This version of the ESI replaces the previous version published on 18.05.2018 to correctly display the 13C NMR of 4e on page 47.

Supporting information

for

Towards Environmentally Friendlier Suzuki-Miyaura Reactions with Pd-NHC (NHC = N-Heterocyclic Carbene) Complexes

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General information

All aryl halides and boronic acids were used as received. All bases were used as received (in air) or dried under vacuum at 100 °C (under inert atmosphere). All solvents were used as received when experiments were conducted in air. Degassed solvents were used when experiments were conducted under inert atmosphere. All [NHC·H][Pd(η^3-R-allyl)Cl_2] were prepared from commercially available NHC·HCl and [Pd(η^3-R-allyl)(μ-Cl)]$_2$. Flash chromatography was performed on silica gel 60 Å pore diameter and 40-63 μm particles size. ^{1}H, ^{19}F{^{1}H} and ^{13}C{^{1}H} Nuclear Magnetic Resonance (NMR) spectra were recorded on Bruker-400 and 500 MHz spectrometers at ambient temperature in $CDCl_3$ purchased from Sigma Aldrich and dried over molecular sieves. Chemical shifts (ppm) are referenced to the residual solvent peak. Coupling constants, *J*, are given in hertz. Abbreviations used in the designation of the signals: s = singlet, d = doublet, dd = doublet of doublets, ddd = doublet of doublet of doublets, dt = doublet of triplets, t = triplet, td = triplet of doublets, m = multiplet. Elemental analyses were performed at London Metropolitan University.

Synthesis of palladates

Solvent screening - General procedure. In air, the corresponding NHC·HCl, [Pd(η^3-R-allyl)(μ-Cl)]$_2$ and a magnetic stir bar were charged in a vial and solvent (1 mL) was added. The mixture was stirred at 60 °C for 1 hour. The reaction was allowed to cool for 1 min and the sample was concentrated to 1/3 of the original volume under reduced pressure. Microcrystalline product was collected by filtration and washed with minimum amount of cold acetone or ethanol if necessary. Solid dried under vacuum.

Table S-1: Solvent optimization **[IPr·H][Pd(□^{3}-cin)Cl_2]**

Entry	**Solvents**	**Isolated yield (%)**
1	Acetone	99
2	Cyclopentyl methyl ether	99
3	Pentane	99
4	Dichloromethane	99
5	Chloroform	99
6	Water	99
7	Ethyl acetate	99
8	Ethanol	99

Synthesis of Pd-NHC complexes from palladates

One-pot large scale synthesis of [Pd(IPr)(η^3-cin)Cl]. In a round-bottom flask equipped with a stir bar, IPr·HCl (1.64 g, 3.86 mmol) and [Pd(η^3-cin)(μ-Cl)]$_2$ (1.00 g, 1.93 mmol) were added, followed by ethanol (50 mL). K_2CO_3 (320 mg, 2.32 mmol) was added and the reaction was heated to 60 °C for 5 h. The solvent was removed from the crude product which was dissolved in dichloromethane (20 mL) and filtered through a pad of silica. A yellow crystalline solid was obtained in 98% (2.45 g) yield.

Synthesis of [Pd(IPr)(η^3-cin)Cl] from palladate. In a round-bottom flask equipped with a stir bar, [IPr·H][Pd(η^3-cin)Cl_2] (500 mg, 0.73 mmol) followed by ethanol (25 mL) and K_2CO_3 (140 mg, 1.01 mmol) were added. The reaction was heated to 60 °C for 5 h. The solvent was removed from the crude product which was dissolved in dichloromethane (10 mL) and filtered through a pad of silica. A yellow crystalline solid was obtained in 64% (300 mg) yield.

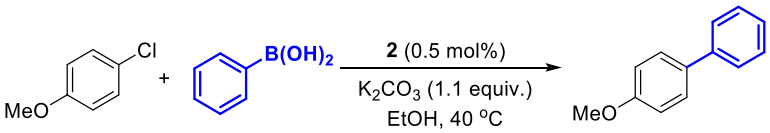
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.50 (t, *J* = 7.7 Hz, 2H), 7.48-7.28 (d, *J* = 7.7 Hz, 4H), 7.12 (m, 5H), 5.09 (m, 1H), 4.36 (d, *J* = 12.9 Hz, 1H), 3.06 (m, 5H), 1.77 (d, *J* = 11.4

Hz, 1H), 1.43-1.36 (m, 12H), 1.16 (d, J = 7.1 Hz, 12H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 184.8 (C, carbene), 145.9 (C), 137.7 (C), 135.7 (C), 129.7 (CH) 128.0 (CH), 127.9 (CH), 127.1 (CH), 126.5 (CH), 124.0 (CH), 123.6 (CH), 108.6 CH), 90.0 (CH), 46.1 (CH_2), 33.9 (CH_2), 28.4 (CH), 26.0 (CH_3), 22.8 (CH_3).

Suzuki-Miyaura coupling

Pre-catalyst Optimization. The general procedure was followed using phenylboronic acid (60.9 mg, 0.5 mmol), 4-chloroanisole (61 µL, 0.5 mmol) with K_2CO_3 (76 mg, 0.55 mmol) in ethanol (1 mL). The GC yield was determined using mesitylene as internal standard.

Table S-3: Optimisation of the pre-catalyst



[Pd] precatalyst (0.5 mol%)	GC yield[a] (%)
[IPr·H][Pd(η^3-cinnamyl)Cl_2]	93
[IPr·H][Pd(η^3-allyl)Cl_2]	55
[IPr*·H][Pd(η^3-cinnamyl)Cl_2]	88
[SIPr·H][Pd(η^3-cinnamyl)Cl_2]	30
[IPr·H][Pd(η^3-2-Me-allyl)Cl_2]	80
[IPr·H] [Pd(η^3-crotyl)Cl_2]	8
[IPr·H][Pd(Ind^{tBu})Cl_2]	n.r.
[IPent·H][Pd(η^3-cinnamyl)Cl_2]	n.r.

[a] The GC yield was determined using mesitylene as internal standard. Average of two runs.

Effect of the boron source. [IPr·H][Pd(η^3-cin)Cl_2] (0.5 mol%), K_2CO_3 (0.7 mmol) and a stirring bar were added to a screw-cap vial. Ethanol (1 mL) was then added. Afterwards, 4-chloroanisole (0.5 mmol) and the corresponding aryl boron source (0.55 mmol) were added through an ethanol solution (1 mL). The reaction was left to stir at 40 °C for 16 h. The GC yield was determined using mesitylene as internal standard.

Table S-2: Boron source effect

Entry	**Boron source (0.55 mmol)**	**GC yield (%)**	**GC yield (%)[a]**
1	Phenyl boronic acid	0	99
2	Potassium phenyltrifluoroborate	8	90
3	Aryl boronic pinacol ester	40	94

[a]An activation step of 1 h was used: [IPr·H][Pd(η^3-cin)Cl_2] and K_2CO_3 were stirred for 1 h in ethanol, before the substrates were added.

Solvent screening. The general procedure was followed using [IPr·H][Pd(η^3-cin)Cl_2] (0.5 mol%), phenylboronic acid (60.9 mg, 0.5 mmol), 4-chloroanisole (61 μL, 0.5 mmol) with K_2CO_3 (76 mg, 0.55 mmol) in the corresponding solvent (1 mL). The GC yield was determined using mesitylene as internal standard.

Table S-4: Solvent screening

Entries	**Solvent (1 mL)**	**GC yield (%)[b]**
1	Ethanol	92
2	*Iso*-propanol	45
3	*n*-butanol	53
4	Acetone	n.r.
5	Water	trace
6	Toluene	n.r.
7	Dioxane	n.r.
8	THF	n.r.
9	Methanol	5
10	Ethanol:water 1:1	35
11	Ethanol:water 2:1	55
12	Ethanol:water 9:1	73
13[a]	*Iso*-propanol	23
14[a]	*n*-butanol	trace
15[a]	Toluene	n.r.

[a]Temperature used in the activation step was altered to the boiling point of the corresponding solvents. [b] GC yield determined using mesitylene as internal standard. Average of two runs.

Base screening. The general procedure was followed using [IPr·H][Pd(η^3-cin)Cl_2] (0.5 mol%), phenyl boronic acid (60.9 mg, 0.5 mmol), 4-chloroanisole (61 μL, 0.5 mmol) with the corresponding base (0.55 mmol) in the corresponding solvent (1 mL). The GC yield was determined using mesitylene as internal standard.

Table S-5: Base screening in ethanol

Entries	**Base (0.55 mmol)**	**GC yield (%)[a]**
1	K_2CO_3	92
2	Na_2CO_3	5
3	Cs_2CO_3	27
4	$KHCO_3$	trace
5	$NaHCO_3$	trace
6	KOH	72
7	NaOH	80
8	LiOH	20
9	$NaHPO_4$	n.r.
10	K_2HPO_4	n.r.
11	K_3PO_4	40
12	KO^{t}Am	78
13	KO^{t}Bu	75
14	NaOOCH	n.r.
15	Imidazole	n.r.

[a] The GC yield was determined using mesitylene as internal standard. Average of two runs.

Table S-6: Base screening in *iso*-propanol

Entries	Base (1.1 equiv.)	GC yield (%)[a]
1	K_2CO_3	47
2	Na_2CO_3	0
3	Cs_2CO_3	0
4	$KHCO_3$	0
5	$NaHCO_3$	0
6	KOH	55
7	NaOH	60
8	LiOH	trace
9	$NaHPO_4$	0
10	K_2HPO_4	0
11	K_3PO_4	55
12	KO^{t}Am	70
13	KO^{t}Bu	72
14	NaOOCH	trace
15	Imidazole	trace

[a] The GC yield was determined using mesitylene as internal standard. Average of two runs.

Table S-7: Base screening in *n*-butanol

Entries	Base (1.1 equiv.)	GC yield (%)[a]
1	K_2CO_3	53
2	Na_2CO_3	n.r.
3	Cs_2CO_3	17
4	$KHCO_3$	trace
5	$NaHCO_3$	0
6	KOH	65
7	NaOH	80
8	LiOH	17
9	$NaHPO_4$	0
10	K_2HPO_4	0
11	K_3PO_4	trace

[a] The GC yield was determined using mesitylene as internal standard. Average of two runs.

Aryl boronic acid stoichiometry. The general procedure was followed using [IPr·H][Pd(η^3-cin)Cl_2] (0.5 mol%), phenyl boronic acid (varying equivalences), 4-chloroanisole (61 µL, 0.5 mmol) with K_2CO_3 (76 mg, 0.55 mmol) in the corresponding solvent (1 mL). The GC yield was determined using mesitylene as internal standard.

Table S-8: Aryl boronic acid optimisation

Entries	$PhB(OH)_2$ (equiv.)	GC yield (%)[a]
1	1.0	90
2	1.1	82
3	1.2	87
4	1.3	82
5	1.4	85

[a] The GC yield was determined using mesitylene as internal standard. Average of four runs.

Base stoichiometry. The general procedure was followed using [IPr·H][Pd(η^3-cin)Cl_2] (0.5 mol%), phenyl boronic acid (60.9 mg, 0.5 mmol), 4-chloroanisole (61 μL, 0.5 mmol) with K_2CO_3 (varying equivalences) in ethanol (1 mL). The GC yield was determined using mesitylene as internal standard.

Table S-9: Optimisation of base stoichiometry

Entries	K_2CO_3 (equiv.)	GC yield (%)[a]
1	1	93
2	1.1	95
3	1.2	93
4	1.3	97
5	1.4	99

[a] The GC yield was determined using mesitylene as internal standard. Average of four runs.

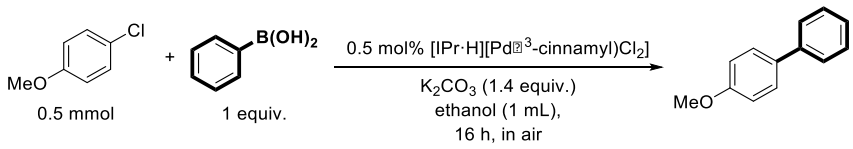
Pre-catalyst loading. The general procedure was followed using [IPr·H][Pd(η^3-cin)Cl_2] (0.1-0.5 mol%), phenyl boronic acid (60.9 mg, 0.5 mmol), 4-chloroanisole (61 μL, 0.5 mmol) with K_2CO_3 (97 mg,0.7 mmol) in ethanol (1 mL). The GC yield was determined using mesitylene as internal standard.

Table S-10: Optimisation of the precatalyst loading

Entries	[IPr·H][Pd(η^3-cin)Cl_2] (mol%)	GC yield (%)
1	0.5	99
2	0.3	99
3	0.2	70
4	0.1	31

[a] The GC yield was determined using mesitylene as internal standard. Average of four runs.

Time and temperature optimisation



The general procedure was followed and aliquots were taken and analysed by Gas chromatography.

Table S-11: Reaction time optimisation at room temperature

Time (min)	GC yield (%)
10	0
30	0
60	0
120	33
180	75
240	88
300	88
360	89
420	90

[a] The GC yield was determined using mesitylene as internal standard. Average of four runs.

Graph S-1: Kinetic profile at room temperature

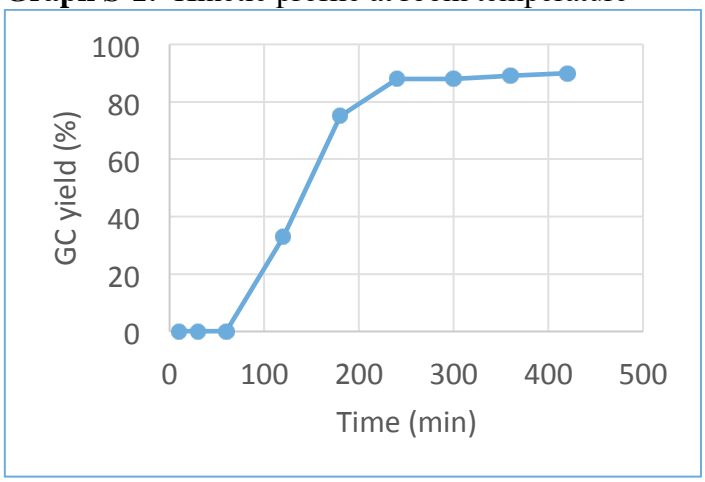


Table S-12: Reaction time optimisation at 40 °C

Time (min)	**GC yield (%)**
10	0
30	19
60	66
120	91
180	99
240	99
300	99

[a] The GC yield was determined using mesitylene as internal standard. Average of four runs.

Graph S-2: Reaction time optimisation at 40 °C.

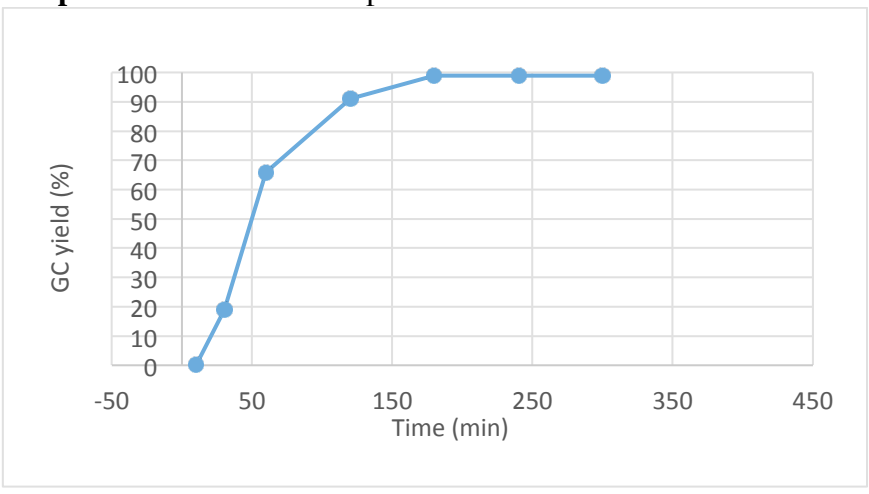
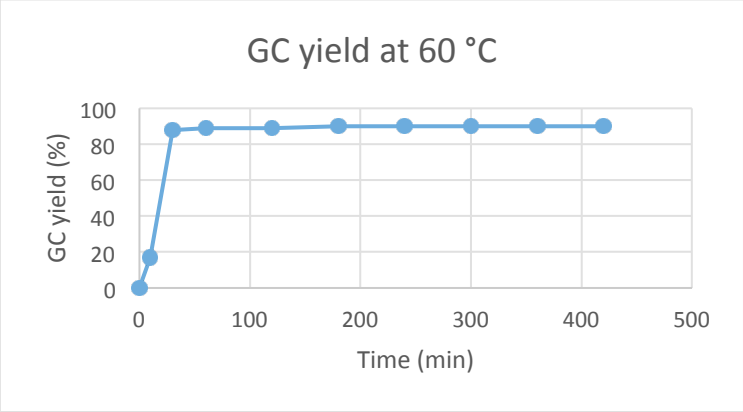


Table S-13: Reaction time optimisation at 60 °C

Time (min)	GC yield (%)
0	0
10	17
30	88
60	89
120	89
180	90
240	90
300	90
360	90
420	90

[a] The GC yield was determined using mesitylene as internal standard. Average of four runs.

Graph S-3: Reaction time optimisation at 60 °C.



Products of the Suzuki-Miyaura reaction (Scheme 6)

3a. Following the general procedure, from phenylboronic acid (60.9 mg, 0.5 mmol) and 4-chloroanisole (61 µL, 0.5 mmol), the product yielded 90 mg (97%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.57 (m, *J* = 8.1 Hz, 4H), 7.42 (m, *J* = 7.3 Hz, 2H), 7.31 (m, *J* = 7.5 Hz, 1H), 7.00 (t, *J* = 2.9 Hz, 1H), 6.98 (t, *J* = 2.1 Hz, 1H), 3.86 (s, 3H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 159.3 (C_{Ar}), 141.0 (C_{Ar}), 133.9 (C_{Ar}), 128.9 (CH_{Ar}), 128.3 (CH_{Ar}), 126.9 (CH_{Ar}), 126.8 (CH_{Ar}), 114.3 (CH_{Ar}), 55.5 (CH_3). Analytical data obtained were in agreement with the reported values.[1]

3b. Following the general procedure, from phenylboronic acid (60.9 mg, 0.5 mmol) and 1-chloro-4-trifluoromethyl benzene (70 µL, 0.5 mmol), the product yielded 105 mg (98%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.70 (s, 4H), 7.61-7.60 (m, 2H), 7.50-7.48 (m, 2H), 7.41 (m, 1H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 144.9 (C_{Ar}), 139.9 (C_{Ar}), 129.5 (q, *J* = 32.5 Hz, C_{Ar}-$_{CF3}$), 129.1 (CH_{Ar}), 128.3 (CH_{Ar}), 127.6 (CH_{Ar}), 127.4 (CH_{Ar}), 125.9 (q, *J* = 3.8 Hz, CH_{Ar}), 124.5(q, *J* = 271.8 Hz, CF_3). Analytical data obtained were in agreement with the reported values.[2]

3c. Following the general procedure, from *p*-tolylboronic acid (68 mg, 0.5 mmol) and 4-chloro-nitrobenzene (79 mg, 0.5 mmol), the product yielded 88.7 mg (89%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.30 (d, *J* = 8.5 Hz, 2H), 7.73 (d, *J* = 9.3 Hz, 2H), 7.54 (d, *J* = 9.3 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 2H), 2.43 (s, 3H). ^{13}C {^{1}H} NMR (100 MHz,

$CDCl_3$): δ (ppm) = 147.7 (C_{Ar}), 147.0 (C_{Ar}), 139.2 (C_{Ar}), 136.0 (C_{Ar}), 130.0 (CH_{Ar}), 127.6 (CH_{Ar}), 127.4 (CH_{Ar}), 124.3 (CH_{Ar}), 21.4 (CH_3). Analytical data obtained were in agreement with the reported values.[2]

3d. Following the general procedure, from *p*-tolylboronic acid (68 mg, 0.5 mmol) and 4-chloroacetophenone (64 μL, 0.5 mmol), the product yielded 100 mg (95%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.03 (d, *J* = 8.2 Hz, 2H), 7.69 (d, *J* = 8.6 Hz, 2H), 7.55 (d, *J* = 8.6 Hz, 2H), 7.29 (d, *J* = 8.6 Hz, 2H), 2.64 (s, 3H), 2.41 (s, 3H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 197.9 (COMe), 145.9 (C_{Ar}), 138.4 (C_{Ar}), 137.1 (C_{Ar}), 135.7 (C_{Ar}), 129.8 (CH_{Ar}), 129.1 (CH_{Ar}), 127.2 (CH_{Ar}), 127.1 (CH_{Ar}), 26.8 (CH_3), 21.3 (CH_3). Analytical data obtained were in agreement with the reported values.[3]

3e. Following the general procedure, from phenylboronic acid (61 mg, 0.5 mmol) and 4-chlorobenzonitrile (69 mL, 0.5 mmol), the product yielded 80.7 mg (89%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.75-7.67 (m, 4H), 7.61-7.58 (m, 2H), 7.52-7.46 (m, 2H), 7.45-7.42 (dt, *J* = 5.2, 2.1 Hz, 2H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 145.8 (C_{Ar}), 139.3 (C_{Ar}), 132.7 (CH_{Ar}), 129.3 (CH_{Ar}), 128.8 (CH_{Ar}), 127.9 (CH_{Ar}), 127.4 (CH_{Ar}), 119.1 (CN), 111.1 (C_{Ar}-$_{CN}$). Analytical data obtained were in agreement with the reported values.[2]

3f. Following the general procedure, from *p*-tolyl boronic acid (68 mg, 0.5 mmol) and 2-chloroanisole (61 μL, 0.5 mmol), the product yielded 88.4 mg (89%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.49 (d, *J* = 8.7 Hz, 2H), 7.35 (t, *J* = 7.1 Hz, 2H), 7.29 (d, *J* = 8.6 Hz, 2H), 7.09-7.01 (m, 2H), 3.85 (s, 3H), 2.44 (s, 3H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 156.6 (C_{Ar}), 136.7 (C_{Ar}), 135.7 (C_{Ar}), 130.9 (CH_{Ar}), 130.8 (C_{Ar}), 129.5 (CH_{Ar}), 128.9 (CH_{Ar}), 128.5 (CH_{Ar}), 120.9 (CH_{Ar}), 111.3 (CH_{Ar}), 55.6 (CH_3), 21.3 (CH_3). Analytical data obtained were in agreement with the reported values.[3]

3g. Following the general procedure, from phenylboronic acid (61 mg, 0.5 mmol) and 2-chloroaniline (64 mg, 0.5 mmol), the product yielded 68 mg (80%) as a brown solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.27 (d, *J* = 7.1 Hz, 1H), 7.59-7.36 (m, 4H), 7.23-7.04 (m, 2H), 6.86-6.67 (m, 2H), 4.02 (m, 2H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 143.6 (C_{Ar}), 139.6 (C_{Ar}), 135.8 (CH_{Ar}), 132.8 (CH_{Ar}), 130.6 (CH_{Ar}), 129.2 (CH_{Ar}), 128.9 (CH_{Ar}), 128.6 (CH_{Ar}), 128.1 (CH_{Ar}), 127.8 (C_{Ar}), 127.3 (CH_{Ar}), 118.8 (CH_{Ar}), 115.8 (CH_{Ar}). Analytical data obtained were in agreement with the reported values.[3]

3h. Following the general procedure, from 2-tolylboronic acid (68 mg, 0.5 mmol) and 2-chlorotoluene (67 μL, 0.5 mmol), the product yielded 82.5 mg (90%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.28-7.22 (m, 6H), 7.13 (d, *J* = 7.2 Hz, 2H), 2.07 (s, 6H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 141.7 (C_{Ar}), 135.9 (C_{Ar}), 129.9 (CH_{Ar}), 129.4 (CH_{Ar}), 127.3 (CH_{Ar}), 125.7 (CH_{Ar}), 20.0 (CH_3). Analytical data obtained were in agreement with the reported values.[1]

3i. Following the general procedure, from 2-tolylboronic acid (68 mg, 0.5 mmol) and 2-chloroanisole (61 μL, 0.5 mmol), the product yielded 96.7 mg (97%) as a yellowish/white oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.41-7.35 (m, 1H), 7.29-7.18 (m, 5H), 7.08-6.99 (m, 2H), 3.80 (s, 3H), 2.19 (s, 3H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 156.7 (C_{Ar}), 138.8 (C_{Ar}), 137.0 (C_{Ar}), 131.1 (CH_{Ar}), 131.0 (C_{Ar}), 130.1 (CH_{Ar}), 129.7 (CH_{Ar}), 128.7 (CH_{Ar}), 127.4 (CH_{Ar}), 125.6 (CH_{Ar}), 120.6 (CH_{Ar}), 110.8 (CH_{Ar}), 55.5 (CH_3), 20.1 (CH_3). Analytical data obtained were in agreement with the reported values.[5]

3j. Following the general procedure, from phenylboronic acid (61 mg, 0.5 mmol) and 2-chloro-6-trifluoromethyl pyridine (91 mg, 0.5 mmol), the product yielded 112 mg (99%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.09-8.06 (m, 2H), 7.92-7.91 (m, 2H),

7.62-7.60 (m, 1H), 7.52 – 7.46 (m, 3H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 157.9 (C_{Ar}), 148.5 (q, J = 34.5 Hz, C_{Py}-CF_3), 138.2 (CH_{Ar}), 137.9 (C_{Ar}), 129.9 (CH_{Ar}), 129.0 (CH_{Ar}), 127.3 (CH_{Ar}), 122.9 (CH_{Ar}), 121.7 (q, J = 274.3 Hz, CF_3), 118.6 (d, J = 2.7 Hz, CH_{Ar}). Analytical data obtained were in agreement with the reported values.[6]

3k. Following the general procedure, from phenylboronic acid (61 mg, 0.5 mmol) and 2-chloropyridine (68 μL, 0.5 mmol), the product yielded 69 mg (90%) as a brown solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.71 (m, J = 4.5 Hz, 1H), 8.01 (m, 2H), 7.77 (m, 2H), 7.50 (m, 2H), 7.45 (m, 1H), 7.25 (m, 1H) ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 158.0 (C_{Ar}), 148.5 (C_{Ar}), 148.1 (CH_{Ar}), 138.2 (CH_{Ar}), 137.9 (CH_{Ar}), 129.9 (CH_{Ar}), 129.1 (CH_{Ar}), 127.3 (CH_{Ar}), 123.0 (CH_{Ar}), 120.4 (CH_{Ar}), 118.6 (CH_{Ar}). Analytical data obtained were in agreement with the reported values.[1]

3l. Following the general procedure, from 4-methoxyphenylboronic acid (79 mg, 0.5 mmol) and 4-chlorotoluene (67 μL, 0.5 mmol), the product yielded 84 mg (85%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.53-7.50 (m, 2H), 7.49-7.44 (m, 2H), 7.24 (d, J = 8.5 Hz, 2H), 6.98-6.96 (m, 2H), 3.85 (s, 3H), 2.39 (s, 3H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 159.1 (C_{Ar}), 138.1 (C_{Ar}), 136.5 (CH_{Ar}), 133.9 (C_{Ar}), 129.6 (CH_{Ar}), 128.1 (CH_{Ar}), 127.9 (C_{Ar}), 126.7 (CH_{Ar}), 114.3 (CH_{Ar}), 55.5 (CH_3), 21.2 (CH_3). Analytical data obtained were in agreement with the reported values.[7]

3m. Following the general procedure, from 4-methoxy phenylboronic acid (76 mg, 0.5 mmol) and 4-chloro-nitrobenzene (79 mg, 0.5 mmol), the product yielded 105 mg (91 %) as a beige solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.82 (d, J = 7.8 Hz, 2H), 7.71 (d, J = 8.9 Hz, 2H), 7.60 (d, J = 6.9 Hz, 2H), 7.03 (d, J = 9.7 Hz, 2H), 3.88 (s, 3H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 160.6 (C_{Ar}), 147.4 (C_{Ar}), 146.7 (C_{Ar}), 131.2 (C_{Ar}), 128.7 (CH_{Ar}), 127.2 (CH_{Ar}), 124.3 (CH_{Ar}), 114.8 (CH_{Ar}), 55.6 (CH_3). Analytical data obtained were in agreement with the reported values.[8]

3n. Following the general procedure, from 4-acetylphenyl boronic acid (82 mg, 0.5 mmol) and 4-chloro-nitrobenzene (79 mg, 0.5 mmol), the product yielded 103 mg (86 %) as a beige solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.32 (d, J = 10.8 Hz, 2H), 8.09 (d, J = 8.1 Hz, 2H), 7.78 (d, J = 9.1 Hz, 2H), 7.73 (d, J = 9.1 Hz, 2H), 2.56 (s, 3H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 197.6 (COMe), 147.7 (C_{Ar}), 146.3 (C_{Ar}), 143.2 (C_{Ar}), 137.2 (C_{Ar}), 129.2 (CH_{Ar}), 128.2 (CH_{Ar}), 127.7 (CH_{Ar}), 124.3 (CH_{Ar}), 26.8 (CH_3). Analytical data obtained were in agreement with the reported values.[8]

3o. Following the general procedure, from 4-formylboronic acid (75 mg, 0.5 mmol) and 2-chloropyridine (68 μL, 0.5 mmol), the product yielded 65 mg (70%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 10.09 (s, 1H), 8.75 (d, J = 4.8 Hz, 1H), 8.19 (d, J = 8.7 Hz, 2H), 8.00 (d, J = 8.7 Hz, 2H), 7.82-7.81 (m, 2H), 7.33 (q, J = 4.6 Hz, 1H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 192.1 (CH_{CHO}), 156.0 (C_{Ar}), 150.1 (CH_{Ar}), 145.0 (C_{Ar}), 137.2 (CH_{Ar}), 136.5 (C_{Ar}), 130.5 (CH_{Ar}), 130.3 (CH_{Ar}), 128.1 (CH_{Ar}), 127.6 (CH_{Ar}), 123.3 (CH_{Ar}), 121.4 (CH_{Ar}). Analytical data obtained were in agreement with the reported values.[9]

3p. Following the general procedure, from 1-naphthalene boronic acid (86 mg, 0.5 mmol) and 2-bromopyrimidine (79.5 mL, 0.5 mmol), the product yielded 102.3 mg (99%) as a brown oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 9.31 (s, 1H), 8.90 (s, 2H), 7.98-7.95 (m, 2H), 7.77 (d, J = 8.9 Hz, 1H), 7.61-7.42 (m, 4H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 157.7 (C_{Ar}), 157.4 (C_{Ar}), 134.5 (C_{Ar}), 133.9 (C_{Ar}), 132.5 (CH_{Ar}), 131.3 (CH_{Ar}), 129.5 (CH_{Ar}), 128.8 (CH_{Ar}), 127.8 (CH_{Ar}), 127.2 (CH_{Ar}), 126.5 (CH_{Ar}), 125.5 (CH_{Ar}), 124.6 (CH_{Ar}). Analytical data obtained were in agreement with the reported values.[9]

3q. Following the general procedure, from 1-naphthalene boronic acid (86 mg, 0.5 mmol) and 2-chloropyridine (68 μL, 0.5 mmol), the product yielded 101.9 mg (99%) as a beige oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 8.80 (m, *J* = 4.9, 1.8, 0.9 Hz, 1H), 8.12-8.05 (m, 1H), 7.95-7.89 (m, 2H), 7.84 (m, *J* = 7.7, 1.8 Hz, 1H), 7.63-7.57 (m, 3H), 7.49 (m, *J* = 6.8, 5.4 Hz, 3H), 7.34 (m, *J* = 7.6, 4.9, 1.2 Hz, 1H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 159.4 (C_{Ar}), 149.6 (CH_{Ar}), 138.6 (C_{Ar}), 136.5 (CH_{Ar}), 134.0 (C_{Ar}), 131.3 (C_{Ar}), 129.0 (CH_{Ar}), 128.5 (CH_{Ar}), 127.6 (CH_{Ar}), 126.6 (CH_{Ar}), 125.9 (CH_{Ar}), 125.7 (CH_{Ar}), 125.4 (CH_{Ar}), 125.2 (CH_{Ar}), 122.2 (CH_{Ar}). Analytical data obtained were in agreement with the reported values.[10]

3r. Following the general procedure, from 1-naphthalene boronic acid (86 mg, 0.5 mmol) 2-chloronaphthalene (81.3 mL, 0.5 mmol), the product yielded 126 mg (99%) as a brown oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.96 (dd, *J* = 8.1, 2.6 Hz, 4H), 7.62 (t, *J* = 7.7 Hz, 2H), 7.51-7.45 (m, 4H), 7.41-7.38 (m, 2H), 7.31-7.29 (m, 2H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 138.6 (C_{Ar}), 133.6 (C_{Ar}), 133.0 (C_{Ar}), 128.3 (CH_{Ar}), 128.0 (CH_{Ar}), 128.0 (CH_{Ar}), 126.7 (CH_{Ar}), 126.1 (CH_{Ar}), 125.9 (CH_{Ar}), 125.5 (CH_{Ar}). Analytical data obtained were in agreement with the reported values.[11]

3s. Following the general procedure, from 1-naphthalene boronic acid (86 mg, 0.5 mmol) and 1-chloro-2-,4 difluorobenzene (74.3 mg, 0.5 mmol), the product yielded 95.8 mg (80%) as a brown solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.93 (d, *J* = 8.6 Hz, 2H), 7.64-7.34 (m, 6H), 7.05-6.96 (m, 2H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 162.7 (dd, *J* = 253.0, 11.8 Hz, C_{Ar}-F), 160.3 (dd, *J* = 253.4, 11.7 Hz, C_{Ar}-F), 133.7 (C_{Ar}), 133.2-133.1 (m, C_{Ar} + CH_{Ar}), 132.0 (C_{Ar}), 128.7 (CH_{Ar}), 128.5 (CH_{Ar}), 128.0 (CH_{Ar}), 126.5 (CH_{Ar}), 126.1 (CH_{Ar}), 125.7 (CH_{Ar}), 125.4 (CH_{Ar}), 124.2 (dd, *J* = 16.7, 3.8 Hz, C_{Ar}), 111.5 (dd, *J* = 21.0, 3.7 Hz, CH_{Ar}), 104.2 (t, *J* = 25.8 Hz, CH_{Ar}).Analytical data obtained were in agreement with the reported values.[12]

3t. Following the general procedure, from (*E*)-styrylboronic acid (74 mg, 0.5 mmol) and 1-chloronaphthalene (82 mg, 0.5 mmol), the product yielded 80 mg (69 %) as a beige solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.92-7.75 (m, 2H), 7.61-7.15 (m, 10H), 6.99-6.96 (m, 1H), 6.69-6.66 (m, 1H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 137.8 (C_{Ar}), 137.5 (CH_{Ar}), 135.2 (C_{Ar}), 133.9 (C_{Ar}), 133.0 (CH_{Ar}), 131.9 (CH_{Ar}), 131.5 (C_{Ar}), 129.4 (CH_{Ar}), 128.9 (CH_{Ar}), 128.8 (CH_{Ar}), 127.7 (CH_{Ar}), 126.8 (CH_{Ar}), 126.5 (CH_{Ar}), 126.2 (CH_{Ar}), 126.0 (CH_{Ar}), 125.8 (CH_{Ar}), 123.9 (CH_{Alkene}), 123.8 (CH_{Alkene}). Analytical data obtained were in agreement with the reported values.[7]

3u. Following the general procedure, from (*E*)-styrylboronic acid (74 mg, 0.5 mmol) and 4-chlorobenzonitrile (69 mg, 0.5 mmol), the product yielded 76 mg (74 %) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.65-7.63 (m, 2H), 7.60-7.58 (m, 2H), 7.55-7.53 (m, 2H), 7.41-7.37 (m, 2H), 7.34-7.30 (t, *J* = 7.27 Hz, 1H), 7.22 (d, *J* = 16.3 Hz, 1H), 7.09 (d, *J* = 16.3 Hz, 1H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 142.0 (C_{Ar}), 136.4 (C_{Ar}), 132.6 (CH_{Ar}), 132.5 (CH_{Ar}), 129.0 (CH_{Ar}), 128.8 (CH_{Ar}), 127.1 (CH_{Alkene}), 127.0 (CH_{Alkene}), 126.9 (CH_{Ar}), 119.2 (CN), 110.7 (C_{Ar}-CN). Analytical data obtained were in agreement with the reported values.[13]

3v. Following the general procedure, from (E)-styrylboronic acid (74 mg, 0.5 mmol) and 4-chlorobenzaldehyde (70 mg, 0.5 mmol), the product yielded 100.5 mg (96 %) as a beige solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 10.00 (s, 1H), 7.89 (d, *J* = 8.7 Hz, 2H), 7.67 (d, *J* = 8.1 Hz, 2H), 7.56 (d, *J* = 8.1 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.34 (m, 1H), 7.29 (d, *J* = 4.9 Hz, 1H), 7.15 (d, *J* = 16.3 Hz, 1H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 191.8 (CHO), 143.5 (C_{Ar}), 136.7 (C_{Ar}), 135.4 (C_{Ar}), 132.2 (CH_{Ar}), 130.4 (CH_{Ar}), 129.0 (CH_{Ar}), 128.6 (CH_{Ar}), 127.5 (CH_{Ar}), 127.0 (CH_{Alkene}). Analytical data obtained were in agreement with the reported values.[14]

4a. Following the general procedure, from 4-fluorobenzene boronic acid (70 mg, 0.5 mmol) and 2-bromoanisole (61 μL, 0.5 mmol), the product yielded 90 mg (89 %).^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.40-7.36 (m, 2H, Ar-H), 7.16-7.21 (m, 2H, Ar-H), 6.97-7.10 (m, 2H, Ar-H), 6.85-6.95 (m, 2H, Ar-H), 3.68 (s, 3H, OCH_3). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm) = 156.3, 131.1, 131.0, 130.7, 129.6, 128.4, 120.8, 114.9, 114.7, 111.2, 55.4. Analytical data obtained were in agreement with the reported values.[15]

4b. Following the general procedure, from 4-acetylphenyl boronic acid (82 mg, 0.5 mmol) and 2-bromoanisole (61 μL, 0.5 mmol), the product yielded 86 mg (76 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.92 (d, *J* = 7.6 Hz 1H, Ar-H), 7.55 (d, *J* = 8.0 Hz 1H, Ar-H), 7.24 – 7.32 (m, 2H, Ar-H), 6.97 (t, *J* = 7.6 Hz 1H, Ar-H), 6.93 (d, *J* = 8.4 Hz, 1H, Ar-H), 3.73 (s, 3H, OCH_3), 2.55 (s, 3H, $COCH_3$), ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm) = 197.9, 156.4, 143.6, 135.5, 130.7, 129.7, 128.0, 120.9, 111.3, 55.5, 26.6. Analytical data obtained were in agreement with the reported values.[16]

4c. Following the general procedure, from 4-fluorobenzene boronic acid (70 mg, 0.5 mmol) and 3-bromoanisole (61 μL, 0.5 mmol), the product yielded 87 mg (86 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.43 – 7.48 (m, 2H, Ar-H), 7.24 – 7.29 (m, 1H, Ar-H), 6.98 – 7.06 (m, 4H, Ar-H), 6.80 – 6.83 (m, 1H, Ar-H), 3.77 (s, 3H, OCH_3), ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm) = 159.9, 141.7, 137.2, 129.8, 128.7, 119.5, 115.7, 115.4, 112.8, 112.5, 55.3. Analytical data obtained were in agreement with the reported values.[17]

4d. Following the general procedure, from 4-acetylphenyl boronic acid (82 mg, 0.5 mmol) and 3-bromoanisole (61 μL, 0.5 mmol), the product yielded 91 mg (81 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.04 (d, *J* = 8.4 Hz 2H, Ar-H), 7.69 (d, *J* = 8.4 Hz 2H, Ar-H), 7.40 (t, *J* = 7.6 Hz, 1H, Ar-H), 7.40 (t, *J* = 7.6 Hz, 1H, Ar-H), 7.23 (d, *J* = 7.2 Hz, 1H, Ar-H), 7.16 (s, 1H, Ar-H), 6.98-6.96 (dd, *J* = 2.8, 8.0 Hz, 1H, Ar-H), 3.89 (s, 3H, OCH_3), 2.65 (s, 3H, $COCH_3$), ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm) = 196.7, 158.9, 144.5, 140.3, 134.9, 128.9, 127.8, 126.2, 118.7, 112.5, 112.0, 54.3, 25.6. Analytical data obtained were in agreement with the reported values.[16]

4e. Following the general procedure, from 4-(trifluoromethyl)phenylboronic acid (95 mg, 0.5 mmol) and 3-bromoanisole (61 μL, 0.5 mmol), the product yielded 102 mg (81 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.59 – 7.60 (m, 4H, Ar-H), 7.30 (t, *J* = 8.0 Hz, 1H, Ar-H), 7.03 – 7.10 (m, 2H, Ar-H), 6.87 - 6.85 (dd, *J* = 3.6, 8.0 Hz, 1H, Ar-H), 3.78 (s, 3H, OCH_3), ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ (ppm) = 160.1, 144.6, 141.2, 127.6, 127.3, 125.8, 125.6, 122.9, 119.6, 113.3, 55.2. Analytical data obtained were in agreement with the reported values.[18]

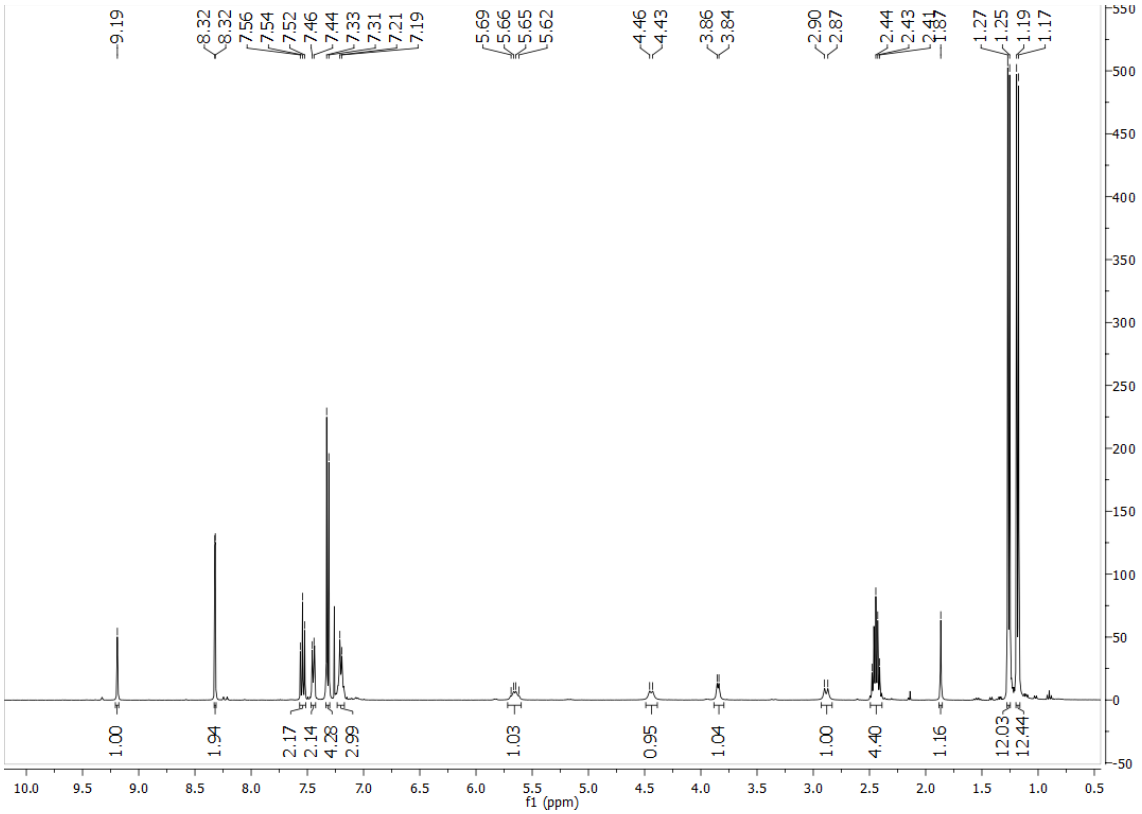
4f. Following the general procedure, from 4-(methoxy)phenylboronic acid (95 mg, 0.5 mmol) and 3-bromoanisole (61 μL, 0.5 mmol), the product yielded 93 mg (87 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.60 (d, J = 8.8 Hz, 2H, Ar-H), 7.55 (d, *J* = 8.8 Hz, 1H, Ar-H), 7.40 (t, *J* = 7.6 Hz, 1H, Ar-H), 7.17 – 7.24 (m, 2H, Ar-H), 7.17 –7.24 (m, 2H, Ar-H), 7.02 – 7.07 (m, 2H, Ar-H), 6.93 (s, 3H, OCH_3), 3.91 (s, 3H, OCH3). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 158.9, 159.2, 158.6, 142.3, 133.4, 128.1, 126.7, 119.1, 114.2, 112.1, 55.2. Analytical data obtained were in agreement with the reported values.[18]

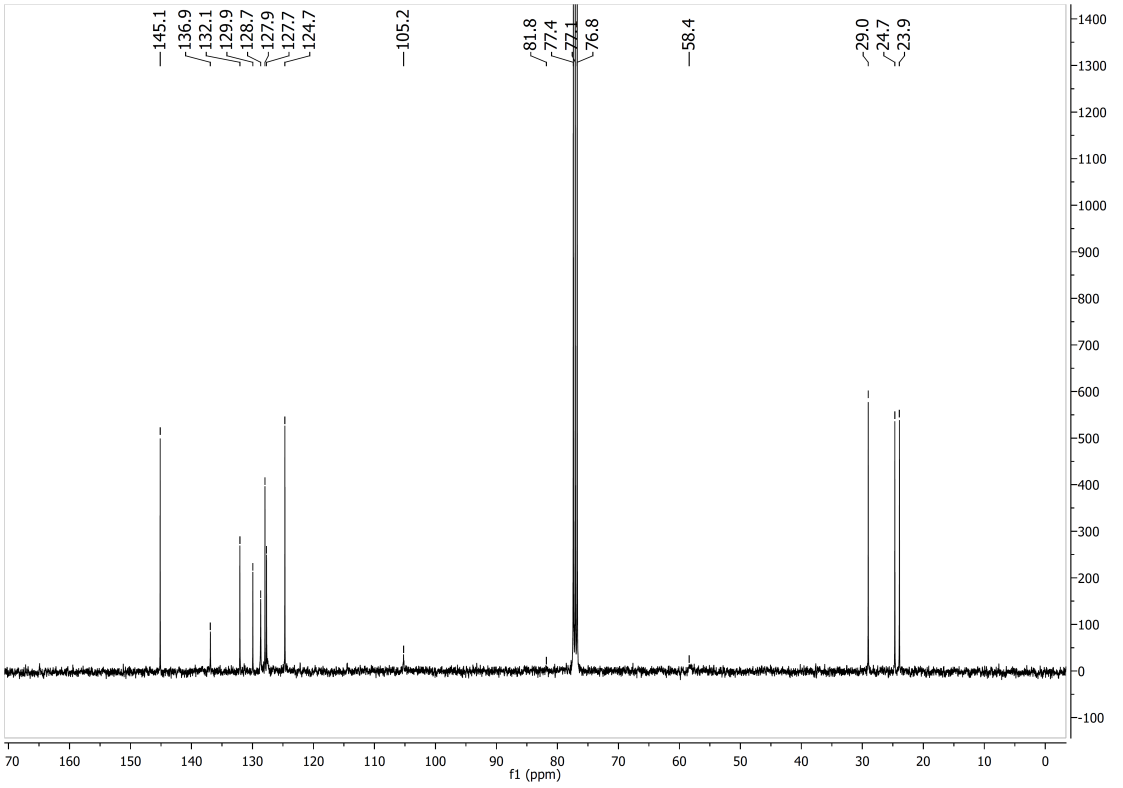
4g. Following the general procedure, from phenylboronic acid (60 mg, 0.5 mmol) and 4-bromoanisole (61 μL, 0.5 mmol), the product yielded 74 mg (85 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.46 (t, *J* = 8.8 Hz, 4H, Ar-H), 7.46 (t, *J* = 8.8 Hz, 4H, Ar-H), 7.34 (t, *J* = 8.0 Hz, 2H, Ar-H), 7.22 (t, *J* = 7.2 Hz, 1H, Ar-H), 6.90 (d, *J* = 6.8 Hz, 2H, Ar-H), 3.77 (s, 3H, OCH_3). Analytical data obtained were in agreement with the reported values.[19]

4h. Following the general procedure, from 4-acetylphenylboronic acid (82 mg, 0.5 mmol) and 2-bromopyridine (79 mg, 0.5 mmol), the product yielded 65 mg (66 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.61 – 8.62 (m, 1H, Ar-H), 7.96 – 7.97 (m, 5H, Ar-H), 7.16 – 7.20 (m, 1H, Ar-H), 2.53 (s, 3H, OCH_3). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 197.7, 155.8, 149.7, 149.6, 143.3, 136.9, 128.7, 128.6, 126.9, 126.8, 122.8, 121.0, 26.6. Analytical data obtained were in agreement with the reported values[20]

NMR spectra of complexes (^{1}H and ^{13}C {^{1}H}, $CDCl_3$)

[IPr·H][Pd(□^{3}-cin)Cl_2] 2a





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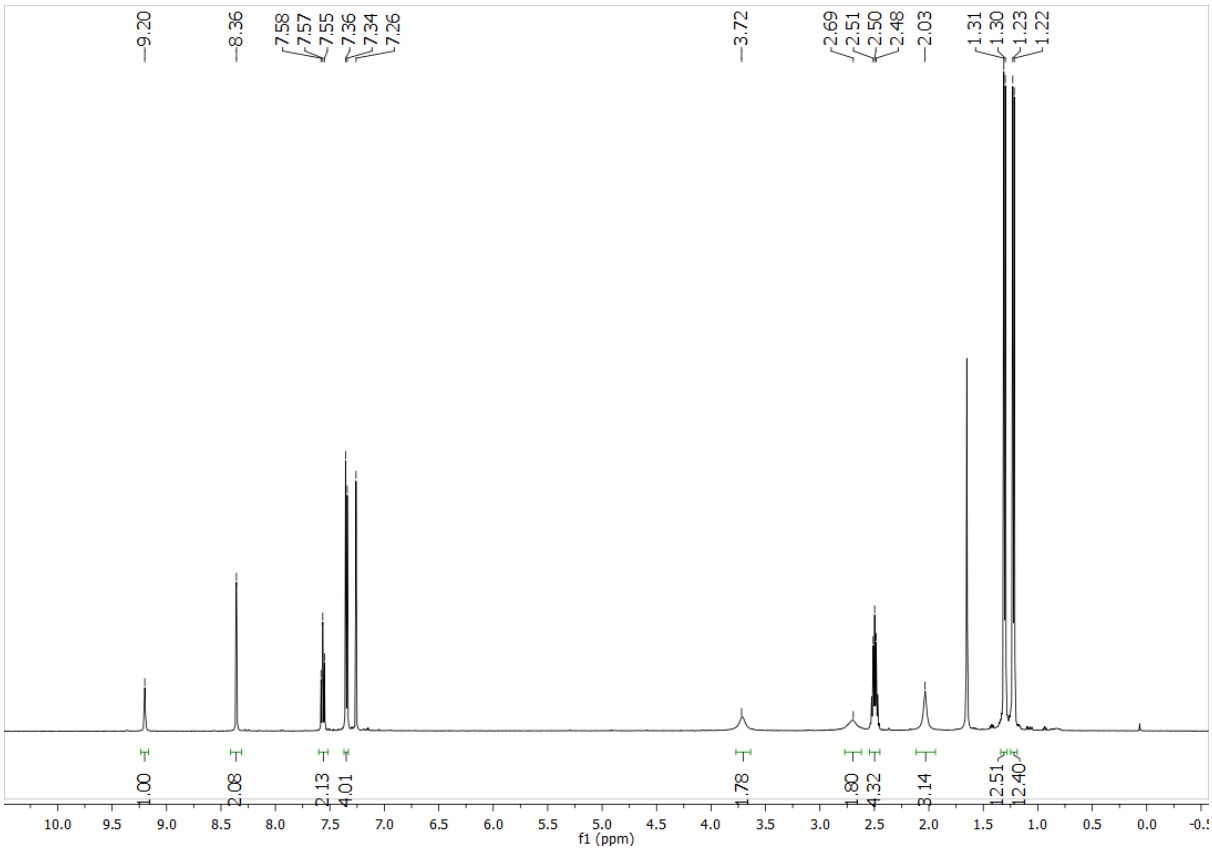

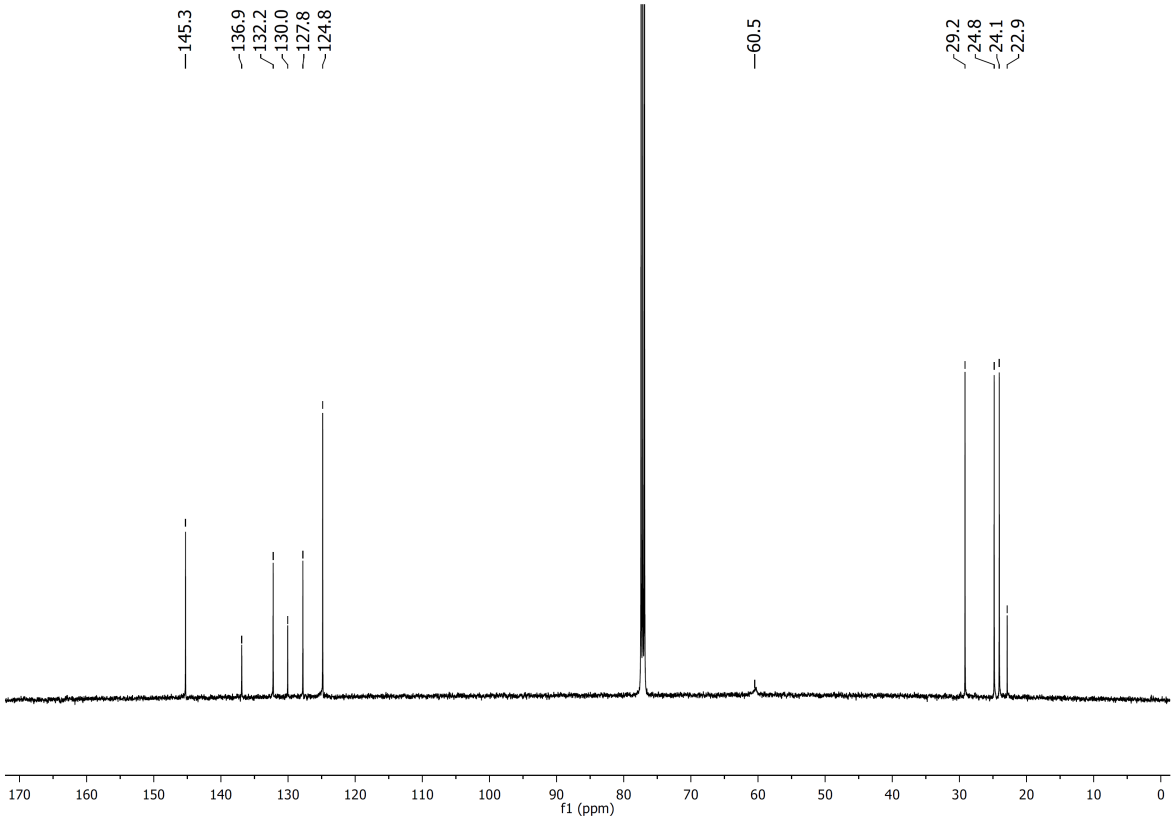

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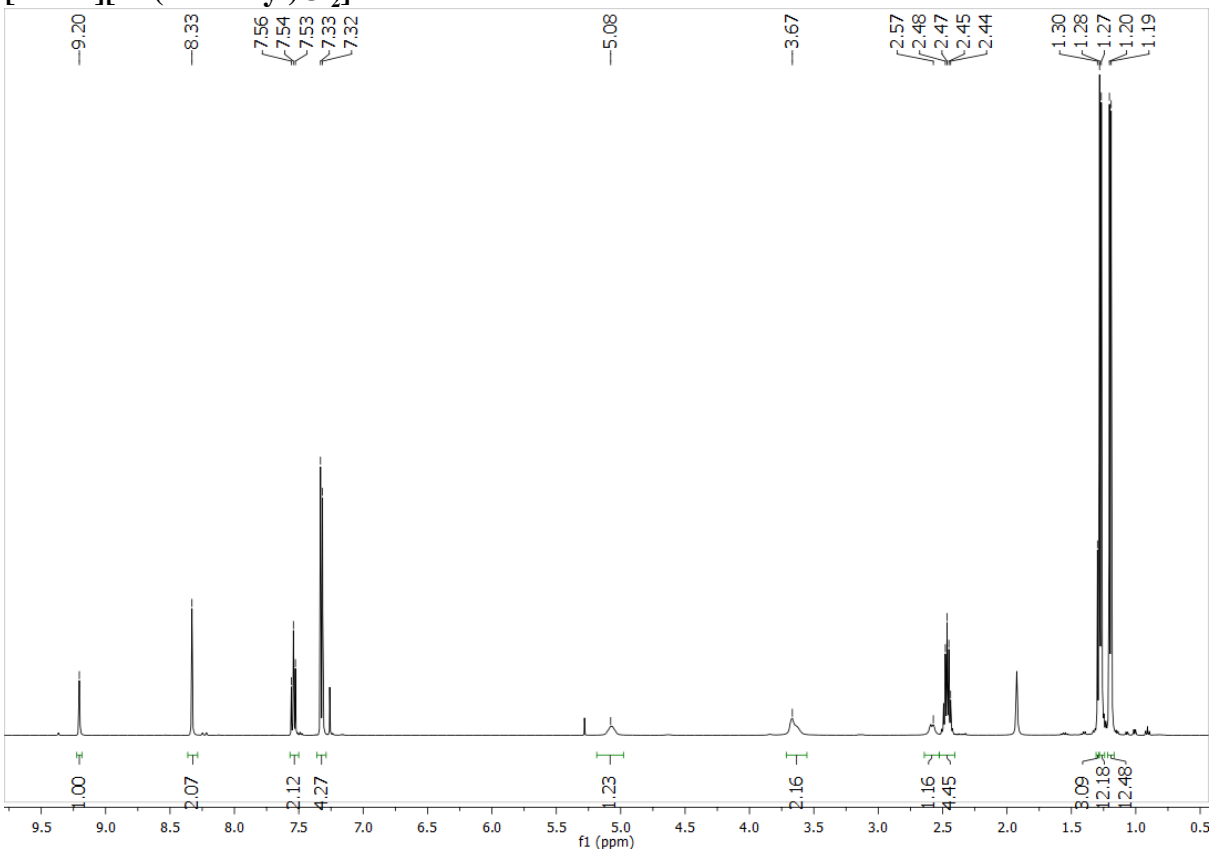
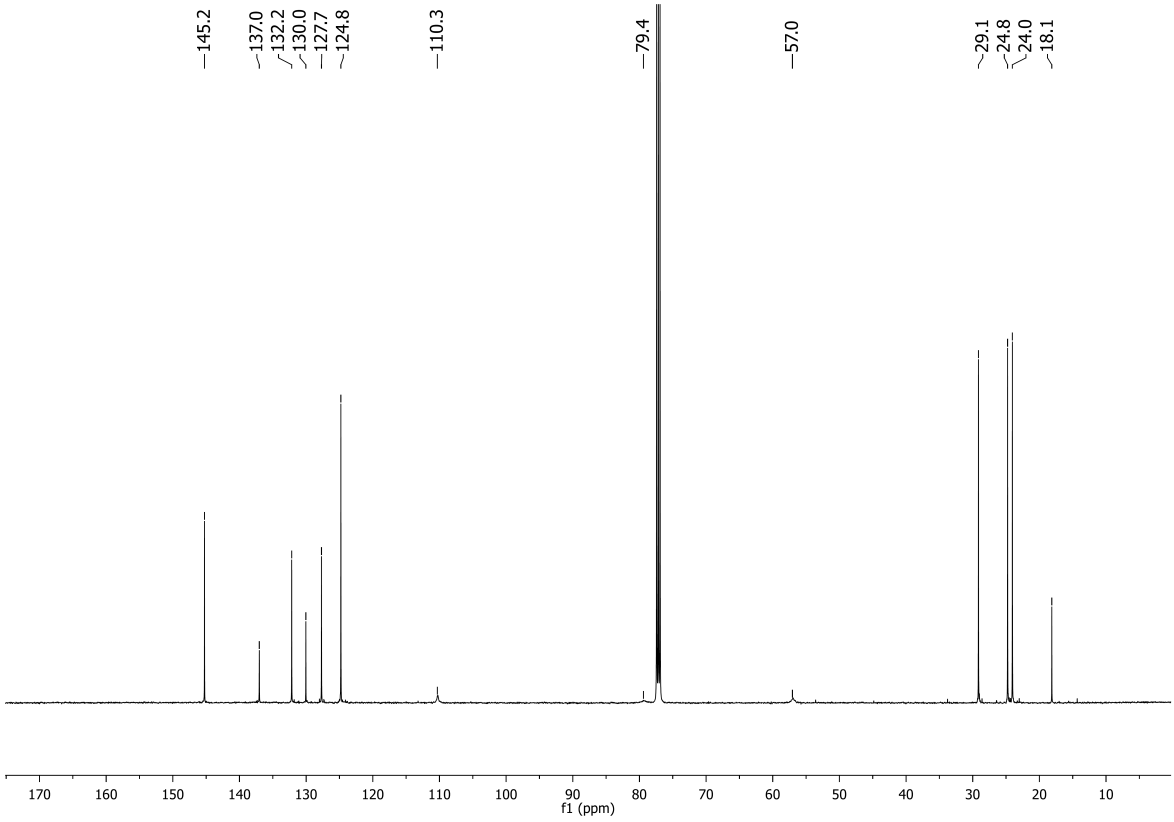
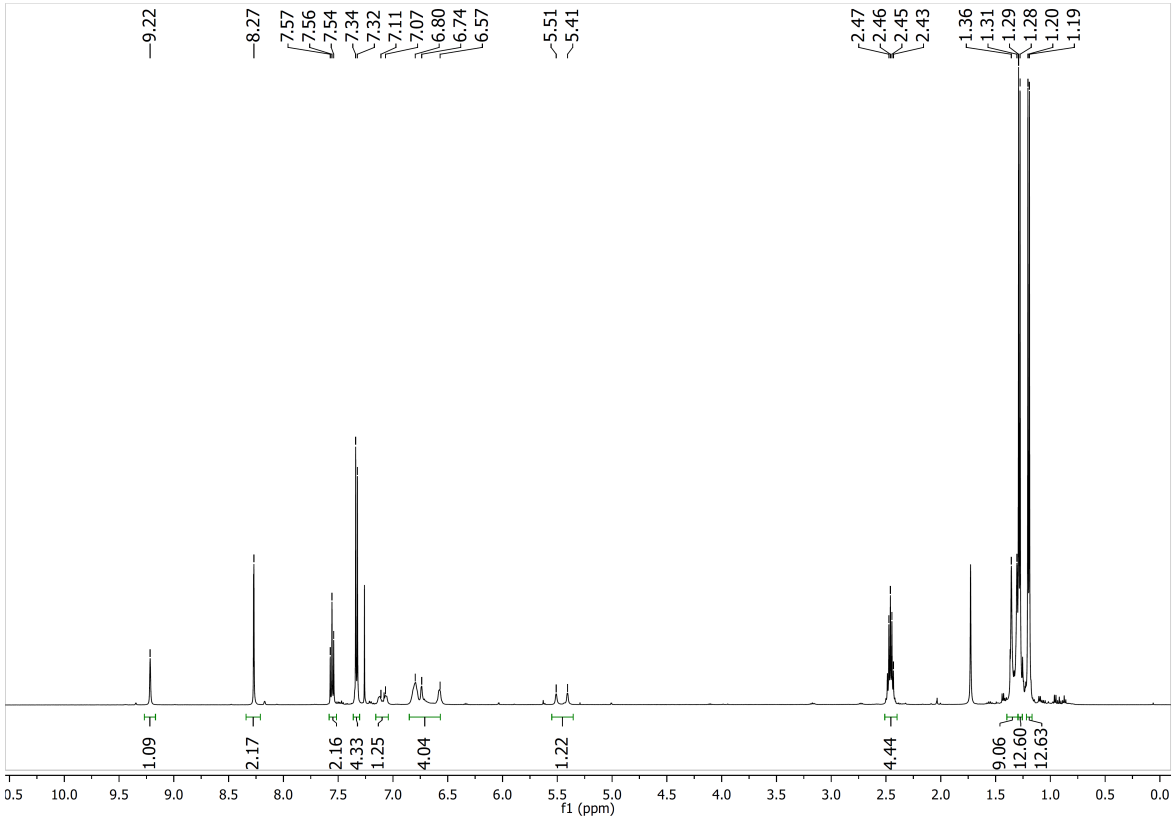
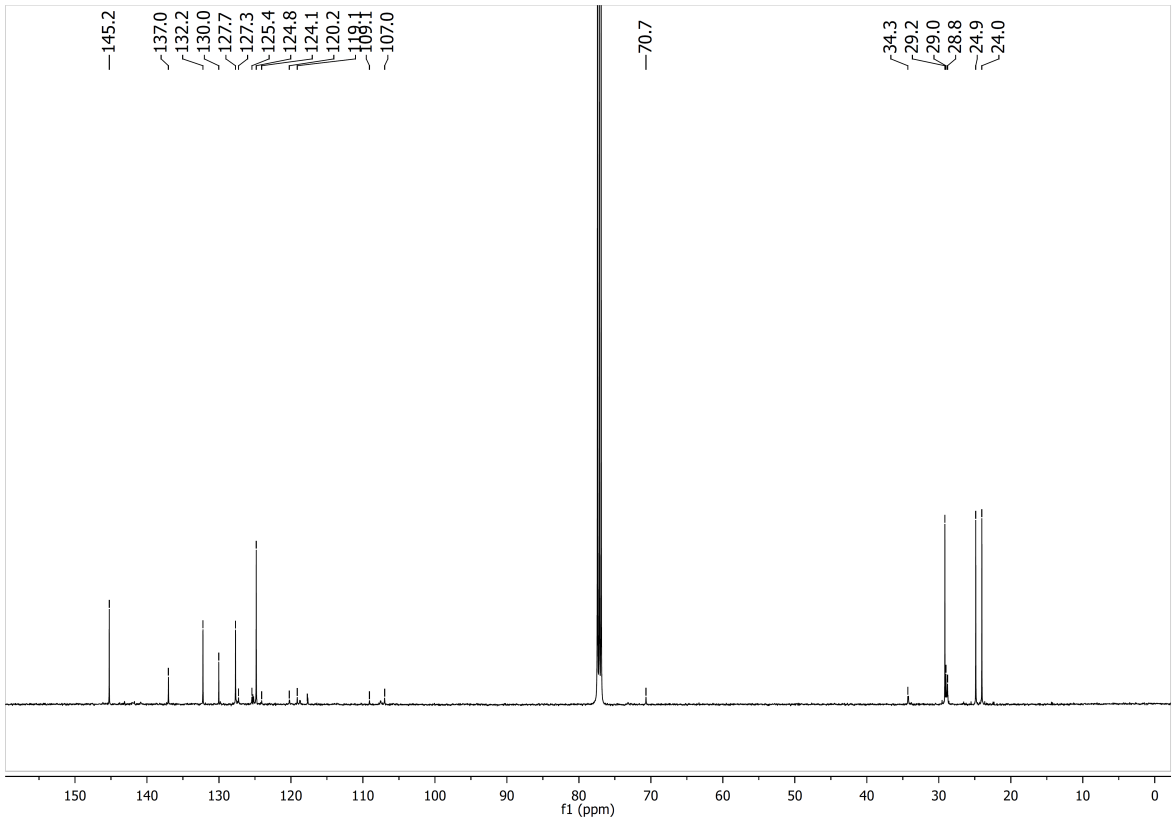


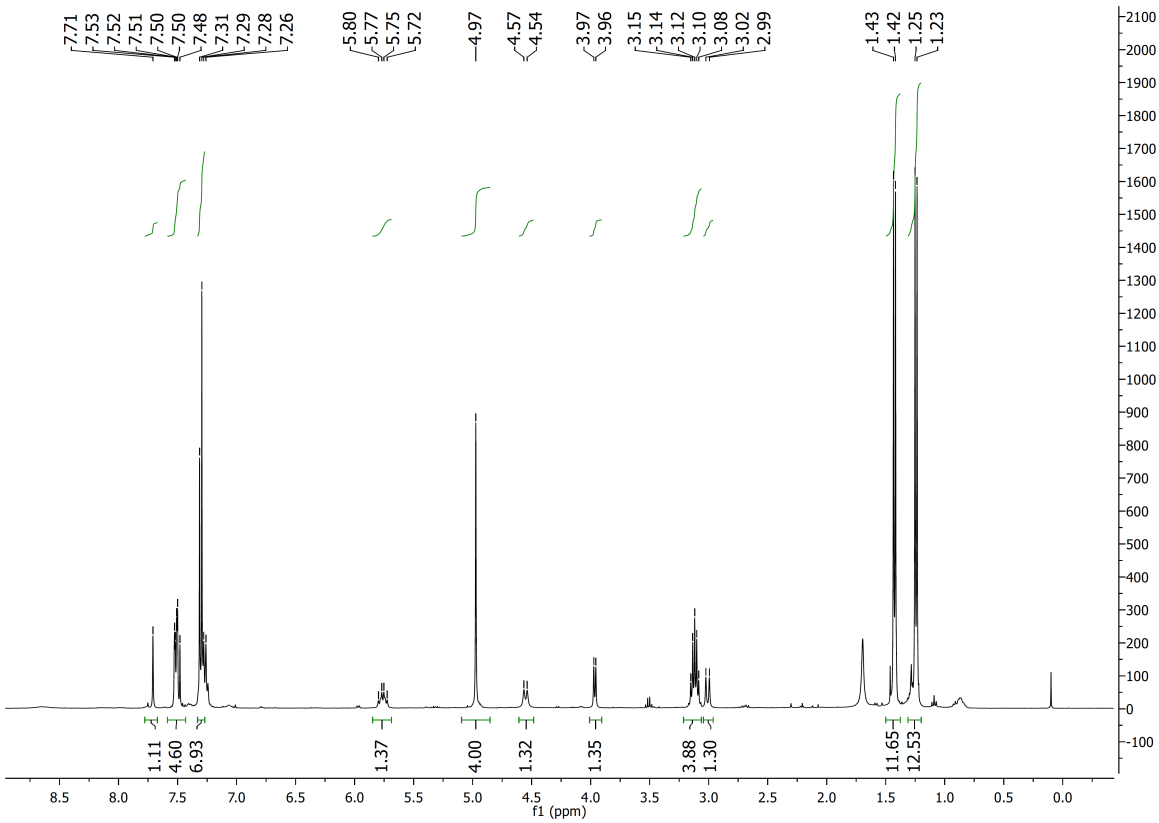


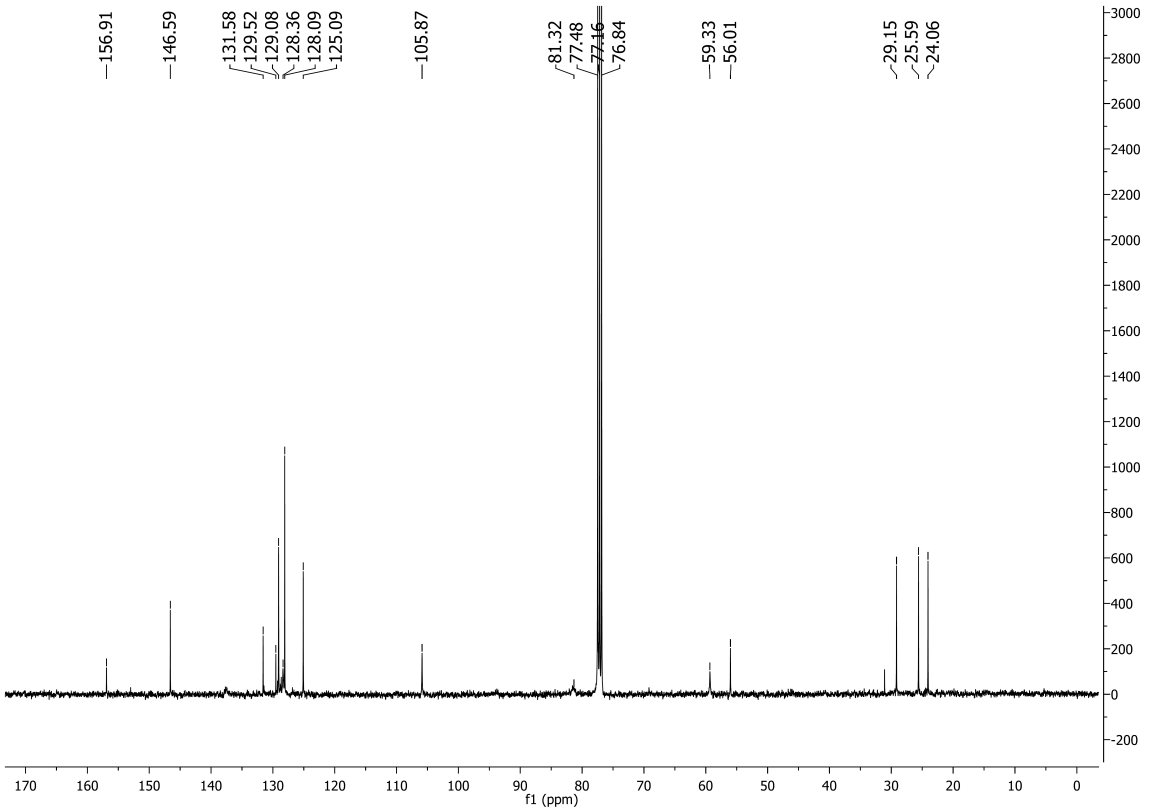
[IPr·H][Pd(η^3-Ind^{t}Bu)Cl$_2$] 2d





[SIPr·H][Pd(□^{3}-cin)Cl$_2$] 2e





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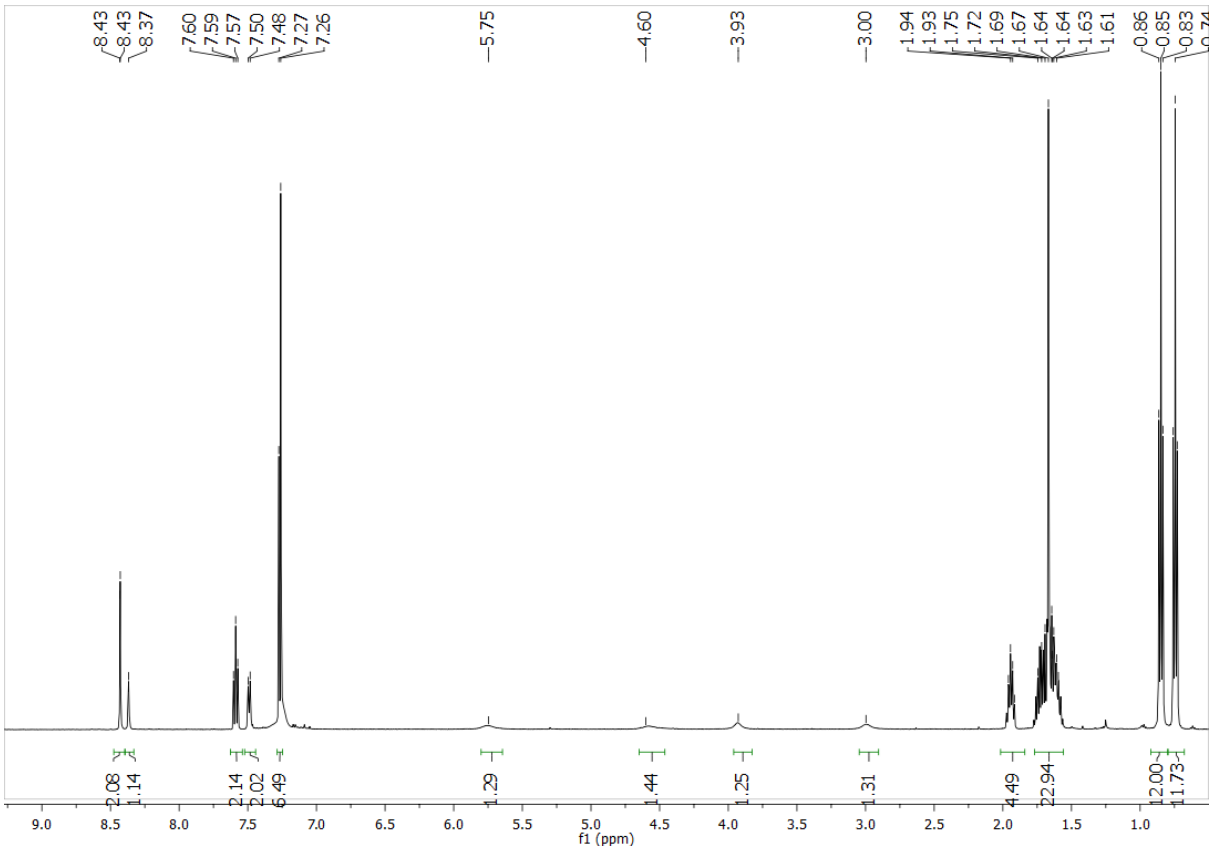

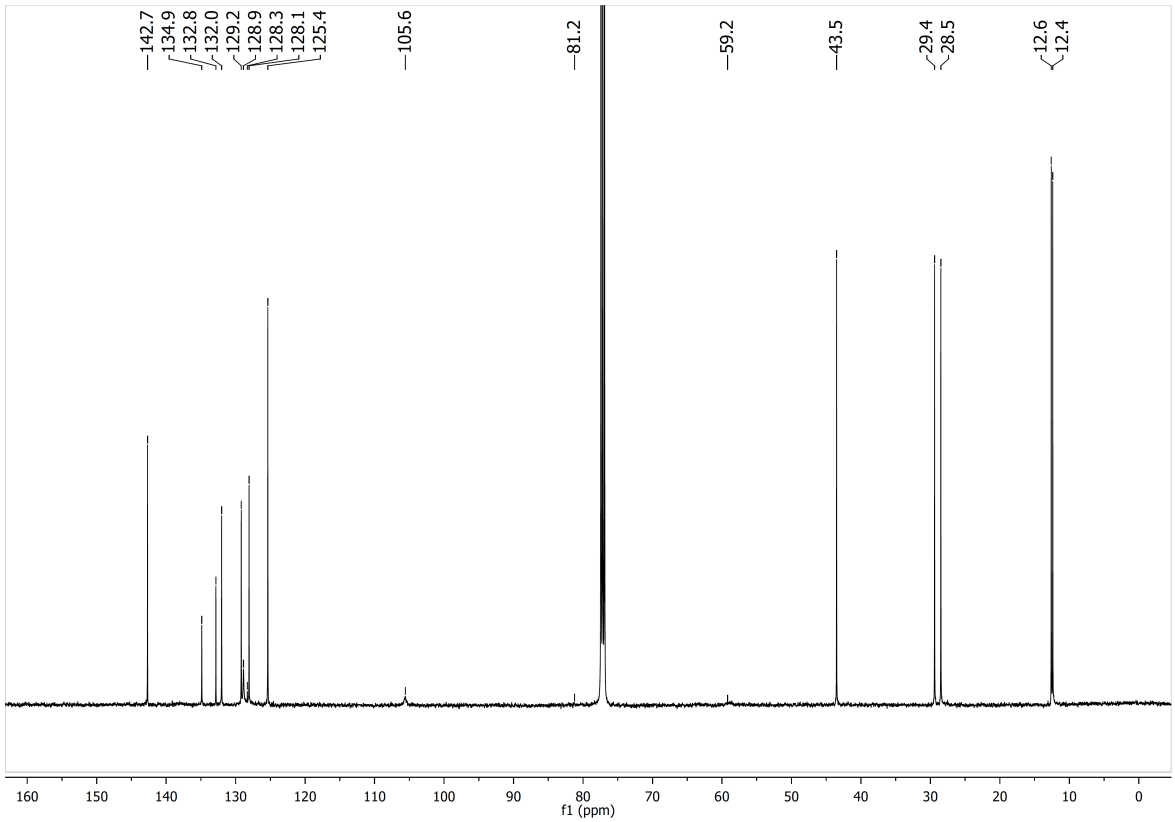

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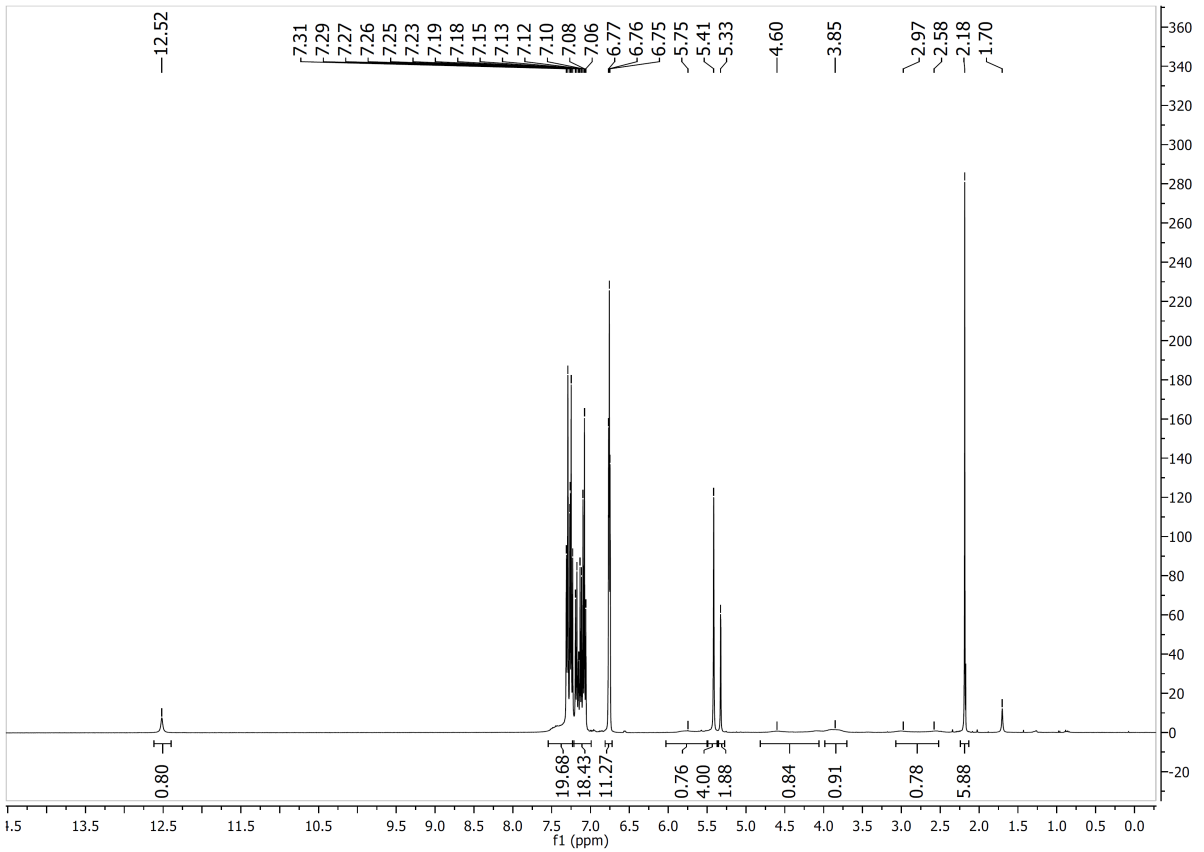
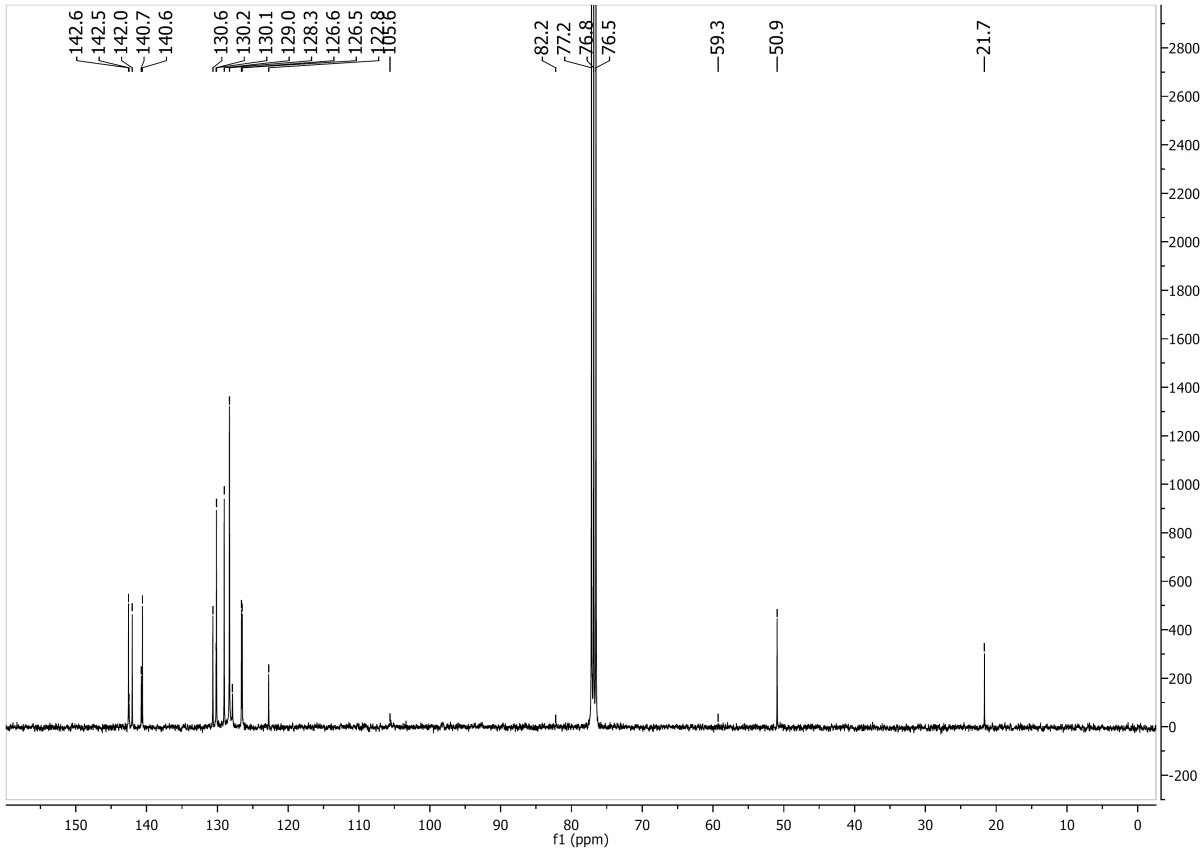
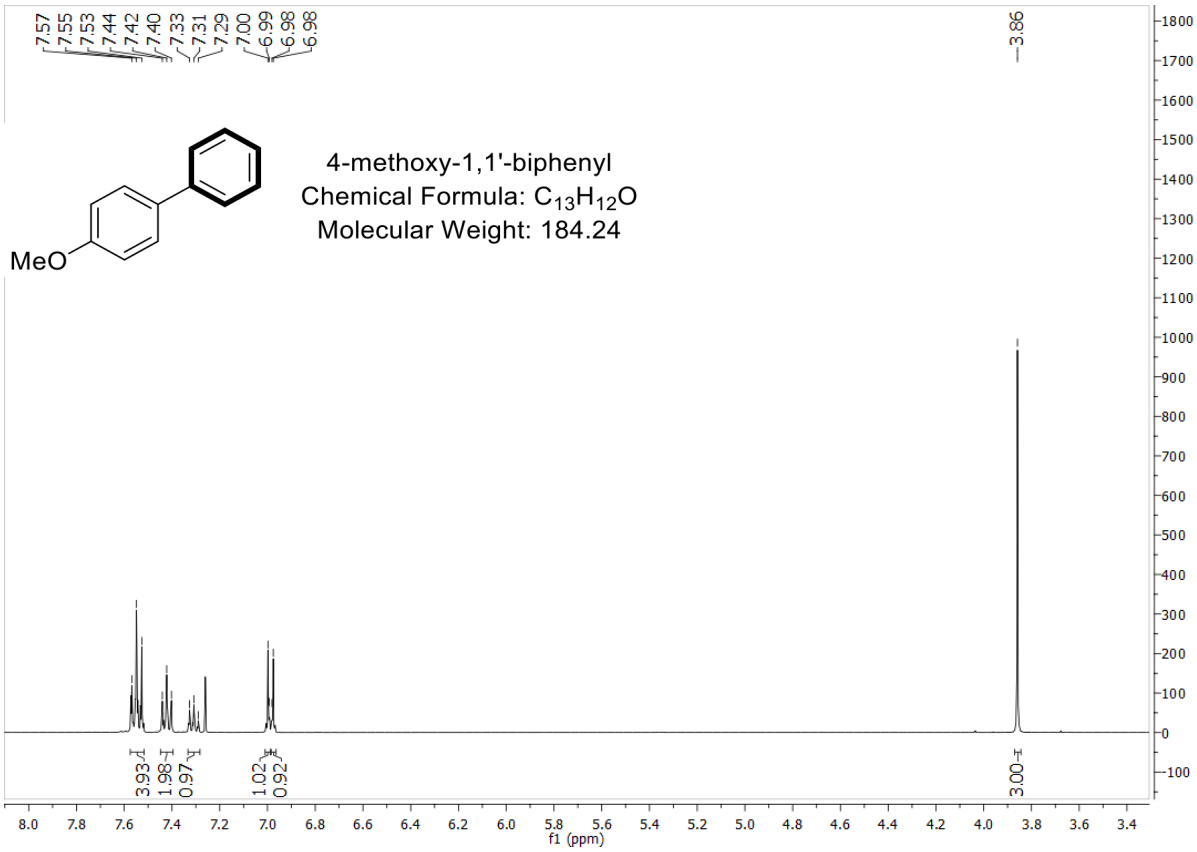
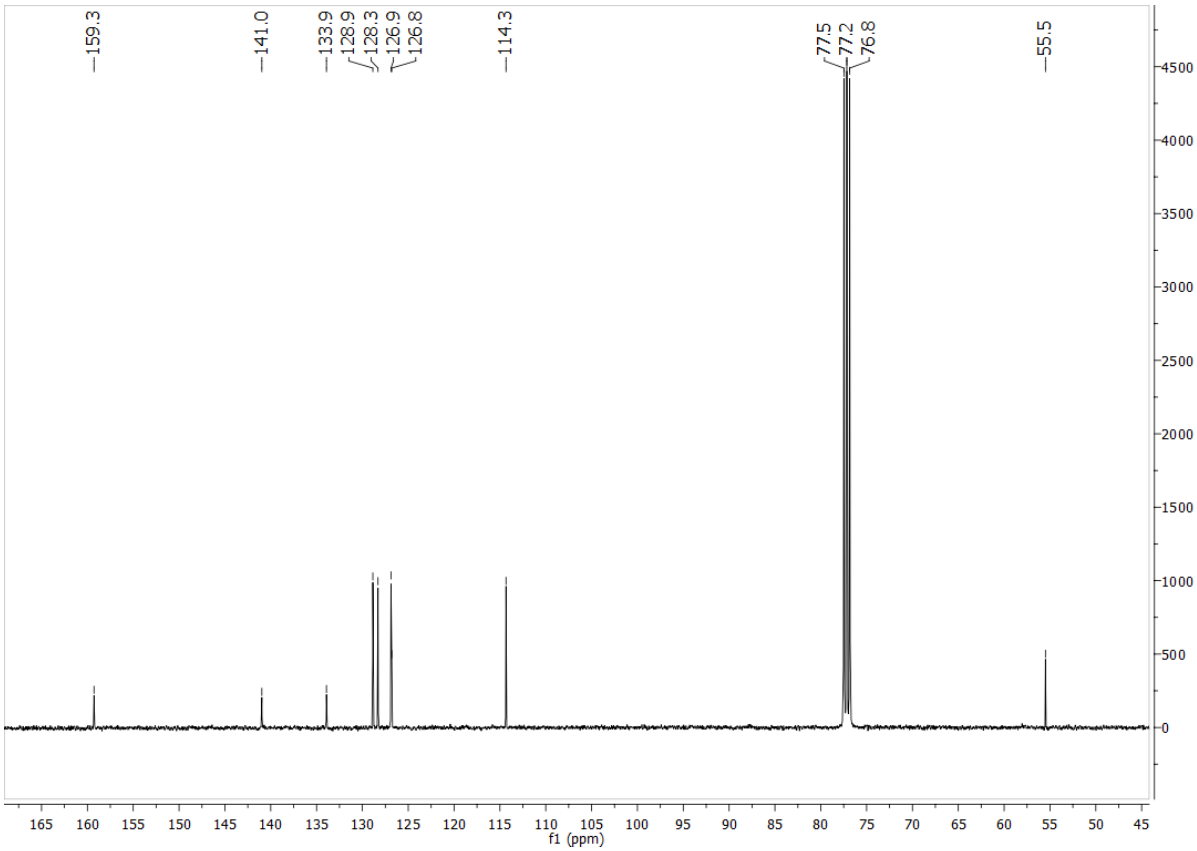


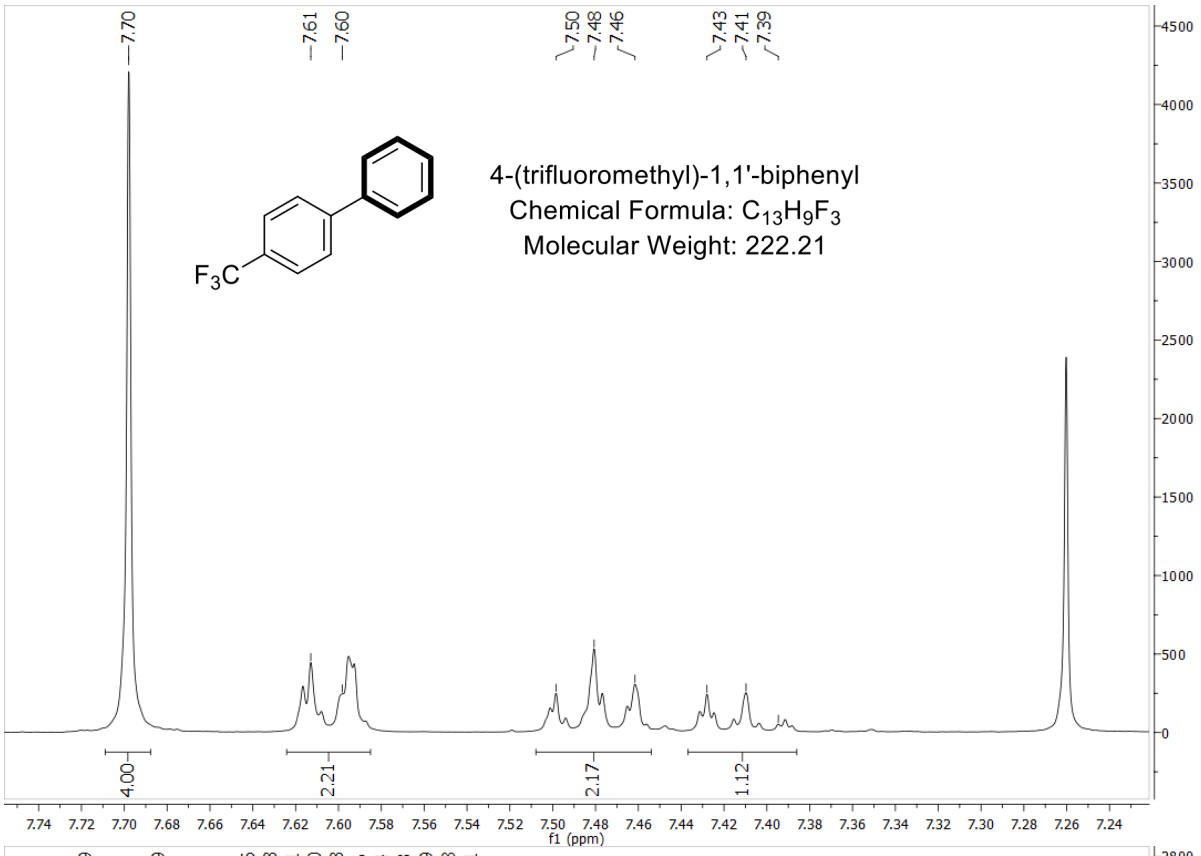


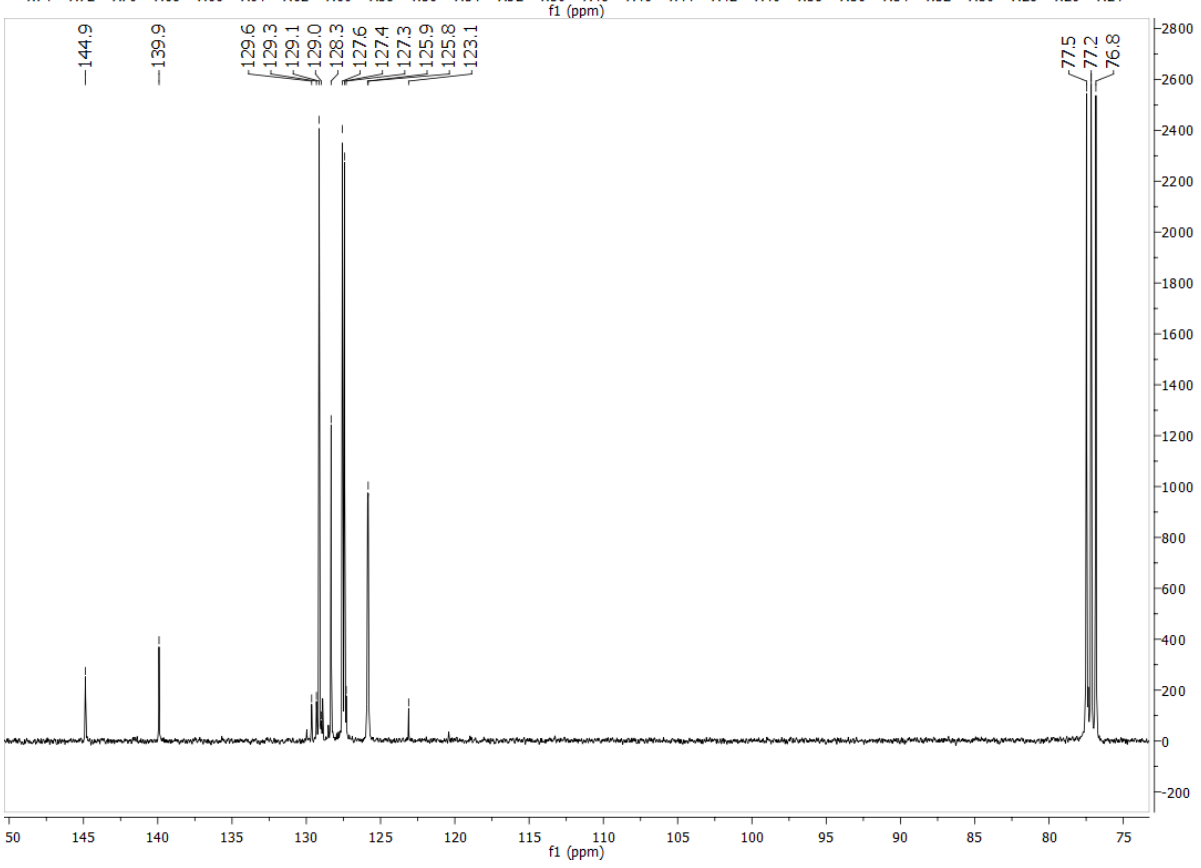
NMR spectra of cross-coupling products (^{1}H and ^{13}C{^{1}H} NMR)
Product, 3a



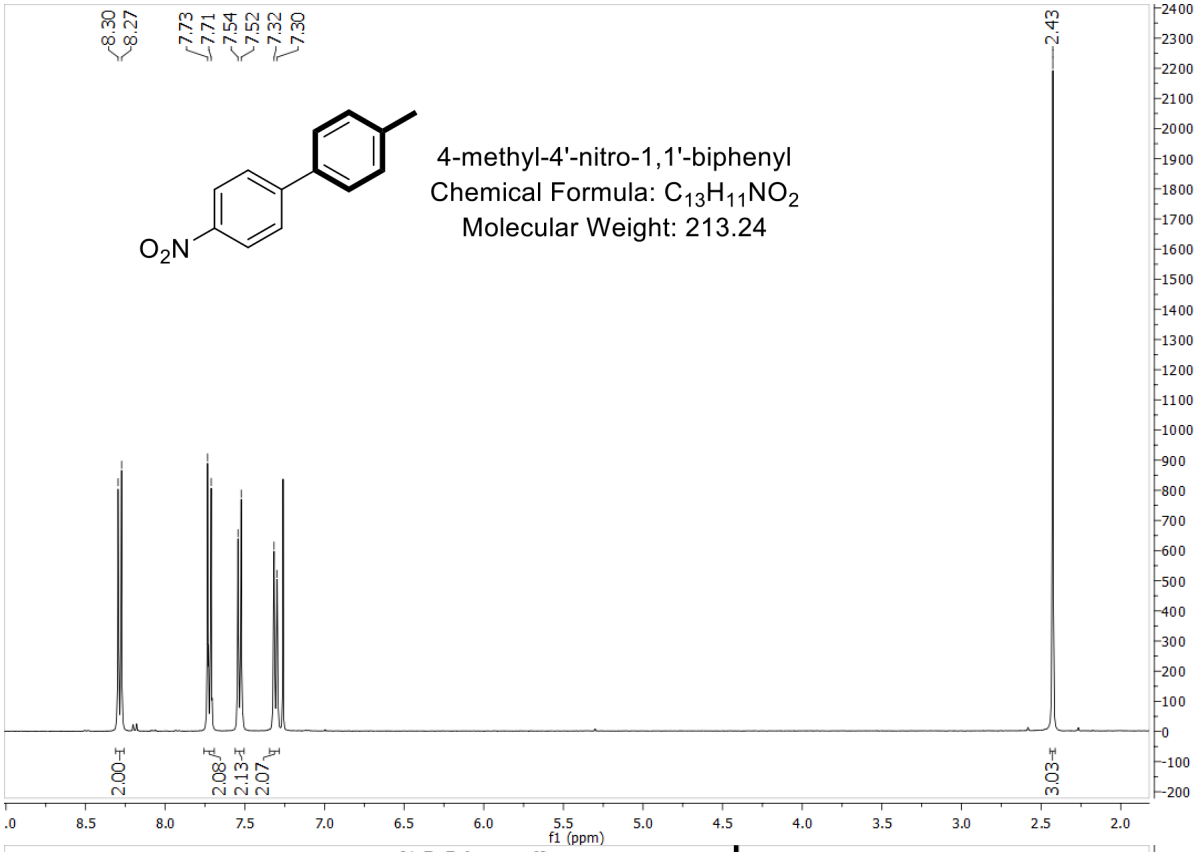


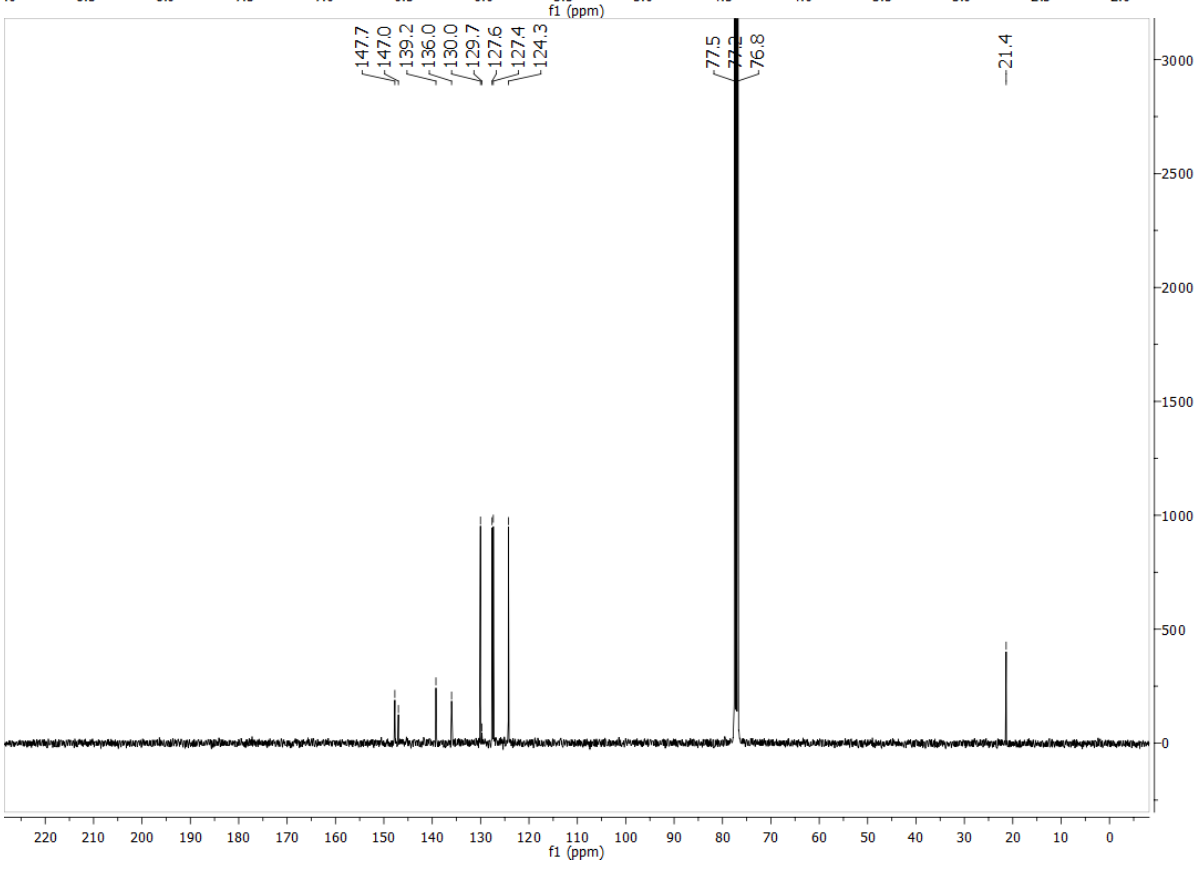
Product, 3b


7.70
7.61
7.60
7.50
7.48
7.46
7.43
7.41
7.39
4-(trifluoromethyl)-1,1'-biphenyl
Chemical Formula: C13H9F3
Molecular Weight: 222.21
F3C
4.00
2.21
2.17
1.12
f1 (ppm)

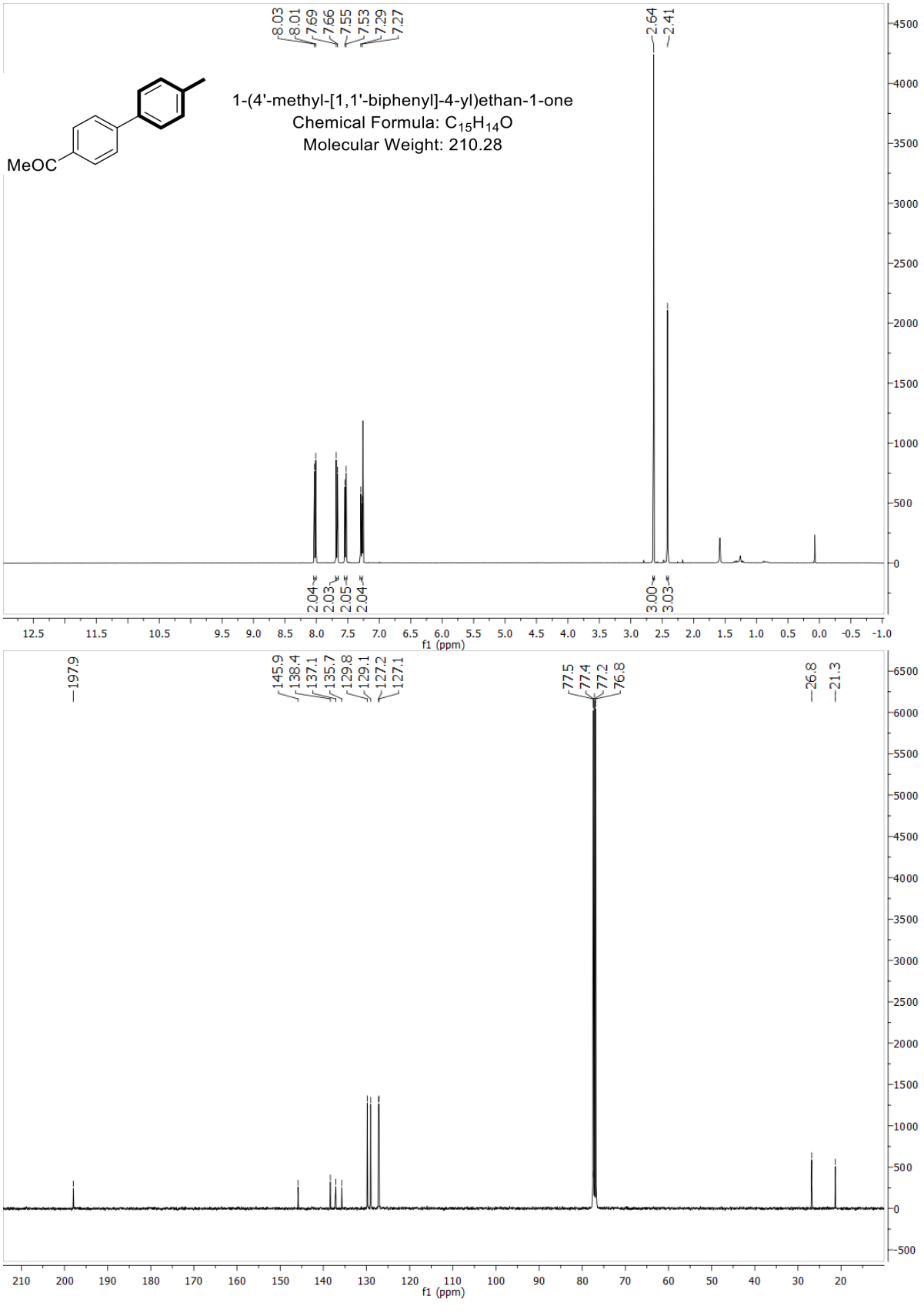

144.9
139.9
129.6
129.3
129.1
129.0
128.3
127.6
127.4
127.3
125.9
125.8
123.1
77.5
77.2
76.8
f1 (ppm)

Product, 3c

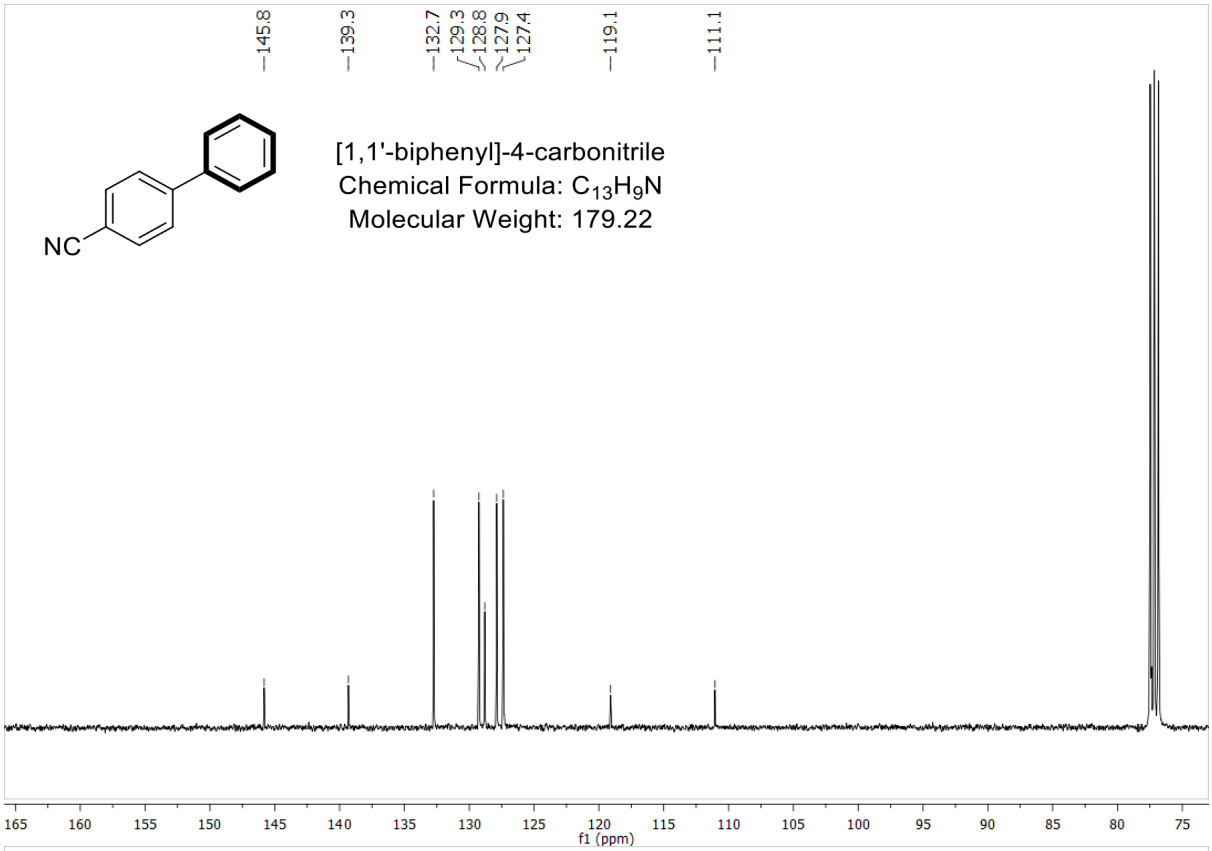

8.30
8.27
7.73
7.71
7.54
7.52
7.32
7.30
2.43
4-methyl-4'-nitro-1,1'-biphenyl
Chemical Formula: $C_{13}H_{11}NO_2$
Molecular Weight: 213.24
O_2N
2.00
2.08
2.13
2.07
3.03
f1 (ppm)

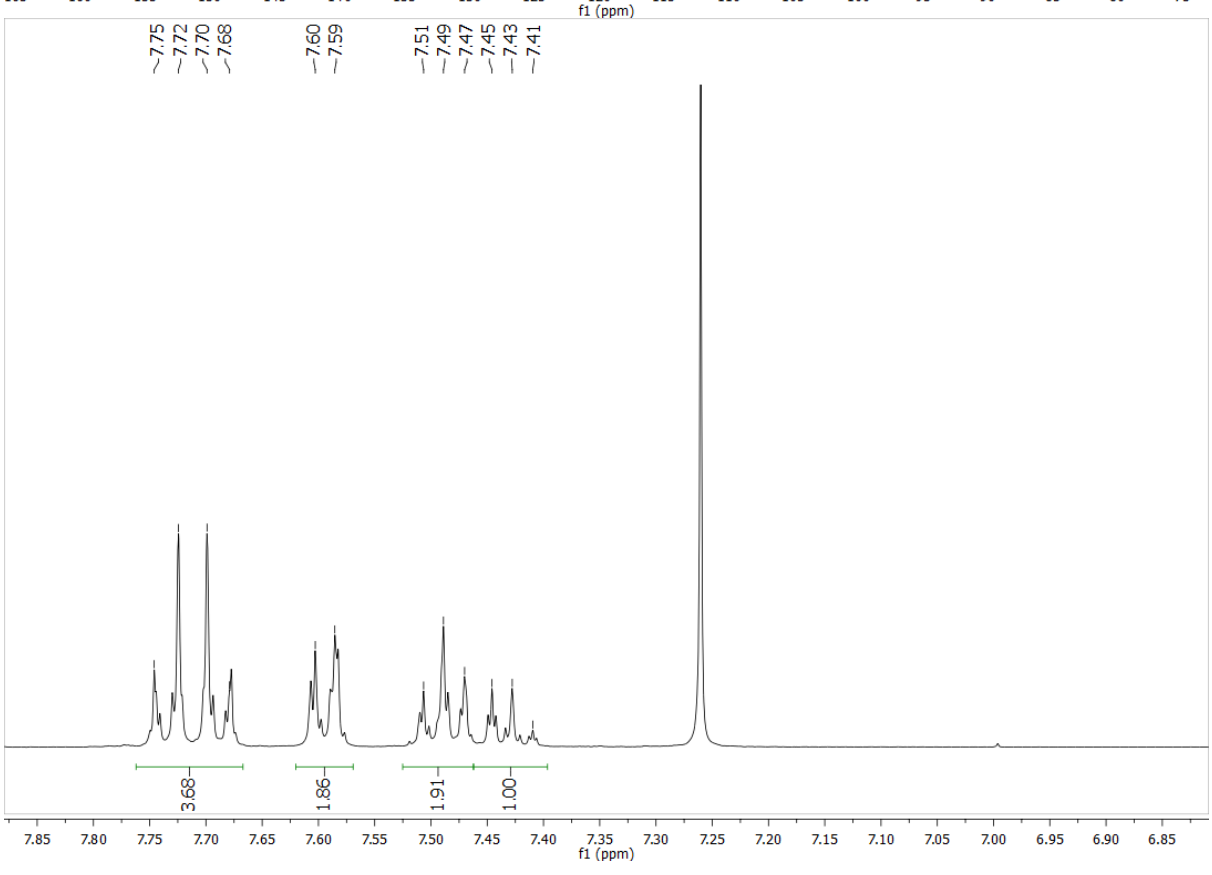

147.7
147.0
139.2
136.0
130.0
129.7
127.6
127.4
124.3
77.5
77.2
76.8
21.4
f1 (ppm)

Product, 3d

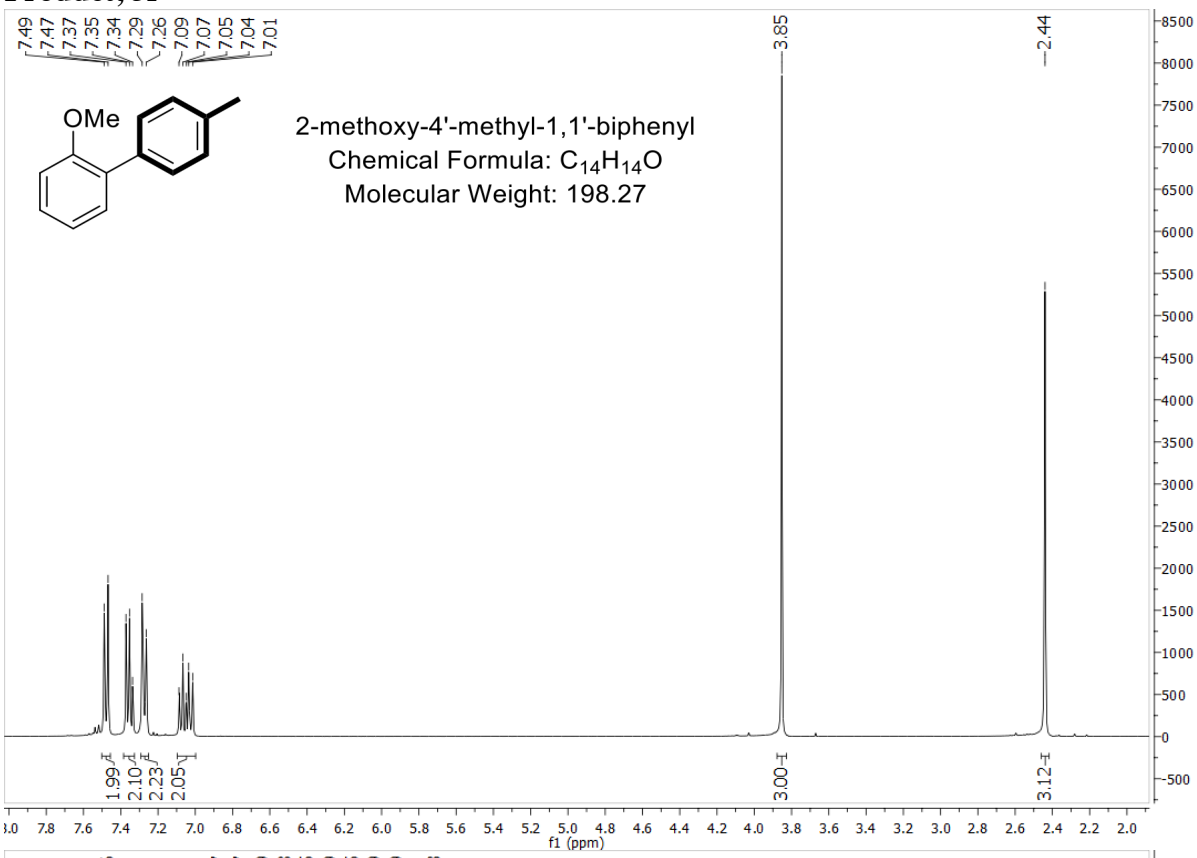

8.03
8.01
7.69
7.66
7.55
7.53
7.29
7.27
2.64
2.41
MeOC
1-(4'-methyl-[1,1'-biphenyl]-4-yl)ethan-1-one
Chemical Formula: C15H14O
Molecular Weight: 210.28
2.04
2.03
2.05
2.04
3.00
3.03
f1 (ppm)
197.9
145.9
138.4
137.1
135.7
129.8
129.1
127.2
127.1
77.5
77.4
77.2
76.8
26.8
21.3
f1 (ppm)

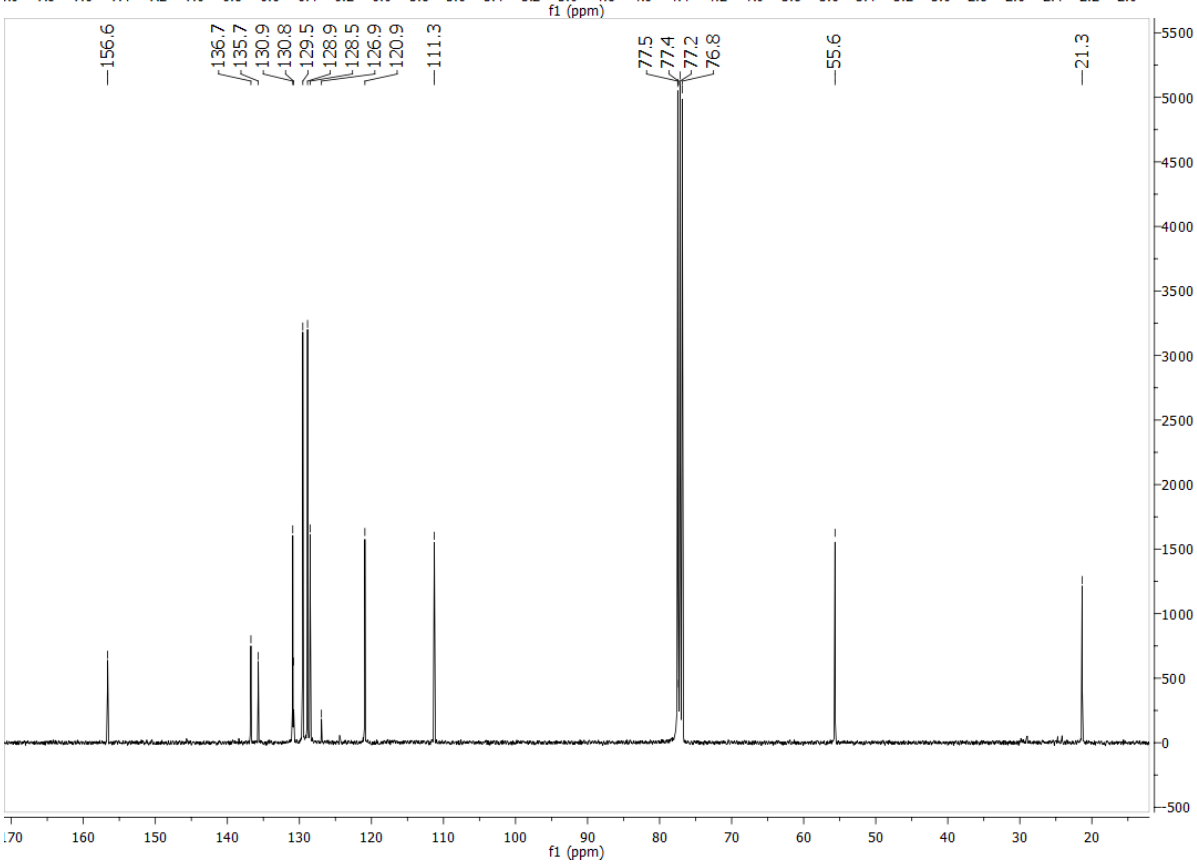
Product, 3e


145.8
139.3
132.7
129.3
128.8
127.9
127.4
119.1
111.1
NC
[1,1'-biphenyl]-4-carbonitrile
Chemical Formula: C13H9N
Molecular Weight: 179.22
f1 (ppm)

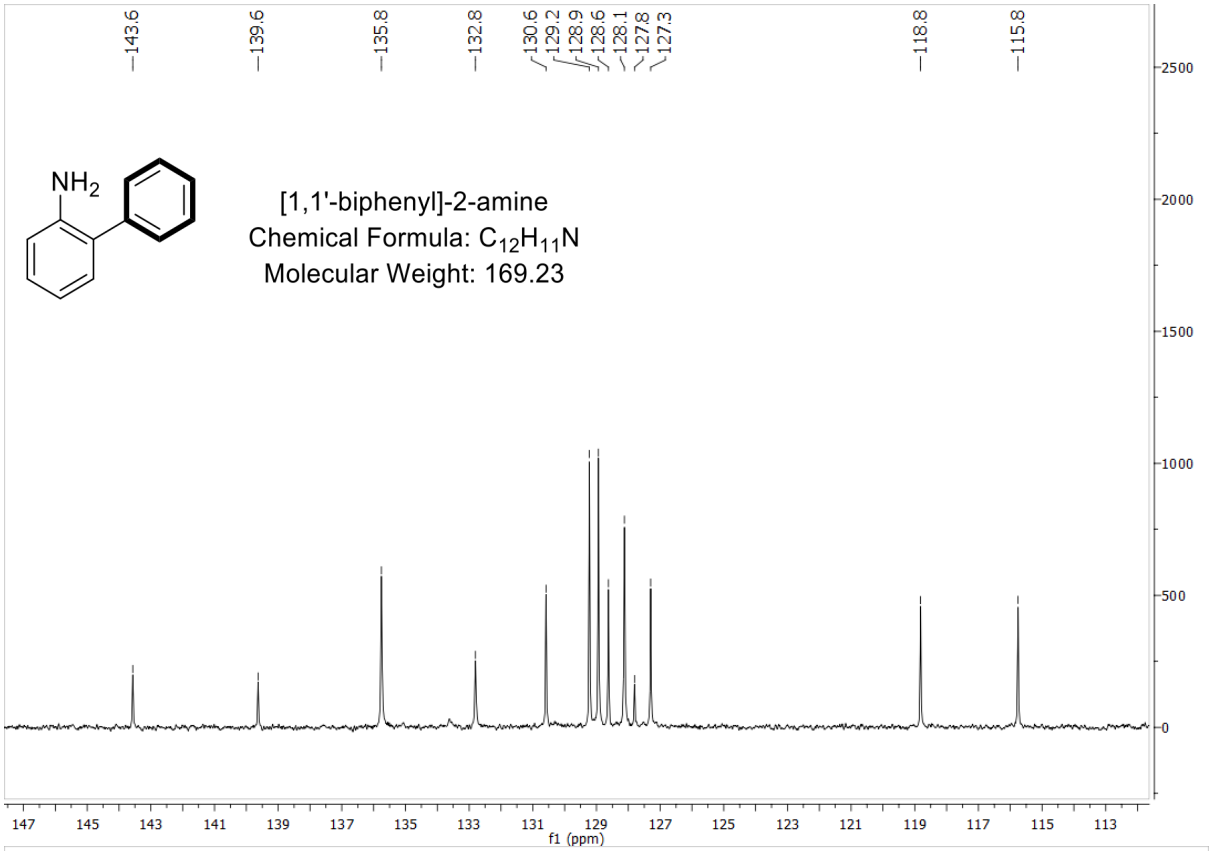

7.75
7.72
7.70
7.68
7.60
7.59
7.51
7.49
7.47
7.45
7.43
7.41
3.68
1.86
1.91
1.00
f1 (ppm)

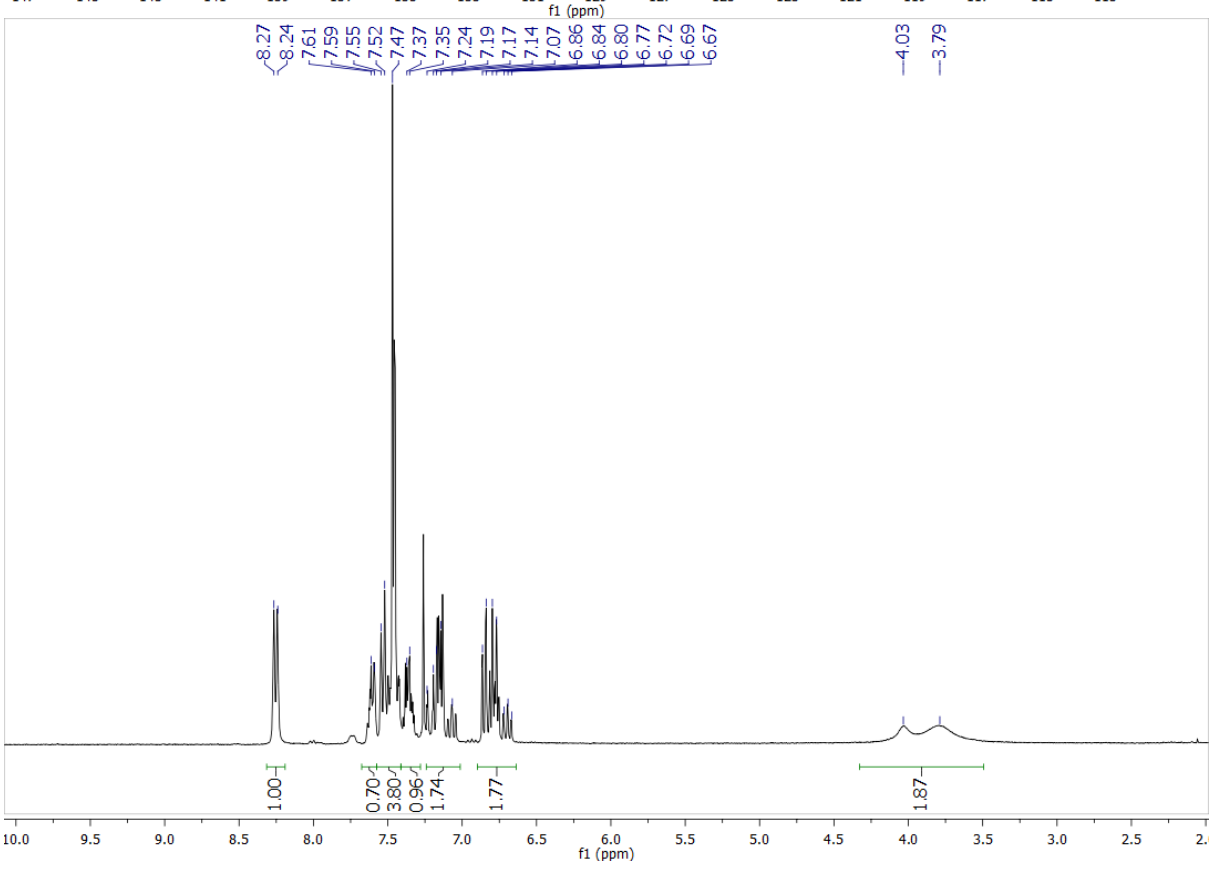
Product, 3f


7.49
7.47
7.37
7.35
7.34
7.29
7.26
7.09
7.07
7.05
7.04
7.01
3.85
2.44
OMe
2-methoxy-4'-methyl-1,1'-biphenyl
Chemical Formula: C14H14O
Molecular Weight: 198.27
1.99
2.10
2.23
2.05
3.00
3.12
f1 (ppm)

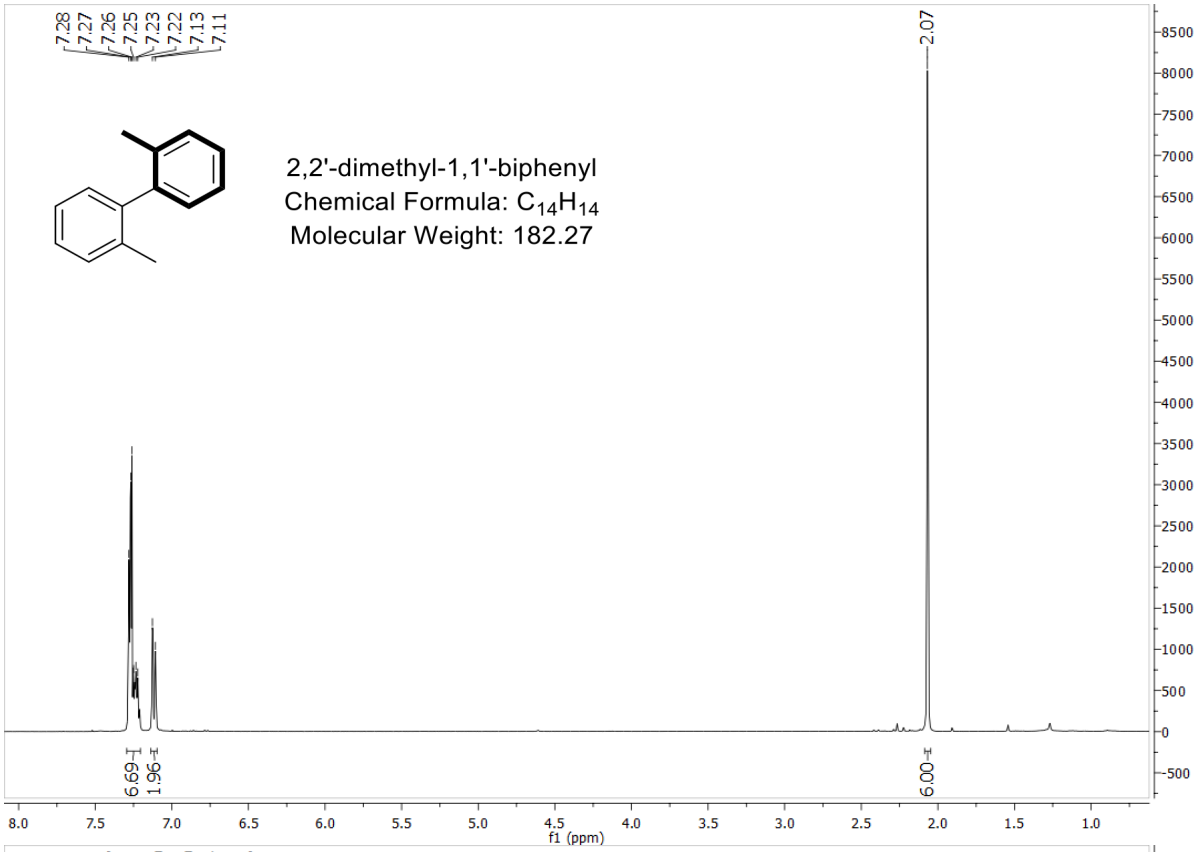

156.6
136.7
135.7
130.9
130.8
129.5
128.9
128.5
126.9
120.9
111.3
77.5
77.4
77.2
76.8
55.6
21.3
f1 (ppm)

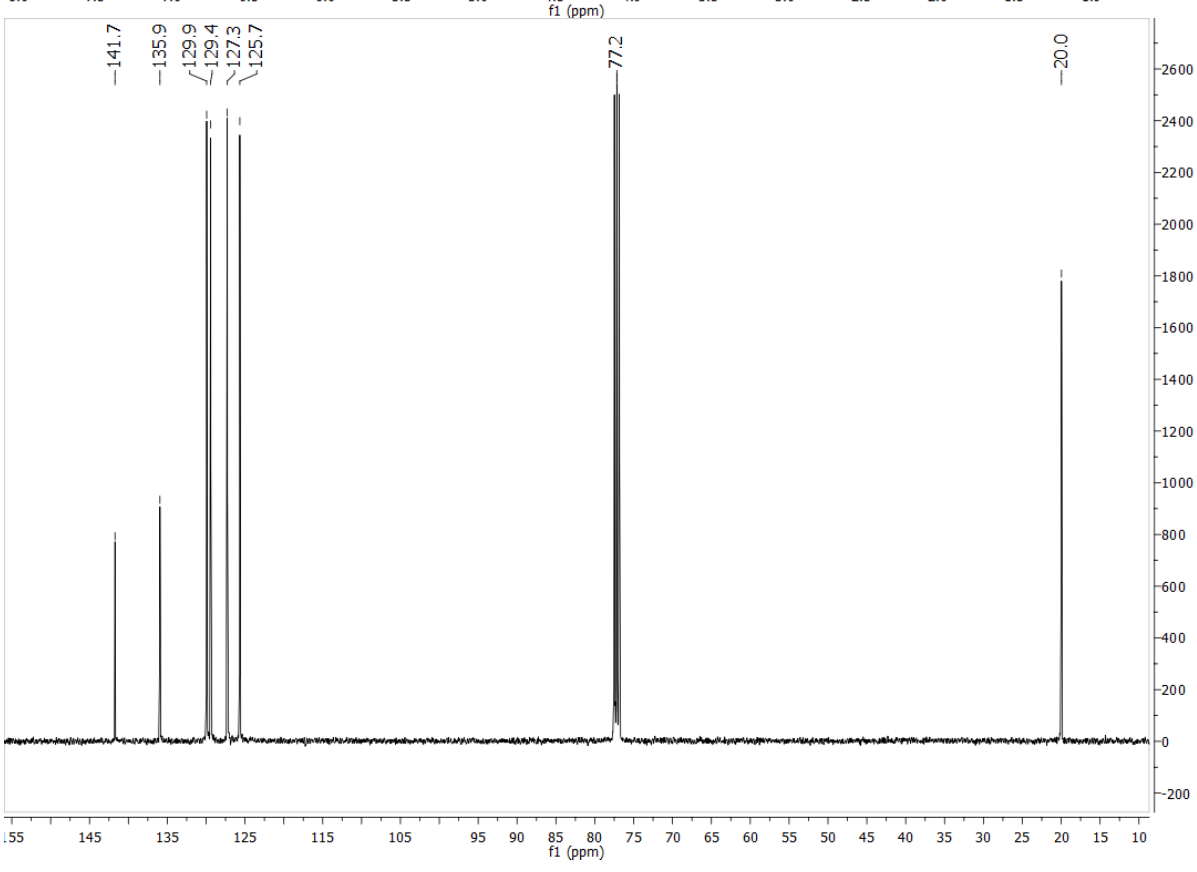
Product, 3g


143.6
139.6
135.8
132.8
130.6
129.2
128.9
128.6
128.1
127.8
127.3
118.8
115.8
NH2
[1,1'-biphenyl]-2-amine
Chemical Formula: C12H11N
Molecular Weight: 169.23
f1 (ppm)

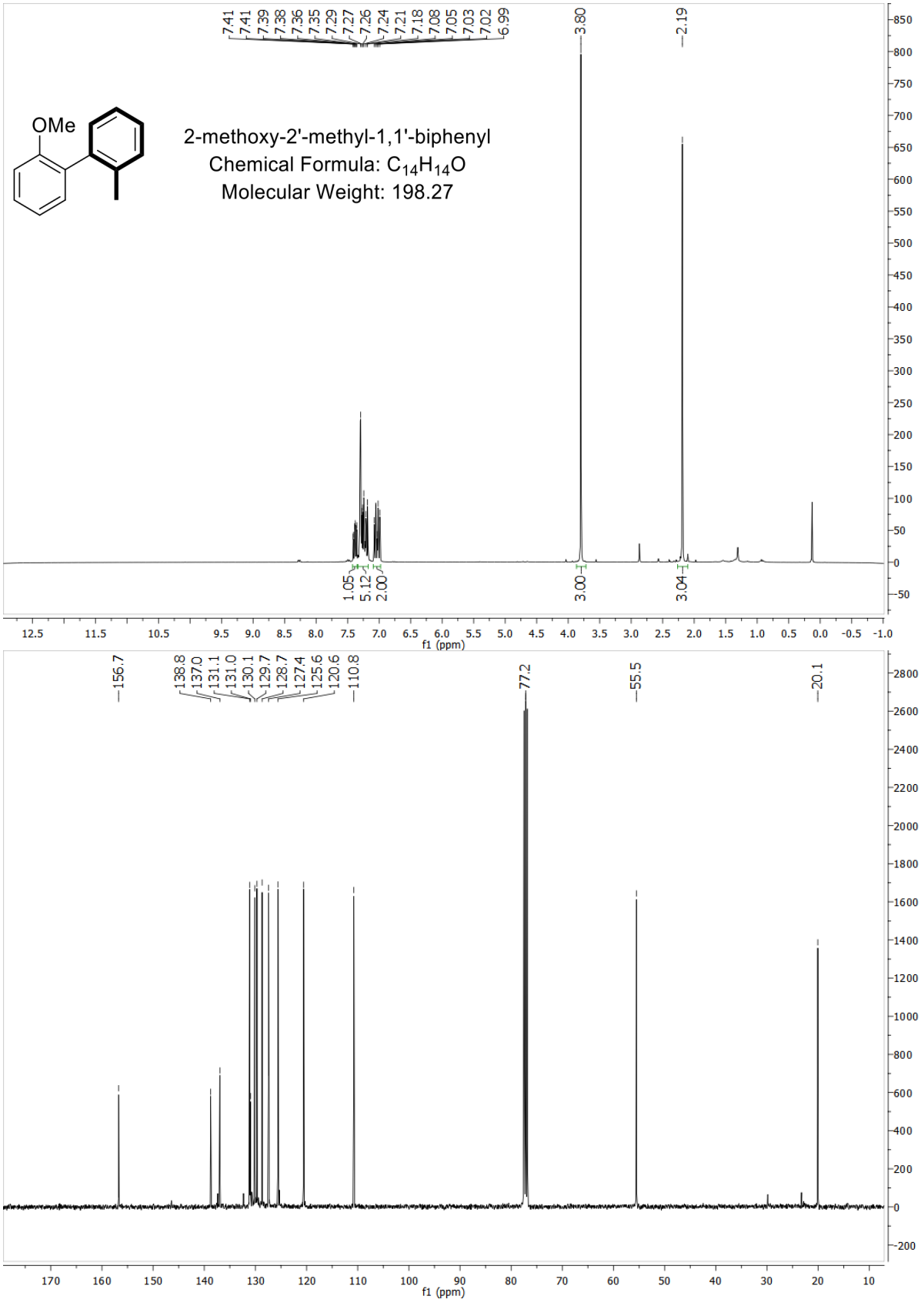

8.27
8.24
7.61
7.59
7.55
7.52
7.47
7.37
7.35
7.24
7.19
7.17
7.14
7.07
6.86
6.84
6.80
6.77
6.72
6.69
6.67
4.03
3.79
1.00
0.70
3.80
0.96
1.74
1.77
1.87
f1 (ppm)

Product, 3h

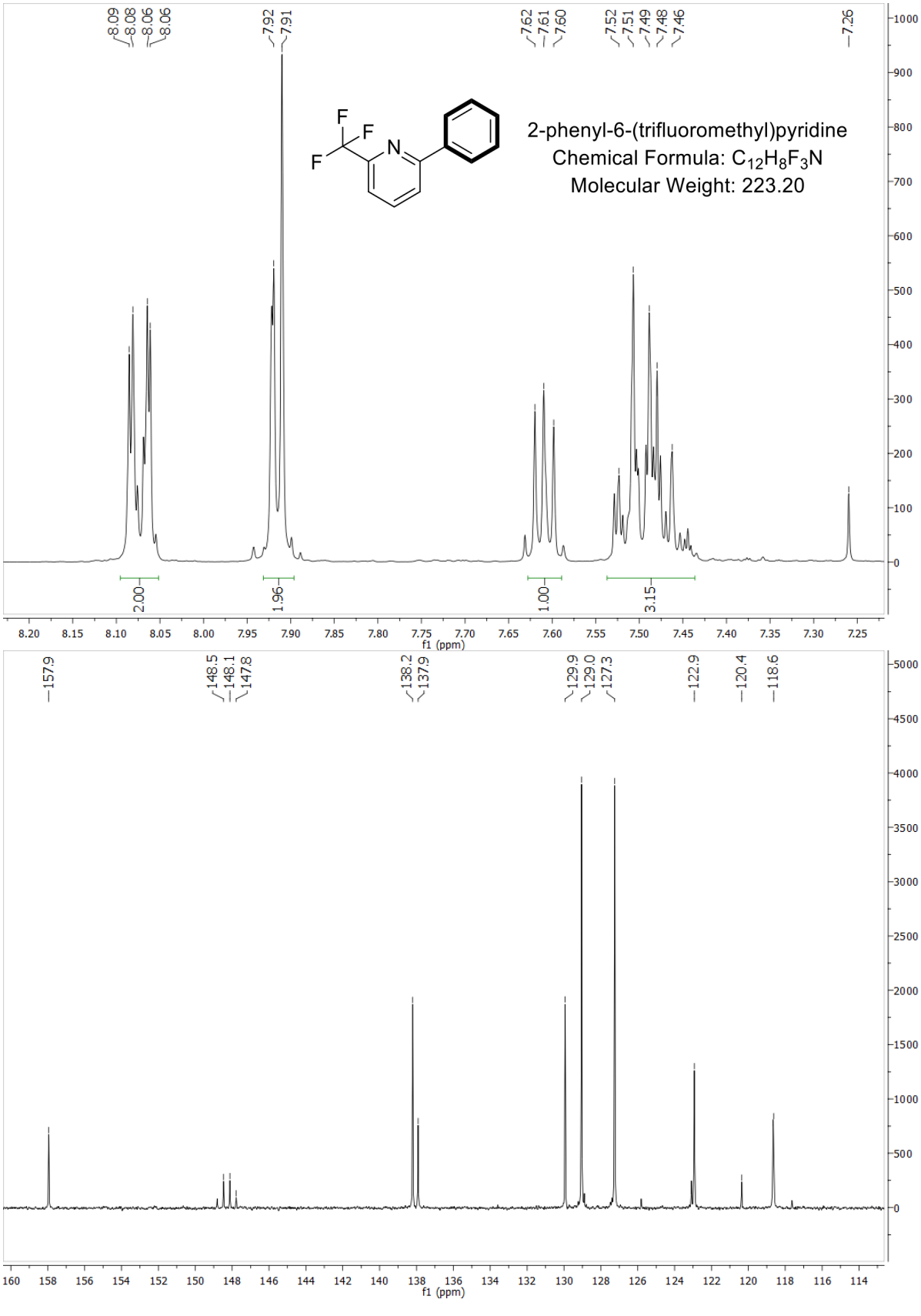

7.28
7.27
7.26
7.25
7.23
7.22
7.13
7.11
2.07
2,2'-dimethyl-1,1'-biphenyl
Chemical Formula: C14H14
Molecular Weight: 182.27
6.69
1.96
6.00
f1 (ppm)


141.7
135.9
129.9
129.4
127.3
125.7
77.2
20.0
f1 (ppm)

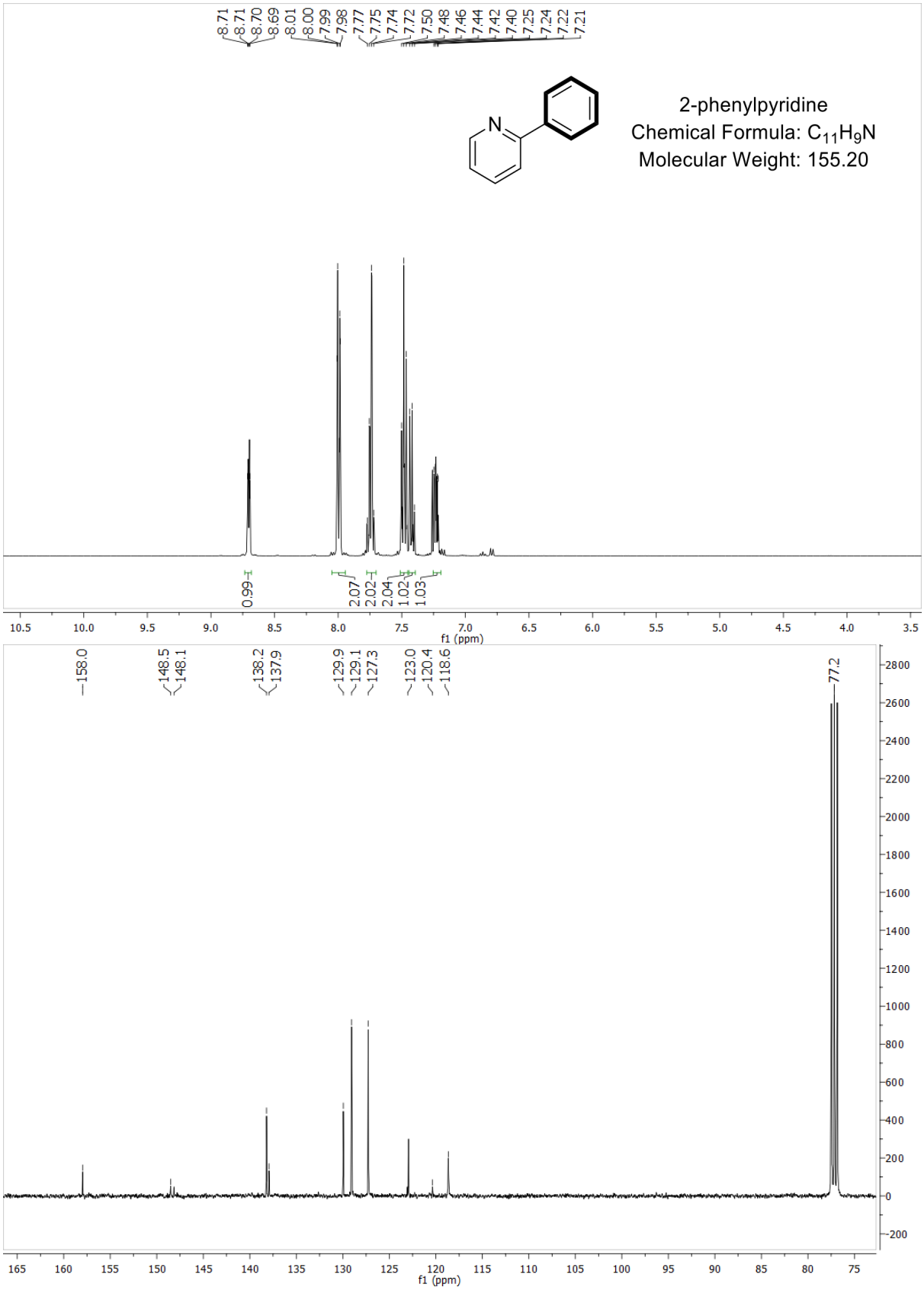
Product, 3i


OMe
2-methoxy-2'-methyl-1,1'-biphenyl
Chemical Formula: C14H14O
Molecular Weight: 198.27
7.41
7.41
7.39
7.38
7.36
7.35
7.29
7.27
7.26
7.24
7.21
7.18
7.08
7.05
7.03
7.02
6.99
3.80
2.19
1.05
5.12
2.00
3.00
3.04
f1 (ppm)
156.7
138.8
137.0
131.1
131.0
130.1
129.7
128.7
127.4
125.6
120.6
110.8
77.2
55.5
20.1
f1 (ppm)

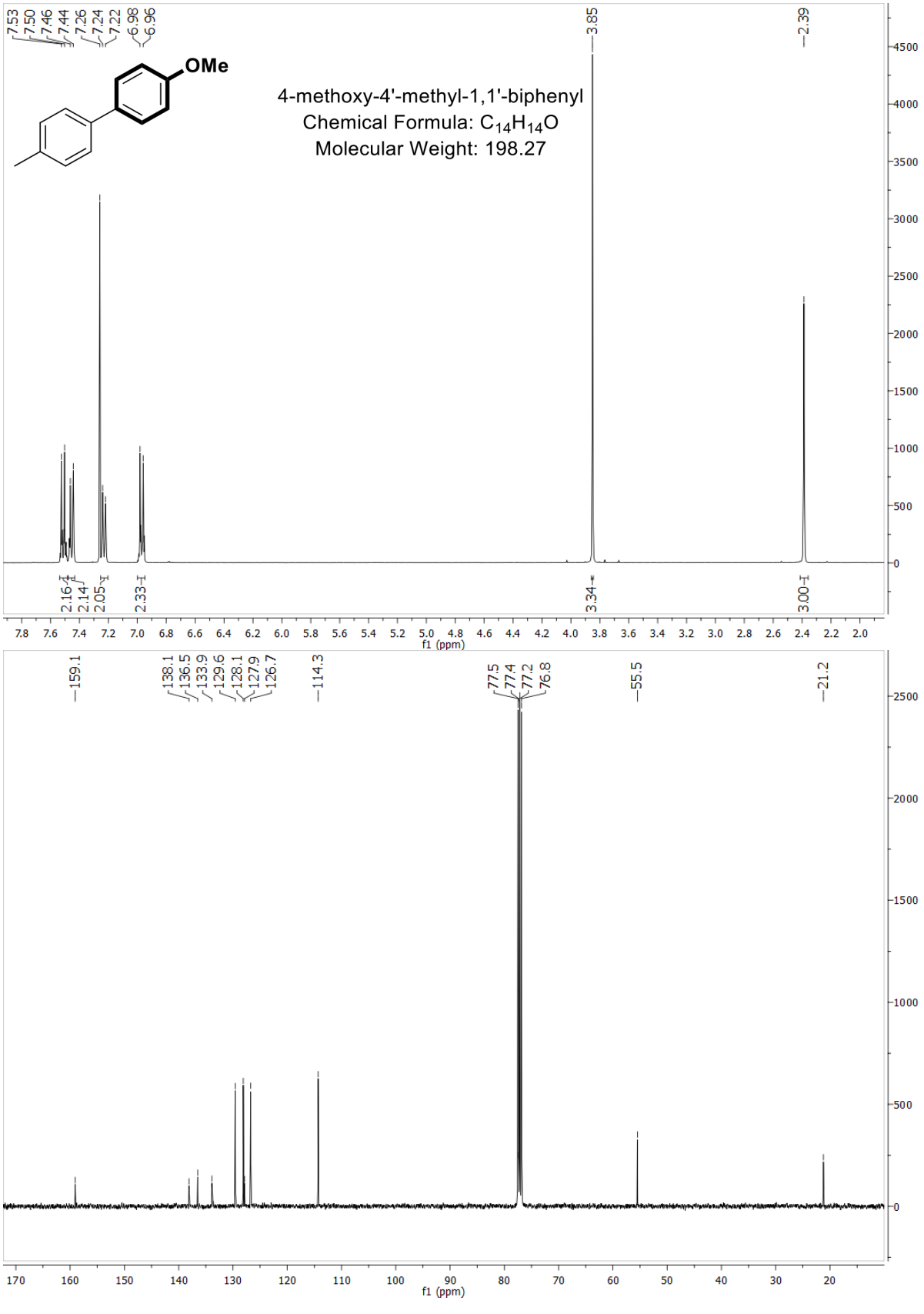
Product, 3j


8.09
8.08
8.06
8.06
7.92
7.91
7.62
7.61
7.60
7.52
7.51
7.49
7.48
7.46
7.26
F
F
F
N
2-phenyl-6-(trifluoromethyl)pyridine
Chemical Formula: C12H8F3N
Molecular Weight: 223.20
2.00
1.96
1.00
3.15
f1 (ppm)
157.9
148.5
148.1
147.8
138.2
137.9
129.9
129.0
127.3
122.9
120.4
118.6
f1 (ppm)

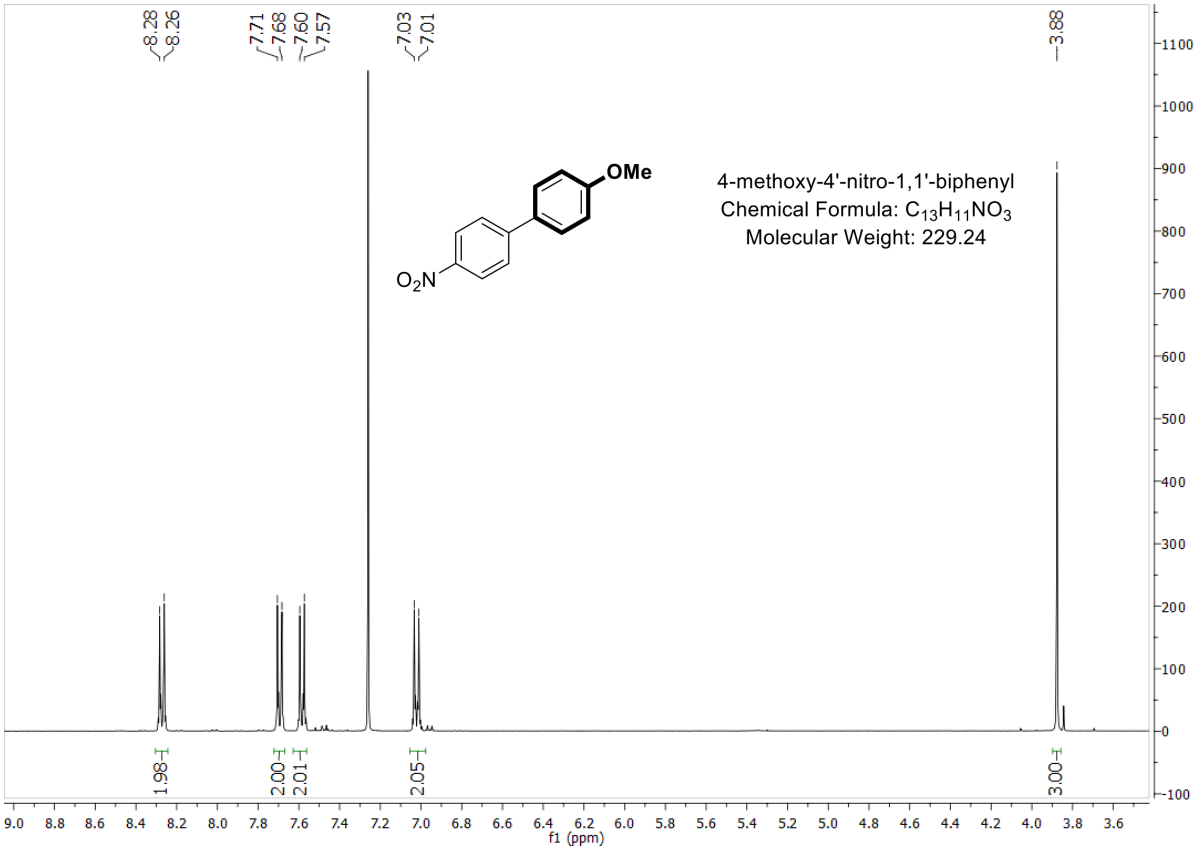
Product, **3k**

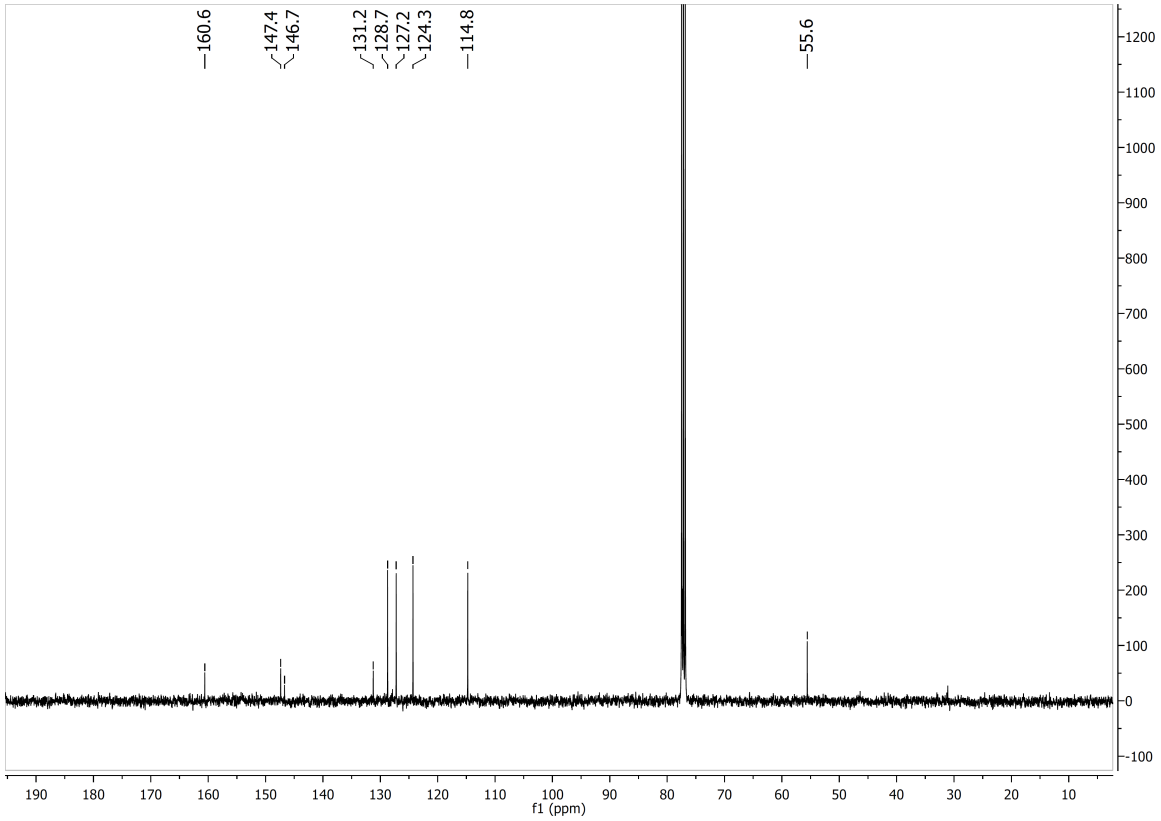

8.71
8.71
8.70
8.69
8.01
8.00
7.99
7.98
7.77
7.75
7.74
7.72
7.50
7.48
7.46
7.44
7.42
7.40
7.25
7.24
7.22
7.21
N
2-phenylpyridine
Chemical Formula: C11H9N
Molecular Weight: 155.20
0.99
2.07
2.02
2.04
1.02
1.03
f1 (ppm)
158.0
148.5
148.1
138.2
137.9
129.9
129.1
127.3
123.0
120.4
118.6
77.2
f1 (ppm)

Product, 3l

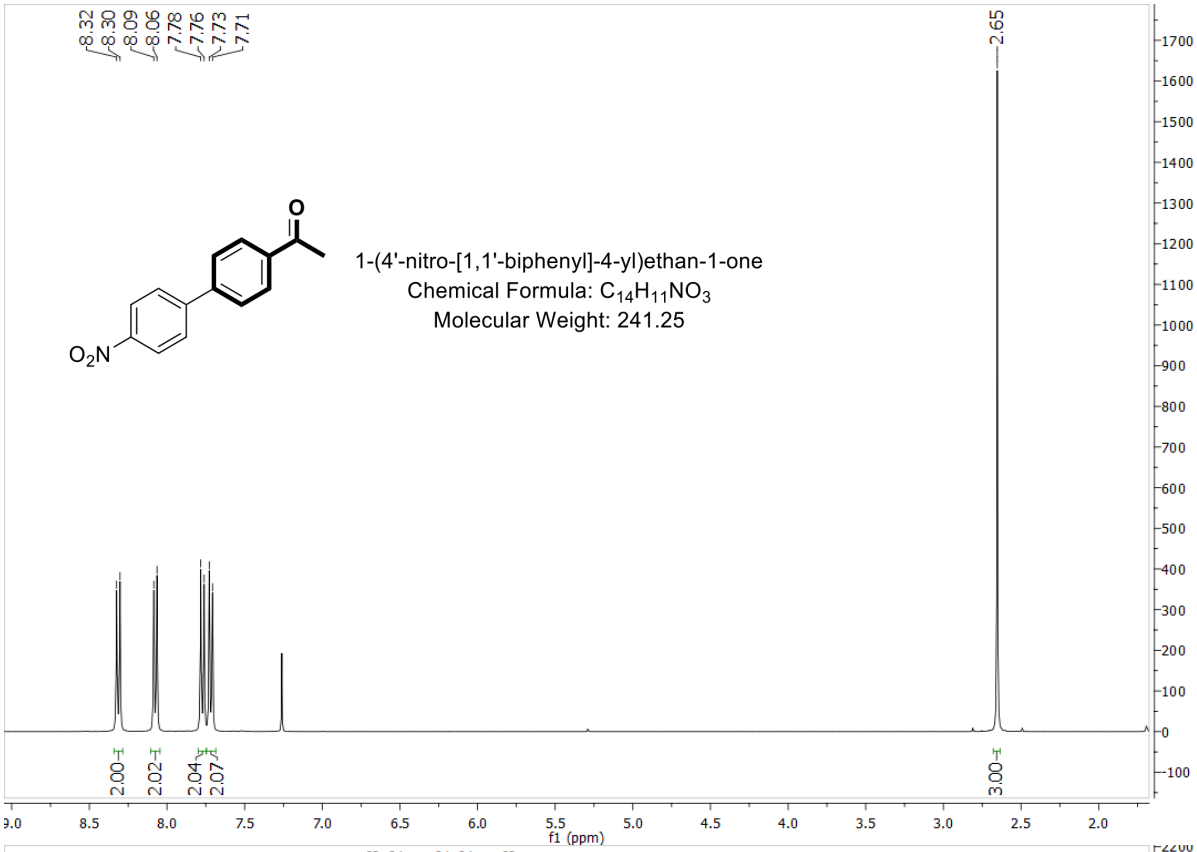

7.53
7.50
7.46
7.44
7.26
7.24
7.22
6.98
6.96
3.85
2.39
OMe
4-methoxy-4'-methyl-1,1'-biphenyl
Chemical Formula: C14H14O
Molecular Weight: 198.27
2.16
2.14
2.05
2.33
3.34
3.00
f1 (ppm)
159.1
138.1
136.5
133.9
129.6
128.1
127.9
126.7
114.3
77.5
77.4
77.2
76.8
55.5
21.2
f1 (ppm)

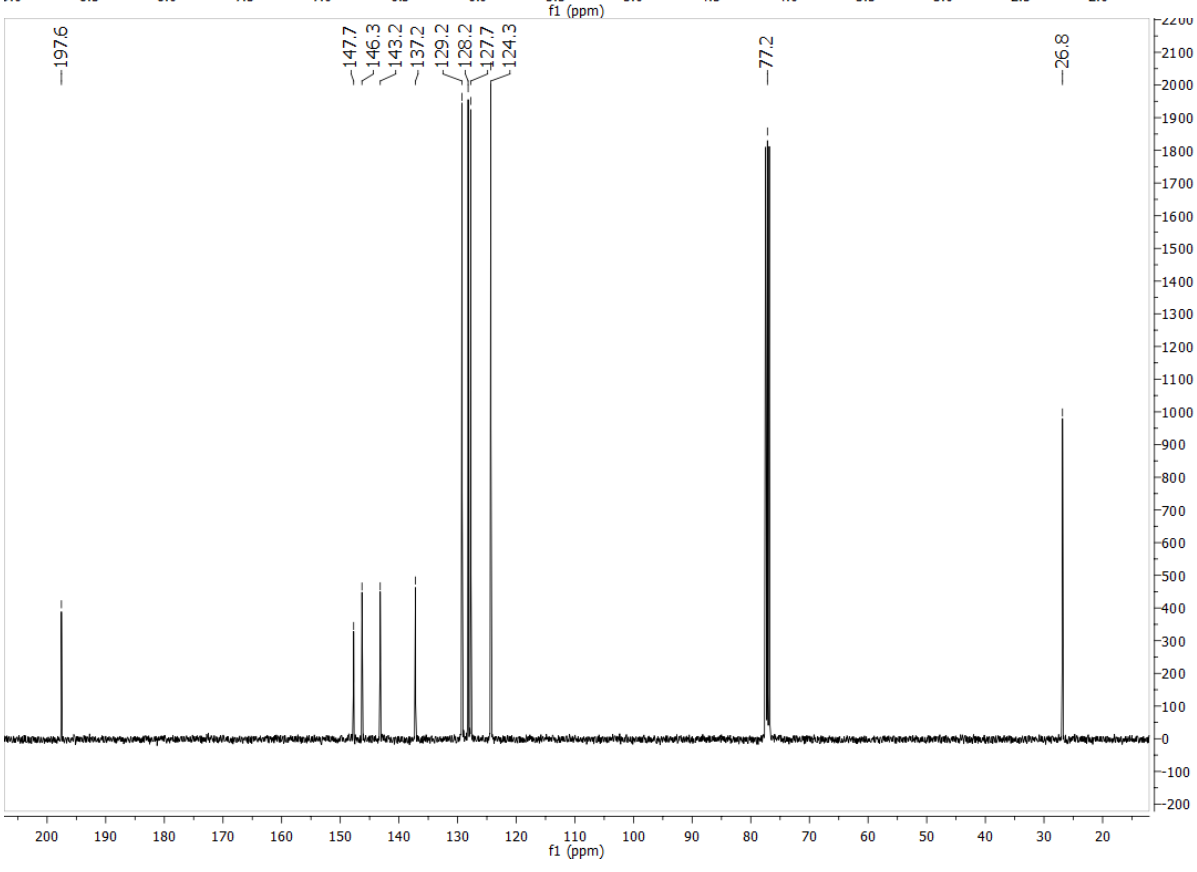
Product, 3m


8.28
8.26
7.71
7.68
7.60
7.57
7.03
7.01
3.88
OMe
O_2N
4-methoxy-4'-nitro-1,1'-biphenyl
Chemical Formula: $C_{13}H_{11}NO_3$
Molecular Weight: 229.24
1.98
2.00
2.01
2.05
3.00
f1 (ppm)

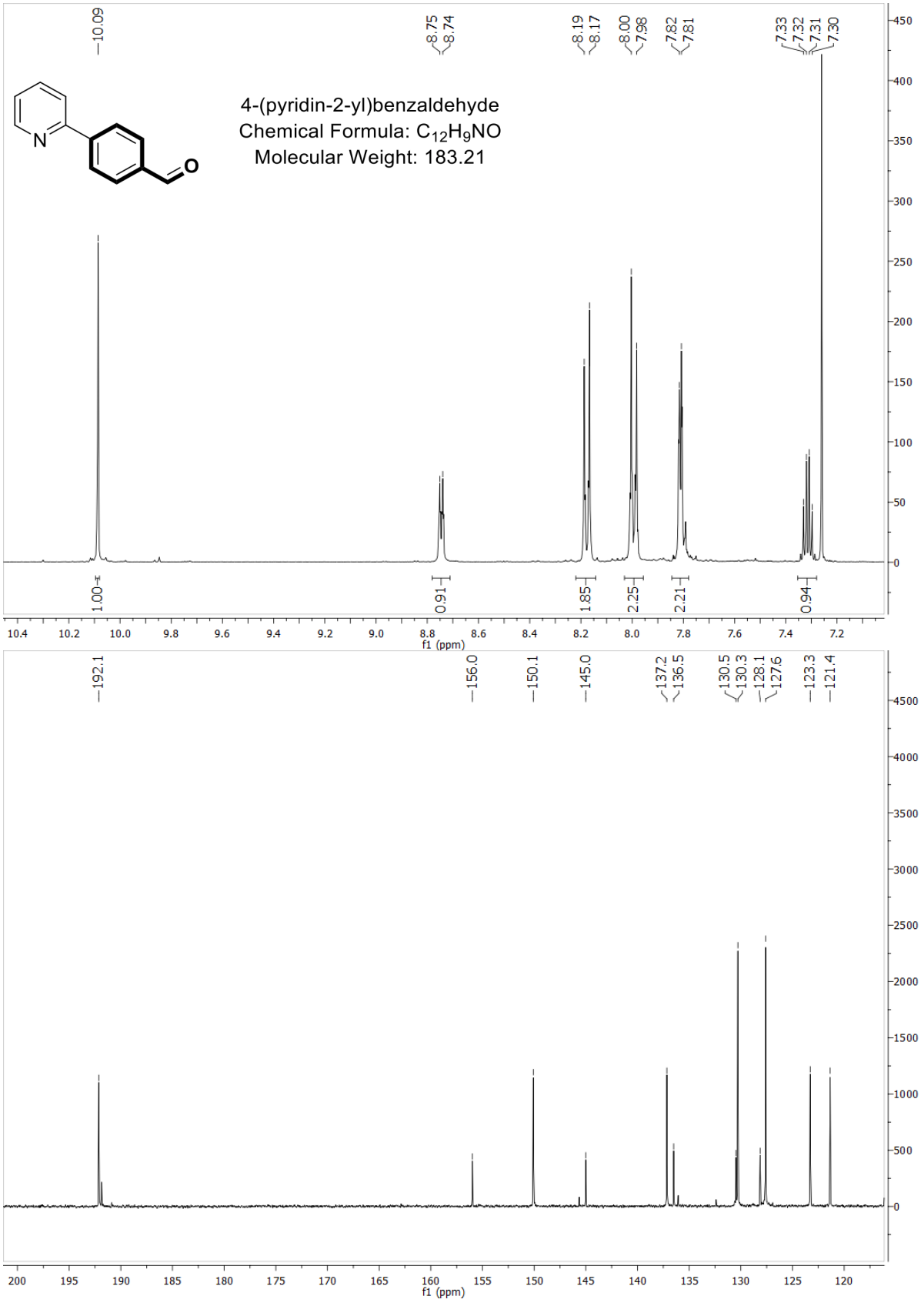

160.6
147.4
146.7
131.2
128.7
127.2
124.3
114.8
55.6
f1 (ppm)

Product, 3n

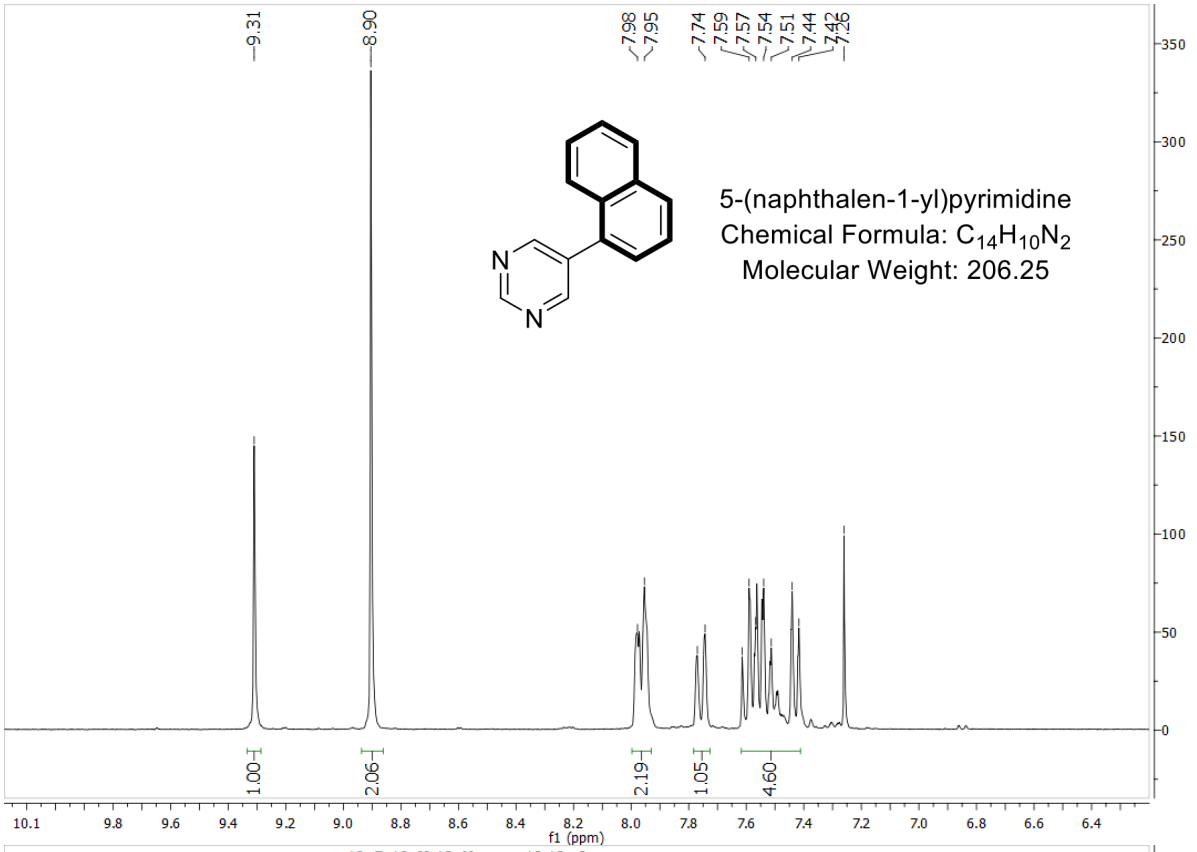

8.32
8.30
8.09
8.06
7.78
7.76
7.73
7.71
2.65
O
O_2N
1-(4'-nitro-[1,1'-biphenyl]-4-yl)ethan-1-one
Chemical Formula: $C_{14}H_{11}NO_3$
Molecular Weight: 241.25
2.00
2.02
2.04
2.07
3.00
f1 (ppm)

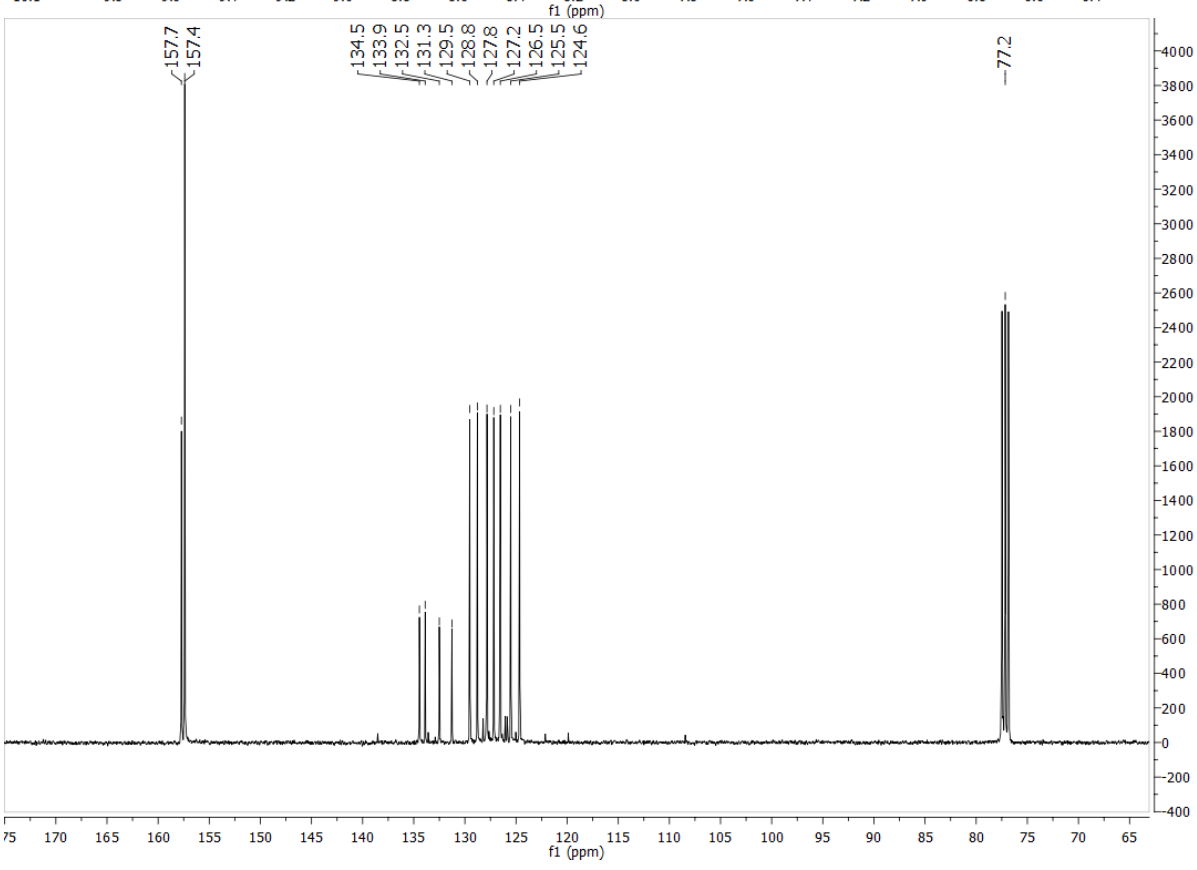

197.6
147.7
146.3
143.2
137.2
129.2
128.2
127.7
124.3
77.2
26.8
f1 (ppm)

Product, 3o

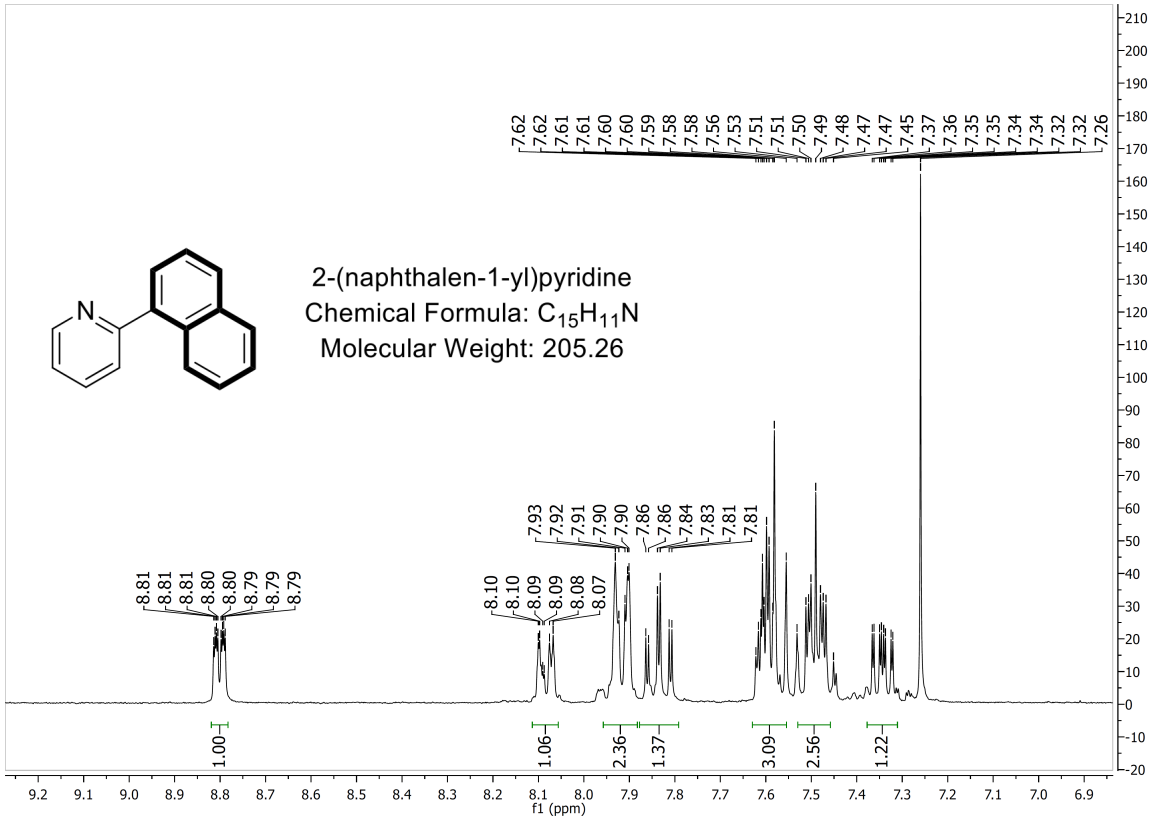

10.09
8.75
8.74
8.19
8.17
8.00
7.98
7.82
7.81
7.33
7.32
7.31
7.30
4-(pyridin-2-yl)benzaldehyde
Chemical Formula: C12H9NO
Molecular Weight: 183.21
1.00
0.91
1.85
2.25
2.21
0.94
f1 (ppm)
192.1
156.0
150.1
145.0
137.2
136.5
130.5
130.3
128.1
127.6
123.3
121.4
f1 (ppm)

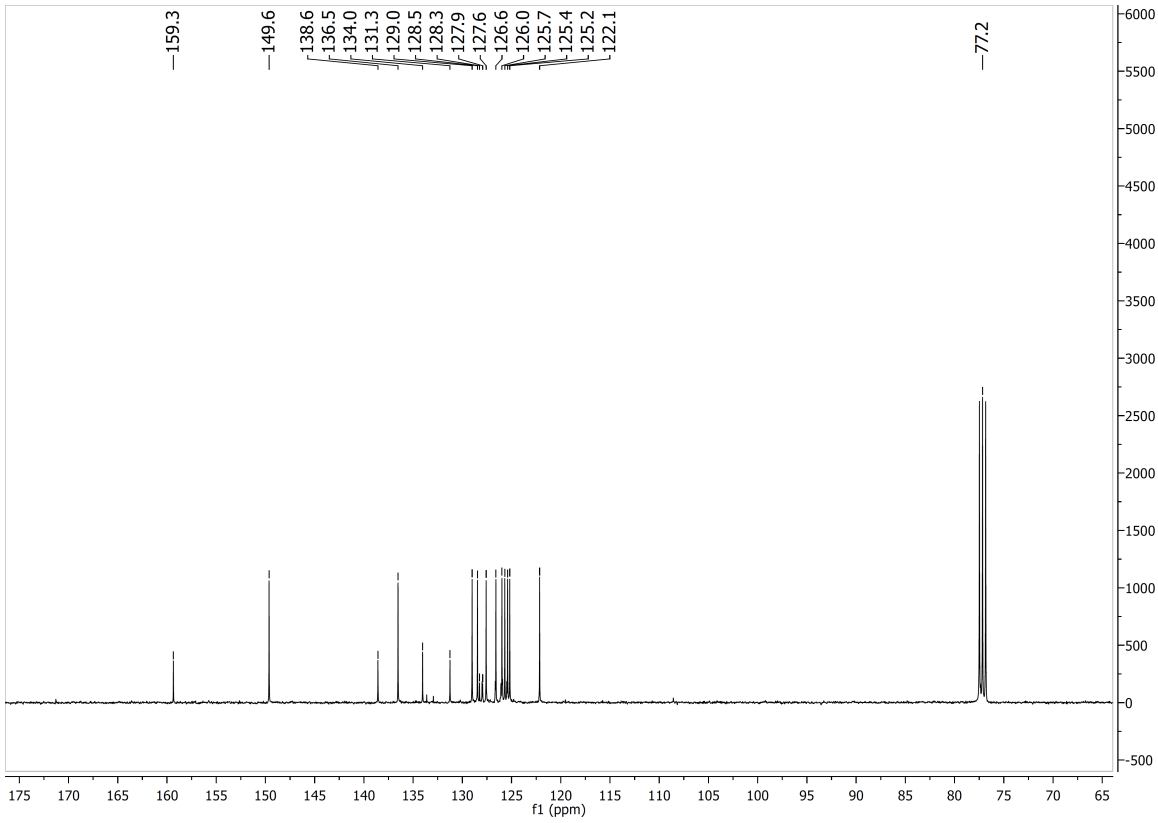
Product, 3p


9.31
8.90
7.98
7.95
7.74
7.59
7.57
7.54
7.51
7.44
7.42
7.26
5-(naphthalen-1-yl)pyrimidine
Chemical Formula: C14H10N2
Molecular Weight: 206.25
1.00
2.06
2.19
1.05
4.60
f1 (ppm)

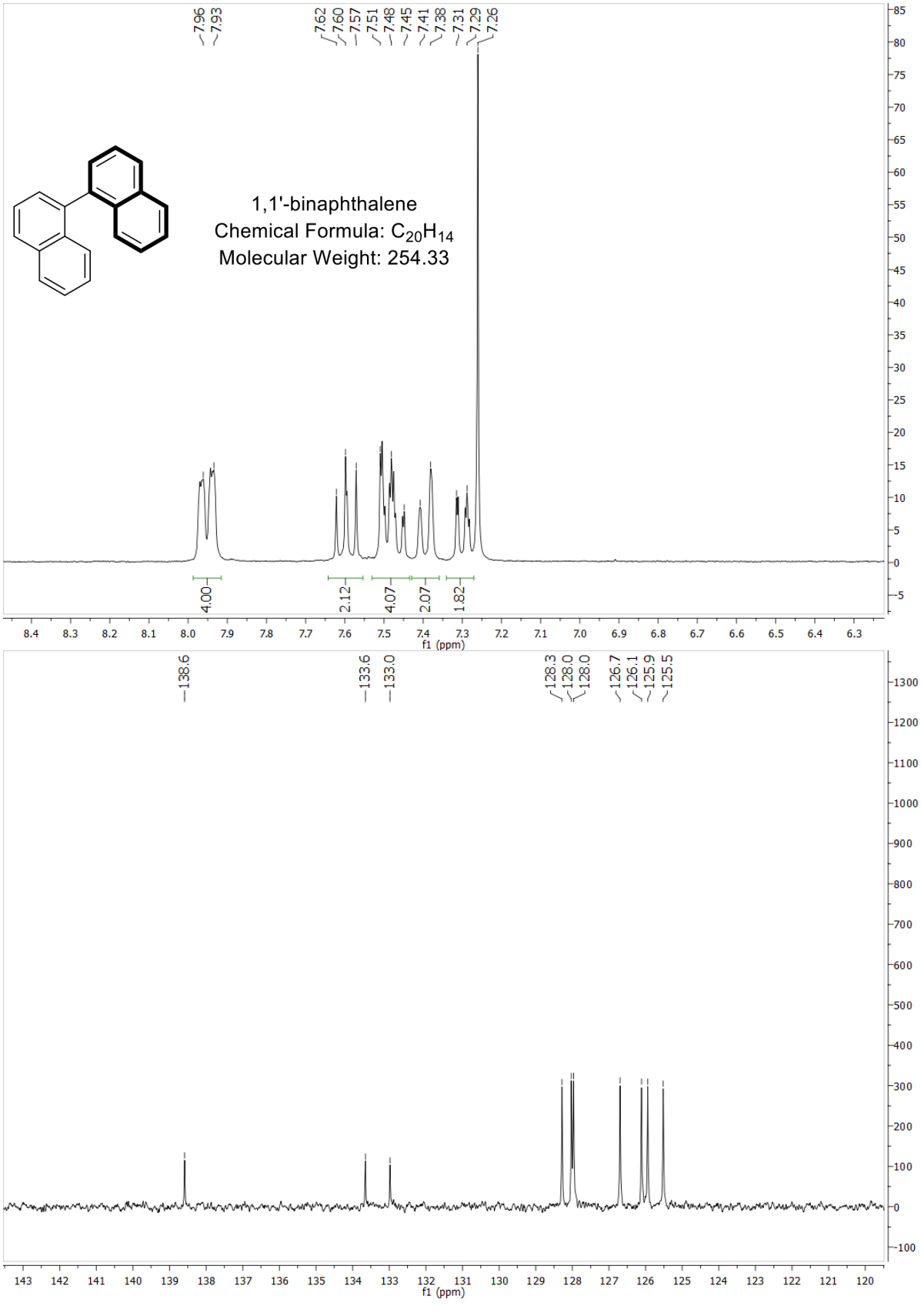

157.7
157.4
134.5
133.9
132.5
131.3
129.5
128.8
127.8
127.2
126.5
125.5
124.6
77.2
f1 (ppm)

Product, 3q

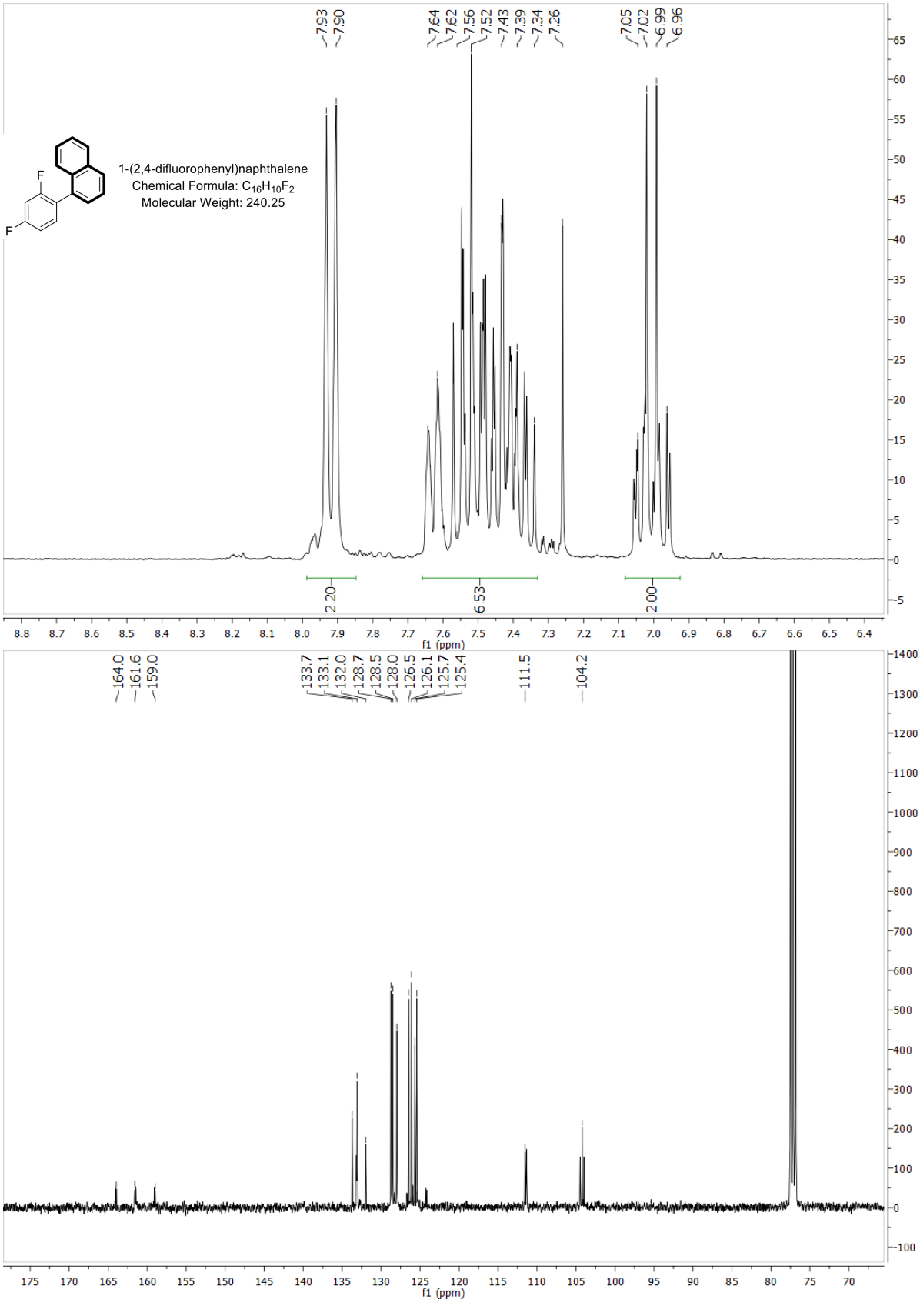

2-(naphthalen-1-yl)pyridine
Chemical Formula: $C_{15}H_{11}N$
Molecular Weight: 205.26
f1 (ppm)


f1 (ppm)

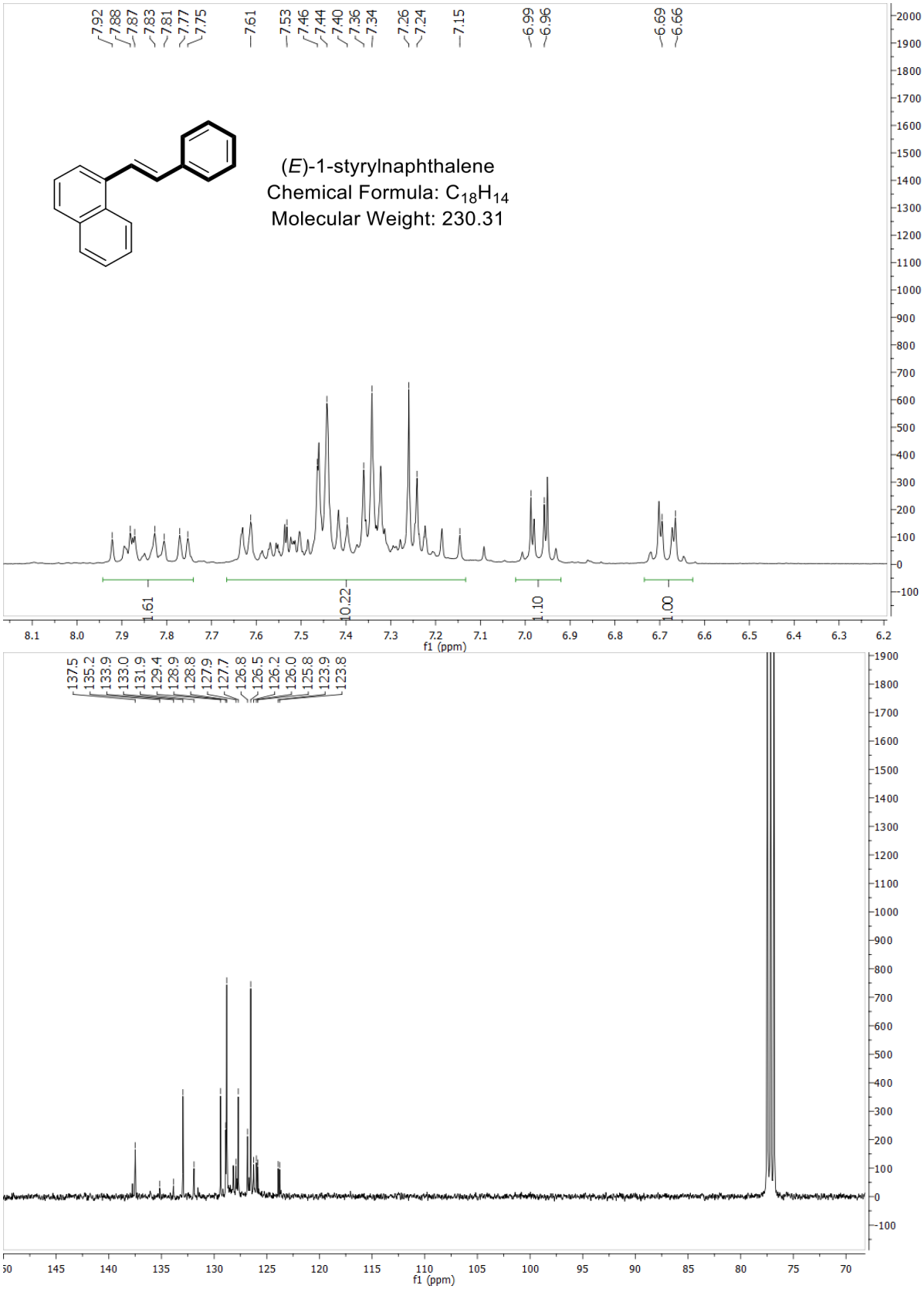
Product, 3r


7.96
7.93
7.62
7.60
7.57
7.51
7.48
7.45
7.41
7.38
7.31
7.29
7.26
1,1'-binaphthalene
Chemical Formula: C20H14
Molecular Weight: 254.33
4.00
2.12
4.07
2.07
1.82
f1 (ppm)
138.6
133.6
133.0
128.3
128.0
128.0
126.7
126.1
125.9
125.5
f1 (ppm)

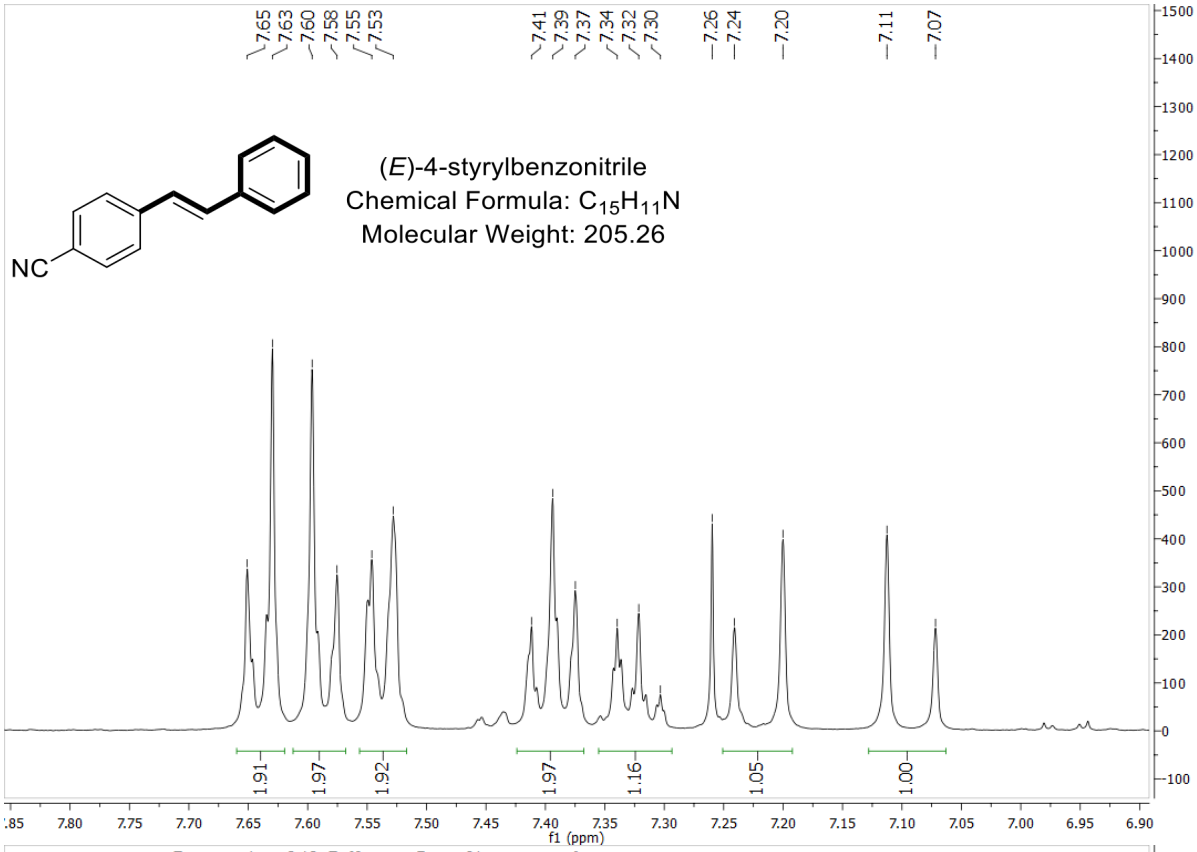
Product, 3s

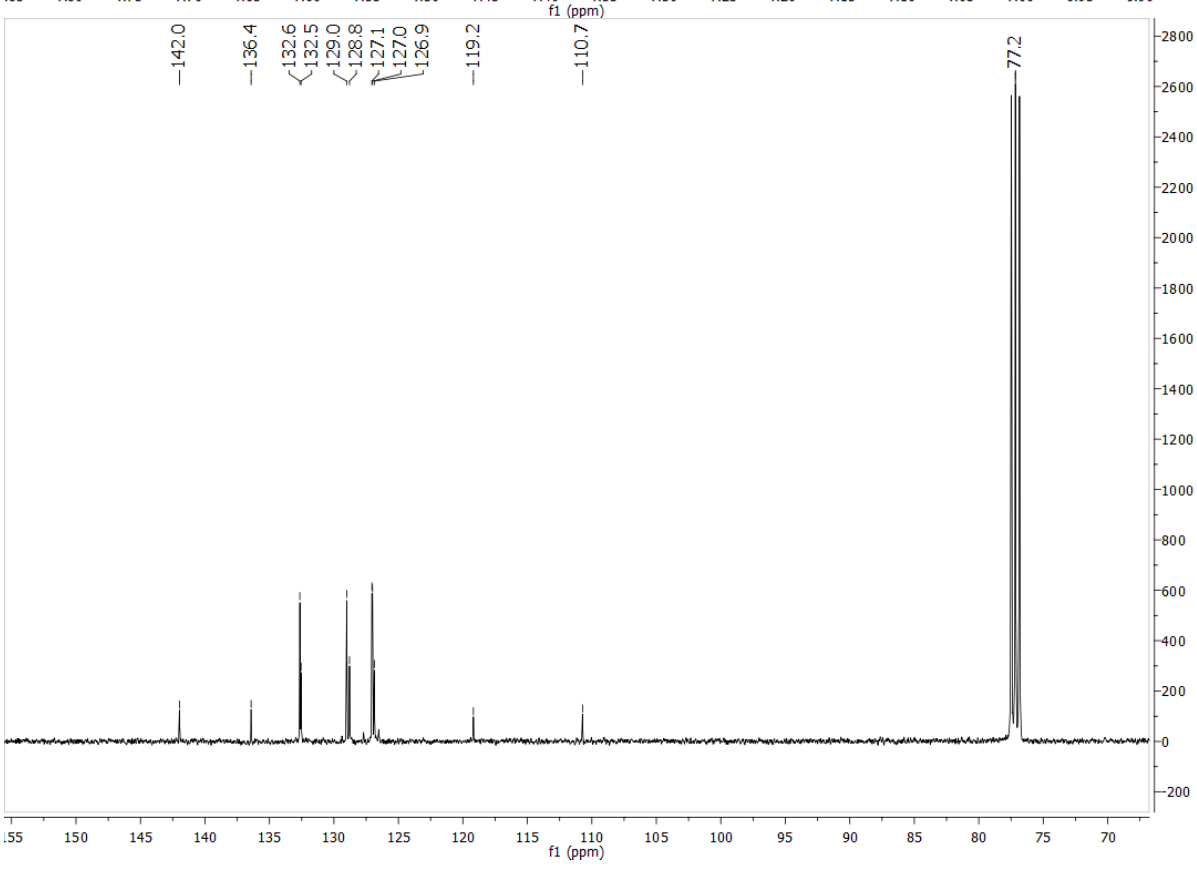

7.93
7.90
7.64
7.62
7.56
7.52
7.43
7.39
7.34
7.26
7.05
7.02
6.99
6.96
F
F
1-(2,4-difluorophenyl)naphthalene
Chemical Formula: C16H10F2
Molecular Weight: 240.25
2.20
6.53
2.00
f1 (ppm)
164.0
161.6
159.0
133.7
133.1
132.0
128.7
128.5
128.0
126.5
126.1
125.7
125.4
111.5
104.2
f1 (ppm)

Product, 3t

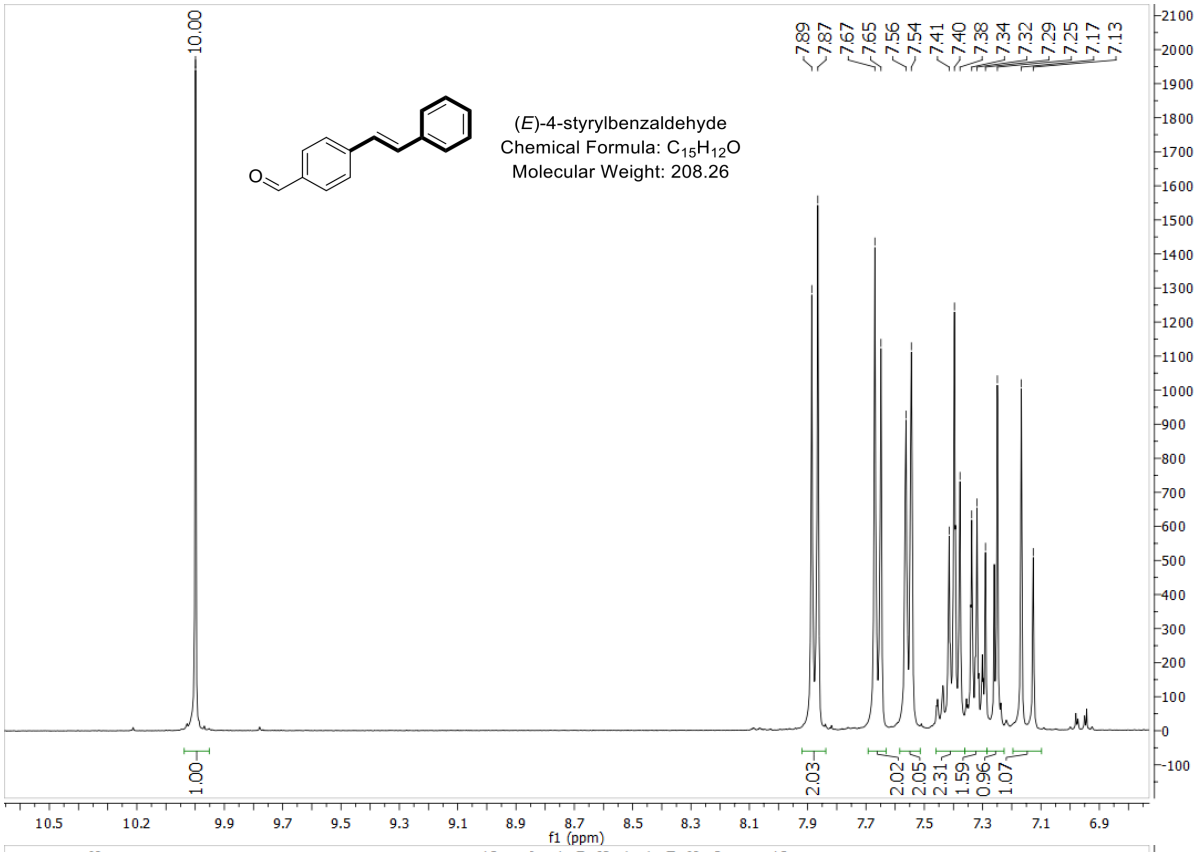

7.92
7.88
7.87
7.83
7.81
7.77
7.75
7.61
7.53
7.46
7.44
7.40
7.36
7.34
7.26
7.24
7.15
6.99
6.96
6.69
6.66
(E)-1-styrylnaphthalene
Chemical Formula: C18H14
Molecular Weight: 230.31
1.61
10.22
1.10
1.00
f1 (ppm)
137.5
135.2
133.9
133.0
131.9
129.4
128.9
128.8
127.9
127.7
126.8
126.5
126.2
126.0
125.8
123.9
123.8
f1 (ppm)

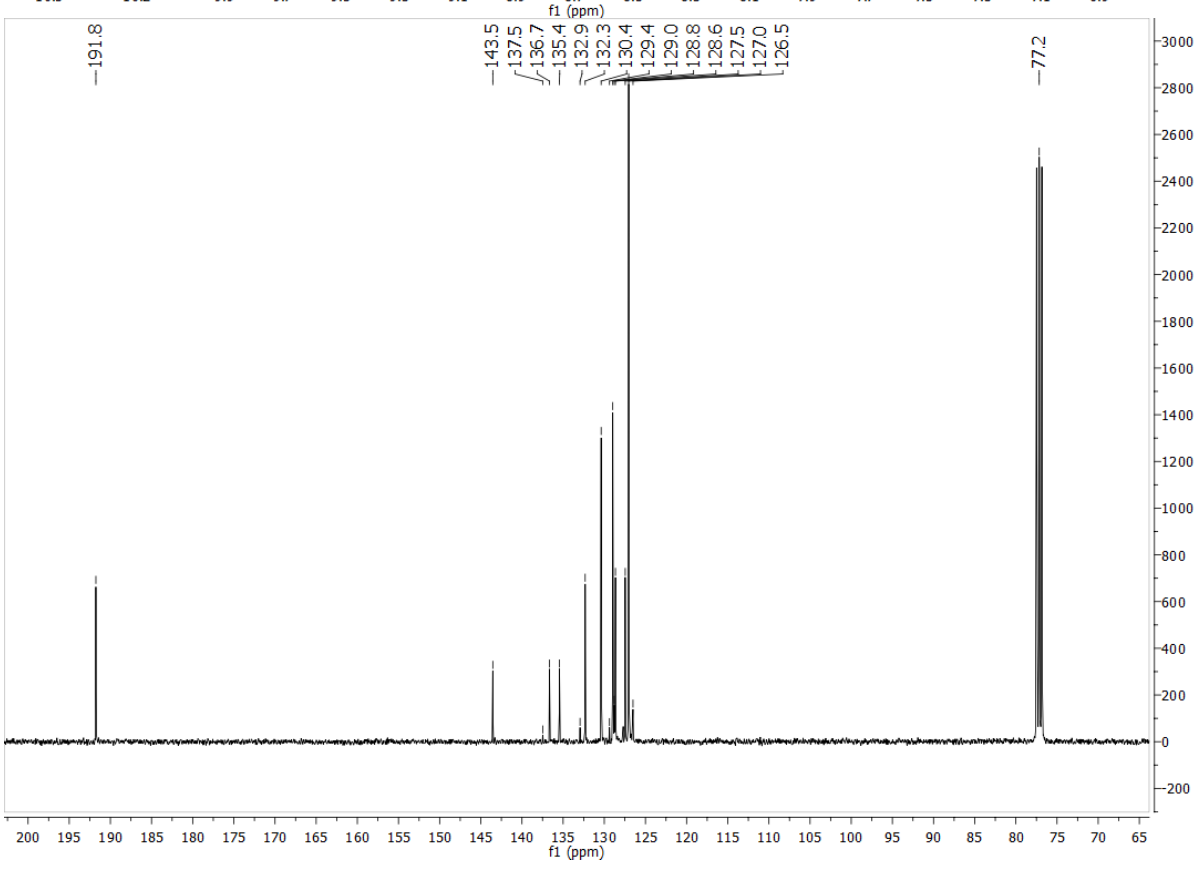
Product, 3u


7.65
7.63
7.60
7.58
7.55
7.53
7.41
7.39
7.37
7.34
7.32
7.30
7.26
7.24
7.20
7.11
7.07
(E)-4-styrylbenzonitrile
Chemical Formula: C15H11N
Molecular Weight: 205.26
NC
1.91
1.97
1.92
1.97
1.16
1.05
1.00
f1 (ppm)

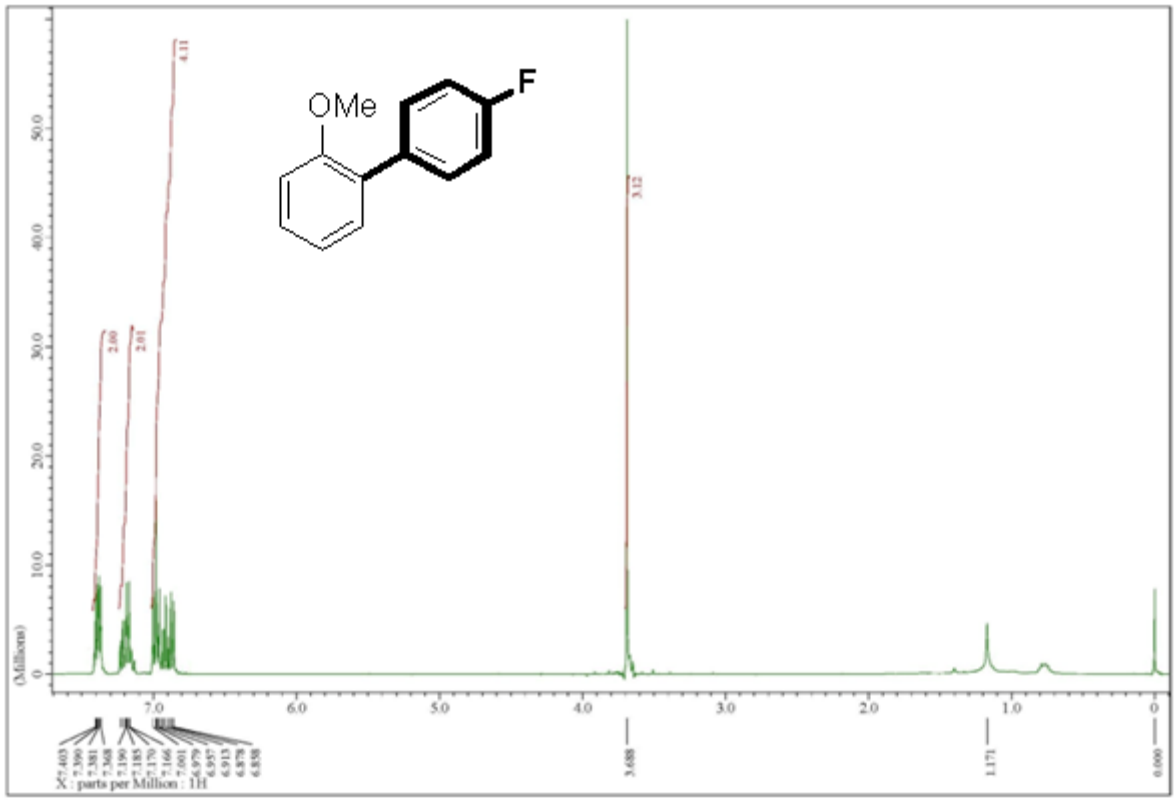

142.0
136.4
132.6
132.5
129.0
128.8
127.1
127.0
126.9
119.2
110.7
77.2
f1 (ppm)

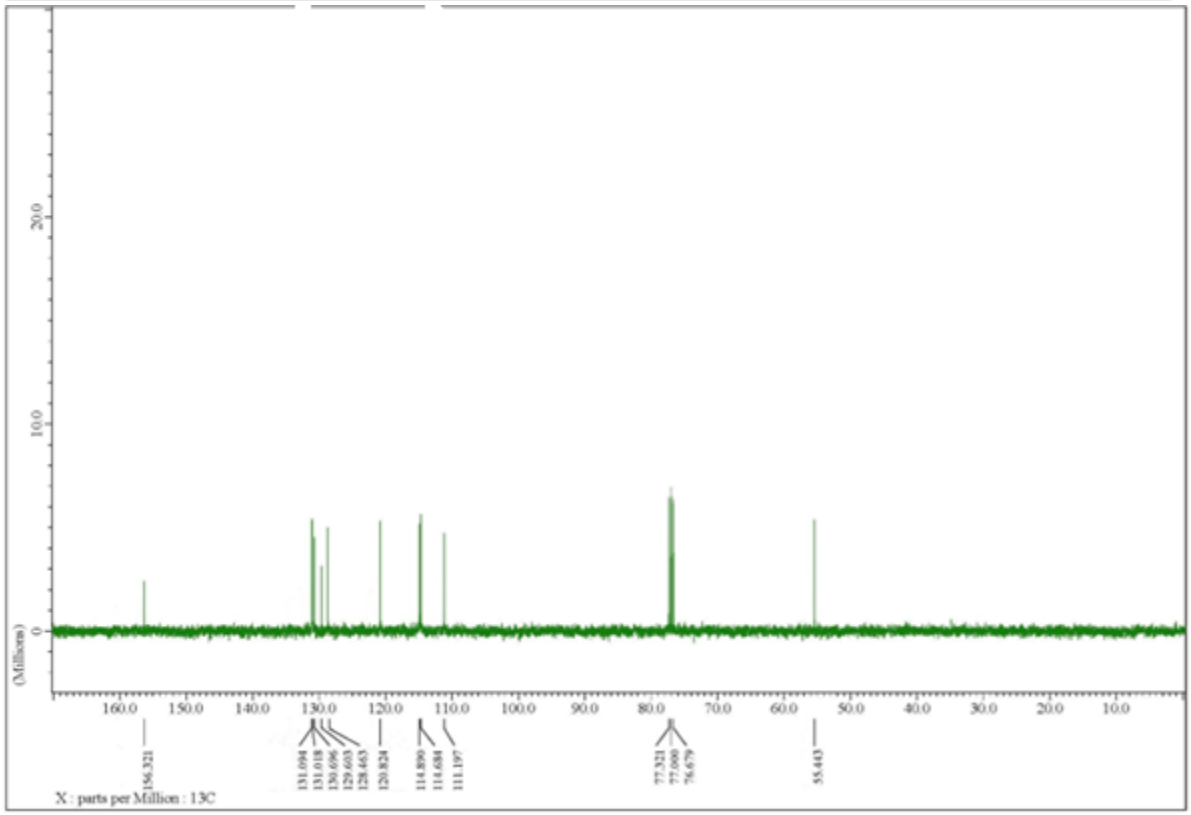
Product, 3v


(E)-4-styrylbenzaldehyde
Chemical Formula: C15H12O
Molecular Weight: 208.26
10.00
7.89
7.87
7.67
7.65
7.56
7.54
7.41
7.40
7.38
7.34
7.32
7.29
7.25
7.17
7.13
1.00
2.03
2.02
2.05
2.31
1.59
0.96
1.07
f1 (ppm)

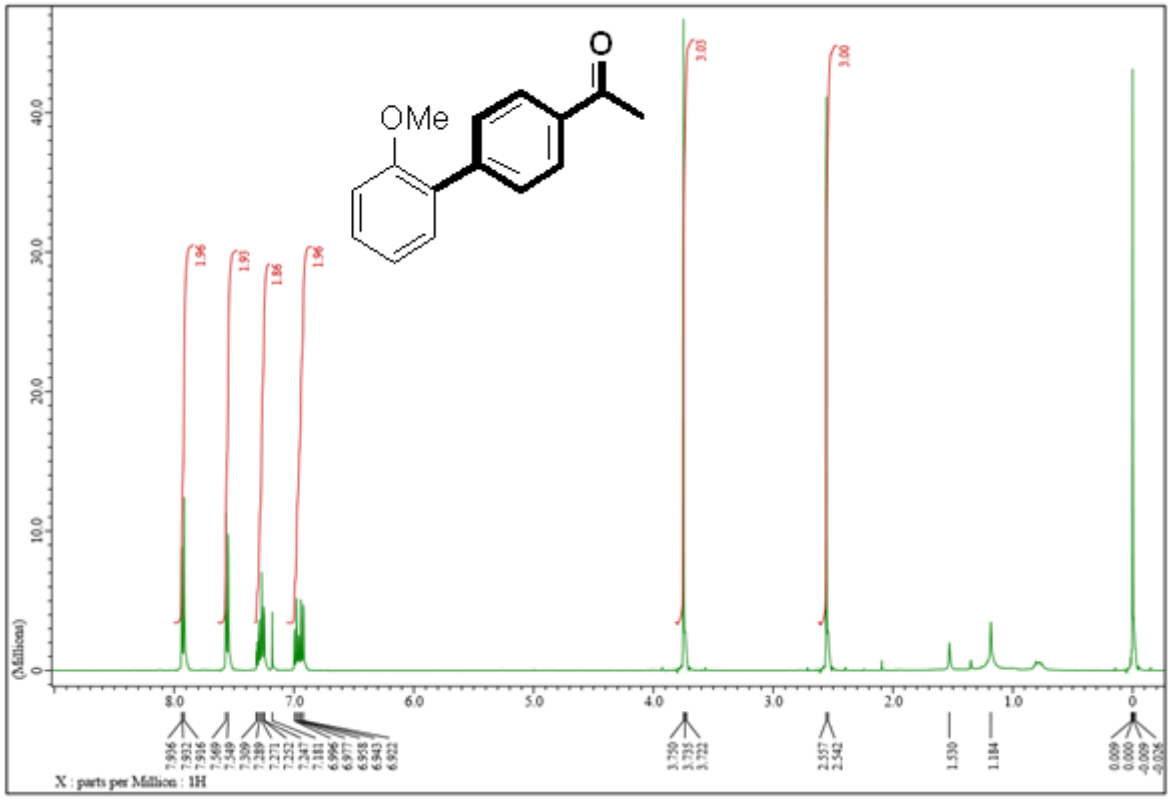

191.8
143.5
137.5
136.7
135.4
132.9
132.3
130.4
129.4
129.0
128.8
128.6
127.5
127.0
126.5
77.2
f1 (ppm)

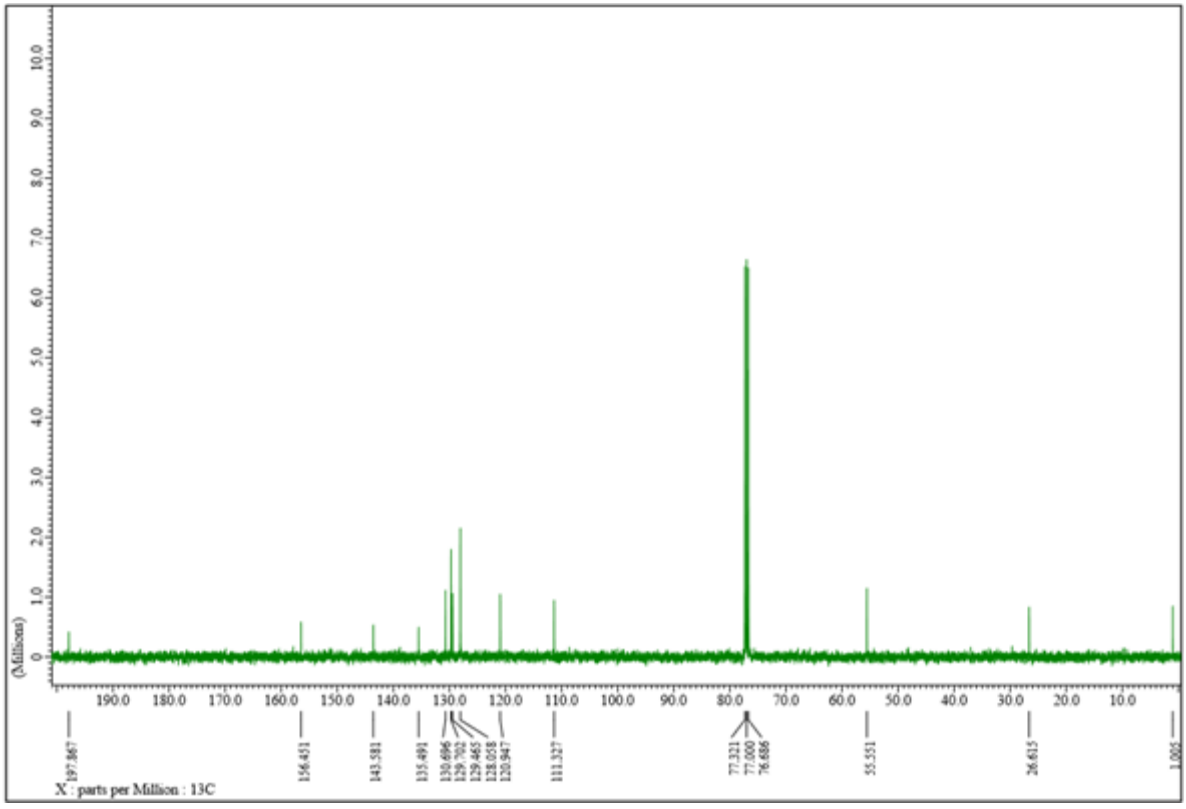
Product, 4a:


OMe
F
4.11
3.12
2.00
2.01
(Millions)
X : parts per Million : 1H

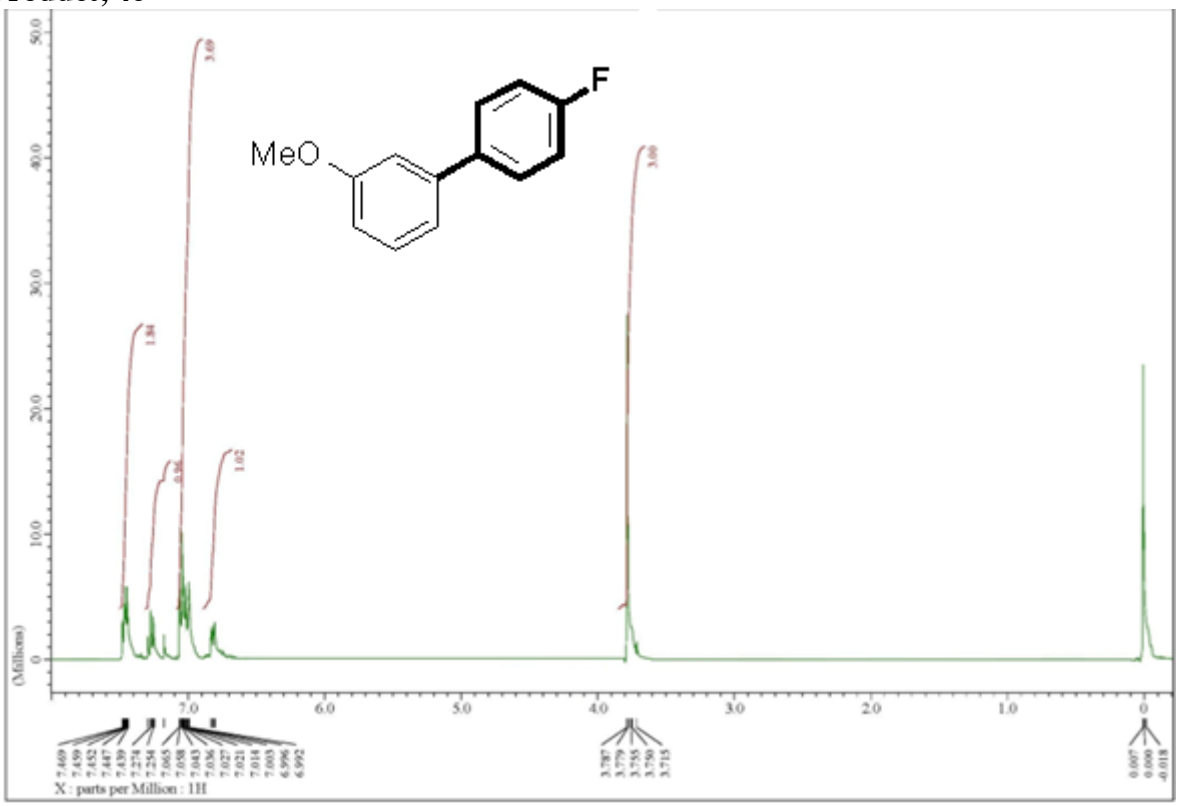

(Millions)
X : parts per Million : 13C

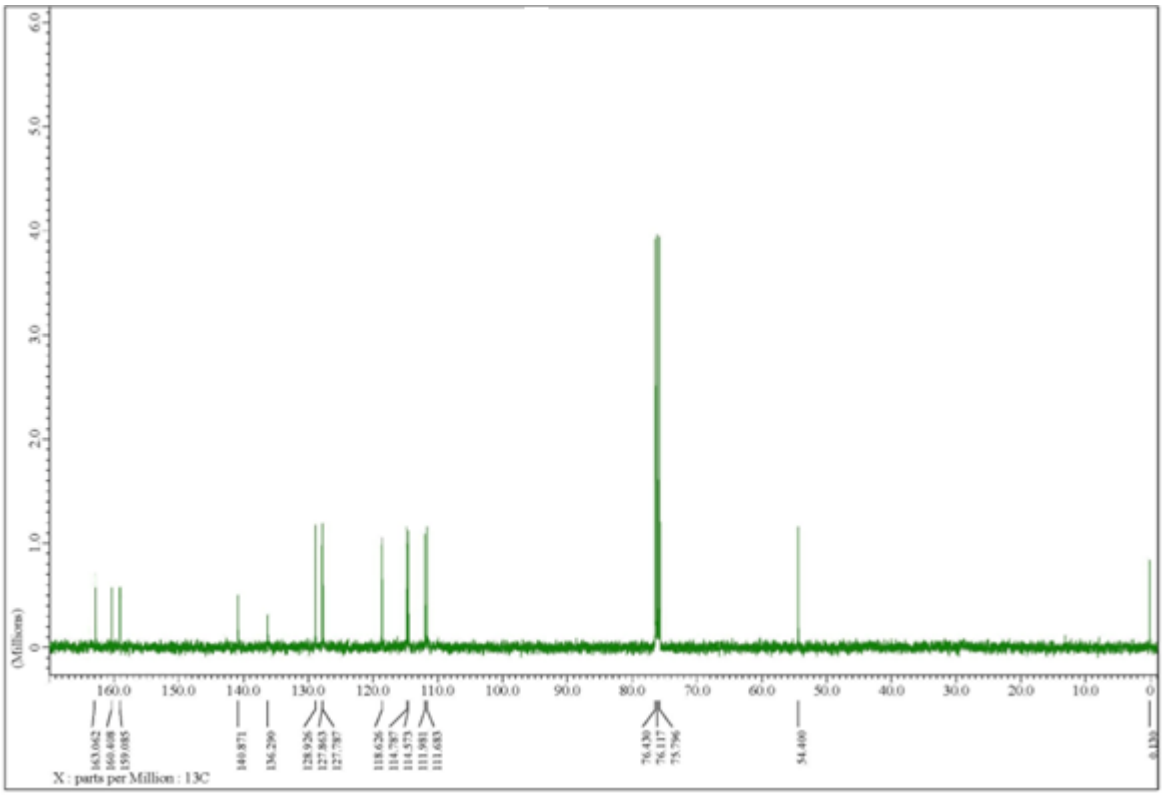
Product, 4b:


OMe
O
3.03
3.00
1.96
1.93
1.86
1.96
X : parts per Million : 1H

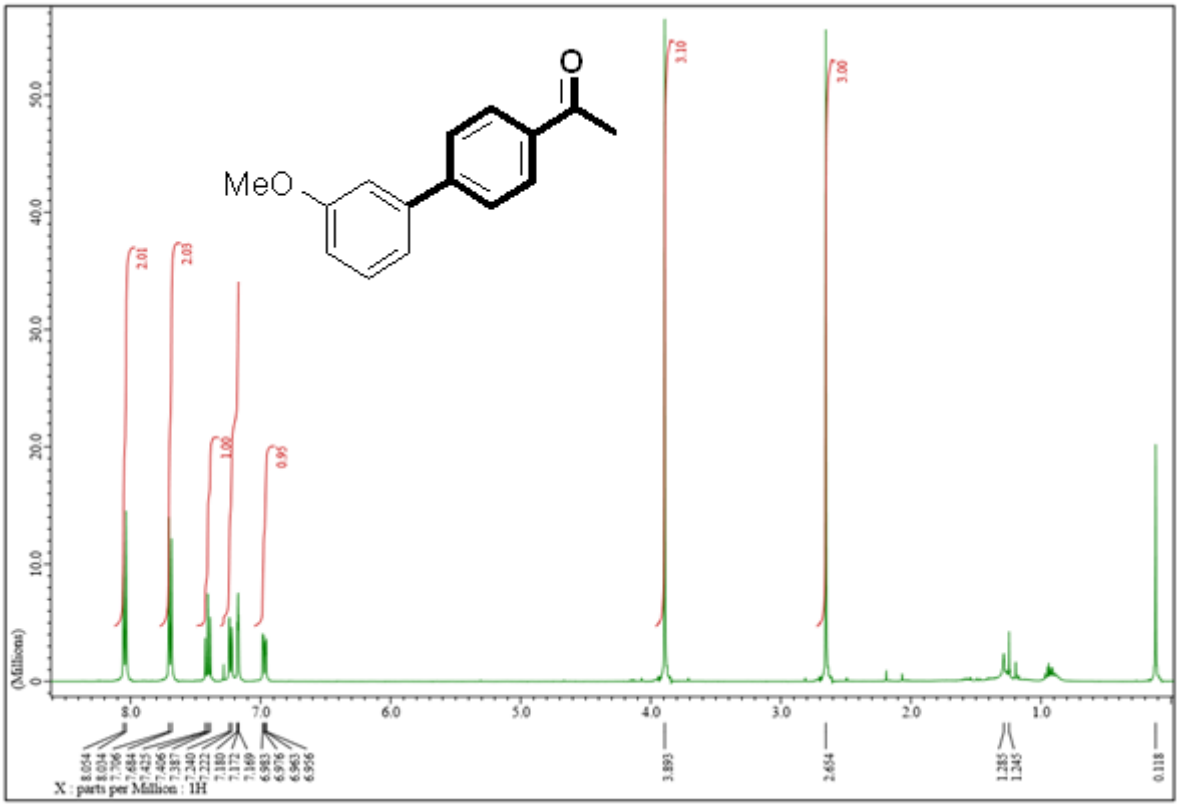

X : parts per Million : 13C

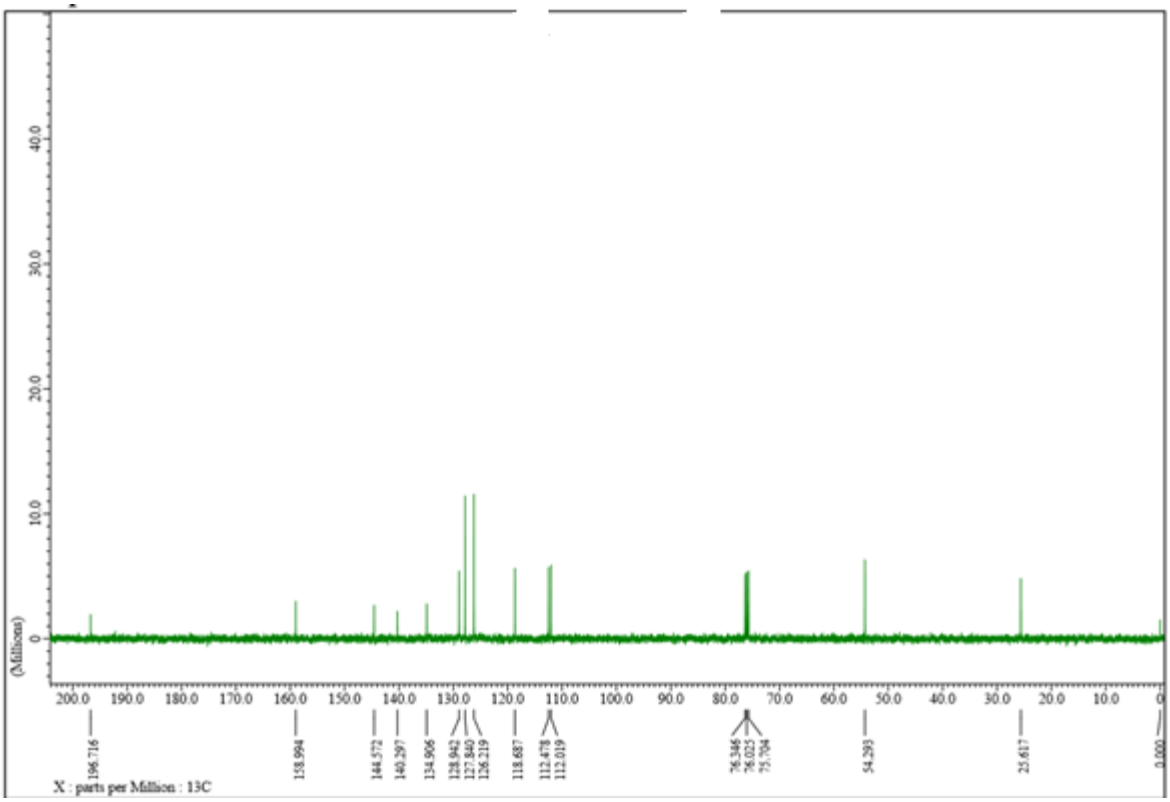
Product, 4c



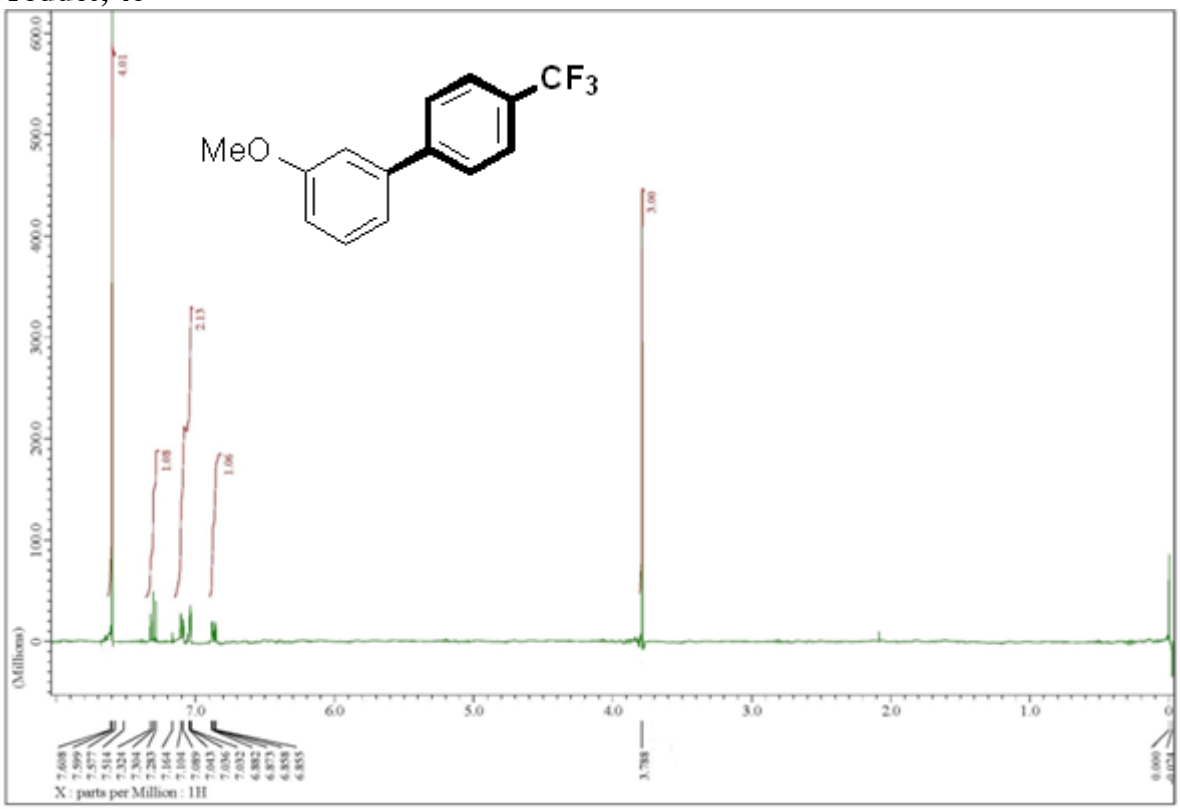


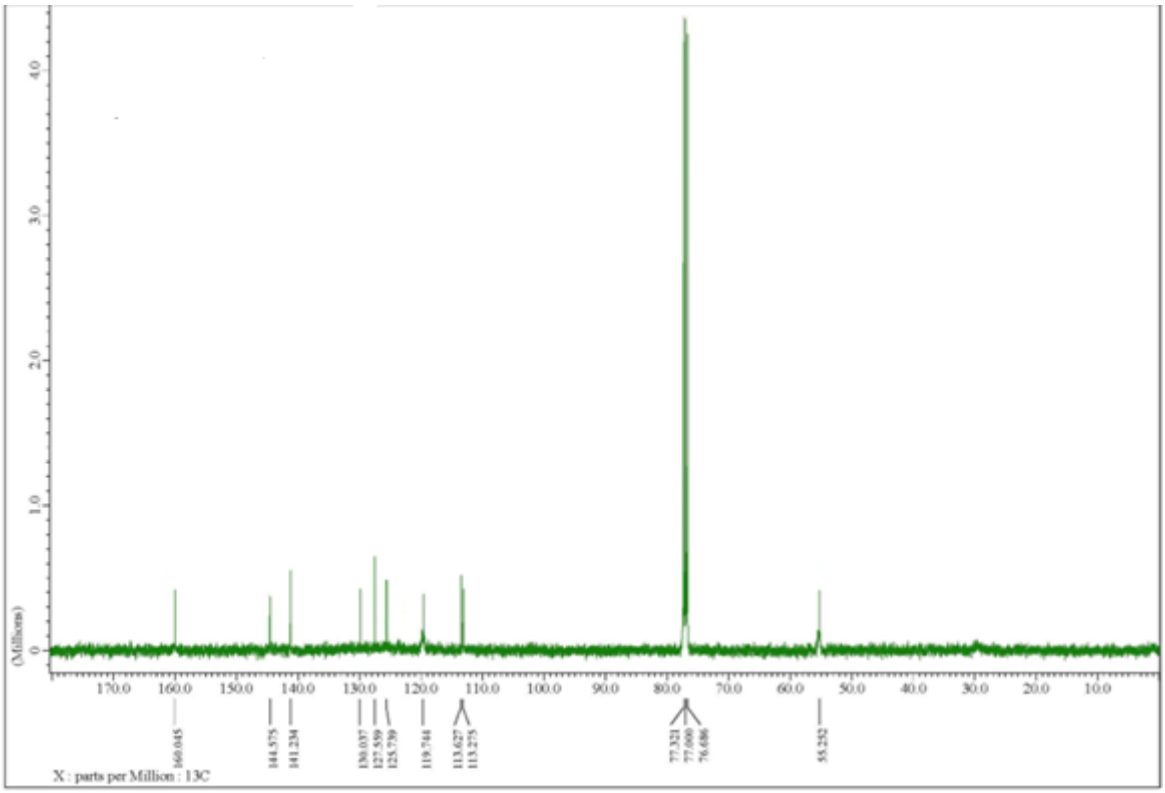
Product, 4d



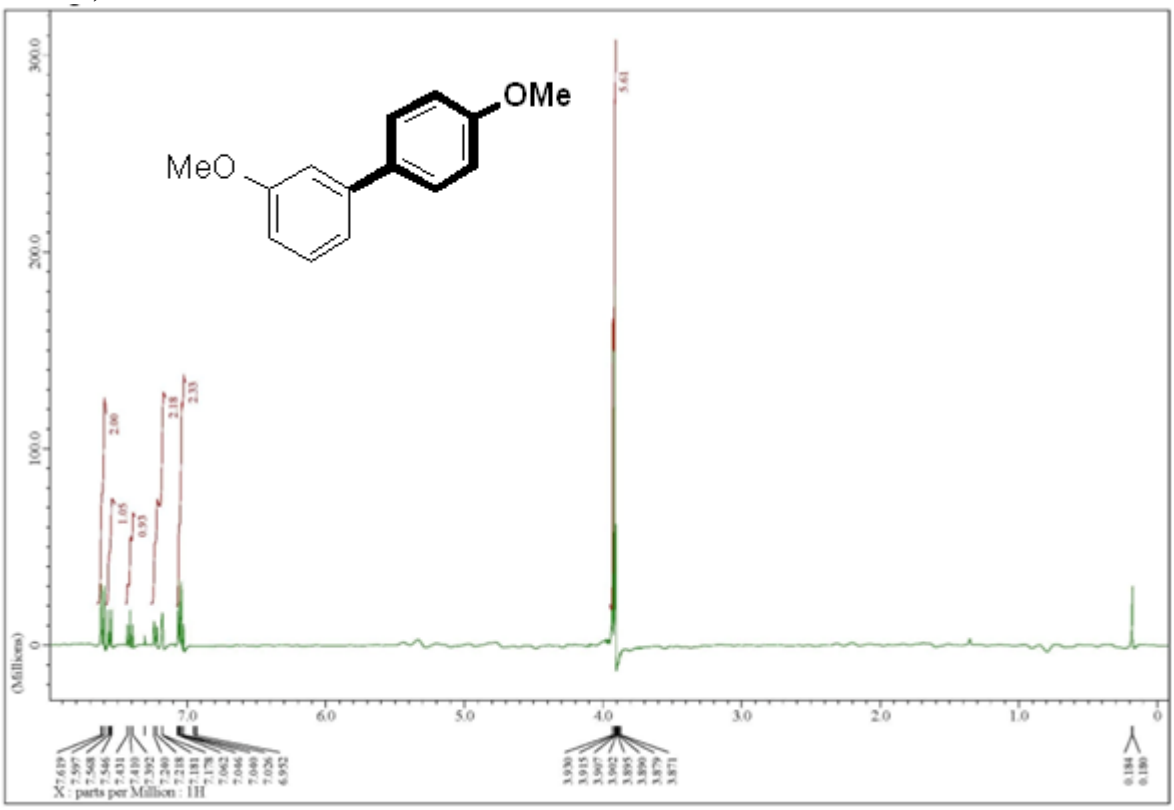


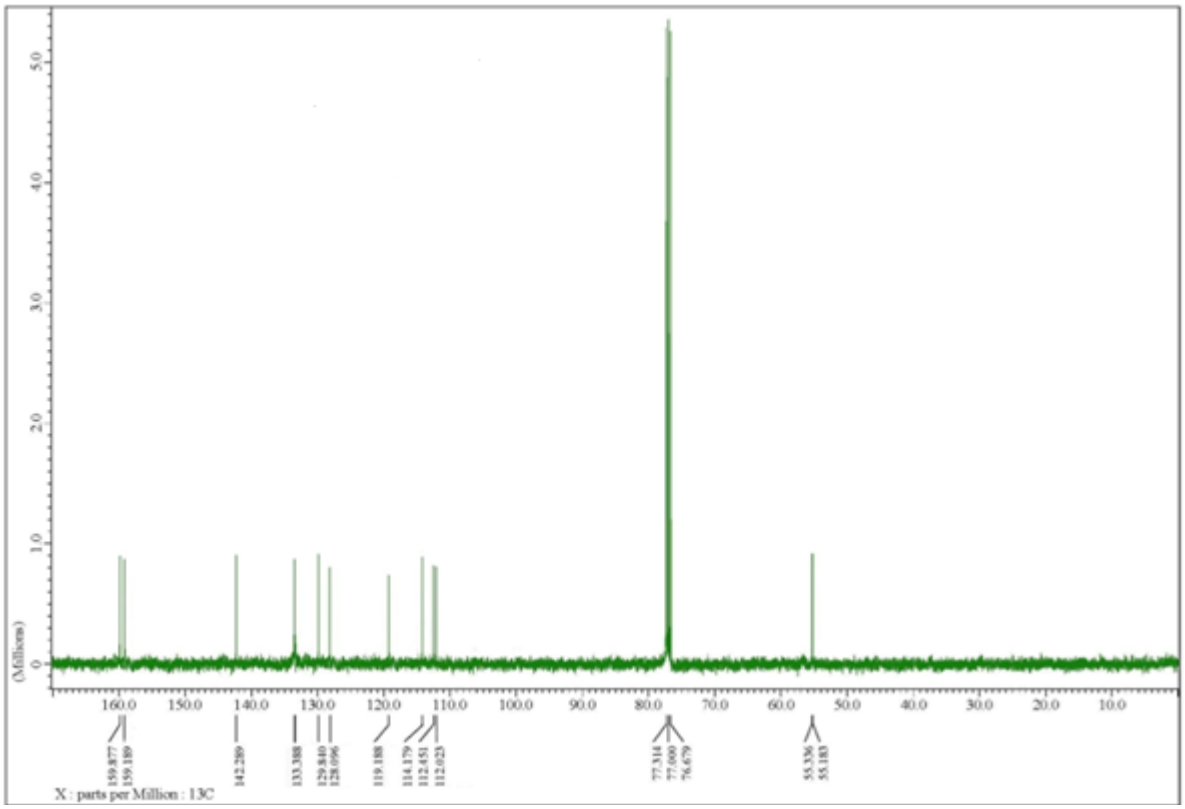
Product, 4e



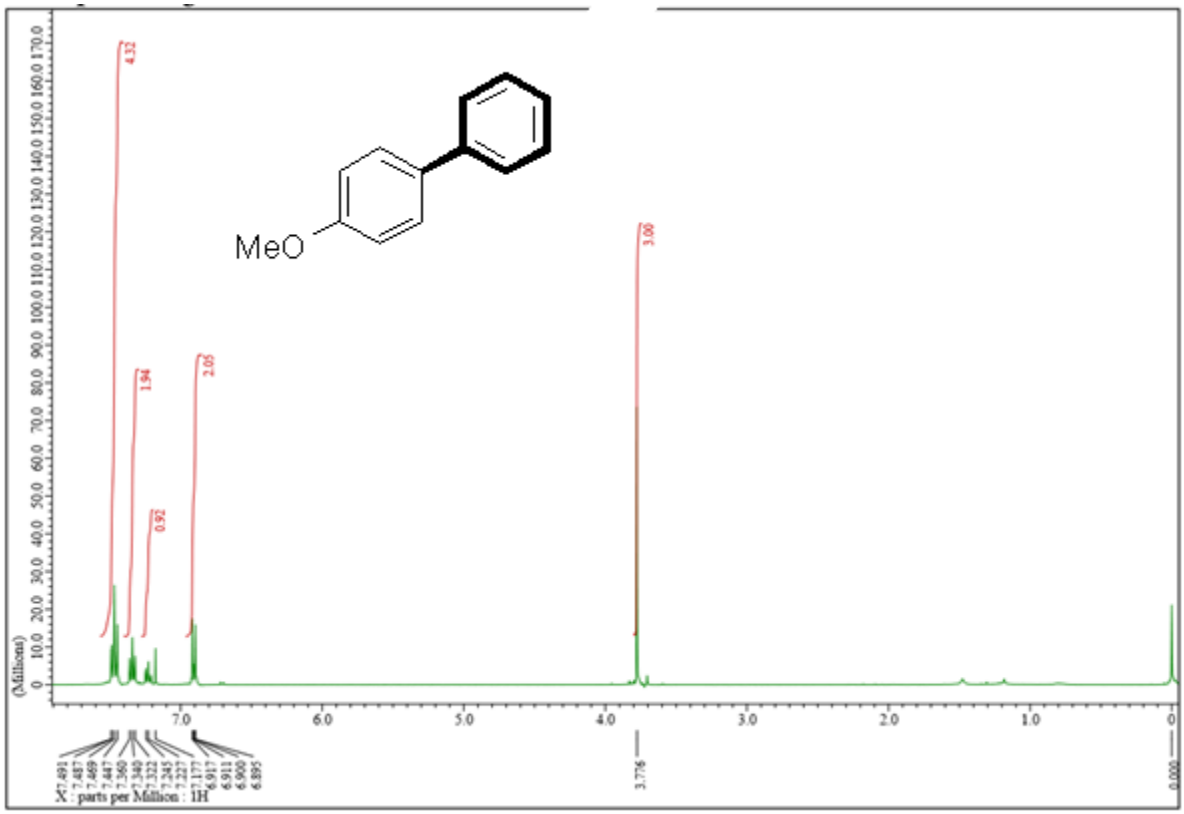


Product, 4f

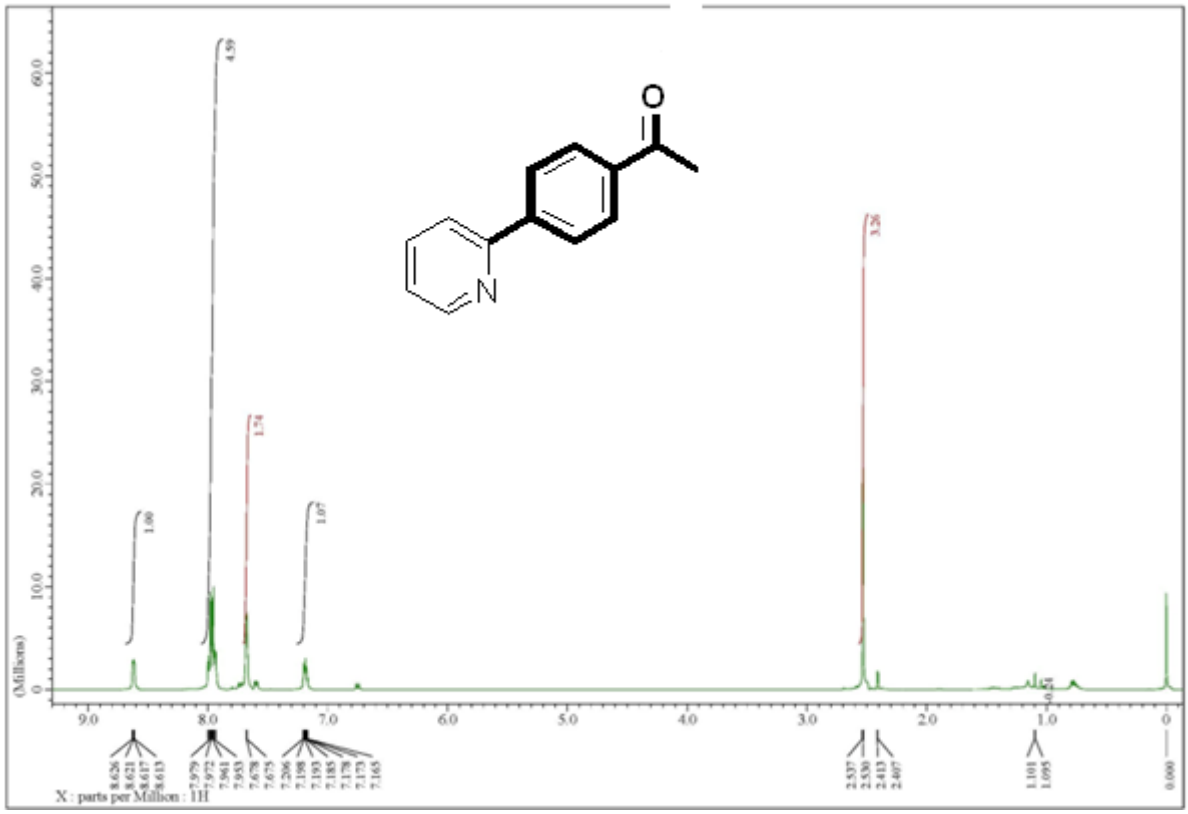


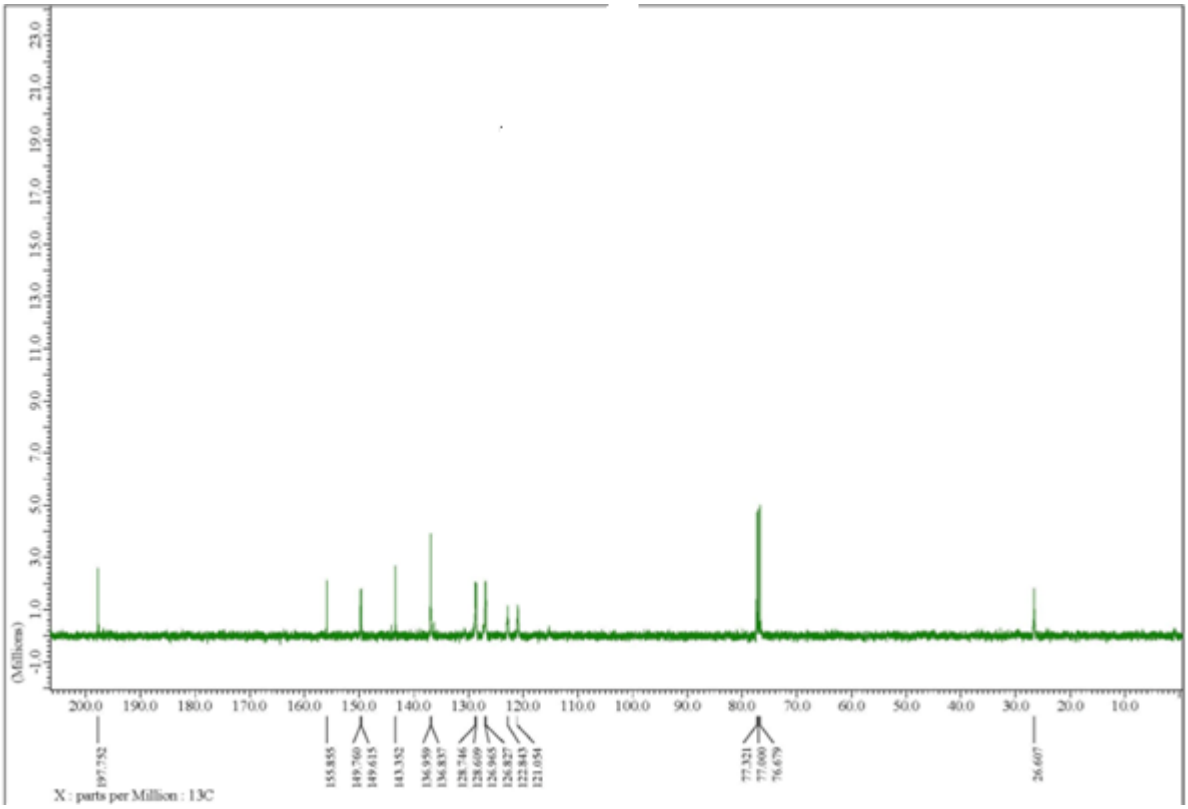


Product, 4g



Product, 4h




(Millions)
23.0
21.0
19.0
17.0
15.0
13.0
11.0
9.0
7.0
5.0
3.0
1.0
-1.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
197.752
155.855
149.760
149.615
143.352
136.959
136.837
128.746
128.659
126.965
126.827
122.843
121.054
77.321
77.000
76.679
26.607
X : parts per Million : 13C

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