Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

Catalyst-Free Three-Component Synthesis of Highly Functionalized 2,3-Dihydropyrroles

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1. General Experimental

The preparation experiments were performed under an argon atmosphere in oven dried glassware. Solvents used as reaction media were distilled immediately before use: THF and ether were distilled from Na/benzophenone ketyl, dichloromethane was distilled from calcium hydride, DMF was obtained from vacuum distillation, EtOH was distilled from Mg and I_2. All reagents were purchased at the highest commercial quality and used without further purification. Reactions were monitored by thin layer chromatography (TLC) using ultra violet light (UV) as the visualizing agent. Nuclear magnetic resonance spectra (NMR) were recorded on Bruker AV-400 instruments and were calibrated using residual undeuterated solvent as an internal reference (^{1}H NMR: $CHC1_3$ 7.26 ppm, MeOH 3.31 ppm). The following abbreviations were used to indicate multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, qui = quintet, sxt = sextet, dd = doublet of doublets, dt = doublet of triplets, ddd = doublet of doublet of doublets, ddt = doublet of doublet of triplets, m = multiplet).

General Procedure A: Preparation of pyruvic amides (3)

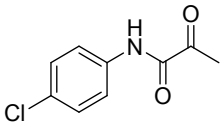
To a solution of pyruvic acid (1.1 equiv) in anhydrous DMF (0.3 M) was added HATU (1.3 equiv) at 0^{o}C. After stirring for 10 minutes, amine (1.0 equiv) and DIEA (3.0 equiv) were slowly added. The resulting reaction mixture was warmed to r.t. and stirred for several hours until the reaction is complete as indicated by TLC. The reaction mixture was diluted with EtOAc and water, the separated organic layer was washed sequentially with 5% citric acid solution, half-saturated aqueous NaCl for five times, dried over Na_2SO_4, filtered and concentrated under reduced pressure to afford the crude product, which was purified by column chromatography on silica gel (PE/EA 100:1).

General Procedure B: Preparation of 2,3-dihydropyrroles (4)

A solution of amine (1.0 equiv), aldehyde (2.0 equiv), pyruvic amide (2.0 equiv) and acetic acid (V_{EtOH} : V_{AcOH} = 12:1) in anhydrous EtOH (amine concentration: 0.025 mol/L) was stirred under reflux for 8 h. After cooled down to r.t., ethanol was removed under vacuum,

and the residue was diluted with EtOAc and water. After separation, the aqueous phase was extracted two more times with EtOAc. The combined organic phases were successively washed with saturated aqueous $KHSO_4$, saturated aqueous $NaHCO_3$, and brine, dried over $MgSO_4$, concentrated *in vacuo* and chromatographed gradiently on silica gel with PE/EA (5:1~3:1) to give the dihydropyrrole products.

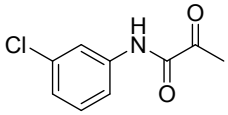
2. Preparation Procedure for 3, 4, 5 and 6



3a

***N*-(4-Chlorophenyl)-2-oxopropanamide (3a)**

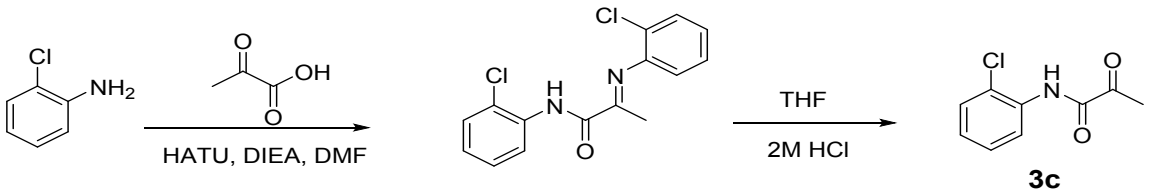
Using 4-chloroaniline (1.0 g, 7.8 mmol), in accordance with General Procedure A, the title compound **3a** was obtained (810 mg, 52% yield) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (s, 1H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 2.57 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.1, 157.6, 135.0, 130.6, 129.5, 121.1, 24.2. HRMS (ESI-TOF) *m/z* calcd. for $C_9H_7NO_2Cl^-$ [M-H]$^-$: 196.0171, found 196.0170.



3b

***N*-(3-Chlorophenyl)-2-oxopropanamide (3b)**

Using 3-chloroaniline (1.0 g, 7.8 mmol), in accordance with General Procedure A, the title compound **3b** was obtained (900 mg, 59% yield) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (s, 1H), 7.78 (t, *J* = 2.0 Hz, 1H), 7.46 (dd, *J* = 1.6, 8.0 Hz, 1H), 7.29 (t, *J* = 8.0 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 1H), 2.57 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 157.7, 137.5, 135.1, 130.4, 125.5, 120.0, 117.9, 24.1. HRMS (ESI-TOF) *m/z* calcd. for $C_9H_7NO_2Cl^-$ [M-H]$^-$: 196.0171, found 196.0172.

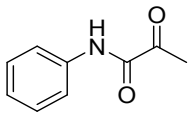


3c

***N*-(2-Chlorophenyl)-2-oxopropanamide (3c)**

To a solution of pyruvic acid (2.8 g, 31.4 mmol) in anhydrous DMF (30 ml) was added HBTU (11.9 g, 31.4 mmol) at 0 ℃. After stirring for 10 minutes, 2-chloroaniline (2.0 g, 15.7 mmol) and DIEA (6.1 g, 47.1 mmol) were slowly added. The resulting reaction mixture was warmed to r.t. and stirred for several hours until the reaction is complete as indicated by TLC. The reaction mixture was diluted with EtOAc and water, the separated organic layer was washed sequentially with 5% citric acid solution, half-saturated aqueous NaCl for five times, dried over Na_2SO_4, filtered and concentrated under reduced pressure to afford the crude product, which was purified by column chromatography on silica gel (PE/EA 100:1) to produce the imine intermediate (~ 600 mg).

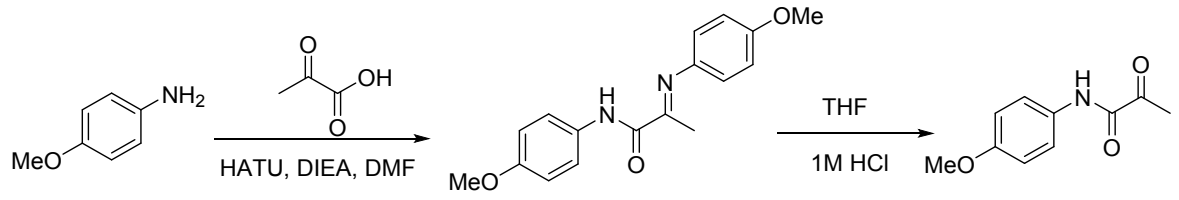
A solution of the intermediate (500 mg) in THF (12 ml) and 2 M HCl (5 ml) was stirred under reflux for 3 h. The reaction mixture was diluted with EtOAc and water, the separated organic layer was washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure to afford **3c** (316 mg, 98% yield) as a pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.38 (s, 1H), 8.45 (d, *J* = 8.4 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.32 (t, *J* = 8.0 Hz, 1H), 7.11 (t, *J* = 8.0 Hz, 1H), 2.58 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.7, 157.7, 133.3, 129.5, 128.0, 125.8, 123.9, 121.1, 24.1. HRMS (ESI-TOF) *m/z* calcd. for $C_9H_7NO_2Cl^-$ $[M-H]^-$: 196.0171, found 196.0166.



3d

2-Oxo-*N*-phenylpropanamide (3d)

Using aniline (3.0 g, 7.8 mmol), in accordance with General Procedure A, the title compound **3d** was obtained (3.0 g, 57% yield) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (s, 1H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 8.0 Hz, 2H), 7.18 (t, *J* = 7.6 Hz, 1H), 2.57 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.5, 157.7, 136.4, 129.4, 125.4, 119.8, 24.2. HRMS (ESI-TOF) *m/z* calcd. for $C_9H_{10}NO_2$ $[M+H]^+$: 164.0706, found 164.0712.

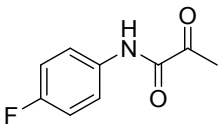


3e

***N*-(4-Methoxyphenyl)-2-oxopropanamide (3e)**

To a solution of pyruvic acid (1.2 g, 13.6 mmol) in anhydrous DMF (20 ml) was added HATU (6.7 g, 17.7 mmol) at 0 °C. After stirring for 10 minutes, *p*-anisidine (3.0 g, 24.4 mmol) and DIEA (5.3 g, 41.0 mmol) were slowly added. The resulting reaction mixture was warmed to r.t. and stirred for several hours until the reaction is complete as indicated by TLC. The reaction mixture was diluted with EtOAc and water, the separated organic layer was washed sequentially with 5% citric acid solution, and half-saturated aqueous NaCl for five times, dried over Na_2SO_4, filtered and concentrated under reduced pressure to afford the crude product, which was purified by column chromatography on silica gel (PE/EA 100:1~50:1) to produce the imine intermediate (~1.6 g).

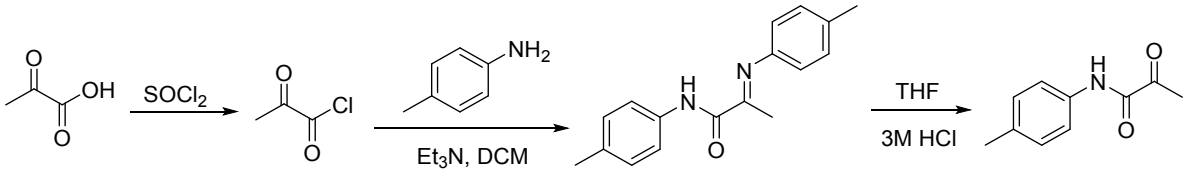
A solution of the imine intermediate (1.2 g, 4.0 mmol) in THF (45 ml) and 1 M HCl (24 ml) was stirred under reflux for 3 h. The reaction mixture was diluted with EtOAc and water, the separated organic layer was washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure to afford the crude product, which was purified by column chromatography on silica gel (PE/EA 10:1) to afford **3e** (720 mg, 93% yield) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (s, 1H), 7.56 (d, J = 8.8 Hz, 2H), 6.90 (d, J = 8.8 Hz, 2H), 3.81 (s, 3H), 2.56 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.7, 157.4, 157.2, 129.6, 121.4, 114.5, 55.6, 24.3. HRMS (ESI-TOF) *m/z* calcd. for $C_{10}H_{10}NO_3^-$ [M-H]$^-$: 192.0666, found 192.0665.



3f

***N*-(4-Fluorophenyl)-2-oxopropanamide (3f)**

Using *p*-fluoroaniline (1.0 g, 9.0 mmol), in accordance with General Procedure A, the title compound **3f** was obtained (350 mg, 22% yield) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (s, 1H), 7.61 (dd, *J* = 4.8, 8.8 Hz, 2H), 7.06 (t, *J* = 8.8 Hz, 2H), 2.56 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 161.2, 158.2 (d, *J* = 119.0 Hz), 132.5 (d, *J* = 2.0 Hz), 121.6 (d, *J* = 8.0 Hz), 116.1 (d, *J* = 23.0 Hz), 24.2. HRMS (ESI-TOF) *m/z* calcd. for $C_9H_7NO_2F^-$ $[M-H]^-$: 180.0466, found 180.0461.



3g

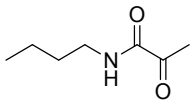
2-Oxo-*N*-(p-tolyl)propanamide (3g)

A solution of pyruvic acid (5.0 g, 57 mmol) in $SOCl_2$ (30 ml) was refluxed for 2 h. After cooled down to r.t., $SOCl_2$ was removed under vacuum to afford the acyl chloride intermediate.

To a cold (0 ℃) solution of acyl chloride in dichloromethane (15 ml) was added *p*-toluidine (15.3 g, 143 mmol) and Et_3N (23 g, 228 mmol). The medium was stirred at room temperature for several hours until the reaction is complete as indicated by TLC. The reaction mixture was diluted with dichloromethane and water, the separated organic layer was washed with 1 M HCl, brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure to afford the crude product, which was purified by column chromatography on silica gel (PE/EA 50:1) to give the imine intermediate (~4.0 g).

A solution of the imine intermediate (4.0 g) in THF (20 ml) and 3 M HCl (20 ml) was stirred under reflux for 3 h. The reaction mixture was diluted with EtOAc and water, the separated organic layer was washed with brine, dried over Na_2SO_4, filtered and concentrated under vacum to afford the crude product, which was purified by column chromatography on silica gel (PE/EA 10:1) to afford **3g** (2.2 g, 82% yield) as a pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (s, 1H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.17 (d, *J* = 8.4 Hz, 2H), 2.56 (s, 3H), 2.34 (s,

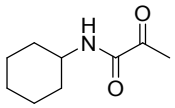
3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 157.6, 135.2, 133.9, 129.9, 119.8, 24.2, 21.1. HRMS (ESI-TOF) *m/z* calcd. for $C_{10}H_{10}NO_2^-$ [M-H]$^-$: 176.0717, found 176.0724.



3h

***N*-Butyl-2-oxopropanamide (3h)**

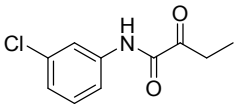
Using *n*-butylamine (1.0 g, 13.7 mmol), in accordance with General Procedure A, the title compound **3h** was obtained (504 mg, 26% yield) as a purple solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.96 (s, 1H), 3.29-3.24 (m, 2H), 2.45 (s, 3H), 1.54-1.47 (m, 2H), 1.34 (sxt, *J* = 7.2 Hz, 2H), 0.91 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 160.2, 39.0, 31.2, 24.4, 19.9, 13.6. HRMS (ESI-TOF) *m/z* calcd. for $C_7H_{14}NO_2$ [M+H]$^+$: 144.1019, found 144.1018.



3i

***N*-Cyclohexyl-2-oxopropanamide (3i)**

Using cyclohexylamine (1.0 g, 10.1 mmol), in accordance with General Procedure A, the title compound **3i** was obtained (1.0 g, 61% yield) as a brown crystal. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.81 (s, 1H), 3.76-3.67 (m, 1H), 2.46 (s, 3H), 1.92-1.88 (m, 2H), 1.75-1.64 (m, 2H), 1.63-1.60 (m, 2H), 1.42-1.32 (m, 2H), 1.25-1.16 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.8, 159.3, 48.5, 32.8, 25.5, 24.8, 24.5. HRMS (ESI-TOF) *m/z* calcd. for $C_9H_{16}NO_2$ [M+H]$^+$: 170.1176, found 170.1179.

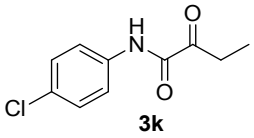


3j

***N*-(3-Chlorophenyl)-2-oxobutanamide (3j)**

Using 3-chloroaniline (1.5 g, 11.8 mmol) and 2-oxobutyric acid (1.3 g, 13 mmol) in accordance with General Procedure A, the title compound **3j** was obtained (270 mg, 11% yield) as a pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (s, 1H), 7.79 (t, *J* = 2.0 Hz, 1H), 7.47 (dd, *J* = 1.2, 8.0 Hz, 1H), 7.29 (t, *J* = 8.0 Hz, 1H), 7.15 (dd, *J* = 1.2, 8.0 Hz, 1H),

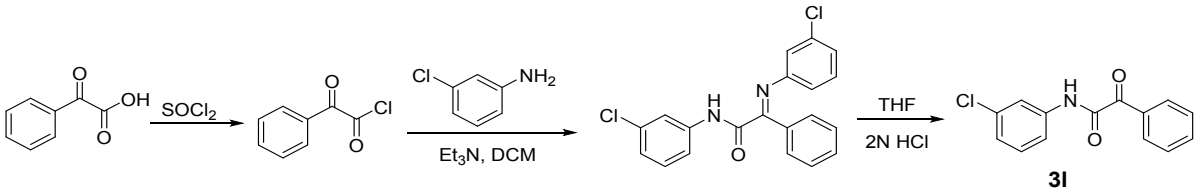
3.05 (q, J = 7.2 Hz, 2H), 1.17 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.6, 157.7, 137.6, 135.1, 130.4, 125.5, 120.0, 117.9, 30.1, 7.3. HRMS (ESI-TOF) *m/z* calcd. for $C_{10}H_9NO_2Cl^-$ [M-H]$^-$: 210.0327, found 210.0326.



3k

***N*-(4-chlorophenyl)-2-oxobutanamide (3k)**

Using 4-chloroaniline (2.6 g, 20.2 mmol) and 2-oxobutyric acid (3.3 g, 32.3 mmol) in accordance with General Procedure A, the title compound **3k** was obtained (900 mg, 20% yield) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (s, 1H), 7.60 (d, J = 8.8 Hz, 2H), 7.33 (d, J = 8.8 Hz, 2H), 3.04 (q, J = 7.2 Hz, 2H), 1.61 (t, J = 7.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.8, 157.6, 135.1, 130.5, 129.4, 121.1, 30.1, 7.3. HRMS (ESI-TOF) *m/z* calcd. for $C_{10}H_9NO_2Cl^-$ [M-H]$^-$: 210.0327, found 210.0327.



3l

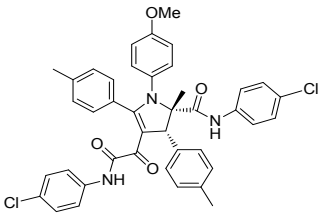
***N*-(3-chlorophenyl)-2-oxo-2-phenylacetamide (3l)**

A solution of benzoylformic acid (3.0 g, 20 mmol) in $SOCl_2$ (20 ml) was refluxed for 2 h. After cooled down to r.t., $SOCl_2$ was removed under vacuum to afford the acyl chloride intermediate.

To a cold (0 ℃) solution of acyl chloride in dichloromethane (10 ml) was added 3-chloroaniline (2.8 g, 22 mmol) and Et_3N (8.0 g, 80 mmol). The medium was stirred at room temperature for several hours until the reaction is complete as indicated by TLC. The reaction mixture was diluted with dichloromethane and water, the separated organic layer was washed with 1 M HCl, brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure to afford the crude product, which was purified by column chromatography on silica gel (PE/EA 50:1) to give the imine intermediate (~2.7 g).

A solution of the imine intermediate (2.4 g) in THF (30 ml) and 2 M HCl (20 ml) was stirred under reflux for 3 h. The reaction mixture was diluted with EtOAc and water, the separated

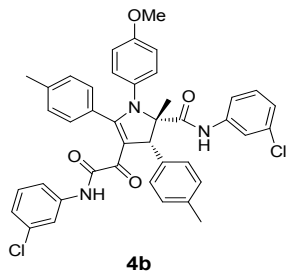
organic layer was washed with brine, dried over Na_2SO_4, filtered and concentrated under vacum to afford the crude product, which was purified by column chromatography on silica gel (PE/EA 10:1) to afford **3l** (1.5 g, 88% yield) as a pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (s, 1H), 8.42 (d, *J* = 7.6 Hz, 2H), 7.872-7.868 (m, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.53 (t, *J* = 8.0 Hz, 3H), 7.34 (t, *J* = 8.0 Hz, 1H), 7.18 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.0, 158.9, 137.9, 135.1, 135.0, 133.0, 131.7, 130.4, 128.8, 125.5, 120.2, 118.0. HRMS (ESI-TOF) *m/z* calcd. for $C_{14}H_9NO_2Cl^-$ [M-H]$^-$: 258.0327, found 258.0339.



4a

(2S,3R)-*N*-(4-Chlorophenyl)-4-(2-((4-chlorophenyl)amino)-2-oxoacetyl)-1-(4-methoxyphenyl)-2-methyl-3,5-di-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4a)

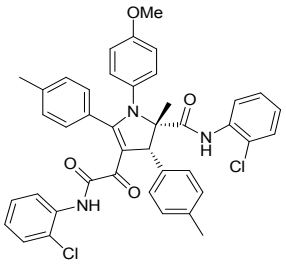
Using *p*-anisidine (31 mg, 0.25 mmol), *p*-tolualdehyde (60 mg, 0.5 mmol), and **3a** (100 mg, 0.5 mmol) in accordance with General Procedure B, the title compound was obtained (89 mg, 51% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (s, 1H), 8.03 (s, 1H), 7.20-7.15 (m, 6H), 7.10 (d, *J* = 8.4 Hz, 4H), 7.03 (d, *J* = 8.4 Hz, 2H), 6.97 (d, *J* = 8.0 Hz, 4H), 6.86 (d, *J* = 9.2 Hz, 2H), 6.68 (d, *J* = 8.8 Hz, 2H), 5.11 (s, 1H), 3.70 (s, 3H), 2.22 (s, 3H), 2.19 (s, 3H), 1.67 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.4, 168.3, 166.3, 162.4, 158.3, 140.5, 137.3, 135.8, 135.6, 134.2, 130.8, 129.6, 129.33, 129.26, 129.21, 129.1, 128.84, 128.77, 128.69, 128.3, 128.0, 121.6, 121.1, 114.4, 111.0, 78.6, 61.0, 55.4, 23.5, 21.5, 21.1. HRMS (ESI-TOF) *m/z* calcd. for $C_{41}H_{36}N_3O_4Cl_2$ [M+H]$^+$: 704.2077, found 704.2052.



4b

(2S,3R)-*N*-(3-Chlorophenyl)-4-(2-((3-chlorophenyl)amino)-2-oxoacetyl)-1-(4-methoxyphenyl)-2-methyl-3,5-di-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4b)

Using *p*-anisidine (31 mg, 0.25 mmol), *p*-tolualdehyde (60 mg, 0.5 mmol), and **3b** (100 mg, 0.5 mmol), in accordance with General Procedure B, the title compound was obtained (87 mg, 49% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (s, 1H), 7.79 (s, 1H), 7.22-7.20 (m, 3H), 7.18-7.13 (m, 4H), 7.11-7.09 (m, 1H), 7.05-6.95 (m, 8H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.68 (d, *J* = 8.8 Hz, 2H), 5.16 (s, 1H), 3.71 (s, 3H), 2.28 (s, 3H), 2.20 (s, 3H), 1.70 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.2, 168.4, 166.5, 162.6, 162.5, 158.3, 140.6, 138.3, 138.1, 137.5, 134.4, 134.3, 130.9, 129.73, 129.67, 129.4, 129.3, 129.1, 128.9, 128.3, 128.0, 124.8, 124.3, 120.8, 120.1, 118.7, 118.0, 114.4, 111.0, 78.7, 60.8, 55.4, 23.7, 21.4, 21.1. HRMS (ESI-TOF) *m/z* calcd. for $C_{41}H_{36}N_3O_4Cl_2$ $[M+H]^+$: 704.2077, found 704.2076.

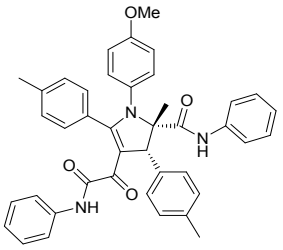


4c

(2S,3R)-*N*-(2-Chlorophenyl)-4-(2-((2-chlorophenyl)amino)-2-oxoacetyl)-1-(4-methoxyphenyl)-2-methyl-3,5-di-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4c)

Using *p*-anisidine (31 mg, 0.25 mmol), *p*-tolualdehyde (60 mg, 0.5 mmol), and **3c** (100 mg, 0.5 mmol), in accordance with General Procedure B, the title compound was obtained (109 mg, 62% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (s, 1H), 8.79 (s, 1H), 7.70 (dd, *J* = 8.0, 14.0 Hz, 2H), 7.37-7.35 (m, 1H), 7.32-7.29 (m, 2H), 7.271-7.269 (m, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.14-7.06 (m, 4H), 7.02-6.97 (m, 1H), 6.94 (d, *J* = 8.8 Hz, 3H), 6.90 (d, *J* = 7.6 Hz, 2H), 6.66 (d, *J* = 8.8 Hz, 2H), 5.28 (s, 1H), 3.70 (s, 3H), 2.28 (s, 3H), 2.10 (s, 3H), 1.65 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.8, 168.6, 166.0, 161.5, 158.3, 140.2, 137.1, 135.2, 134.1, 133.9, 131.5, 129.40, 129.35, 129.23, 129.18, 129.10, 128.9, 128.5, 128.3, 127.6, 127.4, 124.83, 124.76, 123.5, 122.9, 121.23, 121.20, 114.4, 111.8, 78.9, 61.5,

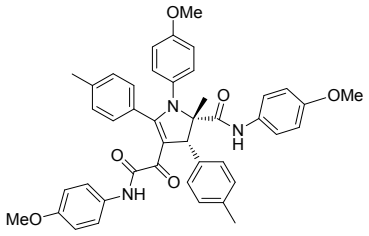
55.4, 24.3, 21.6, 21.0. HRMS (ESI-TOF) *m/z* calcd. for $C_{41}H_{36}N_3O_4Cl_2$ $[M+H]^+$: 704.2077, found 704.2079.



4d

(2S,3R)-1-(4-Methoxyphenyl)-2-methyl-4-(2-oxo-2-(phenylamino)acetyl)-*N*-phenyl-3,5-di-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4d)

Using *p*-anisidine (74 mg, 0.6 mmol), *p*-tolualdehyde (144 mg, 1.2 mmo), and **3d** (200 mg, 1.2 mmol), in accordance with General Procedure B, the title compound was obtained (75 mg, 20% yield) as a yellow solid. ^{1}H NMR (400 MHz, CD_3OD) δ 7.32-7.28 (m, 4H), 7.21-7.14 (m, 4H), 7.12-7.07 (m, 3H), 7.05-6.99 (m, 5H), 6.93 (d, *J* = 8.0 Hz, 2H), 6.86 (d, *J* = 8.0 Hz, 2H), 6.70 (d, *J* = 8.4 Hz, 2H), 4.83 (s, 1H), 3.64 (s, 3H), 2.22 (s, 3H), 2.04 (s, 3H), 1.75 (s, 3H). ^{13}C NMR (100 MHz, CD_3OD) δ 185.8, 170.6, 169.5, 167.4, 160.2, 141.4, 138.8, 138.1, 137.9, 135.9, 132.0, 131.5, 131.1, 130.1, 129.7, 129.6, 129,29, 129.26, 128.7, 126.3, 125.4, 124.1, 121.5, 115.1, 111.7, 79.7, 60.9, 55.8, 25.0, 21.3, 21.1. HRMS (ESI-TOF) *m/z* calcd. for $C_{41}H_{38}N_3O_4$ $[M+H]^+$: 636.2857, found 636.2840.

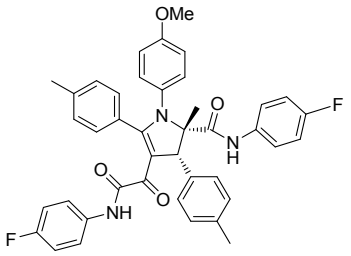


4e

(2S,3R)-1-Butyl-*N*-(3-chlorophenyl)-4-(2-((3-chlorophenyl)amino)-2-oxoacetyl)-2-methyl-3,5-di-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4e)

Using *p*-anisidine (62 mg, 0.5 mmol), *p*-tolualdehyde (120 mg, 1.0 mmol), and **3e** (200 mg, 1.0 mmol), in accordance with General Procedure B, the title compound was obtained (105 mg, 30% yield) as a yellow crystalline solid. ^{1}H NMR (400 MHz, CD_3OD) δ 7.32-7.26 (m,

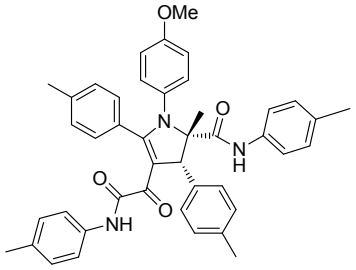
4H), 7.05 (d, J = 10.0 Hz, 3H), 7.01 (d, J = 4.0 Hz, 2H), 6.99 (s, 1H), 6.89 (d, J = 8.0 Hz, 2H), 6.74 (s, 4H), 6.72-6.70 (m, 4H), 4.83 (s, 1H), 3.73 (s, 3H), 3.72 (s, 3H), 3.66 (s, 3H), 2.26 (s, 3H), 2.09 (s, 3H), 1.73 (s, 3H). ^{13}C NMR (100 MHz, CD_3OD) δ 185.9, 170.7, 169.4, 167.1, 160.2, 158.8, 158.0, 141.3, 137.9, 136.03, 136.01, 132.1, 131.8, 131.5, 131.1, 130.9, 130.2, 129.7, 129.6, 128.8, 126.0, 123.1, 115.1, 114.5, 111.8, 79.5, 61.0, 55.82, 55.81, 55.80, 25.1, 21.3, 21.2. HRMS (ESI-TOF) *m/z* calcd. for $C_{43}H_{42}N_3O_6$ $[M+H]^+$: 696.3068, found 696.3066.



4f

(2S,3R)-*N*-(4-Fluorophenyl)-4-(2-((4-fluorophenyl)amino)-2-oxoacetyl)-1-(4-methoxyphenyl)-2-methyl-3,5-di-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4f)

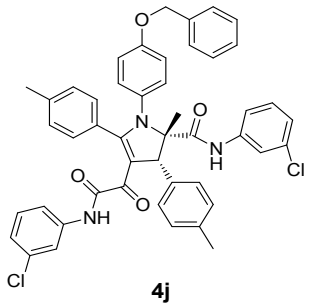
Using *p*-anisidine (62 mg, 0.5 mmol), *p*-tolualdehyde (120 mg, 1.0 mmol), and **3f** (180mg, 1.0 mmol), in accordance with General Procedure B, the title compound was obtained (85 mg, 25% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, J = 12.0 Hz, 1H), 7.89 (d, J = 7.6 Hz, 1H), 7.22 (d, J = 8.0 Hz, 2H), 7.16 (d, J = 8.0 Hz, 2H), 7.11-7.03 (m, 6H), 6.98 (d, J = 7.6 Hz, 2H), 6.93-6.87 (m, 6H), 6.68 (d, J = 8.8 Hz, 2H), 5.20 (s, 1H), 3.71 (s, 3H), 2.29 (s, 3H), 2.19 (s, 3H), 1.69 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.9, 168.3, 166.1, 161.6, 161.0, 160.7, 158.5, 158.4, 158.3, 140.4, 137.4, 134.9, 133.10, 133.06, 131.2, 129.4, 129.2, 128.9, 128.5, 128.4, 122.3 (d, J = 7.0 Hz), 121.6 (d, J = 8.0 Hz), 115.7 (d, J = 4.0 Hz), 115.5 (d, J = 4.0 Hz), 114.5, 78.7, 61.3, 55.5, 23.8, 21.6, 21.2. HRMS (ESI-TOF) *m/z* calcd. for $C_{41}H_{36}N_3O_4F_2$ $[M+H]^+$: 672.2668, found 672.2681.



4g

(2S,3R)-1-(4-Methoxyphenyl)-2-methyl-4-(2-oxo-2-(p-tolylamino)acetyl)-*N*,3,5-tri-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4g)

Using *p*-anisidine (172 mg, 1.4 mmol), *p*-tolualdehyde (336 mg, 2.8 mmol), and **3g** (500 mg, 2.8 mmol), in accordance with General Procedure B, the title compound was obtained (238 mg, 23% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (s, 1H), 7.91 (s, 1H), 7.22 (d, *J* = 7.6 Hz, 2H), 7.18 (d, *J* = 7.6 Hz, 2H), 7.07-6.97 (m, 12H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.66 (d, *J* = 8.8 Hz, 2H), 5.21 (s, 1H), 3.70 (s, 3H), 2.28 (s, 6H), 2.26 (s, 3H), 2.19 (s, 3H), 1.68 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.8, 168.0, 165.8, 162.2, 162.1, 158.0, 140.0, 136.8, 134.54, 134.50, 134.3 134.0, 133.6, 131.0, 129.2, 129.1, 129.0, 128.9, 128.8, 128.3, 128.1, 120.5, 119.8, 114.1, 111.2, 78.3, 60.8, 55.2, 23.5, 21.3, 21.0, 20.80, 20.79. HRMS (ESI-TOF) *m/z* calcd. for $C_{43}H_{42}N_3O_4$ $[M+H]^+$: 664.3170, found 664.3168.

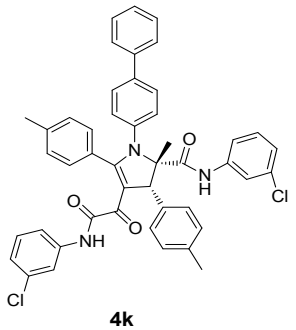


4j

(2S,3R)-1-(4-(Benzyloxy)phenyl)-*N*-(3-chlorophenyl)-4-(2-((3-chlorophenyl)amino)-2-oxoacetyl)-2-methyl-3,5-di-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4j)

Using $BnOPhNH_2$ (50 mg, 0.25 mmol), *p*-tolualdehyde (60 mg, 0.5 mmol), and **3b** (100 mg, 0.5 mmol) in accordance with General Procedure B, the title compound was obtained (73 mg, 37% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.35 (m, 4H), 7.21(d, *J* = 8.4 Hz, 3H), 7.17-7.11 (m, 5H), 7.07 (d, *J* = 8.4 Hz, 3H), 7.03-6.94 (m, 6H), 6.88 (d, *J* = 8.8

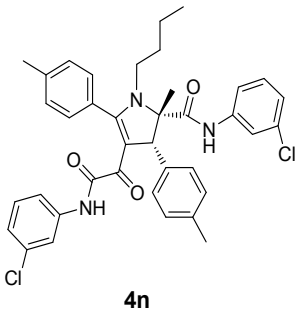
Hz, 2H), 6.75 (d, *J* = 8.8 Hz, 2H), 5.19 (s, 1H), 4.94 (s, 2H), 2.31 (s, 3H), 2.20 (s, 3H), 1.71 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.0, 168.3, 166.4, 162.1, 162.0, 157.5, 140.6, 138.2, 138.0, 137.6, 136.4, 134.6, 134.5, 134.4, 131.2, 129.79, 129.76, 129.42, 129.35, 129.2, 128.9, 128.7, 128.24, 128.15, 127.6, 124.8, 124.4, 120.5, 120.0, 118.4, 117.9, 115.4, 111.1, 78.8, 70.3, 60.9, 23.6, 21.5, 21.0. HRMS (ESI-TOF) *m/z* calcd. for $C_{47}H_{40}Cl_2N_3O_4$ $[M+H]^+$: 780.2390, found 780.2401.



4k

(2S,3R)-1-([1,1'-Biphenyl]-4-yl)-*N*-(3-chlorophenyl)-4-(2-((3-chlorophenyl)amino)-2-oxoacetyl)-2-methyl-3,5-di-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4k)

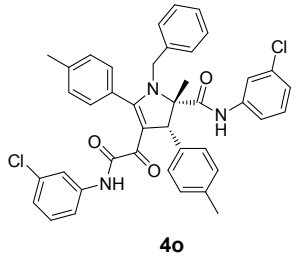
Using 4-aminobiphenyl (42 mg, 0.25 mmol), *p*-tolualdehyde (60 mg, 0.5 mmol), and **3b** (100 mg, 0.5 mmol), in accordance with General Procedure B, the title compound was obtained (49 mg, 26% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (s, 1H), 7.84 (s, 1H), 7.48 (d, *J* = 7.2 Hz, 2H), 7.41-7.38 (m, 4H), 7.34-7.30 (m, 1H), 7.27 (s, 1H), 7.25 (s, 1H), 7.22 (s, 1H), 7.18-7.13 (m, 5H), 7.11-7.07 (m, 3H), 7.03-6.97 (m, 7H), 5.21 (s, 1H), 2.30 (s, 3H), 2.21 (s, 3H), 1.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.3, 168.4, 165.4, 161.7, 140.9, 139.6, 139.5, 138.2, 138.1, 137.7, 137.6, 134.51, 134.49, 134.3, 129.9, 129.8, 129.5, 129.4, 129.0, 128.27, 128.25, 128.1, 127.81, 127.77, 127.3, 126.9, 124.9, 124.6, 120.7, 120.1, 118.6, 118.0, 111.9, 78.8, 61.3, 23.6, 21.6, 21.2. HRMS (ESI-TOF) *m/z* calcd. for $C_{46}H_{38}Cl_2N_3O_3$ $[M+H]^+$: 750.2285, found 750.2258.



4n

(2S,3R)-1-Butyl-*N*-(3-chlorophenyl)-4-(2-((3-chlorophenyl)amino)-2-oxoacetyl)-2-methyl-3,5-di-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4n)

Using butylamine (19 mg, 0.25 mmol), *p*-tolualdehyde (60 mg, 0.5 mmol), and **3b** (100 mg, 0.5 mmol), in accordance with General Procedure B, except that no acetic acid was added in the reaction media, the title compound was obtained (87 mg, 51% yield) as a yellow crystalline solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (s, 1H), 7.46-7.38 (m, 2H), 7.29 (s, 2H), 7.15 (d, *J* = 7.6 Hz, 2H), 7.12-7.07 (m, 3H), 7.04-6.97 (m, 5H), 6.90 (s, 1H), 6.83 (d, *J* = 8.0 Hz, 1H), 5.04 (s, 1H), 3.25-3.18 (m, 1H), 3.12-3.05 (m, 1H), 2.43 (s, 3H), 2.18 (s, 3H), 1.88 (s, 3H), 1.33-1.30 (m, 2H), 1.01 (sxt, *J* = 7.2 Hz, 2H), 0.66 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.6, 169.2, 168.5, 162.0, 140.2, 138.4, 137.84, 137.83, 137.5, 136.4, 134.5, 134.4, 129.8, 129.7, 129.6, 128.7, 127.9, 124.9, 124.3, 120.8, 120.7, 119.8, 118.6, 117.7, 110.1, 79.1, 58.4, 45.5, 32.4, 23.3, 21.7, 21.0, 20.3, 13.4. HRMS (ESI-TOF) *m/z* calcd. for $C_{38}H_{37}N_3O_3Cl_2Na^+$ $[M+Na]^+$: 676.2104, found 676.2092.

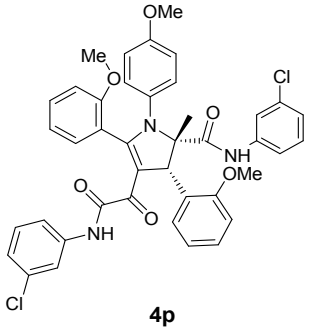


4o

(2S,3R)-1-Benzyl-*N*-(3-chlorophenyl)-4-(2-((3-chlorophenyl)amino)-2-oxoacetyl)-2-methyl-3,5-di-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4o)

Using benzylamine (54 mg, 0.5 mmol), *p*-tolualdehyde (120 mg, 1.0 mmol), and **3b** (200 mg, 1.0 mmol), in accordance with General Procedure B, the title compound was obtained (94 mg, 28% yield) as a yellow solid. The single crystal was obtain by wap crystallization. ^{1}H NMR

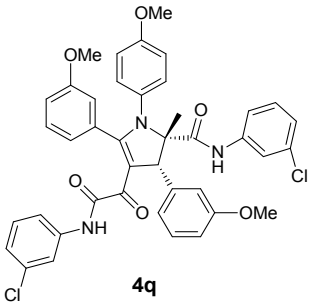
(400 MHz, $CDCl_3$) δ 8.63 (s, 1H), 7.29 (s, 1H), 7.24-7.18 (m, 7H), 7.11-7.05 (m, 4H), 7.03-6.95 (m, 6H), 6.66-6.59 (m, 3H), 5.10 (s, 1H), 4.57 (d, *J* = 16.4 Hz, 1H), 4.34 (d, *J* = 16.0 Hz, 1H), 2.37 (s, 3H), 2.17 (s, 3H), 1.79 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 181.0, 169.7, 168.0, 161.8, 140.1, 138.3, 137.7, 137.6, 137.4, 136.4, 134.5, 134.1, 129.8, 129.65, 129.64, 129.62, 129.5, 128.9, 128.6, 128.0, 127.8, 127.3, 124.7, 124.4, 120.5, 119.8, 118.4, 117.7, 110.5, 79.6, 58.8, 48.7, 23.5, 21.6, 21.0. HRMS (ESI-TOF) *m/z* calcd. for $C_{41}H_{36}N_3O_3Cl_2$ $[M+H]^+$: 688.2128, found 688.2119.



4p

(2S,3R)-*N*-(3-Chlorophenyl)-4-(2-((3-chlorophenyl)amino)-2-oxoacetyl)-3,5-bis(2-methoxyphenyl)-1-(4-methoxyphenyl)-2-methyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4p)

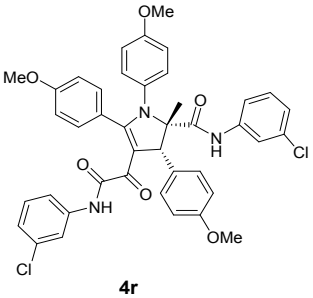
Using *p*-anisidine (31 mg, 0.25 mmol), 2-methoxy-benzaldehyde (68 mg, 0.5 mmol), and **3b** (100 mg, 0.5 mmol), in accordance with General Procedure B, the title compound was obtained (63 mg, 34% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.38 (s, 1H), 7.46 (s, 1H), 7.35-7.34 (m, 2H), 7.21-7.17 (m, 3H), 7.13-7.06 (m, 4H), 6.99 (d, *J* = 8.0 Hz, 1H), 6.94-6.92 (m, 2H), 6.87-6.83 (m, 4H), 6.64 (d, *J* = 8.8 Hz, 2H), 6.53-6.49 (m, 1H), 5.79 (s, 1H), 3.92(s, 3H), 3.69 (s, 3H), 3.65 (s, 3H), 1.70 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.4, 168.9, 163.1, 161.4, 158.4, 158.2, 156.1, 139.0, 138.2, 134.7, 134.6, 131.8, 130.7, 130.0, 129.8, 128.6, 127.9, 127.8, 124.5, 124.4, 121.3, 121.1, 120.4, 120.2, 120.06, 120.05, 118.2, 117.9, 113.99, 113.97, 112.7, 111.9, 111.0, 78.8, 56.3, 55.7, 55.4, 53.8, 22.7. HRMS (ESI-TOF) *m/z* calcd. for $C_{41}H_{36}Cl_2N_3O_6$ $[M+H]^+$: 736.1976, found 736.1986.



4q

(2S,3R)-*N*-(3-Chlorophenyl)-4-(2-((3-chlorophenyl)amino)-2-oxoacetyl)-3,5-bis(3-methoxyphenyl)-1-(4-methoxyphenyl)-2-methyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4q)

Using *p*-anisidine (31 mg, 0.25 mmol), 3-methoxy-benzaldehyde (68 mg, 0.5 mmol), and **3b** (100 mg, 0.5 mmol), in accordance with General Procedure B, the title compound was obtained (69 mg, 38% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 7.65 (s, 1H), 7.27 (s, 1H), 7.22-7.20 (m, 2H), 7.18-7.10 (m, 3H), 7.03 (t, *J* = 8.8 Hz, 3H), 6.96 (d, *J* = 8.4 Hz, 1H), 6.91-6.83 (m, 7H), 6.69-6.65 (m, 3H), 5.19 (s, 1H), 3.71 (s, 3H), 3.64 (s, 3H), 3.59 (s, 3H), 1.73 (s, 3H). ^{13}C NMR (100 MHz, CD_3OD) δ 185.2, 170.6, 169.0, 167.3, 161.0, 160.42, 160.36, 140.4, 140.2, 139.6, 134.9, 134.8, 132.7, 131.79, 131.78, 131.51, 131.49, 130.7, 130.6, 130.13, 130.10, 130.05, 130.04, 126.0, 125.1, 123.8, 121.9, 121.3, 119.5, 115.12, 115.11, 113.7, 111.6, 79.8, 61.3, 55.8, 55.6, 55.5, 24.7. HRMS (ESI-TOF) *m/z* calcd. for $C_{41}H_{36}Cl_2N_3O_6$ $[M+H]^+$: 736.1976, found 736.1974.

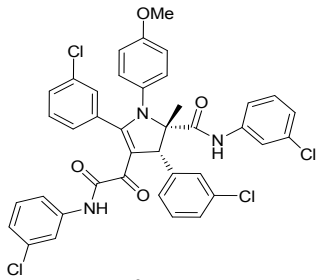


4r

(2S,3R)-*N*-(3-Chlorophenyl)-4-(2-((3-chlorophenyl)amino)-2-oxoacetyl)-1,3,5-tris(4-methoxyphenyl)-2-methyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4r)

Using *p*-anisidine (31 mg, 0.25 mmol), 4-methoxy-benzaldehyde (68 mg, 0.5 mmol), and **3b** (100 mg, 0.5 mmol), in accordance with General Procedure B, the title compound was

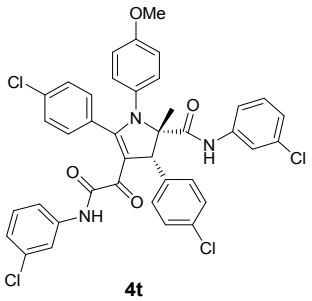
obtained (73 mg, 40% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (s, 1H), 8.14 (s, 1H), 7.25-7.23 (m, 4H), 7.21-7.17 (m, 2H), 7.15-7.11 (m, 1H), 7.09-7.05 (m, 2H), 7.03-6.96 (m, 4H), 6.86 (d, *J* = 8.8 Hz, 2H), 6.70-6.67 (m, 5H), 5.06 (s, 1H), 3.71 (s, 3H), 3.68 (s, 3H), 3.65 (s, 3H), 1.65 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.1, 168.6, 166.2, 162.54, 162.50, 161.2, 159.2, 158.4, 138.4, 138.25, 138.23, 134.5, 131.24, 131.23, 131.1, 129.8, 129.5, 129.0, 124.8, 124.5, 123.2, 120.8, 120.1, 118.7, 118.0, 114.6, 114.1, 113.9, 110.9, 78.6, 60.7, 55.5, 55.34, 55.27, 23.9. HRMS (ESI-TOF) *m/z* calcd. for $C_{41}H_{36}Cl_2N_3O_6$ $[M+H]^+$: 736.1976, found 736.1956.



4s

(2S,3R)-*N*,3,5-Tris(3-chlorophenyl)-4-(2-((3-chlorophenyl)amino)-2-oxoacetyl)-1-(4-methoxyphenyl)-2-methyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4s)

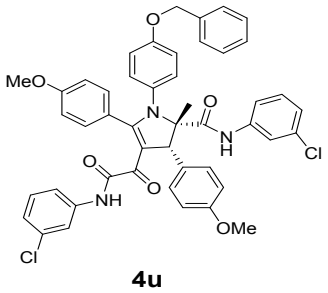
Using *p*-anisidine (31 mg, 0.25 mmol), 3-chlorobenzaldehyde (70 mg, 0.5 mmol), and **3b** (100 mg, 0.5 mmol), in accordance with General Procedure B, the title compound was obtained (56 mg, 30% yield) as a yellow crystalline solid. ^{1}H NMR (400 MHz, CD_3OD) δ 7.47 (d, *J* = 10.4 Hz, 2H), 7.36-7.32 (m, 2H), 7.29 (s, 1H), 7.22-7.18 (m, 2H), 7.17-7.13 (m, 2H), 7.11-7.06 (m, 7H), 7.04-6.98 (m, 2H), 6.74 (d, *J* = 8.8 Hz, 2H), 4.86 (s, 1H), 3.66 (s, 3H), 1.80 (s, 3H). ^{13}C NMR (100 MHz, CD_3OD) δ 184.8, 170.0, 167.7, 167.1, 160.6, 141.4, 140.0, 139.4, 135.1, 135.0, 134.90, 134.89, 133.4, 131.9, 131.1, 131.0, 130.8, 130.7, 130.6, 130.51, 130.45, 129.4, 128.5, 126.1, 125.3, 123.6, 121.7, 121.12, 121.11, 119.3, 115.22, 115.21, 111.3, 80.0, 60.7, 55.8, 24.4. HRMS (ESI-TOF) *m/z* calcd. for $C_{39}H_{30}Cl_4N_3O_4$ $[M+H]^+$: 744.0985, found 744.0984.



4t

(2S,3R)-*N*-(3-Chlorophenyl)-3,5-bis(4-chlorophenyl)-4-(2-((3-chlorophenyl)amino)-2-oxoacetyl)-1-(4-methoxyphenyl)-2-methyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4t)

Using *p*-anisidine (31 mg, 0.25 mmol), 4-chlorobenzaldehyde (70 mg, 0.5 mmol), and **3b** (100 mg, 0.5 mmol), in accordance with General Procedure B, the title compound was obtained (55 mg, 30% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (s, 1H), 7.57 (s, 1H), 7.28-7.21 (m, 7H), 7.17-7.13 (m, 5H), 7.09-6.99 (m, 3H), 6.88 (d, *J* = 8.4 Hz, 3H), 6.70 (d, *J* = 8.4 Hz, 2H), 5.23 (s, 1H), 3.72 (s, 3H), 1.72 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.7, 167.8, 165.7, 161.3, 158.8, 137.9, 137.6, 136.7, 136.4, 134.7, 133.8, 130.6, 130.2, 130.06, 130.05, 129.7, 129.6, 129.29, 129.28, 128.90, 128.88, 125.3, 124.9, 120.6, 119.9, 118.4, 117.8, 114.7, 110.8, 79.0, 60.7, 55.5, 23.9. HRMS (ESI-TOF) *m/z* calcd. for $C_{39}H_{30}Cl_4N_3O_4$ $[M+H]^+$: 744.0985, found 744.0968.

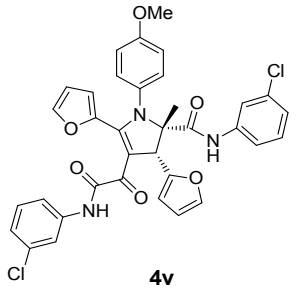


4u

(2S,3R)-1-(4-(Benzyloxy)phenyl)-*N*-(3-chlorophenyl)-4-(2-((3-chlorophenyl)amino)-2-oxoacetyl)-3,5-bis(4-methoxyphenyl)-2-methyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4u)

Using $BnOPhNH_2$ (76 mg, 0.38 mmol), 4-methoxy-benzaldehyde (103 mg, 0.76 mmol), and **3b** (150 mg, 0.76 mmol), in accordance with General Procedure B, the title compound was obtained (100 mg, 32% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (s, 1H),

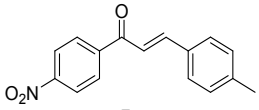
7.86 (s, 1H), 7.36-7.35 (m, 6H), 7.25-7.23 (m, 3H), 7.18 (d, *J* = 8.4 Hz, 2H), 7.15-7.09 (m, 2H), 7.05-6.97 (m, 4H), 6.86 (d, *J* = 8.4 Hz, 2H), 6.77-6.69 (m, 6H), 5.11 (s, 1H), 4.95 (s, 2H), 3.71 (s, 3H), 3.65 (s, 3H), 1.68 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.1, 168.5, 166.1, 162.4, 161.2, 159.2, 157.6, 138.4, 138.2, 136.4, 134.52, 134.45, 131.3, 131.19, 131.17, 129.88, 129.84, 129.5, 128.8, 128.7, 128.3, 127.6, 124.8, 124.5, 123.1, 120.6, 120.0, 118.5, 118.0, 115.5, 114.1, 114.0, 110.9, 78.6, 70.3, 60.7, 55.4, 55.3, 23.7. HRMS (ESI-TOF) *m/z* calcd. for $C_{47}H_{39}Cl_2N_3O_6Na^+$ $[M+Na]^+$: 834.2108, found 834.2102.



4v

(2S,3R)-*N*-(3-Chlorophenyl)-4-(2-((3-chlorophenyl)amino)-2-oxoacetyl)-3,5-di(furan-2-yl)-1-(4-methoxyphenyl)-2-methyl-2,3-dihydro-1H-pyrrole-2-carboxamide (4v)

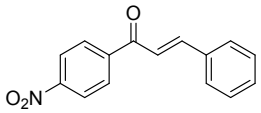
Using *p*-anisidine (31 mg, 0.25 mmol), furan-2-carbaldehyde (48 mg, 0.5 mmol), and **3b** (100 mg, 0.5 mmol), in accordance with General Procedure B, the title compound was obtained (31 mg, 19% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (s, 1H), 8.49 (s, 1H), 7.57-7.55 (m, 2H), 7.32 (s, 1H), 7.28-7.26 (m, 2H), 7.23-7.18 (m, 3H), 7.09-7.06 (m, 2H), 6.99 (d, *J* = 8.8 Hz, 2H), 6.81 (d, *J* = 8.8 Hz, 2H), 6.38-6.37 (m, 1H), 6.28-6.27 (m, 1H), 6.21 (s, 2H), 5.16 (s, 1H), 3.78 (s, 3H), 1.62 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.0, 168.3, 161.6, 159.2, 153.2, 150.5, 144.9, 144.2, 142.6, 138.7, 138.5, 134.8, 134.6, 131.1, 130.1, 130.0, 128.7, 124.73, 124.69, 120.5, 119.8, 118.5, 117.8, 116.6, 114.8, 112.4, 110.8, 109.0, 107.2, 76.9, 55.6, 55.0, 22.9. HRMS (ESI-TOF) *m/z* calcd. for $C_{35}H_{28}Cl_2N_3O_6$ $[M+H]^+$: 656.1350, found 656.1348.



5a

(E)-1-(4-Nitrophenyl)-3-(p-tolyl)prop-2-en-1-one (5a)

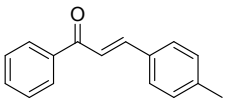
4-Tolualdehyde (0.73 g, 6.05 mmol) and a 6 M NaOH aqueous solution (50 μL, 0.3 mmol) were successively added to a solution of 4-nitroacetophenone (1.0 g, 6.05 mmol) in methanol (4 ml). The reaction was stirred for 4h at r.t. The precipitate was flitrered, washed with MeOH and dried in vacuo to provide chalcone **5a** as a white solid (1.2 g, 75% yield). The spectroscopic data are consistent with material from commercial sources. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, J = 8.8 Hz, 2H), 8.13 (d, J = 8.8 Hz, 2H), 7.82 (d, J = 15.6 Hz, 1H), 7.56 (d, J = 8.0 Hz, 2H), 7.44 (d, J = 15.6 Hz, 1H), 7.25 (d, J = 8.4 Hz, 2H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.2, 150.1, 147.0, 143.4, 142.1, 131.7, 130.0, 129.5, 128.9, 123.9, 120.4, 21.7.



5b

(E)-1-(4-Nitrophenyl)-3-phenylprop-2-en-1-one (5b)

4-Nitroacetophenone (1.0 g, 6.05 mmol) and benzaldehyde (642 mg, 6.05 mmol) were dissolved in methanol (30 ml). An aqueous solution of sodium hydroxide (5 % w/v, 15 ml) was added slowly and the reaction mixture was stirred at room temperature for 12 h. The obtained solid was filtered, washed with water (15 ml) and crystallized from methanol to provide chalcone **5b** as a yellow solid (1.2 g, 80% yield). The spectroscopic data are consistent with material from commercial sources. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, J = 8.8 Hz, 2H), 8.15 (d, J = 8.8 Hz, 2H), 7.85 (d, J = 15.6 Hz, 1H), 7.67-7.65 (m, 2H), 7.51-7.45 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.2, 150.2, 146.9, 143.2, 134.4, 131.4, 129.5, 129.3, 128.8, 124.0, 121.4.

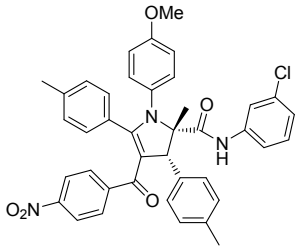


5c

(E)-1-phenyl-3-(p-tolyl)prop-2-en-1-one (5c)

Acetophenone (2.0 g, 16.6 mmol) and *p*-tolualdehyde (2.0 g, 16.6 mmol) were dissolved in methanol (80 ml). An aqueous solution of sodium hydroxide (5 % w/v, 40 ml) was added slowly and the reaction mixture was stirred at room temperature for 12 h. The obtained solid was filtered, washed with water (15 ml) and crystallized from methanol to provide chalcone **5c** as a yellow solid (2.7 g, 73% yield). The spectroscopic data are consistent with previously

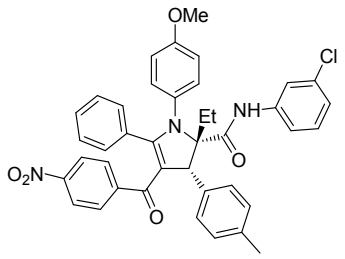
reported.[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-8.01 (m, 2H), 7.80 (d, *J* = 16.0 Hz, 1H), 7.61-7.48 (m, 6H), 7.23 (d, *J* = 8.0 Hz, 2H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.8, 145.1, 141.3, 138.5, 132.8, 132.3, 129.9, 128.7, 128.63, 128.62, 121.2, 21.7.



6a

(2S,3R)-*N*-(3-Chlorophenyl)-1-(4-methoxyphenyl)-2-methyl-4-(4-nitrobenzoyl)-3,5-di-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (6a)

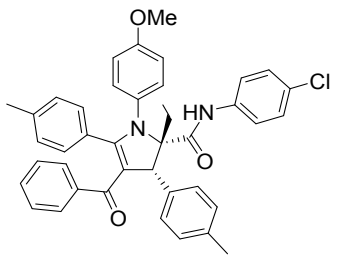
A solution of 4-anisidine (63 mg, 0.51 mmol), 4-tolualdehyde (123 mg, 1.02 mmol), pyruvic amide **3b** (200 mg, 1.02 mmol) and chalcone **5a** (272 mg, 1.02 mmol) in EtOH (19 ml) and HOAc (1.6 ml) was stirred under reflux for 8 h. After cooled down to r.t., ethanol was removed under vacuum, and the residue was diluted with EtOAc and water. After separation, the aqueous phase was extracted two more times with EtOAc. The combined organic phases were successively washed with saturated aqueous $KHSO_4$, saturated aqueous $NaHCO_3$, and brine, dried over $MgSO_4$, concentrated *in vacuo* and chromatographed gradiently on silica gel with pentane/diethyl ether (5:1~1:1) to give the dihydropyrrole **6a** (80 mg, 23% yield) as a yellow solid, and **4b** (80 mg, 23% yield) as a yellow solid. **6a**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.21-7.18 (m, 2H), 7.06-7.02 (m, 3H), 6.92-6.85 (m, 7H), 6.70 (d, *J* = 7.2 Hz, 2H), 6.65 (d, *J* = 8.8 Hz, 2H), 4.95 (s, 1H), 3.69 (s, 3H), 2.23 (s, 3H), 2.08 (s, 3H), 1.70 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.0, 169.3, 162.8, 158.0, 148.0, 146.3, 140.2, 137.9, 137.8, 135.2, 134.4, 131.6, 130.4, 129.75, 129.73, 129.6, 129.1, 128.6, 127.9, 127.7, 125.0, 122.4, 121.0, 118.9, 114.7, 114.4, 77.7, 62.4, 55.4, 23.7, 21.3, 21.1. HRMS (ESI-TOF) *m/z* calcd. for $C_{40}H_{35}N_3O_5Cl$ $[M+H]^+$: 672.2260, found 672.2245.



6b

(2S,3R)-*N*-(3-Chlorophenyl)-2-ethyl-1-(4-methoxyphenyl)-4-(4-nitrobenzoyl)-3,5-di-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (6b)

A solution of 4-anisidine (117 mg, 0.95 mmol), 4-tolualdehyde (114 mg, 0.95 mmol), pyruvic amide **3j** (200 mg, 0.95 mmol) and chalcone **5b** (240 mg, 0.95 mmol) in EtOH (38 ml) and HOAc (3.0 ml) was stirred under reflux for 8 h. After cooled down to r.t., ethanol was removed under vacuum, and the residue was diluted with EtOAc and water. After separation, the aqueous phase was extracted two more times with EtOAc. The combined organic phases were successively washed with saturated aqueous $KHSO_4$, saturated aqueous $NaHCO_3$, and brine, dried over $MgSO_4$, concentrated *in vacuo* and chromatographed gradiently on silica gel with PE/EA (5:1~3:1) to give the dihydropyrrole product **6b** as a yellow solid (98 mg, 16% yield). ^{1}H NMR (400 MHz, CD_3OD) δ 7.76 (d, *J* = 8.4 Hz, 2H), 7.41-7.36 (m, 4H), 7.23-7.21 (m, 2H), 7.18-7.14 (m, 2H), 7.07-7.02 (m, 2H), 6.97 (d, *J* = 8.8 Hz, 3H), 6.89 (d, *J* = 7.6 Hz, 2H), 6.74-6.72 (m, 1H), 6.67 (d, *J* = 9.2 Hz, 3H), 5.16 (s, 1H), 3.66 (s, 3H), 2.52-2.46 (m, 1H), 2.16-2.09 (m, 1H), 2.05 (s, 3H), 1.16 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, CD_3OD) δ 190.6, 170.9, 168.5, 159.5, 149.0, 148.2, 141.0, 140.1, 139.7, 134.7, 132.5, 130.6, 130.5, 130.4, 129.3, 129.22, 129.21, 129.18, 128.3, 125.9, 123.8, 123.37, 123.35, 121.9, 115.8, 114.8, 83.1, 57.5, 55.8, 27.2, 21.1, 8.6. HRMS (ESI-TOF) *m/z* calcd. for $C_{40}H_{35}N_3O_5Cl$ $[M+H]^+$: 672.2260, found 672.2262.

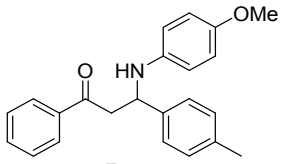


6c

(2S,3R)-4-benzoyl-*N*-(4-chlorophenyl)-2-ethyl-1-(4-methoxyphenyl)-3,5-di-p-tolyl-2,3-dihydro-1H-pyrrole-2-carboxamide (6c)

A solution of *p*-anisidine (58 mg, 0.47 mmol), *p*-tolualdehyde (56 mg, 0.47 mmol), **3k** (100 mg, 0.47 mmol), and **5c** (105 mg, 0.47 mmol) in EtOH (9.2 ml) and HOAc (0.74 ml) was stirred under reflux for 8 h. After cooled down to r.t., ethanol was removed under vacuum, and the residue was diluted with ethyl acetate and water. After separation, the aqueous phase was extracted two more times with ethyl acetate. The combined organic phases were successively washed with saturated aqueous $KHSO_4$, saturated aqueous $NaHCO_3$, and brine, dried over $MgSO_4$, concentrated *in vacuo* and chromatographed gradiently on silica gel with PE/EA (5:1~3:1) to give the dihydropyrrole product **6c** as a yellow solid (53 mg, 18% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.31 (d, *J* = 7.2 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 7.08 (t, *J* = 7.2 Hz, 2H), 6.96-6.93 (m, 5H), 6.90 (d, *J* = 8.4 Hz, 2H), 6.78 (d, *J* = 9.2 Hz, 2H), 6.70 (d, *J* = 7.2 Hz, 2H), 6.60 (d, *J* = 8.8 Hz, 2H), 5.26 (s, 1H), 3.68 (s, 3H), 2.37-2.21 (m, 1H), 2.19 (s, 3H), 3.12 (s, 3H), 2.09-2.03 (m, 1H), 1.07 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.1, 169.6, 160.4, 157.1, 140.4, 139.2, 137.0, 135.64, 135.61, 132.2, 130.3, 129.9, 129.7, 129.4, 128.9, 128.8, 128.5, 128.3, 128.1, 127.8, 127.3, 121.7, 114.8, 114.0, 80.3, 57.2, 55.4, 26.5, 21.3, 21.1, 8.3. HRMS (ESI-TOF) *m/z* calcd. for $C_{41}H_{38}N_2O_3Cl$ $[M+H]^+$: 641.2565, found 641.2558.

3. Mechanism studies



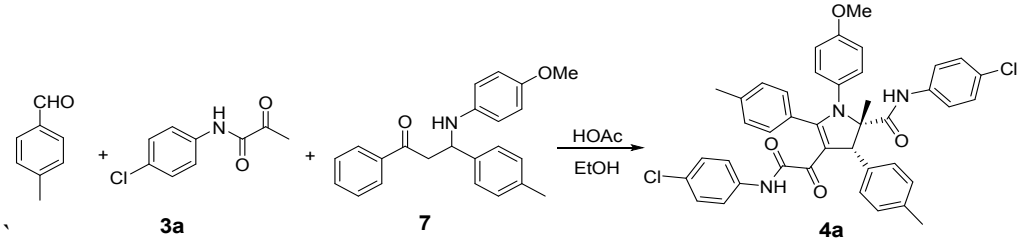
7

(E)-4-(4-methoxyphenyl)-1-phenyl-3-(p-tolyl)but-2-en-1-one (7)

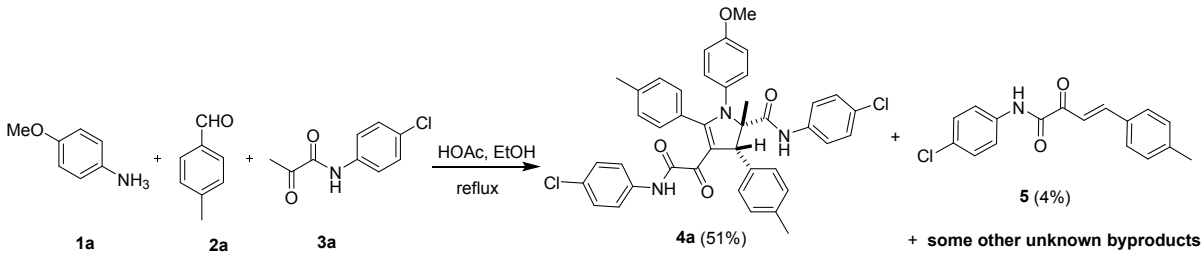
Compound **7** was prepared following the known method[2].

To a solution of **5c** (1.3 g, 6.0 mmol) in anhydrous EtOH (3 ml) was added 4-methoxyaniline (1.1 g, 9.0 mmol) and K_3PO_4 (192 mg). After stirring for five hours at r.t., the reaction mixture was diluted with ethyl acetate and water. After separation, the aqueous phase was extracted two more times with ethyl acetate. The combined organic phase was washed with

brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure to afford the crude product, which was purified by column chromatography on silica gel with PE/EA (50:1), the title compound was obtained (550 mg, 27% yield) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.6 Hz, 2H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.33 (d, *J* = 3.6 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.69 (d, *J* = 8.8 Hz, 2H), 6.54 (d, *J* = 8.8 Hz, 2H), 4.91 (t, *J* = 7.2 Hz, 1H), 4.27 (s, 1H), 3.69 (s, 3H), 3.48 (dd, *J* = 5.2, 16.0 Hz, 1H), 3.39 (dd, *J* = 7.6, 16.0 Hz, 1H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.6, 152.4, 141.4, 140.4, 137.0, 136.9, 133.5, 129.6, 128.8, 128.3, 126.5, 115.5, 114.8, 55.8, 55.5, 46.6, 21.2. HRMS (ESI-TOF) *m/z* calcd. for $C_{23}H_{24}NO_2$ $[M+H]^+$: 346.1802, found 346.1786.

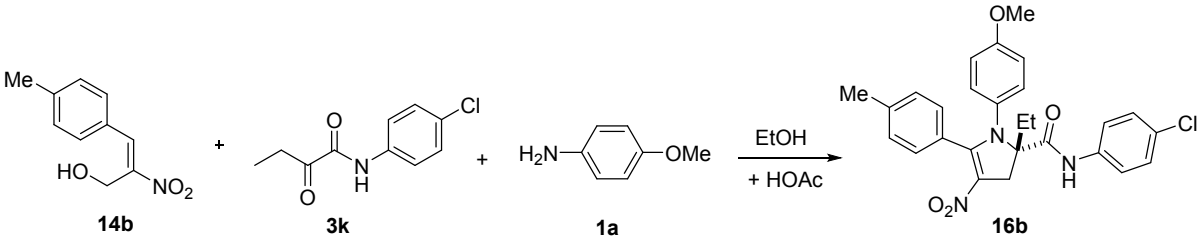


Using *p*-tolualdehyde (49 mg, 0.41 mmol), **3a** (80 mg, 0.41 mmol), and **7** (140 mg, 0.41 mmol) in EtOH (8 ml) and HOAc (0.64 ml) was stirred under reflux for 8 h. After cooled down to r.t., ethanol was removed under vacuum, and the residue was diluted with ethyl acetate and water. After separation, the aqueous phase was extracted two more times with ethyl acetate. The combined organic phases were successively washed with saturated aqueous $KHSO_4$, saturated aqueous $NaHCO_3$, and brine, dried over $MgSO_4$, concentrated *in vacuo* and chromatographed gradiently on silica gel with PE/EA 5:1~3:1 to give the dihydropyrrole product **4a** as a yellow solid (64 mg, 45%).

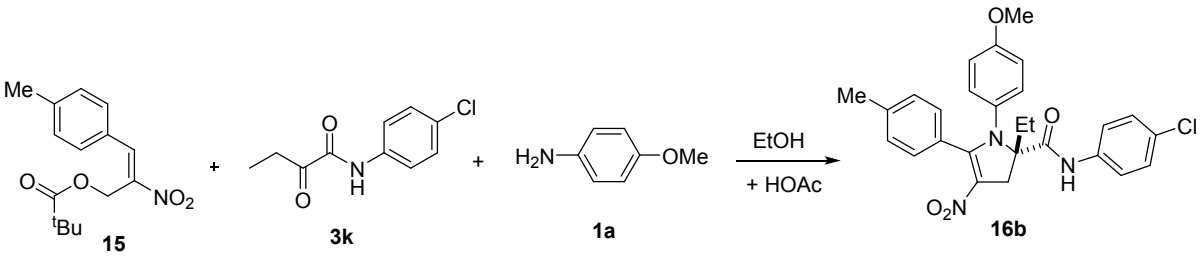


Using p-anisidine (31 mg, 0.25 mmol), p-tolualdehyde (60 mg, 0.5 mmol), and **3a** (100 mg, 0.5 mmol) in accordance with General Procedure B, the title compound was obtained (89 mg,

51% yield) as a yellow solid, and the aldol condensation product **5** was obtained (6 mg, 4% yield) as a yellow solid, along with unknown byproducts. Spectra data of the aldol product: ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.01 (d, *J* = 16.0 Hz, 1H), 7.82 (d, *J* = 16.0 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.60 (d, *J* = 7.2 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.26-7.24 (m, 2H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.2, 159.1, 149.4, 142.9, 135.4, 131.7, 130.4, 130.1, 129.6, 129.4, 121.1, 116.8, 21.8. HRMS (ESI-TOF) *m/z* calcd. for $C_{17}H_{14}ClNO_2Na$ $[M+Na]^+$: 322.0605, found 322.0602.

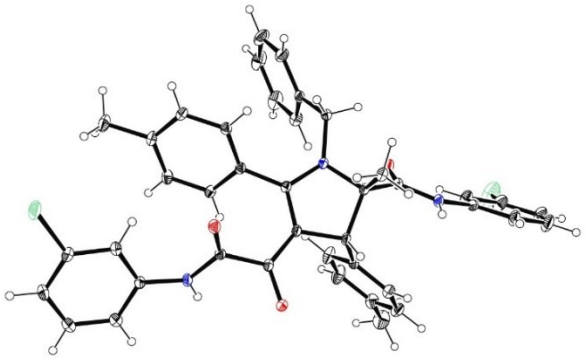


Using *p*-anisidine (58 mg, 0.47 mmol), **14b** (91 mg, 0.47 mmol), and **3k** (100 mg, 0.47 mmol), in accordance with General Procedure B, the title compound was obtained (45 mg, 19% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (s, 1H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.4 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.98 (d, *J* = 7.6 Hz, 2H), 6.78 (d, *J* = 8.4 Hz, 2H), 6.61 (d, *J* = 8.4 Hz, 2H), 3.70-3.66 (m, 4H), 3.52 (d, *J* = 16.4 Hz, 1H), 2.26 (s, 3H), 2.07-2.02 (m, 1H), 1.89-1.83 (m, 1H), 1.06 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.8, 161.3, 159.0, 140.3, 136.7, 129.7, 129.6, 129.3, 129.0, 128.7, 125.9, 122.3, 121.4, 114.3, 75.7, 55.4, 36.9, 27.8, 21.7, 7.5. HRMS (ESI-TOF) *m/z* calcd. for $C_{27}H_{25}N_3O_4Cl$ $[M-H]^-$: 490.1539, found 490.1535.

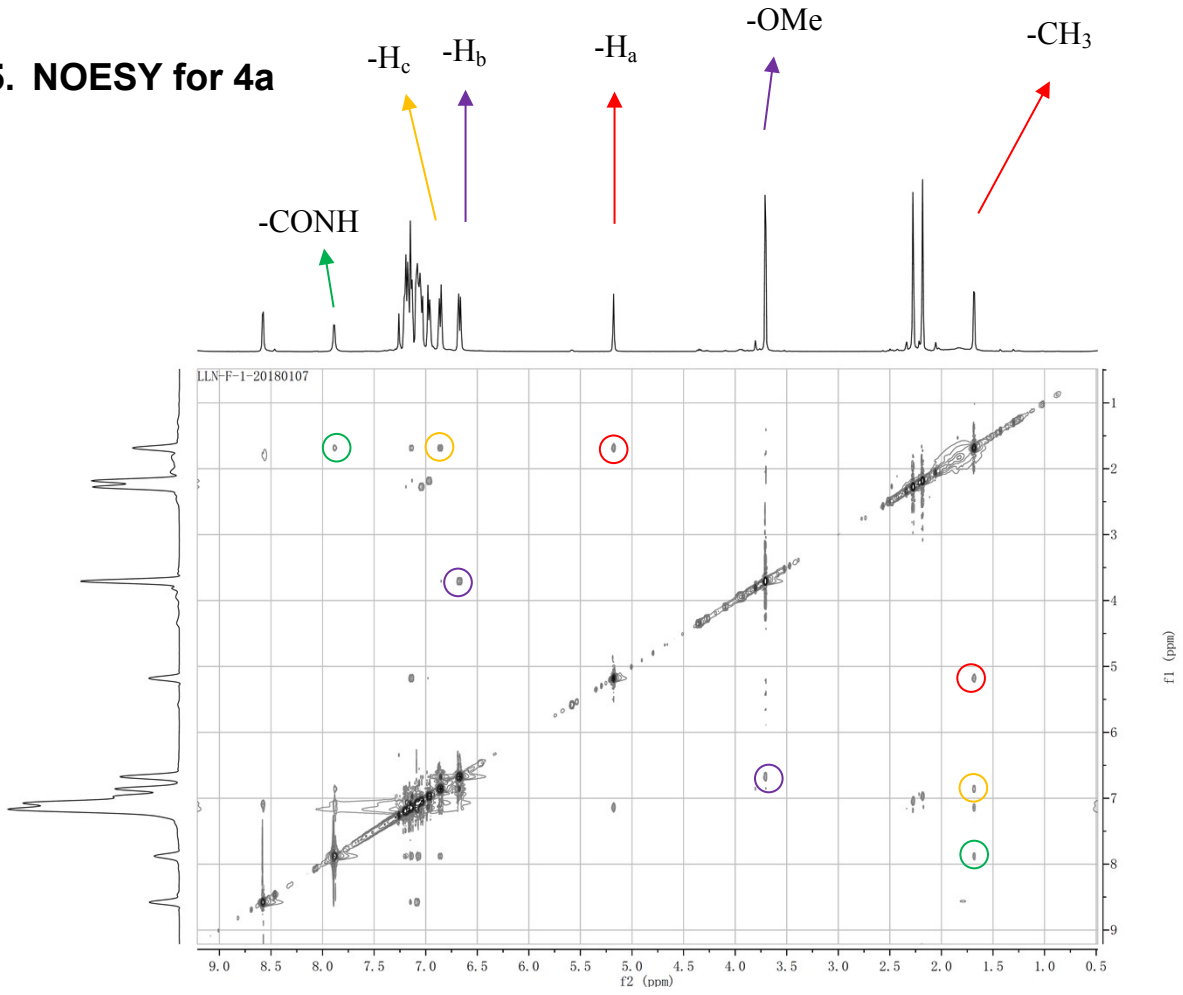


Using *p*-anisidine (58 mg, 0.47 mmol), **15** (130 mg, 0.47 mmol), and **3k** (100 mg, 0.47 mmol), in accordance with General Procedure B, the title compound was obtained (55 mg, 23% yield) as a yellow solid.

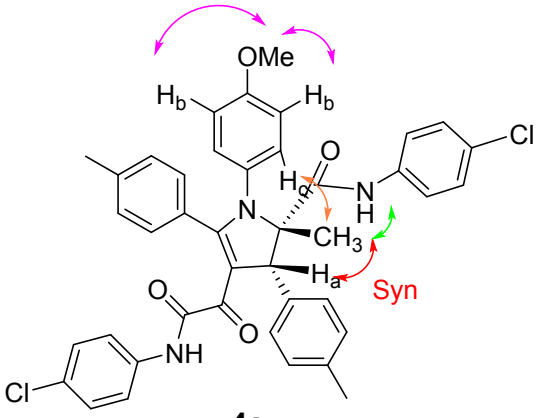
4. ORTEP Drawing for 4o



5. NOESY for 4a



The correlation between the methyl group and the proton was observed:



4a

6. Kinetics of α-Glucosidase Inhibition

The commercially available α-glucosidase from baker's yeast (Sigma, G5003) was selected as the target protein using *p*-nitrophenyl-α-D-glucopyranoside (pNGP, Sigma, N1377) as the substrate. The compounds and acarbose were dissolved in DMSO. The enzyme and the substrate were dissolved in 0.05 M potassium phosphate buffer with pH 6.8. The enzymatic reaction mixture composed of 20 μL α-glucosidase (0.03 U/ml), 30 μL of substrate (0.6, 1.2, 2.4 mM), 10 μL of test compounds (0, 0.62, 5 μM) or acarbose (0, 0.19, 0.39 mM), and 140 μL of potassium phosphate buffer was incubated at 37 °C for 20 min. The enzymatic activity was detected by spectrophotometer at the wavelength of 405 nm. The inhibitory kinetics of the investigated compounds on α-glucosidase was analyzed using the Lineweaver-Burk plot of the substrate concentration and velocity. Results are the average of three independent experiments, each performed in duplicate.

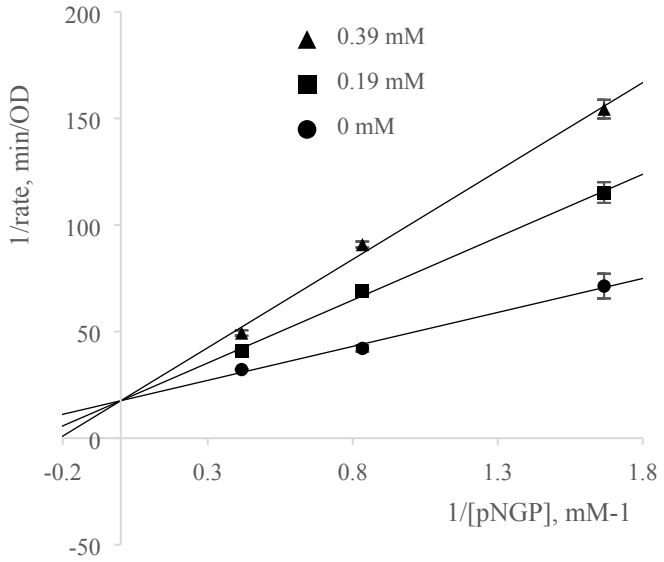


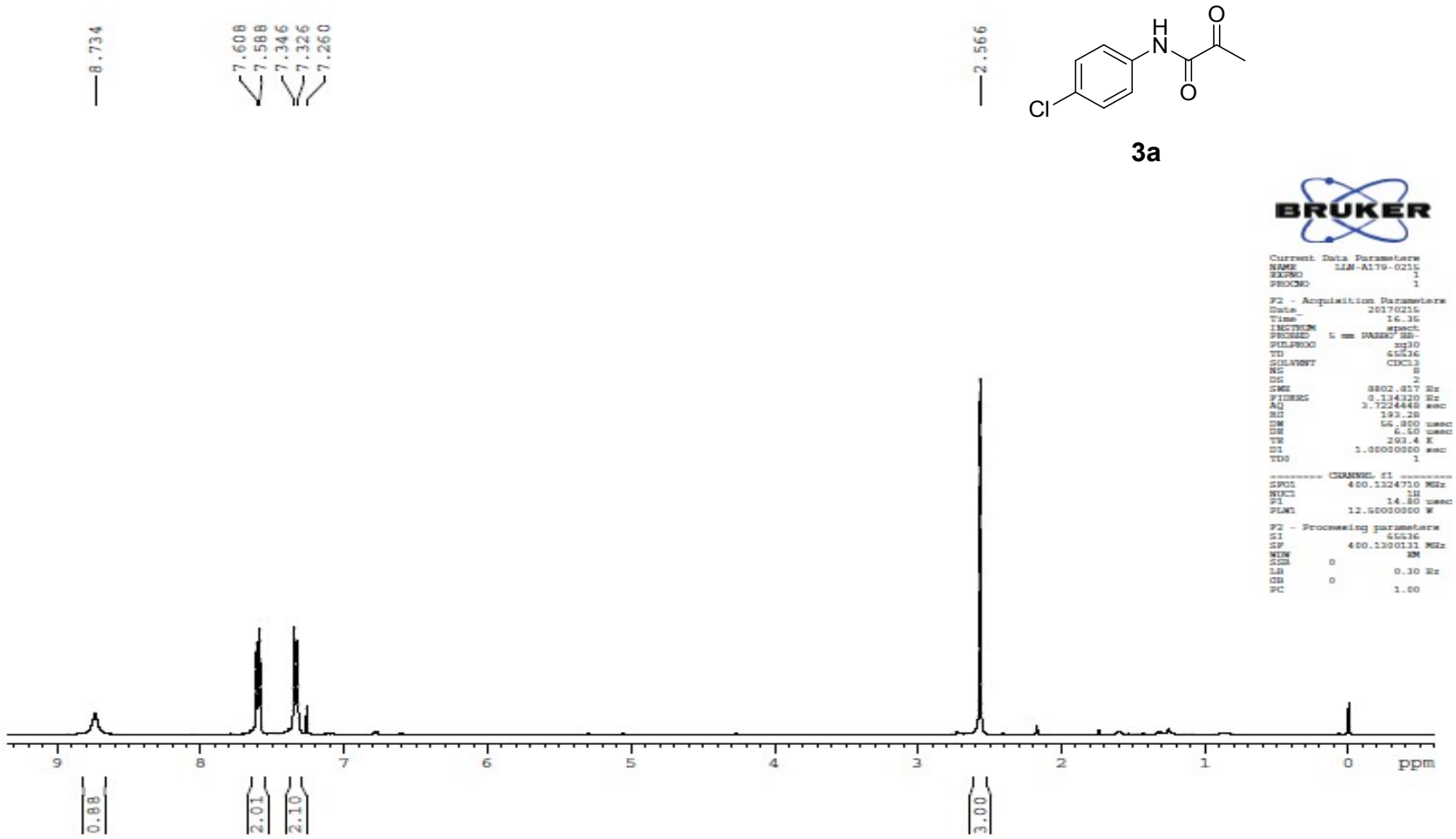
Fig. S1 Lineweaver-Burk plot of acarbose

7. Reference

1. Jin-Lin Zuo, Jia-Xiang Yang, Fu-ZhiWang, Xiang-Nan Dang, Jian-Liang Sun, De-Chun Zou,Yu-Peng Tian, Na Lin, Xu-Tang Tao, Min-Hua Jiang. Journal of Photochemistry and Photobiology A: Chemistry. **2008**, *199,* 322-329.
2. Barahman Movassagh, Sakineh Khosousi. Monatshefte fuer Chemie. **2012**, *143*, 1503-1506.

8. Spectra Data

Spectra data are shown from the next page.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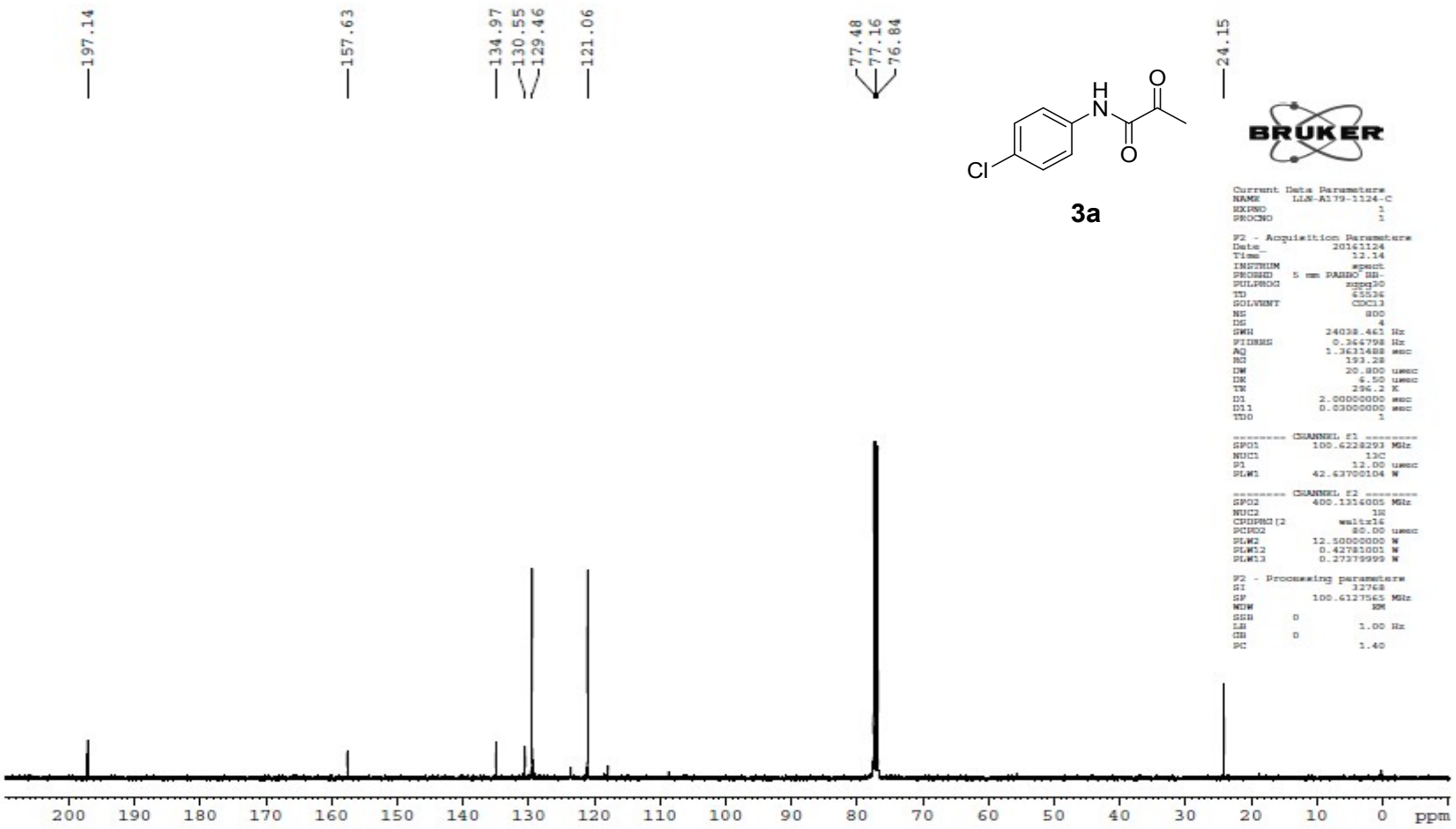
2.10
3.00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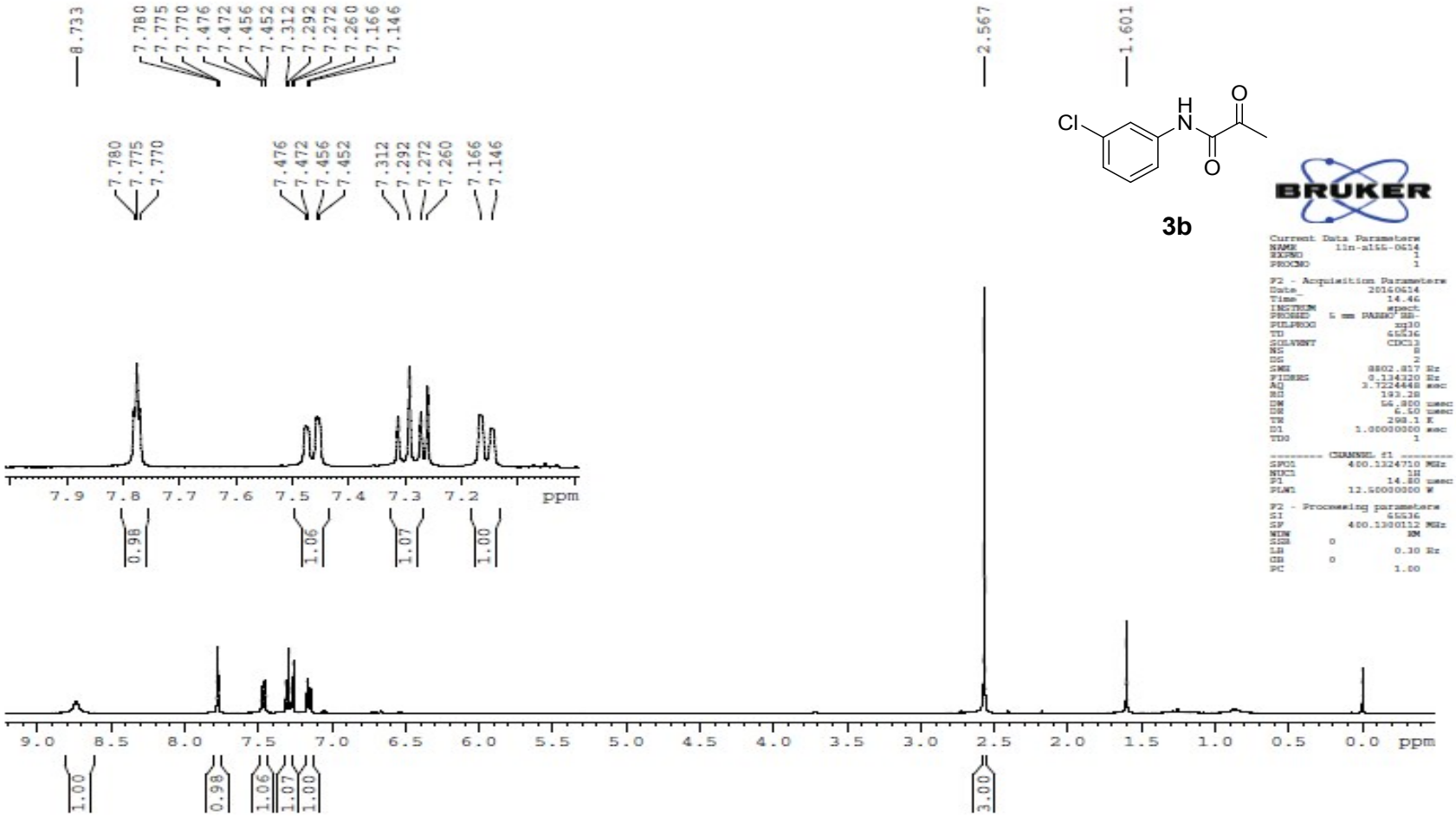
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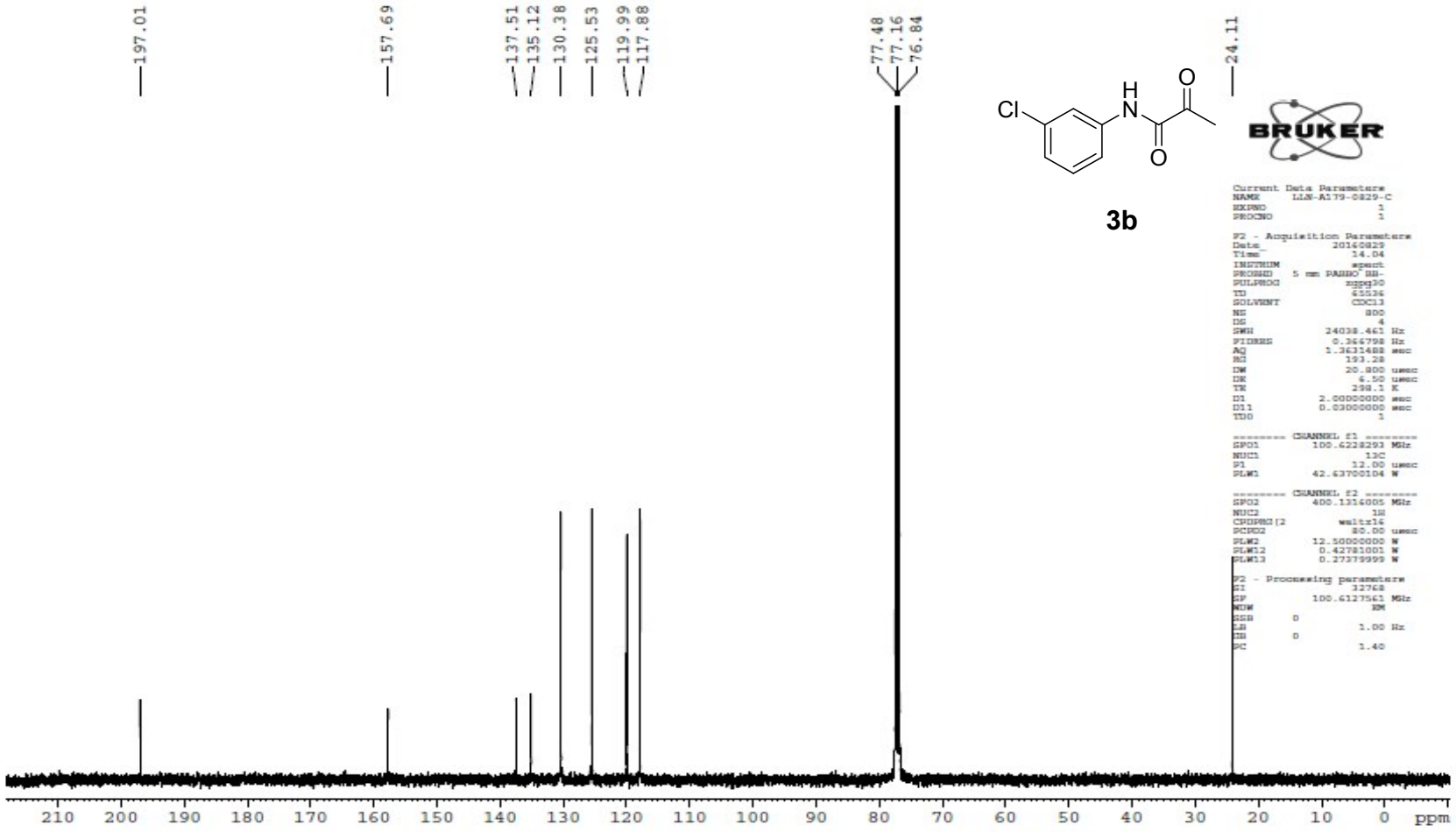
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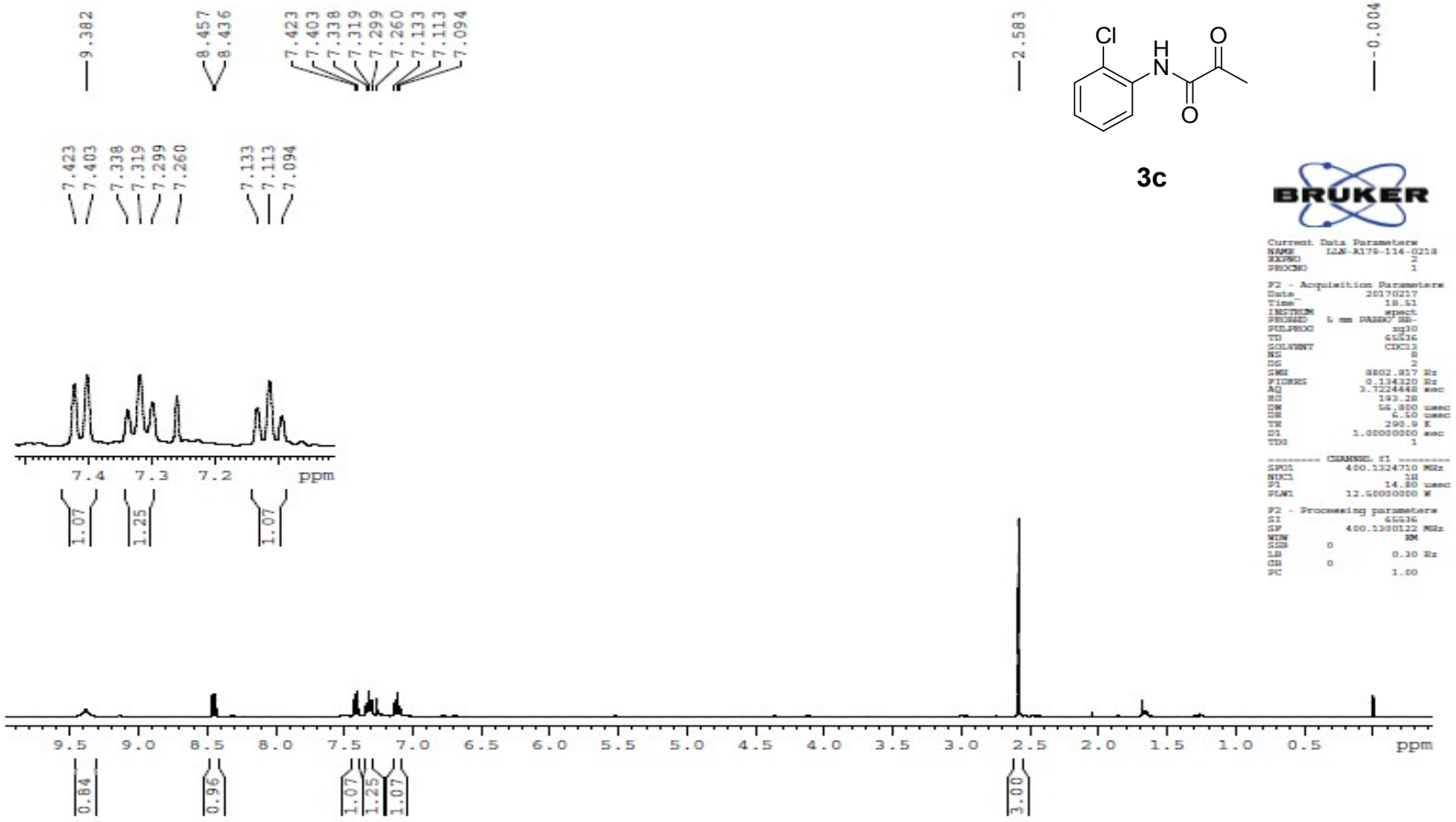
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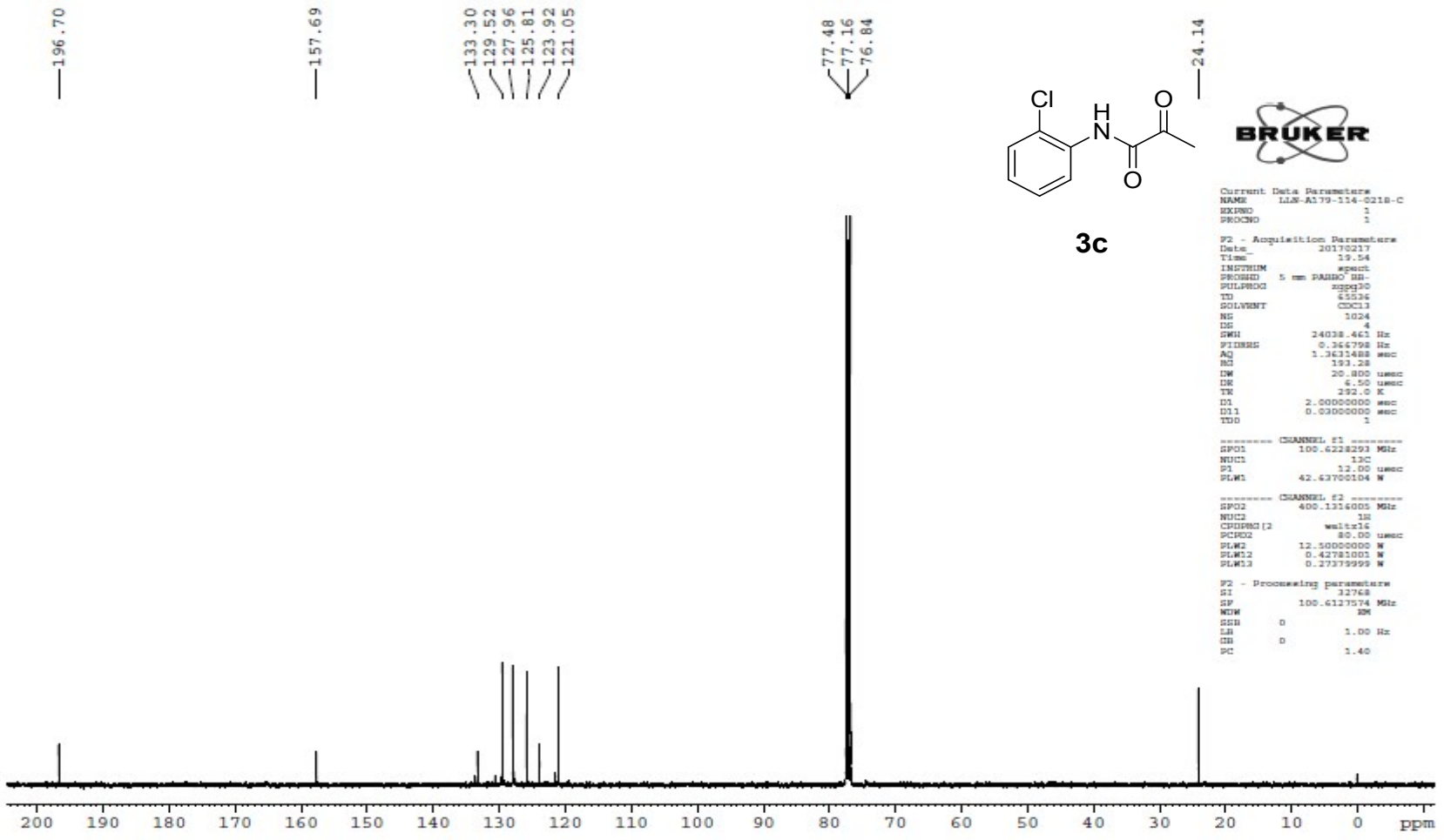
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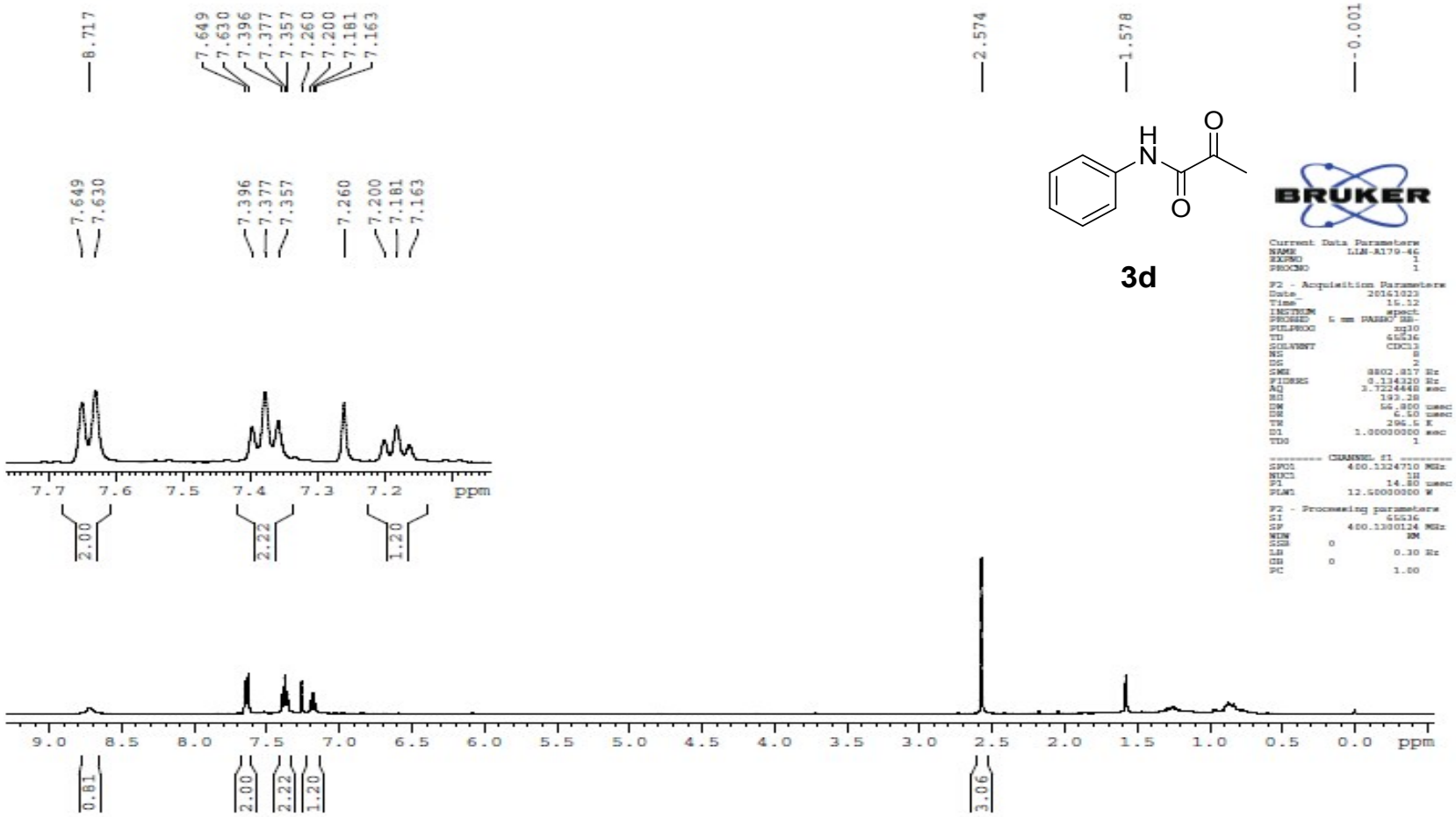
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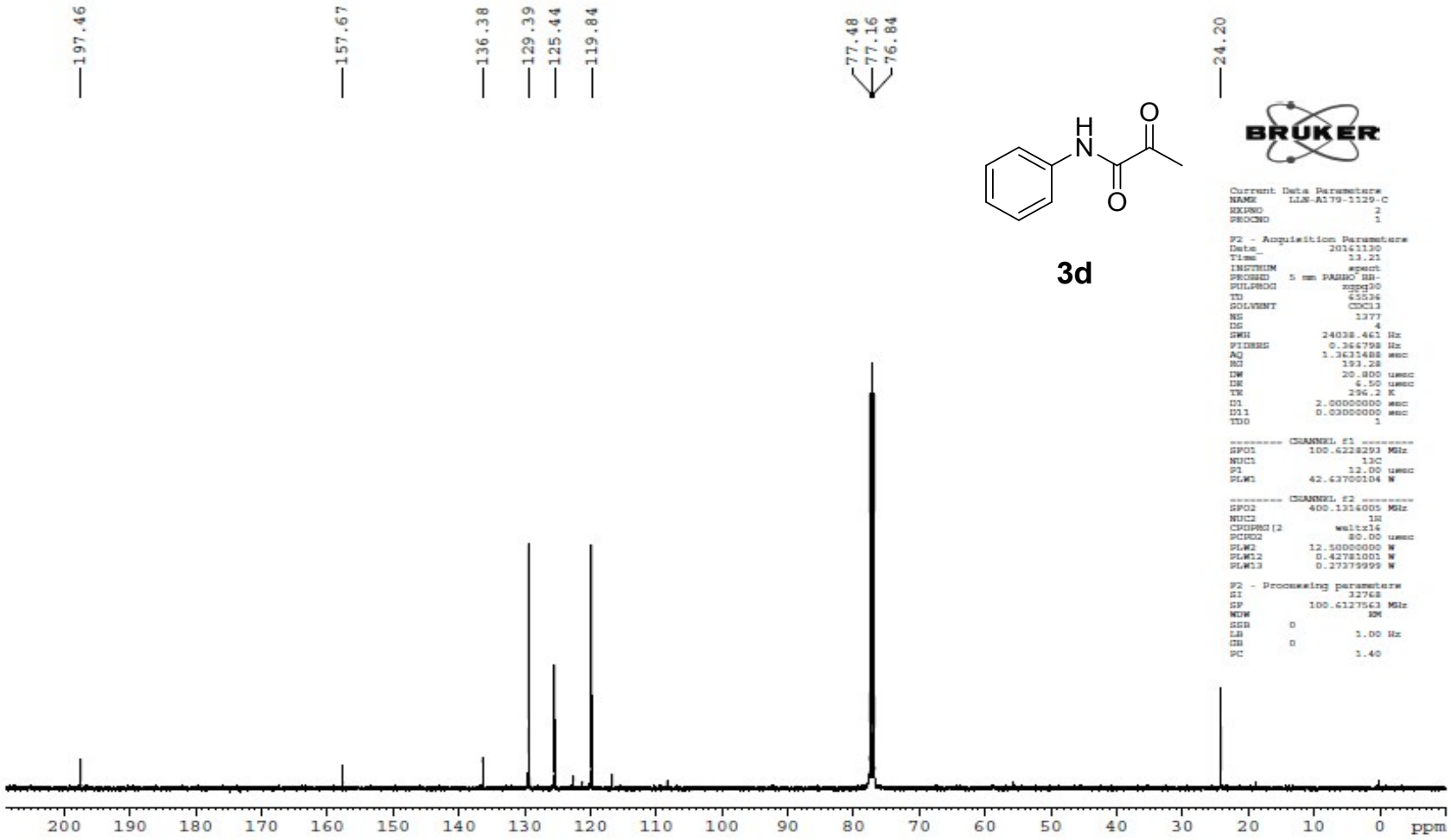
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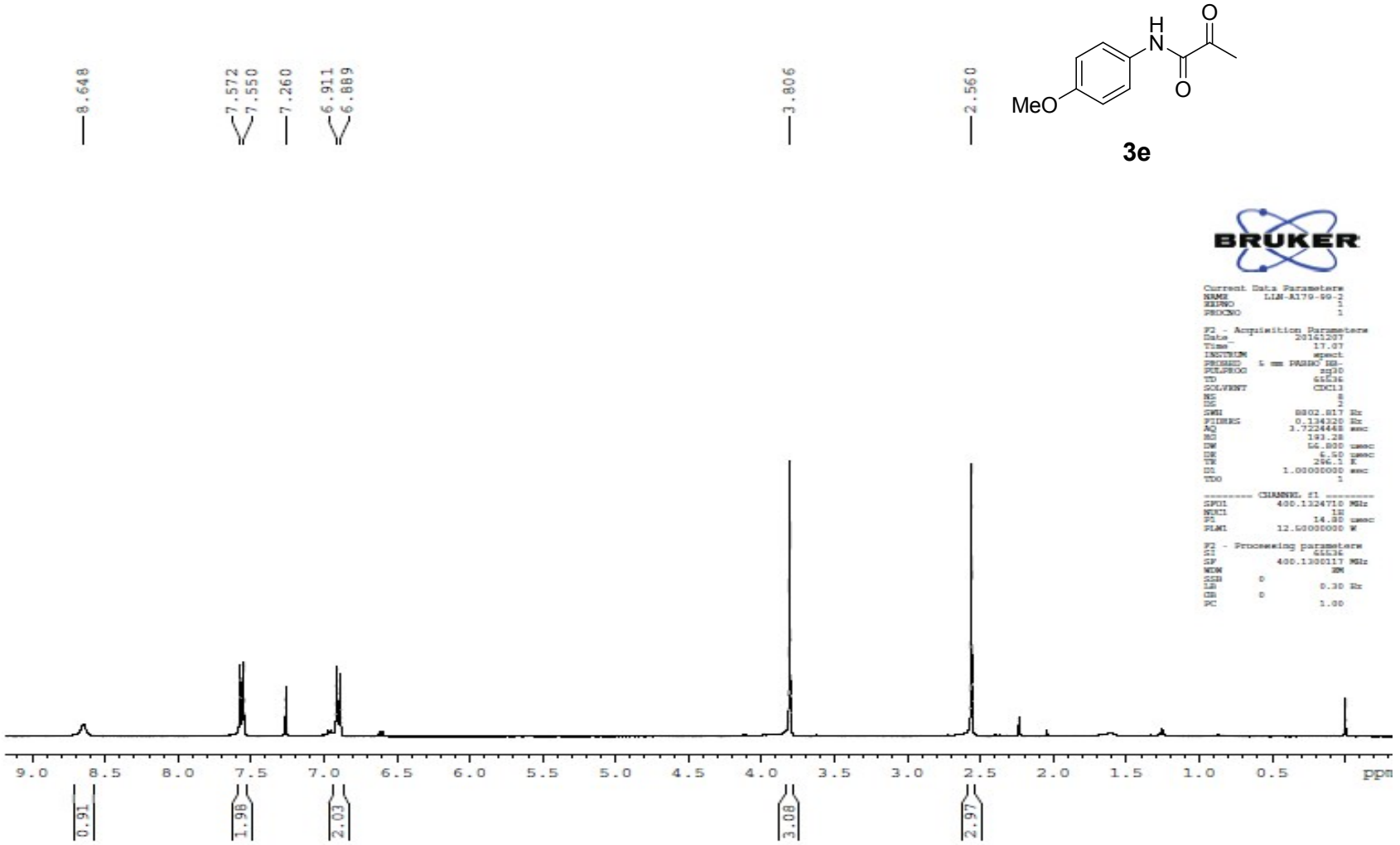
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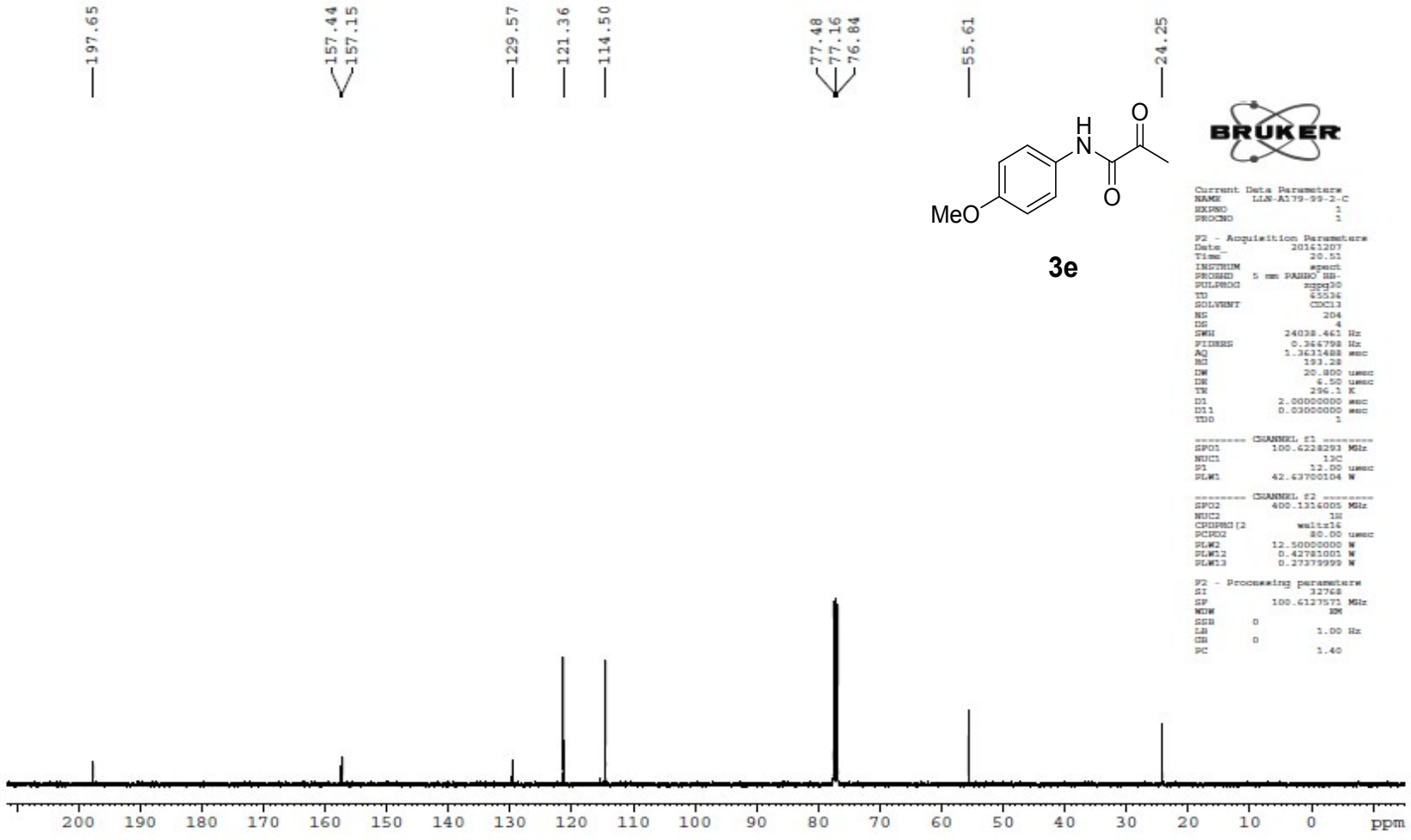
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CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
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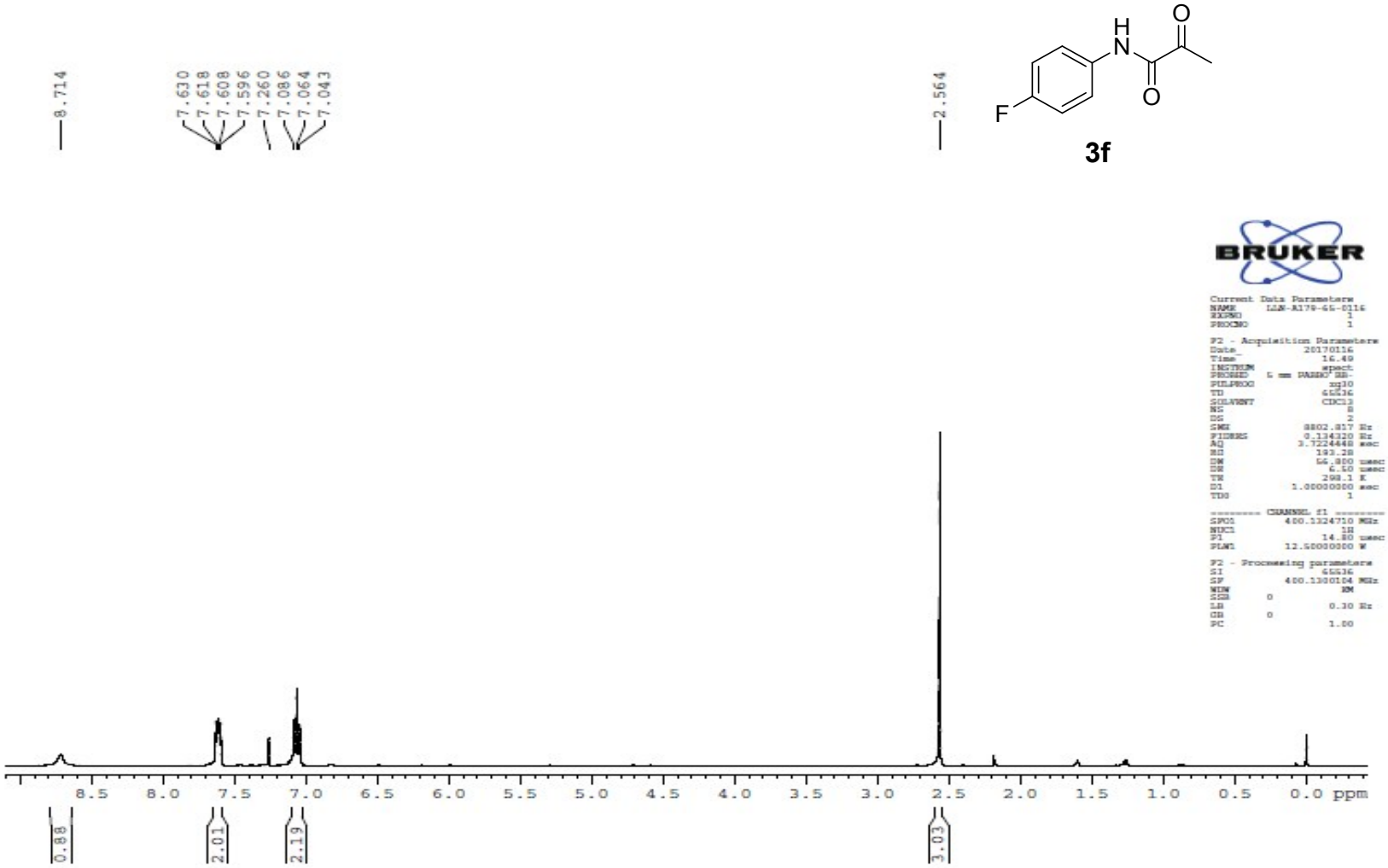
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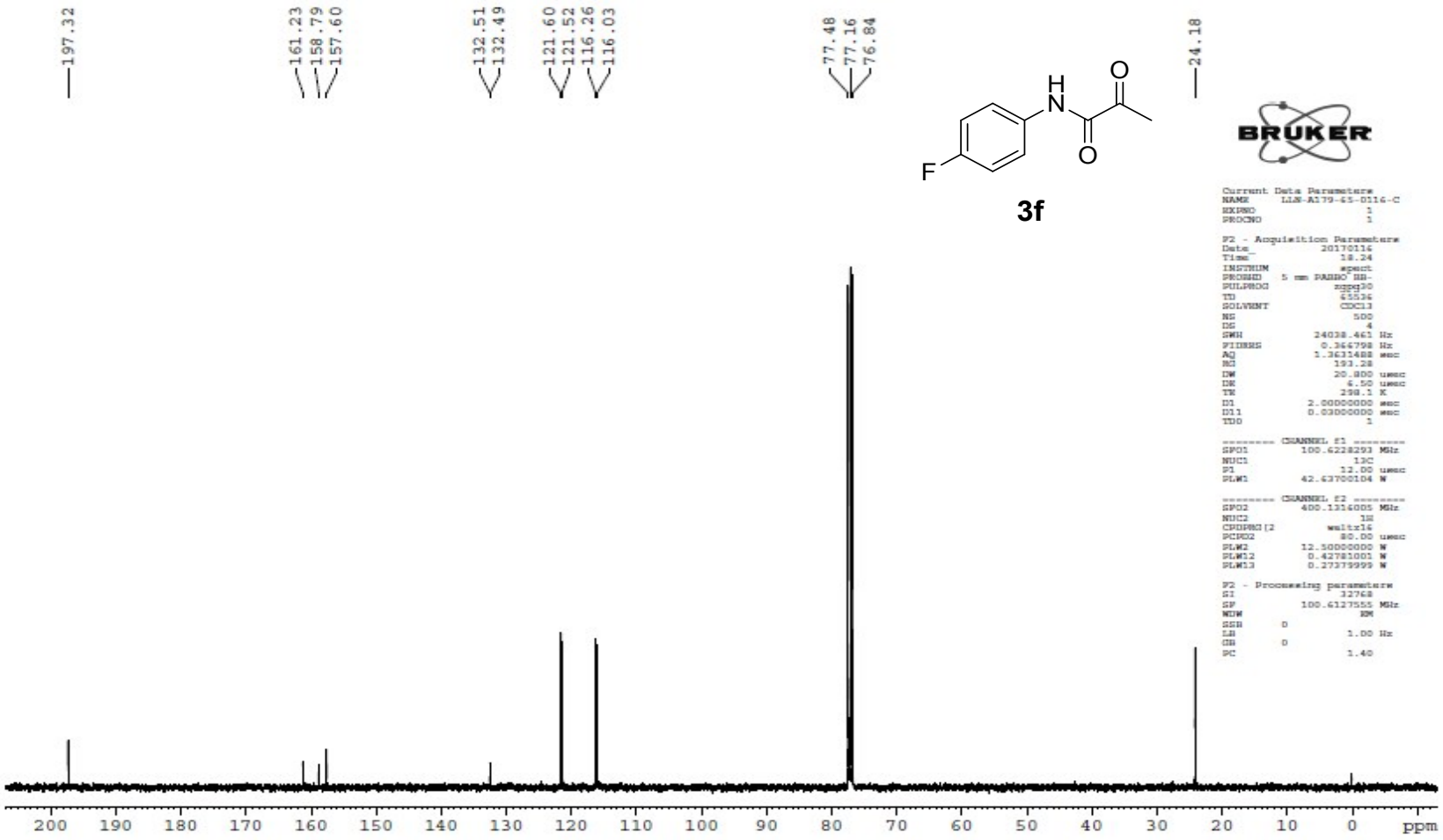
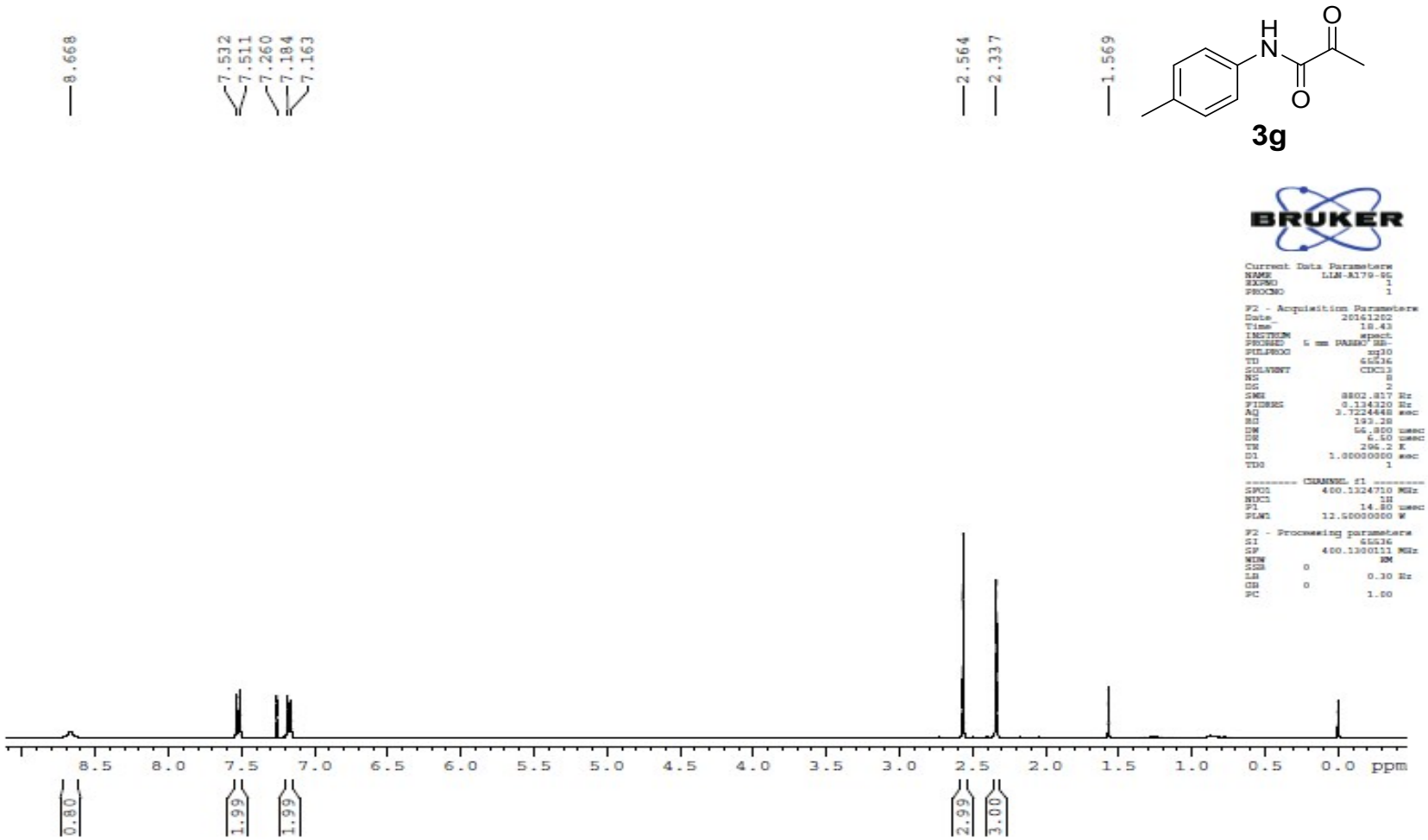
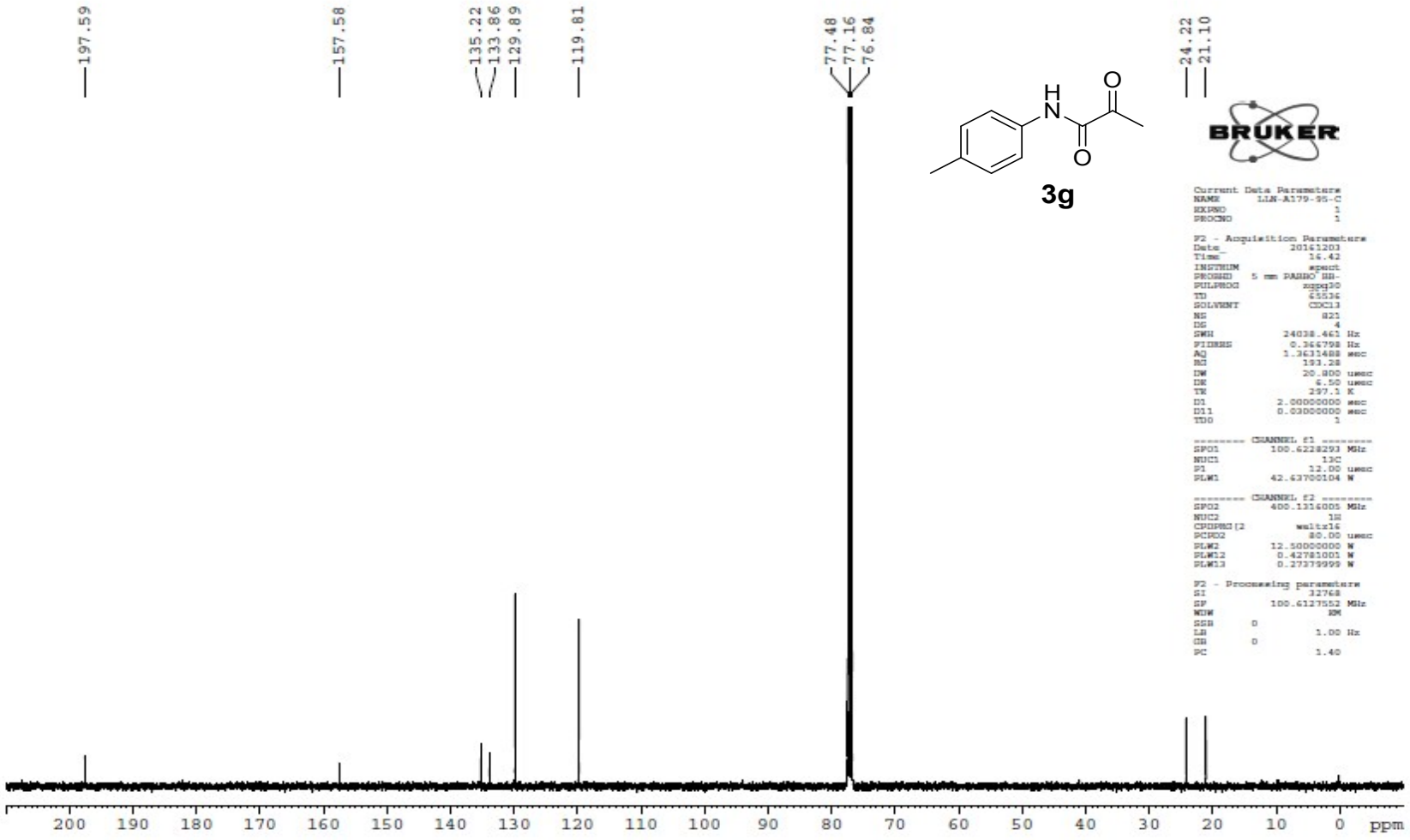
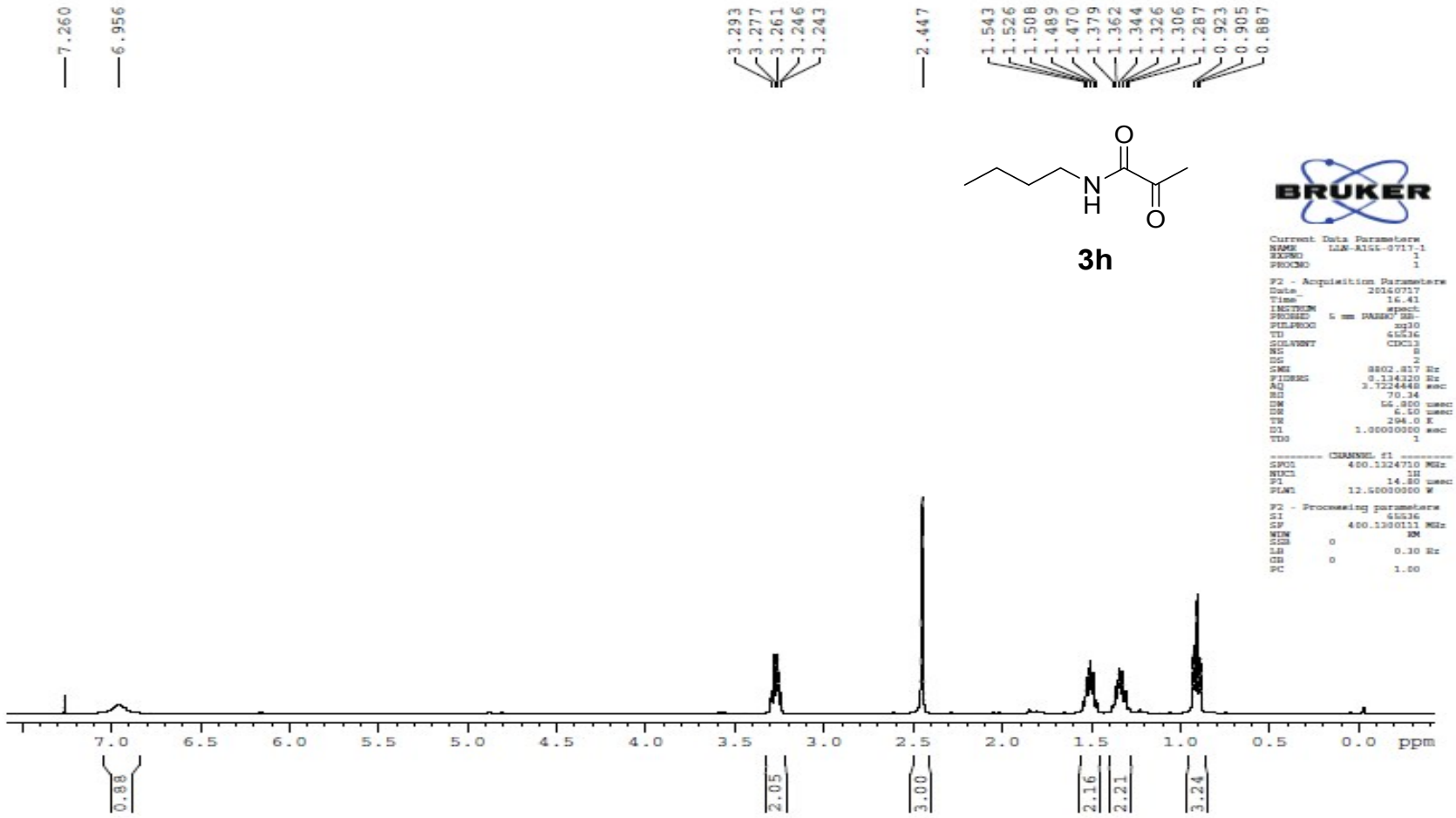
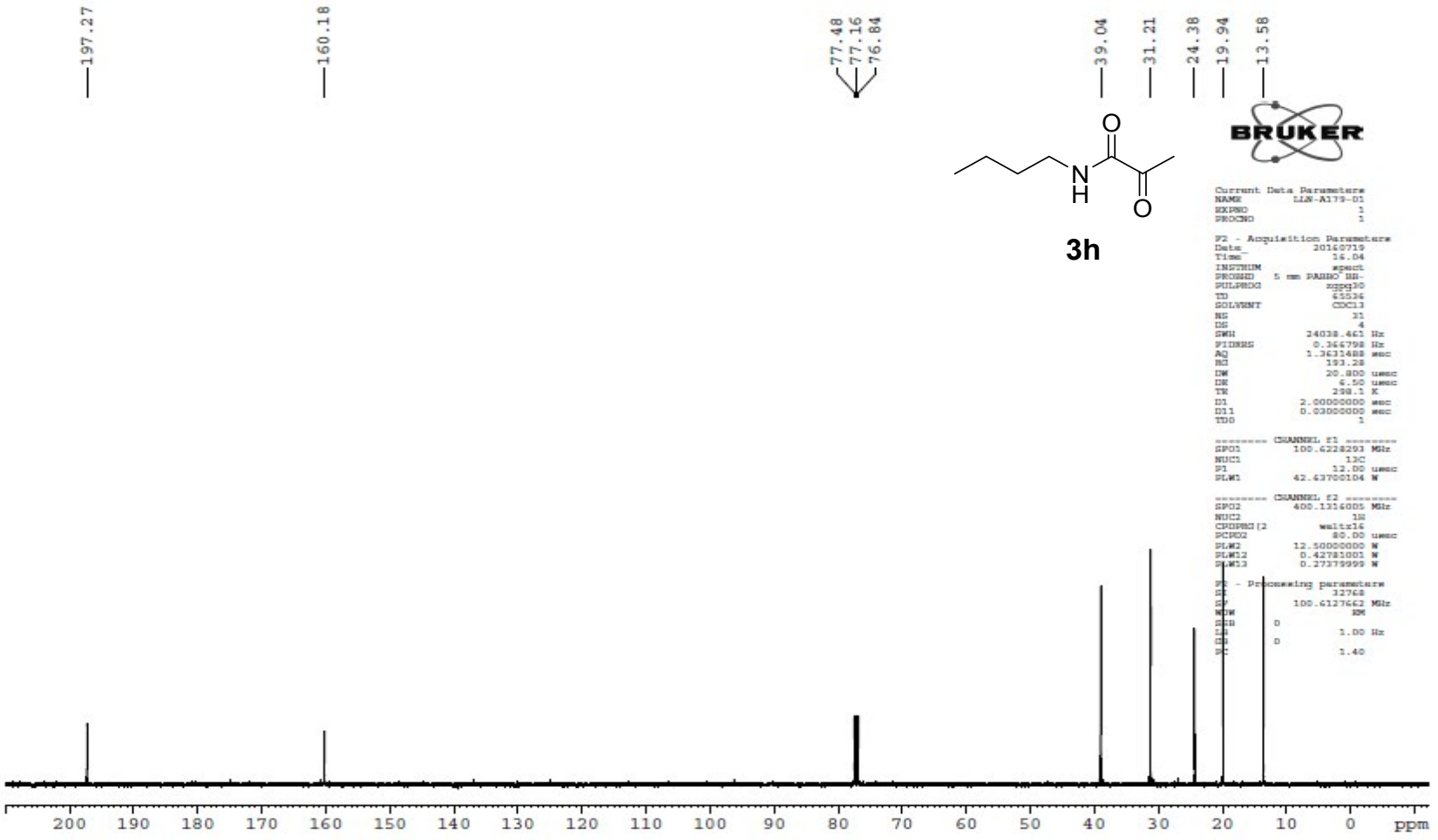
BRUKER
Current Data Parameters
NAME LLN-A179-6L-0116
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170116
Time 16.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 193.28
DW 56.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
0.88
2.01
2.19
3.03

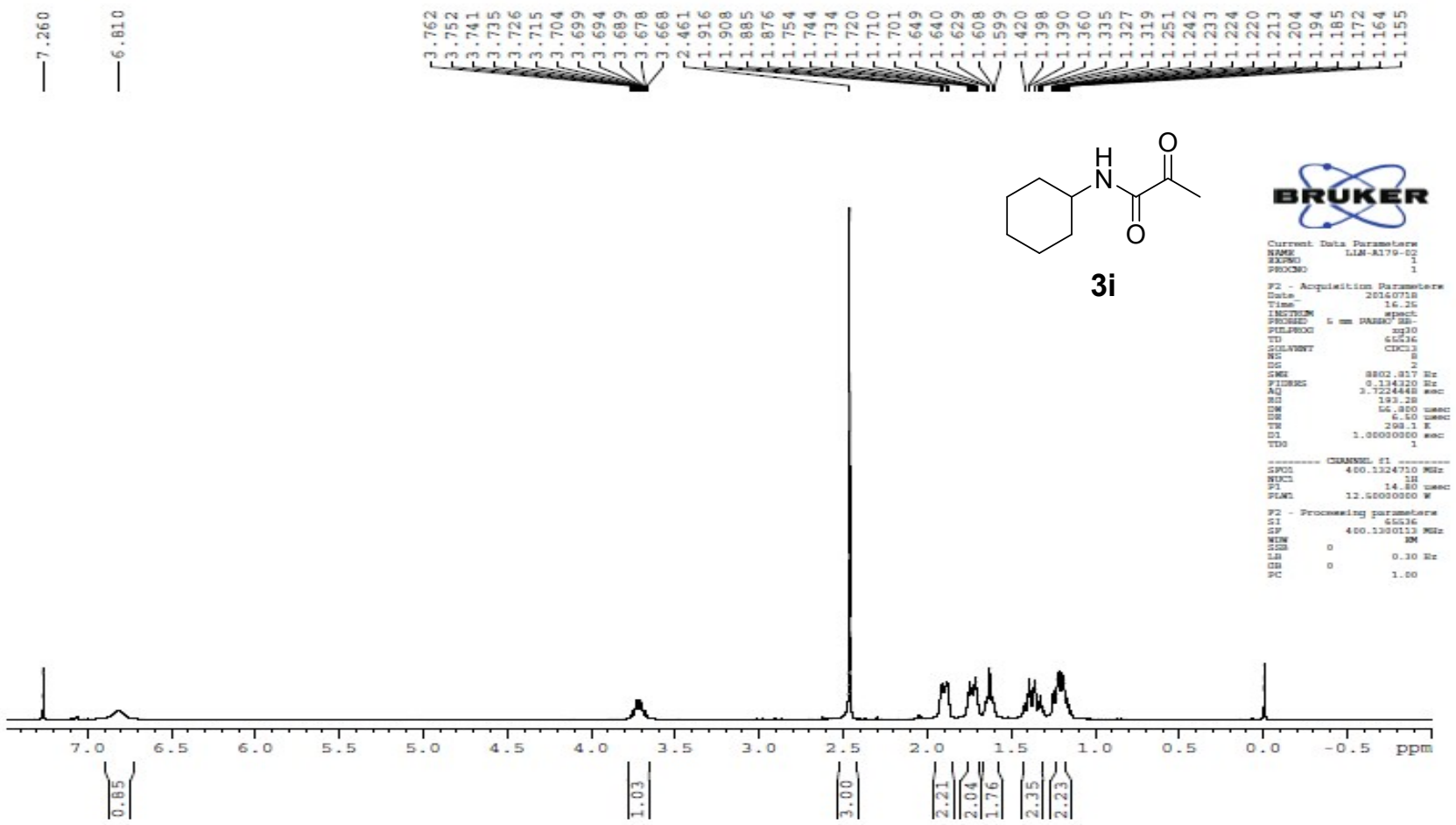

197.32
161.23
158.79
157.60
132.51
132.49
121.60
121.52
116.26
116.03
77.48
77.16
76.84
24.18
3f
BRUKER
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

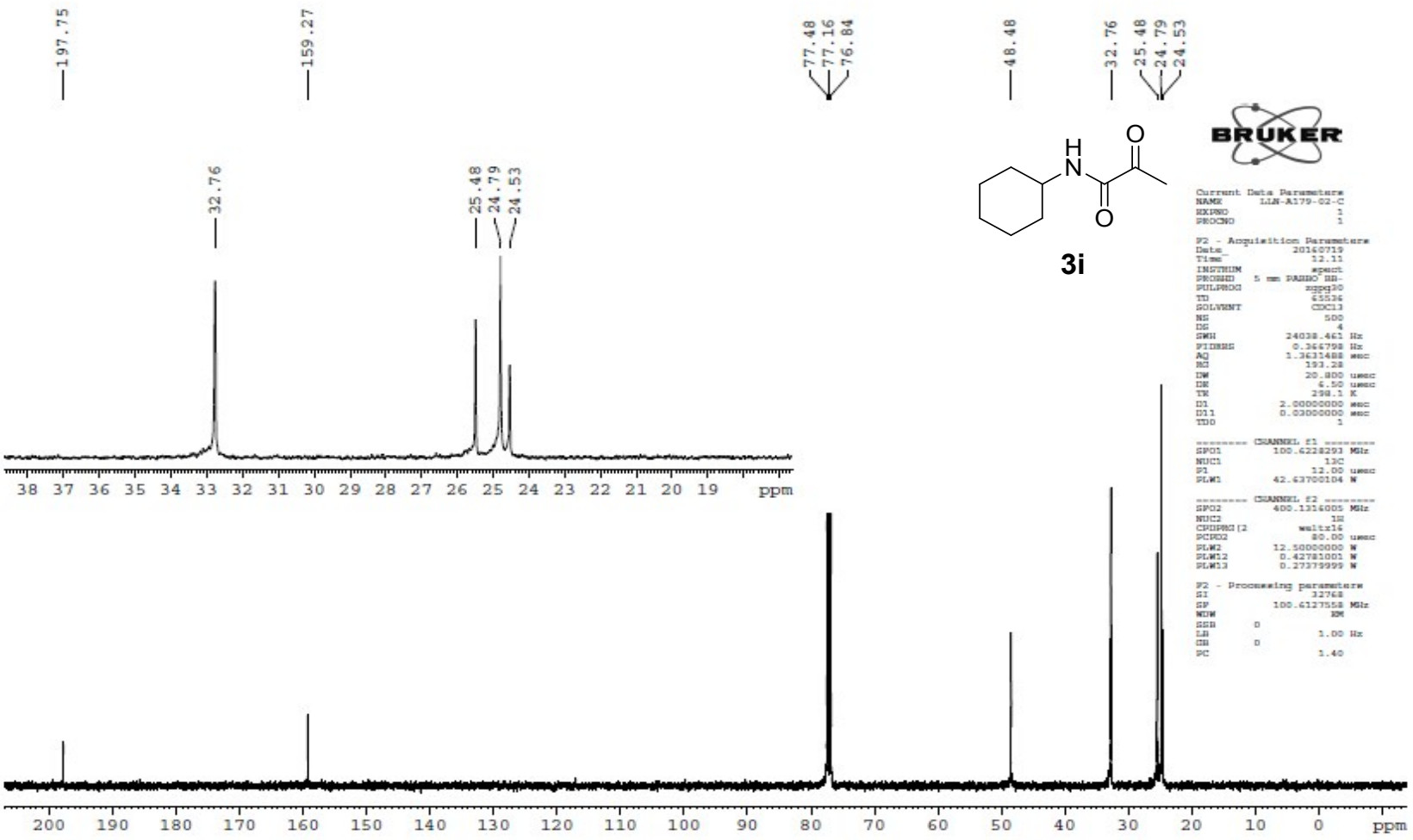

8.668
7.532
7.511
7.260
7.184
7.163
2.564
2.337
1.569
3g
BRUKER
Current Data Parameters
NAME LLM-A179-9S
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20161202
Time 18.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 193.28
DW 56.800 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
0.80
1.99
1.99
2.99
3.00

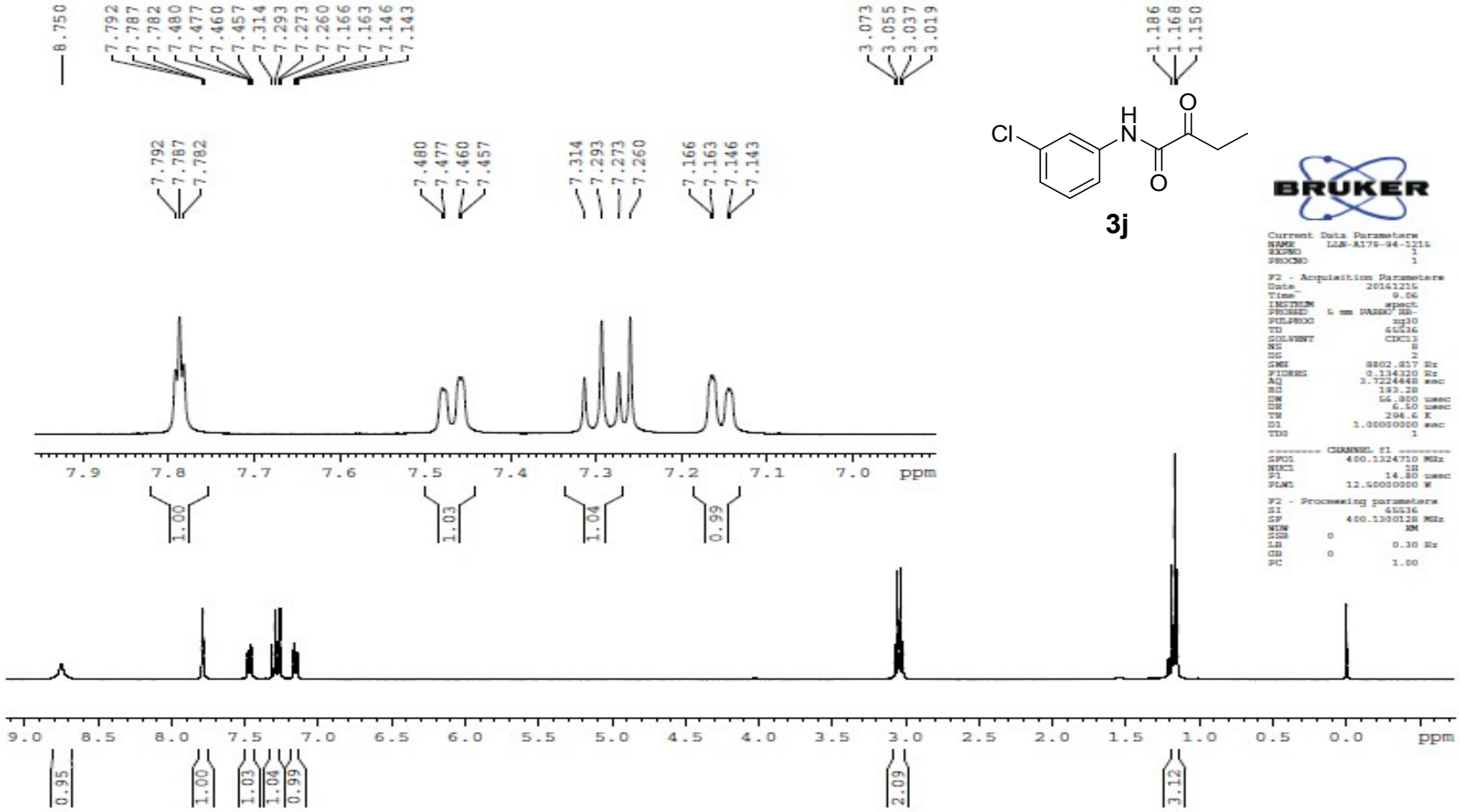

197.59
157.58
135.22
133.86
129.89
119.81
77.48
77.16
76.84
24.22
21.10
H
N
O
O
3g
BRUKER
Current Data Parameters
NAME LLN-A179-95-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161203
Time 14.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 821
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127552 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

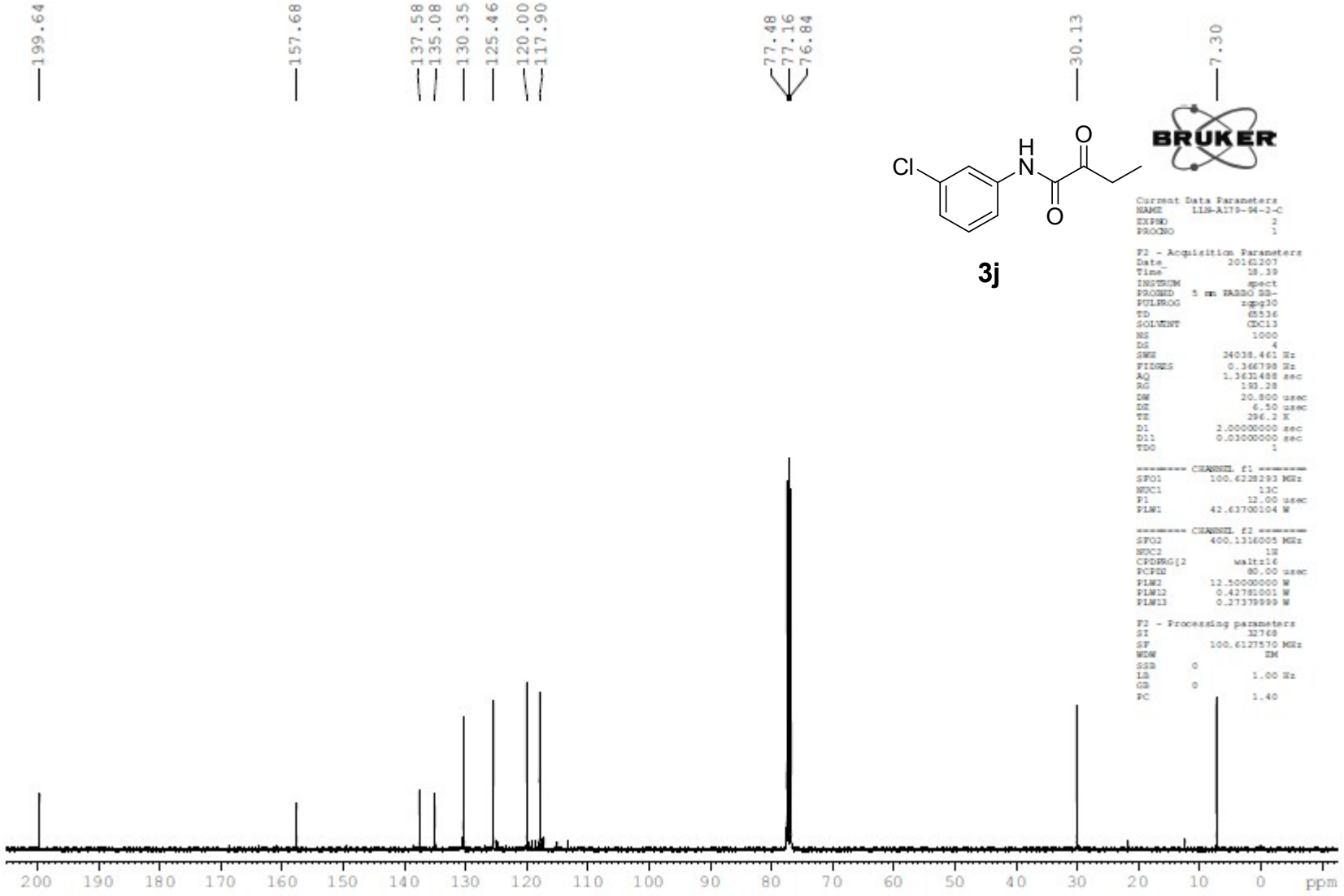

7.260
6.956
3.293
3.277
3.261
3.246
3.243
2.447
1.543
1.526
1.508
1.489
1.470
1.379
1.362
1.344
1.326
1.306
1.287
0.923
0.905
0.887
O
N
H
O
3h
BRUKER
Current Data Parameters
NAME LLW-A155-0717-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160717
Time 16.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 70.34
DW 56.800 usec
DE 6.50 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.88
2.05
3.00
2.16
2.21
3.24

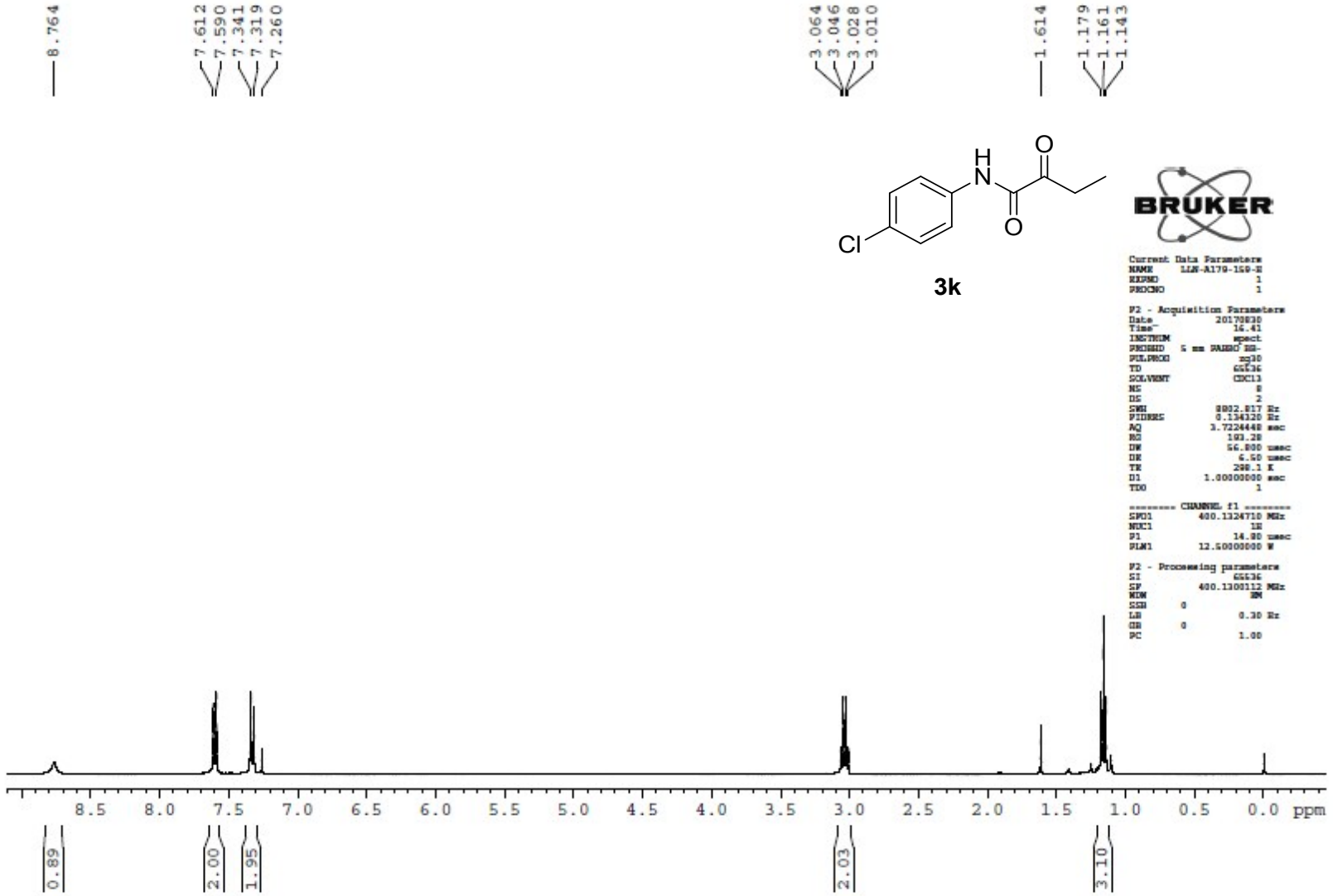

197.27
160.18
77.48
77.16
76.84
39.04
31.21
24.38
19.94
13.58
O
N
H
O
3h
BRUKER
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

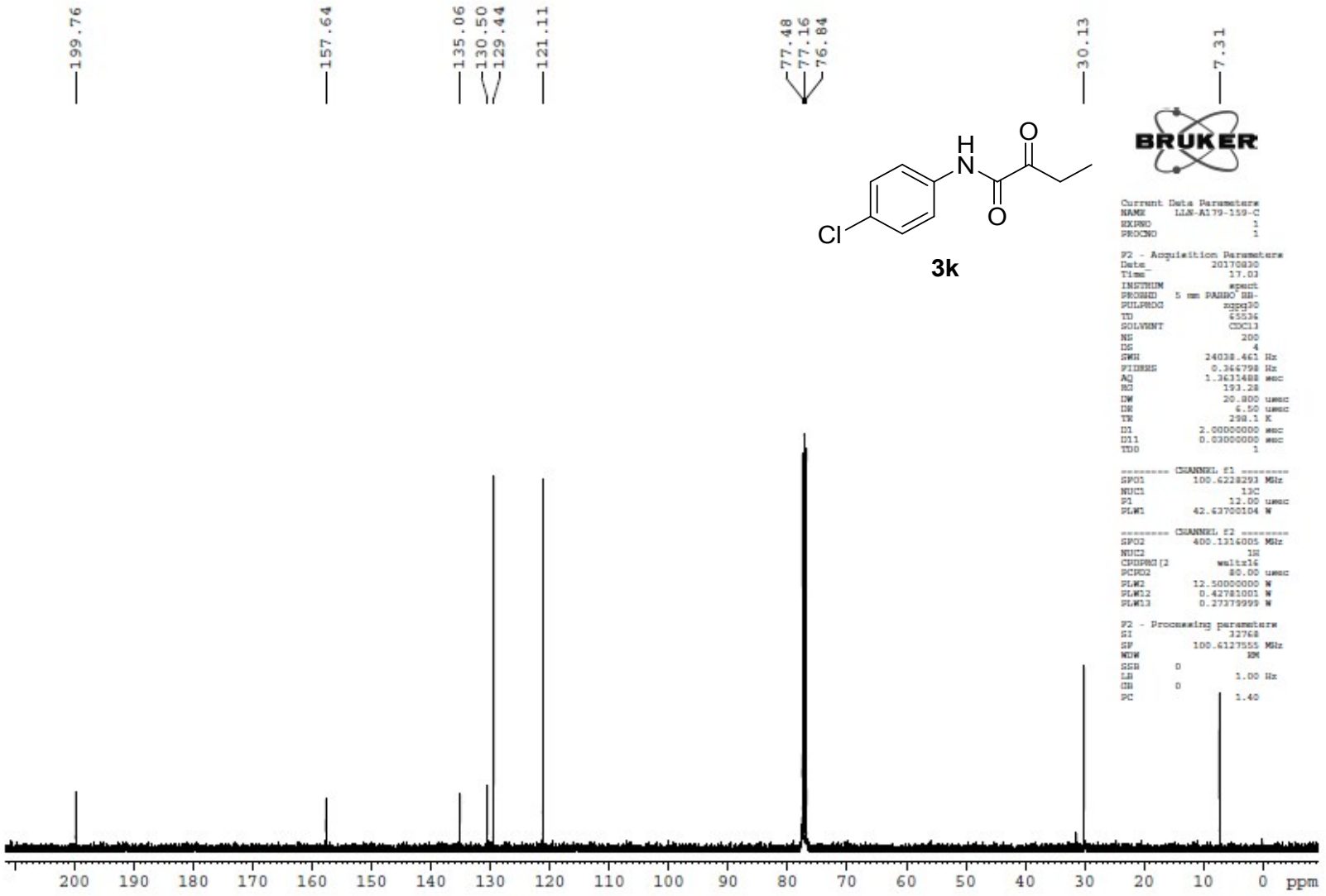

7.260
6.810
3.762
3.752
3.741
3.735
3.726
3.715
3.704
3.699
3.694
3.689
3.678
3.668
2.461
1.916
1.908
1.885
1.876
1.754
1.744
1.734
1.720
1.710
1.701
1.649
1.640
1.629
1.608
1.599
1.420
1.398
1.390
1.360
1.335
1.327
1.319
1.251
1.242
1.233
1.224
1.220
1.213
1.204
1.194
1.185
1.172
1.164
1.155
H
N
O
O
3i
BRUKER
Current Data Parameters
NAME LIM-A179-02
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160718
Time 16.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 193.28
DW 56.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
0.85
1.03
3.00
2.21
2.04
1.76
2.35
2.23

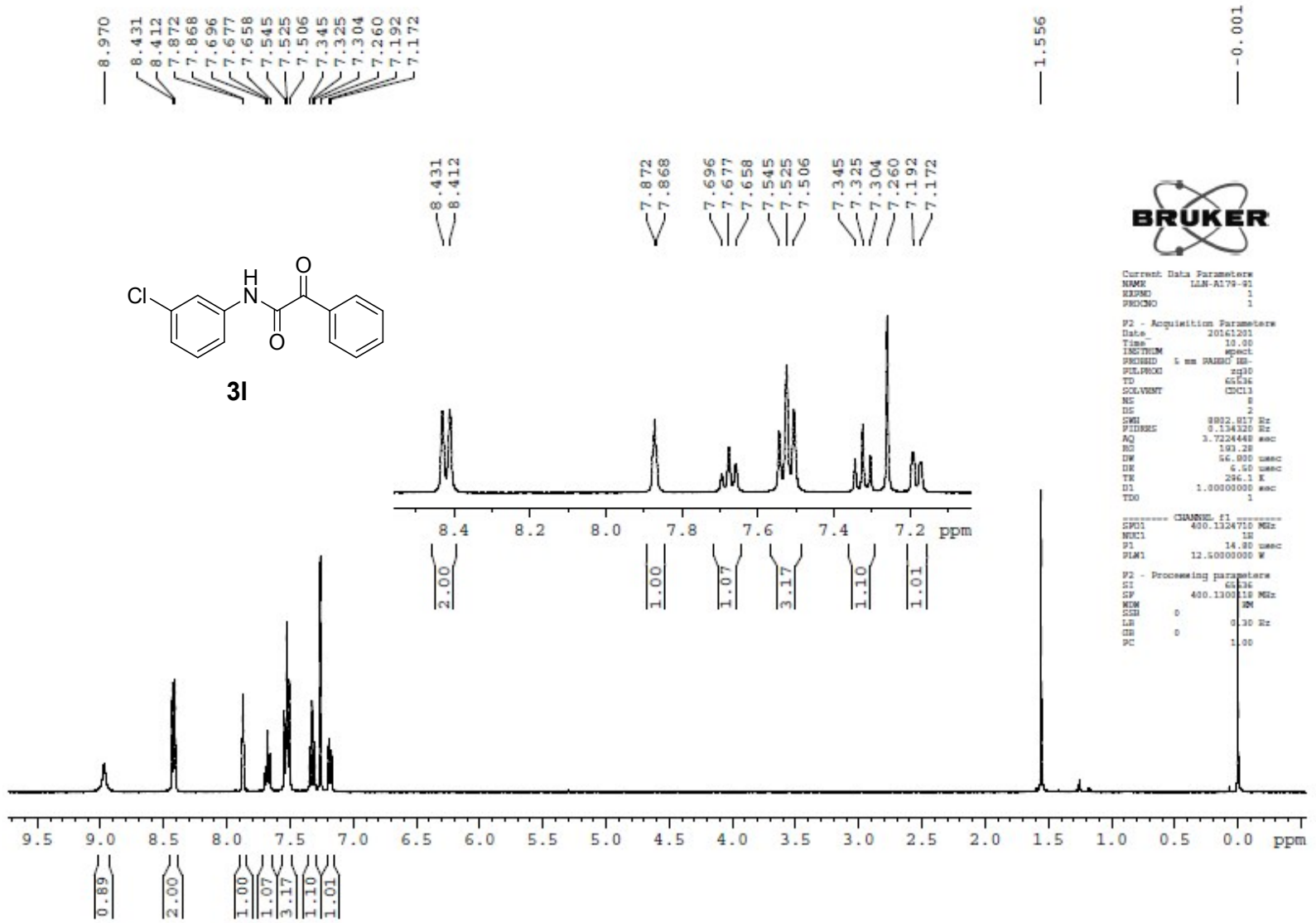

197.75
159.27
77.48
77.16
76.84
48.48
32.76
25.48
24.79
24.53
3i
BRUKER
ppm

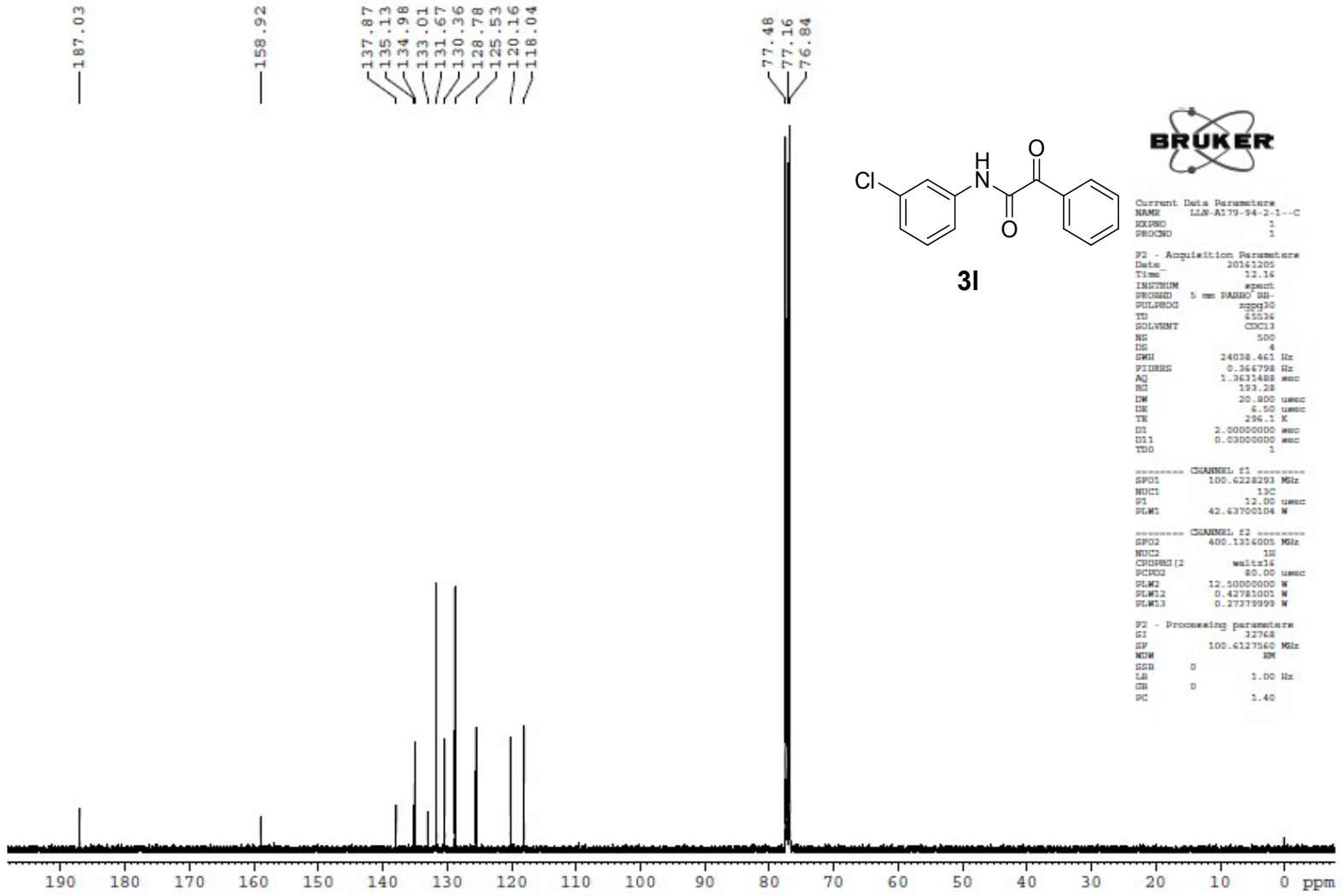

8.750
7.792
7.787
7.782
7.480
7.477
7.460
7.457
7.314
7.293
7.273
7.260
7.166
7.163
7.146
7.143
3.073
3.055
3.037
3.019
1.186
1.168
1.150
Cl
H
N
O
O
3j
BRUKER
ppm
1.00
1.03
1.04
0.99
0.95
2.09
3.12

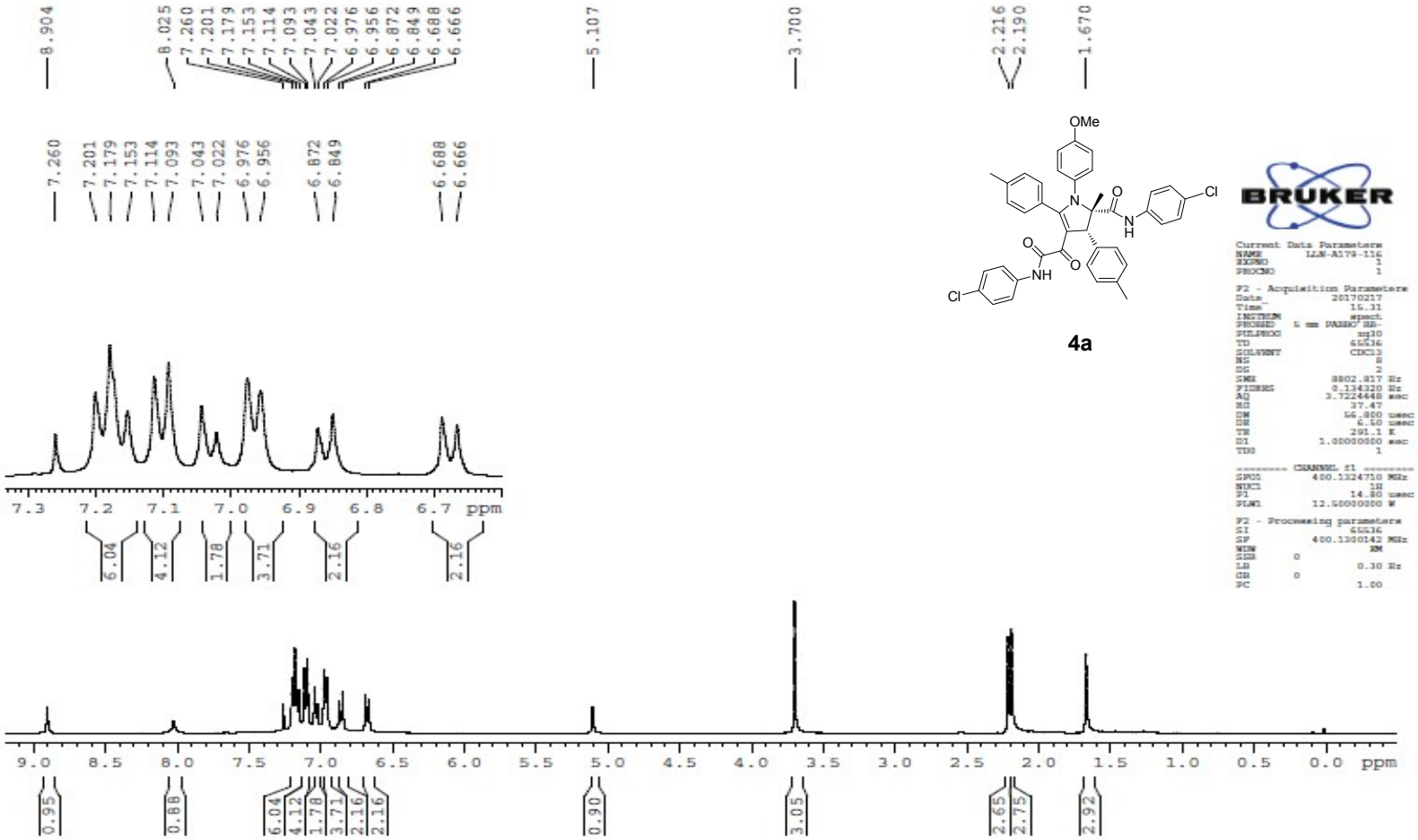

199.64
157.68
137.58
135.08
130.35
125.46
120.00
117.90
77.48
77.16
76.84
30.13
7.30
Cl
H
N
O
O
3j
BRUKER
Current Data Parameters
NAME LLB-A179-04-2-C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161207
Time 18.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127570 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

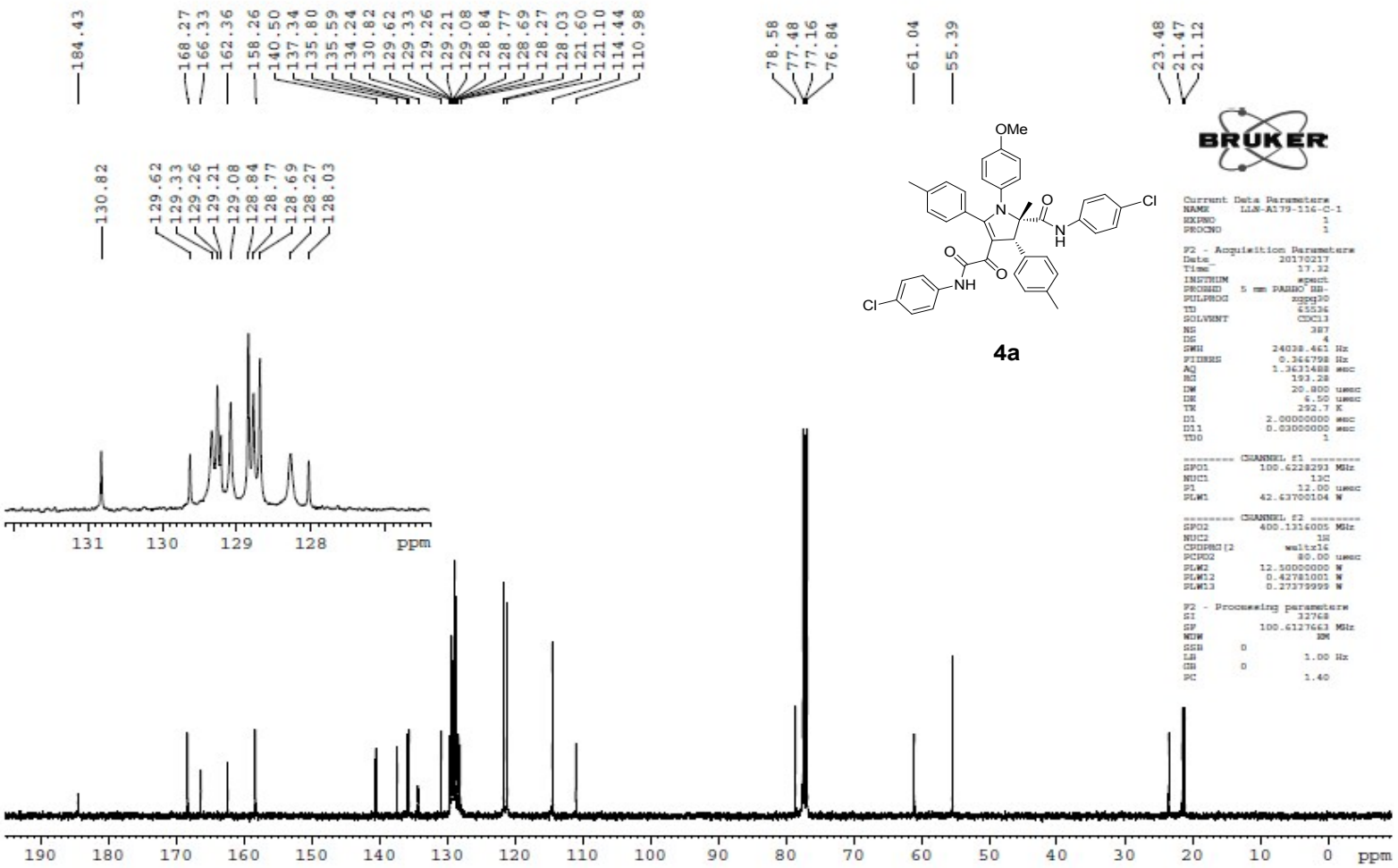

8.764
7.612
7.590
7.341
7.319
7.260
3.064
3.046
3.028
3.010
1.614
1.179
1.161
1.143
Cl
H
N
O
O
3k
BRUKER
Current Data Parameters
NAME LLW-A179-159-H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170830
Time 16.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 193.28
DW 56.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.89
2.00
1.95
2.03
3.10

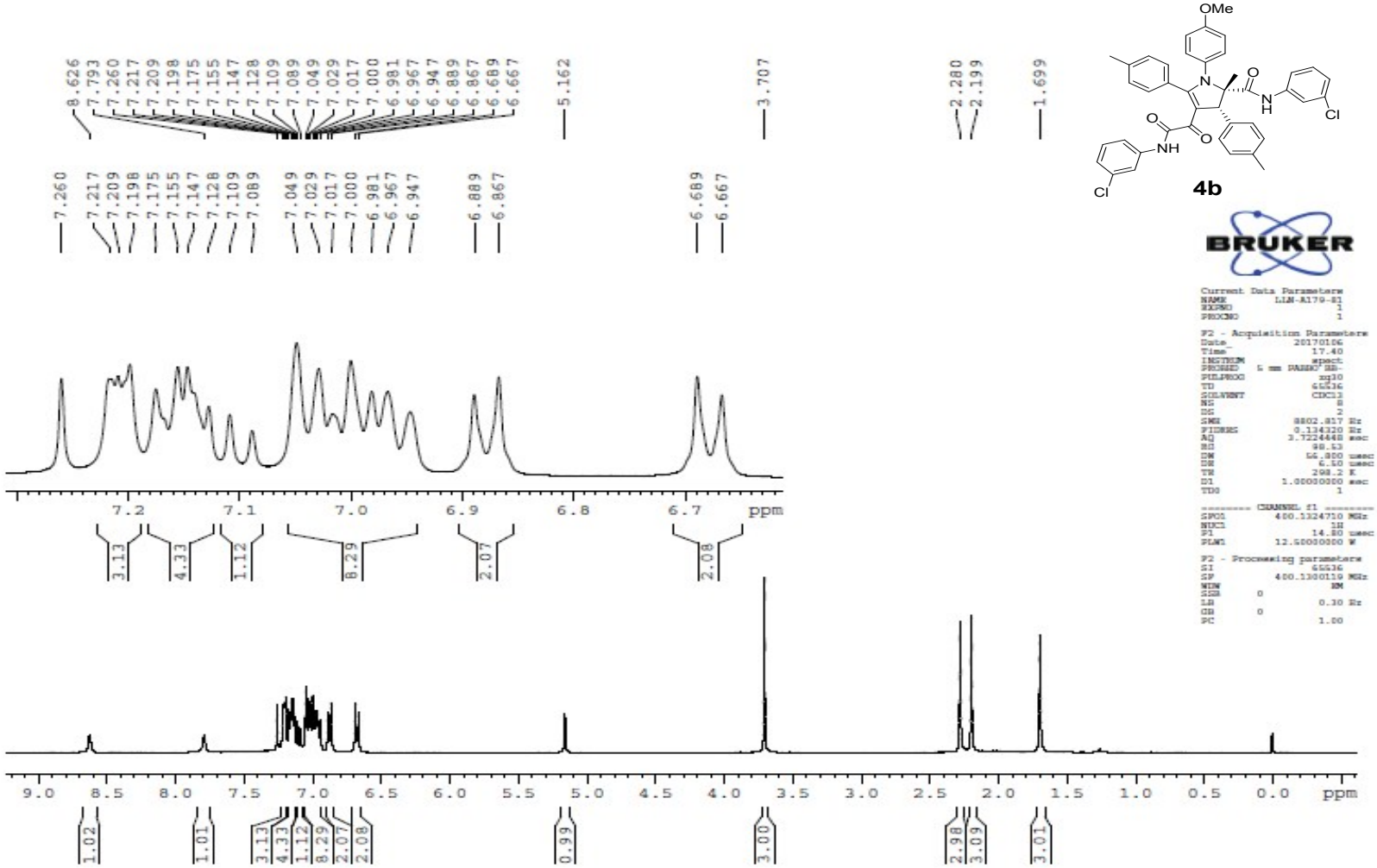

199.76
157.64
135.06
130.50
129.44
121.11
77.48
77.16
76.84
30.13
7.31
BRUKER
Cl
H
N
O
O
3k
Current Data Parameters
NAME LLN-A179-159-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170830
Time 17.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

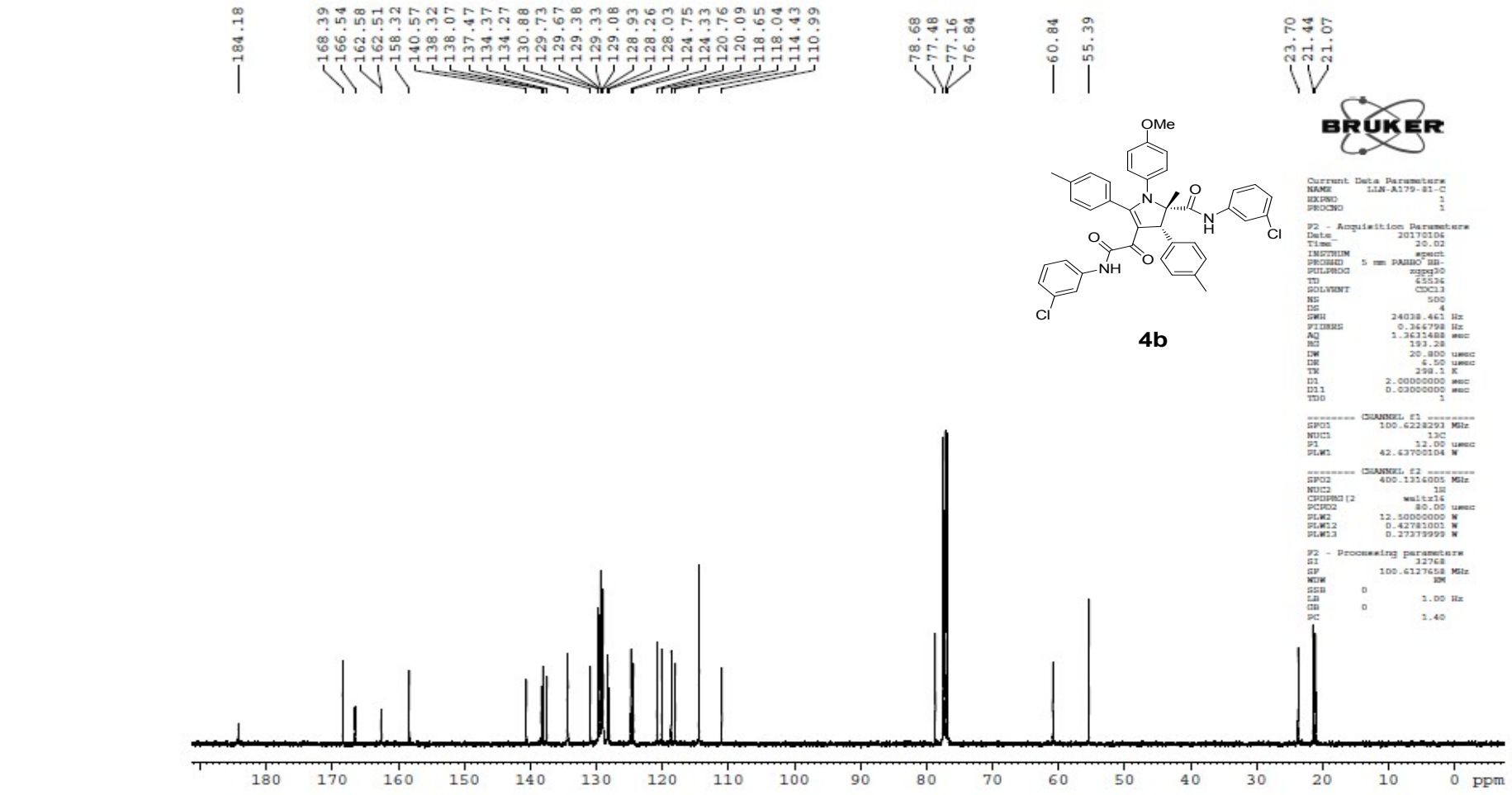

8.970
8.431
8.412
7.872
7.868
7.696
7.677
7.658
7.545
7.525
7.506
7.345
7.325
7.304
7.260
7.192
7.172
1.556
-0.001
Cl
H
N
O
O
3l
BRUKER
ppm
0.89
2.00
1.00
1.07
3.17
1.10
1.01

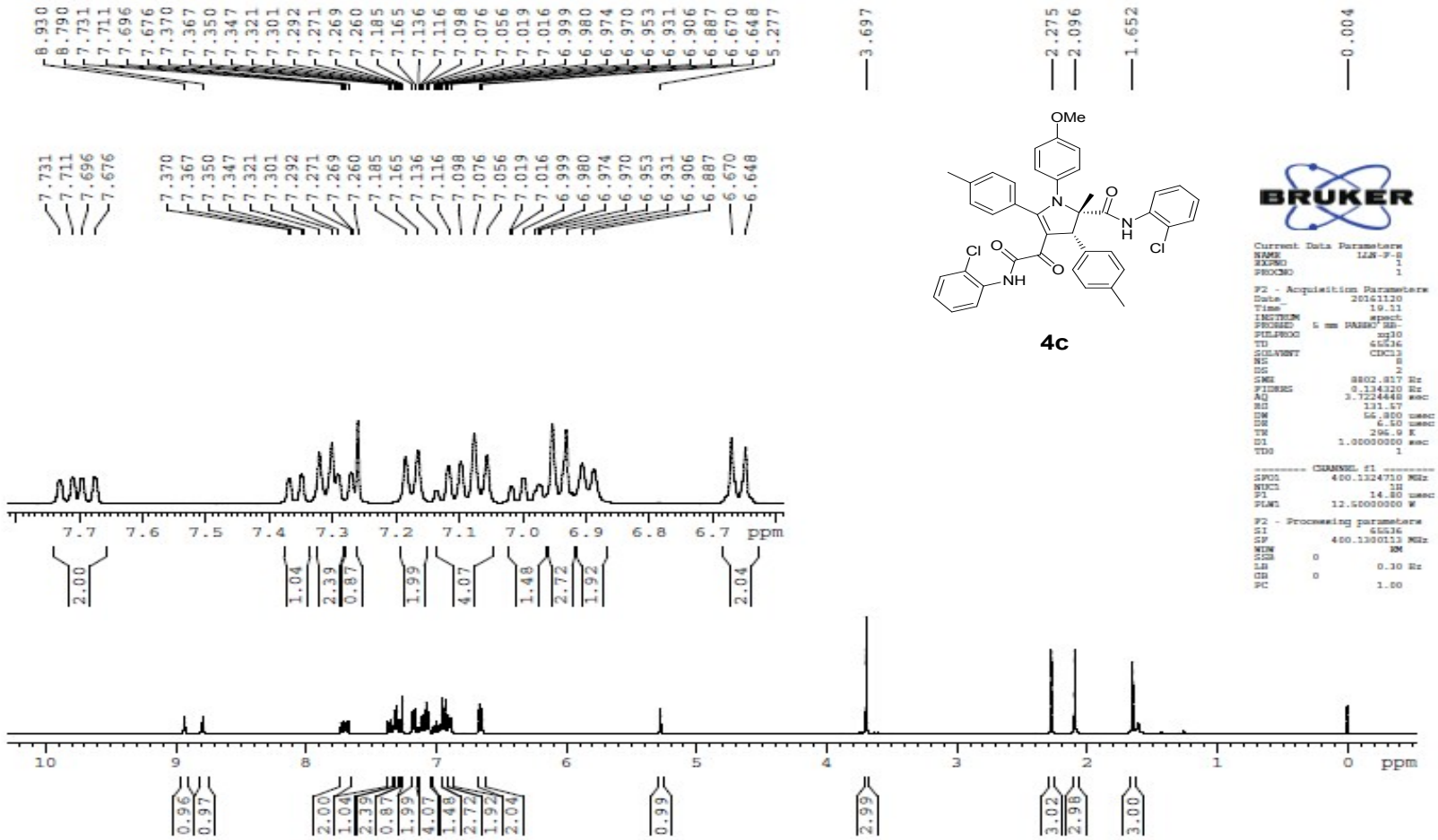

187.03
158.92
137.87
135.13
134.98
133.01
131.67
130.36
128.78
125.53
120.16
118.04
77.48
77.16
76.84
Cl
H
N
O
O
3l
BRUKER
Current Data Parameters
NAME LLN-A179-94-2-1--C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161205
Time 12.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127560 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

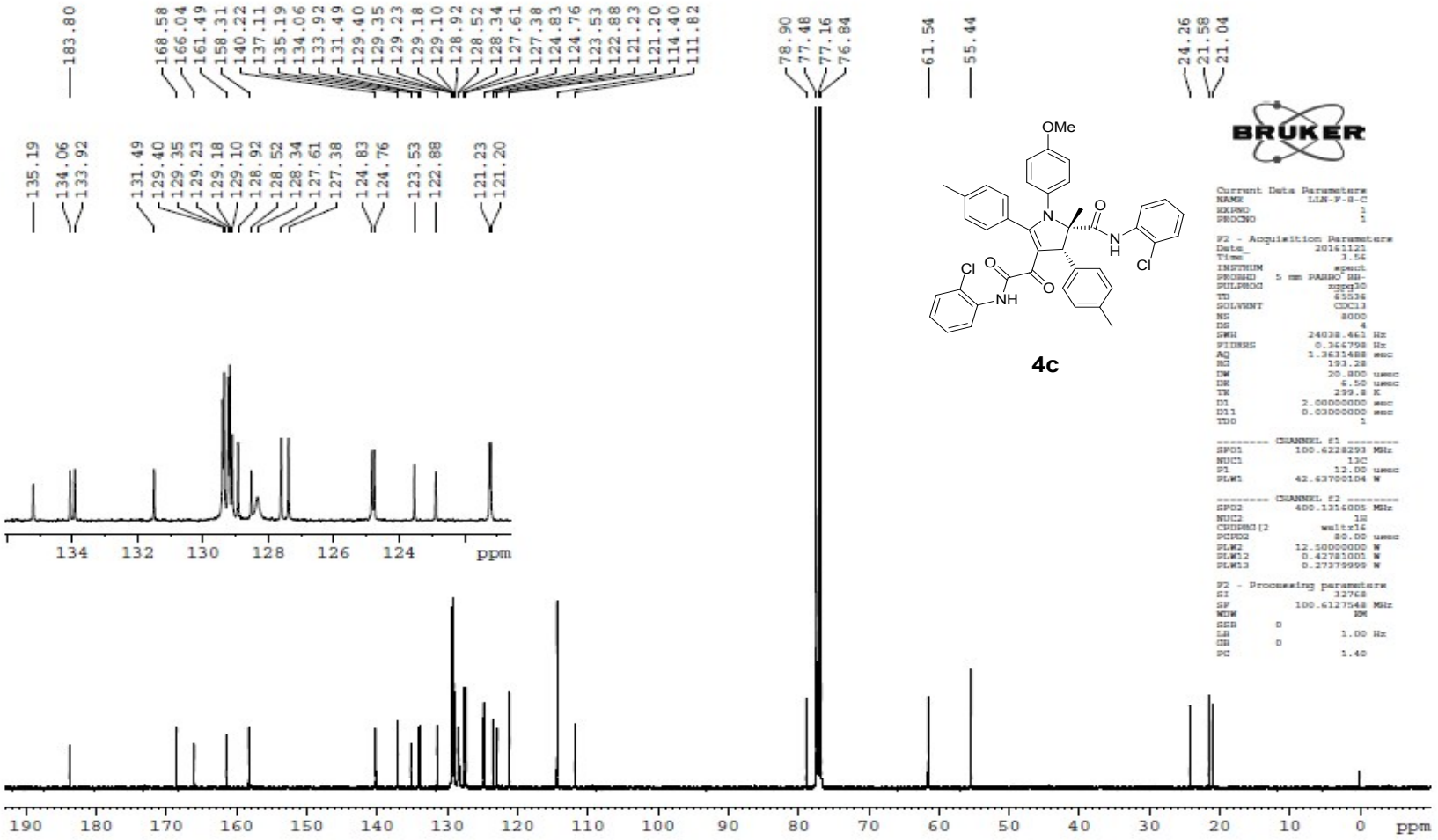

8.904
8.025
7.260
7.201
7.179
7.153
7.114
7.093
7.043
7.022
6.976
6.956
6.872
6.849
6.688
6.666
5.107
3.700
2.216
2.190
1.670
OMe
Cl
NH
O
N
Cl
4a
BRUKER
Current Data Parameters
NAME LLW-A179-116
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170217
Time 15.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 37.47
DW 56.800 usec
DE 6.50 usec
TE 291.1 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PL1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.3 7.2 7.1 7.0 6.9 6.8 6.7 ppm
6.04 4.12 1.78 3.71 2.16 2.16
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.95 0.88 6.04 4.12 1.78 3.71 2.16 2.16 0.90 3.05 2.65 2.75 2.92

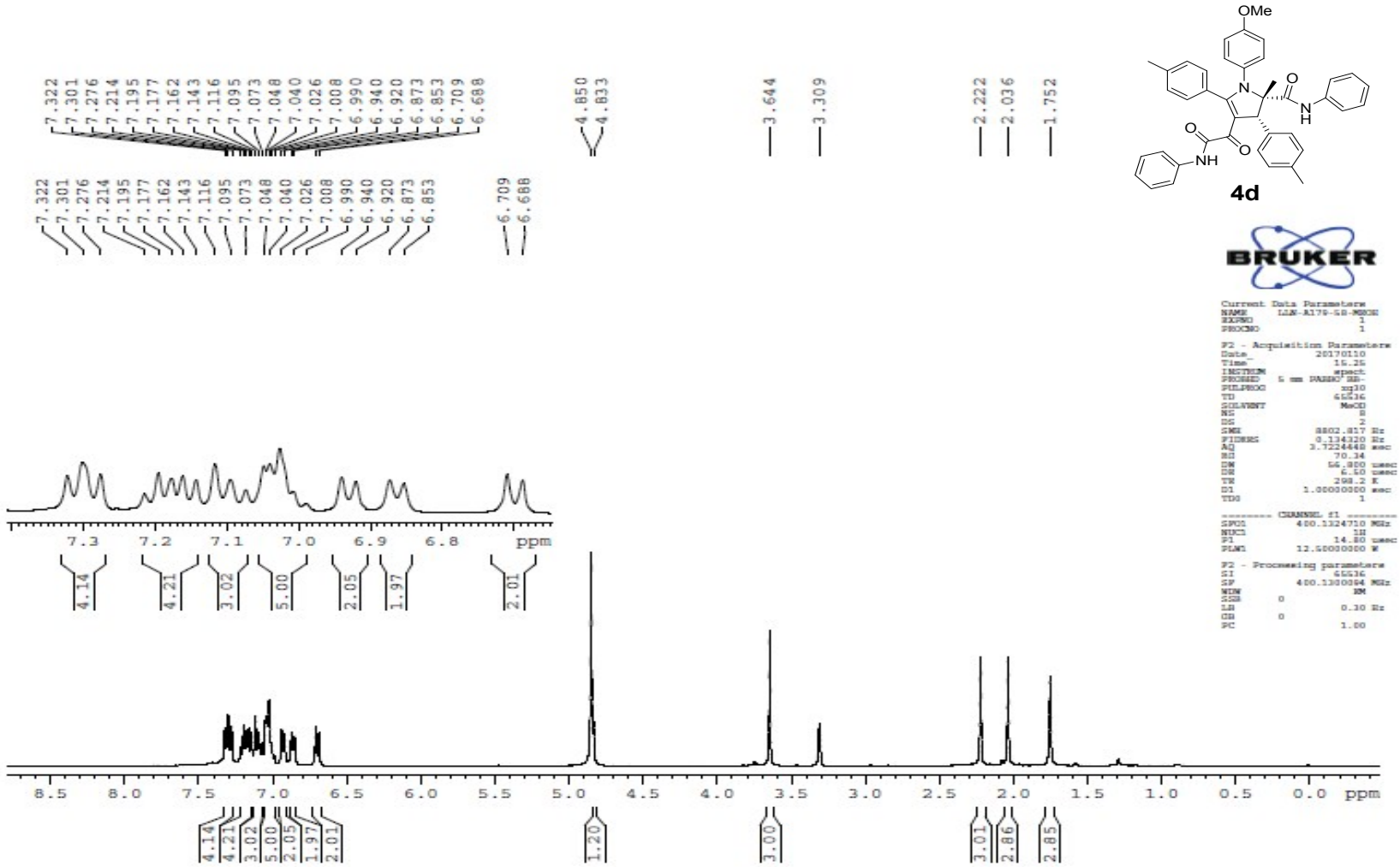

184.43
168.27
166.33
162.36
158.26
140.50
137.34
135.80
135.59
134.24
130.82
129.62
129.33
129.26
129.21
129.08
128.84
128.77
128.69
128.27
128.03
121.60
121.10
114.44
110.98
78.58
77.48
77.16
76.84
61.04
55.39
23.48
21.47
21.12
OMe
Cl
NH
O
N
4a
BRUKER
ppm

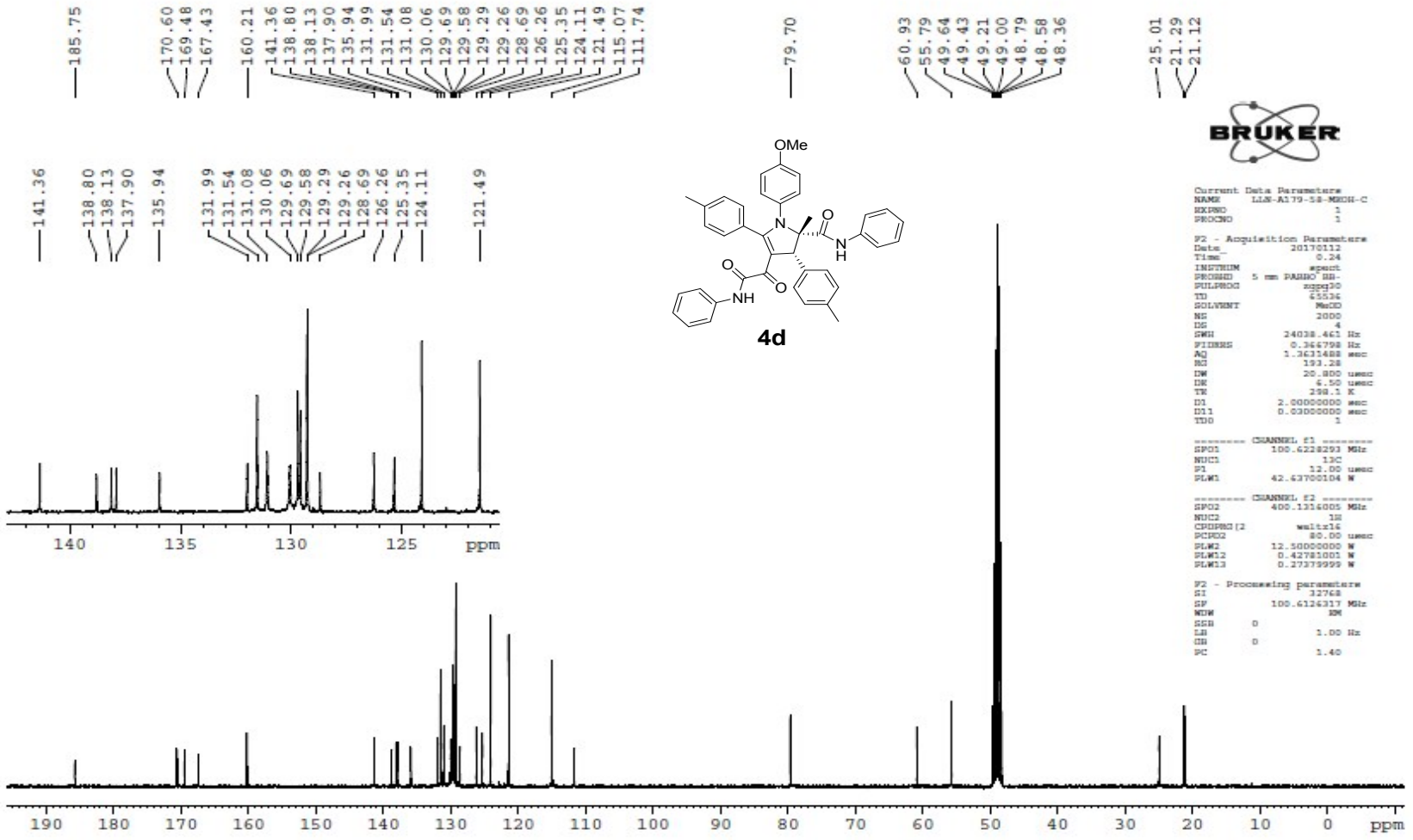

8.626
7.793
7.260
7.217
7.209
7.198
7.175
7.155
7.147
7.128
7.109
7.089
7.049
7.029
7.017
7.000
6.981
6.967
6.947
6.889
6.867
6.689
6.667
5.162
3.707
2.280
2.199
1.699
OMe
Cl
NH
O
N
4b
BRUKER
Current Data Parameters
NAME LLN-A179-01
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170106
Time 17.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 98.53
DW 56.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm
3.13
4.33
1.12
8.29
2.07
2.08
1.02
1.01
0.99
3.00
2.98
3.09
3.01


184.18
168.39
166.54
162.58
162.51
158.32
140.57
138.32
138.07
137.47
134.37
134.27
130.88
129.73
129.67
129.38
129.33
129.08
128.93
128.26
128.03
124.75
124.33
120.76
120.09
118.65
118.04
114.43
110.99
78.68
77.48
77.16
76.84
60.84
55.39
23.70
21.44
21.07
OMe
N
O
N
H
Cl
O
O
NH
Cl
4b
BRUKER
Current Data Parameters
NAME LLN-A179-81-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170106
Time 20.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127658 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

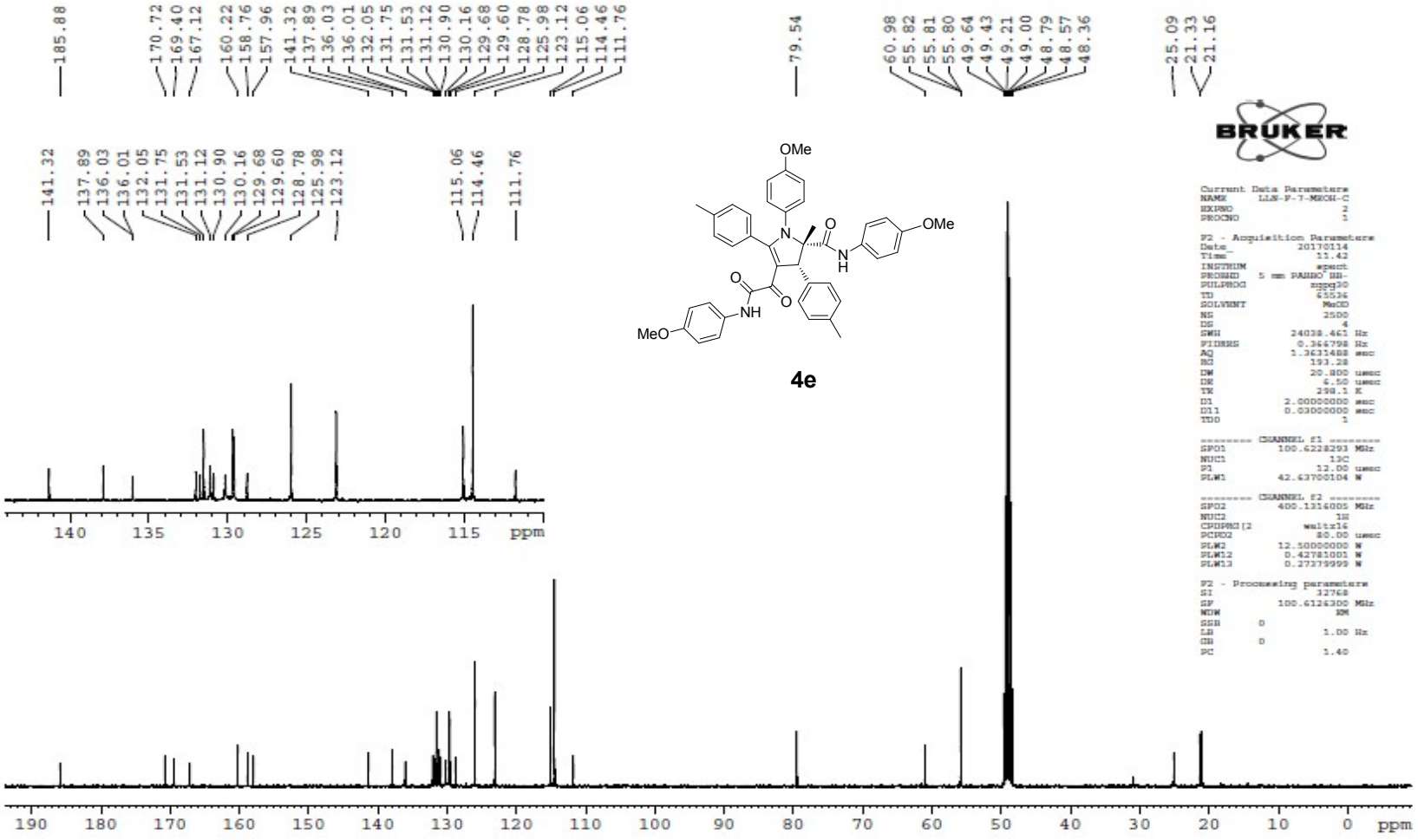

8.930
8.790
7.731
7.711
7.696
7.676
7.370
7.367
7.350
7.347
7.321
7.301
7.292
7.271
7.269
7.260
7.185
7.165
7.136
7.116
7.098
7.076
7.056
7.019
7.016
6.999
6.980
6.974
6.970
6.953
6.931
6.906
6.887
6.670
6.648
5.277
3.697
2.275
2.096
1.652
0.004
OMe
N
O
N
H
Cl
O
NH
Cl
O
4c
BRUKER
Current Data Parameters
NAME LLN-P-8
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161120
Time 19.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 131.57
DW 56.800 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 ppm
2.00 1.04 2.39 0.87 1.99 4.07 1.48 2.72 1.92 2.04
10 9 8 7 6 5 4 3 2 1 0 ppm
0.96 0.97 2.00 1.04 2.39 0.87 1.99 4.07 1.48 2.72 1.92 2.04 0.99 2.99 3.02 2.98 3.00

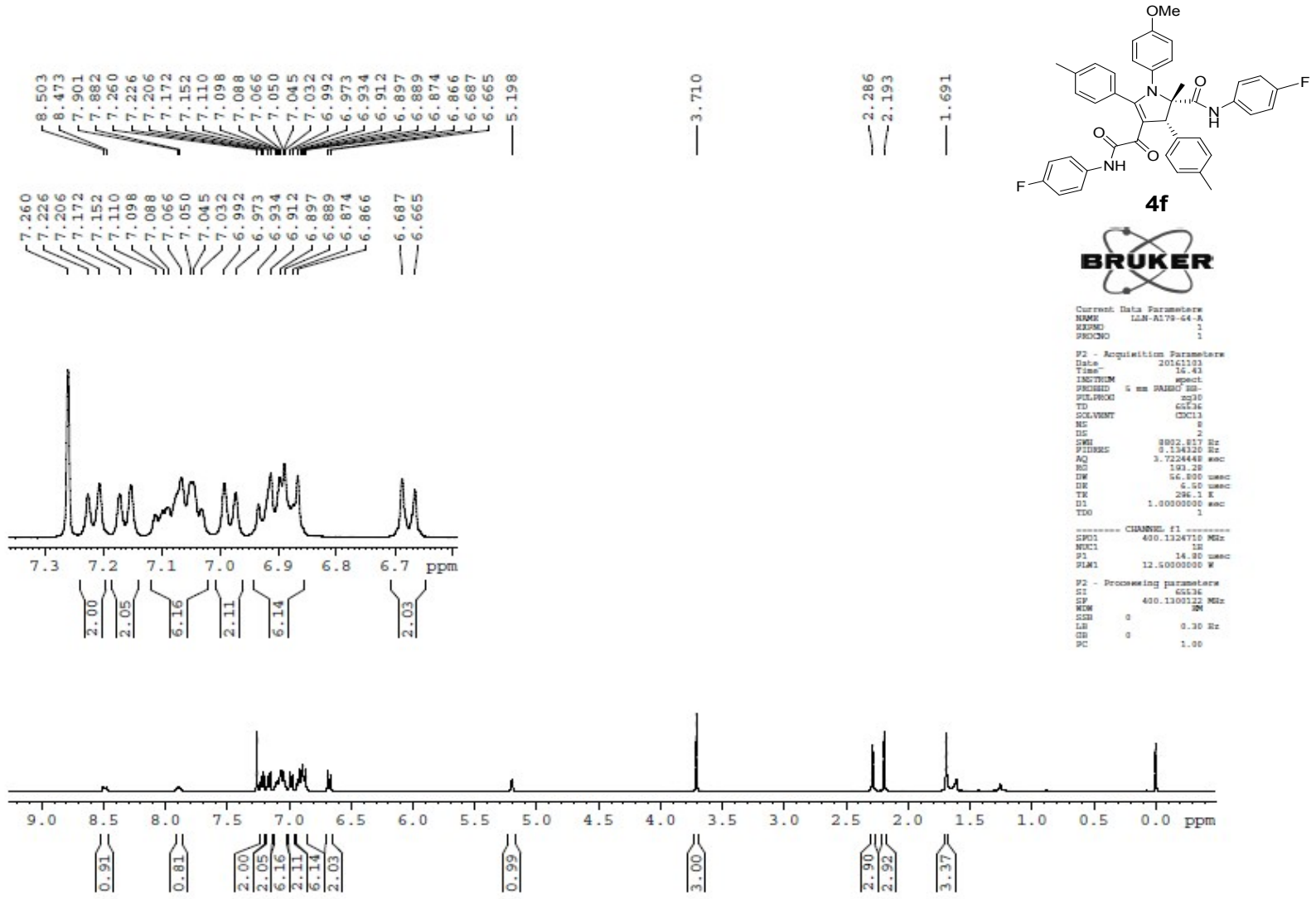

183.80
168.58
166.04
161.49
158.31
140.22
137.11
135.19
134.06
133.92
131.49
129.40
129.35
129.23
129.18
129.10
128.92
128.52
128.34
127.61
127.38
124.83
124.76
123.53
122.88
121.23
121.20
114.40
111.82
78.90
77.48
77.16
76.84
61.54
55.44
24.26
21.58
21.04
OMe
N
O
NH
Cl
4c
BRUKER
Current Data Parameters
NAME LLN-F-8-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161121
Time 3.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 181.28
DW 20.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27279999 W
F2 - Processing parameters
SI 32768
SF 100.6127548 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
134
132
130
128
126
124
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.322
7.301
7.276
7.214
7.195
7.177
7.162
7.143
7.116
7.095
7.073
7.048
7.040
7.026
7.008
6.990
6.940
6.920
6.873
6.853
6.709
6.688
4.850
4.833
3.644
3.309
2.222
2.036
1.752
OMe
N
O
NH
O
O
NH
4d
BRUKER
Current Data Parameters
NAME LLN-A179-SB-MEOH
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170110
Time 15.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 70.34
DW 56.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.3
7.2
7.1
7.0
6.9
6.8
ppm
4.14
4.21
3.02
5.00
2.05
1.97
2.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
4.14
4.21
3.02
5.00
2.05
1.97
2.01
1.20
3.00
3.01
2.86
2.85


185.75
170.60
169.48
167.43
160.21
141.36
138.80
138.13
137.90
135.94
131.99
131.54
131.08
130.06
129.69
129.58
129.29
129.26
128.69
126.26
125.35
124.11
121.49
115.07
111.74
79.70
60.93
55.79
49.64
49.43
49.21
49.00
48.79
48.58
48.36
25.01
21.29
21.12
OMe
N
O
NH
O
O
NH
4d
BRUKER
Current Data Parameters
NAME LLN-A179-58-MEOH-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170112
Time 0.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 181.28
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6124317 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
140
135
130
125
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.315
7.295
7.283
7.263
7.066
7.041
7.018
7.008
6.986
6.902
6.882
6.735
6.719
6.713
6.697
4.849
4.825
3.733
3.720
3.662
3.310
2.264
2.087
1.726
OMe
OMe
MeO
NH
NH
4e
BRUKER
Current Data Parameters
NAME 1LN-P-7-MEOH
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170113
Time 10.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 77.88
DW 56.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.3
7.2
7.1
7.0
6.9
6.8
ppm
4.10
3.24
2.06
1.02
2.07
4.00
4.11
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
4.10
3.24
2.06
1.02
2.07
4.00
4.11
1.10
3.12
2.98
3.05
3.10
3.10
3.06


185.88
170.72
169.40
167.12
160.22
158.76
157.96
141.32
137.89
136.03
136.01
132.05
131.75
131.53
131.12
130.90
130.16
129.68
129.60
128.78
125.98
123.12
115.06
114.46
111.76
79.54
60.98
55.82
55.81
55.80
49.64
49.43
49.21
49.00
48.79
48.57
48.36
25.09
21.33
21.16
OMe
OMe
MeO
NH
NH
O
O
O
N
4e
BRUKER
Current Data Parameters
NAME ILN-F-7-MEOH-C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170114
Time 11.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 2500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6126300 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
140 135 130 125 120 115 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.503
8.473
7.901
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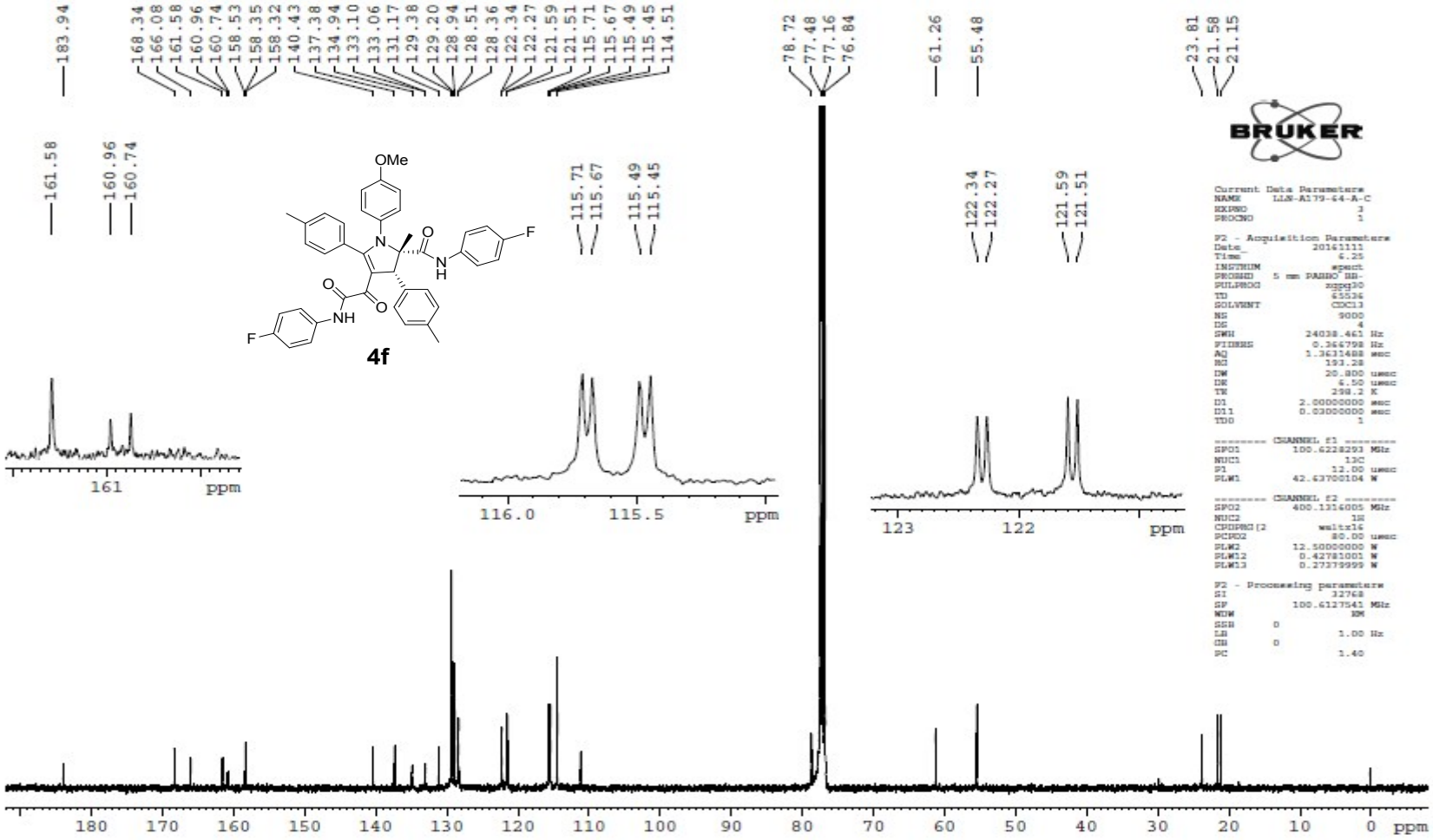
7.226
7.206
7.172
7.152
7.110
7.098
7.088
7.066
7.050
7.045
7.032
6.992
6.973
6.934
6.912
6.897
6.889
6.874
6.866
6.687
6.665
5.198
3.710
2.286
2.193
1.691
OMe
F
O
N
H
O
O
NH
F
4f
BRUKER
Current Data Parameters
NAME LLN-A179-64-A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20161103
Time 16.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 101.28
DW 56.800 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.3
7.2
7.1
7.0
6.9
6.8
6.7
ppm
2.00
2.05
6.16
2.11
6.14
2.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.91
0.81
2.00
2.05
6.16
2.11
6.14
2.03
0.99
3.00
2.90
2.92
3.37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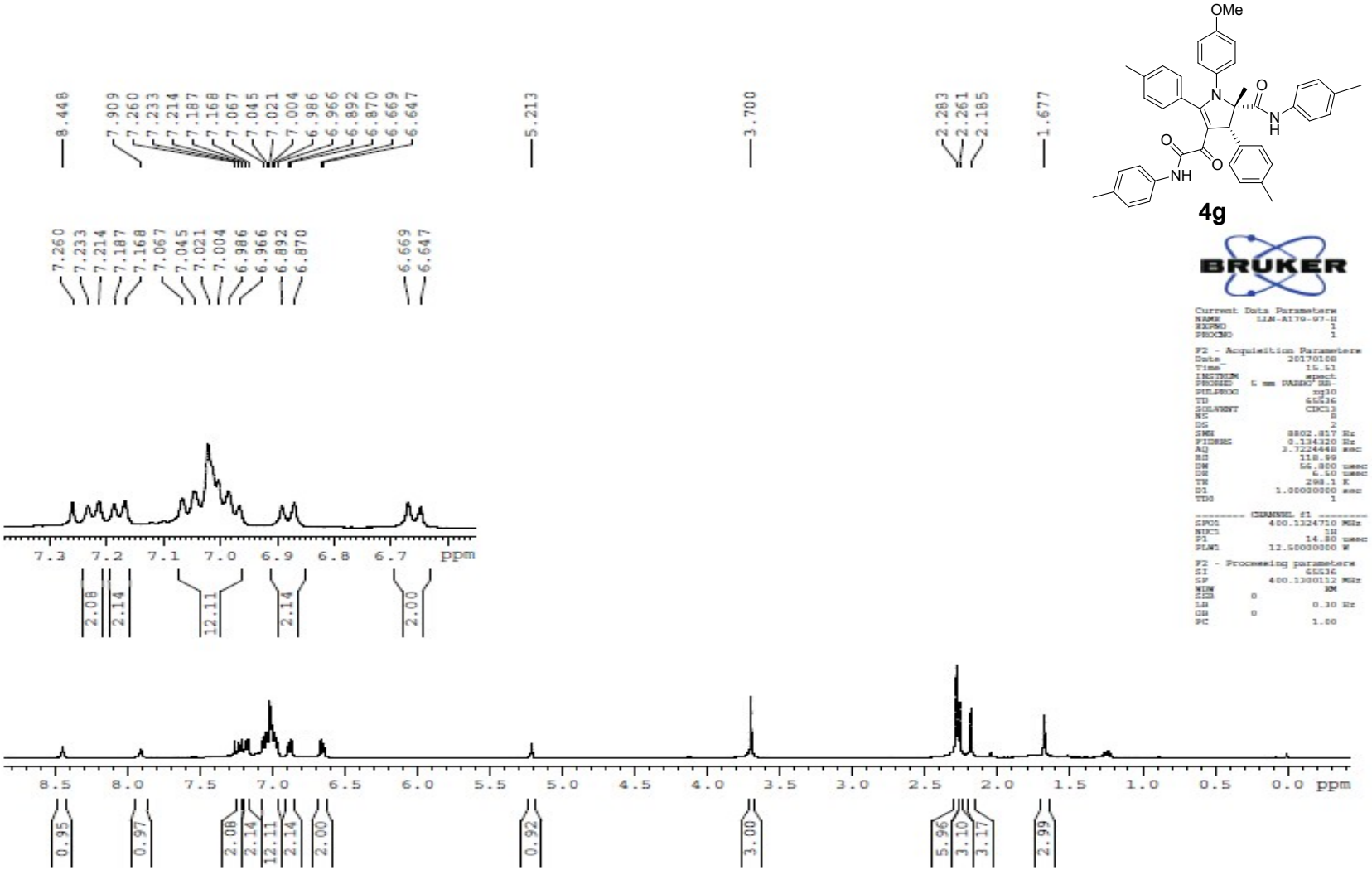
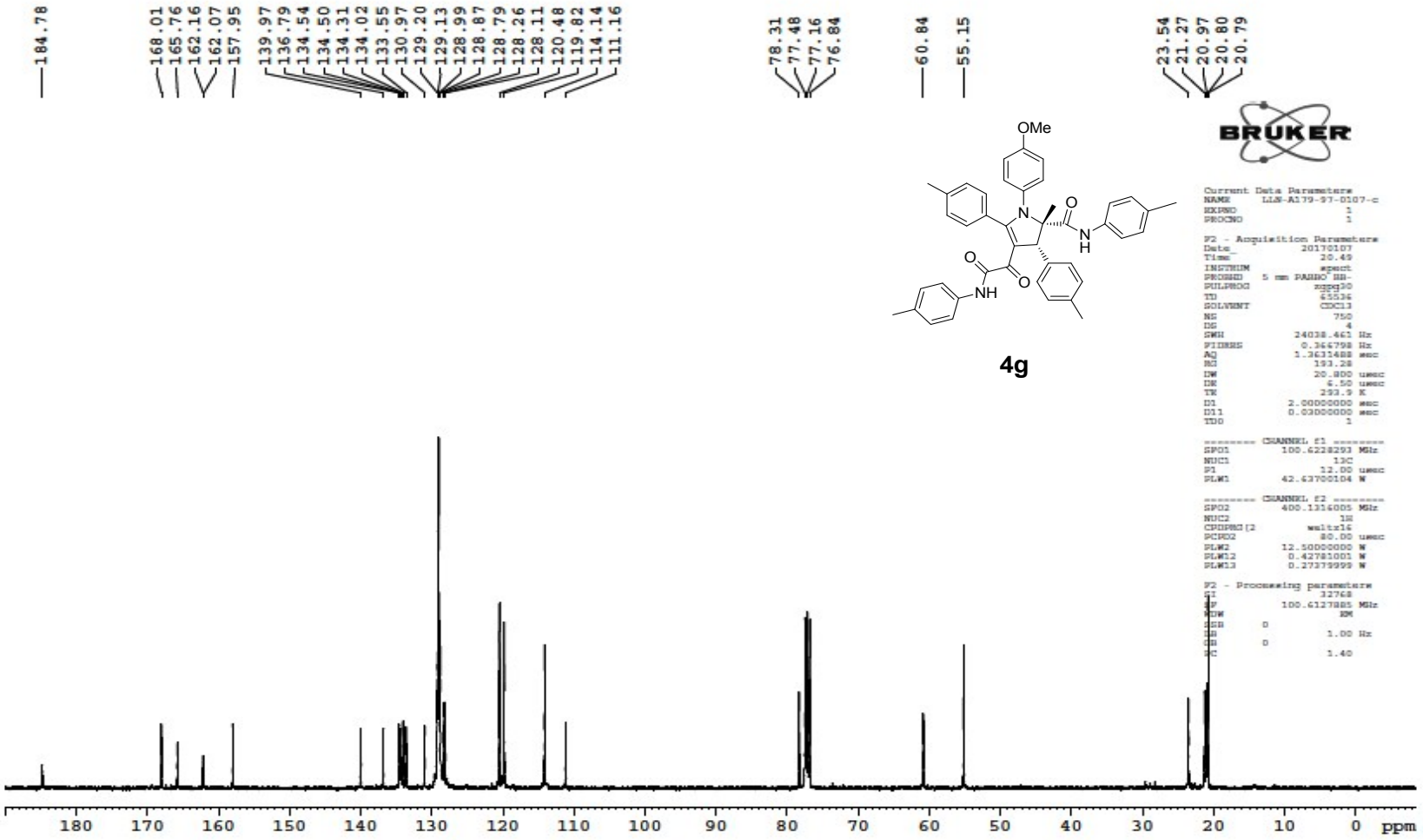
161.58
160.96
160.74
158.53
158.35
158.32
140.43
137.38
134.94
133.10
133.06
131.17
129.38
129.20
128.94
128.51
128.36
122.34
122.27
121.59
121.51
115.71
115.67
115.49
115.45
114.51
78.72
77.48
77.16
76.84
61.26
55.48
23.81
21.58
21.15
OMe
F
NH
O
N
4f
ppm
BRUKER


8.448
7.909
7.260
7.233
7.214
7.187
7.168
7.067
7.045
7.021
7.004
6.986
6.966
6.892
6.870
6.669
6.647
5.213
3.700
2.283
2.261
2.185
1.677
OMe
N
O
NH
O
O
NH
4g
BRUKER
Current Data Parameters
NAME LLM-A179-97-H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170108
Time 16.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 118.99
DW 56.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.3 7.2 7.1 7.0 6.9 6.8 6.7 ppm
2.08
2.14
12.11
2.14
2.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.95
0.97
2.08
2.14
12.11
2.14
2.00
0.92
3.00
5.96
3.10
3.17
2.99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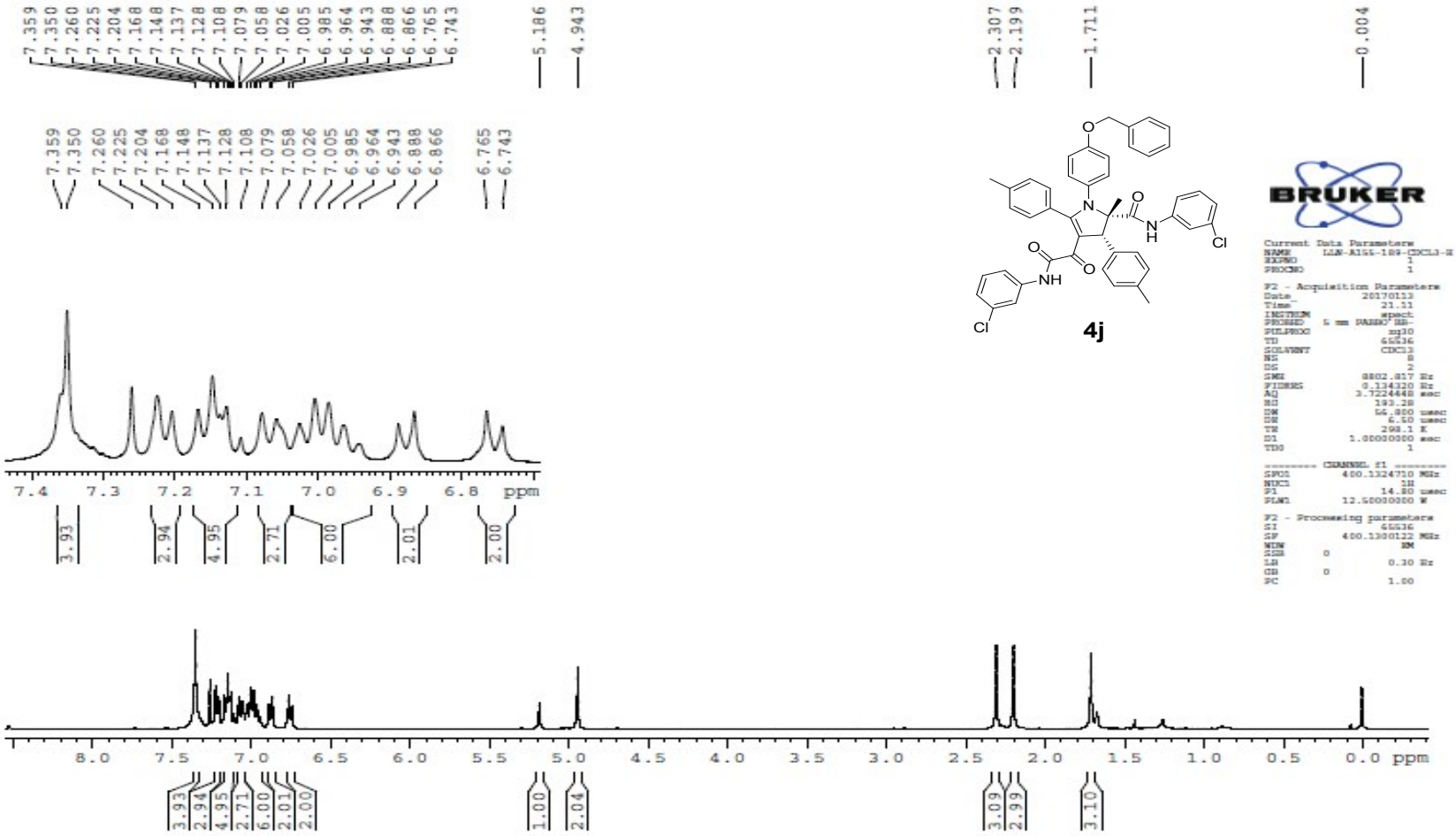
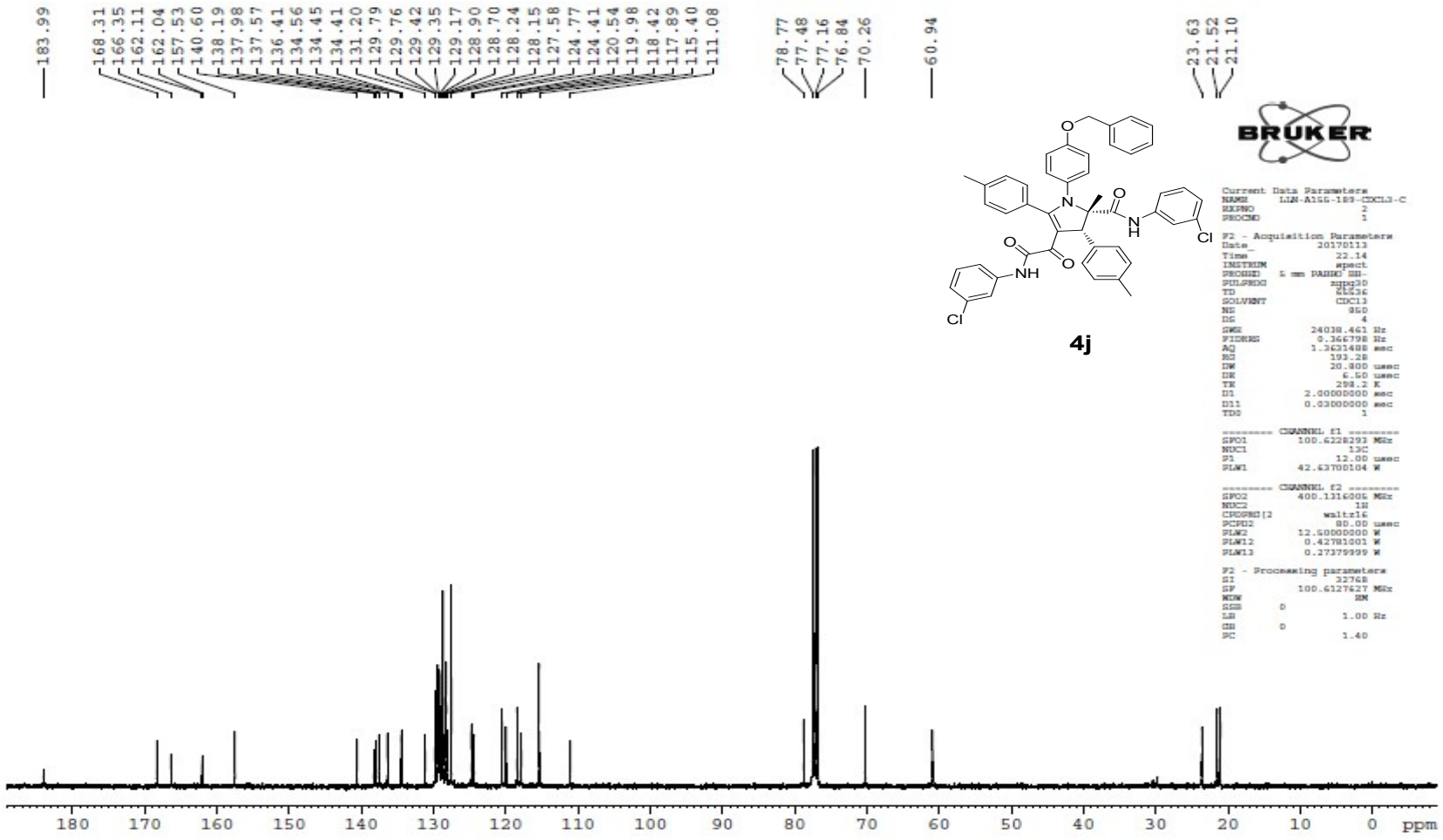
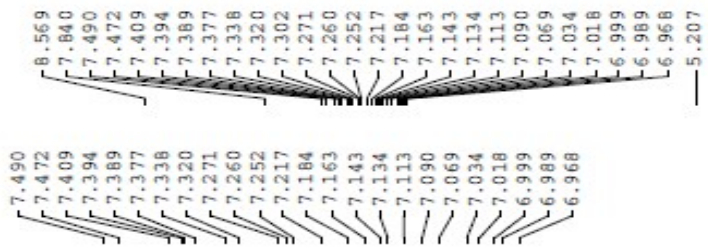
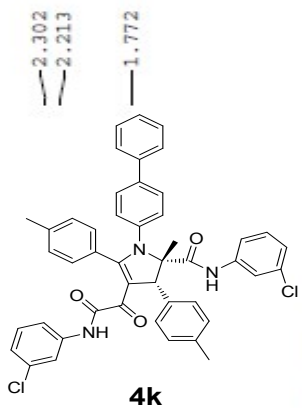
168.01
165.76
162.16
162.07
157.95
139.97
136.79
134.54
134.50
134.31
134.02
133.55
130.97
129.20
129.13
128.99
128.87
128.79
128.26
128.11
120.48
119.82
114.14
111.16
78.31
77.48
77.16
76.84
60.84
55.15
23.54
21.27
20.97
20.80
20.79
OMe
N
O
NH
O
O
NH
4g
BRUKER
Current Data Parameters
NAME LLW-A179-97-0107-c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170107
Time 20.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 750
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 293.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

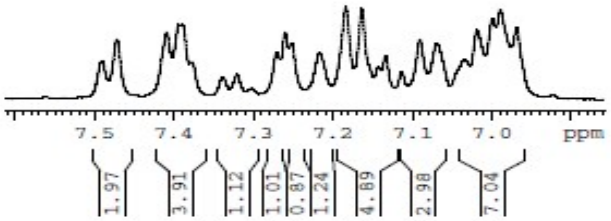

7.359
7.350
7.260
7.225
7.204
7.168
7.148
7.137
7.128
7.108
7.079
7.058
7.026
7.005
6.985
6.964
6.943
6.888
6.866
6.765
6.743
5.186
4.943
2.307
2.199
1.711
0.004
4j
BRUKER
Current Data Parameters
NAME LLW-A155-189-(CDCl3-H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170113
Time 21.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 193.28
DW 56.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.4
7.3
7.2
7.1
7.0
6.9
6.8
ppm
3.93
2.94
4.95
2.71
6.00
2.01
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
1.00
2.04
3.09
2.99
3.10


183.99
168.31
166.35
162.11
162.04
157.53
140.60
138.19
137.98
137.57
136.41
134.56
134.45
134.41
131.20
129.79
129.76
129.42
129.35
129.17
128.90
128.70
128.24
128.15
127.58
124.77
124.41
120.54
119.98
118.42
117.89
115.40
111.08
78.77
77.48
77.16
76.84
70.26
60.94
23.63
21.52
21.10
BRUKER
4j
Current Data Parameters
NAME LIN-A155-189-CDCl3-C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170113
Time 22.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 950
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127627 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm





4k

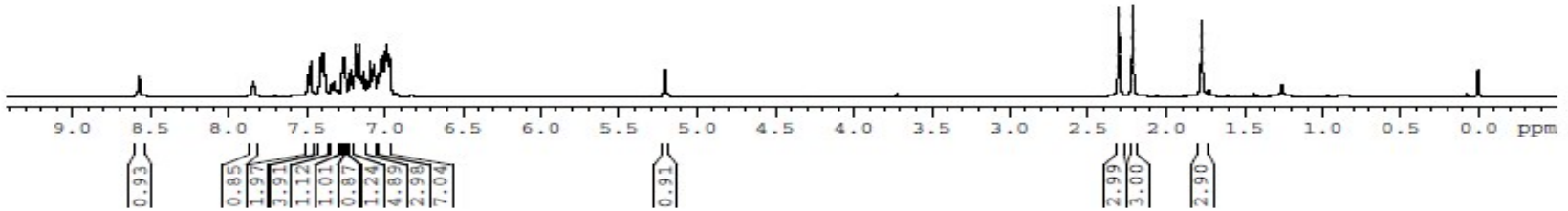


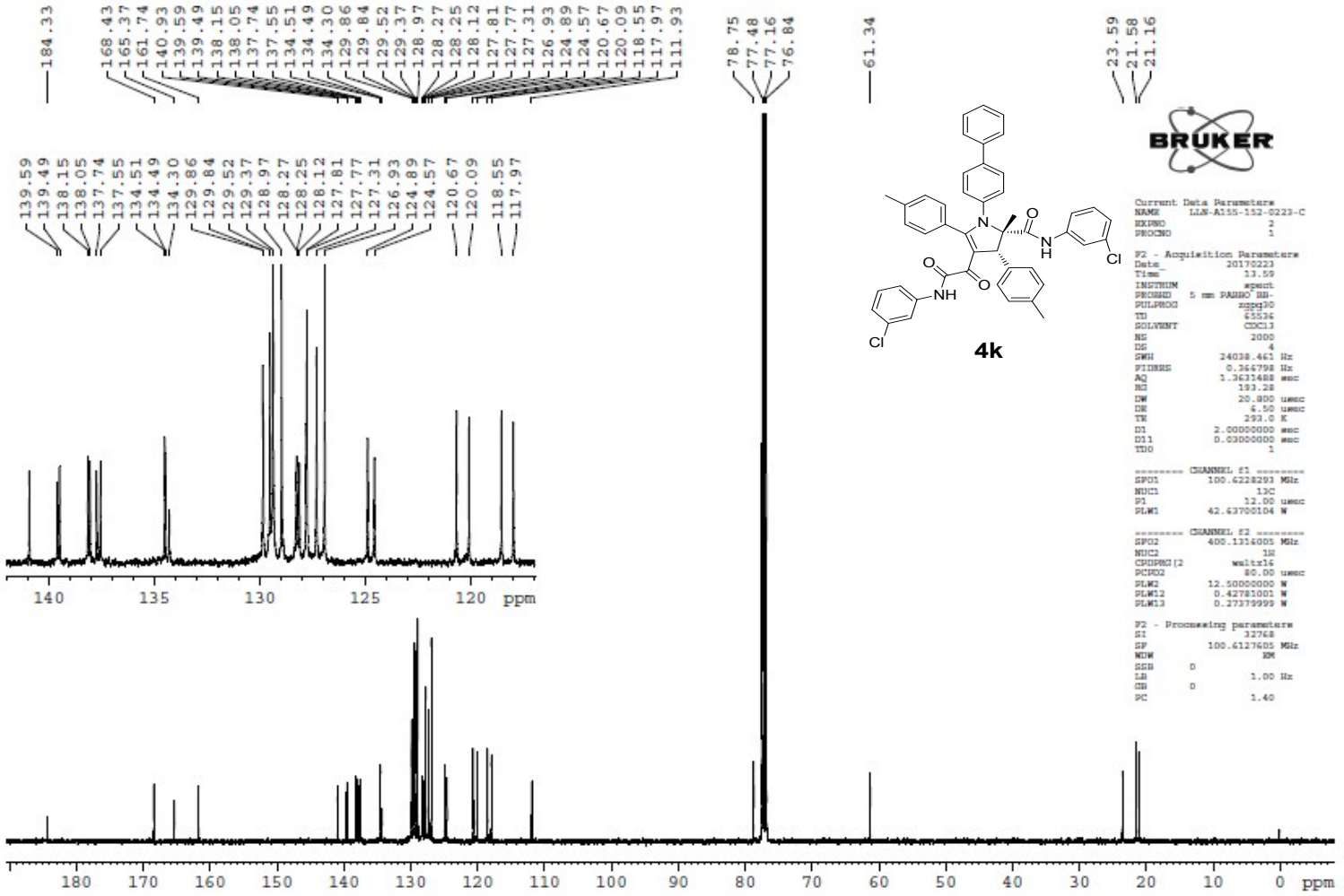
Current Data Parameters
NAME LLW-A155-162-0217
EXPNO 1
PROCNO 1

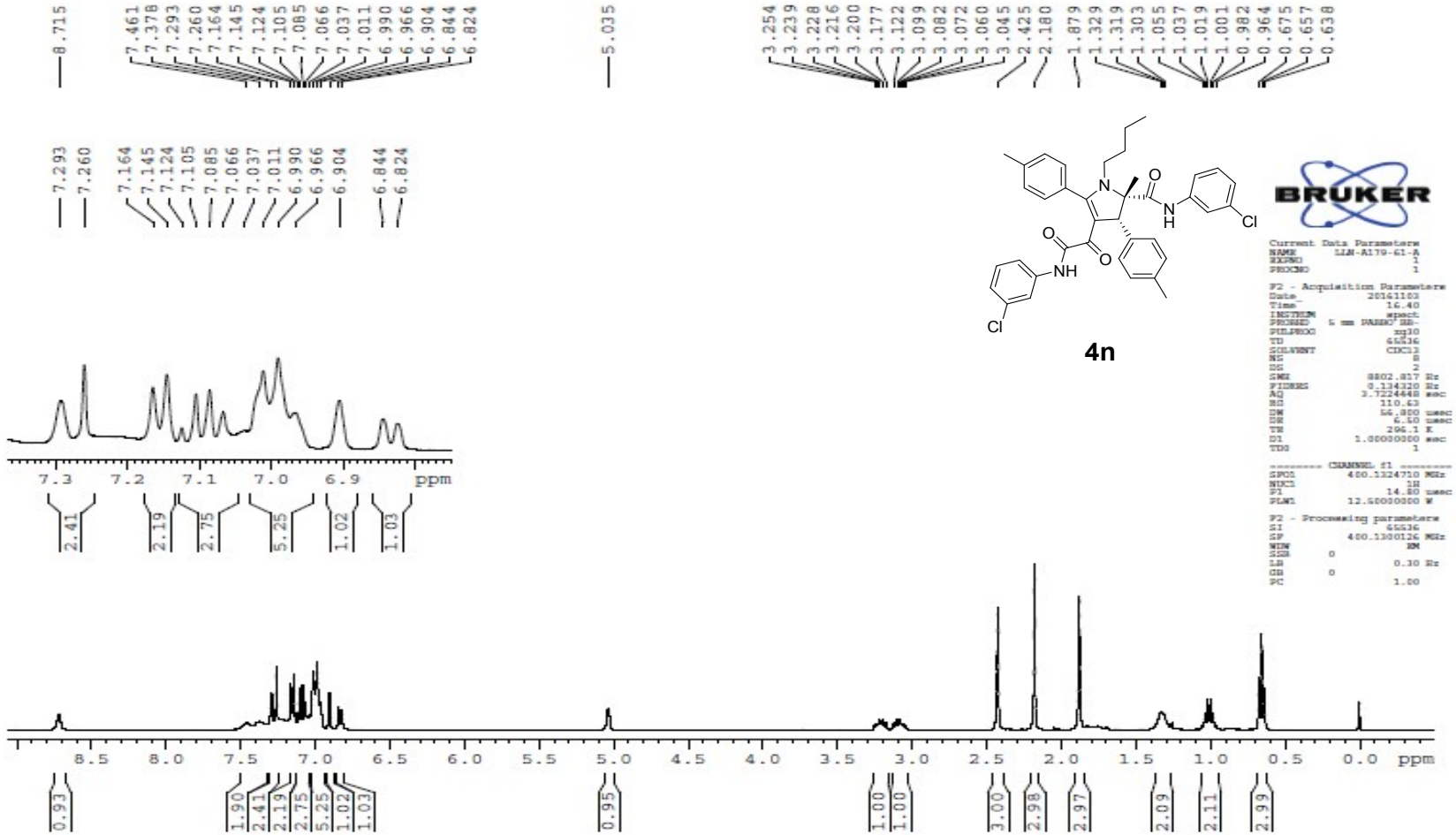
F2 - Acquisition Parameters
Date_ 20170217
Time 20.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 193.28
DW 56.800 usec
DE 6.50 usec
TE 291.0 K
D1 1.00000000 sec
TD0 1

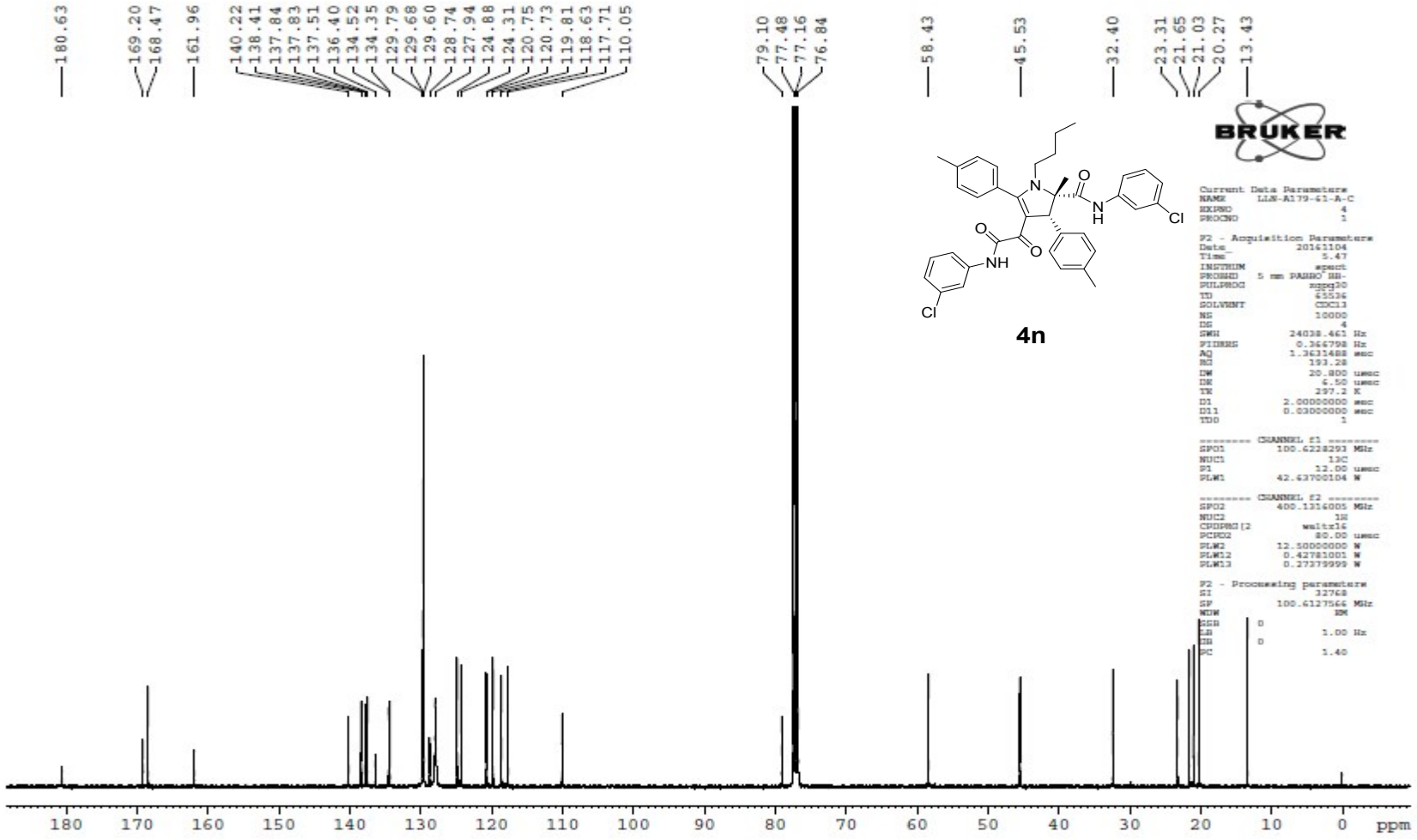
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W

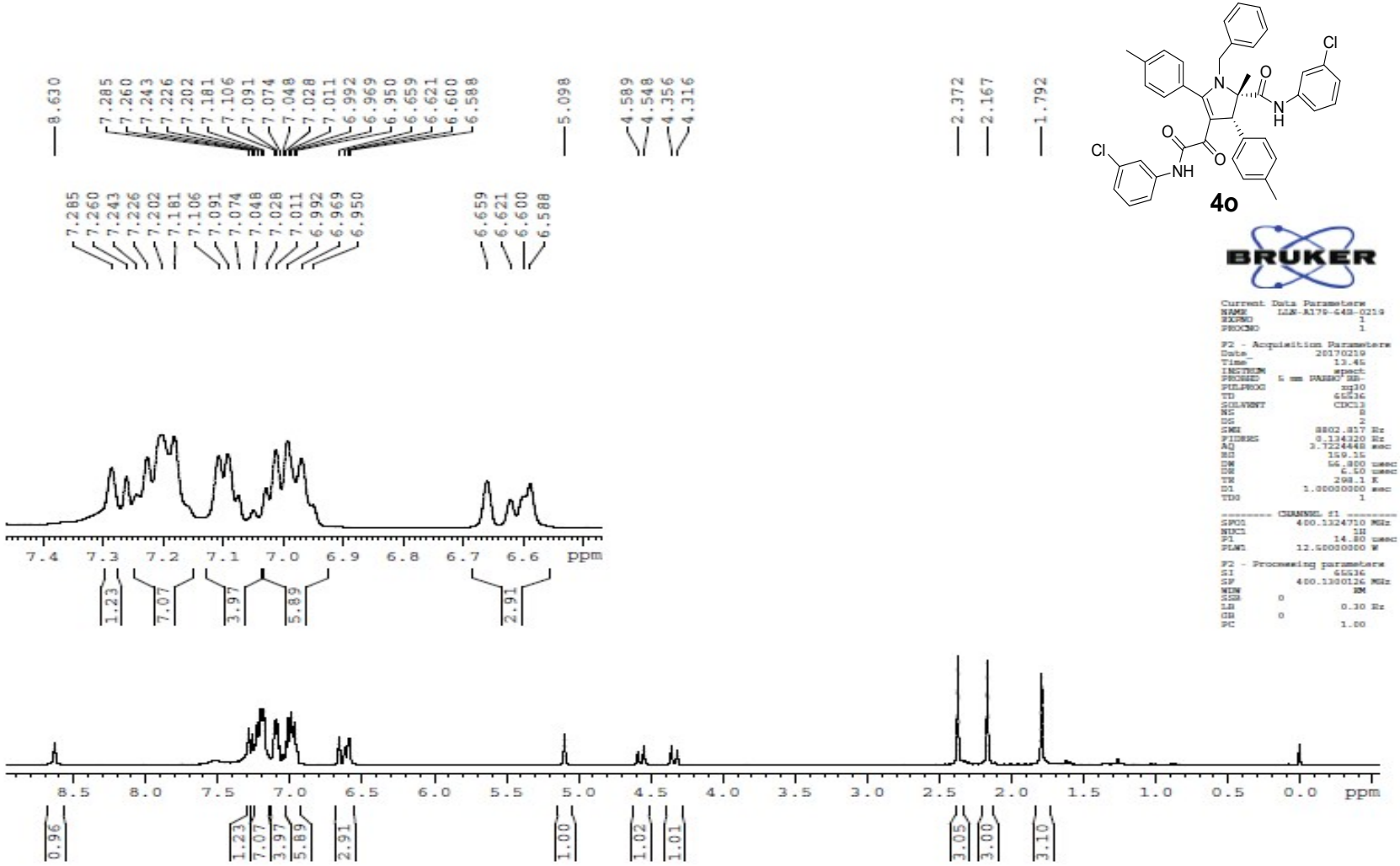
F2 - Processing parameters
SI 65536
SF 400.1300124 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

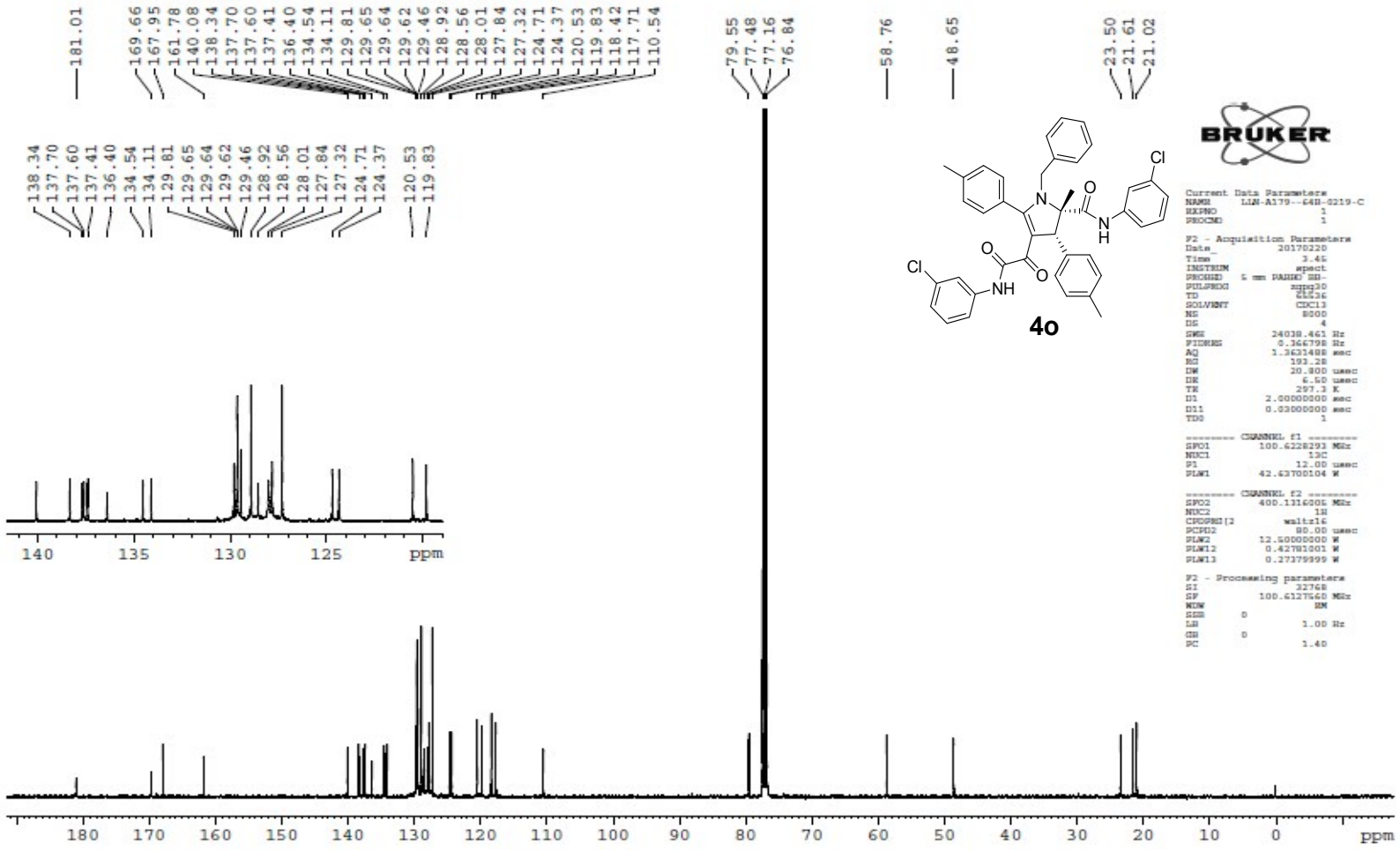


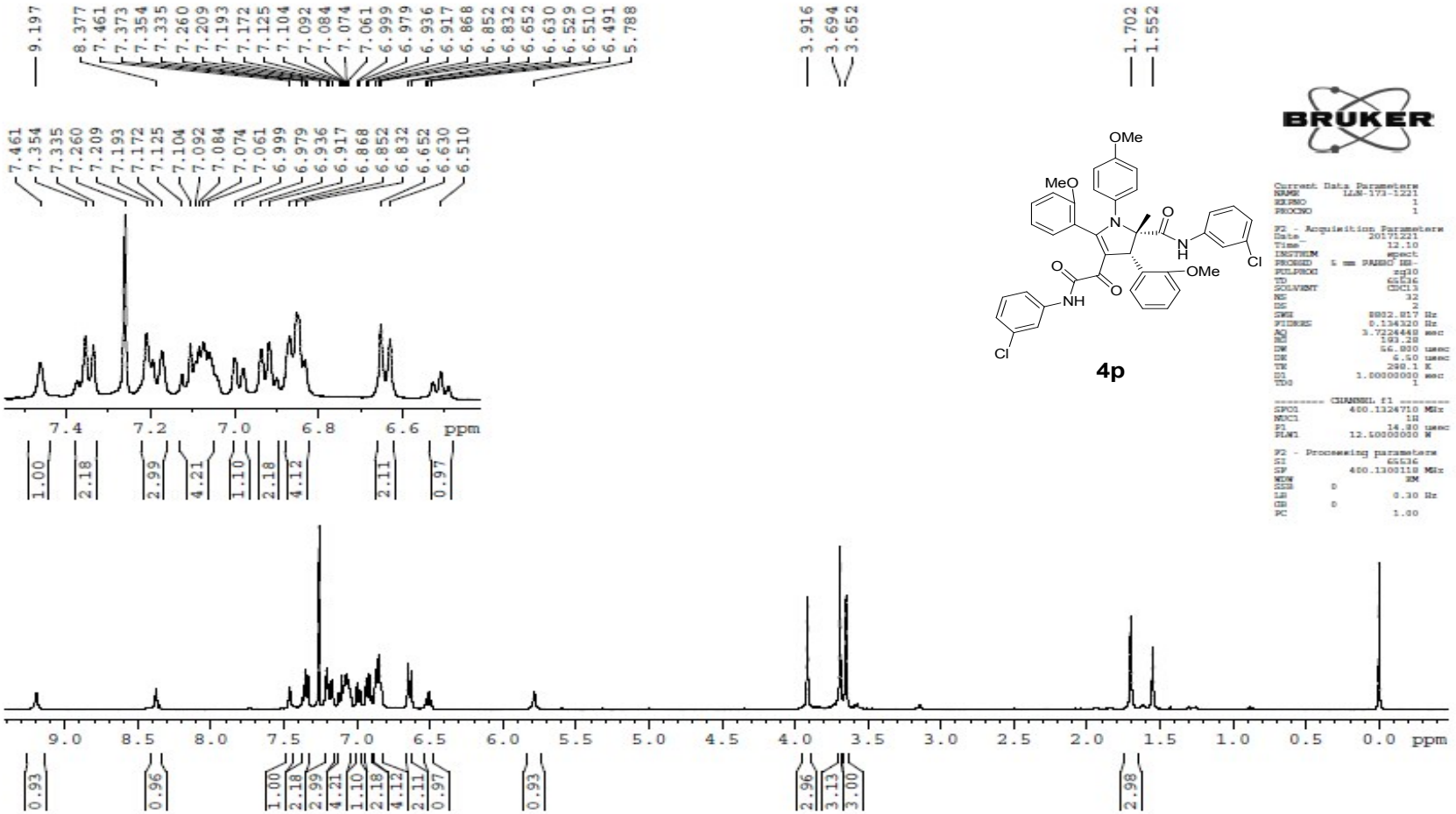

184.33
168.43
165.37
161.74
140.93
139.59
139.49
138.15
138.05
137.74
137.55
134.51
134.49
134.30
129.86
129.84
129.52
129.37
128.97
128.27
128.25
128.12
127.81
127.77
127.31
126.93
124.89
124.57
120.67
120.09
118.55
117.97
111.93
78.75
77.48
77.16
76.84
61.34
23.59
21.58
21.16
4k
BRUKER
Current Data Parameters
NAME LLN-A155-152-0223-C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date 20170223
Time 13.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127605 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
140 135 130 125 120 ppm
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

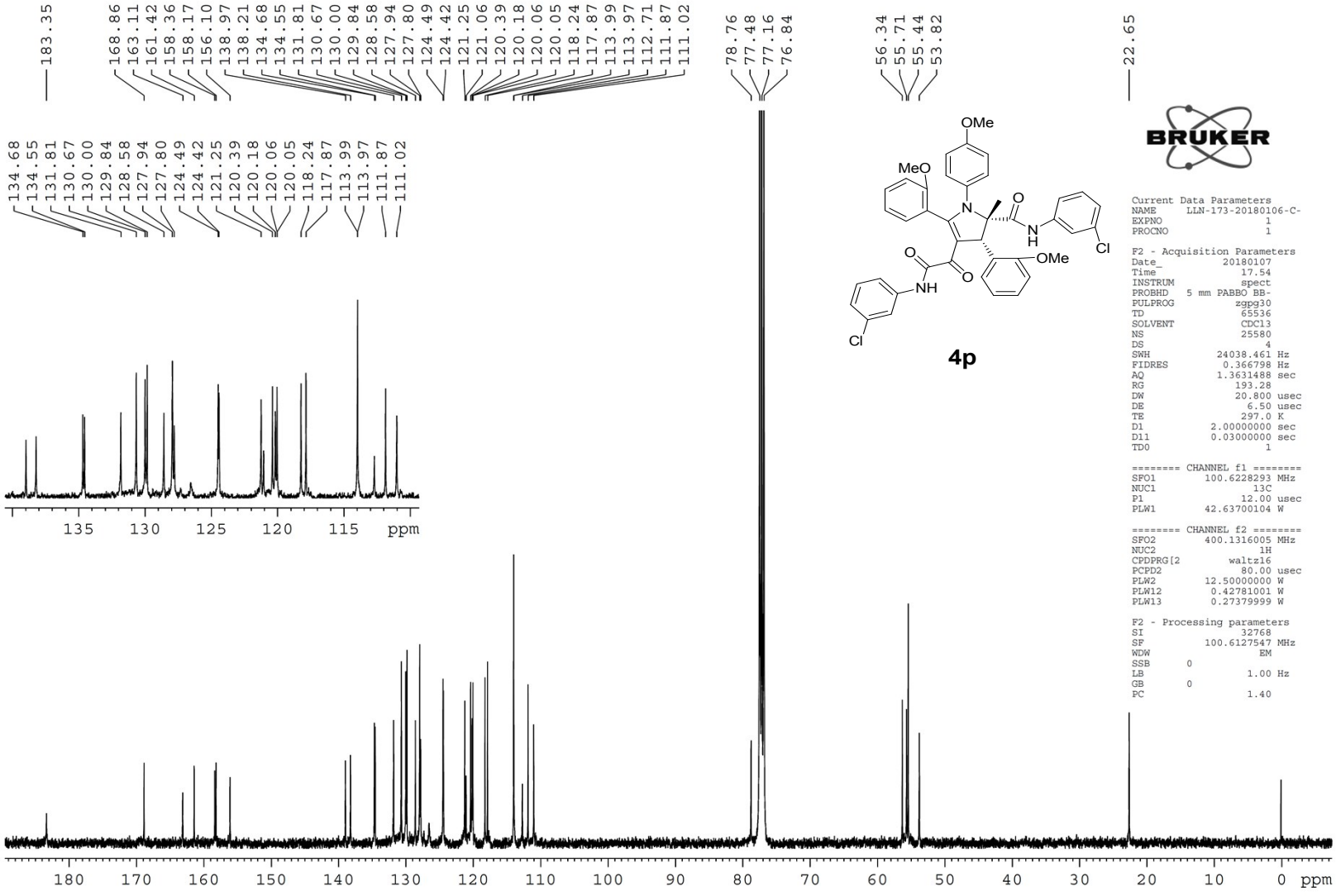

8.715
7.461
7.378
7.293
7.260
7.164
7.145
7.124
7.105
7.085
7.066
7.037
7.011
6.990
6.966
6.904
6.844
6.824
5.035
3.254
3.239
3.228
3.216
3.200
3.177
3.122
3.099
3.082
3.072
3.060
3.045
2.425
2.180
1.879
1.329
1.319
1.303
1.055
1.037
1.019
1.001
0.982
0.964
0.675
0.657
0.638
7.3
7.2
7.1
7.0
6.9
ppm
2.41
2.19
2.75
5.25
1.02
1.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.93
1.90
2.41
2.19
2.75
5.25
1.02
1.03
0.95
1.00
1.00
3.00
2.98
2.97
2.09
2.11
2.99
4n
BRUKER
Current Data Parameters
NAME LLN-AI79-61-A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161103
Time 16.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 110.63
DW 56.800 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

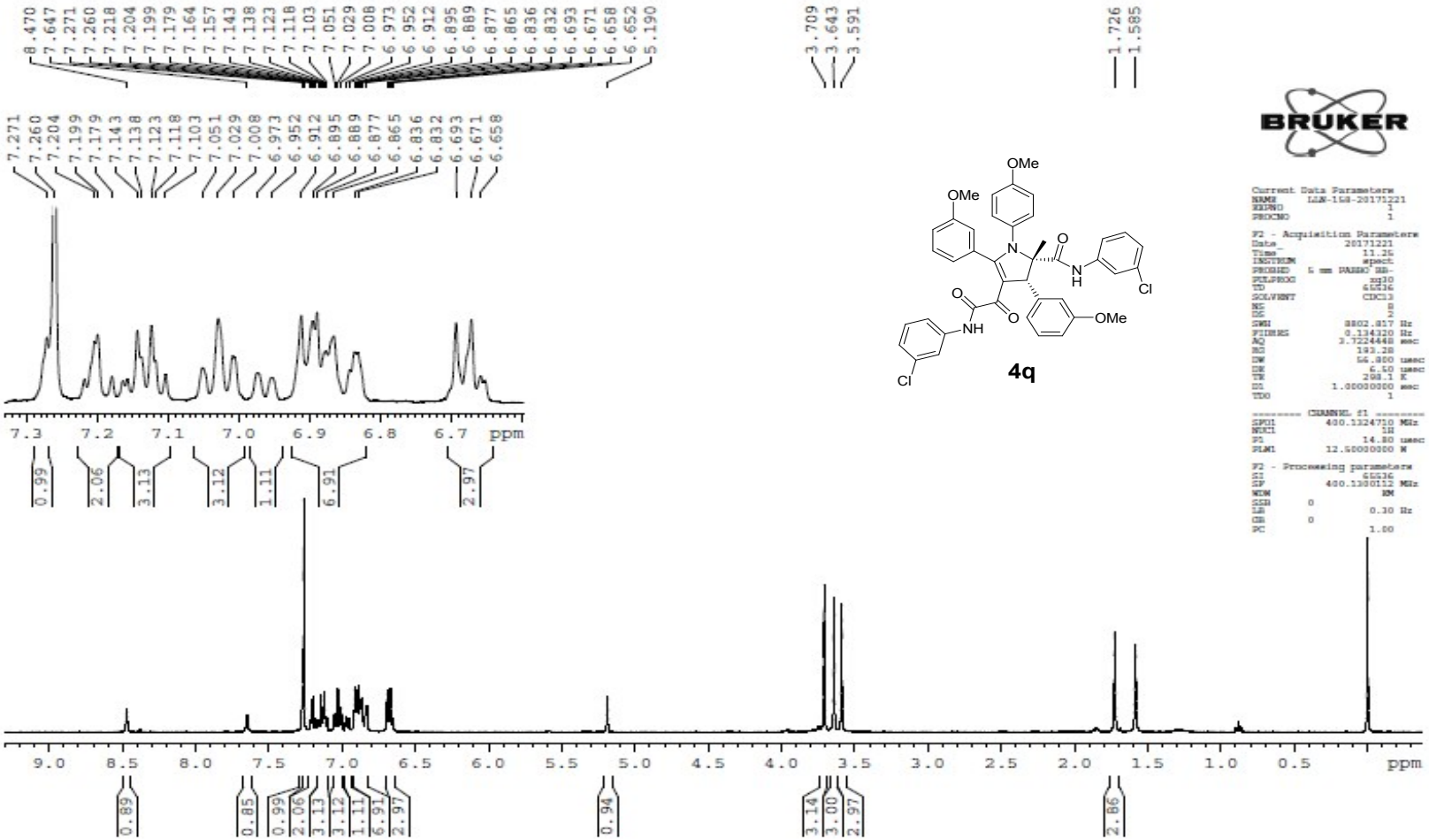

180.63
169.20
168.47
161.96
140.22
138.41
137.84
137.83
137.51
136.40
134.52
134.35
129.79
129.68
129.60
128.74
127.94
124.88
124.31
120.75
120.73
119.81
118.63
117.71
110.05
79.10
77.48
77.16
76.84
58.43
45.53
32.40
23.31
21.65
21.03
20.27
13.43
4n
BRUKER
Current Data Parameters
NAME LLN-A179-61-A-C
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161104
Time 5.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127566 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

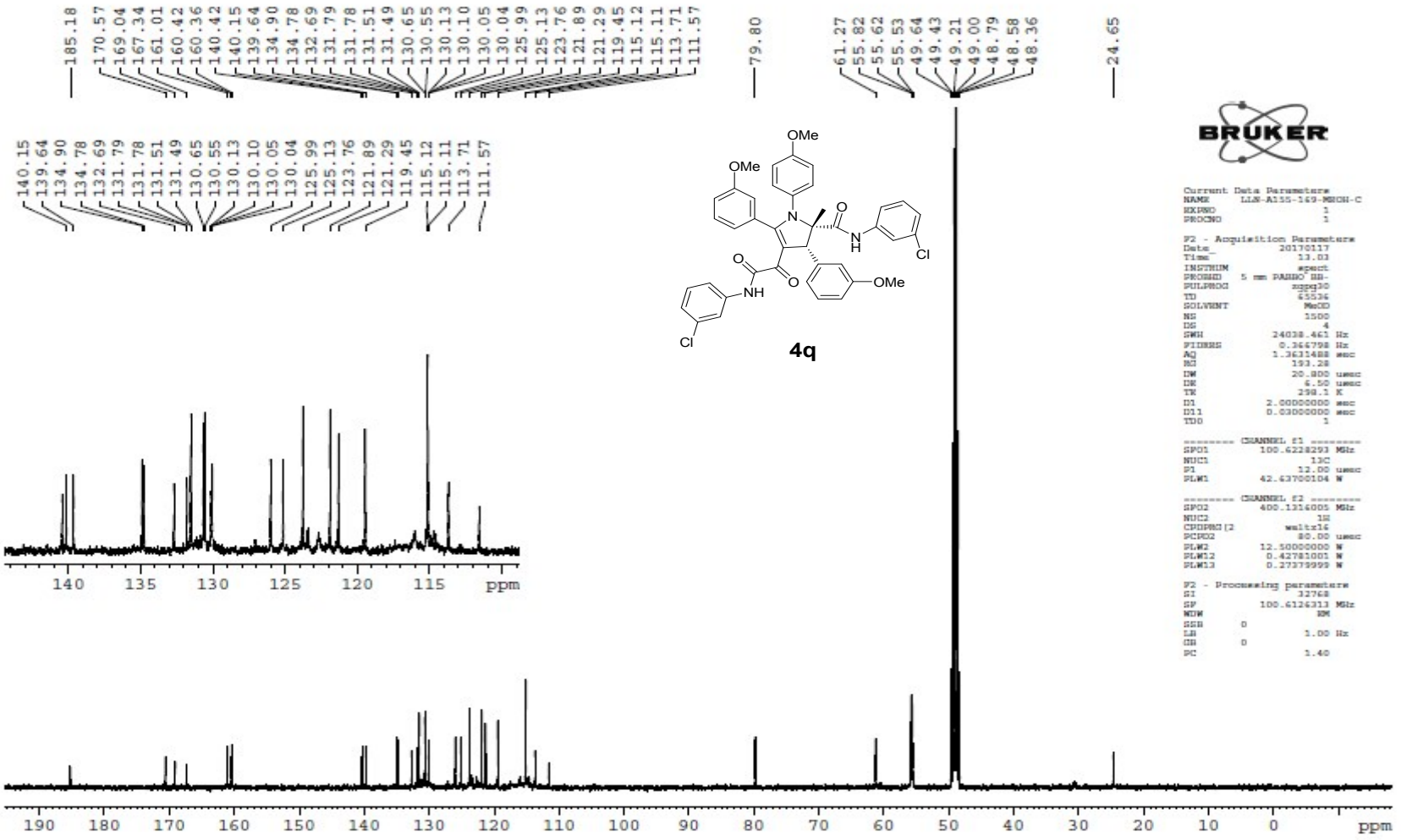

8.630
7.285
7.260
7.243
7.226
7.202
7.181
7.106
7.091
7.074
7.048
7.028
7.011
6.992
6.969
6.950
6.659
6.621
6.600
6.588
5.098
4.589
4.548
4.356
4.316
2.372
2.167
1.792
Cl
N
O
NH
Cl
O
O
4o
BRUKER
Current Data Parameters
NAME IZM-A179-648-0219
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170219
Time 13.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 159.15
DW 56.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
---------- CHANNEL f1 ----------
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 ppm
1.23
7.07
3.97
5.89
2.91
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.96
1.23
7.07
3.97
5.89
2.91
1.00
1.02
1.01
3.05
3.00
3.10

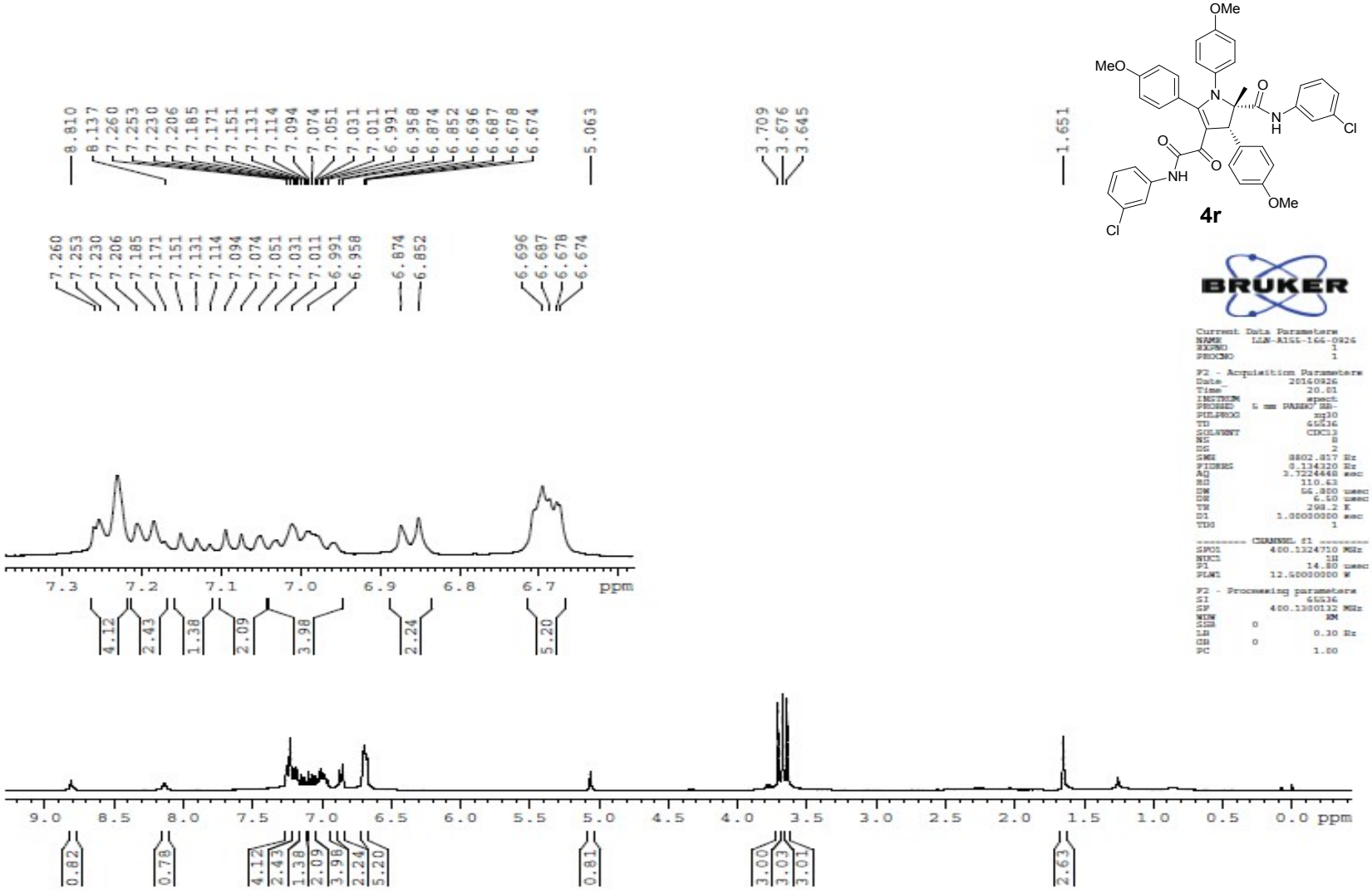

181.01
169.66
167.95
161.78
140.08
138.34
137.70
137.60
137.41
136.40
134.54
134.11
129.81
129.65
129.64
129.62
129.46
128.92
128.56
128.01
127.84
127.32
124.71
124.37
120.53
119.83
118.42
117.71
110.54
79.55
77.48
77.16
76.84
58.76
48.65
23.50
21.61
21.02
4o
BRUKER
ppm

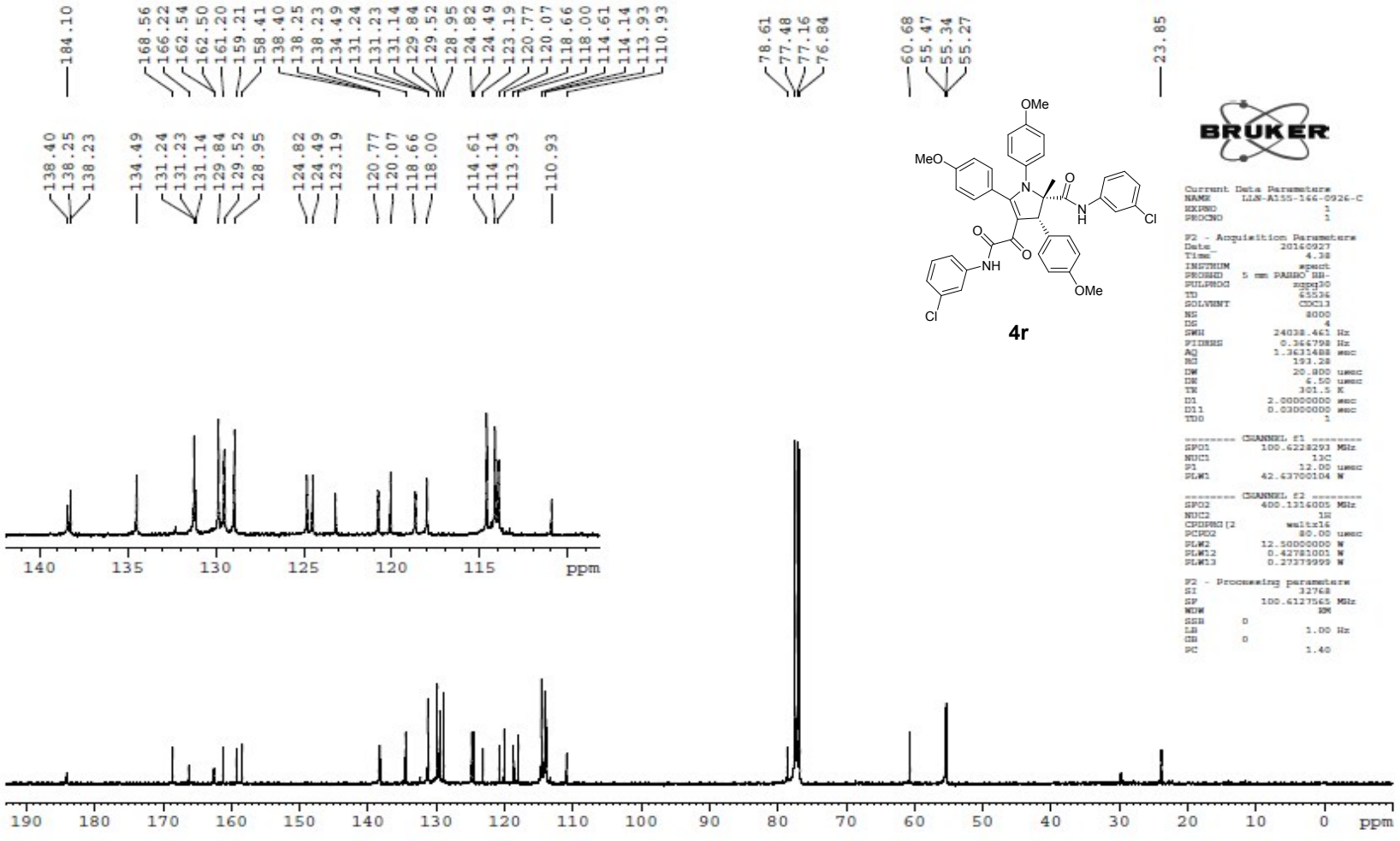

9.197
8.377
7.461
7.373
7.354
7.335
7.260
7.209
7.193
7.172
7.125
7.104
7.092
7.084
7.074
7.061
6.999
6.979
6.936
6.917
6.868
6.852
6.832
6.652
6.630
6.529
6.510
6.491
5.788
3.916
3.694
3.652
1.702
1.552
OMe
MeO
N
O
NH
Cl
OMe
4p
BRUKER
ppm

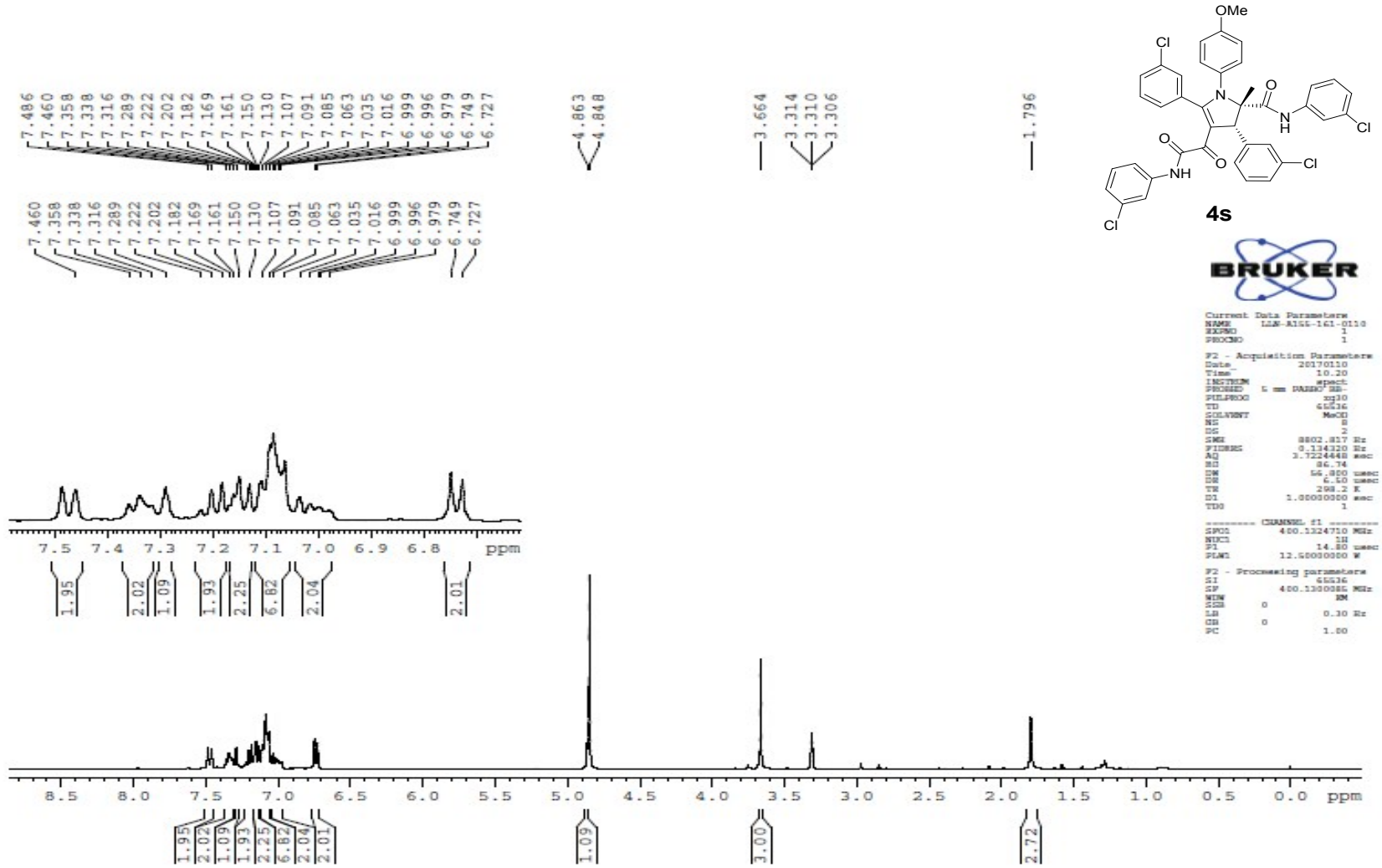

183.35
168.86
163.11
161.42
158.36
158.17
156.10
138.97
138.21
134.68
134.55
131.81
130.67
130.00
129.84
128.58
127.94
127.80
124.49
124.42
121.25
121.06
120.39
120.18
120.06
120.05
118.24
117.87
113.99
113.97
112.71
111.87
111.02
78.76
77.48
77.16
76.84
56.34
55.71
55.44
53.82
22.65
OMe
MeO
N
O
NH
Cl
OMe
O
O
NH
Cl
4p
BRUKER
Current Data Parameters
NAME LLN-173-20180106-C-
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180107
Time 17.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 25580
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127547 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
135
130
125
120
115
ppm
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

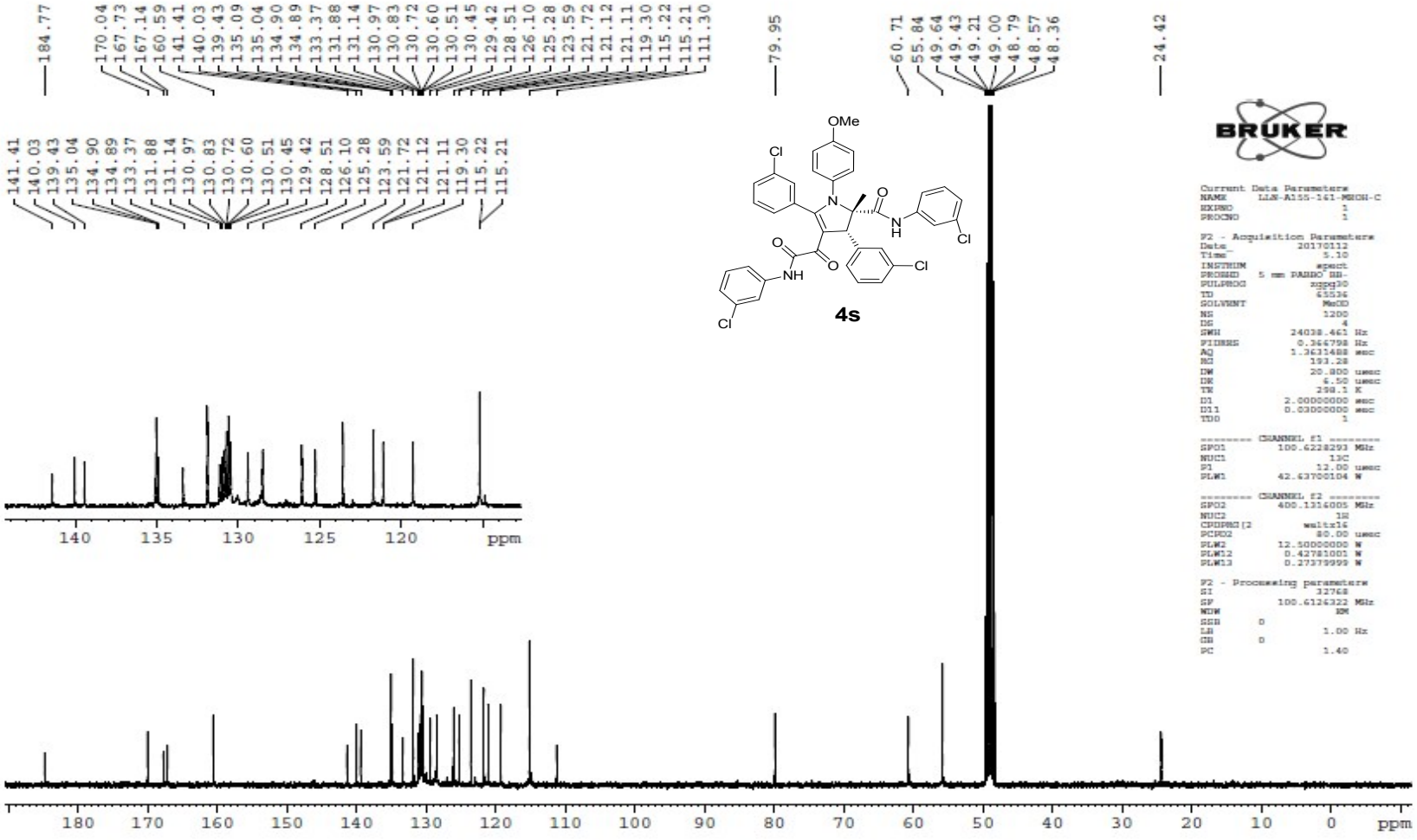

8.470
7.647
7.271
7.260
7.218
7.204
7.199
7.179
7.164
7.157
7.143
7.138
7.123
7.118
7.103
7.051
7.029
7.008
6.973
6.952
6.912
6.895
6.889
6.877
6.865
6.836
6.832
6.693
6.671
6.658
6.652
5.190
3.709
3.643
3.591
1.726
1.585
OMe
OMe
N
O
NH
Cl
O
O
NH
OMe
Cl
4q
BRUKER
Current Data Parameters
NAME LSM-158-20171221
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171221
Time_ 11.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 193.28
DW 56.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.3
7.2
7.1
7.0
6.9
6.8
6.7
ppm
0.99
2.06
3.13
3.12
1.11
6.91
2.97
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.89
0.85
0.99
2.06
3.13
3.12
1.11
6.91
2.97
0.94
3.14
3.00
2.97
2.86

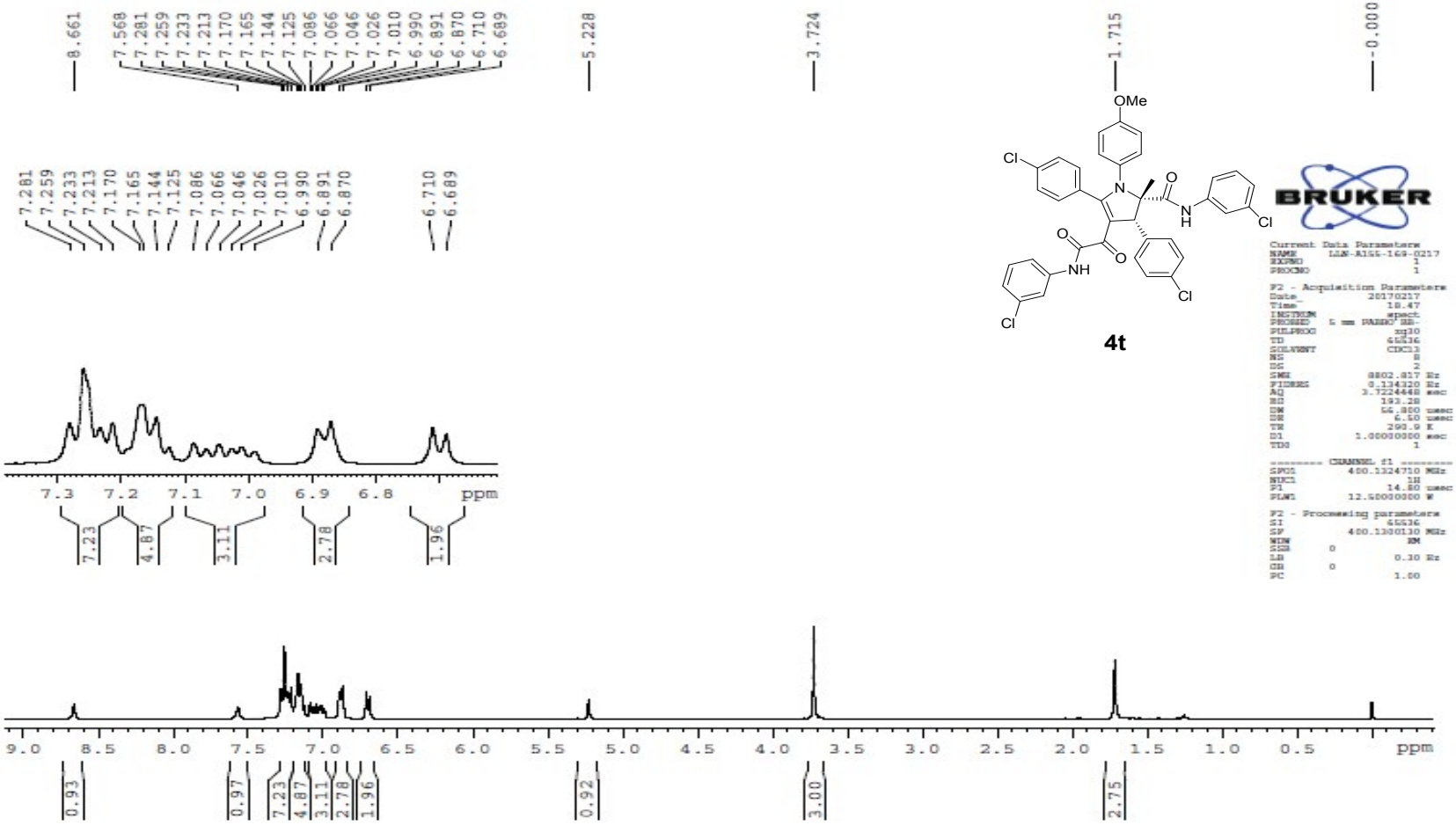

185.18
170.57
169.04
167.34
161.01
160.42
160.36
140.42
140.15
139.64
134.90
134.78
132.69
131.79
131.78
131.51
131.49
130.65
130.55
130.13
130.10
130.05
130.04
125.99
125.13
123.76
121.89
121.29
119.45
115.12
115.11
113.71
111.57
79.80
61.27
55.82
55.62
55.53
49.64
49.43
49.21
49.00
48.79
48.58
48.36
24.65
OMe
OMe
N
O
N
H
Cl
O
O
NH
Cl
OMe
4q
BRUKER
Current Data Parameters
NAME LLW-A155-169-MECN-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170117
Time 13.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 1500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6126311 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
140 135 130 125 120 115 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

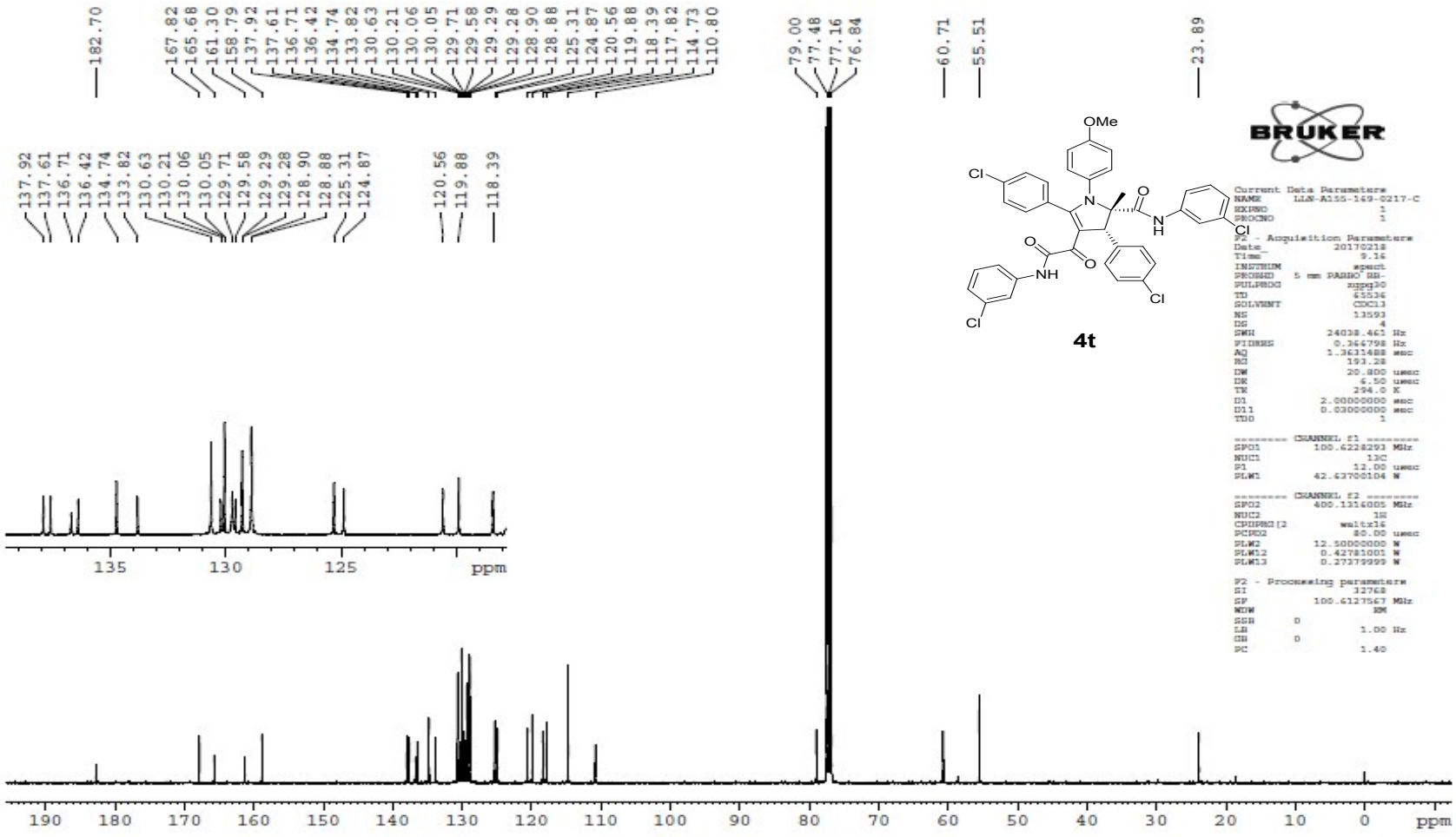

8.810
8.137
7.260
7.253
7.230
7.206
7.185
7.171
7.151
7.131
7.114
7.094
7.074
7.051
7.031
7.011
6.991
6.958
6.874
6.852
6.696
6.687
6.678
6.674
5.063
3.709
3.676
3.645
1.651
OMe
MeO
N
O
NH
Cl
OMe
4r
BRUKER
Current Data Parameters
NAME LLW-A155-166-0926
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160926
Time 20.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 110.63
DW 56.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.3
7.2
7.1
7.0
6.9
6.8
6.7
ppm
4.12
2.43
1.38
2.09
3.98
2.24
5.20
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
0.82
0.78
4.12
2.43
1.38
2.09
3.98
2.24
5.20
0.81
3.00
3.03
3.01
2.63


184.10
168.56
166.22
162.54
162.50
161.20
159.21
158.41
138.40
138.25
138.23
134.49
131.24
131.23
131.14
129.84
129.52
128.95
124.82
124.49
123.19
120.77
120.07
118.66
118.00
114.61
114.14
113.93
110.93
78.61
77.48
77.16
76.84
60.68
55.47
55.34
55.27
23.85
OMe
MeO
N
O
NH
Cl
OMe
4r
BRUKER
Current Data Parameters
NAME LLW-A155-166-0926-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160927
Time 4.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 301.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127565 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
140
135
130
125
120
115
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.486
7.460
7.358
7.338
7.316
7.289
7.222
7.202
7.182
7.169
7.161
7.150
7.130
7.107
7.091
7.085
7.063
7.035
7.016
6.999
6.996
6.979
6.749
6.727
4.863
4.848
3.664
3.314
3.310
3.306
1.796
OMe
Cl
N
O
NH
Cl
4s
BRUKER
Current Data Parameters
NAME LLW-AISS-161-0110
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170110
Time 10.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 86.74
DW 56.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 ppm
1.95 2.02 1.09 1.93 2.25 6.82 2.04 2.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.95 2.02 1.09 1.93 2.25 6.82 2.04 2.01
1.09
3.00
2.72


184.77
170.04
167.73
167.14
160.59
141.41
140.03
139.43
135.09
135.04
134.90
134.89
133.37
131.88
131.14
130.97
130.83
130.72
130.60
130.51
130.45
129.42
128.51
126.10
125.28
123.59
121.72
121.12
121.11
119.30
115.22
115.21
111.30
79.95
60.71
55.84
49.64
49.43
49.21
49.00
48.79
48.57
48.36
24.42
OMe
Cl
N
O
NH
Cl
O
O
NH
Cl
4s
BRUKER
Current Data Parameters
NAME LLN-A155-161-MEOH-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170112
Time 5.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6126322 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
140
135
130
125
120
ppm
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.661
7.568
7.281
7.259
7.233
7.213
7.170
7.165
7.144
7.125
7.086
7.066
7.046
7.026
7.010
6.990
6.891
6.870
6.710
6.689
5.228
3.724
1.715
-0.000
OMe
Cl
N
O
NH
Cl
Cl
4t
BRUKER
Current Data Parameters
NAME LLM-A155-169-0217
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170217
Time 18.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 193.28
DW 56.800 usec
DE 6.50 usec
TE 298.9 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.3
7.2
7.1
7.0
6.9
6.8
ppm
7.23
4.87
3.11
2.78
1.96
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.93
0.97
7.23
4.87
3.11
2.78
1.96
0.92
3.00
2.75



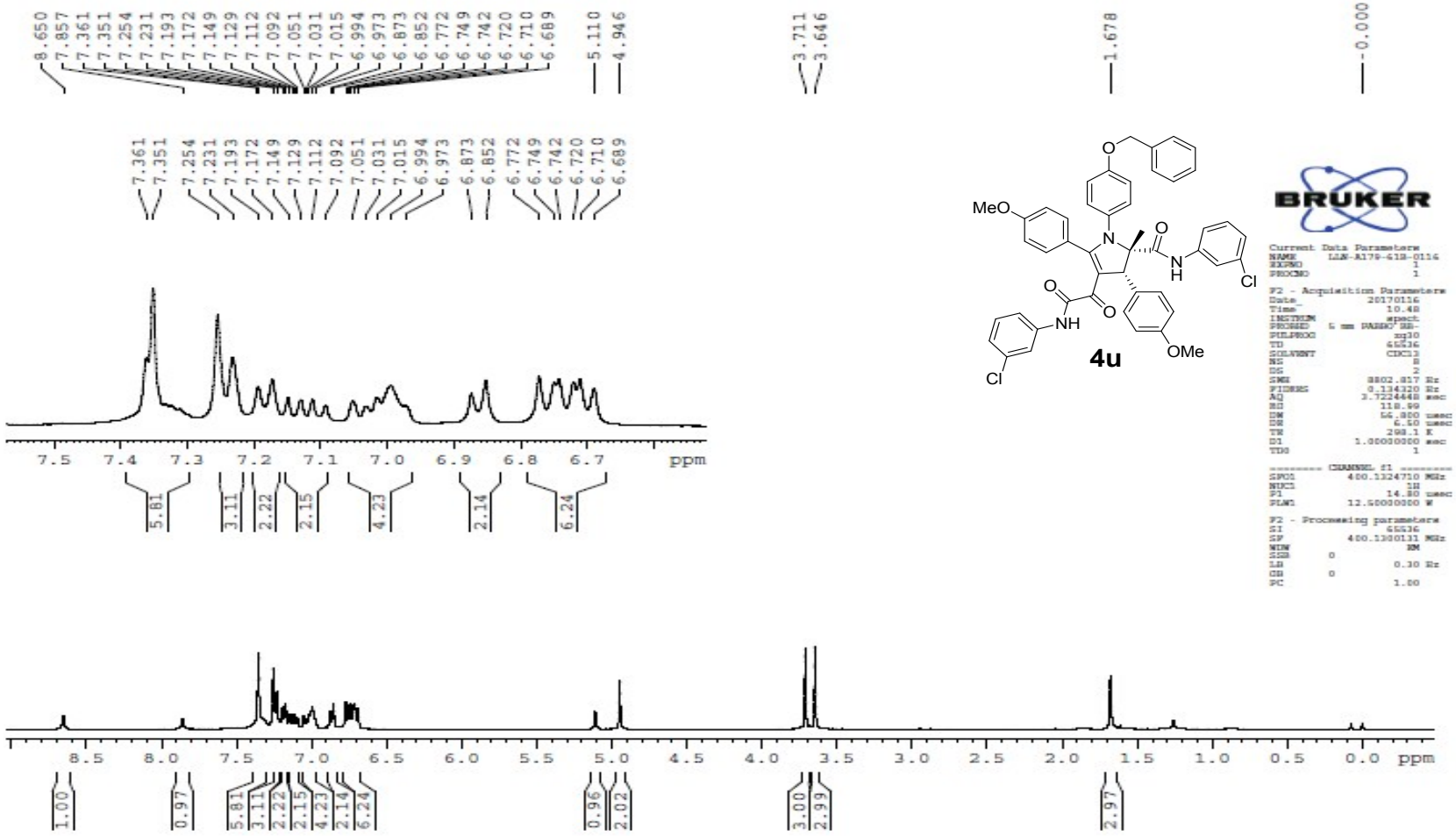
Current Data Parameters
NAME LLW-A155-149-0217-C
EXPNO 1
PROCNO 1

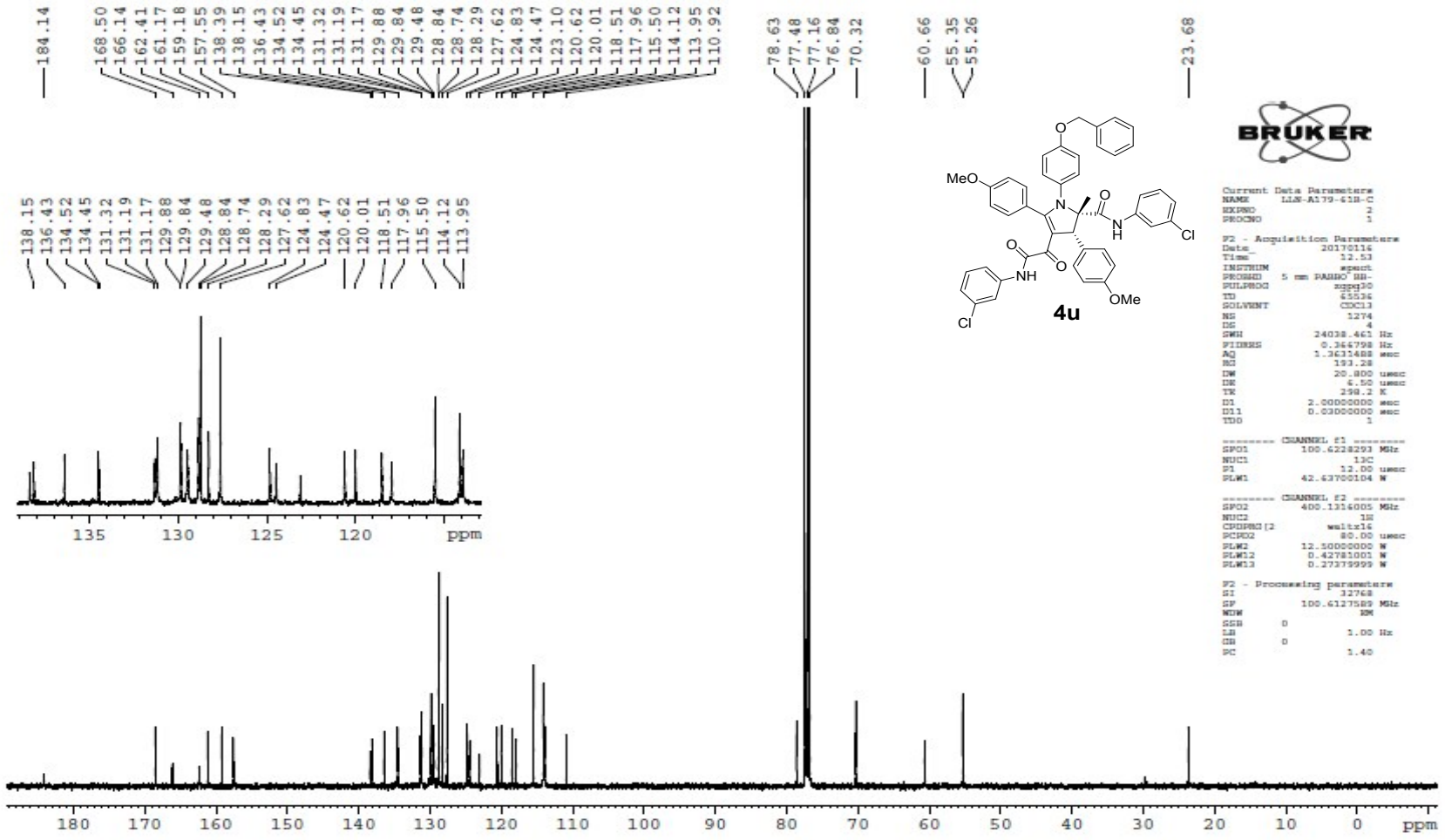
F2 - Acquisition Parameters
Date_ 20170218
Time 9.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 13593
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 294.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

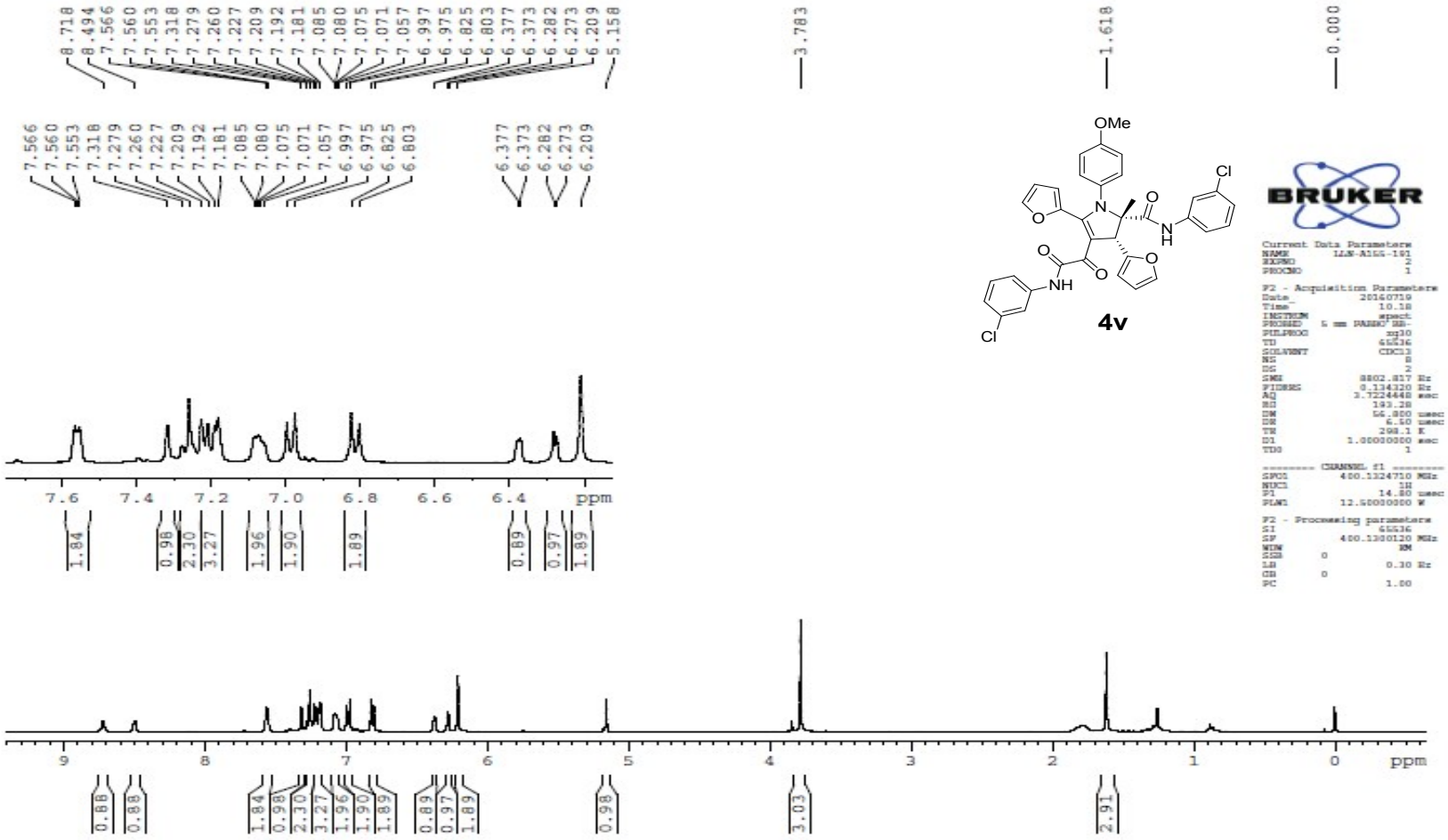
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W

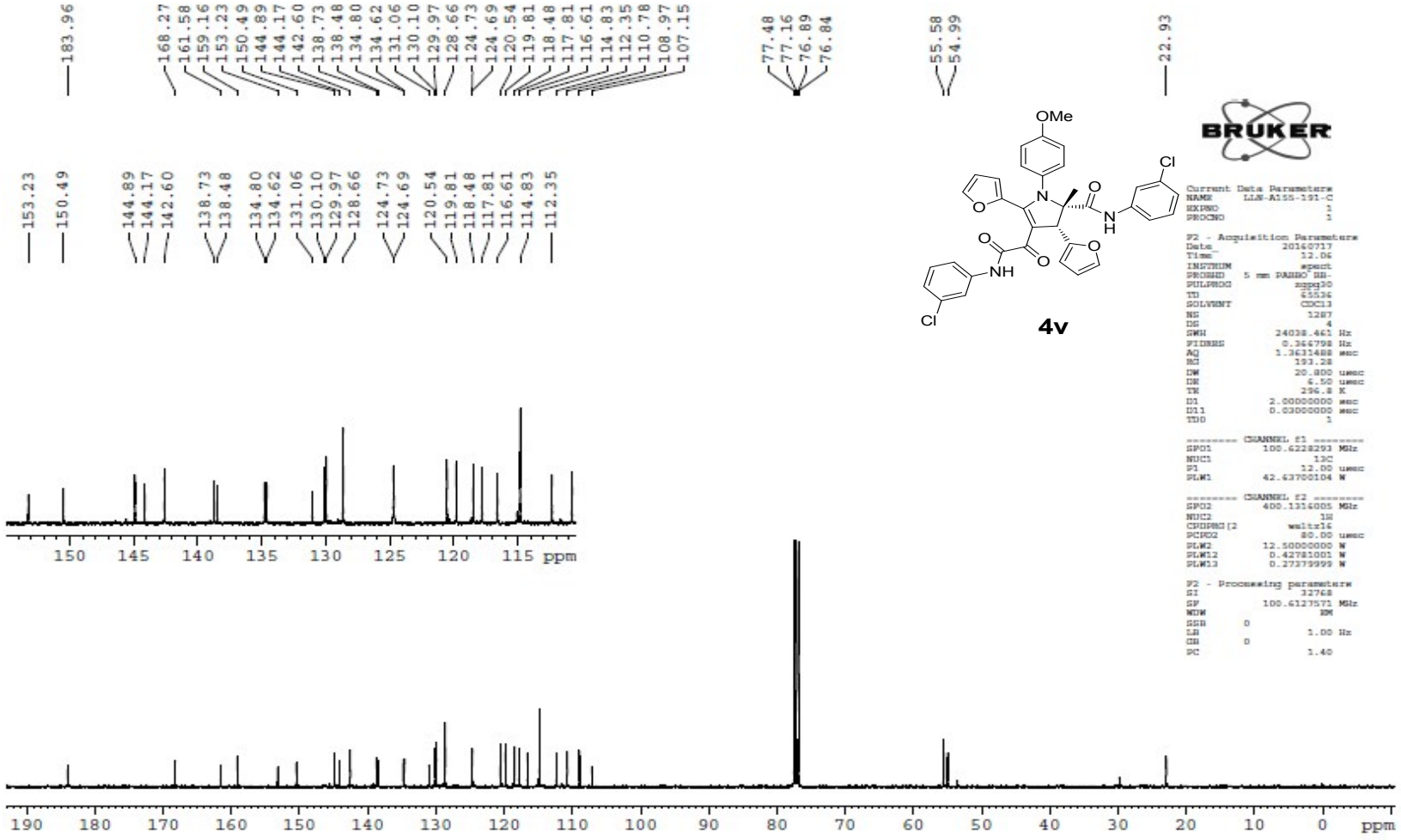
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W

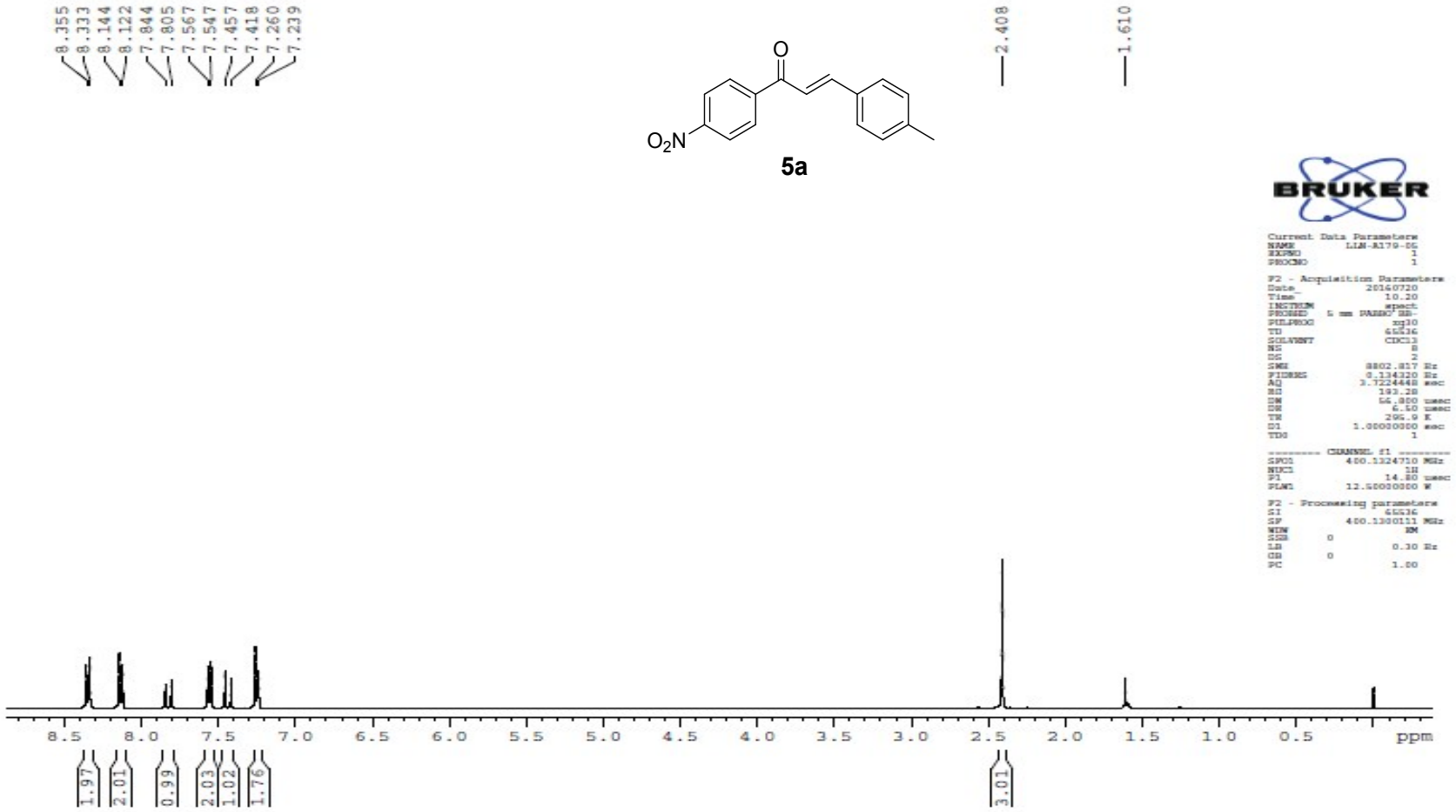
F2 - Processing parameters
SI 32768
SF 100.6127567 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

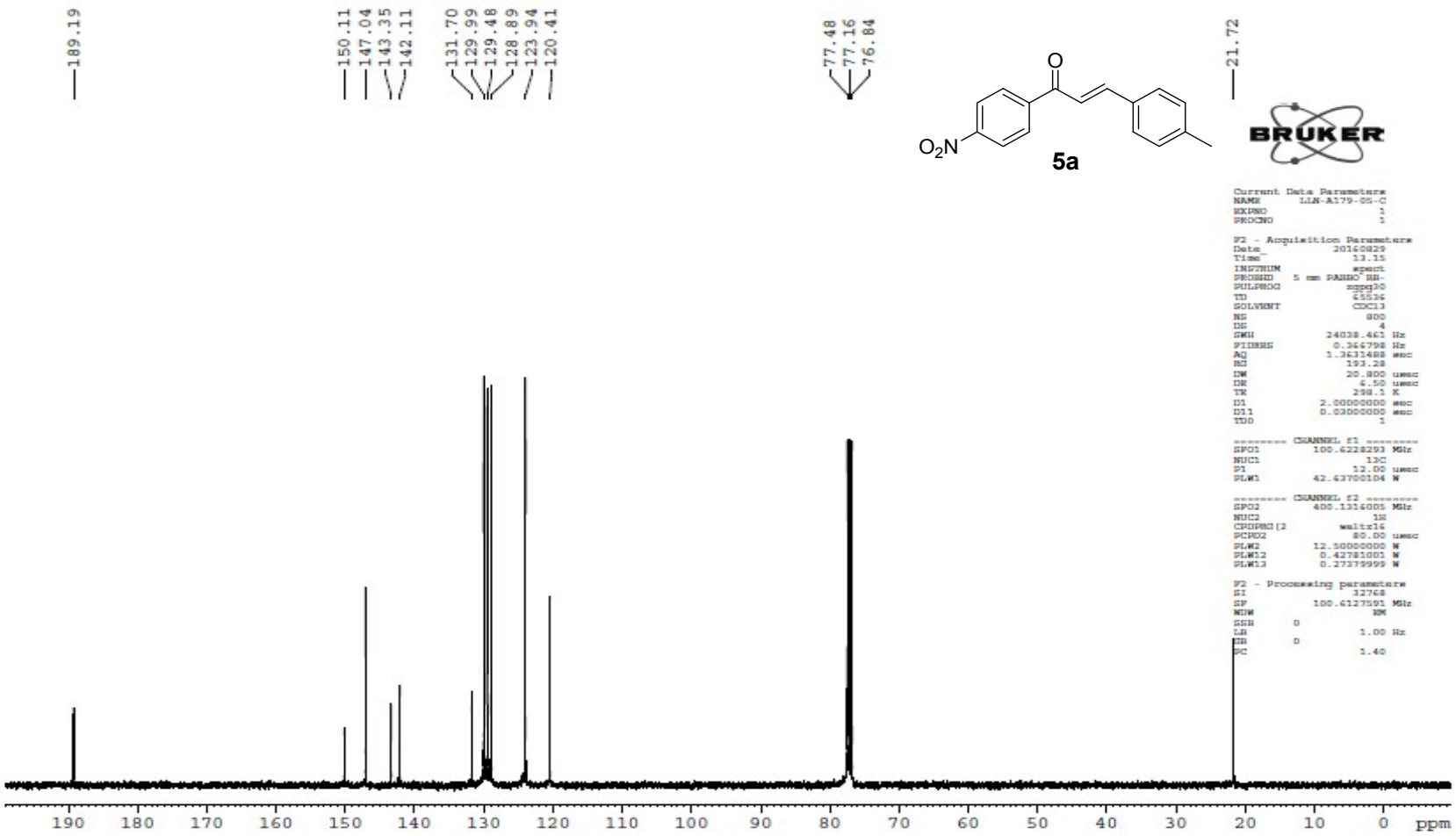

8.650
7.857
7.361
7.351
7.254
7.231
7.193
7.172
7.149
7.129
7.112
7.092
7.051
7.031
7.015
6.994
6.973
6.873
6.852
6.772
6.749
6.742
6.720
6.710
6.689
5.110
4.946
3.711
3.646
1.678
0.000
MeO
OMe
Cl
NH
4u
BRUKER
ppm
5.81
3.11
2.22
2.15
4.23
2.14
6.24
1.00
0.97
0.96
2.02
3.00
2.99
2.97

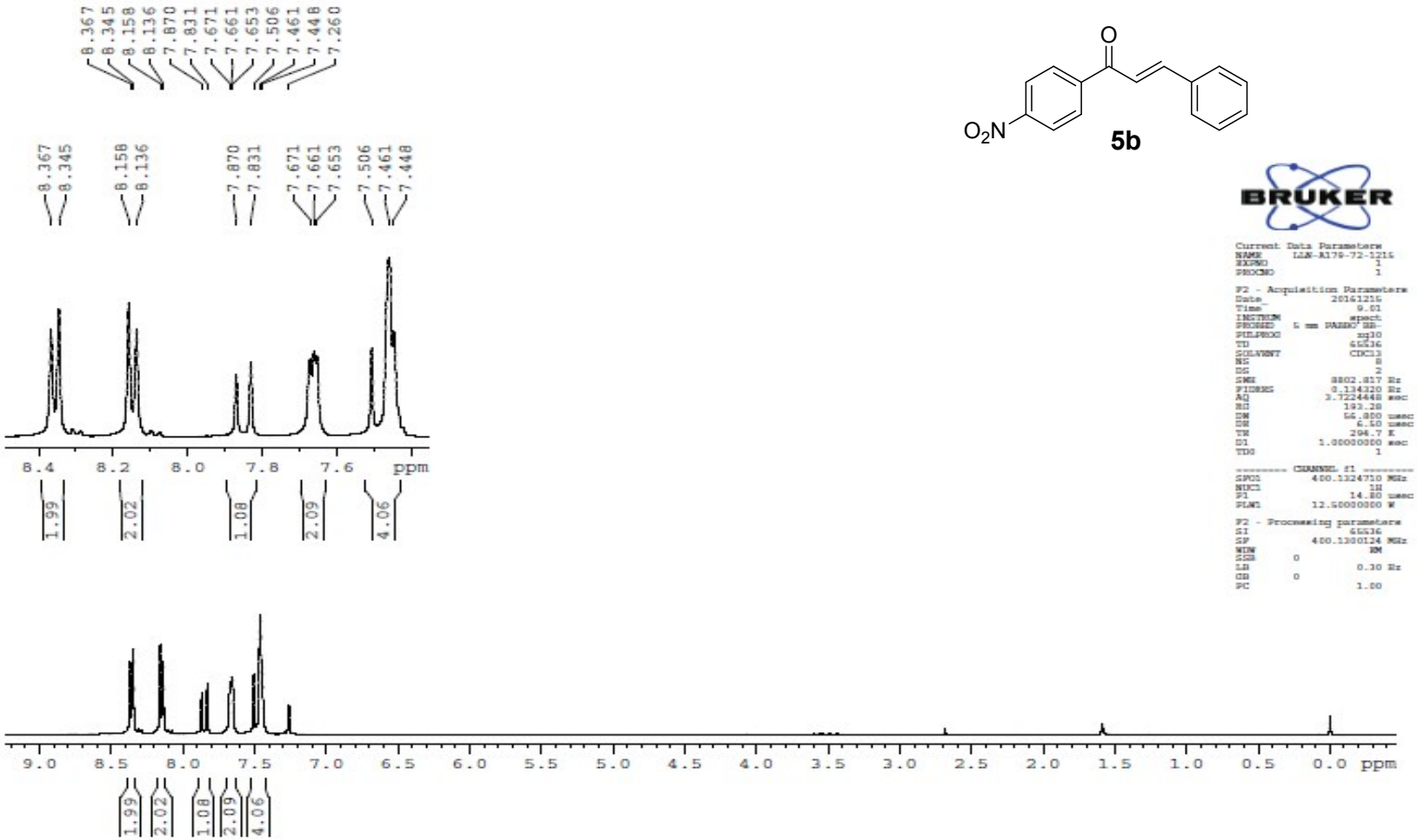

184.14
168.50
166.14
162.41
161.17
159.18
157.55
138.39
138.15
136.43
134.52
134.45
131.32
131.19
131.17
129.88
129.84
129.48
128.84
128.74
128.29
127.62
124.83
124.47
123.10
120.62
120.01
118.51
117.96
115.50
114.12
113.95
110.92
78.63
77.48
77.16
76.84
70.32
60.66
55.35
55.26
23.68
MeO
OMe
Cl
NH
4u
BRUKER
135
130
125
120
ppm
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.718
8.494
7.566
7.560
7.553
7.318
7.279
7.260
7.227
7.209
7.192
7.181
7.085
7.080
7.075
7.071
7.057
6.997
6.975
6.825
6.803
6.377
6.373
6.282
6.273
6.209
5.158
3.783
1.618
0.000
OMe
Cl
N
O
NH
O
O
NH
Cl
4v
BRUKER
Current Data Parameters
NAME LLN-A165-191
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date 20140719
Time 10.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 193.28
DW 56.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.6
7.4
7.2
7.0
6.8
6.6
6.4
ppm
1.84
0.98
2.30
3.27
1.96
1.90
1.89
0.89
0.97
1.89
9
8
7
6
5
4
3
2
1
0
ppm
0.88
0.88
1.84
0.98
2.30
3.27
1.96
1.90
1.89
0.89
0.97
1.89
0.98
3.03
2.91


183.96
168.27
161.58
159.16
153.23
150.49
144.89
144.17
142.60
138.73
138.48
134.80
134.62
131.06
130.10
129.97
128.66
124.73
124.69
120.54
119.81
118.48
117.81
116.61
114.83
112.35
110.78
108.97
107.15
77.48
77.16
76.89
76.84
55.58
54.99
22.93
OMe
Cl
O
N
NH
O
O
O
NH
Cl
4v
BRUKER
Current Data Parameters
NAME LLW-A155-191-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140717
Time 12.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1287
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127571 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
150 145 140 135 130 125 120 115 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.355
8.333
8.144
8.122
7.844
7.805
7.567
7.547
7.457
7.418
7.260
7.239
2.408
1.610
O
O2N
5a
BRUKER
Current Data Parameters
NAME LIN-A179-05
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20160720
Time 10.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 193.28
DW 56.800 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.97
2.01
0.99
2.03
1.02
1.76
3.01


189.19
150.11
147.04
143.35
142.11
131.70
129.99
129.48
128.89
123.94
120.41
77.48
77.16
76.84
21.72
O
O2N
5a
BRUKER
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



5b

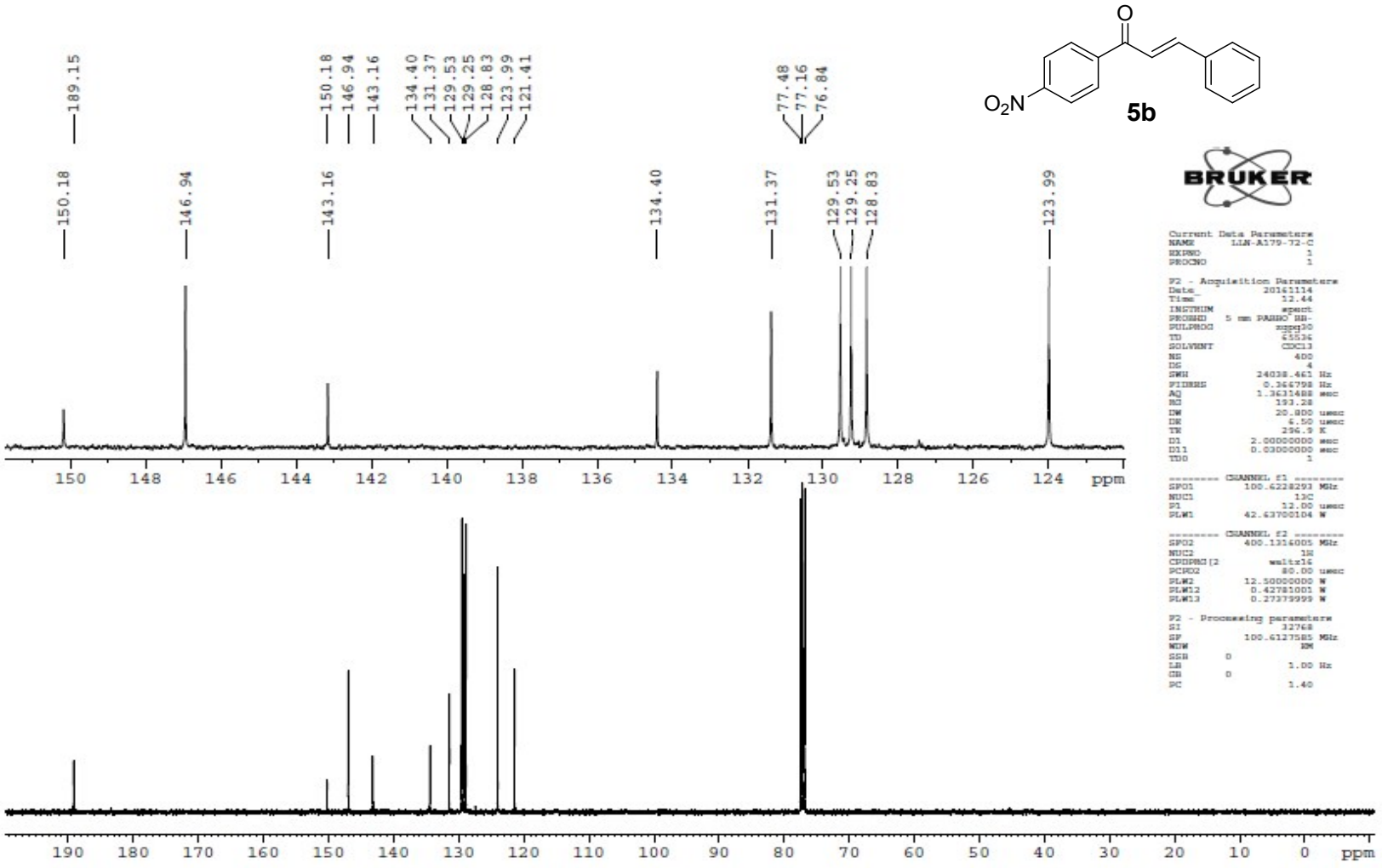
BRUKER

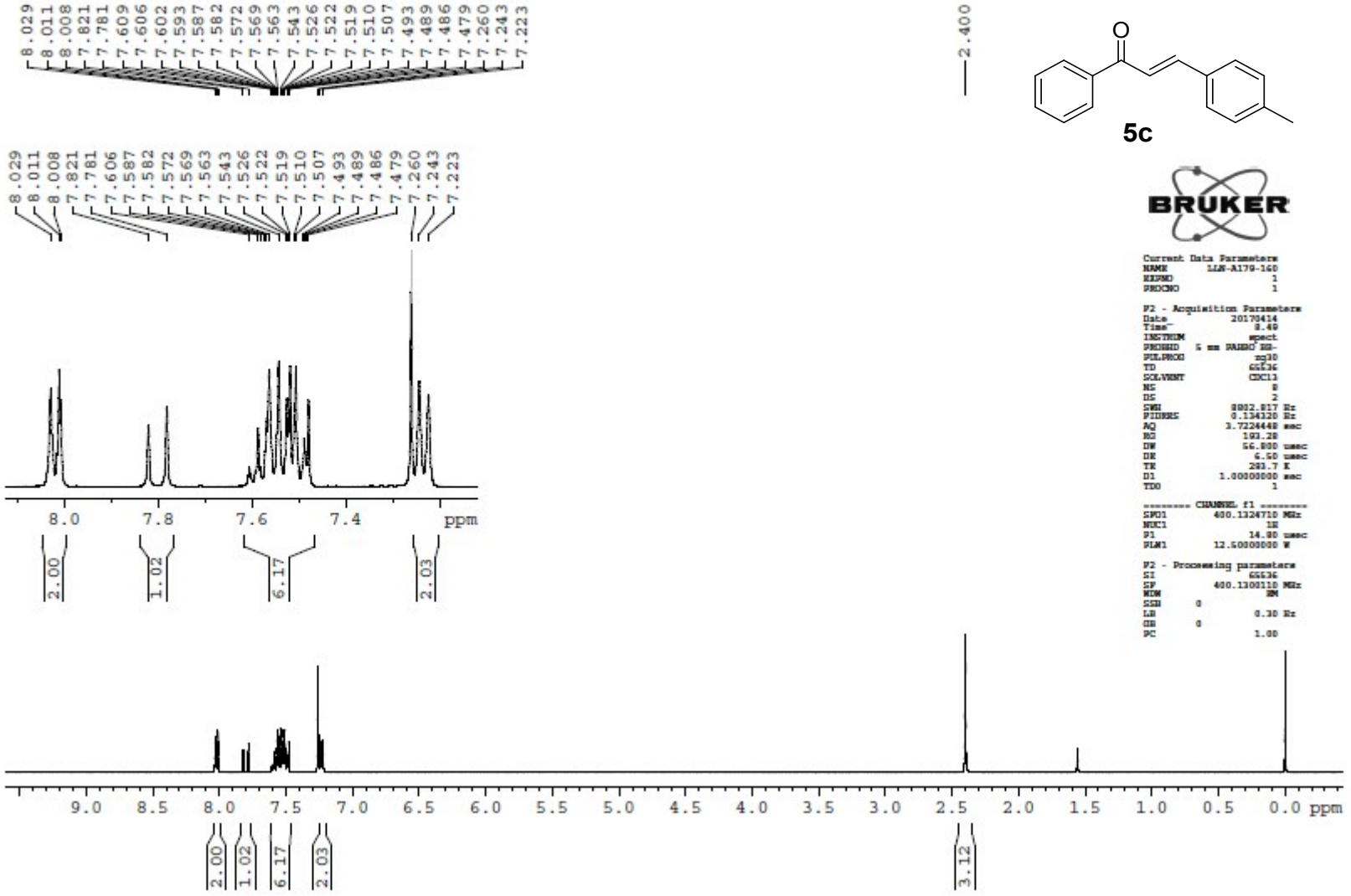
Current Data Parameters
NAME LSR-A179-72-1216
EXPNO 1
PROCNO 1

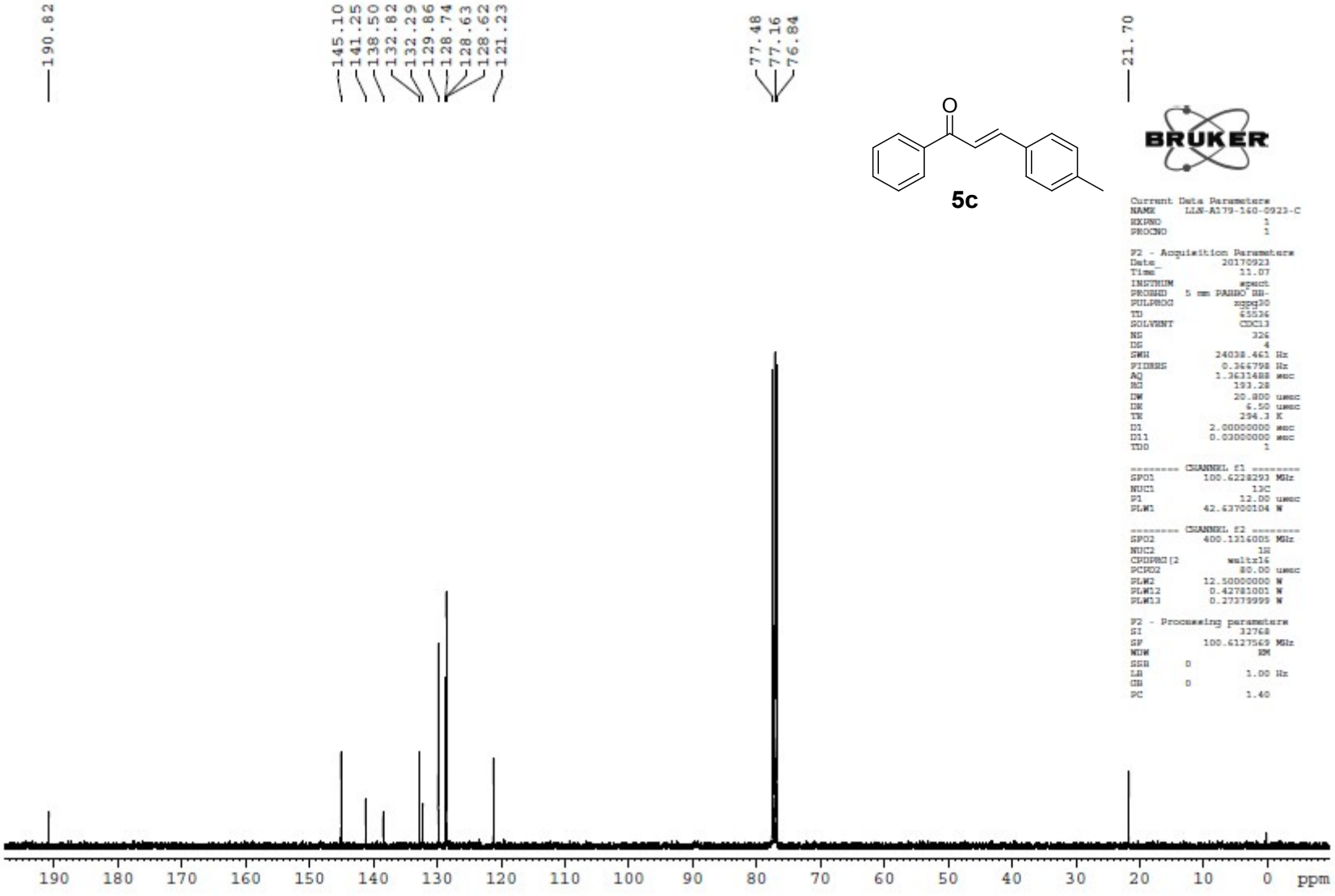
F2 - Acquisition Parameters
Date_ 20161216
Time 9.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 193.28
DW 56.800 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W

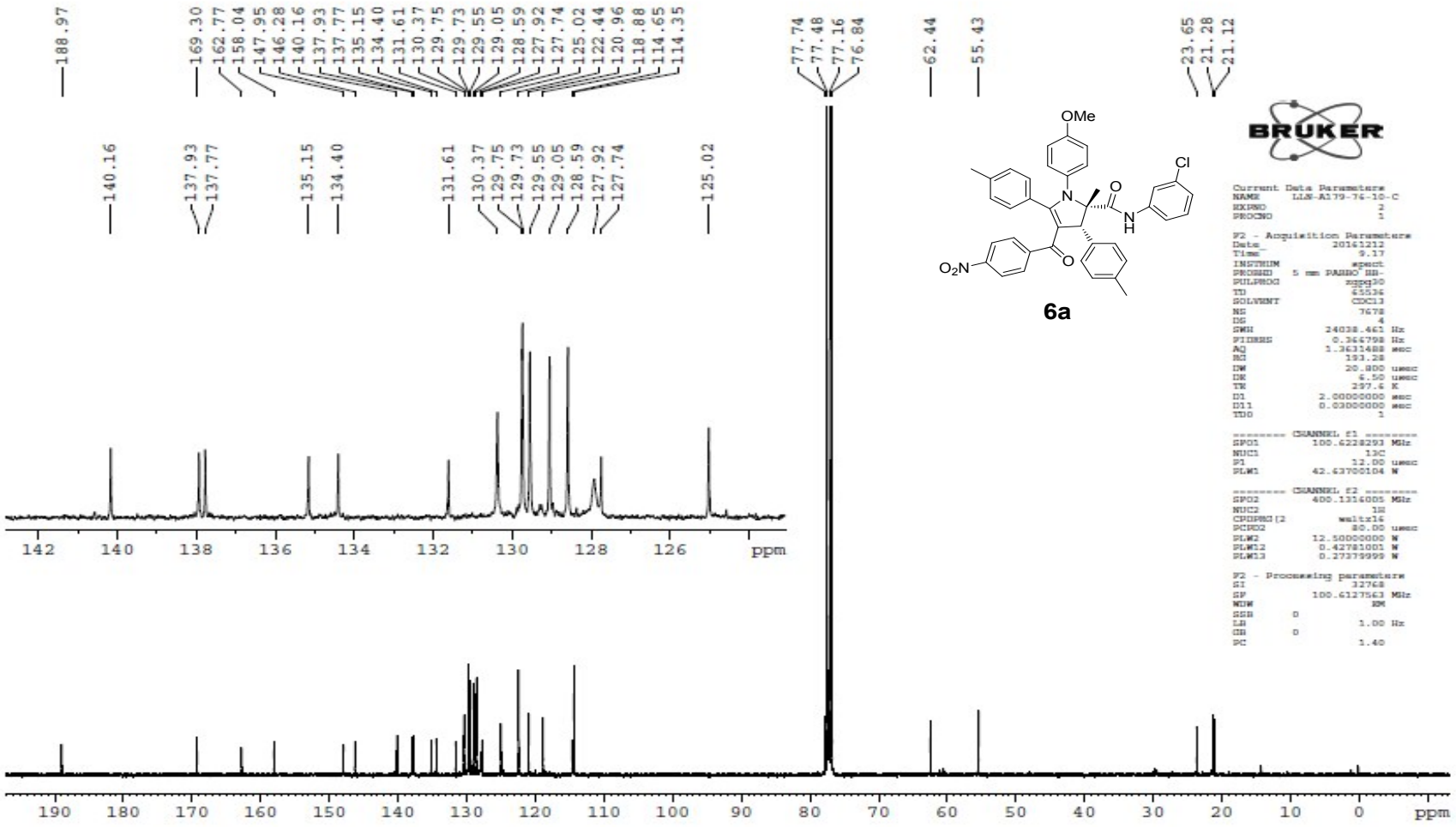
F2 - Processing parameters
SI 65536
SF 400.1300124 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

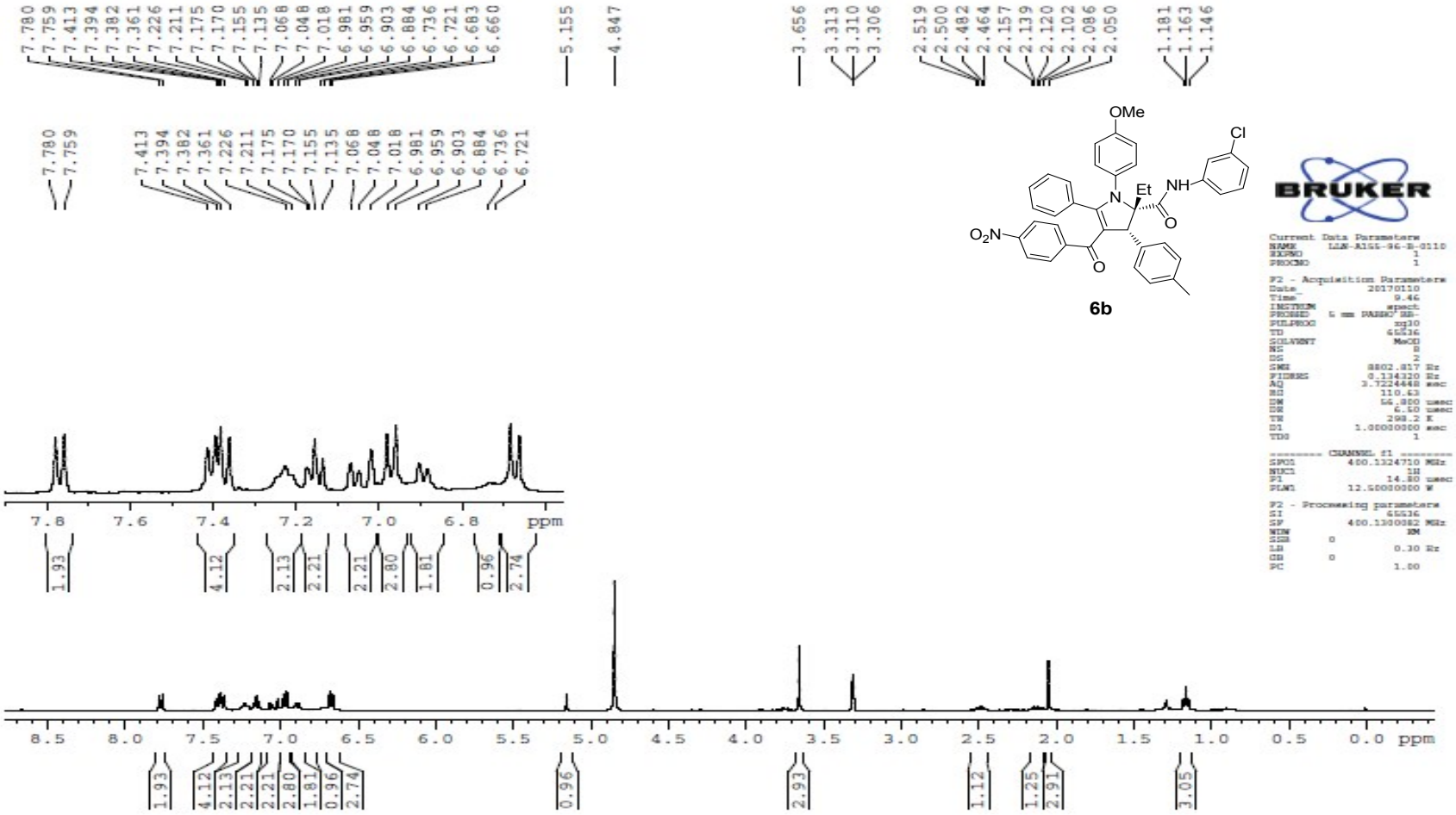

189.15
150.18
146.94
143.16
134.40
131.37
129.53
129.25
128.83
123.99
121.41
77.48
77.16
76.84
O
O_2N
5b
BRUKER
150.18
146.94
143.16
134.40
131.37
129.53
129.25
128.83
123.99
150 148 146 144 142 140 138 136 134 132 130 128 126 124 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Current Data Parameters
NAME LLN-A179-72-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161114
Time 12.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127585 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

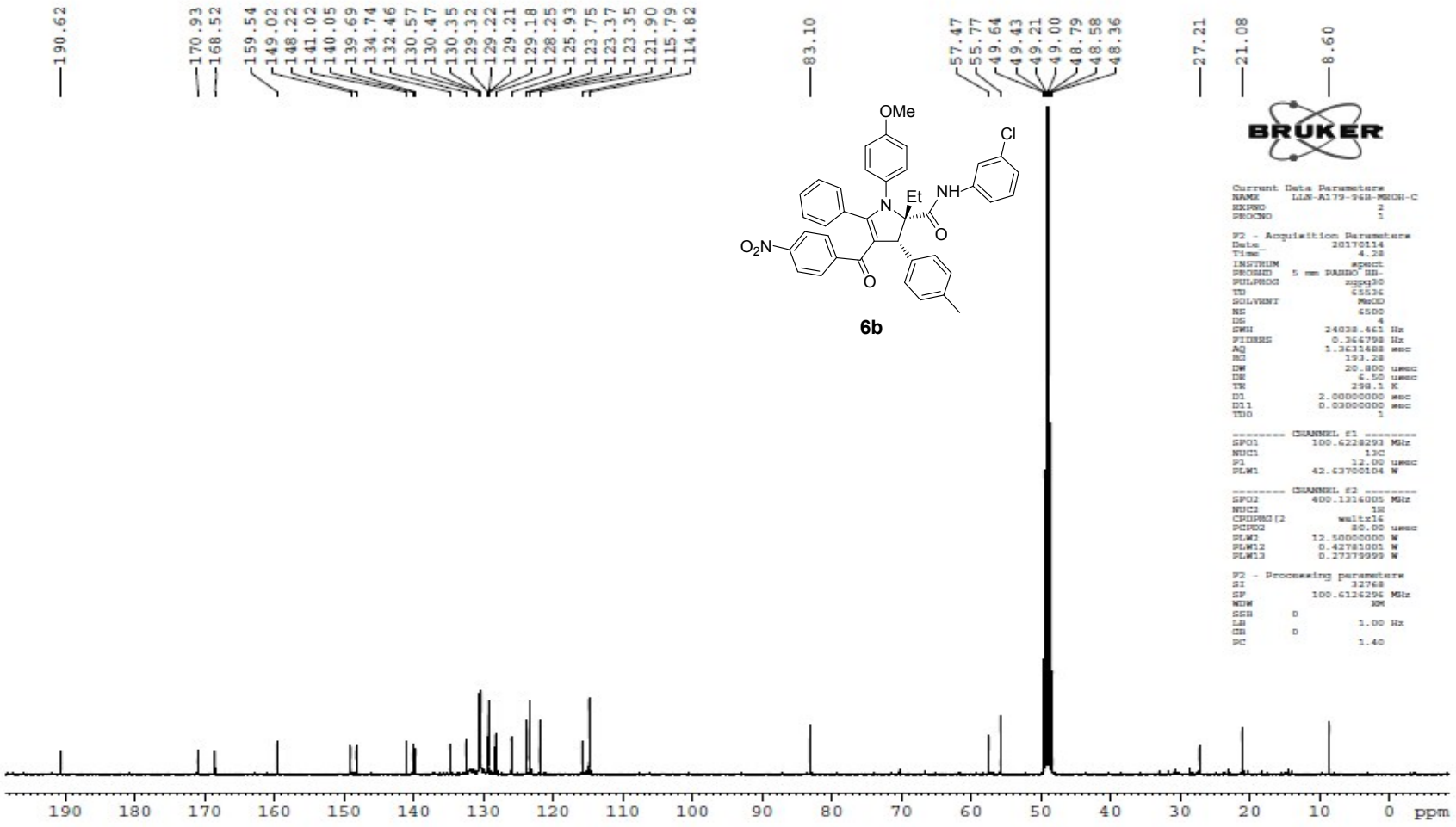

8.029
8.011
8.008
7.821
7.781
7.609
7.606
7.602
7.593
7.587
7.582
7.572
7.569
7.563
7.543
7.526
7.522
7.519
7.510
7.507
7.493
7.489
7.486
7.479
7.260
7.243
7.223
2.400
5c
BRUKER
Current Data Parameters
NAME LLW-A179-160
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20170414
Time 8.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8002.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 181.28
DW 56.800 usec
DE 6.50 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.00 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.0
7.8
7.6
7.4
ppm
2.00
1.02
6.17
2.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
2.00
1.02
6.17
2.03
3.12

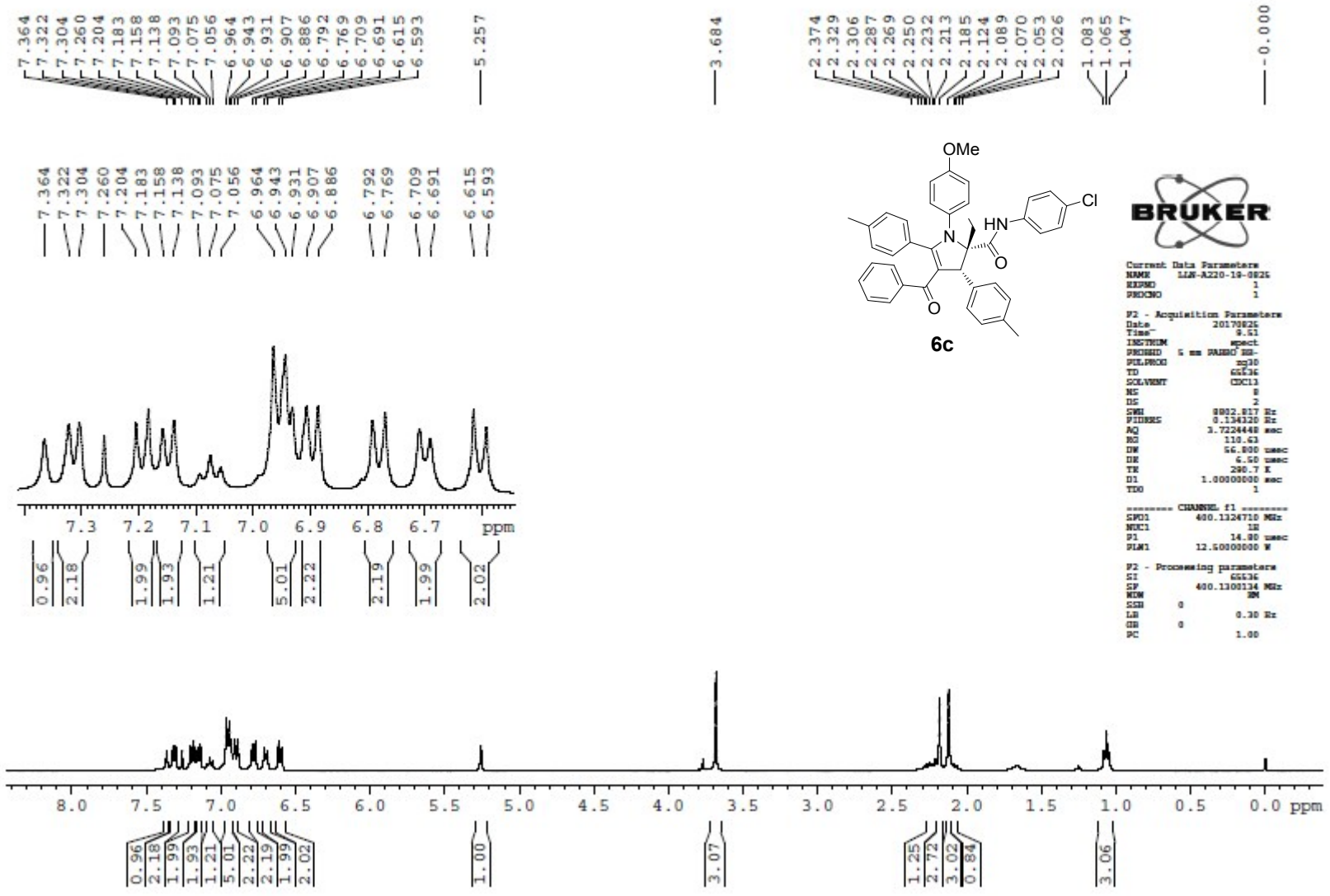

190.82
145.10
141.25
138.50
132.82
132.29
129.86
128.74
128.63
128.62
121.23
77.48
77.16
76.84
21.70
O
5c
BRUKER
Current Data Parameters
NAME LLN-A179-160-0923-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170923
Time 11.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 326
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 294.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127569 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

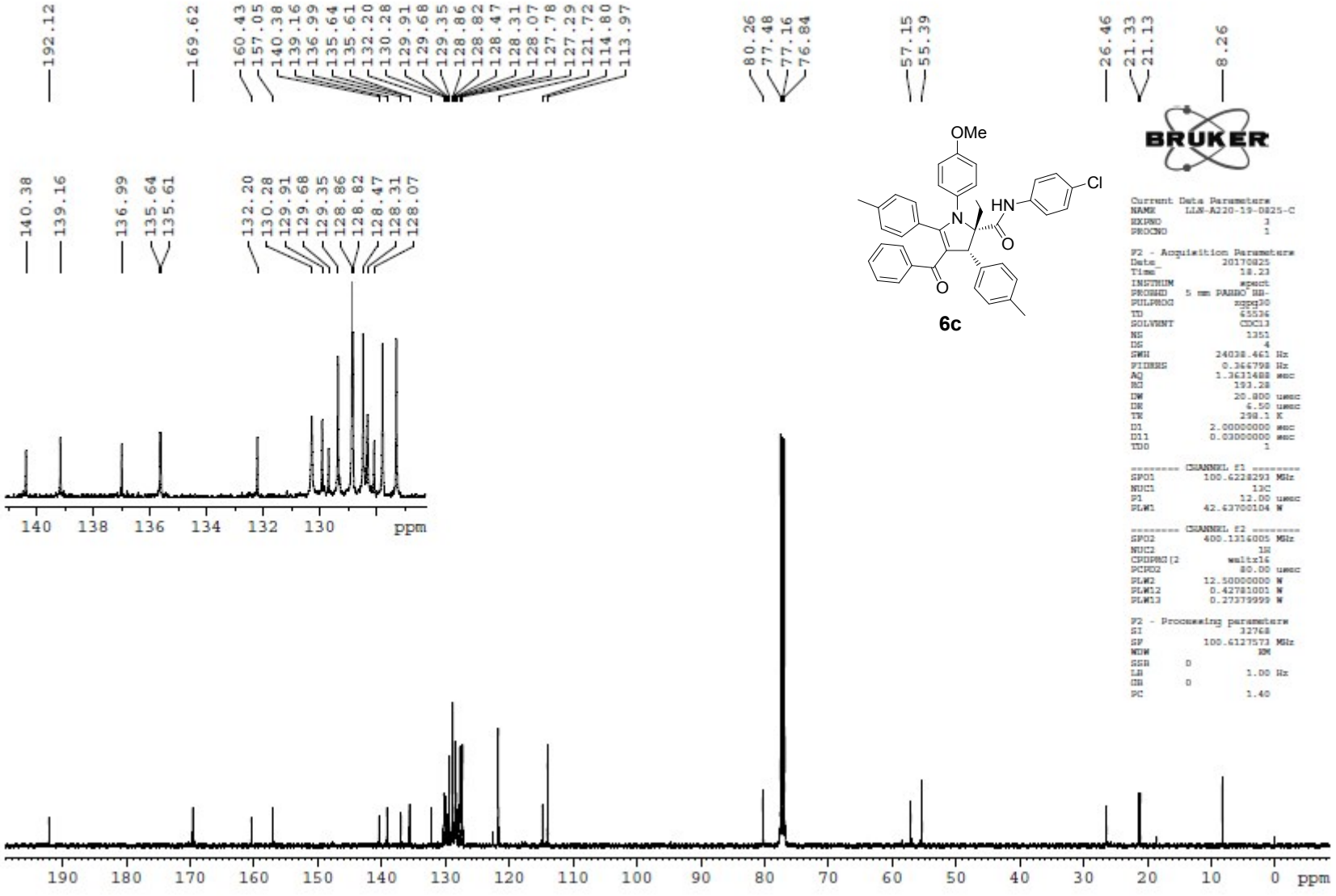

7.773
7.752
7.416
7.395
7.260
7.210
7.190
7.175
7.154
7.134
7.063
7.041
7.021
6.918
6.904
6.899
6.895
6.872
6.860
6.845
6.705
6.687
6.664
6.642
4.946
3.691
2.229
2.082
1.699
OMe
Cl
O
N
H
O2N
6a
BRUKER
Current Data Parameters
NAME LZM-A179-76-10-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161251
Time 19.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 193.28
DW 56.800 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.8
7.6
7.4
7.2
7.0
6.8
ppm
2.04
2.02
2.17
2.94
6.95
2.01
2.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
0.99
3.00
3.03
2.99
3.21

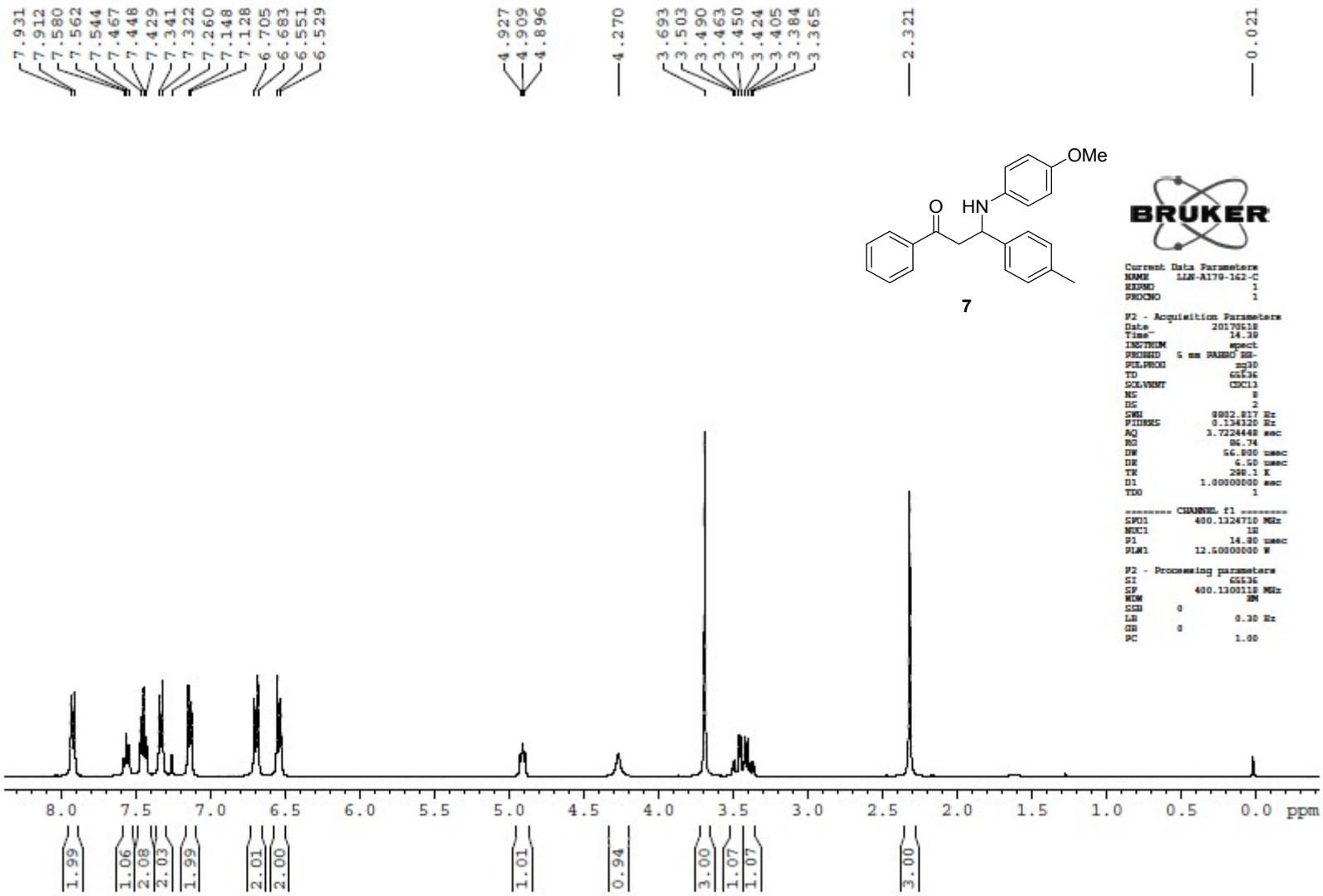

188.97
169.30
162.77
158.04
147.95
146.28
140.16
137.93
137.77
135.15
134.40
131.61
130.37
129.75
129.73
129.55
129.05
128.59
127.92
127.74
125.02
122.44
120.96
118.88
114.65
114.35
77.74
77.48
77.16
76.84
62.44
55.43
23.65
21.28
21.12
OMe
Cl
O
N
H
O2N
6a
BRUKER
Current Data Parameters
NAME LLW-A179-76-10-C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161212
Time 9.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 7678
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 181.28
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127563 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
142 140 138 136 134 132 130 128 126 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.780
7.759
7.413
7.394
7.382
7.361
7.226
7.211
7.175
7.170
7.155
7.135
7.068
7.048
7.018
6.981
6.959
6.903
6.884
6.736
6.721
6.683
6.660
5.155
4.847
3.656
3.313
3.310
3.306
2.519
2.500
2.482
2.464
2.157
2.139
2.120
2.102
2.086
2.050
1.181
1.163
1.146
OMe
Cl
NH
Et
N
O
O2N
O
6b
BRUKER
Current Data Parameters
NAME LLM-A155-96-8-0110
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170110
Time 9.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 110.63
DW 56.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.8
7.6
7.4
7.2
7.0
6.8
ppm
1.93
4.12
2.13
2.21
2.21
2.80
1.81
0.96
2.74
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
1.93
4.12
2.13
2.21
2.21
2.80
1.81
0.96
2.74
0.96
2.93
1.12
1.25
2.91
3.05


190.62
170.93
168.52
159.54
149.02
148.22
141.02
140.05
139.69
134.74
132.46
130.57
130.47
130.35
129.32
129.22
129.21
129.18
128.25
125.93
123.75
123.37
123.35
121.90
115.79
114.82
83.10
57.47
55.77
49.64
49.43
49.21
49.00
48.79
48.58
48.36
27.21
21.08
8.60
OMe
Cl
NH
Et
N
O
O
O2N
6b
BRUKER
Current Data Parameters
NAME LLN-A179-96B-MEOH-C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170114
Time 4.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 6500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3633488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6126296 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.364
7.322
7.304
7.260
7.204
7.183
7.158
7.138
7.093
7.075
7.056
6.964
6.943
6.931
6.907
6.886
6.792
6.769
6.709
6.691
6.615
6.593
5.257
3.684
2.374
2.329
2.306
2.287
2.269
2.250
2.232
2.213
2.185
2.124
2.089
2.070
2.053
2.026
1.083
1.065
1.047
0.000
OMe
Cl
HN
N
O
O
6c
BRUKER
Current Data Parameters
NAME LLW-A220-19-0826
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20170826
Time 9.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 110.63
DW 56.800 usec
DE 6.50 usec
TE 290.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.3 7.2 7.1 7.0 6.9 6.8 6.7 ppm
0.96 2.18 1.99 1.93 1.21 5.01 2.22 2.19 1.99 2.02
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.96 2.18 1.99 1.93 1.21 5.01 2.22 2.19 1.99 2.02 1.00 3.07 1.25 2.72 3.02 0.84 3.06


192.12
169.62
160.43
157.05
140.38
139.16
136.99
135.64
135.61
132.20
130.28
129.91
129.68
129.35
128.86
128.82
128.47
128.31
128.07
127.78
127.29
121.72
114.80
113.97
80.26
77.48
77.16
76.84
57.15
55.39
26.46
21.33
21.13
8.26
OMe
HN
Cl
N
O
O
6c
BRUKER
Current Data Parameters
NAME LLW-A220-19-0825-C
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170825
Time 18.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1351
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127573 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
140.38
139.16
136.99
135.64
135.61
132.20
130.28
129.91
129.68
129.35
128.86
128.82
128.47
128.31
128.07
140 138 136 134 132 130 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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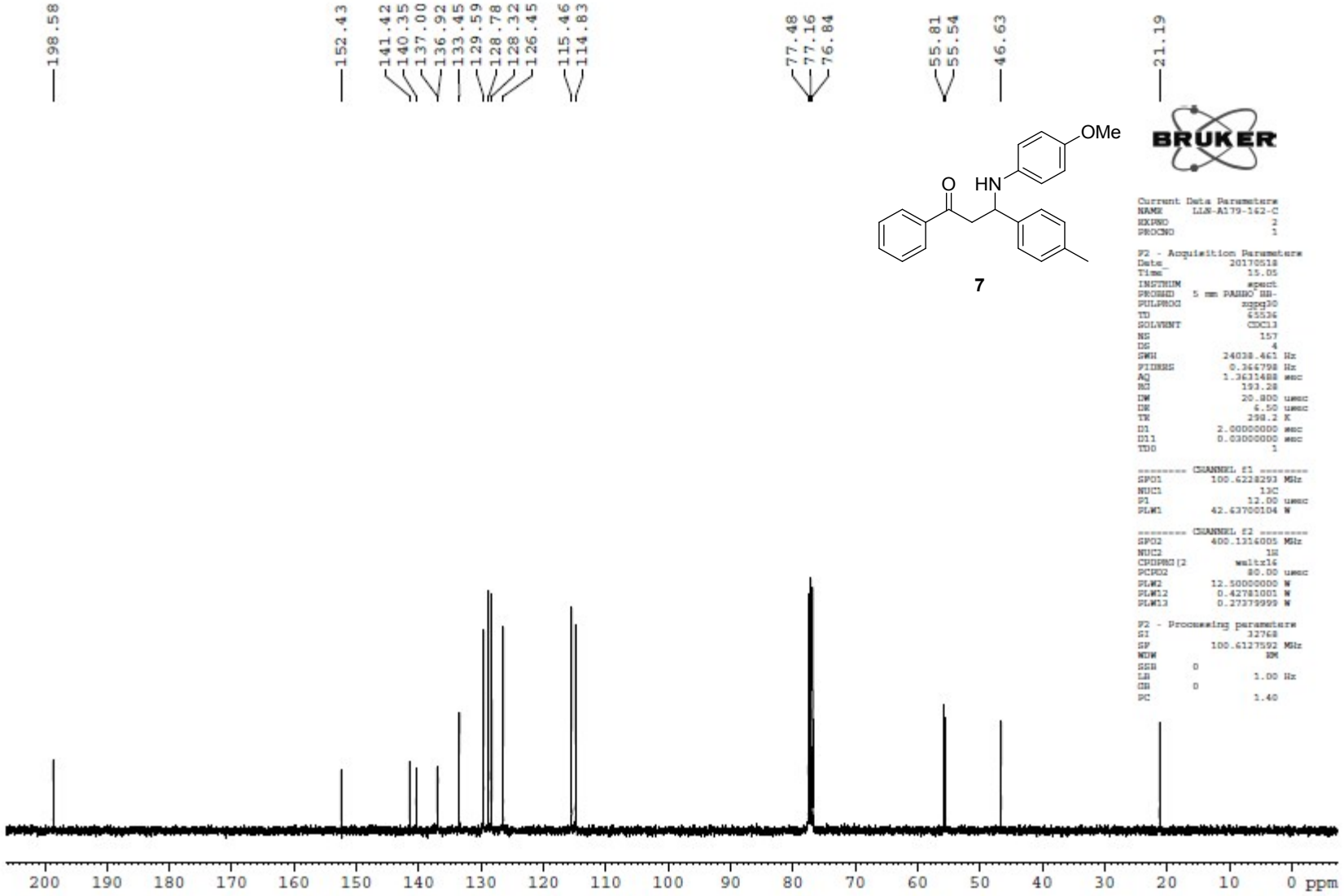
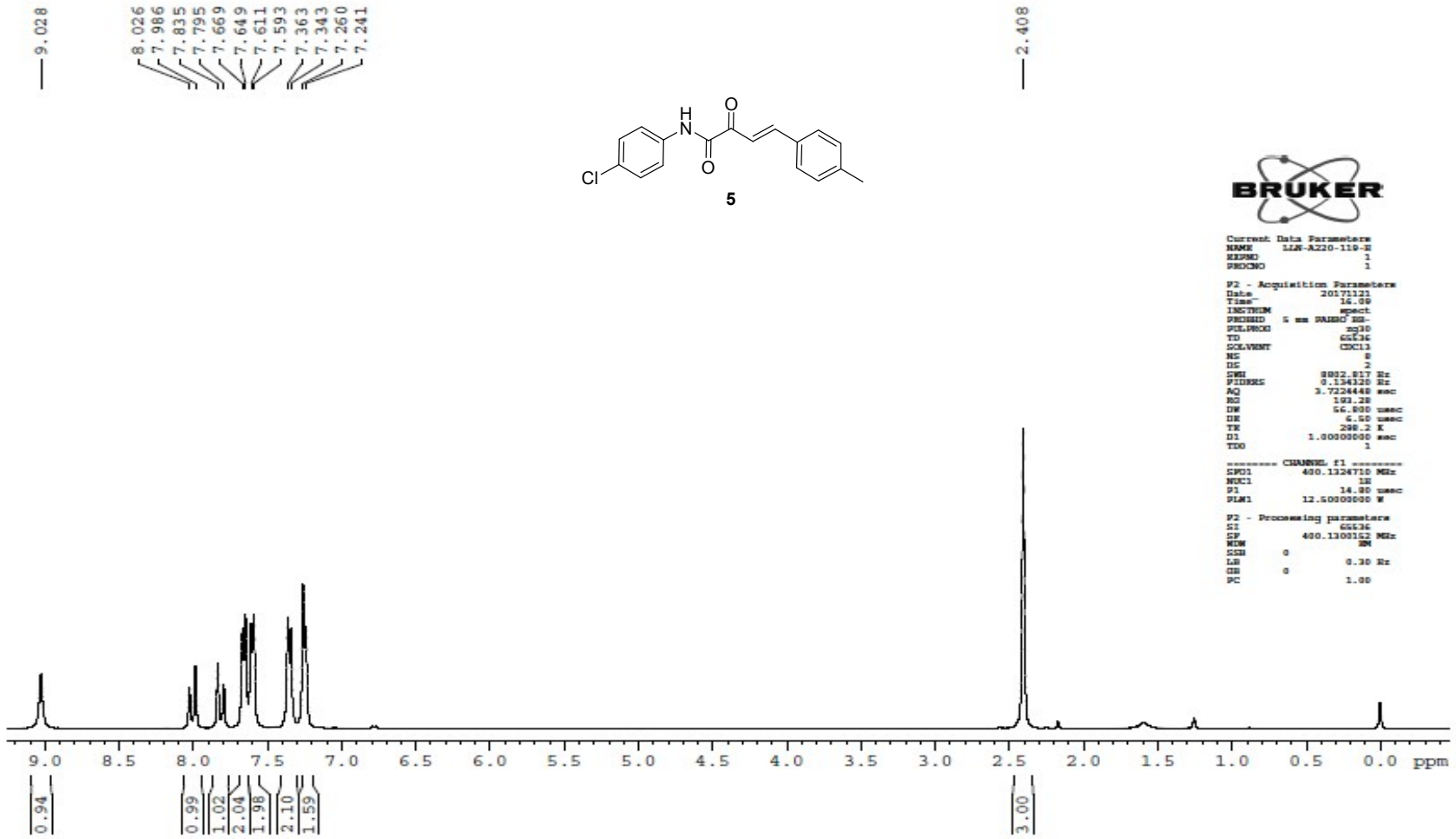
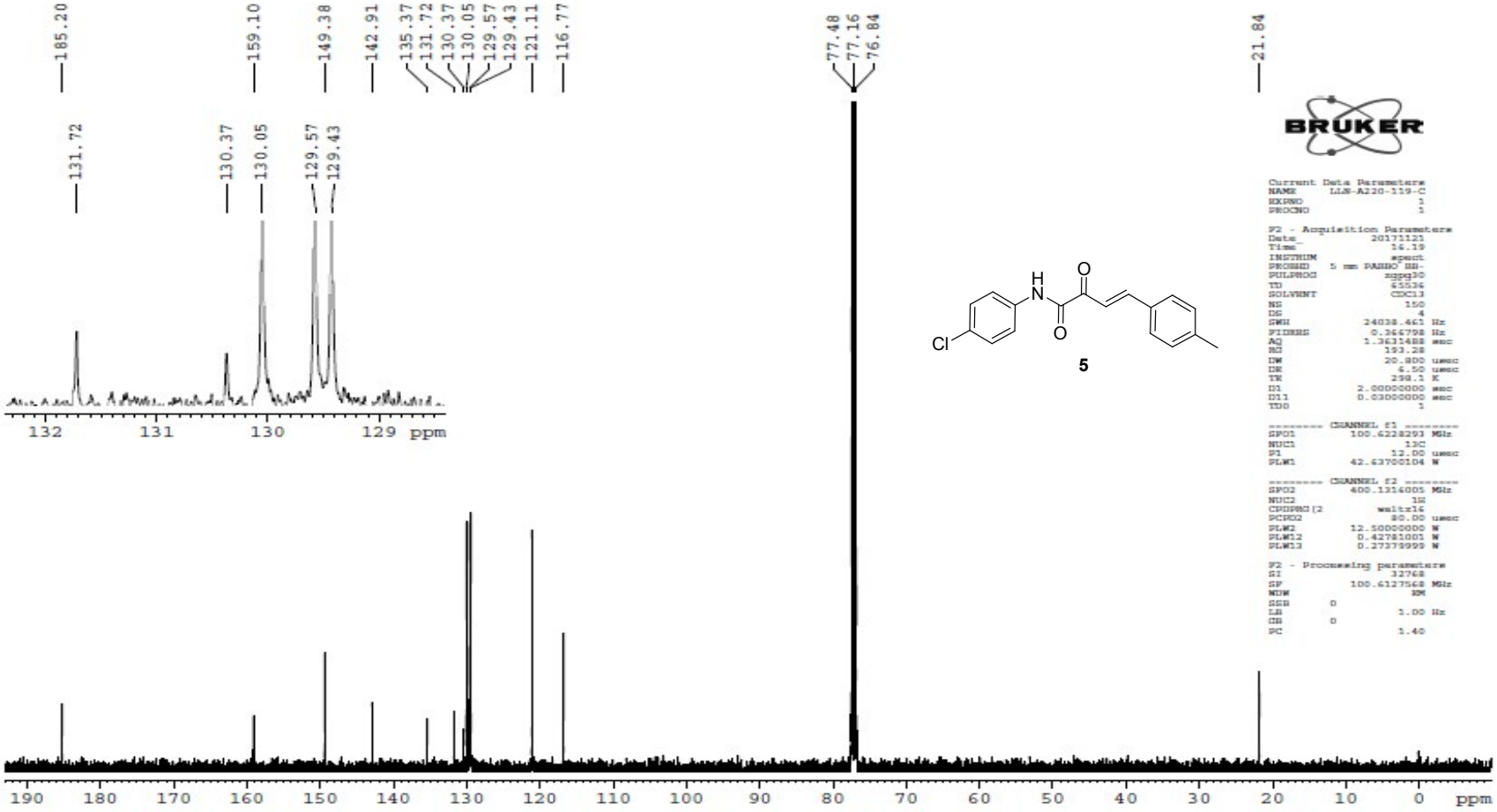
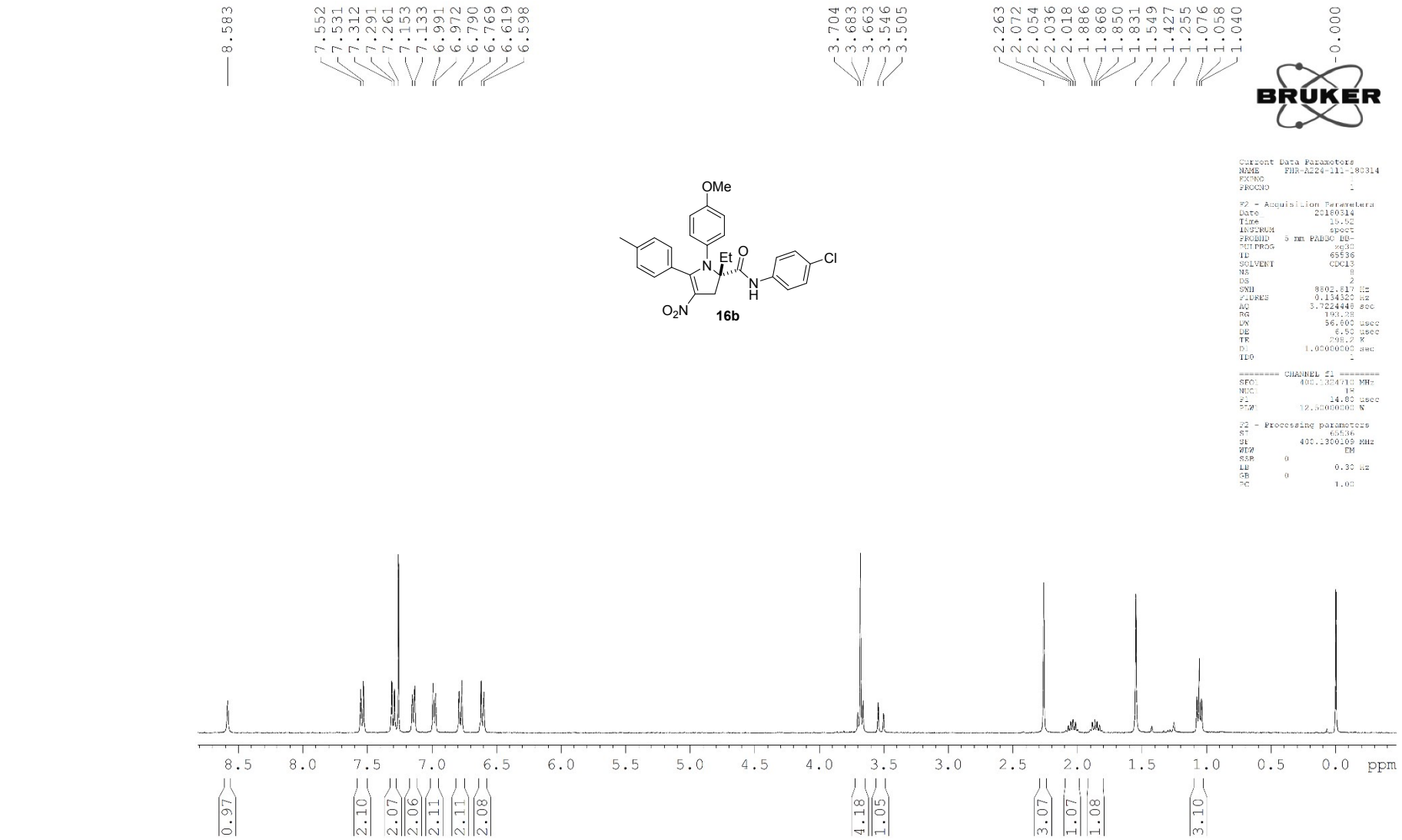
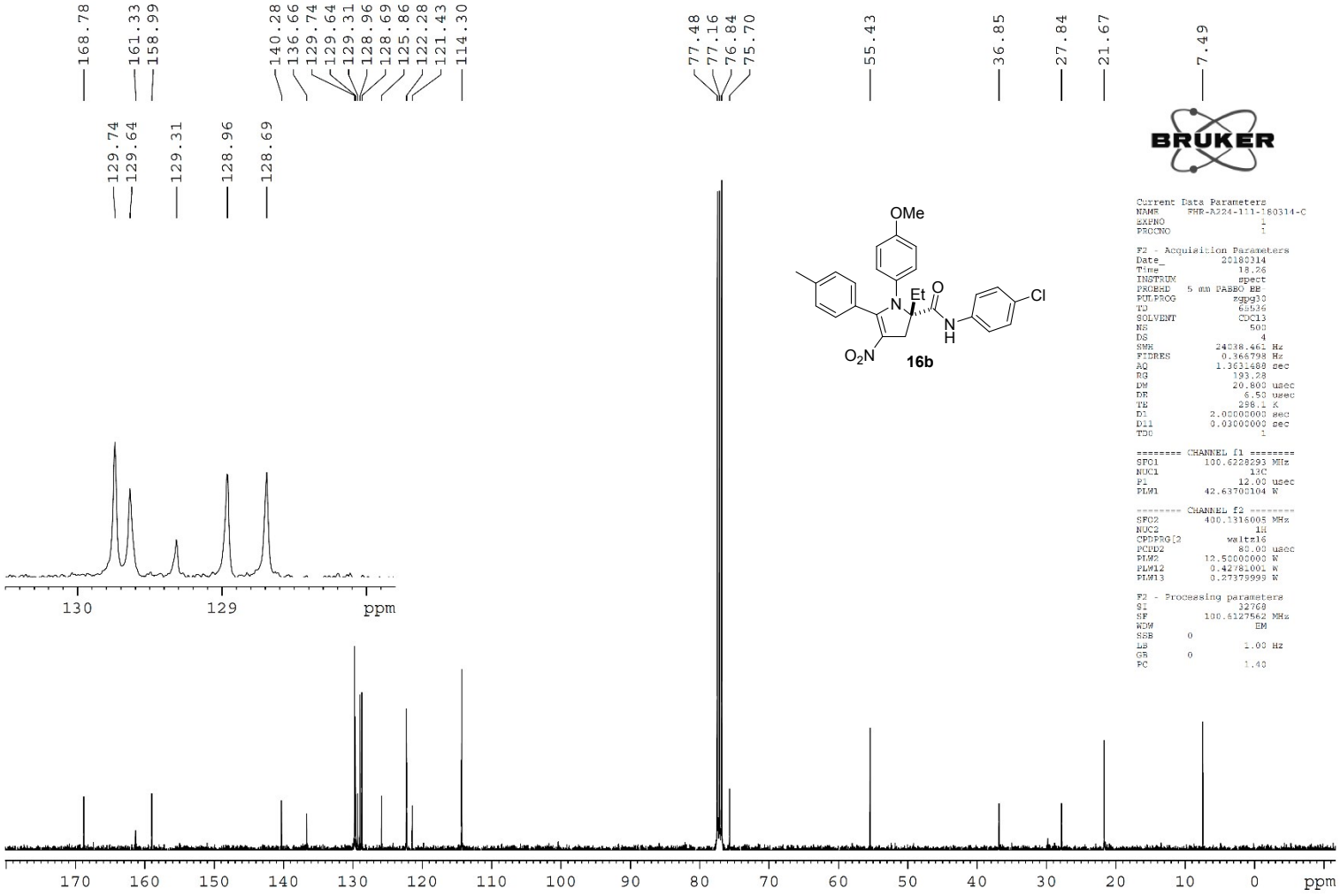
7.912
7.580
7.562
7.544
7.467
7.448
7.429
7.341
7.322
7.260
7.148
7.128
6.705
6.683
6.551
6.529
4.927
4.909
4.896
4.270
3.693
3.503
3.490
3.463
3.450
3.424
3.405
3.384
3.365
2.321
0.021
OMe
O
HN
7
BRUKER
Current Data Parameters
NAME LLW-A179-162-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20170518
Time 14.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8992.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 86.74
DW 55.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.99
1.06
2.08
2.03
1.99
2.01
2.00
1.01
0.94
3.00
1.07
1.07
3.00


198.58
152.43
141.42
140.35
137.00
136.92
133.45
129.59
128.78
128.32
126.45
115.46
114.83
77.48
77.16
76.84
55.81
55.54
46.63
21.19
OMe
HN
O
7
BRUKER
Current Data Parameters
NAME LLN-A179-162-C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170518
Time 15.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 157
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127592 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


9.028
8.026
7.986
7.835
7.795
7.669
7.649
7.611
7.593
7.363
7.343
7.260
7.241
2.408
H
N
O
O
Cl
5
BRUKER
Current Data Parameters
NAME LLW-A220-119-H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20171121
Time 16.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 101.28
DW 56.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300152 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.94
0.99
1.02
2.04
1.98
2.10
1.59
3.00


185.20
159.10
149.38
142.91
135.37
131.72
130.37
130.05
129.57
129.43
121.11
116.77
77.48
77.16
76.84
21.84
131.72
130.37
130.05
129.57
129.43
132
131
130
129 ppm
BRUKER
Current Data Parameters
NAME LLS-A220-119-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171121
Time 16.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 150
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127568 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Cl
H
N
O
O
5
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.583
7.552
7.531
7.312
7.291
7.261
7.153
7.133
6.991
6.972
6.790
6.769
6.619
6.598
3.704
3.683
3.663
3.546
3.505
2.263
2.072
2.054
2.036
2.018
1.886
1.868
1.850
1.831
1.549
1.427
1.255
1.076
1.058
1.040
0.000
BRUKER
OMe
Et
O
N
Cl
N
H
O2N
16b
Current Data Parameters
NAME FHR-A224-111-180314
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20180314
Time 15.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8802.817 Hz
FIDRES 0.134320 Hz
AQ 3.7224448 sec
RG 101.28
DW 56.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1300109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.97
2.10
2.07
2.06
2.11
2.11
2.08
4.18
1.05
3.07
1.07
1.08
3.10


168.78
161.33
158.99
140.28
136.66
129.74
129.64
129.31
128.96
128.69
125.86
122.28
121.43
114.30
77.48
77.16
76.84
75.70
55.43
36.85
27.84
21.67
7.49
129.74
129.64
129.31
128.96
128.69
OMe
Et
O
N
Cl
N
H
O2N
16b
130
129
ppm
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
BRUKER
Current Data Parameters
NAME FHR-A224-III-180314-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180314
Time 18.26
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.28
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 12.00 usec
PLW1 42.63700104 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.42781001 W
PLW13 0.27379999 W
F2 - Processing parameters
SI 32768
SF 100.6127562 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40