

Supporting Information

Spectral Data of Products

4-Acetyl-1,1'-biphenyl (Table 2, Entries 1 and 15)

Obtained (196 mg, 100% for Table 2, Entry 1; 176 mg, 90% for Table 2, Entry 15) from 4-iodoacetophenone (246 mg, 1 mmol) and phenylboronic acid (1.1 mmol, 122 mg) or 4-bromoacetophenone (199 mg, 1 mmol) and phenylboronic acid (1.1 mmol, 122 mg).

^1H NMR (CDCl_3) 2.64 (3H, s), 7.41 (1H, t, $J = 7.2$ Hz), 7.47 (2H, t, $J = 7.2$ Hz), 7.63 (2H, d, $J = 6.8$ Hz), 7.69 (2H, d, $J = 6.8$ Hz), 8.03 (2H, d, $J = 8.4$ Hz); MS (EI) m/z (%) 196 (M^+ , 29), 181 (100).

Ethyl biphenyl-4-carboxylate (Table 2, Entries 2 and 16)

Obtained (226 mg, 100% for Table 2, Entry 2; 176 mg, 78% for Table 2, Entry 16) from ethyl 4-iodobenzoate (276 mg, 1 mmol) and phenylboronic acid (1.1 mmol, 122 mg) or ethyl 4-bromobenzoate (229 mg, 1 mmol) and phenylboronic acid (1.1 mmol, 122 mg).

^1H NMR (CDCl_3) 1.41 (3H, t, $J = 7.6$ Hz), 4.40 (2H, q, $J = 7.6$ Hz), 7.39 (1H, t, $J = 7.6$ Hz), 7.46 (2H, t, $J = 7.6$ Hz), 7.61–7.66 (4H, m), 8.11 (2H, d, $J = 8.8$ Hz); MS (EI) m/z (%) 226 (M^+ , 70), 181 (100).

Ethyl biphenyl-2-carboxylate (Table 2, Entry 3)

Obtained (199 mg, 88% for Table 2, Entry 3) from ethyl 2-iodobenzoate (276 mg, 1 mmol) and phenylboronic acid (1.1 mmol, 122 mg).

^1H NMR (CDCl_3) 0.99 (3H, t, $J = 7.2$ Hz), 4.09 (2H, q, $J = 7.2$ Hz), 7.31–7.42 (7H, m), 7.52 (2H, d, $J = 8.0$ Hz), 7.82 (2H, d, $J = 8.3$ Hz); MS (EI) m/z (%) 226 (M^+ , 40), 181 (100).

4-Methylbiphenyl (Table 2, Entry 4)

Obtained (153 mg, 91% for Table 2, Entry 4) from 4-iodotoluene (218 mg, 1 mmol) and phenylboronic acid (1.1 mmol, 122 mg).

^1H NMR (CDCl_3) 2.40 (3 H, s), 7.25 (2H, d, $J = 8.4$ Hz), 7.34 (1H, t, $J = 8.0$ Hz), 7.43 (2H, t, $J = 8.0$ Hz), 7.49 (2H, d, $J = 8.0$ Hz), 7.58 (2H, m); MS (EI) m/z (%) 168 (M^+ , 100).

4-Methoxybiphenyl (Table 2, Entry 5)

Obtained (149 mg, 81% for Table 2, Entry 5) from 4-iodoanisole (234 mg, 1 mmol) and phenylboronic acid (1.1 mmol, 122 mg).

^1H NMR (CDCl_3) 3.85 (3H, s), 6.98 (2H, d, $J = 8.8$ Hz), 7.30 (1H, t, $J = 7.6$ Hz), 7.41 (2H, t, $J = 7.6$ Hz), 7.52–7.56 (4H, m); MS (EI) m/z (%) 184 (M^+ , 100).

3, 4'-Diacetylbiphenyl (Table 2, Entry 6)

Obtained (236 mg, 99% for Table 2, Entry 6) from 4-iodoacetophenone (246 mg, 1 mmol) and 3-acetyl phenylboronic acid (1.1 mmol, 180 mg). Although the compound has been reported in three papers, the ^1H NMR and ^{13}C NMR data were not found in the literature.

^1H NMR (CDCl_3) 2.65 (3H, s), 2.67 (3 H, s), 7.57 (1H, t, $J = 7.8$ Hz), 7.71 (2H, d, $J = 8.8$ Hz), 7.83 (1H, d, $J = 6.8$ Hz), 7.97 (1H, d, $J = 7.8$ Hz), 8.05 (2H, d, $J = 6.8$ Hz), 8.21 (1H, s); ^{13}C NMR (CDCl_3) 26.6, 26.7, 126.9, 127.3, 128.1, 129.0, 129.2, 131.7, 136.3, 137.7, 140.4, 144.6, 197.6, 197.8 ; MS (EI) m/z (%) 238 (M^+ , 40), 223 (100).

Ethyl 4'-acetyl-[1, 1'-biphenyl]-4-carboxylate (Table 2, Entry 7)

Obtained (244 mg, 91% for Table 2, Entry 7) from ethyl 4-iodobenzoate (276 mg, 1 mmol) and 4-acetylphenylboronic acid (1.1 mmol, 180 mg).

¹H NMR (CDCl₃) 1.42 (3H, t, *J* = 7.2 Hz), 2.64 (3H, s), 4.41 (2H, q, *J* = 7.2 Hz), 7.67–7.71 (4H, m), 8.04 (2H, d, *J* = 8.4 Hz), 8.13 (2H, d, *J* = 8.4 Hz); MS (EI) *m/z* (%) 268 (M⁺, 34), 253 (100).

4-Acetyl-4'-methoxy-1,1'-biphenyl (Table 2, Entries 8 and 9 and 17)

Obtained (219 mg, 97% for Table 2, Entry 8; 201 mg, 89% for Table 2, Entry 9; 219 mg, 97% for Table 2, Entry 17) from 4-iodoanisole (234 mg, 1 mmol) and 4-acetylphenylboronic acid (1.1 mmol, 180 mg) or 4-iodoacetophenone (246 mg, 1 mmol) and 4-methoxyphenylboronic acid (1.1 mmol, 167 mg) or 4-bromoacetophenone (199 mg, 1 mmol) and 4-methoxyphenylboronic acid (1.1 mmol, 167 mg).

¹H NMR (CDCl₃) 2.63 (3H, s), 3.87 (3H, s), 7.00 (2H, d, *J* = 9.0 Hz), 7.58 (2H, d, *J* = 9.0 Hz), 7.65 (2H, d, *J* = 8.4 Hz), 8.00 (2H, d, *J* = 8.4 Hz); MS (EI) *m/z* (%) 226 (M⁺, 50), 211 (100).

4'-Methoxy-biphenyl-4-carboxylic acid ethyl ester (Table 2, Entries 10 and 18)

Obtained (248 mg, 97% for Table 2, Entry 10; 256 mg, 100% for Table 2, Entry 18) from ethyl 4-iodobenzoate (276 mg, 1 mmol) and 4-methoxyphenylboronic acid (1.1 mmol, 167 mg) or ethyl 4-bromobenzoate (229 mg, 1 mmol) and 4-methoxyphenylboronic acid (1.1 mmol, 167 mg).

¹H NMR (CDCl₃) 1.41 (3H, t, *J* = 7.6 Hz), 3.85 (3H, s), 4.40 (2H, q, *J* = 7.6 Hz), 7.00 (2H, d, *J* = 8.8 Hz), 7.56–7.63 (4H, m), 8.08 (2H, d, *J* = 8.8 Hz); MS (EI) *m/z* (%) 256 (M⁺, 100).

4-Methoxy-4'-methylbiphenyl (Table 2, Entry 11)

Obtained (198 mg, 100% for Table 2, Entry 11) from 4-iodotoluene (218 mg, 1 mmol) and 4-methoxyphenylboronic acid (1.1 mmol, 167 mg).

¹H NMR (CDCl₃) 2.38 (3H, s), 3.85 (3H, s), 6.96 (2H, d, *J* = 8.8 Hz), 7.24 (2H, d, *J* = 8.0 Hz), 7.44 (2H, d, *J* = 8.0 Hz), 7.50 (2H, d, *J* = 8.8 Hz); MS (EI) *m/z* (%) 198 (M⁺, 100).

4'-Methoxy-3-methyl-1,1'-biphenyl (Table 2, Entry 12)

Obtained (194 mg, 98% for Table 2, Entry 12) from 3-iodotoluene (218 mg, 1 mmol) and 4-methoxyphenylboronic acid (1.1 mmol, 167 mg).

¹H NMR (CDCl₃) 2.41 (3H, s), 3.85 (3H, s), 6.96 (2H, d, *J* = 8.4 Hz), 7.12 (1H, d, *J* = 6.4 Hz), 7.26–7.36 (3H, m), 7.52 (2H, d, *J* = 8.4 Hz); MS (EI) *m/z* (%) 198 (M⁺, 100).

4'-Methoxy-2-methyl-1,1'-biphenyl (Table 2, Entry 13)

Obtained (198 mg, 100% for Table 2, Entry 13) from 2-iodotoluene (218 mg, 1 mmol) and 4-methoxyphenylboronic acid (1.1 mmol, 167 mg).

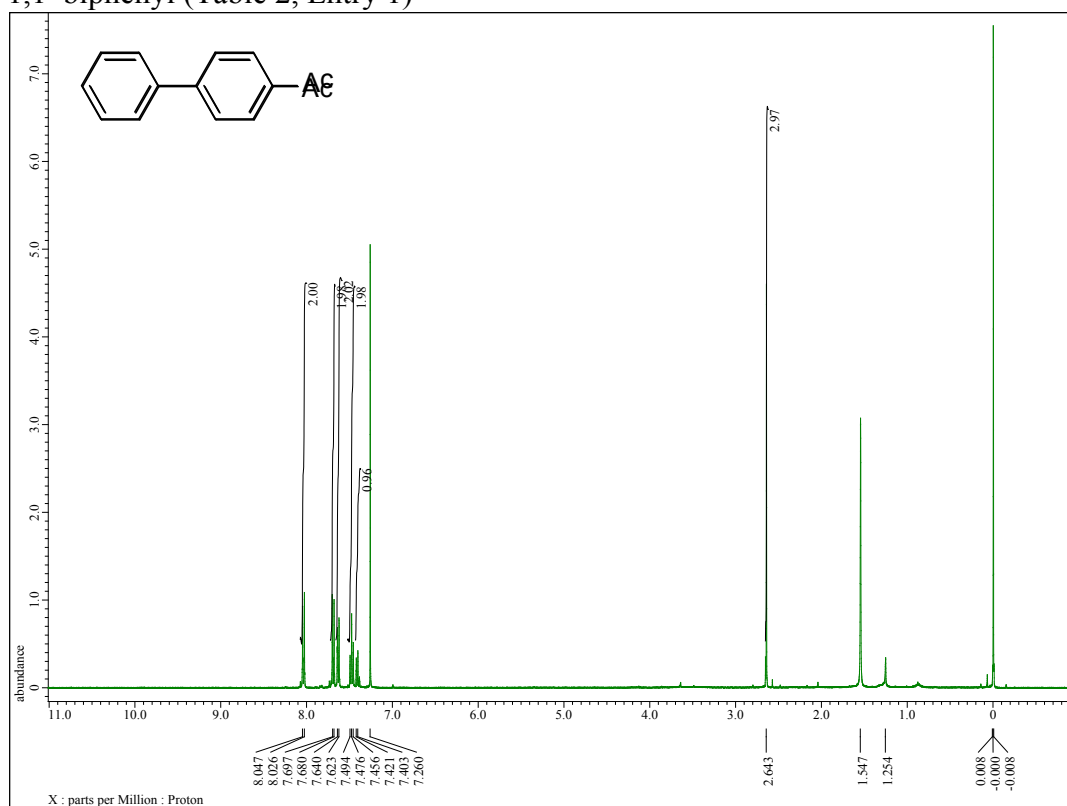
¹H NMR (CDCl₃) 2.28 (3H, s), 3.85 (3H, s), 6.94 (2H, d, *J* = 8.8 Hz), 7.21–7.26 (6H, m); MS (EI) *m/z* (%) 198 (M⁺, 100).

2, 4, 4'-Dimethoxy-1,1'-biphenyl (Table 2, Entry 14)

Obtained (190 mg, 78% for Table 2, Entry 14) from 4-iodoanisole (234 mg, 1 mmol) and 2, 4-dimethoxyphenylboronic acid (1.1 mmol, 200 mg).

^1H NMR (CDCl_3) 3.78–3.83 (9H, m), 6.54 (2H, m), 6.93 (2H, m), 7.22 (1H, m), 7.42 (2H, m); MS (EI) m/z (%) 244 (M^+ , 100).

4-Acetyl-1,1'-biphenyl (Table 2, Entry 1)



Ethyl biphenyl-4-carboxylate (Table 2, Entry 2)

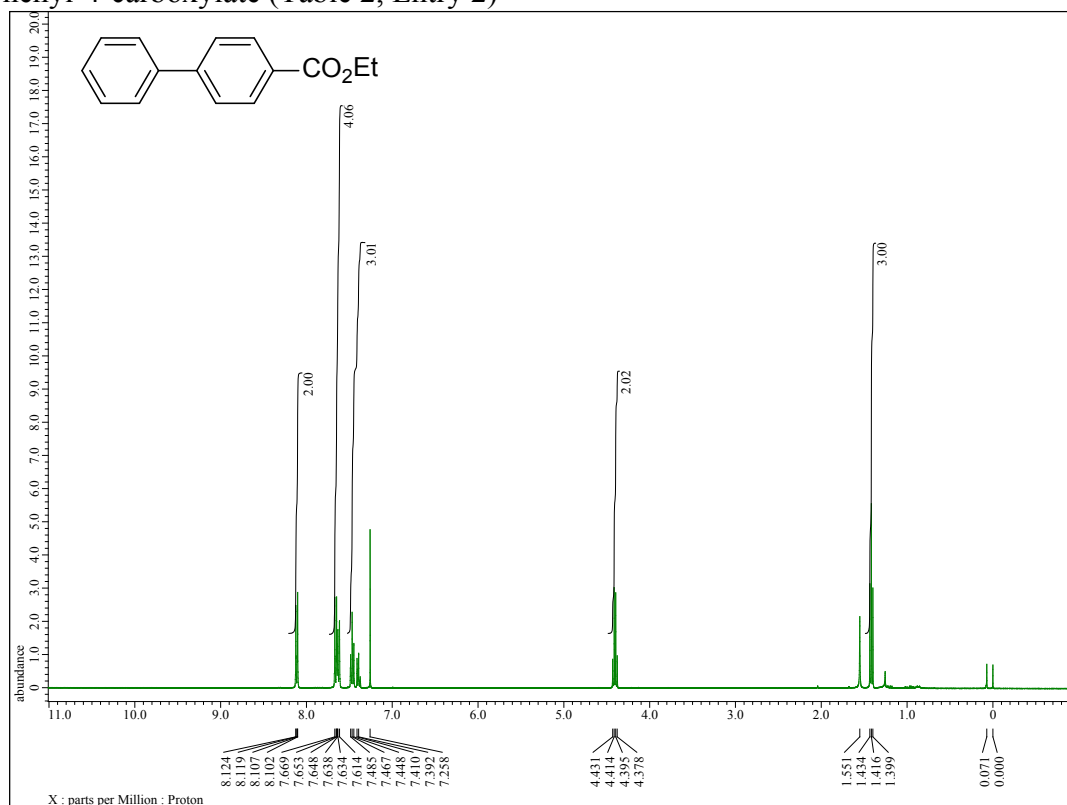
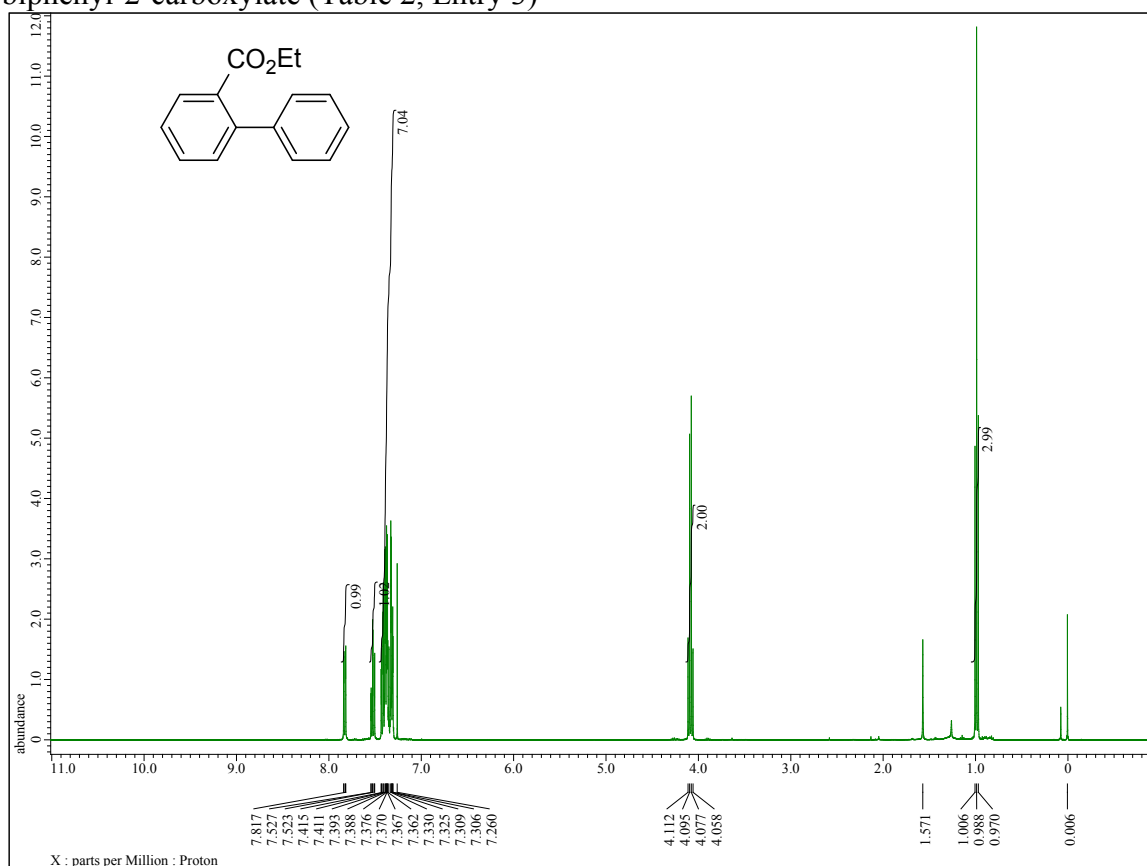


Figure S1. Cont.

Ethyl biphenyl-2-carboxylate (Table 2, Entry 3)



4-Methylbiphenyl (Table 2, Entry 4)

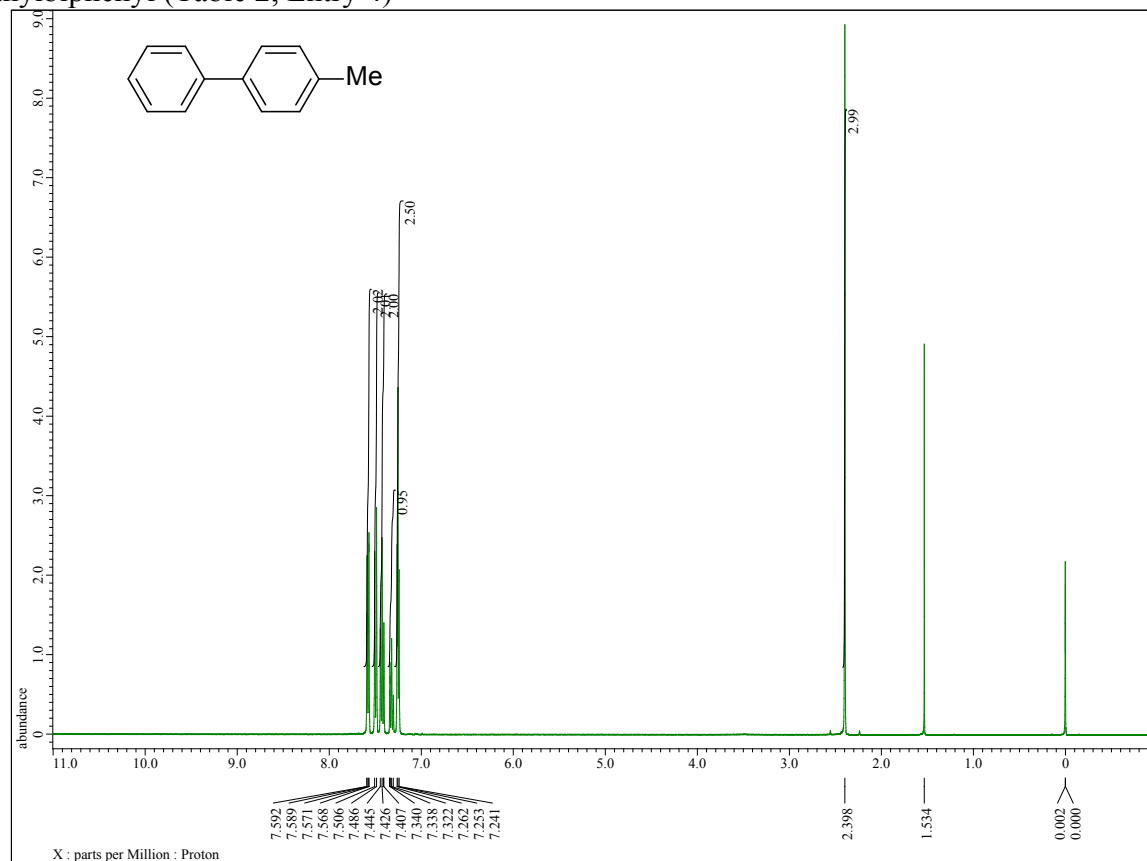
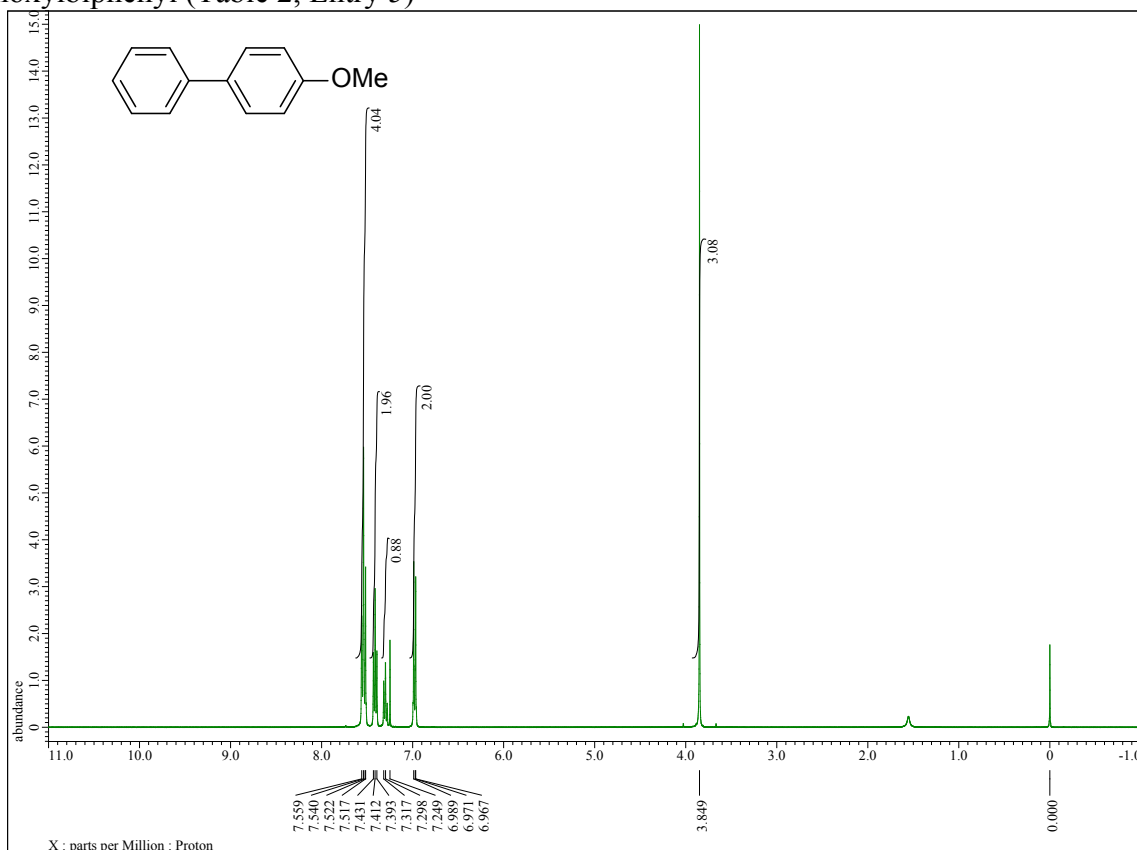


Figure S1. Cont.

4-Methoxybiphenyl (Table 2, Entry 5)



3, 4'-Diacetylbiphenyl (Table 2, Entry 6)

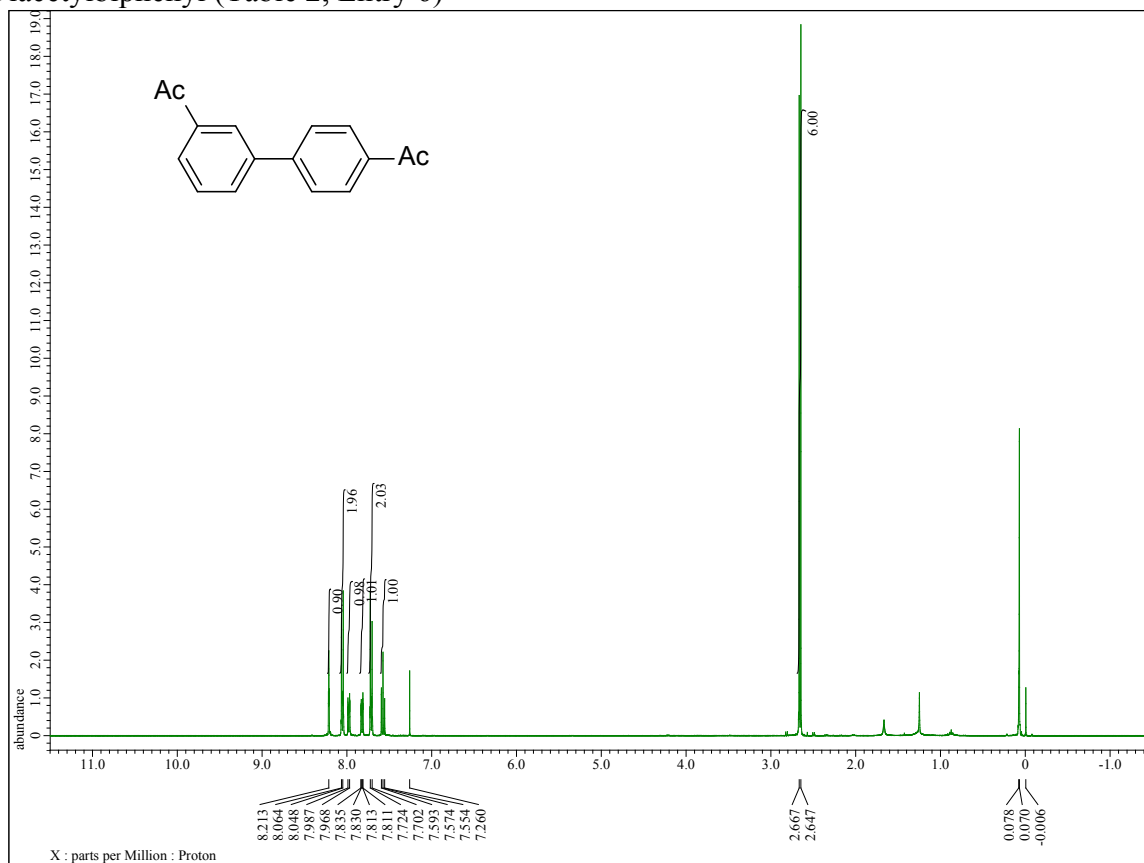
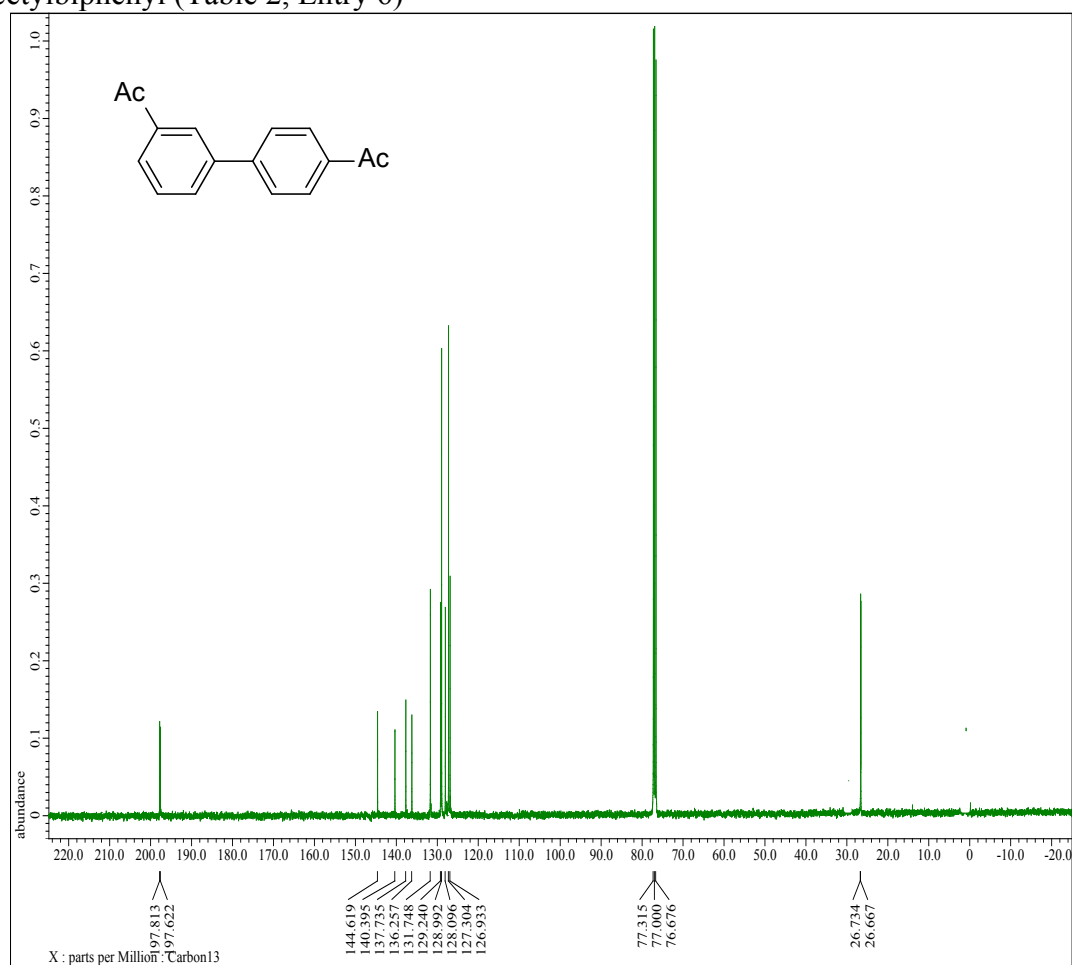


Figure S1. Cont.

3, 4'-Diacetylbiphenyl (Table 2, Entry 6)



Ethyl 4'-acetyl-[1,1'-biphenyl]-4-carboxylate (Table 2, Entry 7)

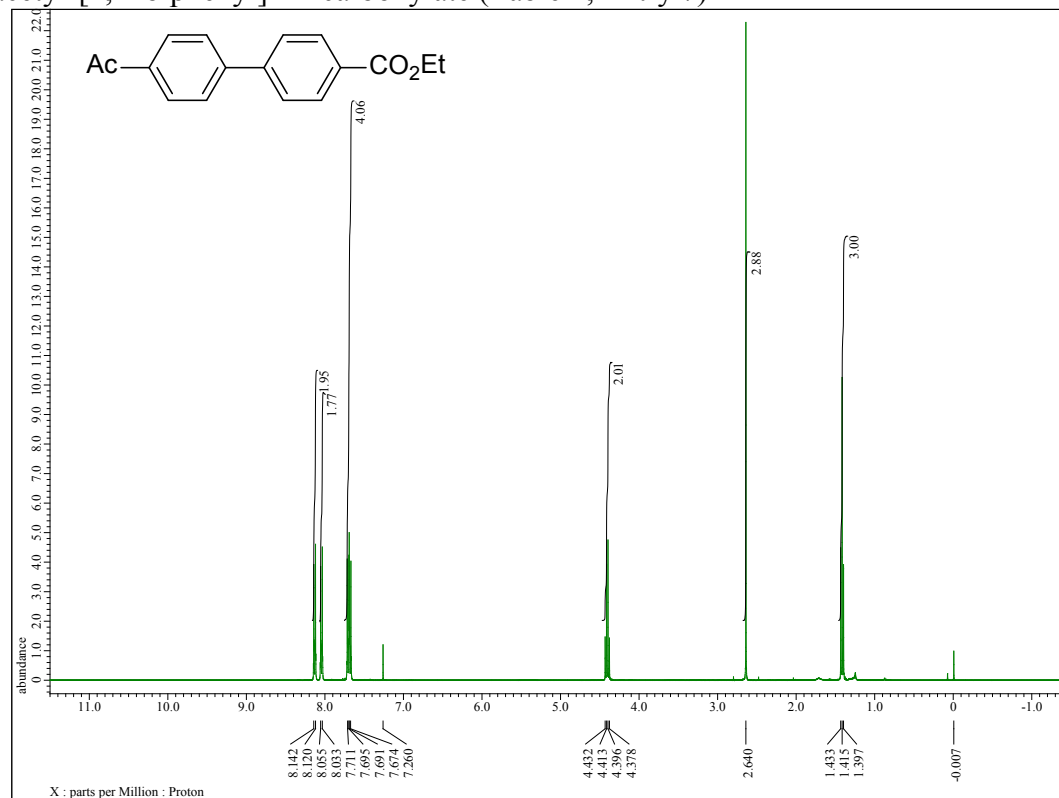
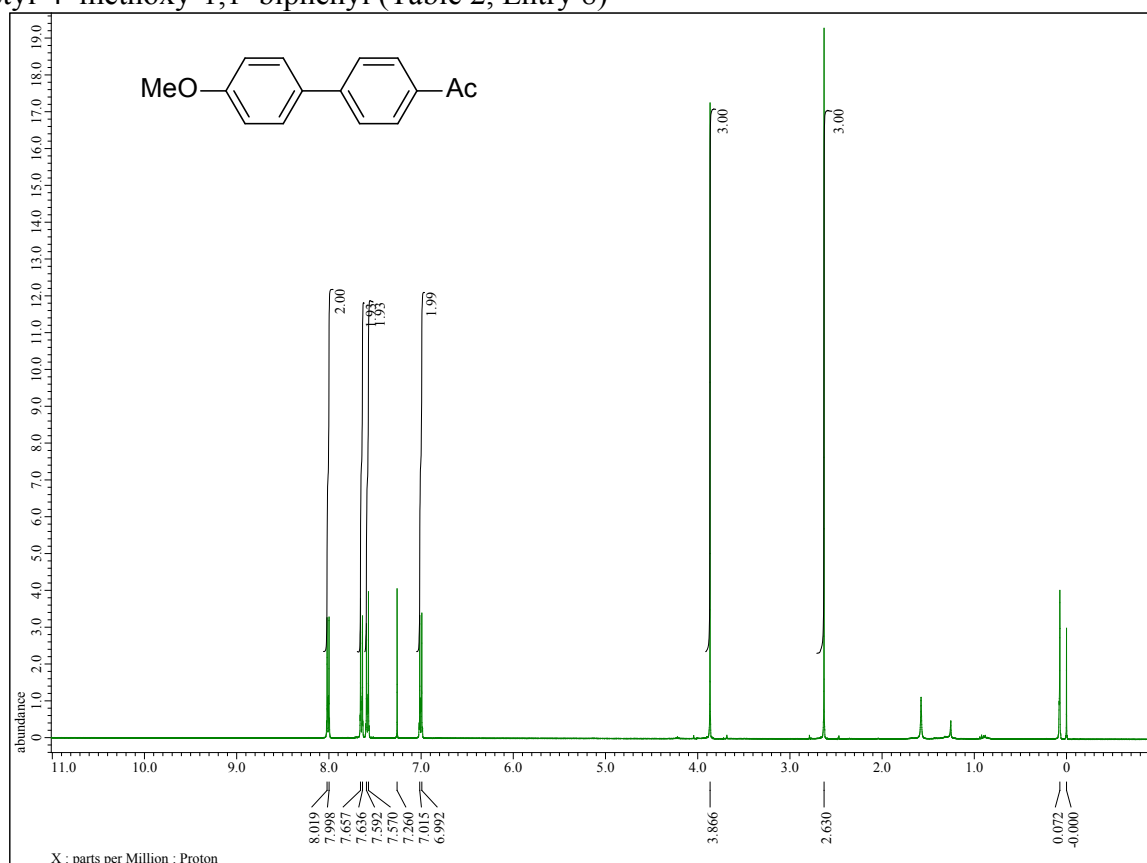


Figure S1. Cont.

4-Acetyl-4'-methoxy-1,1'-biphenyl (Table 2, Entry 8)



4-Acetyl-4'-methoxy-1,1'-biphenyl (Table 2, Entry 9)

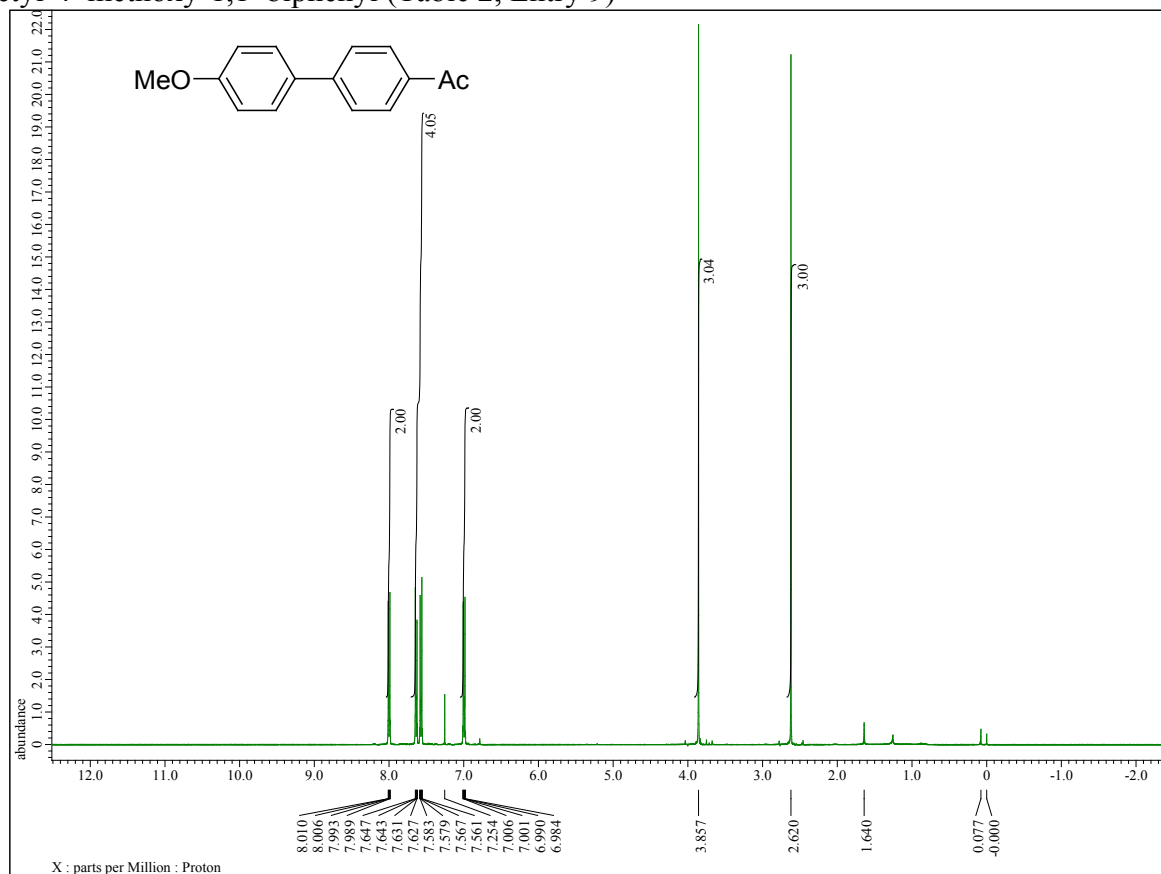
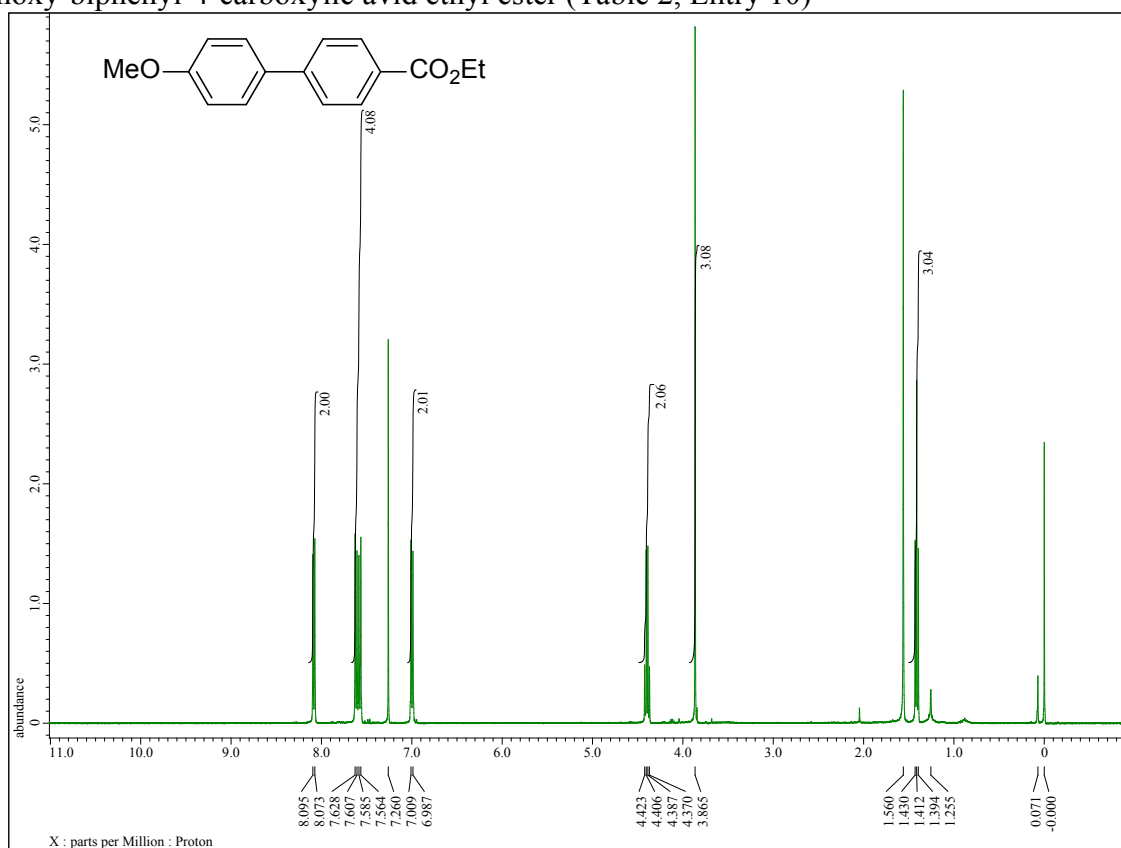


Figure S1. Cont.

4'-Methoxy-biphenyl-4-carboxylic acid ethyl ester (Table 2, Entry 10)



4-Methoxy-4'-methylbiphenyl (Table 2, Entry 11)

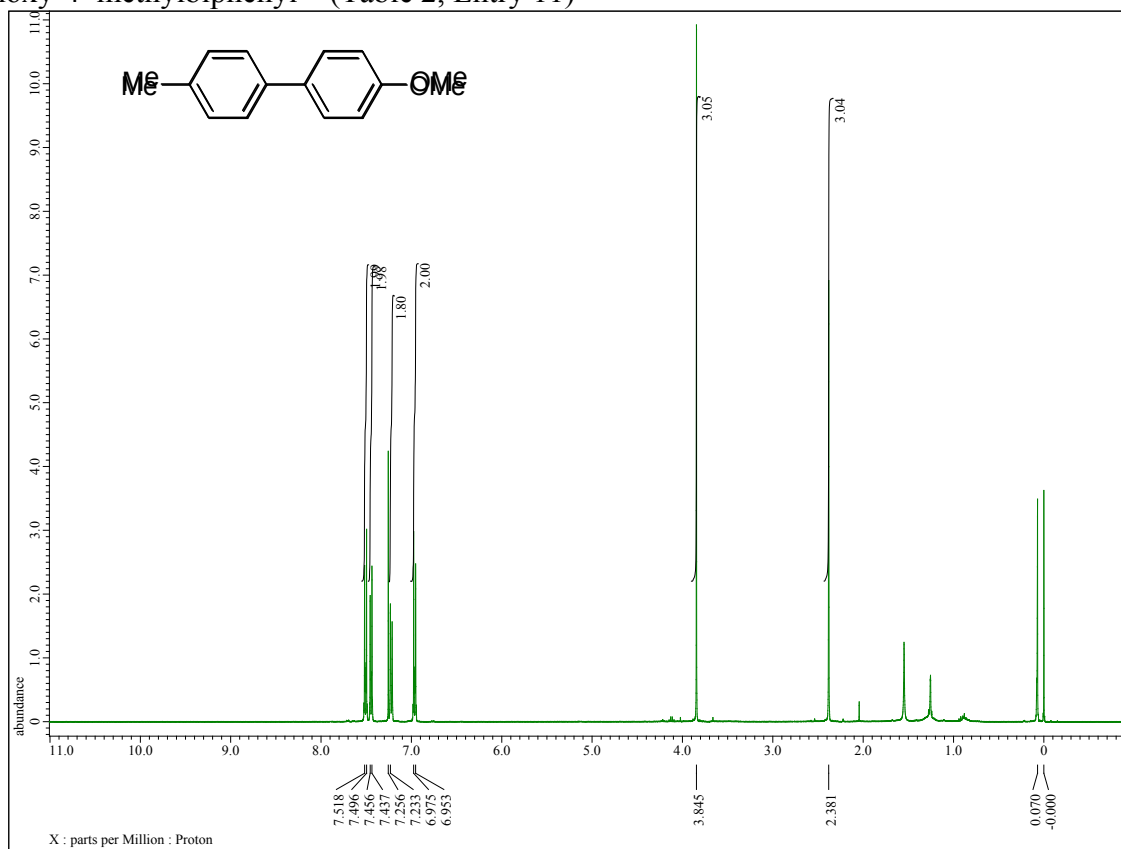
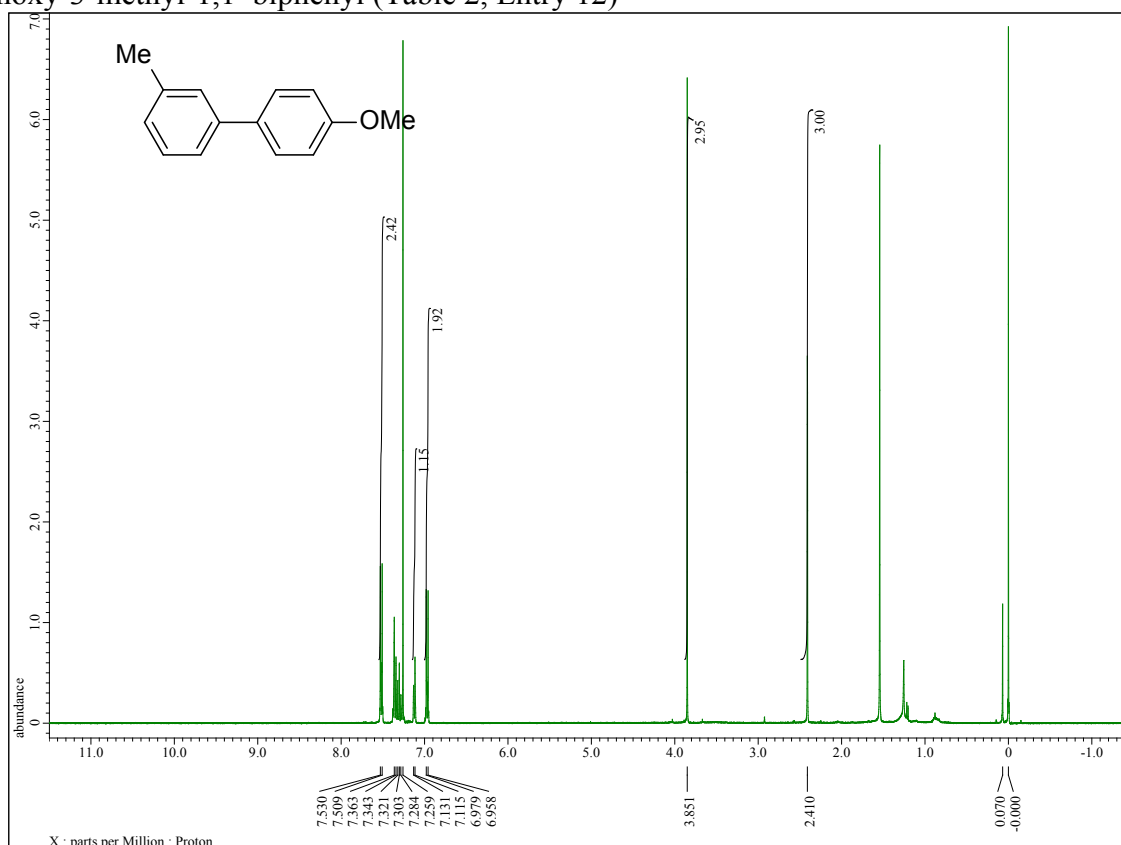


Figure S1. Cont.

4'-Methoxy-3-methyl-1,1'-biphenyl (Table 2, Entry 12)



4'-Methoxy-2-methyl-1,1'-biphenyl (Table 2, Entry 13)

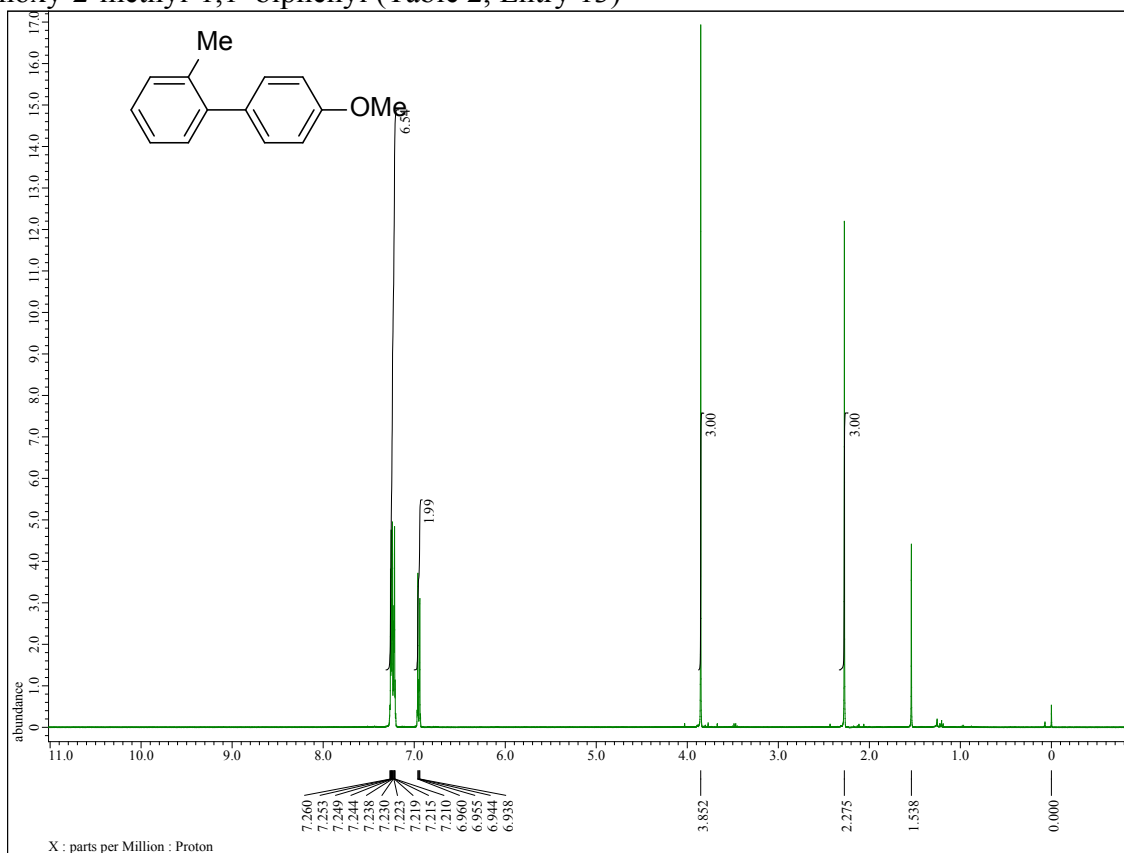
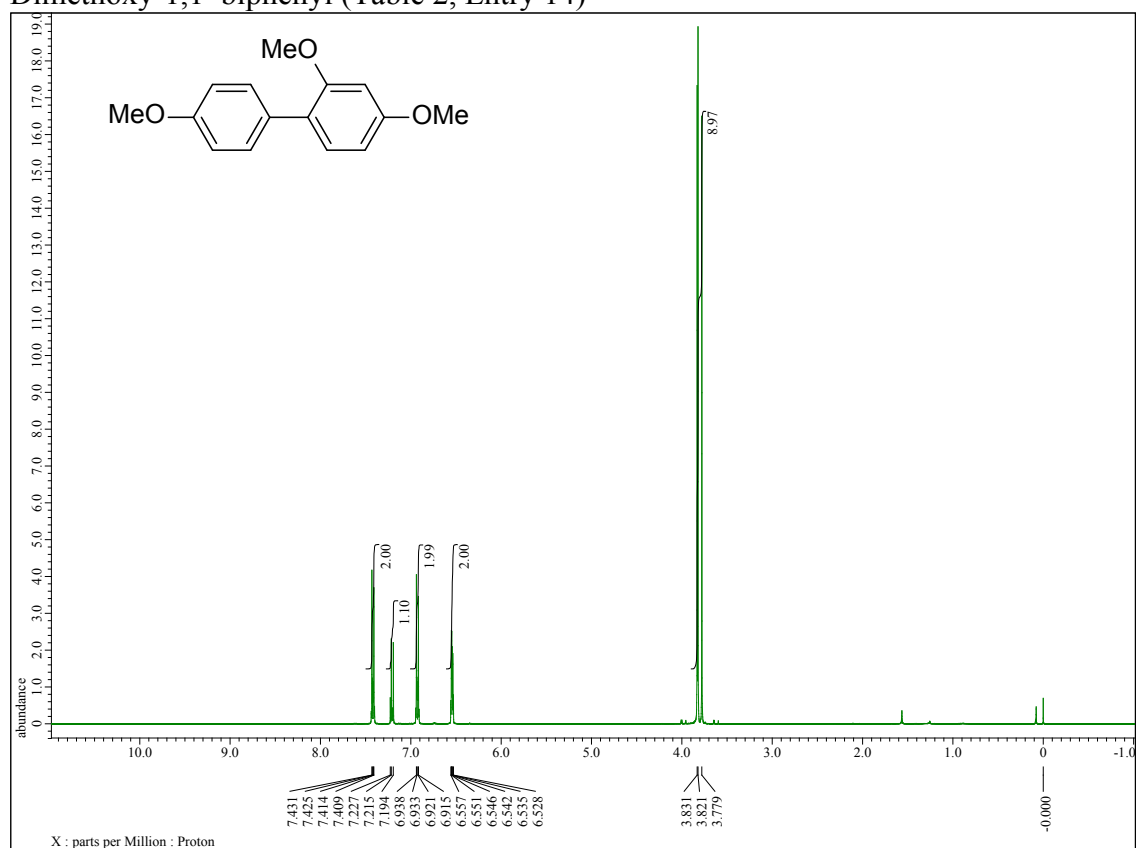


Figure S1. Cont.

2, 4, 4'-Dimethoxy-1,1'-biphenyl (Table 2, Entry 14)



4-Acetyl-1,1'-biphenyl (Table 2, Entry 15)

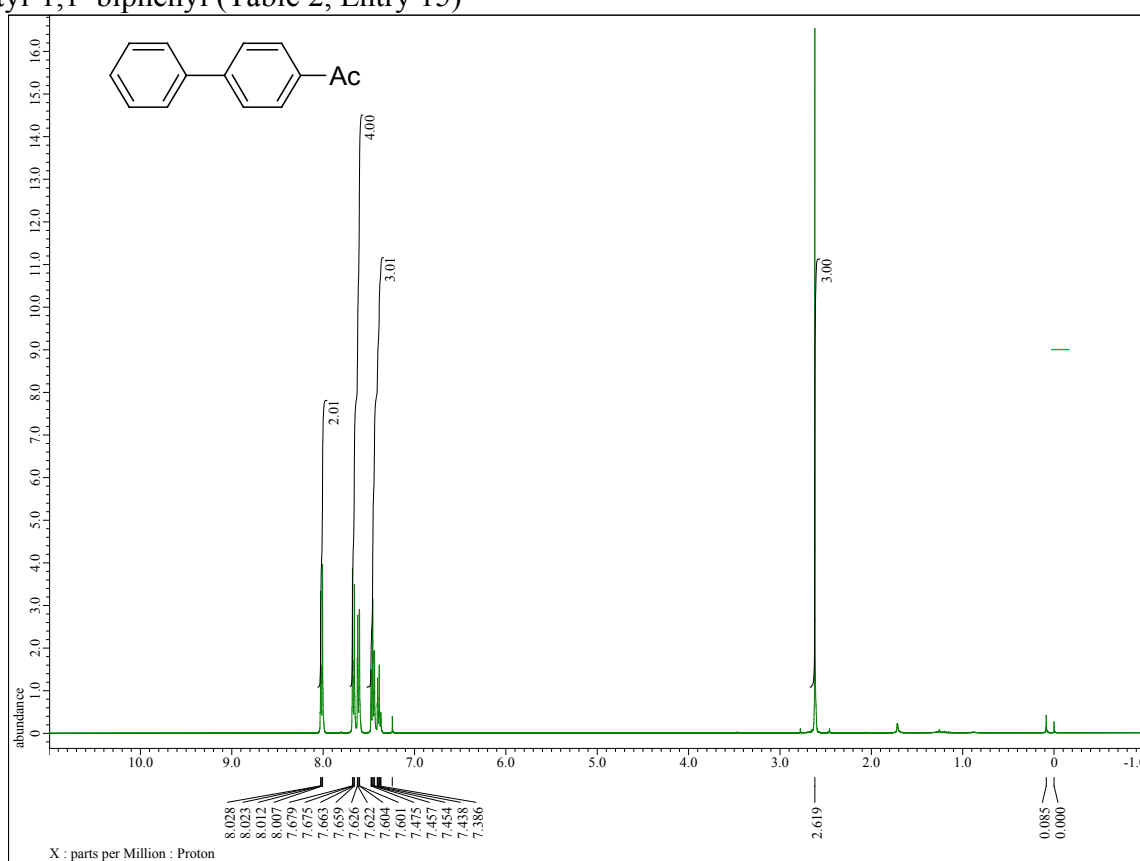
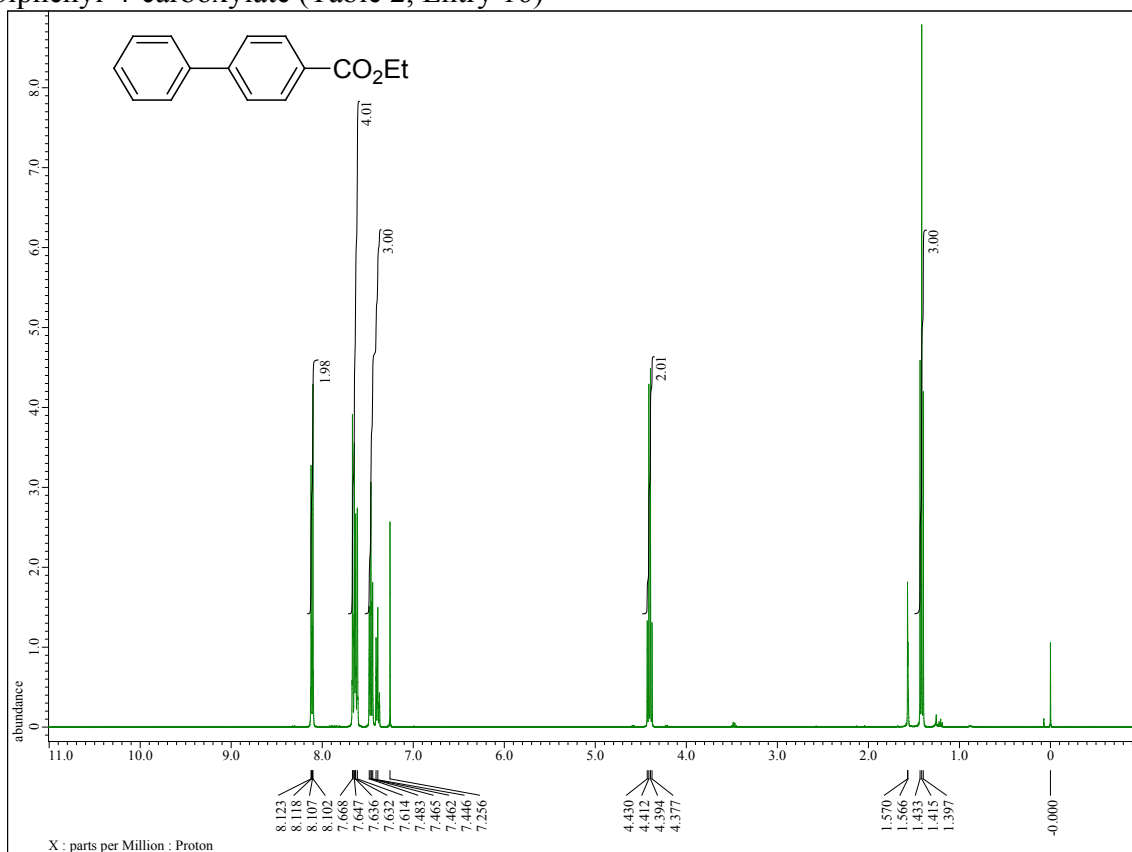


Figure S1. Cont.

Ethyl biphenyl-4-carboxylate (Table 2, Entry 16)



4-Acetyl-4'-methoxy-1,1'-biphenyl (Table 2, Entry 17)

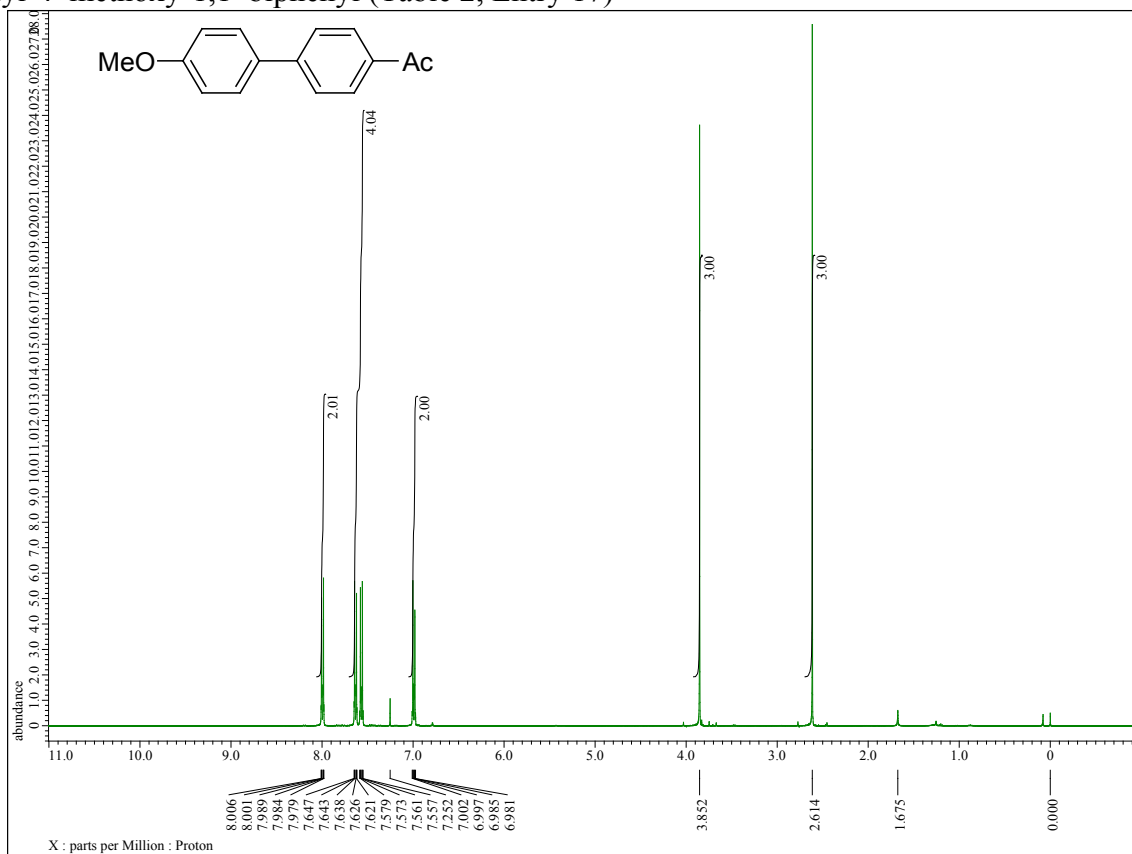


Figure S1. Cont.

4'-Methoxy-biphenyl-4-carboxylic acid ethyl ester (Table 2, Entry 18)

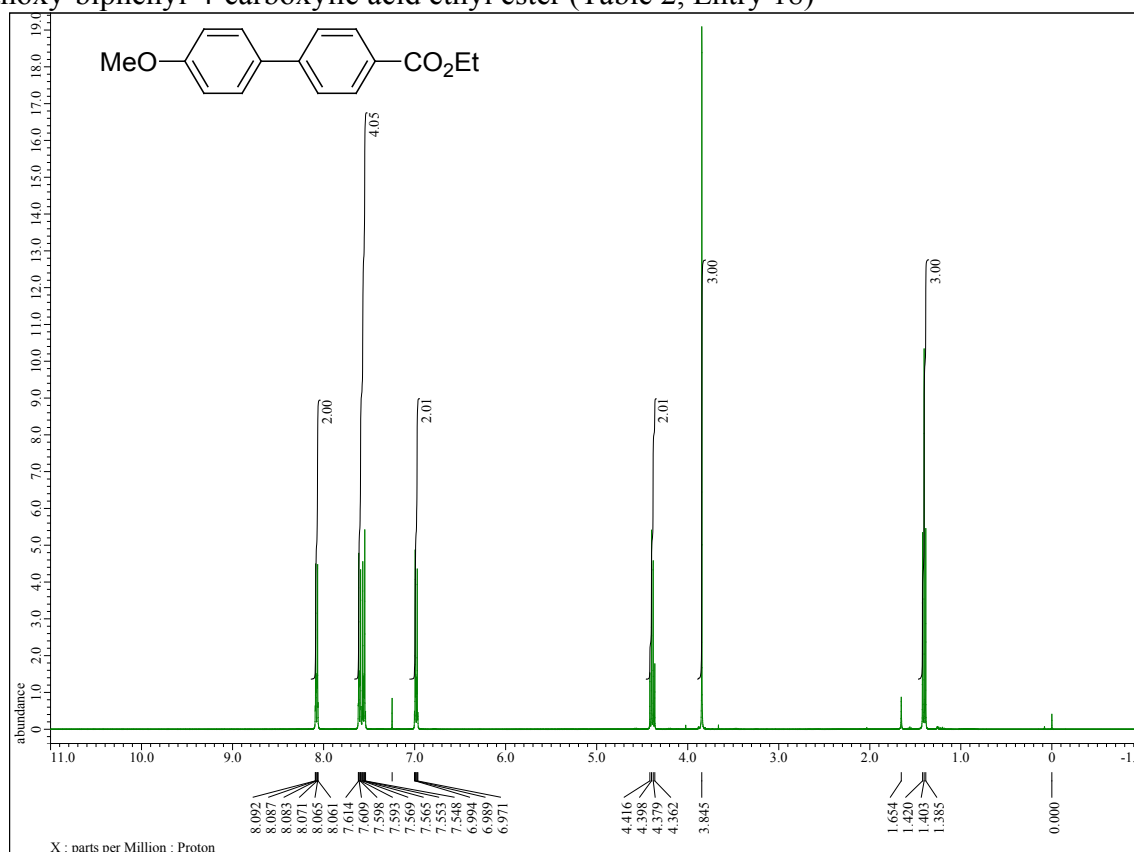
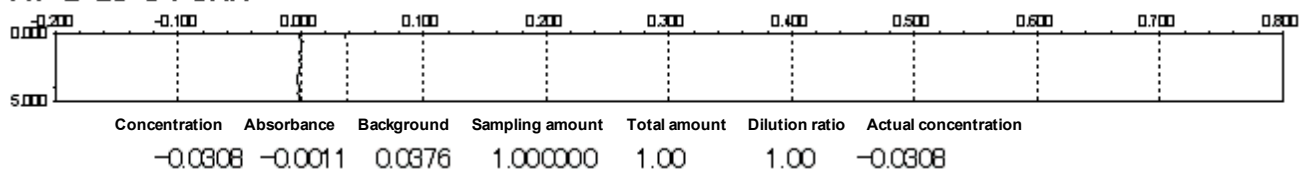


Figure S1. Copies of NMR spectra.

Organic Layer

AT-2-28-d : UNK



Aqueous layer

AT-2-28-d : UNK

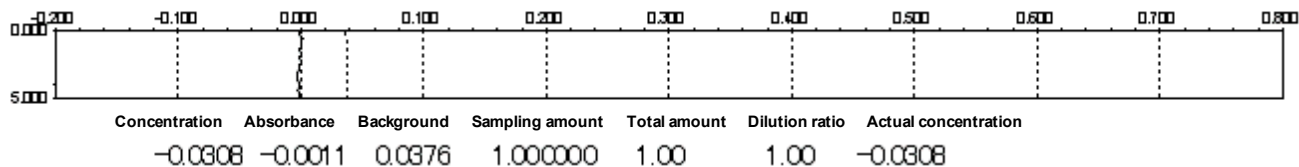


Figure S2. Leaching test of palladium.

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