Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Cp*Co^{III}-Catalyzed C2-Alkylation of Indole Derivatives with Substituted Cyclopropanols

*Kuppan Ramachandran and Pazhamalai Anbarasan**

Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India.

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1. General Comments:

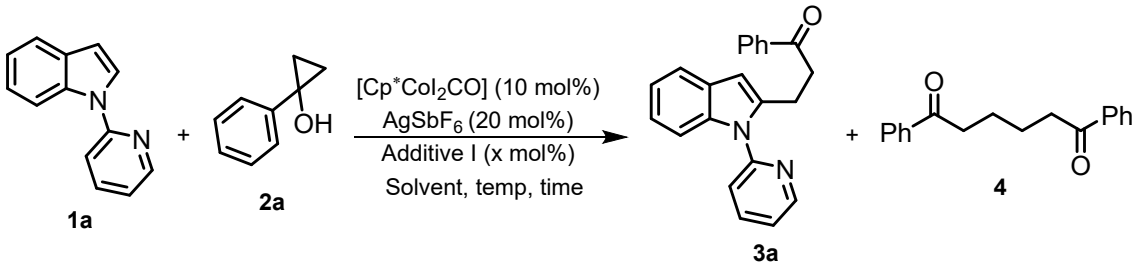
All reactions were carried out in pressure tube under dry nitrogen atmosphere. All the *N*-pyridylindole[1] and cyclopropanol[2] derivatives were synthesized according to the literature procedure. $[Cp^*CoI_2CO]$,[3a] $[Cp^*CoI_2]_2$[3b], $[Cp^*Co(MeCN)_3](SbF_6)_2$[3c], and $[Cp^*Co(MeCN)_3](SbF_6)_2$[3d] were synthesized according to the literature procedure. Dry solvents were prepared through standard procedure and stored over using molecular sieves 4Å under N_2 atmosphere. Column chromatography was performed using silica gel (100-200 mesh) and ethyl acetate-hexanes with various percentage of polarity depending on the nature of the substrate as an eluent, unless otherwise specified.

2. Analytical Methods:

NMR data were recorded on 400 and 500 MHz spectrometers. ^{1}Hand ^{13}C NMR spectra were referenced to signals of either deuterated solvents or residual protiated solvents. Infrared spectra were recorded on a Thermo Nicolet iS10 FT and Jasco ATR-IR spectrometer. HRMS were recorded by electron spry ionization (ESI) method on a Q-TOF Micro with lock spray source.

1. Whyte, A.; Torelli, A.; Mirabi, B.; Prieto, L.; Rodríguez, J. F.; Lautens, M. *J. Am. Chem. Soc.* **2020**, *142*, 9510.
2. Kulinkovich, O. G.; Sviridov, S. V.; Vasilevski, D. A.; Prityts kaya, T. S. *Zh. Org. Khim.* **1989**, *25*, 2244-2245 (*J. Org. Chem. USSR (Engl. Transl.)* **1989**, *25*, 2027.
3. a) Sun, B.; Yoshino, T.; Matsunaga, S.; Kanai, M. *Adv. Synth.Catal*. **2014**, *356*, 1491.; b) Sun, B.; Yoshino, T.; Matsunaga, S.; Kanai, M. *Chem. Commun.* **2015**, *51*, 4659.; c) Yu, D.-G.; Gensch, T.; Azambuja, F.; Vásquez-Céspedes, S.; and Glorius, F. *J. Am. Chem. Soc.* **2014**, *136*, 17722; d) White, C.; Thompson, S. J.; Maitlis, P. M. *J. Chem. Soc., Dalton Trans.* **1977,** 1654.

3. Optimization: Cobalt(III)-catalyzed alkylation of 1a with 2a

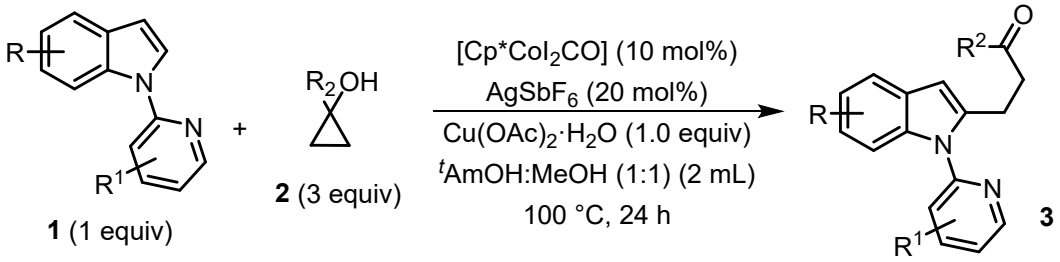


Entry	Additive I (x mol%)	Solvent	Temp (°C)	Time (h)	Yield 3a/4 (%)
1	NaOAc [10]	DCE	100	24	-/-
2	NaOAc [10]	MeOH	100	24	19/-
3	NaOAc [10]	^{t}AmOH	100	24	25/-
4	KOAc [10]	^{t}AmOH	100	24	38/-
5	KOAc [50]	^{t}AmOH	100	24	33/-
6	KOAc [200]	^{t}AmOH	100	24	-/-
7	$Cu(OAc)_2$	^{t}AmOH	100	24	23/-
8	$Cu(OAc)_2 \cdot H_2O$[50]	^{t}AmOH	100	24	58/11
9	$Cu(OAc)_2 \cdot H_2O$[100]	^{t}AmOH	100	24	68/24
10	$Cu(OAc)_2 \cdot H_2O$[200]	^{t}AmOH	100	24	33/48
11	$Cu(OAc)_2 \cdot H_2O$[100]	^{t}AmOH	80	24	29/8
12	$Cu(OAc)_2.H_2O$[100]	^{t}AmOH	50	24	8/-
13	$Cu(OAc)_2 \cdot H_2O$[100]	^{t}AmOH	rt	24	-/-
14	$Cu(OAc)_2 \cdot H_2O$[100]	^{t}AmOH	100	16	66/22
15[a]	$Cu(OAc)_2 \cdot H_2O$[100]	^{t}AmOH	100	24	56/18
16[b]	$Cu(OAc)_2 \cdot H_2O$[100]	^{t}AmOH	100	24	45/10
17[c]	$Cu(OAc)_2 \cdot H_2O$[100]	^{t}AmOH	100	24	36/7
18[d]	$Cu(OAc)_2 \cdot H_2O$[100]	^{t}AmOH	100	8	10/-
19[e]	$Cu(OAc)_2 \cdot H_2O$[100]	^{t}AmOH	100	8	-/-
20	$Cu(OAc)_2 \cdot H_2O$[100]	^{i}PrOH	100	24	10/5
21	$Cu(OAc)_2 \cdot H_2O$[100]	EtOH	100	24	24/5
22	$Cu(OAc)_2 \cdot H_2O$[100]	^{t}BuOH	100	24	21/10
23	$Cu(OAc)_2 \cdot H_2O$[100]	^{t}BuOH: ^{t}AmOH	100	24	18/15
25[f]	$Cu(OAc)_2 \cdot H_2O$[100]	MeOH: ^{t}AmOH	100	24	63/10
26	$Cu(OAc)_2 \cdot H_2O$[200]	MeOH: ^{t}AmOH	100	24	21/18

27	$Cu(OAc)_2 \cdot H_2O$[10]	MeOH: ^{t}AmOH	100	24	14/5
28[g]	**$Cu(OAc)_2 \cdot H_2O$[100]**	**MeOH: ^{t}AmOH**	**100**	**24**	**80**
29	$Cu(OAc)_2.H_2O$[100]	DMF	100	24	-
30	$Cu(OAc)_2 \cdot H_2O$[100]	DMSO	100	24	-
31	$Cu(OAc)_2 \cdot H_2O$[100]	CH_3CN	100	24	11
32	$Cu(OAc)_2 \cdot H_2O$[100]	chlorobenzene	100	24	-/-
33	$Cu(OAc)_2 \cdot H_2O$[100]	DCM	100	24	-/-
34[h]	$Cu(OAc)_2 \cdot H_2O$[100]	^{t}AmOH	100	24	-/10
35[i]	$Cu(OAc)_2 \cdot H_2O$[100]	^{t}AmOH	100	24	-/-
36	AgOAc [20]	^{t}AmOH	100	24	-/-
37	$AgNO_3$ [20]	^{t}AmOH	100	24	-/-
38	Ag_2CO_3 [20]	^{t}AmOH	100	24	-/-
39[j]	$Cu(OAc)_2 \cdot H_2O$[100]	MeOH: ^{t}AmOH	100	24	20/6
40	KOPiv [100]	MeOH: ^{t}AmOH	100	24	41/8
41	$Cu(OPiv)_2$ [100]	MeOH: ^{t}AmOH	100	24	61/9
42	$Cu(acac)_2$ [100]	MeOH: ^{t}AmOH	100	24	11/8
43	AgO_2CF_3 [100]	MeOH: ^{t}AmOH	100	24	17/15
44	$Cu(TFA)_2$	MeOH: ^{t}AmOH	100	24	27/5
45[k]	AgOAc [20]	MeOH: ^{t}AmOH	100	24	-/5
46	$Cu(OTf)_2$ [20]	MeOH: ^{t}AmOH	100	24	5/-
47[k]	AgOTf [20]	MeOH: ^{t}AmOH	100	24	24/14
48	$Cu(CH_3CN)_4BF_4$	MeOH: ^{t}AmOH	100	24	-/9
49[k]	AgF [20]	MeOH: ^{t}AmOH	100	24	-/17

Reaction condition: **1a** (1.0 equiv.), **2a** (2.0 equiv.), [Cp*CoI_2(CO)] (10 mol%), $Cu(OAc)_2 \cdot H_2O$[100], solvent-MeOH: ^{t}AmOH (2mL), 100 °C. [a] with 20 mol% TEMPO. [b] with 50 mol% TEMPO. [c] with 100 mol% TEMPO. [d] with 20 mol% of benzoyl peroxide. [e] with 20 mol% of H_2O_2. [f] $[Cp^*CoCl_2]_2$ (10 mol%). [g] **2a** (3.0 equiv). [h] $Co(acac)_3$ (20 mol%) instead of [Cp*CoI_2CO]. [i] $CoBr_2$ (20 mol%) instead of [Cp*CoI_2CO]. [j] $[Cp^*Co(CH_3CN)_3(SbF_6)_2]$ (10 mol%) instead of [Cp*CoI_2CO] and w/o $AgSbF_6$. [K] $Cu(OAc)_2 \cdot H_2O$ (100 mol%).

4. Typical procedure for the cobalt-catalyzed alkylation of heteroarenes:

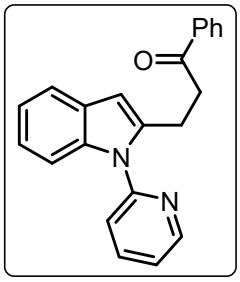


Oven dried sealed tube was charged with indole derivative **1** (0.26 mmol), (1.0 equiv), cyclopropanols **2** (0.78 mmol, 3 equiv), [Cp*CoI_2CO] (10 mol%), $AgSbF_6$ (20 mol%) and $Cu(OAc)_2 \cdot H_2O$ (100 mol%). The inner atmosphere was made inert through repeated (thrice) evacuation and refilled with nitrogen. Dry (MeOH:^{t}AmOH) (1:1), (2 mL) was added to the reaction mixture and the reaction mixture stirred at 100 °C temperature for 24 h. After completion of the reaction (monitored by TLC), the reaction mixture was cooled to room temperature, filtered through a pad of celite, and concentrated to get the crude product. The crude product was purified by column chromatography through silica gel to afford the expected product **3** in good to excellent yield.

5. Properties of isolated C2-alkylindoles

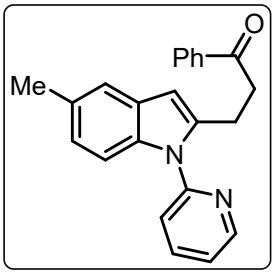
3-(1*H*-Indol-2-yl)-1-phenylpropan-1-one (3a):

Yield: 80%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3055, 2900, 1683, 1469, 1261, 972, 750; ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.63 (dd, J = 4.9, 1.9 Hz, 1H), 7.95-7.87 (m, 3H), 7.66 (s, 1H), 7.54 (t, J = 8.2 Hz, 1H), 7.47-7.40 (m, 3H), 7.33 (m, 1H), 7.17 (m, 2H), 6.41 (s, 1H), 3.37 (t, J = 9.4 Hz, 2H), 3.22 (t, J = 9.7 Hz, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 199.0, 151.5, 149.8, 140.4, 138.5, 137.4, 136.9, 133.2, 128.7, 128.6, 128.2, 128.1, 122.3, 122.0, 121.2, 120.8, 120.1, 110.2, 102.5, 38.3, 22.2; HRMS: (ESI) m/z calcd. for $C_{23}H_{18}N_2O$, 327.1492 $[M+H]^+$; found 327.1494.



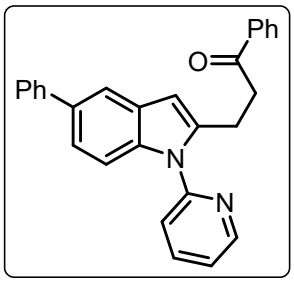
3-(5-Methyl-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one (3b):

Yield: 69%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3006, 2886, 1675, 1471, 1275, 970, 758; ^1H NMR (500 MHz, $CDCl_3$, 24 °C): δ 7.88-7.79 (m, 3H), 7.47 (t, J = 8.4 Hz, 1H), 7.36 (t, J = 7.8 Hz, 3H), 7.30-7.20 (m,



2H),), 7.15 (d, J = 8.0 Hz, 1H) 6.88 (d, J = 7.7 Hz, 1H) 6.33 (s, 1H), 3.35-3.27 (m, 2H), 3.24-3.14 (m, 2H), 2.35 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 199.1, 140.4, 138.5, 136.8, 135.7, 133.6, 133.2, 130.1, 128.9, 128.6, 128.2, 123.4, 119.9, 109.9, 102.2, 38.3, 22.3, 21.5; HRMS: (ESI) *m*/*z* calcd. for $C_{23}H_{20}N_2O$, 341.1648 $[M+H]^+$; found 341.1643.

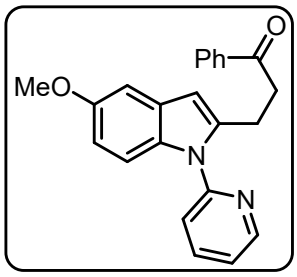
1-Phenyl-3-(5-phenyl-1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one (3c):



Yield: 68%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3007, 2860, 1683, 1468, 1256, 755; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.65 (d, J = 4.8 Hz, 1H), 7.97-7.90 (m, 3H), 7.78 (s, 1H), 7.64 (d, J = 7.5 Hz, 2H), 7.58-7.50 (m, 2H), 7.49-7.38 (m, 6H), 7.37-7.28 (m, 2H), 6.54 (s, 1H), 3.41 (t, J = 9.0 Hz, 2H), 3.26 (t, J = 9.3 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 199.0, 151.4, 149.9, 142.5, 141.1, 138.7, 136.9, 136.8, 134.4, 133.3, 129.2, 128.8, 128.7, 128.2, 127.5, 126.5, 122.4, 121.7, 121.2, 118.7, 110.6, 102.8, 38.3, 22.3.; HRMS: (ESI) *m*/*z* calcd. for $C_{28}H_{22}N_2O$, 403.1805 $[M+H]^+$; found 403.1816.

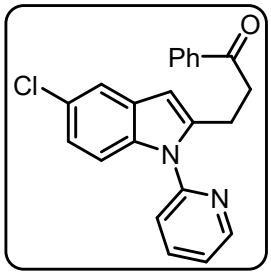
3-(5-Methoxy-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one (3d):

Yield: 84%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 2994, 1683, 1582, 1438, 1275, 760; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.62 (dd, J = 8.6, 2.0 Hz, 1H), 7.94 (dd, J = 8.3, 1.1 Hz, 1H), 7.88 (dt, J = 7.8, 2.0 Hz, 1H), 7.55 (dt, J = 7.5, 1.5 Hz, 1H), 7.47-7.43 (m, 3H), 7.30 (dd, J = 7.3, 1.0 Hz, 1H), 7.25 (d, J = 8.6 Hz, 1H), 7.04 (d, J = 2.4 Hz, 1H), 6.79 (dd, J = 8.9, 2.4 Hz, 1H), 6.42 (s, 1H), 3.85 (s, 3H), 3.39 (t, J = 9.2 Hz, 2H), 3.26 (t, J = 9.0 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 199.1, 154.9, 151.5, 149.8, 140.9, 138.5, 136.8, 133.2, 132.5, 128.7, 128.2, 122.1, 120.9, 111.5, 111.1, 102.4, 102.3, 55.9, 38.4, 22.4; HRMS: (ESI) *m*/*z* calcd. for $C_{23}H_{19}N_2O_2$, 357.1698 $[M+H]^+$; found 357.1605.



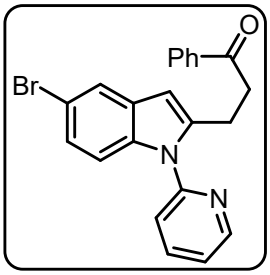
3-(5-Chloro-1-(pyridin-2-yl)-1H-indol-2-yl)-1-phenylpropan-1-one (3e):

Yield: 63%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3006, 2965, 1680, 1585, 1439, 1254, 755; IR (ν_{max}, cm^{-1}): 2994, 1683, 1582, 1438, 1275, 760. ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.62 (dd, J = 8.6, 2.0 Hz, 1H),



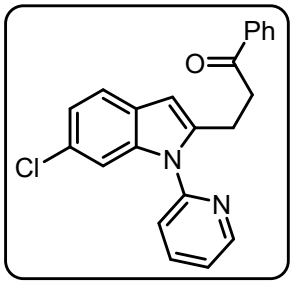
7.94 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.88 (dt, *J* = 7.8, 2.0 Hz, 1H), 7.55 (dt, *J* = 7.5, 1.5 Hz, 1H), 7.47-7.43 (m, 4H), 7.30 (dd, *J* = 7.3, 1.0 Hz, 1H), 7.25 (d, *J* = 8.6 Hz, 1H), 7.04 (d, *J* = 2.4 Hz, 1H), 6.79 (dd, *J* = 8.9, 2.4 Hz, 1H), 6.42 (s, 1H), 3.85 (s, 2H), 3.26 (t, *J* = 9.0 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): *δ* 199.1, 154.9, 151.5, 149.8, 140.9, 138.5, 136.8, 133.2, 132.5, 128.7, 128.2, 122.1, 120.9, 111.5, 111.1, 102.4, 102.3, 55.9, 38.4, 22.4; HRMS: (ESI) *m*/*z* calcd. for $C_{22}H_{18}ClN_2O$, 361.1102 $[M+H]^+$; found 361.1112.

3-(5-Bromo-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one (3f):



Yield: 65%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3007, 2862, 1683, 1466, 1265, 988, 756; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): *δ* 8.64 (d, *J* = 4.8 Hz, 1H), 7.96-7.89 (m, 3H), 7.67 (s, 1H), 7.55 (t, *J* = 7.9 Hz, 1H), 7.49-7.42 (m, 3H), 7.35 (t, *J* = 7.7 Hz, 1H), 7.22-7.16 (m, 2H) 6.42 (s, 1H) 3.38 (t, *J* = 7.9 Hz, 2H), 3.23 (t, *J* = 9.0 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): *δ* 198.7, 150.9, 149.9, 141.7, 138.7, 136.7, 136.1, 133.3, 130.3, 128.7, 128.1, 124.7, 122.6, 121.3, 113.9, 111.7, 101.8, 38.0, 22.4, 20.1; HRMS: (ESI) *m*/*z* calcd. for $C_{22}H_{17}BrN_2O$, 405.0597 $[M+H]^+$; found 405.0605.

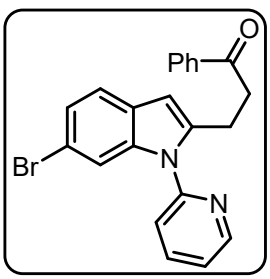
3-(6-Chloro-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one (3g):



Yield: 73%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3008, 1678, 1545, 1477, 1223, 751; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): *δ* 8.56 (s, 1H), 7.87-7.80 (m, 3H), 7.46 (t, *J* = 8.3 Hz, 1H), 7.39-7.30 (m, 4H), 7.26 (s, 1H), 7.19-7.10 (m, 2H), 6.35 (s, 1H), 3.28 (t, *J* = 7.8 Hz, 2H), 3.13 (t, *J* = 8.9 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): *δ* 198.7, 150.8, 150.0, 141.1, 138.8, 138.2, 136.7, 133.3, 128.7, 128.1, 127.4, 124.0, 122.7, 121.3, 115.5, 113.3, 102.3, 37.9, 22.1; HRMS: (ESI) *m*/*z* calcd. for $C_{22}H_{18}ClN_2O$, 361.1102 $[M+H]^+$; found 361.1067.

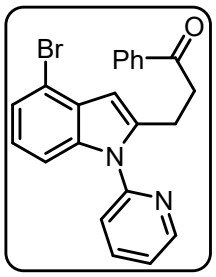
3-(6-Bromo-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one (3h):

Yield: 77%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 2990, 1689, 1567, 1470, 1234, 755; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): *δ* 8.56 (s, 1H), 7.87-7.80 (m, 3H), 7.46 (t, *J* = 8.3 Hz, 1H), 7.39-7.30 (m, 4H), 7.26 (s, 1H), 7.19-7.10 (m, 2H), 6.35 (s, 1H), 3.28 (t, *J* = 7.8 Hz, 2H), 3.13 (t, *J* =



8.9 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 198.7, 150.8, 150.0, 141.1, 138.8, 138.2, 136.7, 133.3, 128.7, 128.1, 127.4, 124.0, 122.7, 121.3, 115.5, 113.3, 102.3, 37.9, 22.1; HRMS: (ESI) *m*/*z* calcd. for $C_{22}H_{17}BrN_2O$, 405.0597 $[M+H]^+$; found 405.0568.

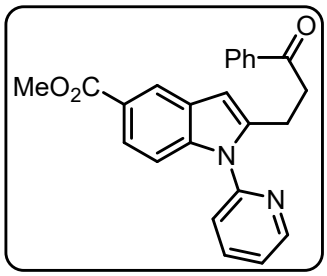
3-(4-Bromo-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one (3i):



Yield: 52%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3003, 1682, 1580, 1460, 1272, 941, 756; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.56 (s, 1H), 7.90-7.80 (m, 3H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.32-7.25 (m, 1H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 8.5 Hz, 1H), 6.46 (s, 1H), 3.34 (t, *J* = 8.4 Hz, 2H), 3.14 (t, *J* = 8.8 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 198.7, 150.9, 149.9, 141.2, 138.7, 137.6, 136.7, 133.3, 129.2, 128.7, 128.1, 123.6, 122.8, 121.4, 114.0, 109.5, 102.3, 37.9, 22.1; HRMS: (ESI) *m*/*z* calcd. for $C_{22}H_{18}BrN_2O$, 405.0597 $[M+H]^+$; found 405.0605.

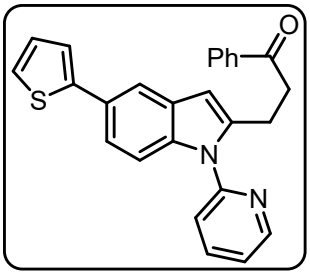
Methyl 2-(3-oxo-3-phenylpropyl)-1-(pyridin-2-yl)-1*H*-indole-5-carboxylate (3j):

Yield: 55 %; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 2937, 1685, 1583, 1468, 1262, 755; ^{1}H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.67 (dd, *J* = 4.8, 1.7 Hz, 1H), 8.00 (t, *J* = 0.9 Hz, 1H), 7.98-7.92 (m, 3H), 7.83 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.59-7.54 (m, 2H), 7.51 (dt, *J* = 8.0, 1.1 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.39 (dt, *J* = 7.5, 0.9 Hz, 1H), 6.53 (s, 1H), 3.88 (s, 3H), 3.42 (t, *J* = 8.1 Hz, 2H), 3.27 (t, *J* = 9.0 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 198.7, 168.2, 150.1, 144.1, 138.9, 136.8, 136.7, 133.4, 132.4, 128.7, 128.2, 123.6, 122.9, 122.1, 121.6, 111.7, 102.7, 52.0, 37.9, 22.2; HRMS: (ESI) *m*/*z* calcd. for $C_{24}H_{20}N_2O_3$, 385.1547 $[M+H]^+$; found 385.1554.



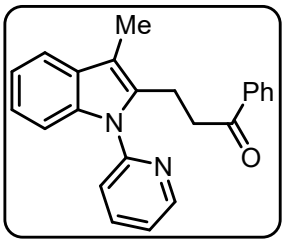
1-Phenyl-3-(1-(pyridin-2-yl)-5-(thiophen-2-yl)-1*H*-indol-2-yl)propan-1-one (3k):

Yield: 49 %; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 2990, 2857, 1683, 1587, 1470, 1261, 751; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.64 (d, *J* = 4.7 Hz, 1H), 7.96-7.86 (m, 3H), 7.77 (s, 1H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.51-7.26 (m, 8H), 6.50 (s, 1H), 3.39 (t, *J* = 9.1 Hz, 2H), 3.26 (t, *J* = 9.2 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ



198.9, 141.1, 138.6, 136.8, 136.7, 133.2, 129.1, 129.0, 128.7, 128.2, 126.8, 125.9, 122.4, 121.2, 121.2, 119.0, 117.9, 110.5, 102.7, 38.3, 22.2; HRMS: (ESI) *m*/*z* calcd. for $C_{26}H_{20}N_2OS$, 409.1369 $[M+H]^+$; found 409.1384.

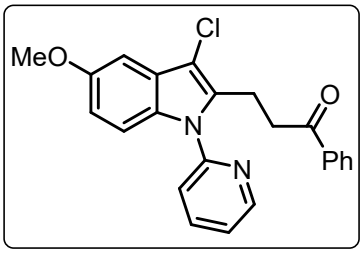
3-(3-Methyl-1-(pyridin-2-yl)-1H-indol-2-yl)-1-phenylpropan-1-one (3l):



Yield: 61% (Yield was calculated based on ^{1}H NMR); yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3056, 2993, 1680, 1518, 1262, 755; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.62 (s, 1H), 7.87 (d, J = 7.1 Hz, 1H), 7.56-7.47 (m, 3H), 7.44–7.38 (m, 2H), 7.37-7.33 (m, 2H), 7.15 (t, J = 7.2, 1.0 Hz, 2H), 3.26 (s, 4H), 2.33 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 199.5, 138.4, 136.8, 136.6, 135.8, 133.1, 129.6, 128.7, 128.6, 128.4, 128.3, 128.1, 122.1, 120.5, 118.5, 110.5, 109.9, 38.9, 20.2, 8.8; HRMS: (ESI) *m*/*z* calcd. for $C_{23}H_{20}N_2O$, 341.1648 $[M+H]^+$; found 341.1654.

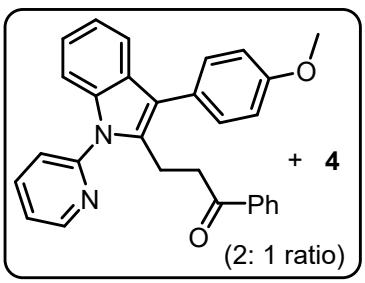
3-(3-Chloro-5-methoxy-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one (3m):

Yield: 61%; yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3020, 2860, 1680, 1567, 1234, 751; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.48 (d, J = 3.1 Hz, 1H), 7.89-7.76 (m, 3H), 7.45 (t, J = 8.1 Hz, 1H), 7.39–7.31 (m, 3H), 7.21 (dd, J = 7.1, 4.8 Hz, 1H), 7.16 (d, J = 8.5 Hz, 1H), 6.96 (d, J = 2.3 Hz, 1H), 6.75 (dd, J = 8.6, 2.4 Hz, 1H), 3.80 (s, 3H), 3.34-3.27 (m, 2H), 3.17 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 198.9, 155.5, 150.8, 149.8, 138.6, 136.6, 135.8, 133.2, 130.3, 128.2, 126.7, 122.5, 120.7, 113.3, 111.6, 106.6, 99.4, 55.9, 37.9, 20.2; HRMS: (ESI) *m*/*z* calcd. for $C_{23}H_{19}ClN_2O_2$, 391.1208 $[M+H]^+$; found 391.1300.



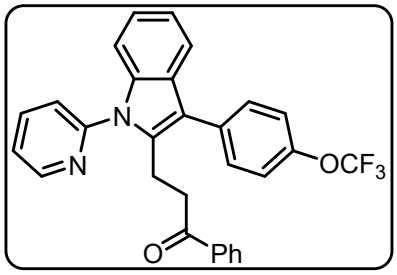
3-(3-Chloro-5-methoxy-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one (3n):

Yield: 48% (Yield was calculated based on ^{1}H NMR); (2: 1 ratio of **3m** and **4**); yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3006, 2856, 1670, 1567, 1234, 755; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.47 (d, J = 3.8 Hz, 1H), 7.87-7.83 (m, 3H), 7.80 (d, J = 7.6 Hz, 1H),



7.72–7.69 (m, 3H), 7.46-7.7.41 (m, 2H), 7.37-7.32 (m, 2H), 7.32 (dt, J = 8.5, 1.0 Hz, 2H), 7.05 (dt, J = 7.2, 0.6 Hz, 2H), 3.75 (s, 3H), 3.75 (s, 3H), 3.27 (s, 4H); 2.93-2.90 (m, 2H), 1.74-1.72 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 200.7, 198.3, 158.6, 152.3, 149.0, 138.4, 137.0, 135.7, 133.2, 133.0, 128.9, 128.7, 128.3, 128.1, 127.2, 127.1, 126.8, 123.5, 122.8,121.6, 120.5, 120.1, 120.0, 114.6, 114.3, 113.3, 58.3, 38.7, 38.4, 27.7, 23.9; HRMS: (ESI) *m*/*z* calcd. for $C_{29}H_{24}N_2O_2$, 433.1911 $[M+H]^+$; found 433.1923.

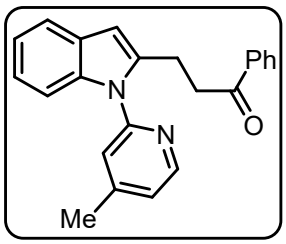
1-Phenyl-3-(1-(pyridin-2-yl)-3-(4-(trifluoromethoxy)phenyl)-1H-indol-2-yl)propan-1-one (3o):



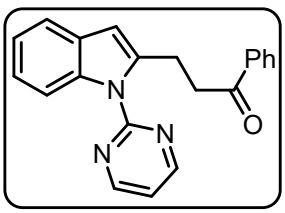
Yield: 45%; yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3008, 2987, 1678, 1446, 1245, 987, 750; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.64 (d, J = 4.6 Hz, 1H), 7.99-7.88 (m, 4H), 7.55-7.53 (m, 3H), 7.52–7.29 (m, 4H), 7.16-7.15 (m, 2H), 7.13 (d, J = 6.5 Hz, 2H), 6.49 (s, 1H), 3.42–3.37 (m, 2H), 3.29-3.24 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 199.1, 151.5, 149.8, 140.4, 138.6, 137.4, 136.8, 133.2, 128.7, 128.3, 128.2, 124.9, 122.3, 122.0, 121.3, 120.9, 120.2, 110.3, 102.5, 38.3, 20.3; HRMS: (ESI) *m*/*z* calcd. for $C_{29}H_{21}F_3N_2O_2$, 487.1628 $[M+H]^+$; found 487.1623.

3-(1-(4-Methylpyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one (3p):

Yield: 64 %; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3007, 1684, 1456, 1273, 754; ^{1}H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.49 (d, J = 4.9 Hz, 1H), 7.94 (d, J = 7.6 Hz, 2H), 7.60-7.54 (m, 2H), 7.45 (t, J = 7.9 Hz, 2H), 7.33-7.28 (m, 2H), 7.17-7.11 (m, 3H), 6.48 (s, 1H), 3.40 (t, J = 9.5 Hz, 2H), 3.25 (t, J = 9.4 Hz, 2H), 2.46 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 199.1, 151.4, 150.1, 149.4, 140.4, 137.5, 136.8, 133.2, 128.7, 128.6, 128.2, 123.5, 122.0, 121.8, 120.7, 120.1, 102.2, 38.3, 22.2, 21.2; HRMS: (ESI) *m*/*z* calcd. for $C_{23}H_{20}N_2O$, 341.11648 $[M+H]^+$; found 341.1661.



1-Phenyl-3-(1-(pyrimidin-2-yl)-1*H*-indol-2-yl)propan-1-one (3q):

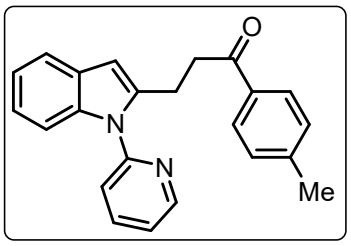


Yield: 74%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3008, 2912, 1678, 1589, 1448, 1234, 690; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.77 (d, J = 4.8 Hz, 2H), 8.32 (d, J = 8.3 Hz, 1H),

7.99 (d, J = 8.4 Hz, 2H), 7.58-7.50 (m, 2H), 7.46 (t, J = 8.4 Hz, 2H), 7.25-7.18 (m, 2H), 7.13 (t, J = 5.0 Hz, 1H), 6.53 (s, 1H), 3.59 (t, J = 8.6 Hz, 2H), 3.46 (t, J = 8.0 Hz, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 199.4, 158.3, 140.9, 137.1, 133.1, 129.4, 128.7, 128.2, 122.1, 119.9, 117.2, 114.3, 106.3, 72.9, , 38.9, 24.3; HRMS: (ESI) m/z calcd. for $C_{21}H_{17}N_3O$, 328.1444 $[M+H]^+$; found 328.1456.

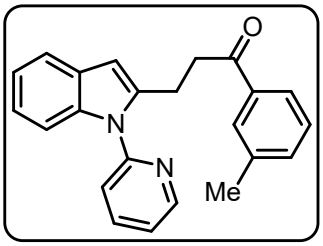
3-(1-(Pyridin-2-yl)-1*H*-indol-2-yl)-1-(p-tolyl)propan-1-one (3r):

Yield: 72%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3008, 2912, 1680, 1469, 1427, 1181, 752; ^1H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.64 (dd, J = 4.8, 1.3 Hz, 1H), 7.89 (dt, J = 7.6, 2.0 Hz, 1H), 7.83 (d, J = 8.1 Hz, 2H), 7.57 (dd, J = 7.6, 3.0 Hz, 1H), 7.48 (d, J = 8.1 Hz, 1H), 7.35-7.30 (m, 2H), 7.24 (d, J = 8.1 Hz, 2H), 7.15-7.11 (m, 2H), 6.48 (s, 1H), 3.36 (t, J = 8.1 Hz, 2H), 3.24 (t, J = 7.6 Hz, 2H), 2.40 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 198.7, 151.4, 149.8, 144.0, 140.5, 138.6, 137.4, 134.4, 129.4, 128.7, 128.3, 122.3, 121.9, 121.3, 120.8, 120.1, 110.3, 102.4, 38.1, 22.3, 21.7; HRMS: (ESI) m/z calcd. for $C_{23}H_{20}N_2O$, 341.1648 $[M+H]^+$; found 341.1653.



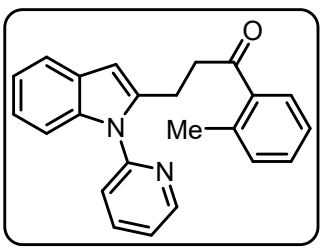
3-(1-(Pyridin-2-yl)-1*H*-indol-2-yl)-1-(*p*-tolyl)propan-1-one (3s):

Yield: 53%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3008, 2912, 1680, 1469, 1427, 1181, 752; ^1H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.64 (dd, J = 4.8, 1.3 Hz, 1H), 7.89 (dt, J = 7.6, 2.0 Hz, 1H), 7.83 (d, J = 8.1 Hz, 2H), 7.57 (dd, J = 7.6, 3.0 Hz, 1H), 7.48 (d, J = 8.1 Hz, 1H), 7.35-7.30 (m, 2H), 7.24 (d, J = 8.1 Hz, 2H), 7.15-7.11 (m, 2H), 6.48 (s, 1H), 3.36 (t, J = 8.1 Hz, 2H), 3.24 (t, J = 7.6 Hz, 2H), 2.40 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 198.7, 151.4, 149.8, 144.0, 140.5, 138.6, 137.4, 134.4, 129.4, 128.7, 128.3, 122.3, 121.9, 121.3, 120.8, 120.1, 110.3, 102.4, 38.1, 22.3, 21.7; HRMS: (ESI) m/z calcd. for $C_{23}H_{20}N_2O$, 341.1648 $[M+H]^+$; found 341.1653.



3-(1-(Pyridin-2-yl)-1*H*-indol-2-yl)-1-(*o*-tolyl)propan-1-one (3t):

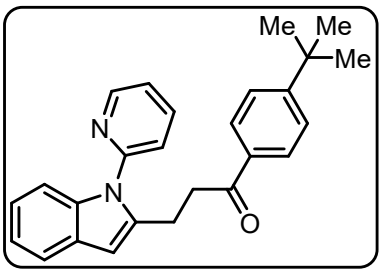
Yield: 48%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3008, 2993, 1668, 1445, 1260, 751; ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.63 (dd, J = 8.6, 2.0 Hz, 1H), 7.89 (dt, J = 7.8, 1.9 Hz, 1H), 7.75-7.71 (m, 2H),



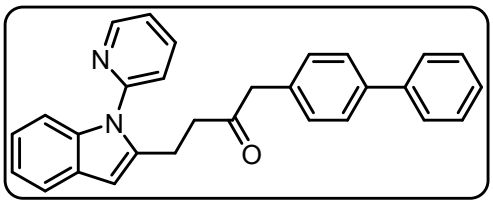
7.56 (dd, *J* = 7.6, 2.6 Hz, 1H), 7.48 (d, *J* = 7.9 Hz, 1H), 7.37-7.30 (m, 4H), 7.15-7.11 (m, 2H), 6.49 (s, 1H), 3.39-3.35 (m, 2H), 3.27-3.23 (m, 2H), 2.38 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 199.3, 151.4, 149.8, 140.4, 138.6, 138.6, 138.5, 137.4, 136.8, 133.9, 128.7, 128.7, 128.6, 125.4, 122.3, 121.9, 121.3, 120.8, 120.1, 102.4, 38.3, 22.6, 21.5; HRMS: (ESI) *m*/*z* calcd. for $C_{23}H_{20}N_2O$, 341.1648 $[M+H]^+$; found 341.1651.

1-(4-(*tert*-Butyl)phenyl)-3-(1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one (3u):

Yield: 87%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3020, 2880, 1676, 1554, 1245, 990, 750; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.50 (d, *J* = 4.4 Hz, 1H), 7.76 (d, *J* = 8.5 Hz, 2H), 7.72 (d, *J* = 7.5 Hz, 1H), 7.44 (dd, *J* = 5.9, 2.7 Hz, 1H), 7.37-7.30 (m, 3H), 7.22 (t, *J* = 4.8 Hz, 1H), 7.15 (t, *J* = 7.6 Hz, 1H), 7.01 (dd, *J* = 5.7, 2.5 Hz, 2H), 6.37 (s, 1H), 3.24 (t, *J* = 9.5 Hz, 2H), 3.14 (t, *J* = 9.3 Hz, 2H), 1.21 (s, 9H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 198.5, 156.8, 151.3, 149.7, 140.4, 138.4, 137.3, 134.2, 128.6, 128.0, 122.2, 121.8, 121.2, 120.7, 120.1, 110.2, 102.3, 38.0, 35.1, 31.1, 22.2; HRMS: (ESI) *m*/*z* calcd. for $C_{26}H_{26}N_2O$, 405.1937 $[M+Na]^+$; found 405.1929.



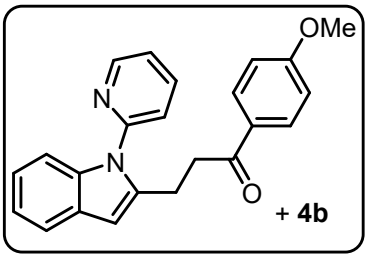
1-([1,1'-Biphenyl]-4-yl)-3-(1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one (3v) and 1-phenylpropan-1-ol:



Yield: 67% (Yield was calculated based on ^{1}H NMR); yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3006, 2990, 1670, 1545, 1424, 991, 760; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.63 (d, *J* = 4.8 Hz, 1H), 7.99 (d, *J* = 8.8 Hz, 2H), 7.88 (t, *J* = 7.9 Hz, 1H), 7.68-7.54 (m, 12H), 7.50-7.38 (m, 12H), 7.36-7.31 (m, 3H) 7.16-7.11 (m, 2H) 6.50 (s, 1H), 4.46 (t, *J* = 7.1 Hz, 1H), 3.43-3.37 (m, 2H), 3.30-3.25 (m, 2H), 1.88-1.77 (m, 1H), 0.94 (t, *J* = 7.3 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 198.6, 151.4, 149.8, 145.8, 143.7, 140.9, 140.5, 140.4, 139.9, 138.6, 137.8, 135.5, 129.1, 128.8, 128.7, 128.3, 127.3, 127.2, 127.1, 126.5, 122.0, 121.3, 120.8, 120.1, 110.2, 102.4, 75.8, 38.3, 31.9, 22.2, 10.3; HRMS: (ESI) *m*/*z* calcd. for $C_{29}H_{24}N_2O$, 403.1805 $[M+H]^+$; found 403.1796.

3-(5-Methoxy-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-(4-methoxyphenyl)propan-1-one (3w):

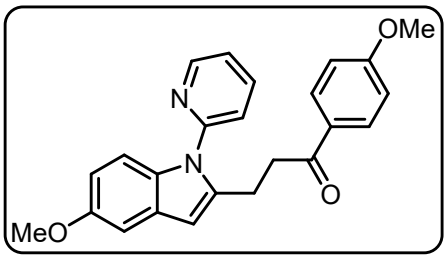
Yield: 81% (Yield was calculated based on ^{1}H NMR); (2: 1) ratio of **3w** and **4b**; yellow liquid;



Rf= 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3009, 2990, 1670, 1559, 1270, 984, 751; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.55 (d, J = 3.8 Hz, 1H), 7.88-7.72 (m, 5H), 7.47 (dd, J = 5.7, 2.7 Hz, 1H), 7.39 (d, J = 8.0 Hz, 1H), 7.26-7.20 (m, 2H), 6.82 (dd, J = 8.1, 6.1 Hz, 4H) 6.39 (s, 1H) 3.76 (s, 3H) 3.26 (s, 2H), 3.27-3.21 (m, 2H), 3.19-3.12 (m, 2H), 2.91-2.85 (m, 1.6H), 1.76-1.70 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 198.8, 197.6, 163.6, 151.4, 149.7, 140.5, 138.6, 137.4, 130.4, 128.6, 122.3, 121.9, 121.3, 120.8, 120.1, 113.8, 113.7, 110.2, 102.4, 55.5, 38.8, 37.8, 24.3, 22.3; HRMS: (ESI) *m*/*z* calcd for $C_{23}H_{19}N_2O_2$, 379.1417 $[M+Na]^+$; found 379.1409.

3-(5-Methoxy-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-(4-methoxyphenyl)propan-1-one (3x):

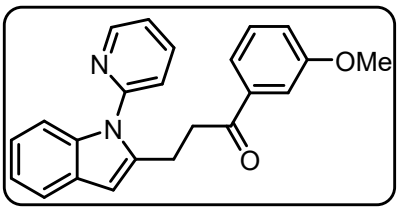
Yield: 68% (Yield was calculated based on ^{1}H NMR); (20: 1) ratio of 3ax and 4x; yellow liquid;



R_f = 0.50 in 2:8 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3007, 2964, 1675, 1445, 1234, 751; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.66 (s, 1H), 7.94-7.90 (m, 4H), 7.67 (s, 1H), 7.54 (dd, J = 7.5, 8.1 Hz, 1H), 7.45 (d, J = 7.5 Hz, 1H), 7.35 (d, J = 7.3 Hz, 1H), 7.19 (s, 1H), 6.95-6.89 (m, 2H), 6.41 (s, 1H), 3.86 (s, 6H), 3.32 (t, J = 8.1 Hz, 2H), 3.22 (t, J = 8.2 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 197.2, 163.6, 141.7, 138.7, 136.0, 130.6, 130.3, 129.7, 124.6, 122.6, 122.5, 113.9, 113.8, 113.8, 113.7, 111.6, 55.6, 55.5, 37.4, 22.2; HRMS: (ESI) *m*/*z* calcd. for $C_{24}H_{22}N_2O_3$, 387.1703 $[M+H]^+$; found 387.1714.

1-(4-Methoxyphenyl)-3-(1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one (3y):

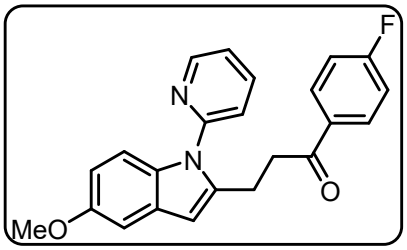
Yield: 60%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3012, 2903, 1683, 1279, 751; ^{1}H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.55 (d, J = 4.0 Hz, 1H), 7.78 (t, J = 7.8 Hz, 1H), 7.47 (dd, J = 6.5, 2.5 Hz, 3H), 7.42-7.36 (m, 3H), 7.26-7.19 (m, 3H), 7.05-6.97 (m, 3H), 6.39 (s, 1H), 3.72 (s, 3H), 3.27 (t, J = 8.7 Hz, 2H), 3.16 (t, J =



8.7 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 198.8, 159.9, 151.3, 149.7, 140.3, 138.6, 138.5, 138.2, 137.3, 129.6, 128.6, 122.3, 121.9, 121.3, 120.8, 120.7, 120.1, 119.6, 114.4, 112.4, 110.2, 102.4, 55.5, 38.3, 22.3; HRMS: (ESI) *m/z* calcd. for $C_{23}H_{20}N_2O_2$, 357.1598 $[M+H]^+$; found 357.1603.

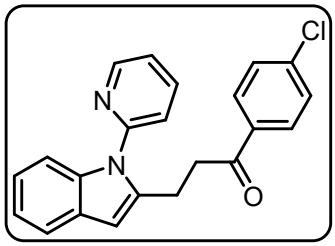
1-(4-Fluorophenyl)-3-(5-methoxy-1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one (3z):

Yield: 68%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3008, 2998, 1678, 1588, 1465, 1224, 750; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.52 (d, *J* = 4.6 Hz, 1H), 7.86 (dd, *J* = 7.4, 3.0 Hz, 2H), 7.97 (dt, *J* = 8.6, 1.8 Hz, 1H), 7.36 (d, *J* = 7.9 Hz, 1H), 7.20 (dd, *J* = 6.8, 2.3 Hz, 1H), 7.16 (d, *J* = 9.1 Hz, 1H), 7.01 (t, *J* = 8.9 Hz, 2H), 6.94 (d, *J* = 2.1 Hz, 1H), 6.70 (dd, *J* = 8.7, 2.5 Hz, 1H), 6.31 (s, 1H), 3.75 (s, 3H), 3.26 (t, *J* = 9.3 Hz, 2H), 3.15 (t, *J* = 8.6 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 197.5, 167.1, 164.6, 154.9, 151.5, 149.7, 140.8, 138.5, 133.3, 133.2, 132.4, 130.8, 130.7, 129.2, 122.1, 120.9, 115.8, 115.7, 111.6, 111.1, 110.5, 102.3, 55.9, 38.3, 22.3; HRMS: (ESI) *m/z* calcd. for $C_{23}H_{19}FN_2O_2$, 375.1503 $[M+H]^+$; found 375.1535.



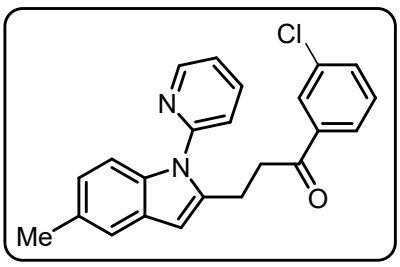
1-(4-Chlorophenyl)-3-(1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one (3aa):

Yield: 66%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3008, 2860, 1687, 1468, 1234, 990, 751; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.55 (dd, *J* = 4.8, 2.0 Hz, 1H), 7.85-7.77 (m, 3H), 7.49 (dd, *J* = 5.7, 3.1 Hz, 1H), 7.41 (dt, *J* = 7.8, 1.1 Hz, 1H), 7.34 (d, *J* = 7.3 Hz, 2H), 7.27-7.24 (m, 2H) 7.07-7.05 (m, 2H), 6.40 (s, 1H) 3.31-3.27 (m, 2H), 3.19-3.15 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 197.8, 151.4, 149.8, 140.1, 139.7, 138.6, 137.3, 135.1, 129.6, 129.0, 128.6, 127.5, 122.3, 121.2, 120.9, 120.2, 110.3, 102.6, 38.3, 22.2; HRMS: (ESI) *m/z* calcd. for $C_{22}H_{17}ClN_2O$, 361.1102 $[M+H]^+$; found 361.1094.



1-(3-Chlorophenyl)-3-(5-methyl-1-(pyridin-2-yl)-1H-indol-2-yl)propan-1-one (3ab):

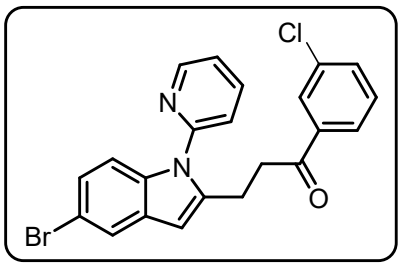
Yield: 71%; yellow liquid; *Rf*= 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3079, 2918, 1689, 1584, 1469, 1202, 785; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.61 (d, *J* = 3.7 Hz, 1H), 7.92-7.86 (m, 2H), 7.80 (d, *J* = 7.7



Hz, 1H), 7.49-7.45 (m, 2H), 7.40-7.33 (m, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.23-7.20 (m, 2H), 6.96 (d, *J* = 8.4 Hz, 1H), 6.40 (s, 1H), 3.36 (t, *J* = 9.0 Hz, 2H), 3.24 (t, *J* = 8.7 Hz, 2H), 2.43 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 197.9, 151.5, 149.7, 140.1, 138.5, 138.4, 135.6, 135.0, 133.1, 130.2, 128.9, 128.9, 128.3, 126.2, 123.5, 122.1, 120.9, 119.9, 109.9, 102.3, 38.5, 22.2, 21.5; HRMS: (ESI) *m*/*z* calcd for $C_{23}H_{19}ClN_2O$, 397.1070 $[M+Na]^+$; found 397.1073.

3-(5-Bromo-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-(3-chlorophenyl)propan-1-one (3ac):

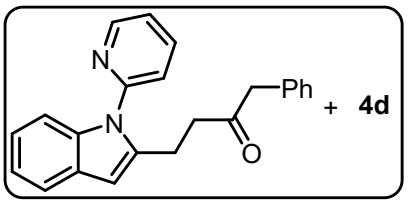
Yield: 67%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3072, 2934, 1689,



1575, 1472, 1337, 1200, 787; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.65 (d, *J* = 4.2 Hz, 1H), 7.95-7.88 (m, 2H), 7.80 (d, *J* = 7.7 Hz, 1H), 7.67-7.45 (s, 1H), 7.52 (t, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.42-7.34 (m, 2H), 7.23-7.15 (m, 2H), 6.41 (s, 1H), 3.36 (t, *J* = 9.1 Hz, 2H), 3.22 (t, *J* = 8.7 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 197.9, 150.9, 149.9, 141.3, 138.8, 138.3, 136.0, 135.1, 133.2, 130.3, 128.2, 126.2, 124.8, 122.7, 122.6, 121.2, 114.0, 111.7, 101.9, 38.2, 22.1; HRMS: (ESI) *m*/*z* calcd. for $C_{22}H_{16}BrClN_2O$, 439.0207 $[M+H]^+$; found 441.0316.

1-Phenyl-4-(1-(pyridin-2-yl)-1*H*-indol-2-yl)butan-2-one (3ad):

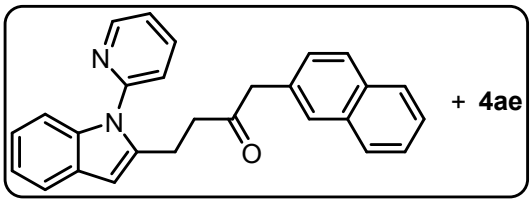
Yield: 79% (Yield was calculated based on ^{1}H NMR); (1: 1) ratio of **3ad** and **4d**; yellow liquid;



R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3059, 2933, 1710, 1585, 1461, 1211, 1090, 701; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.65 (d, *J* = 4.4 Hz, 1H), 7.83 (t, *J* = 7.8 Hz, 1H), 7.52 (t, *J* = 4.7 Hz, 1H), 7.37 (t, *J* = 7.9 Hz, 1H), 7.33-7.21 (m, 9H), 7.19-7.07 (m, 6H), 6.31 (s, 1H), 3.63 (s, 2H), 3.62 (s, 2H), 3.05 (t, *J* = 8.7 Hz, 2H), 2.82 (t, *J* = 7.9 Hz, 2H), 2.41-2.35 (m, 2H), 1.49-1.43 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 208.1, 207.1, 151.2, 149.7, 139.9, 138.4, 137.2, 134.3, 134.1, 129.4, 128.8, 128.5, 127.1, 127.0, 122.2, 121.9, 121.1, 120.8, 120.8, 120.1, 110.1, 102.3, 50.2, 50.1, 41.6, 41.1, 23.0, 21.7; HRMS: (ESI) *m*/*z* calcd. for $C_{23}H_{20}N_2O$, 341.1648 $[M+H]^+$; found 341.1618.

1-(Naphthalen-2-yl)-4-(1-(pyridin-2-yl)-1*H*-indol-2-yl)butan-2-one (3ae):

Yield: 72% (Yield was calculated based on ^{1}H NMR); (4: 1) ratio of **3ae** and **4ae**; yellow liquid;

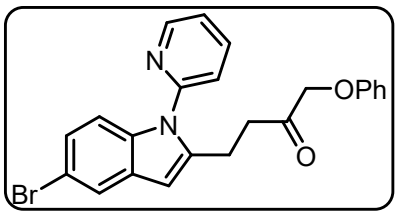


R_f= 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3056,

2912, 1679, 1554, 1443, 1224, 755; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.36 (dd, J = 4.8, 1.6 Hz, 1H), 7.71-7.60 (m, 7H), 7.50 (s, 0.7H), 7.46 (s, 1H), 7.39-7.31 (m, 5H), 7.19-7.10 (m, 5H), 7.05(dd, J = 7.5, 0.7 Hz, 1H), 7.00-6.96 (m, 2H), 6.19 (s, 1H), 3.67 (s, 2H), 3.64 (s, 1.4H), 2.96 (t, J = 9.3 Hz, 2H), 2.70 (t, J = 9.3 Hz, 2H), 2.31-2.28 (m, 1.3 H), 1.38-1.35 (m, 1.3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 208.1, 207.1, 151.2, 149.6, 139.8, 138.3, 137.2, 133.6, 132.5, 131.8, 131.6, 128.5, 128.4, 128.1, 127.8, 127.7, 127.5, 127.4, 126.3, 125.9, 125.8, 122.3, 121.9, 120.9, 120.7, 120.1, 110.1, 102.5, 50.4, 50.3, 41.6, 43.1, 23.0, 21.7; HRMS: (ESI) *m*/*z* calcd. for $C_{27}H_{22}N_2O$, 391.1805 $[M+H]^+$; found 391.1818.

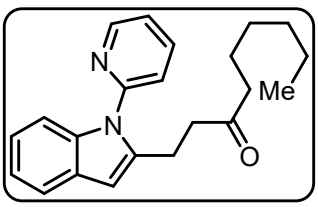
4-(5-Bromo-1-(pyridin-2-yl)-*1H*-indol-2-yl)-1-phenoxybutan-2-one (3af):

Yield: 54%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3072, 2934, 1689, 1575, 1472, 1337, 1200, 787; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.53 (s, 1H), 7.81 (t, J = 8.7 Hz, 1H), 7.59 (s, 1H), 7.33-7.23 (m, 2H), 7.22-7.16 (m, 2H), 7.15-7.05 (m, 2H), 6.91 (t, J = 7.9 Hz, 1H), 6.74 (d, J = 8.2 Hz, 2H), 6.28 (s, 1H), 4.44 (s, 2H), 3.05 (t, J = 8.5 Hz, 2H), 2.92 (t, J = 8.7 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 206.7, 157.7, 141.1, 138.7, 135.9, 130.3, 130.2, 129.8, 129.8, 129.7, 128.9, 124.8, 122.7, 121.9, 114.5, 114.0, 111.7, 101.9, 72.9, 38.3, 22.0; HRMS: (ESI) *m*/*z* calcd. for $C_{23}H_{19}BrN_2O_2$, 457.0522 $[M+Na]^+$; found 457.0522.



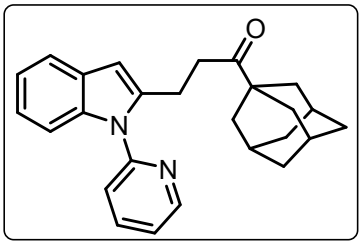
1-(1-(Pyridin-2-yl)-1*H*-indol-2-yl)nonan-3-one (3ag):

Yield: 77%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3119, 2926, 1712, 1276, 1461, 1276, 1173, 758; ^{1}H NMR (500 MHz, $CDCl_3$, 24 °C): δ 8.61 (dd, J = 5.0, 1.7 Hz, 1H), 7.85 (dt, J = 8.0, 1.9 Hz, 1H), 7.54 (dd, J = 7.5, 3.0 Hz, 1H), 7.42 (d, J = 8.0 Hz, 1H), 7.32-7.26 (m, 2H), 7.13-7.09 (m, 2H), 6.31 (s, 1H), 3.01 (t, J = 9.4 Hz, 2H), 2.76 (t, J = 9.2 Hz, 2H), 2.35 (t, J = 8.3 Hz, 2H), 1.56-1.49 (m, 2H), 1.32-1.20 (m, 8H), 0.86 (t, J = 7.3 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C): δ 209.9, 167.1, 151.3, 149.7, 140.2, 138.4, 138.4, 137.3, 128.6, 122.2, 121.9, 121.1, 120.8, 120.0, 110.2, 102.3, 42.9, 41.8, 31.6, 28.9, 23.8, 22.5, 21.7, 14.1; HRMS: (ESI) *m*/*z* calcd. for $C_{22}H_{26}N_2O$, 335.2118 $[M+H]^+$; found 335.2132.



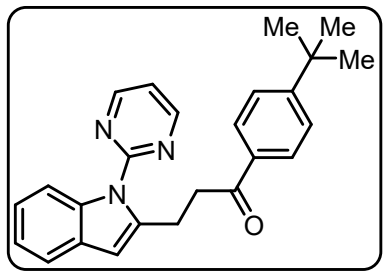
1-Adamantan-1-yl)-3-(1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one (3ah):

Yield: 55%; yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^1): 3008, 2912, 1680, 1460, 1427, 1181, 752; ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.64 (d, J = 4.7 Hz, 1H), 7.89 (td, J = 8.4, 1.6 Hz, 1H), 7.56 (dd, J = 5.6, 3.2 Hz, 1H), 7.46 (d, J = 7.7 Hz, 1H), 7.32 (m, 2H), 7.12 (dd, J = 5.8, 3.2 Hz, 2H), 6,42 (s, 1H), 3.03 (t, J = 9.5 Hz, 2H), 2.85 (t, J = 8.0 Hz, 2H), 2.02 (m, 3H), 1.76 (m, 7H), 1.72-1.70 (m , 2H), 1.65 (m, 5H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 214.5, 151.5, 149.8, 140.7, 138.5, 137.4, 128.7, 122.3, 121.9, 121.9, 121.3, 120.8, 120.1, 110.3, 102.2, 46.4, 38.3, 36.7, 35.8, 28.0, 21.8; HRMS: (ESI) *m*/*z* calcd. for $C_{26}H_{29}N_2O$, 385.2274 $[M+H]^+$; found 385.2280.



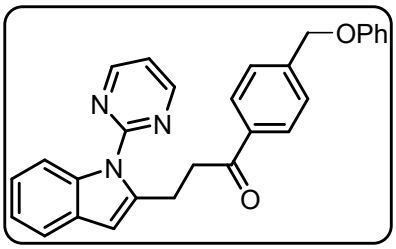
1-(4-(*tert*-Butyl)phenyl)-3-(1-(pyrimidin-2-yl)-1*H*-indol-2-yl)propan-1-one (3ai):

Yield: 72%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 2993, 1680, 1574, 1476, 1250, 690; ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.76 (d, J = 7.5 Hz, 2H), 8.30 (d, J = 8.2 Hz, 1H), 7.91 (d, J = 8.3 Hz, 2H), 7.52 (d, J = 7.6 Hz, 2H), 7.23-7.15 (m, 2H), 7.12 (t, J = 4.8 Hz, 1H), 6.52 (s, 1H), 3.58 (t, J = 8.1 Hz, 2H), 3.42 (t, J = 7.1 Hz, 2H), 1.33 (s, 9H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 199.1, 158.3, 156.9, 141.1, 137.1, 134.5, 129.4, 128.2, 125.6, 122.8, 122.1, 119.8, 117.2, 114.2, 106.3, 38.8, 35.2, 31.2, 24.3; HRMS: (ESI) *m*/*z* calcd. for $C_{25}H_{25}N_3O$, 384.2070 $[M+H]^+$; found 384.2084.



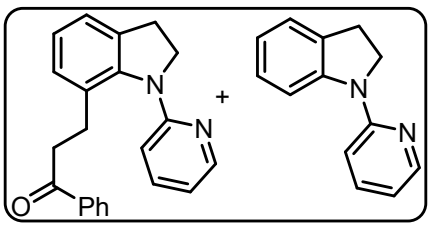
1-(4-(phenoxymethyl)phenyl)-3-(1-(pyrimidin-2-yl)-1H-indol-2-yl)propan-1-one (3aj):

Yield: 73%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3007, 2912, 1689, 1555, 1470, 1220, 755; ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.73 (d, J = 5.5 Hz, 2H), 8.30 (d, J = 8.2 Hz, 1H), 7.51 (d, J = 6.8 Hz, 1H), 7.22-7.11 (m, 2H), 6.98 (t, J = 8.1 Hz, 1H), 6.84 (d, J = 6.9 Hz, 6.46 (s, 1H), 4.56 (s, 2H), 3.48 (t, J = 8.4 Hz, 2H), 3.08 (t, J = 8.7 Hz, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 207.0, 157.8, 140.3, 137.0, 129.7, 122.9, 122.1, 121.8, 119.9, 117.1, 114.6, 114.3, 106.5, 72.9, , 39.2, 23.3; HRMS: (ESI) *m*/*z* calcd. for $C_{28}H_{23}N_3O_2$, 434.1863 $[M+H]^+$; found 434.1860.



1-(4-(phenoxymethyl)phenyl)-3-(1-(pyrimidin-2-yl)-1*H*-indol-2-yl)propan-1-one (3ak):

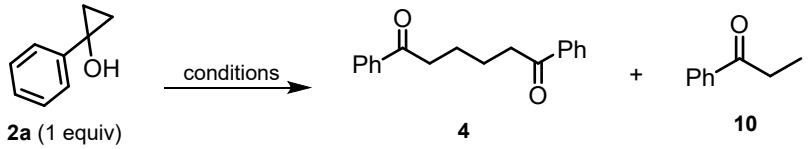
Yield: 12% (Yield was calculated based on ^{1}H NMR); yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 3067, 3008, 2980, 1676, 1554, 1260, 750; ^{1}H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.57 (d, J = 4.4 Hz, 0.2H), 8.34 (d, J = 4.0 Hz, 1H), 8.20 (d, J = 8.5 Hz, 0.2H), 8.17 (d, J = 8.1 Hz, 1H), 8.57 (dt, J = 8.1, 1.9 Hz, 0.2H), 7.72 (d, J = 3.4, 0.2 Hz, 0.2H), 7.66 (d, J = 7.4 Hz, 0.2H), 7.58 (dt, J = 8.7, 1.6 Hz, 1H), 7.39–7.31 (m, 3H), 7.21 (dd, J = 7.1, 4.8 Hz, 1H), 7.16 (d, J = 8.5 Hz, 1H), 6.96 (d, J = 2.3 Hz, 1H), 7.4 (d, J = 7.8 Hz, 0.2H), 7.21-7.15 (m, 2.5H), 6.86 (d, J = 7.5 Hz, 1H), 6.80-6.75 (m, 2H), 6.71 (d, J = 3.2 Hz, 0.2H), 4.04 (t, J = 8.9 Hz, 2.2H), 3.21 (t, J = 8.8 Hz, 2.2H); HRMS: (ESI) m/z calcd. for $C_{23}H_{21}N_2O$, 328.1696 $[M+H]^+$; found 328.1684.



6. Mechanistic investigation

6.1 Control experiment with cyclopropanol 2a:

General experimental procedure was followed for the control experiment reactions.

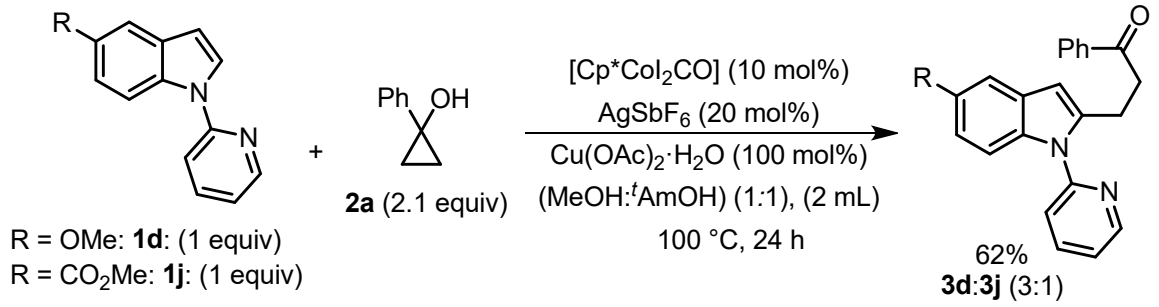


2a (1 equiv) **4** **10**

Entry	Cp*CoI_2CO [10 mol%]	$AgSbF_6$ [20 mol%]	$Cu(OAc)_2 \cdot H_2O$ [100 mol%]	Yield (%)[a]	
				4	**10**
1	✓	✓	✓	17	41
2	-	✓	✓	51	4
3	✓	-	✓	33	11
4	✓	✓	-	16	ND

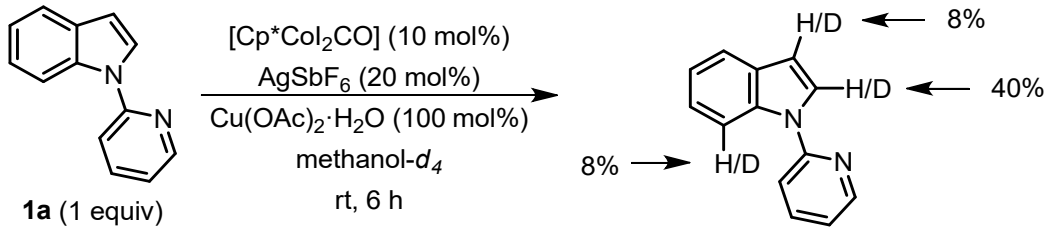
[a] All are isolated yield.

6.2 Intermolecular competitive experiment with *N*-pyridylindoles

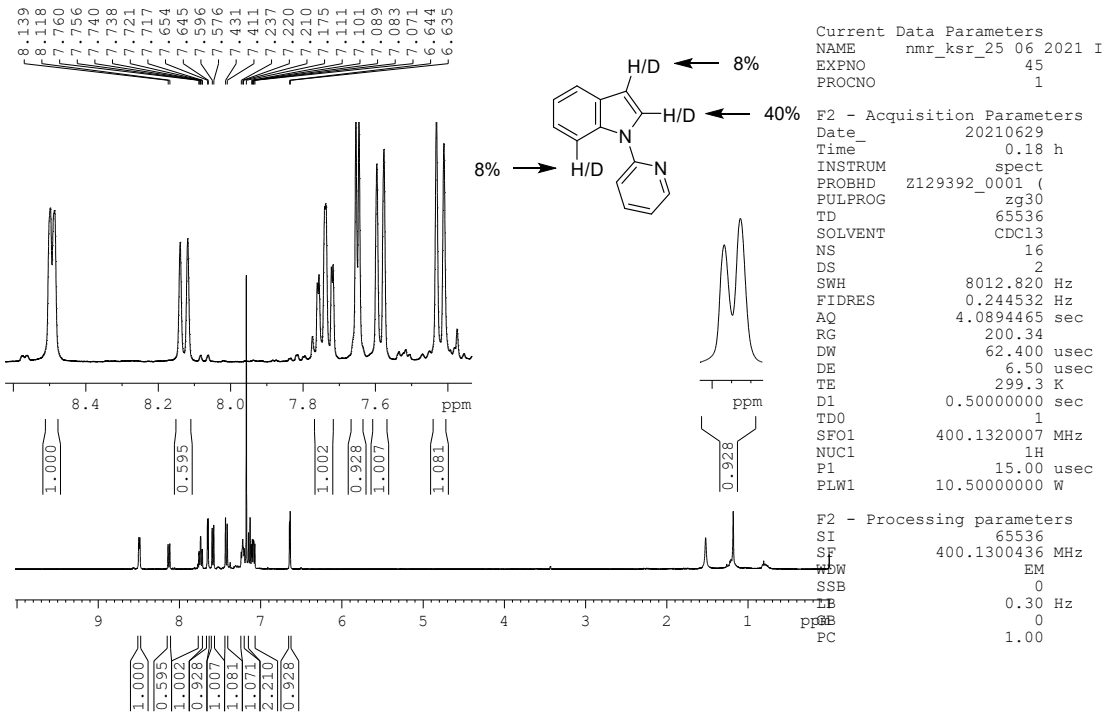


Oven-dried sealed tube was charged with 5-methoxy-1-(pyridin-2-yl)-1*H*-indole **1d** (0.22 mmol), (1.0 equiv)**,** methyl-1-(pyridin-2-yl)-1*H*-indole-5-carboxylate **1j** (0.22 mmol), (1.0 equiv), 1-phenylcyclopropan-1-ol **2a** (0.46 mmol, 2.1 equiv), [Cp*CoI_2CO] (10 mol%), $AgSbF_6$ (20 mol%) and $Cu(OAc)_2 \cdot H_2O$ (100 mol%). The inner atmosphere was made inert through repeated (thrice) evacuation and refilled with nitrogen. Dry (MeOH:^{t}AmOH) (1:1), (2 mL) was added to the reaction mixture and the reaction mixture was stirred at 100 °C temperature for 4 h. After completion of the reaction (monitored by TLC), the reaction mixture was cooled to room temperature, filtered through a pad of celite, and concentrated to get the crude product. The crude product was purified by column chromatography through silica gel to afford the expected products (**3d**:**3j**) in 62% in 3:1 ratio.

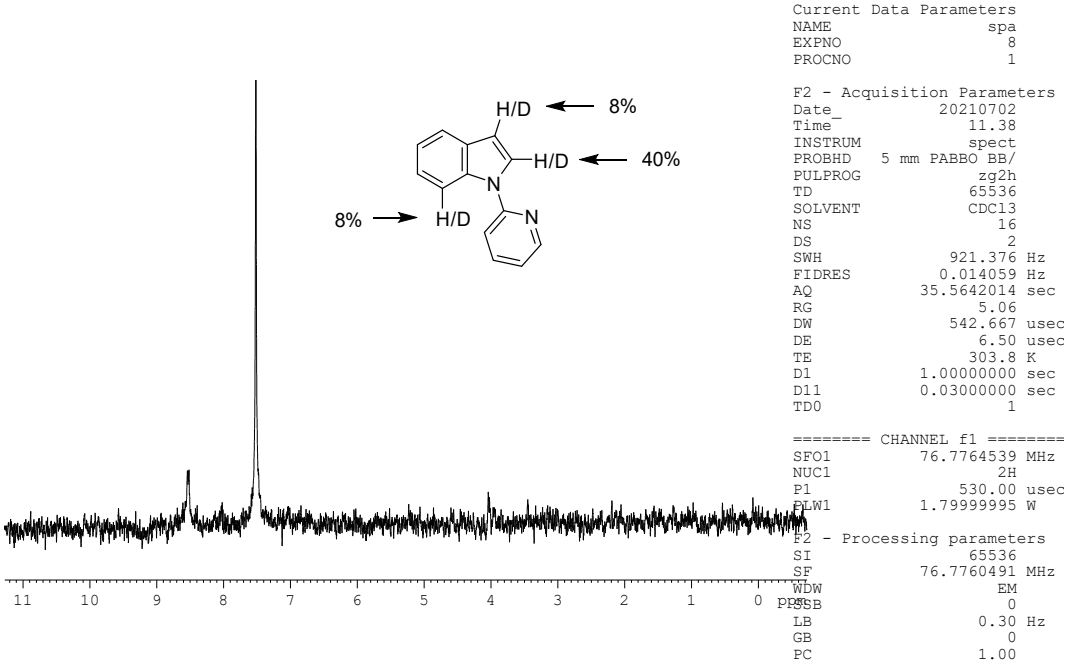
6.3 Deuterium experiment



1-(pyridin-2-yl)-1*H*-indole **1a** (50 mg) (1 equiv), [Cp*CoI_2CO], (10 mol %), $Cu(OAc)_2 \cdot H_2O$ (100 mol%) and $AgSbF_6$ (20 mol%) were taken in a 15 mL reaction tube, followed by methanol-d_4 (2 mL) was added. The reaction mixture was allowed to stir at room temperature for 6 h. After 6 h, the reaction was diluted with DCM, filtered through celite, and the filtrate was concentrated. The crude residue was purified by column chromatography using hexane: ethyl acetate (2:8). The recovered **1a** (93%) had deuterium incorporation at C2, C3, and C7-position in 40%, 8%, and 8%, respectively.

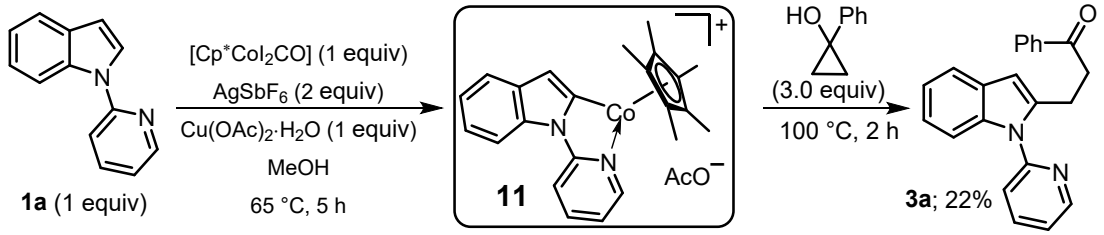


^{1}H NMR (500 MHz, $CDCl_3$, 24 °C) deuterated compound **1a**/**1a'**

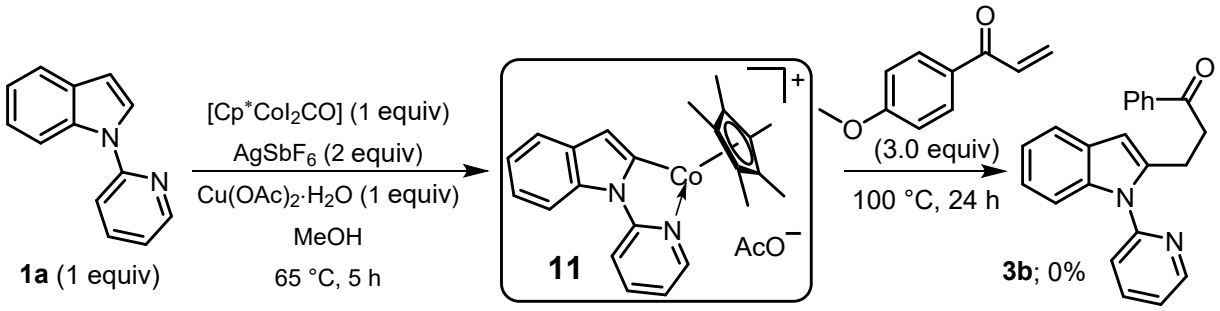


Deuterium NMR (500 MHz, $CHCl_3$, 24 °C) of the compound **1a/1a'**

6.4 Stoichiometric experiments

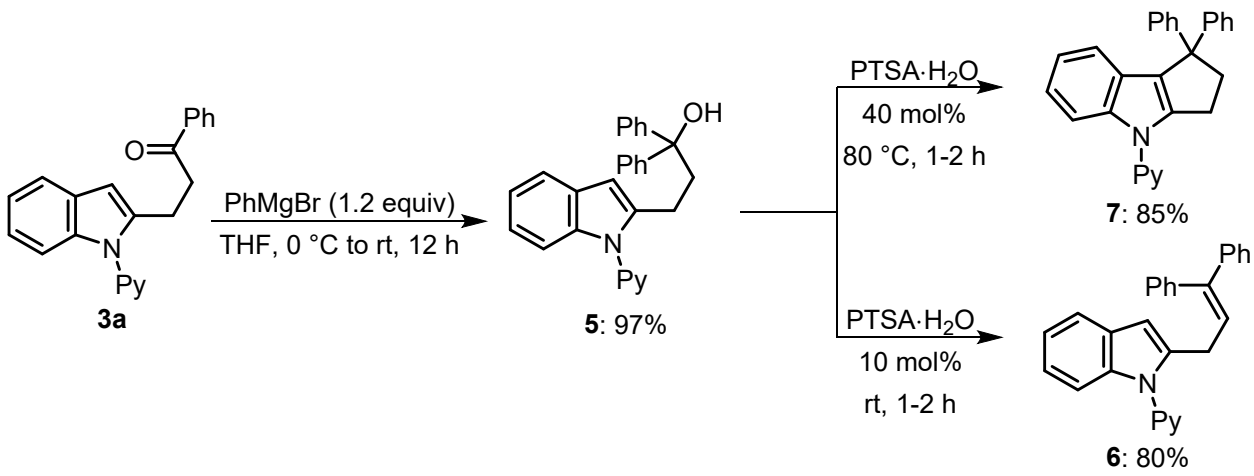


Oven-dried Schlenk tube was charged with **1a** (1 equiv, 0.26 mmol), $Cu(OAc)_2 \cdot H_2O$ (1 equiv), $AgSbF_6$ (2 equiv) and [Cp*CoI_2CO] (1 equiv). The charged Schlenk tube was made inert through repeated (thrice) evacuation and refilling with nitrogen. And 3 mL of dry MeOH (3mL) was added, then reaction mixture was stirred at 65 °C in a pre-heated oil bath for 5 h. Then, the reaction was cooled to room temperature and complex **11** was identified by HRMS. Subsequently, the compound **11** was transferred to pressure tube under inert atmosphere and **2a** (3 equiv) was added followed by stirring at 100 °C for 2 h. The reaction mixture was brought to room temperature, filtered through a pad of celite and concentrated to get the crude product. The crude product was purified by column chromatography through silica gel to afford the expected product **3a** in 22% yield.



Similarly, an oven-dried Schlenk tube was charged with **1a** (1 equiv, 0.26 mmol), $Cu(OAc)_2 \cdot H_2O$ (1 equiv), $AgSbF_6$ (2 equiv) and [Cp*CoI_2CO] (1 equiv). The charged Schlenk tube was made inert through repeated (thrice) evacuation and refilling with nitrogen and 3 mL of dry MeOH (3mL) was added. The reaction mixture was stirred at 65 °C in a pre-heated oil bath for 5 h. Subsequently, compound **11** was transferred to pressure tube under inert atmosphere and 1-(4-methoxyphenyl)prop-2-en-1-one (3 equiv) was added followed by stirring at 100 °C for 24 h. The desired product **3b** did not formed and **1a** and 1-(4-methoxyphenyl)prop-2-en-1-one were recovered.

7. Synthetic of 1,1-Diphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydro cyclopenta-[*b*]indole (6) and 2-(3,3-diphenylallyl)-1-(pyridin-2-yl)-1*H*-indole (7):

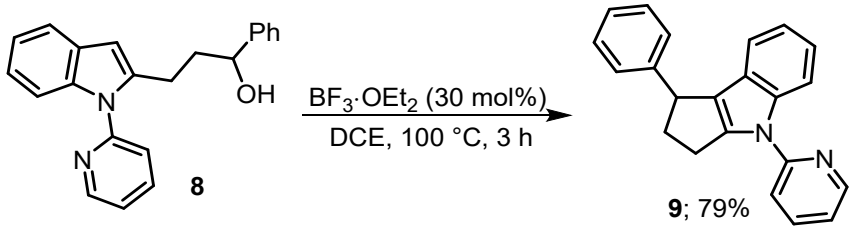


A 25 mL round-bottom flask was charged with alkylated indole **3a** (0.60 mmol, 1.0 equiv) and dry THF (5 mL), subsequently, phenyl magnesium bromide (0.72 mmol, 1.2 equiv) was added dropwise. The reaction mixture was stirred at room temperature. Once the reaction was completed (monitored by TLC), the reaction mixture was quenched with ammonium chloride solution. The mixture was extract with DCM and washed with water. The collected organic layer was concentrated to get the crude product. The crude product was purified by column chromatography to afford the expected product **5** in 97% yield.

The alcohol **5** was treated with PTSA·H_2O (10 mol%) in DCE at room temperature for 2 h. The progress of the reaction was monitored by TLC. The reaction mixture was quenched with $NaHCO_3$ solution. The mixture was extracted with DCM and washed using water. The collected organic layer was concentrated to get the crude product. The crude product was purified by column chromatography through silica gel to afford the expected product **6** in 80% yield.

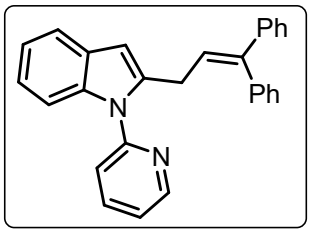
On the other hand, the mixture of alcohol **5** and 40 mol% of PTSA·H_2O in DCE was heated at 80 °C for 2 h. After the reaction was completed, the reaction mixture was quenched with $NaHCO_3$ solution, extracted with DCM and washed with water. The collected organic layer was concentrated to get the crude product. The crude was subjected silica gel column chromatography to give **7** in 85% of yield.

7.1 Synthetic of 1-Phenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[*b*]indole (9):



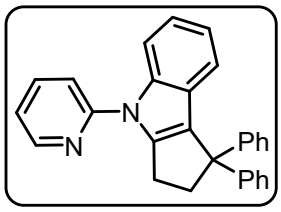
Oven dried 15 mL reaction tube was charged with alcohol **8** (0.15 mmol, 1.0 equiv) and dry DCE (2 mL). Subsequently, $BF_3{\cdot}OEt_2$ (0.044 mmol, 50 mol%) was added and closed with stopper. The reaction tube was kept in a preheated oil bath at 100 °C. After completion of the reaction (monitored by TLC), the reaction mixture was cooled to room temperature and quenched with $NaHCO_3$ solution, extracted with DCM and washed with water. The collected organic layer was concentrated to get the crude product. The crude product was purified by column chromatography through silica gel to afford the expected product **9** in 79% yield.

2-(3,3-Diphenylallyl)-1-(pyridin-2-yl)-1*H*-indole (6):



Yield: 80%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 2939, 1725, 1678, 1403, 1234, 678; ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.53 (d, J = 4.3 Hz, 1H), 7.77 (t, J = 8.1 Hz, 1H), 7.57 (dd, J = 4.1, 2.4 Hz, 1H), 7.35-7.27 (m, 5H), 7.26-7.19 (m, 5H), 7.16-7.11 (m, 5H), 6.53 (s, 1H), 6.16 (t, J = 7.6 Hz, 1H), 3.70 (d, J = 7.6 Hz, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 159.4, 149.7, 143.2, 142.6, 139.9, 139.5, 138.4, 137.5, 129.9, 128.7, 128.3, 128.2, 127.6, 127.3, 127.2, 125.5, 122.0, 121.9, 121.0, 120.8, 120.2, 110.4, 103.2, 28.7; HRMS: (ESI) *m/z* calcd. for $C_{28}H_{22}N_2$, 387.1856 $[M+H]^+$; found 387.1857.

1,1-Diphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[*b*]indole (7):

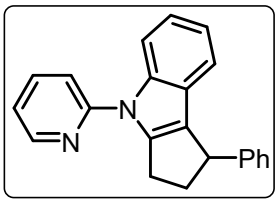


Yield: 85%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 2922, 1735, 1567, 1471, 1224, 750; ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.46 (d, J = 4.6 Hz, 1H), 7.85 (t, J = 8.3 Hz, 1H), 7.67 (t, J = 8.0 Hz, 1H), 7.33 (d, J = 7.3 Hz, 1H), 7.32-7.27 (m, 4H), 7.24 (d, J = 8.0 Hz, 1H), 7.20-7.13 (m, 4H), 7.12-6.94 (m, 5H), 3.18 (t, J = 6.9 Hz, 2H), 3.09 (t, J = 7.6 Hz, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 152.2, 149.2, 148.3, 143.8, 142.5, 140.2, 138.3,

137.8, 128.2, 127.9, 127.6, 126.0, 125.6, 122.7, 121.9, 121.3, 120.4, 119.5, 116.5, 112.8, 57.4, 47.3, 27.8; HRMS: (ESI) *m*/*z* calcd. for $C_{28}H_{22}N_2$, 387.1856 $[M+H]^+$; found 387.1853.

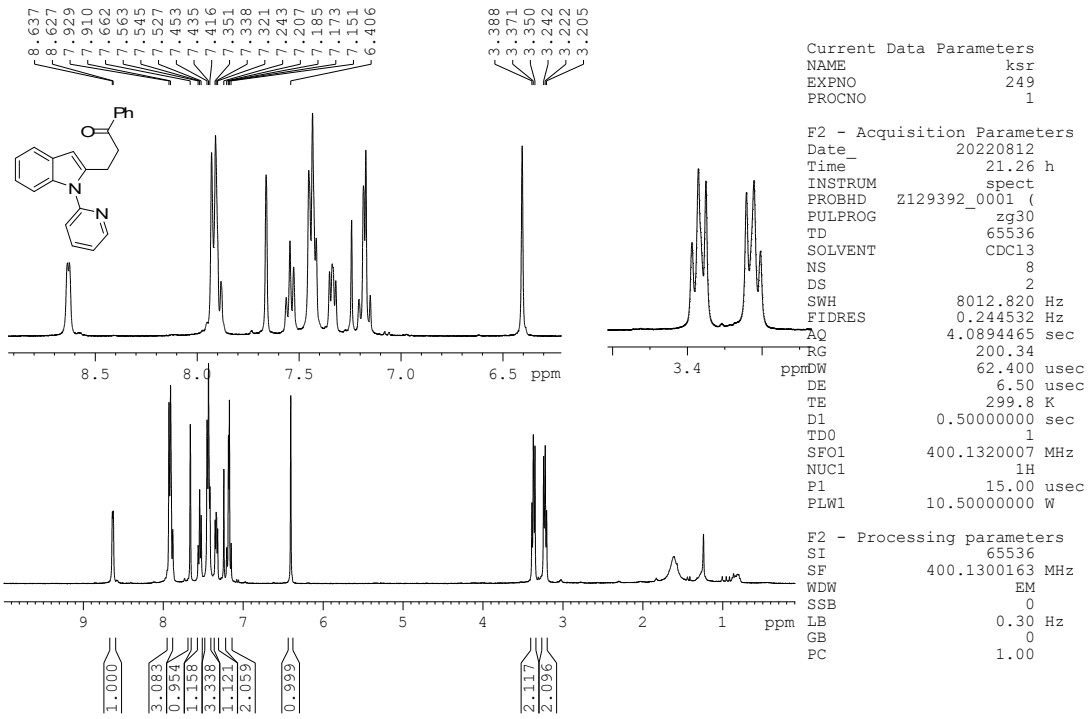
1,1-Diphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[*b*]indole (9):

Yield: 79%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane; IR (ν_{max}, cm^{-1}): 2990, 1656, 1555, 1445, 1224, 750; ^1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.54 (d, J = 4.4 Hz, 1H), 7.94 (d, J = 8.0 Hz, 1H), 7.78 (t, J = 8.3 Hz, 1H), 7.45 (d, J = 8.3 Hz, 1H), 7.26 (d, J = 3.6 Hz, 1H), 7.21-7.20 (m, 3H), 7.18-7.08 (m 4H), 7.00 (t, J = 7.9 Hz, 1H), 4.46 (t, J = 8.5 Hz, 1H), 3.28-3.18 (m, 1H), 3.14-2.98 (m, 2H), 2.41-2.32 (m, ^1H); $^{13}C\{1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 152.5, 149.3, 145.8, 145.2, 140.4, 138.3, 128.5, 127.5, 126.6, 125.7, 124.6, 121.9, 121.1, 120.2, 119.0, 116.1, 112.8, 44.5, 40.0, 27.8; HRMS: (ESI) *m*/*z* calcd. for $C_{22}H_{18}N_2$, 333.1362 $[M+Na]^+$; found 333.1357.

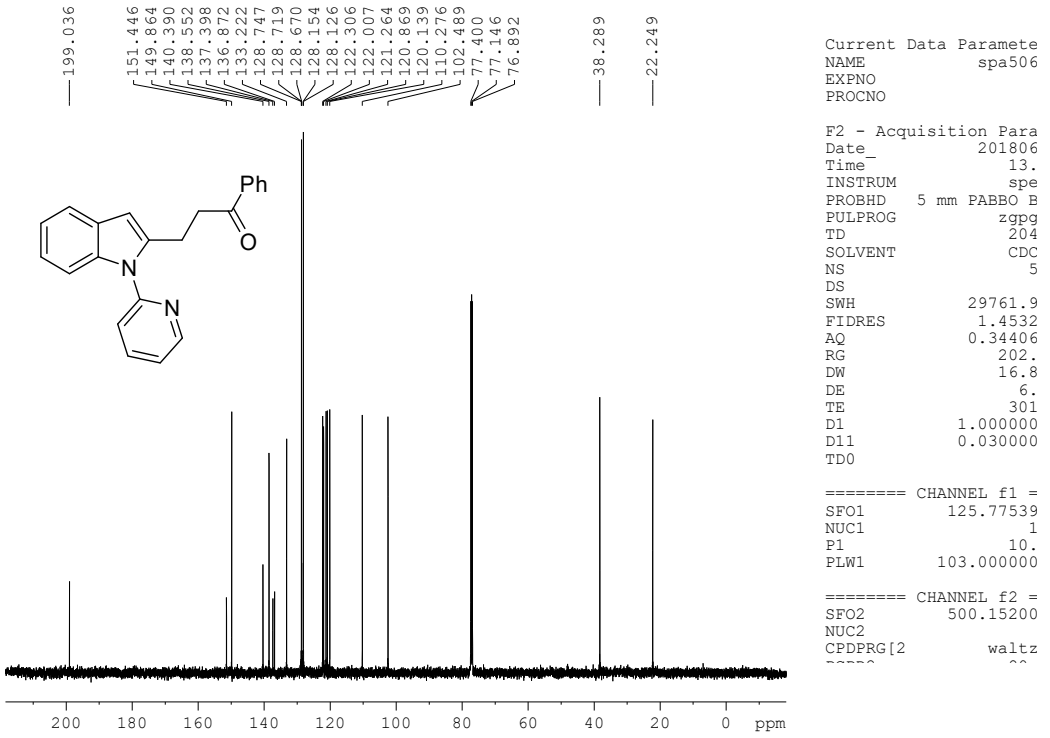


8. Spectral data

3-(1*H*-Indol-2-yl)-1-phenylpropan-1-one: 3a

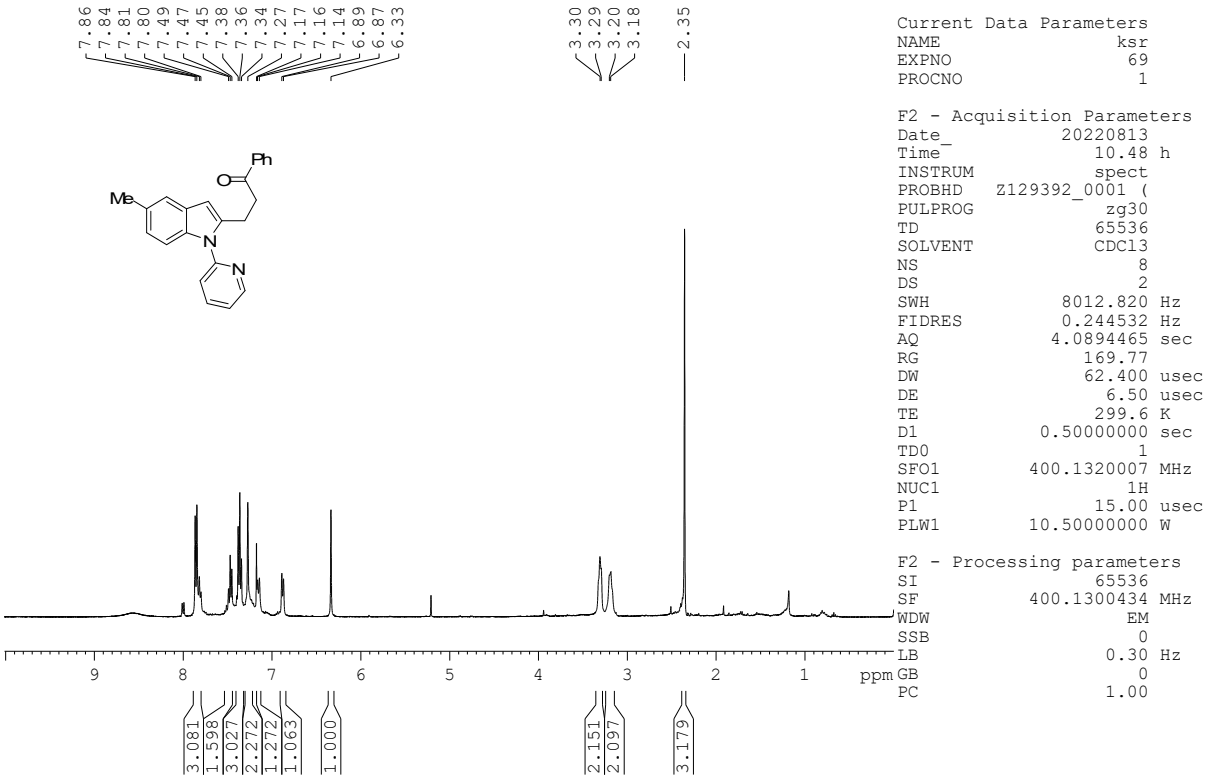


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound: **3a**

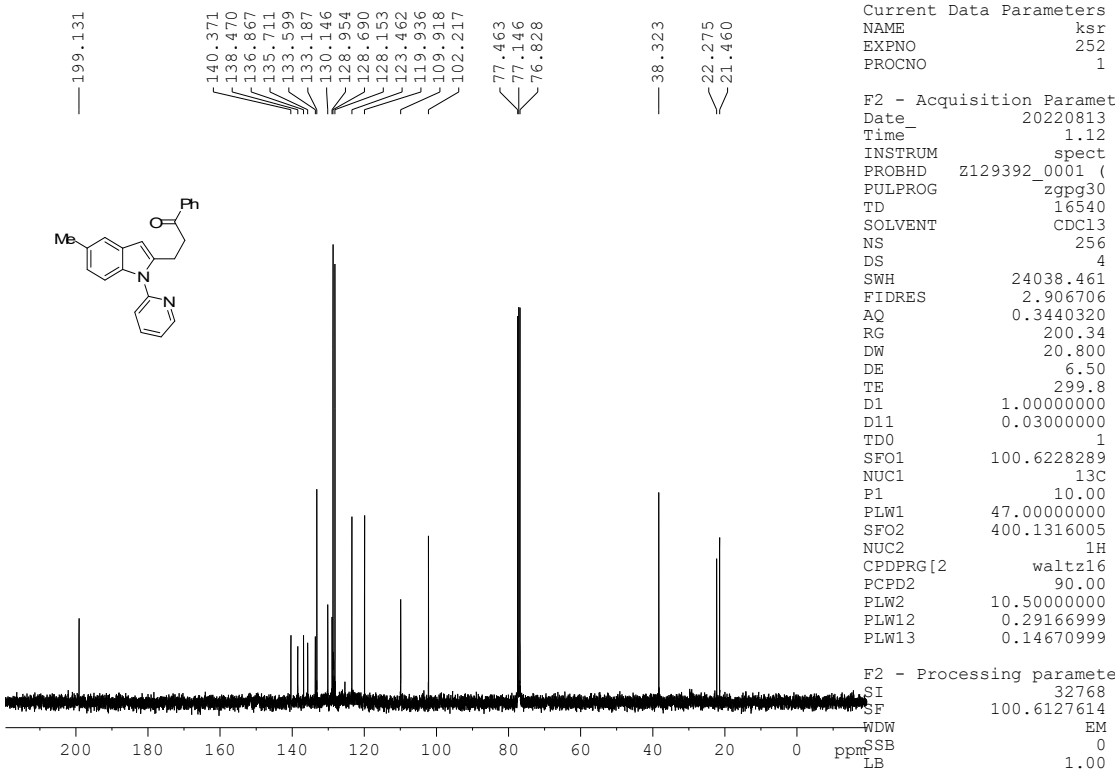


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3a**

3-(5-Methyl-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one: 3b

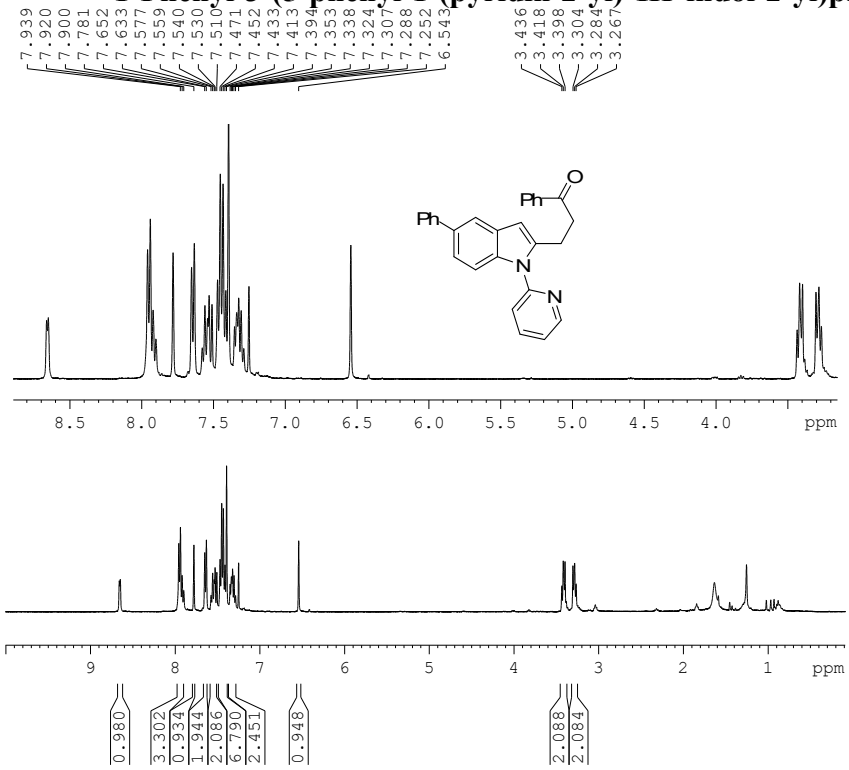


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound: **3b**



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

1-Phenyl-3-(5-phenyl-1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one: 3c

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DE                  6.50 usec
TE                 295.4 K
D1              0.50000000 sec
TD0                    1

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P1                  15.70 usec
PLW1          7.75000000 W

F2 - Processing parameters
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WDW                    EM
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GB                      0
PC                   1.00
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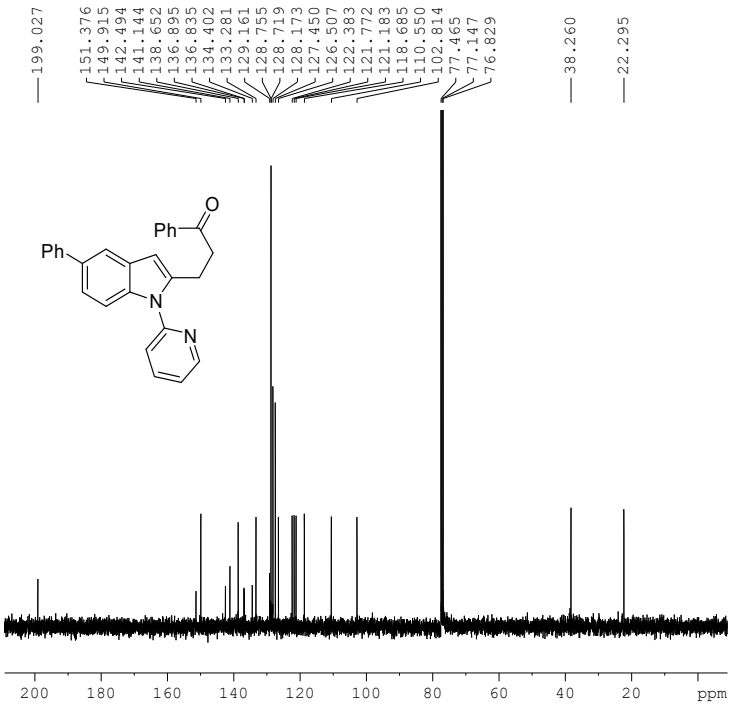
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound: **3c**

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DE                  6.50 usec
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D1              1.00000000 sec
D11             0.03000000 sec
TD0                    1

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NUC1                   13C
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NUC2                   1H
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PCPD2              90.00 usec
PLW2          7.75000000 W
PLW12         0.23583999 W
PLW13         0.11863000 W

F2 - Processing parameters
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SF           100.6127587 MHz
WDW                    EM
SSB                     0
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GB                      0
PC                   1.40
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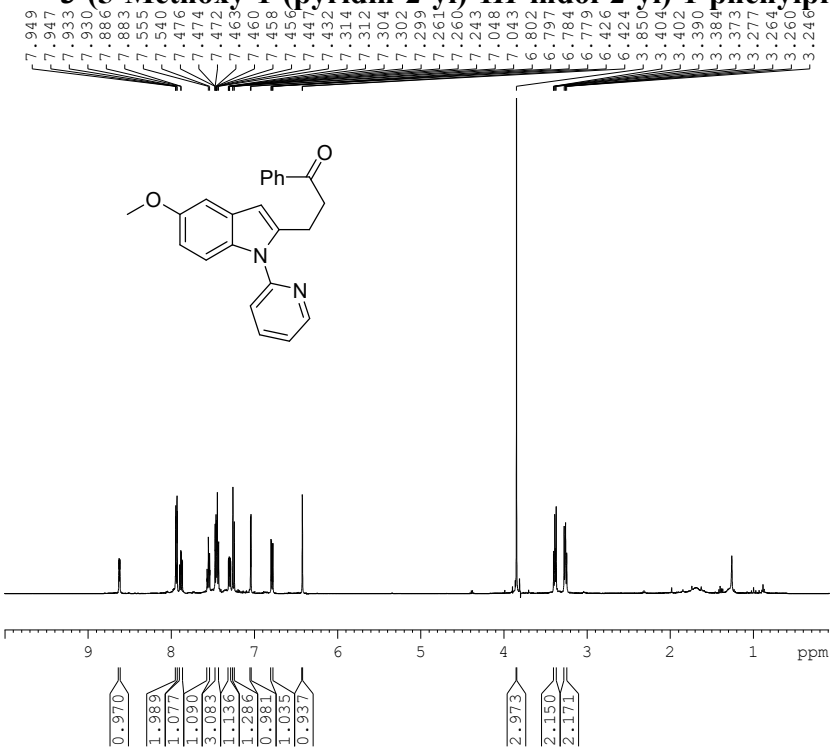
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3c**

3-(5-Methoxy-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one: 3d

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PC                  1.00
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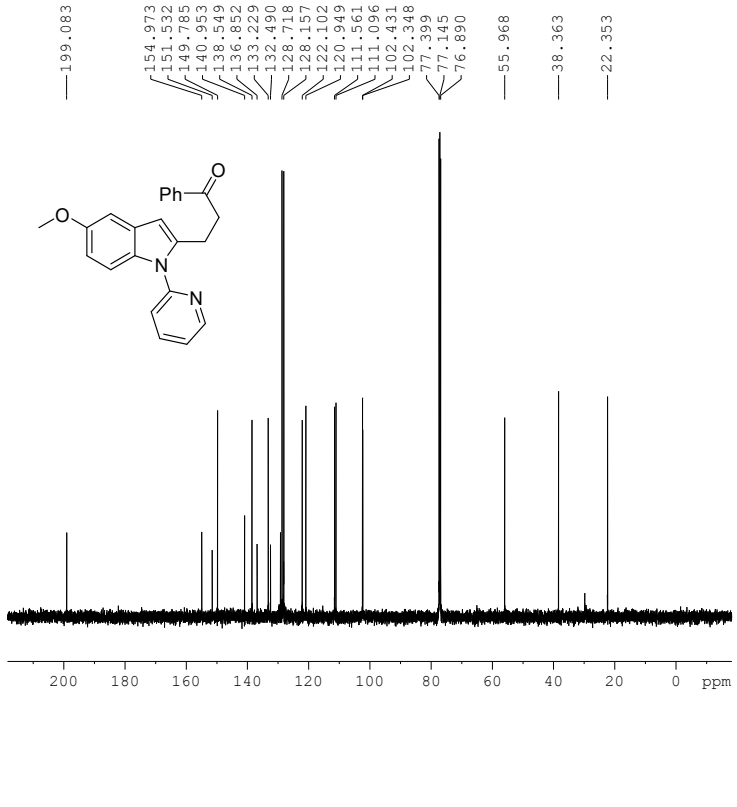
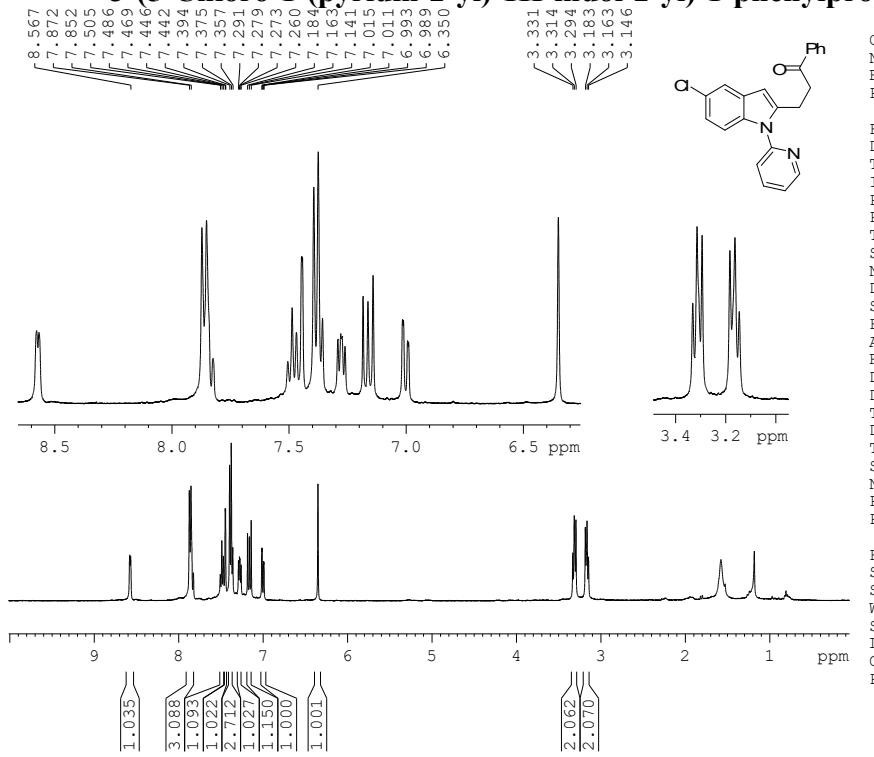
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3d**




```
Current Data Parameters
NAME      1444 5 ome ind
EXPNO                 48
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180816
Time               18.54
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 20480
SOLVENT            CDCl3
NS                   256
DS                     4
SWH           29761.904 Hz
FIDRES         1.453218 Hz
AQ            0.3440640 sec
RG                202.34
DW                16.800 usec
DE                 6.50 usec
TE                299.4 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         0.38863000 W
PLW13         0.19548000 W

F2 - Processing parameters
SI                 32768
SF          125.7628060 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

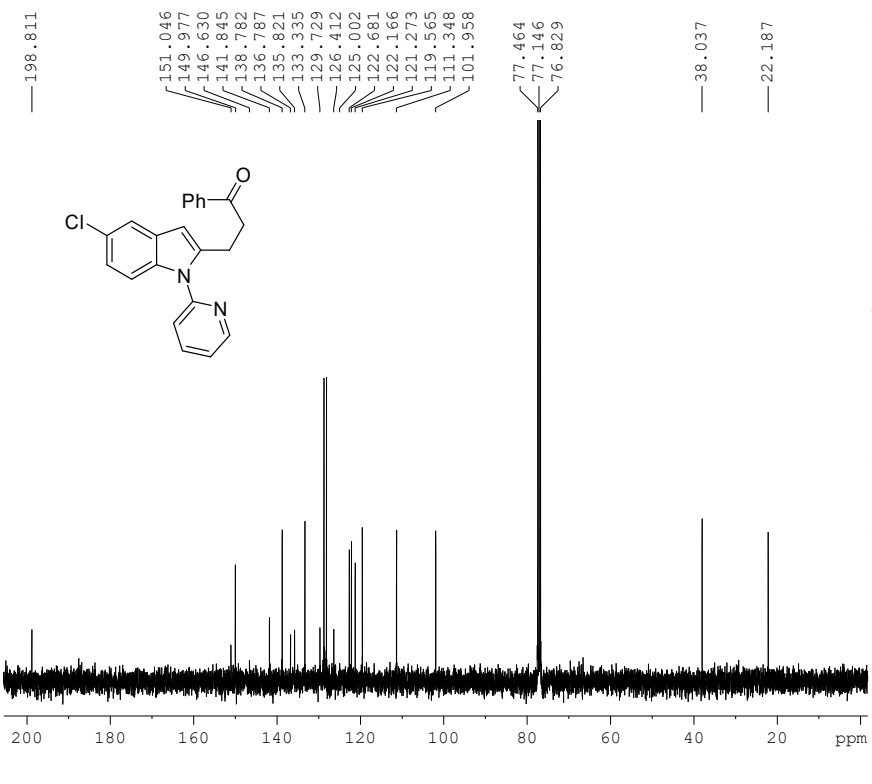
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3d**

3-(5-Chloro-1-(pyridin-2-yl)-1H-indol-2-yl)-1-phenylpropan-1-one: 3e




```
Current Data Parameters
NAME      2779 5CL IND cy oh
EXPNO                  171
PROCNO                   1

F2 - Acquisition Parameters
Date_           20211209
Time                1.24 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                298.7 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           400.1300401 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

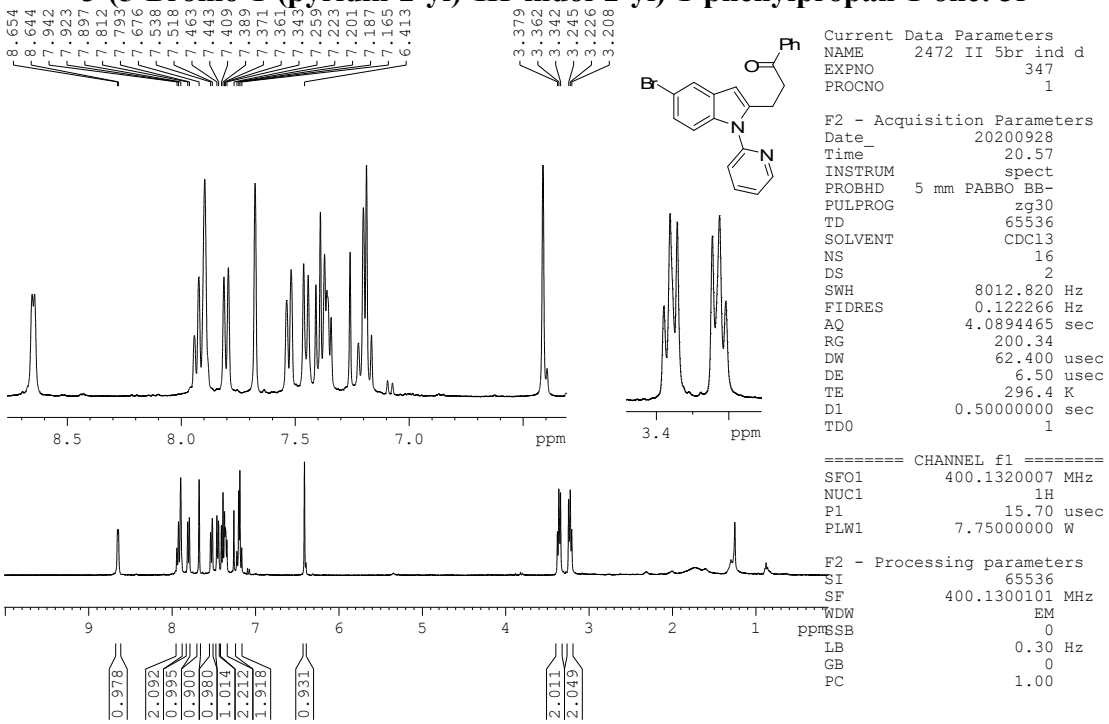
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound: **3e**




```
Current Data Parameters
NAME      2779 5CL IND cy oh
EXPNO                  172
PROCNO                   1

F2 - Acquisition Parameters
Date_           20211209
Time                1.31 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG          zgpg30
TD                 16540
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            24038.461 Hz
FIDRES          2.906706 Hz
AQ              0.3440320 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE                298.8 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           100.6127571 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

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

3-(5-Bromo-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one: 3f



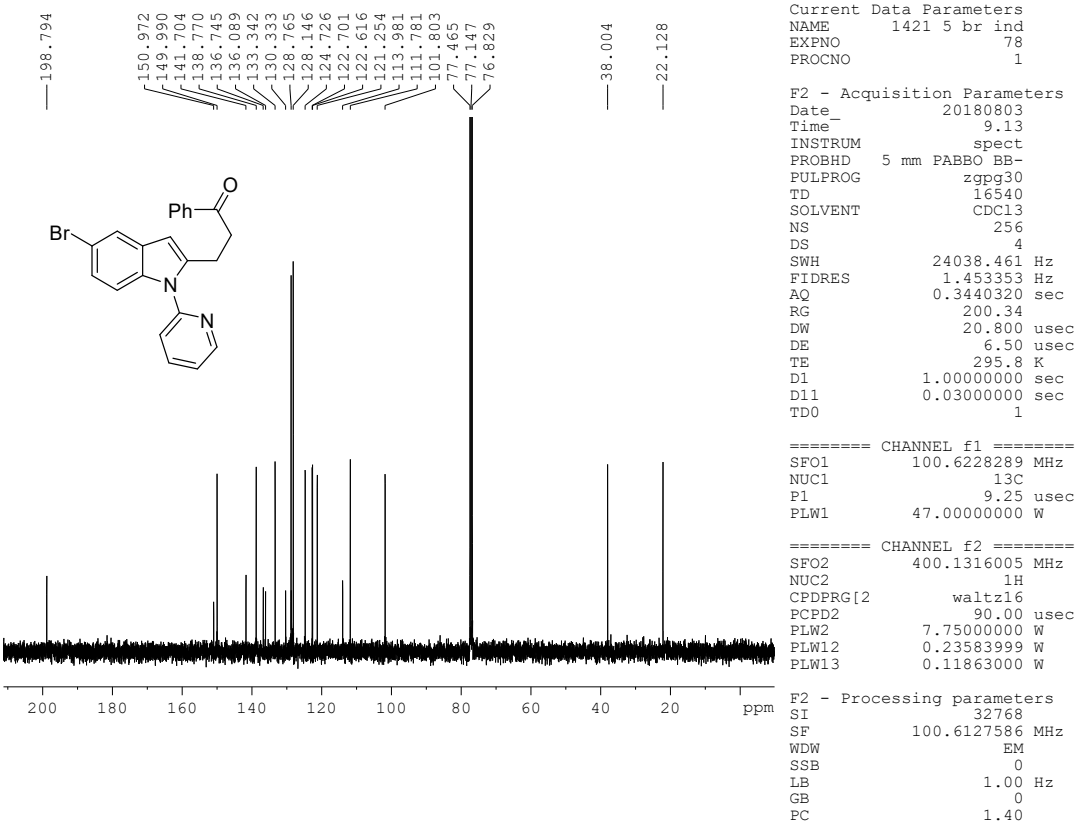
Current Data Parameters
NAME 2472 II 5br ind d
EXPNO 347
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200928
Time 20.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 296.4 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300101 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 **3f**



Current Data Parameters
NAME 1421 5 br ind
EXPNO 78
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180803
Time 9.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

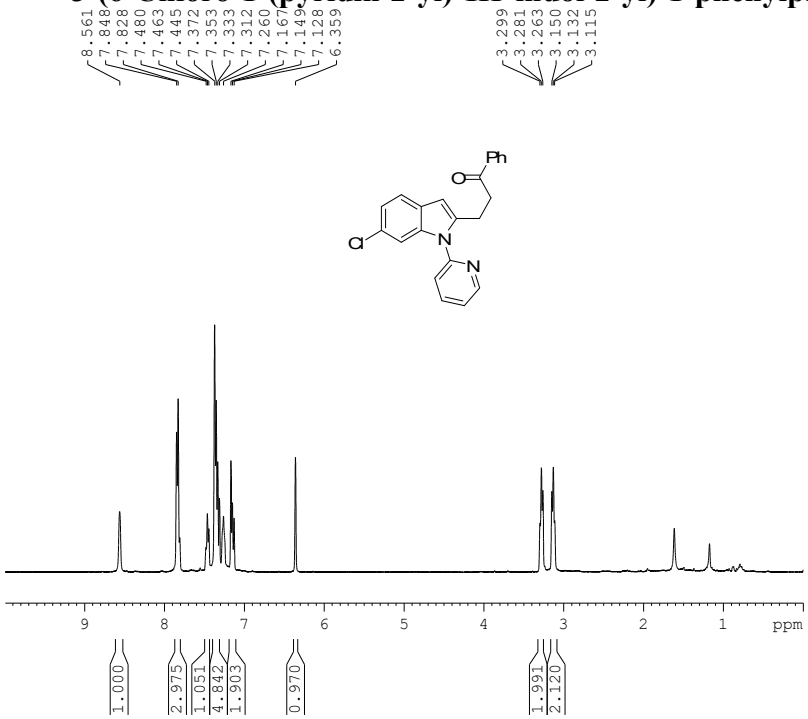
======== CHANNEL f1 ========
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

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

F2 - Processing parameters
SI 32768
SF 100.6127586 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

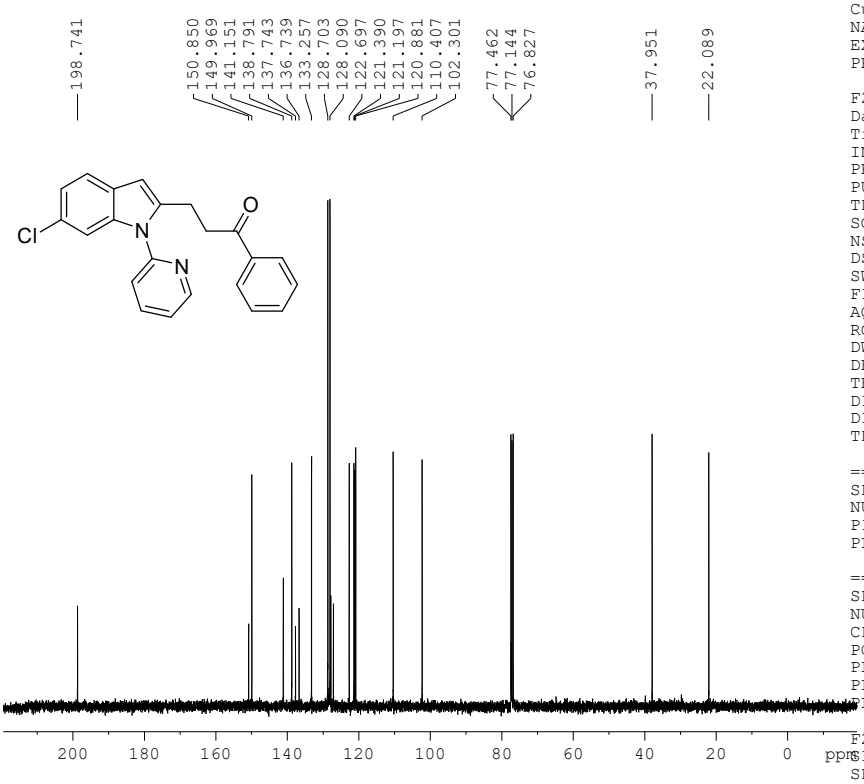
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3f**

3-(6-Chloro-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one: 3g




```
Current Data Parameters
NAME                  2653 d
EXPNO                    521
PROCNO                     1

F2 - Acquisition Parameters
Date_              20210420
Time                 10.57
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                   138.85
DW                   62.400 usec
DE                    6.50 usec
TE                   299.7 K
D1              0.50000000 sec
TD0                        1

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

F2 - Processing parameters
SI                   65536
SF              400.1300485 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

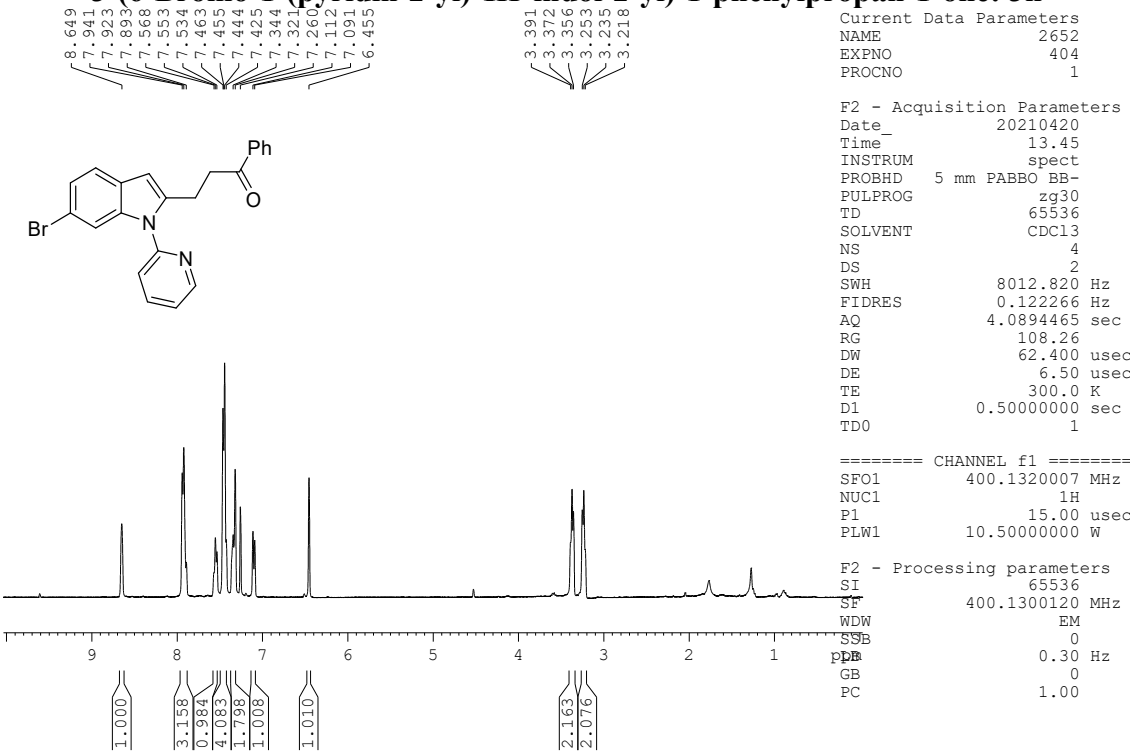
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3g**




```
Current Data Parameters
NAME                  2652 d
EXPNO                    405
PROCNO                     1

F2 - Acquisition Paramet
Date_              20210420
Time                 13.51
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   16540
SOLVENT              CDCl3
NS                     256
DS                       4
SWH              24038.461
FIDRES            1.453353
AQ                0.3440320
RG                   200.34
DW                   20.800
DE                     6.50
TE                    300.4
D1              1.00000000
D11             0.03000000
TD0                        1

======== CHANNEL f1 ====
SFO1           100.6228289
NUC1                    13C
P1                    10.00
PLW1           47.00000000

======== CHANNEL f2 ====
SFO2           400.1316005
NUC2                     1H
CPDPRG[2          waltz16
PCPD2                 90.00
PLW2           10.50000000
PLW12           0.29166999
PLW13           0.14670999

F2 - Processing paramete
SI                   32768
SF              100.6127643
```

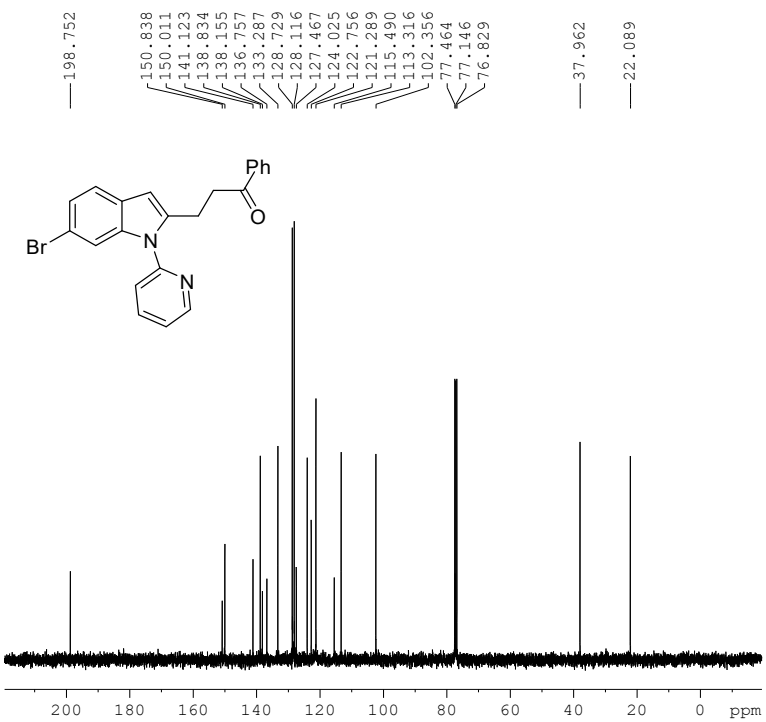
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3g**

3-(6-Bromo-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one: 3h




```
Current Data Parameters
NAME                  2652
EXPNO                  404
PROCNO                   1

F2 - Acquisition Parameters
Date_            20210420
Time                13.45
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      4
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                  108.26
DW                  62.400 usec
DE                    6.50 usec
TE                   300.0 K
D1              0.50000000 sec
TD0                     1

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

F2 - Processing parameters
SI                    65536
SF           400.1300120 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

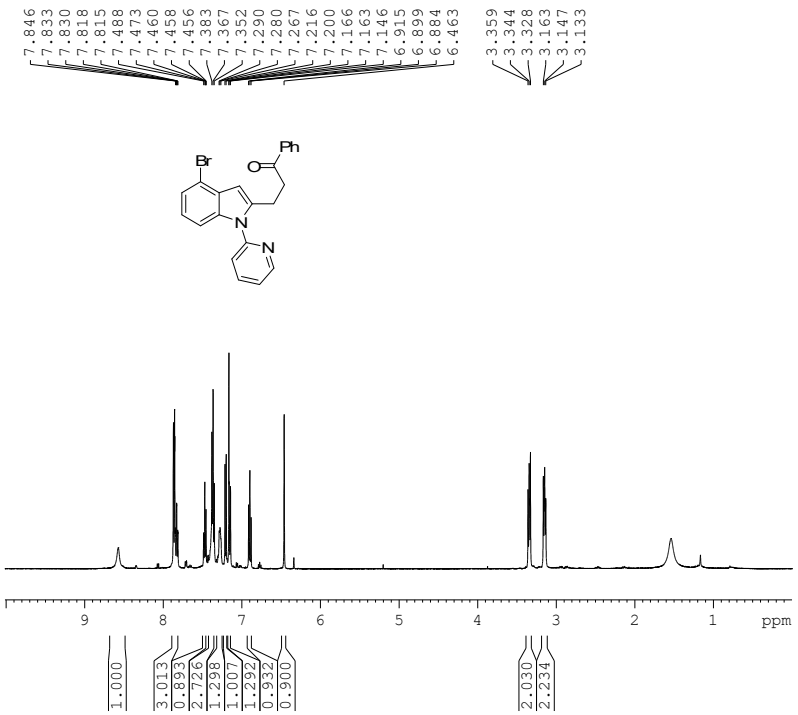
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3h**




```
Current Data Parameters
NAME     2651 2652 2648
EXPNO                522
PROCNO                 1

F2 - Acquisition Parameters
Date_          20210420
Time              10.59
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                16540
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24038.461 Hz
FIDRES         1.453353 Hz
AQ            0.3440320 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE                300.1 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228289 MHz
NUC1                  13C
P1                10.00 usec
PLW1         47.00000000 W

======== CHANNEL f2 ========
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           100.6127613 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

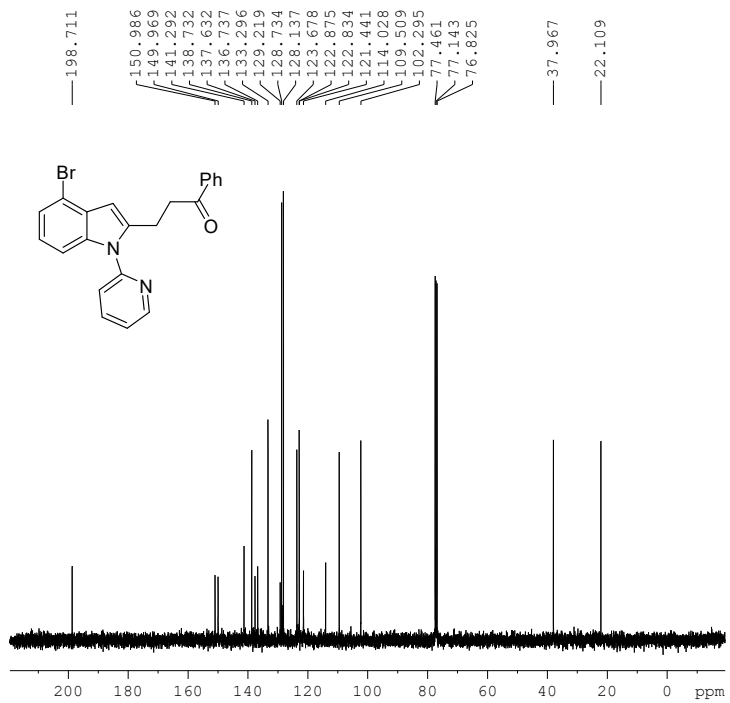
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3h**

3-(4-Bromo-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one: 3i




```
Current Data Parameters
NAME                  spa
EXPNO                  30
PROCNO                  1

F2 - Acquisition Parameters
Date_           20220805
Time               13.21
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                138.53
DW                50.000 usec
DE                 6.50 usec
TE                302.1 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            500.1500588 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

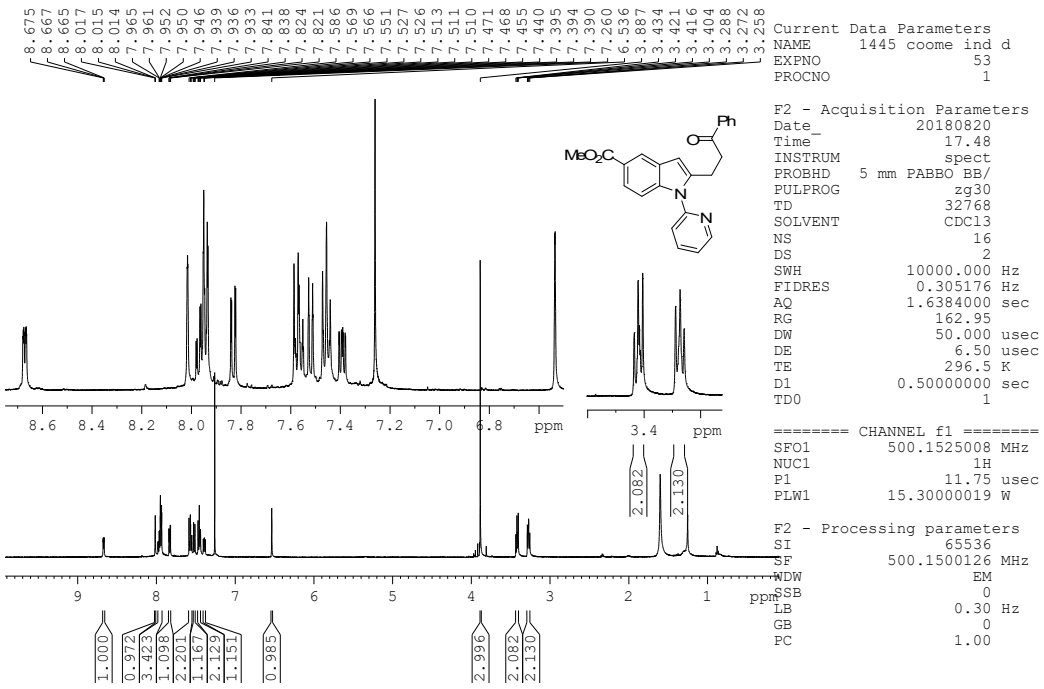
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3i**



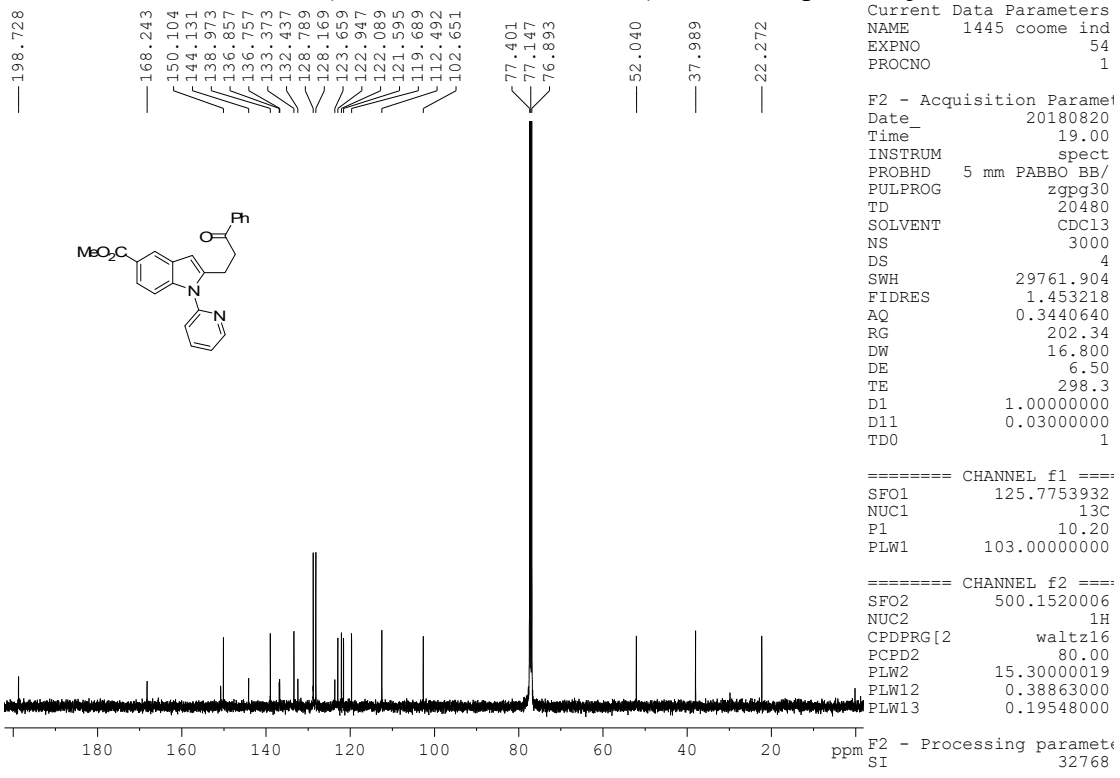

```
Current Data Parameters
NAME     2651 2652 2648
EXPNO                519
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210420
Time               10.49
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 16540
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            24038.461 Hz
FIDRES          1.453353 Hz
AQ             0.3440320 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE                300.1 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228289 MHz
NUC1                  13C
P1                10.00 usec
PLW1         47.00000000 W

======== CHANNEL f2 ========
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           100.6127615 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

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

Methyl 2-(3-oxo-3-phenylpropyl)-1-(pyridin-2-yl)-1*H*-indole-5-carboxylate: 3j

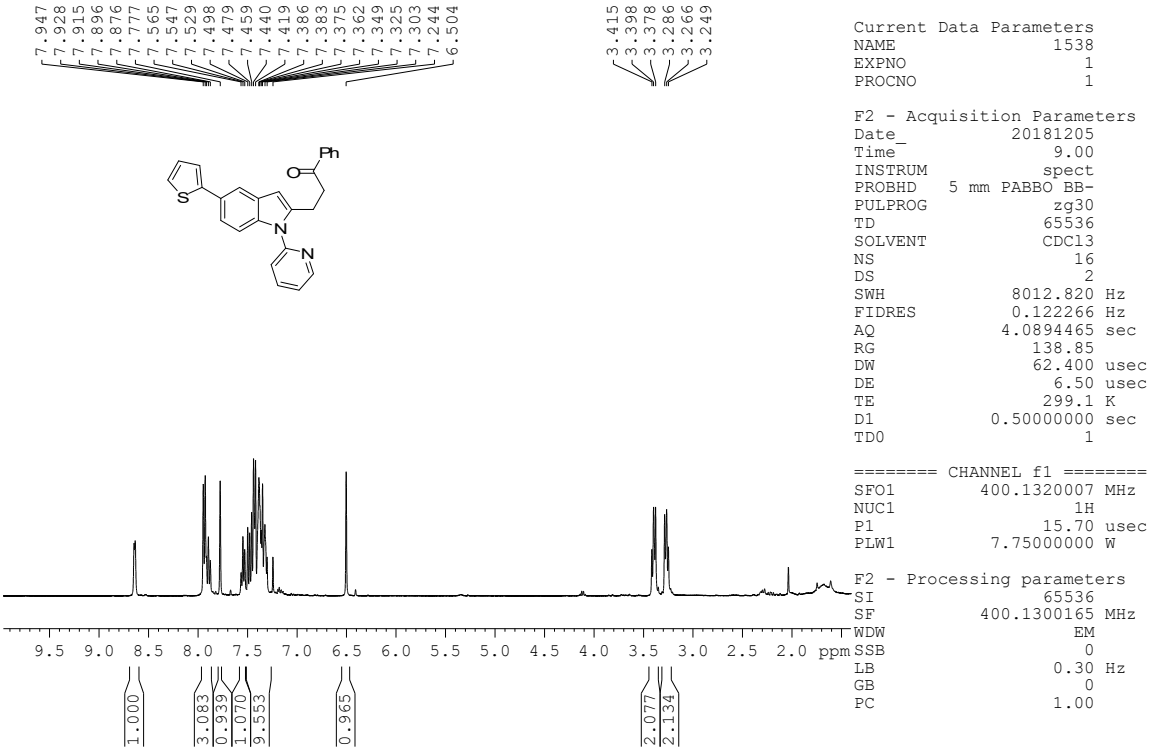


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3j**

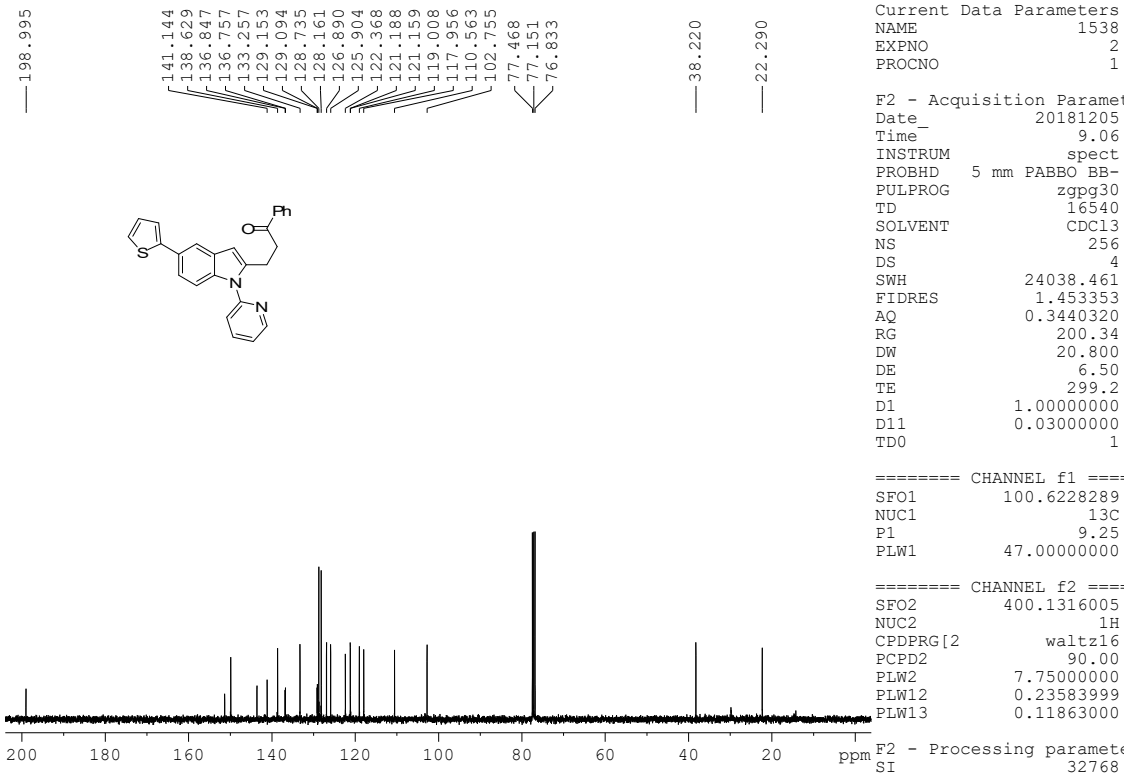


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3j**

1-Phenyl-3-(1-(pyridin-2-yl)-5-(thiophen-2-yl)-1*H*-indol-2-yl)propan-1-one: 3k

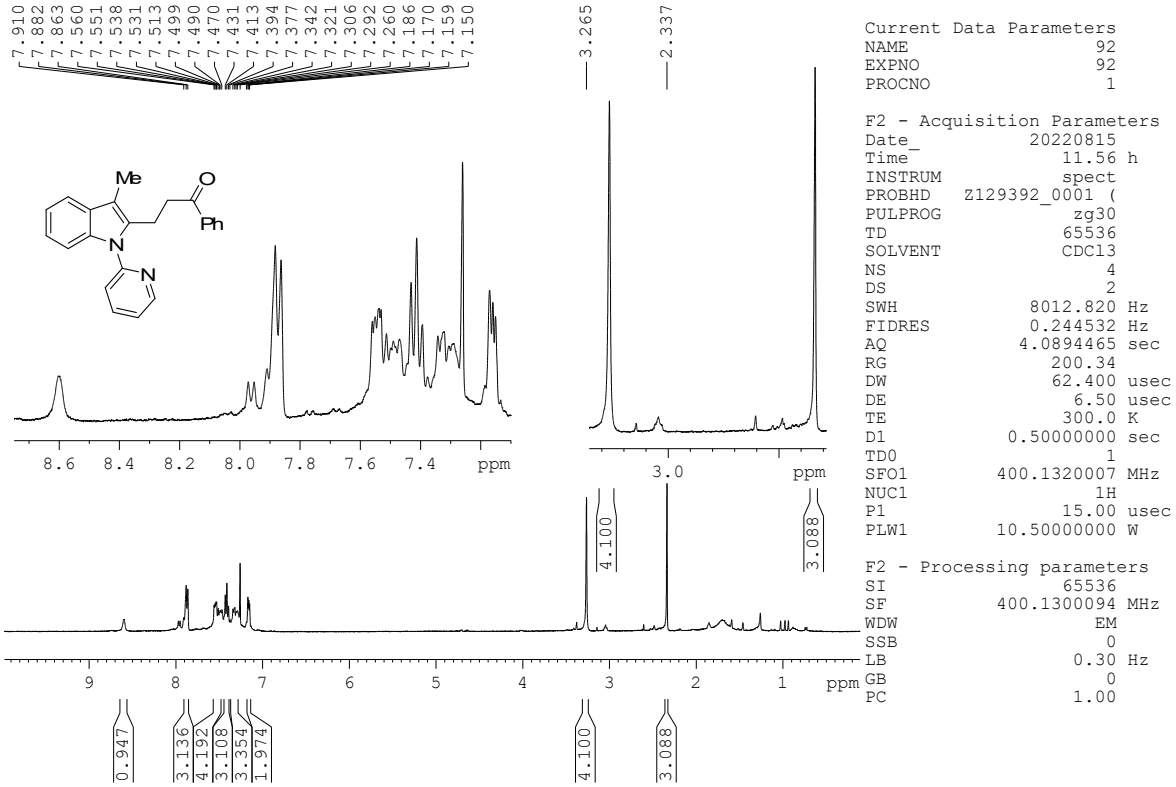


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3k**

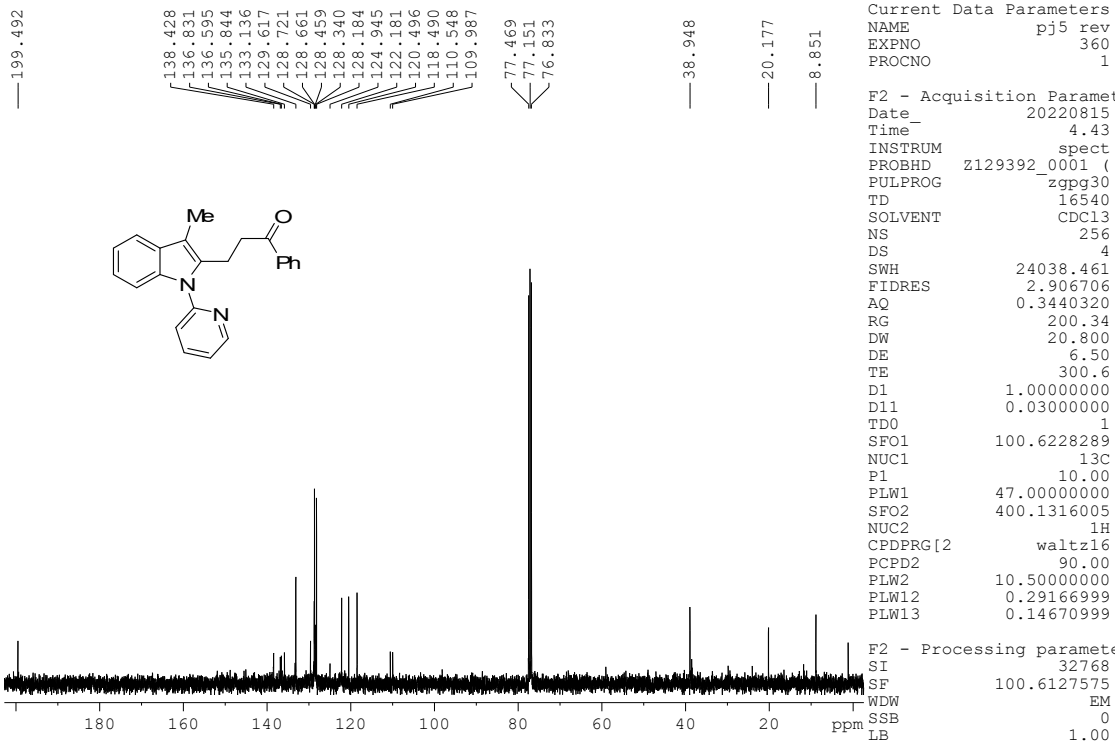


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3k**

3-(3-Methyl-1-(pyridin-2-yl)-1H-indol-2-yl)-1-phenylpropan-1-one: 3l

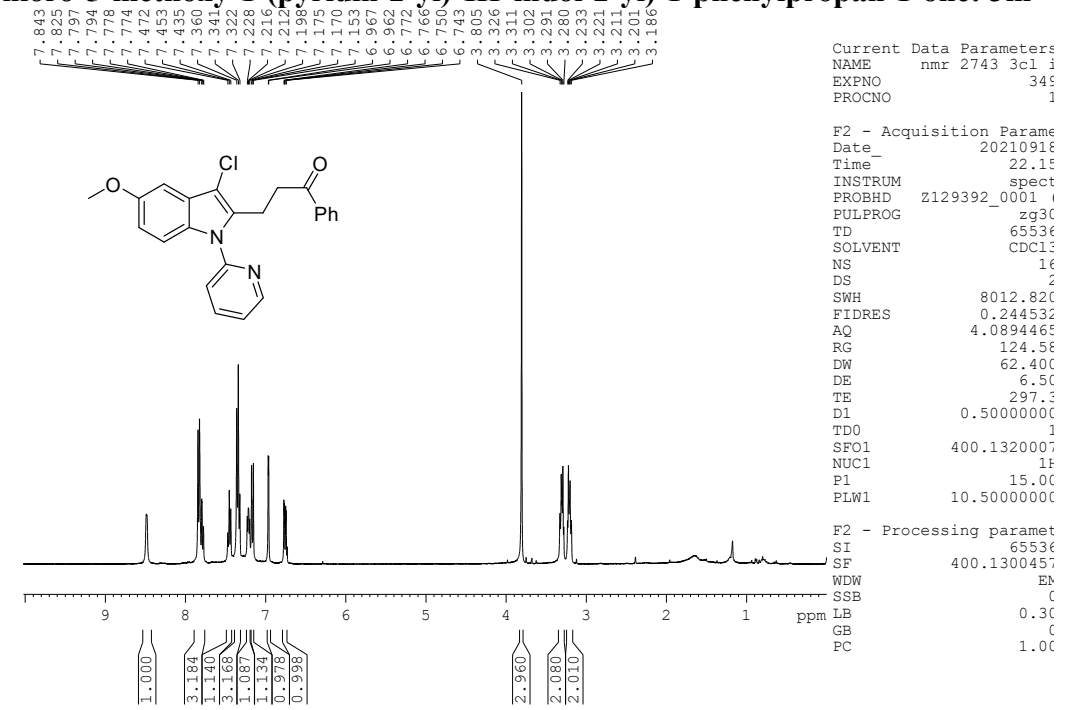


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3l**

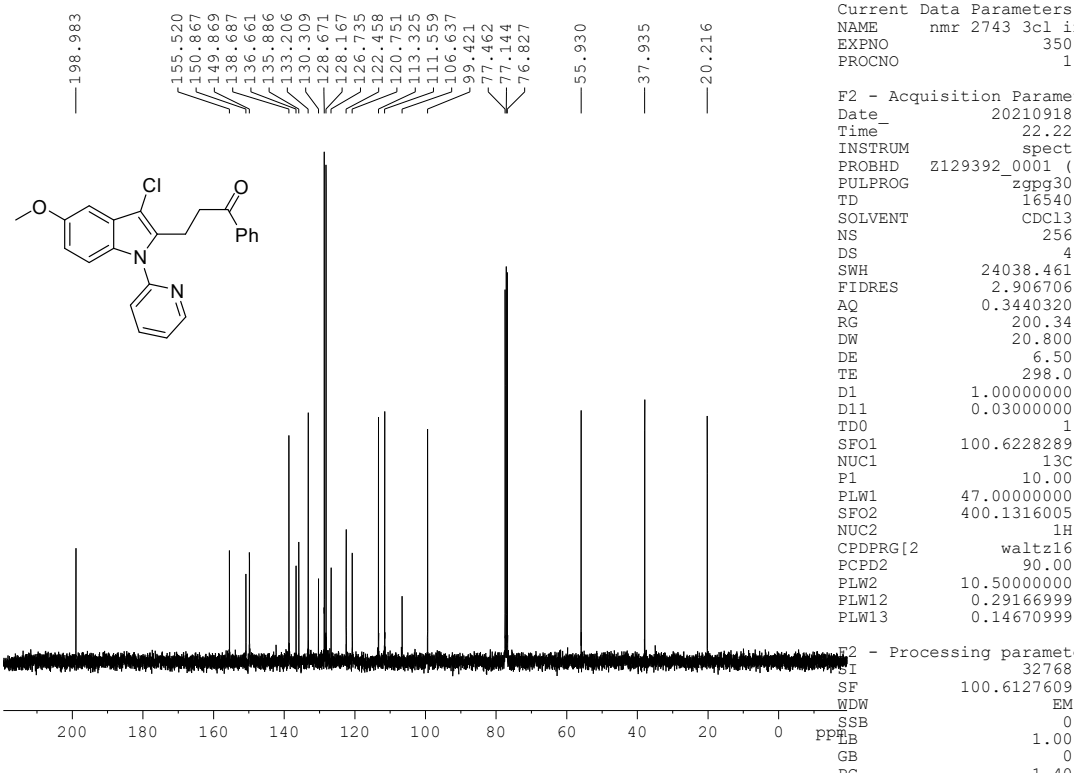


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3l**

3-(3-Chloro-5-methoxy-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one: 3m

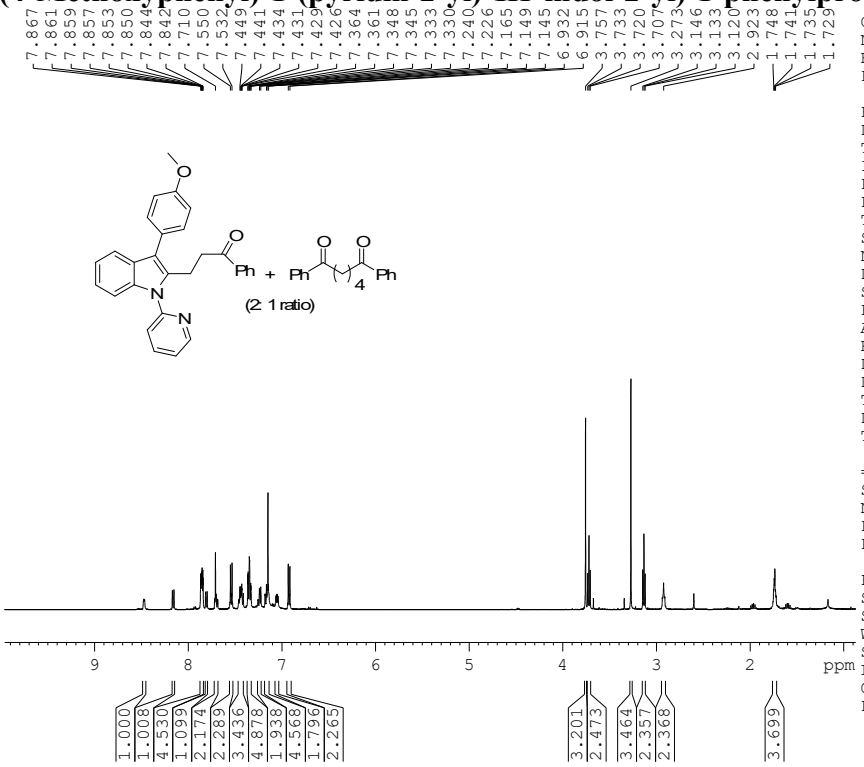


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3m**



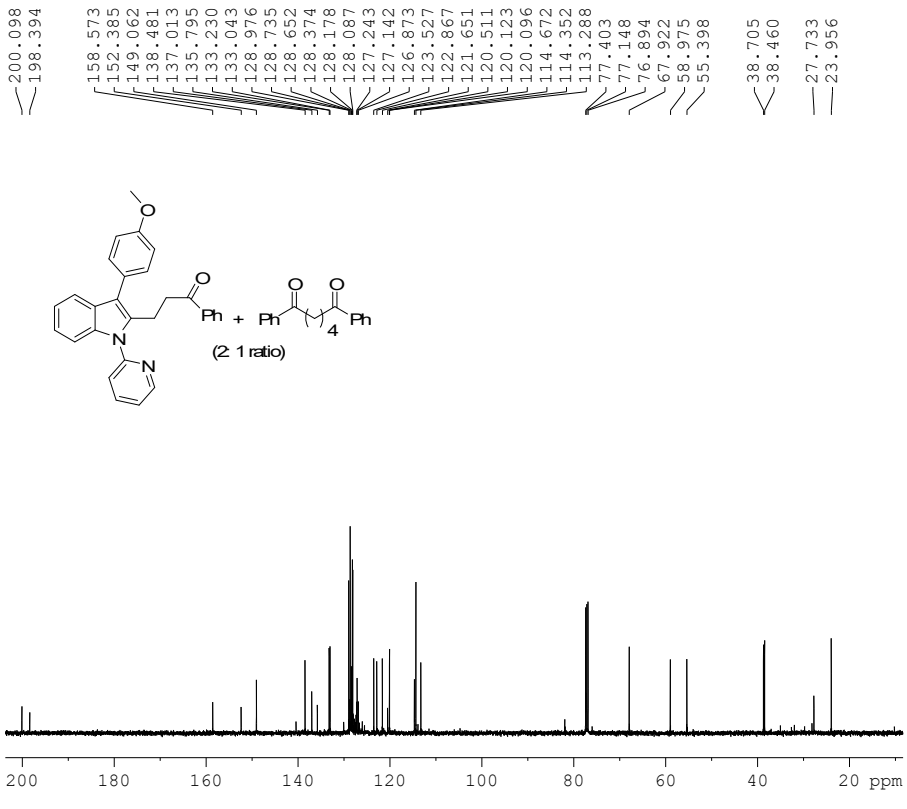
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3m**

3-(3-(4-Methoxyphenyl)-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one: 3n




```
Current Data Parameters
NAME                  spa
EXPNO                  66
PROCNO                  1

F2 - Acquisition Paramet
Date_           20210922
Time               15.06
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     2
SWH            10000.000
FIDRES          0.305176
AQ             1.6384000
RG                 31.24
DW                50.000
DE                  6.50
TE                298.2
D1            0.50000000
TD0                    1

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

F2 - Processing paramete
SI                 65536
SF          500.1500678
WDW                   EM
SSB                    0
LB                  0.30
GB                     0
PC                  1.00
```

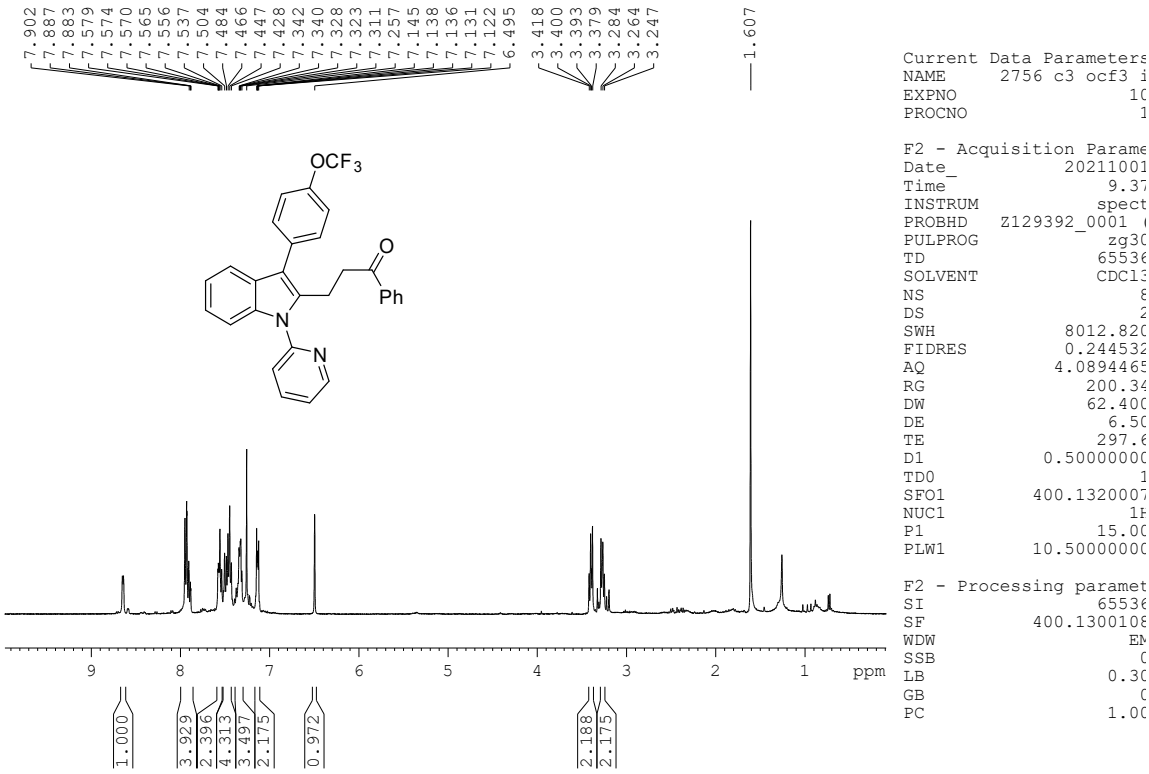
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3n**



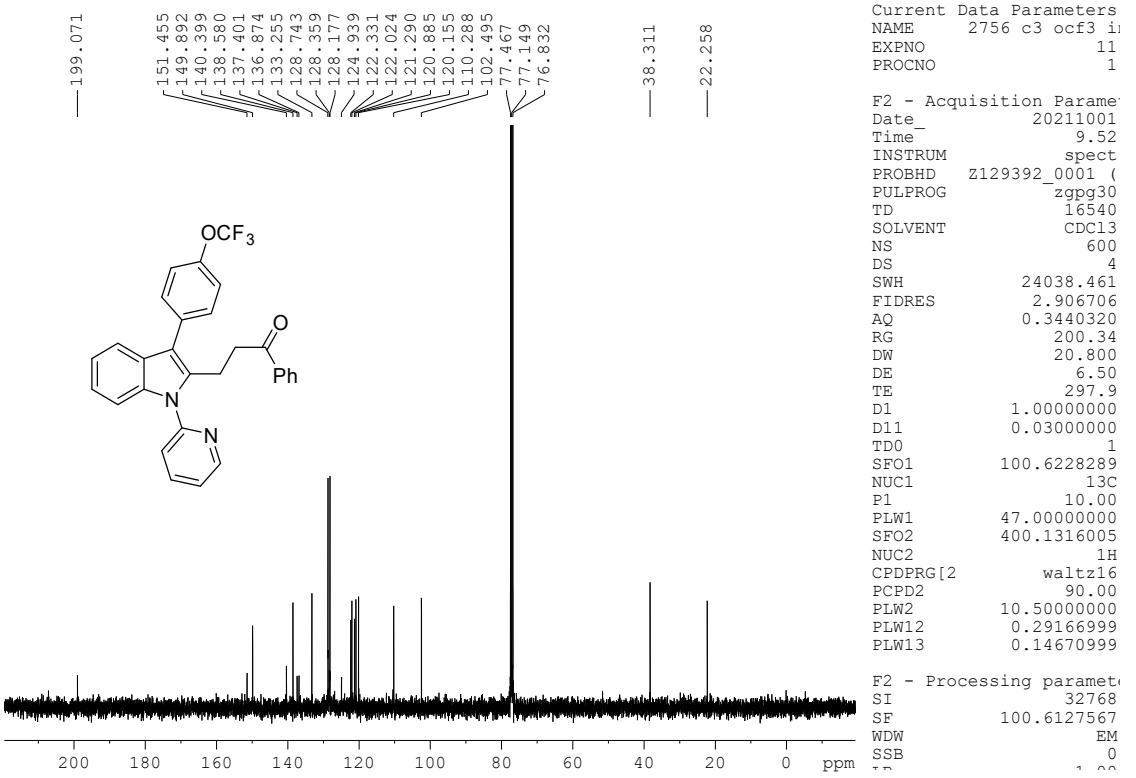

```
Current Data Parameters
NAME                  spa
EXPNO                  67
PROCNO                  1

F2 - Acquisition Paramet
Date_           20210922
Time               15.11
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 20480
SOLVENT            CDCl3
NS                   128
DS                     4
SWH            29761.904
FIDRES          1.453218
AQ             0.3440640
RG                202.34
DW                16.800
DE                  6.50
TE                298.8
D1            1.00000000
D11           0.03000000
TD0                    1

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

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

F2 - Processing paramete
SI                 32768
```

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

1-Phenyl-3-(1-(pyridin-2-yl)-3-(4-(trifluoromethoxy)phenyl)-1*H*-indol-2-yl)propan-1-one: 3o

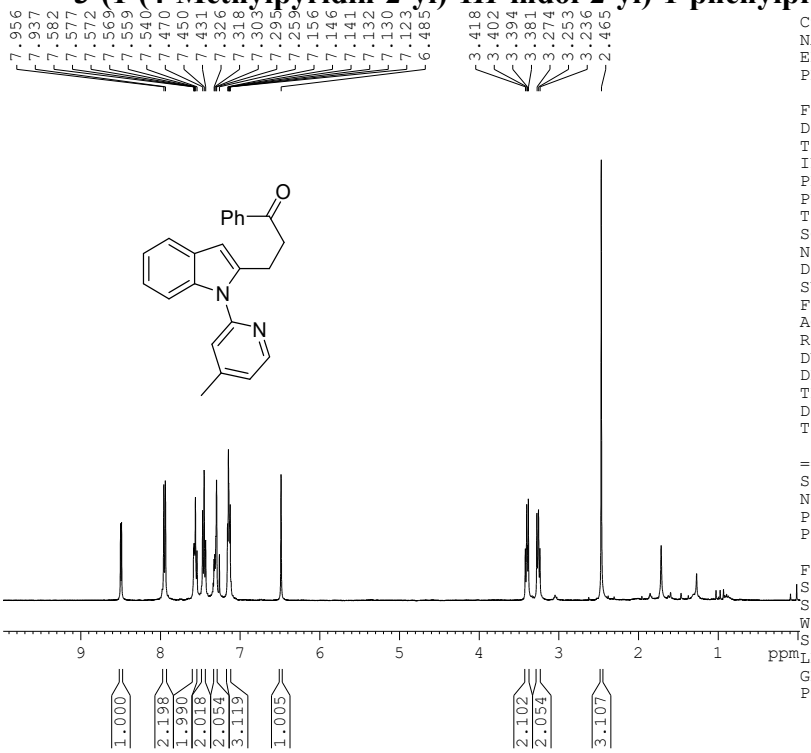


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3o**



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

3-(1-(4-Methylpyridin-2-yl)-1*H*-indol-2-yl)-1-phenylpropan-1-one: 3p



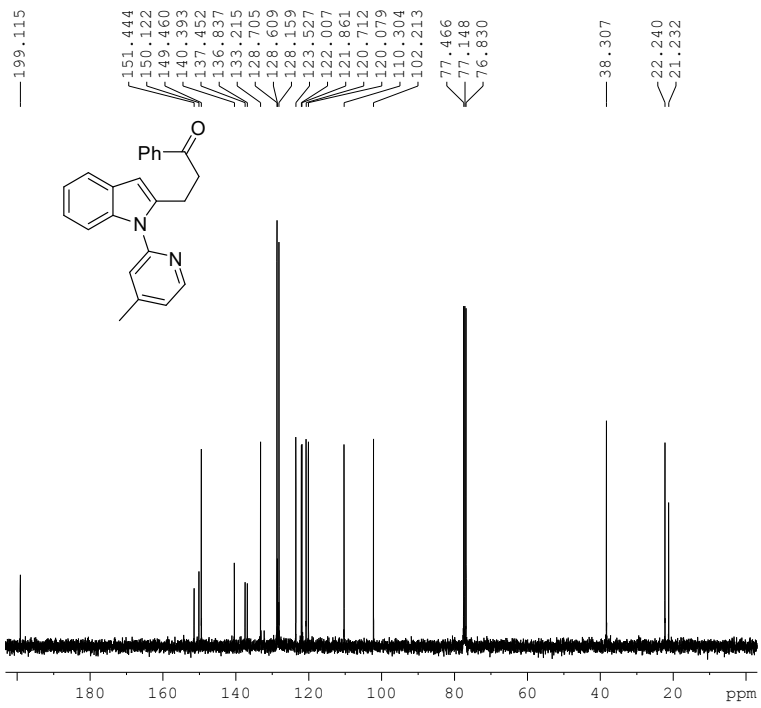
Current Data Parameters
NAME 1450
EXPNO 698
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180821
Time 18.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 124.58
DW 62.400 usec
DE 6.50 usec
TE 296.3 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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



Current Data Parameters
NAME 1450
EXPNO 699
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180821
Time 18.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

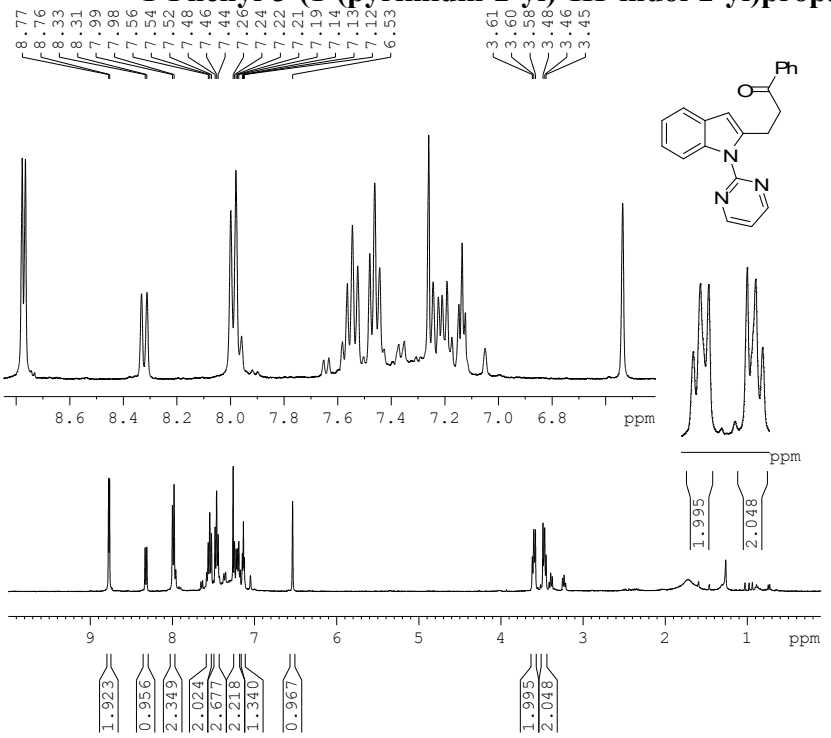
======== CHANNEL f1 ========
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

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

F2 - Processing parameters
SI 32768
SF 100.6127609 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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

1-Phenyl-3-(1-(pyrimidin-2-yl)-1*H*-indol-2-yl)propan-1-one: 3q

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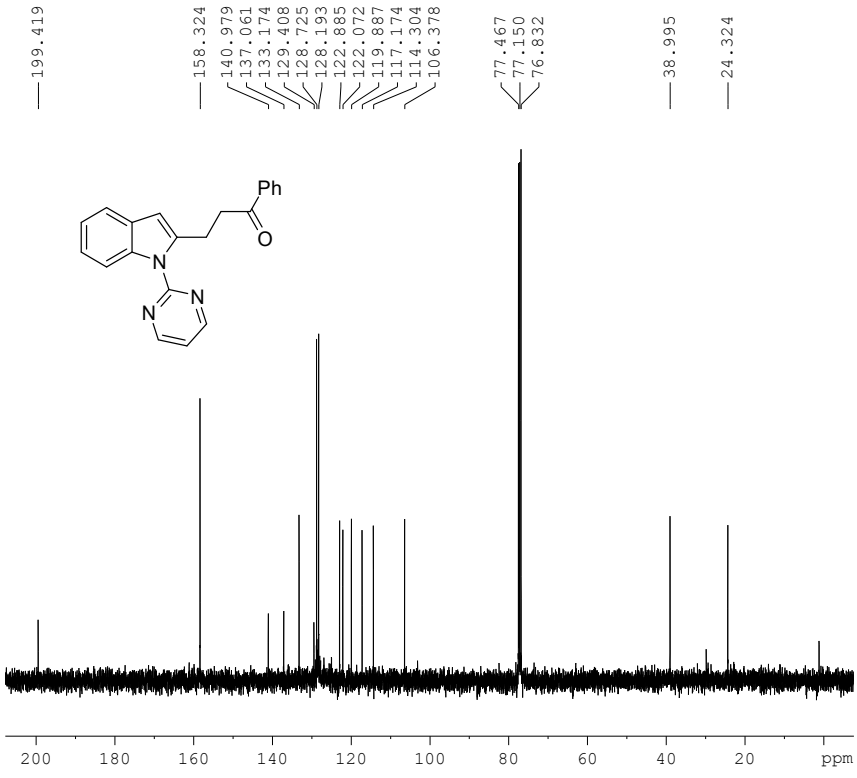
Current Data Parameters
NAME                  pj5
EXPNO                 371
PROCNO                  1

F2 - Acquisition Parameters
Date_           20220815
Time                9.49 h
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
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                299.8 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          400.1300094 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 **3q**

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Current Data Parameters
NAME     2688 I PYM PAREN
EXPNO                 31
PROCNO                 1

F2 - Acquisition Paramete
Date_           20210704
Time              15.10 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                301.0 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
SI                 32768
SF          100.6127579 M
WDW                   EM
SSB                    0
```
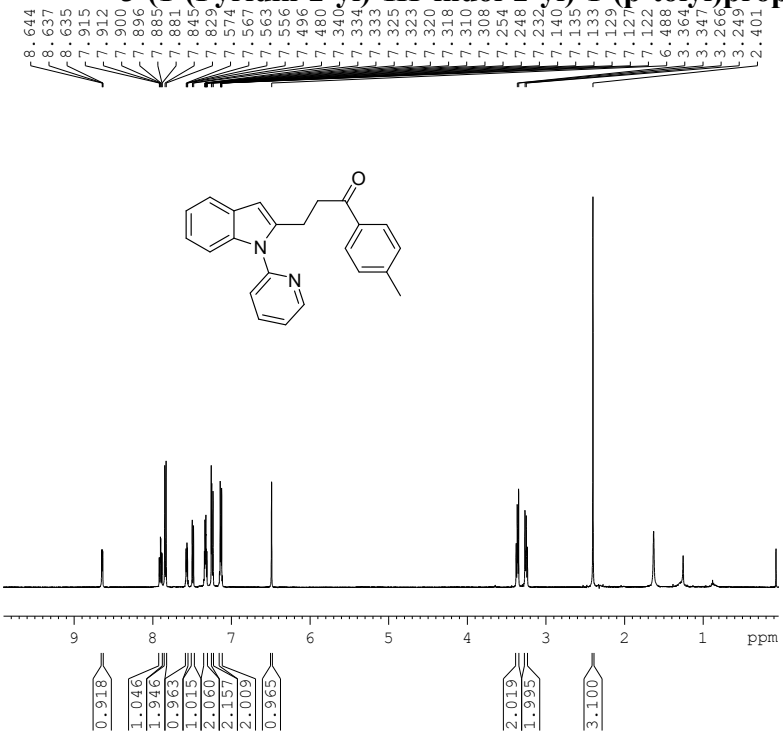

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3q**

3-(1-(Pyridin-2-yl)-1*H*-indol-2-yl)-1-(p-tolyl)propan-1-one: 3r

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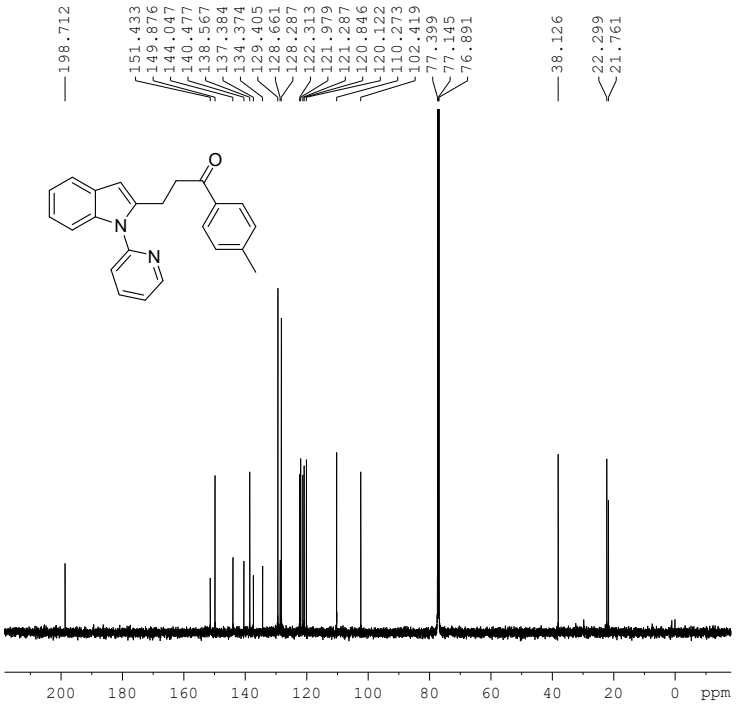
Current Data Parameters
NAME                  pure
EXPNO                   25
PROCNO                   1

F2 - Acquisition Parameters
Date_              20181207
Time                   3.28
INSTRUM               spect
PROBHD   5 mm PABBI 1H/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               10000.000 Hz
FIDRES                0.305176 Hz
AQ                1.6384000 sec
RG                   124.08
DW                   50.000 usec
DE                    6.50 usec
TE                   295.9 K
D1                0.50000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            500.1525008 MHz
NUC1                     1H
P1                    9.65 usec
PLW1             9.30000019 W

F2 - Processing parameters
SI                       65536
SF              500.1500151 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

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




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

F2 - Acquisition Parameters
Date_              20181207
Time                   4.17
INSTRUM               spect
PROBHD   5 mm PABBI 1H/
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                   296.1 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                      1

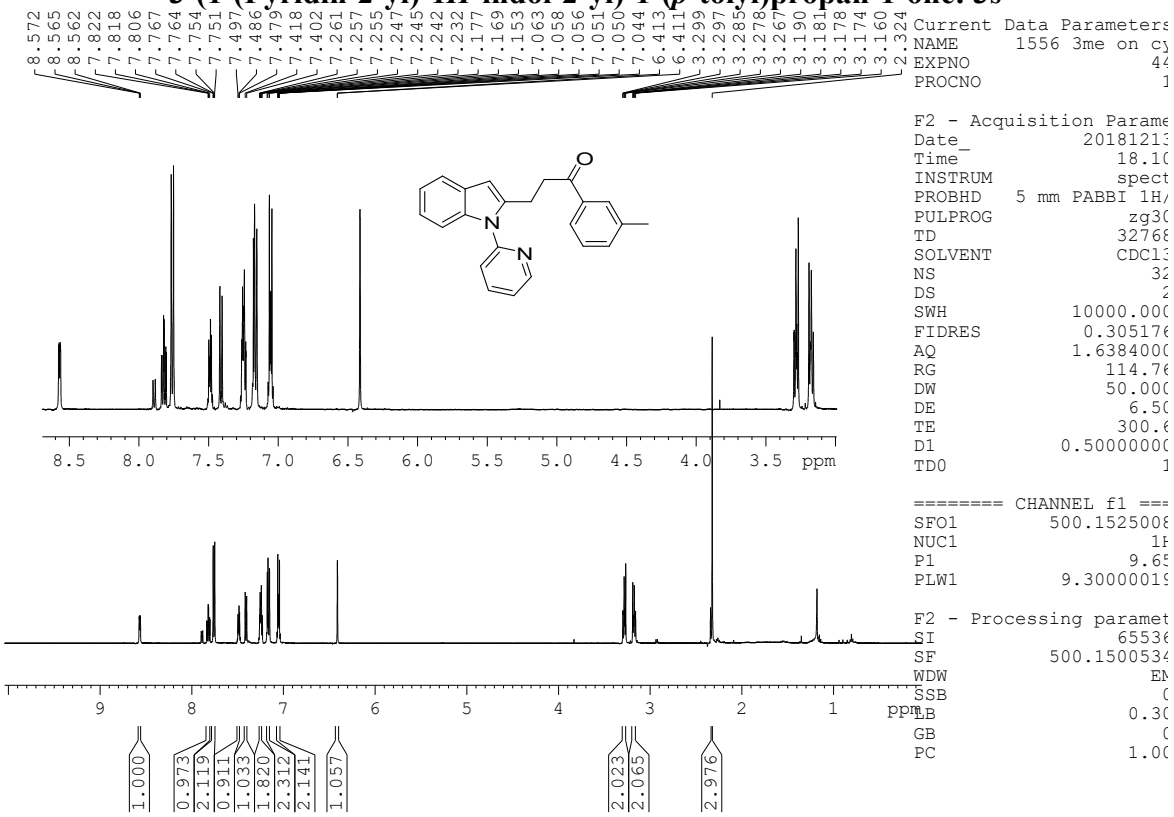
======== CHANNEL f1 ========
SFO1            125.7753932 MHz
NUC1                    13C
P1                   14.60 usec
PLW1           100.00000000 W

======== CHANNEL f2 ========
SFO2            500.1520006 MHz
NUC2                     1H
CPDPRG[2             waltz16
PCPD2                 80.00 usec
PLW2              9.30000019 W
PLW12             0.13531999 W
PLW13             0.06806400 W

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

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

3-(1-(Pyridin-2-yl)-1*H*-indol-2-yl)-1-(*p*-tolyl)propan-1-one: 3s



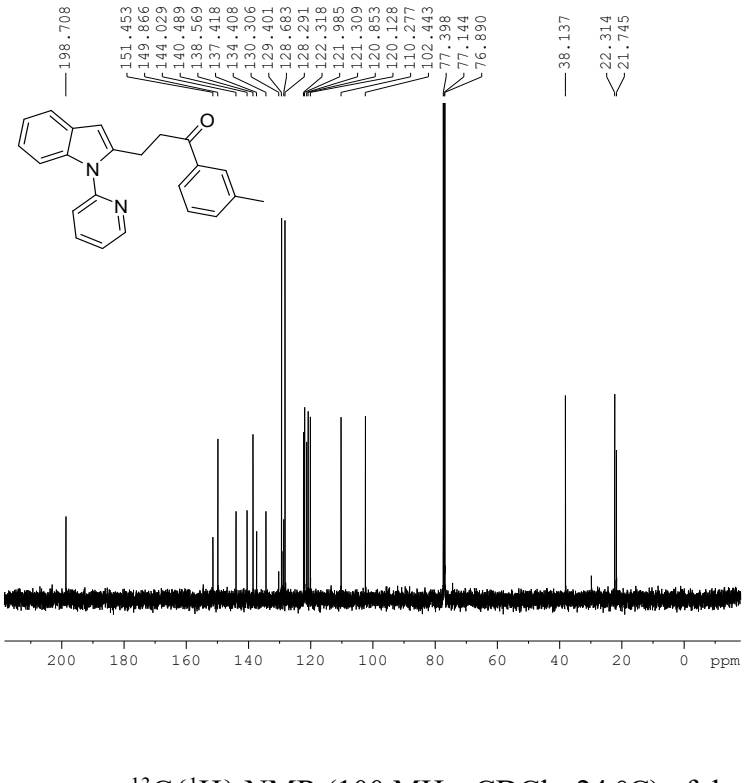

```
Current Data Parameters
NAME      1556 3me on cy
EXPNO                 44
PROCNO                 1

F2 - Acquisition Parame
Date_           20181213
Time_              18.10
INSTRUM            spect
PROBHD   5 mm PABBI 1H/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    2
SWH           10000.000
FIDRES         0.305176
AQ            1.638400
RG               114.76
DW               50.000
DE                 6.50
TE                300.6
D1            0.50000000
TD0                    1

======== CHANNEL f1 ===
SFO1         500.152500
NUC1                 1H
P1                 9.65
PLW1          9.3000001

F2 - Processing paramet
SI                65536
SF          500.150053
WDW                  EM
SSB                   0
LB                 0.30
GB                    0
PC                 1.00
```

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




```
Current Data Parameters
NAME      1556 3me on cy oh
EXPNO                   45
PROCNO                   1

F2 - Acquisition Parameters
Date_           20181213
Time_              18.25
INSTRUM            spect
PROBHD   5 mm PABBI 1H/
PULPROG          zgpg30
TD                20480
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           29761.904 Hz
FIDRES         1.453218 Hz
AQ            0.3440640 sec
RG               202.34
DW               16.800 usec
DE                 6.50 usec
TE                300.9 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1

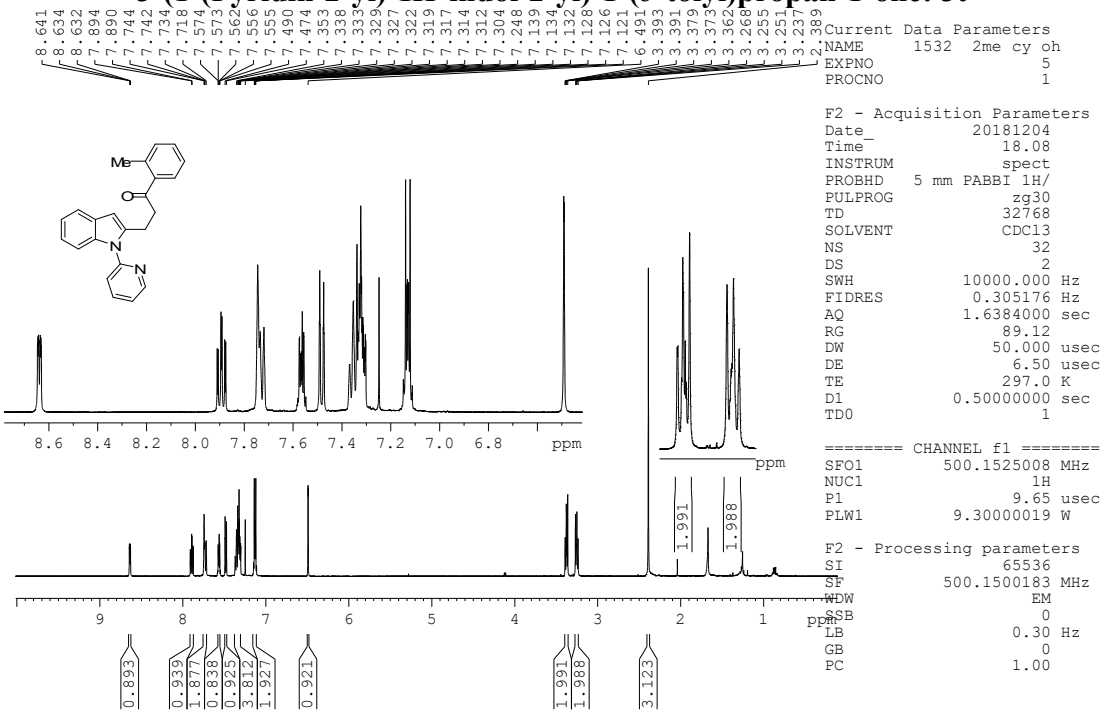
======== CHANNEL f1 ========
SFO1        125.7753932 MHz
NUC1                  13C
P1                 14.60 usec
PLW1       100.00000000 W

======== CHANNEL f2 ========
SFO2        500.1520006 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2          9.30000019 W
PLW12         0.13531999 W
PLW13         0.06806400 W

F2 - Processing parameters
SI                32768
SF          125.7628044 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

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

3-(1-(Pyridin-2-yl)-1*H*-indol-2-yl)-1-(*o*-tolyl)propan-1-one: 3t



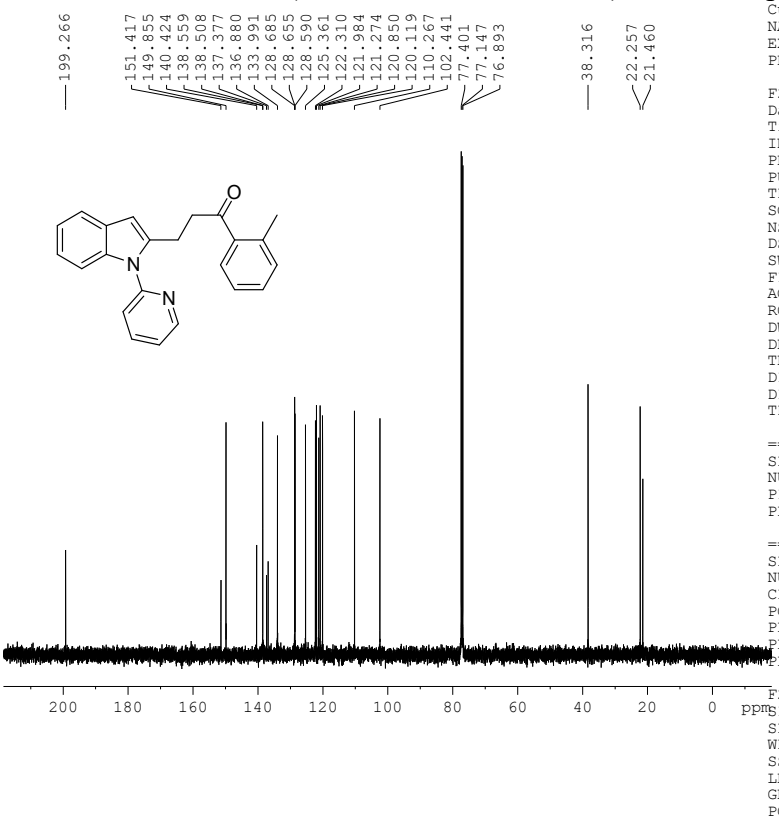

```
Current Data Parameters
NAME      1532  2me cy oh
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181204
Time               18.08
INSTRUM            spect
PROBHD   5 mm PABBI 1H/
PULPROG            zg30
TD                32768
SOLVENT            CDCl3
NS                    32
DS                     2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ            1.6384000 sec
RG                89.12
DW               50.000 usec
DE                6.50 usec
TE                297.0 K
D1           0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        500.1525008 MHz
NUC1                   1H
P1                  9.65 usec
PLW1         9.30000019 W

F2 - Processing parameters
SI                 65536
SF          500.1500183 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

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




```
Current Data Parameters
NAME      1532  2me cy oh
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181204
Time               18.21
INSTRUM            spect
PROBHD   5 mm PABBI 1H/
PULPROG          zgpg30
TD                20480
SOLVENT            CDCl3
NS                   512
DS                     4
SWH           29761.904 Hz
FIDRES         1.453218 Hz
AQ            0.3440640 sec
RG                202.34
DW               16.800 usec
DE                6.50 usec
TE                297.4 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1

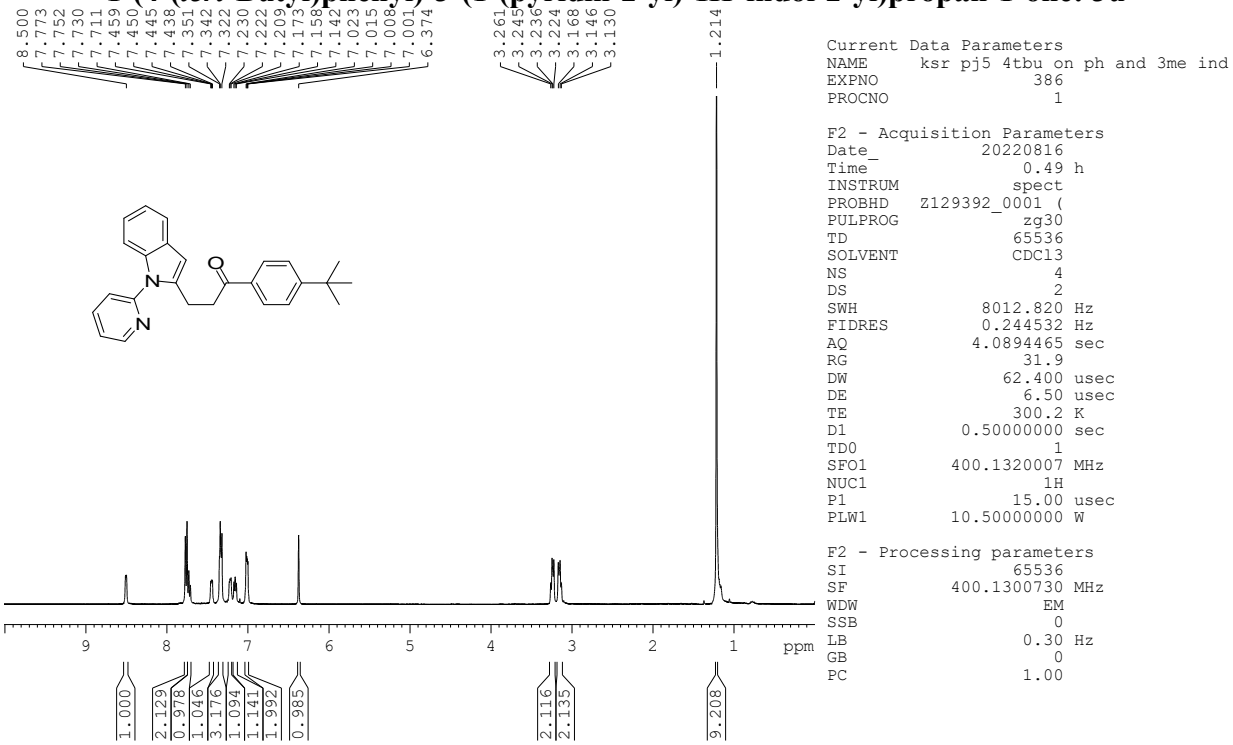
======== CHANNEL f1 ========
SFO1        125.7753932 MHz
NUC1                  13C
P1                14.60 usec
PLW1       100.00000000 W

======== CHANNEL f2 ========
SFO2        500.1520006 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          9.30000019 W
PLW12         0.13531999 W
PLW13         0.06806400 W

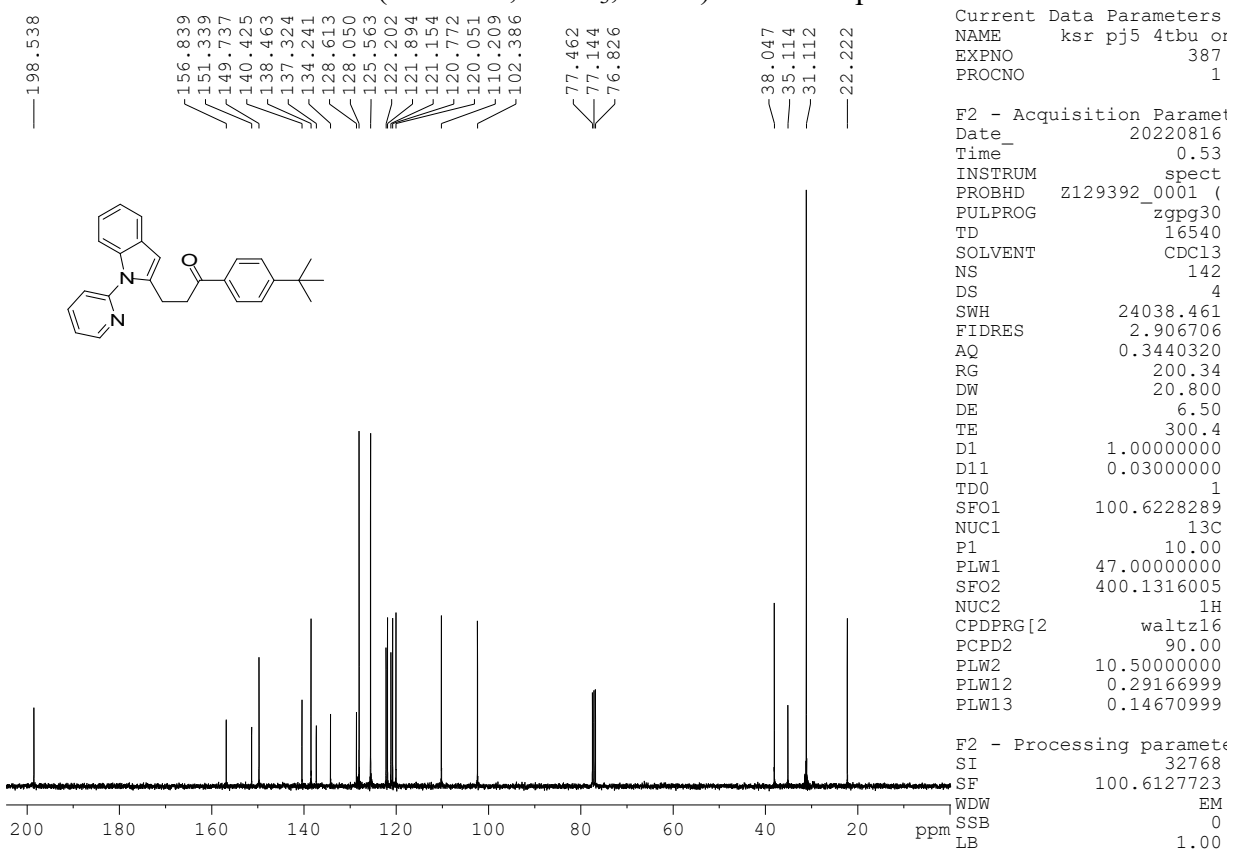
F2 - Processing parameters
SI                 32768
SF          125.7628074 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

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

1-(4-(*tert*-Butyl)phenyl)-3-(1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one: 3u

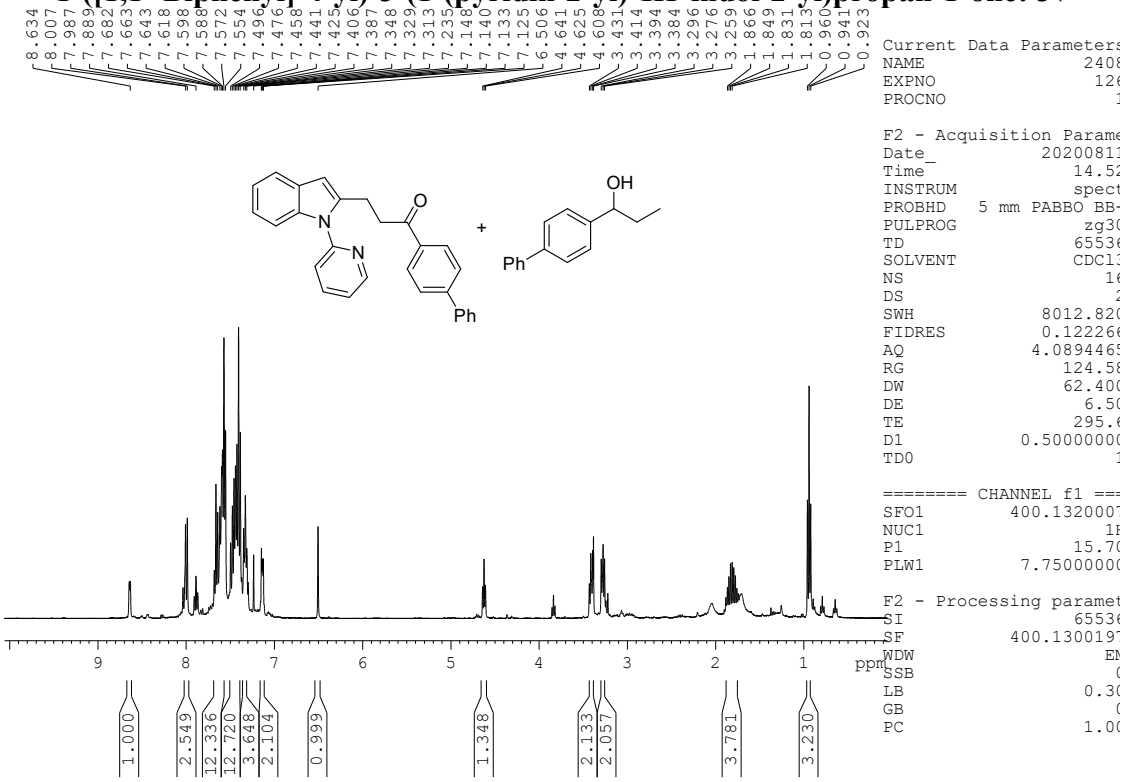


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3u**

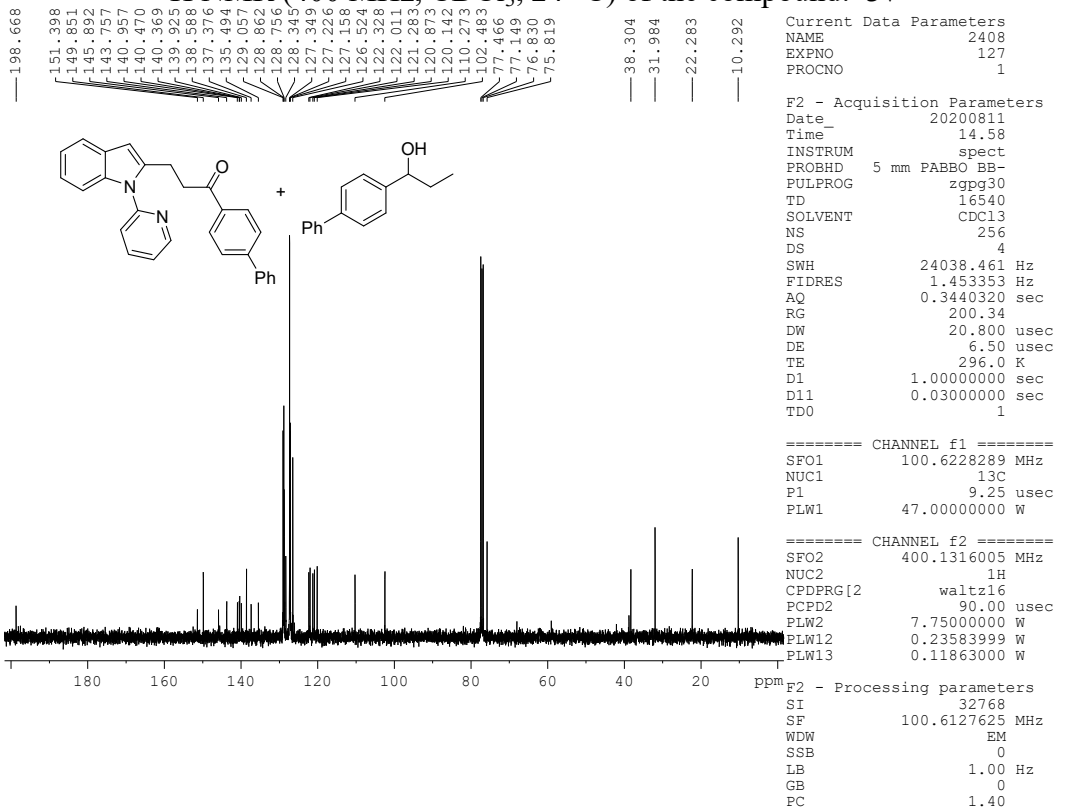


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3u**

1-([1,1'-Biphenyl]-4-yl)-3-(1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one: 3v

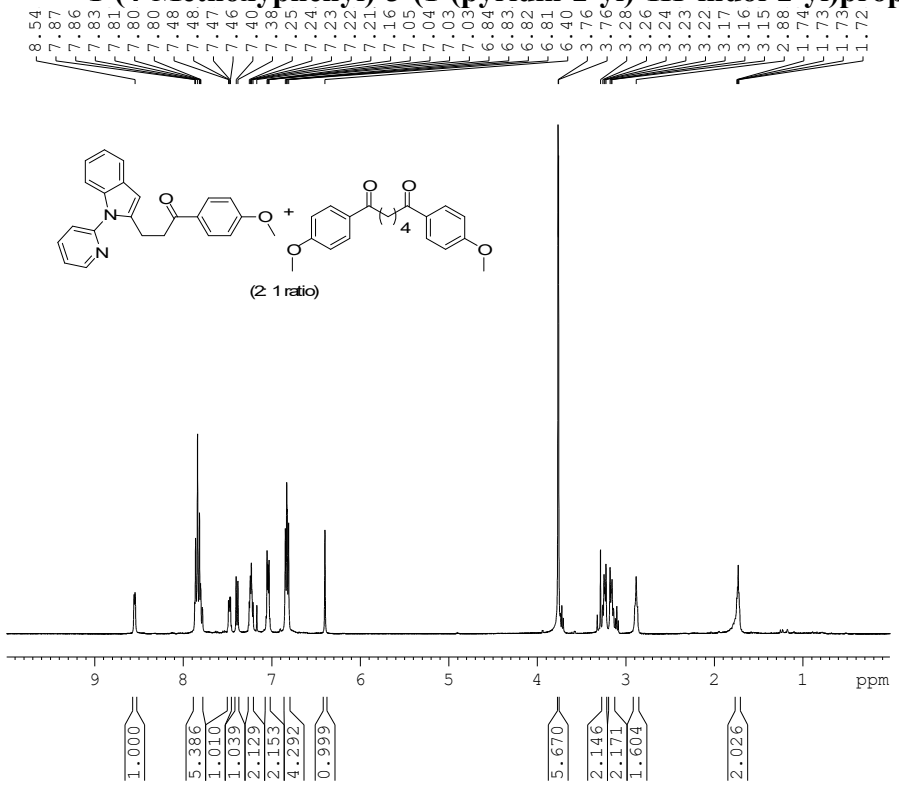


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound: **3v**



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

1-(4-Methoxyphenyl)-3-(1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one: 3w

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Current Data Parameters
NAME      2777 4OMe Ph c
EXPNO                 84
PROCNO                 1

F2 - Acquisition Parame
Date_           20211205
Time                0.14
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     2
SWH             8012.820
FIDRES          0.244532
AQ             4.0894465
RG                 95.73
DW                62.400
DE                  6.50
TE                298.2
D1           0.50000000
TD0                    1
SFO1         400.1320007
NUC1                1H
P1                 15.00
PLW1         10.50000000

F2 - Processing paramet
SI                 65536
SF          400.1300458
WDW                   EM
SSB                    0
LB                  0.30
GB                     0
PC                  1.00
```
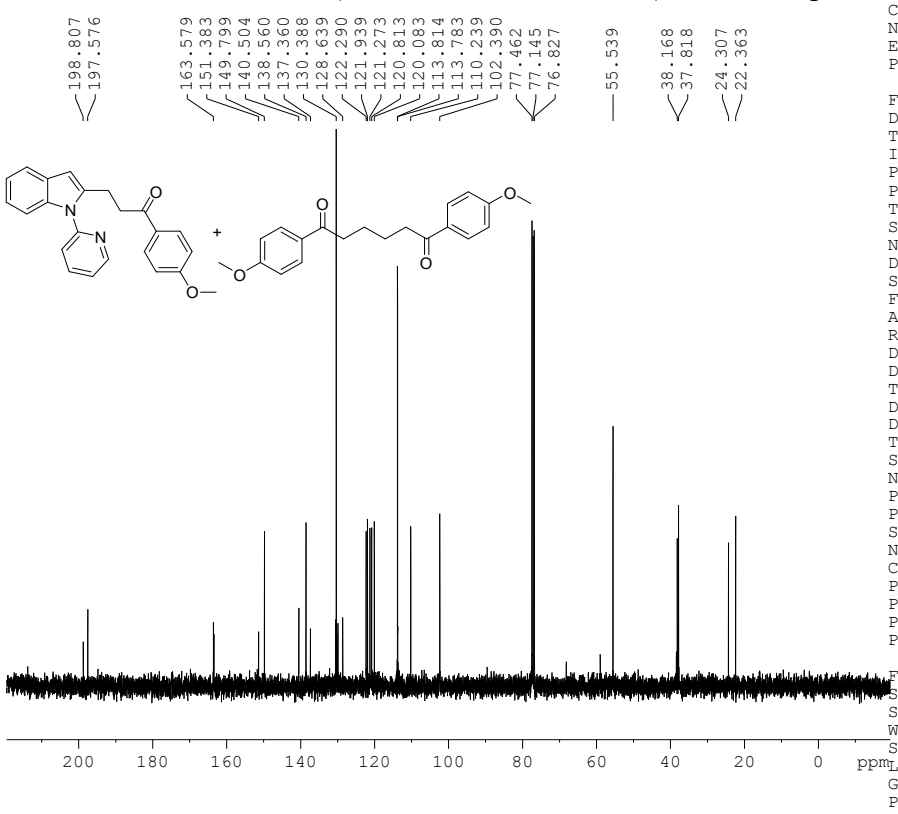
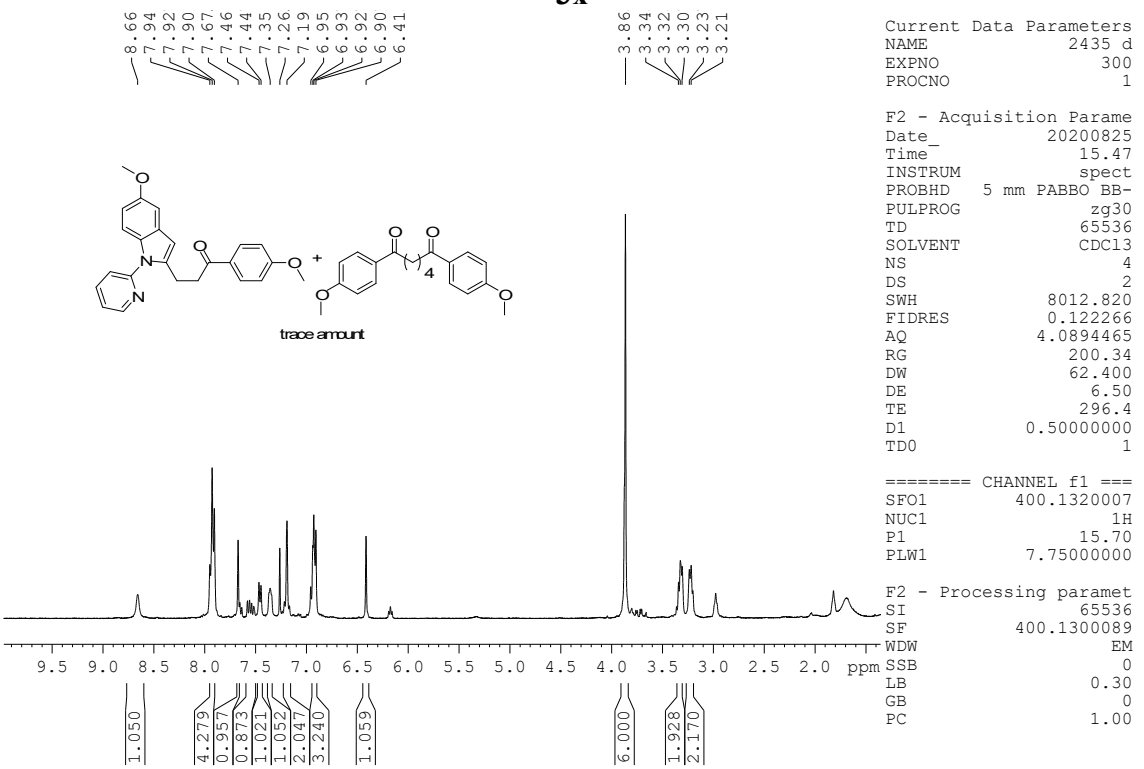

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3w**



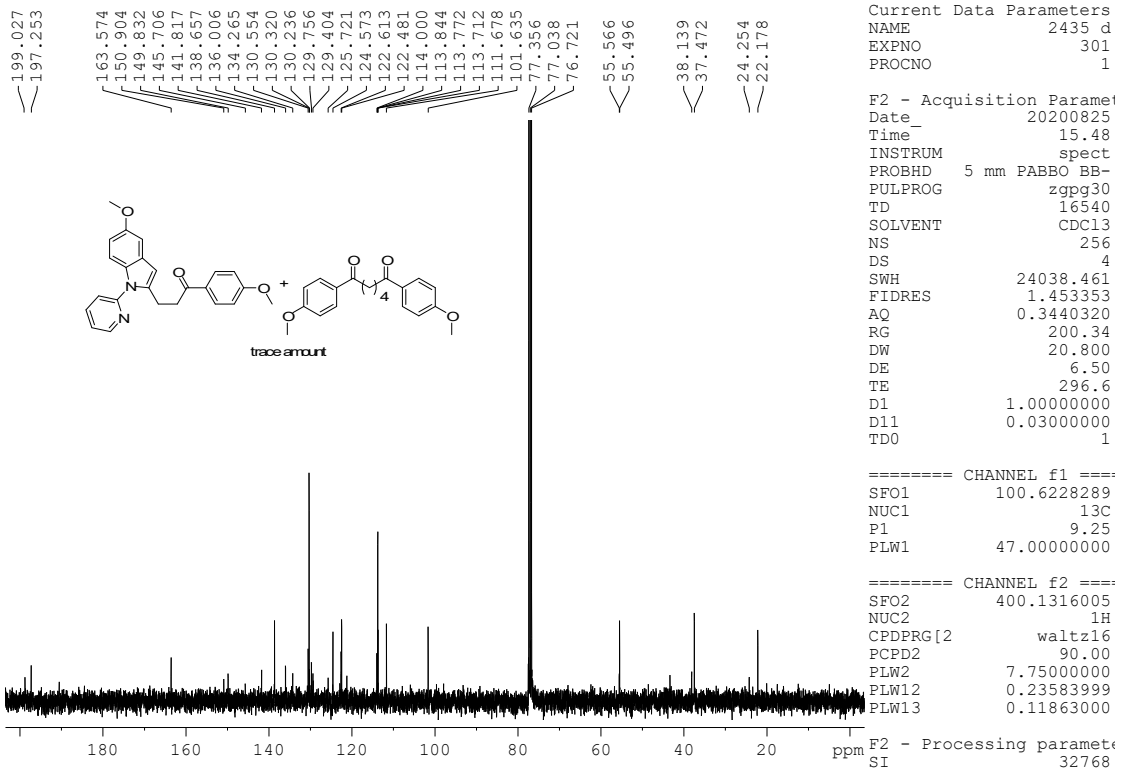

```
Current Data Parameters
NAME      2777 4OMe Ph c
EXPNO                 85
PROCNO                 1

F2 - Acquisition Parame
Date_           20211205
Time                0.17
INSTRUM            spect
PROBHD   Z129392_0001 (
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                    80
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 paramet
SI                 32768
SF          100.6127629
WDW                   EM
SSB                    0
LB                  1.00
GB                     0
PC                  1.40
```

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

3-(5-Methoxy-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-(4-methoxyphenyl)propan-1-one: 3x

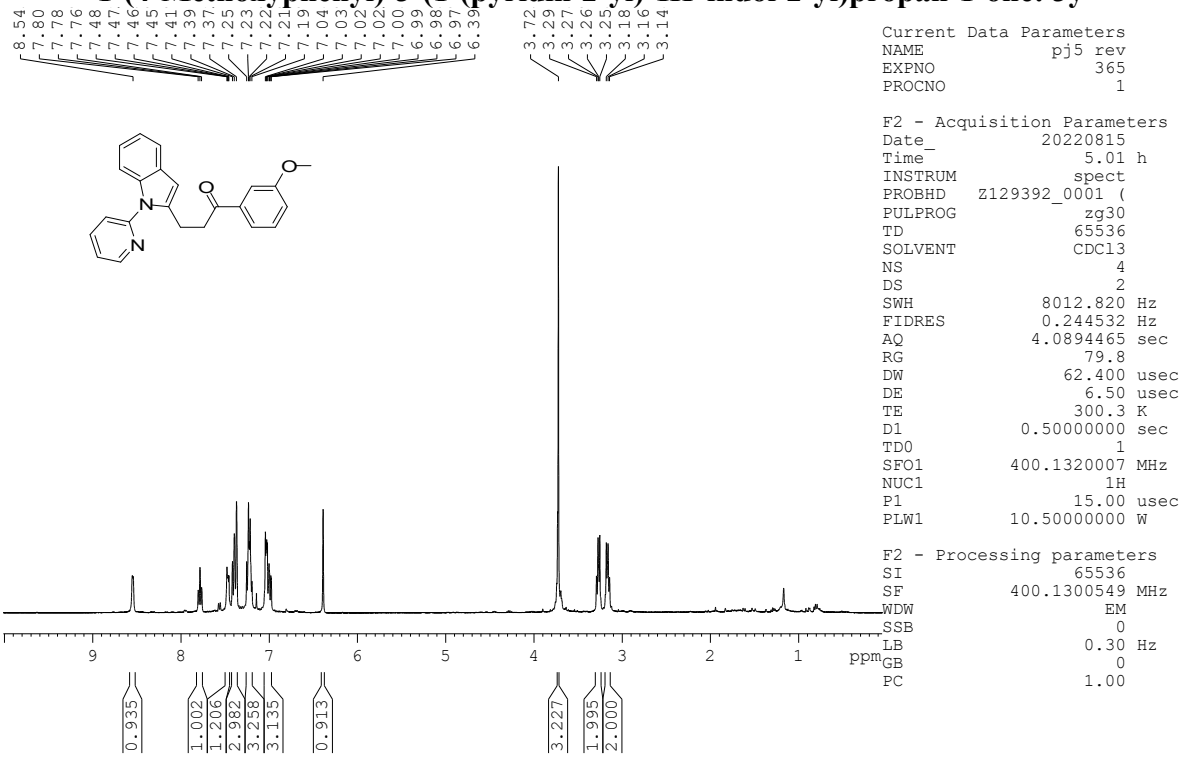


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3x**

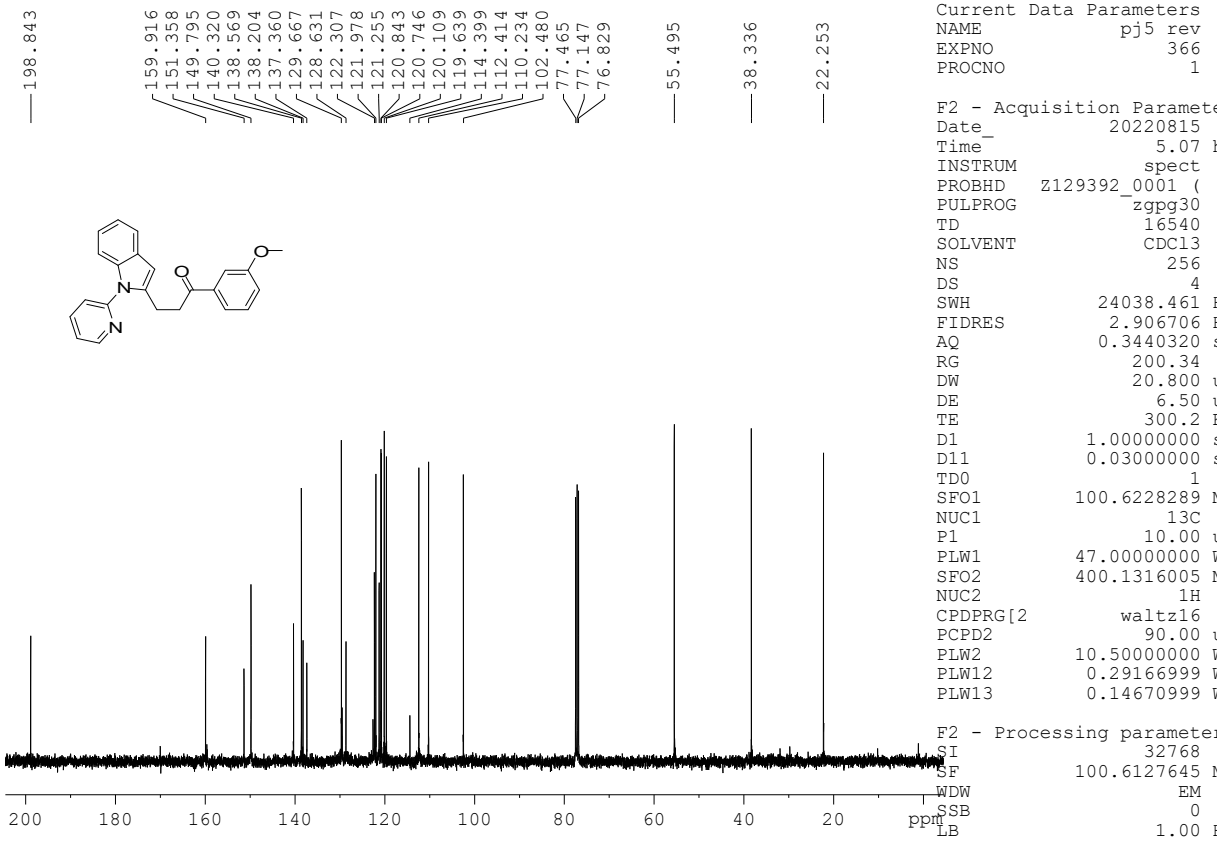


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3x**

1-(4-Methoxyphenyl)-3-(1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one: 3y

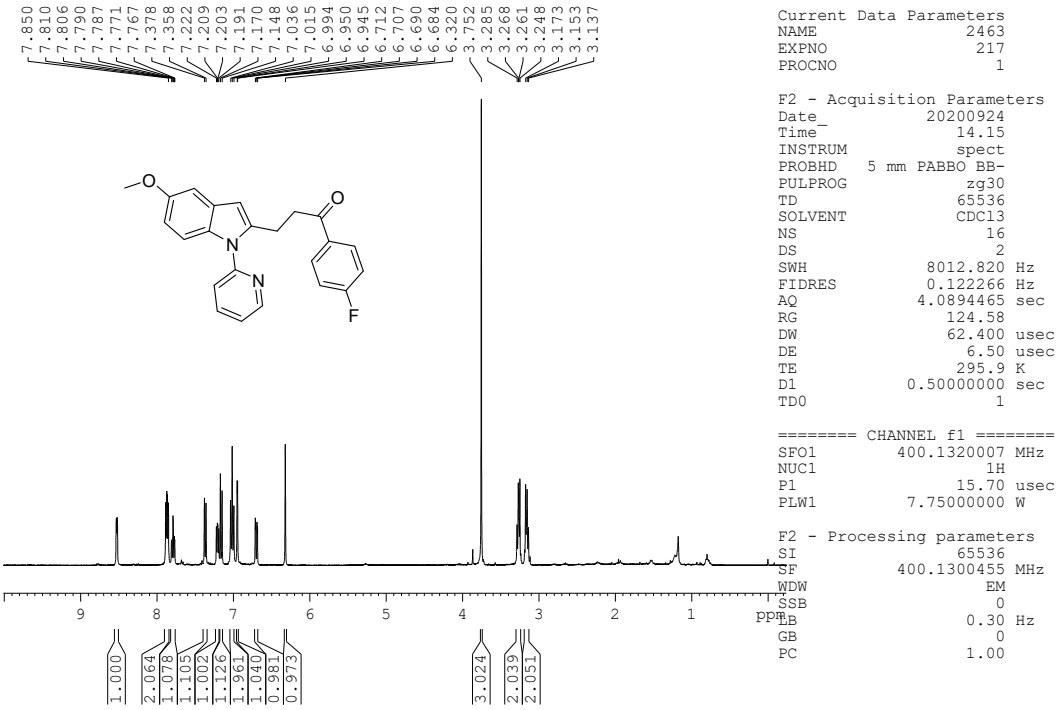


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3y**



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

1-(4-Fluorophenyl)-3-(5-methoxy-1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one: 3z



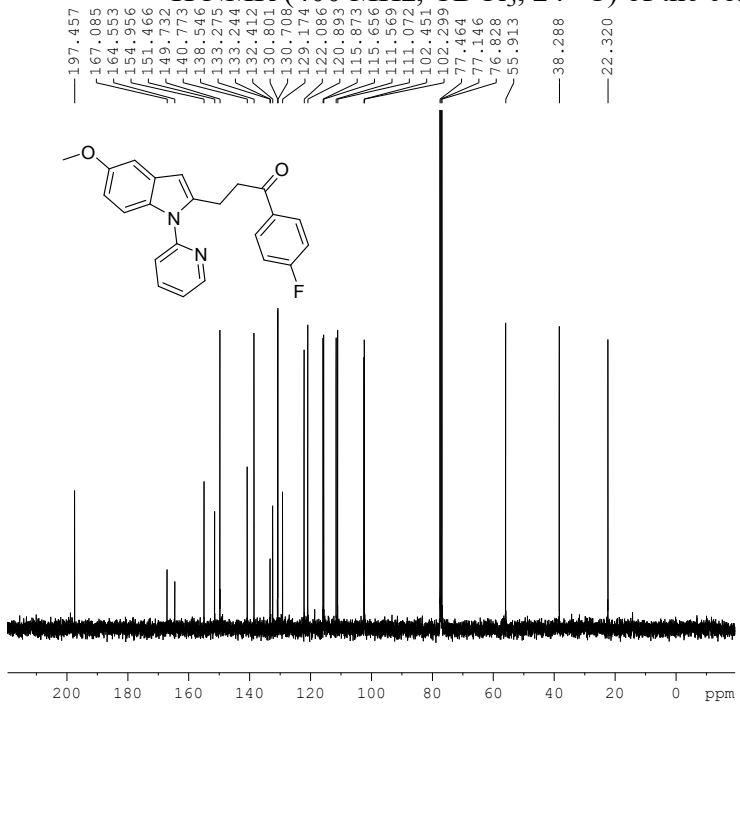
Current Data Parameters
NAME 2463
EXPNO 217
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200924
Time 14.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 124.58
DW 62.400 usec
DE 6.50 usec
TE 295.9 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300455 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 **3z**



Current Data Parameters
NAME 2463
EXPNO 232
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200924
Time 16.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

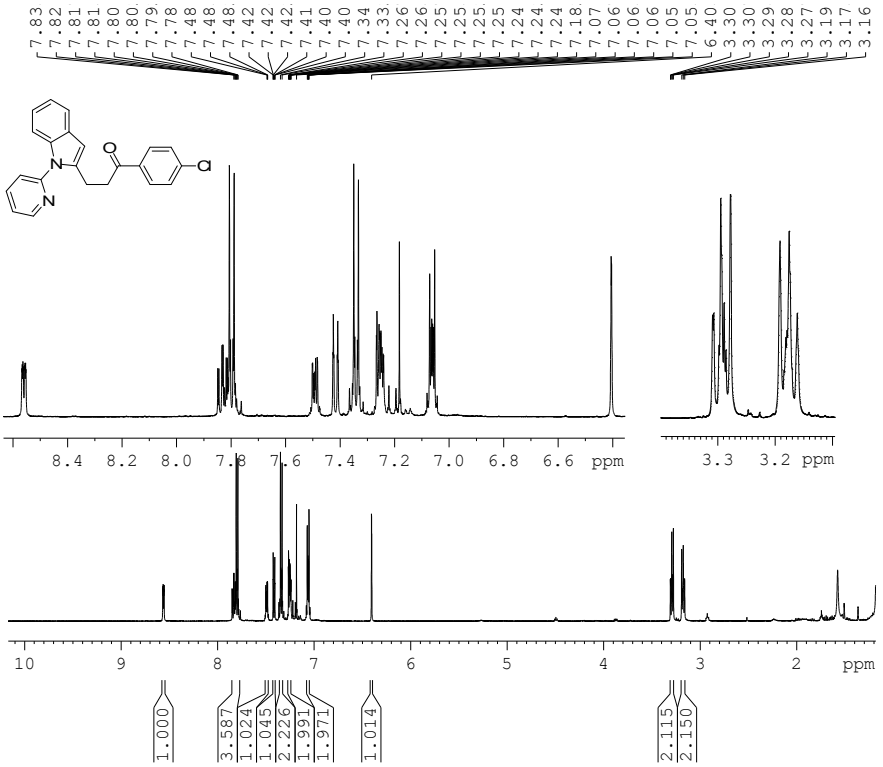
======== CHANNEL f1 ========
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

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

F2 - Processing parameters
SI 32768
SF 100.6127624 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

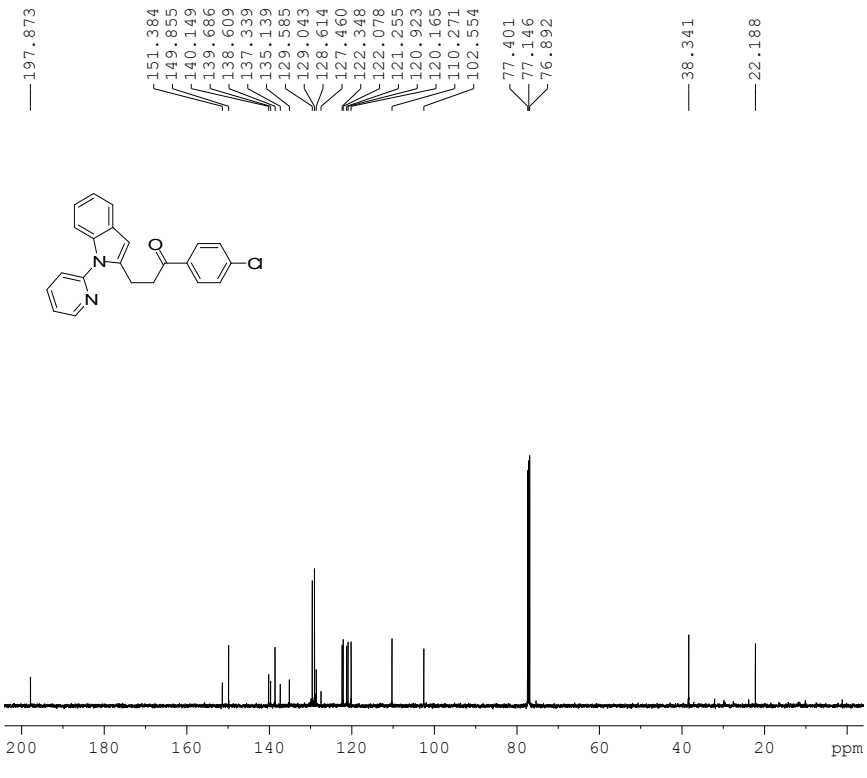
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3z**

1-(4-Chlorophenyl)-3-(1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one: 3aa




```
Current Data Parameters
NAME      1539 4cl on cy oh
EXPNO                   22
PROCNO                   1

F2 - Acquisition Parameters
Date_           20181207
Time               2.38
INSTRUM           spect
PROBHD   5 mm PABBI 1H/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            1.6384000 sec
RG                124.08
DW                50.000 usec
DE                 6.50 usec
TE                296.0 K
D1            0.50000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.1525008 MHz
NUC1                1H
P1                9.65 usec
PLW1          9.30000019 W

F2 - Processing parameters
SI                65536
SF          500.1500508 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

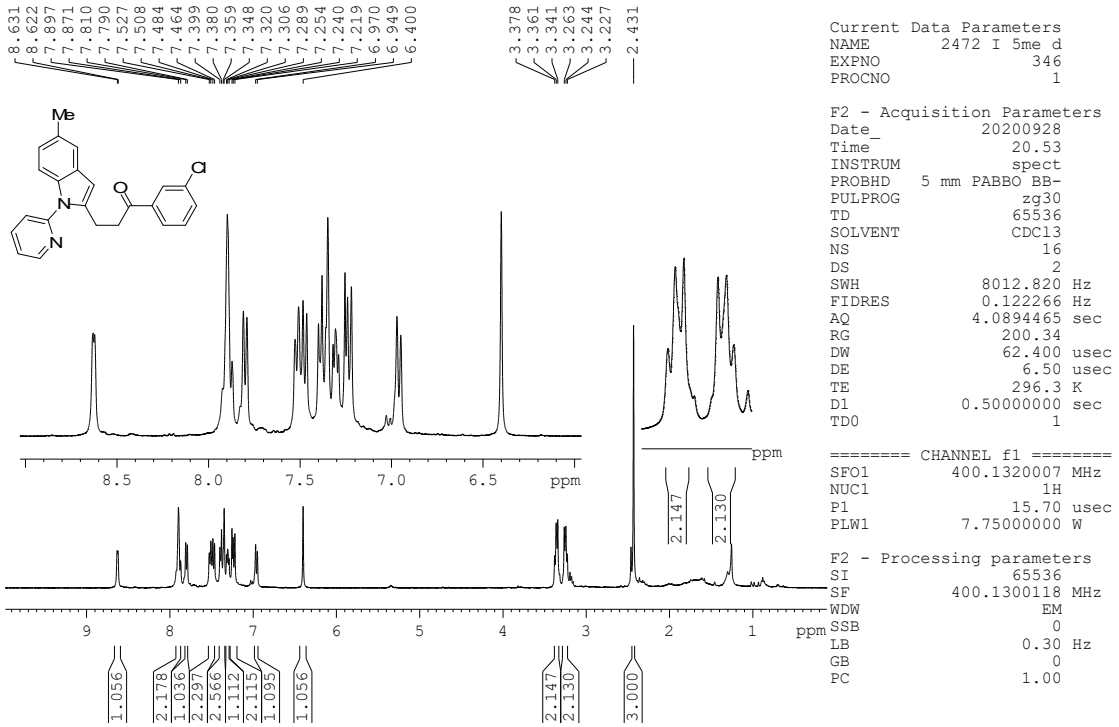
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3aa**



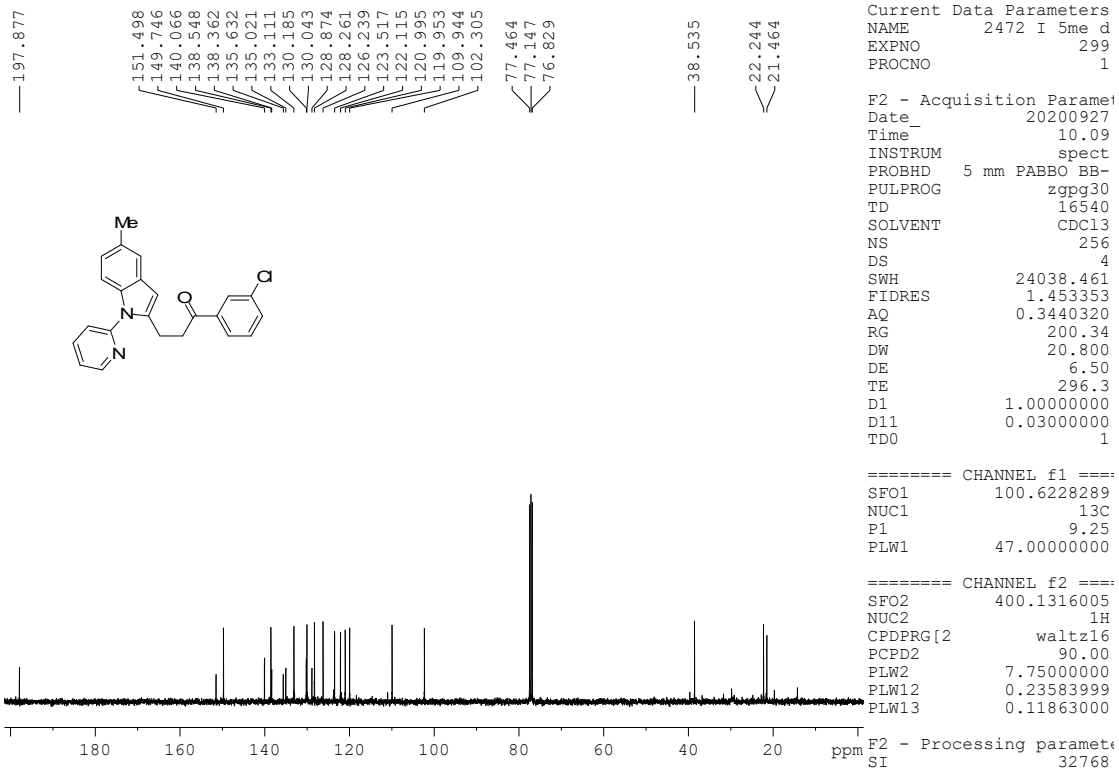

```
Current Data Parameters
NAME      1539 4cl on cy
EXPNO                  23
PROCNO                  1

F2 - Acquisition Parame
Date_           20181207
Time               3.15
INSTRUM           spect
PROBHD   5 mm PABBI 1H/
PULPROG          zgpg30
TD                20480
SOLVENT           CDCl3
NS                 1500
DS                    4
SWH           29761.904
FIDRES         1.453218
AQ            0.3440640
RG                202.34
DW                16.800
DE                 6.50
TE                296.2
D1            1.00000000
D11           0.03000000
TD0                   1

======== CHANNEL f1 ===
SFO1         125.7753932
NUC1                13C
P1                14.60
PLW1        100.00000000

======== CHANNEL f2 ===
SFO2         500.1520006
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00
PLW2          9.30000019
PLW12         0.13531999
PLW13         0.06806400

F2 - Processing paramet
SI                32768
```

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

1-(3-Chlorophenyl)-3-(5-methyl-1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one: 3ab

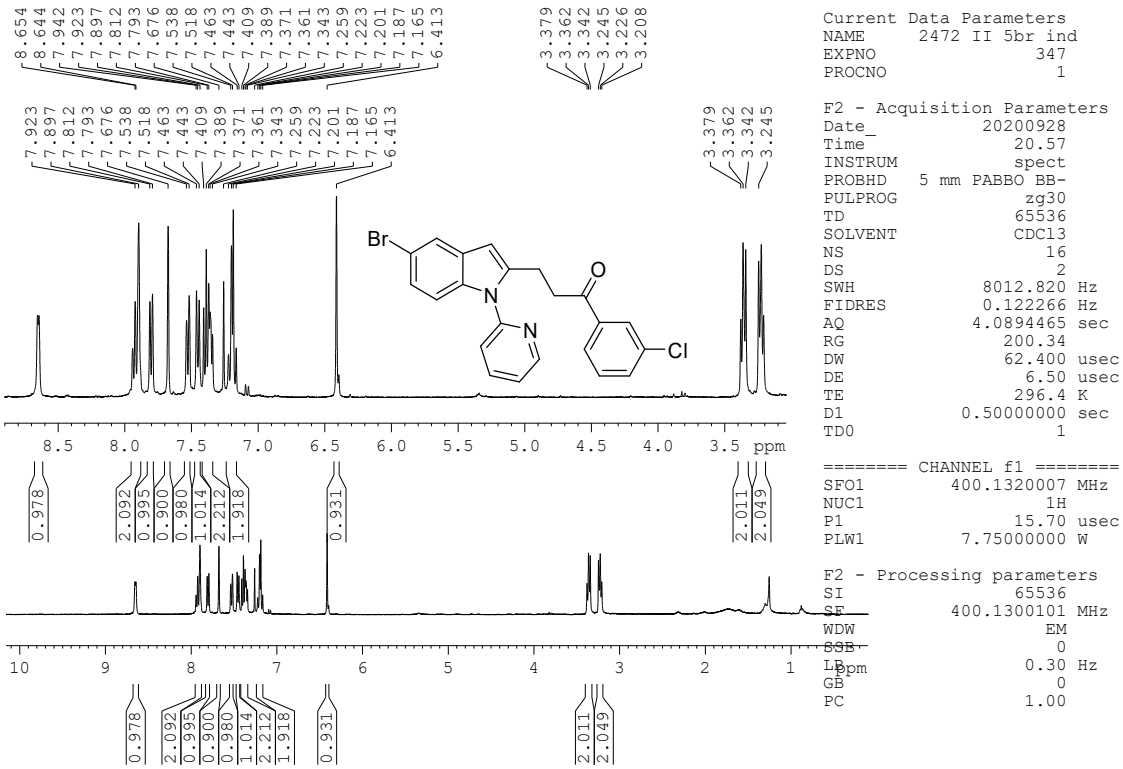


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3ab**



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

3-(5-Bromo-1-(pyridin-2-yl)-1*H*-indol-2-yl)-1-(3-chlorophenyl)propan-1-one: 3ac



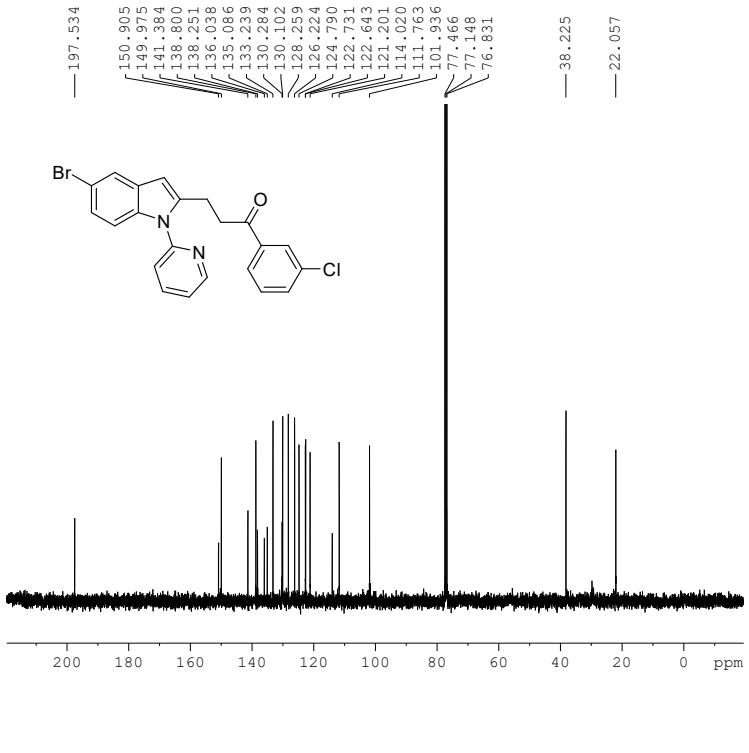
Current Data Parameters
NAME 2472 II 5br ind
EXPNO 347
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200928
Time 20.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 296.4 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300101 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 **3ac**



Current Data Parameters
NAME 2472 II 5br ind
EXPNO 302
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200927
Time 10.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

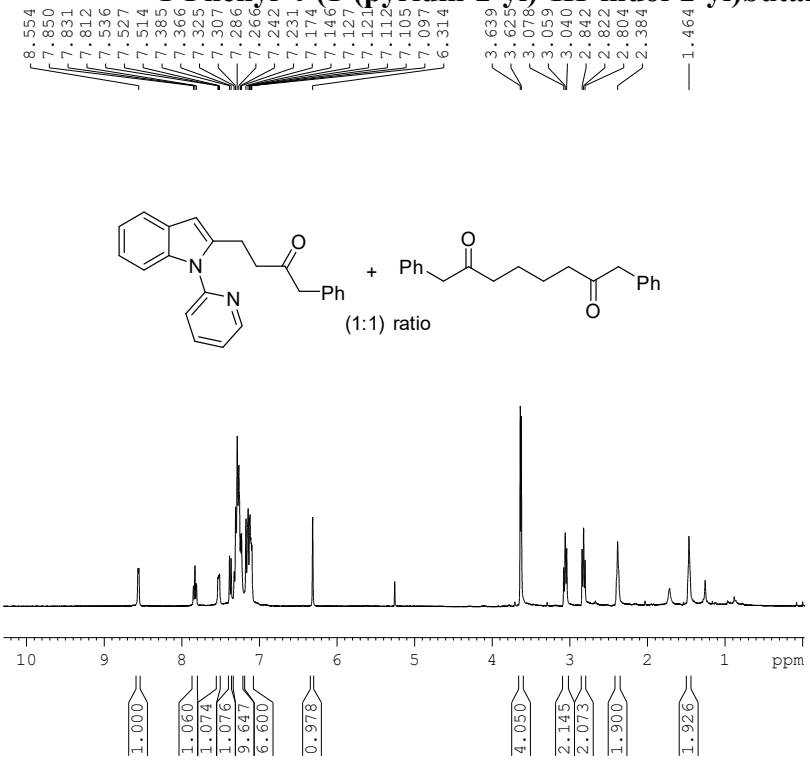
======== CHANNEL f1 ========
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

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

F2 - Processing parameters
SI 32768
SF 100.6127601 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

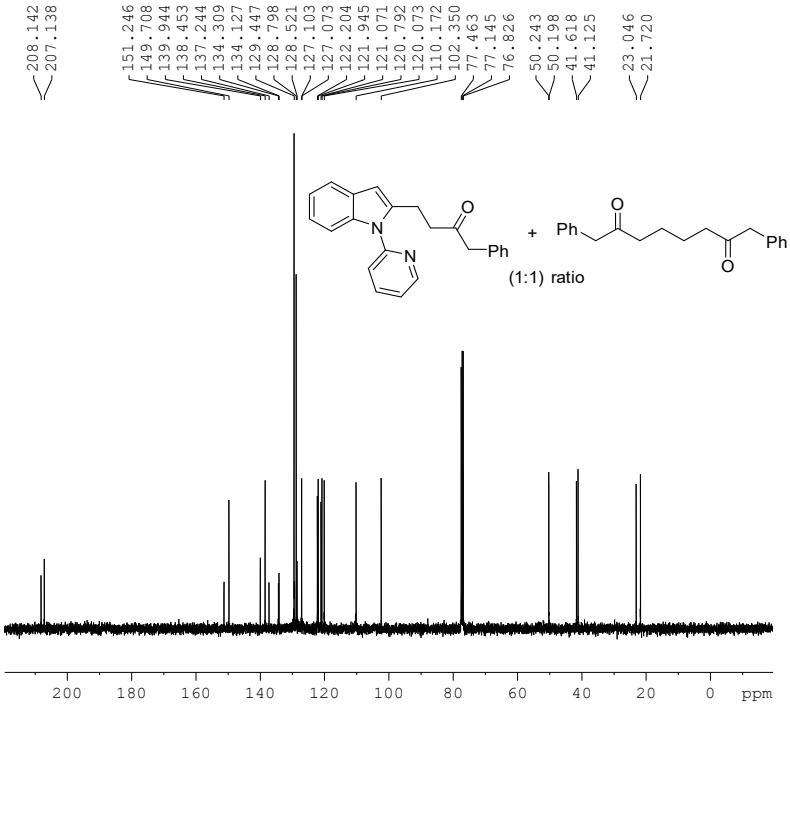
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3ac**

1-Phenyl-4-(1-(pyridin-2-yl)-1*H*-indol-2-yl)butan-2-one: 3ad




```
Current Data Parameters
NAME                  2554
EXPNO                  160
PROCNO                   1

F2 - Acquisition Parameters
Date_              20201212
Time                 20.33
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ               4.0894465 sec
RG                   95.73
DW                 62.400 usec
DE                  6.50 usec
TE                  296.4 K
D1              0.50000000 sec
TD0                      1

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

F2 - Processing parameters
SI                   65536
SF            400.1300220 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

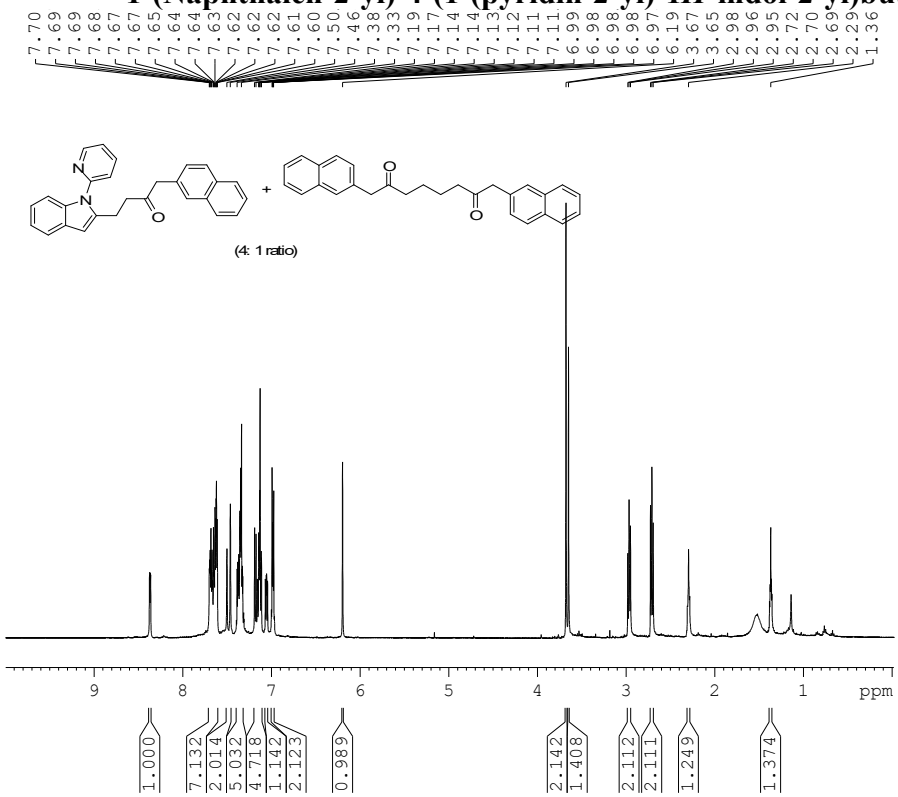
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3ad**




```
Current Data Parameters
NAME                  2554
EXPNO                  161
PROCNO                   1

F2 - Acquisition Parameters
Date_              20201212
Time                 20.34
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   16540
SOLVENT              CDCl3
NS                     227
DS                       4
SWH              24038.461 Hz
FIDRES            1.453353 Hz
AQ               0.3440320 sec
RG                   200.34
DW                 20.800 usec
DE                  6.50 usec
TE                  296.5 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                      1

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

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

F2 - Processing parameters
SI                   32768
SF            100.6127660 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

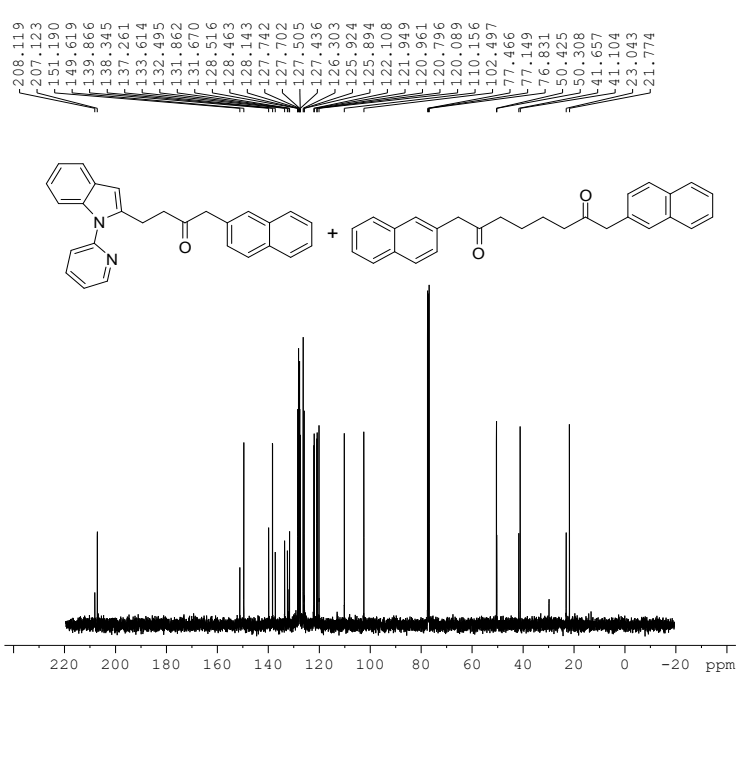
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3ad**

1-(Naphthalen-2-yl)-4-(1-(pyridin-2-yl)-1*H*-indol-2-yl)butan-2-one: 3ae




```
Current Data Parameters
NAME                  spa
EXPNO                  31
PROCNO                  1

F2 - Acquisition Parameters
Date_           20220805
Time               13.26
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                 101.5
DW                50.000 usec
DE                 6.50 usec
TE                301.9 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           500.1500778 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

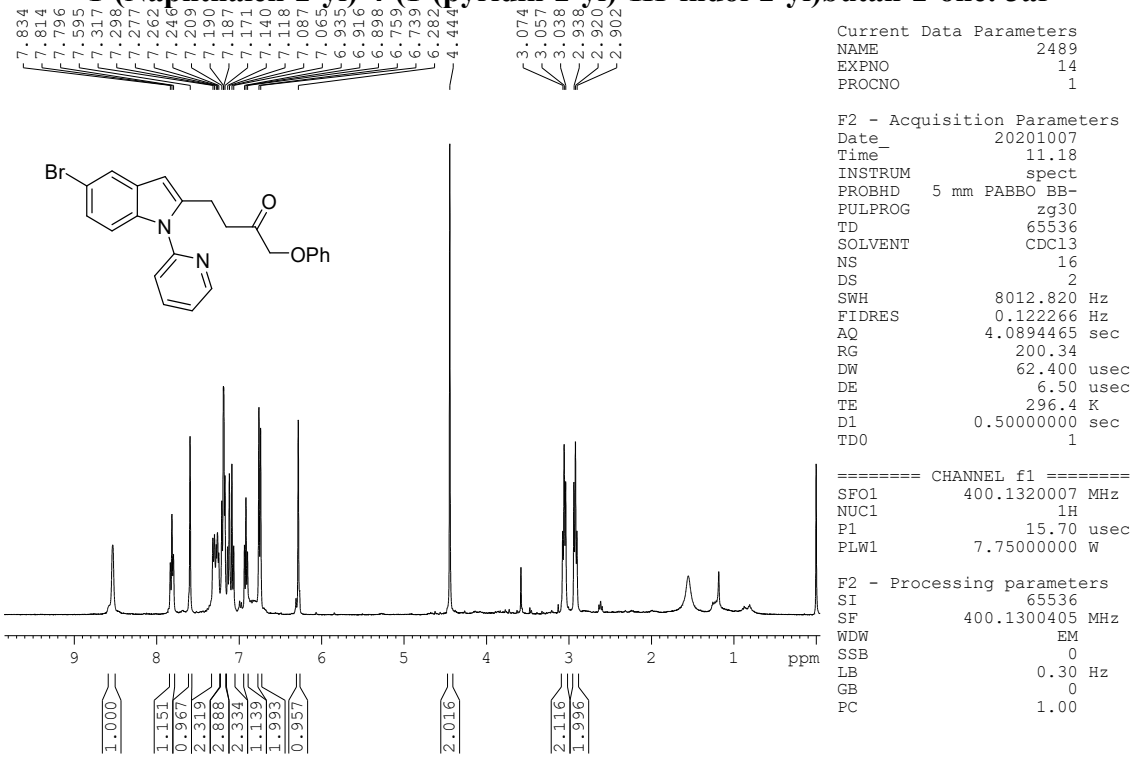
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3ae**




```
Current Data Parameters
NAME     2662 2663 2664 2667
EXPNO                  768
PROCNO                   1

F2 - Acquisition Parameters
Date_           20210430
Time                3.53
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            24038.461 Hz
FIDRES          1.453353 Hz
AQ             0.3440320 sec
RG                 200.34
DW                20.800 usec
DE                 6.50 usec
TE                299.1 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228289 MHz
NUC1                  13C
P1                10.00 usec
PLW1         47.00000000 W

======== CHANNEL f2 ========
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           100.6127668 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

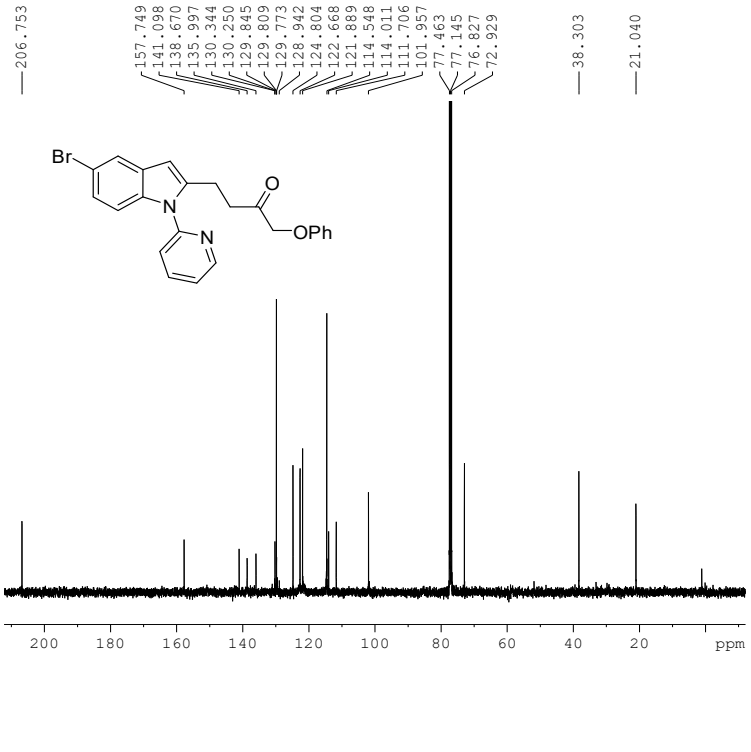
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3ae**

1-(Naphthalen-2-yl)-4-(1-(pyridin-2-yl)-1*H*-indol-2-yl)butan-2-one: 3af




```
Current Data Parameters
NAME                  2489
EXPNO                   14
PROCNO                   1

F2 - Acquisition Parameters
Date_           20201007
Time                11.18
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                200.34
DW                62.400 usec
DE                 6.50 usec
TE                296.4 K
D1             0.50000000 sec
TD0                    1

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

F2 - Processing parameters
SI                 65536
SF            400.1300405 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

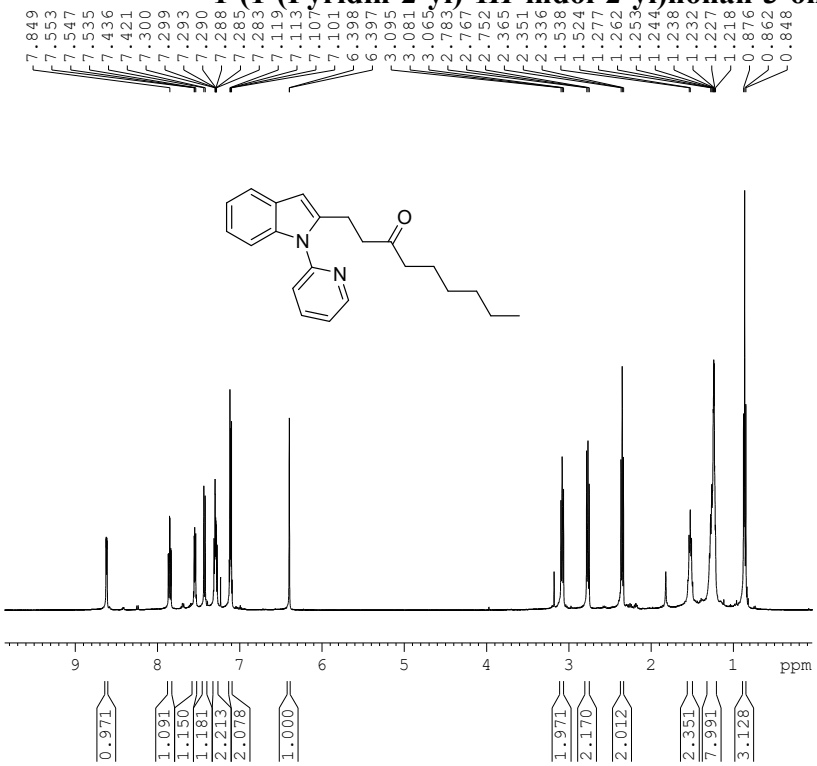
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3af**




```
Current Data Parameters
NAME                  2489
EXPNO                  134
PROCNO                   1

F2 - Acquisition Parameters
Date_           20201006
Time                21.10
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                  1500
DS                     4
SWH            24038.461 Hz
FIDRES          1.453353 Hz
AQ              0.3440320 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE                297.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1

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

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

F2 - Processing parameters
SI                 32768
SF            100.6127601 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

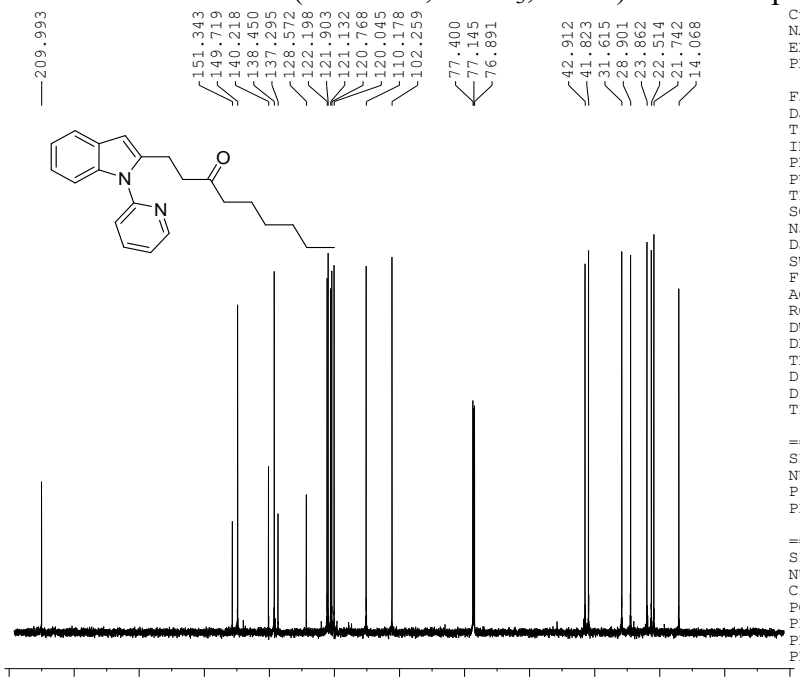
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3af**

1-(1-(Pyridin-2-yl)-1*H*-indol-2-yl)nonan-3-one: 3ag




```
Current Data Parameters
NAME                  2525
EXPNO                   31
PROCNO                   1

F2 - Acquisition Parameters
Date_              20201112
Time                 15.27
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                   31.24
DW                  50.000 usec
DE                   6.50 usec
TE                  302.2 K
D1               0.50000000 sec
TD0                      1

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

F2 - Processing parameters
SI                    65536
SF             500.1500254 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

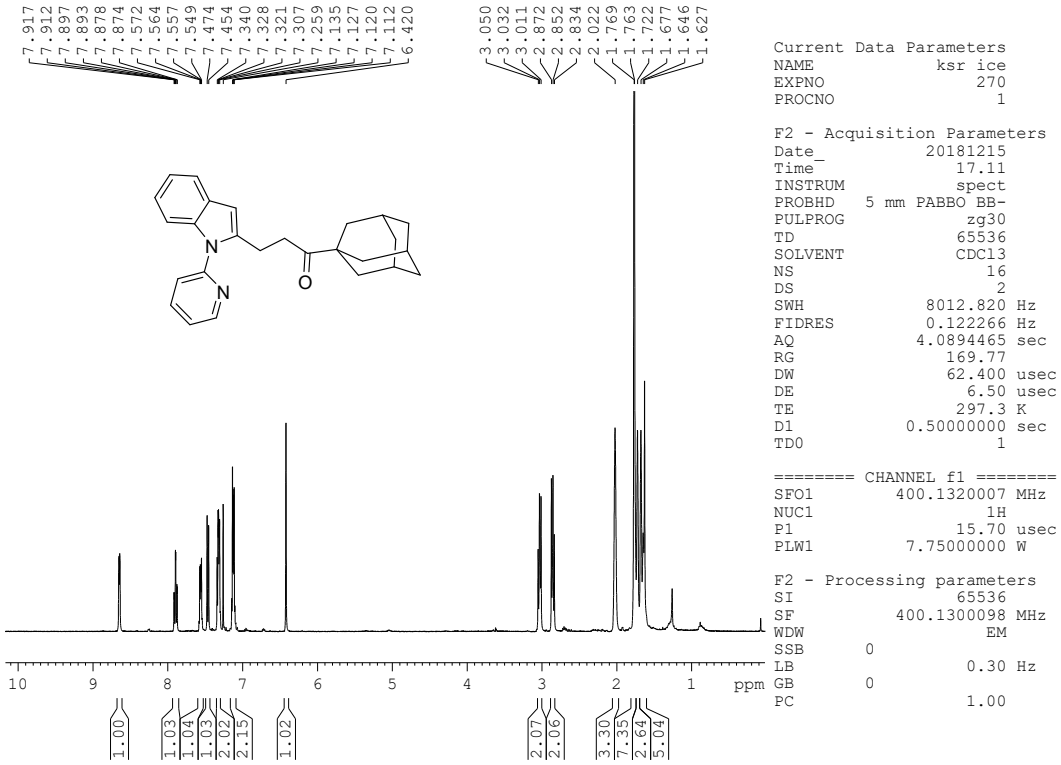
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3ag**



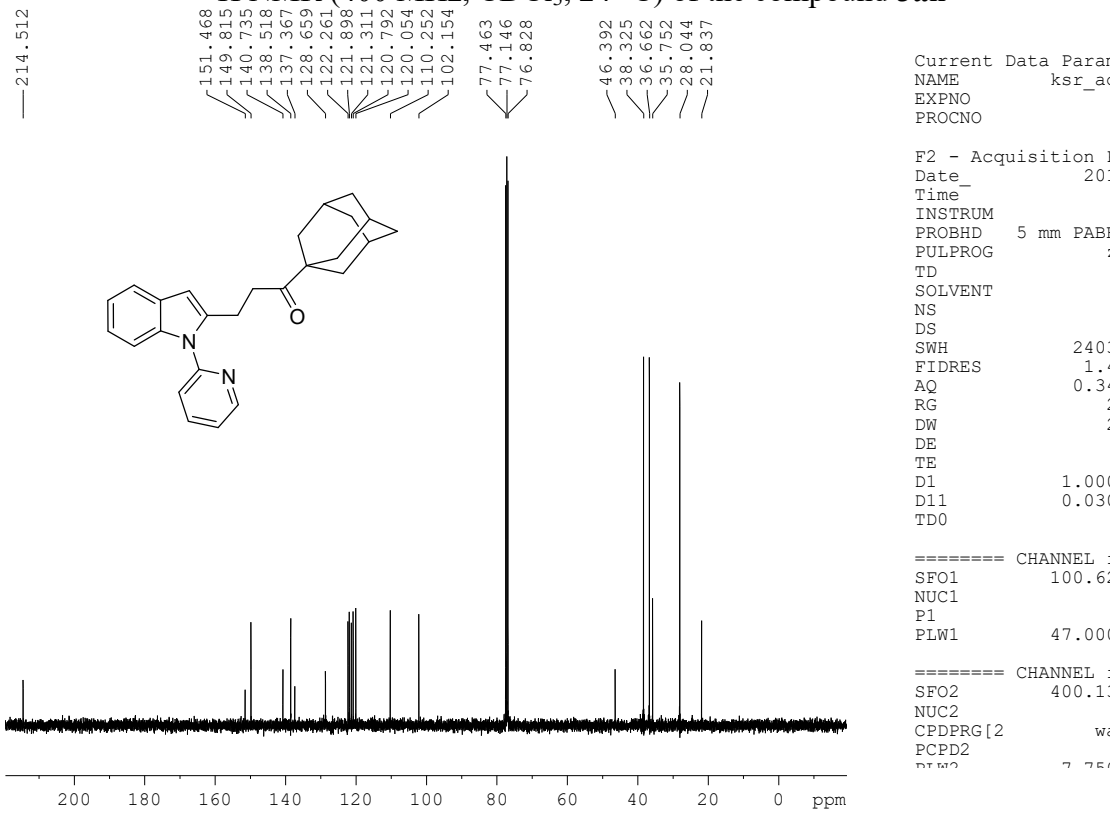

```
Current Data Parameters
NAME                  2525
EXPNO                   32
PROCNO                   1

F2 - Acquisition Parameters
Date_              20201112
Time                 15.35
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   20480
SOLVENT              CDCl3
NS                     256
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                  302.8 K
D1               1.00000000 sec
D11              0.03000000 sec
TD0                      1

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

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

F2 - Processing parameters
SI                    32768
SF             125.7628157 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

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

1-((3r,5r,7r)-Adamantan-1-yl)-3-(1-(pyridin-2-yl)-1*H*-indol-2-yl)propan-1-one: 3ah

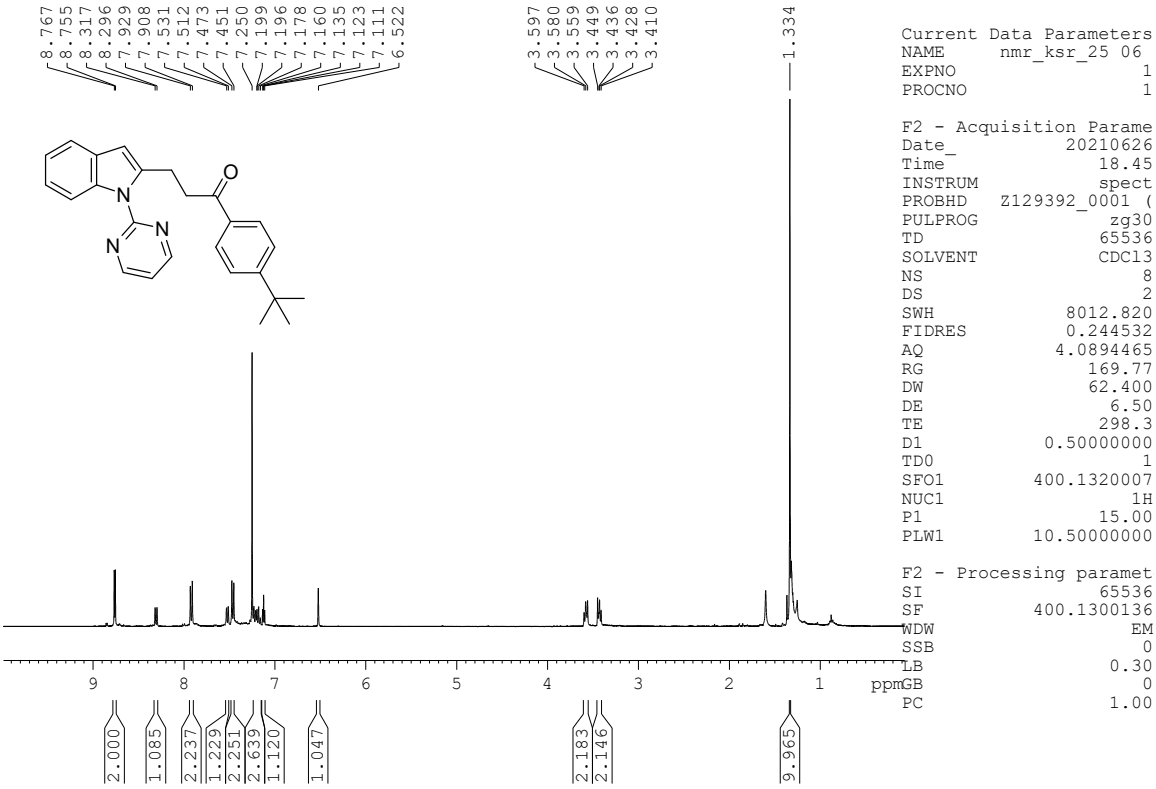


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3ah**

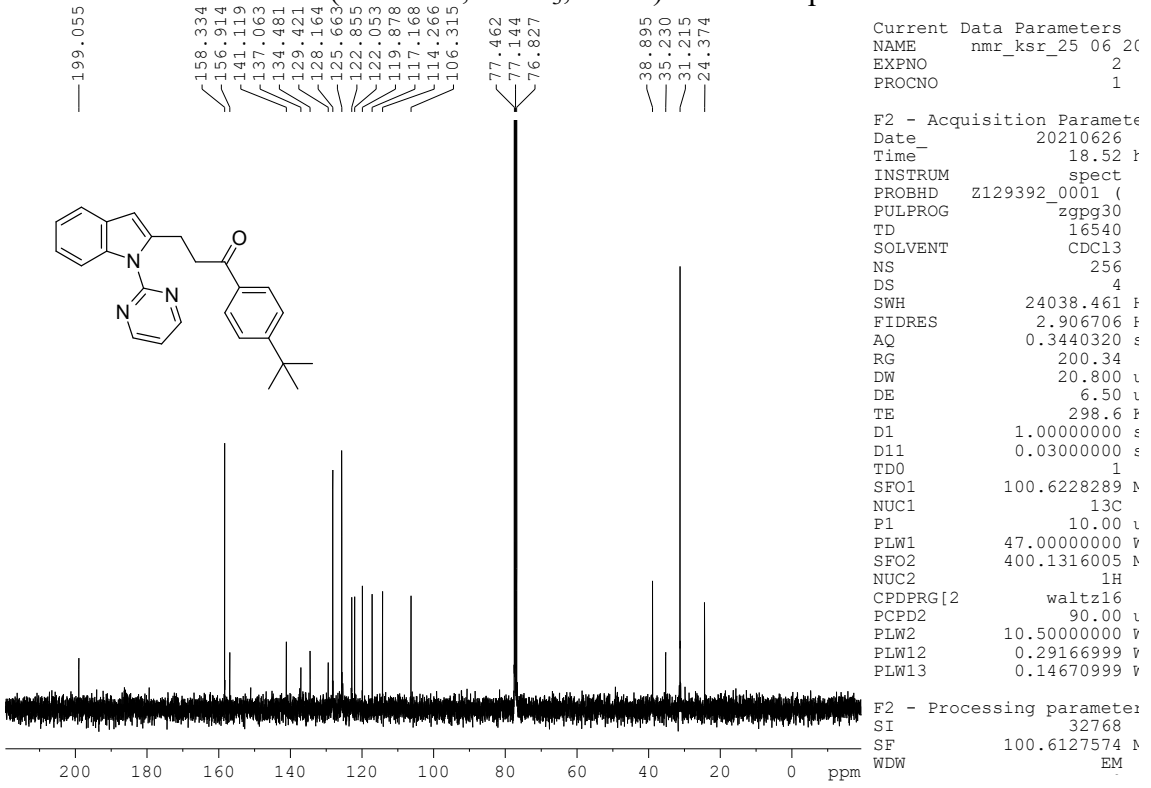


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3ah**

1-(4-(*tert*-Butyl)phenyl)-3-(1-(pyrimidin-2-yl)-1*H*-indol-2-yl)propan-1-one: 3ai

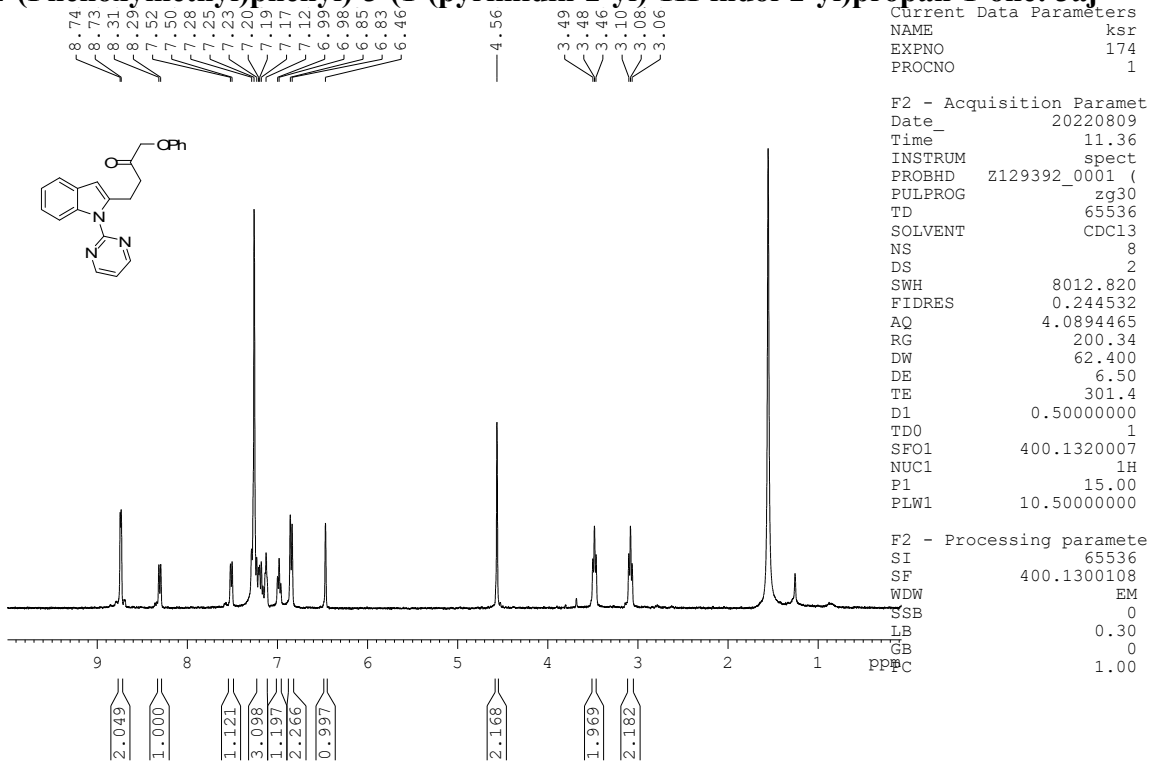


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3ai**

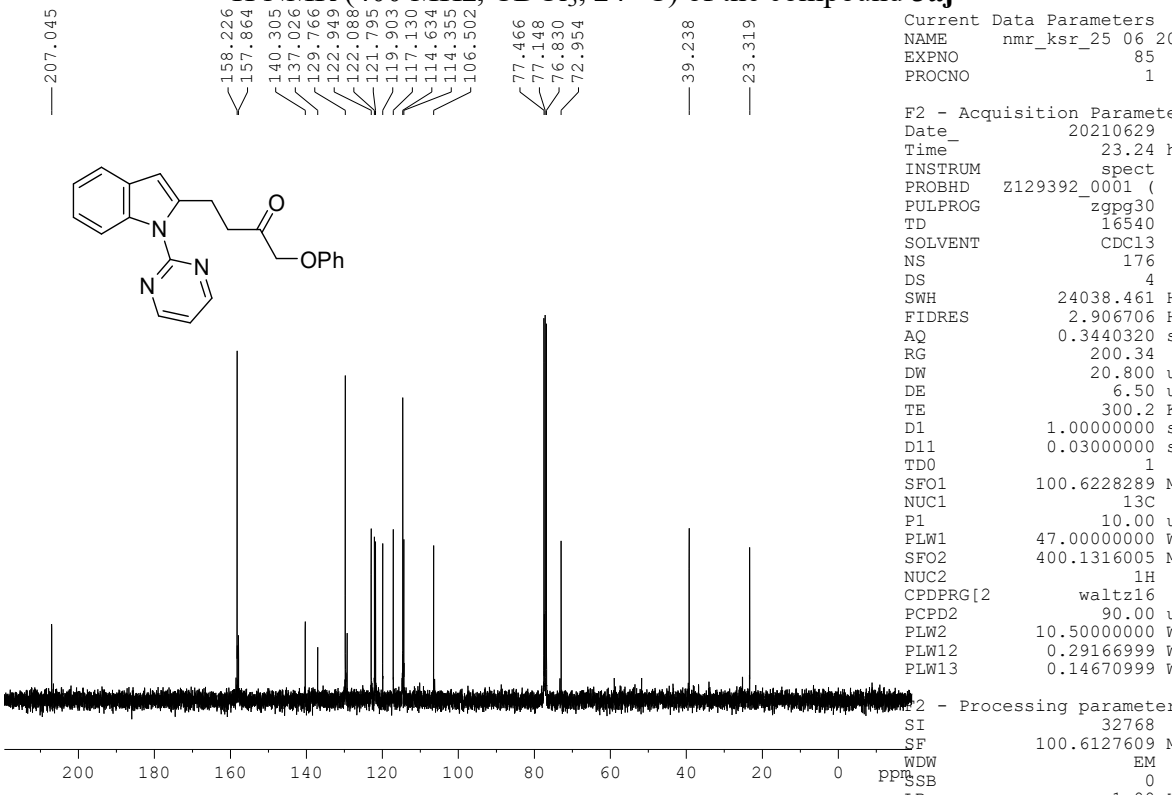


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3ai**

1-(4-(Phenoxymethyl)phenyl)-3-(1-(pyrimidin-2-yl)-1H-indol-2-yl)propan-1-one: 3aj

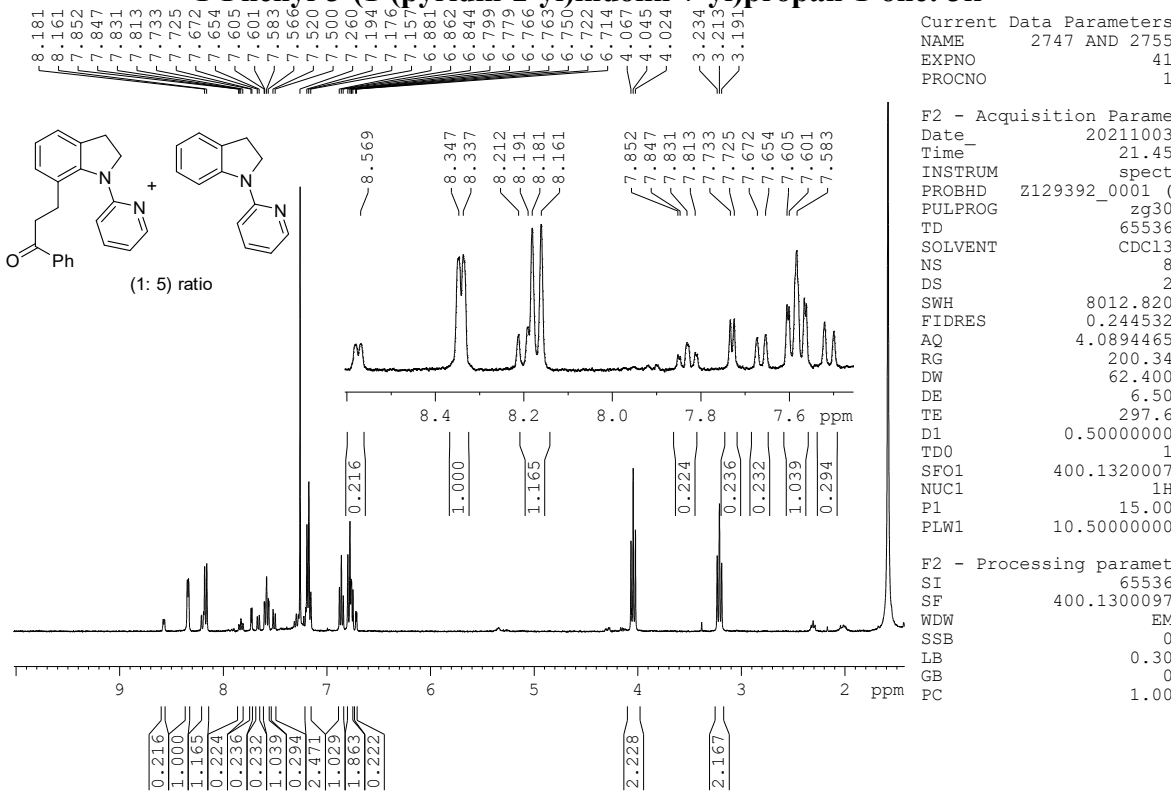


^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **3aj**



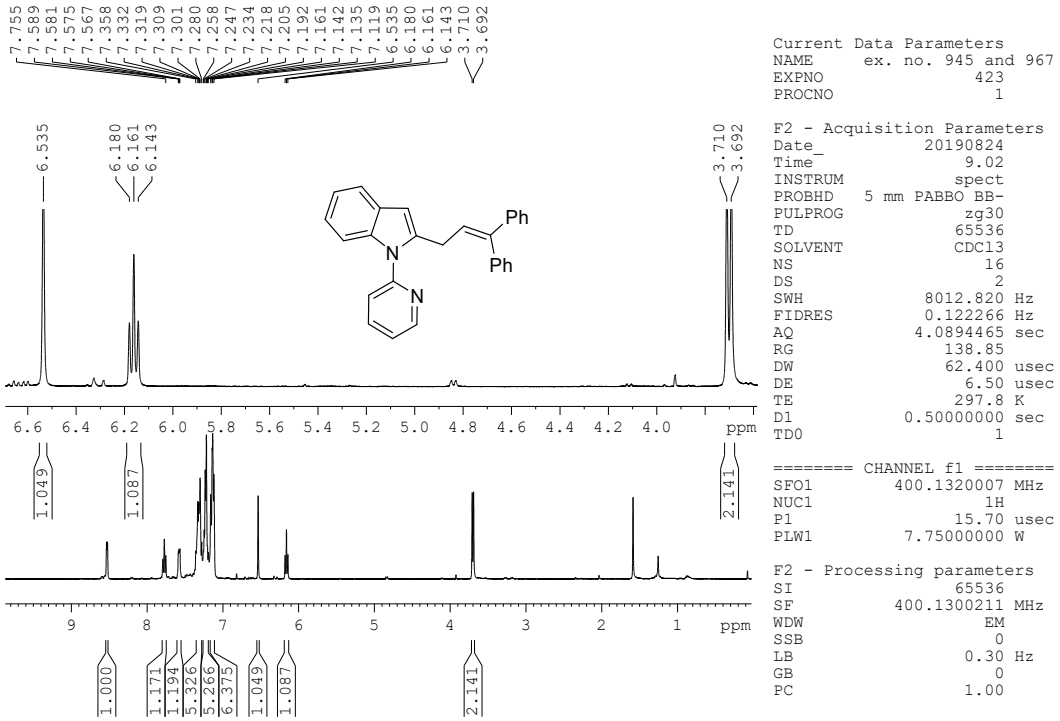
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **3aj**

1-Phenyl-3-(1-(pyridin-2-yl)indolin-7-yl)propan-1-one: 3k



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

2-(3,3-Diphenylallyl)-1-(pyridin-2-yl)-1*H*-indole (6)

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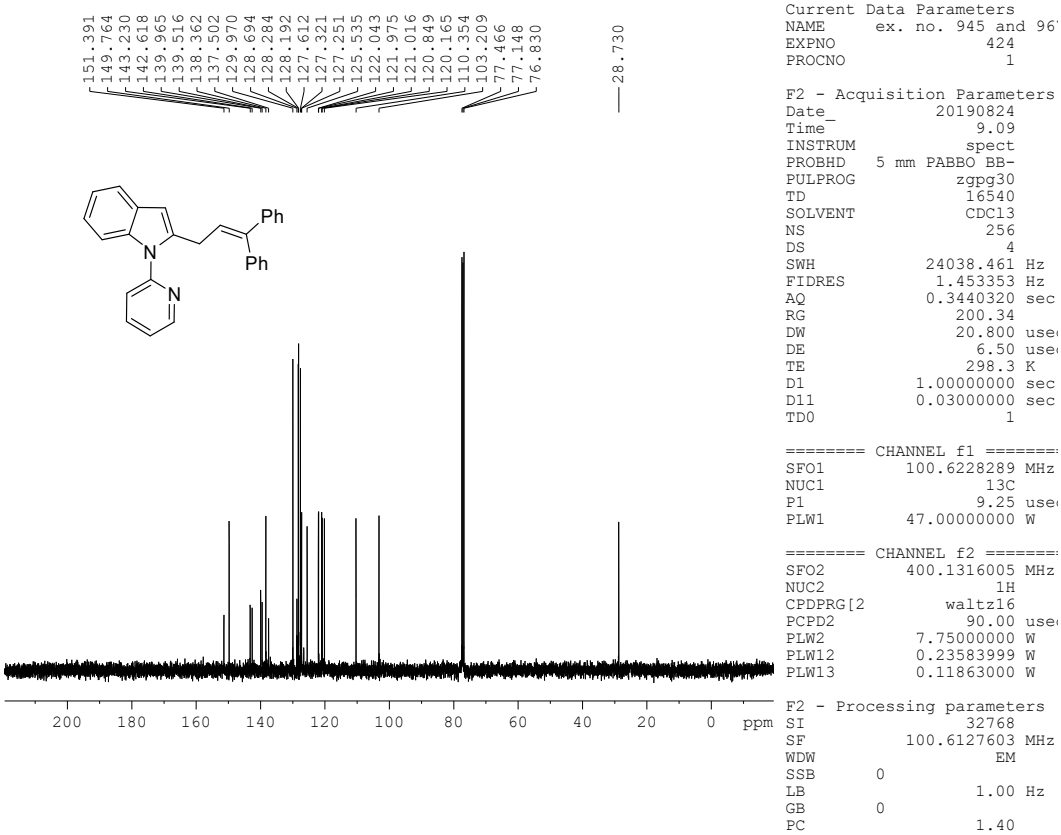
Current Data Parameters
NAME      ex. no. 945 and 967
EXPNO                 423
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190824
Time               9.02
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                138.85
DW                62.400 usec
DE                 6.50 usec
TE                297.8 K
D1           0.50000000 sec
TD0                   1

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

F2 - Processing parameters
SI                65536
SF           400.1300211 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 **6**

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Current Data Parameters
NAME      ex. no. 945 and 96
EXPNO                 424
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190824
Time               9.09
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                16540
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24038.461 Hz
FIDRES         1.453353 Hz
AQ             0.3440320 sec
RG                200.34
DW                20.800 use
DE                 6.50 use
TE                298.3 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

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

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

F2 - Processing parameters
SI                32768
SF           100.6127603 MHz
WDW                  EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```
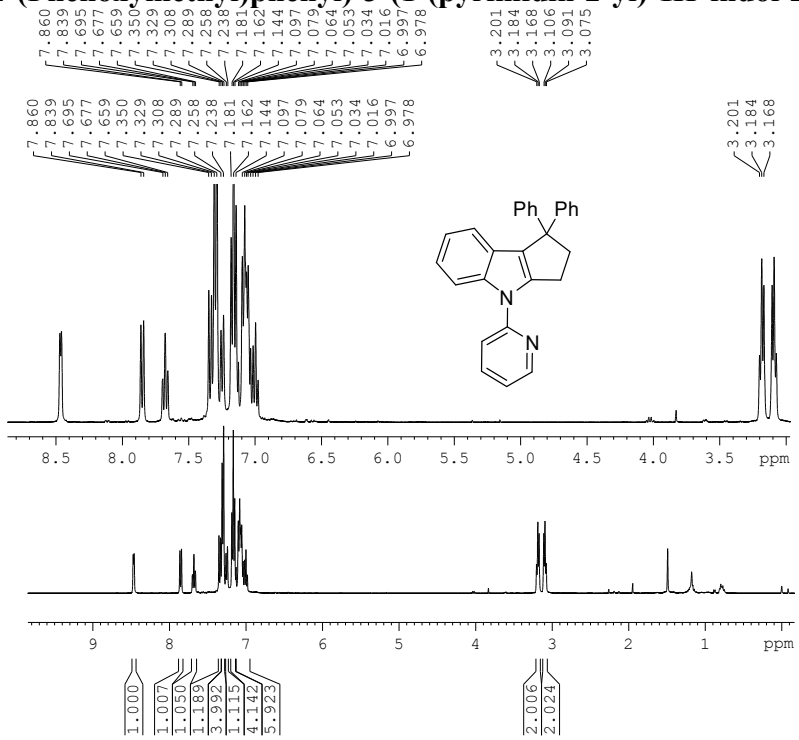

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **6**

1-(4-(Phenoxymethyl)phenyl)-3-(1-(pyrimidin-2-yl)-1*H*-indol-2-yl)propan-1-one (7):

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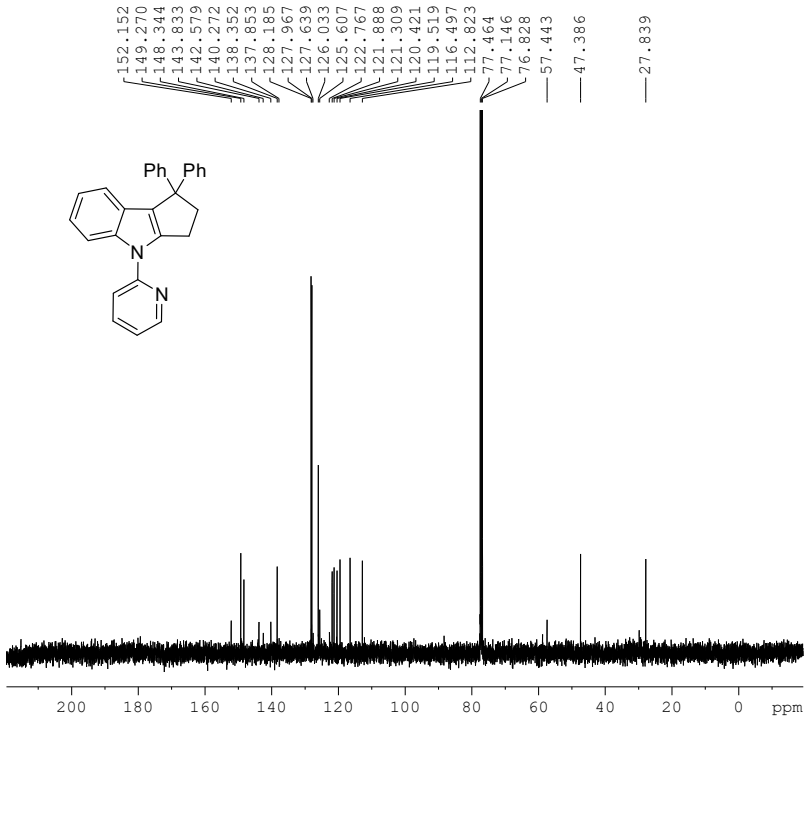
Current Data Parameters
NAME      1859 apllication parent d
EXPNO                 426
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190824
Time                9.16
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 95.73
DW                62.400 usec
DE                 6.50 usec
TE                297.9 K
D1             0.50000000 sec
TD0                    1

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

F2 - Processing parameters
SI                 65536
SF           400.1300634 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

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

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Current Data Parameters
NAME          nmr_1440 p1
EXPNO                 292
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180815
Time               12.47
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            24038.461 Hz
FIDRES          1.453353 Hz
AQ              0.3440320 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE                295.7 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1

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

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

F2 - Processing parameters
SI                 32768
SF           100.6127579 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```
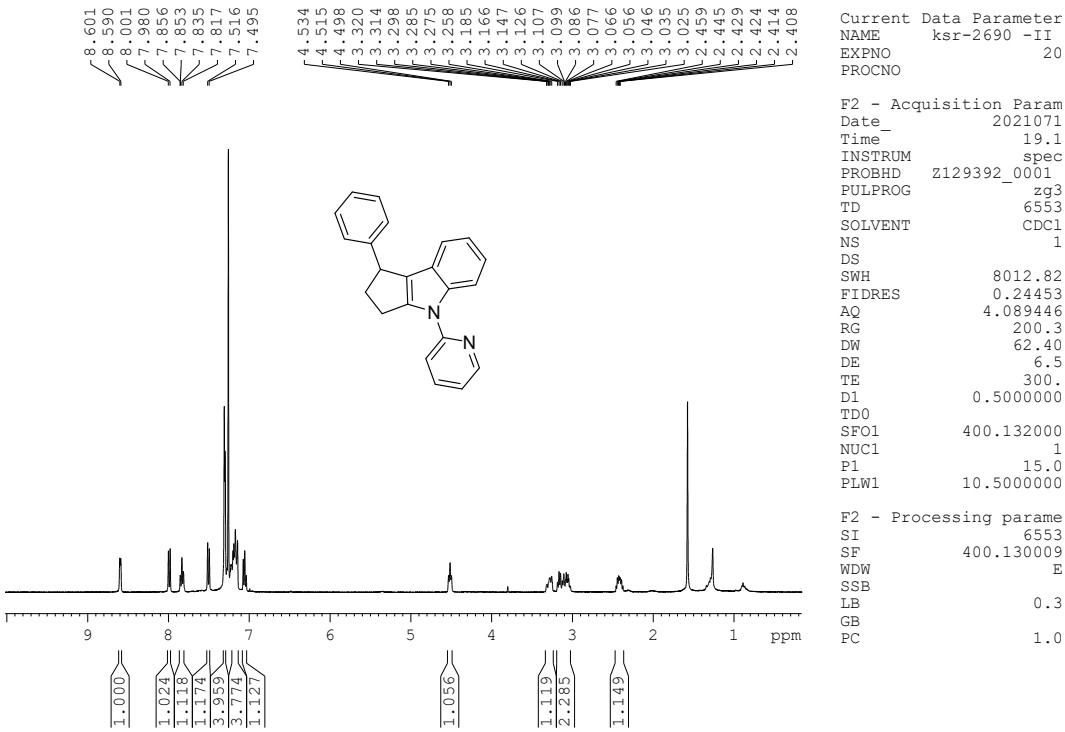
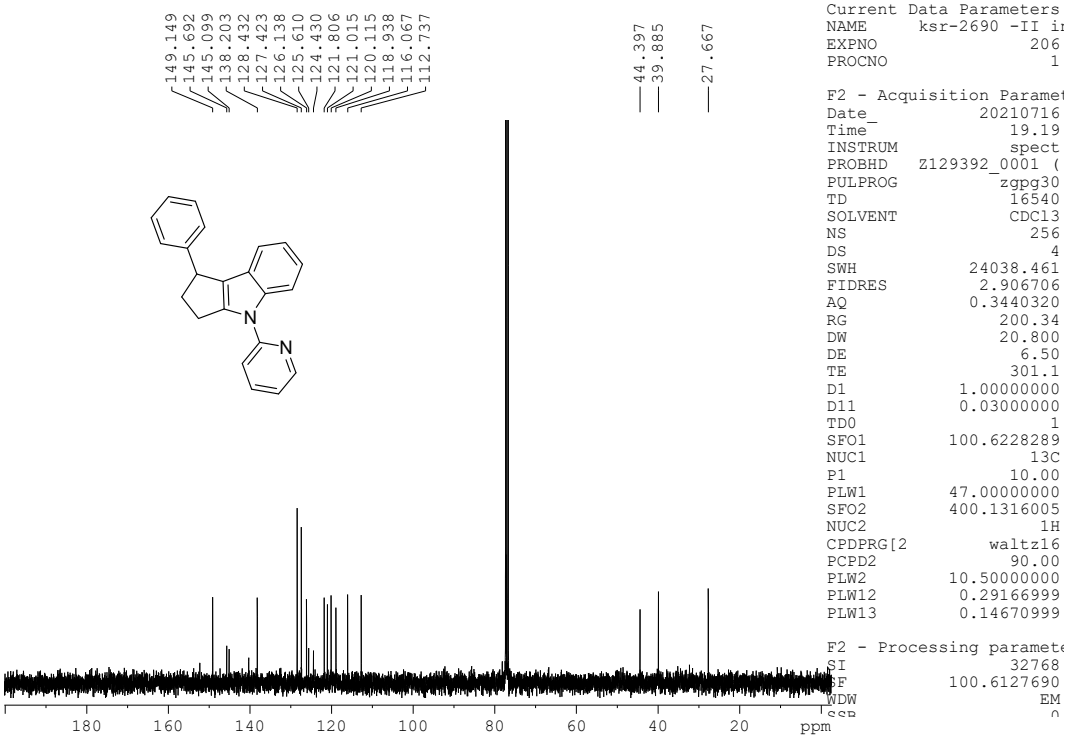

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of the compound **7**

1-Phenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[*b*]indole 9



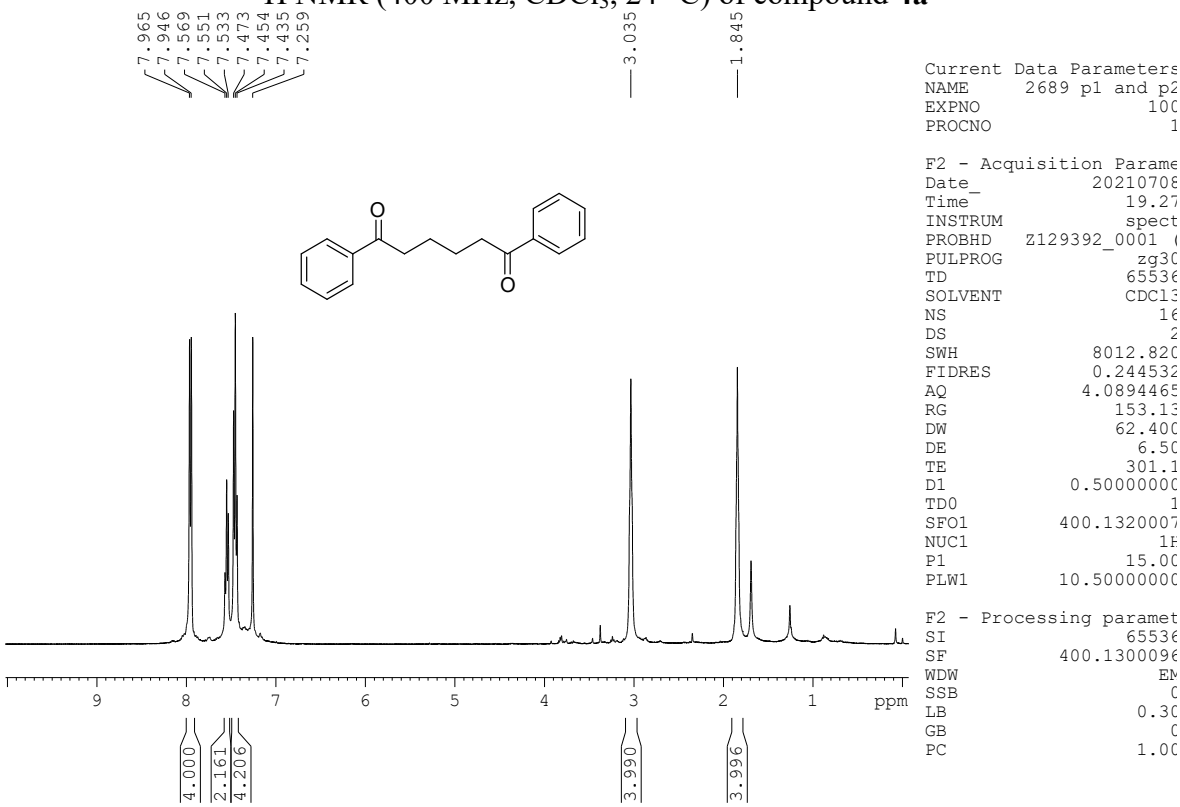
^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of the compound **9**



^{13}C{^{1}H} NMR (100 MHz, CDCl3, 24 °C) of the compound **9**

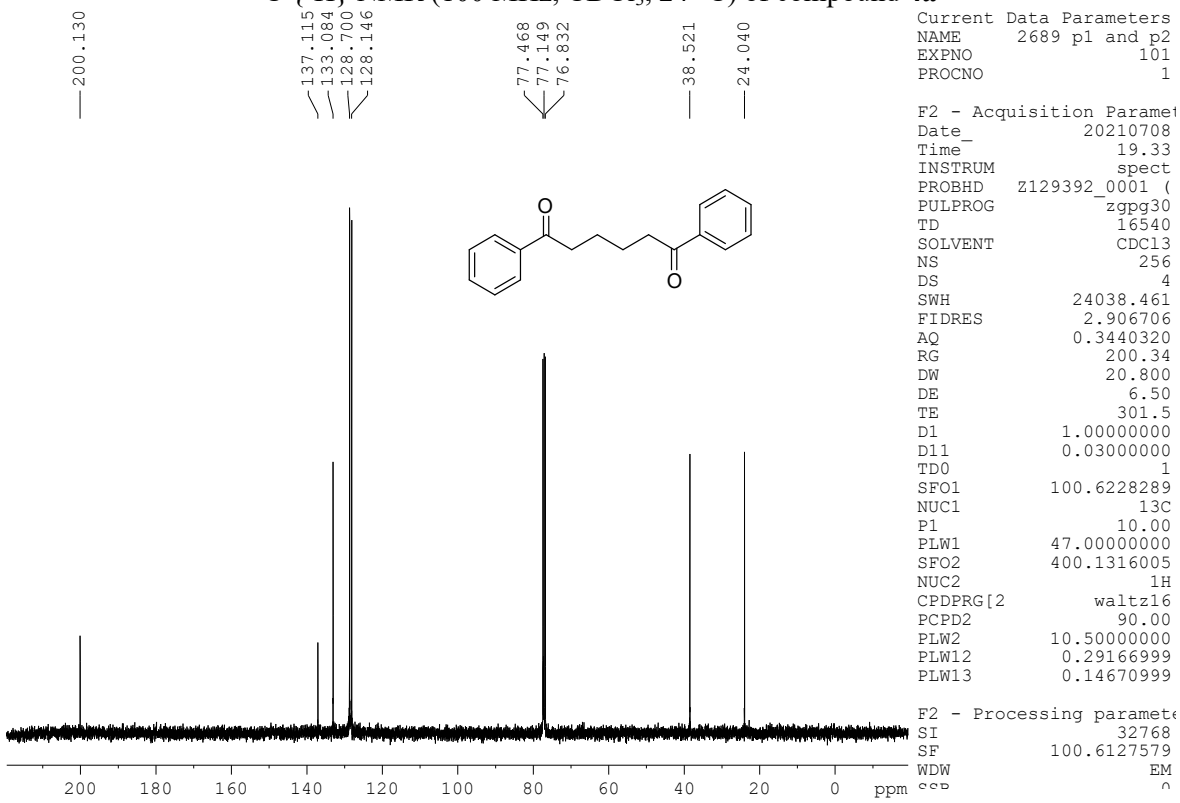
1,6-Diphenylhexane-1,6-dione (4a)

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C) of compound **4a**




```
Current Data Parameters
NAME      2689 p1 and p2
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parame
Date_           2021070
Time              19.2
INSTRUM           spect
PROBHD   Z129392_0001 (
PULPROG            zg3
TD                6553
SOLVENT           CDCl
NS                  1
DS                  2
SWH            8012.82
FIDRES        0.24453
AQ            4.08944
RG              153.1
DW              62.40
DE                6.5
TE              301.1
D1           0.500000
TD0                 1
SFO1        400.13200
NUC1               1H
P1              15.00
PLW1        10.500000

F2 - Processing paramet
SI                6553
SF          400.13000
WDW                EM
SSB                 0
LB               0.30
GB                  0
PC               1.00
```

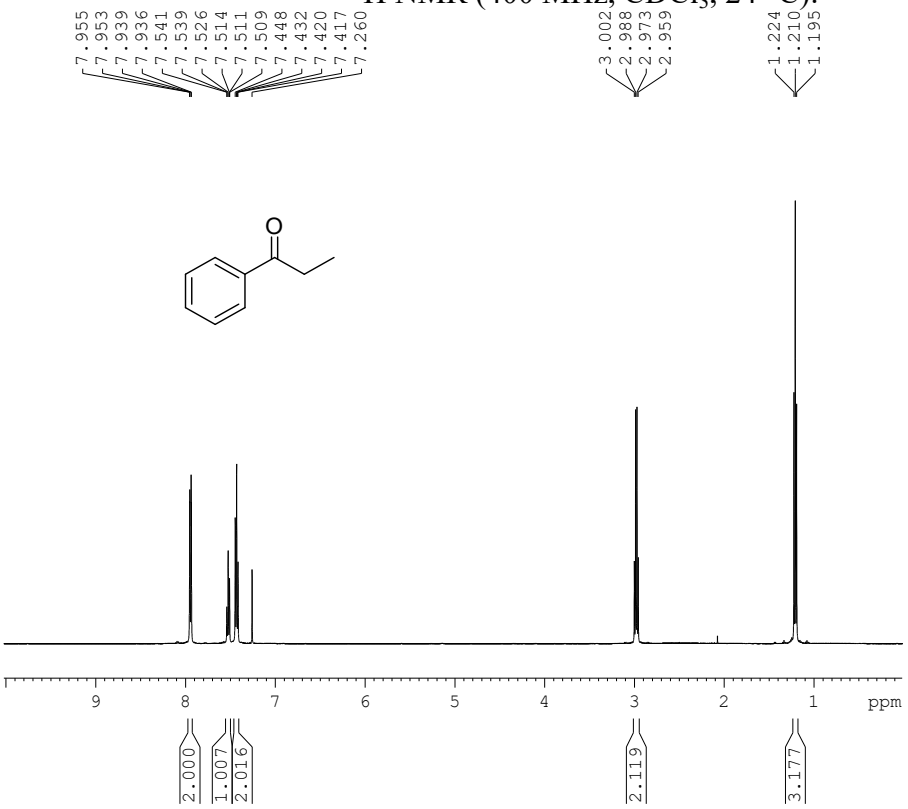
^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$, 24 °C) of compound **4a**




```
Current Data Parameters
NAME      2689 p1 and p2
EXPNO                101
PROCNO                 1

F2 - Acquisition Parame
Date_           20210708
Time              19.33
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              301.5
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
SF          100.6127579
WDW                EM
SSB                 0
```

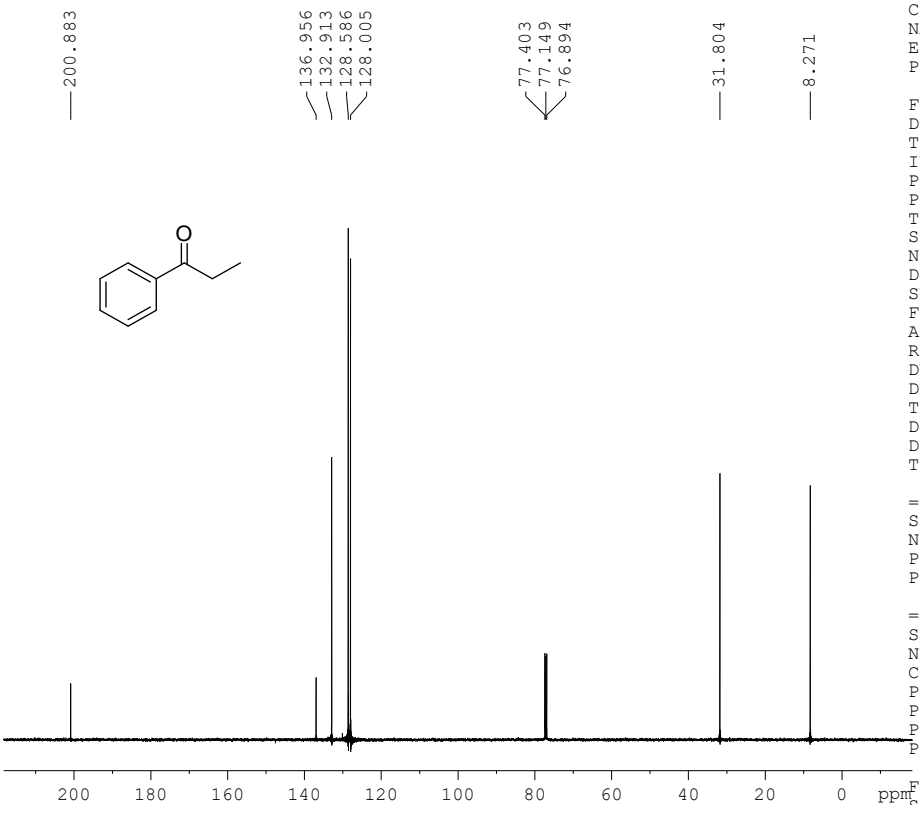
Propiophenone:

^{1}H NMR (400 MHz, $CDCl_3$, 24 °C):




```
Current Data Parameters
NAME                  spa
EXPNO                  65
PROCNO                  1

F2 - Acquisition Parame
Date_           20211026
Time              16.18
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     2
SWH            10000.000
FIDRES         0.305176
AQ             1.6384000
RG                31.24
DW                50.000
DE                 6.50
TE                299.7
D1             0.5000000
TD0                    1

======== CHANNEL f1 ===
SFO1         500.1525008
NUC1                1H
P1                 11.75
PLW1         15.3000001

F2 - Processing paramet
SI                 65536
SF           500.1500112
WDW                   EM
SSB                    0
LB                  0.30
GB                     0
PC                  1.00
```

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




```
Current Data Parameters
NAME                  spa
EXPNO                  66
PROCNO                  1

F2 - Acquisition Paramet
Date_           20211026
Time              16.24
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 20480
SOLVENT            CDCl3
NS                   150
DS                     4
SWH            29761.904
FIDRES         1.453218
AQ             0.3440640
RG                202.34
DW                16.800
DE                 6.50
TE                300.4
D1             1.0000000
D11            0.0300000
TD0                    1

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

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

F2 - Processing paramete
```