

Supporting information

Cp*Co(III)-Catalyzed Selective Alkylation of C-H Bonds of Arenes and Heteroarenes with α -Diazocarbonyl Compounds

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1) General Comments:

All reactions were carried out in reaction tube under dry nitrogen atmosphere. All diazoesters were synthesized from corresponding esters, according to the literature procedure.¹ All the *N*-pyridyl indole derivatives were synthesized according to the literature procedure.² [Cp*CoI₂CO],^{3a} [Cp*CoI₂]₂^{3b} and [Cp*Co(MeCN)₃](SbF₆)₂^{3c} were synthesized from Co₂CO₈ according to the literature procedure. Dry toluene was prepared by distilling over sodium ketyl and stored over using molecular sieves 4Å under N₂ atmosphere. Column chromatography was performed using silica gel (100-200 mesh) and ethylacetate-hexanes with various percentage of polarity depending on the nature of the substrate as an eluent, unless otherwise specified.

Caution: Diazo compounds can decompose violently with the loss of nitrogen. Although no problems were faced in the present study, the appropriate precautions should be taken.

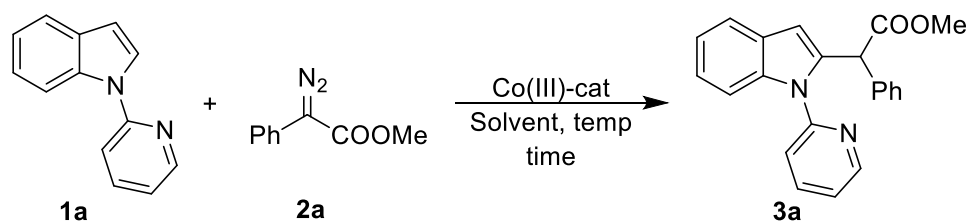
2. Analytical Methods:

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

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1. Ghorai, J.; Anbarasan, P. *J. Org. Chem.* **2015**, *80*, 3455.
 2. Ackermann, L.; Lygin, A. V. *Org. Lett.* **2011**, *13*, 3332.
 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

3.1. Cp*Co(III)-Catalyzed Selective Alkylation of Indoles 1a: Optimization

One oven dried Schlenk tube was charged with *N*-pyridyl indole **1a** (50 mg, 0.25 mmol, 1 equiv), diazo compound **2a** (0.31 mmol, 1.2 equiv) and Cp*Co(III)–catalyst (y mol%). The inner atmosphere was made inert through repeated (thrice) evacuation and refilled with nitrogen. Dry solvent (1.5 mL) was added to the reaction mixture and the reaction mixture stirred at same temperature throughout a mentioned time period. After completion of the reaction (monitored by TLC) the reaction mixture was cooled to room temperature and passes 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**.

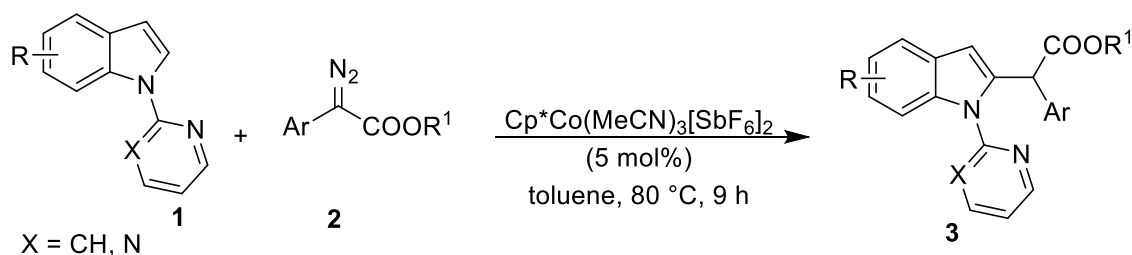


Entry	Catalyst (y mol %)	Solvent	Temp. (°C)	Time (h)	Conv. 1a (%)	Yield (%) ^a
1	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	Toluene	120	6	73	61
2	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	Toluene	100	6	89	70
3	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	Toluene	80	9	100	86
4	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	Toluene	60	12	93	77
5	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	Toluene	30	24	0	0
6	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (3)	Toluene	80	9	83	52
7	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	PhCF ₃	80	9	95	84
8	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	DCE	80	9	100	59
9	[Cp*CoI ₂ CO] (5)	Toluene	80	12	79	61
10	[Cp*CoI ₂] ₂ (5)	Toluene	80	12	67	52
11	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (7.5)	Toluene	80	8	100	86

12	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	THF	80	9	91	73
13	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	PhCl	80	9	85	69
14	Co(acac) ₃	Toluene	80	14	41	23
15	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	MeCN	80	9	91	59
16 ^b	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	Toluene	80	9	96	85
17 ^c	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	Toluene	80	9	100	88
18 ^d	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	Toluene	80	9	94	80
19	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	Toluene	70	11	100	84
20	[Cp*Co(MeCN) ₃][SbF ₆] ₂ (5)	Toluene	90	8	100	80

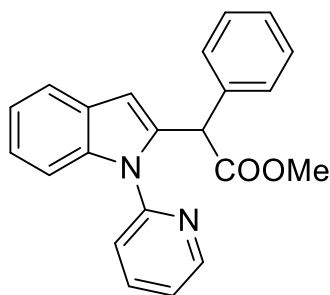
Reaction conditions: **1a** (0.25 mmol, 1 equiv), **2a** (0.31 mmol, 1.2 equiv), [Cp*Co(MeCN)₃][SbF₆]₂ (5 mol%), solvent (1.5 mL for 0.25 mmol), temp, Time. ^a all are isolated yields. ^b diazoester was added slowly over a period of 30 minutes, ^c 1.5 equiv of diazoester was used, ^d 1.0 equiv. of diazoester was used.

3.2. Typical procedure of Cp*Co(III)-catalyzed selective alkylation of indoles:



One dry reaction tube was charged with *N*-pyridyl indole **1** (0.25 mmol, 1 equiv), diazo compound **2** (0.31 mmol, 1.2 equiv) and Cp*Co(MeCN)₃[SbF₆]₂ (5 mol%). The inner atmosphere was made inert through repeated (thrice) evacuation and refilled with nitrogen. Dry toluene (1.5 mL) was added under nitrogen atmosphere and the reaction tube was sealed with glass stopper and kept in a preheated oil bath at 80 °C and stirred at same temperature for 9 hours. After completion of the reaction, the reaction mixture was cooled to room temperature and passes through a pad of celite, concentrated to get the crude product. The crude product was purified by column chromatography to afford the C-2 alkyl indole **3**.

3.2.1. Methyl 2-phenyl-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3a):



Yield: 86 %; colourless liquid; R_f = 0.55 in 2:3 EtOAc/Hexane.

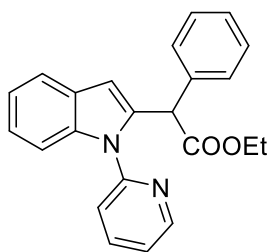
IR ($\nu_{\max}$, cm^{-1}): 2933, 1739, 1654, 1481, 1459, 1273, 912, 658.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.60 (d, J = 3.2 Hz, 1H, ArH), 7.78 (t, J = 7.5 Hz, 1H, ArH), 7.56 (d, J = 7.2 Hz, 1H, ArH), 7.32 (d, J = 7.8 Hz, 2H, ArH), 7.24–7.11 (m, 8H, ArH), 6.44 (s, 1H, ArH), 5.63 (s, 1H, CH), 3.60 (s, 3H, CH_3),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.9, 151.3, 149.4, 138.4, 138.1, 137.3, 136.8, 129.0, 128.6, 128.1, 127.7, 122.7, 122.0, 121.0, 120.9, 110.1, 105.6, 52.4, 50.7.

HRMS: m/z : $[\text{M}+\text{Na}]^+$ Calculated for $\text{C}_{23}\text{H}_{20}\text{N}_2\text{NaO}_3$, 365.1266, found 365.1264.

3.2.2. Ethyl 2-phenyl-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate(3b):



Yield: 82 %; colourless liquid; R_f = 0.55 in 2:3 EtOAc/Hexane.

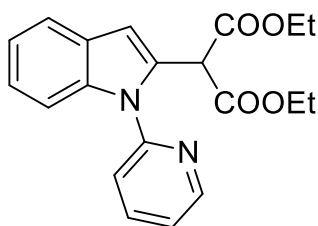
IR ($\nu_{\max}$, cm^{-1}): 2921, 1742, 1660, 1472, 1465, 1280, 925, 654.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.60 (d, J = 4.7 Hz, 1H, ArH), 7.75 (td, J = 7.6, 1.8 Hz, 1H, ArH), 7.55 (d, J = 6.1 Hz, 1H, ArH), 7.32–7.29 (m, 2H, ArH), 7.26–7.23 (m, 6H, ArH), 7.15–7.12 (m, 2H, ArH), 6.43 (s, 1H, ArH), 5.62 (s, 1H, CH), 4.06 (q, J = 6.9 Hz, 2H, CH_2), 1.13 (t, J = 7.0 Hz, 3H, CH_3),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.4, 151.3, 149.4, 138.3, 138.2, 137.3, 136.9, 129.0, 128.5, 128.1, 127.6, 122.6, 122.0, 121.0, 120.9, 120.9, 110.1, 105.5, 61.3, 50.8, 14.1.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{23}\text{H}_{21}\text{N}_2\text{O}_2$, 357.1603, found 357.1607.

3.2.3. Diethyl 2-(1-(pyridin-2-yl)-1*H*-indol-2-yl)malonate (3c):



Yield: 79 %; colourless liquid; R_f = 0.59 in 2:3 EtOAc/Hexane.

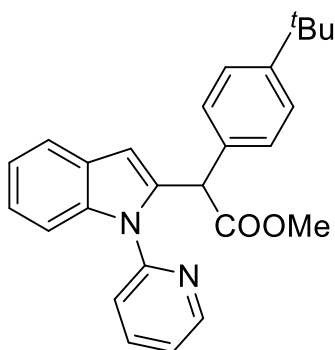
IR (ν_{max} , cm^{-1}): 2958, 1741, 1674, 1469, 1401, 1285, 896, 685.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.57–8.55 (m, 1H, ArH), 7.88 (td, J = 7.6, 1.9 Hz, 1H, ArH), 7.66–7.63 (m, 1H, ArH), 7.56 (d, J = 8.0 Hz, 1H, ArH), 7.45 (d, J = 8.0 Hz, 1H, ArH), 7.29–7.25 (m, 1H, ArH), 7.23–7.15 (m, 2H, ArH), 6.80 (s, 1H, ArH), 5.33 (s, 1H, CH), 4.22 (q, J = 7.1 Hz, 4H, 2CH_2), 1.24 (t, J = 7.1 Hz, 6H, 2CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 167.3, 151.0, 149.3, 138.5, 136.7, 131.8, 128.3, 123.0, 121.8, 121.2, 121.2, 120.2, 110.4, 105.8, 61.9, 52.0, 14.1.

HRMS: m/z : $[\text{M}+\text{Na}]^+$ Calculated for $\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_4\text{Na}$, 375.1321, found 375.1323.

3.2.4. Methyl 2-(4-(tert-butyl)phenyl)-2-(1-(pyridin-2-yl)-1*H*-indol-2-yl)acetate (3d):



Yield: 83 %; pale yellow liquid; R_f = 0.57 in 2:3 EtOAc/Hexane.

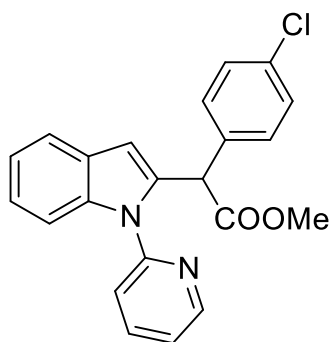
IR ($\nu_{\max}$, cm^{-1}): 2935, 1736, 1645, 1484, 1462, 1280, 936, 625.

^1H NMR (500 MHz, CDCl_3 , 24 °C): δ 8.59 (d, J = 4.8 Hz, 1H, ArH), 7.76 (td, J = 7.8, 1.8 Hz, 1H, ArH), 7.55–7.54 (m, 1H, ArH), 7.34–7.23 (m, 5H, ArH), 7.18–7.10 (m, 4H, ArH), 6.43 (s, 1H, ArH), 5.58 (s, 1H, ArH), 3.57 (s, 3H, CH), 1.28 (s, 9H, 3 CH_3)

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 172.0, 151.3, 150.4, 149.4, 138.3, 138.3, 137.2, 133.7, 128.6, 128.1, 125.5, 122.5, 121.9, 121.0, 120.9, 120.8, 110.1, 105.5, 52.2, 50.2, 34.5, 31.3.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{26}\text{H}_{27}\text{N}_2\text{O}_2$, 399.2073, found 399.2083.

3.2.5. Methyl 2-(4-chlorophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3e):



Yield: 84 %; brown liquid; R_f = 0.52 in 2:3 EtOAc/Hexane.

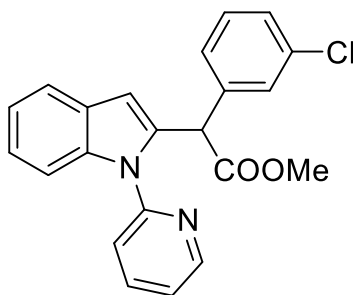
IR ($\nu_{\max}$, cm^{-1}): 2936, 1745, 1675, 1460, 1450, 1265, 896, 725, 645.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.51 (dd, J = 4.8, 1.8 Hz, 1H, ArH), 7.71 (td, J = 7.9, 1.9 Hz, 1H, ArH), 7.51–7.45 (m, 1H, ArH), 7.25–7.07 (m, 6H, ArH), 6.39 (s, 1H, ArH), 5.56 (s, 1H, CH), 3.54 (s, 3H, CH_3)

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.6, 151.1, 149.4, 138.5, 137.4, 137.3, 135.4, 133.6, 130.3, 128.7, 128.0, 122.9, 122.1, 121.1, 121.0, 120.9, 110.2, 105.5, 52.5, 50.0.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{22}\text{H}_{18}\text{ClN}_2\text{O}_2$, 377.1057, found 377.1052.

3.2.6. Methyl 2-(3-chlorophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3f):



Yield: 76 %; yellow liquid; R_f = 0.55 in 2:3 EtOAc/Hexane.

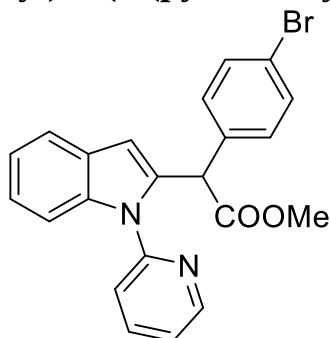
IR ($\nu_{\max}$, cm^{-1}): 2954, 1736, 1661, 1468, 1470, 1246, 945, 714, 661.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.61 (d, J = 4.8 Hz, 1H, ArH), 7.79 (td, J = 7.6, 1.9 Hz, 1H, ArH), 7.61–7.59 (m, 1H, ArH), 7.34–7.27 (m, 3H, ArH), 7.22–7.11 (m, 6H, ArH), 6.51 (s, 1H, ArH), 5.64 (s, 1H, CH), 3.64 (s, 3H, CH_3)

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.3, 151.1, 149.5, 138.8, 138.4, 137.2, 137.2, 134.3, 129.7, 129.1, 128.1, 127.9, 127.2, 122.9, 122.1, 121.1, 121.0, 120.9, 110.2, 105.6, 52.6, 50.2.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{22}\text{H}_{18}\text{ClN}_2\text{O}_2$, 377.1057, found 377.1052.

3.2.7. Methyl 2-(4-bromophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3g):



Yield: 65 %; brown liquid; R_f = 0.57 in 2:3 EtOAc/Hexane.

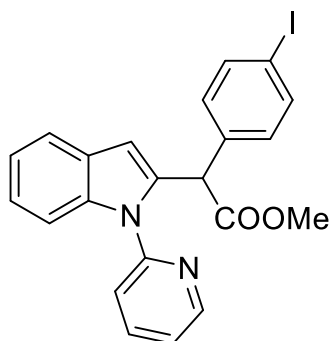
IR ($\nu_{\max}$, cm^{-1}): 2931, 1741, 1652, 1481, 1457, 1241, 896, 645, 612.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.61 (d, J = 4.8 Hz, 1H, ArH), 7.80 (td, J = 7.6, 1.9 Hz, 1H, ArH), 7.61–7.59 (m, 1H, ArH), 7.40–7.35 (m, 4H, ArH), 7.29–7.26 (m, 1H, ArH), 7.19–7.11 (m, 4H, ArH), 6.48 (s, 1H, ArH), 5.65 (s, 1H, CH), 3.63 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.5, 151.1, 149.4, 138.5, 137.3, 137.2, 135.9, 131.7, 130.7, 128.0, 122.8, 122.1, 121.7, 121.1, 120.9, 120.8, 110.1, 105.5, 52.5, 50.0.

HRMS: m/z : $[\text{M}+\text{Na}]^+$ Calculated for $\text{C}_{22}\text{H}_{17}\text{BrN}_2\text{O}_2\text{Na}$, 443.0371, found 443.0370.

3.2.8. Methyl 2-(4-iodophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3h):



Yield: 71 %; brown liquid; R_f = 0.52 in 2:3 EtOAc/Hexane.

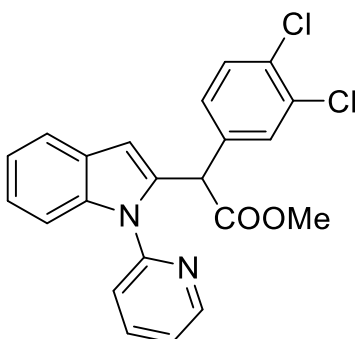
IR (ν_{max} , cm^{-1}): 2936, 1731, 1653, 1487, 1457, 1277, 919, 650, 596.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.58 (d, J = 4.9 Hz, 1H, ArH), 7.78 (td, J = 7.5, 1.9 Hz, 1H, ArH), 7.57 (d, J = 8.2 Hz, 3H, ArH), 7.32 (d, J = 7.9 Hz, 2H, ArH), 7.27–7.23 (m, 1H, ArH), 7.18–7.11 (m, 2H, ArH), 6.97 (d, J = 8.3 Hz, 2H, ArH), 6.45 (s, 1H, ArH), 5.60 (s, 1H, CH), 3.60 (s, 3H, CH_3)

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.4, 151.0, 149.4, 138.5, 137.6, 137.3, 137.2, 136.5, 130.9, 128.0, 122.8, 122.1, 121.1, 120.9, 120.8, 110.1, 105.6, 93.4, 52.5, 50.1.

HRMS: m/z : $[\text{M}+\text{Na}]^+$ Calculated for $\text{C}_{22}\text{H}_{17}\text{IN}_2\text{O}_2\text{Na}$, 491.0232, found 491.0231.

3.2.9. Methyl 2-(3,4-dichlorophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3i):



Yield: 81 %; colourless solid; R_f = 0.46 in 2:3 EtOAc/Hexane.

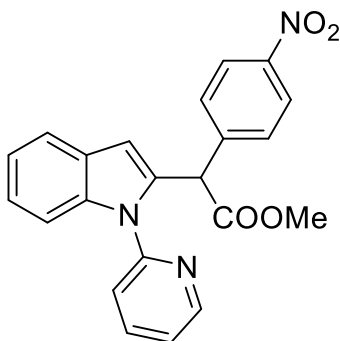
IR ($\nu_{\max}$, cm^{-1}): 2936, 1740, 1666, 1475, 1462, 1277, 917, 714, 630.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.59 (d, J = 4.8 Hz, 1H, ArH), 7.80 (td, J = 7.5, 1.3 Hz, 1H, ArH), 7.60 (d, J = 8.0 Hz, 1H, ArH,), 7.33–7.05 (m, 8H, ArH), 6.51 (s, 1H, ArH), 5.64 (s, 1H, CH), 3.64 (s, 3H, CH).

^{13}C {1H} NMR (100 MHz, CDCl_3 , 24 °C): δ 171.1, 150.9, 149.4, 138.6, 137.2, 137.0, 136.7, 132.5, 131.8, 130.9, 130.4, 128.3, 127.9, 123.0, 122.2, 121.2, 121.0, 120.8, 110.2, 105.5, 52.7, 49.6.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{23}\text{H}_{19}\text{Cl}_2\text{N}_2\text{O}_2$, 425.8024, found 425.8021.

3.2.10. Methyl 2-(4-nitrophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3j):



Yield: 87 %; yellow solid; R_f = 0.45 in 2:3 EtOAc/Hexane.

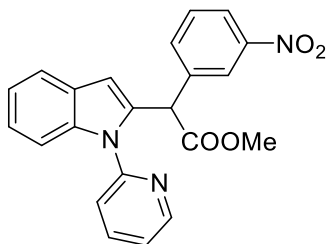
IR ($\nu_{\max}$, cm^{-1}): 2938, 1737, 1659, 1558, 1369, 1487, 1453, 1277, 919, 651.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.59 (d, J = 8.5 Hz, 1H, ArH), 8.09 (d, J = 7.4 Hz, 2H, ArH), 7.80 (t, J = 7.7 Hz, 1H, ArH), 7.61 (d, J = 7.5 Hz, 1H, ArH), 7.40–7.33 (m, 4H, ArH), 7.29–7.27 (m, 1H, ArH), 7.21–7.16 (m, 2H, ArH), 6.54 (s, 1H, ArH), 5.84 (s, 1H, CH), 3.68 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 170.8, 150.9, 149.4, 147.3, 144.2, 138.6, 137.2, 136.2, 129.9, 127.9, 123.6, 123.2, 122.2, 121.3, 121.0, 120.7, 110.2, 105.7, 52.8, 50.2.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{22}\text{H}_{18}\text{N}_3\text{O}_4$, 388.1297, found 388.1296.

3.2.11. Methyl 2-(3-nitrophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3k):



Yield: 89 %; yellow solid; R_f = 0.49 in 2:3 EtOAc/Hexane.

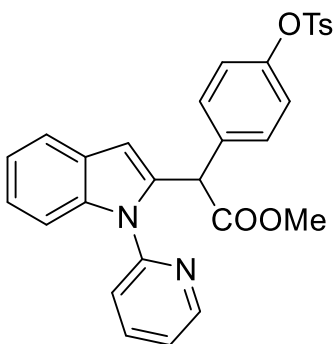
IR (ν_{max} , cm^{-1}): 1746, 1660, 1525, 1478, 1455, 1278, 928, 641.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.61 (d, J = 4.9 Hz, 1H, ArH), 8.09–8.06 (m, 1H, ArH), 8.03 (s, 1H, ArH), 7.78 (td, J = 7.6, 1.9 Hz, 1H, ArH), 7.62–7.59 (m, 2H, ArH), 7.41 (t, J = 7.9 Hz, 1H, ArH), 7.34–7.25 (m, 3H, ArH), 7.20–7.15 (m, 2H, ArH), 6.55 (s, 1H, ArH), 5.82 (s, 1H, CH), 3.68 (s, 3H, CH_3)

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.0, 150.9, 149.5, 148.2, 139.0, 138.6, 137.2, 136.5, 135.2, 129.4, 128.0, 124.1, 123.2, 122.7, 122.3, 121.3, 121.1, 120.8, 110.2, 105.5, 52.8, 50.0.

HRMS: m/z : $[\text{M}+\text{Na}]^+$ Calculated for $\text{C}_{22}\text{H}_{17}\text{N}_3\text{NaO}_4$, 410.1117, found 410.1117.

3.2.12. Methyl 2-(1-(pyridin-2-yl)-1H-indol-2-yl)-2-(4-(tosyloxy)phenyl)acetate (3l):



Yield: 83 %; colourless solid; R_f = 0.43 in 2:3 EtOAc/Hexane.

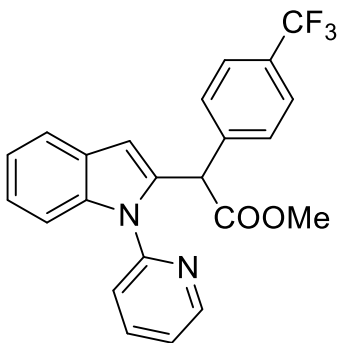
IR ($\nu_{\max}$, cm^{-1}): 2937, 1744, 1651, 1489, 1475, 1339, 1260, 1035, 925, 640.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.57 (dd, J = 5.2, 1.9 Hz, 1H, ArH), 7.77 (td, J = 7.6, 1.9 Hz, 1H, ArH), 7.68 (d, J = 8.3 Hz, 2H, ArH), 7.58–7.56 (m, 1H, ArH), 7.30–7.11 (m, 9H, ArH), 6.85 (d, J = 8.7 Hz, 2H, ArH,), 6.41 (s, 1H, ArH), 5.63 (s, 1H, CH), 3.61 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.4, 151.1, 149.5, 149.0, 145.5, 138.5, 137.4, 137.2, 135.8, 132.5, 130.2, 129.8, 128.5, 128.0, 122.9, 122.4, 122.1, 121.1, 120.9, 120.9, 110.1, 105.4, 52.5, 49.9, 21.8.

HRMS: m/z : $[\text{M}+\text{Na}]^+$ Calculated for $\text{C}_{29}\text{H}_{24}\text{N}_2\text{O}_5\text{SNa}$, 535.1304, found 535.1301.

3.2.13. Methyl 2-(1-(pyridin-2-yl)-1H-indol-2-yl)-2-(4-(trifluoromethyl)phenyl)acetate (3m):



Yield: 81 %; brown gummy liquid; R_f = 0.55 in 2:3 EtOAc/Hexane.

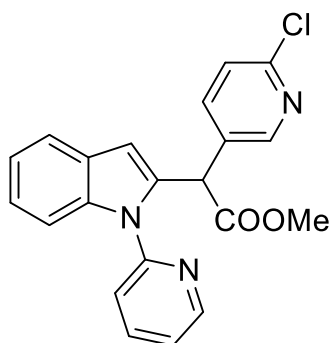
IR ($\nu_{\max}$, cm^{-1}): 2954, 1747, 1678, 1469, 1412, 1318, 1265, 921, 640.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.62 (d, J = 4.8 Hz, 1H, ArH), 7.77 (td, J = 7.8, 1.8 Hz, 1H, ArH), 7.63 (d, J = 7.0 Hz, 1H, ArH,), 7.49–7.19 (m, 9H, ArH), 6.54 (s, 1H, ArH), 5.78 (s, 1H, CH), 3.68 (s, 3H, CH_3).

$^{13}\text{C}\{1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.3, 151.0, 149.4, 138.5, 137.8, 137.1, 132.5, 129.0, 128.0, 125.8, 124.5, 123.9 (q, J = 273 Hz,), 122.9, 122.2, 121.1, 121.0, 120.9, 110.1, 105.4, 52.6, 50.3.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{23}\text{H}_{18}\text{F}_3\text{N}_2\text{O}_2$, 411.1320, found 411.1323.

3.2.14. Methyl 2-(6-chloropyridin-3-yl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3n):



Yield: 83 %; brown gummy liquid; R_f = 0.47 in 2:3 EtOAc/Hexane.

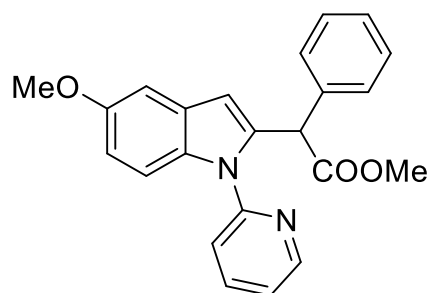
IR (ν_{max} , cm^{-1}): 2949, 1744, 1661, 1489, 1471, 1270, 916, 645.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.60 (dd, J = 4.8, 1.4 Hz, 1H, ArH), 8.13 (d, J = 2.4 Hz, 1H, ArH), 7.80 (td, J = 7.7, 1.8 Hz, 1H, ArH), 7.64–7.60 (m, 2H, ArH), 7.35–7.27 (m, 3H, ArH), 7.23–7.14 (m, 3H, ArH), 6.54 (s, 1H, ArH), 5.73 (s, 1H, CH), 3.67 (s, 3H, CH_3).

$^{13}\text{C}\{1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 170.8, 150.8, 150.6, 149.7, 149.5, 139.4, 138.6, 137.1, 136.2, 131.8, 127.9, 124.1, 123.2, 122.3, 121.3, 121.0, 120.7, 110.2, 105.4, 52.7, 47.2.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{21}\text{H}_{17}\text{ClN}_3\text{O}_2$, 378.1009, found 378.1005.

3.2.15. Methyl 2-(5-methoxy-1-(pyridin-2-yl)-1H-indol-2-yl)-2-phenylacetate (3o):



Yield: 89 %; colourless solid; R_f = 0.50 in 2:3 EtOAc/Hexane.

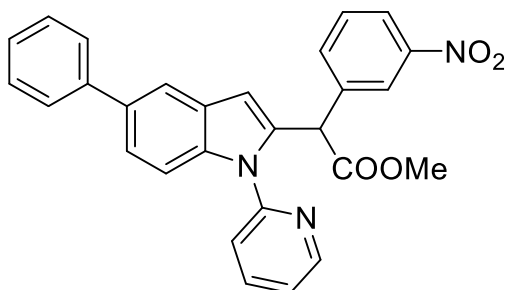
IR ($\nu_{\max}$, cm^{-1}): 2928, 1745, 1659, 1475, 1442, 1425, 1269, 919, 685.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.61 (d, J = 4.0 Hz, 1H, ArH), 7.80 (t, J = 7.9 Hz, 1H, ArH), 7.35–7.33 (m, 7H, ArH), 7.05 (s, 1H, ArH), 6.83 (dd, J = 8.9, 2.0 Hz, 1H, ArH), 6.38 (s, 1H, ArH), 5.64 (s, 1H, CH), 3.85 (s, 3H, CH_3), 3.63 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.9, 155.0, 151.4, 149.4, 138.5, 138.4, 136.9, 132.3, 129.0, 128.7, 128.6, 127.6, 121.8, 120.6, 112.5, 111.0, 105.5, 102.7, 55.9, 52.4, 50.8.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{23}\text{H}_{21}\text{N}_2\text{O}_3$, 373.1552, found 373.1557.

3.2.16. Methyl 2-(3-nitrophenyl)-2-(5-phenyl-1-(pyridin-2-yl)-1H-indol-2 yl) acetate (3p):



Yield: 85 %; colourless solid; R_f = 0.49 in 2:3 EtOAc/Hexane.

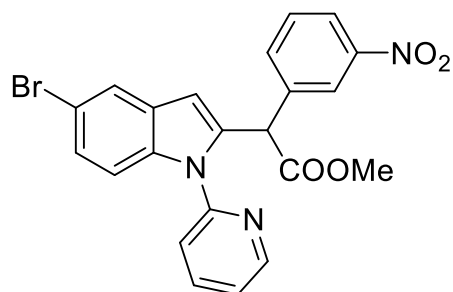
IR ($\nu_{\max}$, cm^{-1}): 2939, 1746, 1651, 1557, 1484, 1463, 1277, 925, 684.

^1H NMR (500 MHz, CDCl_3 , 24 °C): δ 8.63 (d, J = 4.8 Hz, 1H, ArH), 8.10–8.06 (m, 2H, ArH), 7.82–7.79 (m, 2H, ArH), 7.63 (d, J = 7.98 Hz, 3H, ArH), 7.46–7.28 (m, 8H, ArH), 6.62 (s, 1H, ArH), 5.85 (s, 1H, CH), 3.71 (s, 3H, CH_3)

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 °C): δ 170.9, 150.9, 149.6, 148.2, 142.1, 139.0, 138.6, 137.2, 136.7, 135.2, 134.9, 129.4, 128.8, 128.5, 127.4, 126.7, 124.1, 122.9, 122.7, 122.4, 120.7, 119.5, 110.5, 105.9, 52.8, 50.1.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{29}\text{H}_{24}\text{N}_3\text{O}_4$, 478.1767, found 478.1762.

3.2.17. Methyl 2-(5-bromo-1-(pyridin-2-yl)-1*H*-indol-2-yl)-2-(3-nitrophenyl) acetate (3q):



Yield: 88 %; yellow solid; R_f = 0.45 in 2:3 EtOAc/Hexane.

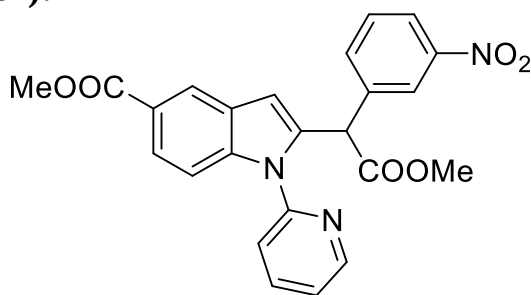
IR (ν_{max} , cm^{-1}): 2938, 1733, 1657, 1562, 1488, 1472, 1457, 1316, 1276, 911, 657, 647.

^1H NMR (500 MHz, CDCl_3 , 24 °C): δ 8.61 (d, J = 4.8 Hz, 1H, ArH), 8.09 (d, J = 8.1 Hz, 1H, ArH), 8.01 (t, J = 1.9 Hz, 1H, ArH), 7.80 (td, J = 7.6, 1.9 Hz, 1H, ArH), 7.72 (d, J = 1.8 Hz, 1H, ArH), 7.58 (d, J = 7.8 Hz, 1H, ArH), 7.43 (t, J = 7.9 Hz, 1H, ArH), 7.32–7.29 (m, 1H, ArH), 7.27–7.25 (m, 2H, ArH), 7.17 (d, J = 8.8 Hz, 1H, ArH), 6.50 (s, 1H, ArH), 5.77 (s, 1H, CH), 3.68 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 °C): δ 170.7, 150.5, 149.7, 148.2, 138.8, 138.7, 137.7, 135.9, 135.1, 129.5, 126.0, 124.0, 123.6, 122.8, 122.7, 120.8, 114.4, 111.7, 104.8, 52.9, 49.9.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{23}\text{H}_{19}\text{BrN}_3\text{O}_4$, 480.0559, found 480.0554.

3.2.18. Methyl 2-(2-methoxy-1-(3-nitrophenyl)-2-oxoethyl)-1-(pyridin-2-yl)-1H-indole-5-carboxylate (3r):



Yield: 85 %; colourless gummy liquid; R_f = 0.45 in 2:3 EtOAc/Hexane.

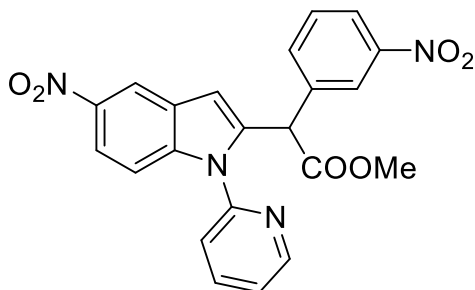
IR ($\nu_{\max}$, cm^{-1}): 2925, 1739, 1657, 1532, 1474, 1467, 1341, 1270, 927, 663.

^1H NMR (500 MHz, CDCl_3 , 24 °C): δ 8.63 (d, J = 4.66 Hz, 1H, ArH), 8.09 (d, J = 8.4 Hz, 1H, ArH), 8.04–8.03 (m, 2H, ArH), 7.84 (td, J = 8.1, 1.4 Hz, 2H, ArH), 7.63–7.59 (m, 2H, ArH), 7.43 (t, J = 7.7 Hz, 1H, ArH), 7.35–7.32 (m, 2H, ArH), 6.60 (s, 1H, ArH), 5.81 (s, 1H, CH), 3.88 (s, 3H, CH_3), 3.68 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 °C): δ 170.6, 167.8, 150.3, 149.7, 148.2, 139.8, 139.0, 138.5, 136.7, 135.1, 131.5, 129.6, 124.9, 124.1, 122.9, 122.4, 121.1, 120.7, 112.4, 105.6, 52.9, 52.1, 50.0.

HRMS: m/z : $[\text{M}+\text{Na}]^+$ Calculated for $\text{C}_{24}\text{H}_{19}\text{N}_3\text{O}_6\text{Na}$, 468.1172, found 468.1174.

3.2.19. Methyl 2-(5-nitro-1-(pyridin-2-yl)-1H-indol-2-yl)-2-(3-nitrophenyl)acetate (3s):



Yield: 79 %; yellow solid; R_f = 0.39 in 2:3 EtOAc/Hexane.

IR ($\nu_{\max}$, cm^{-1}): 2931, 1736, 1659, 1533, 1483, 1451, 1378, 1242, 936, 647.

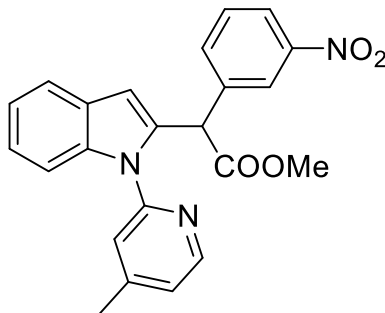
^1H NMR (500 MHz, CDCl_3 , 24 °C): δ 8.67–8.66 (m, 1H, ArH), 8.55 (d, J = 2.1 Hz, 1H, ArH), 8.13–8.07 (m, 2H, ArH), 8.00 (t, J = 2.0 Hz, 1H, ArH), 7.87 (td, J = 7.7, 1.9 Hz, 1H, ArH), 7.60 (d, J = 7.7 Hz, 1H,

ArH), 7.47 (t, $J = 7.8$ Hz, 1H, ArH), 7.41–7.38 (m, 1H, ArH), 7.32–7.28 (m, 2H, ArH), 6.72 (s, 1H, ArH), 5.73 (s, 1H, CH), 3.68 (s, 3H, CH₃).

¹³C{¹H} NMR (125 MHz, CDCl₃, 24 °C): δ 170.3, 150.0, 149.9, 148.3, 142.8, 140.1, 140.0, 139.1, 138.1, 135.0, 129.8, 127.2, 124.0, 123.5, 123.1, 121.1, 118.7, 118.0, 110.3, 106.9, 53.1, 49.9.

HRMS: m/z : [M+H]⁺ Calculated for C₂₂H₁₇N₄O₆, 433.1148, found 433.1140.

3.2.20. Methyl 2-(1-(4-methylpyridin-2-yl)-1H-indol-2-yl)-2-(3-nitrophenyl)acetate (3t):



Yield: 87 %; yellow gummy liquid; $R_f = 0.43$ in 2:3 EtOAc/Hexane.

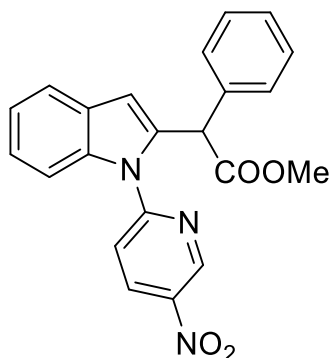
IR ($\nu_{\max}$, cm⁻¹): 2928, 1741, 1675, 1542, 1489, 1447, 1357, 1224, 967, 686.

¹H NMR (500 MHz, CDCl₃, 24 °C): δ 8.45 (d, $J = 4.5$ Hz, 1H, ArH), 8.09 (d, $J = 8.1$ Hz, 1H, ArH), 8.03 (s, 1H, ArH), 7.61 (t, $J = 6.4$ Hz, 2H, ArH), 7.42 (t, $J = 8.0$ Hz, 1H, ArH), 7.33 (d, $J = 7.9$ Hz, 1H, ArH), 7.20–7.11 (m, 4H, ArH), 6.56 (s, 1H, ArH), 5.78 (s, 1H, CH), 3.70 (s, 3H, CH₃), 2.37 (s, 3H, CH₃).

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C): δ 171.0, 150.9, 150.2, 149.1, 148.1, 139.1, 137.2, 136.5, 135.2, 129.3, 127.9, 124.1, 123.5, 123.0, 122.6, 121.4, 121.2, 121.0, 110.3, 105.2, 52.8, 50.0, 21.1.

HRMS: m/z : [M+H]⁺ Calculated for C₂₃H₂₀N₃O₄, 402.1454, found 402.1449.

3.2.21. Methyl 2-(1-(5-nitropyridin-2-yl)-1*H*-indol-2-yl)-2-phenylacetate (3u):



Yield: 81 %; yellow liquid; R_f = 0.45 in 2:3 EtOAc/Hexane.

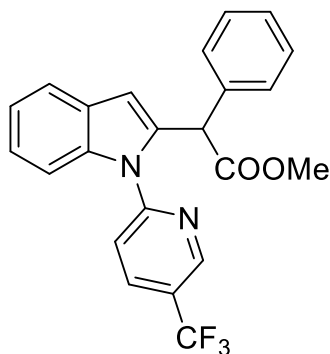
IR ($\nu_{\max}$, cm^{-1}): 2925, 1741, 1669, 1516, 1471, 1469, 1347, 1242, 947, 654.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.61 (dd, J = 4.8, 1.3 Hz, 1H, ArH), 8.09–8.03 (m, 2H, ArH), 7.78 (td, J = 9.6, 1.9 Hz, 1H, ArH), 7.62–7.60 (m, 2H, ArH), 7.42 (t, J = 7.9 Hz, 1H, ArH), 7.34–7.27 (m, 3H, ArH), 7.21–7.15 (m, 2H, ArH), 6.56 (s, 1H, ArH), 5.83 (s, 1H, CH), 3.69 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 170.9, 150.9, 149.5, 148.2, 139.0, 138.6, 137.2, 136.5, 135.2, 129.4, 128.0, 124.1, 123.2, 122.3, 121.3, 120.7, 110.2, 105.5, 52.8, 50.0.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{22}\text{H}_{18}\text{N}_3\text{O}_4$, 388.1297, found 388.1296.

3.2.22. Methyl 2-phenyl-2-(1-(5-(trifluoromethyl)pyridin-2-yl)-1*H*-indol-2-yl)acetate (3v):



Yield: 69 %; colourless liquid; R_f = 0.55 in 2:3 EtOAc/Hexane.

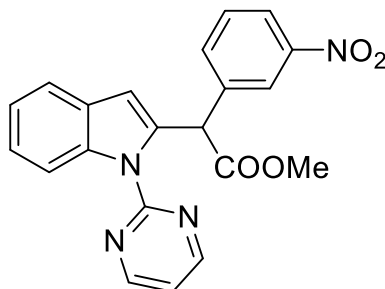
IR ($\nu_{\max}$, cm^{-1}): 2937, 1745, 1621, 1472, 1474, 1314, 1221, 937, 635.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.59 (d, J = 1.9 Hz, 1H, ArH), 7.75 (t, J = 7.9 Hz, 1H, ArH), 7.60–7.15 (m, 10H, ArH), 6.51 (s, 1H, ArH), 5.74 (s, 1H, CH), 3.65 (s, 3H, CH_3).

$^{13}\text{C}\{1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.3, 151.1, 149.5, 138.5, 137.9, 137.3, 137.1, 132.5, 130.7 (q, J = 32.2 Hz), 129.0, 128.0, 125.8 (q, J = 3.7 Hz), 124.5 (q, J = 3.7 Hz), 124.0 (q, J = 272 Hz), 123.0, 122.2, 121.2, 121.0, 120.9, 110.1, 105.4, 52.6, 50.3.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{23}\text{H}_{18}\text{F}_3\text{N}_2\text{O}_2$, 411.1320, found 411.1323.

3.2.23. Methyl 2-(3-nitrophenyl)-2-(1-(pyrimidin-2-yl)-1H-indol-2-yl)acetate (3w):



Yield: 80 %; yellow sticky liquid; R_f = 0.45 in 2:3 EtOAc/Hexane.

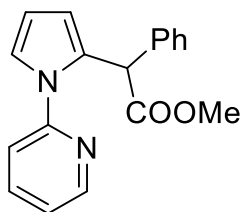
IR (ν_{max} , cm^{-1}): 2939, 1742, 1650, 1545, 1491, 1475, 1360, 1248, 921, 646.

^1H NMR (500 MHz, CDCl_3 , 24 °C): δ 8.72 (d, J = 4.8 Hz, 2H, ArH), 8.51 (d, J = 8.5 Hz, 1H, ArH,), 8.26 (t, J = 1.8 Hz, 1H, ArH), 8.18–8.16 (m, 1H, ArH), 7.71 (d, J = 7.7 Hz, 1H, ArH,), 7.54–7.50 (m, 2H, ArH), 7.30 (td, J = 7.1, 1.1 Hz, 1H, ArH), 7.21 (t, J = 7.1 Hz, 1H, ArH,), 7.11 (t, J = 4.8 Hz, 1H, ArH), 6.28 (s, 1H, ArH), 6.11 (s, 1H, CH), 3.71 (s, 3H, CH_3)

$^{13}\text{C}\{1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.5, 157.9, 148.4, 139.6, 137.2, 136.9, 135.4, 129.6, 128.6, 124.4, 124.1, 122.8, 122.5, 120.6, 117.0, 115.4, 110.3, 52.7, 52.5.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{21}\text{H}_{17}\text{N}_4\text{O}_4$, 389.1250, found 389.1256.

3.2.24. Methyl 2-phenyl-2-(1-(pyridin-2-yl)-1H-pyrrol-2-yl)acetate (3x):



Yield: 73 %; colourless liquid; R_f = 0.55 in 3:7 EtOAc/Hexane.

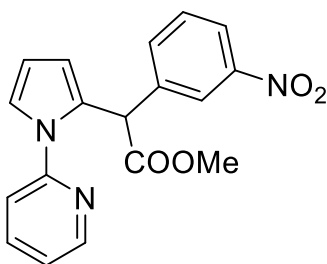
IR ($\nu_{\max}$, cm^{-1}): 2945, 1748, 1667, 1496, 1445, 1261, 911, 614.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.43 (d, J = 4.8 Hz, 1H, ArH), 7.74 (ddd, J = 8.1, 7.5, 1.9 Hz, 1H, ArH), 7.32–7.25 (m, 6H, ArH), 7.15 (ddd, J = 7.47, 5.31, 0.9 Hz, 1H, ArH), 7.08 (dd, J = 2.8, 1.7 Hz, 1H, ArH), 6.22 (t, J = 3.2 Hz, 1H, ArH), 5.89–5.87 (m, 1H, ArH), 5.65 (s, 1H, CH), 3.61 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 172.9, 152.9, 148.1, 138.7, 137.7, 131.4, 129.0, 128.6, 127.5, 121.0, 120.9, 116.1, 112.79, 109.6, 52.3, 51.5.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_2$, 293.1290, found 293.1290.

3.2.25. Methyl 2-(3-nitrophenyl)-2-(1-(pyridin-2-yl)-1H-pyrrol-2-yl)acetate (3y):



Yield: 79 %; yellow liquid; R_f = 0.47 in 3:7 EtOAc/Hexane.

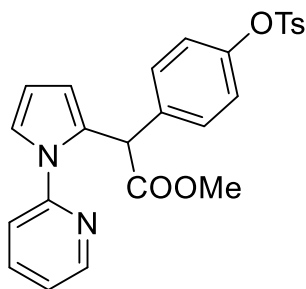
IR ($\nu_{\max}$, cm^{-1}): 2925, 1745, 1648, 1559, 1457, 1462, 1347, 1285, 916, 654.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.41 (d, J = 4.9 Hz, 1H, ArH), 8.16–8.08 (m, 2H, ArH), 7.74 (ddd, J = 8.2, 7.7, 2.0 Hz, 1H, ArH), 7.65 (d, J = 7.7 Hz, 1H, ArH), 7.46 (t, J = 8.0 Hz, 1H, ArH), 7.26–7.06 (m, 3H, ArH), 6.26 (t, J = 3.3 Hz, 1H, ArH), 6.03–6.01 (m, 1H, ArH), 5.89 (s, 1H, CH), 3.66 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.8, 152.5, 148.3, 148.1, 140.1, 138.9, 135.2, 129.7, 129.3, 124.2, 122.4, 121.4, 121.2, 116.1, 112.6, 109.9, 52.5, 50.6.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{18}\text{H}_{16}\text{N}_3\text{O}_4$, 338.1141, found 338.1143.

3.2.26. Methyl 2-(1-(pyridin-2-yl)-1*H*-pyrrol-2-yl)-2-(4-(tosyloxy)phenyl) acetate (3z):



Yield: 73 %; colourless solid; R_f = 0.55 in 3:7 EtOAc/Hexane.

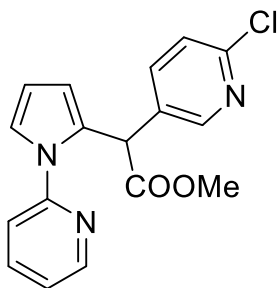
IR (ν_{max} , cm^{-1}): 2912, 1750, 1660, 1489, 1451, 1335, 1269, 915, 602.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.39 (d, J = 4.8 Hz, 1H, ArH), 7.75–7.68 (m, 3H, ArH), 7.29 (d, J = 8.0 Hz, 2H, ArH), 7.23–7.05 (m, 5H, ArH), 6.91 (d, J = 8.6 Hz, 2H, ArH), 6.22 (t, J = 3.2 Hz, 1H, ArH), 5.83–5.81 (m, 1H, ArH), 5.66 (s, 1H, ArH), 3.60 (s, 3H, CH_3), 2.44 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 172.3, 152.7, 148.8, 148.0, 145.4, 138.7, 136.8, 132.4, 130.8, 130.2, 129.8, 128.5, 122.4, 121.2, 121.0, 116.1, 112.5, 109.6, 52.3, 50.7, 21.7.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{25}\text{H}_{23}\text{N}_2\text{O}_5\text{S}$, 463.1328, found 463.1328.

3.2.27. Methyl 2-(6-chloropyridin-3-yl)-2-(1-(pyridin-2-yl)-1*H*-pyrrol-2-yl) acetate (3aa):



Yield: 71 %; yellow liquid; R_f = 0.42 in 3:7 EtOAc/Hexane.

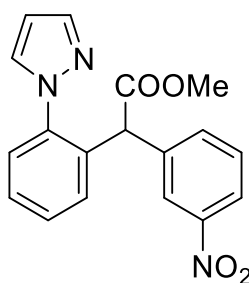
IR (ν_{max} , cm^{-1}): 2941, 1741, 1668, 1472, 1458, 1248, 917, 714, 669.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.40 (d, J = 4.8 Hz, 1H, ArH), 8.26 (d, J = 2.4 Hz, 1H, ArH), 7.77–7.73 (m, 1H, ArH), 7.64 (dd, J = 8.2, 2.5 Hz, 1H, ArH), 7.26–7.06 (m, 4H, ArH), 6.26 (t, J = 3.2 Hz, 1H, ArH), 6.03–6.02 (m, 1H, ArH), 5.80 (s, 1H, CH), 3.64 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.7, 152.5, 150.4, 150.1, 148.0, 139.4, 138.9, 132.8, 129.6, 124.1, 121.4, 121.2, 116.0, 112.5, 109.9, 52.5, 47.9.

HRMS: m/z : $[\text{M}+\text{Na}]^+$ Calculated for $\text{C}_{17}\text{H}_{14}\text{ClN}_3\text{O}_2\text{Na}$, 350.0672, found 350.0677.

3.2.28. Methyl 2-(2-(1*H*-pyrazol-1-yl)phenyl)-2-(3-nitrophenyl)acetate (5a):



Yield: 81 %; yellow liquid; R_f = 0.45 in 3:7 EtOAc/Hexane.

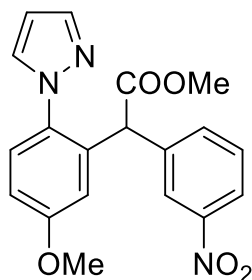
IR (ν_{max} , cm^{-1}): 2951, 1749, 1664, 1547, 1491, 1429, 1351, 1253, 922, 678.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.06 (d, J = 7.9 Hz, 1H, ArH), 8.00 (s, 1H, ArH), 7.76 (s, 1H, ArH), 7.48–7.37 (m, 6H, ArH), 7.30 (d, J = 7.2 Hz, 1H, ArH), 6.40 (t, J = 1.9 Hz, 1H, ArH), 5.58 (s, 1H, CH), 3.70 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.8, 148.3, 141.1, 140.0, 139.5, 135.1, 134.0, 131.0, 129.5, 129.3, 129.2, 128.7, 126.8, 123.8, 122.4, 106.9, 52.7, 50.8.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{18}\text{H}_{16}\text{N}_3\text{O}_4$, 338.1141, found 338.1139.

3.2.29. Methyl 2-(5-methoxy-2-(1H-pyrazol-1-yl)phenyl)-2-(3-nitrophenyl)acetate (5b):



Yield: 82 %; yellow gummy liquid; R_f = 0.43 in 3:7 EtOAc/Hexane.

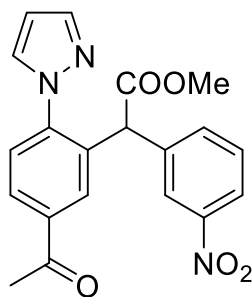
IR ($\nu_{\max}$, cm^{-1}): 2947, 1742, 1689, 1518, 1478, 1445, 1352, 1271, 921, 641.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.06 (d, J = 7.9 Hz, 1H, ArH), 7.99 (s, 1H, ArH), 7.72 (d, J = 1.8 Hz, 1H, ArH), 7.48–7.38 (m, 2H, ArH), 7.34 (d, J = 2.3 Hz, 1H, ArH), 7.23 (d, J = 8.6 Hz, 1H, ArH), 6.96 (d, J = 2.8 Hz, 1H, ArH), 6.88 (dd, J = 8.6, 2.8 Hz, 1H, ArH), 6.36 (t, J = 2.2 Hz, 1H, ArH), 5.40 (s, 1H, CH), 3.81 (s, 3H, CH), 3.69 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 171.1, 159.9, 148.2, 140.8, 139.7, 135.6, 135.0, 132.8, 131.3, 129.3, 128.2, 123.8, 122.4, 115.3, 112.9, 106.6, 55.6, 52.7, 50.7.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{19}\text{H}_{18}\text{N}_3\text{O}_5$, 368.1246, found 368.1241.

3.2.30. Methyl 2-(5-acetyl-2-(1H-pyrazol-1-yl)phenyl)-2-(3-nitrophenyl)acetate (5c):



Yield: 81 %; yellow gummy liquid; R_f = 0.41 in 3:7 EtOAc/Hexane.

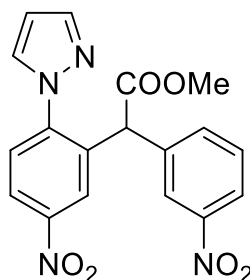
IR ($\nu_{\max}$, cm^{-1}): 2933, 1742, 1725, 1675, 1553, 1489, 1479, 1358, 1261, 891, 614.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.08–7.94 (m, 4H, ArH), 7.77 (s, 1H, ArH), 7.52–7.38 (m, 4H, ArH), 6.43 (s, 1H, ArH), 5.79 (s, 1H, CH), 3.70 (s, 3H, CH_3), 2.57 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 196.5, 171.4, 148.2, 142.8, 141.7, 139.4, 136.9, 134.9, 133.9, 130.8, 129.9, 129.6, 128.7, 126.4, 123.8, 122.6, 107.7, 52.8, 50.9, 26.6.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{20}\text{H}_{18}\text{N}_3\text{O}_5$, 380.1246, found 380.1243.

3.2.31. Methyl 2-(5-nitro-2-(1H-pyrazol-1-yl)phenyl)-2-(3-nitrophenyl)acetate (5d):



Yield: 85 %; yellow solid; R_f = 0.42 in 3:7 EtOAc/Hexane.

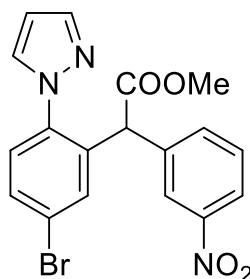
IR (ν_{max} , cm^{-1}): 2937, 1731, 1653, 1551, 1489, 1451, 1367, 1276, 899, 641.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.27–8.14 (m, 3H, ArH), 8.03 (s, 1H, ArH), 7.84 (s, 1H, ArH), 7.60–7.48 (m, 4H, ArH), 6.51 (s, 1H, ArH), 5.90 (s, 1H, CH), 3.72 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 170.9, 148.5, 147.2, 144.0, 142.4, 138.8, 135.2, 134.8, 130.9, 130.0, 126.7, 125.8, 124.0, 124.0, 123.1, 108.4, 53.1, 51.1.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{18}\text{H}_{15}\text{N}_4\text{O}_6$, 383.0992, found 383.0989.

3.2.32. Methyl 2-(5-bromo-2-(1H-pyrazol-1-yl)phenyl)-2-(3-nitrophenyl)acetate (5e):



Yield: 86 %; brown liquid; R_f = 0.46 in 3:7 EtOAc/Hexane.

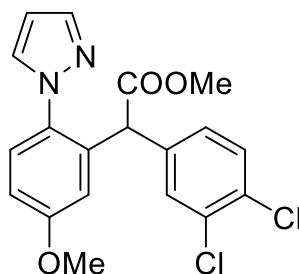
IR (ν_{max} , cm^{-1}): 2942, 1735, 1678, 1541, 1467, 1442, 1357, 1281, 936, 645.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.15–8.12 (m, 1H, ArH), 8.00 (s, 1H, ArH), 7.81 (d, J = 1.6 Hz, 1H, ArH), 7.71–7.42 (m, 6H, ArH), 6.43 (t, J = 2.0 Hz, 1H, ArH), 5.82 (s, 1H, CH), 3.70 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 170.9, 148.5, 142.6, 142.2, 138.8, 135.0, 134.7, 134.2, 132.4, 130.8, 129.9, 126.7, 123.9, 123.0, 117.7, 108.2, 53.1, 50.8.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{18}\text{H}_{15}\text{BrN}_3\text{O}_4$, 416.0246, found 416.0244.

3.2.33. Methyl 2-(3,4-dichlorophenyl)-2-(5-methoxy-2-(1H-pyrazol-1-yl)phenyl) acetate (5f):



Yield: 69 %; yellowish liquid; R_f = 0.49 in 3:7 EtOAc/Hexane.

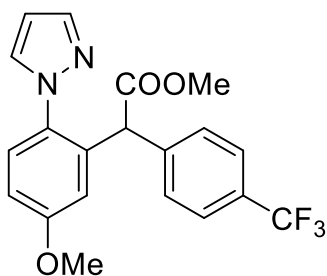
IR (ν_{max} , cm^{-1}): 2937, 1739, 1655, 1485, 1451, 1273, 918, 652, 612.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 7.72 (d, J = 1.85 Hz, 1H, ArH), 7.36 (d, J = 2.3 Hz, 1H, ArH), 7.31 (d, J = 8.3 Hz, 1H, ArH), 7.23–7.21 (m, 2H, ArH), 6.98 (dd, J = 8.3, 2.1 Hz, 1H, ArH), 6.92 (d, J = 2.7 Hz, 1H, ArH), 6.86 (dd, J = 8.6, 2.8 Hz, 1H, ArH), 6.38 (t, J = 2.1 Hz, 1H, ArH), 5.22 (s, 1H, CH), 3.80 (s, 3H, CH_3), 3.66 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 171.8, 159.8, 140.8, 137.8, 135.9, 132.8, 132.6, 131.7, 131.4, 130.7, 130.4, 128.2, 128.1, 115.5, 112.7, 106.5, 55.6, 52.6, 50.3.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{20}\text{H}_{19}\text{Cl}_2\text{N}_2\text{O}_3$, 405.0773, found 405.0769.

3.2.34. Methyl 2-(5-methoxy-2-(1H-pyrazol-1-yl)phenyl)-2-(4-(trifluoromethyl)phenyl)acetate (5g):



Yield: 80 %; colourless liquid; R_f = 0.52 in 3:7 EtOAc/Hexane.

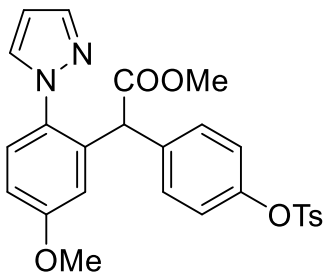
IR ($\nu_{\max}$, cm^{-1}): 2936, 1745, 1651, 1467, 1441, 1212, 1116, 927, 624.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 7.73 (d, J = 1.4 Hz, 1H, ArH), 7.48 (d, J = 6.9 Hz, 1H, ArH), 7.38–7.32 (m, 4H, ArH), 7.22 (d, J = 8.5 Hz, 1H, ArH), 6.92 (d, J = 2.8 Hz, 1H, ArH), 6.87 (dd, J = 8.6, 2.8 Hz, 1H, ArH), 6.37 (t, J = 2.1 Hz, 1H, ArH), 5.34 (s, 1H, CH), 3.80 (s, 3H, CH_3), 3.67 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 172.0, 159.8, 140.8, 138.6, 136.2, 132.8, 132.3, 131.4, 130.9 (q, J = 32 Hz), 129.1, 128.2, 125.6 (q, J = 3.8 Hz), 124.3 (q, J = 3.8 Hz), 124.0 (q, J = 273 Hz), 115.4, 112.8, 106.5, 55.6, 52.6, 51.1.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{21}\text{H}_{20}\text{F}_3\text{N}_2\text{O}_3$, 405.1426, found 405.1424.

3.2.35. Methyl 2-(5-methoxy-2-(1H-pyrazol-1-yl)phenyl)-2-(4-(tosyloxy)phenyl)acetate (5h):



Yield: 69 %; colourless solid; R_f = 0.47 in 3:7 EtOAc/Hexane.

IR ($\nu_{\max}$, cm^{-1}): 2945, 1743, 1661, 1476, 1452, 1341, 1264, 935, 642.

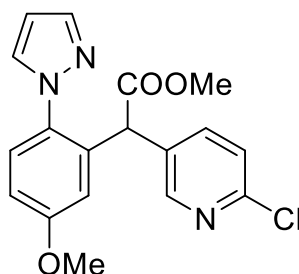
^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 7.70 (d, J = 1.7 Hz, 1H, ArH), 7.67 (d, J = 8.2 Hz, 2H, ArH), 7.32 (d, J = 2.2 Hz, 1H, ArH), 7.28 (d, J = 8.1 Hz, 2H, ArH), 7.20 (d, J = 8.3 Hz, 1H, ArH), 7.06 (d, J = 8.6 Hz,

1H, ArH), 6.89–6.81 (m, 4H, ArH), 6.34 (t, $J = 2.1$ Hz, 1H, ArH), 5.19 (s, 1H, CH), 3.77 (s, 3H, CH₃), 3.62 (s, 3H, CH₃), 2.42 (s, 3H, CH₃).

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C): δ 172.1, 159.7, 148.8, 145.4, 140.7, 136.6, 136.5, 132.7, 132.4, 131.4, 130.0, 129.8, 128.5, 128.1, 122.4, 115.6, 112.5, 106.4, 55.5, 52.5, 50.5, 21.7.

HRMS: m/z : [M+H]⁺ Calculated for C₂₆H₂₅N₂O₆S, 493.1433, found 493.1437.

3.2.36. Methyl 2-(6-chloropyridin-3-yl)-2-(5-methoxy-2-(1H-pyrazol-1-yl)phenyl) acetate (5i):



Yield: 77 %; brown liquid; $R_f = 0.41$ in 3:7 EtOAc/Hexane.

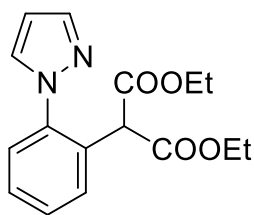
IR ($\nu_{\max}$, cm⁻¹): 2943, 1737, 1674, 1491, 1442, 1274, 936, 642, 712.

¹H NMR (400 MHz, CDCl₃, 24 °C): δ 8.03 (d, $J = 2.5$ Hz, 1H, ArH), 7.72 (d, $J = 1.8$ Hz, 1H, ArH), 7.50 (dd, $J = 8.2, 2.4$ Hz, 1H, ArH), 7.35 (d, $J = 2.3$ Hz, 1H, ArH), 7.22–7.18 (m, 2H, ArH), 6.93 (d, $J = 2.7$ Hz, 1H, ArH), 6.87 (dd, $J = 8.6, 2.8$ Hz, 1H, ArH), 6.38 (t, $J = 2.2$ Hz, 1H, ArH), 5.29 (s, 1H, CH), 3.80 (s, 3H, CH₃), 3.68 (s, 3H, CH₃).

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C): δ 171.6, 159.8, 150.5, 149.7, 140.9, 139.1, 135.5, 132.7, 132.5, 131.3, 128.3, 124.1, 115.1, 112.9, 106.7, 55.7, 52.8, 48.1.

HRMS: m/z : [M+H]⁺ Calculated for C₁₈H₁₇O₃N₃Cl, 258.0958, found 258.0953.

3.2.37. Diethyl 2-(2-(1H-pyrazol-1-yl)phenyl)malonate (5j):



Yield: 86 %; colourless liquid; R_f = 0.55 in 3:7 EtOAc/Hexane.

IR ($\nu_{\max}$, cm^{-1}): 2968, 1733, 1651, 1483, 1474, 1285, 902, 644.

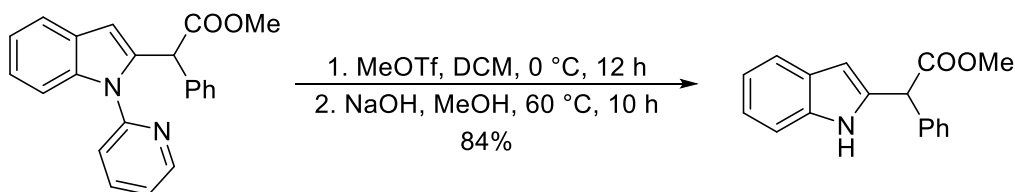
^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 7.69 (d, J = 1.7 Hz, 1H, ArH), 7.64 (dd, J = 2.3, 0.5 Hz, 1H, ArH), 7.62–7.60 (m, 1H, ArH), 7.44–7.37 (m, 2H, ArH), 7.33–7.30 (m, 1H, ArH), 6.42 (t, J = 1.9 Hz, 1H, ArH), 4.88 (s, 1H, CH), 4.17 (q, J = 7.1 Hz, 4H, ArH), 1.21 (t, J = 7.1 Hz, 6H, ArH).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 168.0, 141.0, 139.7, 131.0, 130.2, 129.0, 128.8, 128.5, 126.0, 106.8, 61.8, 52.7, 13.9.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{16}\text{H}_{19}\text{N}_2\text{O}_4$, 303.1345, found 303.1341.

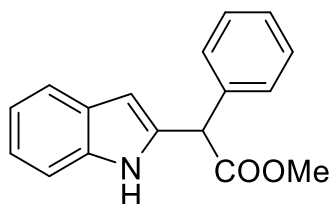
4. Removal of pyridine directing group:

In an oven dried Schlenk tube Methyl trifluoromethanesulfonate (0.175 mmol) was added dropwise to a solution of **3a** (50 mg, 0.146 mmol) in dichloromethane (3 mL) at 0 °C, and the resulting solution was stirred for 12 h at RT. Then the solvent was removed under vacuum, and the residue was dissolved in MeOH (1 mL) and 2 M aq. NaOH solution (0.6 mL) was added, and stirring was continued at 60 °C for 10 h.



After cooling to RT, the solvents were removed under reduced pressure, and the resulting residue was extracted with EtOAc. The combined organic layers were washed with brine, dried over Na_2SO_4 , and concentrated resulted crude product. The residue was purified by column chromatography to provide compound **6** with 84% yield.

4.1. Methyl 2-(1*H*-indol-2-yl)-2-phenylacetate (6):



Yield: 84 %; red liquid; R_f = 0.52 in 2:3 EtOAc/Hexane.

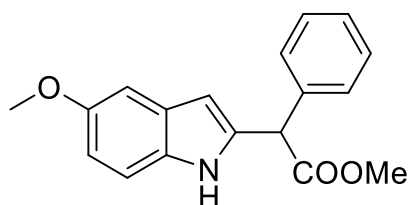
IR ($\nu_{\max}$, cm^{-1}): 3402, 2937, 1731, 1659, 1472, 1271, 910, 657.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.71 (s, br, 1H, NH), 7.54 (d, J = 7.8 Hz, 1H, ArH), 7.31–7.25 (m, 6H, ArH), 7.14 (t, J = 7.9 Hz, 1H, ArH), 7.06 (t, J = 7.6 Hz, 1H, ArH), 6.38 (s, 1H, ArH), 5.20 (s, 1H, CH), 3.76 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 172.4, 137.5, 136.4, 134.6, 128.9, 128.1, 128.0, 127.8, 122.0, 120.5, 120.0, 111.1, 102.3, 52.8, 50.7.

HRMS: m/z : $[\text{M}+\text{H}]^+$ Calculated for $\text{C}_{17}\text{H}_{16}\text{NO}_2$, 266.1181, found 266.1185.

4.2. Methyl 2-(5-methoxy-1*H*-indol-2-yl)-2-phenylacetate (7):



Yield: 69 %; red liquid; R_f = 0.51 in 2:3 EtOAc/Hexane.

IR ($\nu_{\max}$, cm^{-1}): 3457, 2954, 1747, 1649, 1467, 1487, 1246, 941, 671.

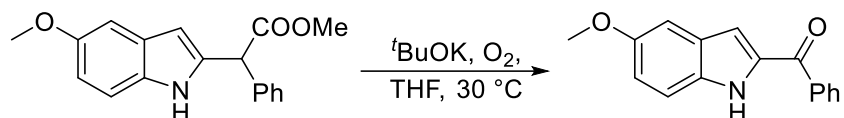
^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.63 (s, br, 1H, NH), 7.40–7.31 (m, 3H, ArH), 7.25–7.20 (m, 3H, ArH), 7.01 (s, 1H, ArH), 6.82 (d, J = 8.5 Hz, 1H, ArH), 6.31 (s, 1H, ArH), 5.18 (s, 1H, CH), 3.82 (s, 3H, CH_3), 3.78 (s, 3H, CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 187.0, 155.0, 138.2, 134.9, 133.1, 132.4, 129.3, 128.5, 128.2, 118.5, 113.2, 112.3, 103.0, 55.8.

HRMS: m/z : $[M+H]^+$ Calculated for $C_{18}H_{18}NO_3$, 296.1287, found 296.1289.

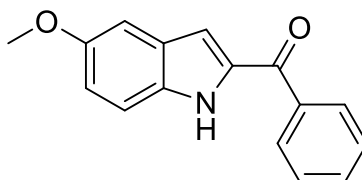
5. Synthesis of (5-methoxy-1*H*-indol-2-yl)(phenyl)methanone (8):

In an oven dried reaction tube compound 7 was added and the reaction tube was flushed with oxygen gas. 0.2 mL of dry THF was added to the reaction tube and followed by 13 mg *t*BuOK was added. The reaction mixture was stirred at RT for 15 minutes the reaction was quenched with saturated ammonium chloride



and the compound was extracted with EtOAc. The combined layer was dried with anhydrous sodium sulphate and concentrated under vacuum to get the crude product. The compound was purified by silica gel column chromatography afforded 17 mg of compound (8).

5.1. (5-methoxy-1*H*-indol-2-yl)(phenyl)methanone (8):



Yield: 68 %; red liquid; R_f = 0.52 in 1:4 EtOAc/Hexane.

IR ($\nu_{\max}$, cm^{-1}): 3396, 3047, 2941, 1735, 1656, 1491, 1474, 1212, 947, 635.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 9.23 (s, br, 1H, NH), 7.98 (d, J = 7.0 Hz, 2H, ArH), 7.61–7.53 (m, 3H, ArH), 7.37 (d, J = 8.8 Hz, 1H, ArH), 7.08–7.05 (m, 3H, ArH), 3.85 (s, 3H, CH_3).

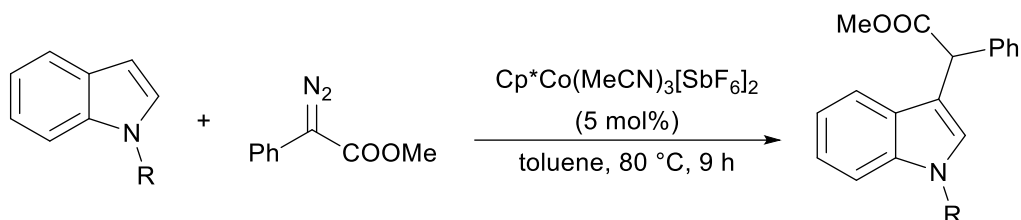
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 187.0, 155.0, 138.2, 134.9, 133.1, 132.4, 129.3, 128.5, 128.2, 118.5, 113.2, 112.3, 103.0, 55.8.

HRMS: m/z : $[M+H]^+$ Calculated for $C_{16}H_{14}NO_2$, 252.1025, found 252.1022.

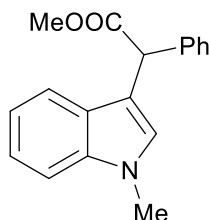
6. Mechanistic investigation for Cp*Co(III)-catalyzed alkylation of indole.

6.1. Influence of directing group.

In order to emphasize the necessity of the directing group *N*-methylindole and *N*-phenylindole were subjected under the optimized reaction conditions. Only selective C3-alkylated product 9a and 9b was isolated, no C2-alkylation occur.



6.1.1. Methyl 2-(1-methyl-1H-indol-3-yl)-2-phenylacetate (9a)

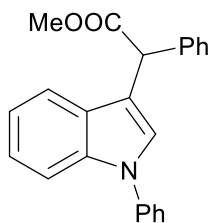


Yield: 69 %; colourless liquid; R_f = 0.49 in 2:3 EtOAc/Hexane.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 7.47–7.43 (m, 3H, ArH), 7.34–7.26 (m, 4H, ArH), 7.24–7.20 (m, H, ArH), 7.09–7.06 (m, 8H, ArH), 5.27 (s, 1H, CH), 3.76 (s, 6H, 2CH₃).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 173.6, 138.8, 137.1, 128.6, 128.5, 128.0, 127.3, 127.1, 121.9, 119.3, 119.1, 112.1, 109.4, 52.4, 48.9, 32.9.

6.1.2. Methyl 2-phenyl-2-(1-phenyl-1H-indol-3-yl)acetate (9b)



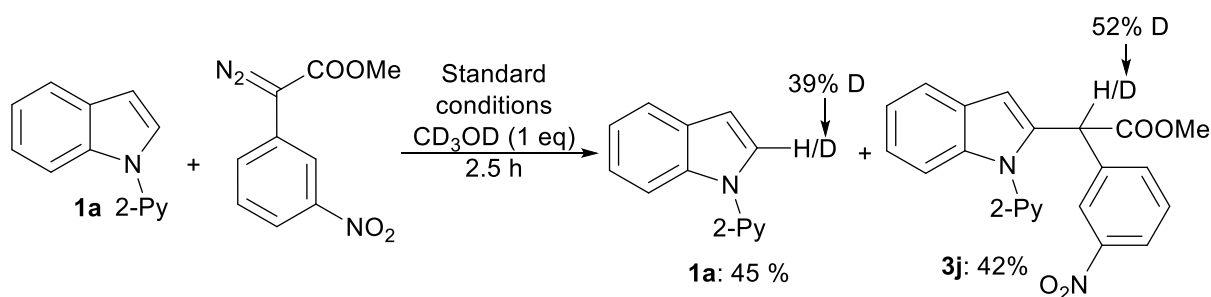
Yield: 63 %; colourless liquid; R_f = 0.50 in 2:3 EtOAc/Hexane.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 7.57–7.48 (m, 8H, ArH), 7.38–7.28 (m, 5H, ArH), 7.22 (t, J = 8.0 Hz, 1H, ArH), 7.13 (t, J = 7.5 Hz, 1H, ArH), 5.33 (s, 1H, CH), 3.78 (s, 3H, 2CH_3).

$^{13}\text{C}\{1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 173.3, 139.7, 138.4, 136.3, 129.7, 128.7, 128.6, 128.1, 127.5, 127.0, 126.5, 124.4, 122.8, 120.4, 119.4, 114.7, 110.8, 52.4, 48.9.

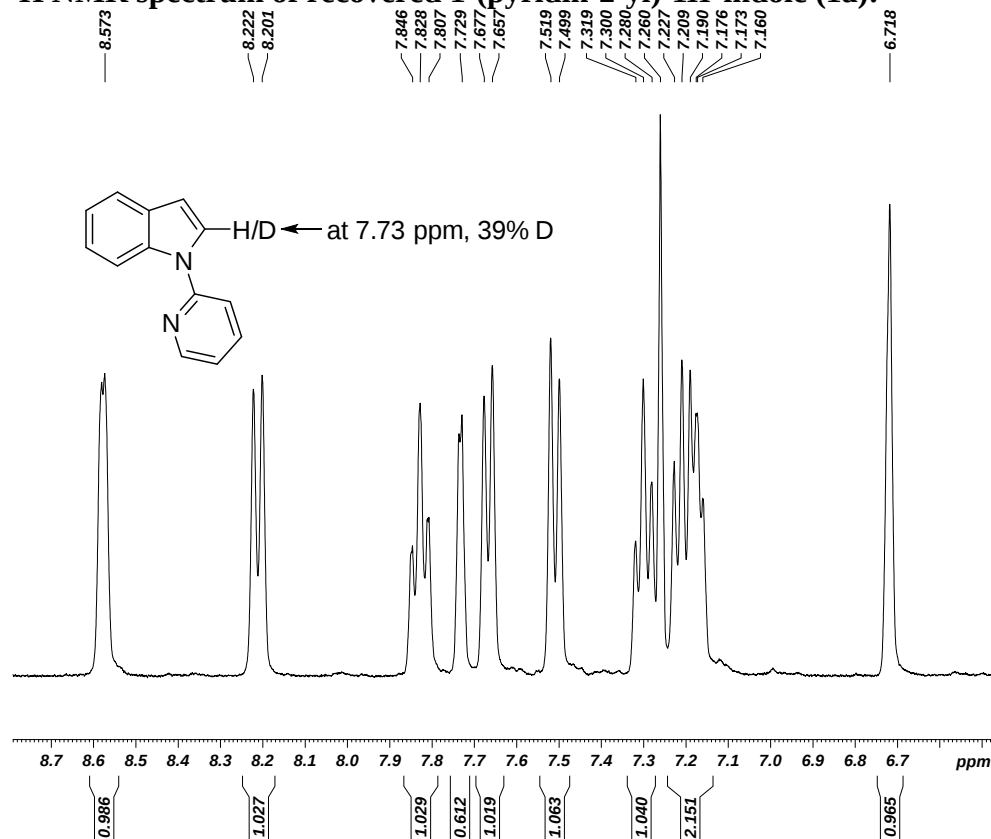
6.2. Deuterium exchange experiment.

One oven dried Schlenk tube was charged with *N*-pyridyl indole **1a** (50 mg, 0.25 mmol, 1 equiv), diazo compound **2j** (0.31 mmol, 1.2 equiv) and $\text{Cp}^*\text{Co}(\text{MeCN})_3[\text{SbF}_6]_2$ (5 mol%). The inner atmosphere was made inert through repeated (thrice) evacuation and refilled with nitrogen. Dry solvent (1.5 mL), followed by CD_3OD (9 mg, 1 equiv) was added to the reaction mixture and the reaction mixture was stirred at 80 °C for 2.5 h.



The reaction mixture was cooled to room temperature and dissolved in 8 mL DCM and filtered through a small pad of Celite. Solvent was evaporated to get the crude reaction mixture, from which starting material and product were isolated through column chromatography. The isolated compounds are analyzed by ^1H NMR. The spectrum indicates that there is about 39% of C2 hydrogen of indole(**1a**) are exchanged with D and about 52% of benzylic H are exchanged with D.

¹H NMR spectrum of recovered 1-(pyridin-2-yl)-1H-indole (1a):



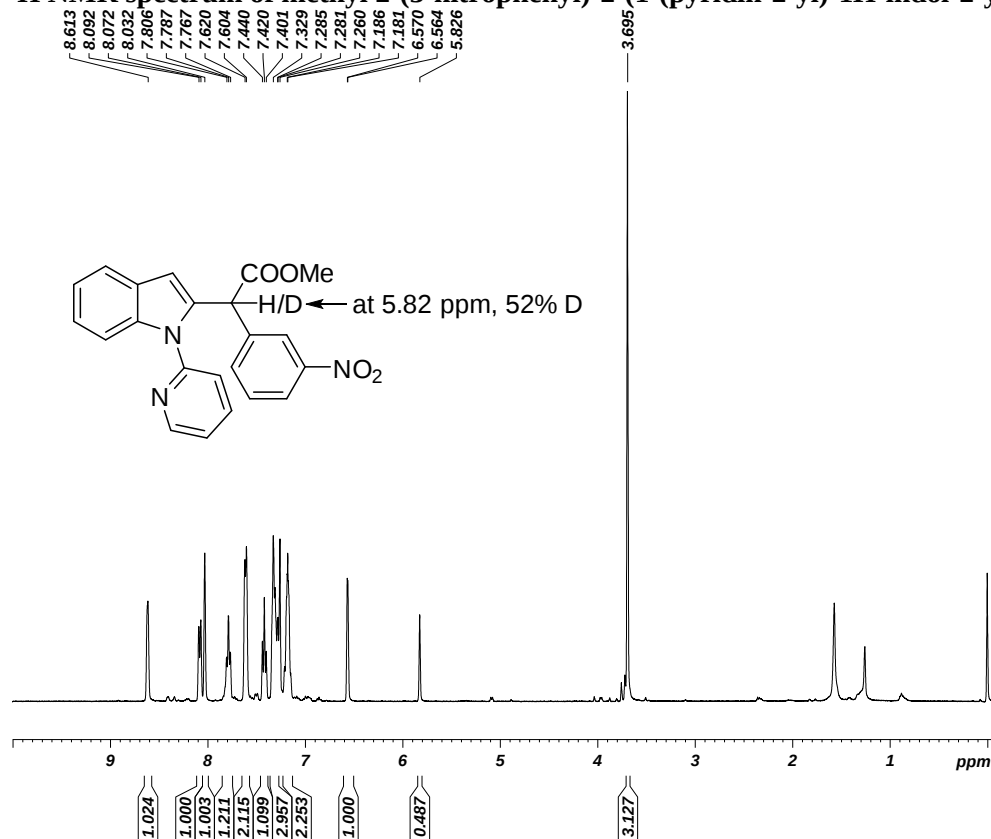
Current Data Parameters
NAME 05.18
EXPNO 466
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180521
Time 13.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 298.1 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 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR spectrum of methyl 2-(3-nitrophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3j):



Current Data Parameters
NAME 05.18
EXPNO 265
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180523
Time 8.04
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 299.2 K
D1 0.50000000 sec
TD0 1

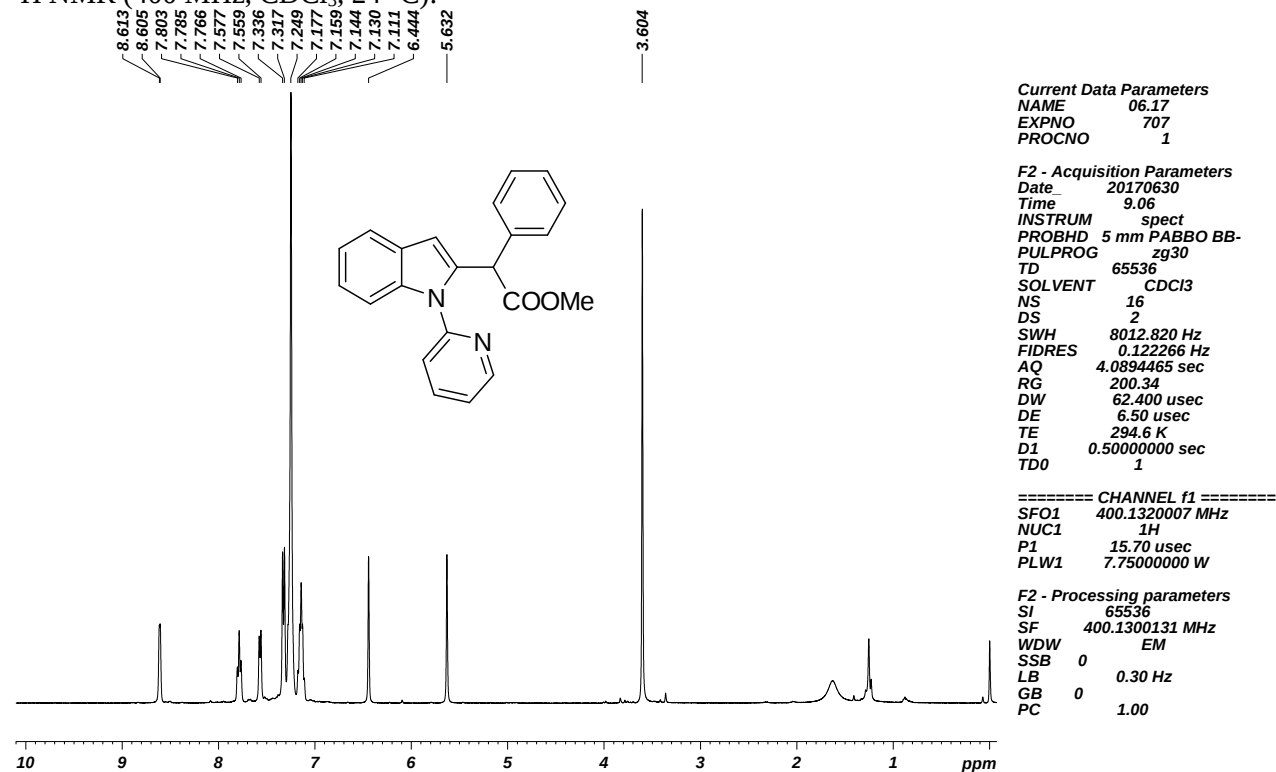
===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

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

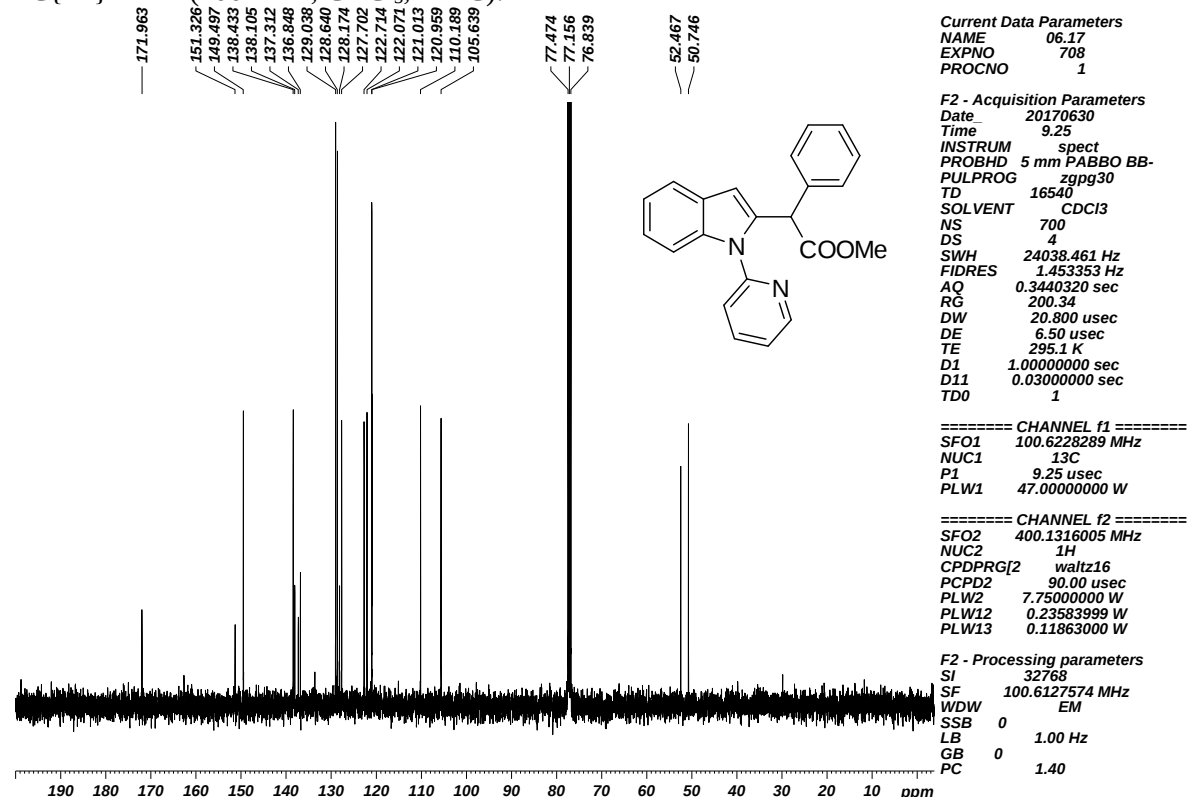
7. Spectral data of synthesized compounds

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

^1H NMR (400 MHz, CDCl_3 , 24 °C):

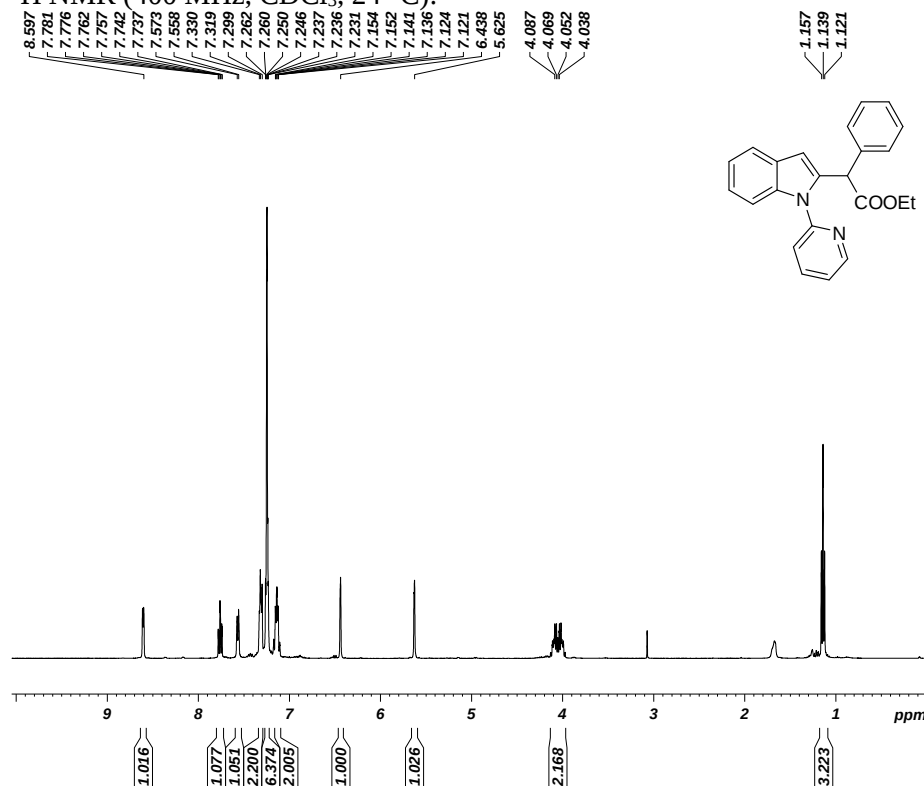


$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C):



Ethyl 2-phenyl-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3b):

¹H NMR (400 MHz, CDCl₃, 24 °C):



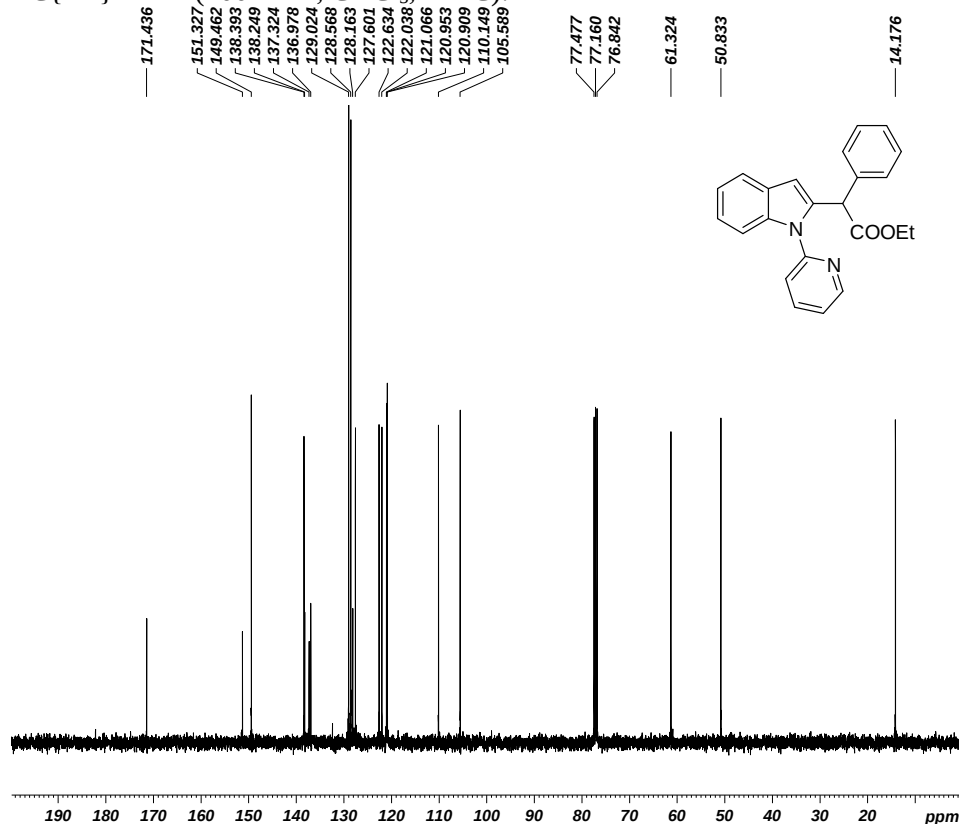
Current Data Parameters
NAME spa41115
EXPNO 196
PROCNO 1

F2 - Acquisition Parameters
Date 20151107
Time 21.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 95.73
DW 62.400 usec
DE 6.50 usec
TE 293.4 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300188 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



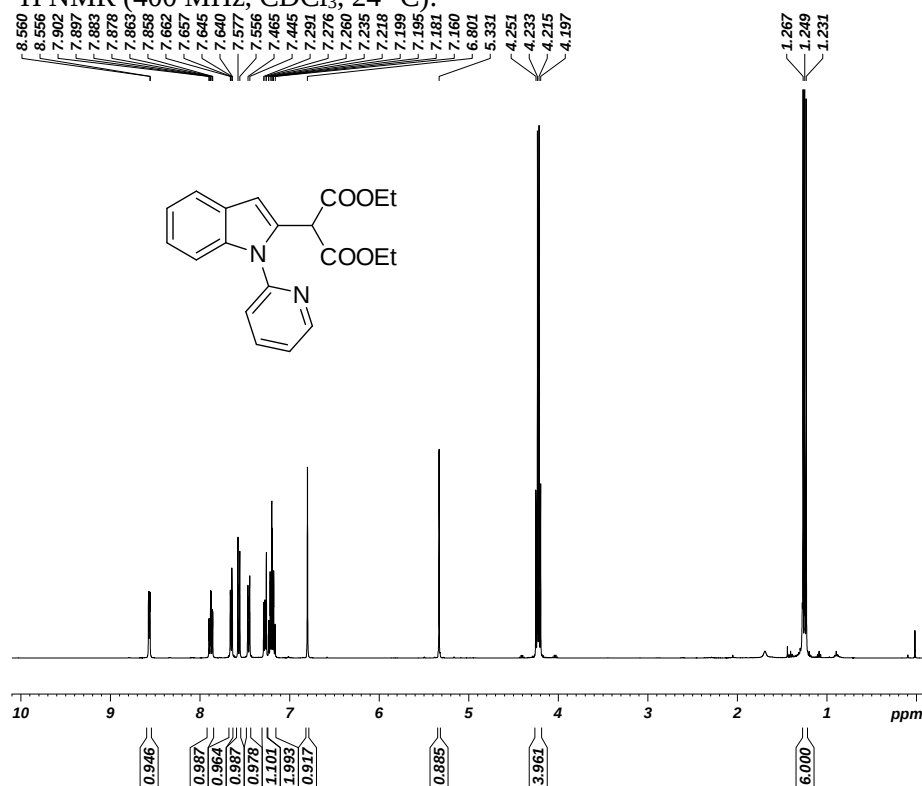
Current Data Parameters
NAME spa41115
EXPNO 197
PROCNO 1

F2 - Acquisition Parameters
Date 20151107
Time 21.41
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 294.1 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W

F2 - Processing parameters
SI 32768
SF 100.6127617 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Diethyl 2-(1-(pyridin-2-yl)-1H-indol-2-yl)malonate (3c):

¹H NMR (400 MHz, CDCl₃, 24 °C):



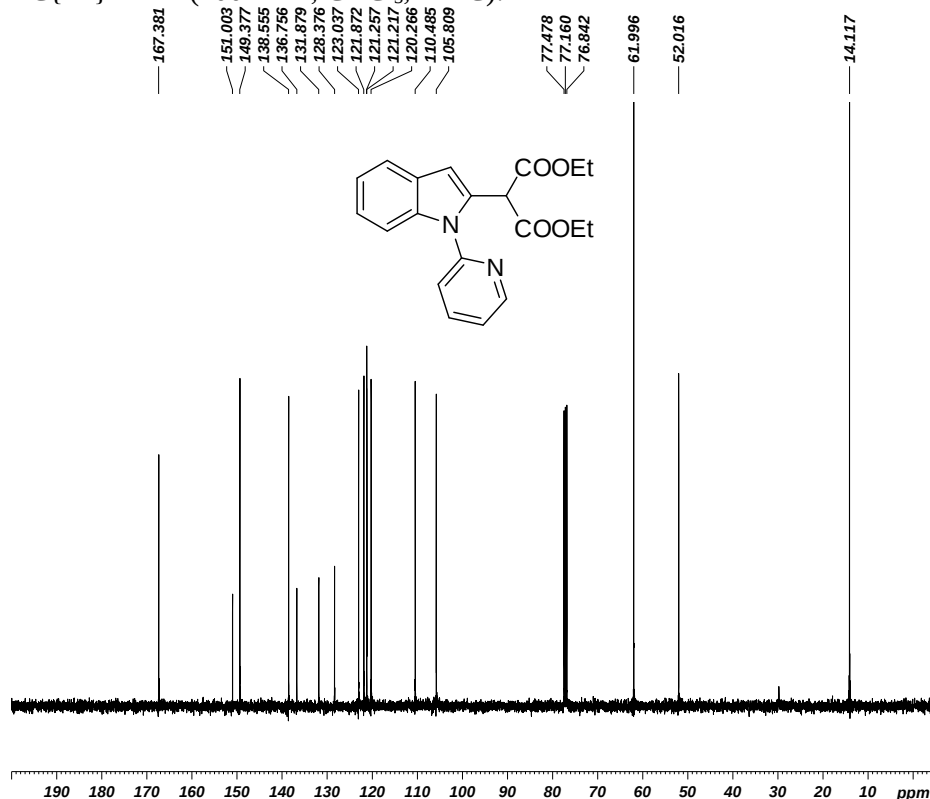
Current Data Parameters
NAME 07.16
EXPNO 77
PROCNO 1

F2 - Acquisition Parameters
Date 20160704
Time 9.19
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 88.51
DW 62.400 usec
DE 6.50 usec
TE 297.7 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 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 07.16
EXPNO 78
PROCNO 1

F2 - Acquisition Parameters
Date 20160704
Time 9.25
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 298.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

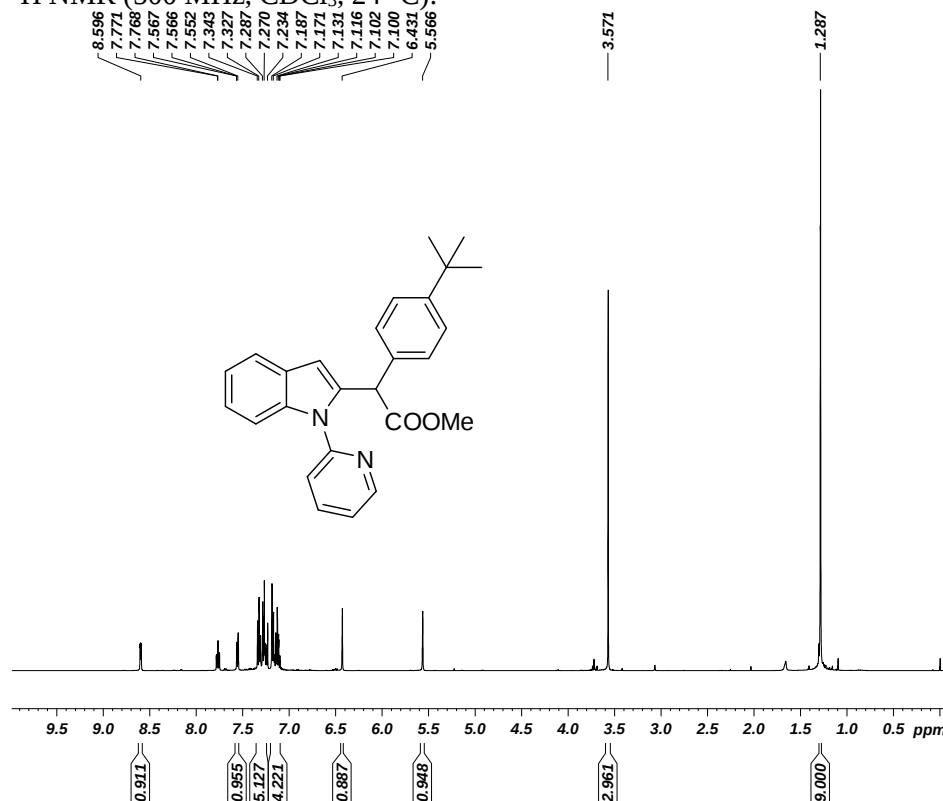
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127615 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(4-(tert-butyl)phenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3d):

^1H NMR (500 MHz, CDCl_3 , 24 °C):



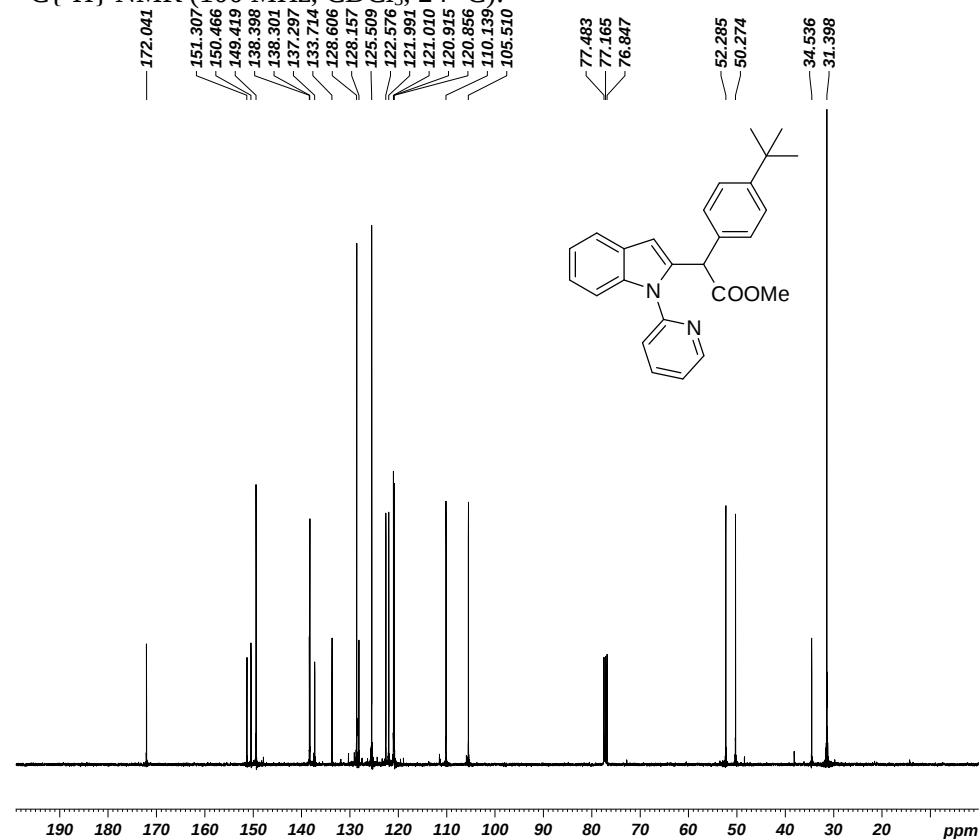
Current Data Parameters
NAME 11.15
EXPNO 188
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151127
Time 7.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl_3
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 55.6
DW 50.000 usec
DE 6.50 usec
TE 294.3 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 500.1500346 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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



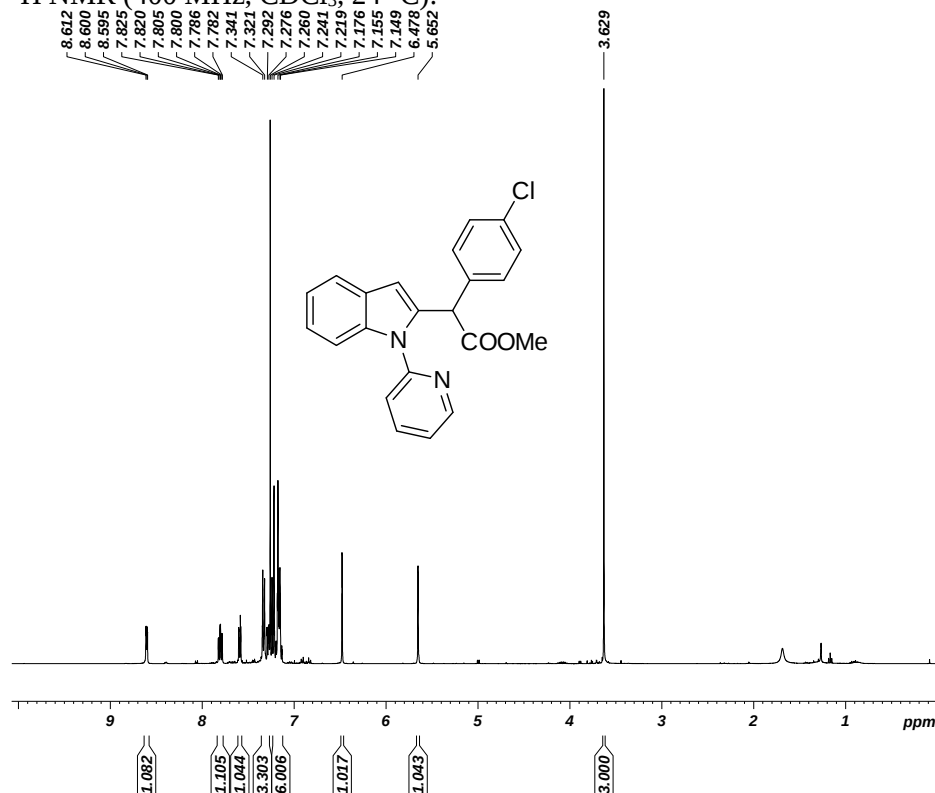
Current Data Parameters
NAME spa41115
EXPNO 411
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151129
Time 8.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl_3
NS 1000
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 299.0 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
SFO1 100.6228289 MHz
NUC1 ^{13}C
P1 9.25 usec
PLW1 47.00000000 W
SFO2 400.1316005 MHz
NUC2 ^1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(4-chlorophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3e):

¹H NMR (400 MHz, CDCl₃, 24 °C):



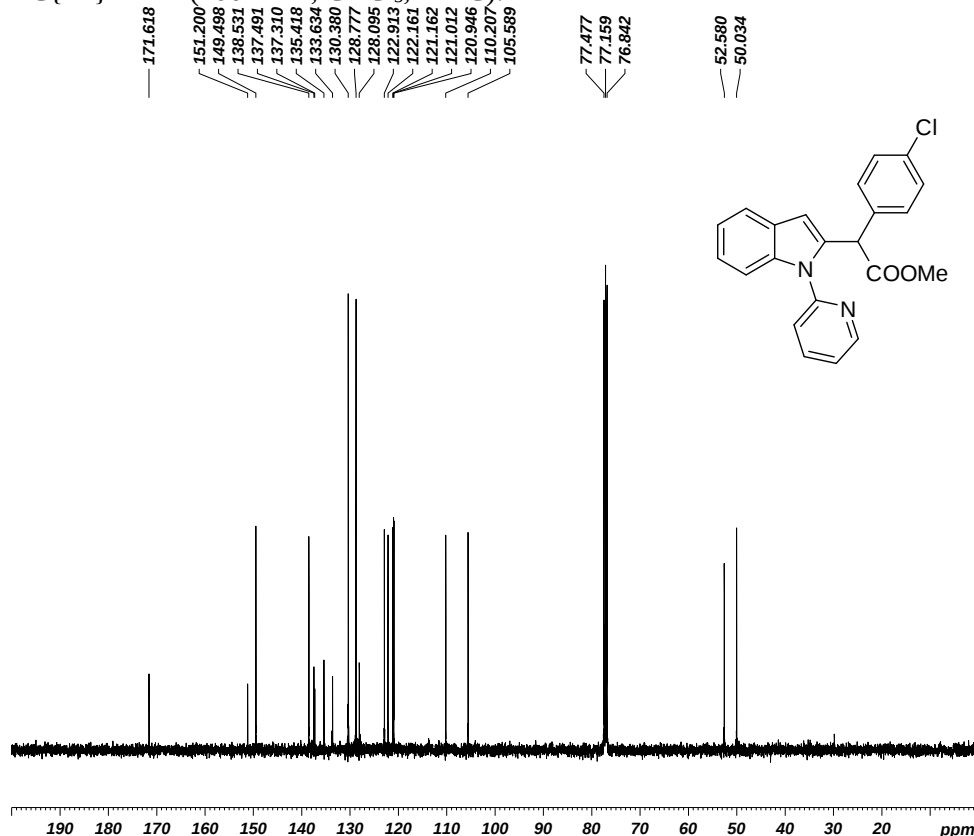
Current Data Parameters
NAME 12.15
EXPNO 369
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151221
Time 1.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 153.13
DW 62.400 usec
DE 6.50 usec
TE 296.7 K
D1 0.50000000 sec
TD0 1

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

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

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



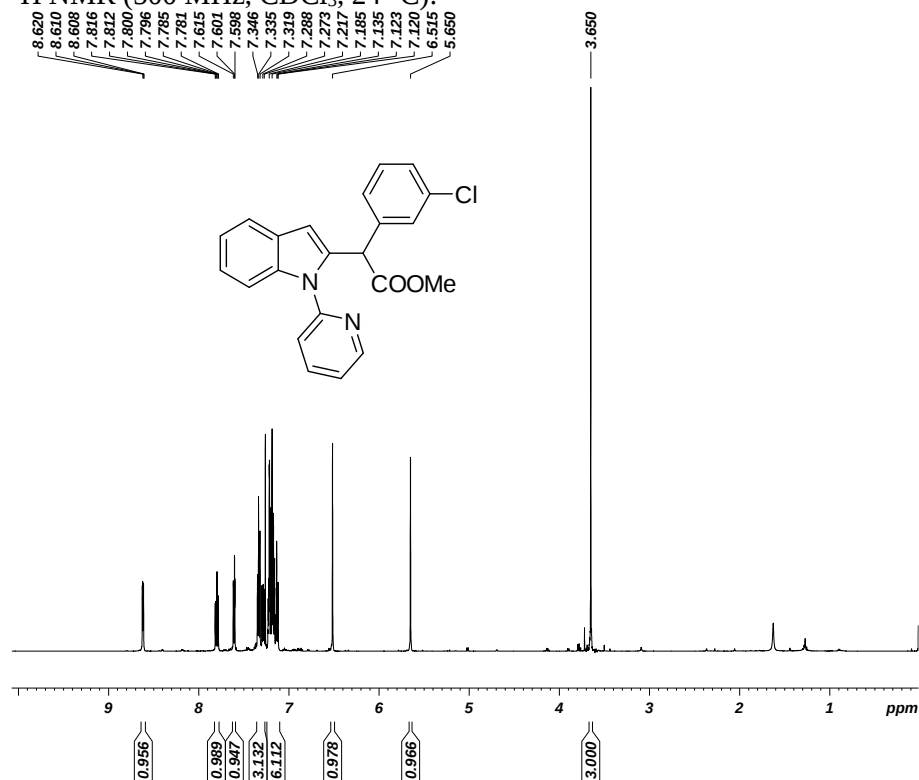
Current Data Parameters
NAME spa41215
EXPNO 370
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151221
Time 1.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 512
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 297.3 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W

F2 - Processing parameters
SI 32768
SF 100.6127573 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(3-chlorophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3f):

¹H NMR (500 MHz, CDCl₃, 24 °C):



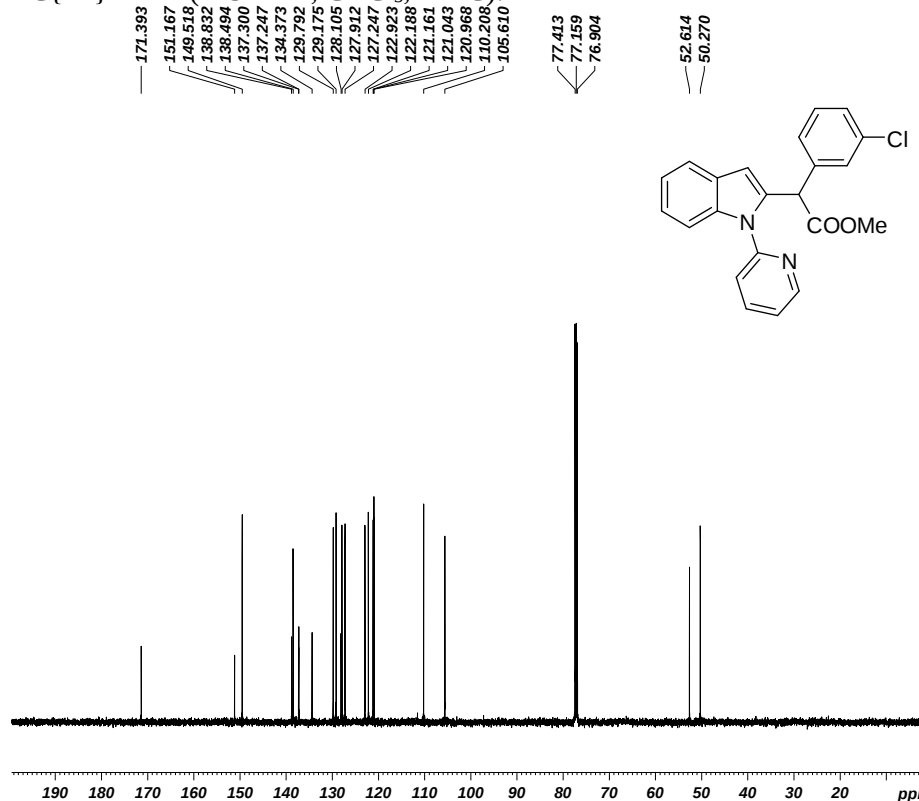
Current Data Parameters
NAME 01.16
EXPNO 227
PROCNO 1

F2 - Acquisition Parameters
Date 20160114
Time 14.18
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 297.9 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 500.1500220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (125 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME spa50116
EXPNO 228
PROCNO 1

F2 - Acquisition Parameters
Date 20160114
Time 14.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 1.453218 Hz
AQ 0.3440640 sec
RG 202.34
DW 16.800 usec
DE 6.50 usec
TE 298.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

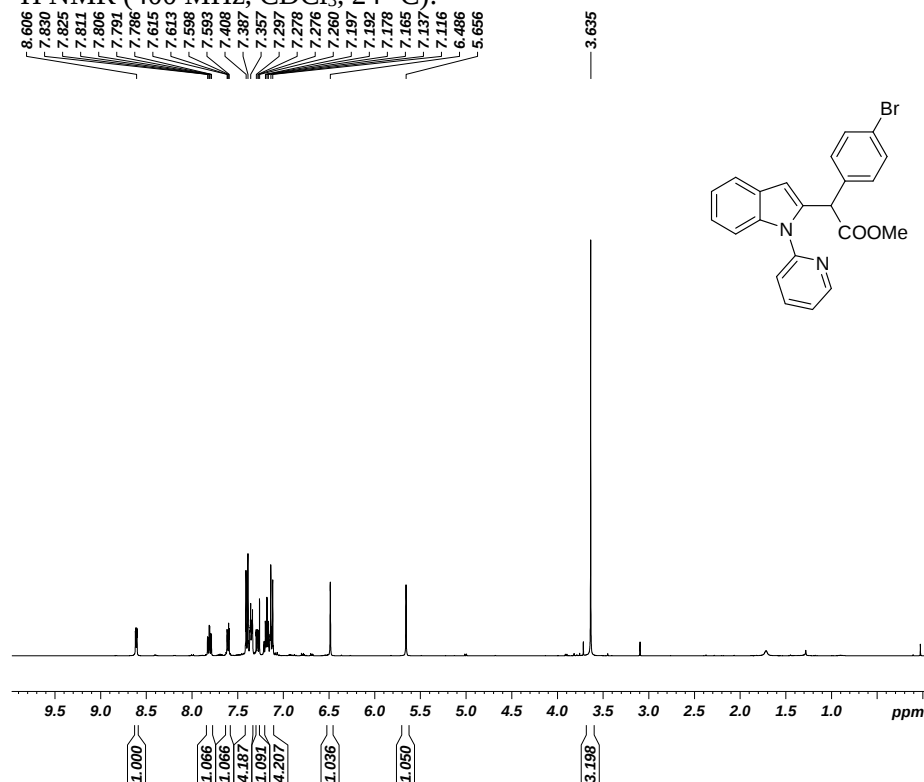
===== CHANNEL f1 =====
SFO1 125.7753932 MHz
NUC1 13C
P1 9.63 usec
PLW1 103.00000000 W

===== CHANNEL f2 =====
SFO2 500.1520006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.30000019 W
PLW12 0.33006001 W
PLW13 0.21123999 W

F2 - Processing parameters
SI 32768
SF 125.7628070 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(4-bromophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3g):

¹H NMR (400 MHz, CDCl₃, 24 °C):



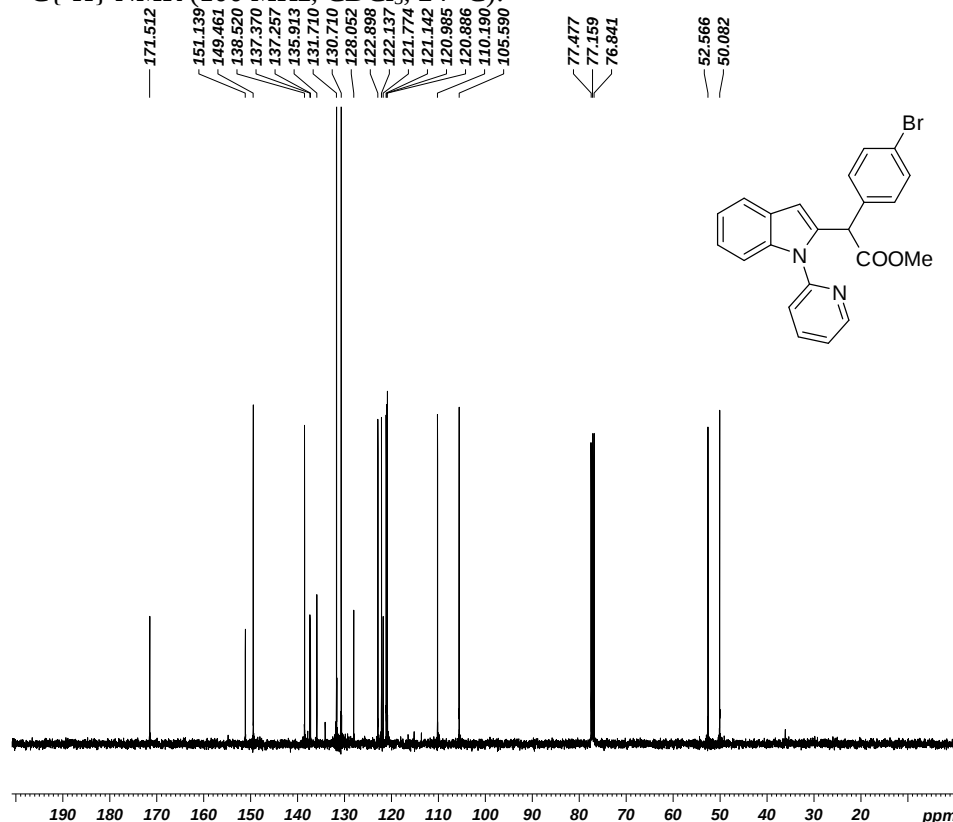
Current Data Parameters
NAME spa41215
EXPNO 133
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151213
Time 1.02
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 95.73
DW 62.400 usec
DE 6.50 usec
TE 290.5 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



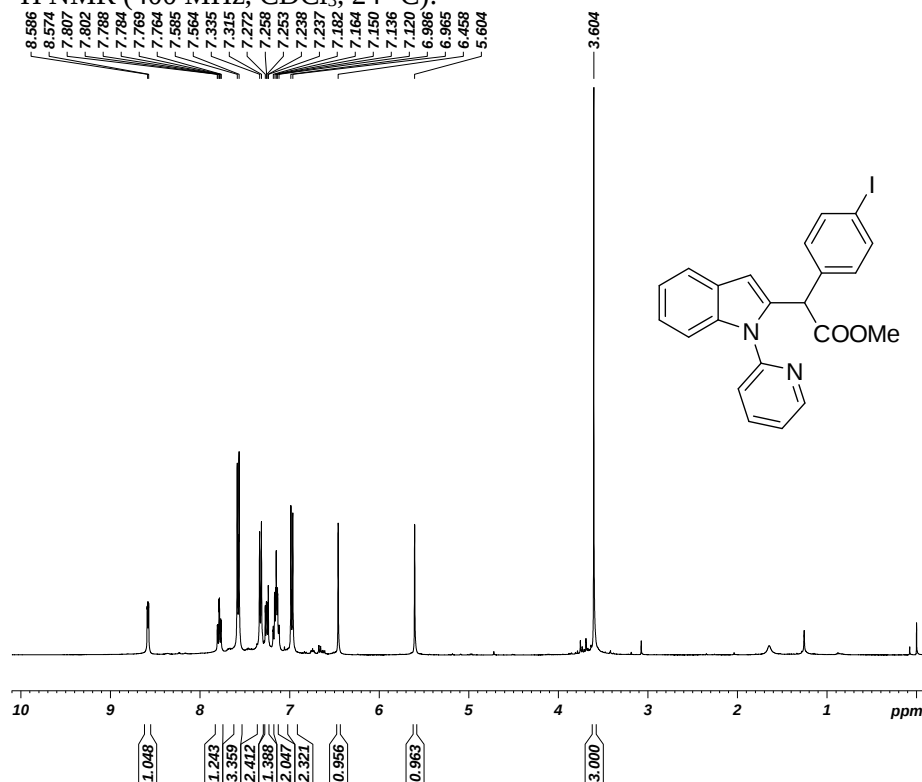
Current Data Parameters
NAME spa41215
EXPNO 144
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151213
Time 13.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 500
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 295.1 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W

F2 - Processing parameters
SI 32768
SF 100.6127623 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(4-iodophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3h):

^1H NMR (400 MHz, CDCl_3 , 24 °C):



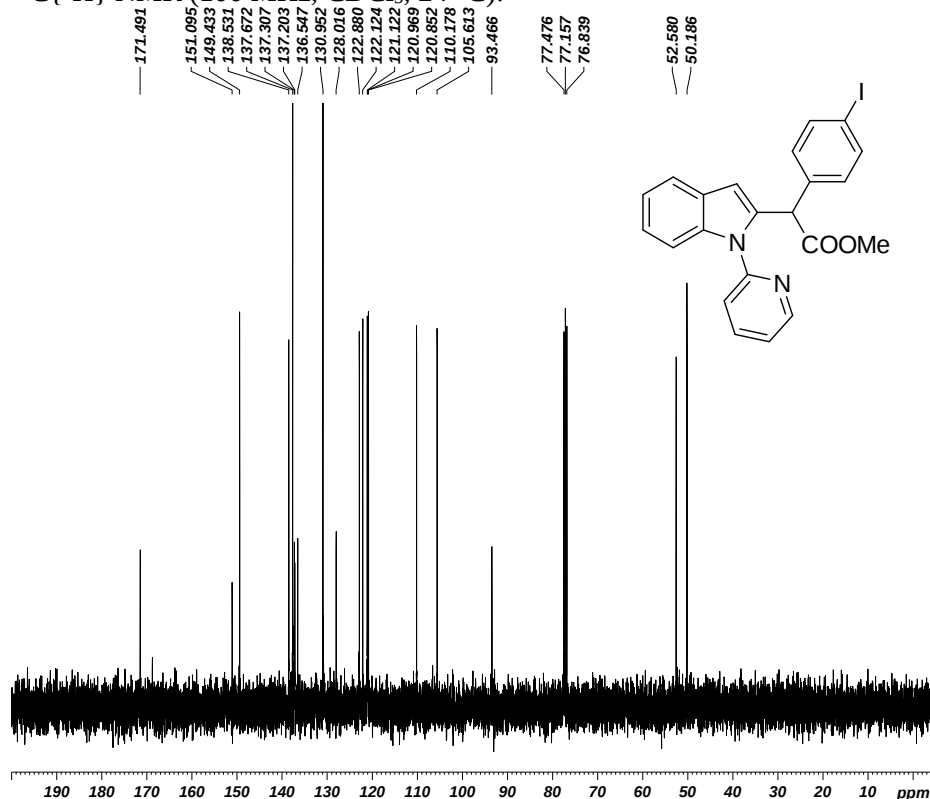
Current Data Parameters
NAME 12.15
EXPNO 38
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151210
Time 8.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 16
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 295.1 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ^1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.132007 MHz

F2 - Processing parameters
SI 65536
SF 400.1300183 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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



Current Data Parameters
NAME 12.15
EXPNO 126
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151212
Time 14.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl_3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 6.15
DW 20.800 usec
DE 6.50 usec
TE 292.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

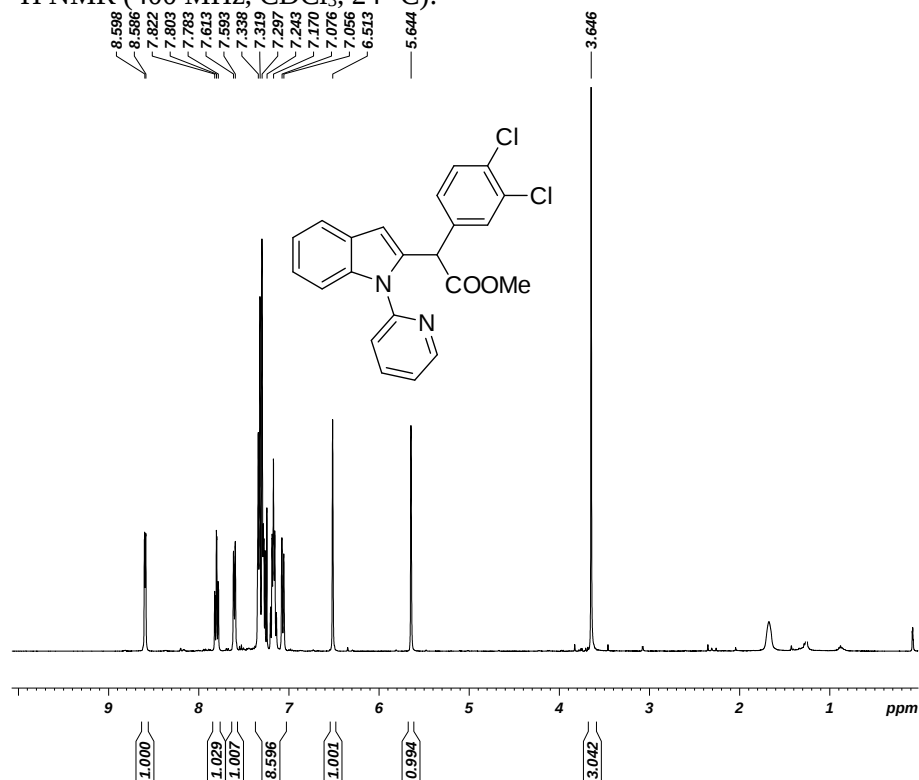
===== CHANNEL f1 =====
NUC1 ^{13}C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ^1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127649 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(3,4-dichlorophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3i):

^1H NMR (400 MHz, CDCl_3 , 24 °C):



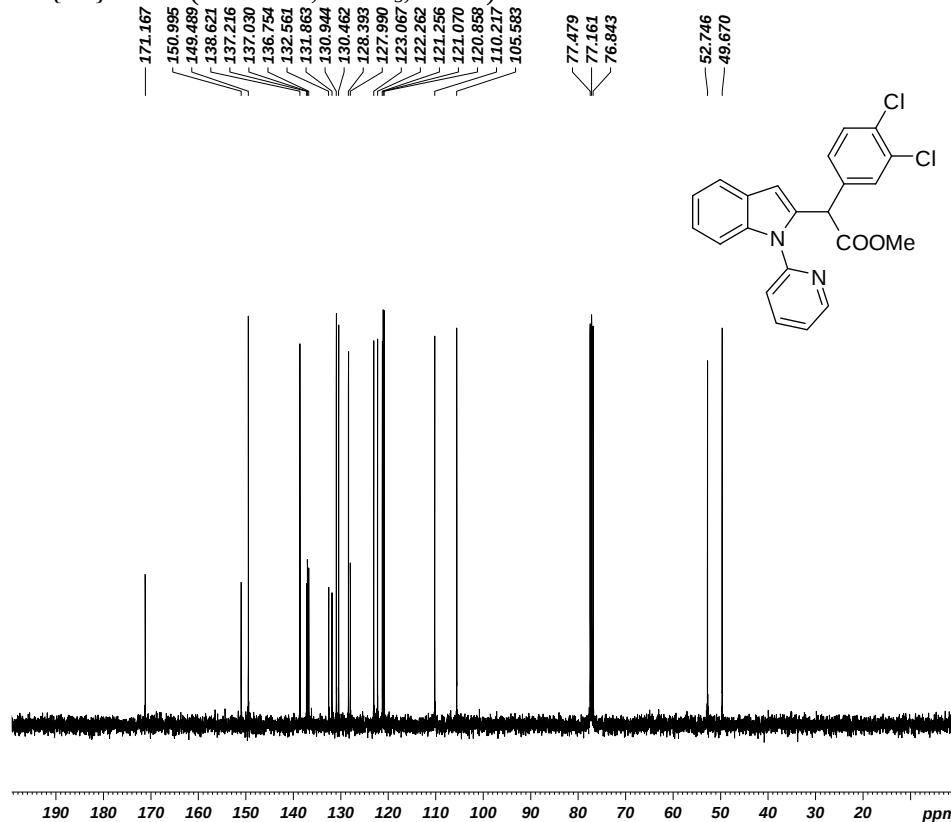
Current Data Parameters
NAME 12.15
EXPNO 327
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151219
Time 0.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl_3
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 291.6 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300158 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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



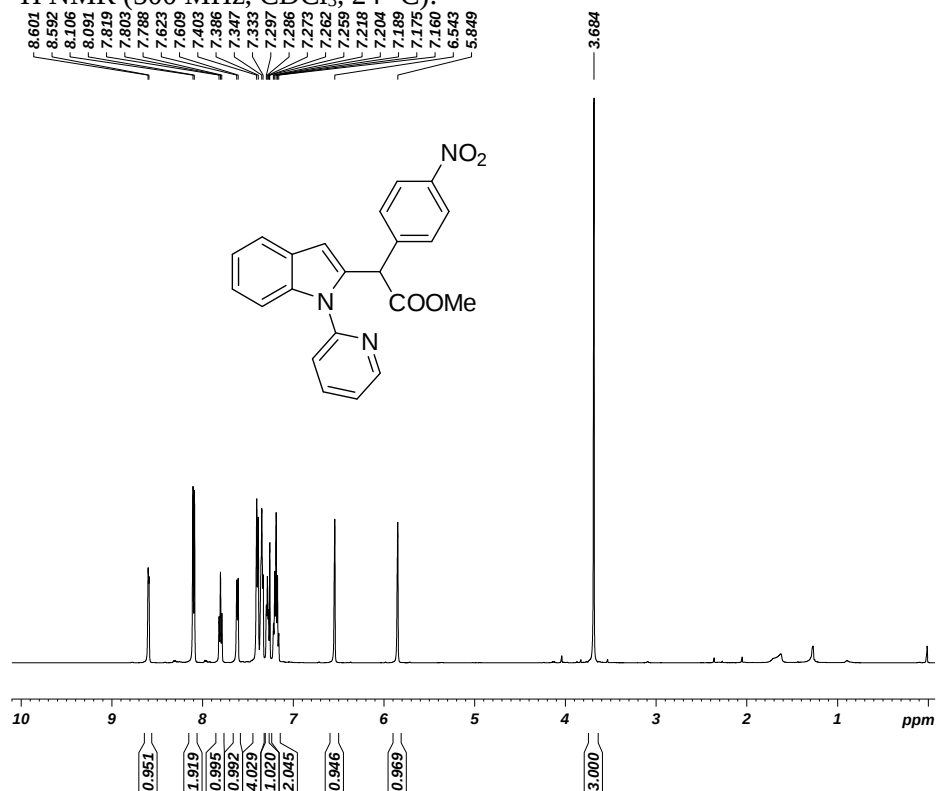
Current Data Parameters
NAME spa41215
EXPNO 328
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151219
Time 0.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl_3
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 292.1 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
SFO1 100.6228289 MHz
NUC1 ^{13}C
P1 9.25 usec
PLW1 47.00000000 W
SFO2 400.1316005 MHz
NUC2 ^1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W

F2 - Processing parameters
SI 32768
SF 100.6127614 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(4-nitrophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3j):

¹H NMR (500 MHz, CDCl₃, 24 °C):



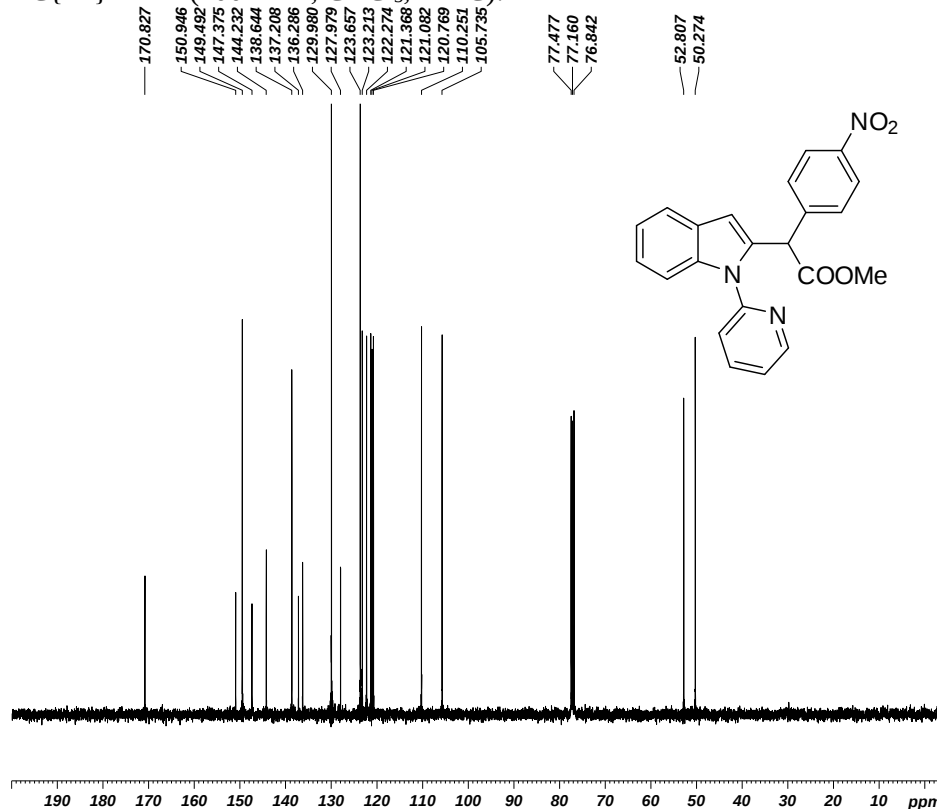
Current Data Parameters
NAME 01.16
EXPNO 229
PROCNO 1

F2 - Acquisition Parameters
Date 20160114
Time 14.45
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 79.04
DW 50.000 usec
DE 6.50 usec
TE 298.3 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 500.1500219 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 01.16
EXPNO 206
PROCNO 1

F2 - Acquisition Parameters
Date 20160119
Time 13.36
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 299.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

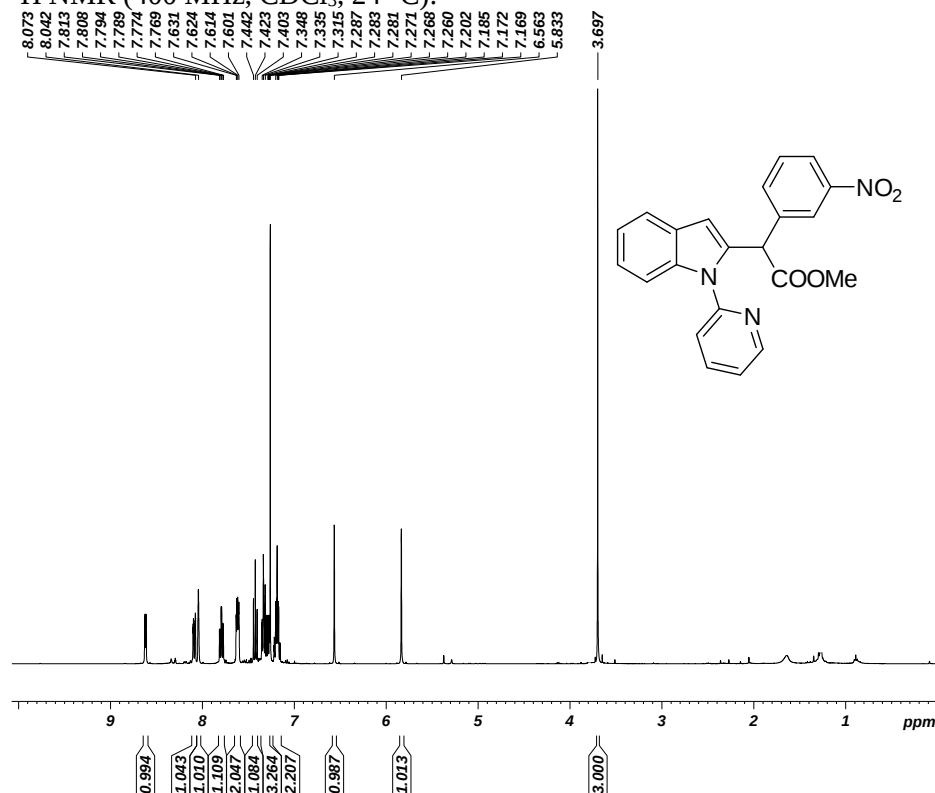
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127622 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(3-nitrophenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3k):

¹H NMR (400 MHz, CDCl₃, 24 °C):



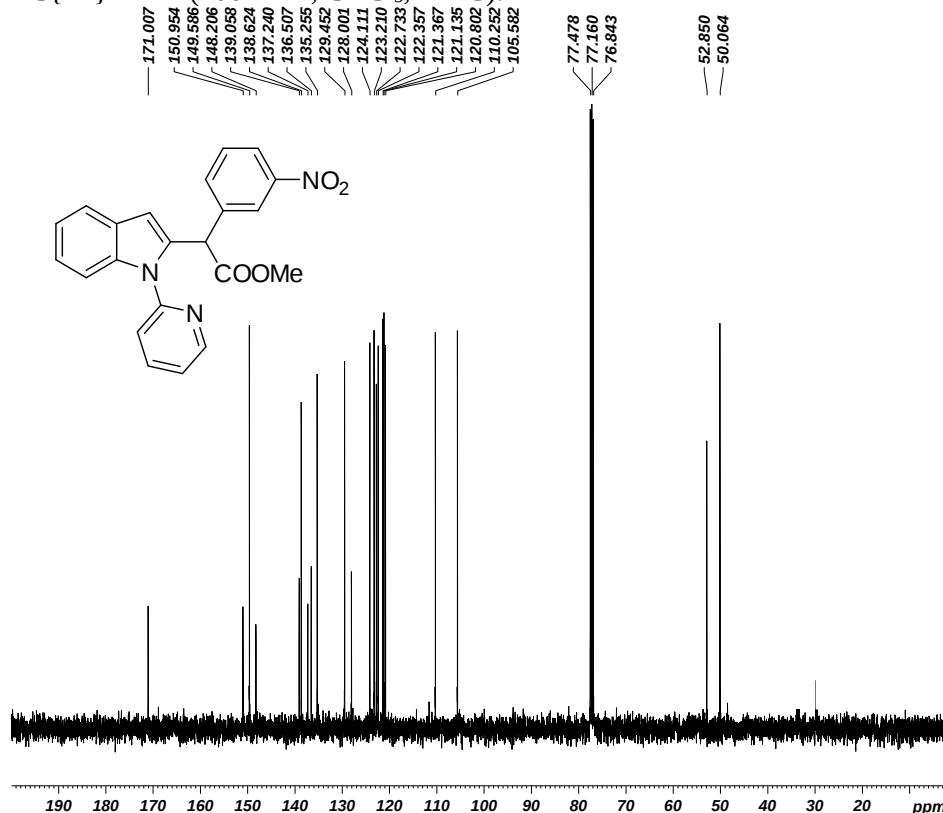
Current Data Parameters
NAME 10.15
EXPNO 658
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151030
Time 19.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 124.58
DW 62.400 usec
DE 6.50 usec
TE 294.9 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 10.15
EXPNO 674
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151031
Time 8.47
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

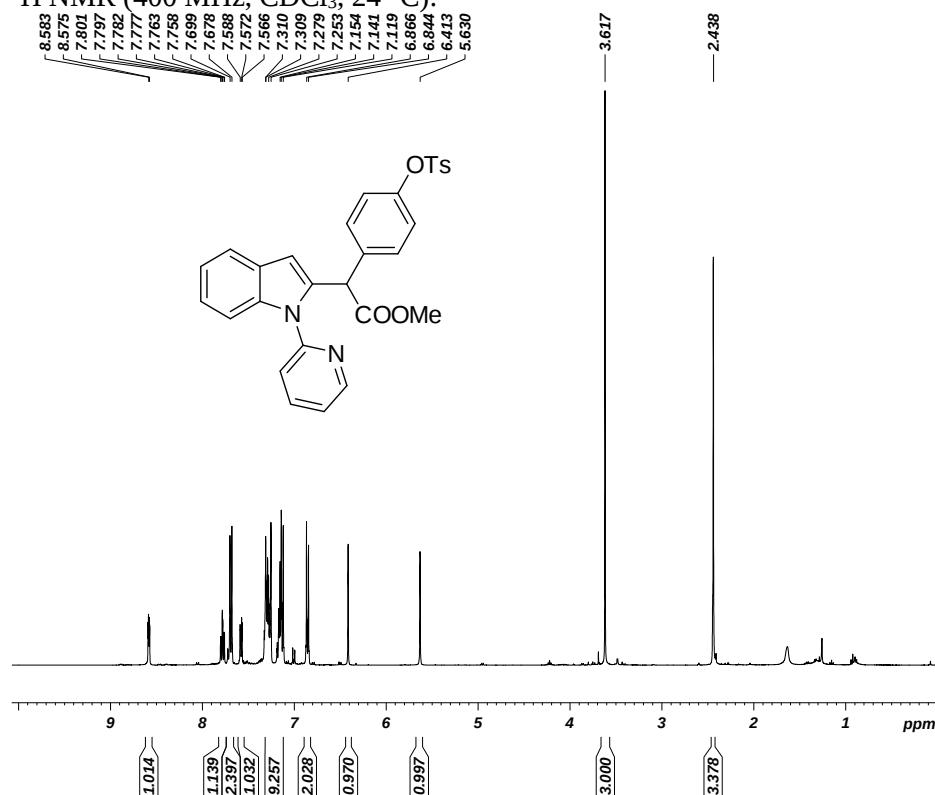
===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127588 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(1-(pyridin-2-yl)-1H-indol-2-yl)-2-(4-(tosyloxy)phenyl)acetate (3l):

¹H NMR (400 MHz, CDCl₃, 24 °C):



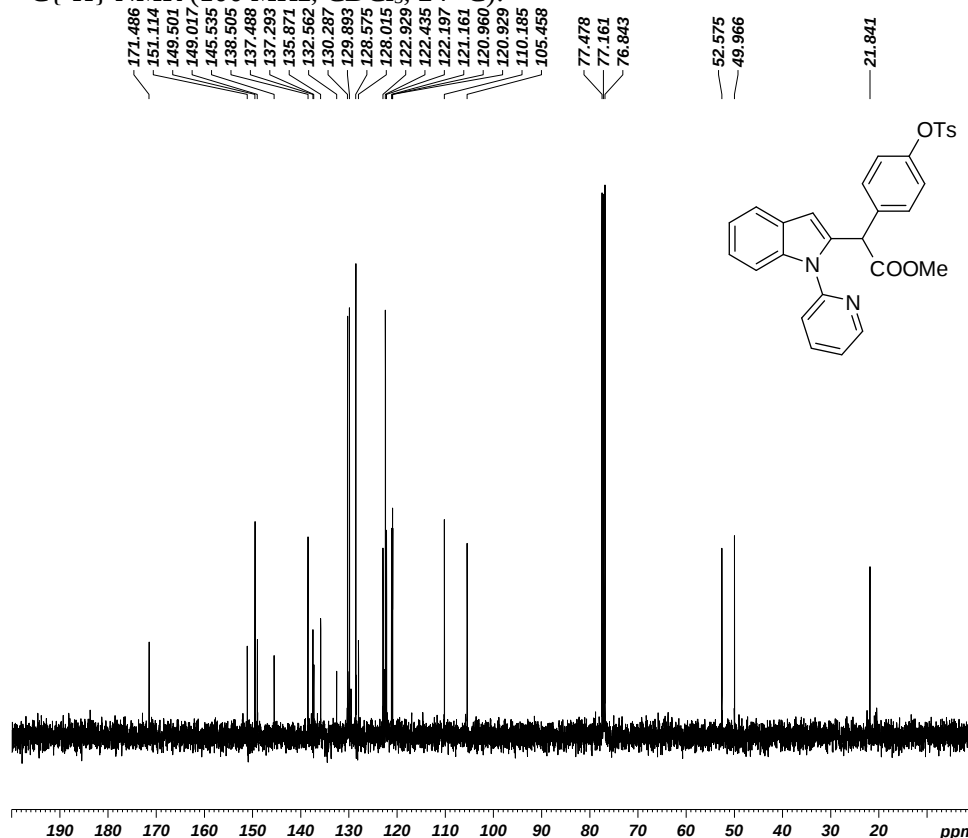
Current Data Parameters
NAME 12.15
EXPNO 438
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151223
Time 11.12
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 297.7 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C {¹H} NMR (100 MHz, CDCl₃, 24 °C):



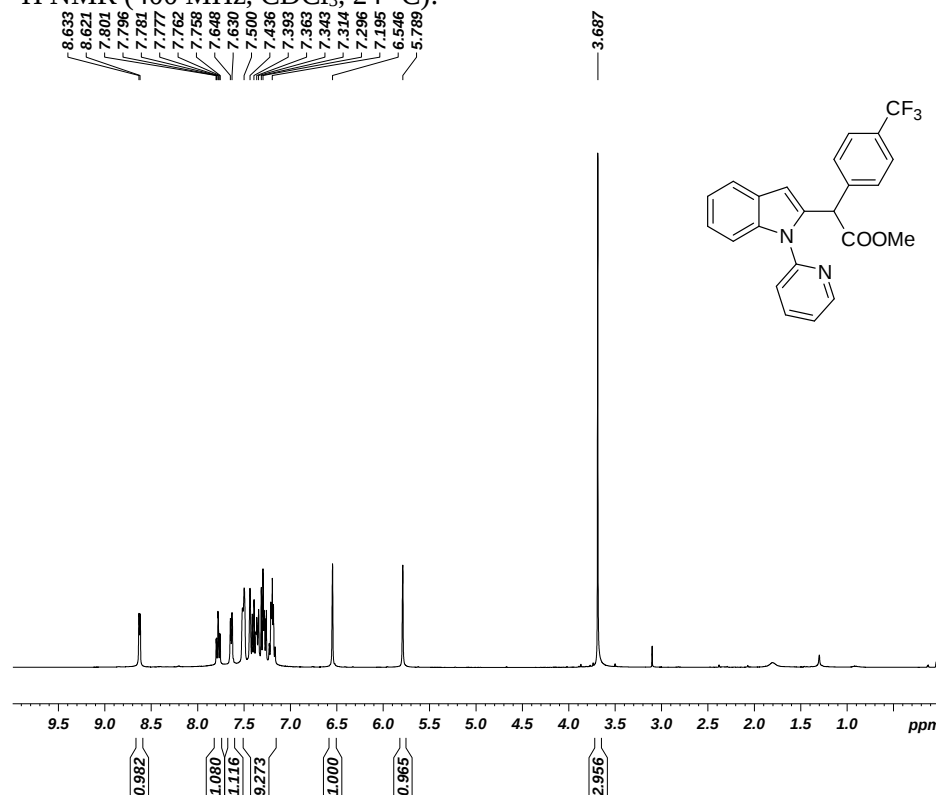
Current Data Parameters
NAME spa41215
EXPNO 439
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151223
Time 11.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 111
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 298.2 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W

F2 - Processing parameters
SI 32768
SF 100.6127584 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(1-(pyridin-2-yl)-1H-indol-2-yl)-2-(4-(trifluoromethyl)phenyl)acetate (3m):

^1H NMR (400 MHz, CDCl_3 , 24 °C):



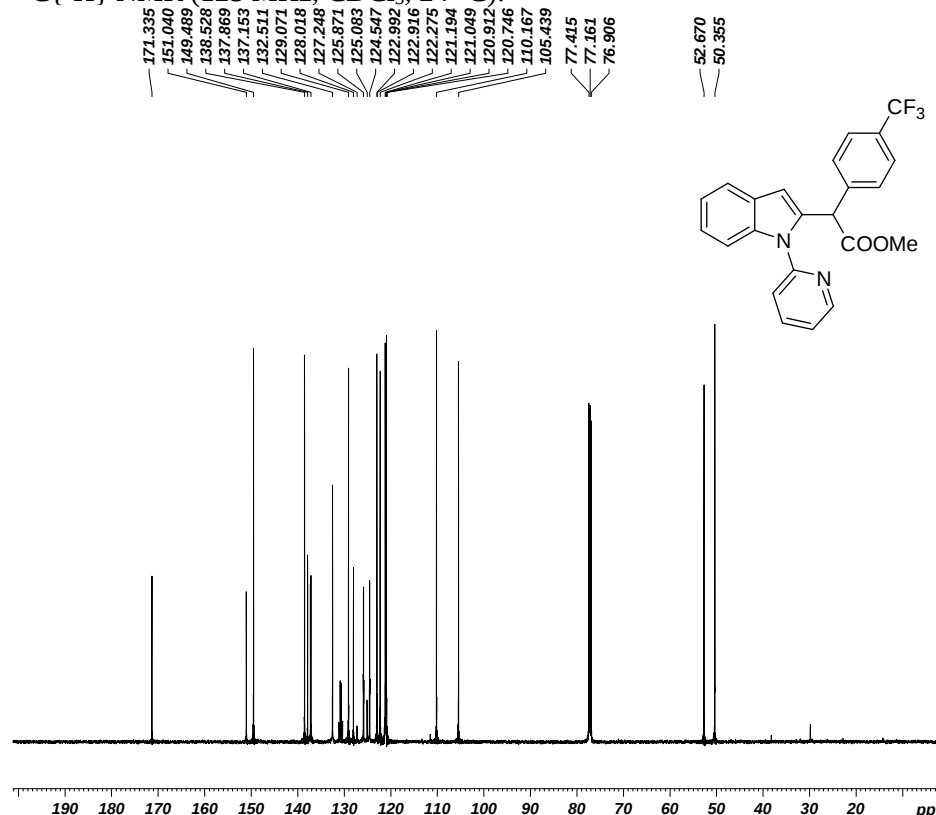
Current Data Parameters
NAME spa40116
EXPNO 78
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160103
Time 8.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 60.89
DW 62.400 usec
DE 6.50 usec
TE 292.1 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 °C):



Current Data Parameters
NAME spa50116
EXPNO 37
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160105
Time 7.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDCl_3
NS 2500
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 293.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

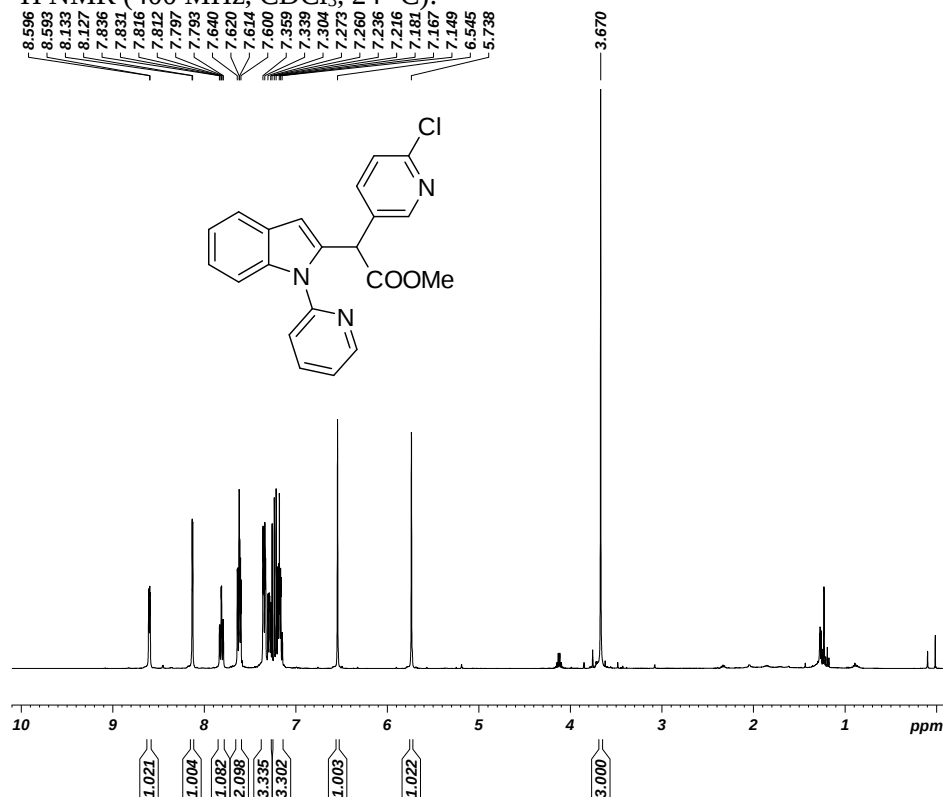
===== CHANNEL f1 =====
SFO1 125.7753932 MHz
NUC1 ^{13}C
P1 9.63 usec
PLW1 103.00000000 W

===== CHANNEL f2 =====
SFO2 500.1520006 MHz
NUC2 ^1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.30000019 W
PLW12 0.33006001 W
PLW13 0.21123999 W

F2 - Processing parameters
SI 32768
SF 125.7628121 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(6-chloropyridin-3-yl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3n):

^1H NMR (400 MHz, CDCl_3 , 24 °C):



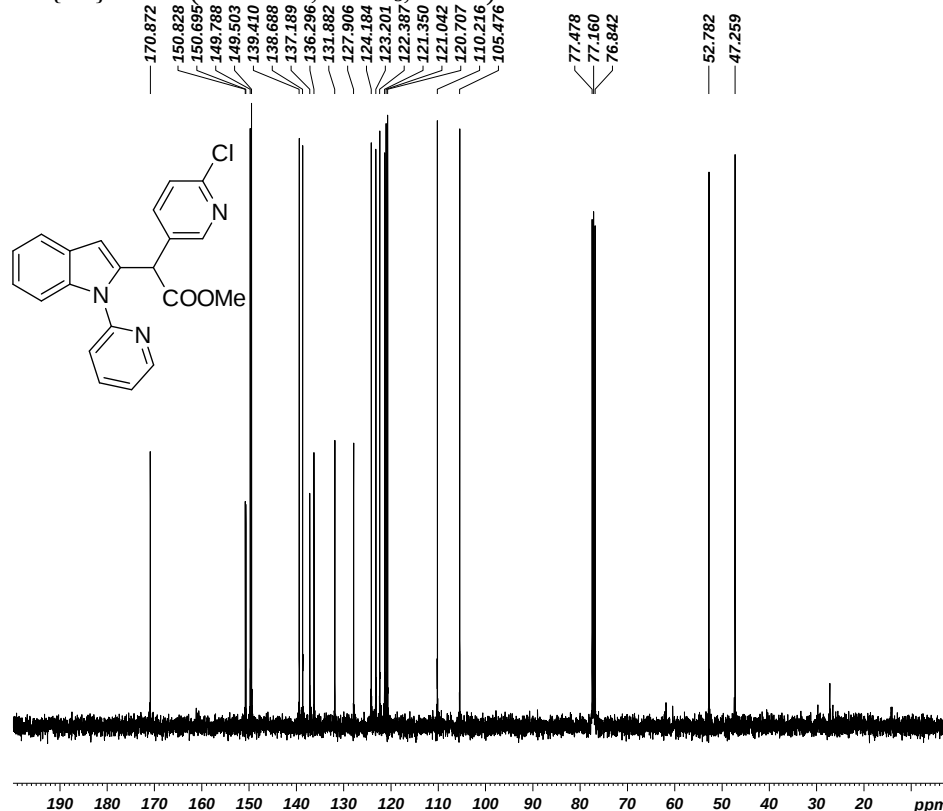
Current Data Parameters
NAME 04.16
EXPNO 233
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160412
Time 8.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 88.51
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 0.50000000 sec
TD0 1

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

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

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



Current Data Parameters
NAME 04.16
EXPNO 234
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160412
Time 8.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl_3
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 299.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

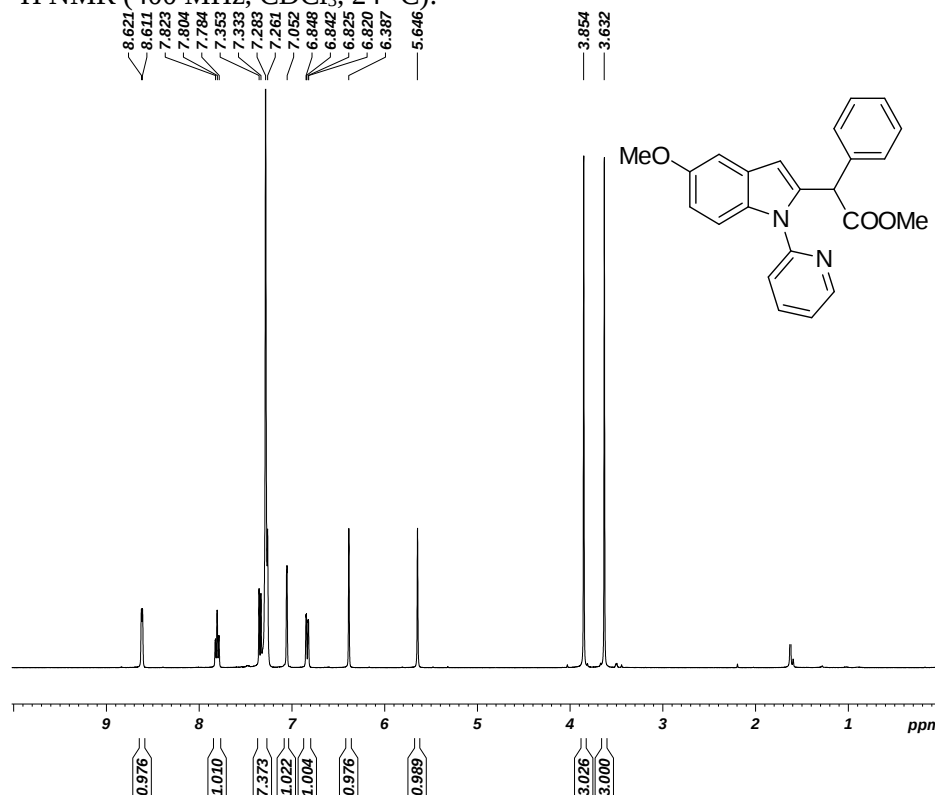
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 ^{13}C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ^1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127641 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(5-methoxy-1-(pyridin-2-yl)-1H-indol-2-yl)-2-phenylacetate (3o):

¹H NMR (400 MHz, CDCl₃, 24 °C):



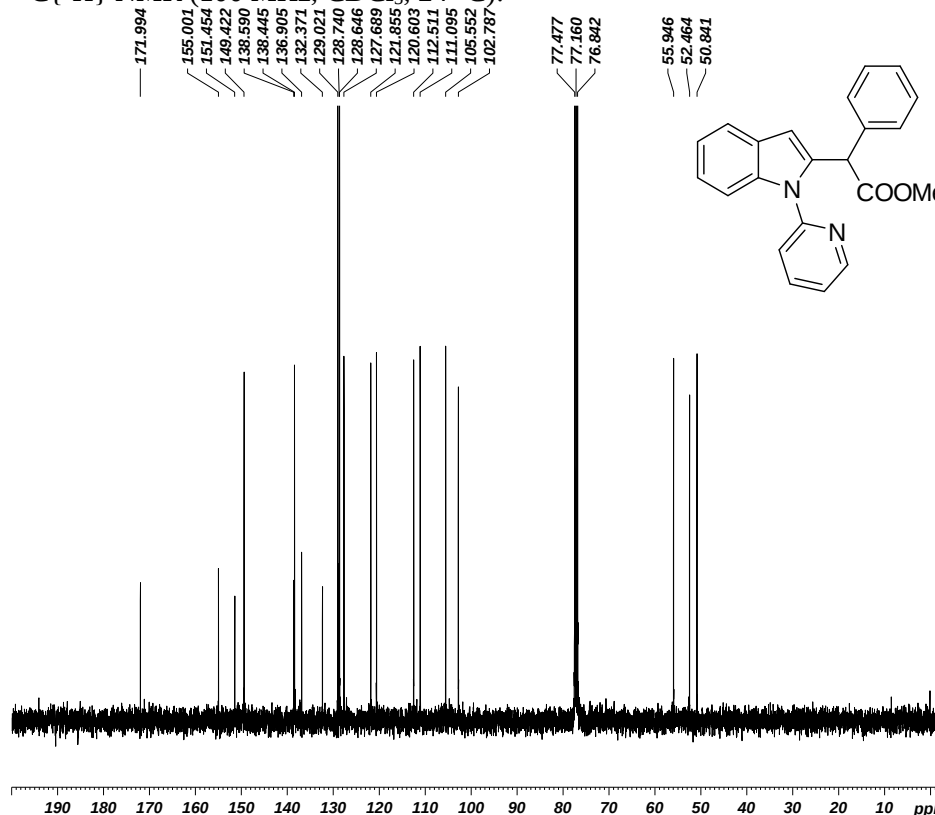
Current Data Parameters
NAME 07.17
EXPNO 237
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170707
Time 7.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 294.0 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300010 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 07.17
EXPNO 104
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170707
Time 6.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 1000
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 294.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

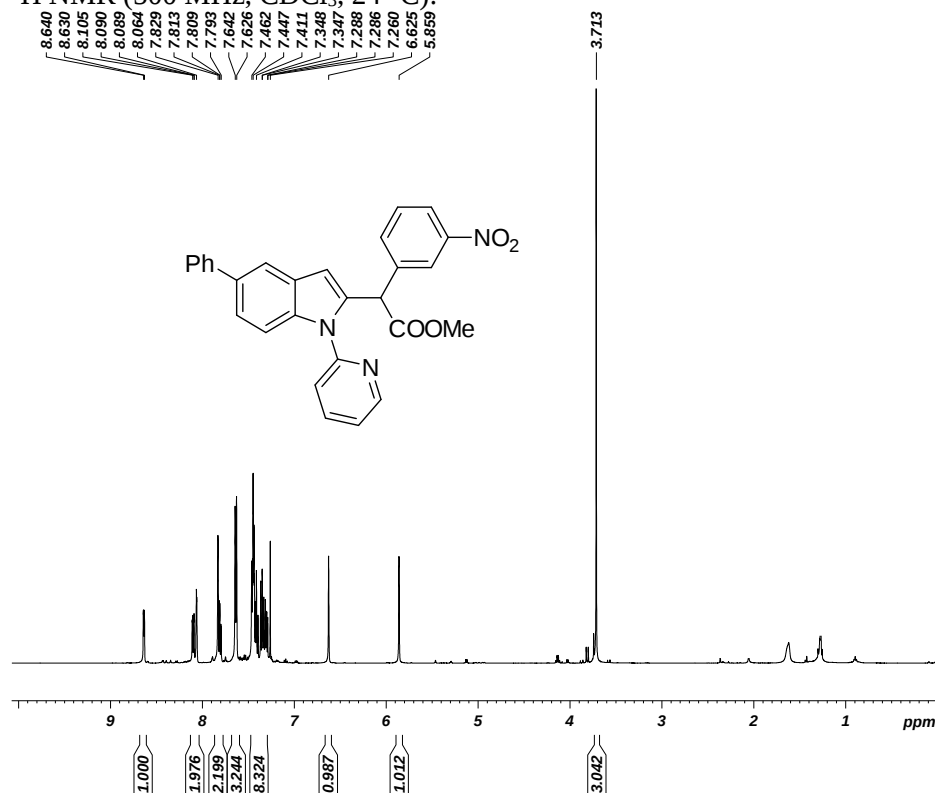
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== 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 100.6127571 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(3-nitrophenyl)-2-(5-phenyl-1-(pyridin-2-yl)-1H-indol-2-yl)acetate (3p):

¹H NMR (500 MHz, CDCl₃, 24 °C):



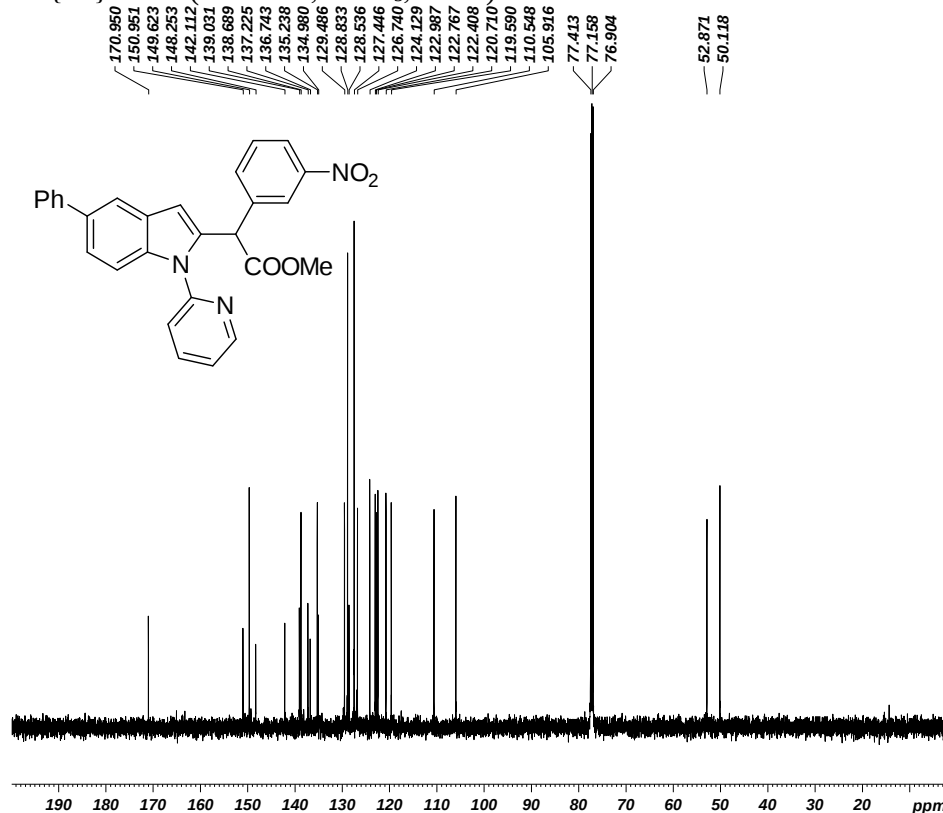
Current Data Parameters
NAME 01.16
EXPNO 111
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160108
Time 11.56
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 299.0 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 500.1500218 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (125 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 01.16
EXPNO 151
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160111
Time 13.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDCl3
NS 200
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 300.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

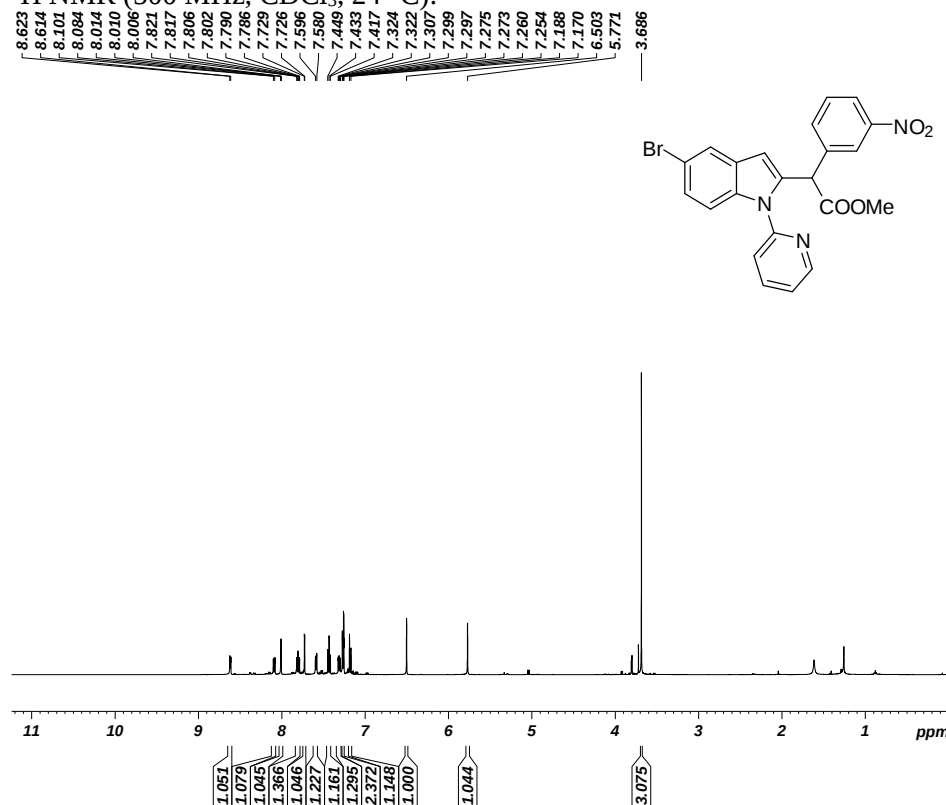
===== CHANNEL f1 =====
SFO1 125.7753932 MHz
NUC1 13C
P1 9.63 usec
PLW1 103.00000000 W

===== CHANNEL f2 =====
SFO2 500.1520006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.30000019 W
PLW12 0.33006001 W
PLW13 0.21123999 W

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

Methyl 2-(5-bromo-1-(pyridin-2-yl)-1H-indol-2-yl)-2-(3-nitrophenyl)acetate (3q):

¹H NMR (500 MHz, CDCl₃, 24 °C):



Current Data Parameters

NAME spa50116
EXPNO 112
PROCNO 1

F2 - Acquisition Parameters

Date_ 20160108
Time 12.03
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 124.08
DW 50.000 usec
DE 6.50 usec
TE 299.0 K
D1 0.50000000 sec
TD0 1

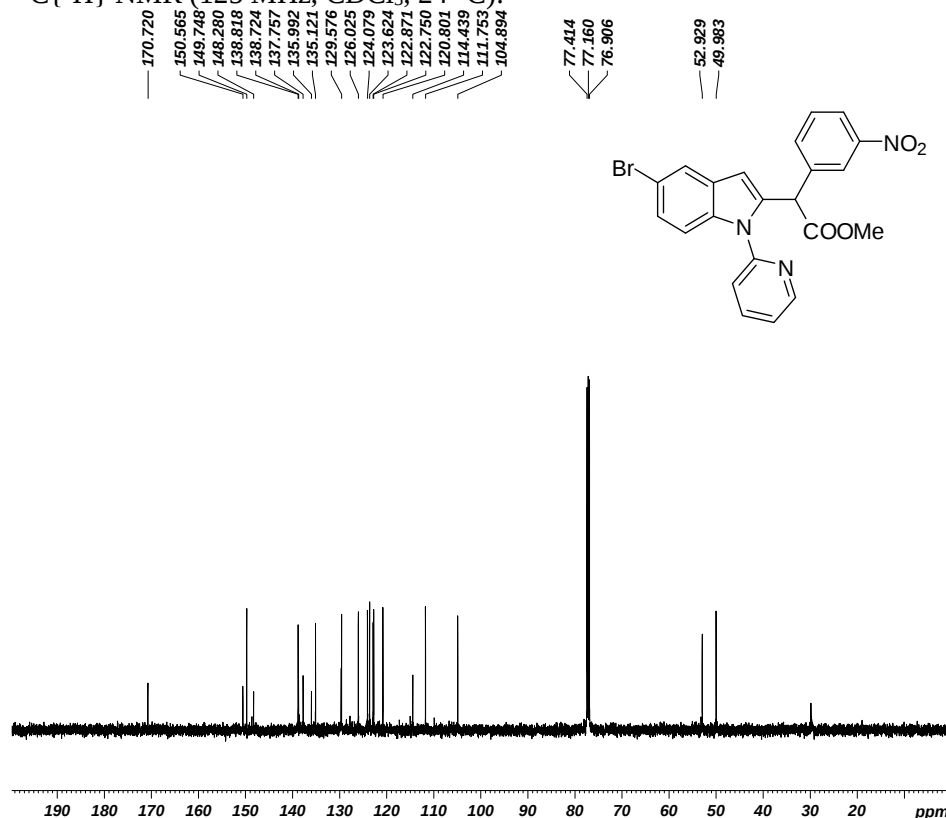
===== CHANNEL f1 =====

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

F2 - Processing parameters

SI 65536
SF 500.1500218 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (125 MHz, CDCl₃, 24 °C):



Current Data Parameters

NAME spa50116
EXPNO 149
PROCNO 1

F2 - Acquisition Parameters

Date_ 20160111
Time 13.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDCl3
NS 200
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 300.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====

SFO1 125.7753932 MHz
NUC1 13C
P1 9.63 usec
PLW1 103.00000000 W

===== CHANNEL f2 =====

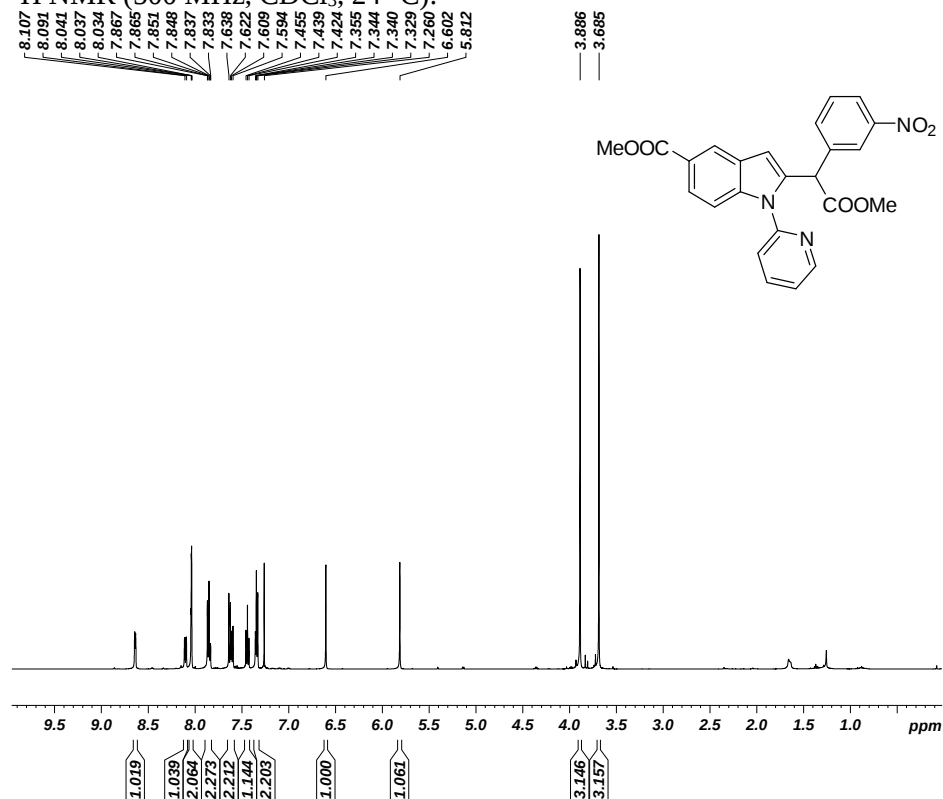
SFO2 500.1520006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.30000019 W
PLW12 0.33006001 W
PLW13 0.21123999 W

F2 - Processing parameters

SI 32768
SF 125.7628053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(2-methoxy-1-(3-nitrophenyl)-2-oxoethyl)-1-(pyridin-2-yl)-1H-indole-5-carboxylate (3r):

¹H NMR (500 MHz, CDCl₃, 24 °C):



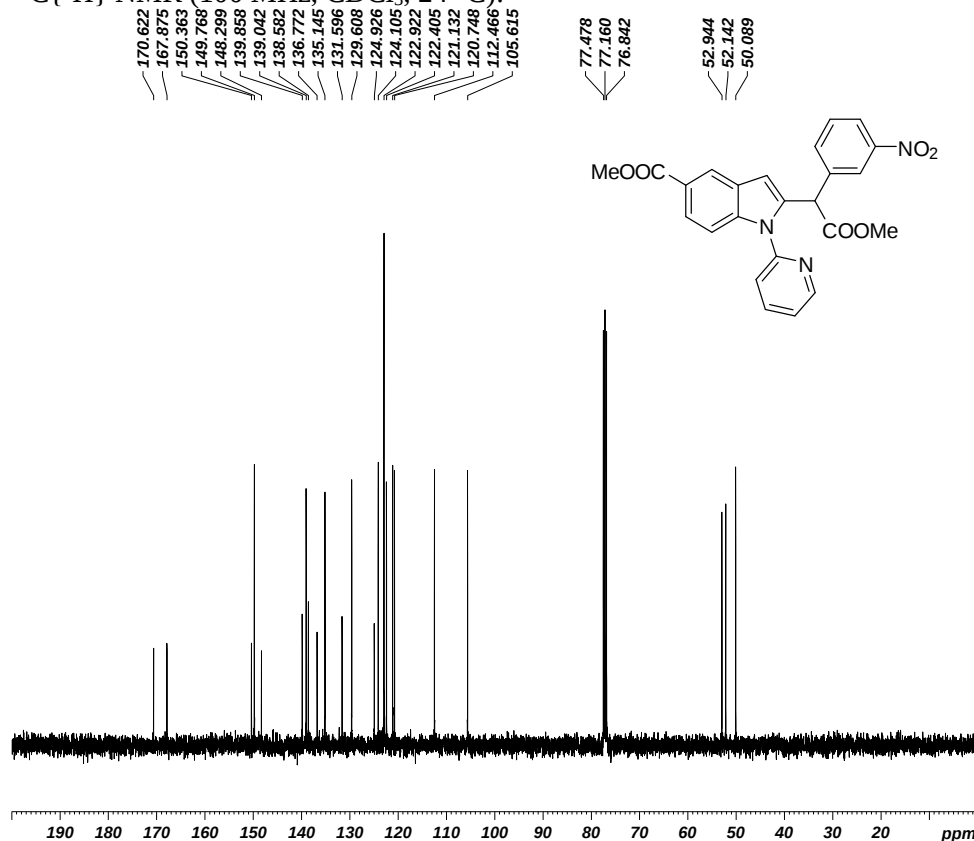
Current Data Parameters
NAME spa50116
EXPNO 203
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160113
Time 15.20
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 299.1 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 500.1500218 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



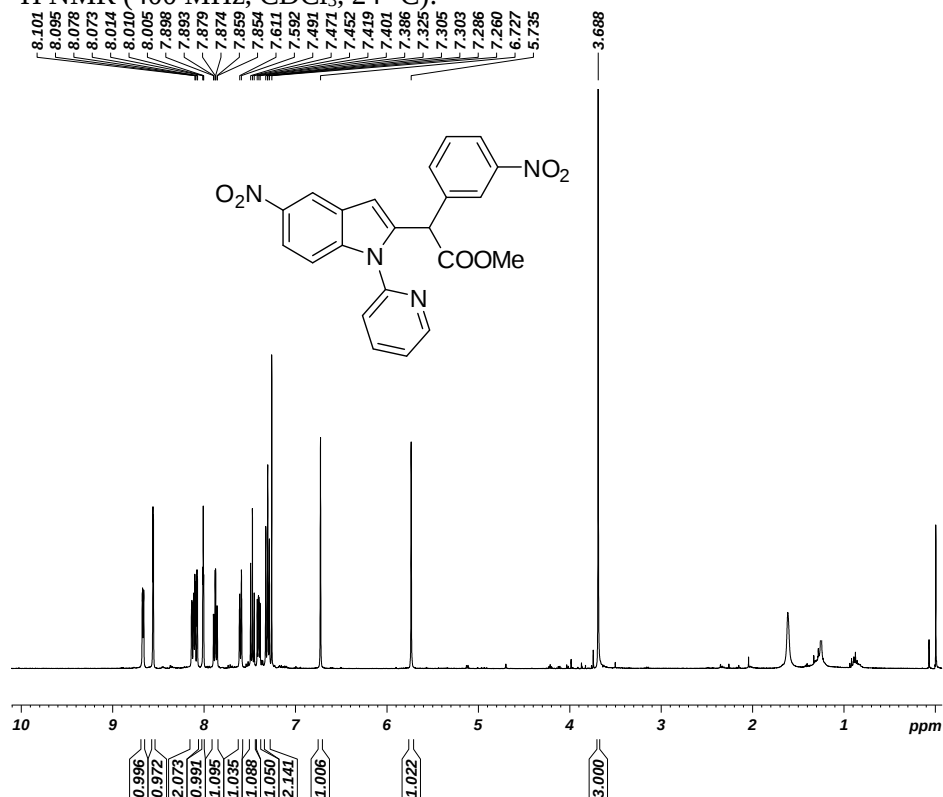
Current Data Parameters
NAME spa40116
EXPNO 127
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160115
Time 8.38
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 298.0 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W

F2 - Processing parameters
SI 32768
SF 100.6127574 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(5-nitro-1-(pyridin-2-yl)-1H-indol-2-yl)-2-(4-nitrophenyl)acetate (3s):

¹H NMR (400 MHz, CDCl₃, 24 °C):



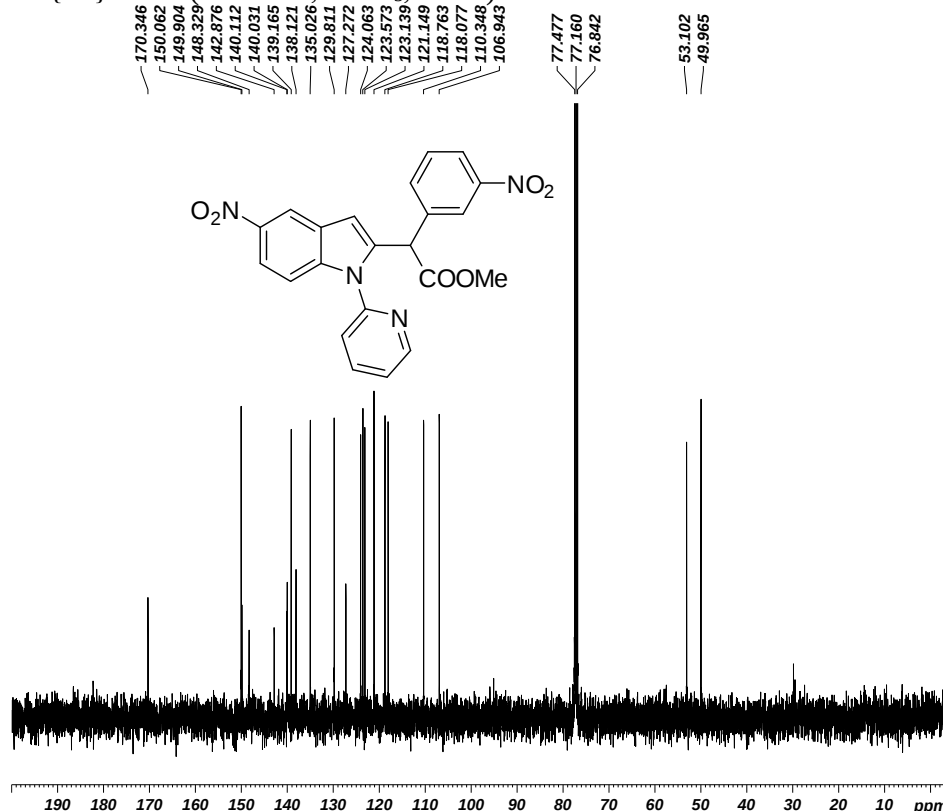
Current Data Parameters
NAME 01.16
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160101
Time 1.42
INSTRUM spect
PROBHD 5 mm PABBO BB-PULPROG
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 292.7 K
D1 0.50000000 sec
TD0 1

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

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

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 01.16
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160101
Time 13.57
INSTRUM spect
PROBHD 5 mm PABBO BB-PULPROG
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 293.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

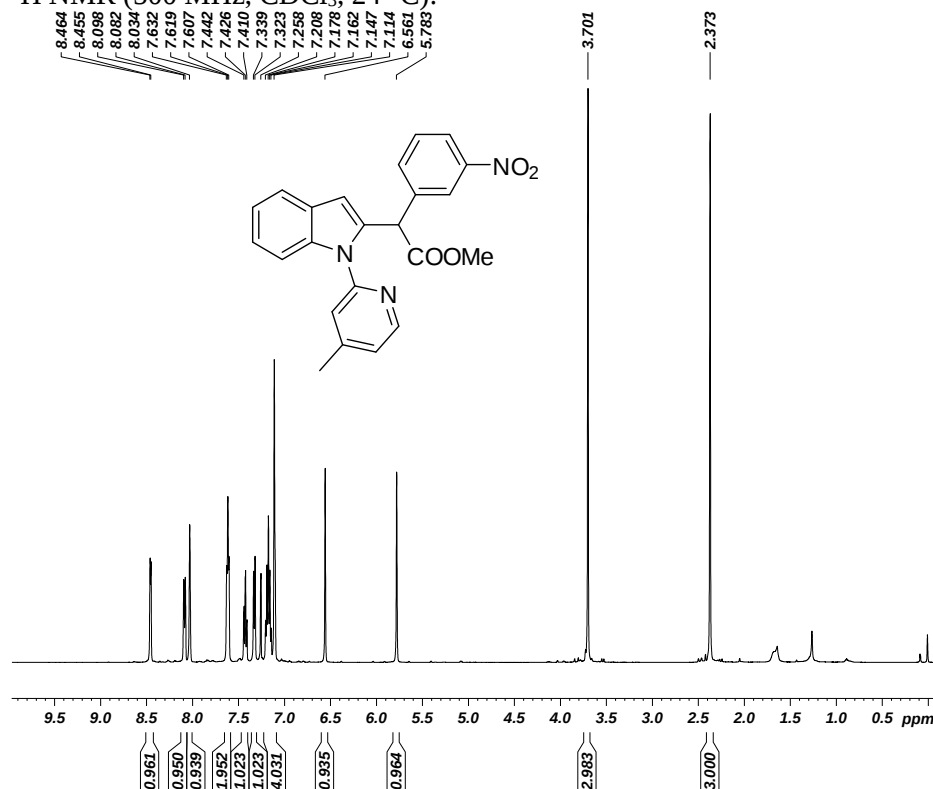
===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127572 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(1-(4-methylpyridin-2-yl)-1H-indol-2-yl)-2-(3-nitrophenyl)acetate (3t):

¹H NMR (500 MHz, CDCl₃, 24 °C):



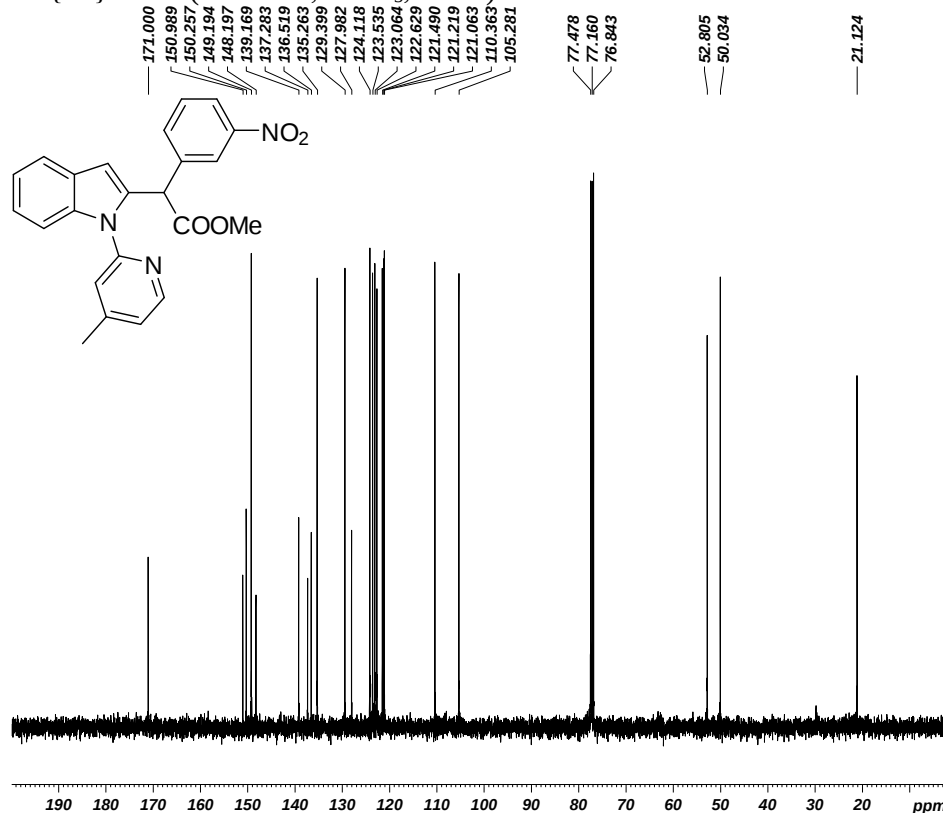
Current Data Parameters
NAME 01.16
EXPNO 183
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160112
Time 23.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 89.12
DW 50.000 usec
DE 6.50 usec
TE 293.7 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 500.1500212 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 01.16
EXPNO 204
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160119
Time 13.22
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 299.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

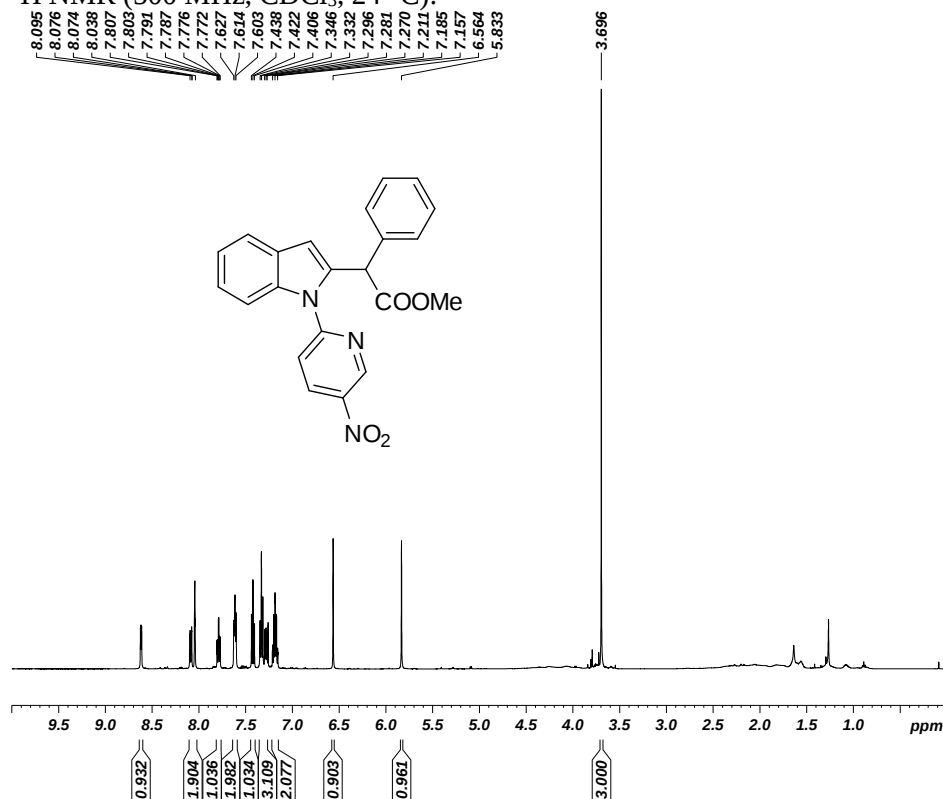
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127599 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(1-(5-nitropyridin-2-yl)-1H-indol-2-yl)-2-phenylacetate (3u):

¹H NMR (500 MHz, CDCl₃, 24 °C):



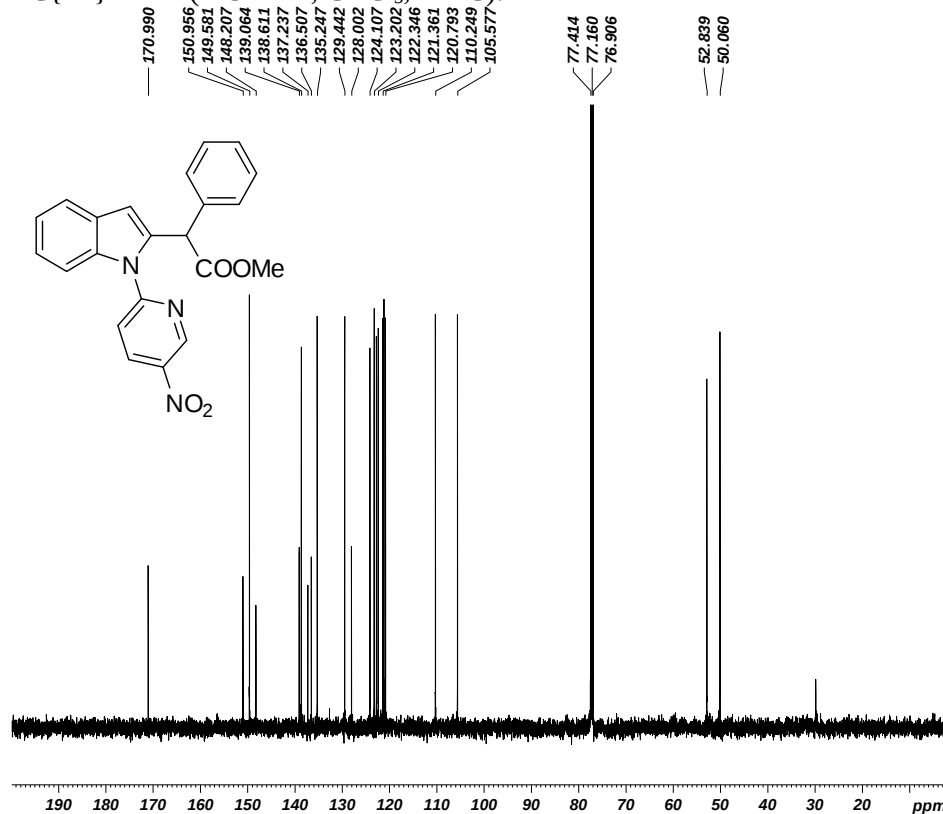
Current Data Parameters
NAME 04.18
EXPNO 191
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180425
Time 12.02
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 64
DW 50.000 usec
DE 6.50 usec
TE 297.5 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008 MHz
NUC1 1H
P1 12.75 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 500.1500119 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (125 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 04.18
EXPNO 192
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180425
Time 12.10
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 298.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

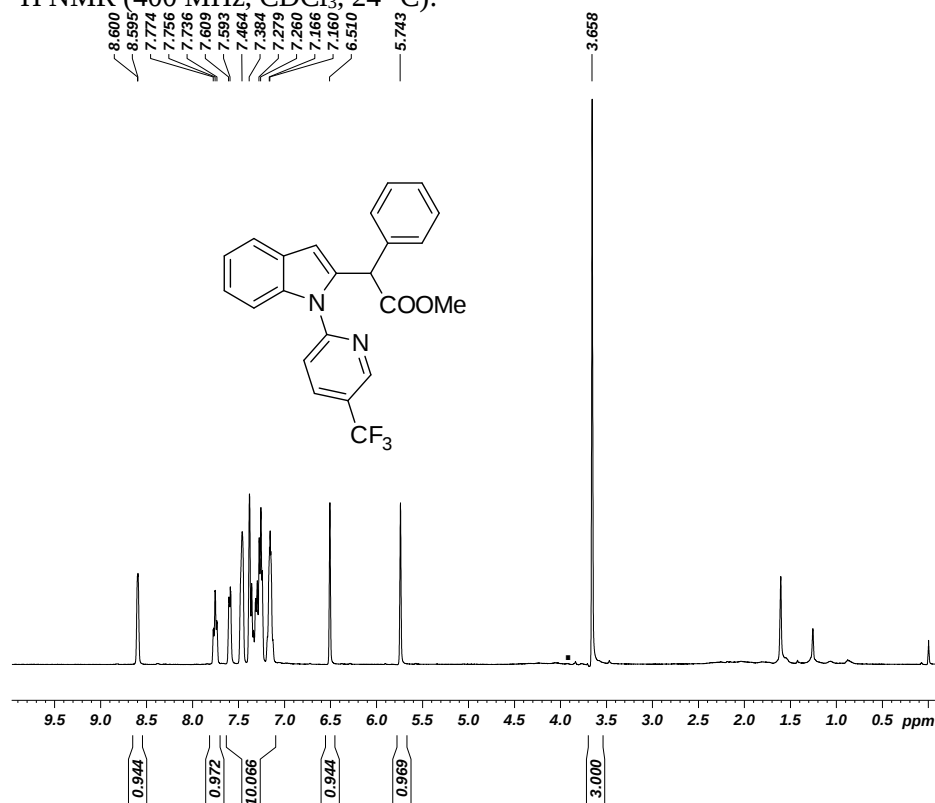
===== CHANNEL f1 =====
SFO1 125.7753932 MHz
NUC1 13C
P1 9.88 usec
PLW1 103.00000000 W

===== CHANNEL f2 =====
SFO2 500.1520006 MHz
NUC2 1H
CPDPRG2 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

Methyl 2-phenyl-2-(1-(5-(trifluoromethyl)pyridin-2-yl)-1H-indol-2-yl)acetate (3v):

¹H NMR (400 MHz, CDCl₃, 24 °C):



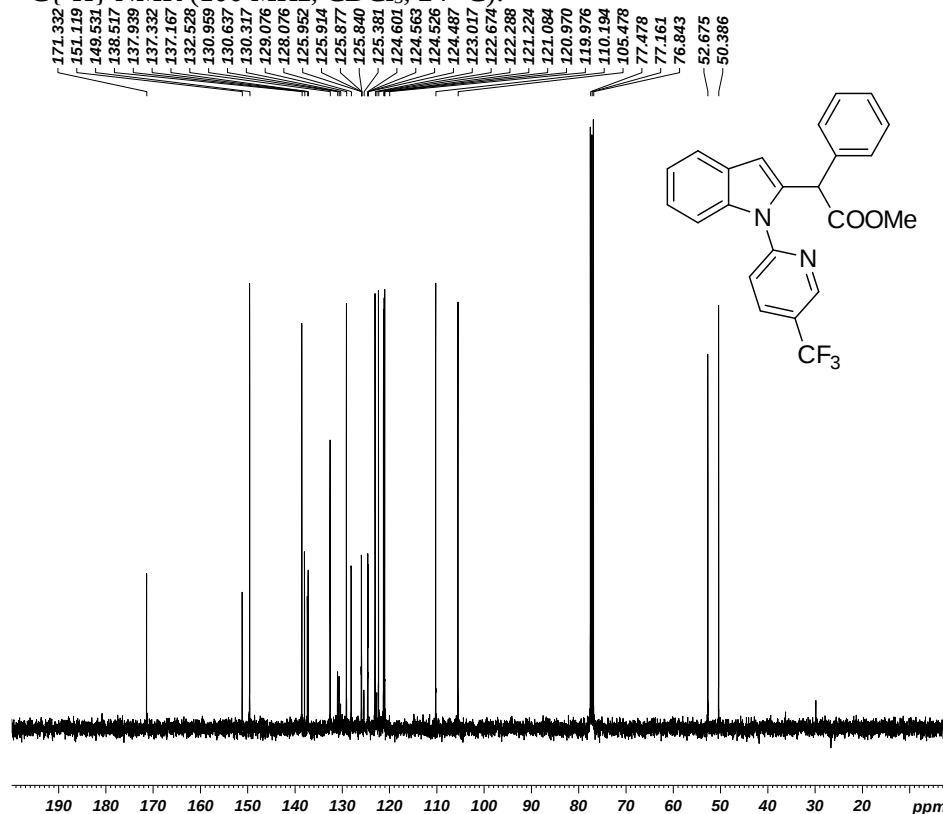
Current Data Parameters
NAME 05.18
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180502
Time 19.22
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 299.4 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 400.1300163 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 05.18
EXPNO 17
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180502
Time 19.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 524
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 299.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

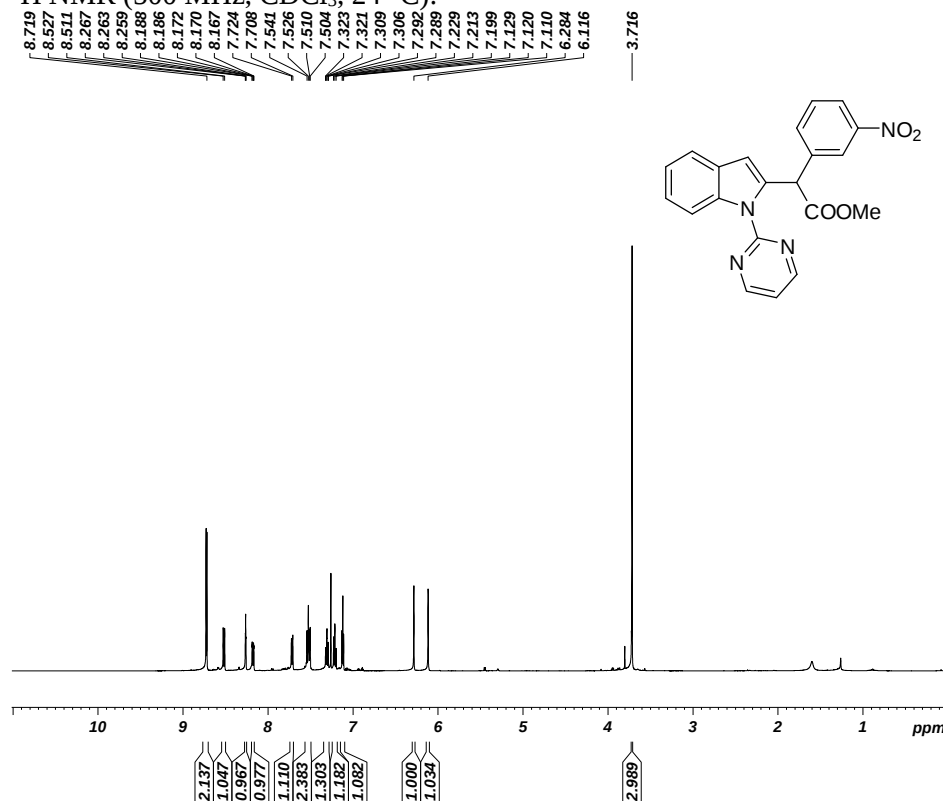
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== 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 100.6127569 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(3-nitrophenyl)-2-(1-(pyrimidin-2-yl)-1H-indol-2-yl)acetate (3w):

^1H NMR (500 MHz, CDCl_3 , 24 °C):



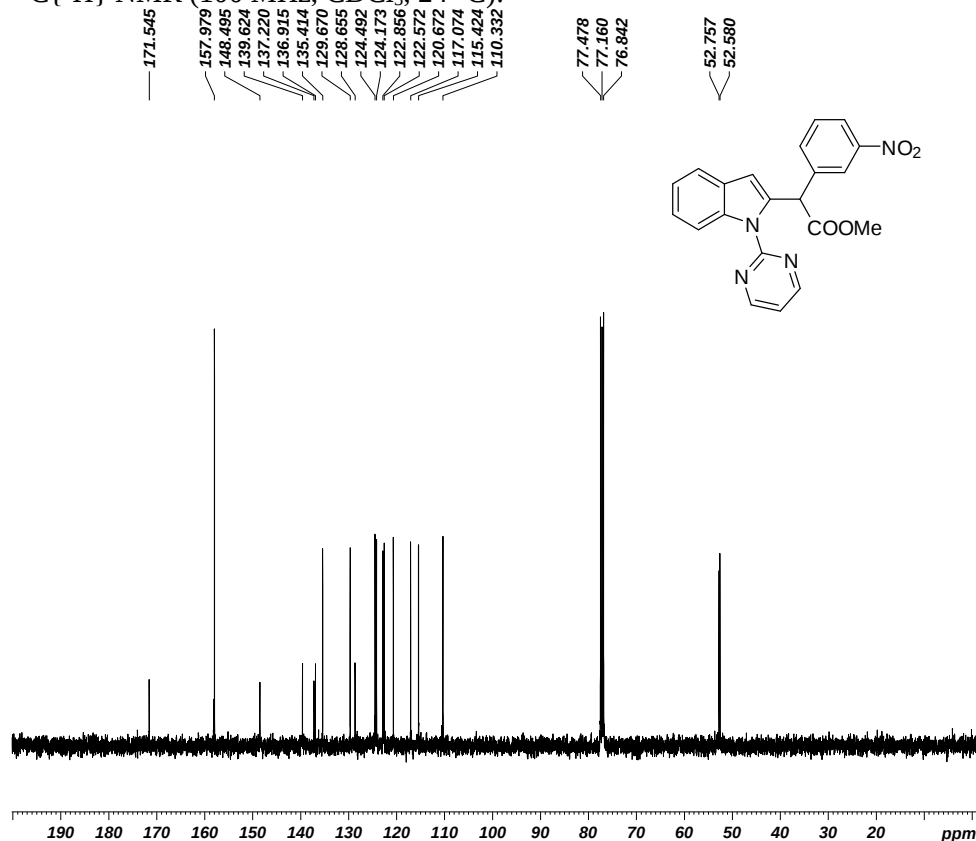
Current Data Parameters
NAME spa50116
EXPNO 204
PROCNO 1

F2 - Acquisition Parameters
Date 20160113
Time 15.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl_3
NS 32
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 299.1 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 500.1500218 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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



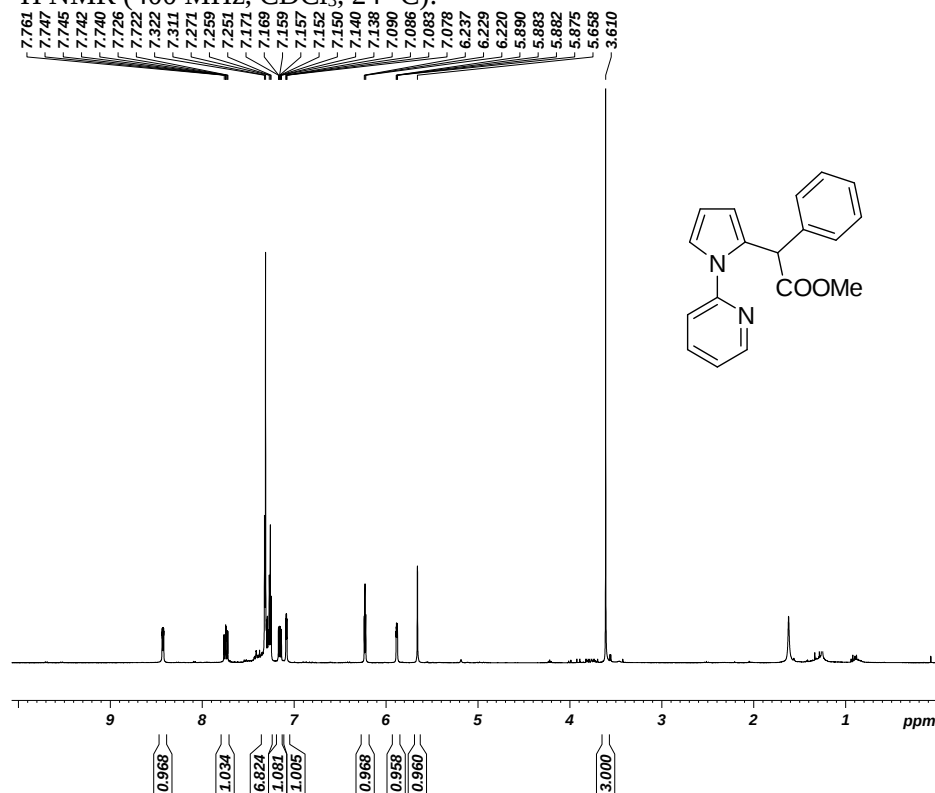
Current Data Parameters
NAME spa40116
EXPNO 129
PROCNO 1

F2 - Acquisition Parameters
Date 20160115
Time 8.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl_3
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 298.1 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
SFO1 100.6228289 MHz
NUC1 ^{13}C
P1 9.25 usec
PLW1 47.00000000 W
SFO2 400.1316005 MHz
NUC2 ^1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W

F2 - Processing parameters
SI 32768
SF 100.6127570 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-phenyl-2-(1-(pyridin-2-yl)-1H-pyrrol-2-yl)acetate (3x):

¹H NMR (400 MHz, CDCl₃, 24 °C):



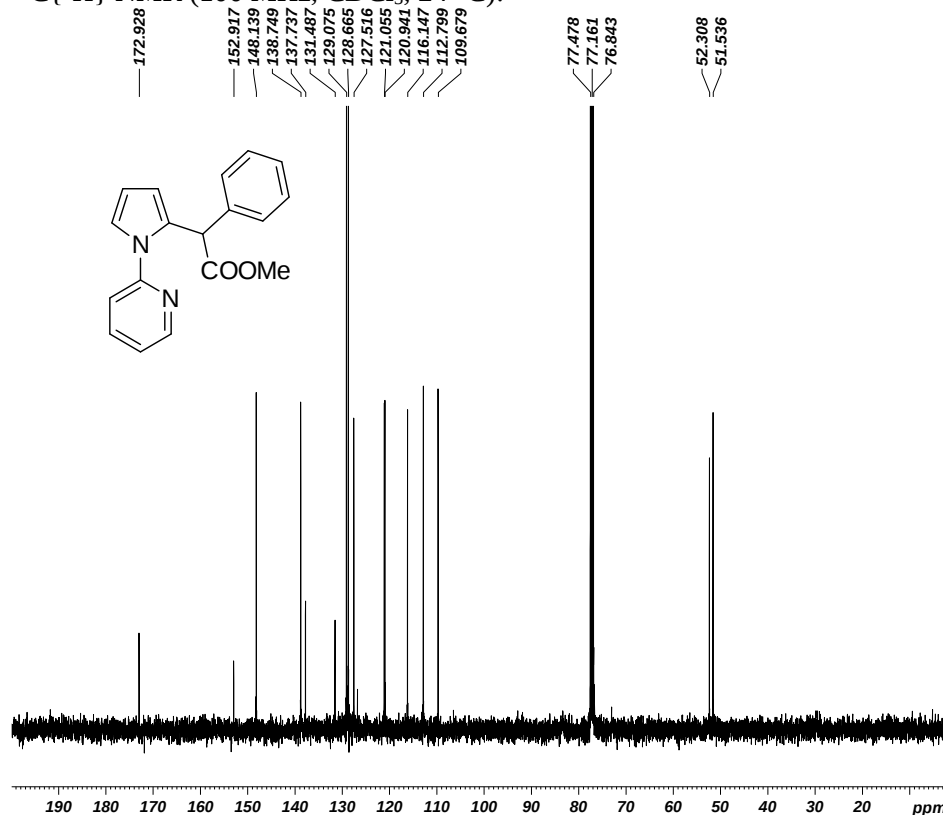
Current Data Parameters
NAME 12.15
EXPNO 166
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151214
Time 7.05
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 291.0 K
D1 0.50000000 sec
TD0 1

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

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

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 12.15
EXPNO 167
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151214
Time 7.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 1000
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 292.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

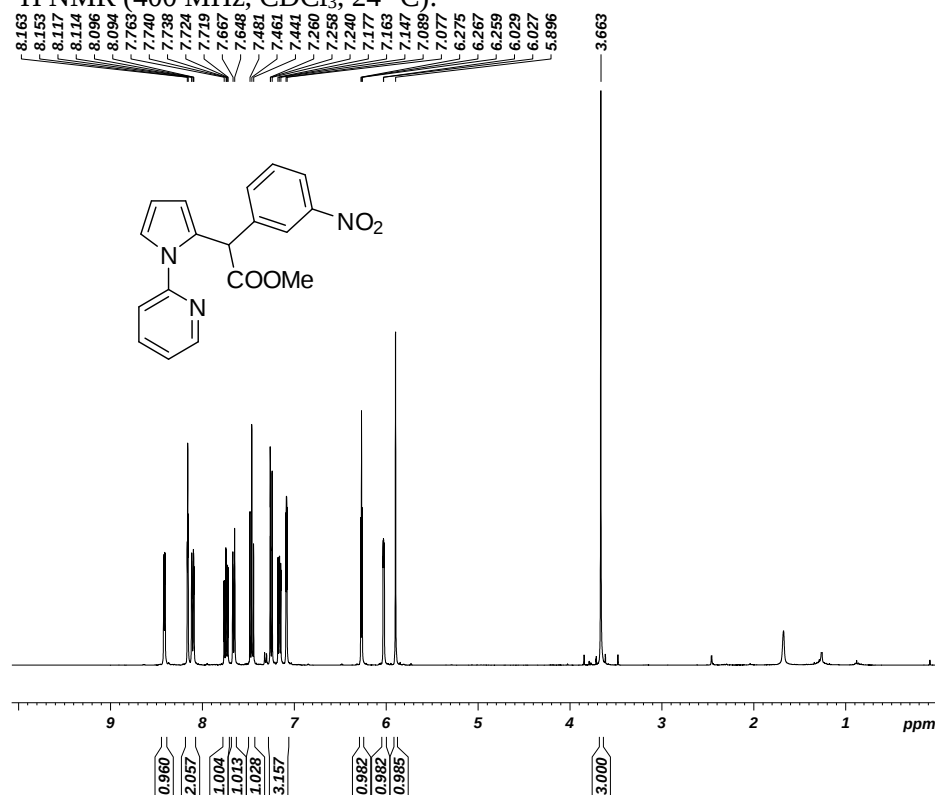
===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127574 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(3-nitrophenyl)-2-(1-(pyridin-2-yl)-1H-pyrrol-2-yl)acetate (3y):

¹H NMR (400 MHz, CDCl₃, 24 °C):



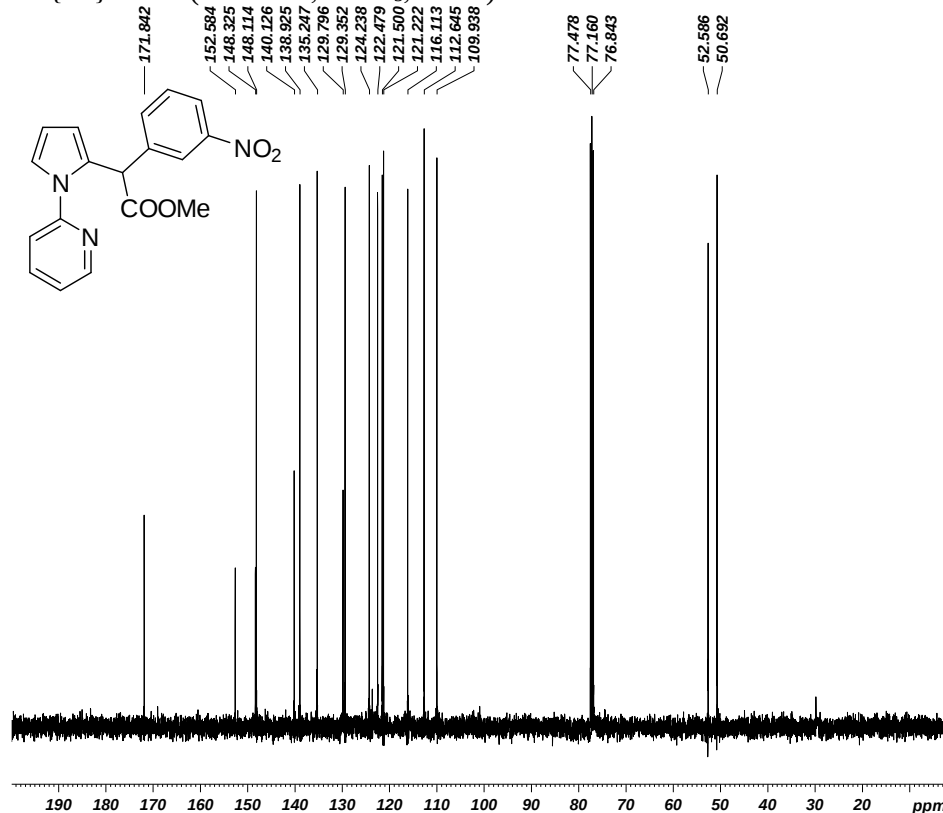
Current Data Parameters
NAME 03.16
EXPNO 421
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160317
Time 10.09
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 108.26
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 0.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 03.16
EXPNO 422
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160317
Time 10.16
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 299.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

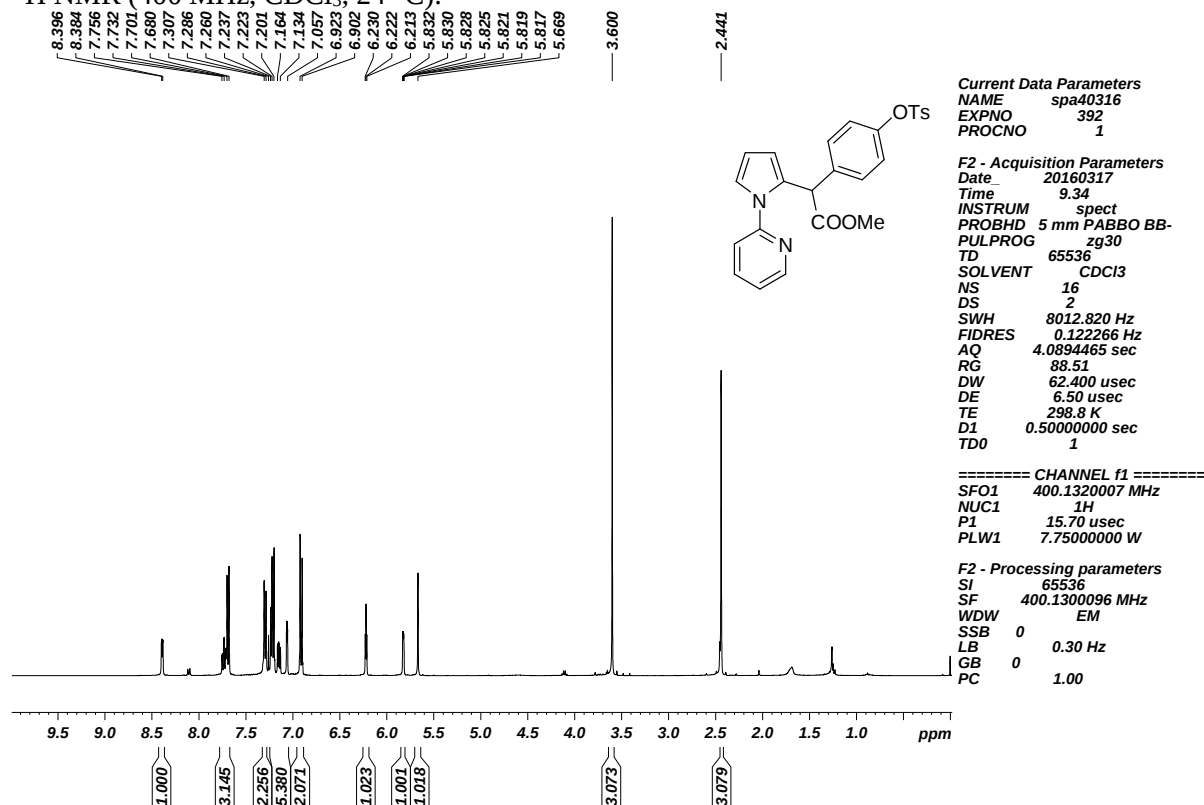
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== 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

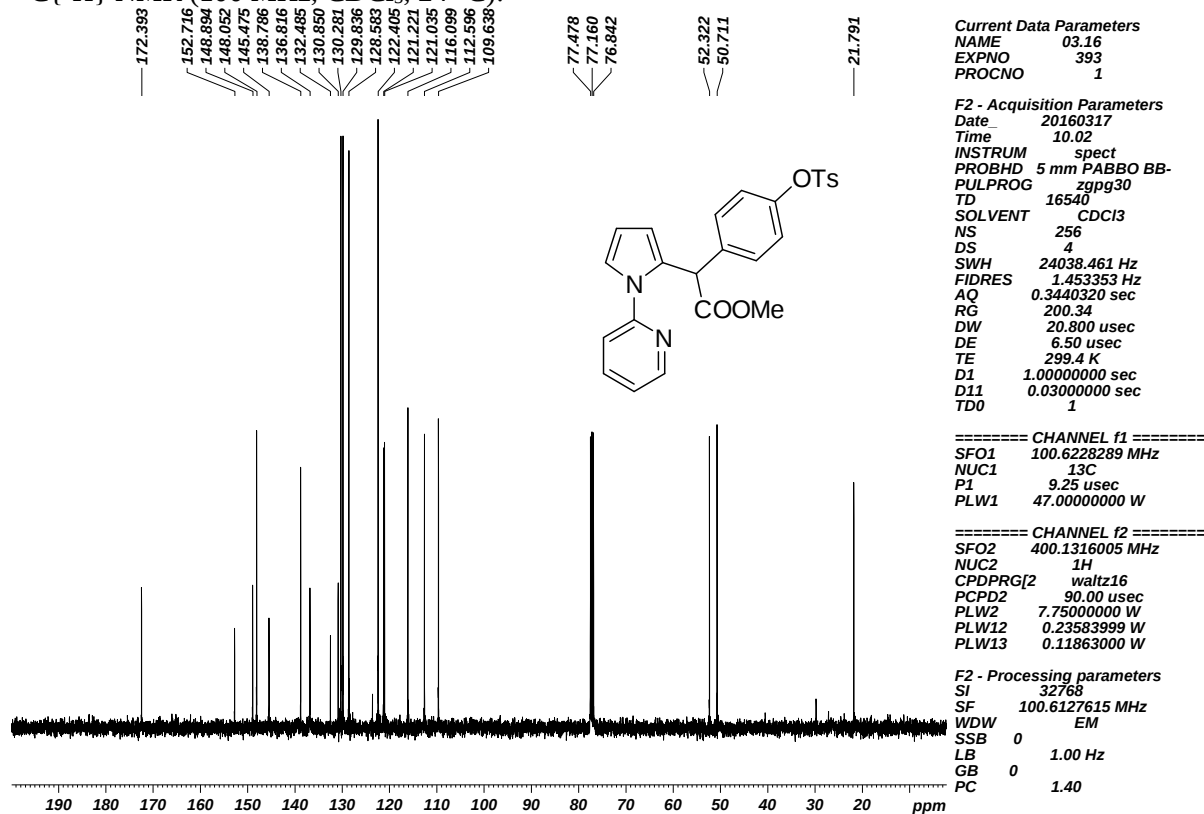
F2 - Processing parameters
SI 32768
SF 100.6127603 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(1-(pyridin-2-yl)-1H-pyrrol-2-yl)-2-(4-(tosyloxy)phenyl)acetate (3z):

¹H NMR (400 MHz, CDCl₃, 24 °C):

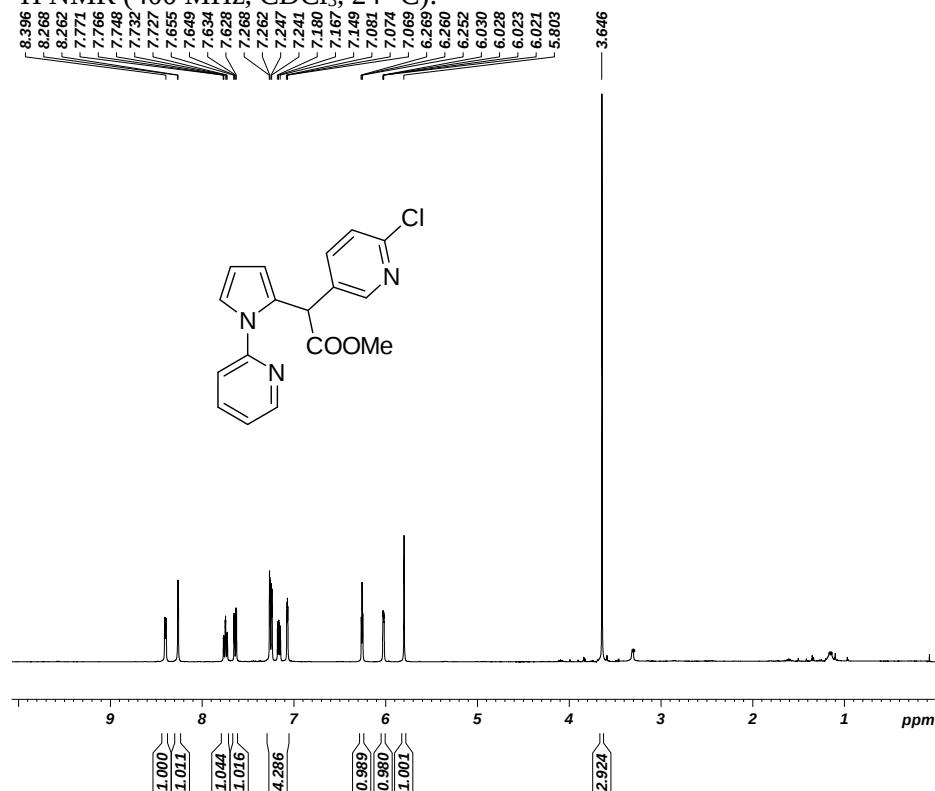


¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Methyl 2-(6-chloropyridin-3-yl)-2-(1-(pyridin-2-yl)-1H-pyrrol-2-yl)acetate (3aa):

¹H NMR (400 MHz, CDCl₃, 24 °C):



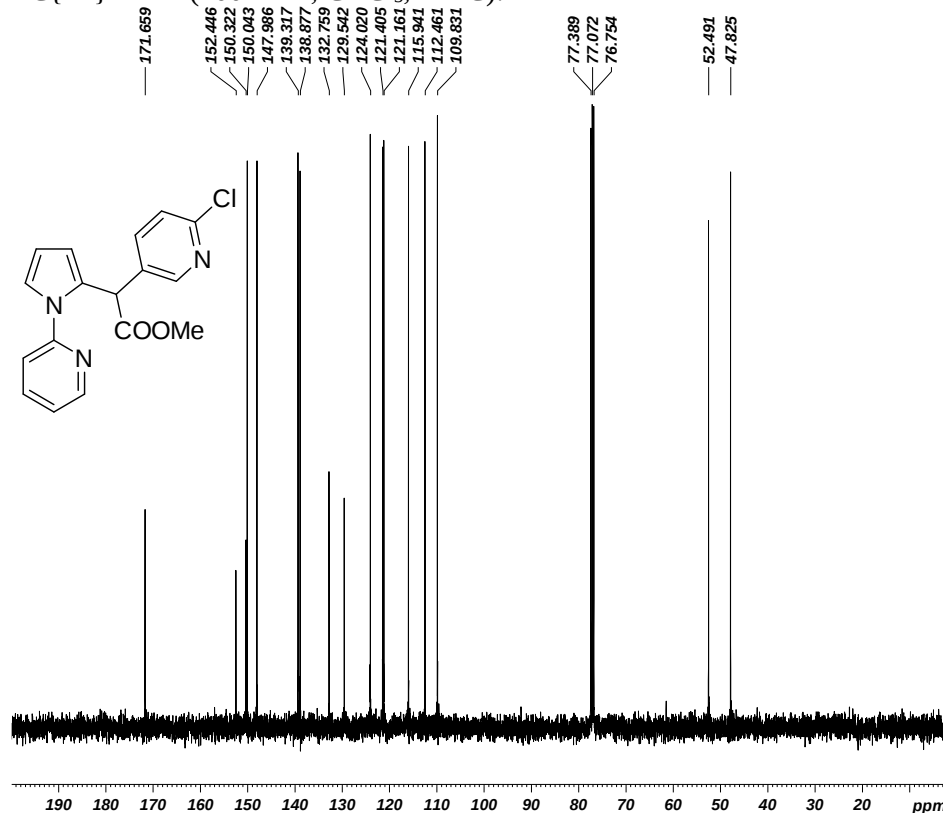
Current Data Parameters
NAME 04.16
EXPNO 46
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160402
Time 9.24
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 108.26
DW 62.400 usec
DE 6.50 usec
TE 298.7 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 400.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 04.16
EXPNO 47
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160402
Time 9.26
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 299.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

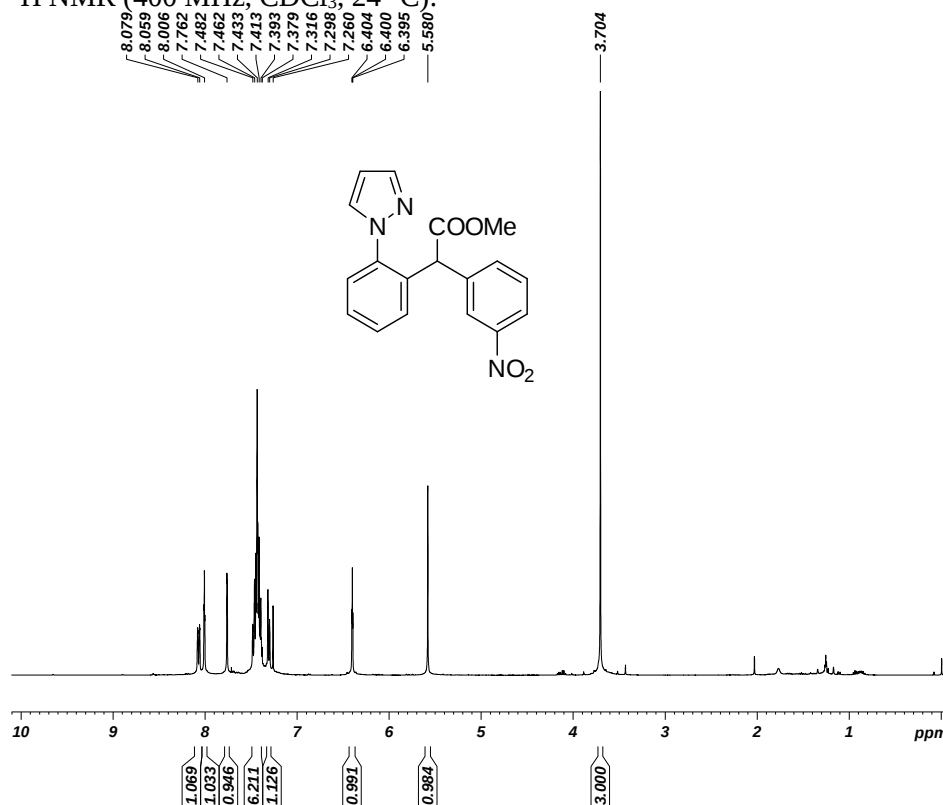
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(2-(1H-pyrazol-1-yl)phenyl)-2-(3-nitrophenyl)acetate (5a):

¹H NMR (400 MHz, CDCl₃, 24 °C):



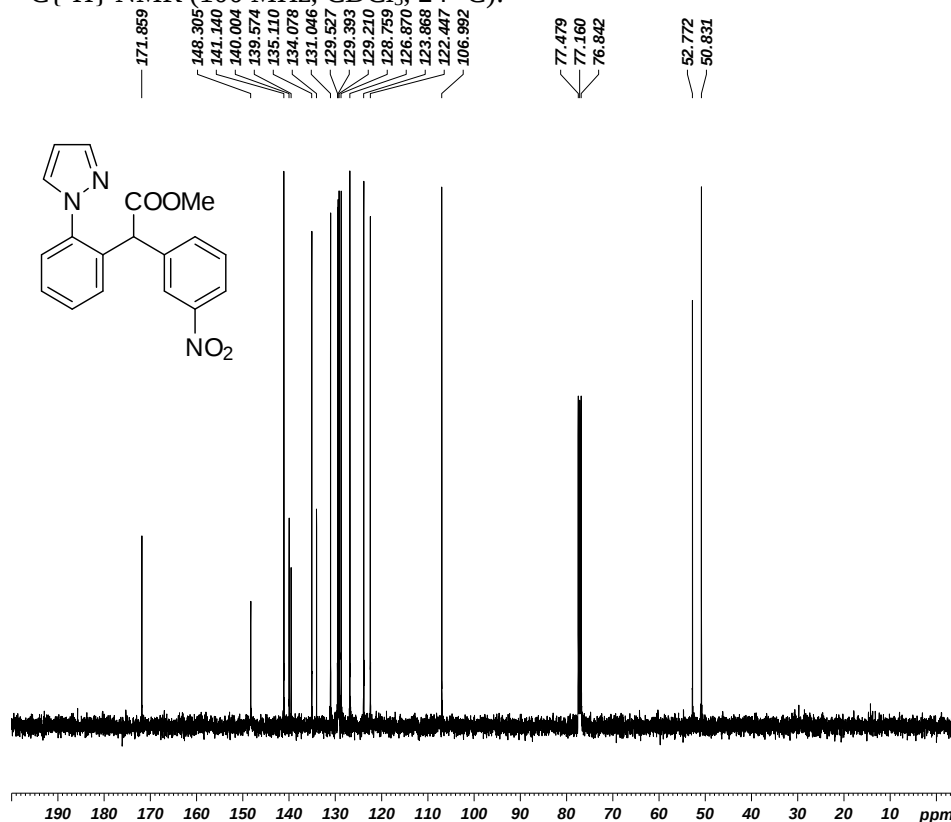
Current Data Parameters
NAME 01.16
EXPNO 710
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161020
Time 10.54
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 88.51
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 0.50000000 sec
TD0 1

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

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

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 01.16
EXPNO 711
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161020
Time 11.01
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 299.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

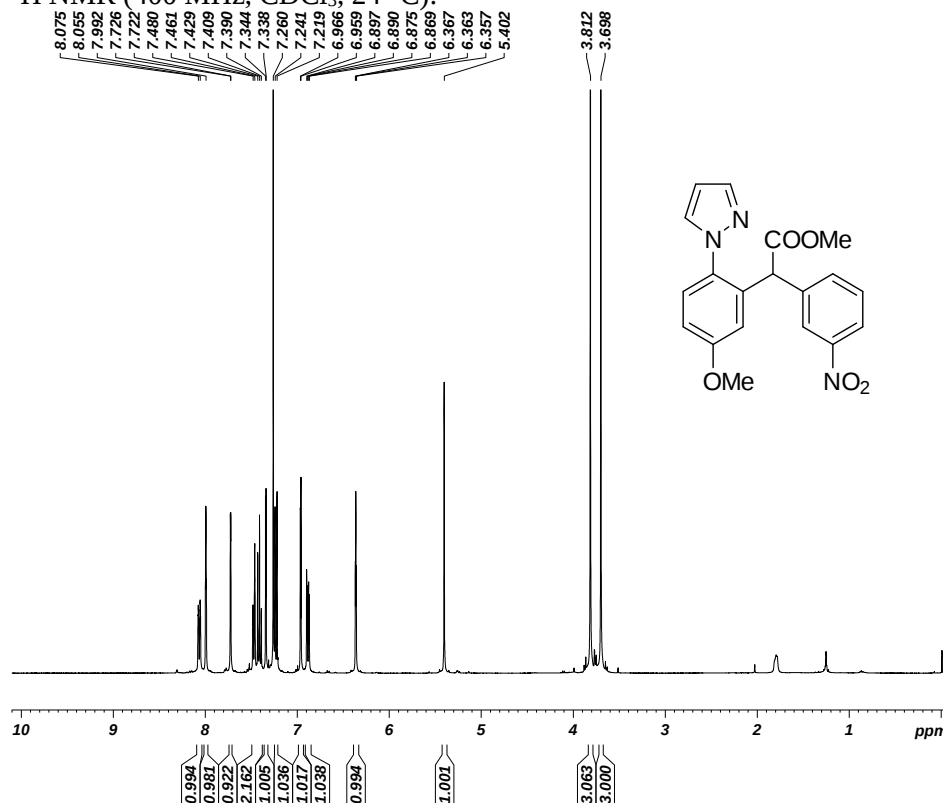
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127612 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(5-methoxy-2-(1H-pyrazol-1-yl)phenyl)-2-(3-nitrophenyl)acetate (5b):

¹H NMR (400 MHz, CDCl₃, 24 °C):



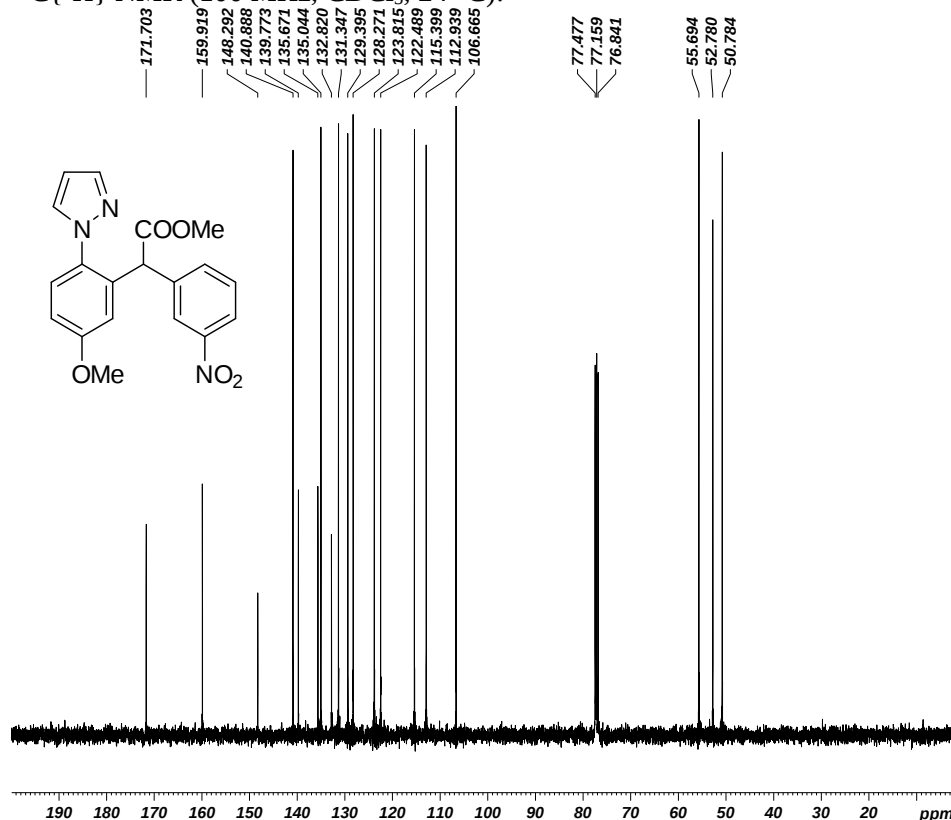
Current Data Parameters
NAME 11.16
EXPNO 476
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161116
Time 9.23
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 88.51
DW 62.400 usec
DE 6.50 usec
TE 301.1 K
D1 0.5000000 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 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 11.16
EXPNO 477
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161116
Time 9.30
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 301.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

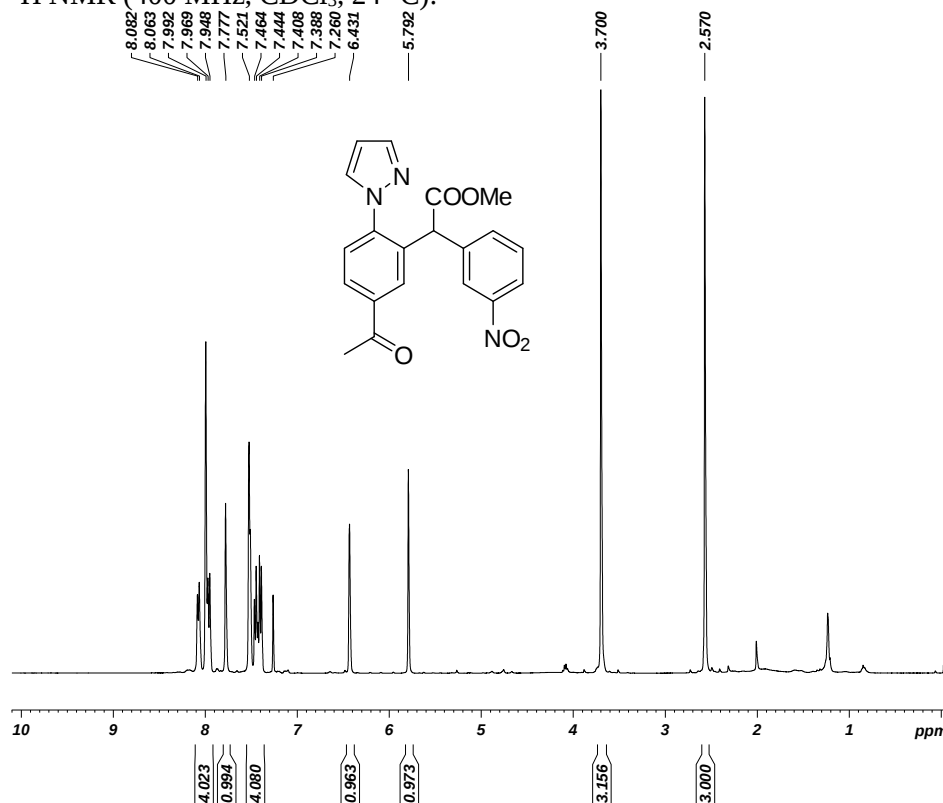
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127611 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(5-acetyl-2-(1H-pyrazol-1-yl)phenyl)-2-(3-nitrophenyl)acetate (5c):

¹H NMR (400 MHz, CDCl₃, 24 °C):



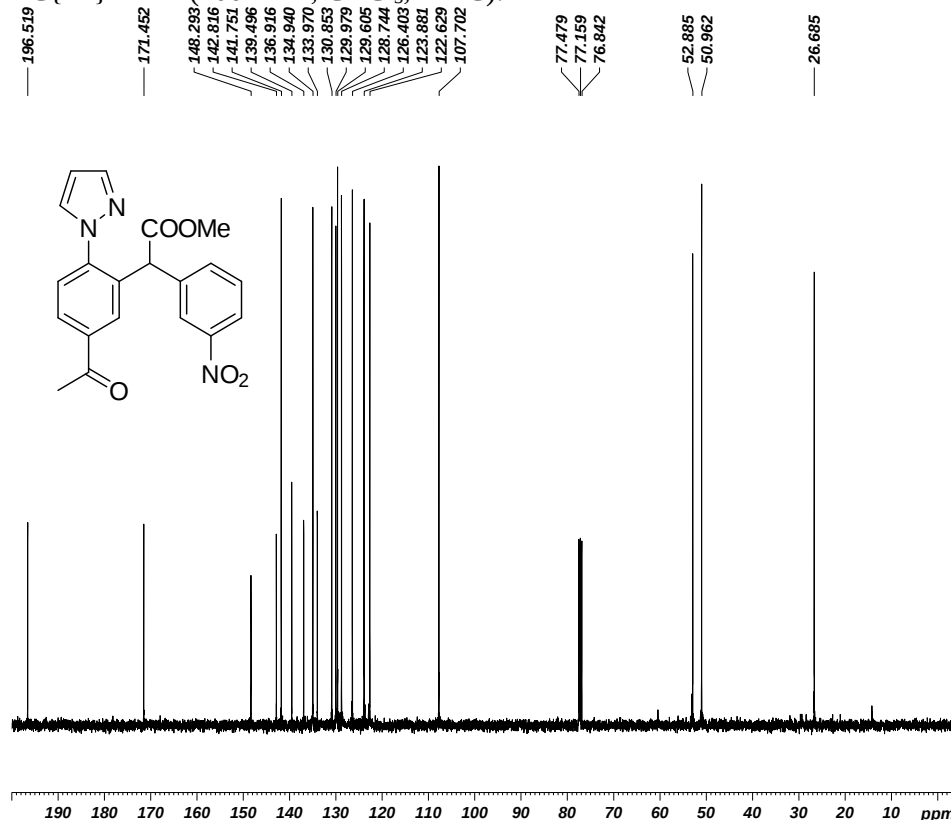
Current Data Parameters
NAME 11.16
EXPNO 253
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161109
Time 10.27
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 60.89
DW 62.400 usec
DE 6.50 usec
TE 297.2 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 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 11.16
EXPNO 254
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161109
Time 10.34
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 297.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

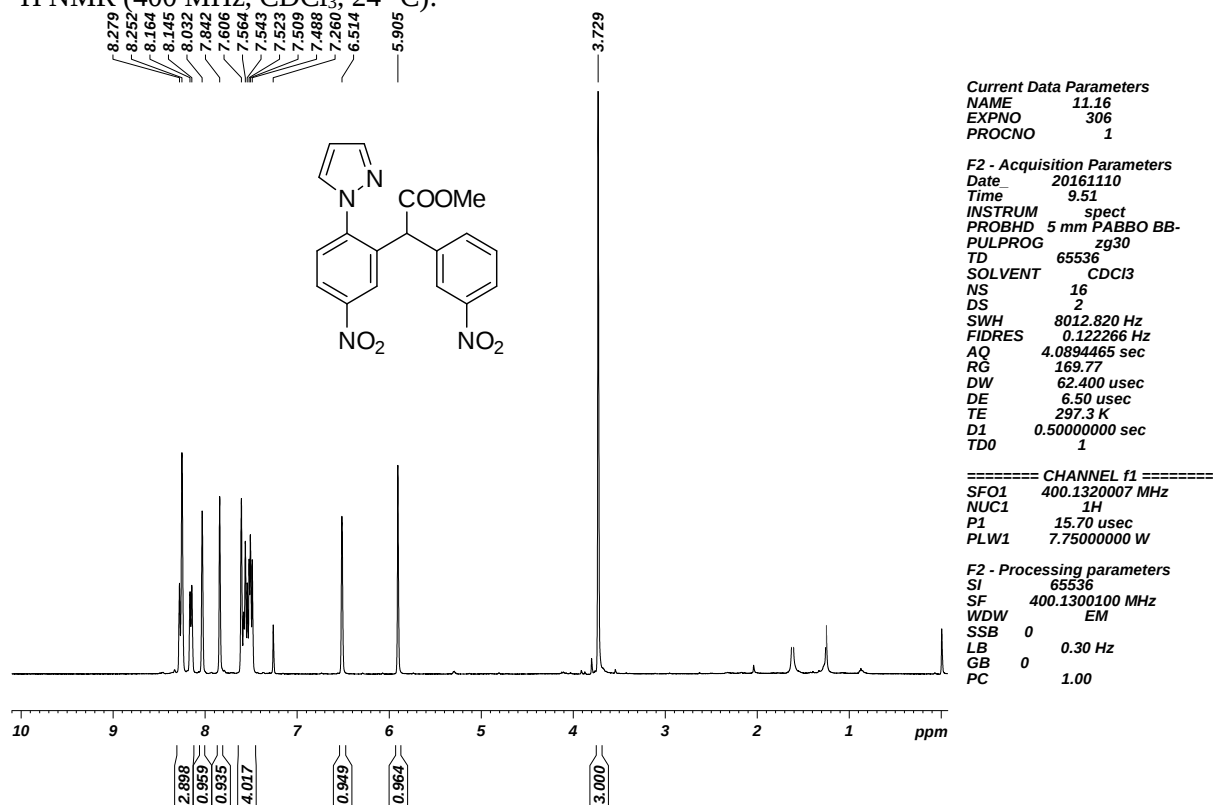
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

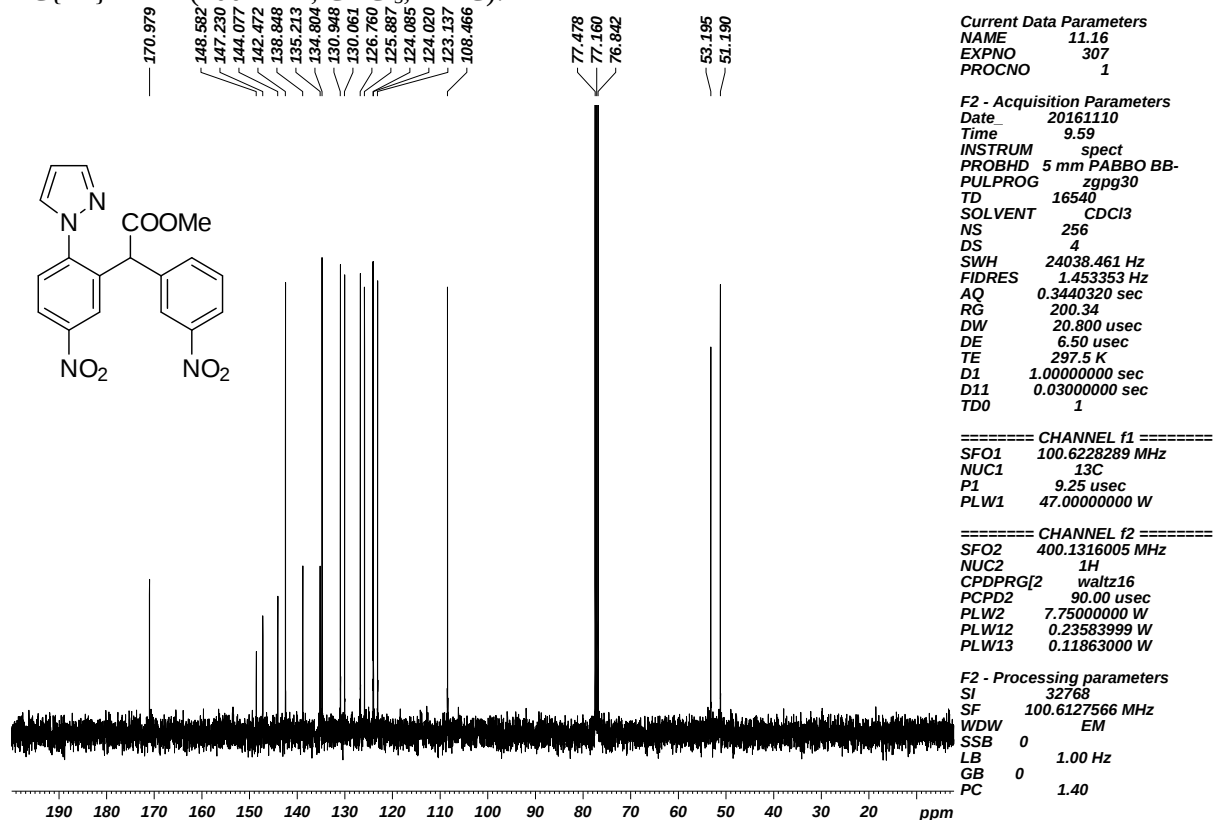
F2 - Processing parameters
SI 32768
SF 100.6127662 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(5-nitro-2-(1H-pyrazol-1-yl)phenyl)-2-(3-nitrophenyl)acetate (5d):

^1H NMR (400 MHz, CDCl_3 , 24 °C):

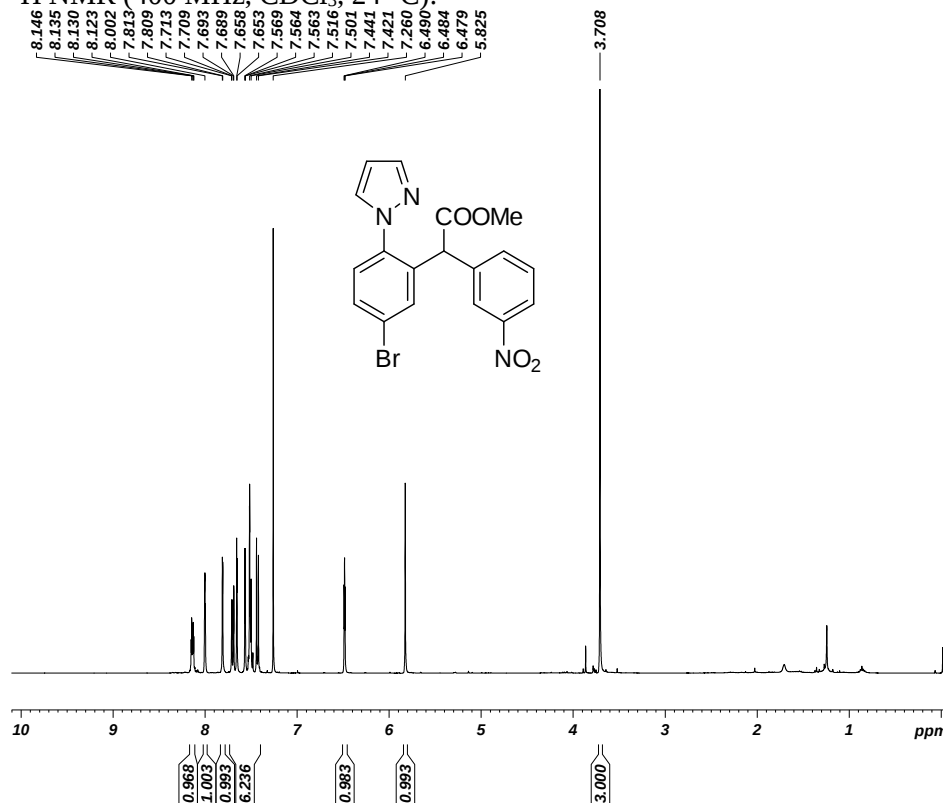


$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C):



Methyl 2-(5-bromo-2-(1H-pyrazol-1-yl)phenyl)-2-(3-nitrophenyl)acetate (5e):

¹H NMR (400 MHz, CDCl₃, 24 °C):



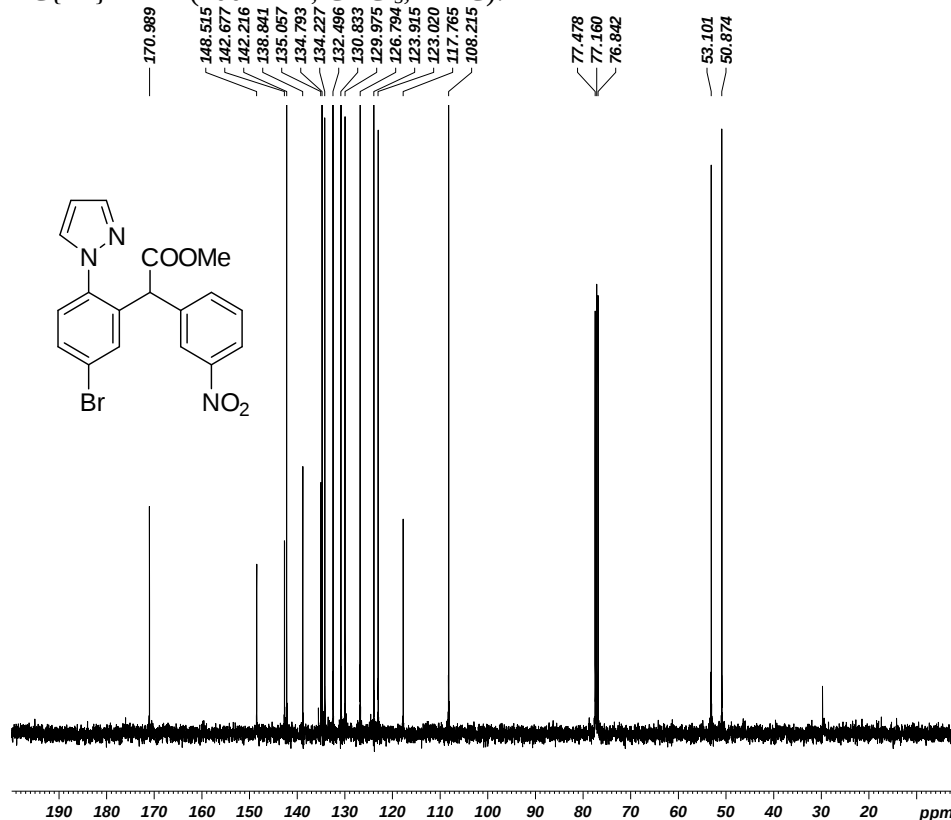
Current Data Parameters
NAME 11.16
EXPNO 303
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161110
Time 9.37
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 88.51
DW 62.400 usec
DE 6.50 usec
TE 297.4 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 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 11.16
EXPNO 304
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161110
Time 9.44
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 297.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

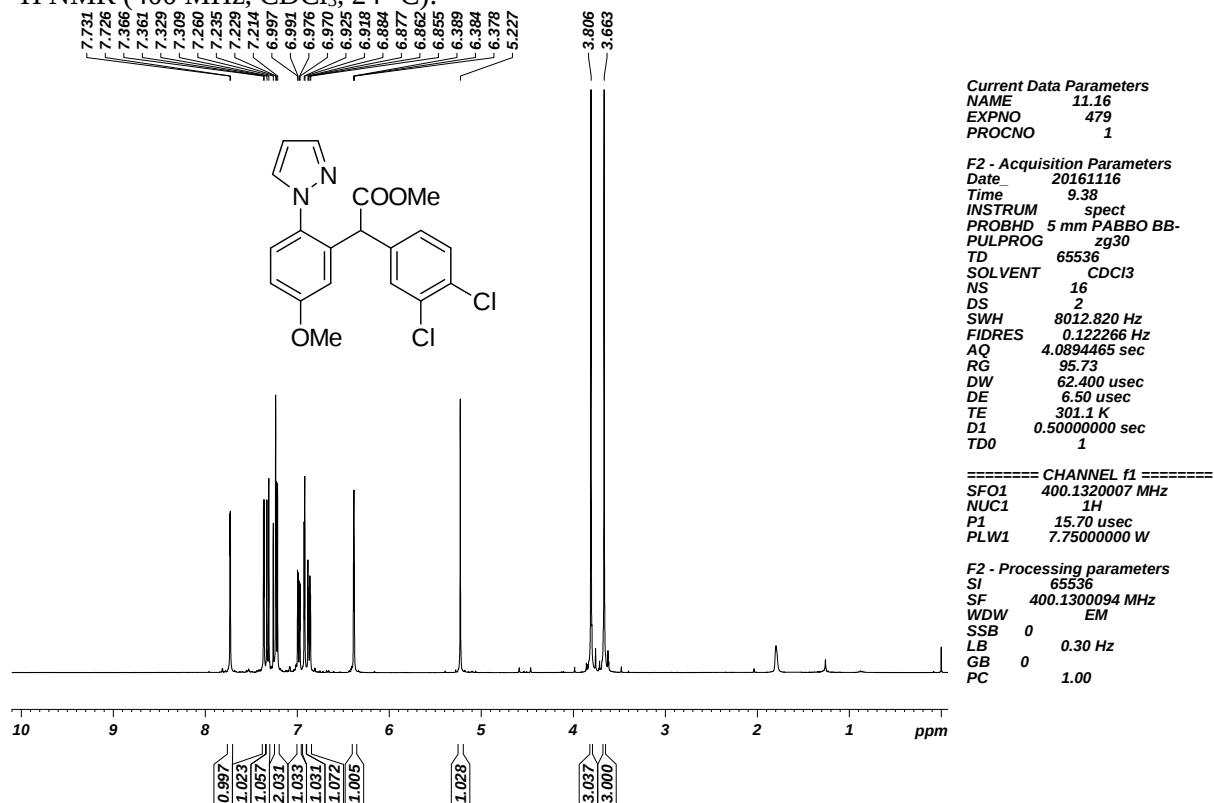
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

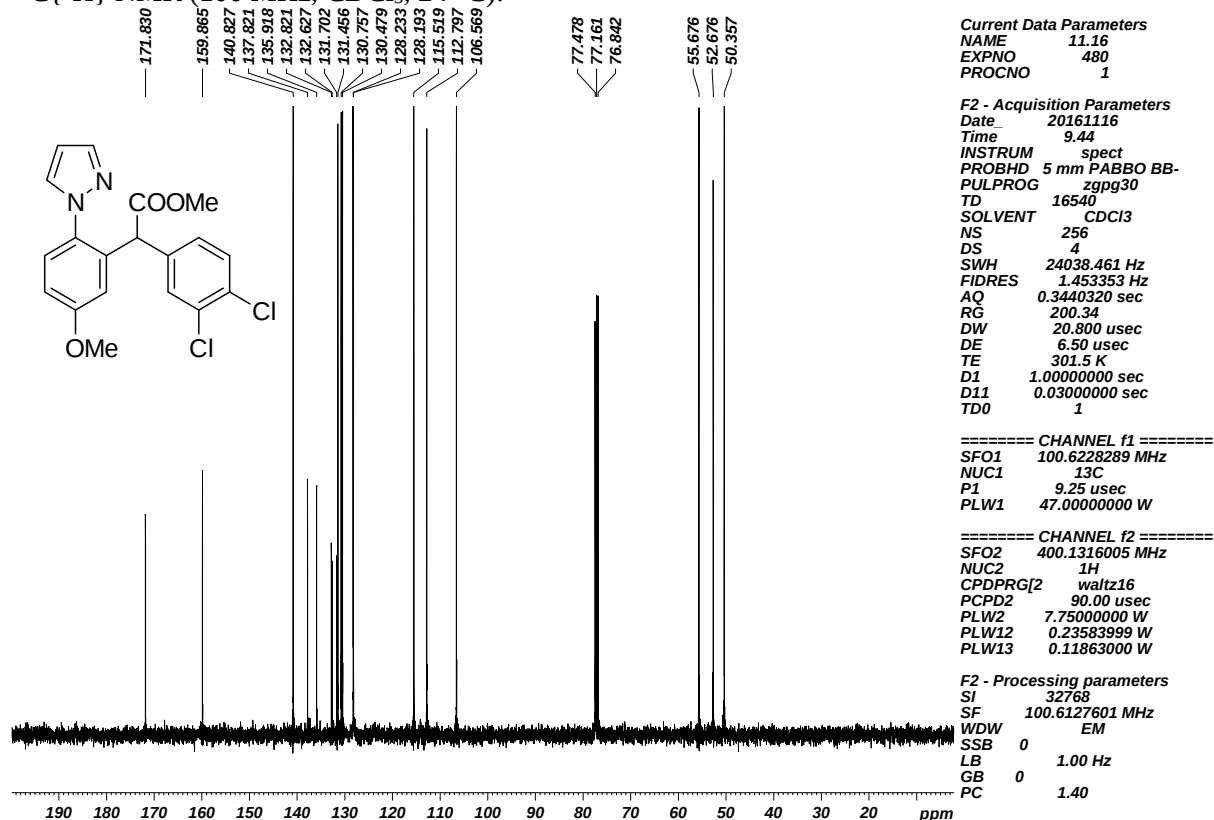
F2 - Processing parameters
SI 32768
SF 100.6127623 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(3,4-dichlorophenyl)-2-(5-methoxy-2-(1H-pyrazol-1-yl)phenyl) acetate (5f):

¹H NMR (400 MHz, CDCl₃, 24 °C):

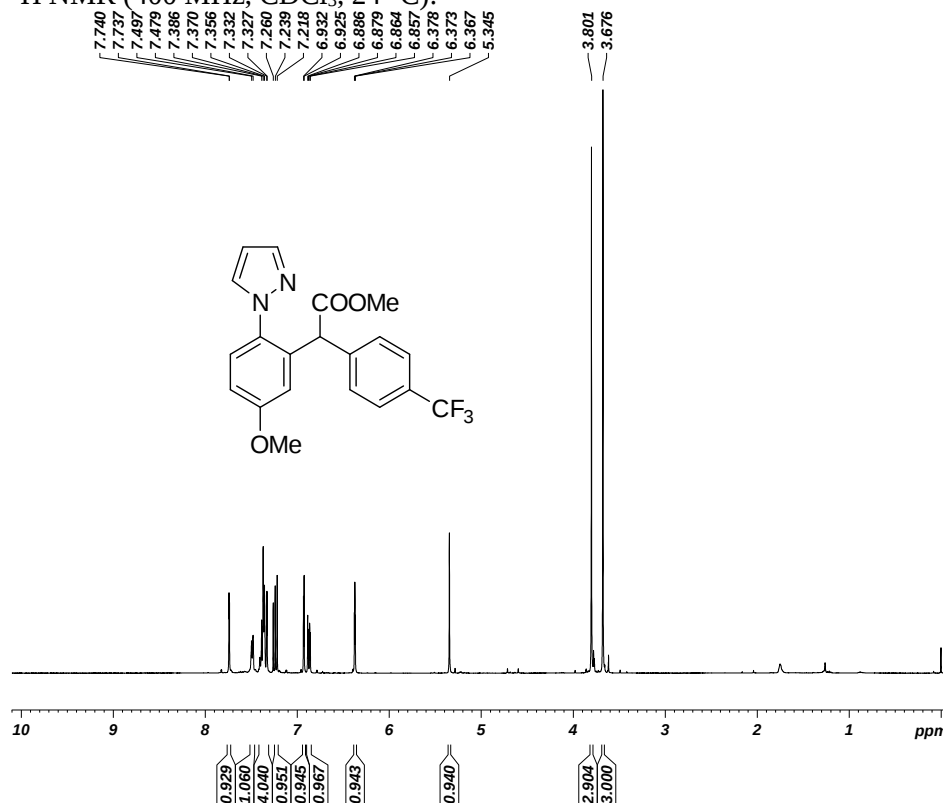


¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Methyl 2-(5-methoxy-2-(1H-pyrazol-1-yl)phenyl)-2-(4 (trifluoromethyl)phenyl) acetate (5g):

¹H NMR (400 MHz, CDCl₃, 24 °C):



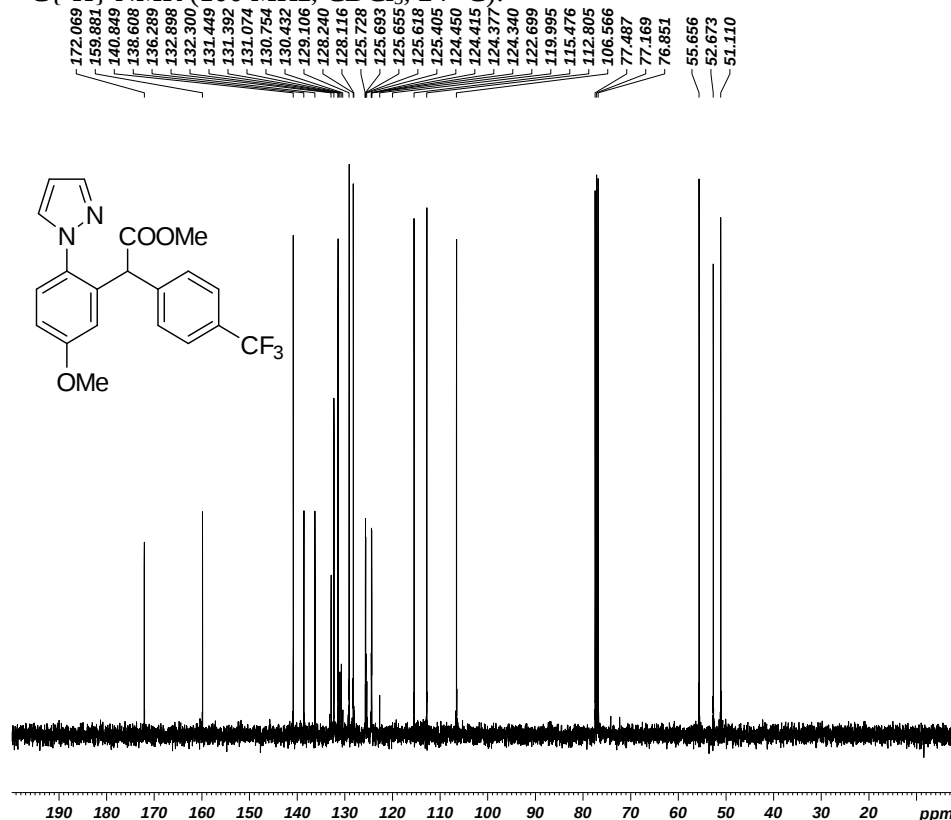
Current Data Parameters
NAME 11.16
EXPNO 561
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161119
Time 6.31
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 108.26
DW 62.400 usec
DE 6.50 usec
TE 297.4 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 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 11.16
EXPNO 562
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161119
Time 6.38
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 297.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

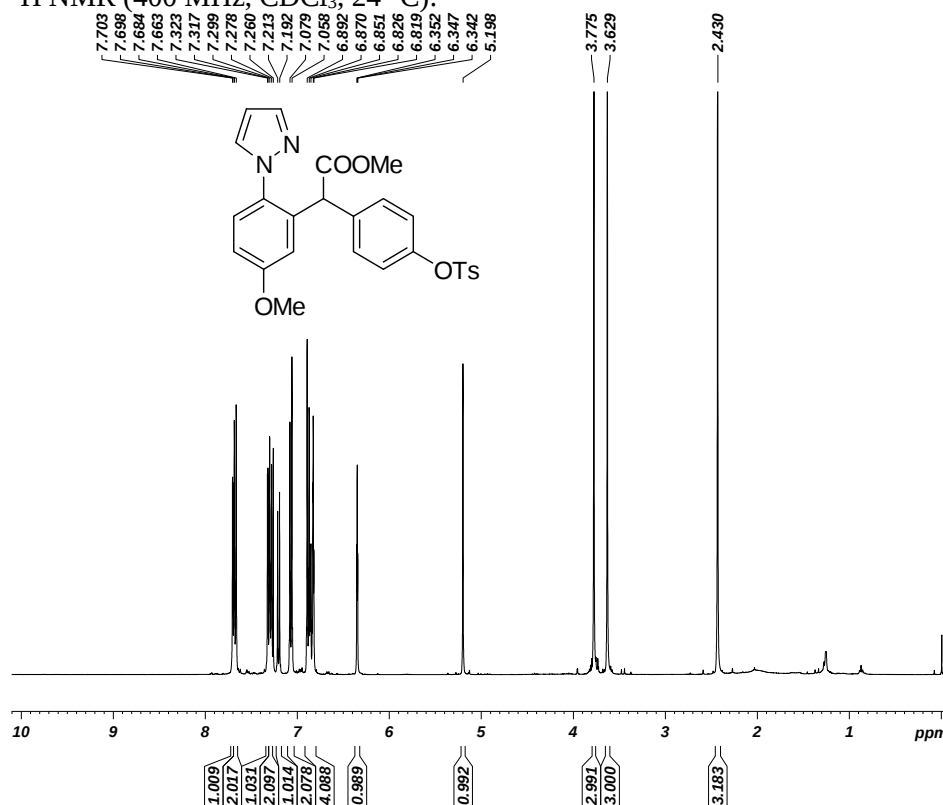
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127569 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(5-methoxy-2-(1*H*-pyrazol-1-yl)phenyl)-2-(4-methoxyphenyl)acetate (5h):

¹H NMR (400 MHz, CDCl₃, 24 °C):



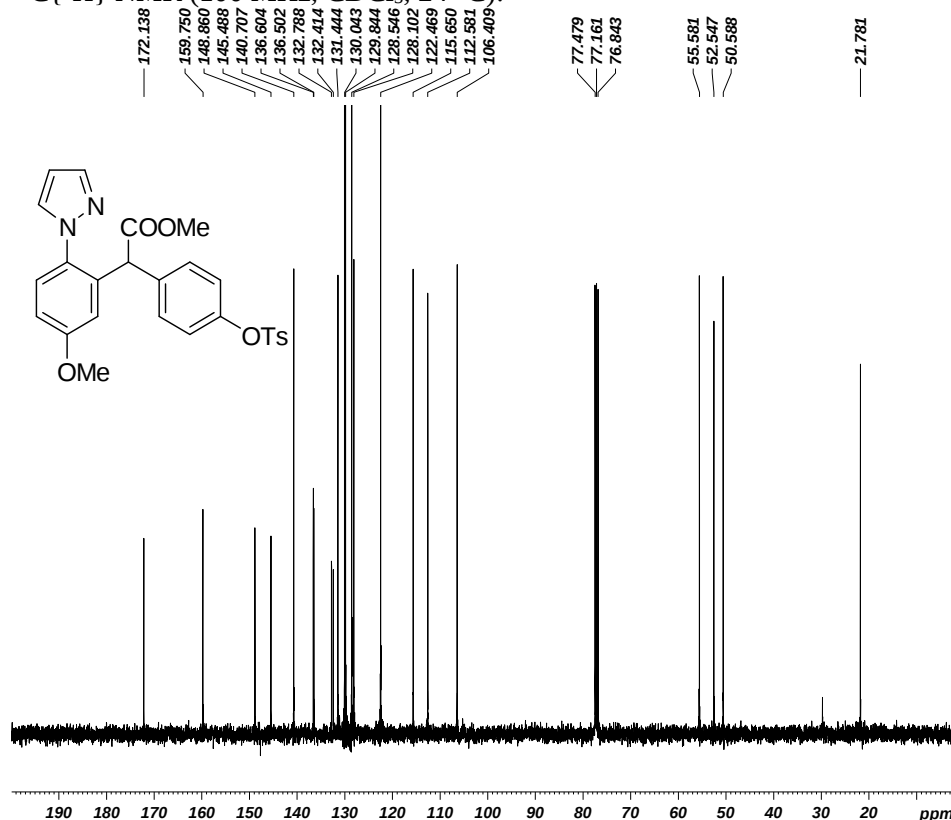
Current Data Parameters
NAME 11.16
EXPNO 564
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161119
Time 6.45
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 79.8
DW 62.400 usec
DE 6.50 usec
TE 297.4 K
D1 0.5000000 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 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 11.16
EXPNO 565
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161119
Time 6.51
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 297.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

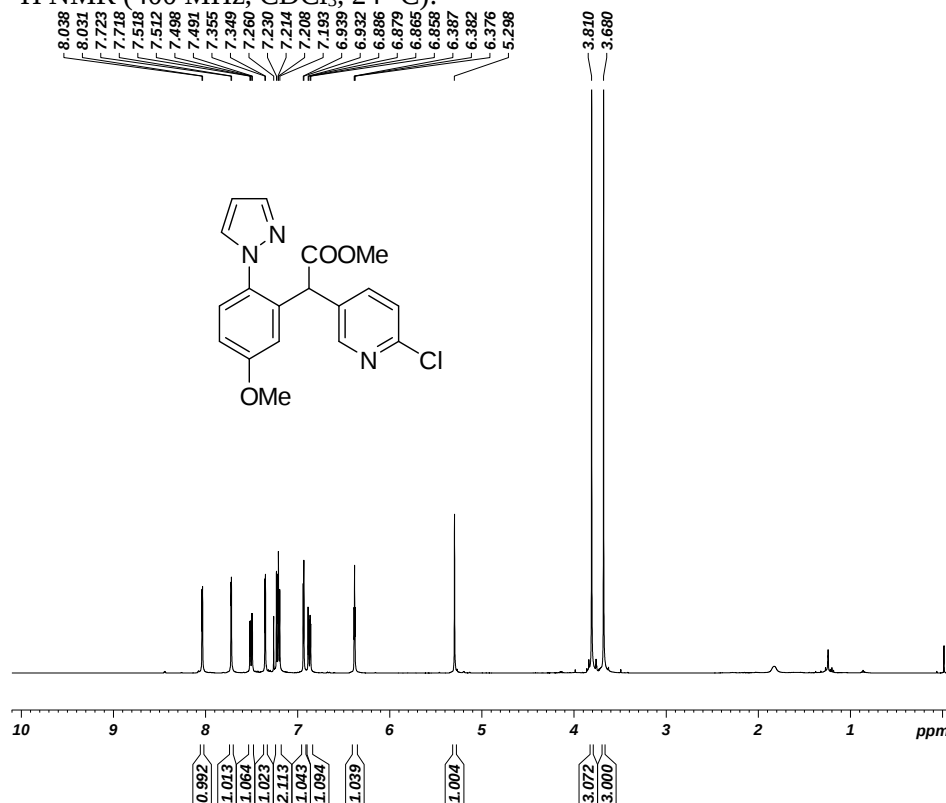
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127626 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(6-chloropyridin-3-yl)-2-(5-methoxy-2-(1H-pyrazol-1-yl)phenyl)acetate (5i):

¹H NMR (400 MHz, CDCl₃, 24 °C):



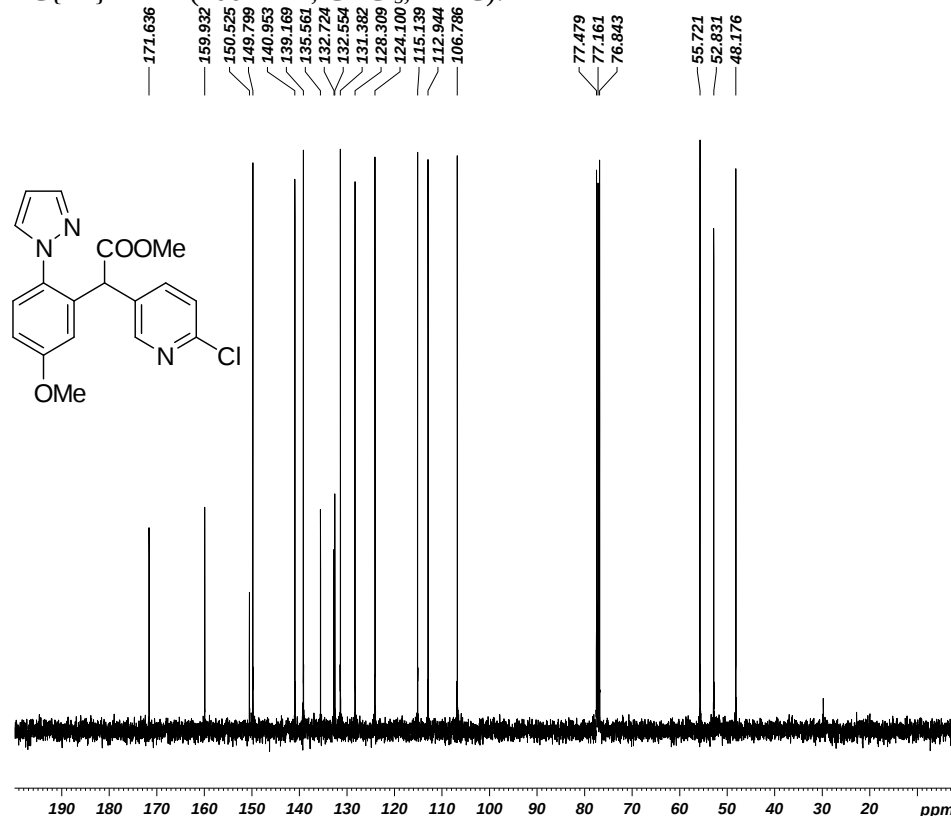
Current Data Parameters
NAME 11.16
EXPNO 567
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161119
Time 6.58
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 108.26
DW 62.400 usec
DE 6.50 usec
TE 297.3 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 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 11.16
EXPNO 568
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161119
Time 7.05
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 297.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

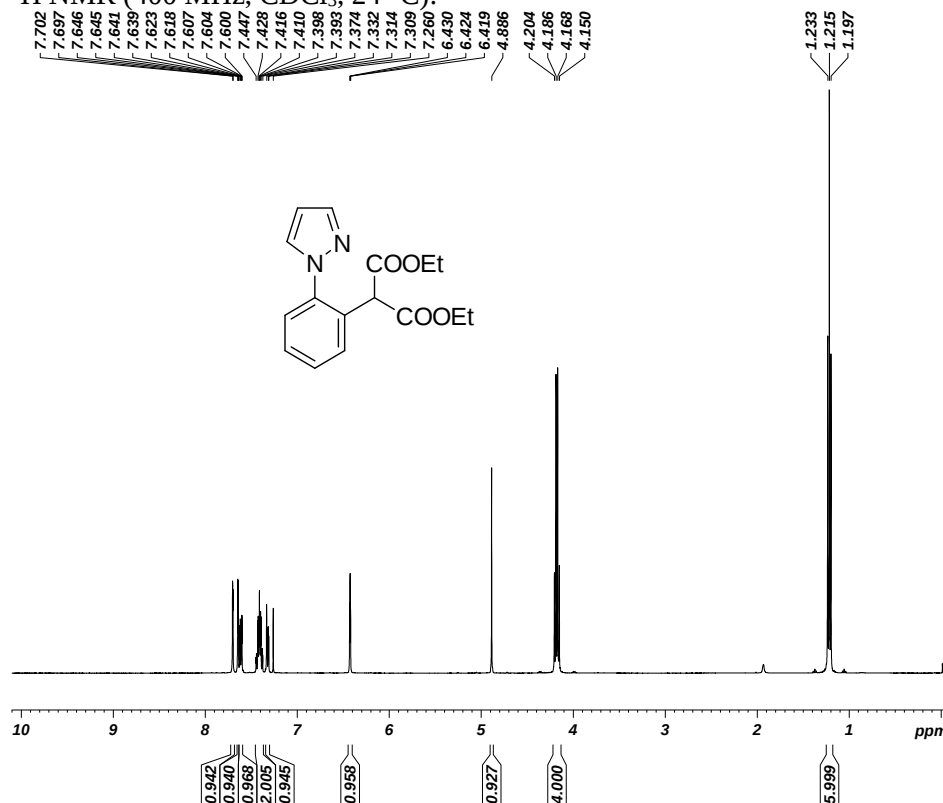
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127598 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Diethyl 2-(2-(1H-pyrazol-1-yl)phenyl)malonate (5j):

^1H NMR (400 MHz, CDCl_3 , 24 °C):



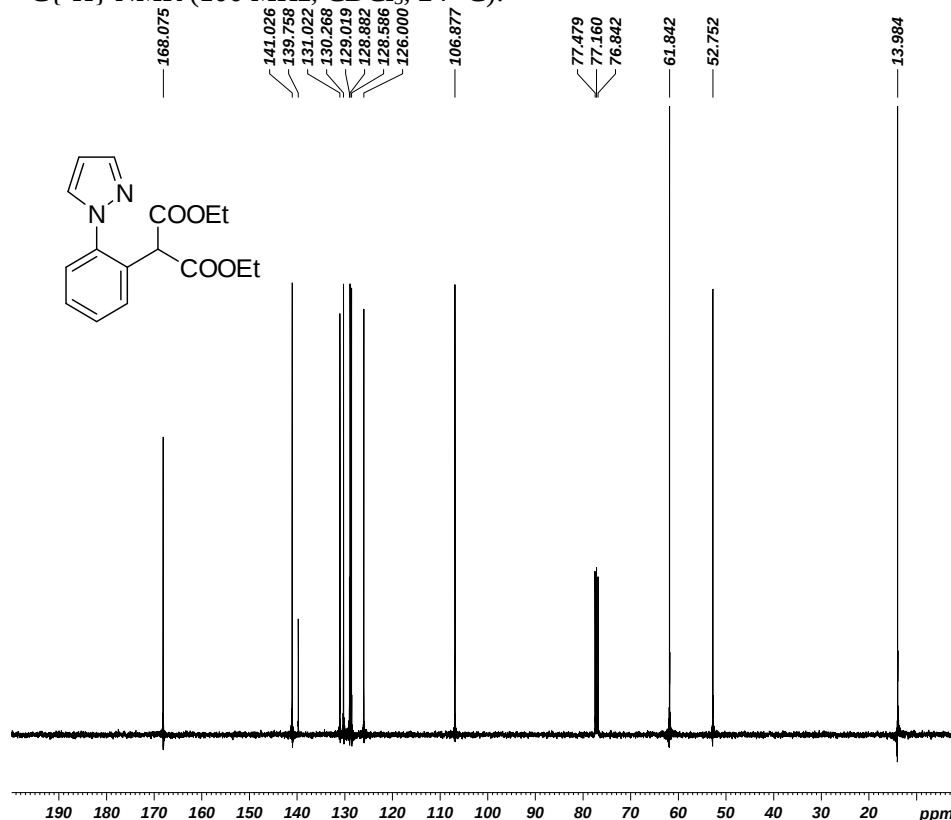
Current Data Parameters
NAME 11.16
EXPNO 570
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161119
Time 7.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.9
DW 62.400 usec
DE 6.50 usec
TE 297.3 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 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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



Current Data Parameters
NAME 11.16
EXPNO 571
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161119
Time 7.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl_3
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 297.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

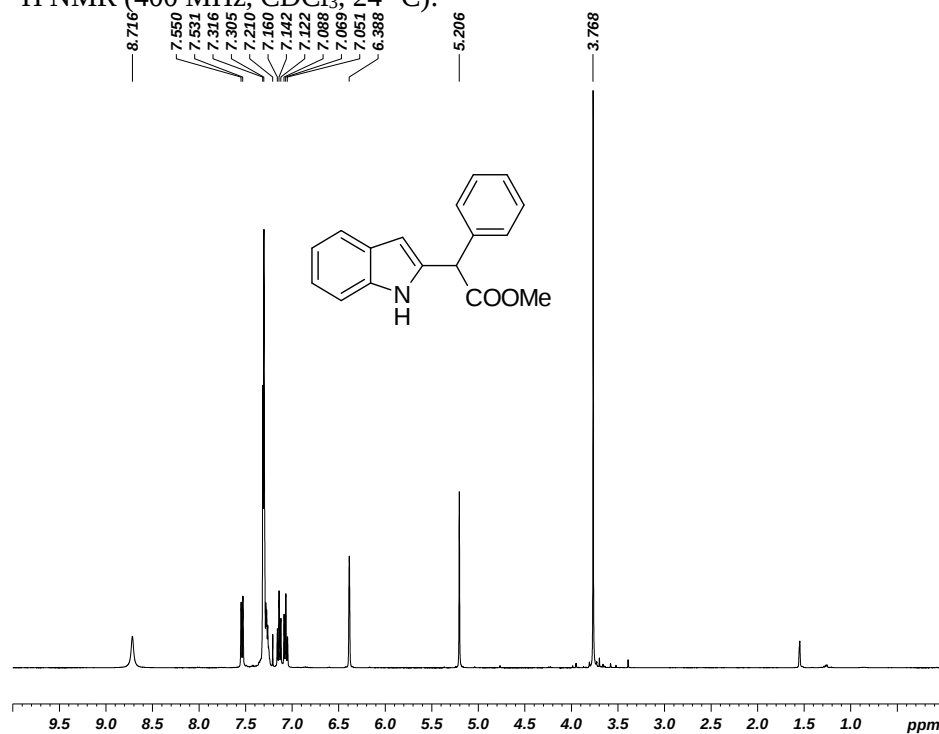
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 ^{13}C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ^1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127684 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(1H-indol-2-yl)-2-phenylacetate (6):

¹H NMR (400 MHz, CDCl₃, 24 °C):



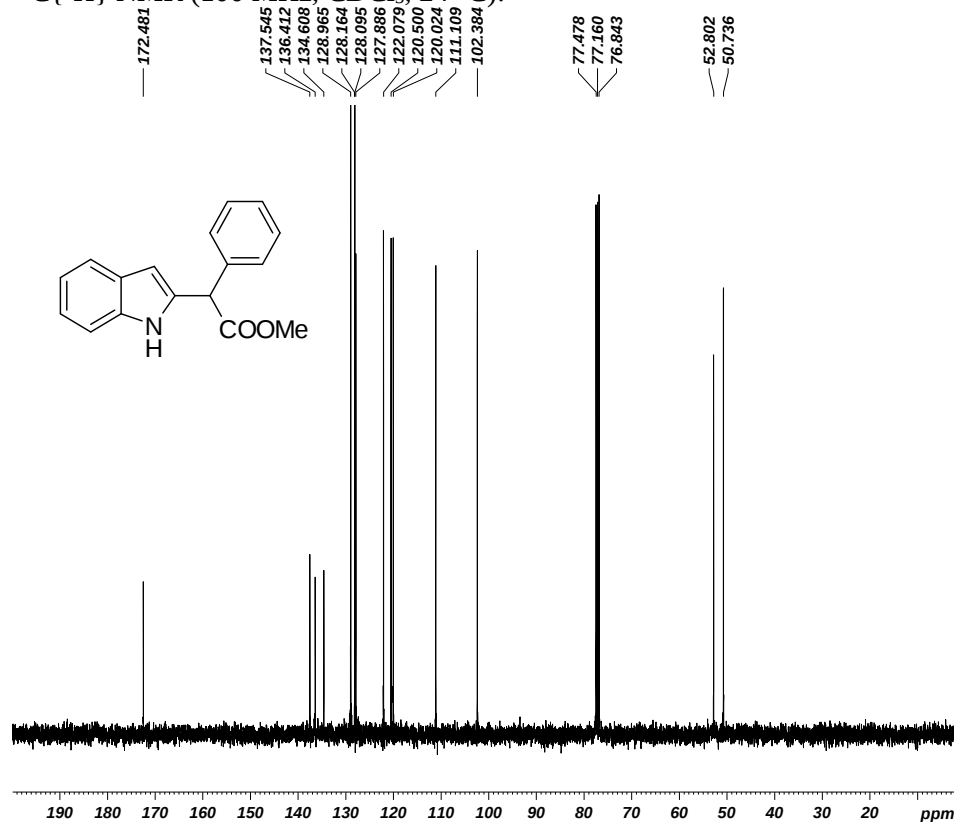
Current Data Parameters
NAME 03.18
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180302
Time 8.14
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 108.26
DW 62.400 usec
DE 6.50 usec
TE 299.6 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 400.1300292 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 03.18
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180302
Time 8.21
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

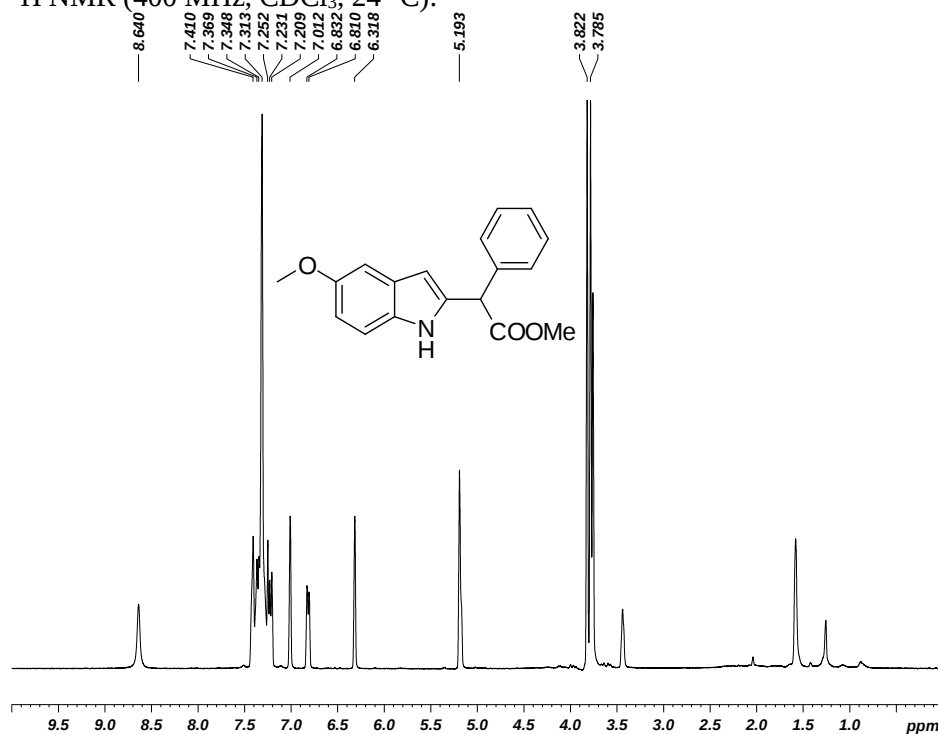
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127606 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(5-methoxy-1H-indol-2-yl)-2-phenylacetate:

¹H NMR (400 MHz, CDCl₃, 24 °C):



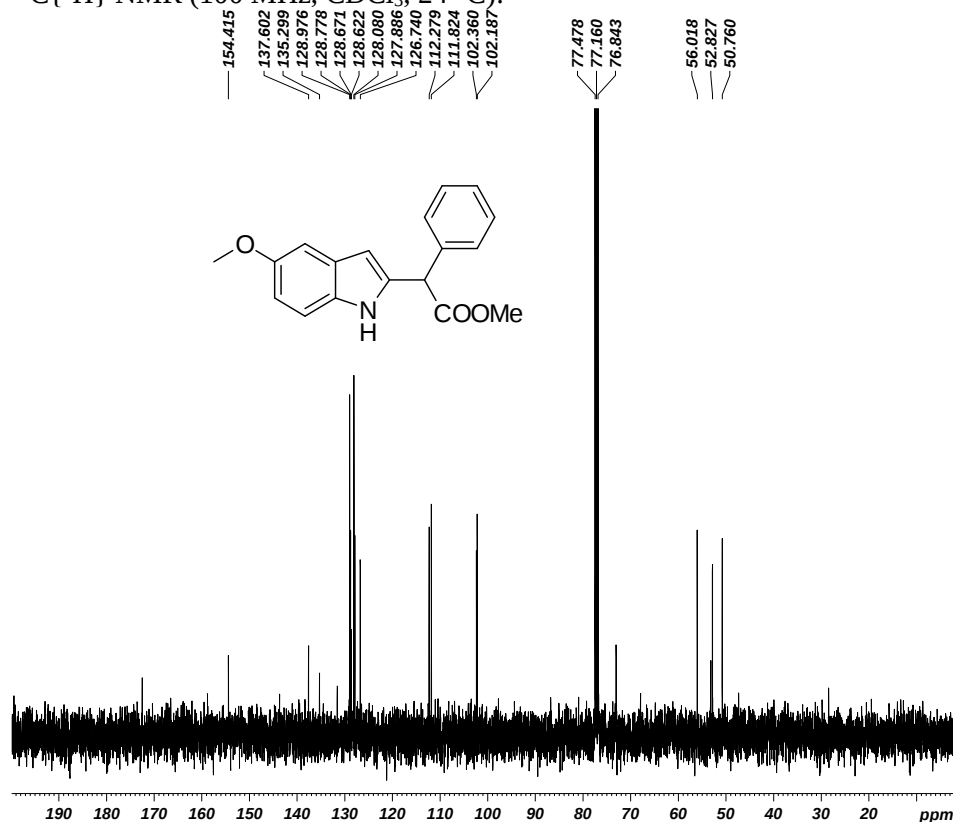
Current Data Parameters
NAME 04.18
EXPNO 604
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180501
Time 12.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 11
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 299.7 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 400.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 04.18
EXPNO 605
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180501
Time 12.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 81
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 299.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

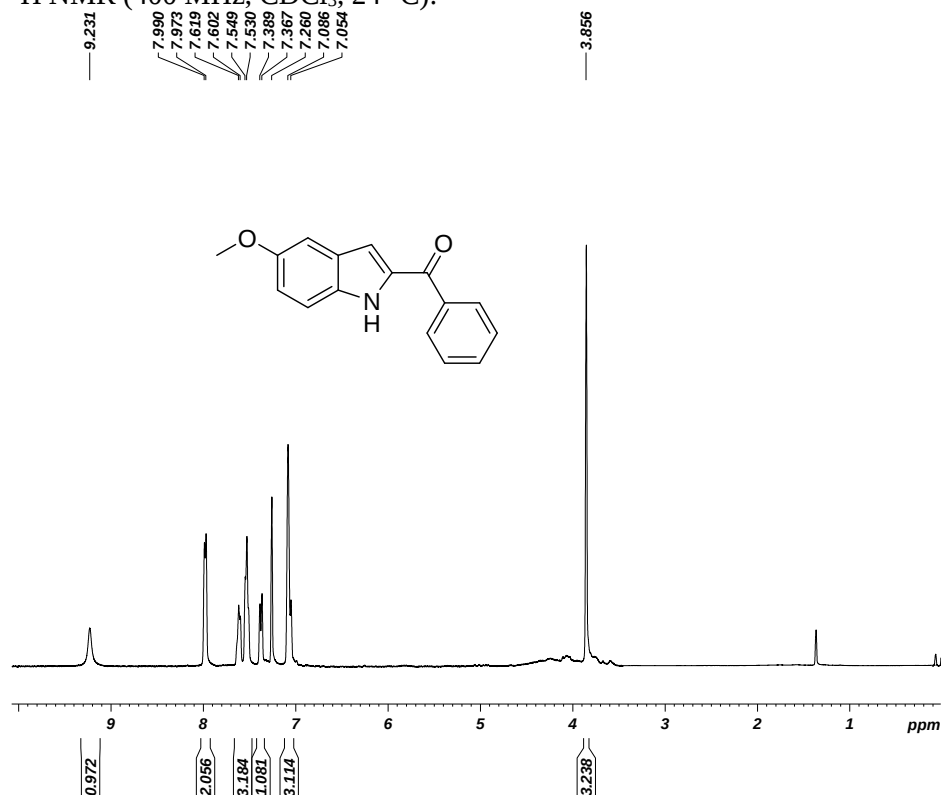
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127556 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

(5-Methoxy-1H-indol-2-yl)(phenyl)methanone (8):

¹H NMR (400 MHz, CDCl₃, 24 °C):



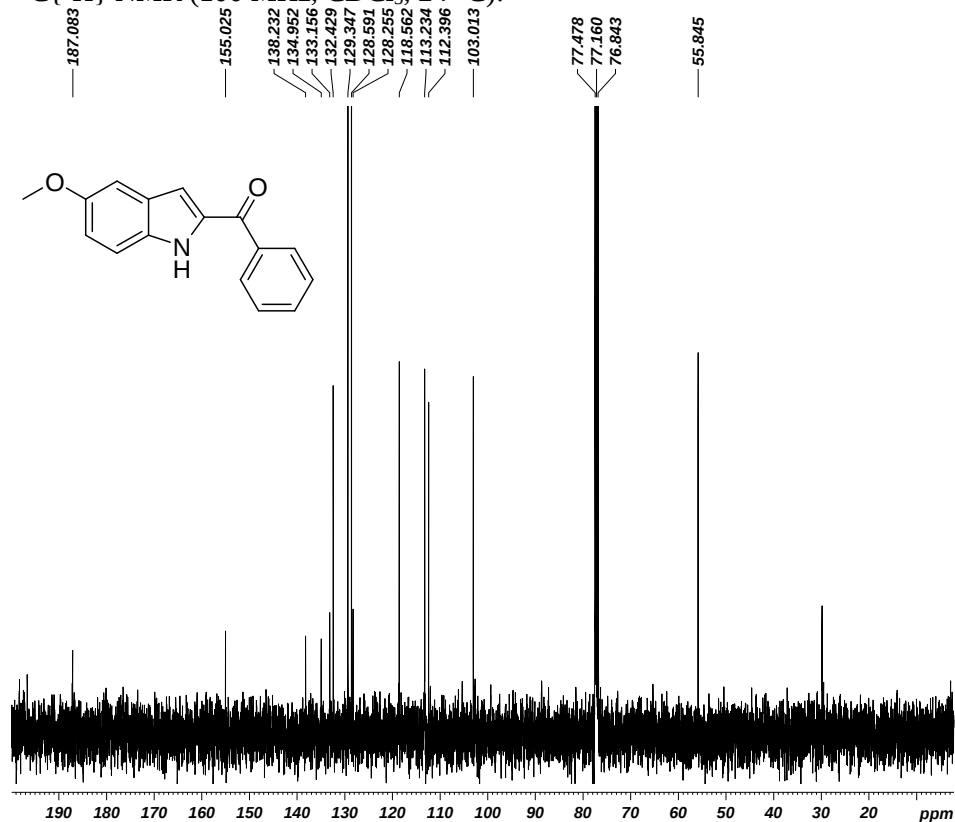
Current Data Parameters
NAME 05.18
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180501
Time 23.34
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 299.6 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 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 05.18
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180502
Time 8.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 1000
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 299.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

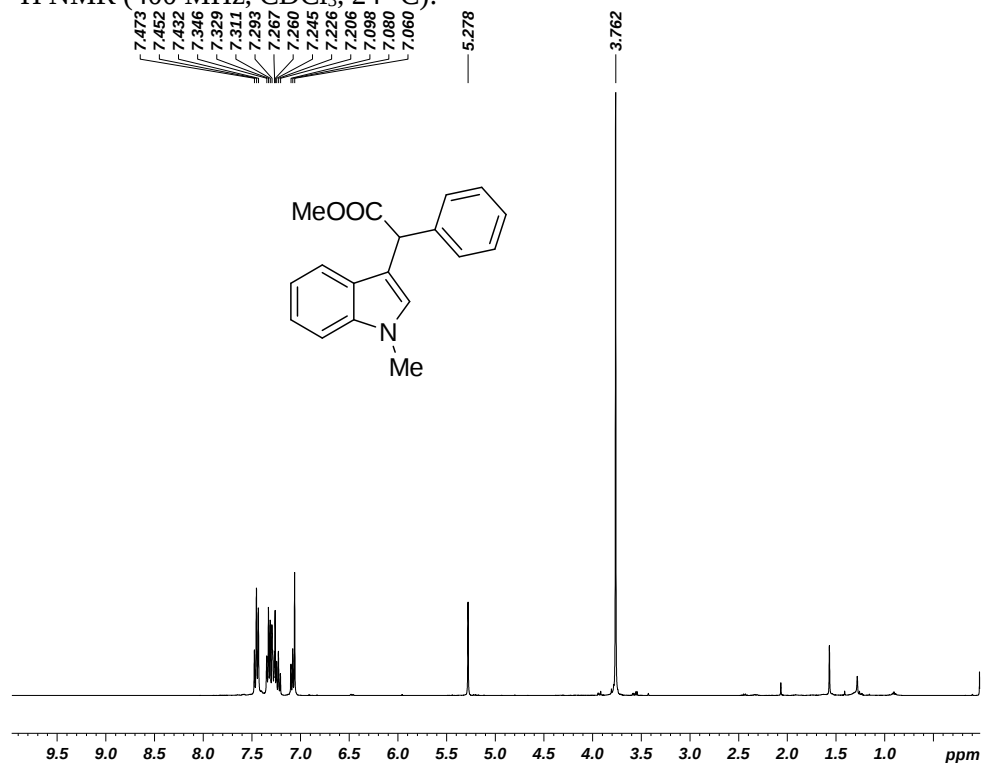
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127539 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-(1-methyl-1H-indol-3-yl)-2-phenylacetate (9a):

^1H NMR (400 MHz, CDCl_3 , 24 °C):



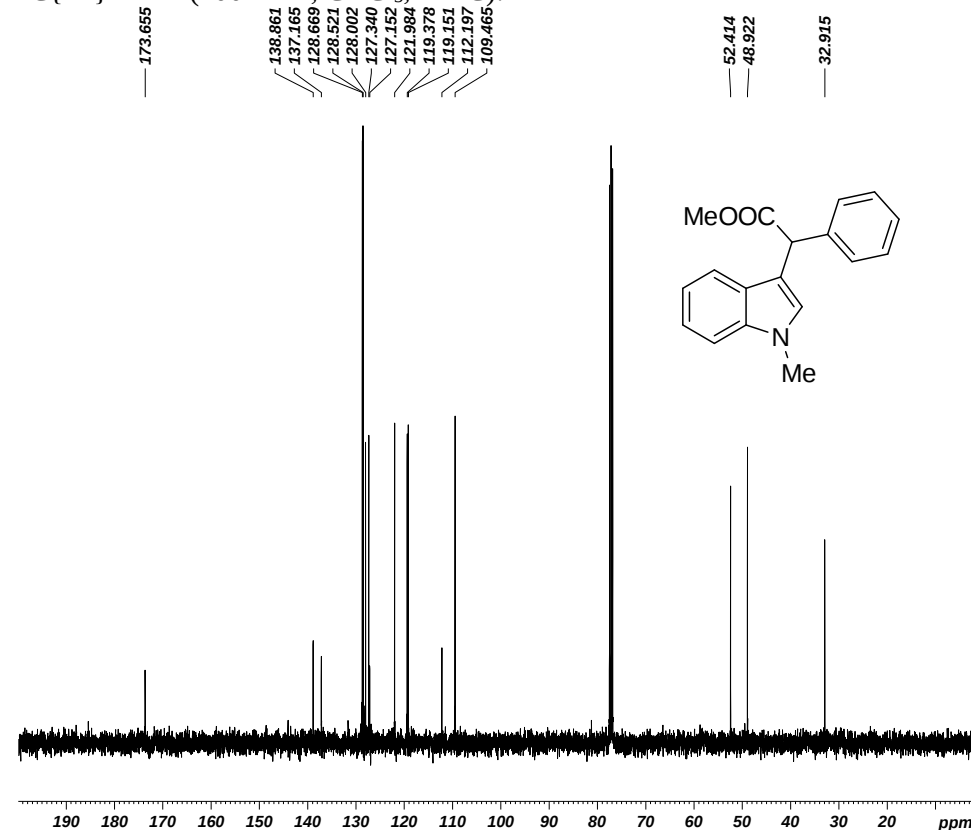
Current Data Parameters
NAME 09.18
EXPNO 402
PROCNO 1

F2 - Acquisition Parameters
Date 20180914
Time 18.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 153.13
DW 62.400 usec
DE 6.50 usec
TE 298.8 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.132007 MHz
NUC1 ^1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.130097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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



Current Data Parameters
NAME 09.18
EXPNO 403
PROCNO 1

F2 - Acquisition Parameters
Date 20180914
Time 18.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl_3
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 298.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

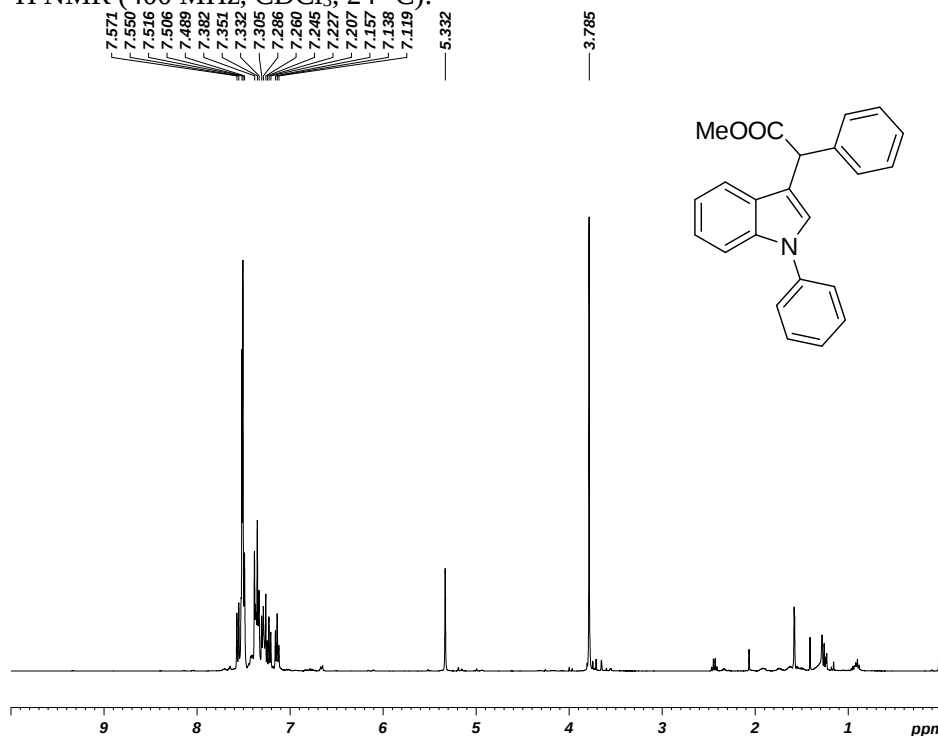
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 ^{13}C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ^1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127574 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Methyl 2-phenyl-2-(1-phenyl-1H-indol-3-yl)acetate (9b):

^1H NMR (400 MHz, CDCl_3 , 24 °C):



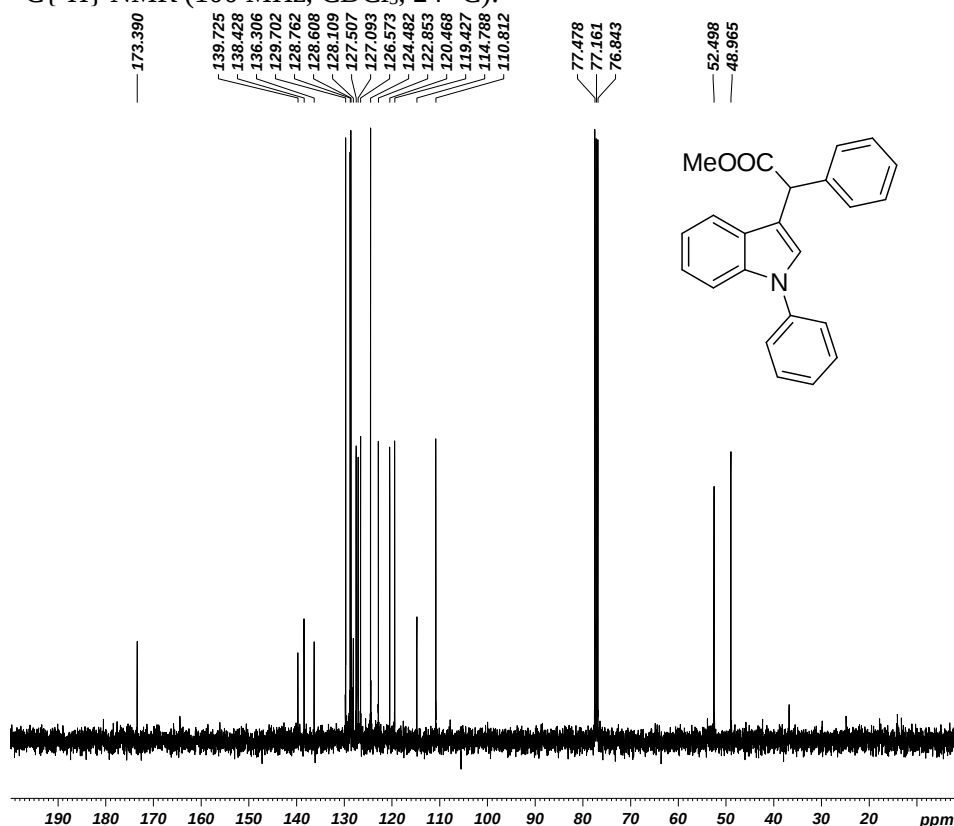
Current Data Parameters
NAME 09.18
EXPNO 404
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180914
Time 18.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl_3
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 298.5 K
D1 0.50000000 sec
TD0 1

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

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

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



Current Data Parameters
NAME 09.18
EXPNO 405
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180914
Time 19.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl_3
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

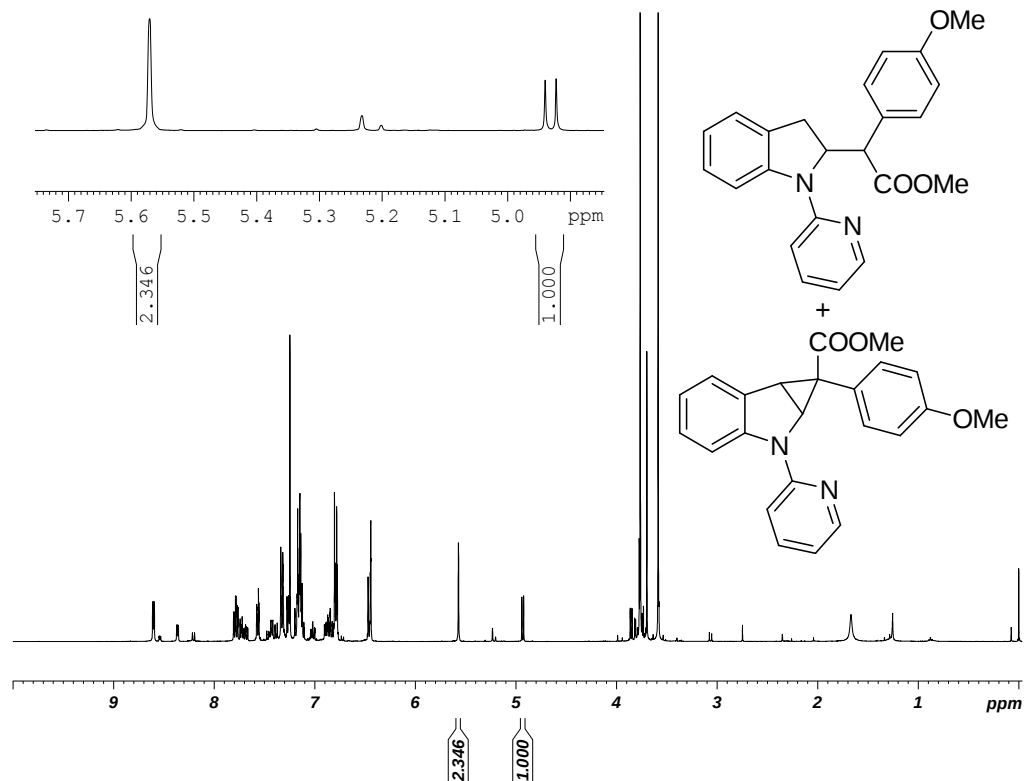
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 ^{13}C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ^1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127575 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Mixture of Methyl 2-(4-methoxyphenyl)-2-(1-(pyridin-2-yl)-1H-indol-2-yl)acetate and methyl 1-(4-methoxyphenyl)-2-(pyridin-2-yl)-1,2-dihydrocyclopropa[b]indole-1-carboxylate

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$):



Current Data Parameters

NAME 11.15
EXPNO 125
PROCNO 1

F2 - Acquisition Parameters

Date_ 20151105
Time 3.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl_3
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 293.5 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====

NUC1 ^1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz

F2 - Processing parameters

SI 65536
SF 400.1300148 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00