), 5.39 (s, 1H), 2.13 (s, 3H).$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 141.4, 140.3, 135.3, 133.6, 129.5, 128.5, 128.2, 127.9, 122.4, 119.3, 119.0, 116.3, 110.8, 110.6, 9.9.

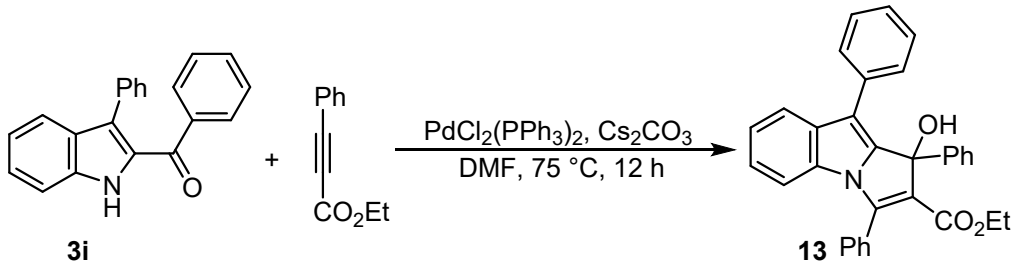
The synthesized olefine derivative **8c** (65 mg, 0.28 mmol, 1 equiv) was taken in 5 mL of CH_3CN in a 25 mL round bottom flask. Tf_2NH (15 mg, 0.06 mmol, 0.2 equiv) was added to the flask followed by Indole (99 mg, 0.56 mmol, 2 equiv)) at room temperature. The reaction mixture was stirred at the same temperature for 48 h. After the reaction was completed as indicated by TLC it was quenched with water and extracted with DCM. The organic layer was then dried over Na_2SO_4 and evaporated under reduced pressure. The crude product was purified by column chromatography over hexane/ethylacetate (10:1) as an eluent to afford the desired product **11** in 82% (80 mg) yield as white solid. m.p. 190-195 °C; R_f= 0.4 in 10% EtOAc; IR (ν_{max}, cm^{-1}): 3438, 3414, 2987, 1460, 1268, 752. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.98 (s, 1H), 7.71 (s, 1H), 7.54-7.53 (m, 1H), 7.38 (d, J = 8.3 Hz, 1H), 7.29 (s, 4H), 7.26-7.22 (m, 2H), 7.19-7.09 (m, 4H), 6.95 (t, J = 7.6 Hz, 1H), 6.59 (s, 1H), 2.36 (s, 3H), 2.08 (s, 3H).$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 146.6, 139.6, 137.1, 133.6, 130.4, 128.1, 127.7, 126.4, 125.9, 123.6, 123.3, 122.1, 121.5, 120.9, 119.6, 118.9, 118.0, 111.3, 110.5, 107.1, 44.9, 28.2, 10.1.

7.5. Synthesis of (4-bromophenyl)(1-methyl-3-phenyl-1H-indol-2-yl)methanone (12)



In an oven dried reaction tube compound, **3ae** (60 mg, 0.16 mmol, 1 equiv) and NaH (5.76 mg, 0.24 mmol, 1.5 equiv) were added in 3 mL of dry DMF followed by MeI (0.24 mmol, 1.5 equiv). The reaction mixture was stirred at room temperature for 12 h. After the reaction was completed, as indicated by TLC, it was extracted with ice cold water and ethyl acetate. The solvent was evaporated under reduced pressure and crude was further purified by column chromatography using ethyl acetate:hexane as an eluent to afford the product **12** in 94% (58 mg) yield as viscous liquid. R_f = 0.5 in 10% EtOAc; IR (ν_{max}, cm^{-1}): 3057, 2939, 1635, 1366, 1255, 952, 747, 704. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.77 (d, J = 8.0 Hz, 1H), 7.53-7.42 (m, 4H), 7.26 -7.20 (m, 5H), 7.18-7.12 (m, 3H), 3.97 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.4, 138.9, 137.1, 133.8, 132.5, 131.6, 131.1, 130.5, 128.2, 127.7, 126.8, 125.9, 125.7, 124.1, 121.6, 121.2, 110.3, 31.7; HRMS (ESI/Q-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{16}BrNO$+H: 390.0494 found 390.0502.

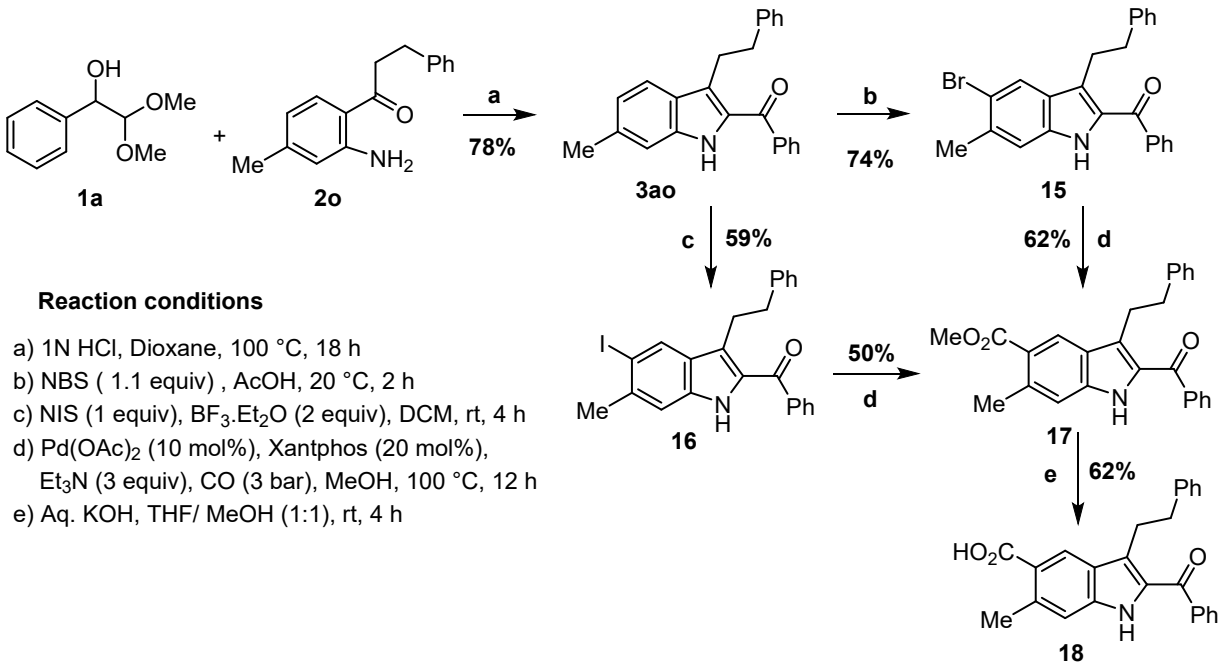
7.6. Synthesis of ethyl 1-hydroxy-1,3,9-triphenyl-1H-pyrrolo[1,2-a]indole-2-carboxylate (13) [9]



In an oven dried reaction tube, compound **3i** (100 mg, 0.34 mmol, 1 equiv), alkyne (59 mg, 0.34 mmol, 1 equiv) and DMF (3 mL) was added followed by, $PdCl_2(PPh_3)_2$ (12 mg, 0.017 mmol, 5 mol%) and Cs_2CO_3 (219 mg, 0.67 mmol, 2 equiv) were introduced. The reaction mixture was then kept in a pre-heated oil bath at 75 °C and stirred at the same temperature for 12 h. After the reaction was completed, as indicated by TLC, it was cooled down to room temperature and the reaction mixture was washed with ice cold water and extracted with ethyl acetate. The solvent was then dried over anhydrous Na_2SO_4 and evaporated under reduced

pressure. It was further purified by column chromatography using ethylacetate:hexane to afford the product **13** in 53% (83 mg) yield as white solid. m.p. 125- 127 °C; R_f=0.5 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3482, 3056, 2982, 1675, 1380, 1084, 752, 701. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 7.77- 7.56 (m, 8H), 7.44 (d, J = 6.5 Hz, 2H), 7.34 (t, J = 7.5 Hz, 2H), 7.29-7.25 (m, 1H), 7.18- 7.12 (m, 4H), 7.04 (t, J = 7.5 Hz, 1H), 6.55 (d, J = 8.2 Hz, 1H), 4.54 (s, 1H), 4.06-3.98 (m, 1H), 3.94- 3.86 (m, 1H), 0.89 (t, J = 7.0 Hz, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 164.3, 149.6, 142.5, 141.5, 132.9, 132.2, 131.9, 130.4, 129.6, 129.0, 128.6, 128.4, 128.1, 127.9, 127.4, 127.1, 125.1, 123.9, 122.1, 121.2, 120.9, 118.7, 111.7, 79.5, 60.1, 13.7; HRMS (ESI/Q-TOF) m/z: $[M + Na]^+$ Calcd for $C_{32}H_{25}NO_3$+Na: 494.1732 found 494.1727.

7.7. Synthesis of anti tumor agent: 18



Step-b: 3ao was synthesized employing the general procedure mentioned earlier. **3ao** (50 mg, 0.15 mmol, 1 equiv) was taken in 3 mL of glacial acetic acid and the reaction mixture was kept at 20 °C. *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 **15** in 74% (45 mg) yield as a yellow solid. m.p. 135-140 °C; R_f= 0.5 in 10% EtOAc; IR (ν_{max}, cm^{-1}): 3317, 1612, 1434, 1276,

748.; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.84 (s, 1H), 7.84 (s, 1H), 7.68 (d, J = 7.6 Hz, 2H), 7.60 (t, J = 7.3 Hz, 1H), 7.49 (t, J = 7.3 Hz, 2H), 7.26 (s, 1H), 7.19-7.11 (m, 3H), 6.86 (d, J = 7.0 Hz, 2H), 2.97 (t, J = 8.8 Hz, 2H), 2.75 (t, J = 7.6 Hz, 2H), 2.51 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.1, 141.2, 139.2, 135.9, 135.8, 132.0, 131.7, 128.6, 128.5, 128.3, 128.2, 128.0, 126.0, 124.3, 123.7, 117.2, 113.2, 37.4, 27.5, 23.9.

Step-c: 3ao (50 mg, 0.15 mmol, 1 equiv) was taken in 5 mL of DCM and $BF_3{\cdot}Et_2O$ (42 mg, 0.3 mmol, 2 equiv) was added to the reaction mixture at room temperature. NIS (33 mg, 0.15 mmol, 1 equiv) was added portion wise to the reaction mixture and it was stirred for 4 h at room temperature. After completion of reaction, as indicated by TLC, it was quenched with water and extracted with DCM. The organic layer was then evaporated under reduced pressure and the crude product was then purified by silica gel chromatography to afford the iodinated product **16** in 59% (40 mg) yield as a yellow solid. m.p. 125-130 °C; R_f = 0.5 in 10% EtOAc; IR (ν_{max}, cm^{-1}): 3324, 1623, 1535, 1434, 744.; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.84 (s, 1H), 8.11 (s, 1H), 7.67 (d, J = 7.4 Hz, 2H), 7.59 (t, J = 7.4 Hz, 1H), 7.49 (t, J = 8.0 Hz, 2H), 7.29 (s, 1H), 7.19-7.13 (m, 3H), 6.86 (d, J = 7.1 Hz, 2H), 2.96 (t, J = 8.3 Hz, 2H), 2.74 (t, J = 7.6 Hz, 2H), 2.53 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 189.1, 141.2, 139.2, 138.4, 136.8, 132.0, 131.5, 131.4, 128.7, 128.6, 128.5, 128.3, 128.2, 126.0, 123.3, 112.3, 91.6, 37.4, 29.0, 27.4.

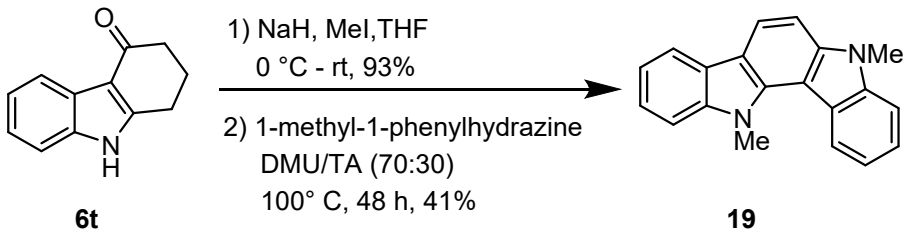
Step-d: The brominated product **15** (0.21 mmol, 1 equiv) or the iodinated product **16** (0.075, 1 equiv) was taken in dry MeOH (3 mL). $Pd(OAc)_2$ (10 mol%), Xantphos (20 mol%), and 3 equiv of Et_3N were added and pressurized 3 bar with CO. The reaction was continued for 12 h at 100 °C. After the 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 **17** in 62% (from bromo compounds) or 50% yield (from iodo compounds), respectively.

Step-e: The ester **17** (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 then dried over Na_2SO_4. Evaporation of solvent followed by

purification of crude product using column chromatography gave the desired product **18** as a white solid in 62% (45 mg) yield.

Properties and spectral data of **17** and **18** were reported in our earlier communication.[7]

7.8. Synthesis of 5,12-dimethyl-5,12-dihydroindolo[3,2-a]carbazole (19):



6t **19**

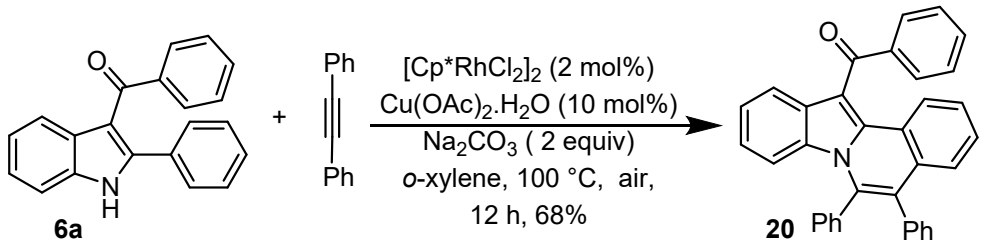
N-methylated starting material was synthesized by treating **6t** (0.54 mmol, 1 equiv) with NaH (1.08 mmol, 2 equiv) in 5 mL of Dry THF at 0 ℃. After 10 min CH_3I (1.62 mmol, 3 equiv) was added dropwise to the reaction mixture and the reaction mixture was gradually allowed to come to room temperature. The reaction mixture was then stirred at the same temperature overnight. After completion of reaction, the reaction mixture was quenched with water and extracted with EtOAc. The organic layer was then dried with Na_2SO_4 and evaporated under reduced pressure. The crude product was then purified by column chromatography over hexane/EtOAc to afford the methylated product as light pink solid**.**

N-methylphenylhydrazine was synthesized according to the literature procedure.[10]

In a 20 mL reaction tube 1.5 g mixture of *N, N′*-dimethylurea/L-(+)-tartaric acid (70:30) was heated to 100 °C to obtain a clear melt. To the clear melt N-methylated starting material (52 mg, 0.26 mmol) and N-methyl phenyl hydrazine (48 mg, 0.39 mmol) was added. The reaction mixture was stirred at 100 °C for 12 h and quenched by adding water to the hot reaction mixture. The reaction mixture was then extracted with DCM and organic layer was dried over Na_2SO_4 and evaporated under vacuum. The crude was then purified by column chromatography over hexane/EtOAc (10:1) to afford the purified product **19** in 41% (30 mg) yield as a white solid. m.p. 220-225 °C; R_f = 0.6 in 15% EtOAc; IR (ν_{max}, cm^{-1}): 3008, 2987, 1469, 1269, 754.; ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.59 (d, J = 8.1 Hz, 1H), 8.16 (d, J = 8.3 Hz, 1H), 8.09 (d, J = 7.6 Hz, 1H), 7.48-7.42 (m, 4H), 7.30-7.24 (m, 3H), 4.50 (s, 3H), 3.93

(s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 141.5, 141.0, 140.3, 137.6, 124.3, 124.2, 123.8, 122.6, 121.0, 119.3, 118.9, 118.8, 118.6, 116.1, 108.8, 108.7, 107.0, 101.5, 34.7, 29.6.

7.9. Synthesis of (5,6-diphenylindolo[2,1-a]isoquinolin-12-yl)(phenyl)methanone (20):



To a 20 mL rection tube **6a** (60 mg, 0.20 mmol, 1equiv) and diphenylacetylene (36 mg, 0.20 mmol, 1 equiv) was added. $[(Cp^*RhCl_2)_2]$ (3 mg, 2 mol %), Cu $(OAc)_2 \bullet H_2O$ (4 mg, 10 mol %), Na_2CO_3 (43 mg, 0.40 mmol, 2 equiv) was added to the reaction tube followed by 5 mL of o-xylene. The reaction was then allowed to stir at 100 ℃ for 12 h under air. After the completion of the reaction as indicated by TLC it was quenched with water and extracted with DCM. The organic layer was then dried over Na_2SO_4 and evaporated under reduced pressure. The crude product was purified by column chromatography over hexane/ethylacetate (10:1) as an eluent to afford the desired product **20** in 68% (65 mg) yield as yellow solid.; m.p. 225-230 ℃, R_f = 0.8 in 10% EtOAc; IR (ν_{max}, cm^{-1}): 3058, 1637, 1446, 1368, 1257, 1164, 1027, 740, 699. ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.32 (d, J = 7.6 Hz, 1H), 8.05 (d, J = 7.6 Hz, 2H), 7.58 (t, J = 7.2 Hz, 1H), 7.47- 7.43 (m, 3H), 7.37- 7.29 (m, 7H), 7.27- 7.22 (m, 3H), 7.20- 7.17 (m, 3H), 7.10 (t, J = 7.7 Hz, 1H), 6.81 (t, J = 7.7 Hz, 1H), 6.02 (t, J = 8.6 Hz, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 195.1, 139.6, 136.3, 136.0, 135.6, 135.0, 133.0, 132.1, 131.6, 130.8, 130.2, 129.7, 129.0, 128.7, 128.6, 128.5, 127.9, 127.1, 127.0, 126.7, 126.3, 124.1, 124.0, 122.7, 121.2, 120.2, 114.9, 109.8.

8. References

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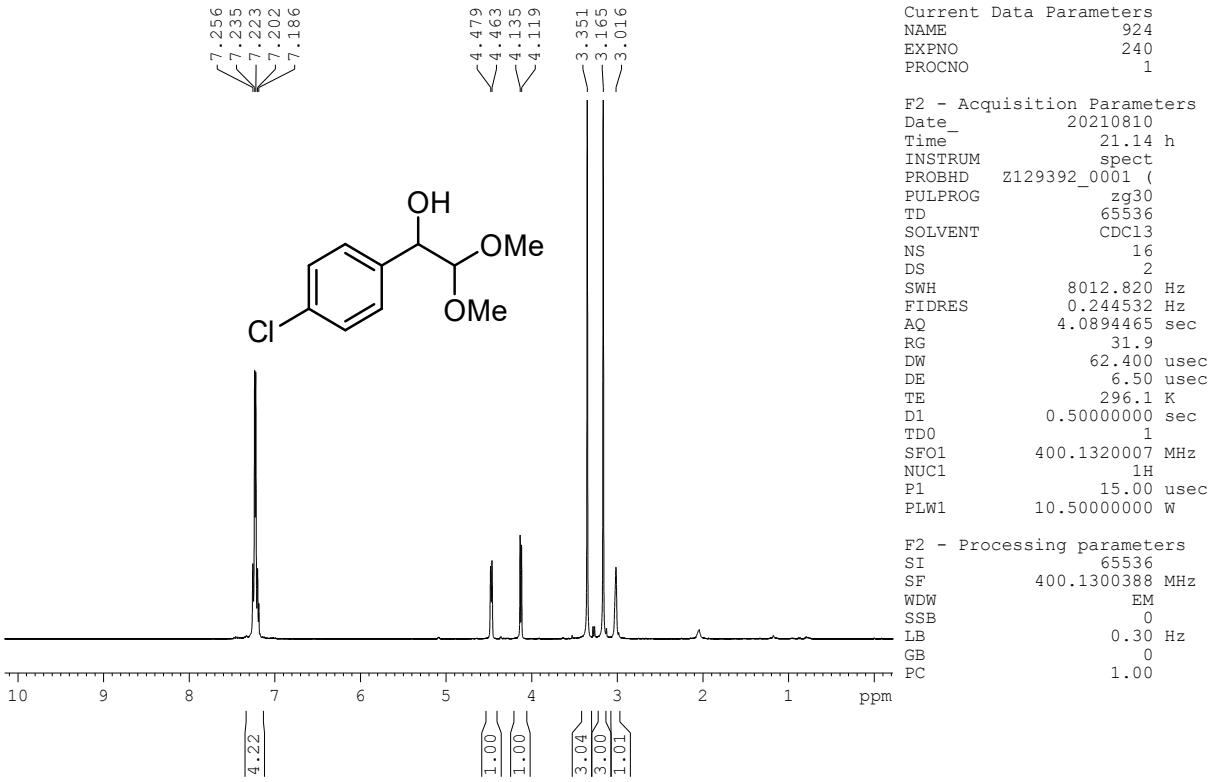
9. Spectral data:

1-(4-chlorophenyl)-2,2-dimethoxyethan-1-ol: 1ad

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PROCNO                  1

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SOLVENT             CDCl3
NS                     16
DS                      2
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FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                   31.9
DW                 62.400 usec
DE                   6.50 usec
TE                  296.1 K
D1              0.50000000 sec
TD0                     1
SFO1           400.1320007 MHz
NUC1                   1H
P1                  15.00 usec
PLW1           10.50000000 W

F2 - Processing parameters
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GB                      0
PC                   1.00
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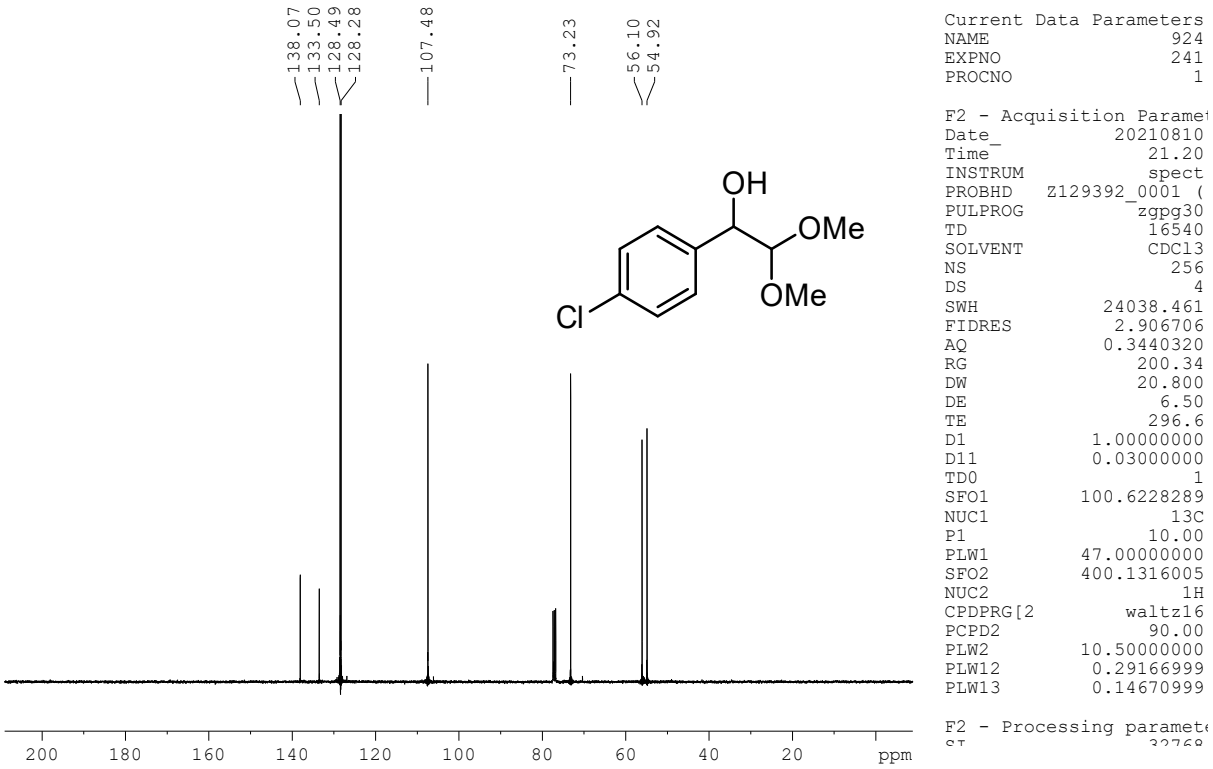
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **1ad**

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EXPNO                 241
PROCNO                  1

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NS                  256
DS                    4
SWH           24038.461
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AQ            0.3440320
RG               200.34
DW               20.800
DE                 6.50
TE                296.6
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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
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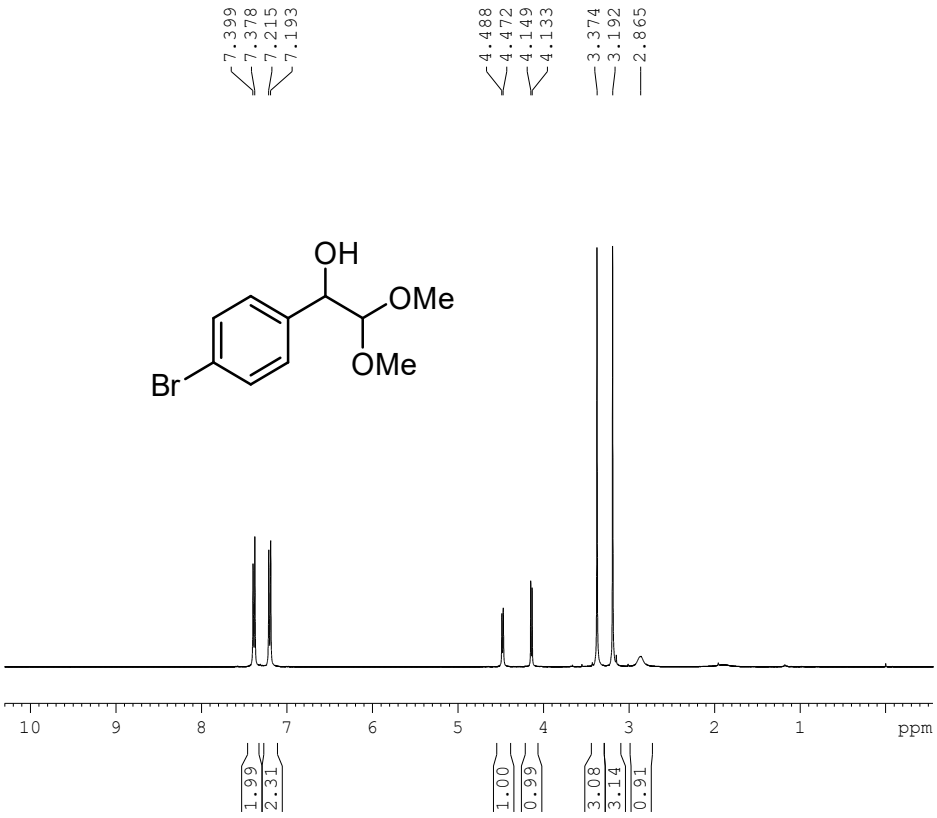
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **1ad**

1-(4-bromophenyl)-2,2-dimethoxyethan-1-ol: 1ae

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PROCNO                1

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TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           8012.820
FIDRES        0.244532
AQ            4.089465
RG                67.99
DW                62.400
DE                 6.50
TE                297.8
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TD0                   1
SFO1         400.1320007
NUC1                1H
P1                15.00
PLW1         10.50000000

F2 - Processing paramet
SI                65536
SF           400.1300369
WDW                  EM
SSB       0
LB                 0.30
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PC                 1.00
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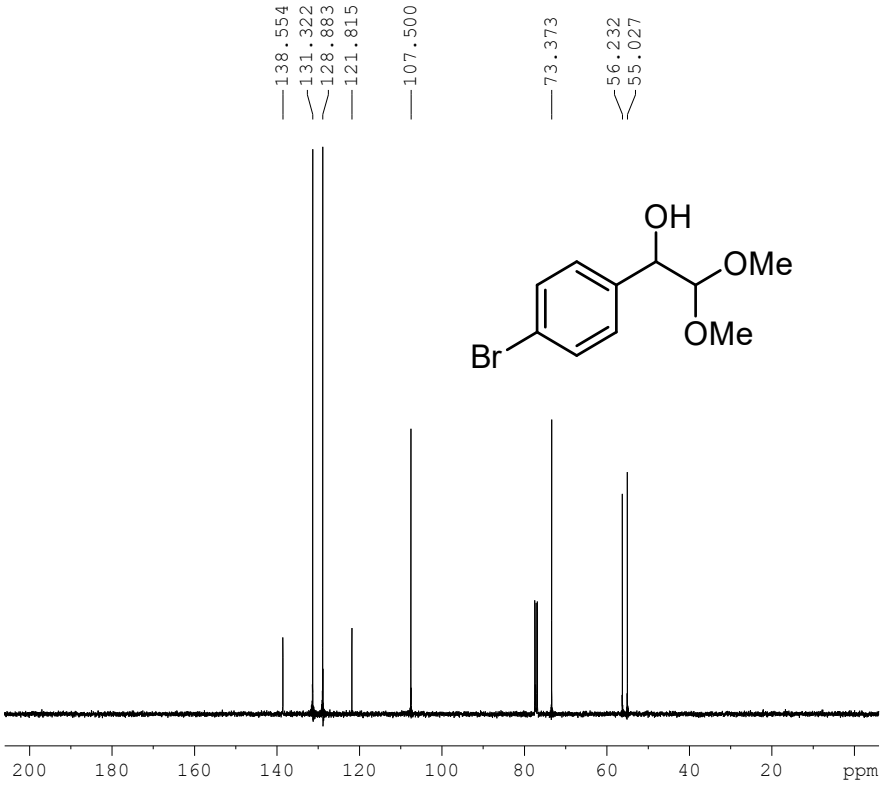
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **1ae**

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PROCNO                 1

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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                 298.3
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
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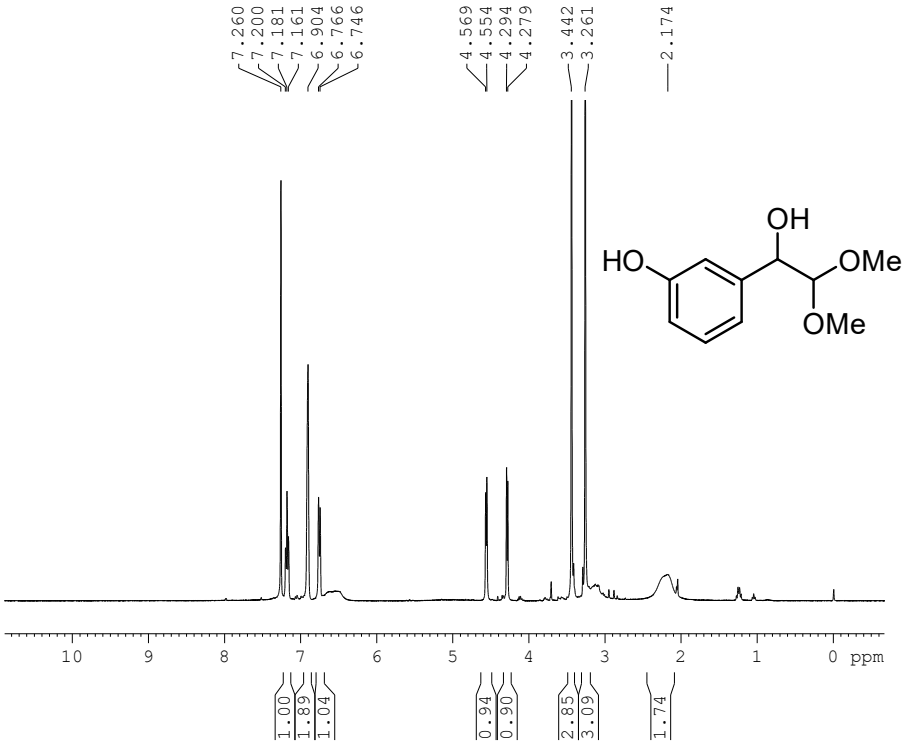
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **1ae**

3-(1-hydroxy-2,2-dimethoxyethyl)phenol : 1ah

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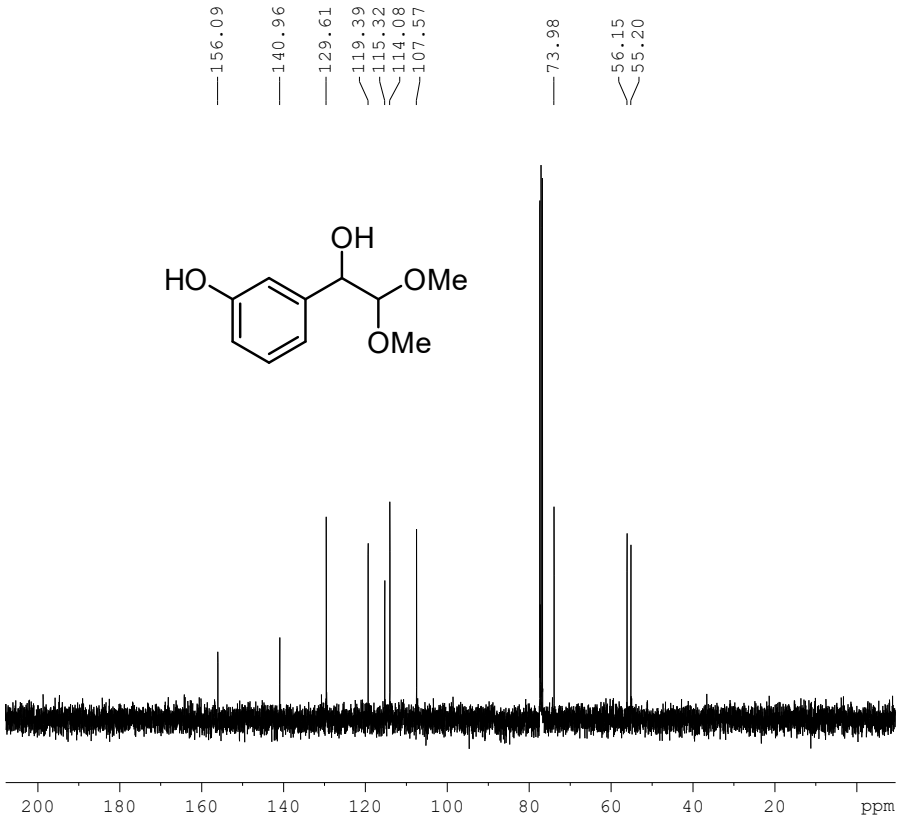
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                169.77
DW                62.400 usec
DE                 6.50 usec
TE                295.6 K
D1           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           400.1300094 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 **1ah**

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EXPNO                  420
PROCNO                   1

F2 - Acquisition Parame
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Time                20.12
INSTRUM             spect
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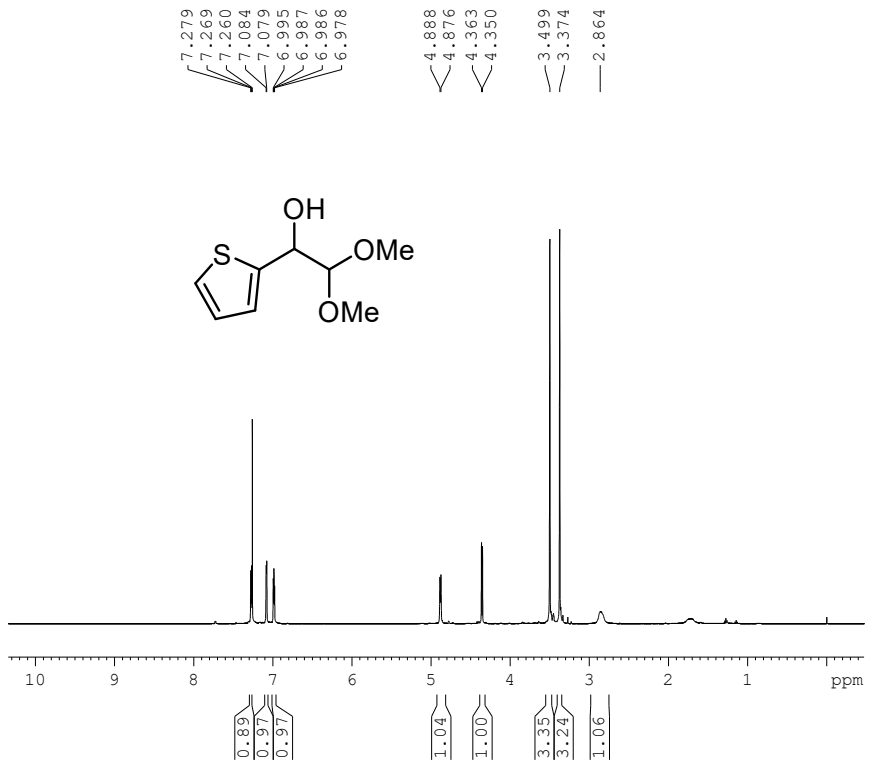
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                    99
DS                     4
SWH             24038.461
FIDRES           2.906706
AQ              0.3440320
RG                200.34
DW                20.800
DE                  6.50
TE                 295.7
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 **1ah**

2,2-dimethoxy-1-(thiophen-2-yl)ethan-1-ol: 1aj

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EXPNO                   12
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PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      2
SWH            10000.000 Hz
FIDRES          0.305176 Hz
AQ             1.6384000 sec
RG                 79.04
DW                50.000 use
DE                 6.50 use
TE                300.5 K
D1            0.50000000 sec
TD0                    1

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

F2 - Processing parameters
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SF           500.1500118 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
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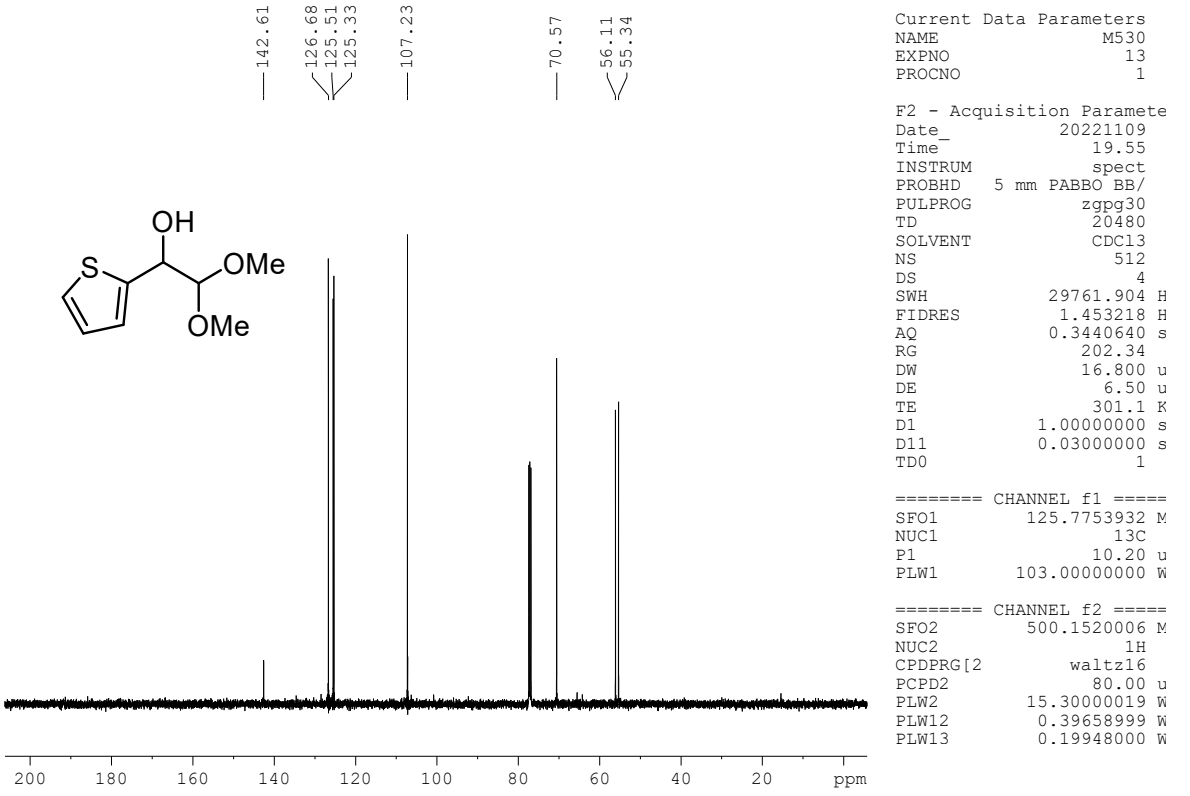
^{1}H NMR (500 MHz, $CDCl_3$, 24 °C) of the compound **1aj**

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EXPNO                   13
PROCNO                   1

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Time                 19.55
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                  301.1 K
D1             1.00000000 s
D11            0.03000000 s
TD0                      1

======== CHANNEL f1 =====
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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
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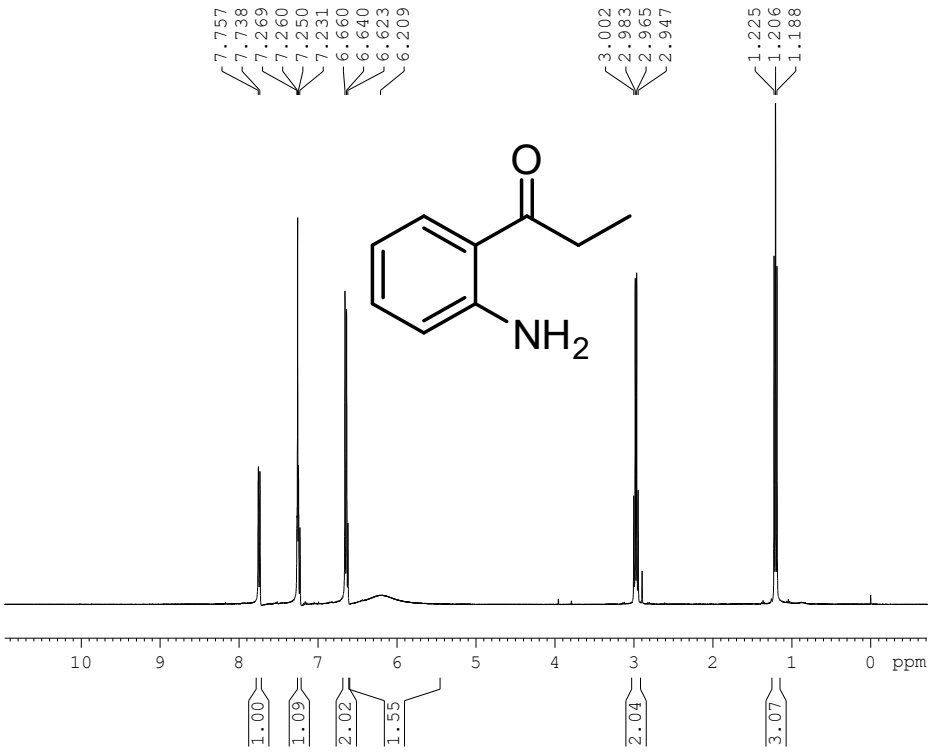
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$, 24 °C) of the compound **1aj**

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

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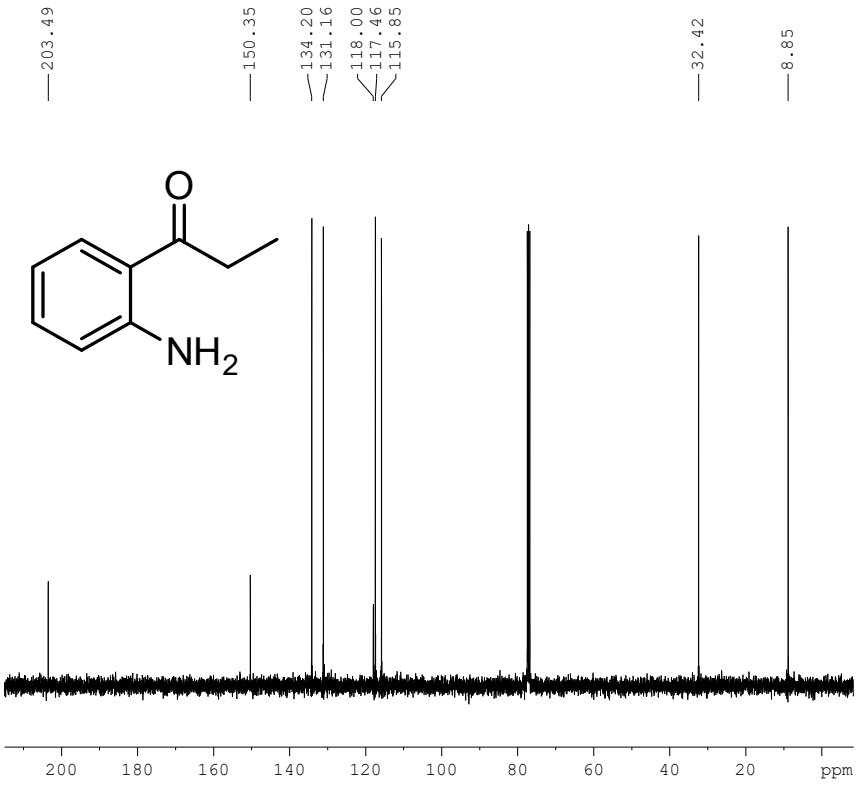
PULPROG              zg30
TD                  65536
SOLVENT              CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                  138.85
DW                  62.400 usec
DE                   6.50 usec
TE                  297.8 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 **2b**

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NS                   256
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SWH            24038.461 H
FIDRES          2.906706 H
AQ              0.3440320 s
RG                200.34
DW                20.800 u
DE                 6.50 u
TE                297.9 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
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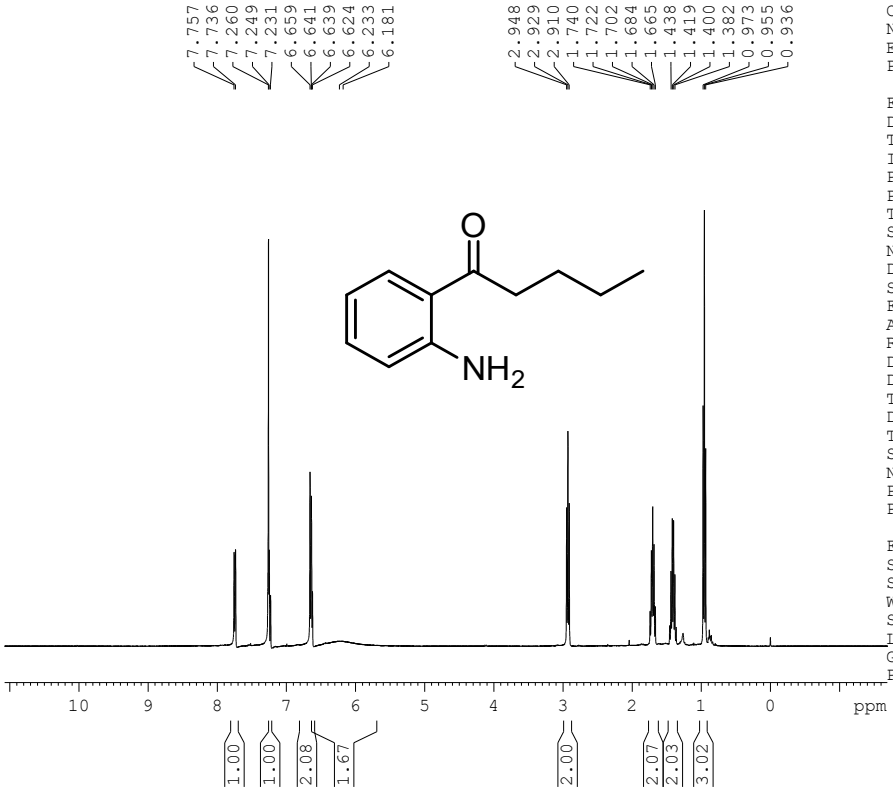
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **2b**

1-(2-aminophenyl)pentan-1-one: 2d

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PROCNO                  1

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TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                153.13
DW                62.400 usec
DE                 6.50 usec
TE                298.4 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            400.1300096 MHz
WDW                  EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
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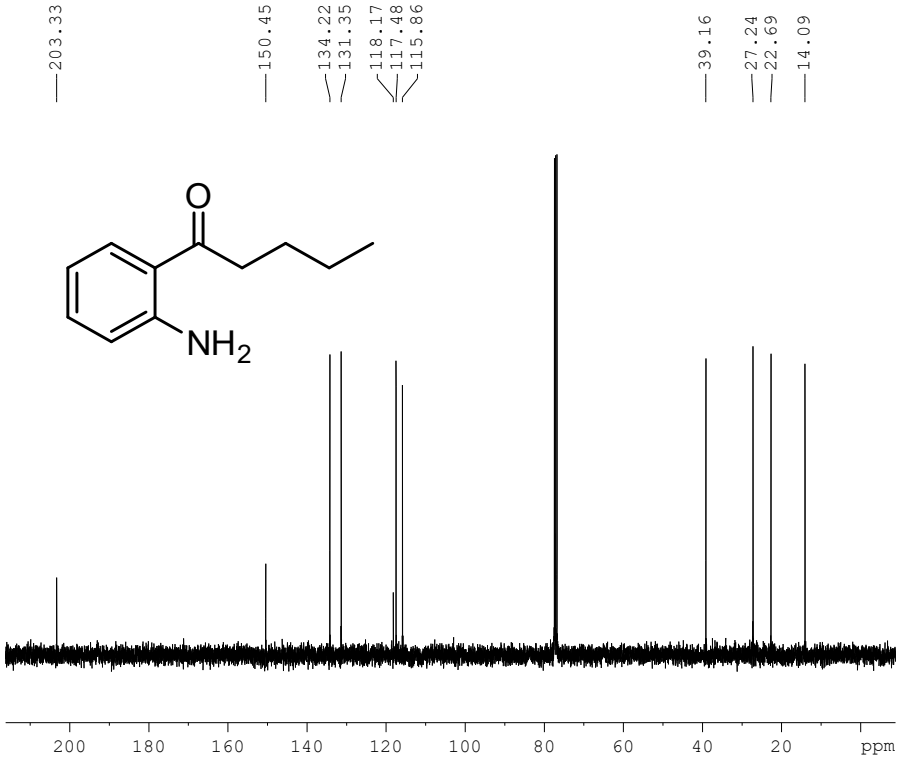
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **2d**

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PROCNO                  1

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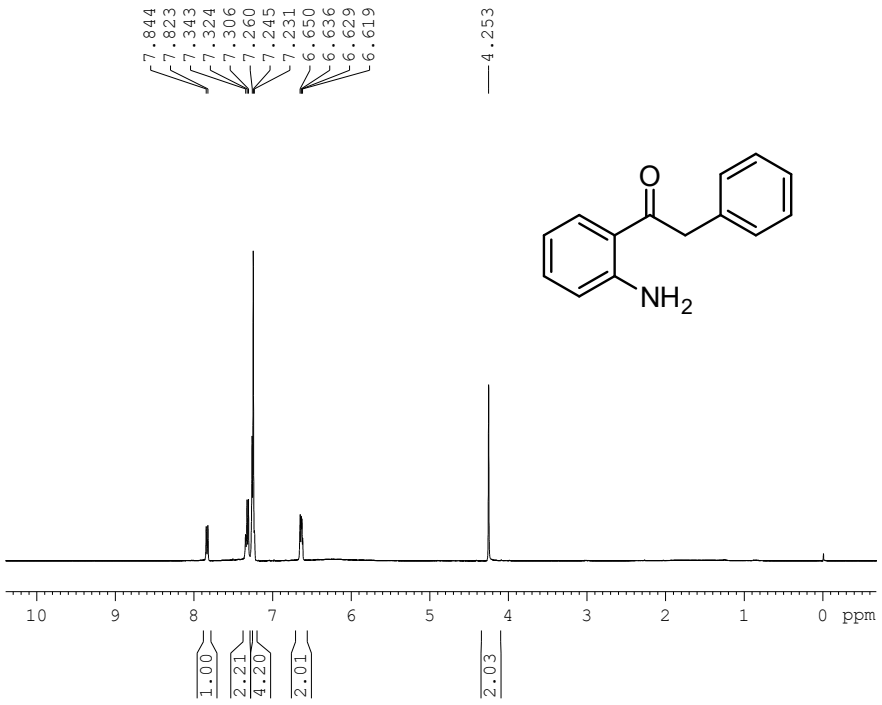
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                   256
DS                     4
SWH           24038.461 H
FIDRES         2.906706 H
AQ             0.3440320 s
RG                200.34
DW                20.800 u
DE                 6.50 u
TE                298.5 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 **2d**

1-(2-aminophenyl)-2-phenylethan-1-one: 2g

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PROCNO                  1

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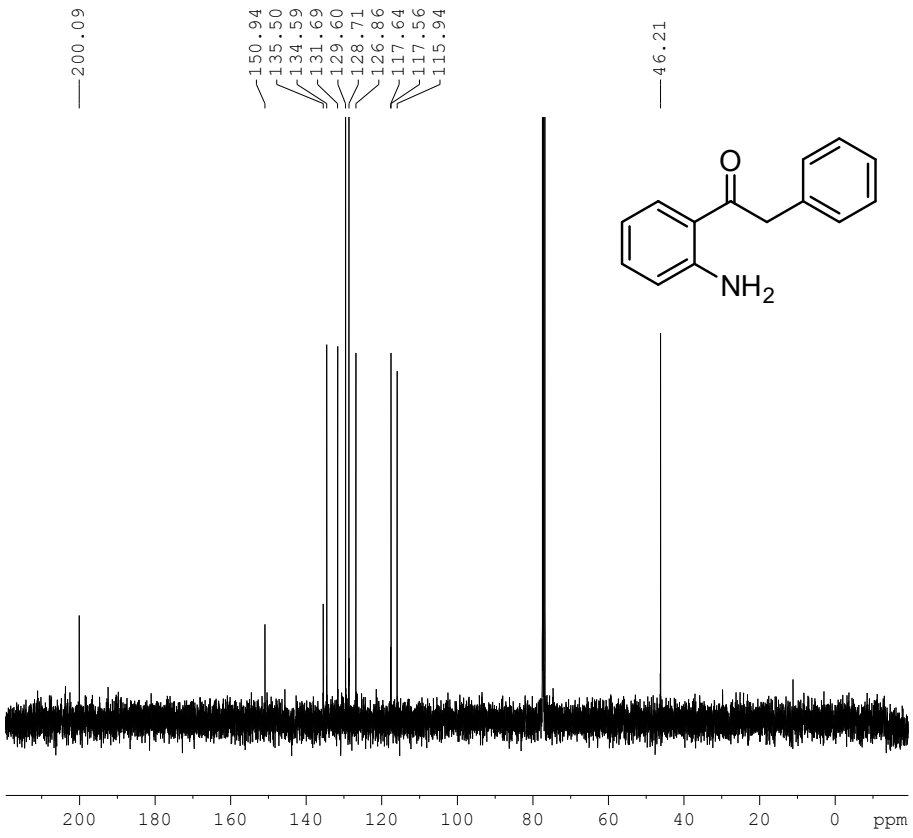
NS                    16
DS                     2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                200.34
DW              62.400 usec
DE                 6.50 usec
TE                297.5 K
D1           0.50000000 sec
TD0                    1
SFO1        400.1320007 MHz
NUC1                1H
P1               15.00 usec
PLW1         10.50000000 W

F2 - Processing parameters
SI                 65536
SF          400.1300157 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 **2g**

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Current Data Parameters
NAME                  954
EXPNO                 123
PROCNO                  1

F2 - Acquisition Parameters
Date_           20210909
Time              21.48 h
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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           100.6127580 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
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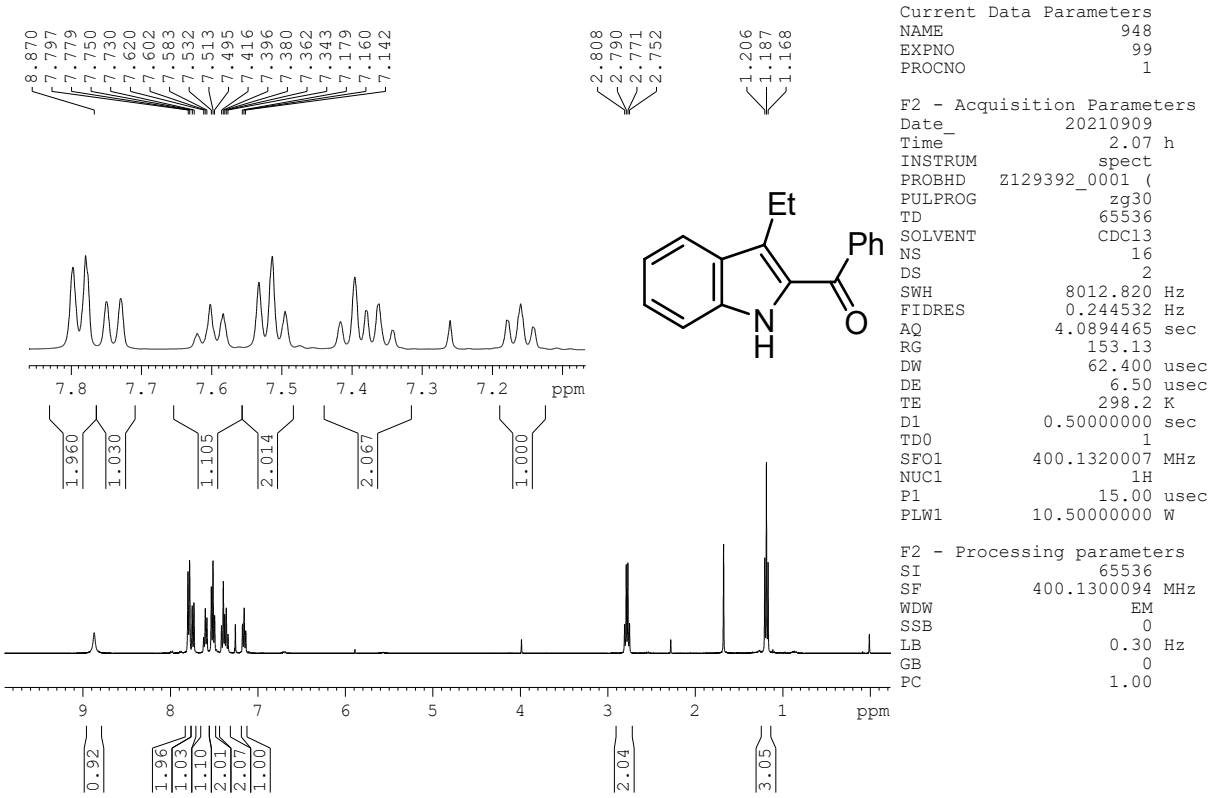
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **2g**

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

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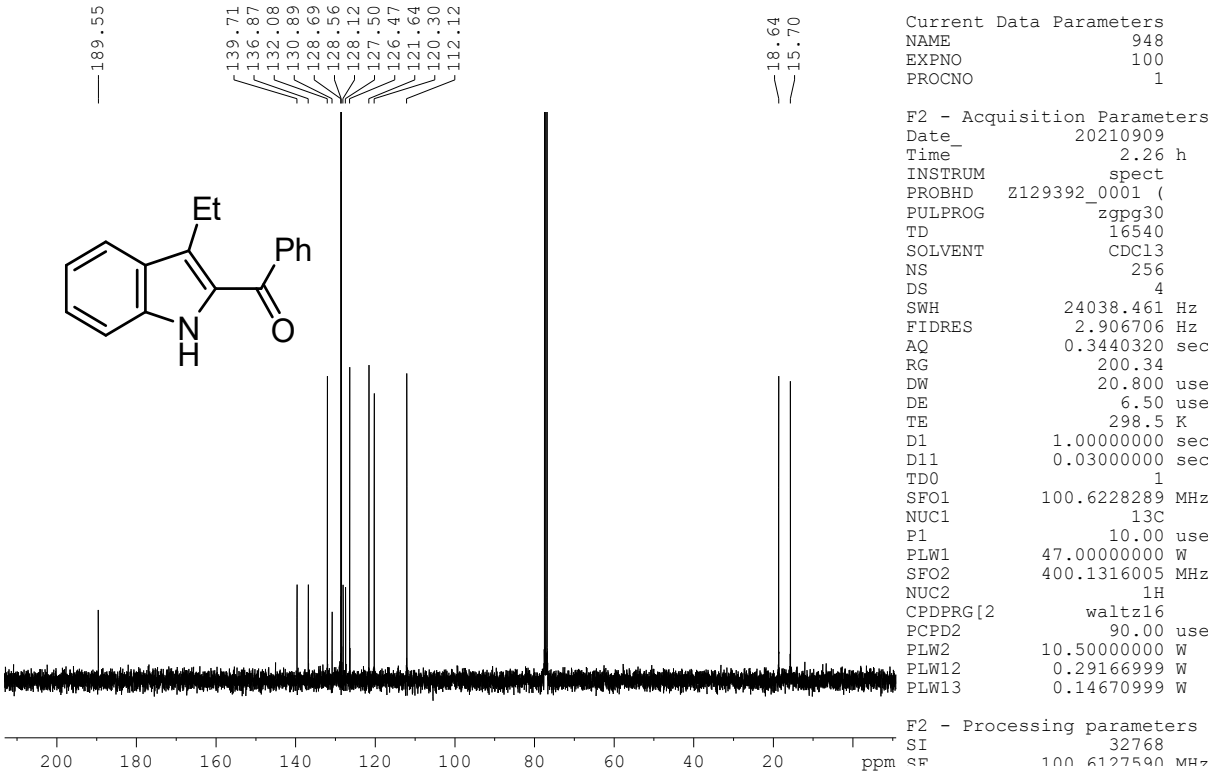
Current Data Parameters
NAME                  948
EXPNO                  99
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210909
Time                2.07 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                  153.13
DW                  62.400 usec
DE                   6.50 usec
TE                  298.2 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 **3b**

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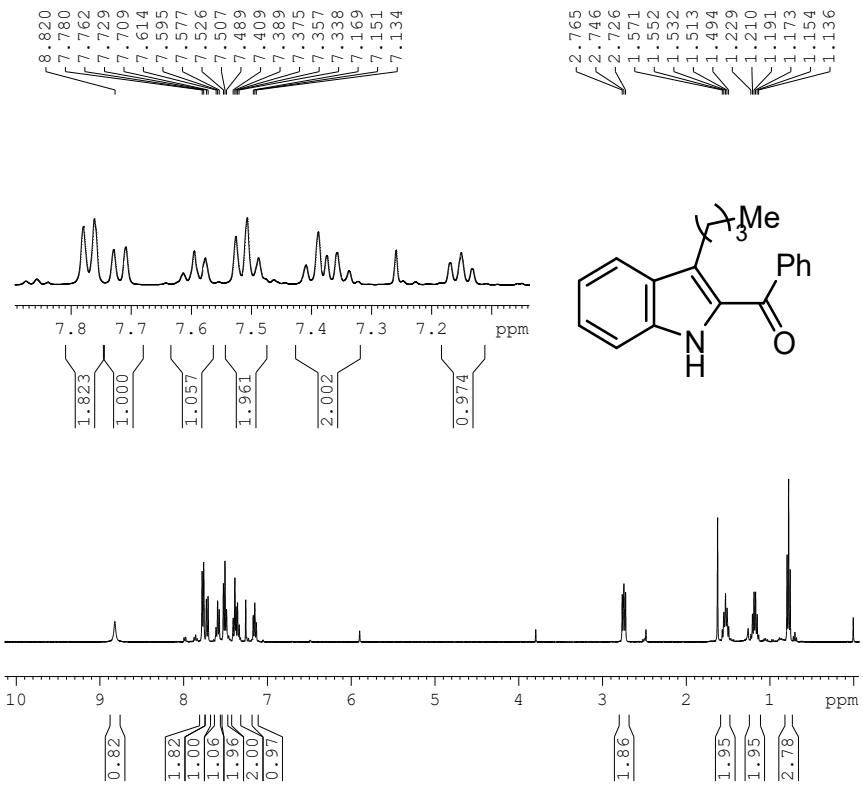
Current Data Parameters
NAME                  948
EXPNO                 100
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210909
Time                2.26 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 use
DE                   6.50 use
TE                  298.5 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                     1
SFO1           100.6228289 MHz
NUC1                   13C
P1                  10.00 use
PLW1           47.00000000 W
SFO2           400.1316005 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2               90.00 use
PLW2           10.50000000 W
PLW12           0.29166999 W
PLW13           0.14670999 W

F2 - Processing parameters
SI                  32768
SF             100.6127590 MHz
```

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

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

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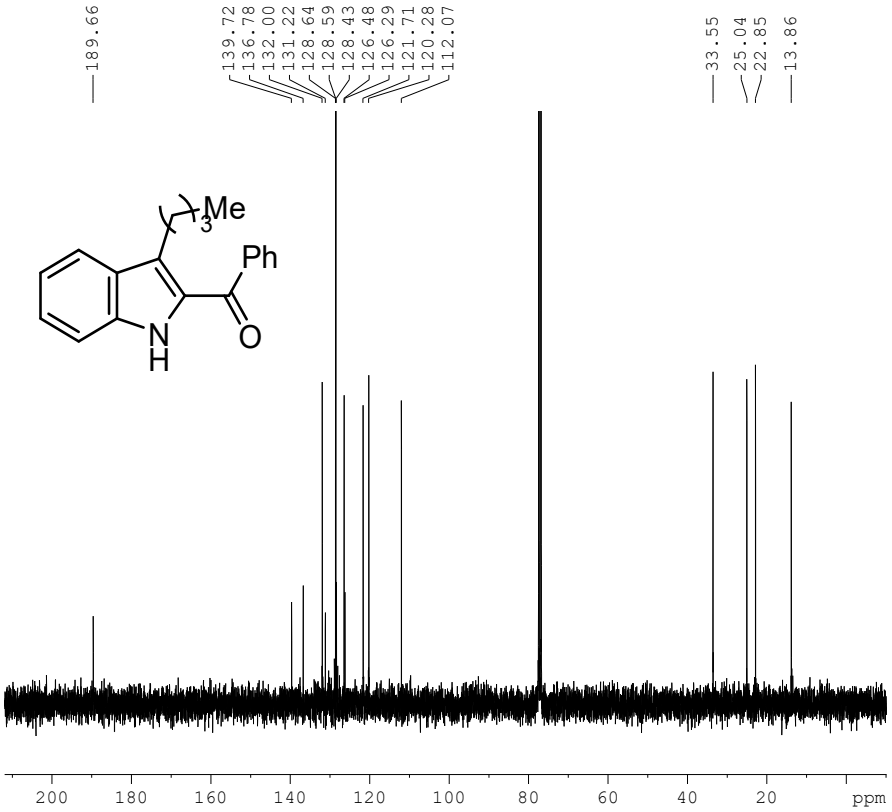
Current Data Parameters
NAME                  951
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210901
Time                18.41 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                 169.77
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            400.1300098 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**

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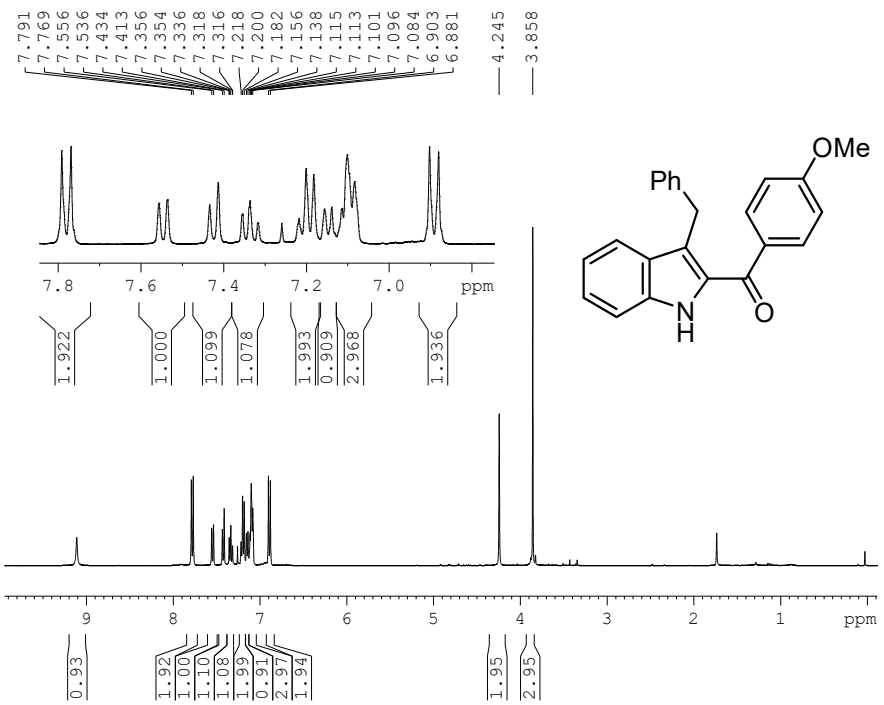
Current Data Parameters
NAME                  951
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameter
Date_            20210901
Time                18.48 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                 298.1 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            100.6127576 MH
WDW                    EM
```

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

(3-benzyl-1H-indol-2-yl)(4-methoxyphenyl)methanone: 3g

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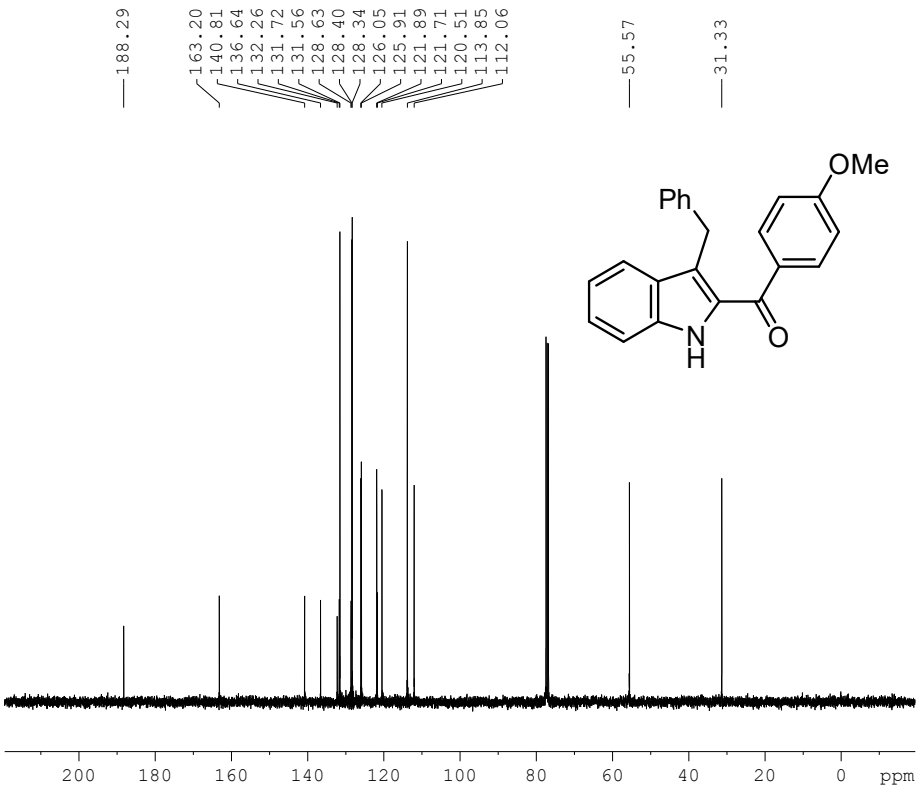
Current Data Parameters
NAME                  978
EXPNO                 453
PROCNO                  1

F2 - Acquisition Parameters
Date_           20211001
Time               5.38 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                108.26
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          400.1300098 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 **3g**

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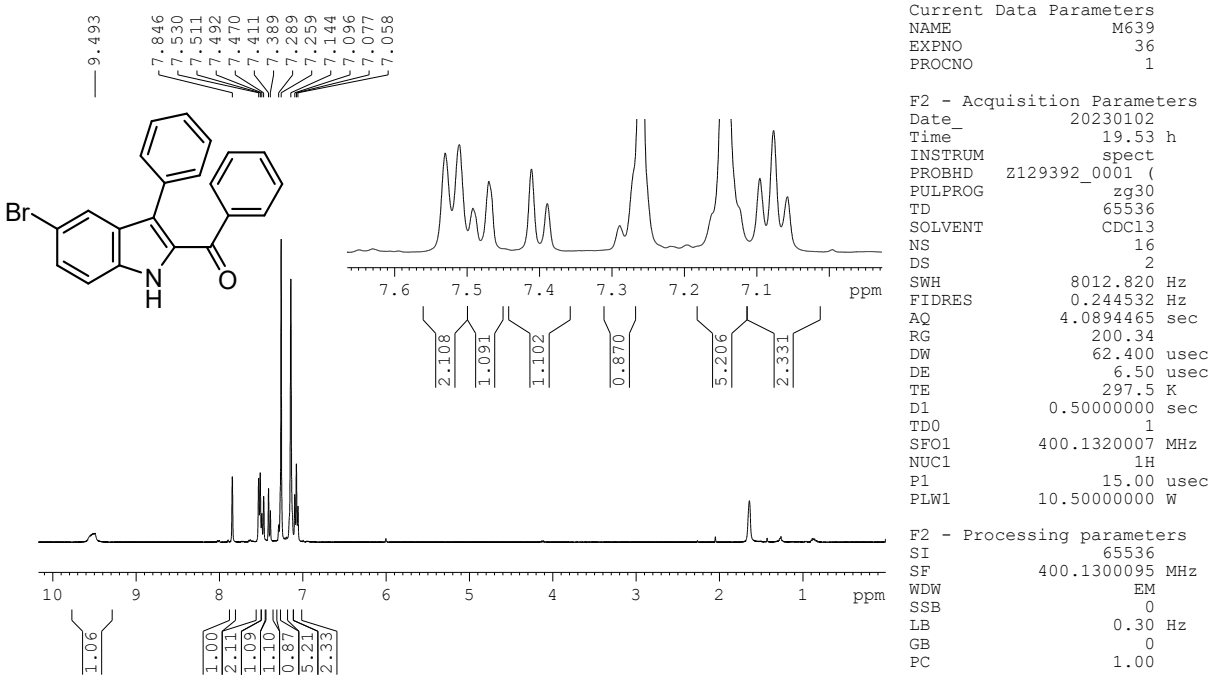
Current Data Parameters
NAME                  978
EXPNO                 454
PROCNO                  1

F2 - Acquisition Paramet
Date_           20211001
Time                5.45
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                298.5
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
SI                32768
```

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

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

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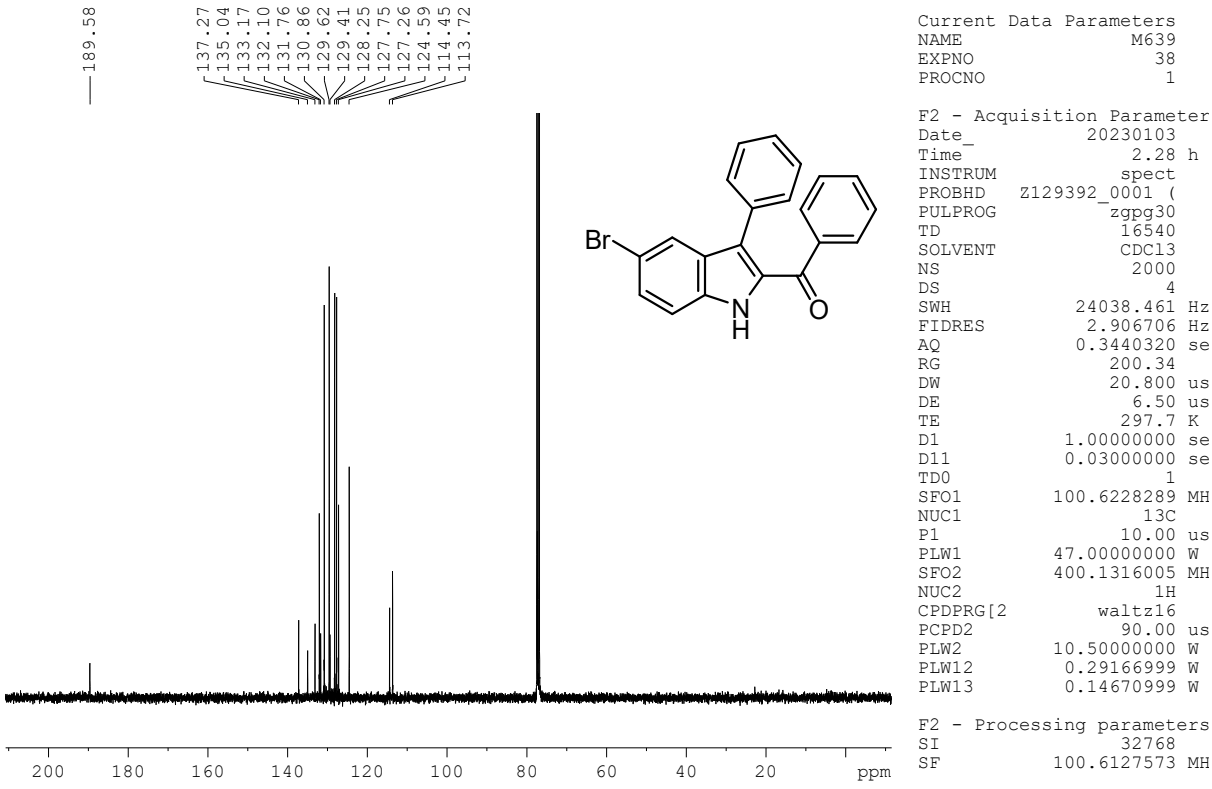
Current Data Parameters
NAME                  M639
EXPNO                   36
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230102
Time                 19.53 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             400.1300095 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 **3n**

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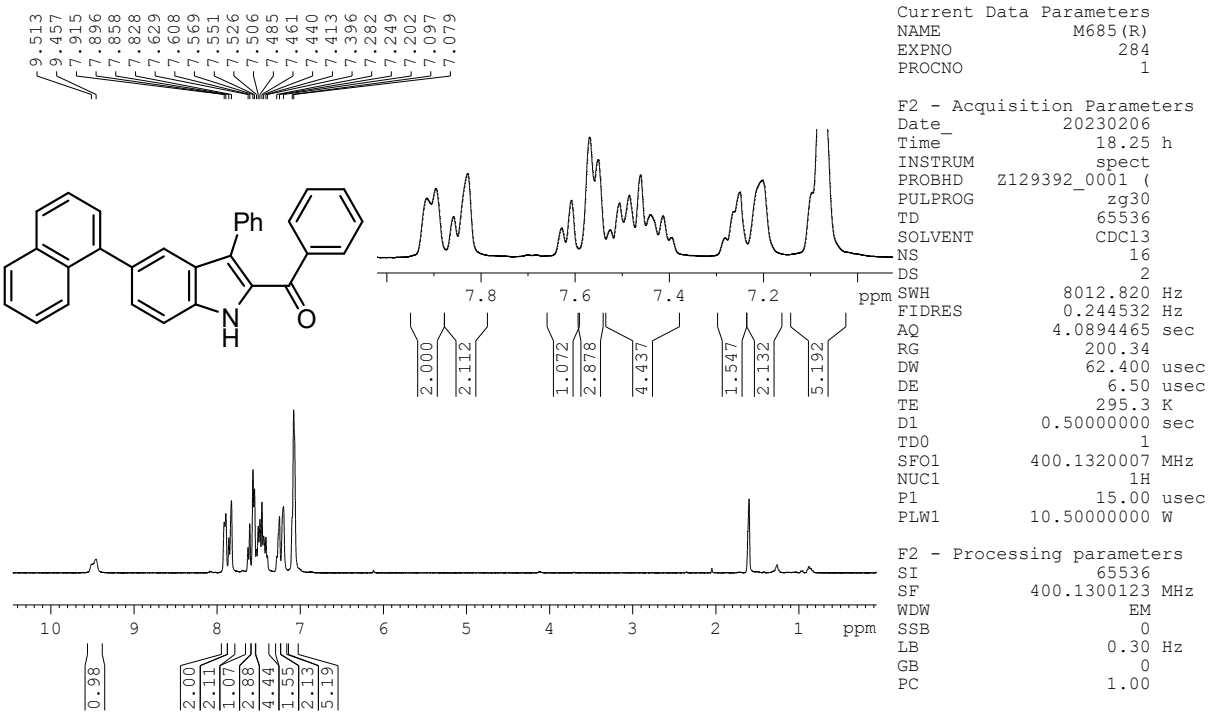
Current Data Parameters
NAME                  M639
EXPNO                   38
PROCNO                   1

F2 - Acquisition Parameter
Date_              20230103
Time                  2.28 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                  297.7 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

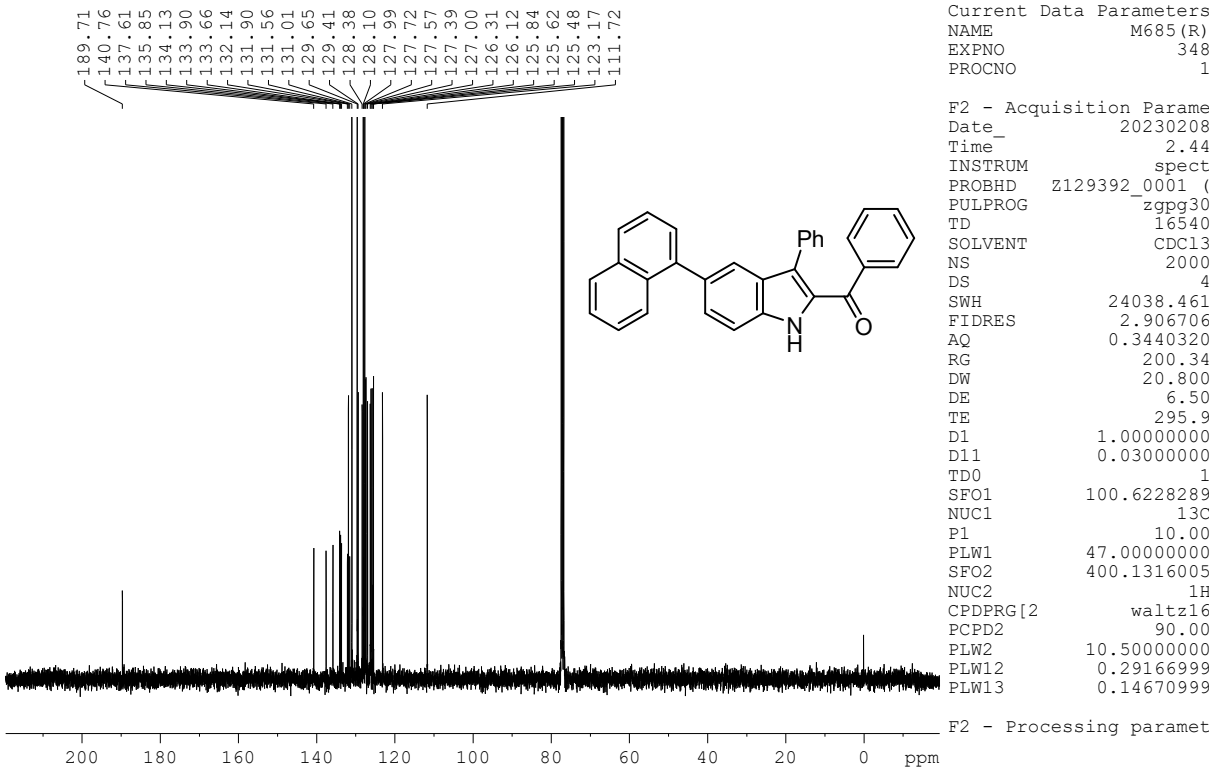
F2 - Processing parameters
SI                  32768
SF             100.6127573 MH
```

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

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

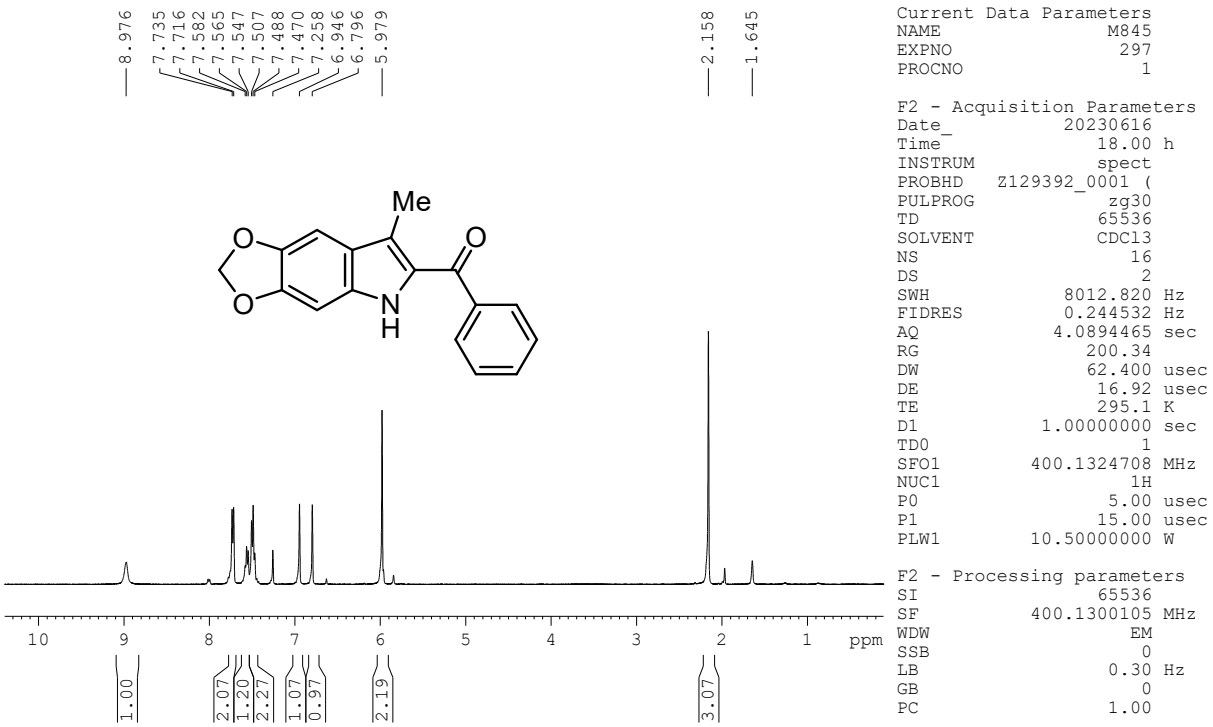


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3q**

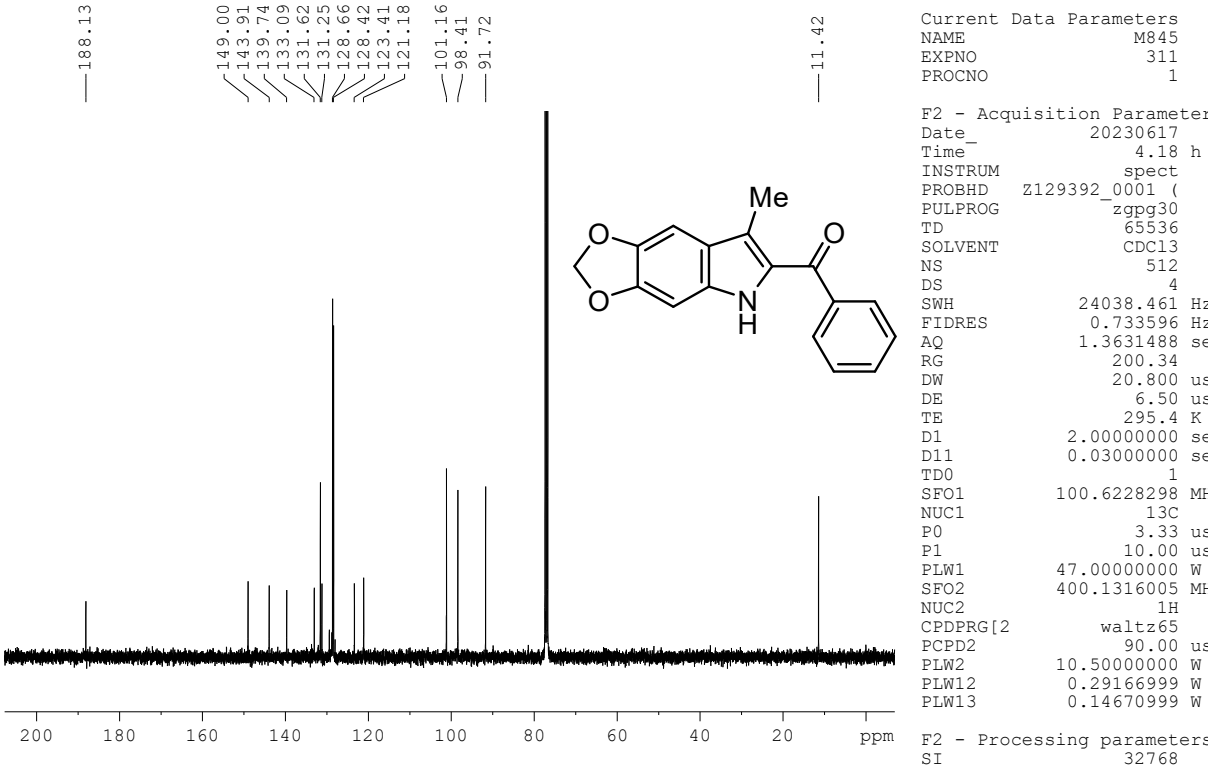


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3q**

(7-methyl-5H-[1,3]dioxolo[4,5-f]indol-6-yl)(phenyl)methanone: 3s

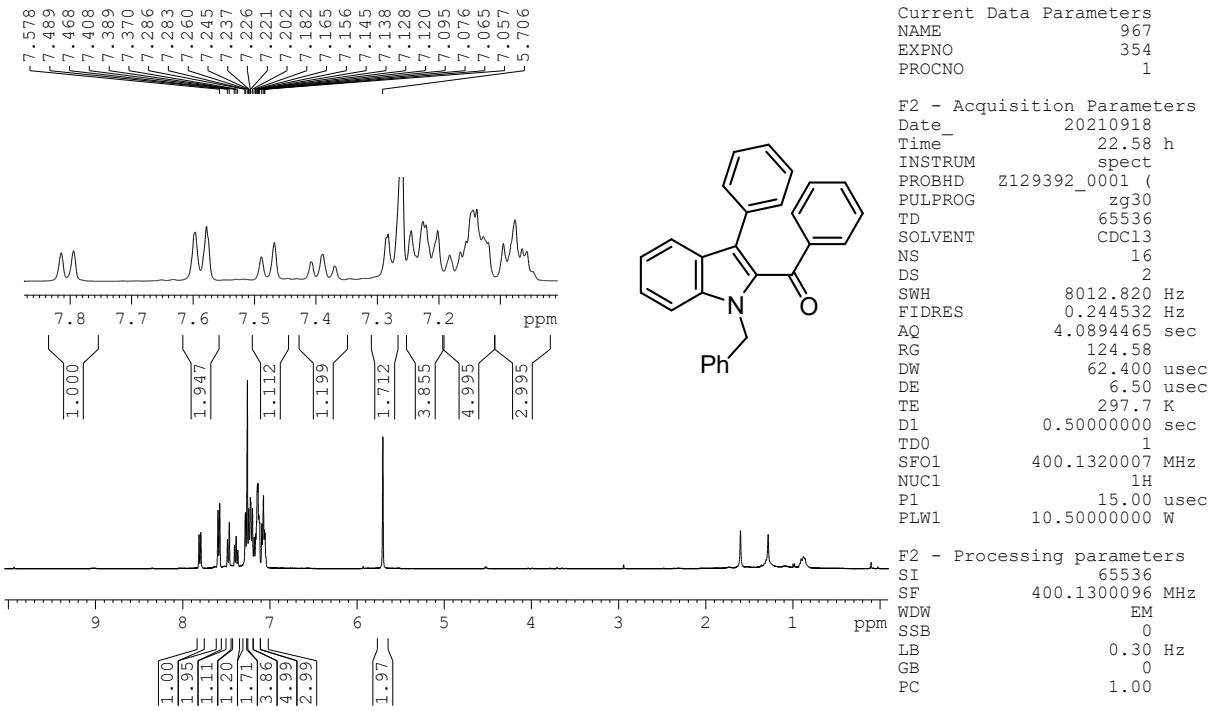


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3s**

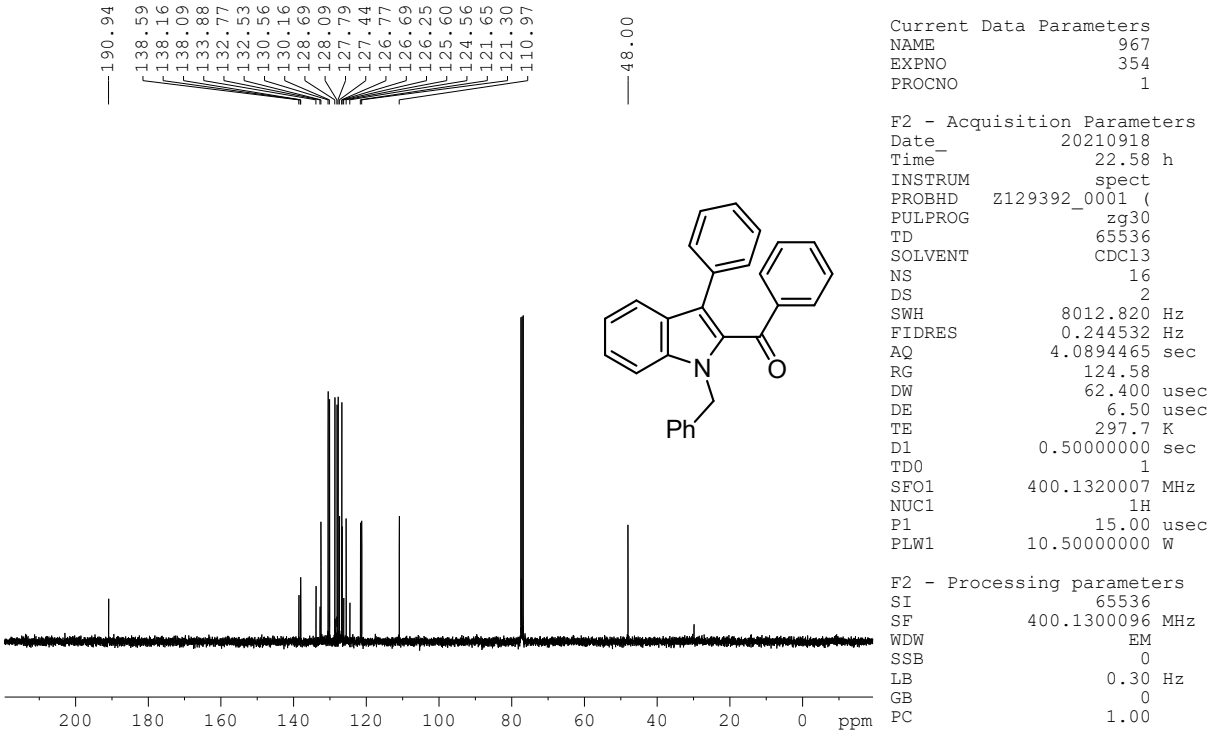


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3s**

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

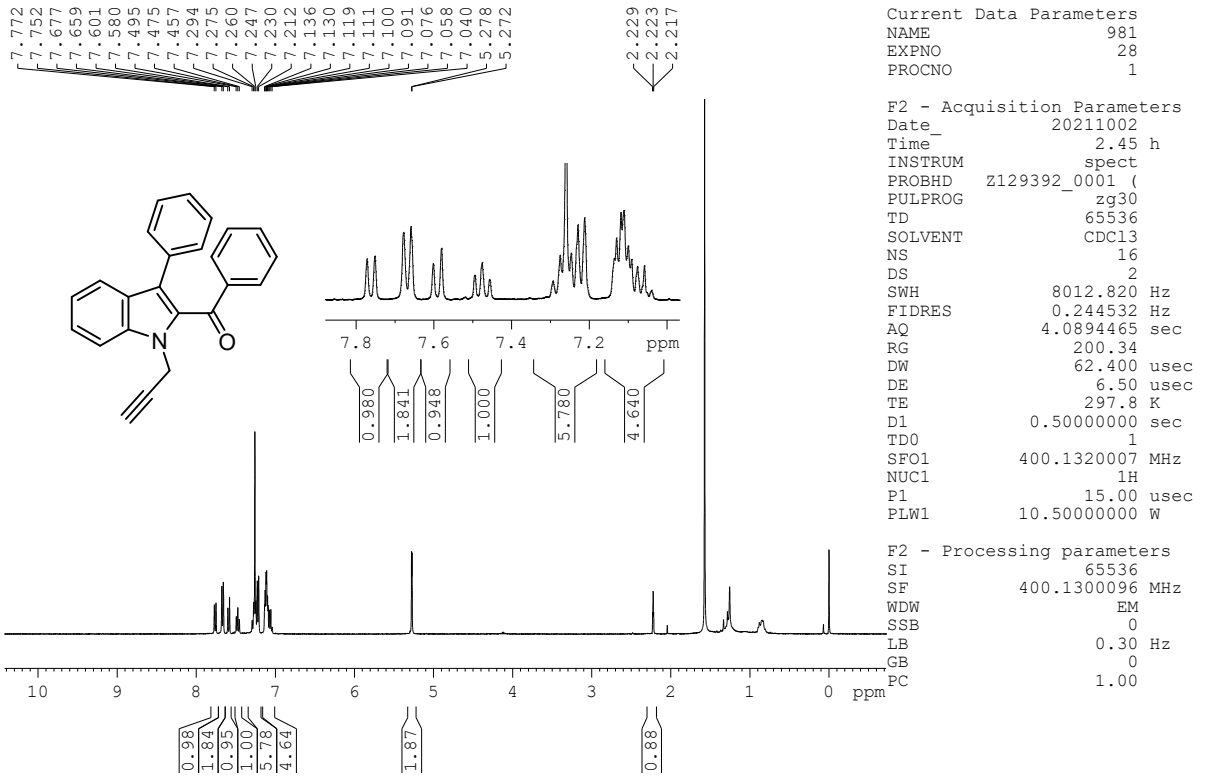


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3v**

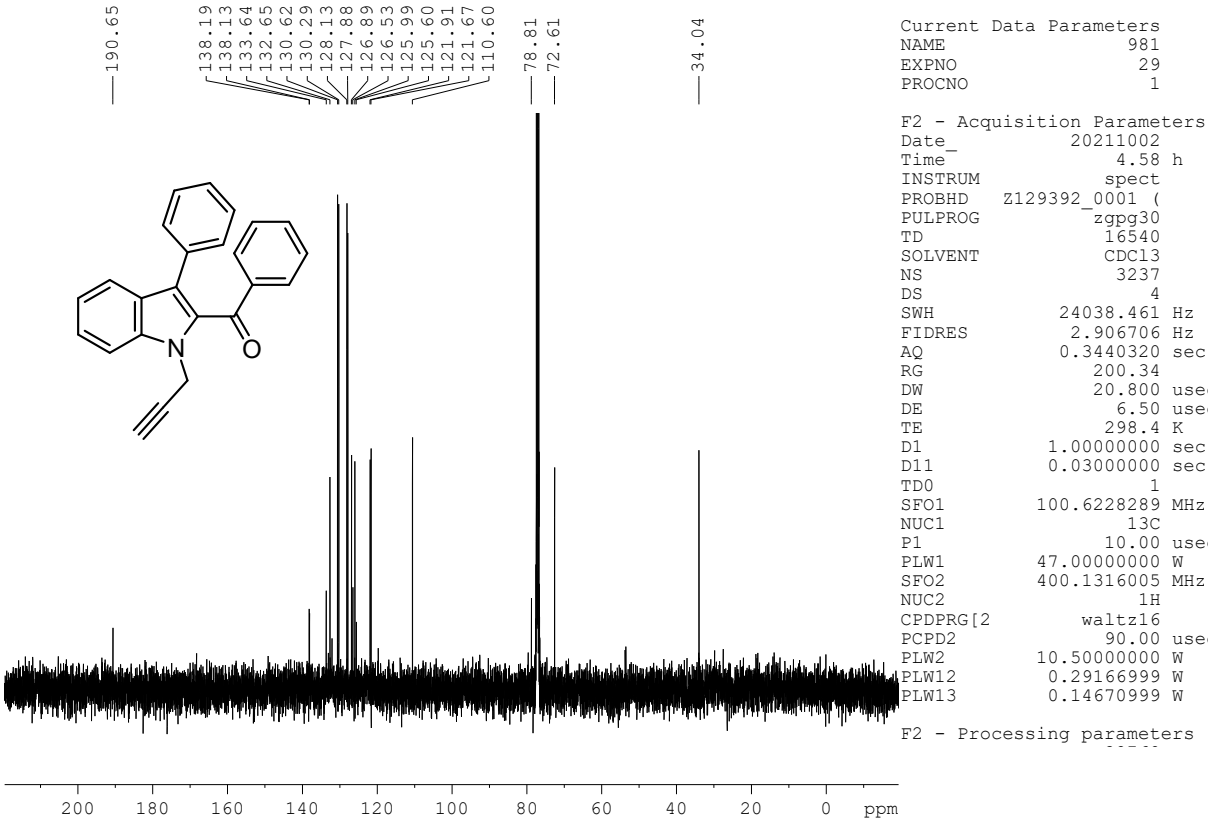


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3v**

phenyl(3-phenyl-1-(prop-2-yn-1-yl)-1H-indol-2-yl)methanone: 3x

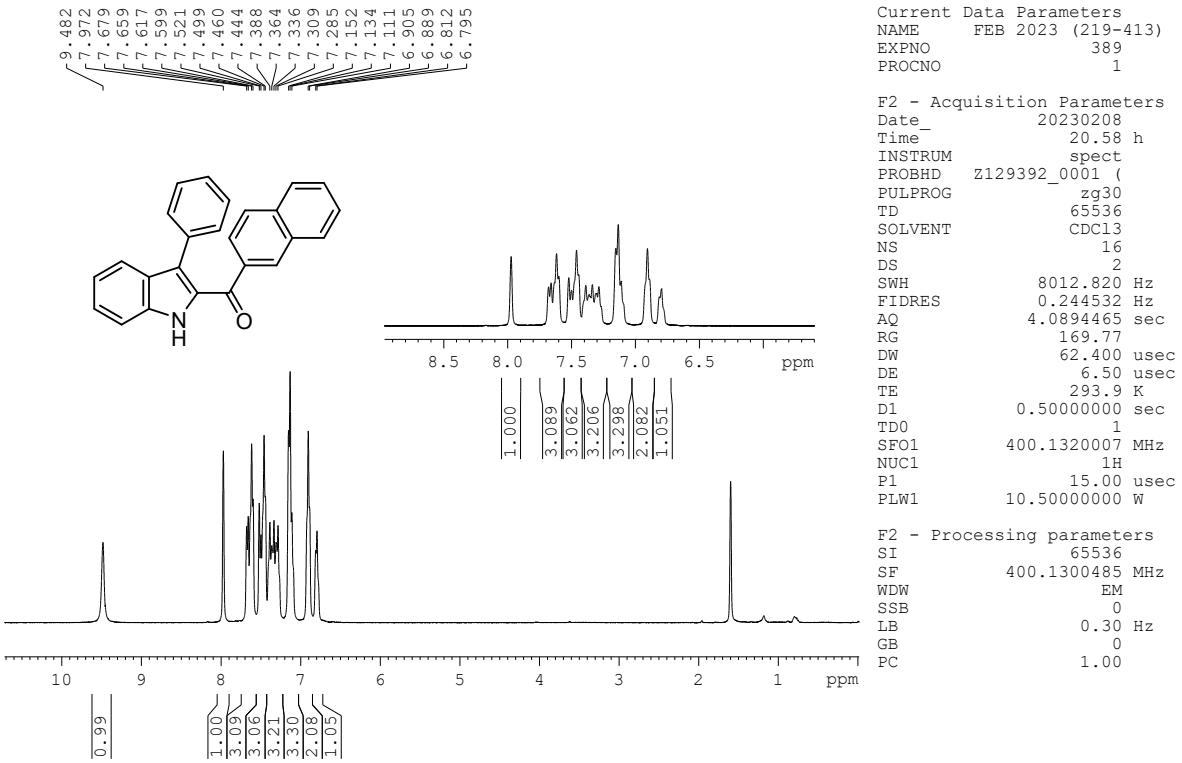


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3x**



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

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

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Current Data Parameters
NAME      FEB 2023 (219-413)
EXPNO                389
PROCNO                 1

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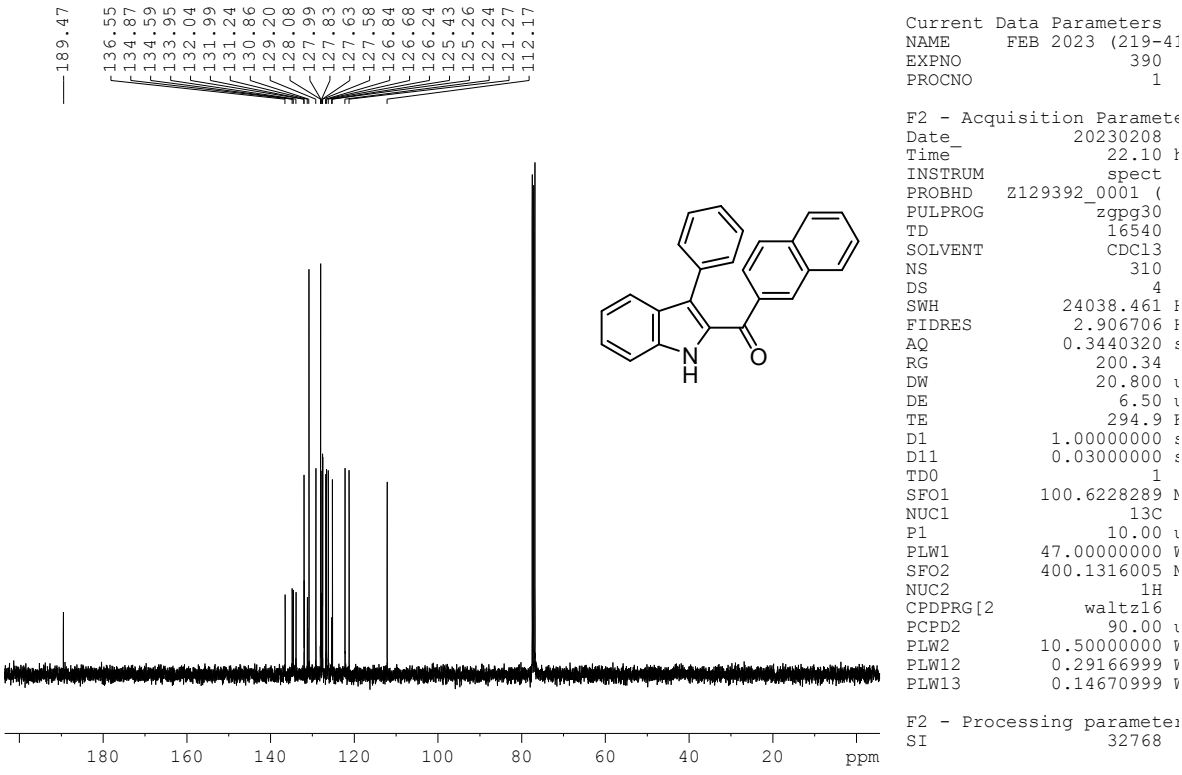
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ             4.0894465 sec
RG                169.77
DW                62.400 usec
DE                 6.50 usec
TE                293.9 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           400.1300485 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 **3y**

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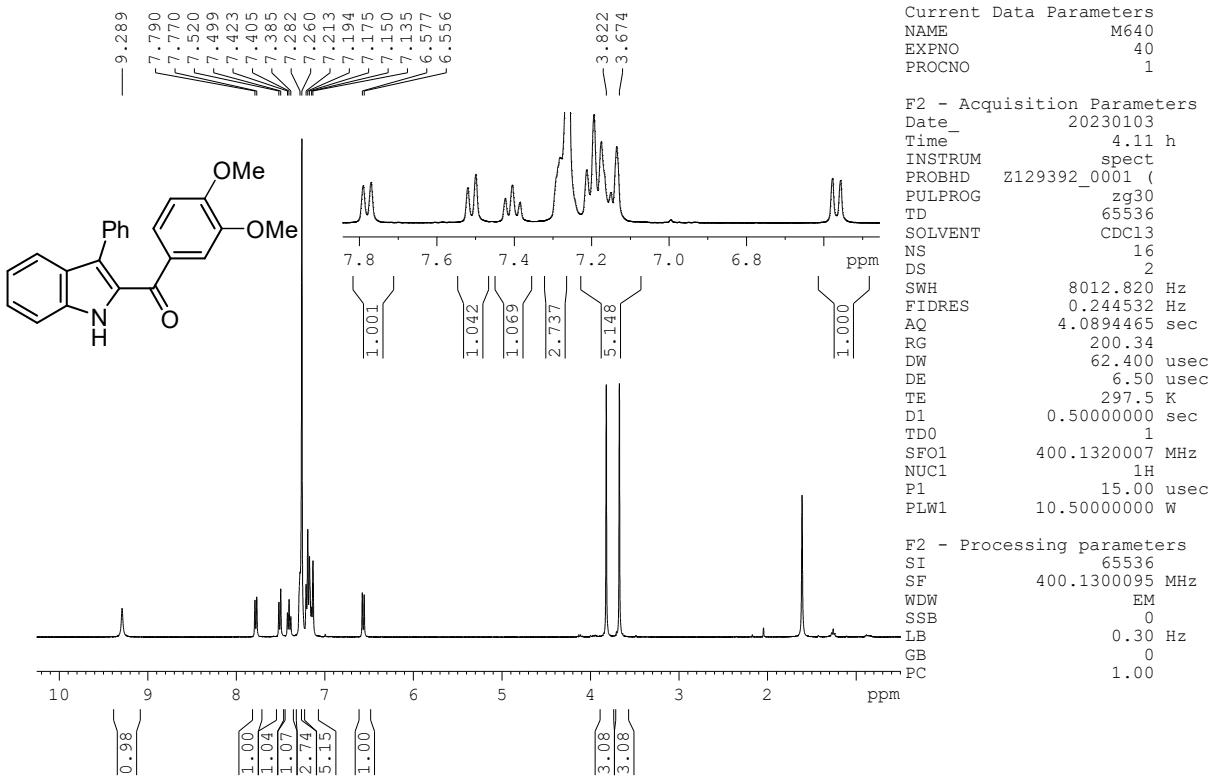
Current Data Parameters
NAME      FEB 2023 (219-41
EXPNO                390
PROCNO                 1

F2 - Acquisition Paramete
Date_           20230208
Time              22.10 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                   310
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                294.9 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

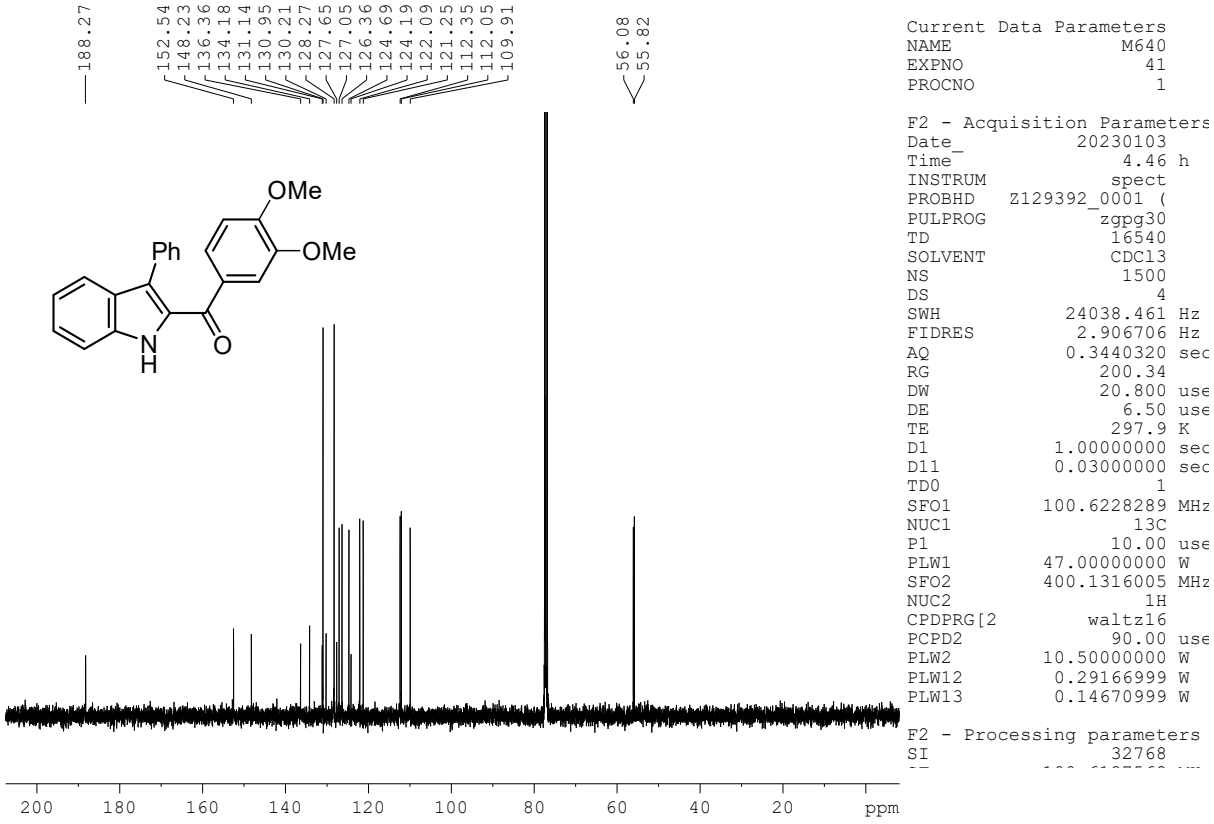
F2 - Processing paramete
SI                 32768
```

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

(2,3-dimethoxyphenyl)(3-phenyl-1H-indol-2-yl)methanone: 3ab

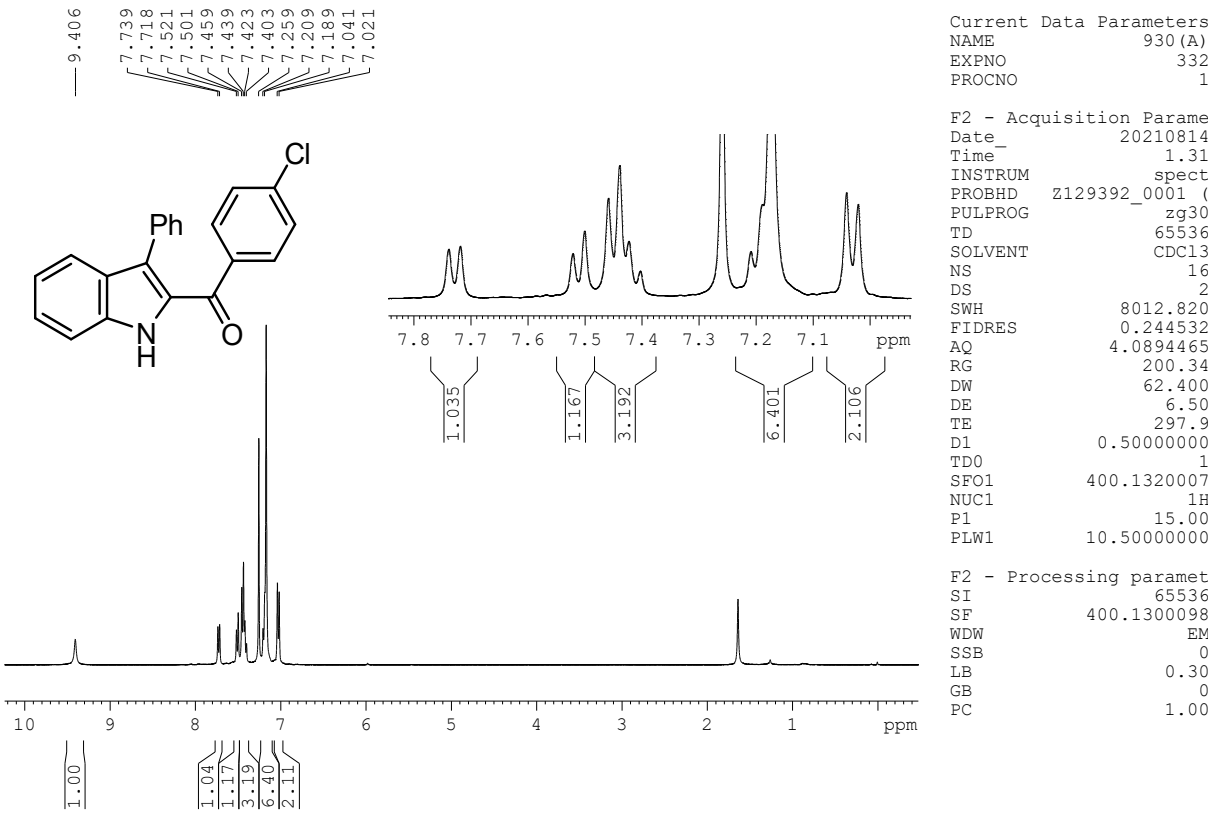


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3ab**

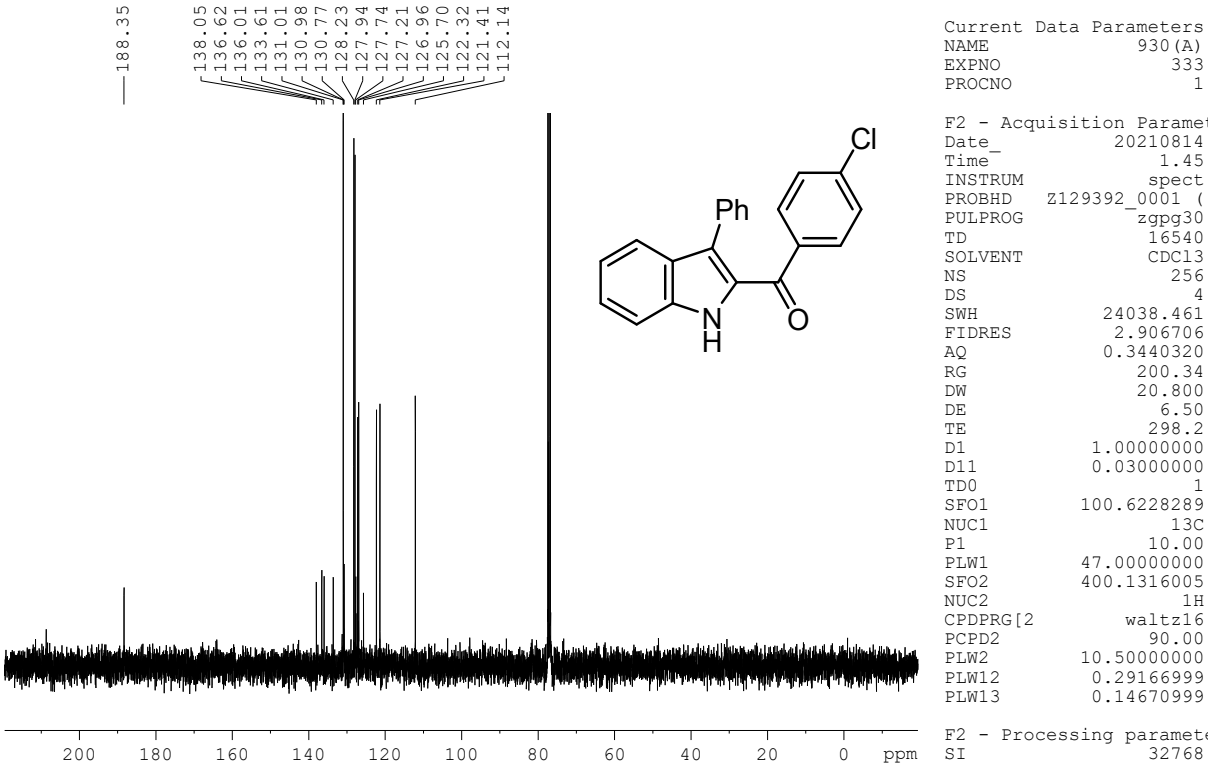


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3ab**

(4-chlorophenyl)(3-phenyl-1H-indol-2-yl)methanone: 3ad

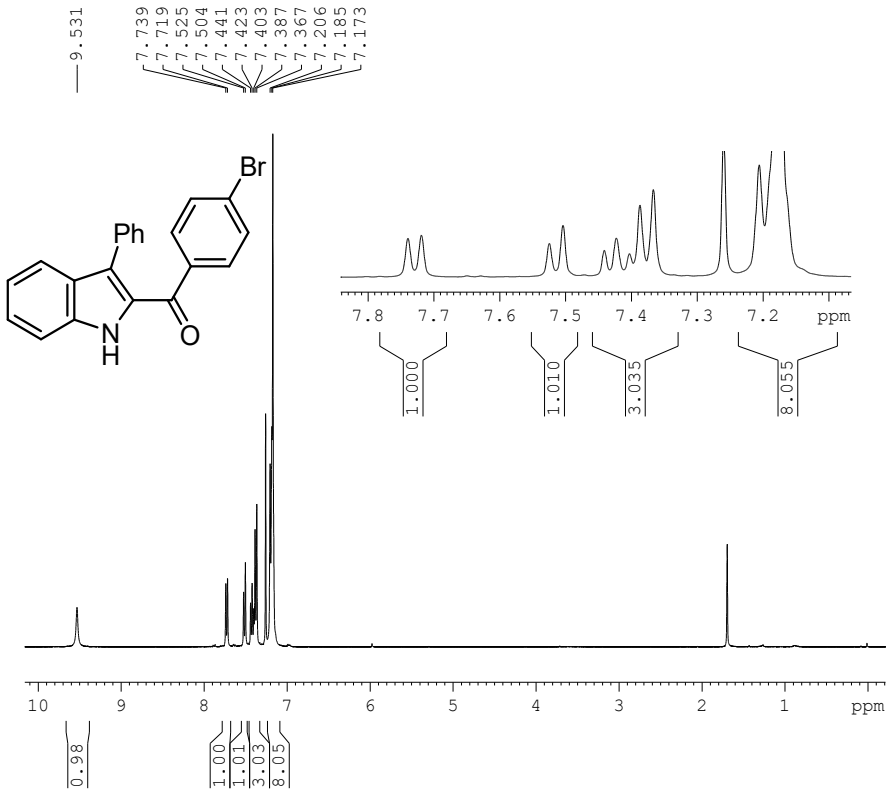


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3ad**



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

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

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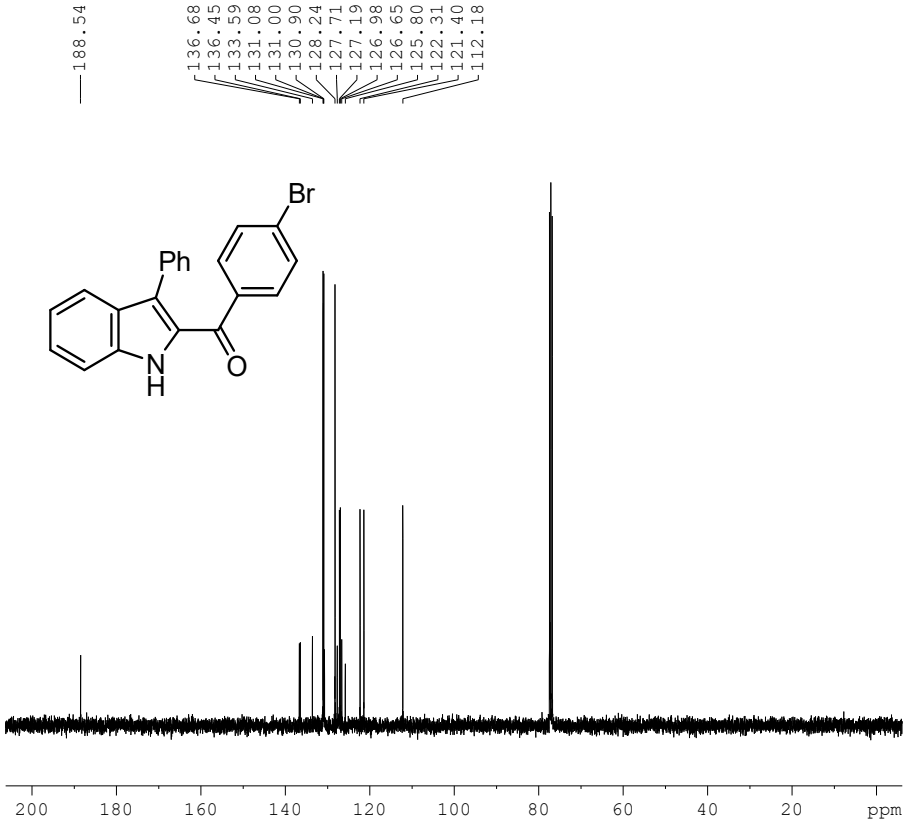
Current Data Parameters
NAME                  M643
EXPNO                   69
PROCNO                   1

F2 - Acquisition Parameters
Date_            20230103
Time                21.47 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                  297.3 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            400.1300096 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 **3ae**

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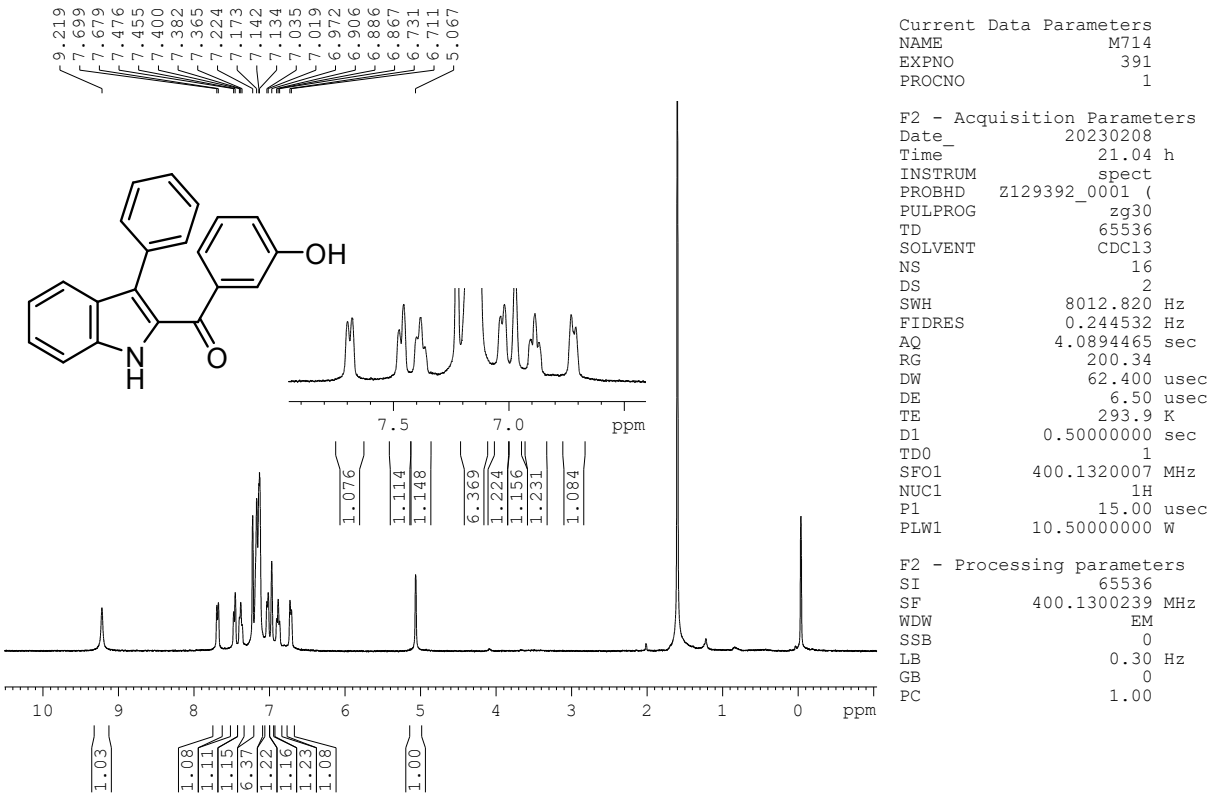
Current Data Parameters
NAME                  M643
EXPNO                   70
PROCNO                   1

F2 - Acquisition Paramete
Date_            20230103
Time                21.54 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                  297.6 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 paramete
SI                   32768
```

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

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

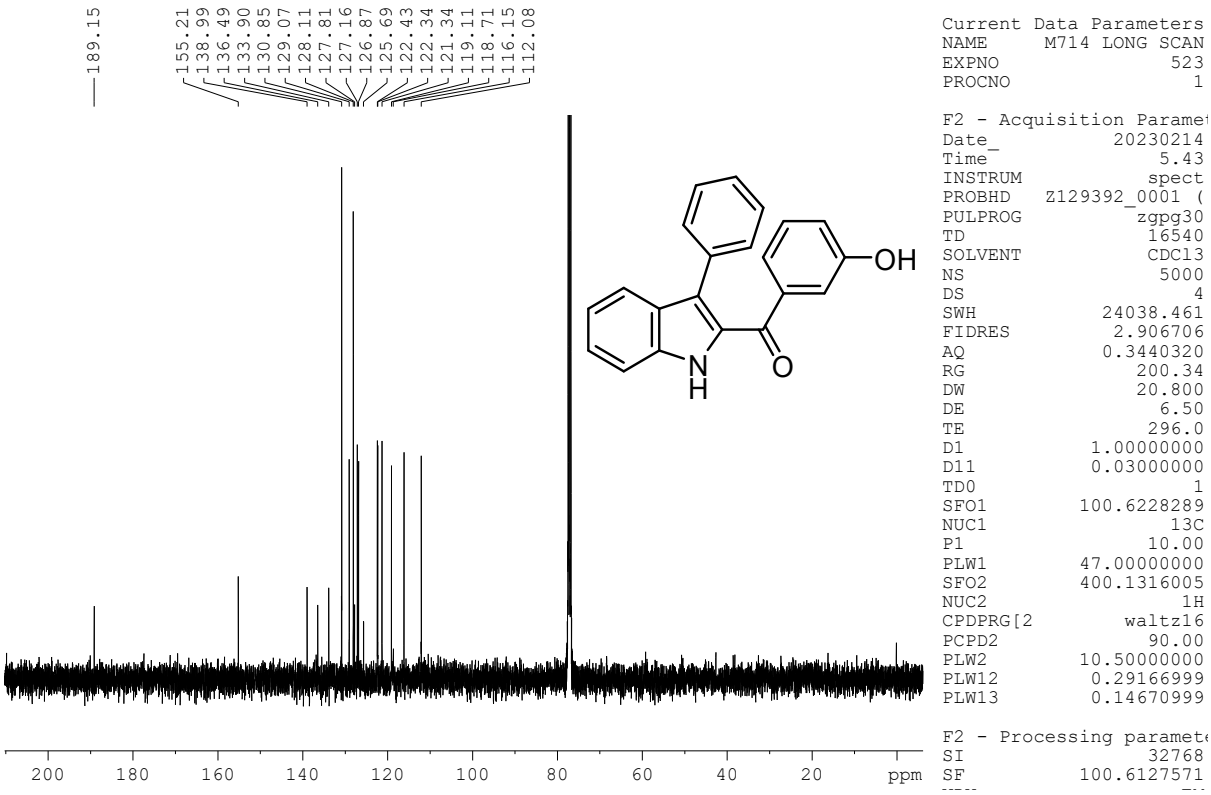


Current Data Parameters
NAME M714
EXPNO 391
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230208
Time 21.04 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 293.9 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 400.1300239 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 **3ah**



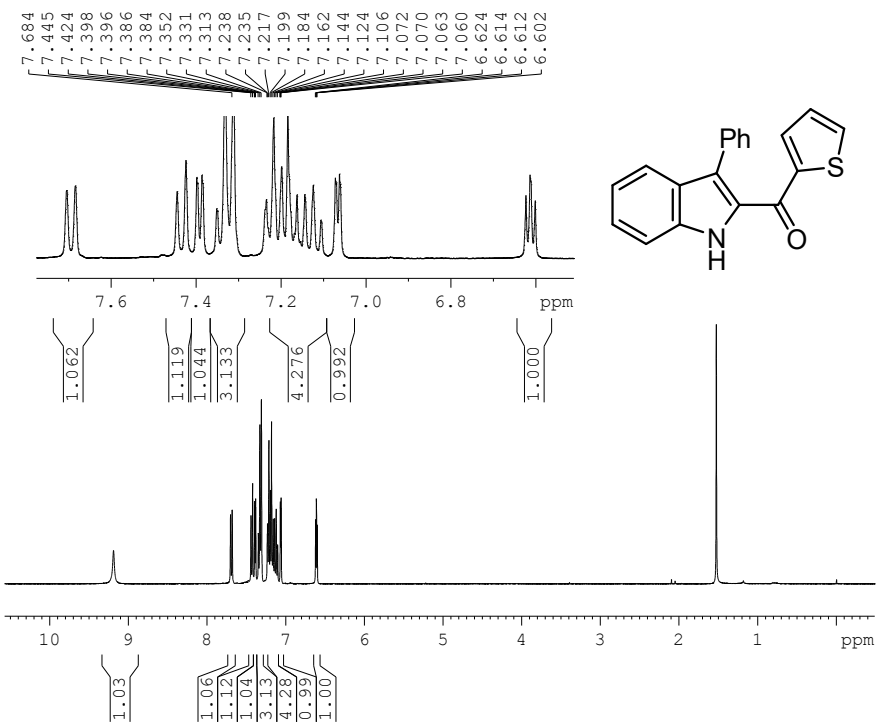
Current Data Parameters
NAME M714 LONG SCAN
EXPNO 523
PROCNO 1

F2 - Acquisition Parame
Date_ 20230214
Time 5.43
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 5000
DS 4
SWH 24038.461
FIDRES 2.906706
AQ 0.3440320
RG 200.34
DW 20.800
DE 6.50
TE 296.0
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 paramet
SI 32768
SF 100.6127571

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

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

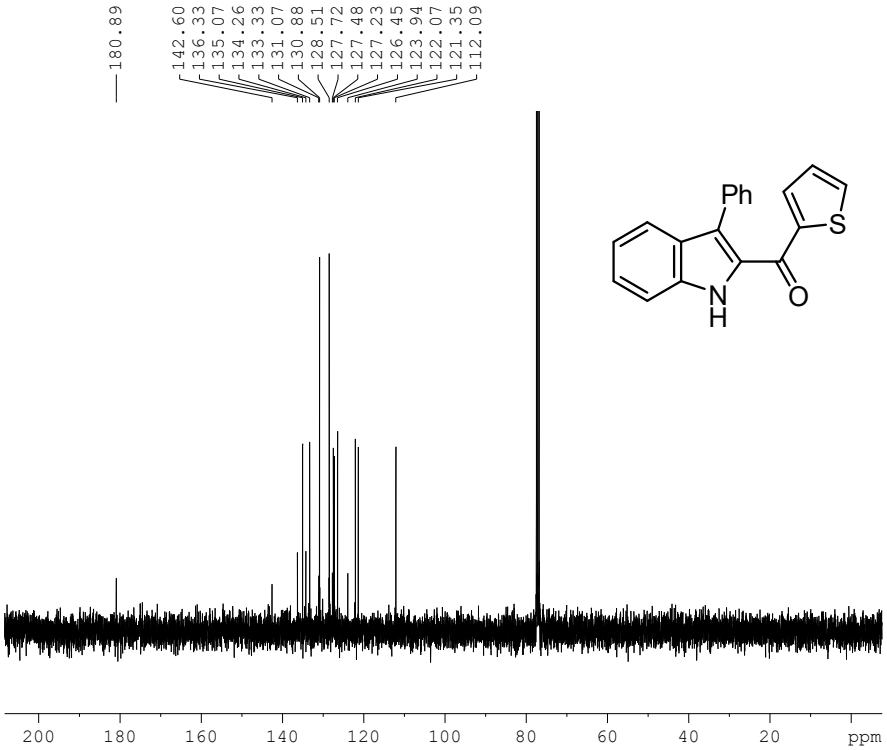



```
Current Data Parameters
NAME                  M153
EXPNO                   26
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220205
Time                  1.39 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             400.1300397 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 **3aj**



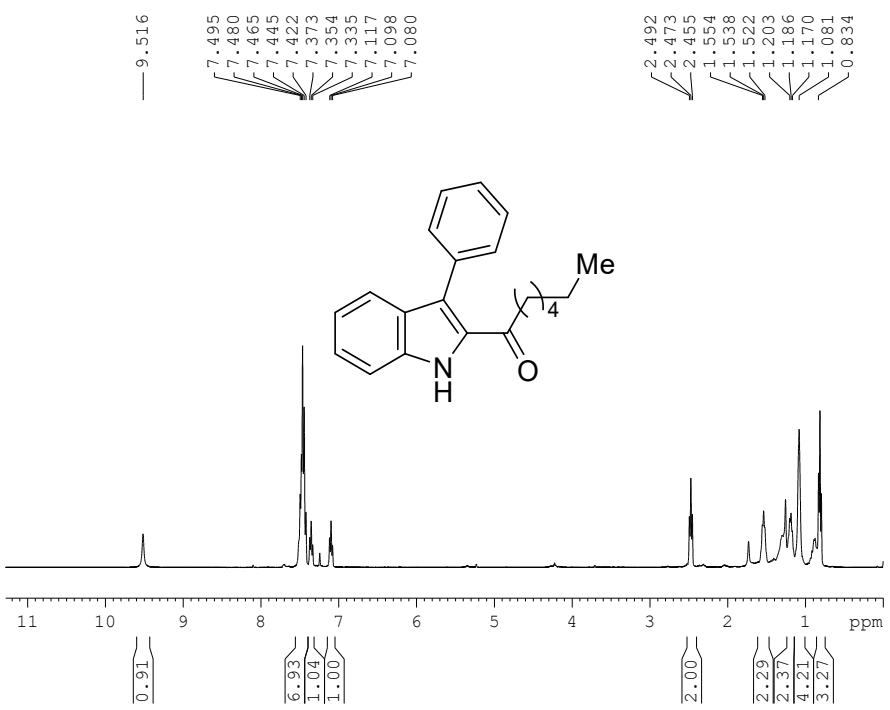

```
Current Data Parameters
NAME                  M153
EXPNO                   27
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220205
Time                  1.46 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                   297.2 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             100.6127571 MHz
```

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

1-(3-phenyl-1H-indol-2-yl)heptan-1-one: 3am

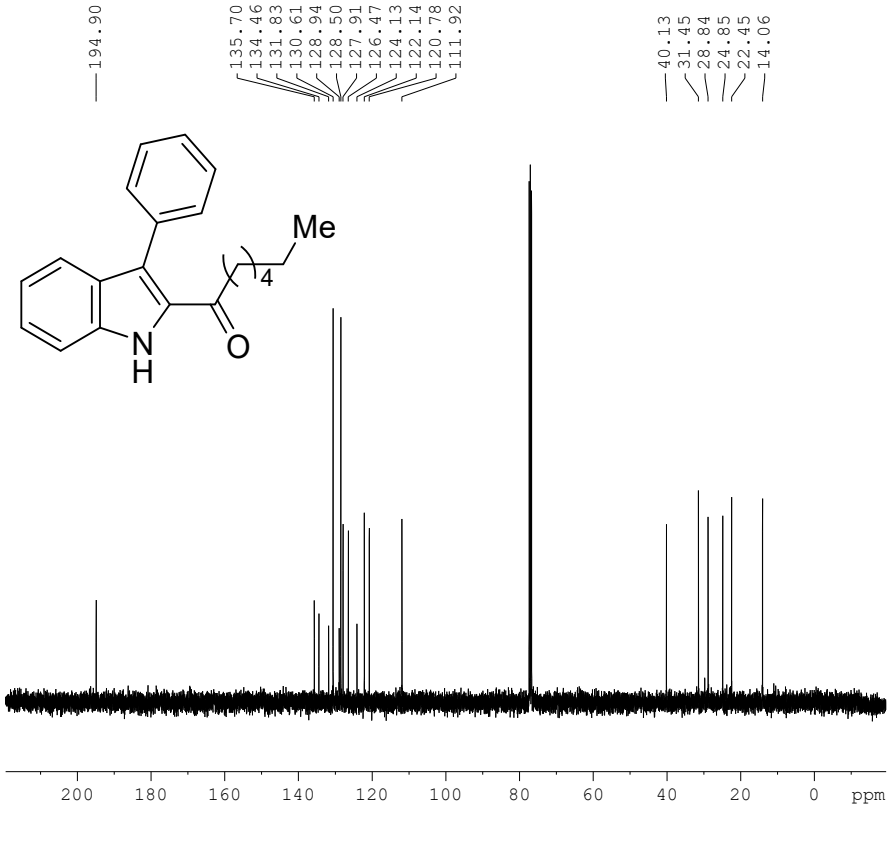



```
Current Data Parameters
NAME                  M813
EXPNO                   49
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230605
Time               10.51 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                 88.51
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            400.1300159 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 **3am**



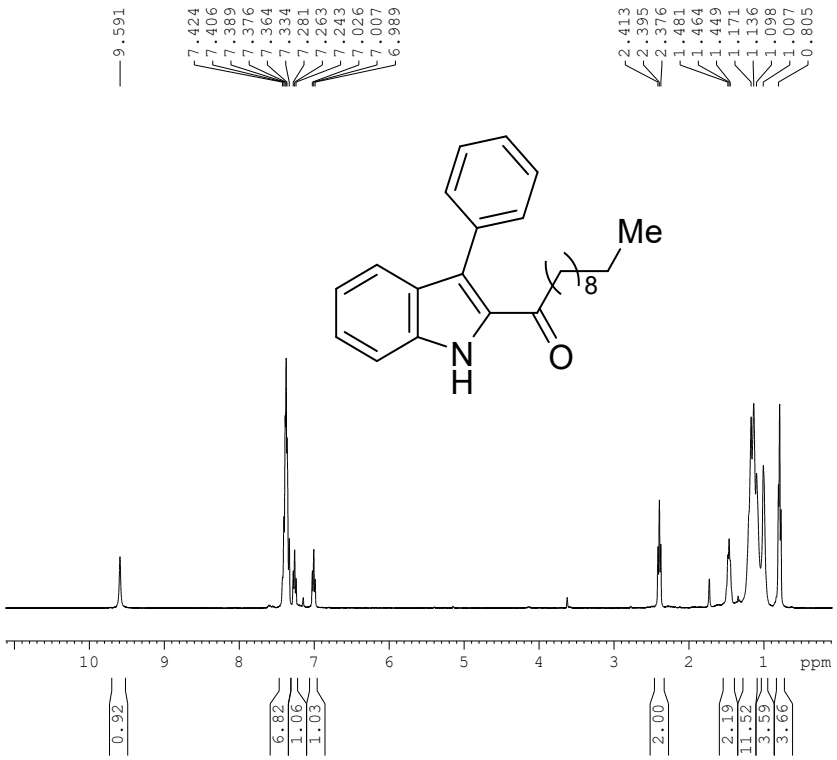

```
Current Data Parameters
NAME                  M813
EXPNO                   50
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230605
Time               10.54 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    36
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                295.2 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
SSB                    0
LB                  1.00 Hz
```

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

1-(3-phenyl-1H-indol-2-yl)undecan-1-one: 3an

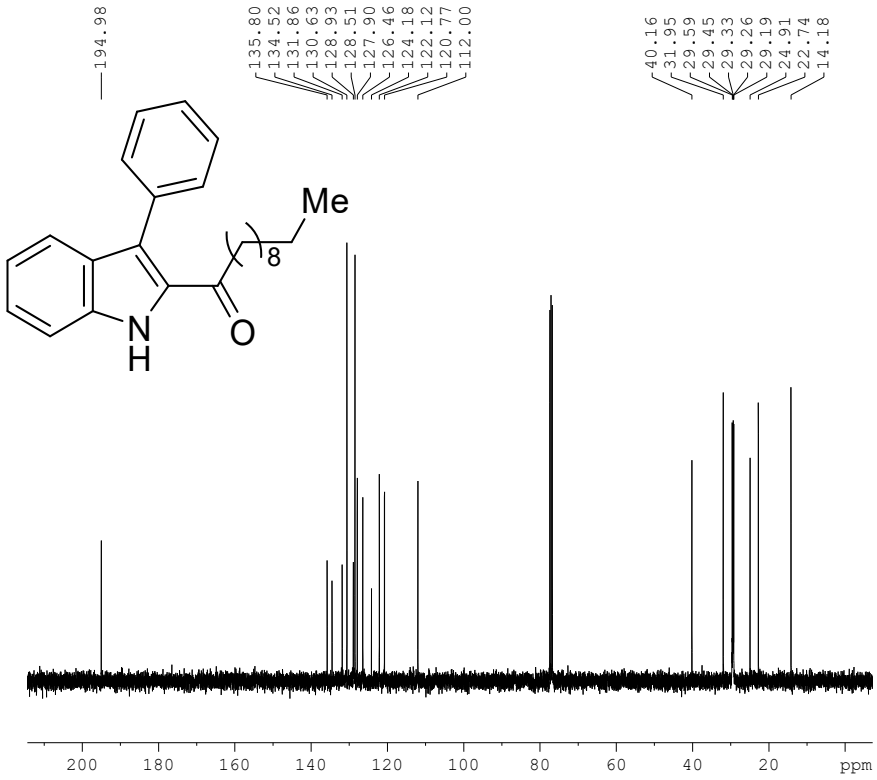



```
Current Data Parameters
NAME                  M814
EXPNO                   51
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230605
Time                 10.58 h
INSTRUM              spect
PROBHD   Z129392_0001 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      6
DS                      2
SWH               8012.820 Hz
FIDRES            0.244532 Hz
AQ               4.0894465 sec
RG                   56.23
DW                  62.400 usec
DE                  16.92 usec
TE                  294.9 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           400.1300542 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 **3an**



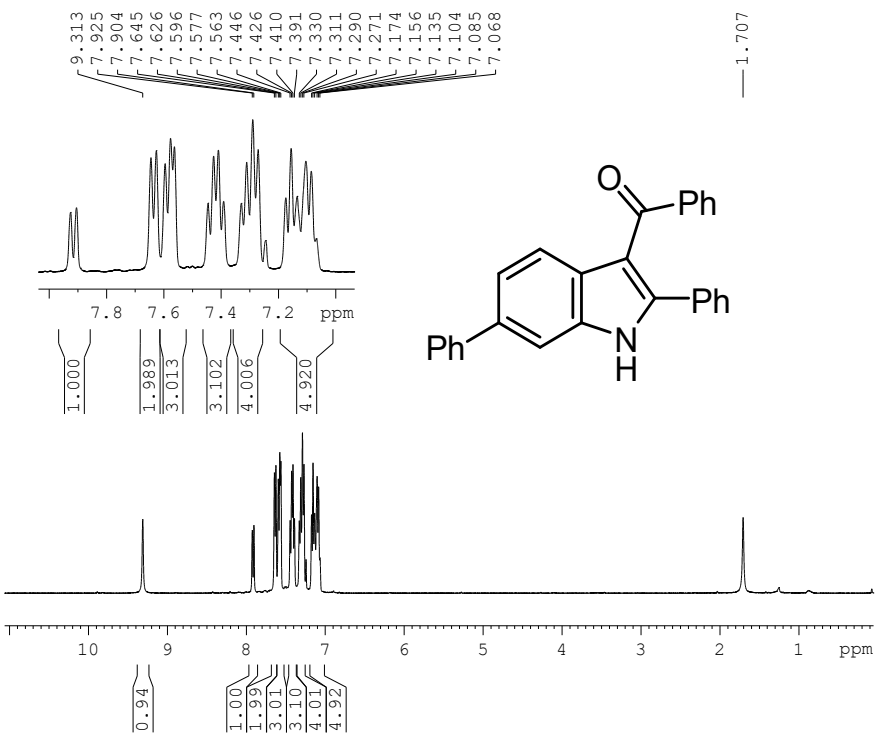

```
Current Data Parameters
NAME                  M814
EXPNO                   52
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230605
Time                 11.01 h
INSTRUM              spect
PROBHD   Z129392_0001 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     33
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                  295.2 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
```

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

(2,6-diphenyl-1H-indol-3-yl)(phenyl)methanone: 6b

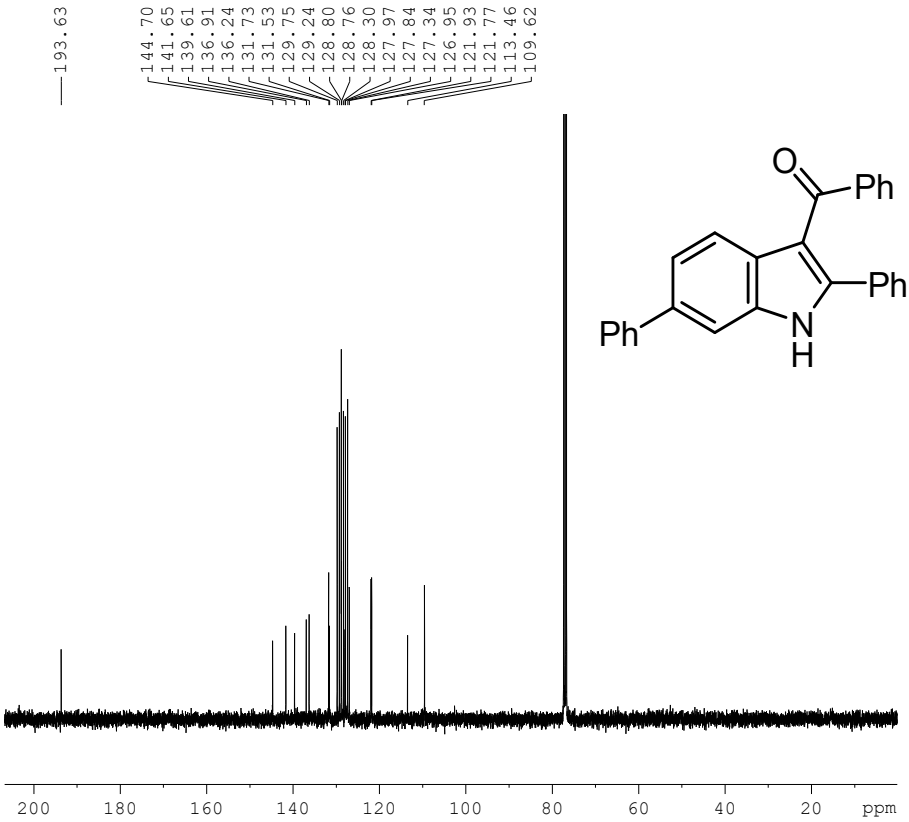



```
Current Data Parameters
NAME                 2152-R
EXPNO                   280
PROCNO                    1

F2 - Acquisition Parameters
Date_             20231124
Time                14.14 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                   293.2 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             400.1300156 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**



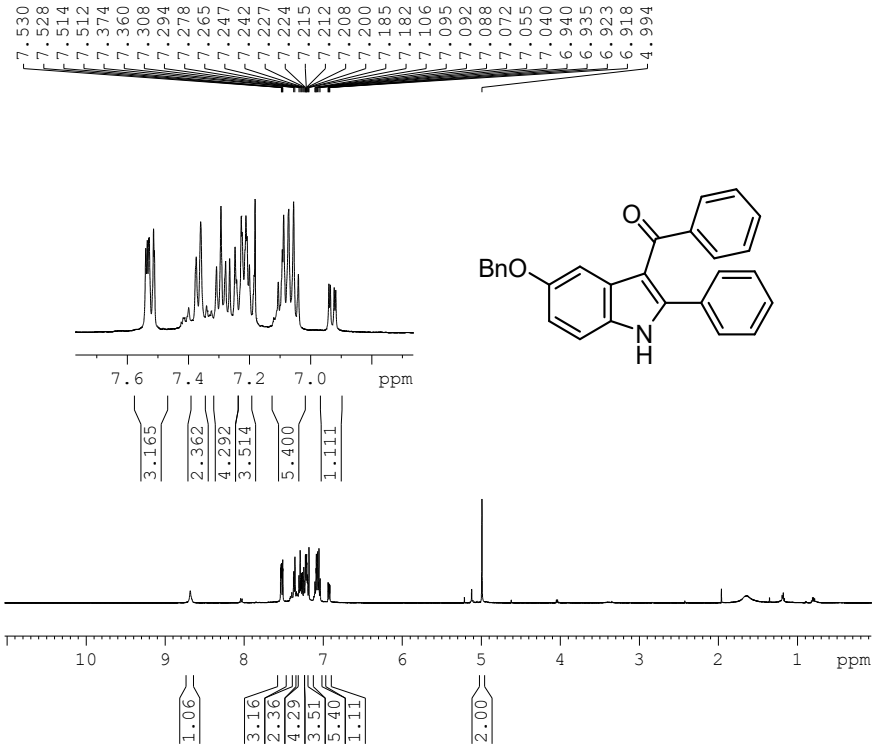

```
Current Data Parameters
NAME                 2152-R
EXPNO                   281
PROCNO                    1

F2 - Acquisition Paramet
Date_             20231124
Time                14.29
INSTRUM              spect
PROBHD    Z129392_0001 (
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     256
DS                       4
SWH              24038.461
FIDRES            0.733596
AQ                1.3631488
RG                   200.34
DW                   20.800
DE                     6.50
TE                   293.5
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 **6b**

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



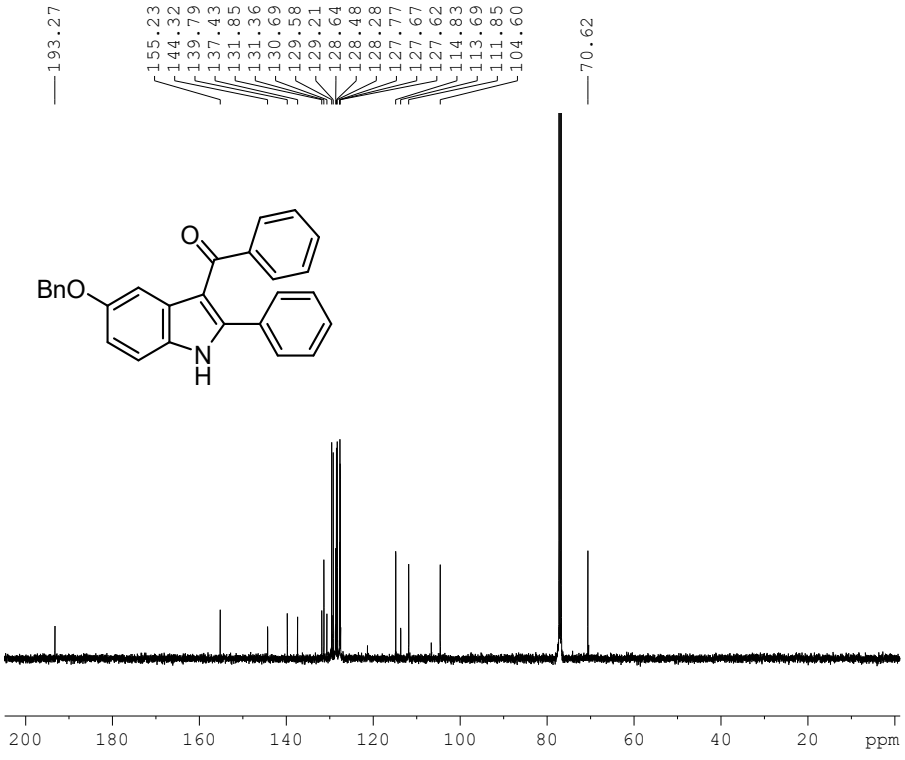

```
Current Data Parameters
NAME          2140-2141
EXPNO                20
PROCNO                1

F2 - Acquisition Parameters
Date_          20231107
Time              22.09
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                162.95
DW                50.000 usec
DE                 6.50 usec
TE                304.7 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           500.1500510 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 **6d**




```
Current Data Parameters
NAME          2140-2141
EXPNO                21
PROCNO                1

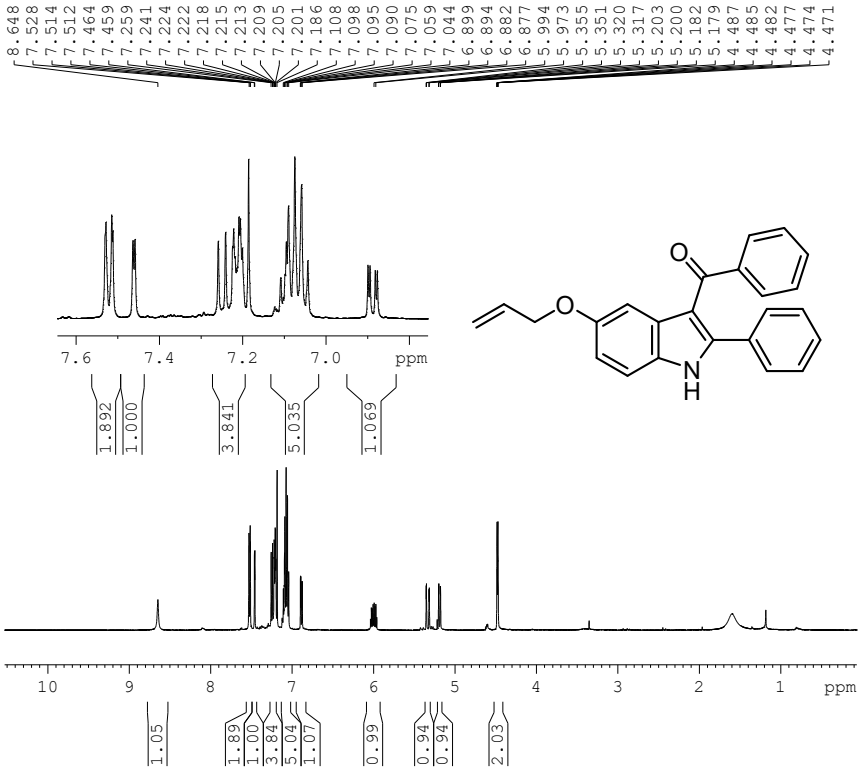
F2 - Acquisition Parameter
Date_          20231107
Time              22.58
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                20480
SOLVENT           CDCl3
NS                 2000
DS                    4
SWH           29761.904 Hz
FIDRES            1.453218 Hz
AQ              0.3440640 se
RG                202.34
DW                16.800 us
DE                 6.50 us
TE                304.9 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
```

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

(5-(allyloxy)-2-phenyl-1H-indol-3-yl)(phenyl)methanone: 6g



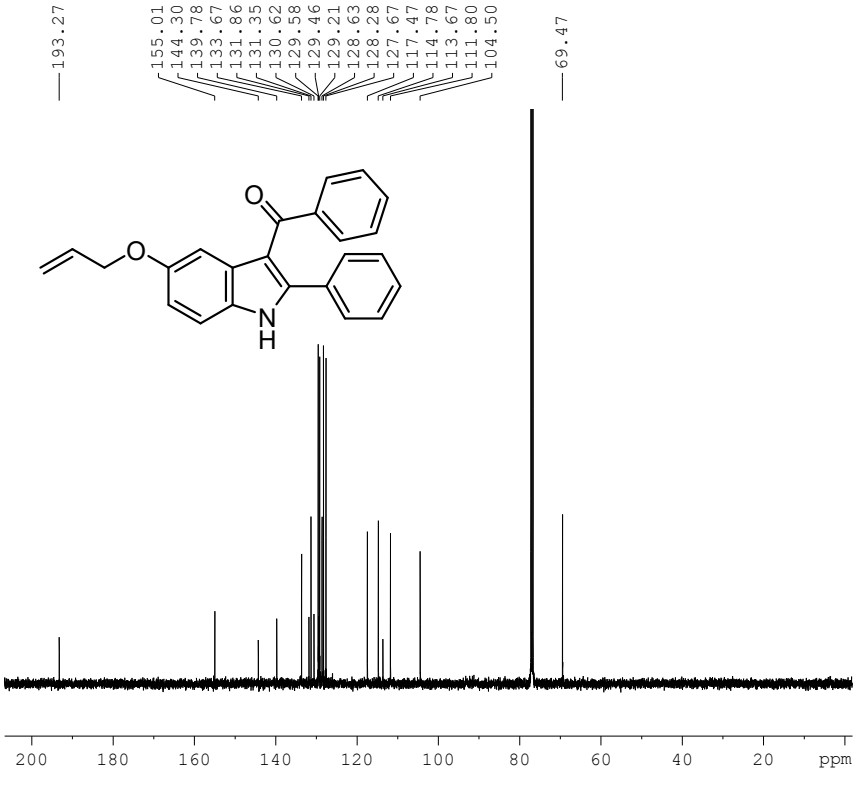

```
Current Data Parameters
NAME          2140-2141
EXPNO                23
PROCNO                1

F2 - Acquisition Parameters
Date_          20231108
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               162.95
DW               50.000 usec
DE                6.50 usec
TE               303.4 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          500.1500485 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 **6g**




```
Current Data Parameters
NAME          2140-2141
EXPNO                24
PROCNO                1

F2 - Acquisition Parameters
Date_          20231108
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               304.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1

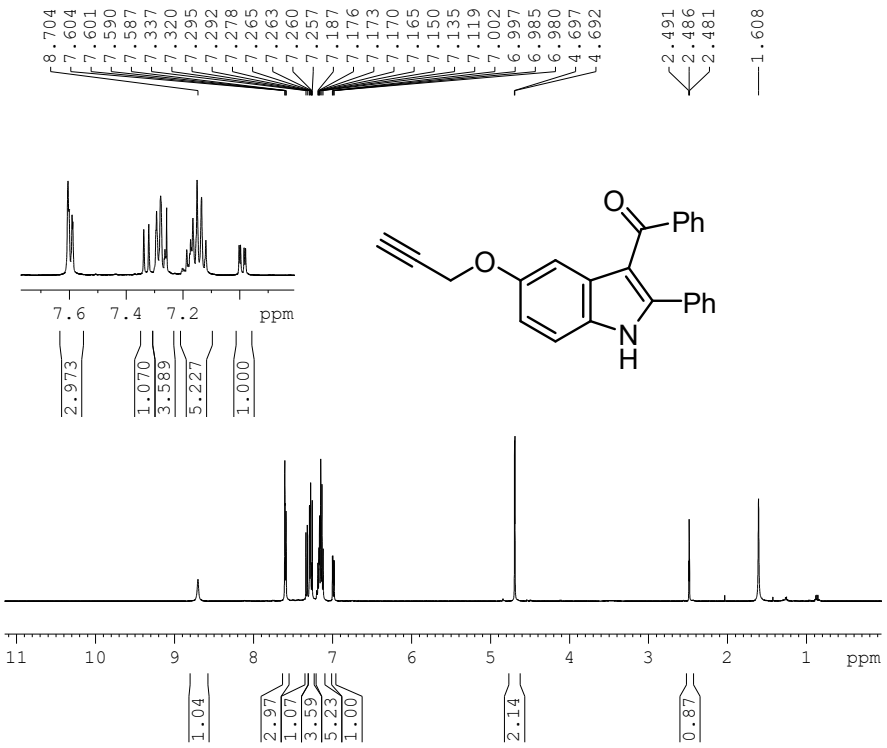
======== CHANNEL f1 ========
SFO1        125.7753932 MHz
NUC1                13C
P1                10.20 usec
PLW1       103.00000000 W

======== 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
```

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

phenyl(2-phenyl-5-(prop-2-yn-1-yloxy)-1H-indol-3-yl)methanone: 6h



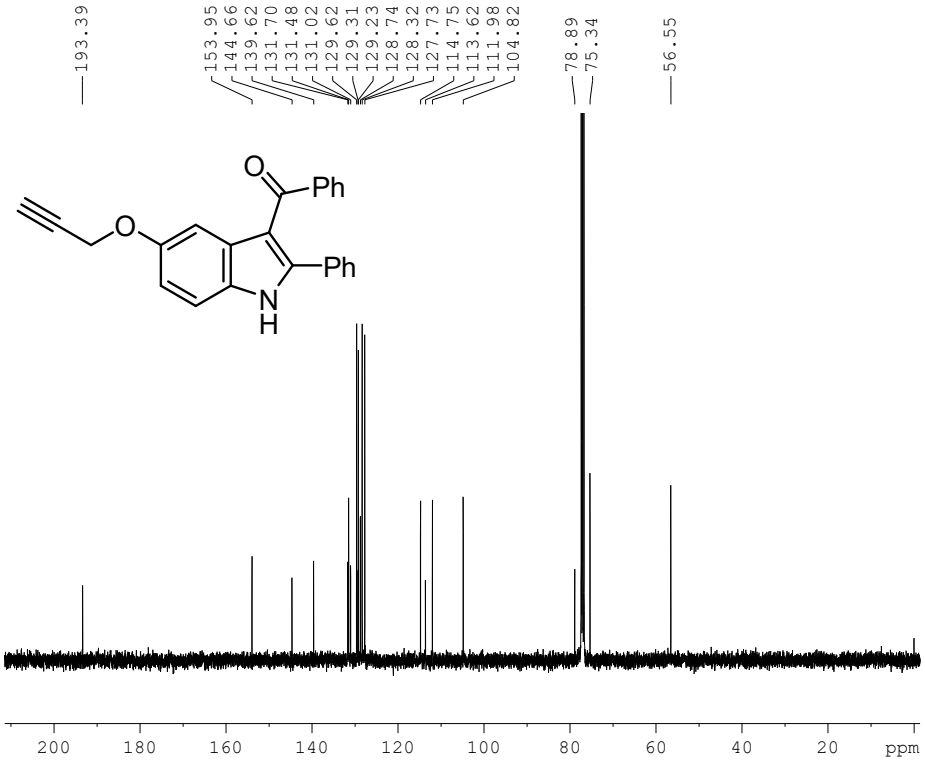

```
Current Data Parameters
NAME                  2160
EXPNO                  108
PROCNO                   1

F2 - Acquisition Parameters
Date_           20231121
Time                16.00
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     16
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                   302.7 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             500.1500130 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 **6h**



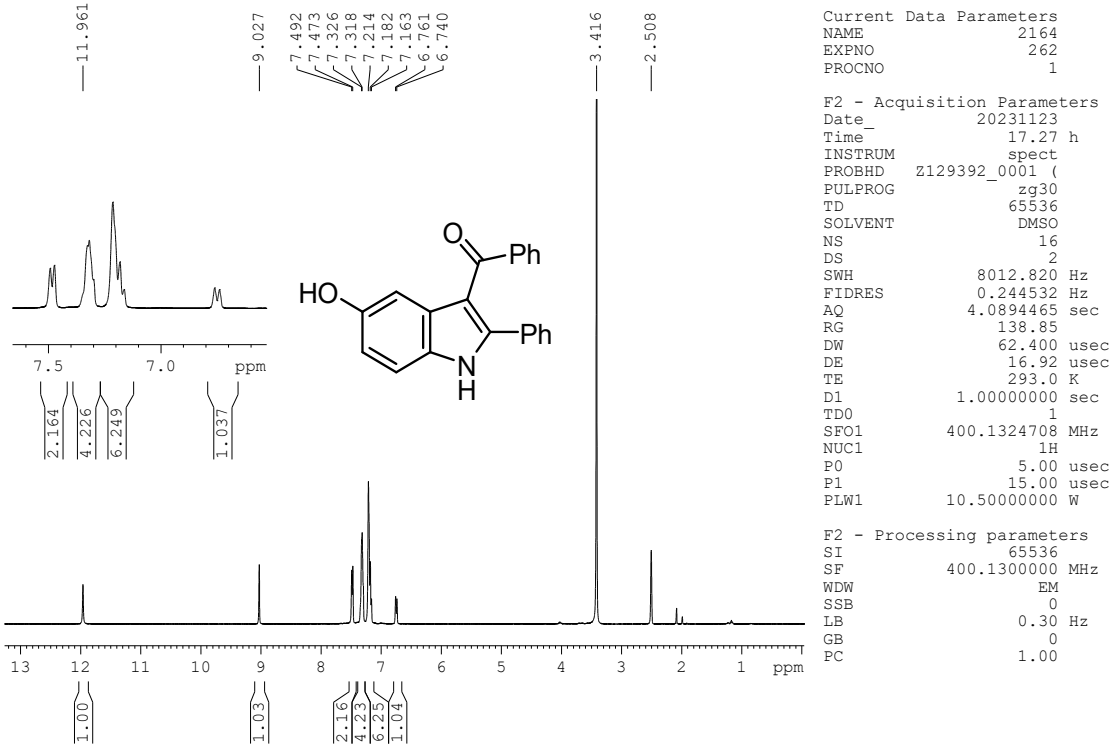

```
Current Data Parameters
NAME                  2160
EXPNO                  271
PROCNO                   1

F2 - Acquisition Parame
Date_           20231124
Time                1.46
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH             24038.461
FIDRES              0.733596
AQ                1.3631488
RG                   200.34
DW                   20.800
DE                    6.50
TE                   293.5
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 paramet
SI                    32768
```

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

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

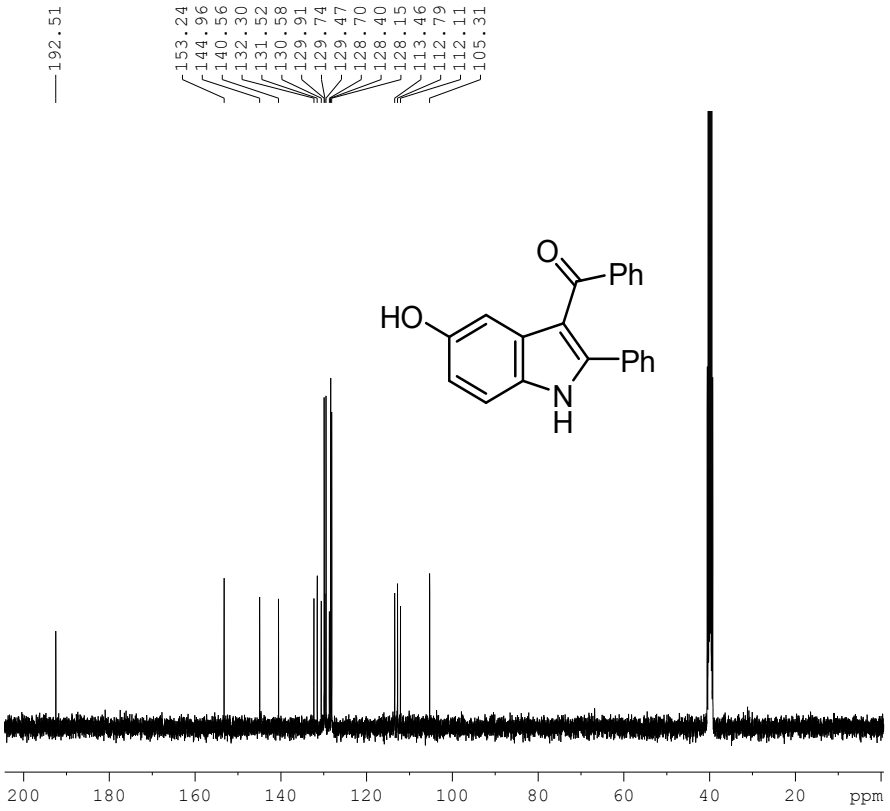


Current Data Parameters
NAME 2164
EXPNO 262
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231123
Time 17.27 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 138.85
DW 62.400 usec
DE 16.92 usec
TE 293.0 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 **6i**



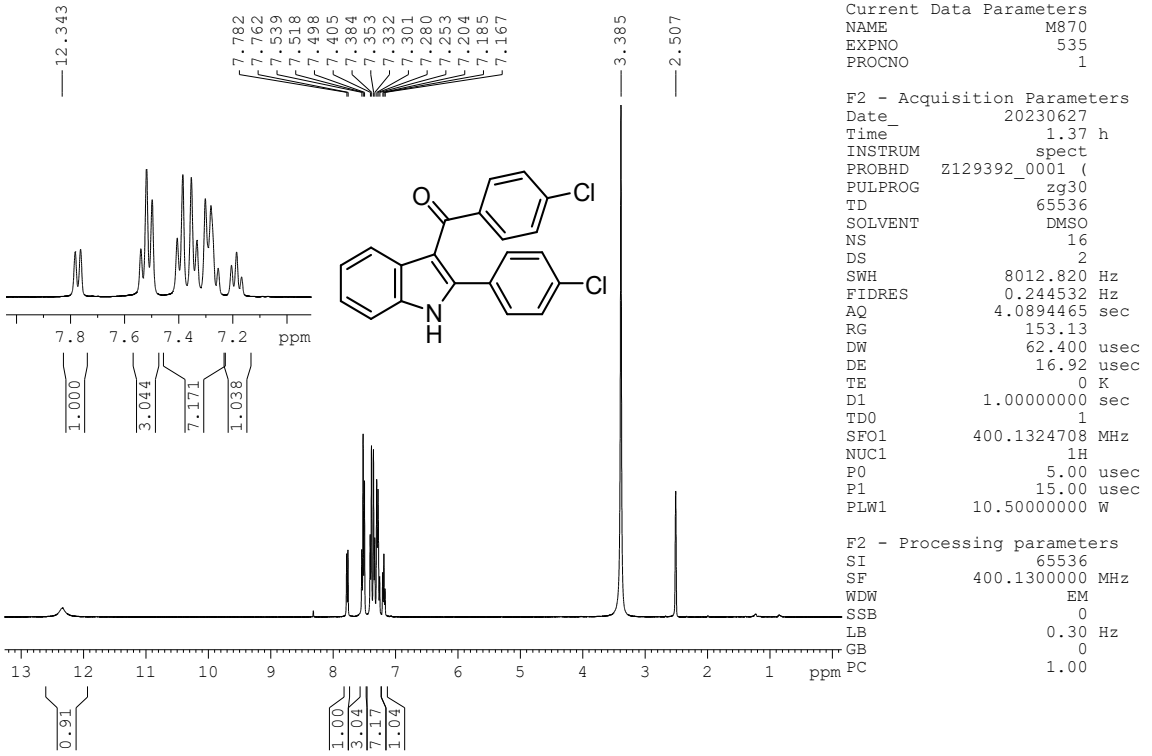
Current Data Parameters
NAME 2164
EXPNO 273
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231124
Time 2.51 h
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 500
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 293.5 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, DMSO-d_6, 24 °C) of the compound **6i**

(4-chlorophenyl)(2-(4-chlorophenyl)-1H-indol-3-yl)methanone: 6m

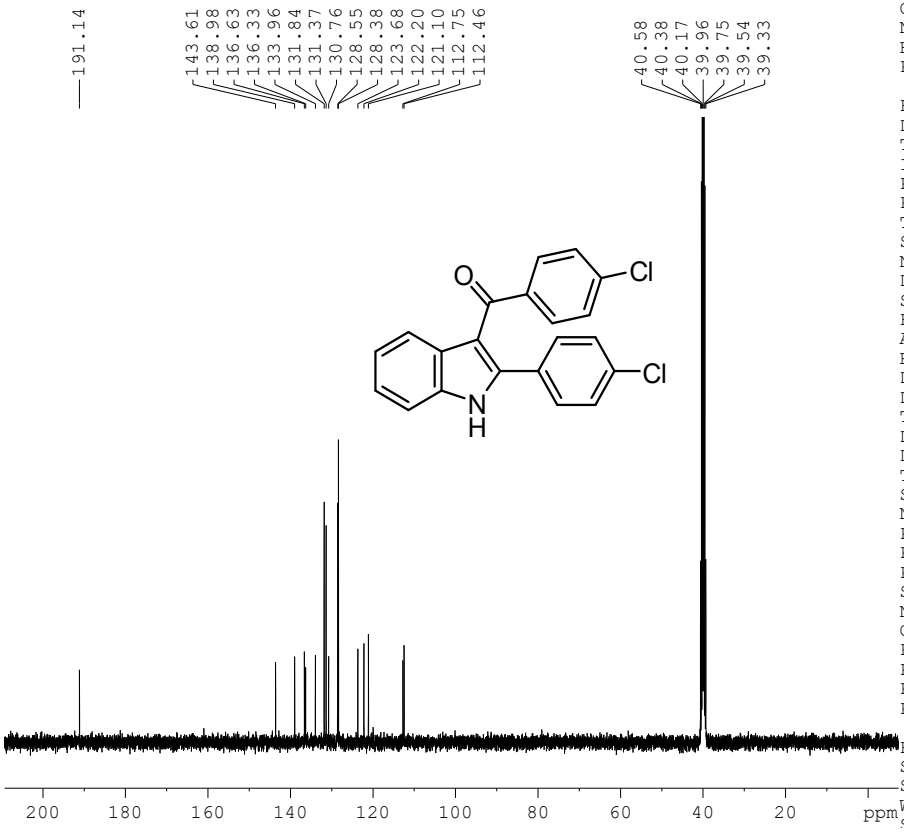


Current Data Parameters
NAME M870
EXPNO 535
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230627
Time 1.37 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 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 **6m**



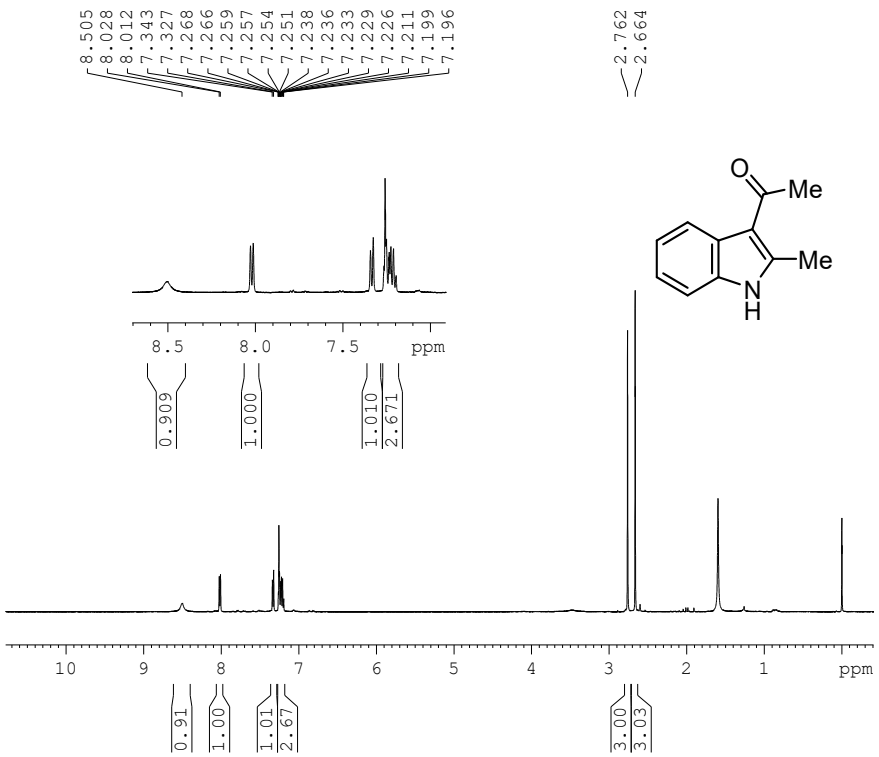
Current Data Parameters
NAME M870
EXPNO 536
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230627
Time 1.53 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 use
DE 6.50 use
TE 0 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
WDW EM
SSB 0

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

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



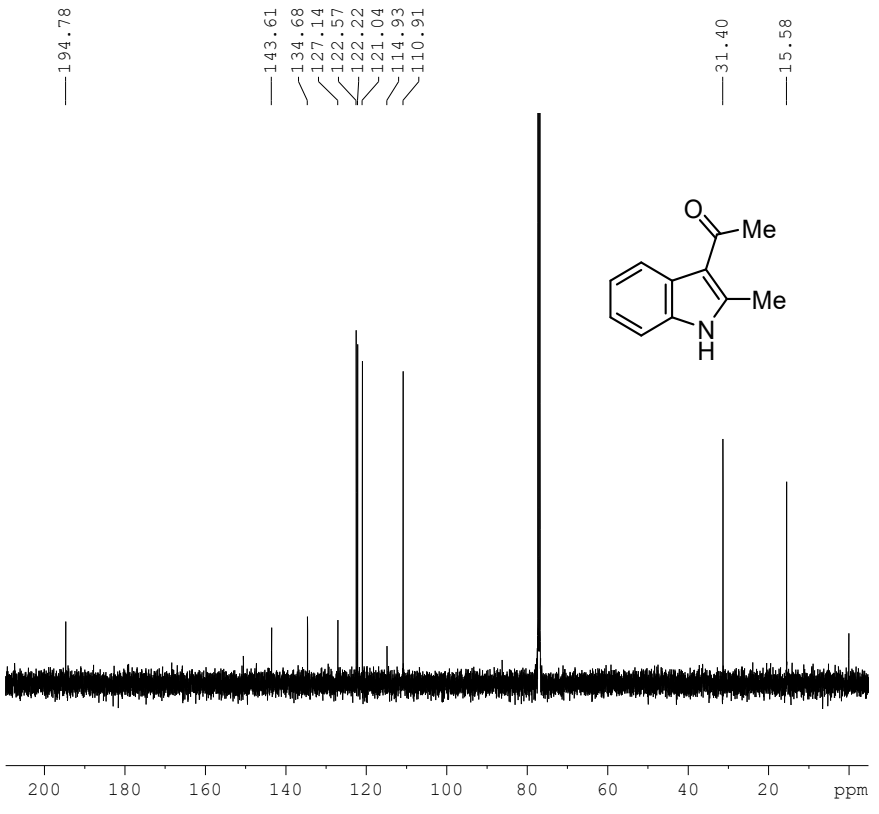
Current Data Parameters
NAME M735
EXPNO 35
PROCNO 1

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 **6o**



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

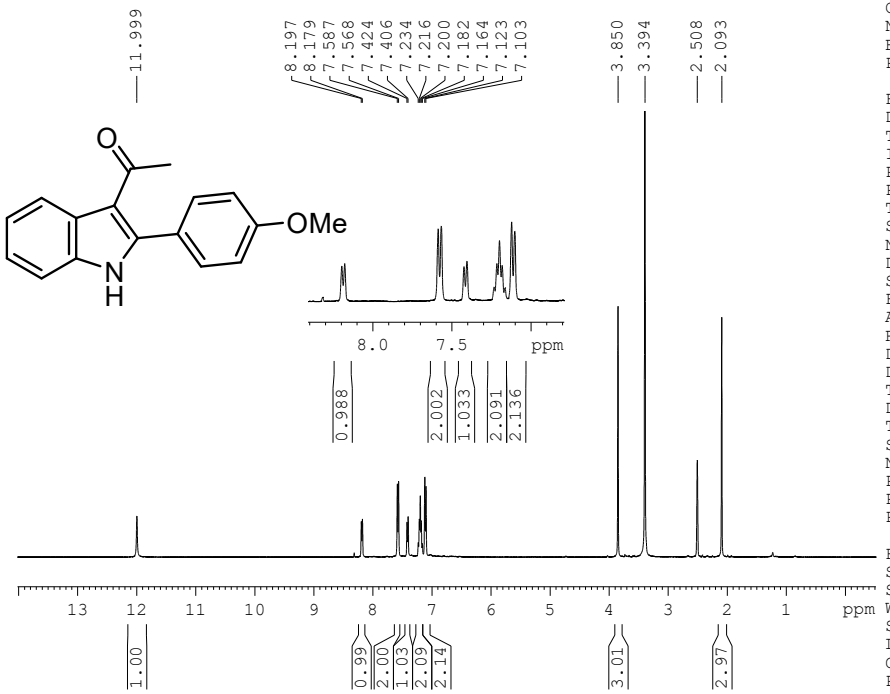
======== CHANNEL f1 ========
SFO1 125.7753932 MHz
NUC1 13C
P1 10.20 usec
PLW1 103.00000000 W

======== 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 **6o**

1-(2-(4-methoxyphenyl)-1H-indol-3-yl)ethan-1-one: 6q

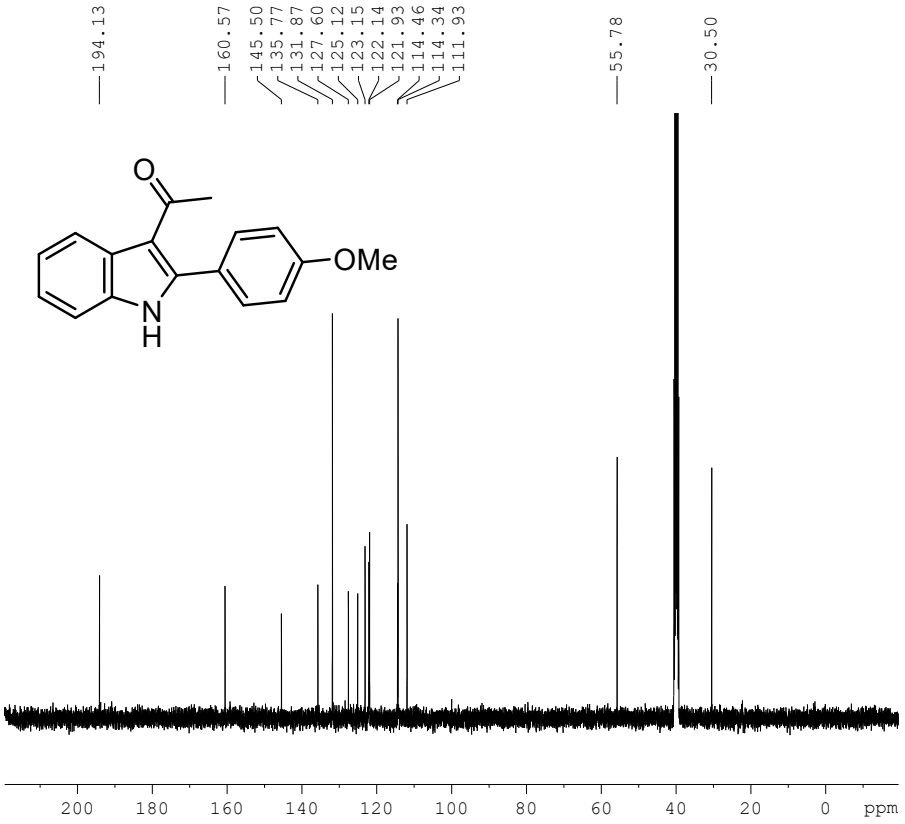



```
Current Data Parameters
NAME             M739(1)
EXPNO                277
PROCNO                 1

F2 - Acquisition Parameter
Date_           20230617
Time                0.20 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8012.820 H
FIDRES          0.244532 H
AQ              4.0894465 s
RG                138.85
DW                62.400 u
DE                16.92 u
TE                295.1 K
D1             1.00000000 s
TD0                    1
SFO1         400.1324708 M
NUC1                  1H
P0                 5.00 u
P1                15.00 u
PLW1         10.50000000 W

F2 - Processing parameter
SI                 65536
SF          400.1300000 M
WDW                   EM
SSB                    0
LB                 0.30 H
GB                     0
PC                  1.00
```

^{1}H NMR (400 MHz, DMSO-d$_6$, 24 °C) of the compound **6q**



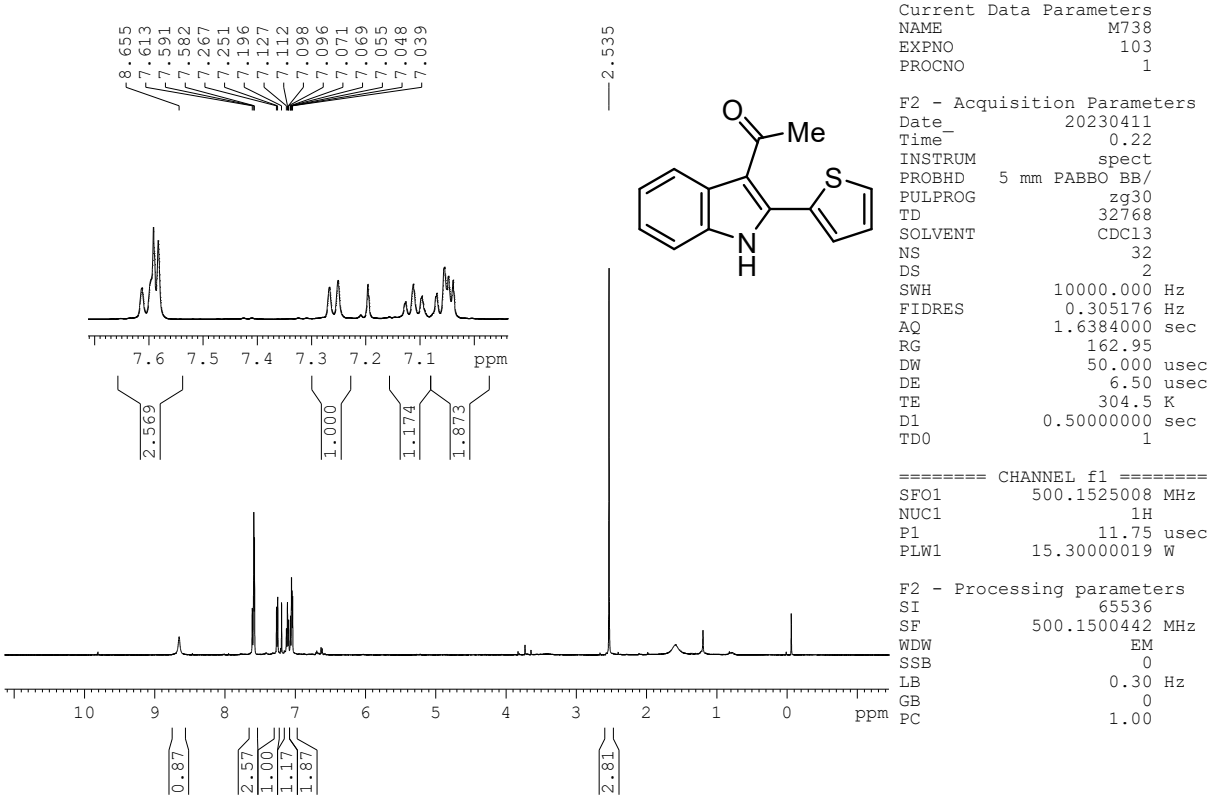

```
Current Data Parameters
NAME             M739(1)
EXPNO                310
PROCNO                 1

F2 - Acquisition Parameter
Date_           20230617
Time                3.44 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 se
RG                200.34
DW                20.800 us
DE                 6.50 us
TE                295.5 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
```

^{13}C{^{1}H} NMR (100 MHz, DMSO-d$_6$, 24 °C) of the compound **6q**

1-(2-(thiophen-2-yl)-1H-indol-3-yl)ethan-1-one: 6r



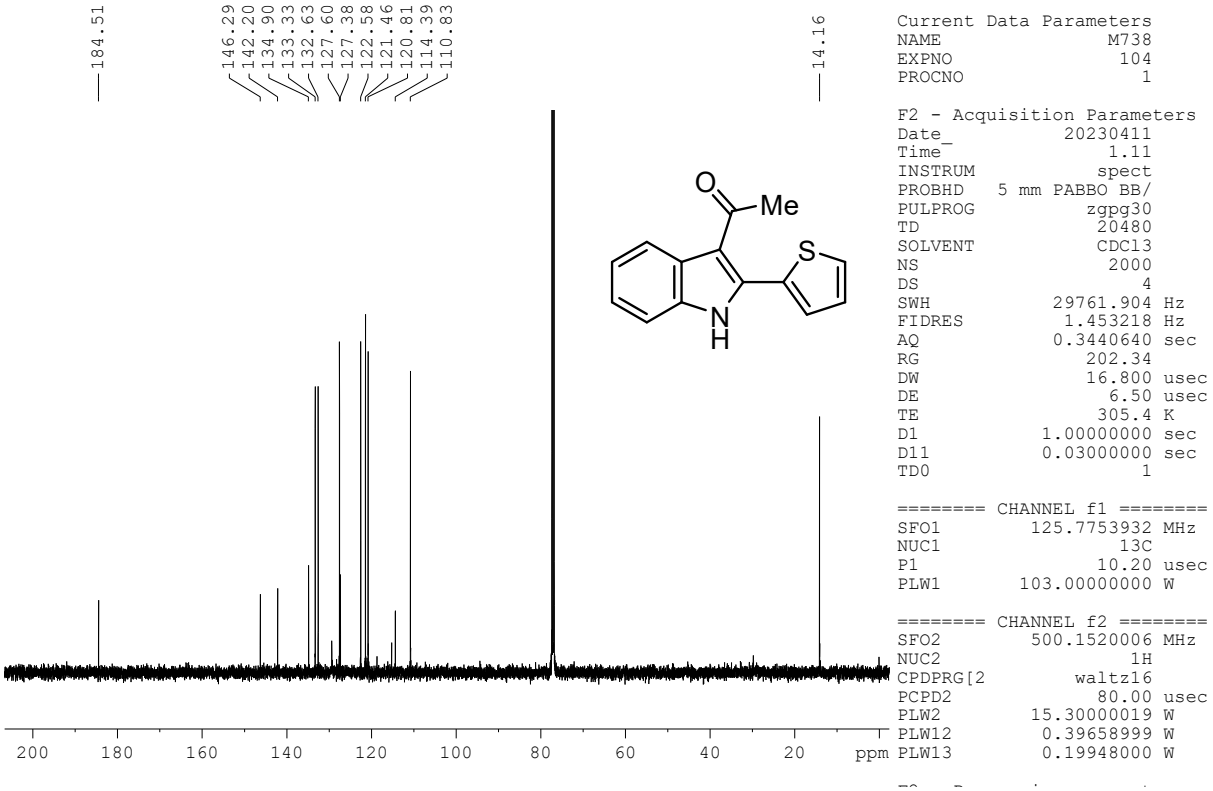

```
Current Data Parameters
NAME                  M738
EXPNO                  103
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230411
Time                   0.22
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                   162.95
DW                   50.000 usec
DE                    6.50 usec
TE                   304.5 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             500.1500442 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 **6r**




```
Current Data Parameters
NAME                  M738
EXPNO                  104
PROCNO                   1

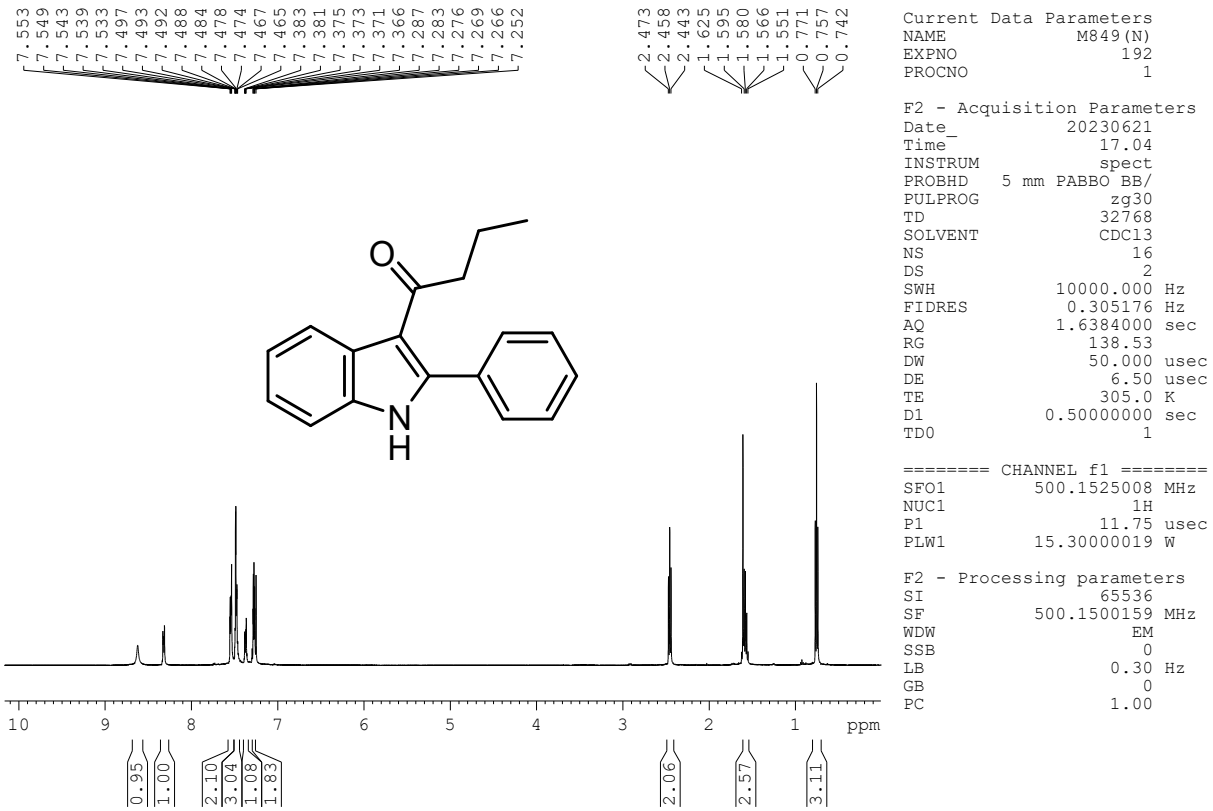
F2 - Acquisition Parameters
Date_              20230411
Time                   1.11
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    20480
SOLVENT               CDCl3
NS                     2000
DS                        4
SWH               29761.904 Hz
FIDRES             1.453218 Hz
AQ                0.3440640 sec
RG                   202.34
DW                   16.800 usec
DE                    6.50 usec
TE                   305.4 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 **6r**

1-(2-phenyl-1H-indol-3-yl)butan-1-one: 6s



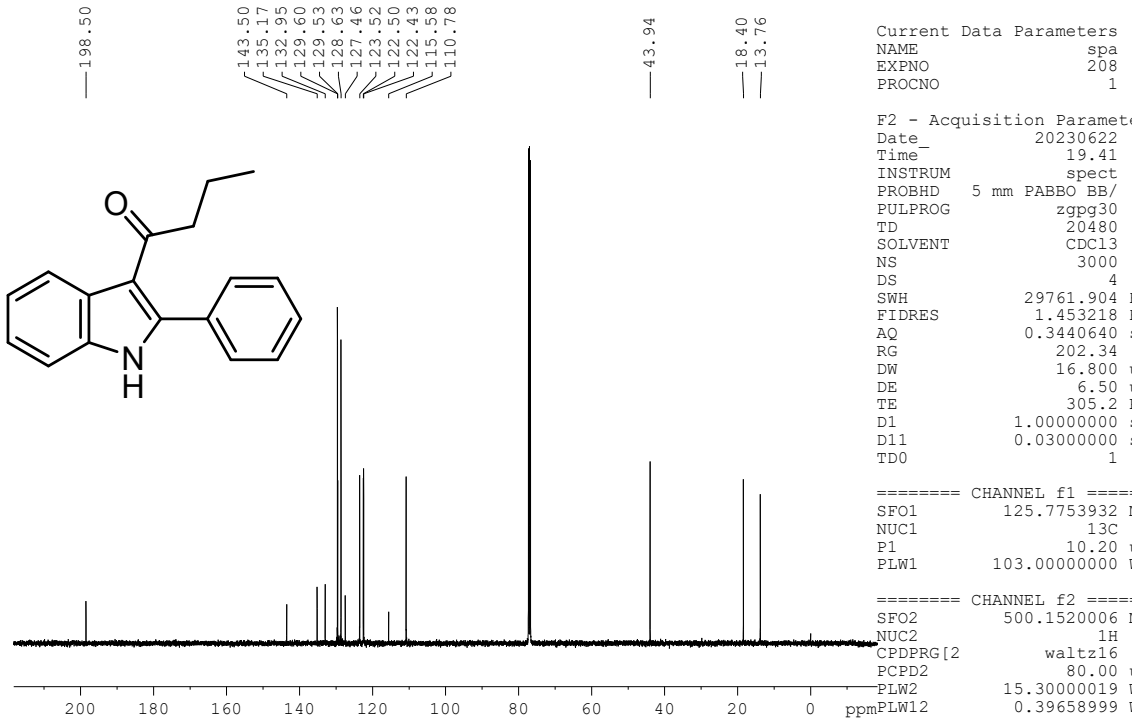

```
Current Data Parameters
NAME              M849(N)
EXPNO                 192
PROCNO                  1

F2 - Acquisition Parameters
Date_           20230621
Time               17.04
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ            1.6384000 sec
RG                138.53
DW                50.000 usec
DE                 6.50 usec
TE                305.0 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           500.1500159 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 **6s**




```
Current Data Parameters
NAME                 spa
EXPNO                208
PROCNO                 1

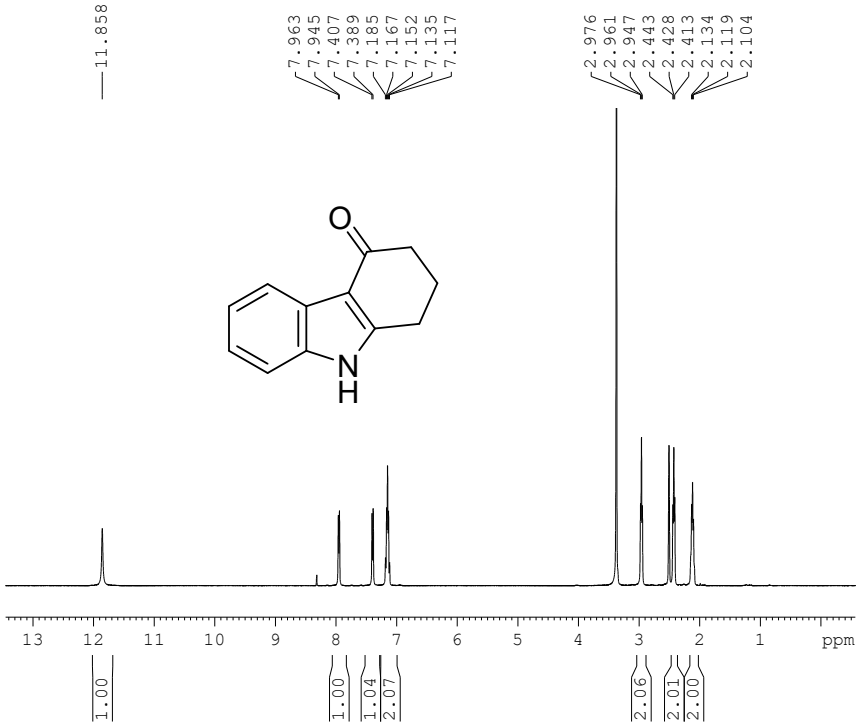
F2 - Acquisition Paramet
Date_           20230622
Time               19.41
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 20480
SOLVENT            CDCl3
NS                  3000
DS                     4
SWH           29761.904 H
FIDRES         1.453218 H
AQ            0.3440640 s
RG                202.34
DW                16.800 u
DE                 6.50 u
TE                305.2 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
```

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

1,2,3,9-tetrahydro-4H-carbazol-4-one: 6t

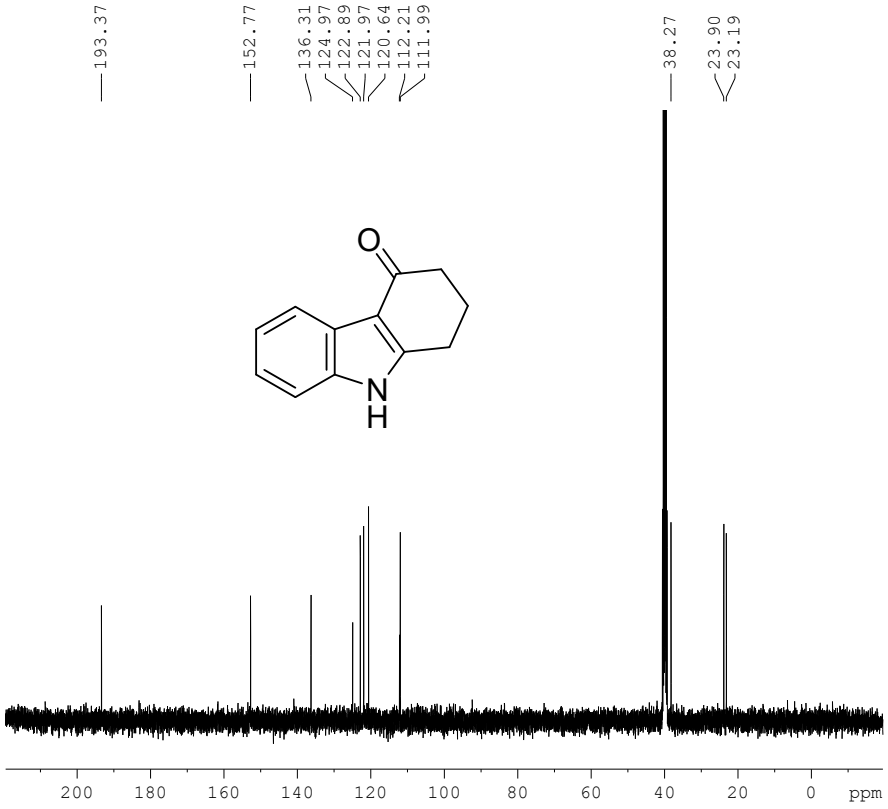



```
Current Data Parameters
NAME                  M795
EXPNO                  231
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230529
Time                 17.23 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                  295.8 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 **6t**



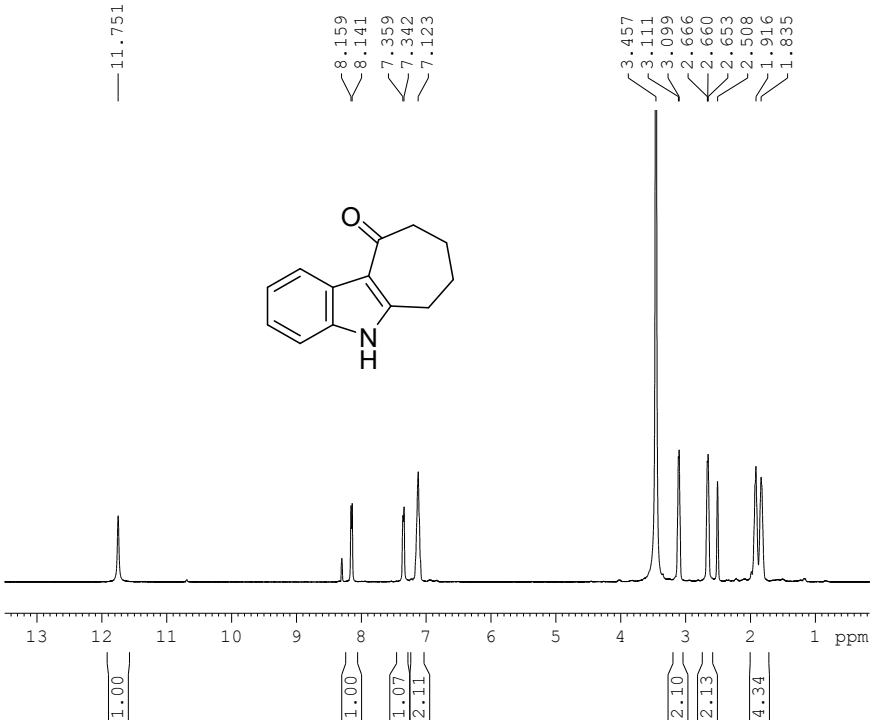

```
Current Data Parameters
NAME                  M795
EXPNO                  232
PROCNO                   1

F2 - Acquisition Parameter
Date_              20230529
Time                 17.31 h
INSTRUM              spect
PROBHD   Z129392_0001 (
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                      128
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                  296.2 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
```

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

6,7,8,9-tetrahydrocyclohepta[b]indol-10(5H)-one: 6u

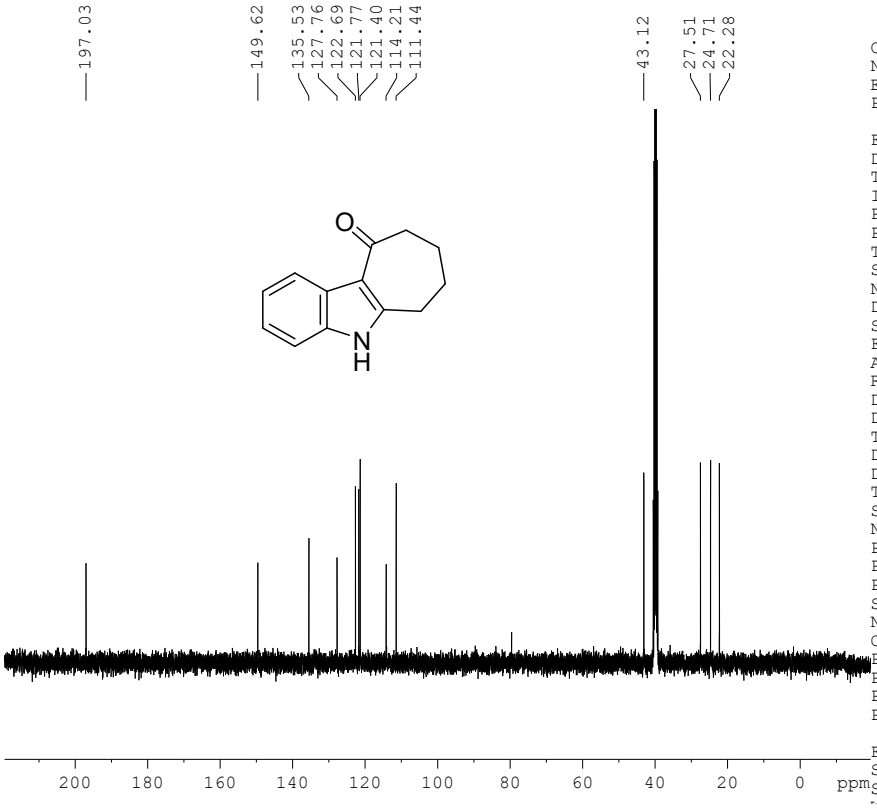



```
Current Data Parameters
NAME                  M787
EXPNO                  187
PROCNO                   1

F2 - Acquisition Parameters
Date_            20230526
Time                20.22 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                  88.51
DW                62.400 usec
DE                16.92 usec
TE                296.3 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 **6u**



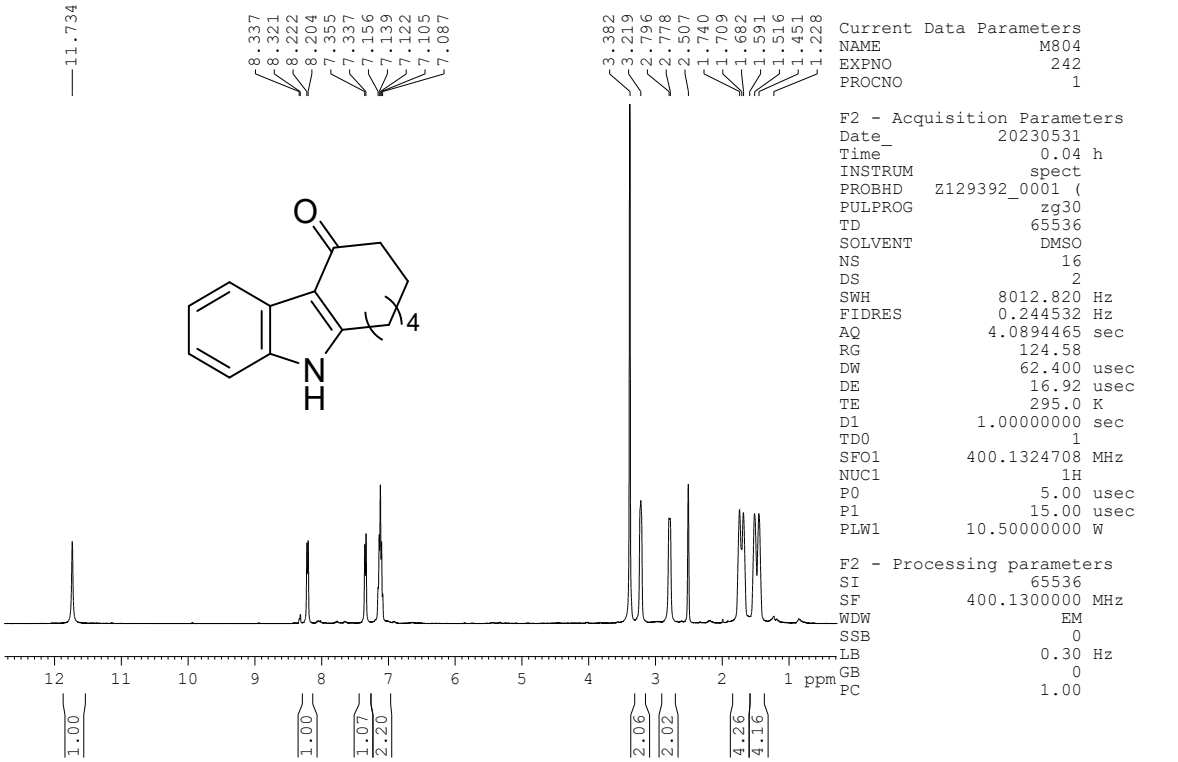

```
Current Data Parameters
NAME                  M787
EXPNO                  188
PROCNO                   1

F2 - Acquisition Parameters
Date_            20230526
Time                20.30 h
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG            zgpg30
TD                  65536
SOLVENT              DMSO
NS                    115
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                296.7 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

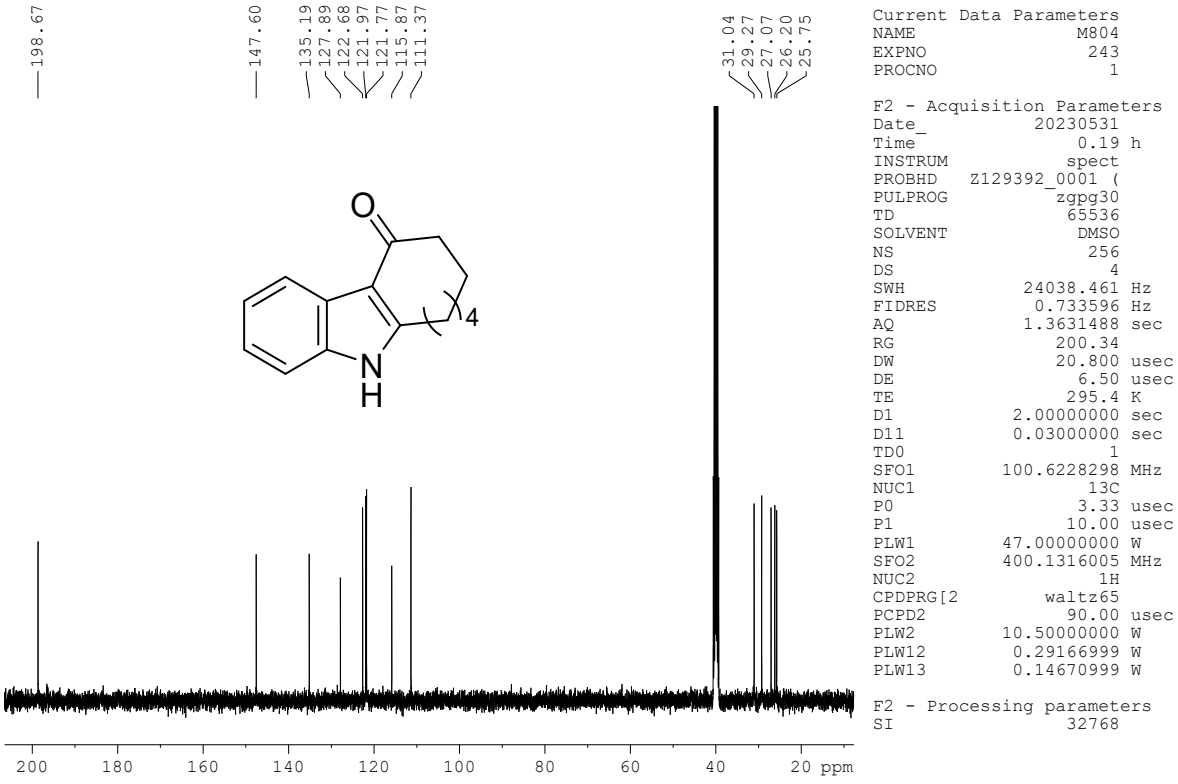
F2 - Processing parameters
SI                  32768
SF            100.6127685 MHz
```

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

6,7,8,9,10,11-hexahydrocyclonona[b]indol-12(5H)-one: 6v

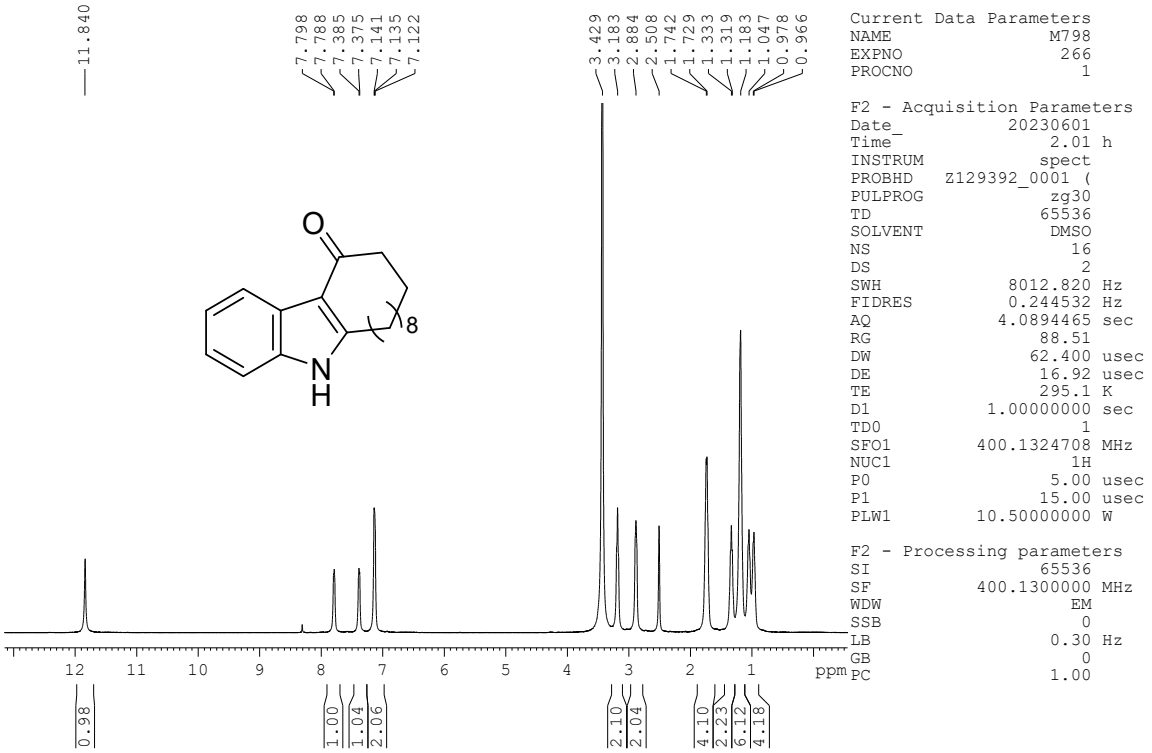


^{1}H NMR (400 MHz, DMSO-d_6, 24 °C) of the compound **6v**

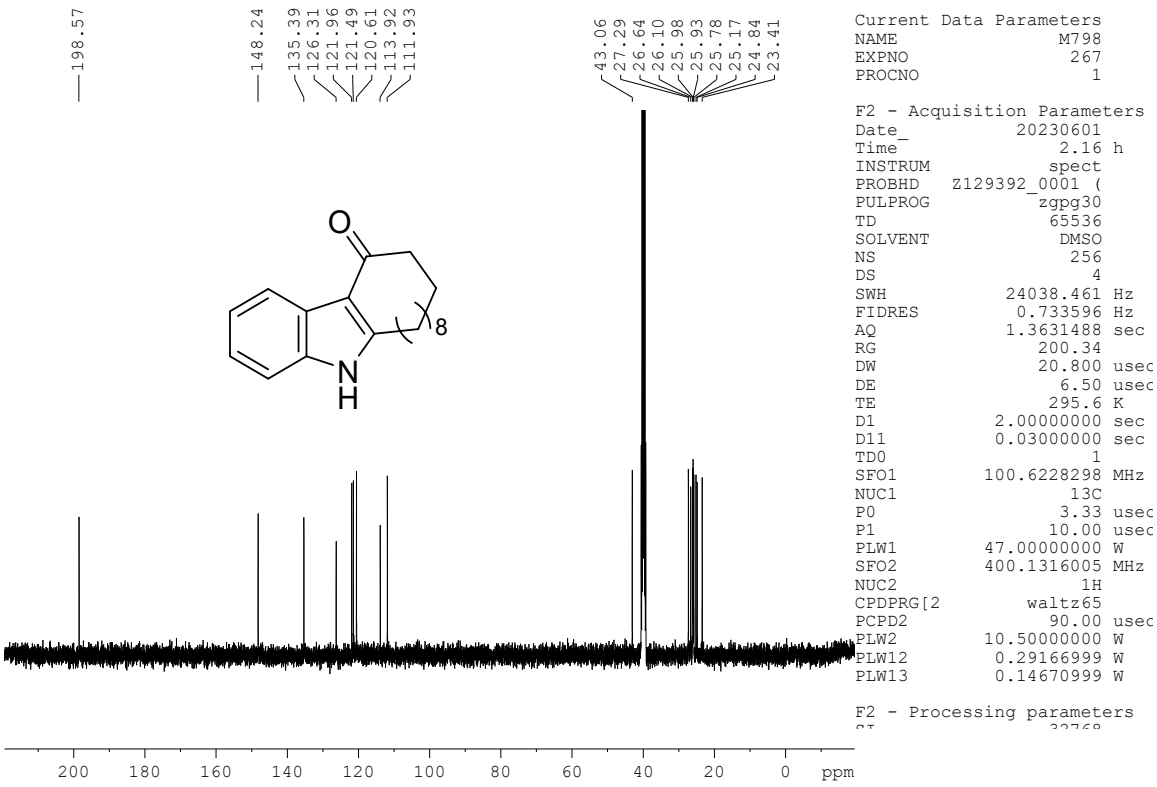


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C) of the compound **6v**

6,7,8,9,10,11,12,13,14,15-decahydrocyclotrideca[b]indol-16(5H)-one: 6w

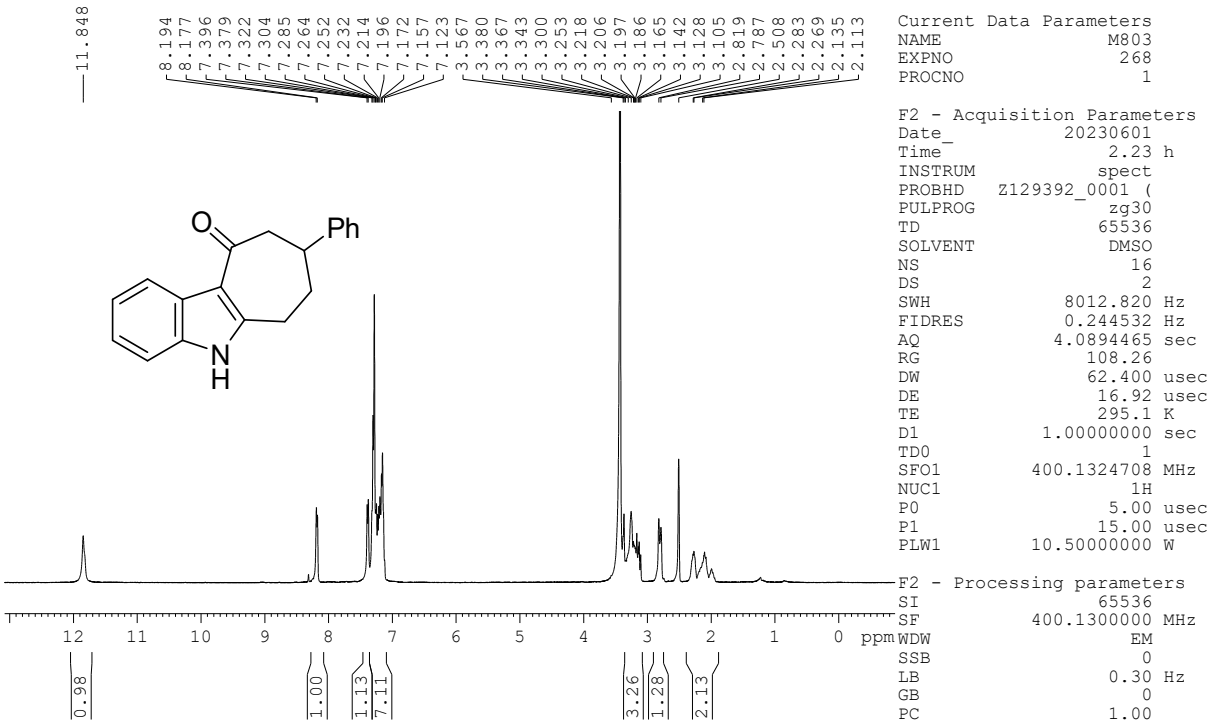


^{1}H NMR (400 MHz, DMSO-d_6, 24 °C) of the compound **6w**

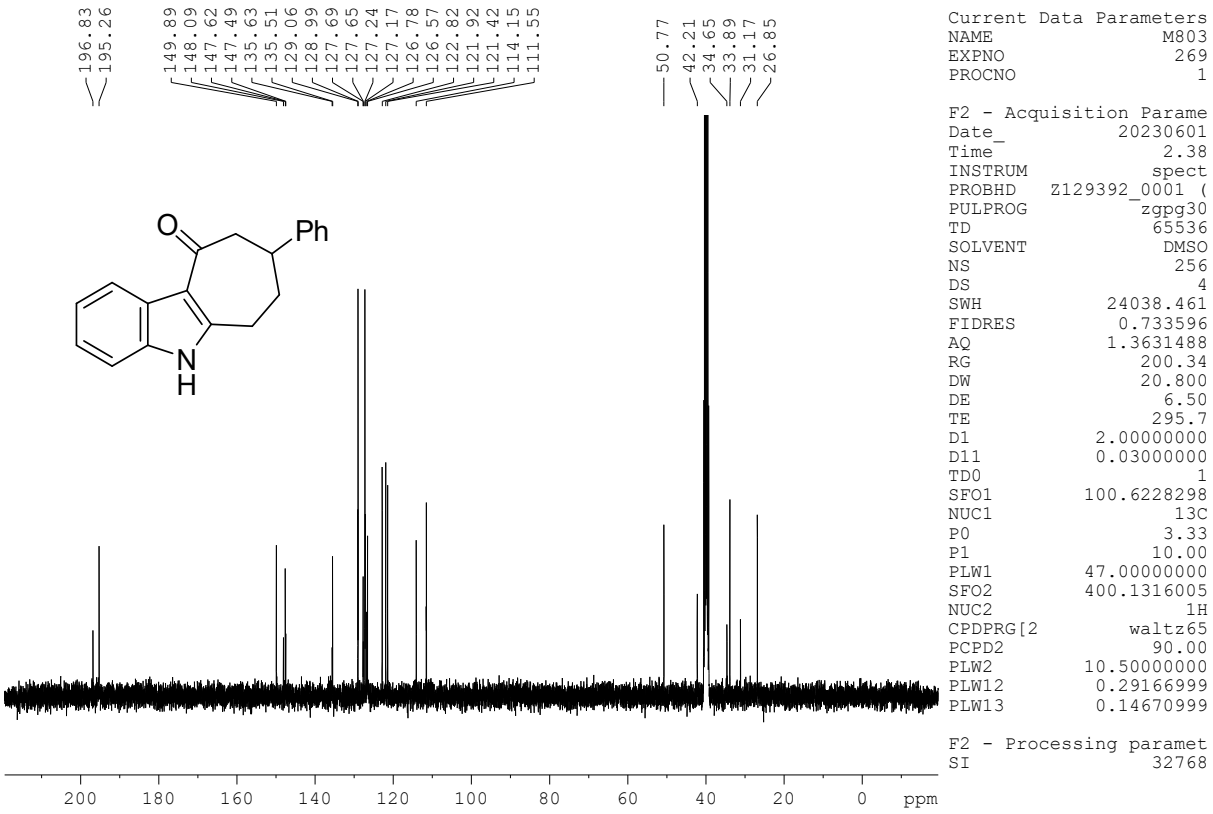


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C) of the compound **6w**

8-phenyl-6,7,8,9-tetrahydrocyclohepta[b]indol-10(5H)-one: 6x

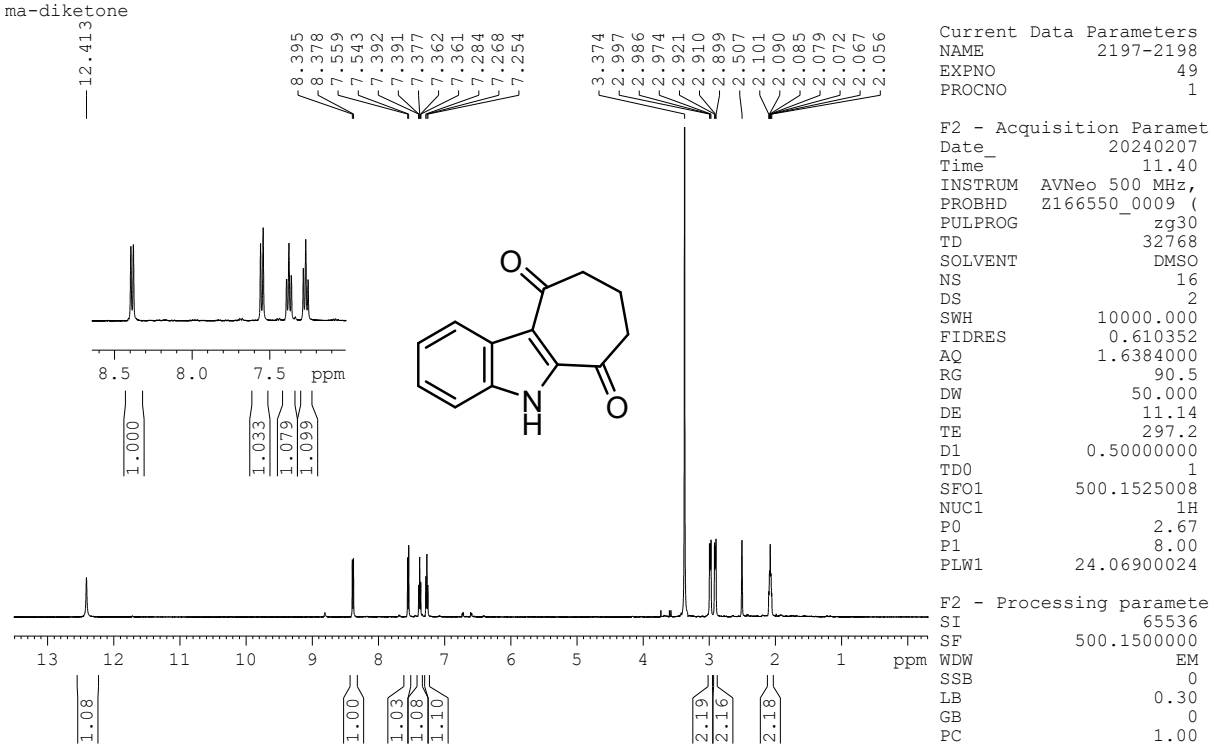


^{1}H NMR (400 MHz, DMSO-d_6, 24 °C) of the compound **6x**

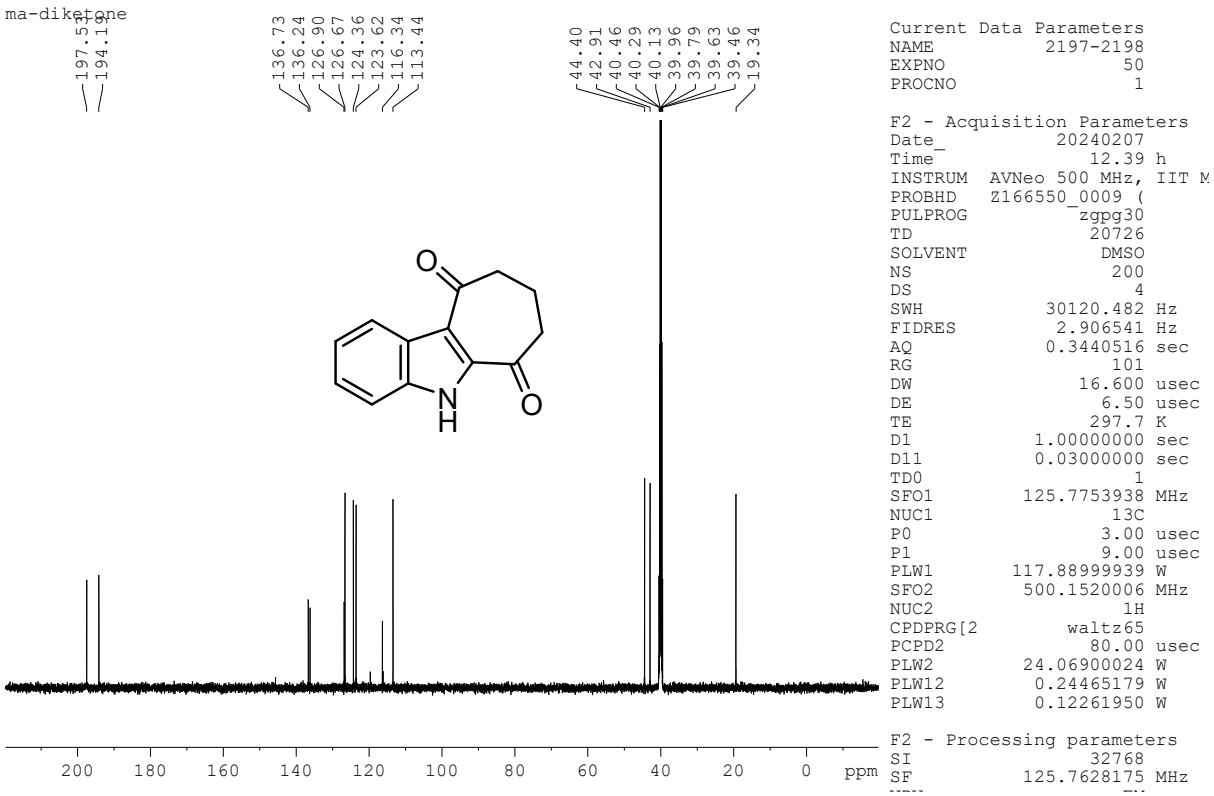


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, 24 °C) of the compound **6x**

8,9-dihydrocyclohepta[b]indole-6,10(5H,7H)-dione: 6y

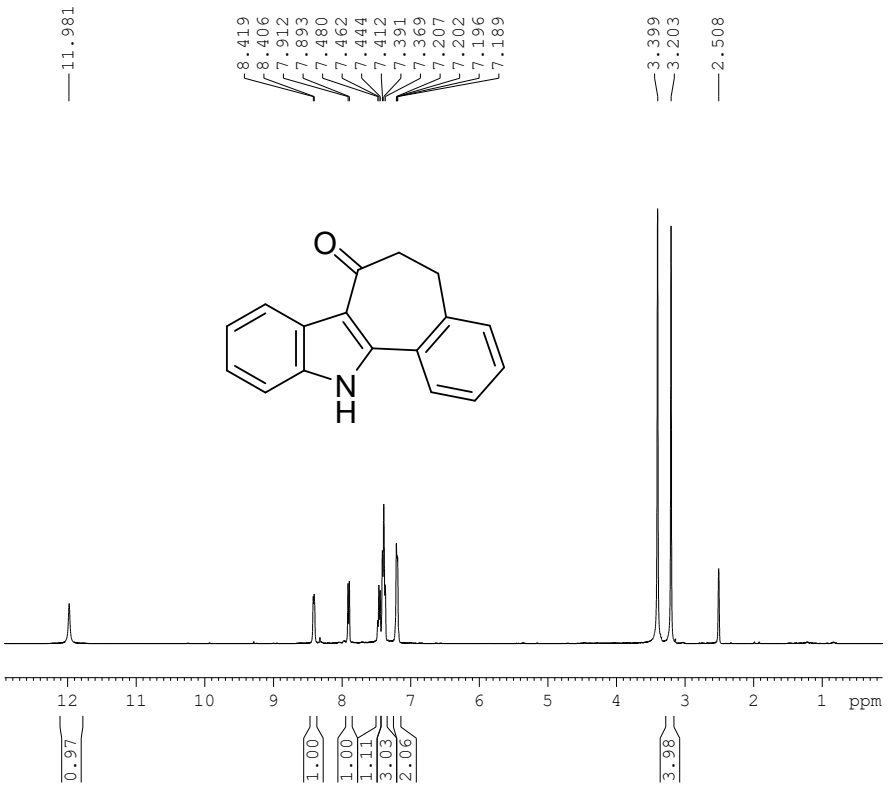


^{1}H NMR (500 MHz, DMSO-d_6, 24 °C) of the compound **6y**



^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6, 24 °C) of the compound **6y**

5,12-dihydrobenzo[6,7]cyclohepta[1,2-b]indol-7(6H)-one: 6z

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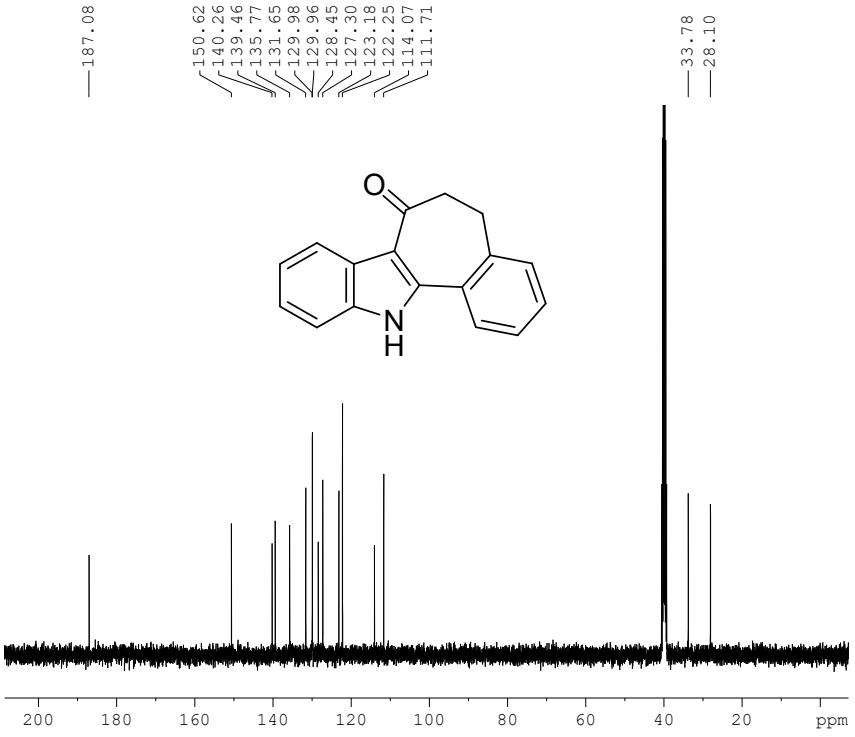
Current Data Parameters
NAME                  M792
EXPNO                  217
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230528
Time                 22.59 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                   295.5 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           400.1300000 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 **6z**



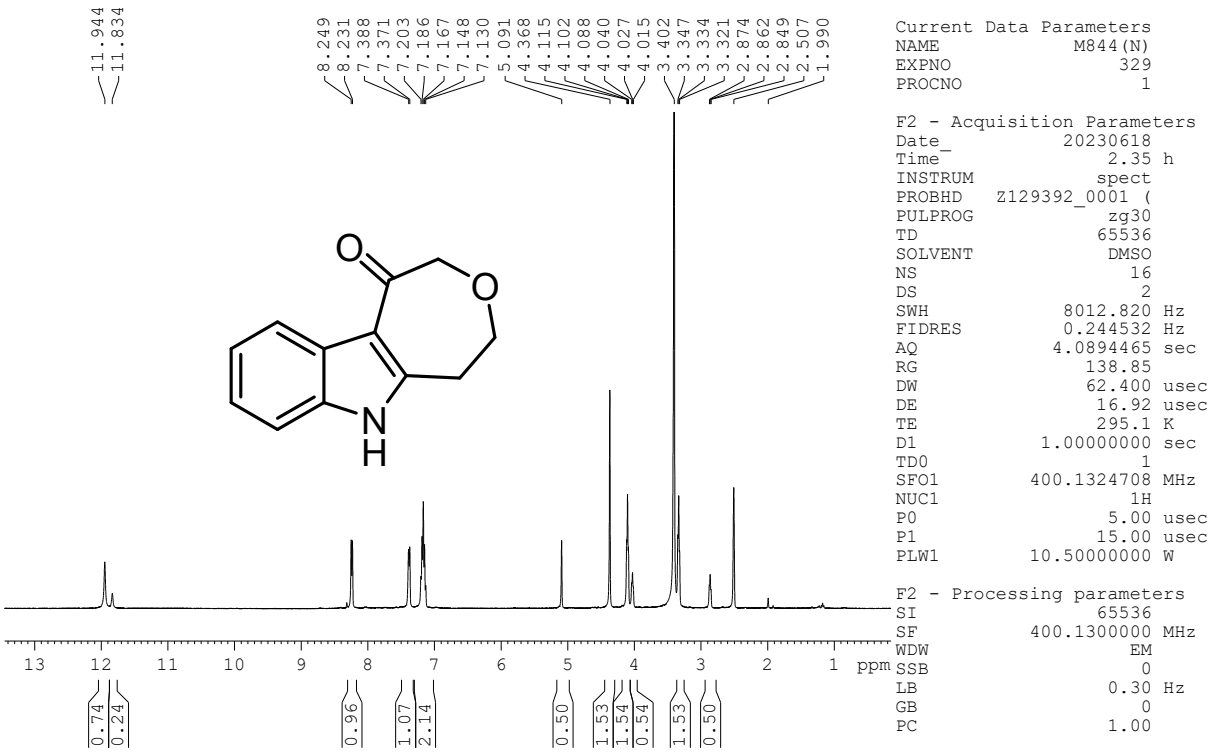

```
Current Data Parameters
NAME                  M792
EXPNO                  218
PROCNO                   1

F2 - Acquisitio Paramete
Date_              20230528
Time                 23.09 h
INSTRUM              spect
PROBHD   Z129392_0001 (
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                     160
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                   295.9 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

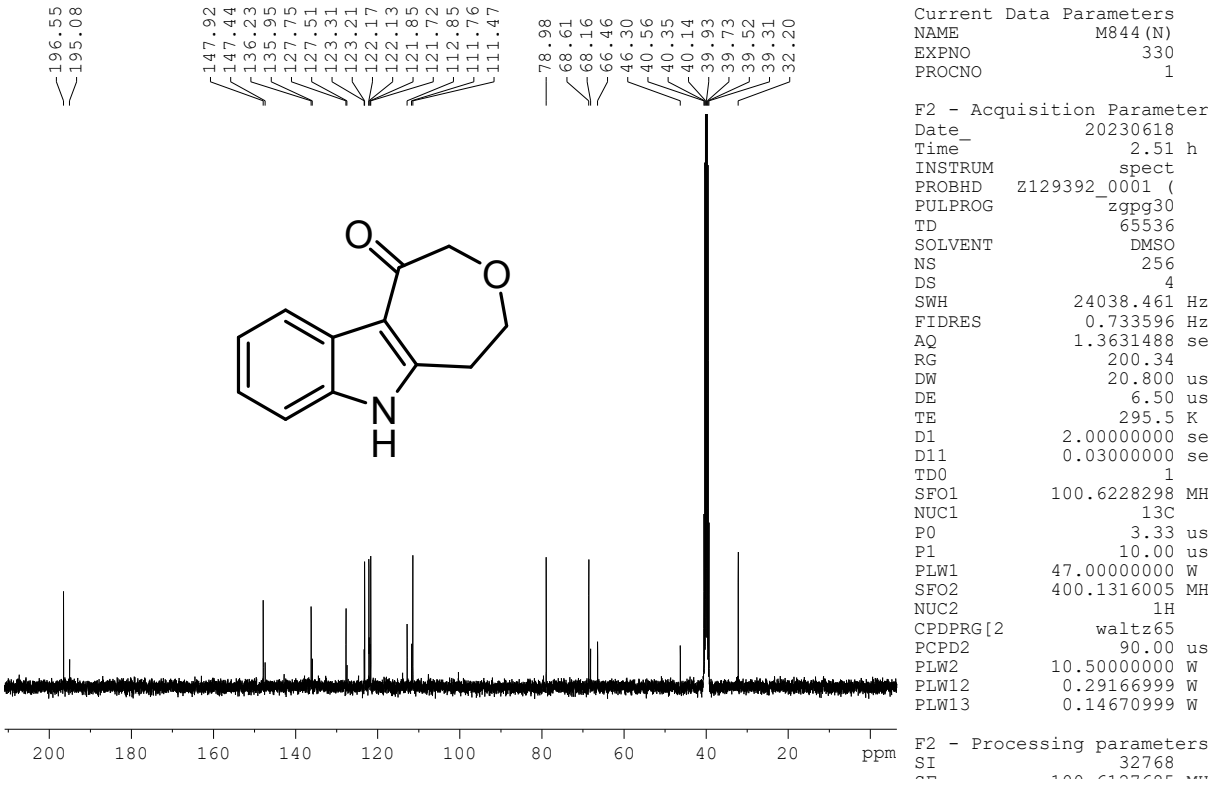
F2 - Processing parameter
SI                   32768
```

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

5,6-dihydro-2H-oxepino[4,5-b]indol-1(4H)-one: 6aa

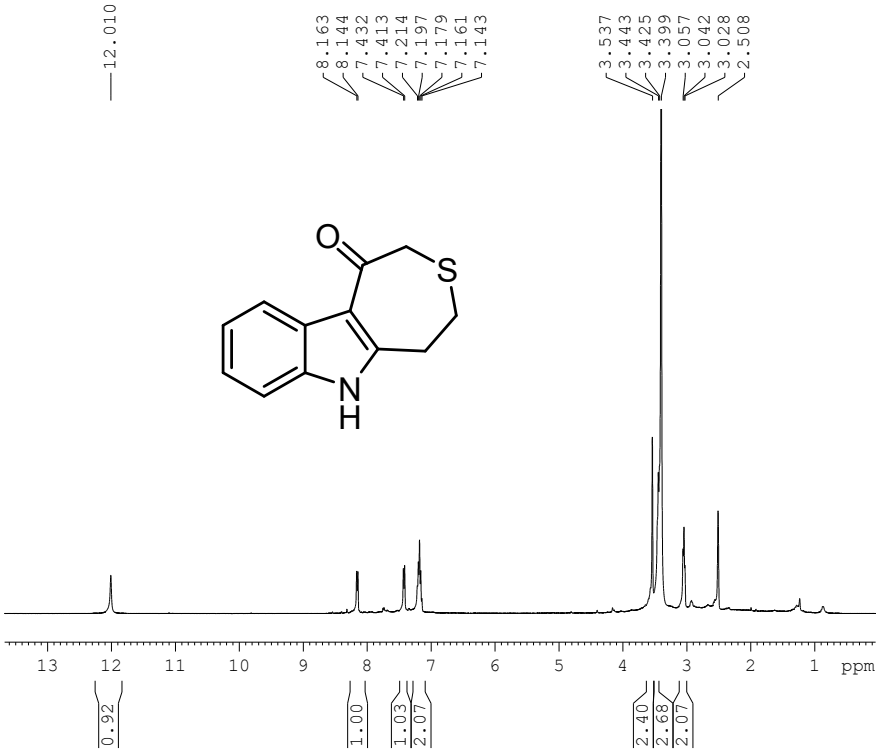


^{1}H NMR (400 MHz, DMSO-d_6, 24 °C) of the compound **6aa**



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

5,6-dihydro-2H-thiepino[4,5-b]indol-1(4H)-one: 6ab

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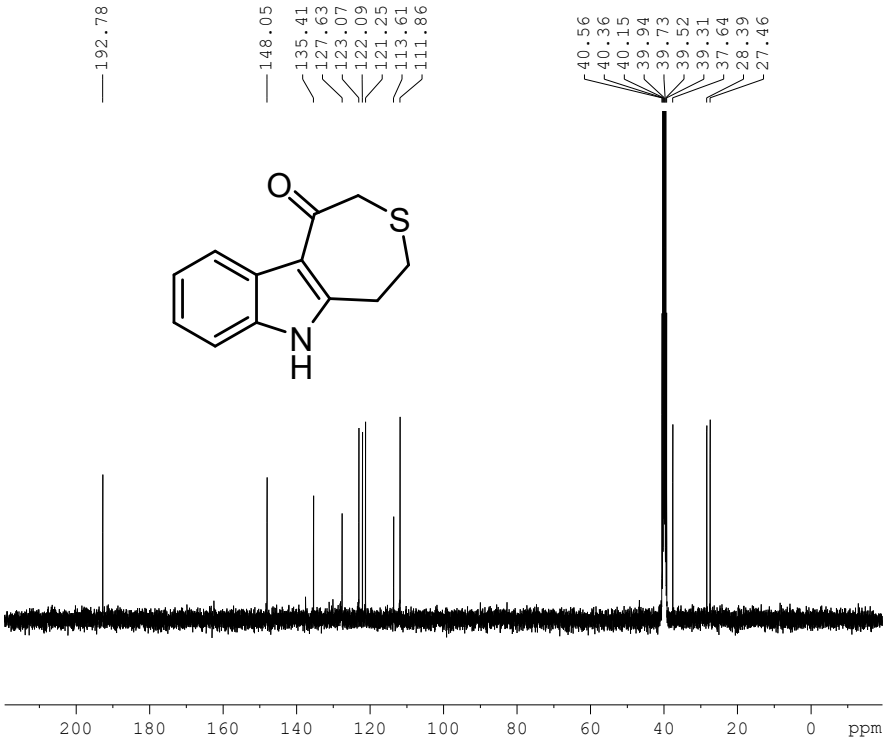
Current Data Parameters
NAME           M841(NMR)
EXPNO                308
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230617
Time                0.58 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                 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          400.1300000 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 **6ab**



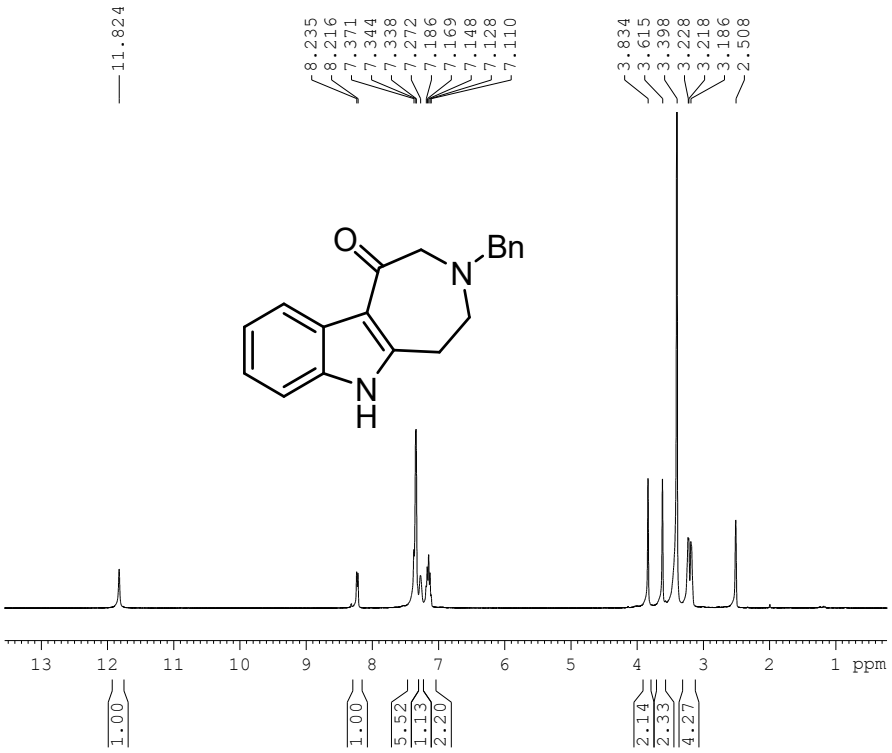

```
Current Data Parameters
NAME           M841(NMR)
EXPNO                308
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230617
Time                0.58 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                 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          400.1300000 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                  1.00
```

^{13}C{^{1}H} NMR (100 MHz, DMSO-d$_6$, 24 °C) of the compound **6ab**

3-benzyl-3,4,5,6-tetrahydroazepino[4,5-b]indol-1(2H)-one: 6ac

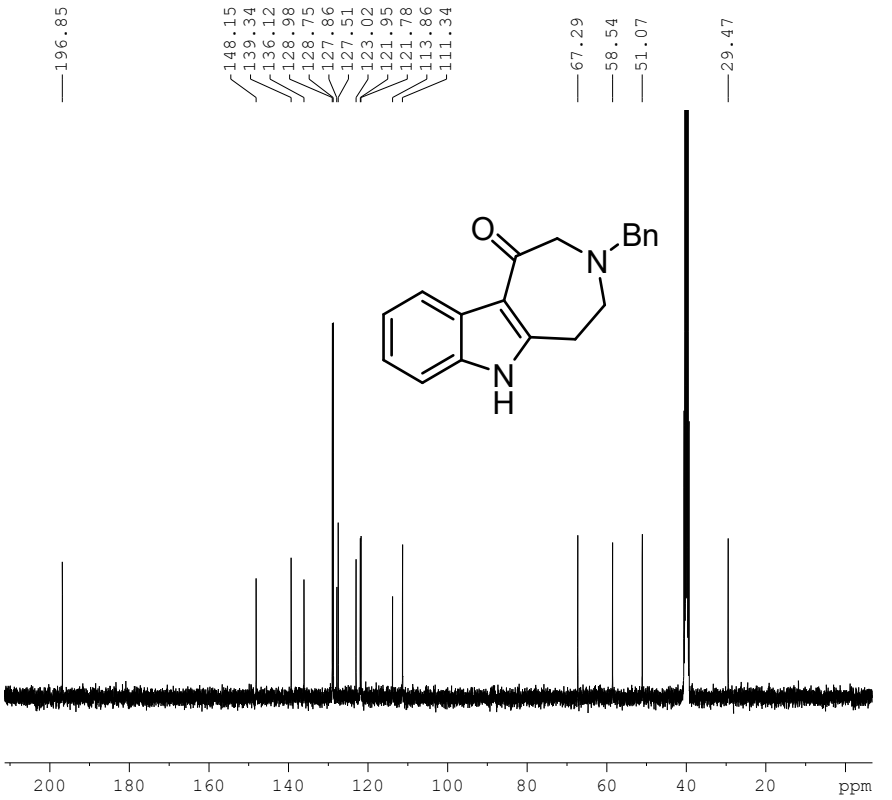



```
Current Data Parameters
NAME            M842(N)
EXPNO               312
PROCNO                1

F2 - Acquisition Parameters
Date_          20230617
Time               1.24 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                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          400.1300000 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 **6ac**



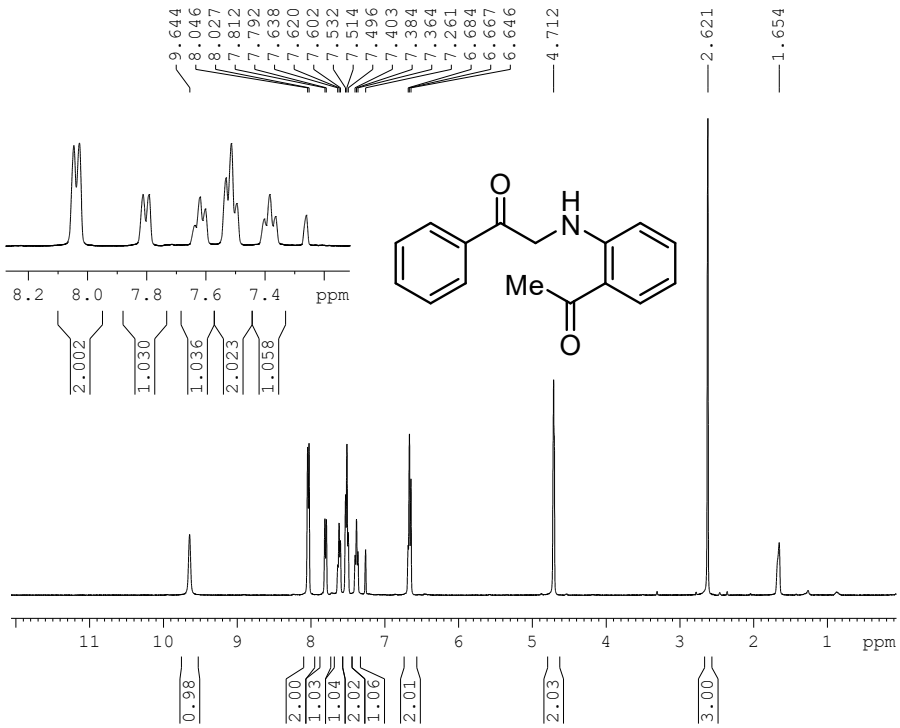

```
Current Data Parameters
NAME            M842(N)
EXPNO               313
PROCNO                1

F2 - Acquisition Parameters
Date_          20230617
Time               1.54 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 use
DE                 6.50 use
TE                295.7 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 **6ac**

2-((2-acetylphenyl)amino)-1-phenylethan-1-one: I

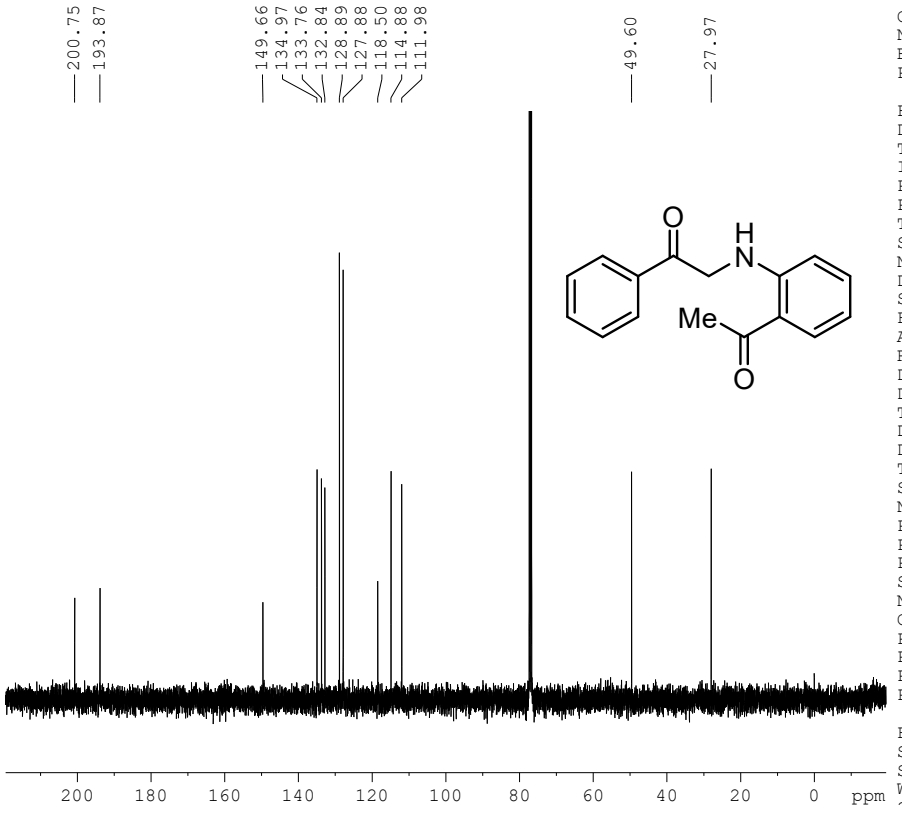



```
Current Data Parameters
NAME                  2170
EXPNO                   38
PROCNO                   1

F2 - Acquisition Parameters
Date_           20240104
Time              20.34 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                 293.9 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            400.1300089 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 **I**



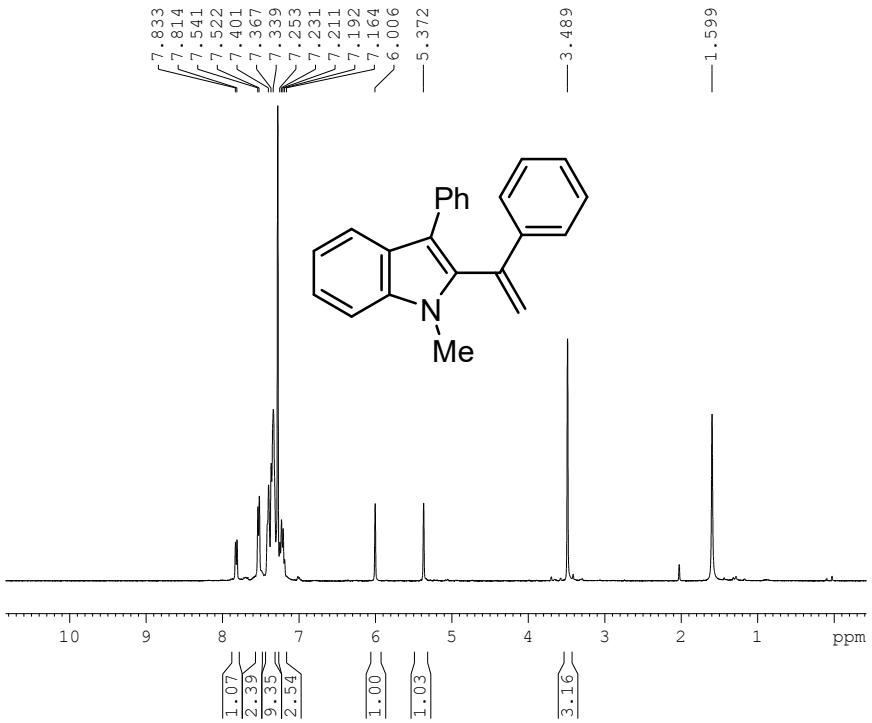

```
Current Data Parameters
NAME                  2170
EXPNO                   39
PROCNO                   1

F2 - Acquisition Parameters
Date_           20240104
Time              22.15 h
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   195
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                 294.1 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, $CDCl_3$, 24 °C) of the compound **I**

1-methyl-3-phenyl-2-(1-phenylvinyl)-1H-indole: 8a

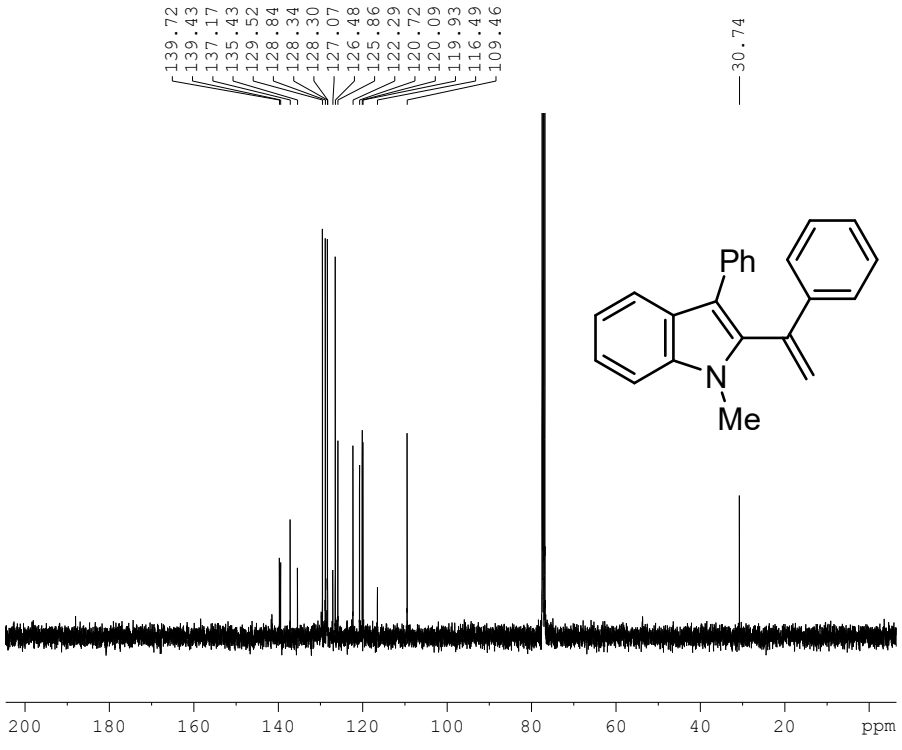



```
Current Data Parameters
NAME                  M653
EXPNO                  519
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230121
Time                 20.56 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                   295.7 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             400.1300011 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 **8a**



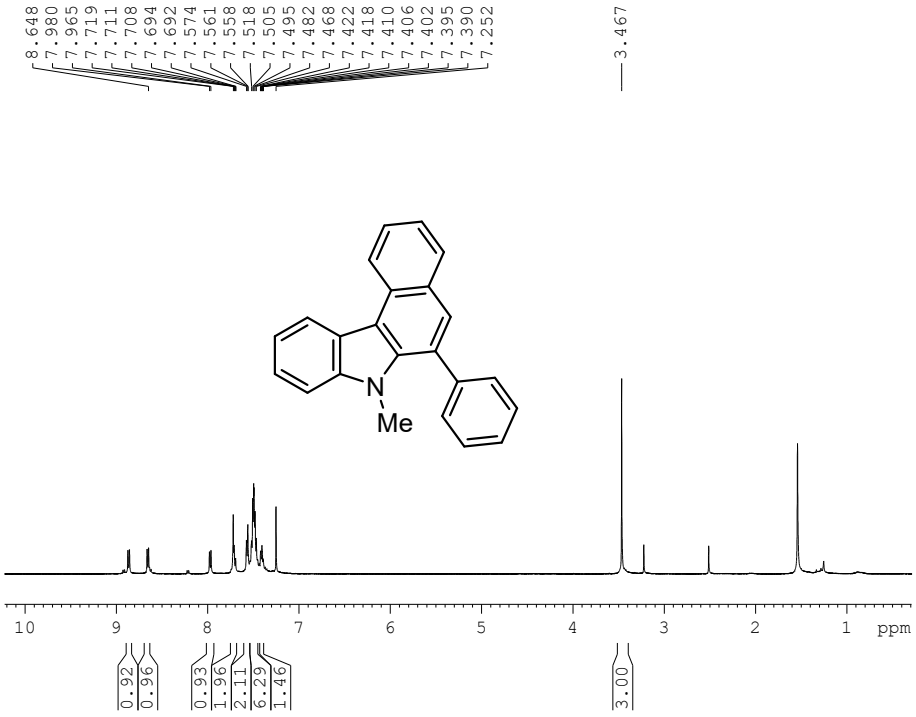

```
Current Data Parameters
NAME                  M653
EXPNO                  547
PROCNO                   1

F2 - Acquisition Paramete
Date_              20230123
Time                  2.37 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                   296.0 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
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **8a**

7-methyl-6-phenyl-7H-benzo[c]carbazole: 9



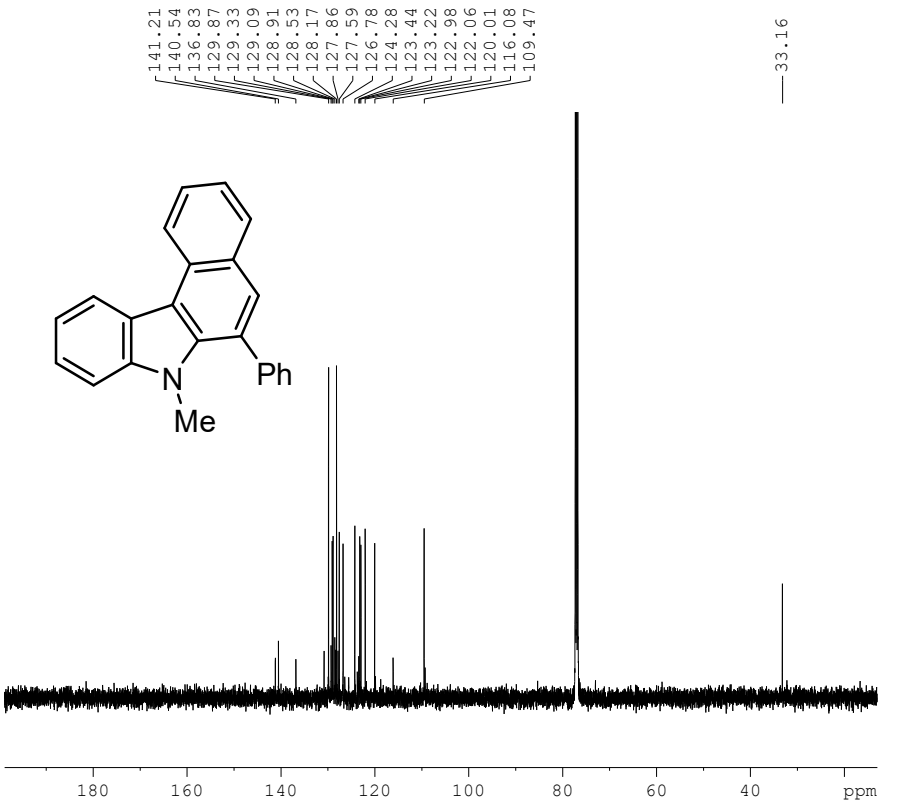

```
Current Data Parameters
NAME                  spa
EXPNO                 226
PROCNO                  1

F2 - Acquisition Parameter
Date_            20230727
Time                11.59
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             10000.000 Hz
FIDRES          0.305176 Hz
AQ              1.6384000 se
RG                 202.34
DW                 50.000 us
DE                  6.50 us
TE                 300.9 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           500.1500160 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 **9**




```
Current Data Parameters
NAME      M750 long scan
EXPNO                239
PROCNO                 1

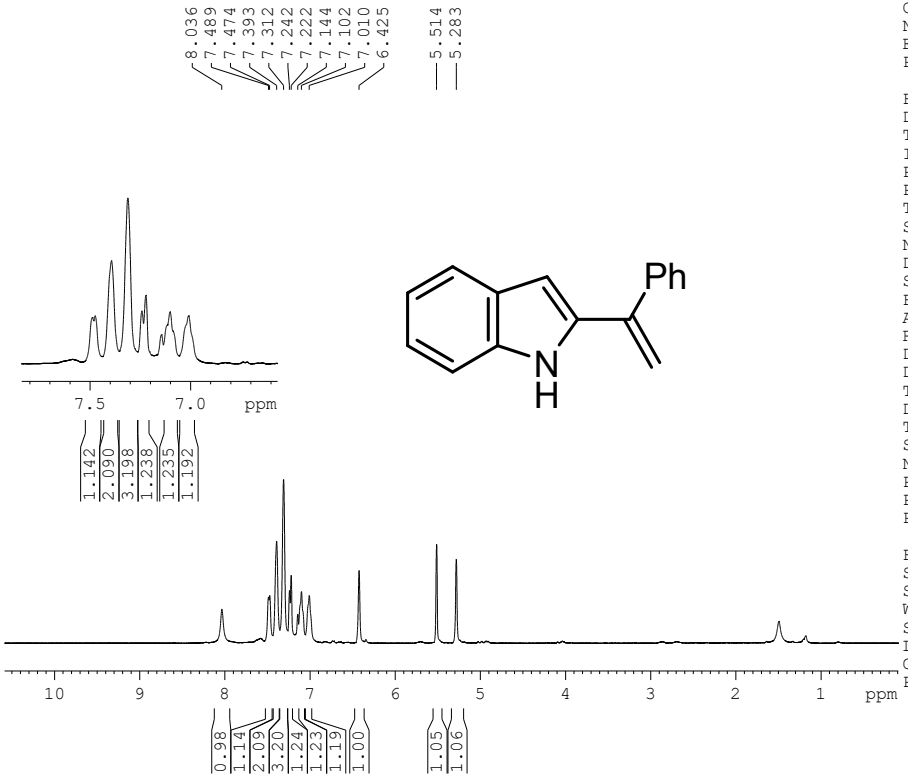
F2 - Acquisition Parameters
Date_            20230727
Time                23.41
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  20480
SOLVENT             CDCl3
NS                   2000
DS                      4
SWH             29761.904 Hz
FIDRES           1.453218 Hz
AQ              0.3440640 sec
RG                 202.34
DW                 16.800 use
DE                  6.50 use
TE                 302.8 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                     1

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

======== CHANNEL f2 =======
SFO2         500.1520006 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              80.00 use
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 **9**

2-(1-phenylvinyl)-1H-indole: 8b

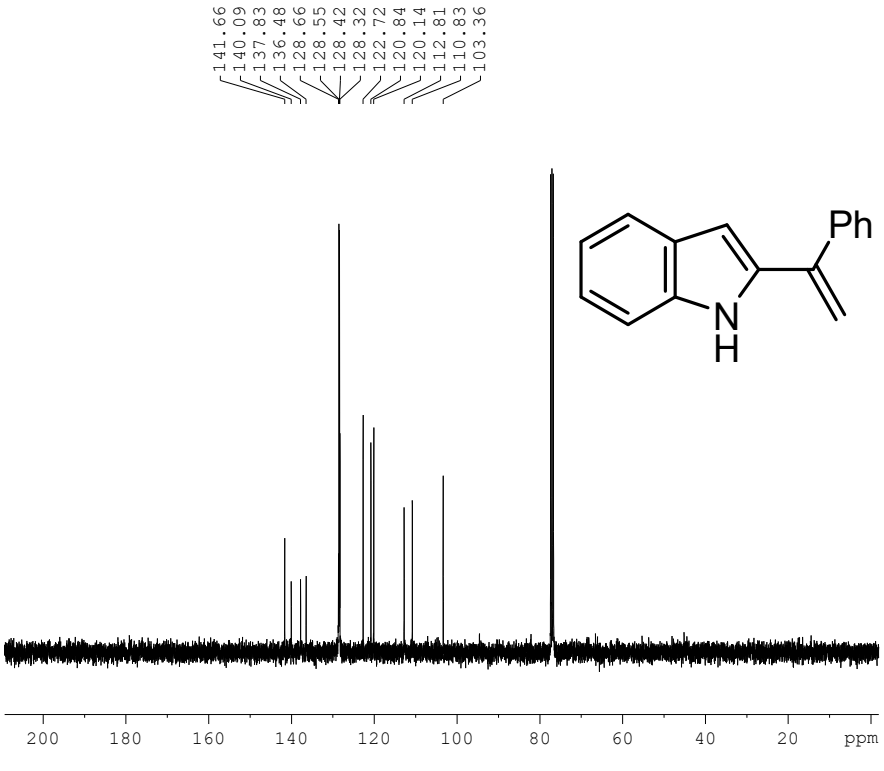



```
Current Data Parameters
NAME          2114-2125
EXPNO               228
PROCNO                1

F2 - Acquisition Parameters
Date_          20240121
Time              19.50 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                16.92 usec
TE                    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           400.1300550 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 **8b**



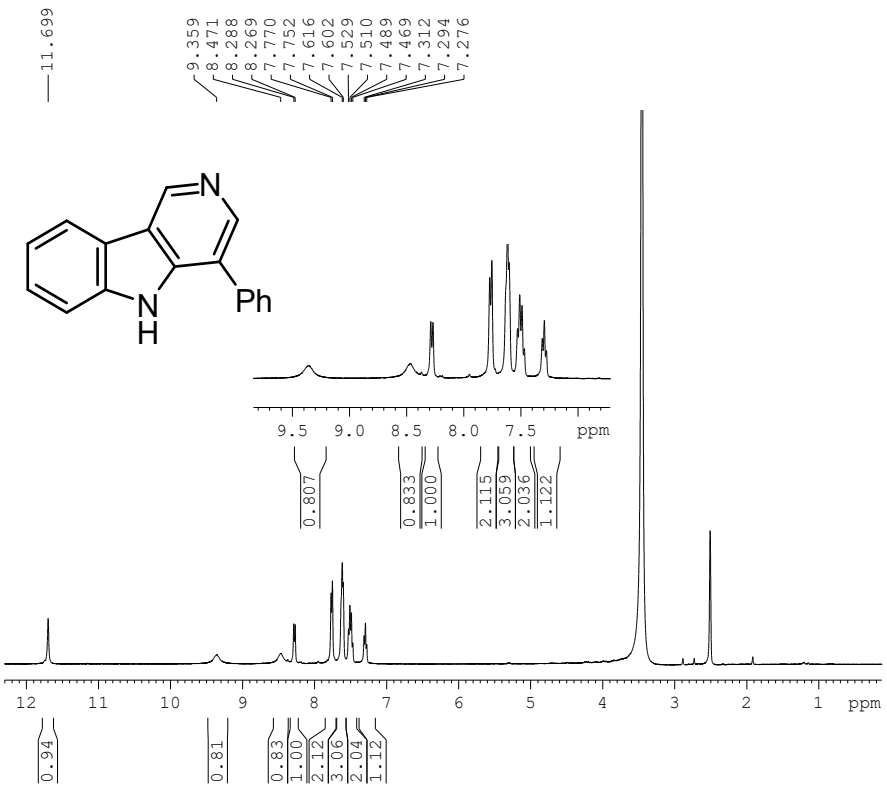

```
Current Data Parameters
NAME          2114-2125
EXPNO               229
PROCNO                1

F2 - Acquisition Parameters
Date_          20240121
Time              20.02 h
INSTRUM           spect
PROBHD   Z129392_0001 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 192
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                    0 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 **8b**

4-phenyl-5H-pyrido[4,3-b]indole: 10

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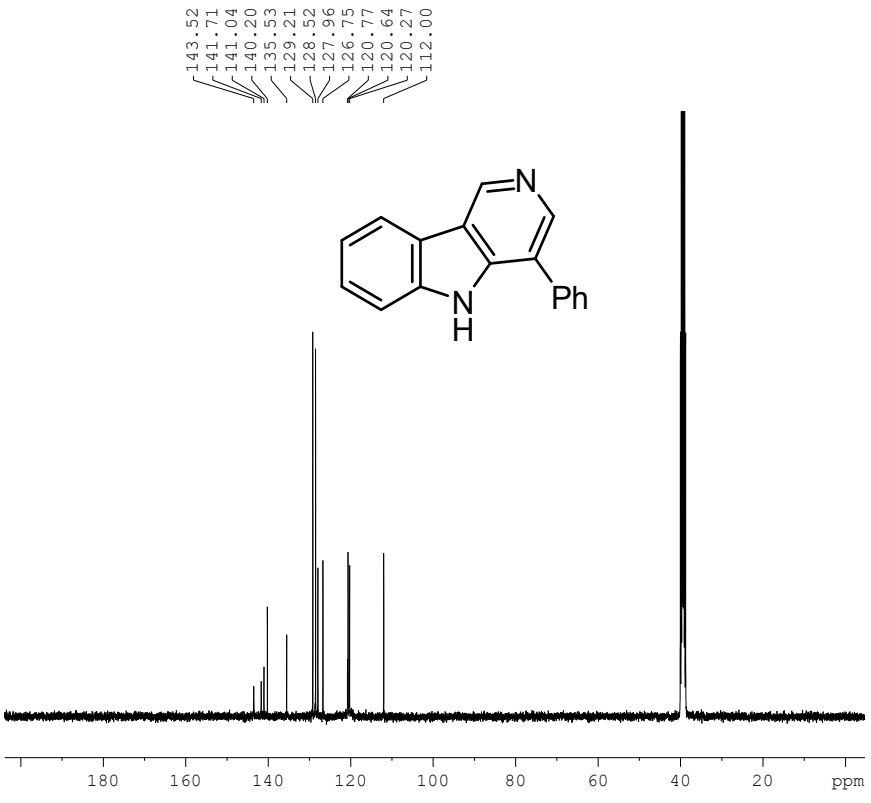
Current Data Parameters
NAME          MM105,2151
EXPNO                104
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231109
Time              21.47 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                293.8 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 **10**



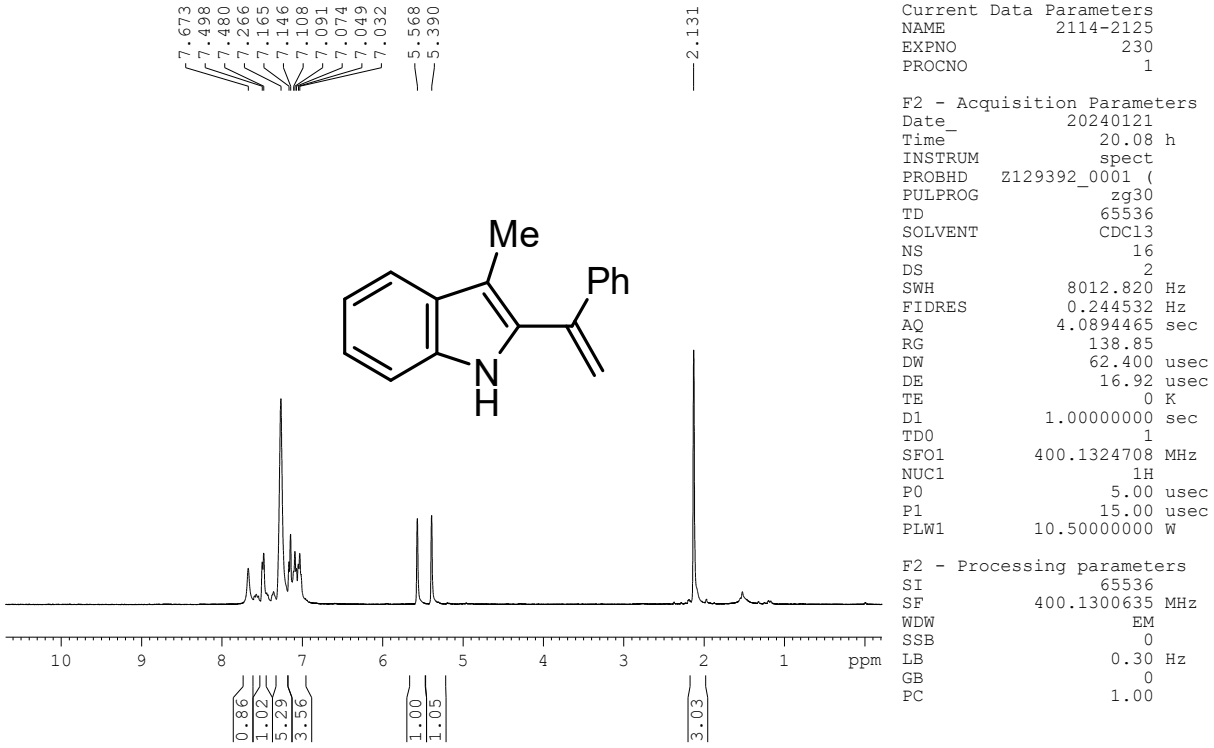

```
Current Data Parameters
NAME          MM105,2151
EXPNO                125
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231111
Time               3.34 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 3000
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                294.2 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

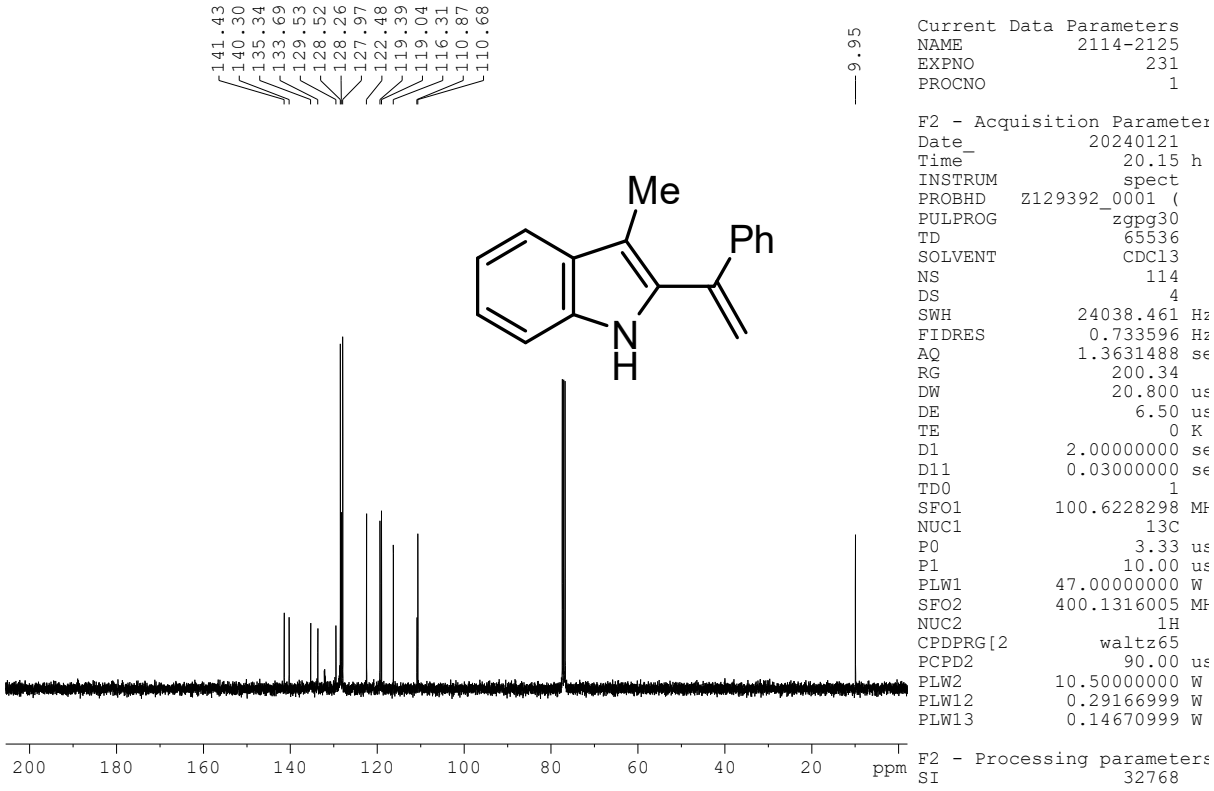
F2 - Processing parameters
SI                 32768
SF            100.6128157 MHz
WDW                   EM
```

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

3-methyl-2-(1-phenylvinyl)-1H-indole: 8c

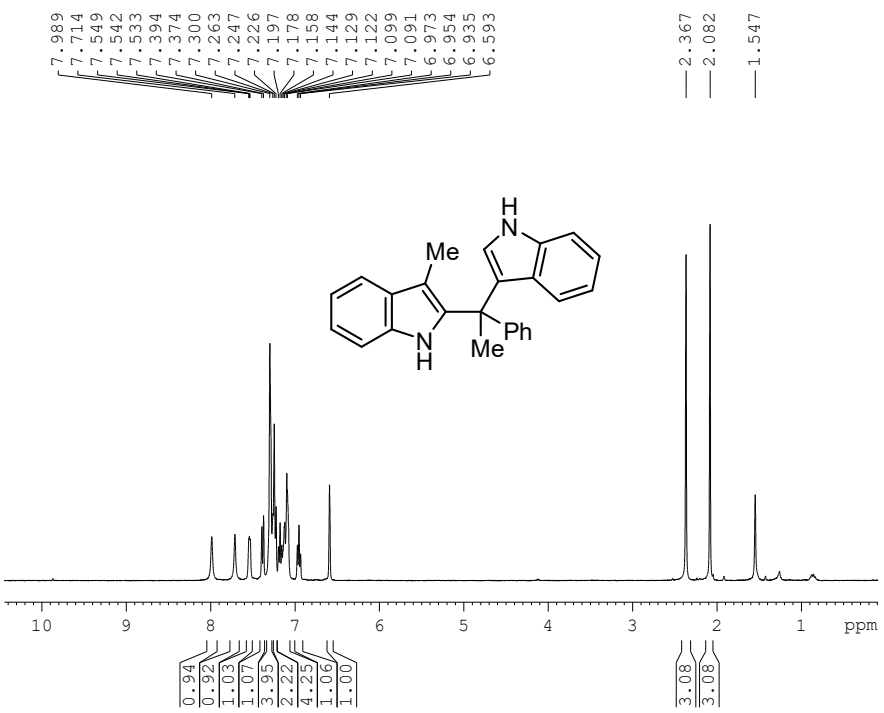


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **8c**



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **8c**

2-(1-(1H-indol-3-yl)-1-phenylethyl)-3-methyl-1H-indole: 11

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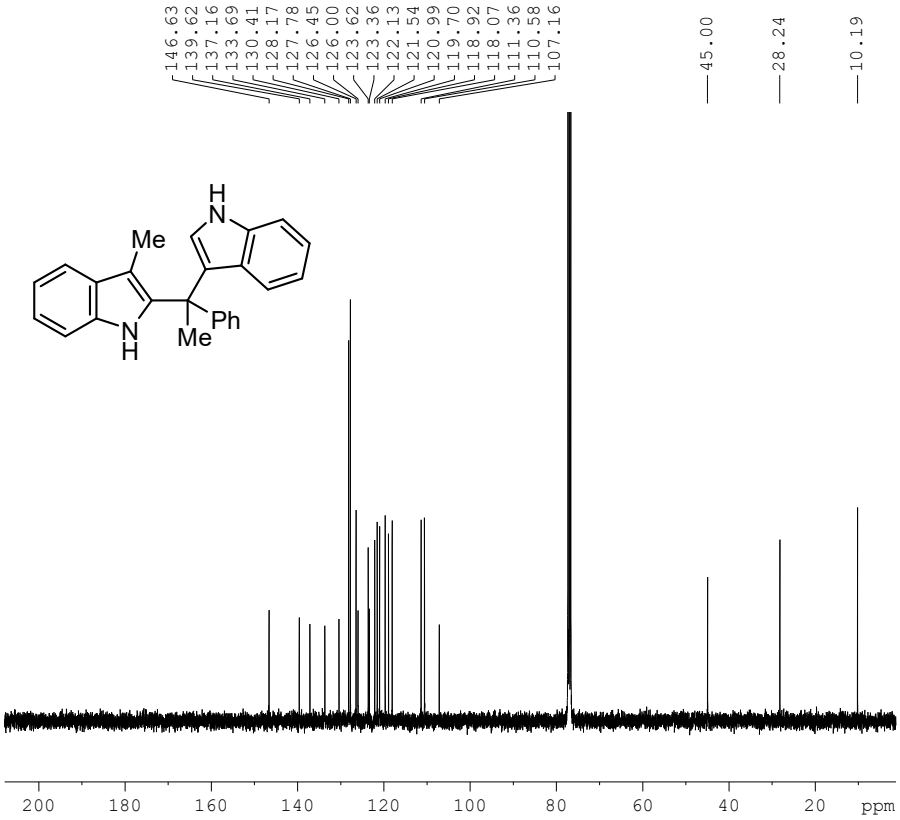
Current Data Parameters
NAME              MA-2132
EXPNO                 191
PROCNO                  1

F2 - Acquisition Parameters
Date_           20231025
Time              11.04 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                293.4 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 **11**



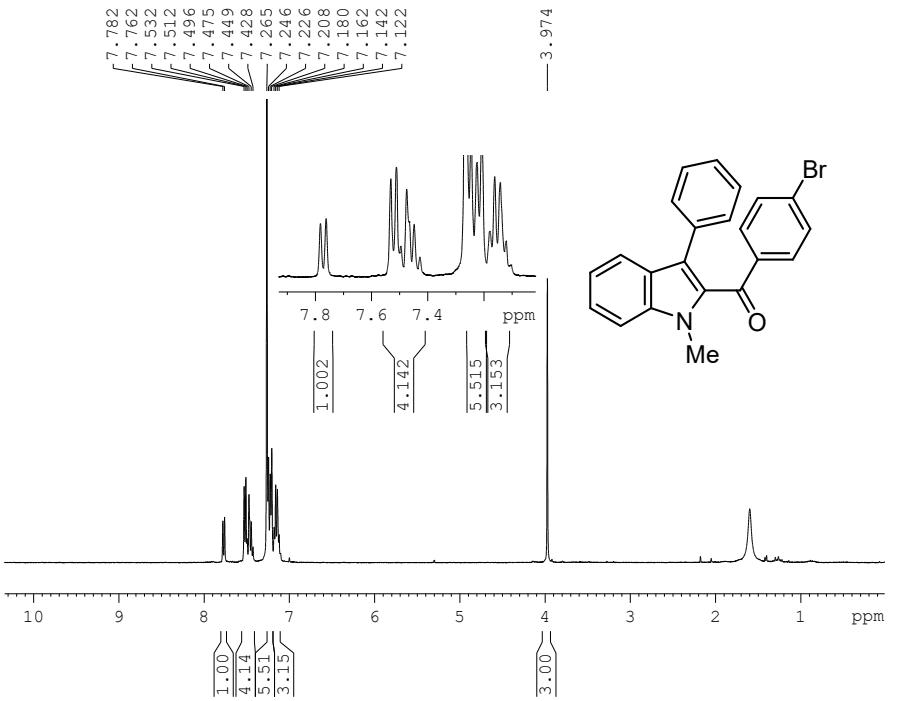

```
Current Data Parameters
NAME           2132-2133
EXPNO                308
PROCNO                 1

F2 - Acquisition Parameter
Date_           20231026
Time              3.33 h
INSTRUM             spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2000
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                294.1 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
SF            100.6127685 MH
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **11**

(4-bromophenyl)(1-methyl-3-phenyl-1H-indol-2-yl)methanone: 12

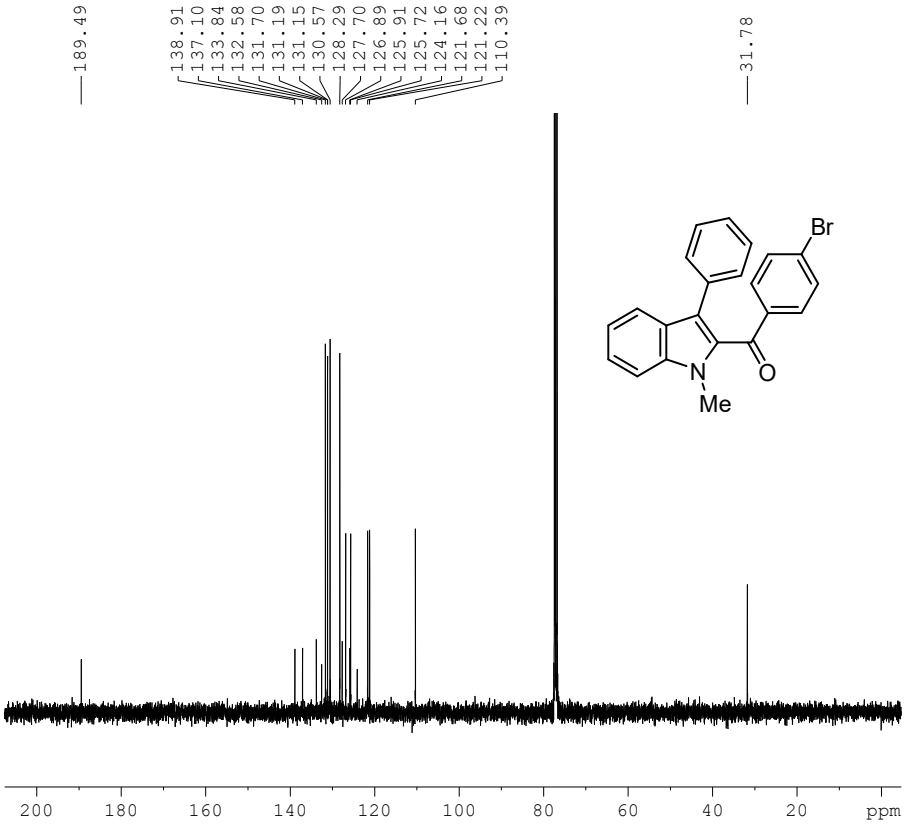



```
Current Data Parameters
NAME      jan 2023(1-185)
EXPNO                 137
PROCNO                  1

F2 - Acquisition Parameters
Date_           20230105
Time              16.42 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                200.34
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          400.1300075 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 **12**



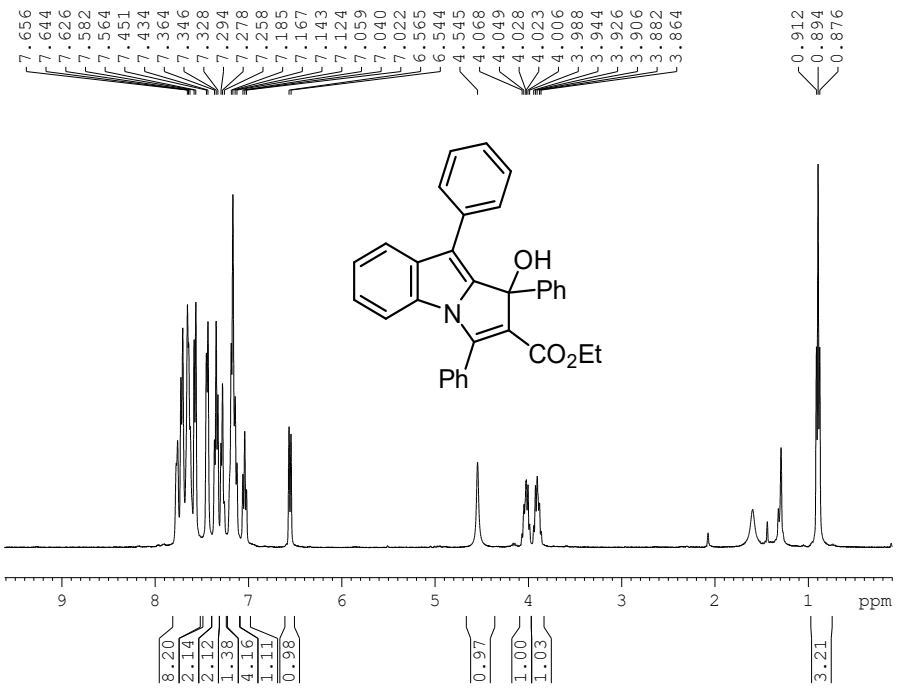

```
Current Data Parameters
NAME      jan 2023(1-185)
EXPNO                 167
PROCNO                  1

F2 - Acquisition Paramet
Date_           20230106
Time                4.16
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                297.8
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 **12**

ethyl 1-hydroxy-1,3,9-triphenyl-1H-pyrrolo[1,2-a]indole-2-carboxylate: 13

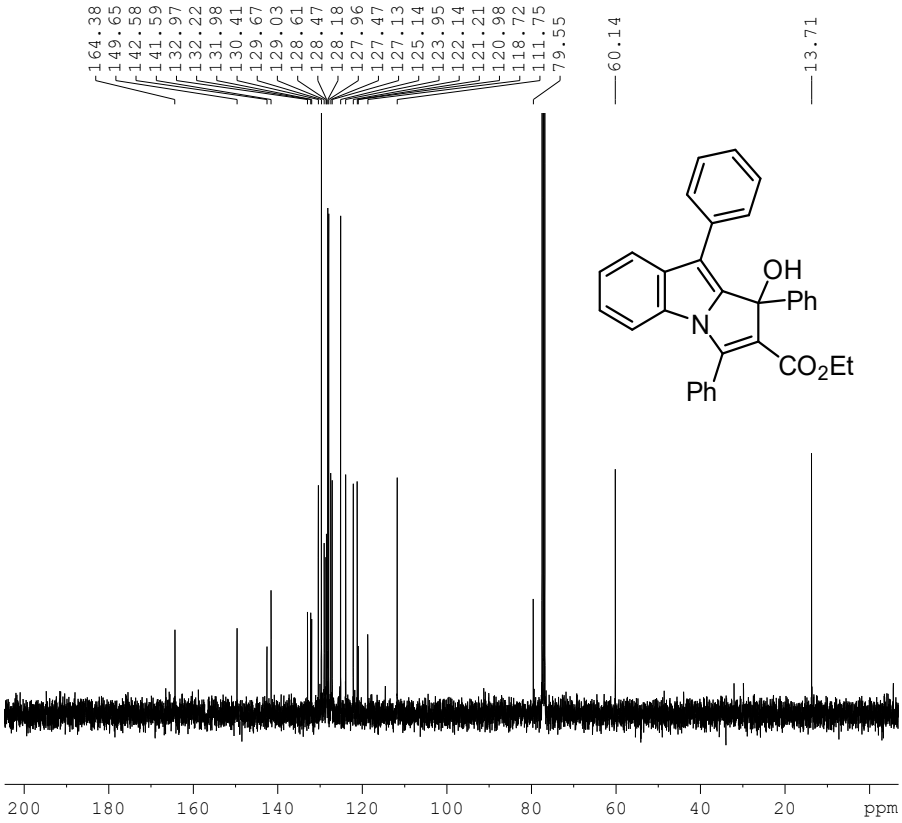



```
Current Data Parameters
NAME                  M676
EXPNO                  537
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230122
Time              21.36 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                153.13
DW                62.400 usec
DE                 6.50 usec
TE                295.6 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          400.1300018 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 **13**



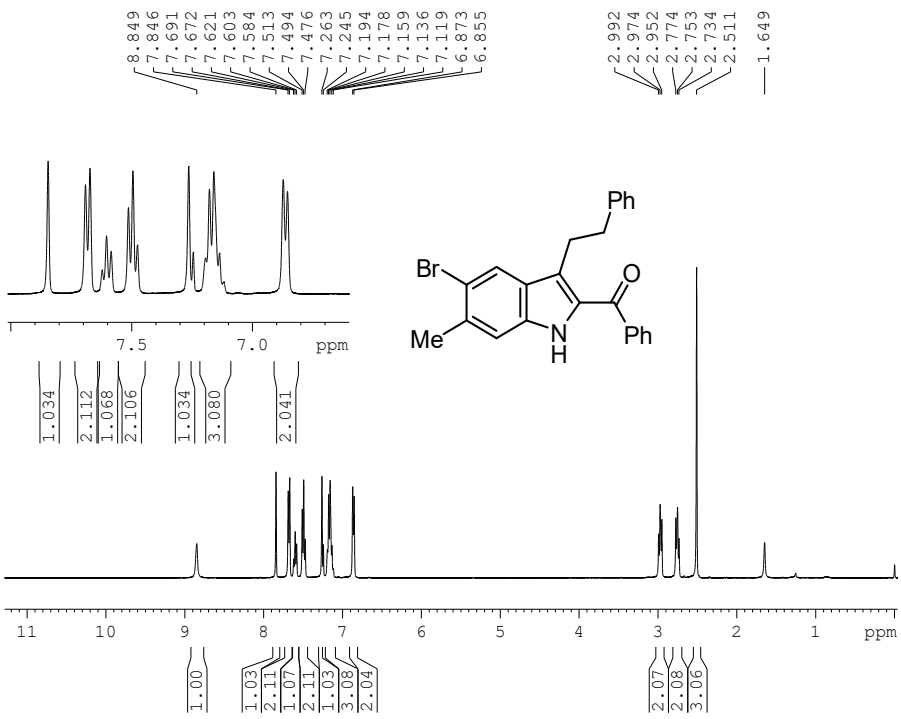

```
Current Data Parameters
NAME                  M676
EXPNO                  538
PROCNO                   1

F2 - Acquisition Parameter
Date_           20230122
Time              21.43 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                295.8 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          100.6127596 MH
```

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

(5-bromo-6-methyl-3-phenethyl-1H-indol-2-yl)(phenyl)methanone: 15

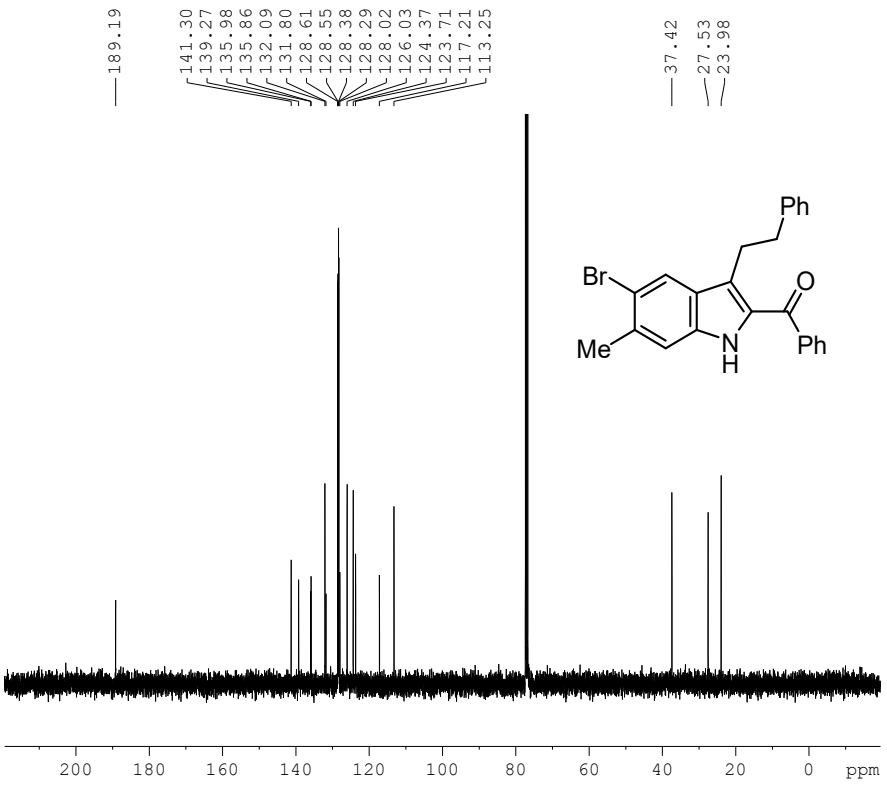



```
Current Data Parameters
NAME      M906  AND M907
EXPNO                 66
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230707
Time                2.01 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                153.13
DW                 62.400 usec
DE                 16.92 usec
TE                 505.1 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            400.1300157 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 **15**



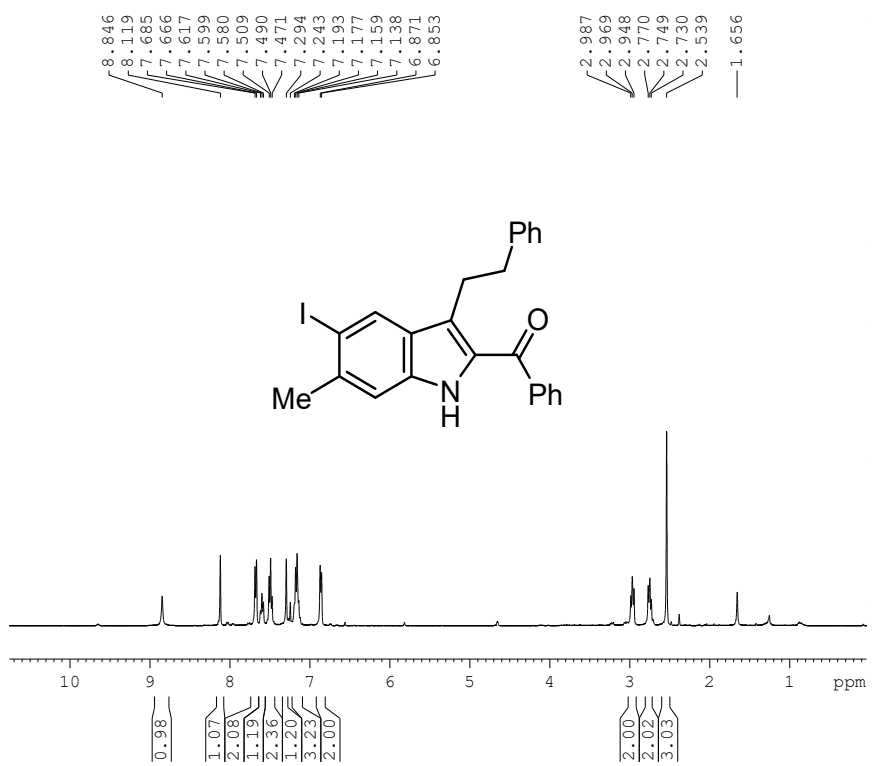

```
Current Data Parameters
NAME      M906  AND M907
EXPNO                 67
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230707
Time                2.07 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    90
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                510.2 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, $CDCl_3$, 24 °C) of the compound **15**

(5-iodo-6-methyl-3-phenethyl-1H-indol-2-yl)(phenyl)methanone: 16

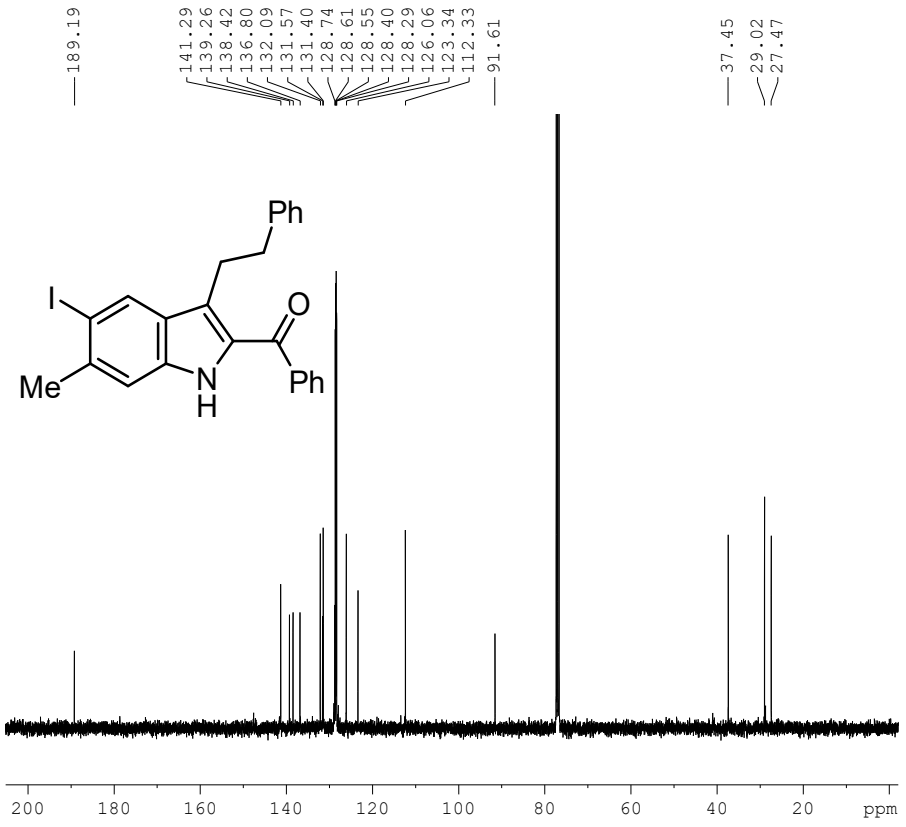



```
Current Data Parameters
NAME      M906  AND M907
EXPNO               63
PROCNO               1

F2 - Acquisition Parameters
Date_          20230707
Time               1.55 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              16.92 usec
TE              496.9 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          400.1300161 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 **16**



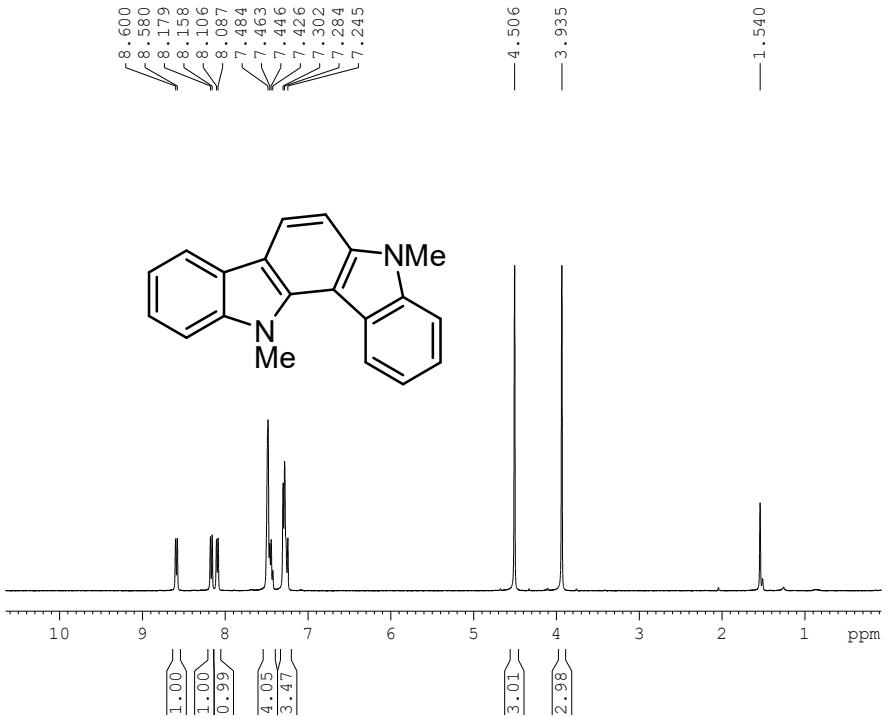

```
Current Data Parameters
NAME      M906  AND M907
EXPNO               64
PROCNO               1

F2 - Acquisition Paramete
Date_          20230707
Time               2.30 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                512.5 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
SF          100.6127685 M
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **16**

5,12-dimethyl-5,12-dihydroindolo[3,2-a]carbazole: 19

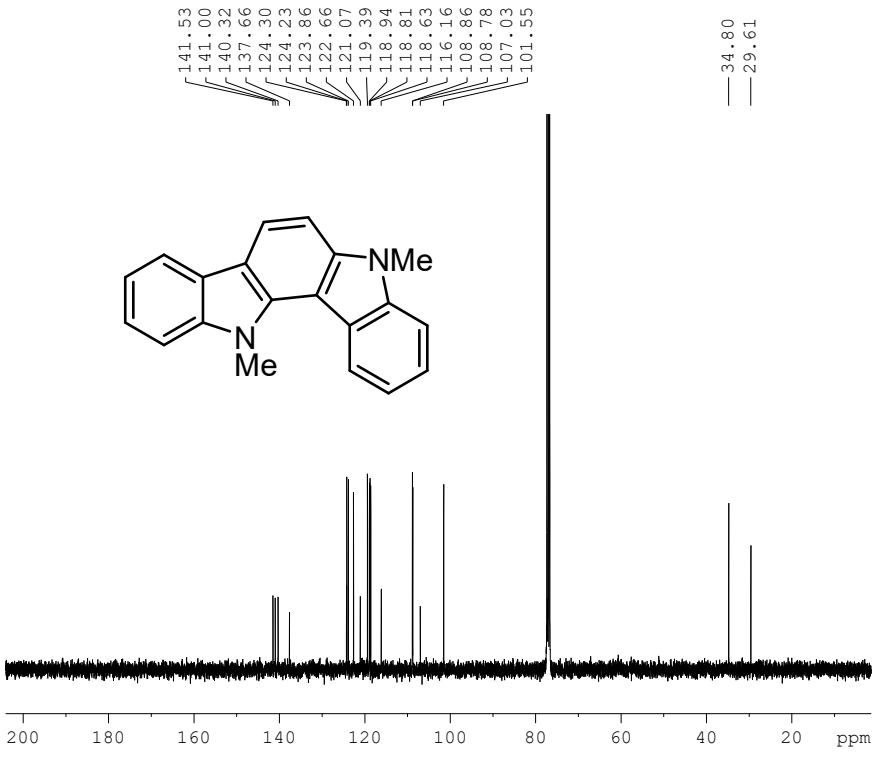



```
Current Data Parameters
NAME          2132-2133
EXPNO               302
PROCNO                1

F2 - Acquisition Parameters
Date_          20231025
Time              20.53 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                293.7 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            400.1300155 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 **19**



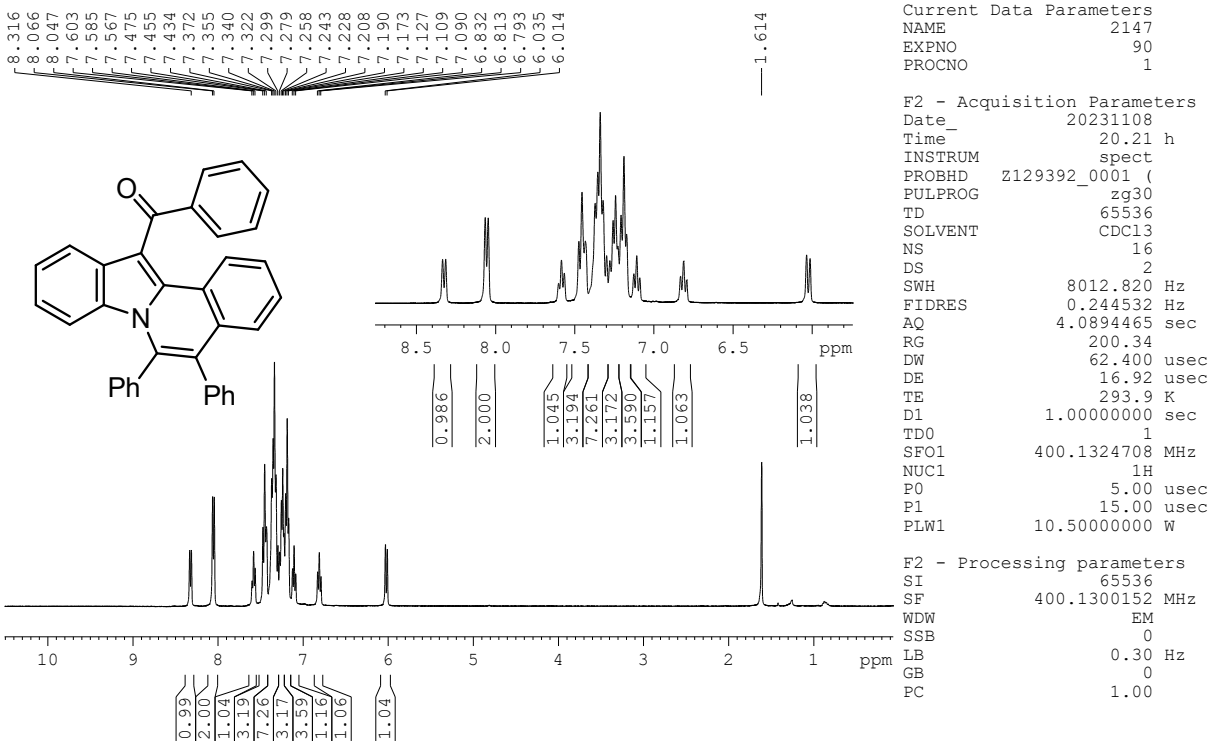

```
Current Data Parameters
NAME          2132-2133
EXPNO               307
PROCNO                1

F2 - Acquisition Parameters
Date_          20231026
Time              1.21 h
INSTRUM           spect
PROBHD   Z129392_0001 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
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                294.1 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
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **19**

(5,6-diphenylindolo[2,1-a]isoquinolin-12-yl)(phenyl)methanone: 20

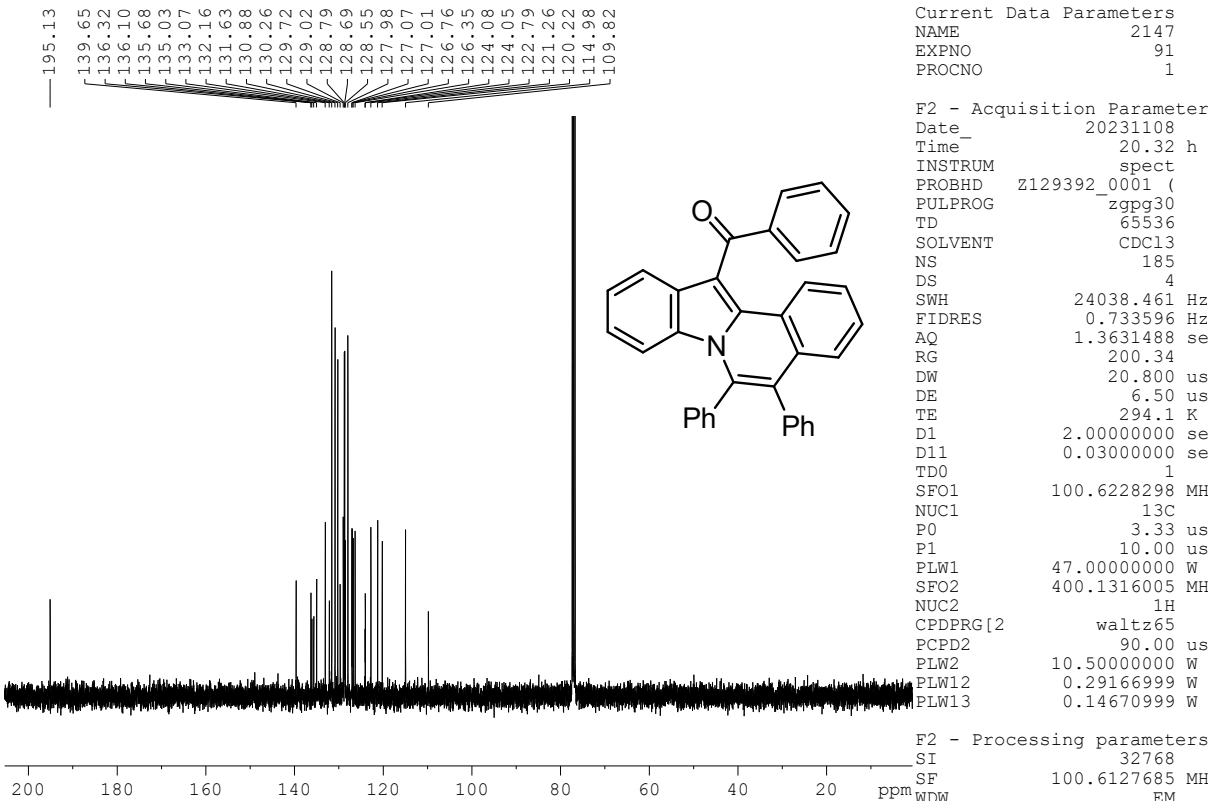



```
Current Data Parameters
NAME                  2147
EXPNO                   90
PROCNO                   1

F2 - Acquisition Parameters
Date_              20231108
Time                 20.21 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                    293.9 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             400.1300152 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 **20**




```
Current Data Parameters
NAME                  2147
EXPNO                   91
PROCNO                   1

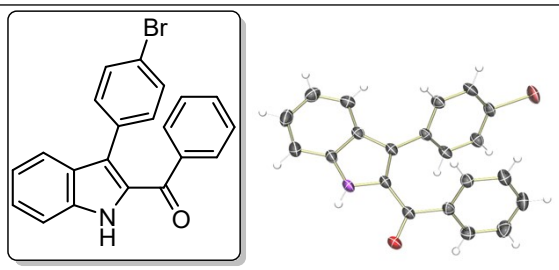
F2 - Acquisition Parameter
Date_              20231108
Time                 20.32 h
INSTRUM              spect
PROBHD   Z129392_0001 (
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     185
DS                       4
SWH              24038.461 Hz
FIDRES               0.733596 Hz
AQ                1.3631488 se
RG                    200.34
DW                    20.800 us
DE                     6.50 us
TE                    294.1 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
SF             100.6127685 MH
WDW                     EM
```

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **20**

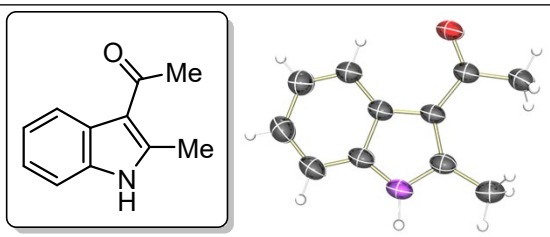
10. XRD data of 3j, 6o, 6p, 6p'

a. Single crystal XRD data of 3j:

DATA	3j
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

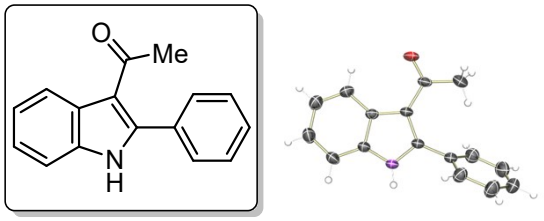
Density (g/mL)	1.498
μ (1/mm)	2.470
F (000)	380
θ(min, max)	2.49 to 26.21
No. of unique reflns	12302
No. of parameters	222
R_obs, wR_2_obs	0.0302, 0.0727
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (eÅ^{-3})	0.0390, 0.0769
GooF	1.040

b. Single crystal XRD data of 6o:

DATA	**6o**
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

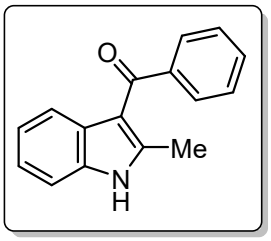
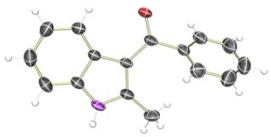
Space group	C 2/c
a (Å)	13.5293(7)
b (Å)	7.3263(3)
c (Å)	19.0986(9)
α (°)	90
β (°)	99.741(3)
γ (°)	90
Volume (Å^3)	1865.75(15)
Z	8
Density (g/mL)	1.233
μ (1/mm)	0.632
F (000)	736
θ(min, max)	4.70 to 71.47
No. of unique reflns	13865
No. of parameters	124
R_obs, wR_2_obs	0.0568, 0.1576
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (eÅ^{-3})	0.0693, 0.1763
GooF	1.065

c. Single crystal XRD data of 6p:

DATA	6p
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

d. Single crystal XRD data of 6p':

DATA	**6p'**
Molecular Structure (ORTEP Structure)	 
Formula	$C_{16}H_{13}NO$
Formula weight	235.27
Color	White colourless
Temperature/K	296(2)
Radiation	Mo Kα
Wavelength/Å	0.71073
Crystal system	monoclinic
Space group	C 1 2/c 1

a (Å)	22.8283(19)
b (Å)	7.6726(6)
c (Å)	14.6984(13)
α (°)	90
β (°)	106.312(3)
γ (°)	90
Volume (Å^3)	2470.8(4)
Z	8
Density (g/mL)	1.265
μ (1/mm)	0.079
F (000)	992
θ(min, max)	2.81 to 23.05
No. of unique reflns	8425
No. of parameters	169
R_obs, wR_2_obs	0.0415, 0.1014
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (eÅ^{-3})	0.0651, 0.1160
GooF	1.031