Electronic Supplementary Information

Synthesis and characterization of trinuclear *N*-heterocyclic carbene-palladium(II) complexes and their applications in the Suzuki-Miyaura cross-coupling reaction

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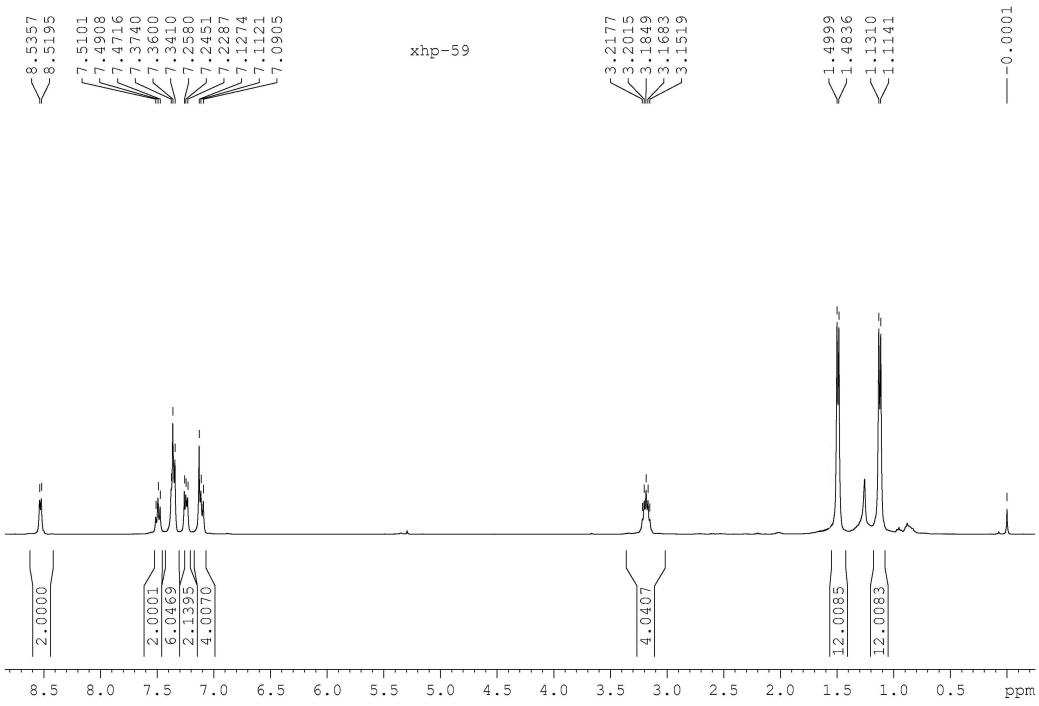
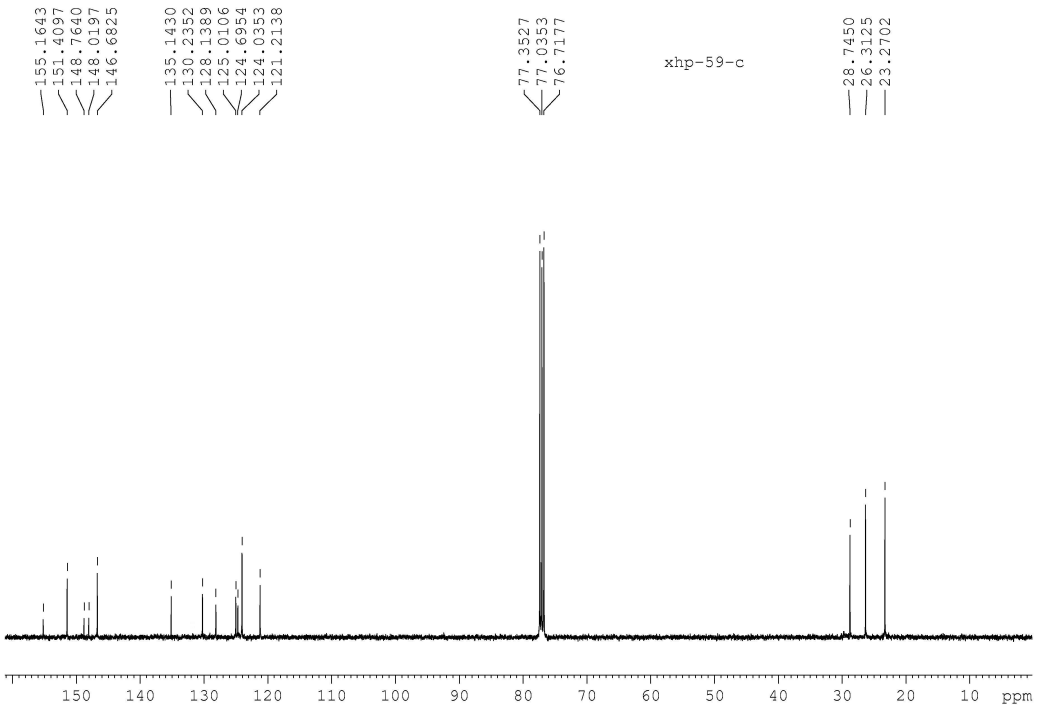
Copies of the ^{1}H and ^{13}C NMR spectra of new complexes 5a-e

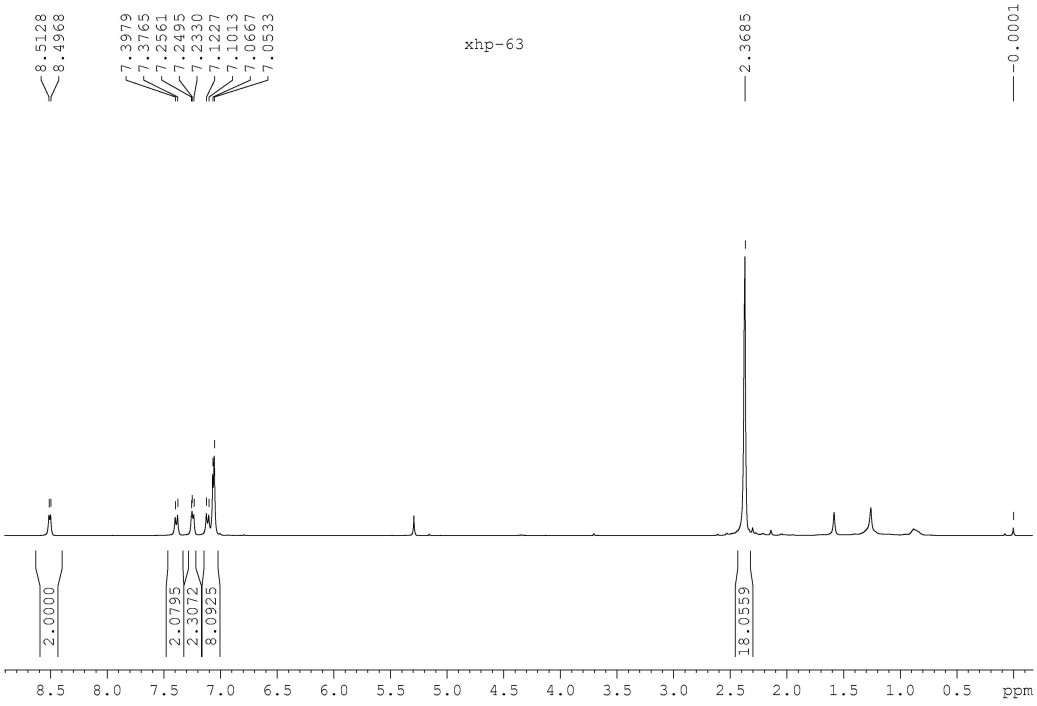
^{1}H NMR(**5a**)



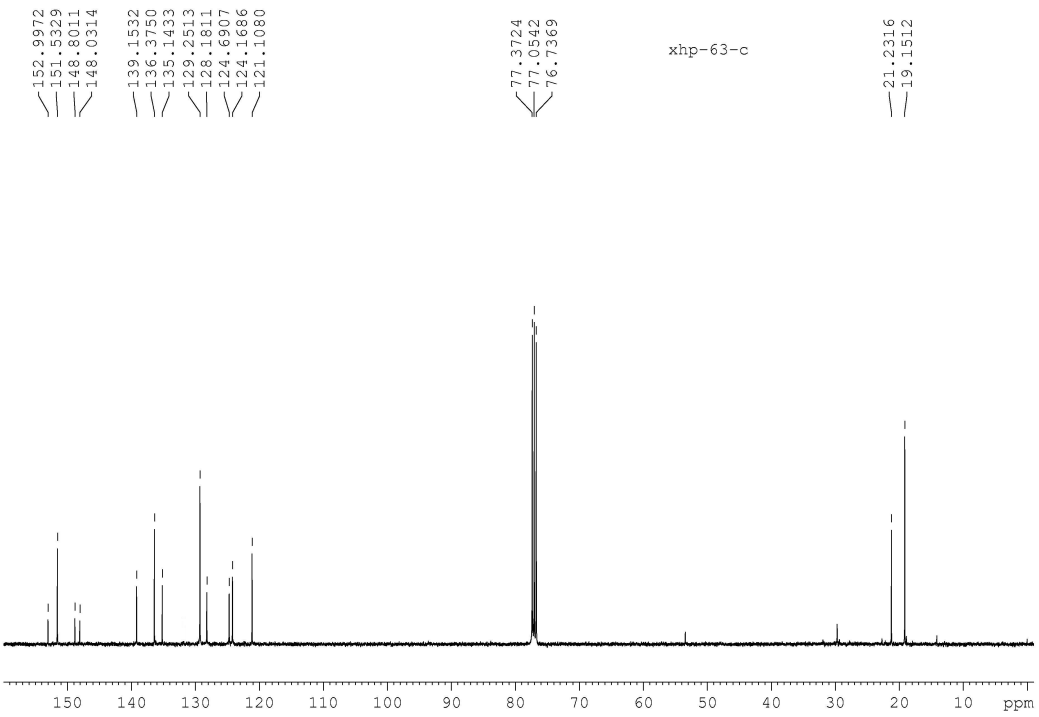
^{13}C NMR(**5a**)



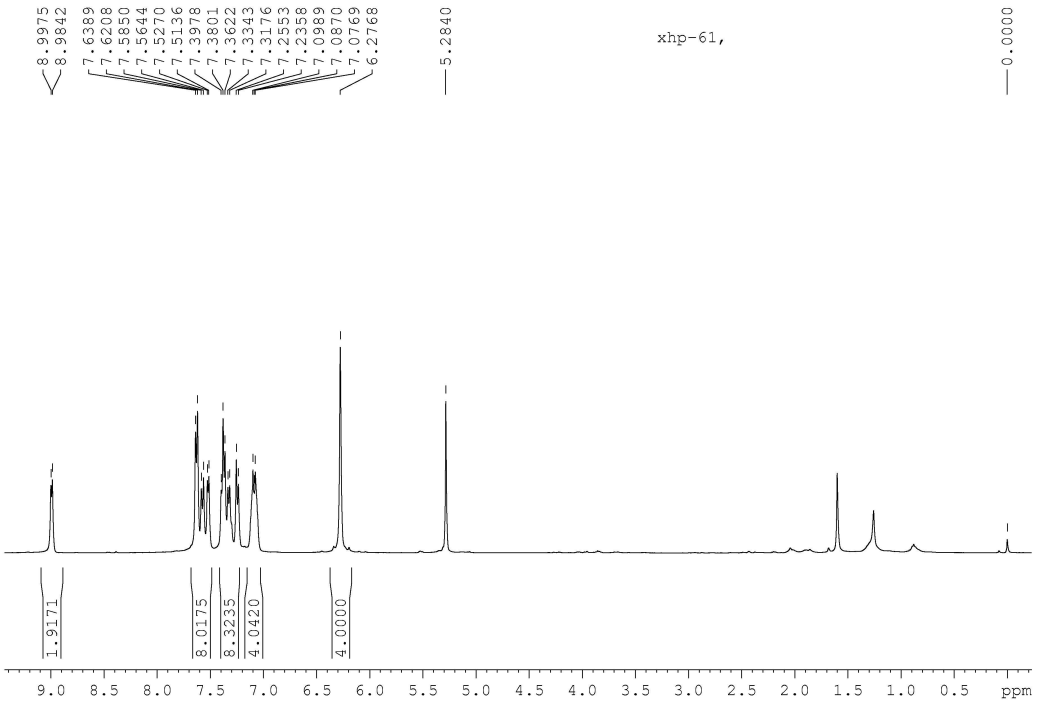
^{1}H NMR(**5b**)



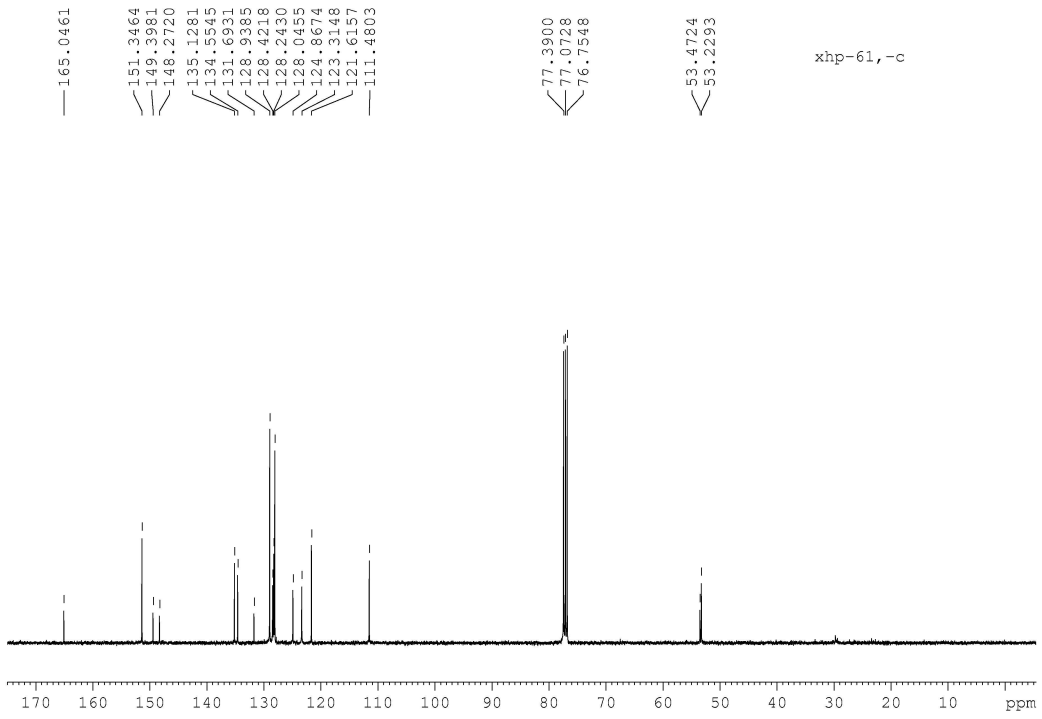
^{13}C NMR(**5b**)



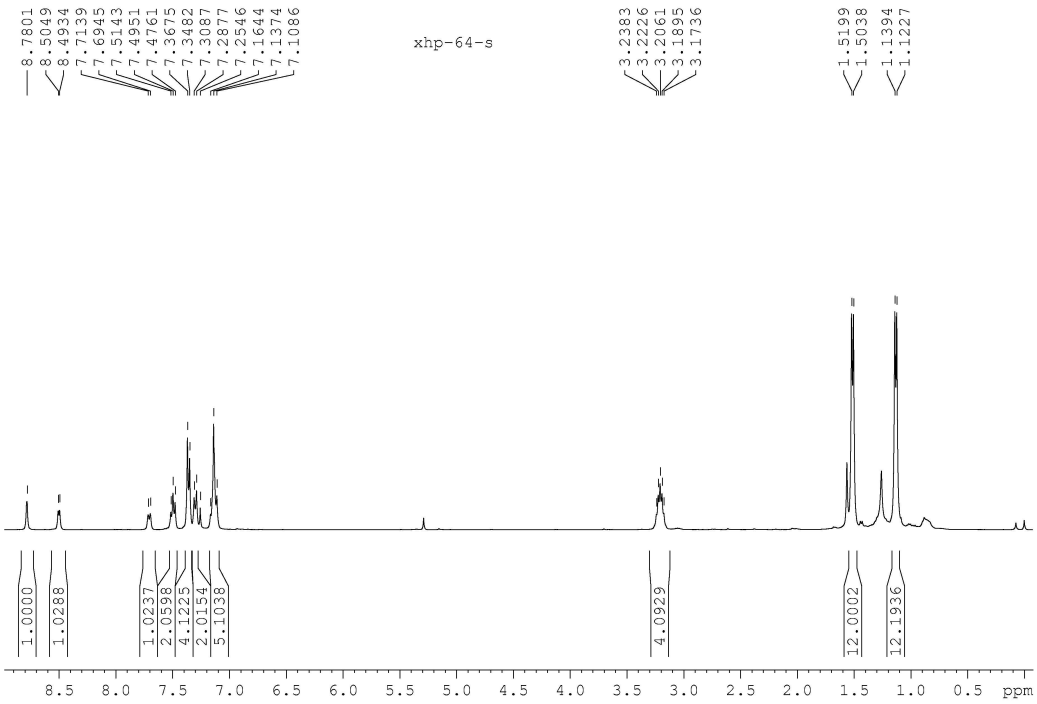
^{1}H NMR(**5c**)



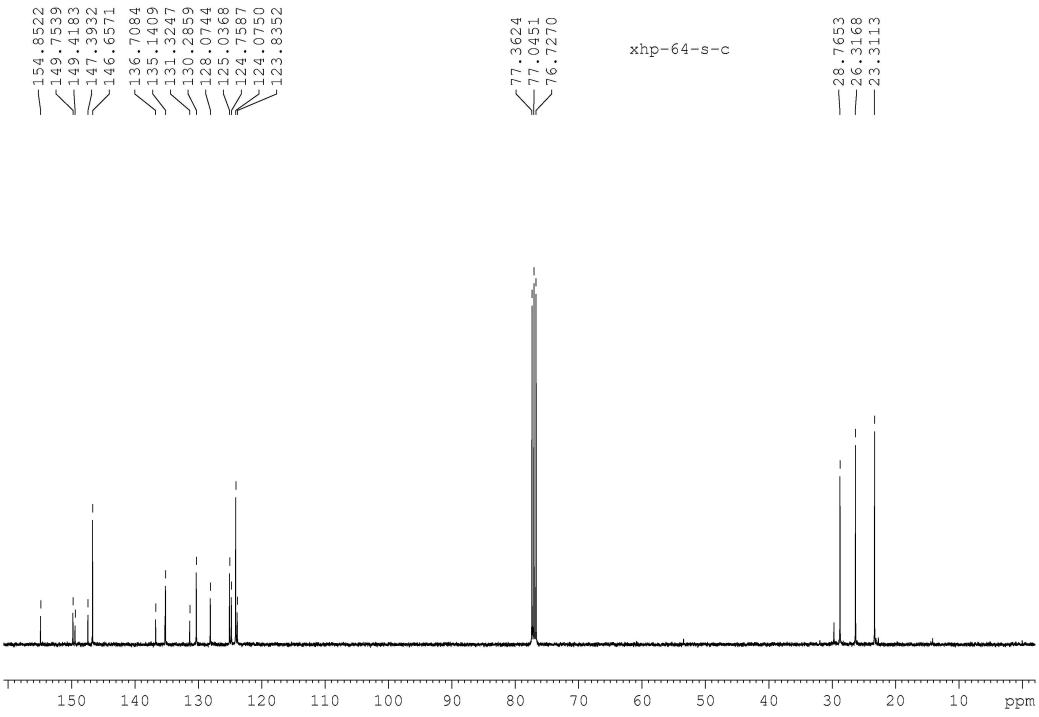
^{13}C NMR(**5c**)



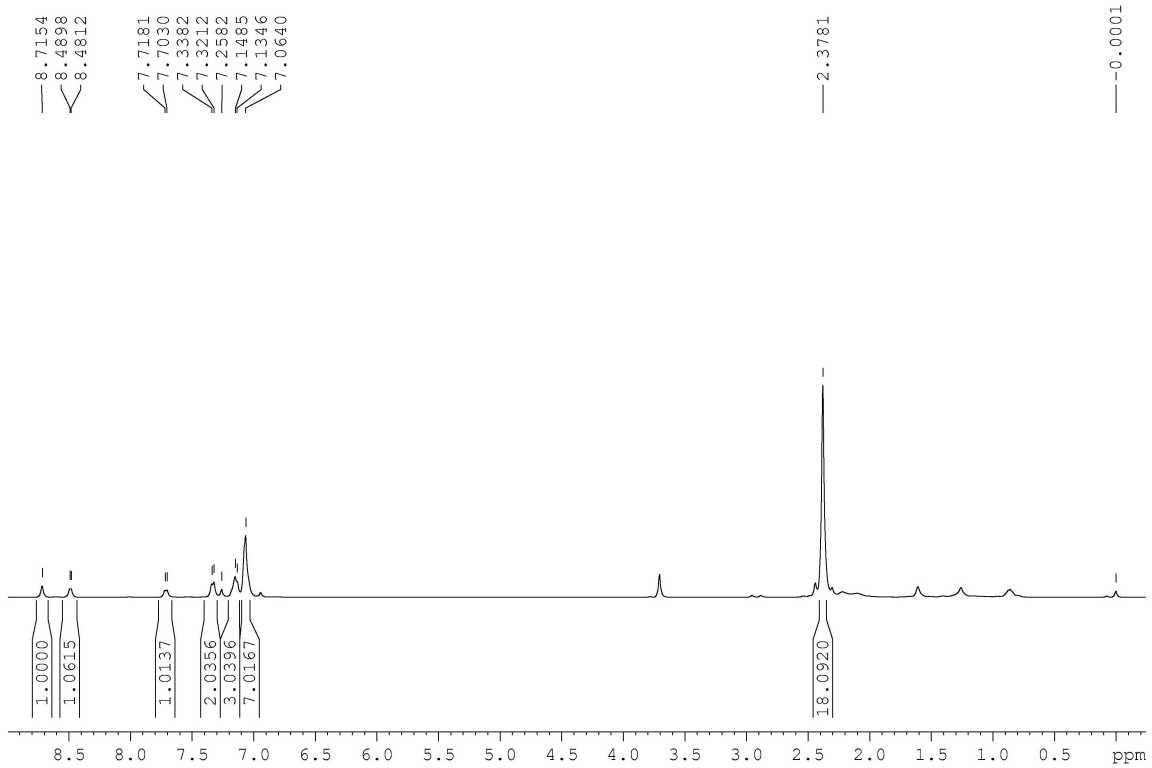
^{1}H NMR(**5d**)



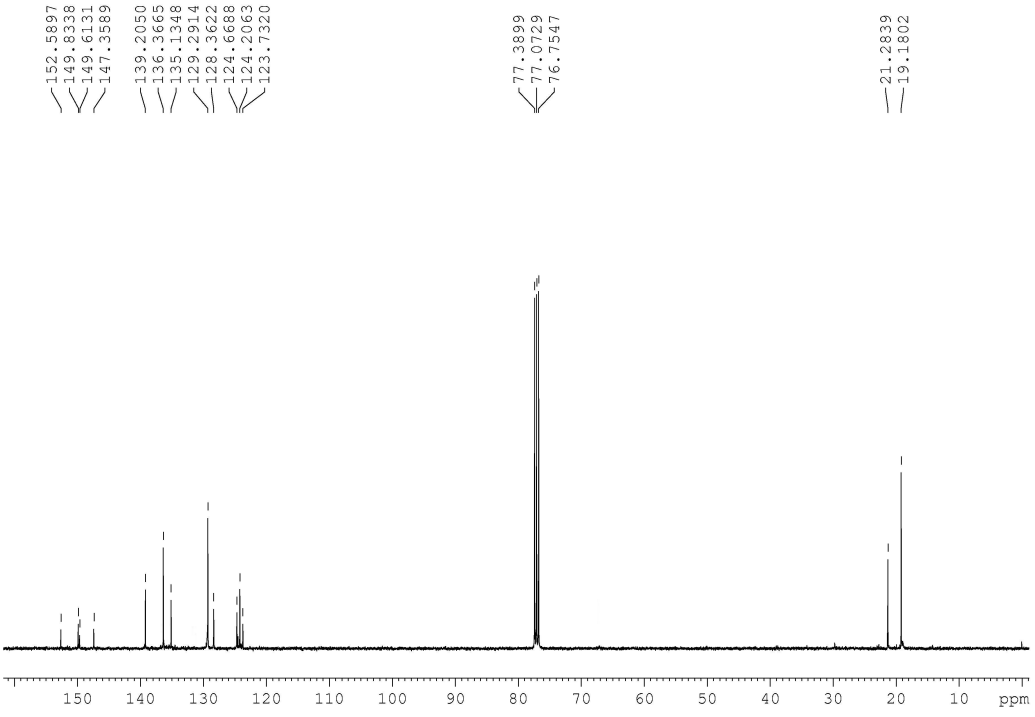
^{13}C NMR(**5d**)



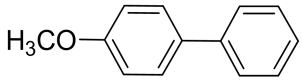
^{1}H NMR(**5e**)



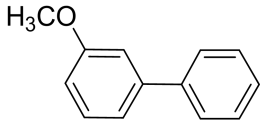
^{13}C NMR(**5e**)



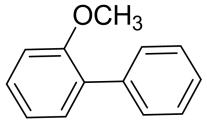
Characterization data of the catalysis products 8 and 10



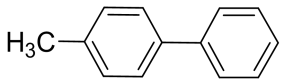
4-methoxy-1,1'-biphenyl (8a)[1-7] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54 (t, *J* = 8.3 Hz, 4H, ArH), 7.41 (t, *J* = 7.6 Hz, 2H, ArH), 7.30 (t, *J* = 7.3 Hz, 1H, ArH), 6.98 (d, *J* = 8.7 Hz, 2H, ArH), 3.85 (s, 3H, OCH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.2, 140.9, 133.8, 128.7, 128.2, 126.8, 126.7, 114.2, 55.4.



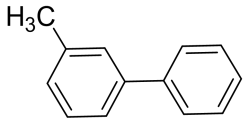
3-methoxy-1,1'-biphenyl (8b)[4] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 5.2 Hz, 2H, ArH), 7.44 (t, *J* = 5.1 Hz, 2H, ArH), 7.37-7.34 (m, 2H, ArH), 7.18 (d, *J* = 5.1 Hz, 1H, ArH), 7.13 (s, 1H, ArH), 6.91-6.89 (m, 1H, ArH), 3.87 (s, 3H, OCH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.0, 142.8, 141.1, 129.8, 128.7, 127.4, 127.2, 119.7, 112.9, 112.7, 55.3.



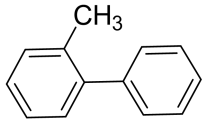
2-methoxy-1,1'-biphenyl (8c)[2,3,5] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52 (d, *J* = 5.0 Hz, 2H, ArH), 7.40 (t, *J* = 5.1 Hz, 2H, ArH), 7.32-7.30 (m, 3H, ArH), 7.02 (t, *J* = 4.9 Hz, 1H, ArH), 6.98 (d, *J* = 5.7 Hz, 1H, ArH), 3.80 (s, 3H, OCH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.5, 138.6, 130.9, 130.8, 129.6, 128.6, 128.0, 126.9, 120.8, 111.3, 55.6.



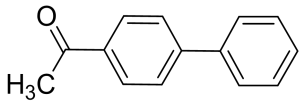
4-methyl-1,1'-biphenyl (8d)[1,3,4,5,6,7] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (d, *J* = 7.1 Hz, 2H, ArH), 7.49 (d, *J* = 8.1 Hz, 2H, ArH), 7.42 (t, *J* = 7.6 Hz, 2H, ArH), 7.34-7.30 (m, 1H, ArH), 7.24 (d, *J* = 8.0 Hz, 2H, ArH), 2.39 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.3, 138.4, 137.1, 129.5, 128.8, 127.3, 127.2, 127.0, 21.2.



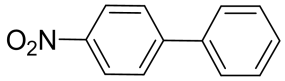
3-methyl-1,1'-biphenyl (8e)[5,7] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59-7.57 (m, 2H, ArH), 7.44-7.38 (m, 4H, ArH), 7.34-7.30 (m, 2H, ArH), 7.15 (d, *J* = 7.4 Hz, 1H, ArH), 2.41 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.3, 138.4, 128.8, 128.73, 128.70, 128.03, 128.02, 127.3, 127.2, 124.3, 21.6.



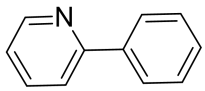
2-methyl-1,1'-biphenyl (8f)[1,2,3,5,6] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45-7.38 (m, 2H, ArH), 7.36-7.31 (m, 3H, ArH), 7.27-7.22 (m, 4H, ArH), 2.27 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.3, 135.4, 130.4, 129.9, 129.3, 128.8, 128.1, 127.3, 126.8, 125.8, 20.5.



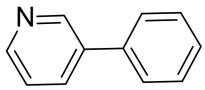
1-([1,1'-biphenyl]-4-yl)ethanone (8g)[1,3,4,7] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 (d, *J* = 8.3 Hz, 2H, ArH), 7.69 (d, *J* = 8.3 Hz, 2H, ArH), 7.63 (d, *J* = 7.2 Hz, 2H, ArH), 7.48 (t, *J* = 7.4 Hz, 2H, ArH), 7.42-7.39 (m, 1H, ArH), 2.64 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.8, 145.8, 139.9, 135.9, 129.0, 128.9, 128.2, 127.3, 127.2, 26.7.



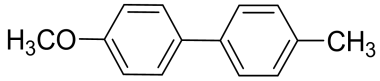
4-nitro-1,1'-biphenyl (8h)[2,3,4,6] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.29 (d, *J* = 8.8 Hz, 2H, ArH), 7.73 (d, *J* = 8.9 Hz, 2H, ArH), 7.64-7.61 (m, 2H, ArH), 7.52-7.42 (m, 3H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.7, 147.1, 138.8, 129.2, 128.9, 127.8, 127.4, 124.1.



2-phenylpyridine (8i)[1,4] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.69 (d, *J* = 3.2 Hz, 1H, ArH), 7.98 (d, *J* = 5.0 Hz, 2H, ArH), 7.75-7.71 (m, 2H, ArH), 7.47 (t, *J* = 5.1 Hz, 2H, ArH), 7.41 (t, *J* = 4.9 Hz, 1H, ArH), 7.22-7.20 (m, 1H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.5, 149.7, 139.4, 136.8, 129.0, 128.8, 126.9, 122.1, 120.6.

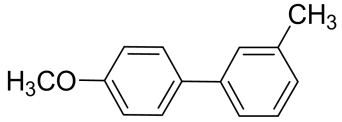


3-phenylpyridine (8j)[3,5] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.86 (s, 1H, ArH), 8.60 (s, 1H, ArH), 7.88 (d, *J* = 5.2 Hz, 1H, ArH), 7.58 (d, *J* = 5.0 Hz, 2H, ArH), 7.49 (t, *J* = 5.1 Hz, 2H, ArH), 7.41 (t, *J* = 4.9 Hz, 1H, ArH), 7.38-7.36 (m, 1H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.4, 148.3, 137.8, 136.7, 134.4, 129.1, 128.1, 127.2, 123.6.

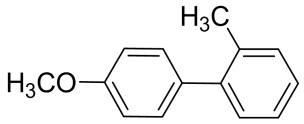


4-methoxy-4'-methyl-1,1'-biphenyl (8k)[4,6] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52-7.49 (m,

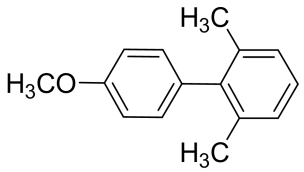
2H, ArH), 7.44 (d, *J* = 8.1 Hz, 2H, ArH), 7.22 (d, *J* = 7.9 Hz, 2H, ArH), 6.98-6.94 (m, 2H, ArH), 3.84 (s, 3H, OCH_3), 2.38 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.9, 138.0, 136.4, 133.8, 129.5, 128.0, 126.6, 114.2, 55.4, 21.1.



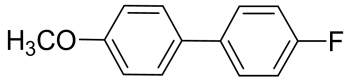
4'-methoxy-3-methyl-1,1'-biphenyl (8l)[6] : ^1H NMR (400 MHz, $CDCl_3$): δ 7.53-7.50 (m, 2H, ArH), 7.36-7.28 (m, 3H, ArH), 7.12 (d, *J* = 7.4 Hz, 1H, ArH), 6.98-6.95 (m, 2H, ArH), 3.84 (s, 3H, OCH_3), 2.41 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.1, 140.8, 138.3, 133.9, 128.6, 128.2, 127.6, 127.4, 123.9, 114.1, 55.4, 21.6.



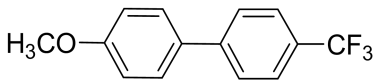
4'-methoxy-2-methyl-1,1'-biphenyl (8m)[6] : ^1H NMR (400 MHz, $CDCl_3$): δ 7.27-7.20 (m, 6H, ArH), 6.97-6.93 (m, 2H, ArH), 3.85 (s, 3H, OCH_3), 2.27 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.5, 140.5, 134.4, 133.3, 129.3, 129.2, 128.9, 125.9, 124.7, 112.4, 54.2, 19.5.



4'-methoxy-2,6-dimethyl-1,1'-biphenyl (8n)[10] : ^1H NMR (400 MHz, $CDCl_3$): δ 7.16-7.04 (m, 5H, ArH), 6.97-6.94 (m, 2H, ArH), 3.84 (s, 3H, OCH_3), 2.04 (s, 6H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.2, 140.5, 135.5, 132.3, 129.0, 126.2, 125.8, 112.8, 54.2, 19.9.

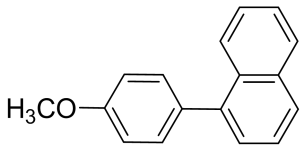


4-fluoro-4'-methoxy-1,1'-biphenyl (8o)[6] : ^1H NMR (400 MHz, $CDCl_3$): δ 7.50-7.46 (m, 4H, ArH), 7.09 (t, *J* = 5.7 Hz, 2H, ArH), 6.97 (d, *J* = 5.7 Hz, 2H, ArH), 3.85 (s, 3H, OCH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.3, 160.9, 159.1, 137.0, 136.9, 132.9, 128.3, 128.2, 128.0, 115.6, 115.4, 114.3, 55.4.

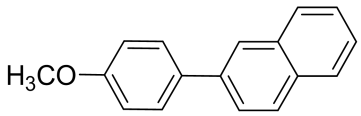


4-methoxy-4'-(trifluoromethyl)-1,1'-biphenyl (8p)[7] : ^1H NMR (400 MHz, $CDCl_3$): δ 7.68-7.63 (m, 4H, ArH), 7.54 (d, *J* = 8.7 Hz, 2H, ArH), 7.00 (d, *J* = 8.8 Hz, 2H, ArH), 3.86

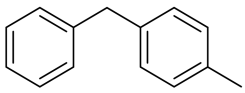
(s, 3H, OCH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.9, 144.3, 132.2, 128.4, 126.9, 125.7, 125.6, 114.4, 55.4.



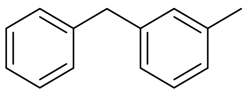
1-(4-methoxyphenyl)naphthalene (8q)[6] : ^1H NMR (400 MHz, $CDCl_3$): δ 7.90 (dd, *J* = 10.5, 5.6 Hz, 2H, ArH), 7.83 (d, *J* = 5.4 Hz, 1H, ArH), 7.52-7.47 (m, 2H, ArH), 7.44-7.40 (m, 4H, ArH), 7.03 (d, *J* = 5.7 Hz, 2H, ArH), 3.89 (s, 3H, OCH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.0, 139.9, 133.9, 133.2, 131.9, 131.1, 128.3, 127.4, 126.9, 126.1, 126.0, 125.7, 125.4, 113.8, 55.4.



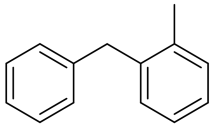
2-(4-methoxyphenyl)naphthalene (8r)[6] : ^1H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 1.3 Hz, 1H, ArH), 7.90-7.83 (m, 3H, ArH), 7.73-7.64 (m, 3H, ArH), 7.51-7.43 (m, 2H, ArH), 7.04-7.00 (m, 2H, ArH), 3.87 (s, 3H, OCH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.3, 138.2, 133.8, 133.7, 132.3, 128.5, 128.4, 128.1, 127.6, 126.3, 125.7, 125.5, 125.1, 114.3, 55.4.



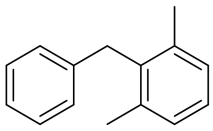
1-benzyl-4-methylbenzene (10a)[1,9] : ^1H NMR (400 MHz, $CDCl_3$): δ 7.46 (d, *J* = 7.2 Hz, 1H, ArH), 7.45-7.17 (m, 4H, ArH), 7.06 (s, 4H, ArH), 3.91 (s, 2H, CH_2), 2.29 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.3, 138.1, 135.6, 129.2, 128.9, 128.8, 128.4, 126.0, 41.5, 21.0.



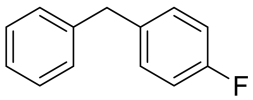
1-benzyl-3-methylbenzene (10b)[9] : ^1H NMR (400 MHz, $CDCl_3$): δ 7.32-7.24 (m, 2H, ArH), 7.18-7.14 (m, 4H, ArH), 6.99 (s, 3H, ArH), 3.92 (s, 2H, CH_2), 2.29 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.3, 129.7, 128.9, 128.8, 128.5, 128.4, 127.3, 127.2, 126.8, 126.0, 41.9, 21.4.



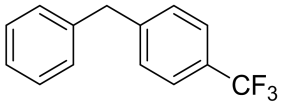
1-benzyl-2-methylbenzene (10c)[1] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27-7.24 (m, 2H, ArH), 7.19-7.10 (m, 7H, ArH), 3.97 (s, 2H, CH_2), 2.23 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.4, 138.9, 136.7, 130.3, 130.0, 128.8, 128.4, 126.5, 126.0, 125.9, 39.5, 19.7.



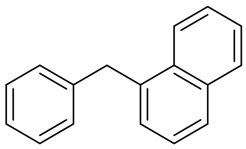
2-benzyl-1,3-dimethylbenzene (10d)[11] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.23-6.99 (m, 8H, ArH), 4.04 (s, 2H, CH_2), 2.23 (s, 6H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.8, 137.2, 136.9, 128.4, 128.1, 127.9, 126.3, 125.7, 35.1, 20.2.



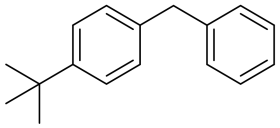
1-benzyl-4-fluorobenzene (10e)[1,9] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47-7.44 (m, 1H, ArH), 7.29-7.25 (m, 2H, ArH), 7.20-7.07 (m, 4H, ArH), 6.96-6.92 (m, 2H, ArH), 3.92 (s, 2H, CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.7, 160.2, 141.3, 141.0, 136.8, 130.3, 130.2, 128.8, 128.6, 127.3, 127.2, 126.2, 115.3, 115.1, 41.1.



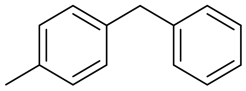
1-benzyl-4-(trifluoromethyl)benzene (10f)[8] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72-7.66 (m, 1H, ArH), 7.52 (d, *J* = 7.6 Hz, 2H, ArH), 7.31-7.15 (m, 6H, ArH), 4.01 (s, 2H, CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.2, 140.0, 129.2, 128.9, 128.7, 127.6, 126.5, 125.4, 29.7.



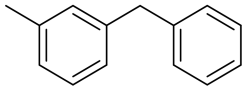
1-benzylnaphthalene (10g)[9]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99-7.97 (m, 1H, ArH), 7.85-7.83 (m, 1H, ArH), 7.74 (d, *J* = 8.1 Hz, 1H, ArH), 7.44-7.38 (m, 3H, ArH), 7.28-7.23 (m, 3H, ArH), 7.18 (d, *J* = 7.1 Hz, 3H, ArH), 4.43 (s, 2H, CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.7, 136.7, 134.0, 132.2, 128.8, 128.7, 128.5, 127.4, 127.2, 126.1, 126.0, 125.6, 124.4, 39.1.



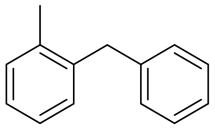
1-benzyl-4-(tert-butyl)benzene (10h)[12] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31-7.10 (m, 9H, ArH), 3.94 (s, 2H, CH_2), 1.29 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.9, 141.3, 138.1, 129.0, 128.5, 128.4, 126.0, 125.4, 41.5, 34.4, 31.4.



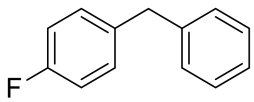
1-benzyl-4-methylbenzene (10i)[1,9] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60-7.18 (m, 5H, ArH), 7.08 (s, 4H, ArH), 3.93 (s, 2H, CH_2), 2.30 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.1, 137.9, 135.3, 128.9, 128.7, 128.6, 128.2, 125.8, 41.3, 20.8.



1-benzyl-3-methylbenzene (10j)[9] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59-7.14 (m, 6H, ArH), 6.99-6.97 (m, 3H, ArH), 3.93 (s, 2H, CH_2), 2.30 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.5, 130.0, 129.2, 129.0, 128.7, 128.6, 127.5, 127.4, 127.1, 126.2, 42.1, 21.6.



1-benzyl-2-methylbenzene (10k)[1] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, J = 7.08 Hz, 1H, ArH), 7.45-7.42 (m, 1H, ArH), 7.41-7.24 (m, 2H, ArH), 7.19-7.10 (m, 5H, ArH), 3.97 (s, 2H, CH_2), 2.23 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.3, 137.9, 135.6, 129.2, 128.9, 127.7, 127.3, 125.4, 124.9, 124.8, 38.4, 18.6.



1-benzyl-4-fluorobenzene (10l)[1,9] : ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, J = 7.08 Hz, 1H, ArH), 7.45-7.42 (m, 1H, ArH), 7.36-7.27 (m, 2H, ArH), 7.22-7.11 (m, 3H, ArH), 6.98-6.94 (m, 2H, ArH), 3.94 (s, 2H, CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.6, 160.2, 141.2, 140.9, 136.7, 130.3, 130.2, 128.7, 128.5, 127.2, 127.1, 126.2, 115.3, 115.1, 41.1.

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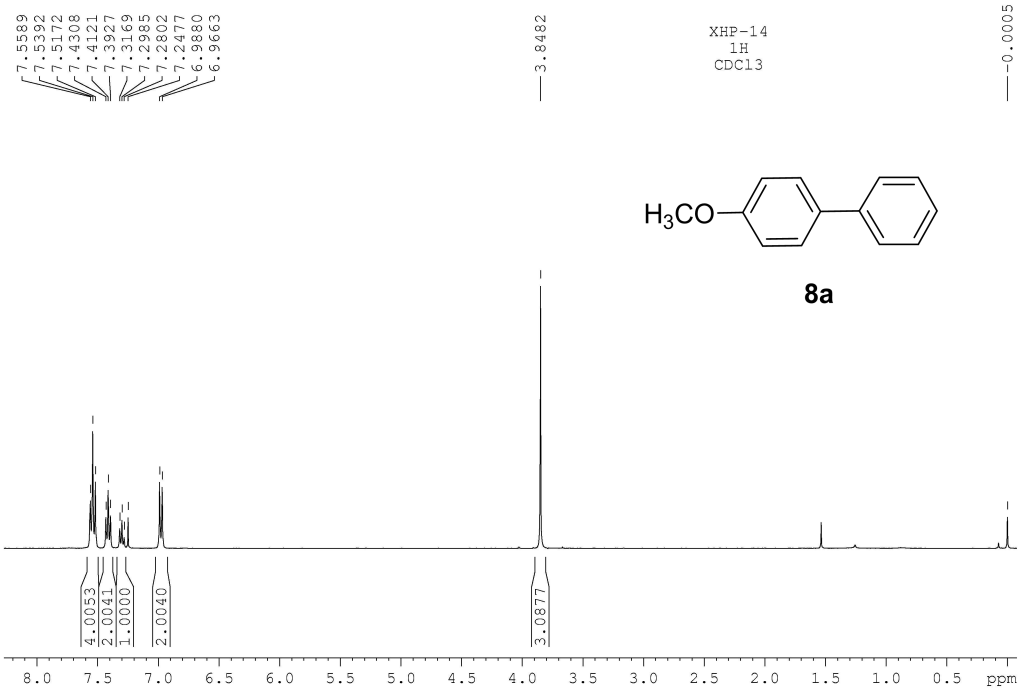
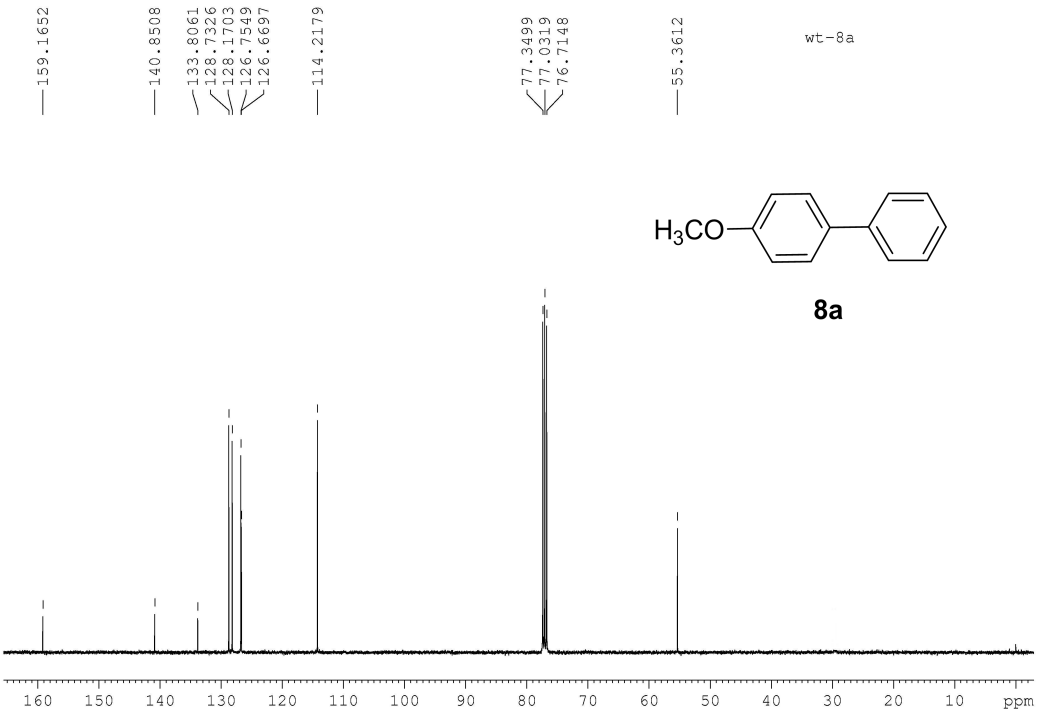
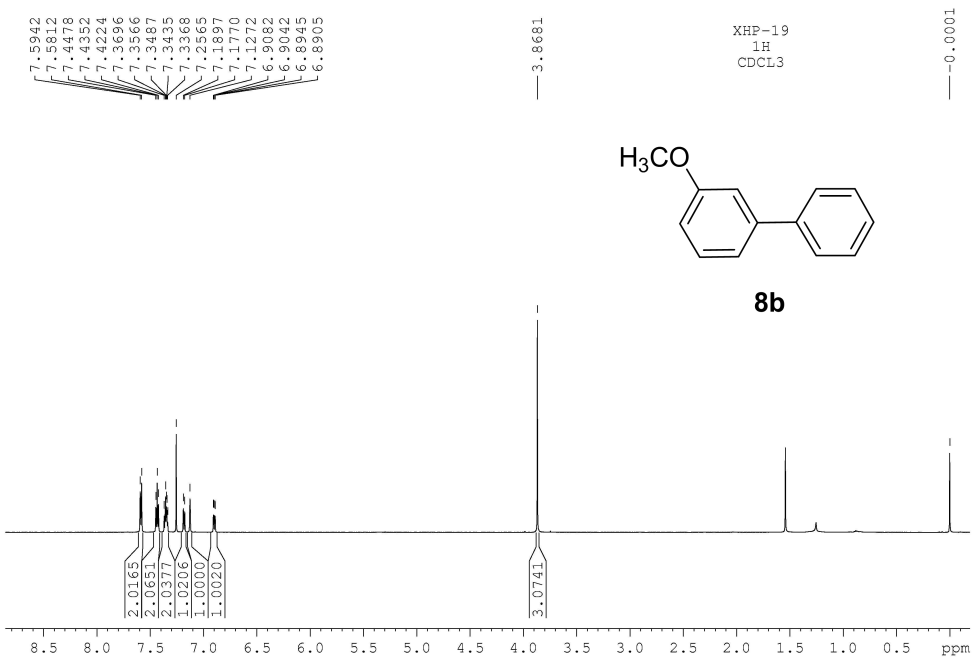
Copies of the NMR spectra of the catalysis products 8 and 10



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7.2565
7.1897
7.1770
7.1272
6.9082
6.9042
6.8945
6.8905
3.8681
XHP-19
1H
CDCL3
0.0001
H3CO
8b
2.0165
2.0651
2.0377
1.0206
1.0000
1.0020
3.0741
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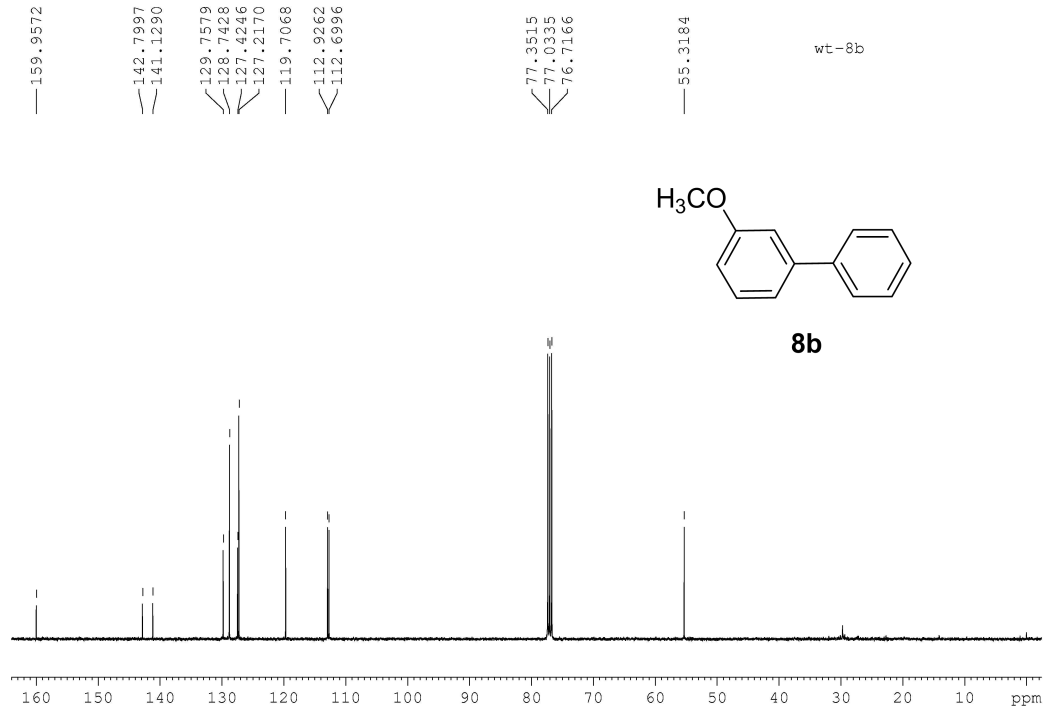
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141.1290
129.7579
128.7428
127.4246
127.2170
119.7068
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112.6996
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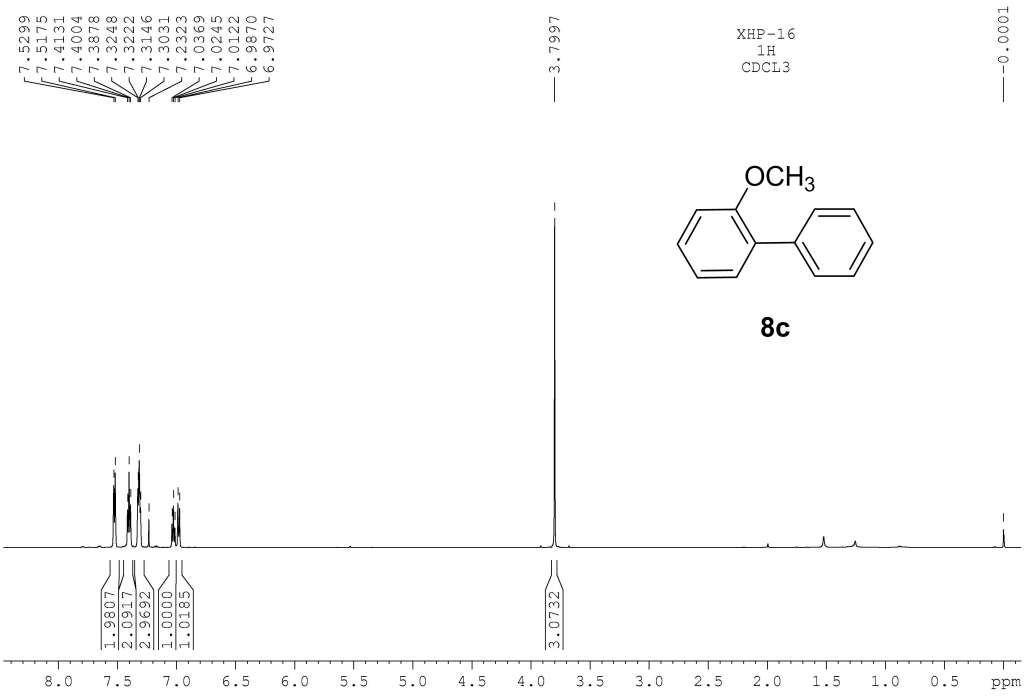
77.0335
76.7166
55.3184
wt-8b
H3CO
8b
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.4131
7.4004
7.3878
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7.3222
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7.0369
7.0245
7.0122
6.9870
6.9727
3.7997
XHP-16
1H
CDCL3
0.0001
OCH3
8c
1.9807
2.0917
2.9692
1.0000
1.0185
3.0732
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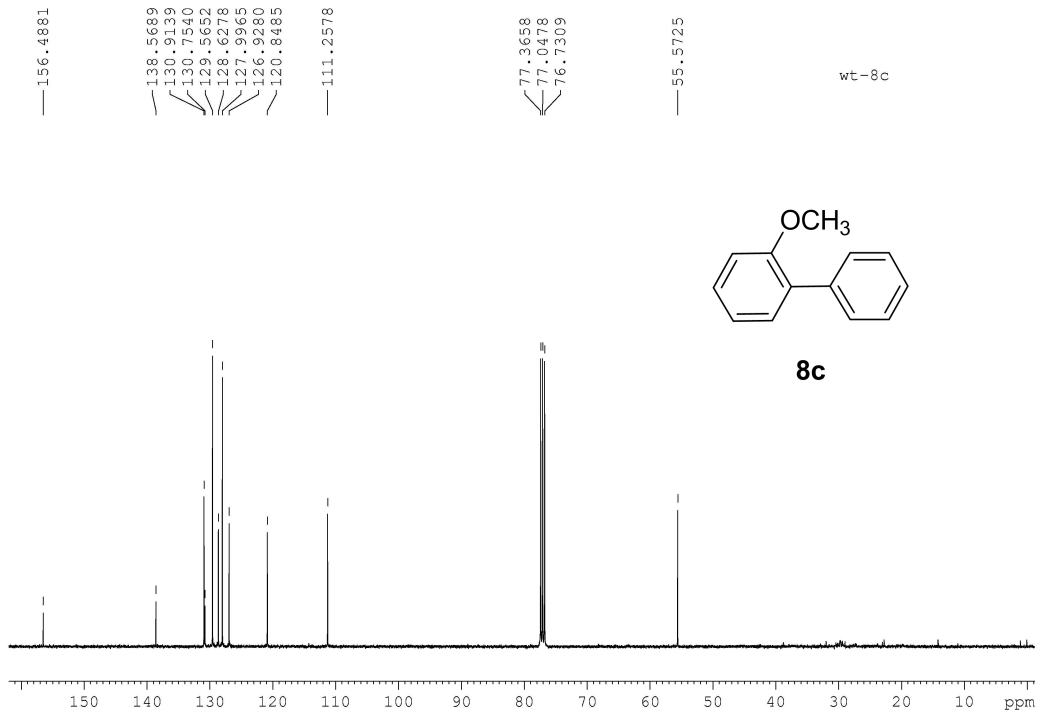
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wt-8c
OCH3
8c
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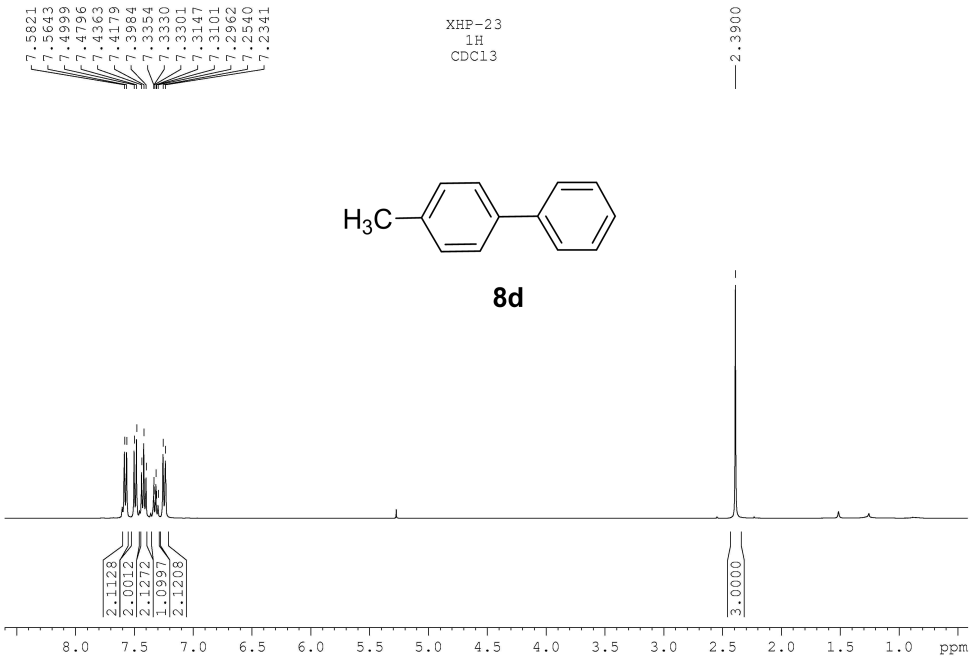
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7.3330
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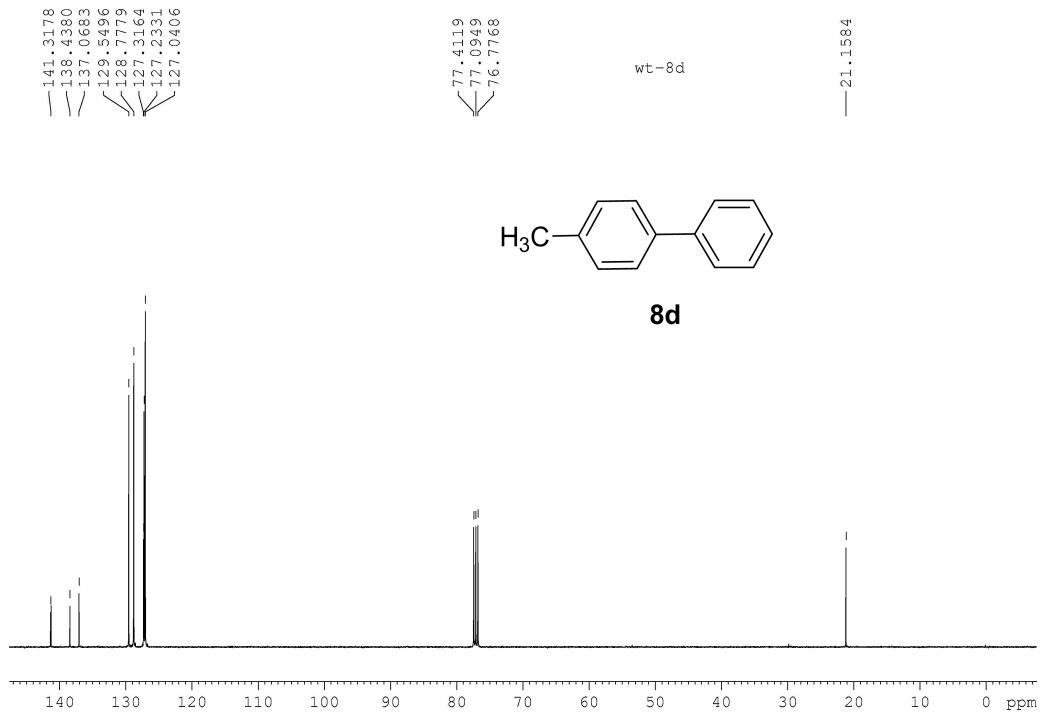
7.3147
7.3101
7.2962
7.2540
7.2341
XHP-23
1H
CDCl3
2.3900
H3C
8d
2.1128
2.0012
2.1272
1.0997
2.1208
3.0000
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm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wt-8d
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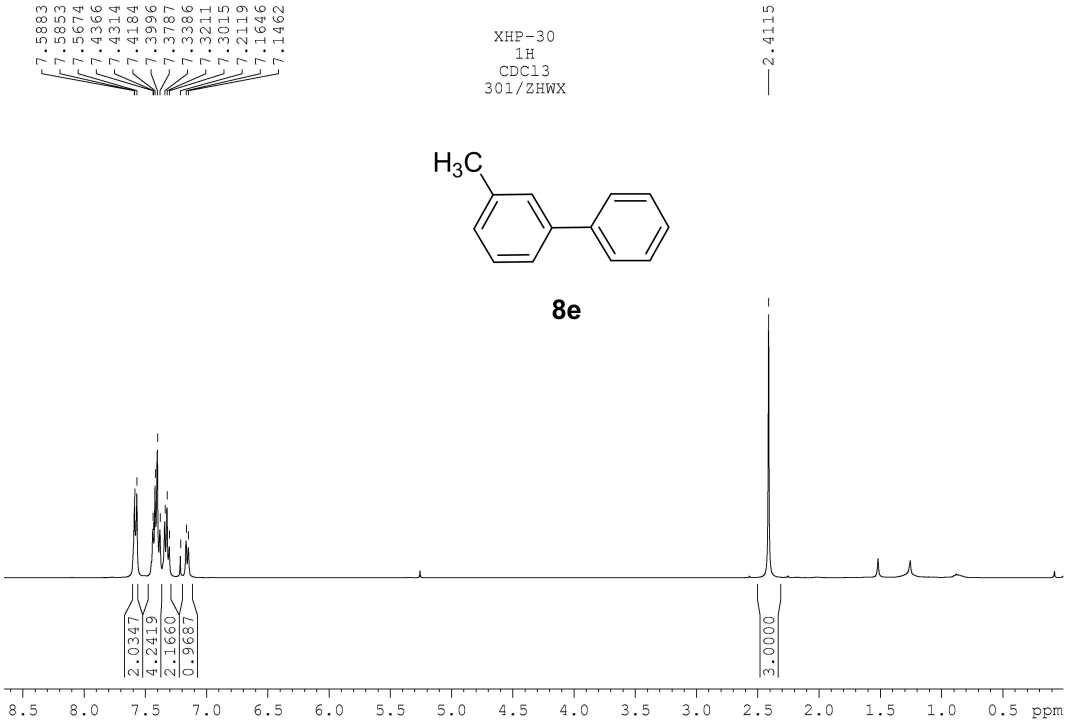
H3C
8d
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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7.2119
7.1646
7.1462
XHP-30
1H
CDCl3
301/ZHWX
2.4115
H3C
8e
2.0347
4.2419
2.1660
0.9687
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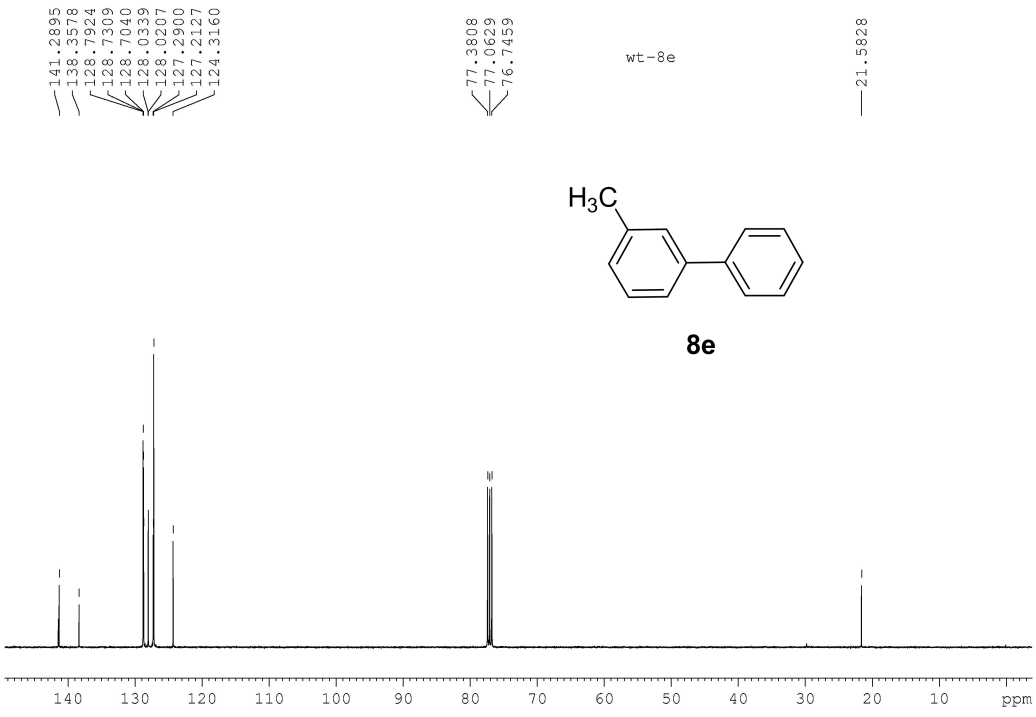
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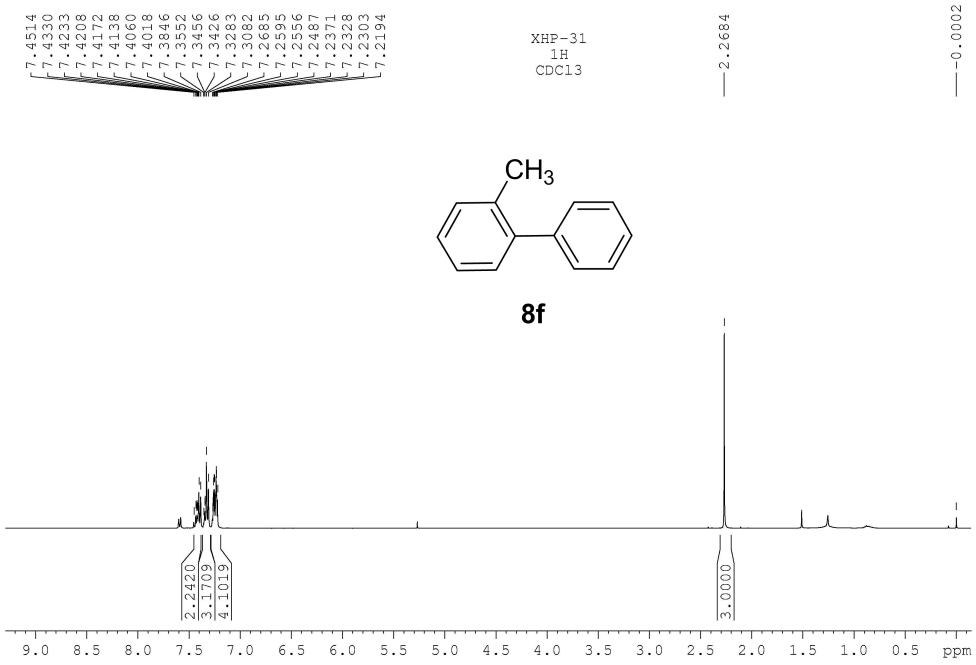
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7.2194
XHP-31
1H
CDCl3
2.2684
0.0002
CH3
2.2420
3.1709
4.1019
3.0000
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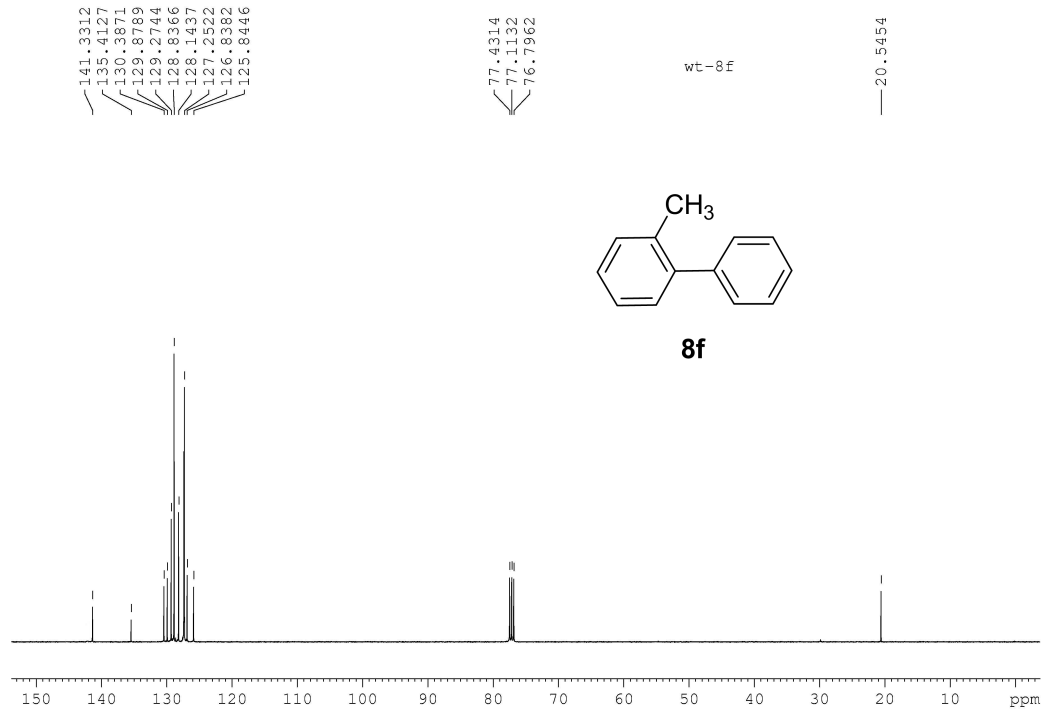
8f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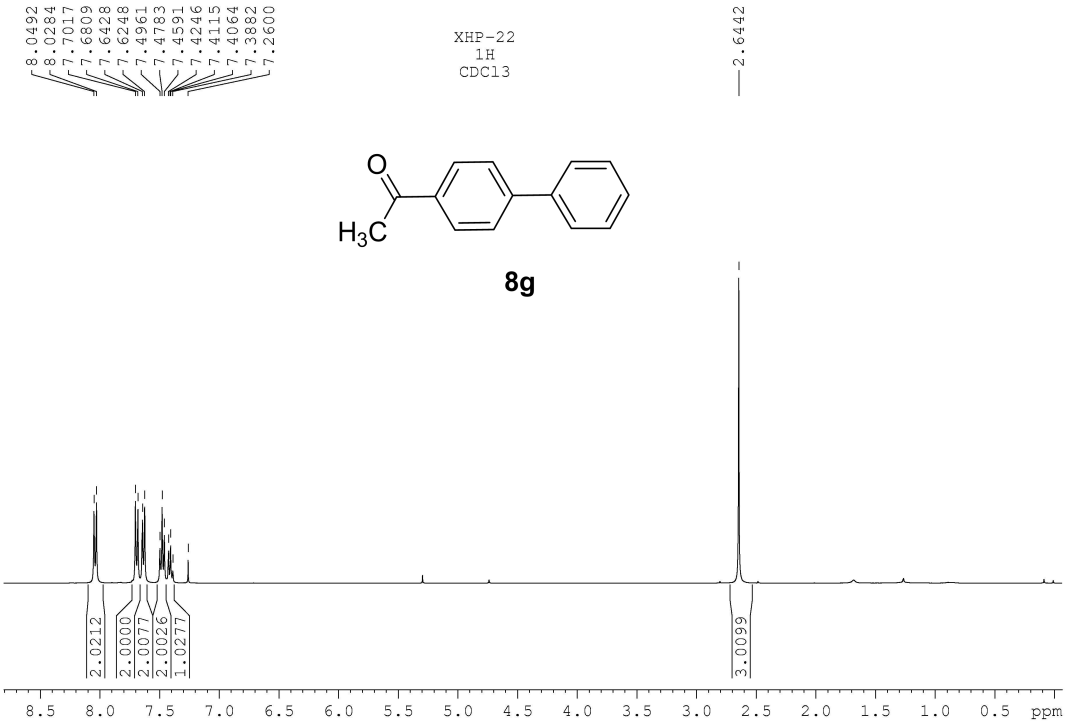
8f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XHP-22
1H
CDCl3
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O
H3C
8g
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2.0000
2.0077
2.0026
1.0277
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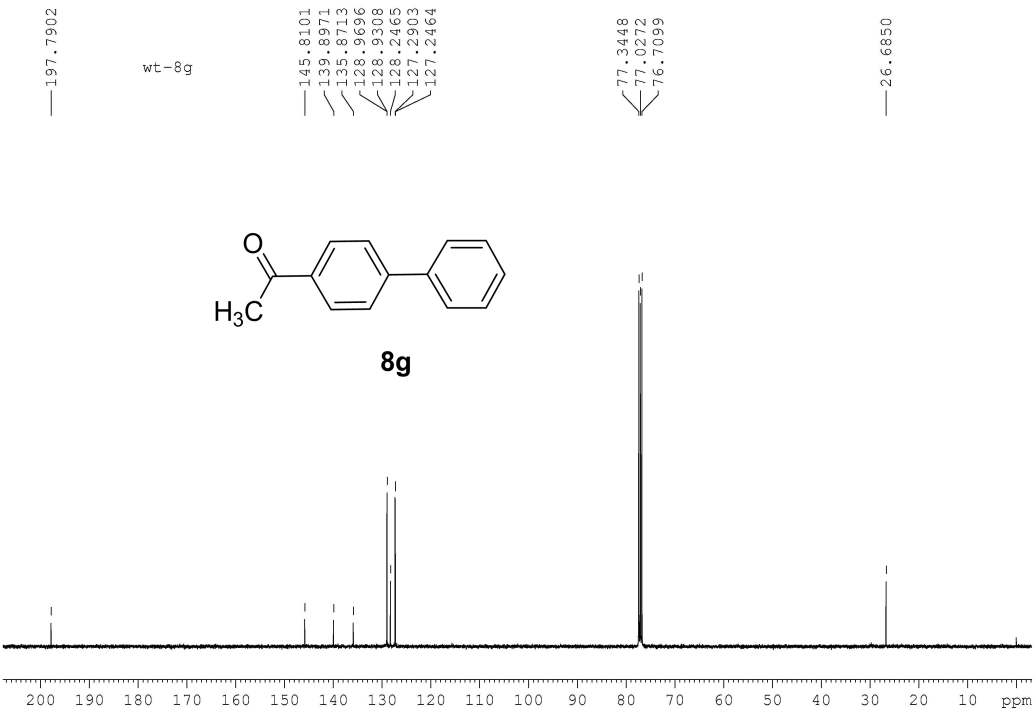
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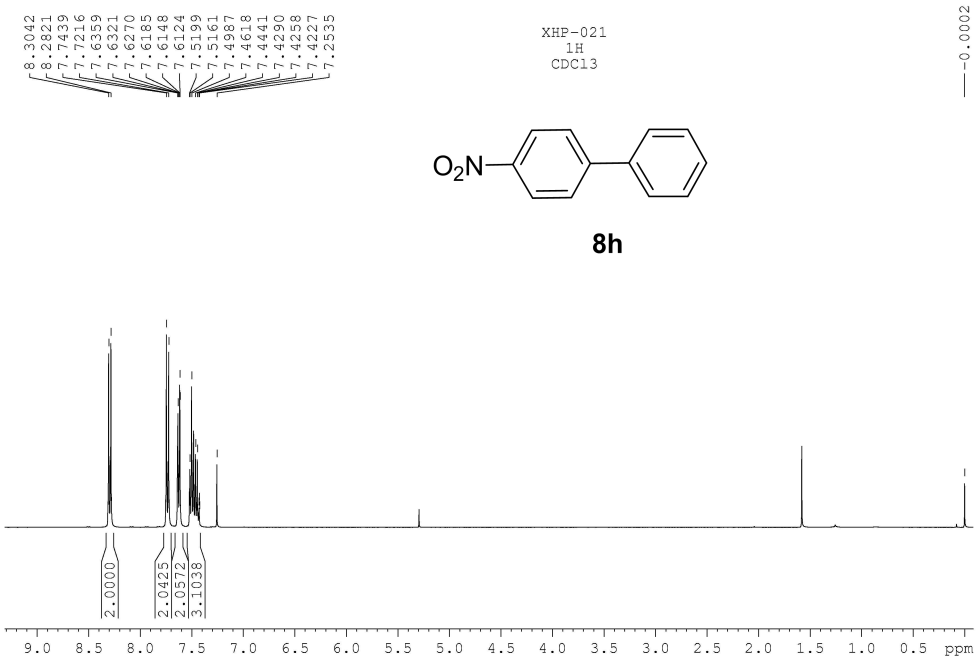
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7.4441
7.4290
7.4258
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XHP-021
1H
CDC13
-0.0002
O2N
8h
2.0000
2.0425
2.0572
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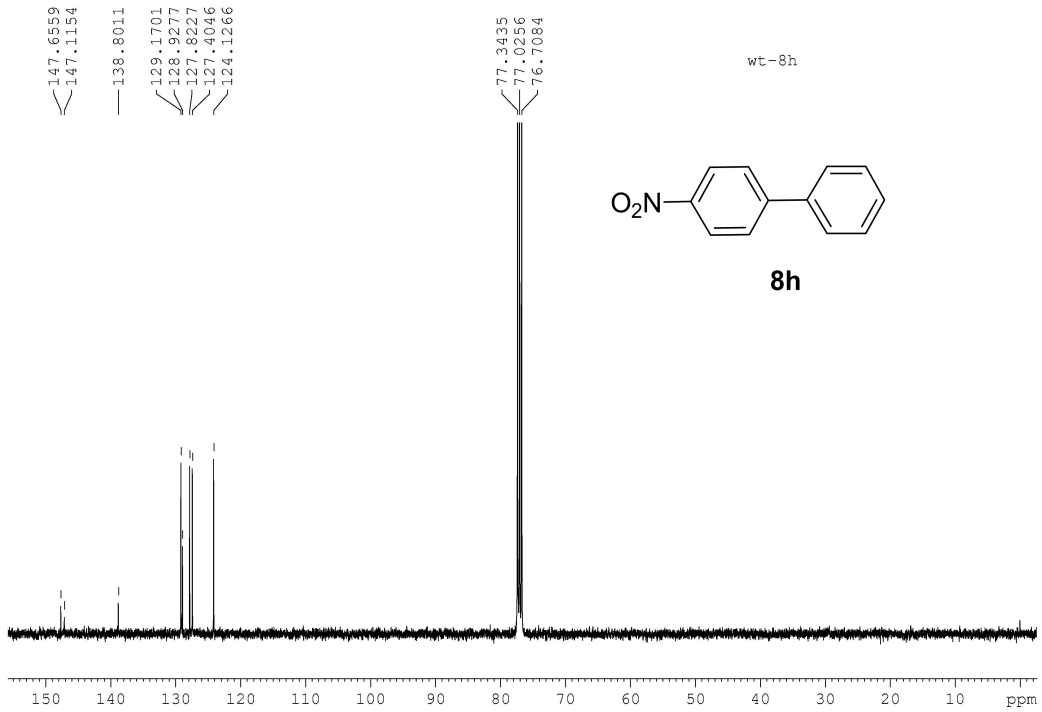
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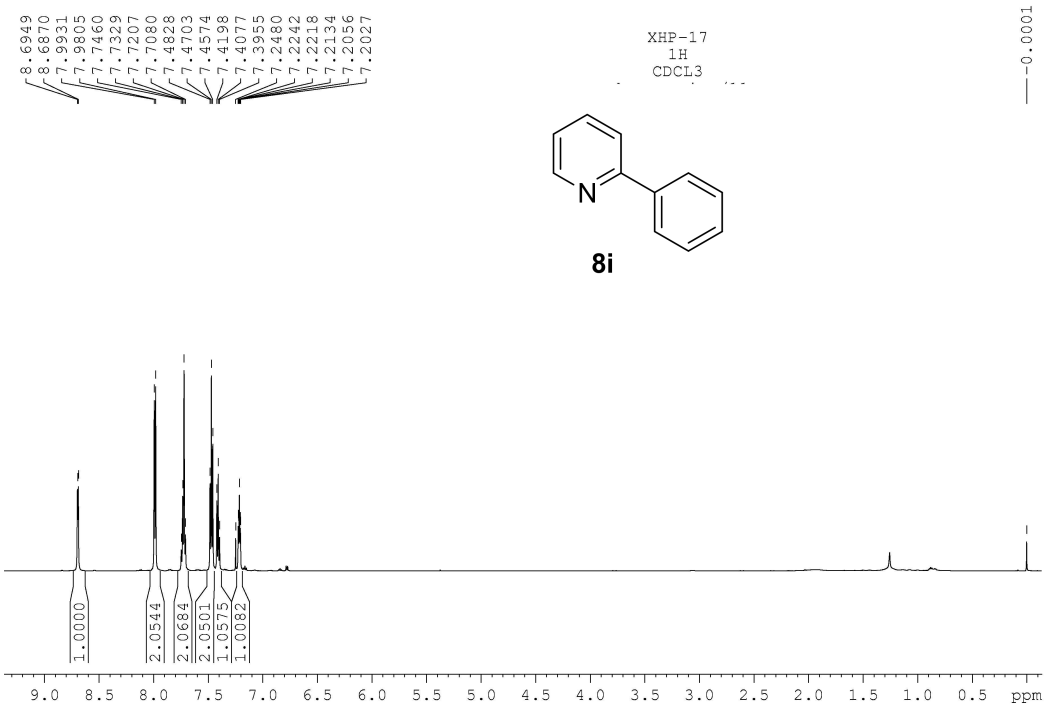
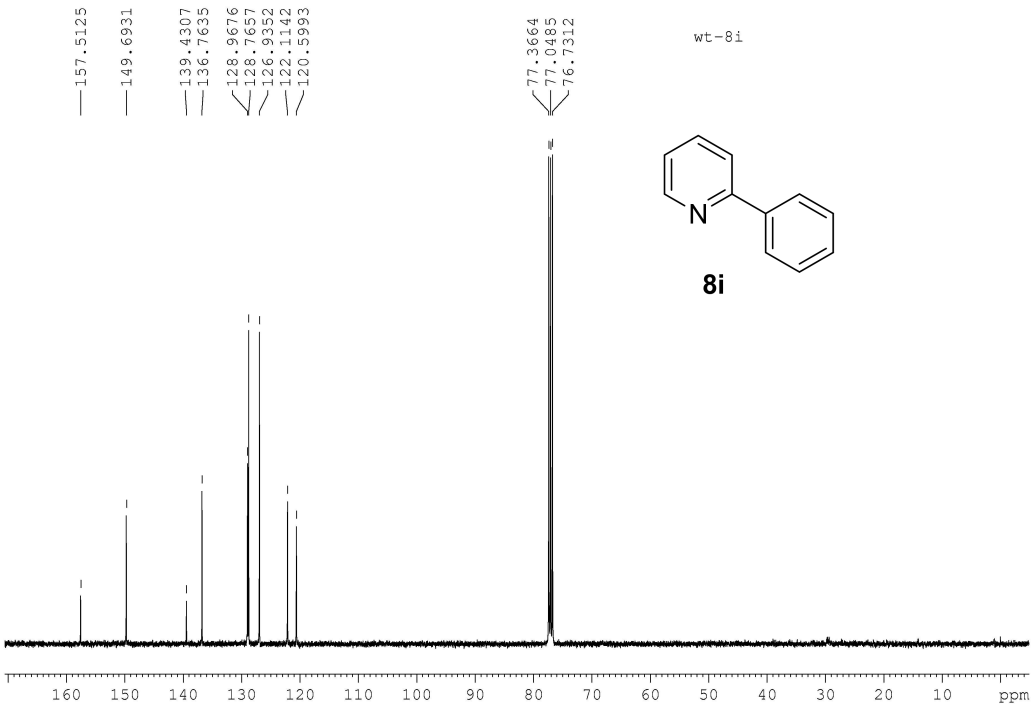
128.9277
127.8227
127.4046
124.1266
77.3435
77.0256
76.7084
wt-8h
O2N
8h
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.6949
8.6870
7.9931
7.9805
7.7460
7.7329
7.7207
7.7080
7.4828
7.4703
7.4574
7.4198
7.4077
7.3955
7.2480
7.2242
7.2218
7.2134
7.2056
7.2027
XHP-17
1H
CDCL3
-0.0001
N
8i
1.0000
2.0544
2.0684
2.0501
1.0575
1.0082
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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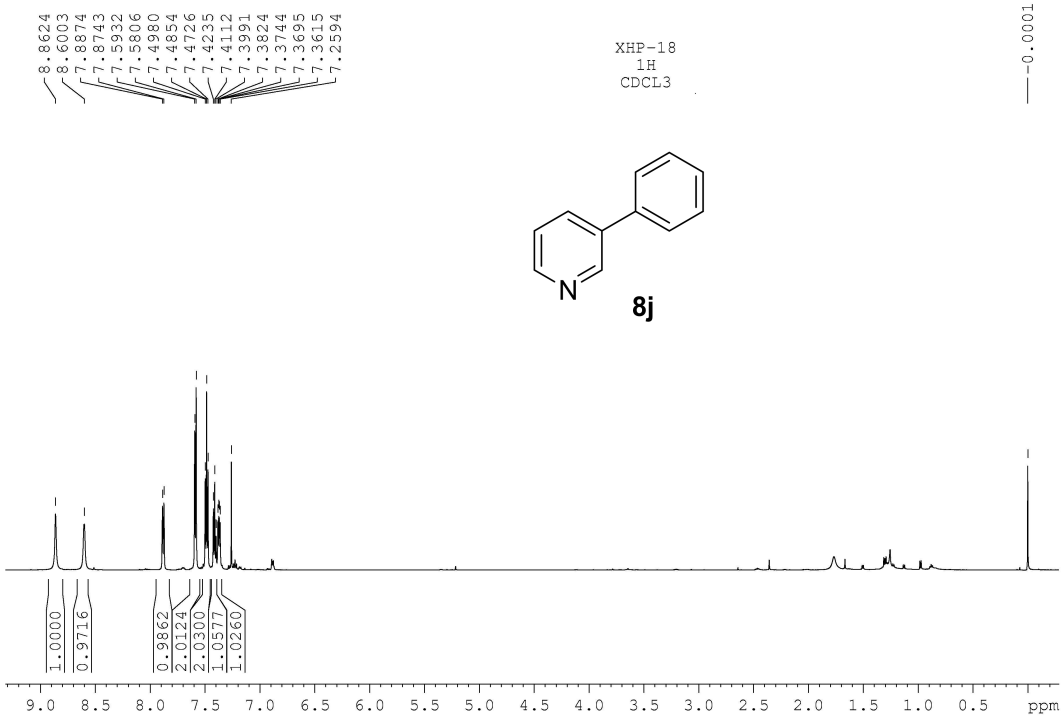
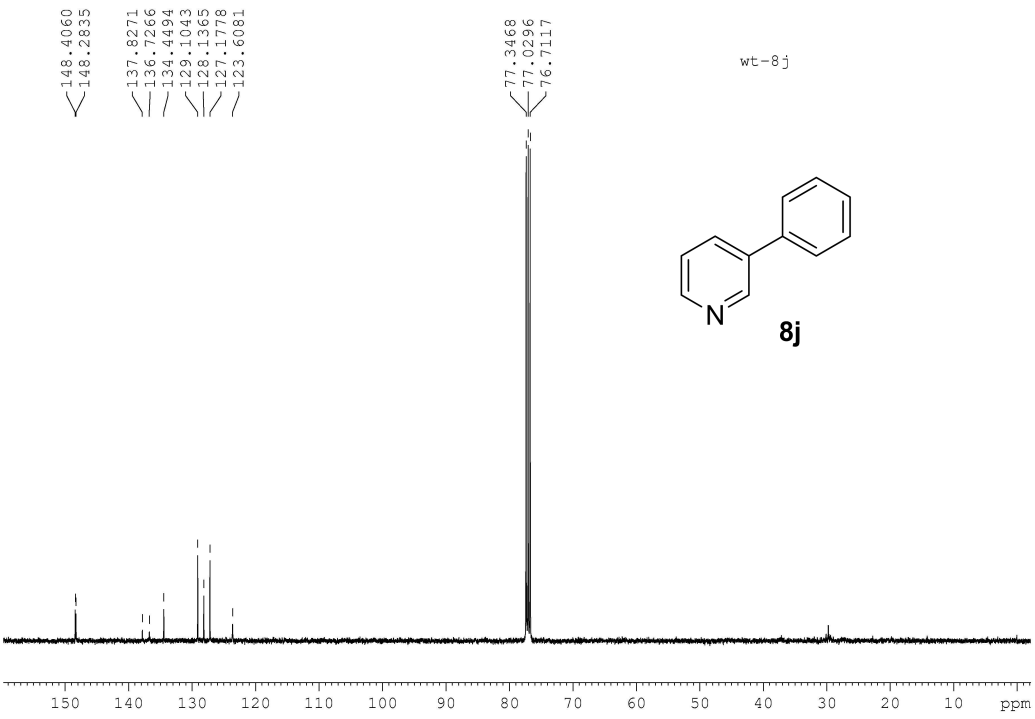
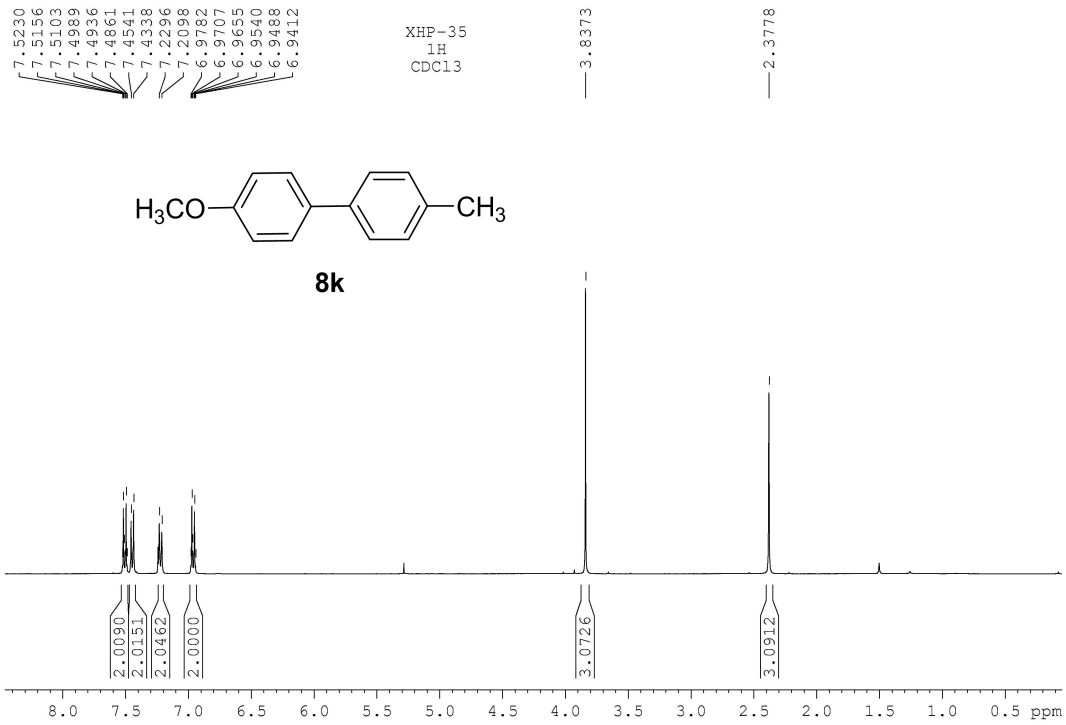
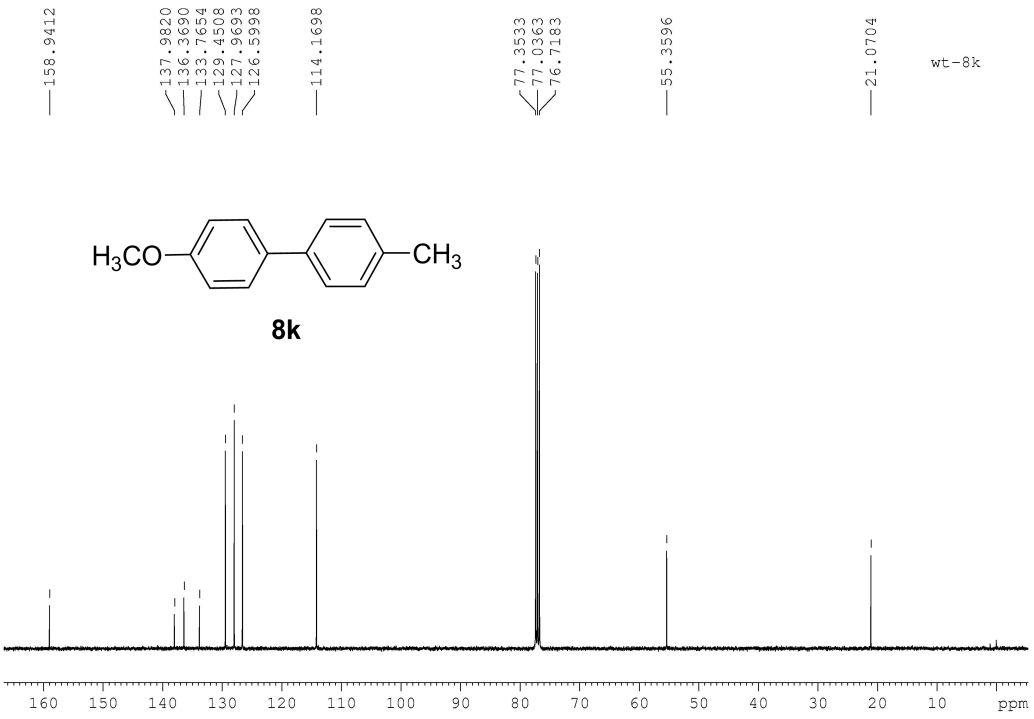
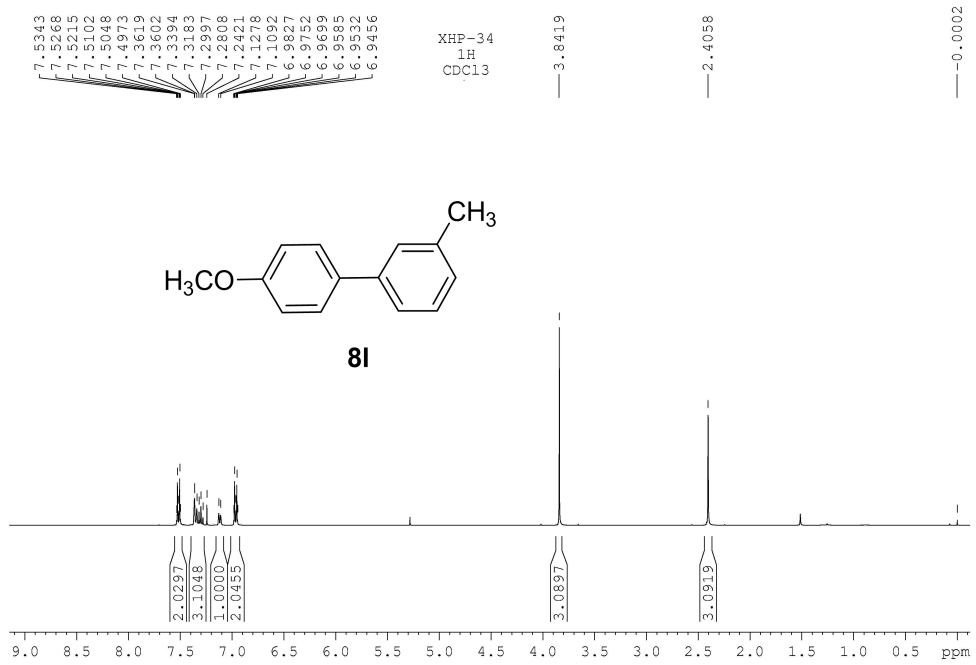
149.6931
139.4307
136.7635
128.9676
128.7657
126.9352
122.1142
120.5993
77.3664
77.0485
76.7312
wt-8i
N
8i
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

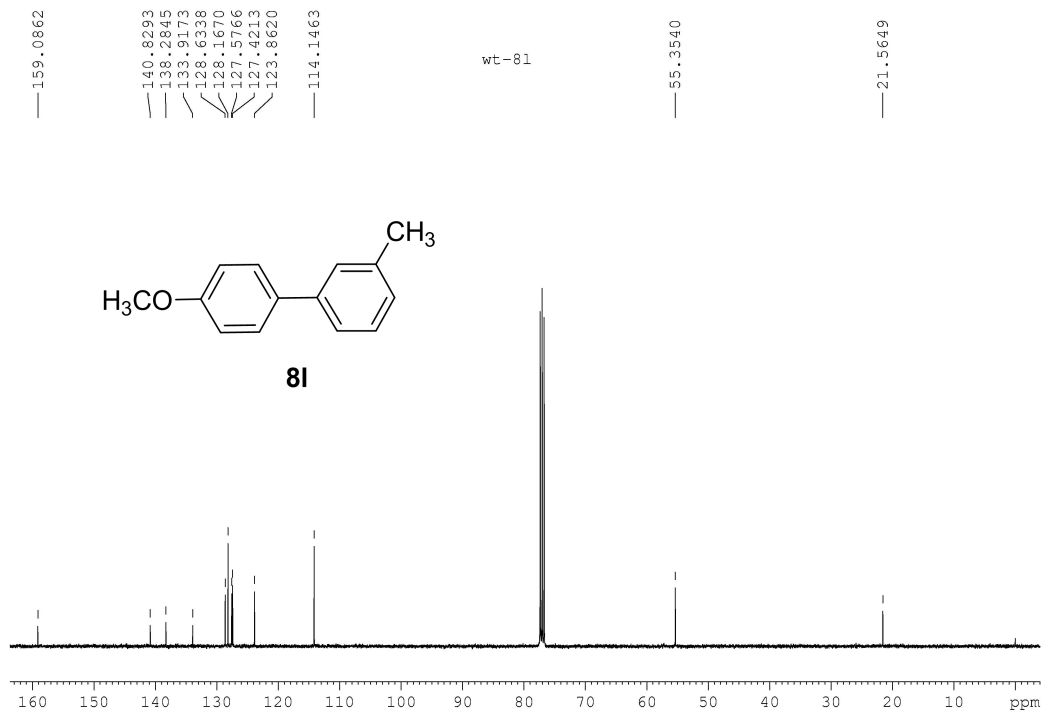

8.8624
8.6003
7.8874
7.8743
7.5932
7.5806
7.4980
7.4854
7.4726
7.4235
7.4112
7.3991
7.3824
7.3744
7.3695
7.3615
7.2594
XHP-18
1H
CDCL3
0.0001
N
8j
1.0000
0.9716
0.9862
2.0124
2.0300
1.0577
1.0260
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

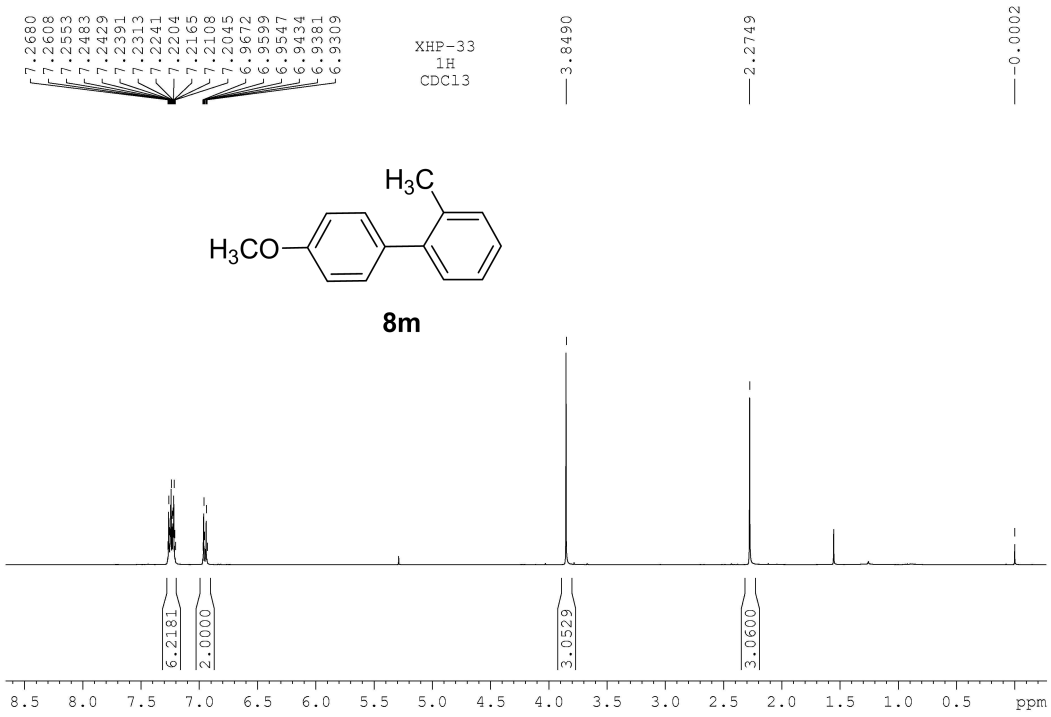

148.4060
148.2835
137.8271
136.7266
134.4494
129.1043
128.1365
127.1778
123.6081
77.3468
77.0296
76.7117
wt-8j
N
8j
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

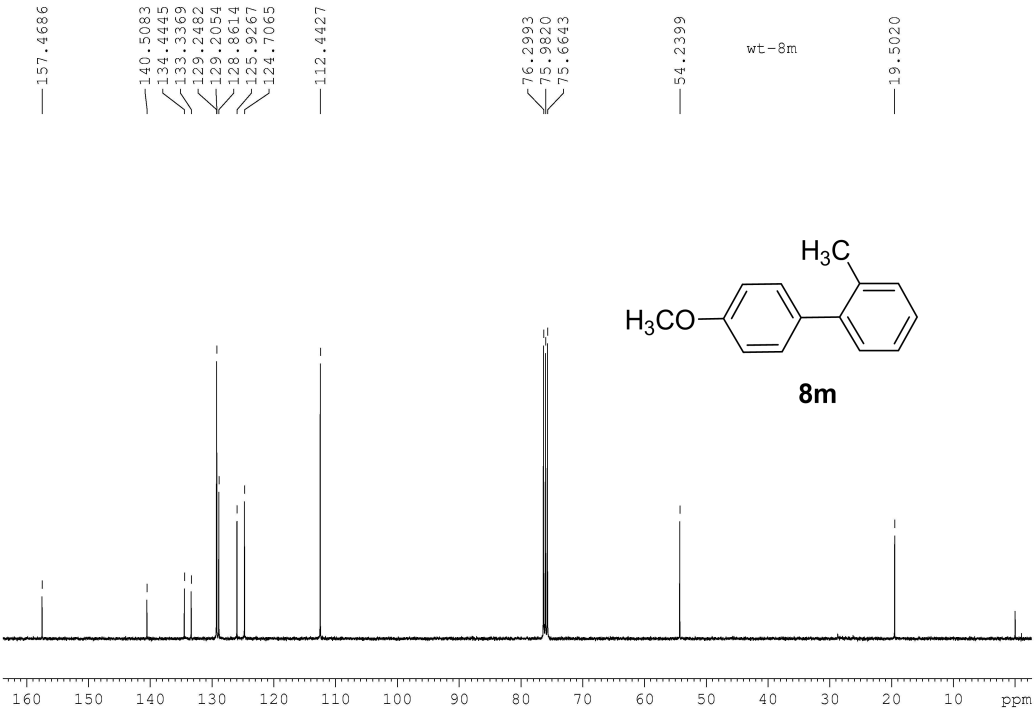

7.5230
7.5156
7.5103
7.4989
7.4936
7.4861
7.4541
7.4338
7.2296
7.2098
6.9782
6.9707
6.9655
6.9540
6.9488
6.9412
XHP-35
1H
CDCl3
3.8373
2.3778
H3CO
CH3
8k
2.0090
2.0151
2.0462
2.0000
3.0726
3.0912
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5 ppm

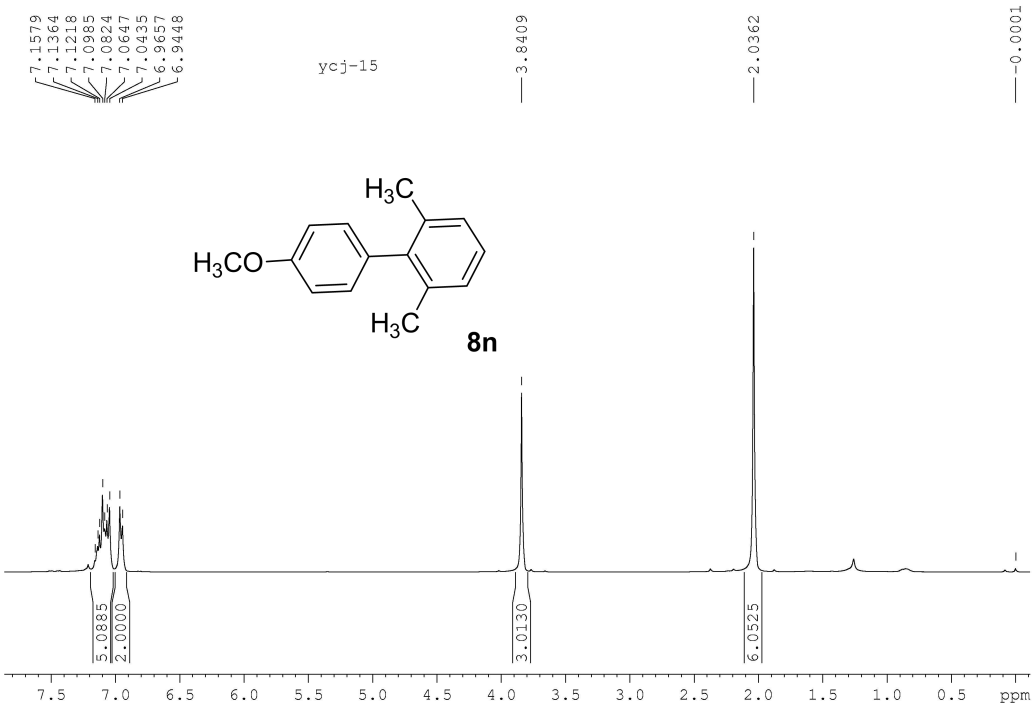

158.9412
137.9820
136.3690
133.7654
129.4508
127.9693
126.5998
114.1698
77.3533
77.0363
76.7183
55.3596
21.0704
wt-8k
H3CO
CH3
8k
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

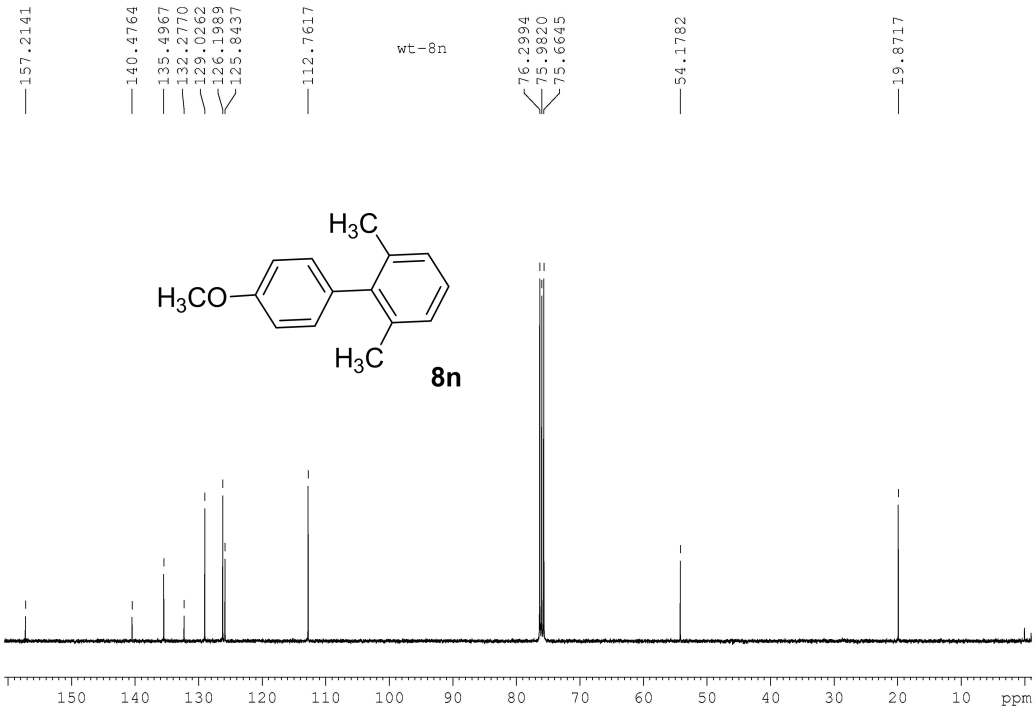

7.5343
7.5268
7.5215
7.5102
7.5048
7.4973
7.3619
7.3602
7.3394
7.3183
7.2997
7.2808
7.2421
7.1278
7.1092
6.9827
6.9752
6.9699
6.9585
6.9532
6.9456
XHP-34
1H
CDCl3
3.8419
2.4058
-0.0002
CH3
H3CO
8l
2.0297
3.1048
1.0000
2.0455
3.0897
3.0919
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

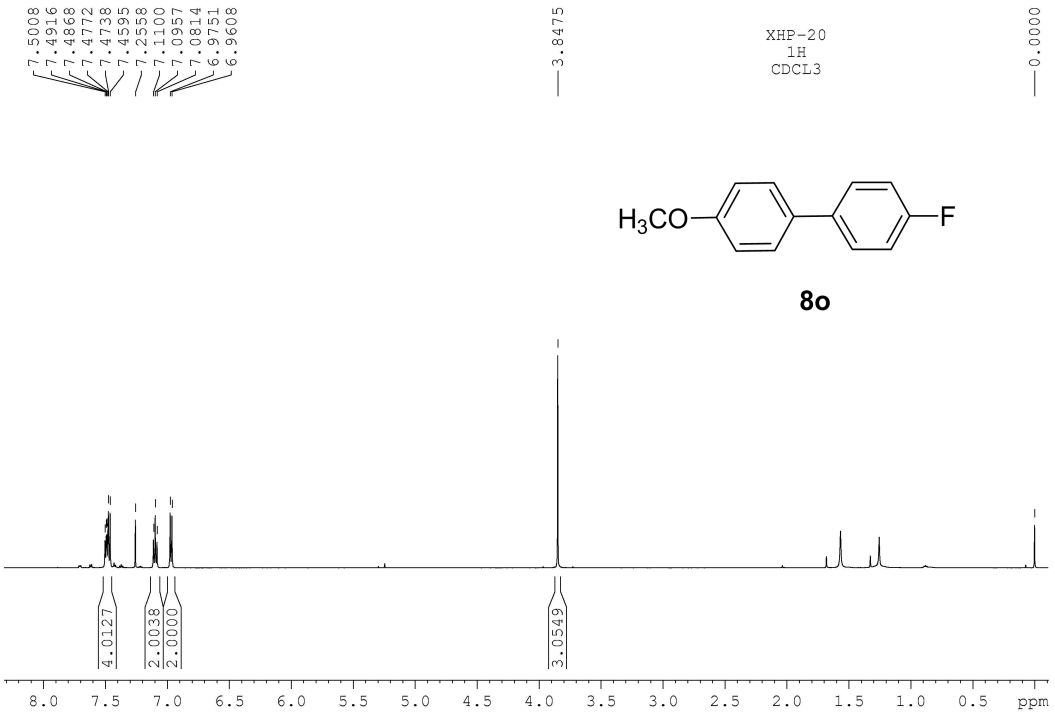

159.0862
140.8293
138.2845
133.9173
128.6338
128.1670
127.5766
127.4213
123.8620
114.1463
wt-8l
55.3540
21.5649
CH3
H3CO
8l
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

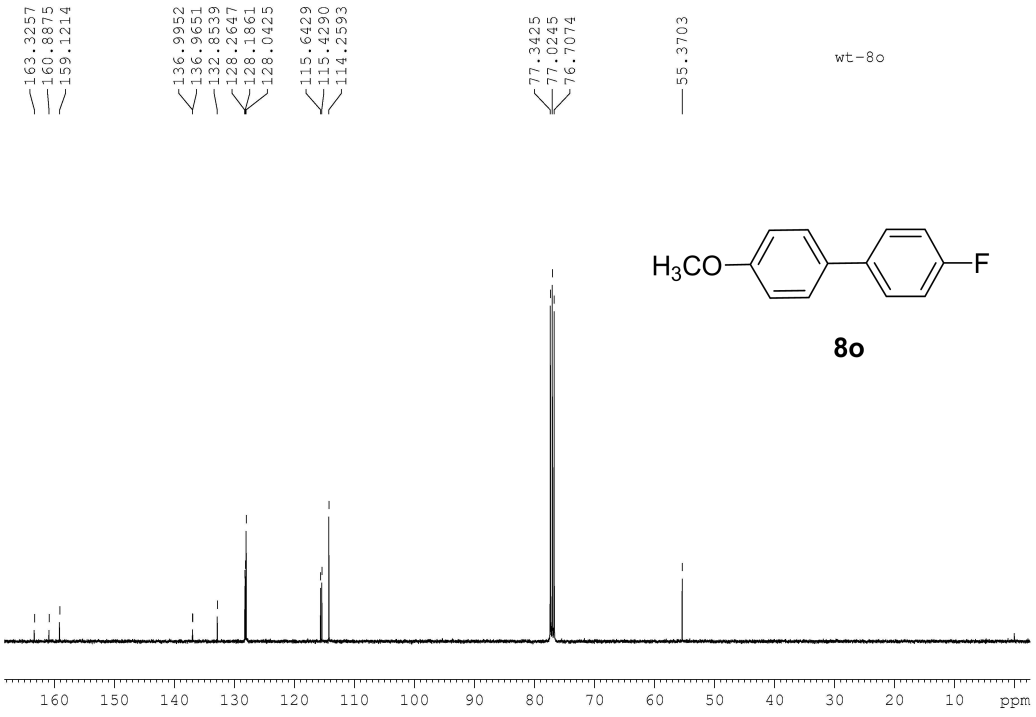

7.2680
7.2608
7.2553
7.2483
7.2429
7.2391
7.2313
7.2241
7.2204
7.2165
7.2108
7.2045
6.9672
6.9599
6.9547
6.9434
6.9381
6.9309
XHP-33
1H
CDCl3
3.8490
2.2749
0.0002
H3C
H3CO
8m
6.2181
2.0000
3.0529
3.0600
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

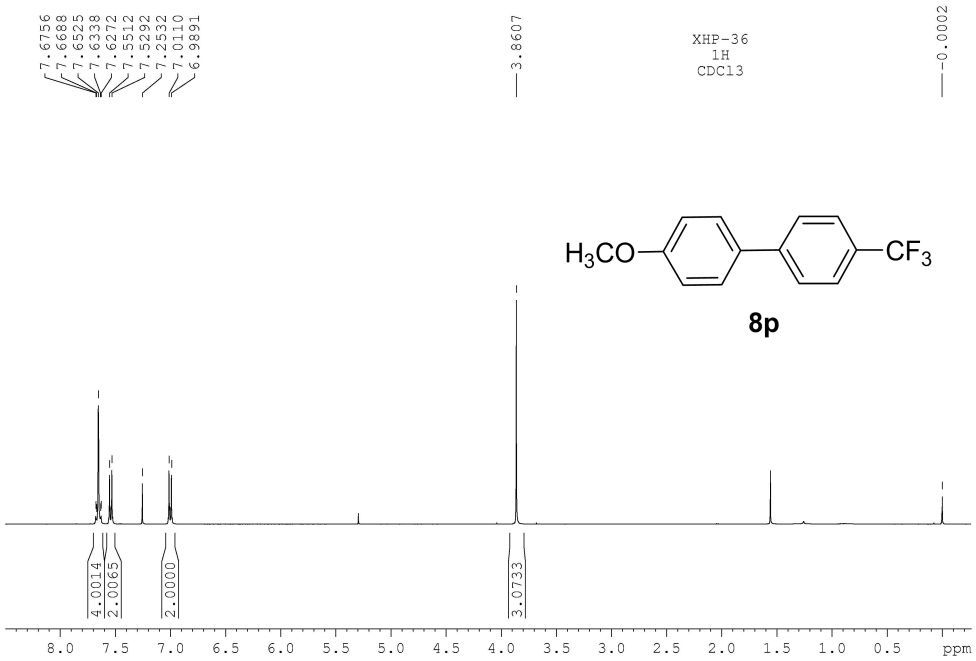

157.4686
140.5083
134.4445
133.3369
129.2482
129.2054
128.8614
125.9267
124.7065
112.4427
76.2993
75.9820
75.6643
54.2399
wt-8m
19.5020
H3C
H3CO
8m
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

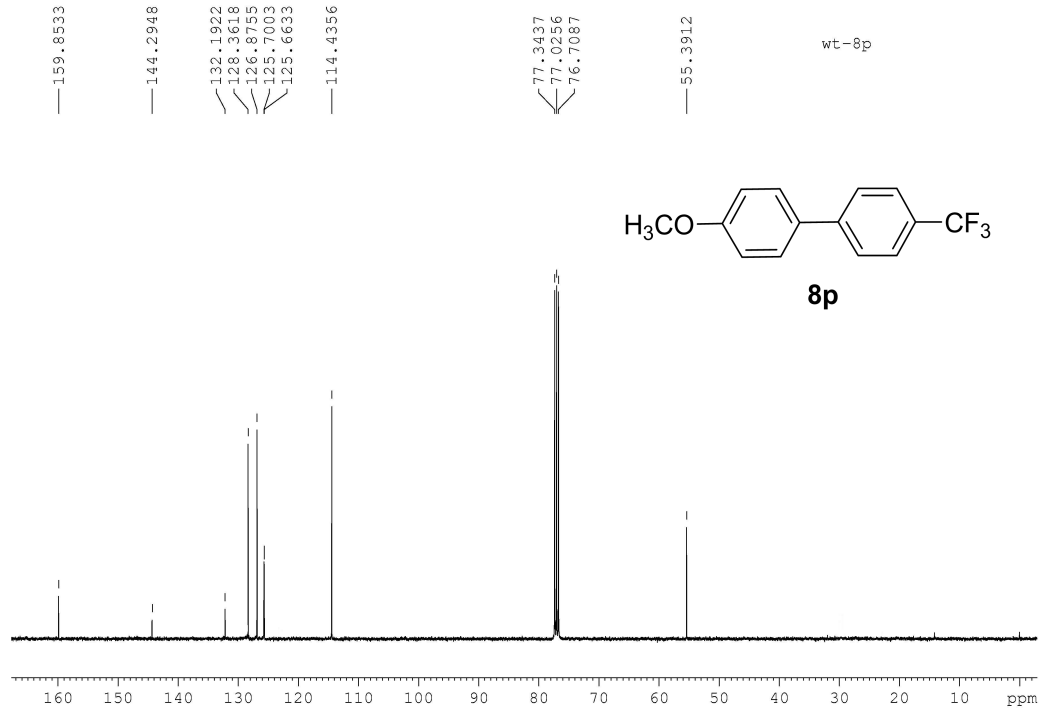

7.1579
7.1364
7.1218
7.0985
7.0824
7.0647
7.0435
6.9657
6.9448
ycj-15
3.8409
2.0362
0.0001
H3C
H3CO
H3C
8n
5.0885
2.0000
3.0130
6.0525
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

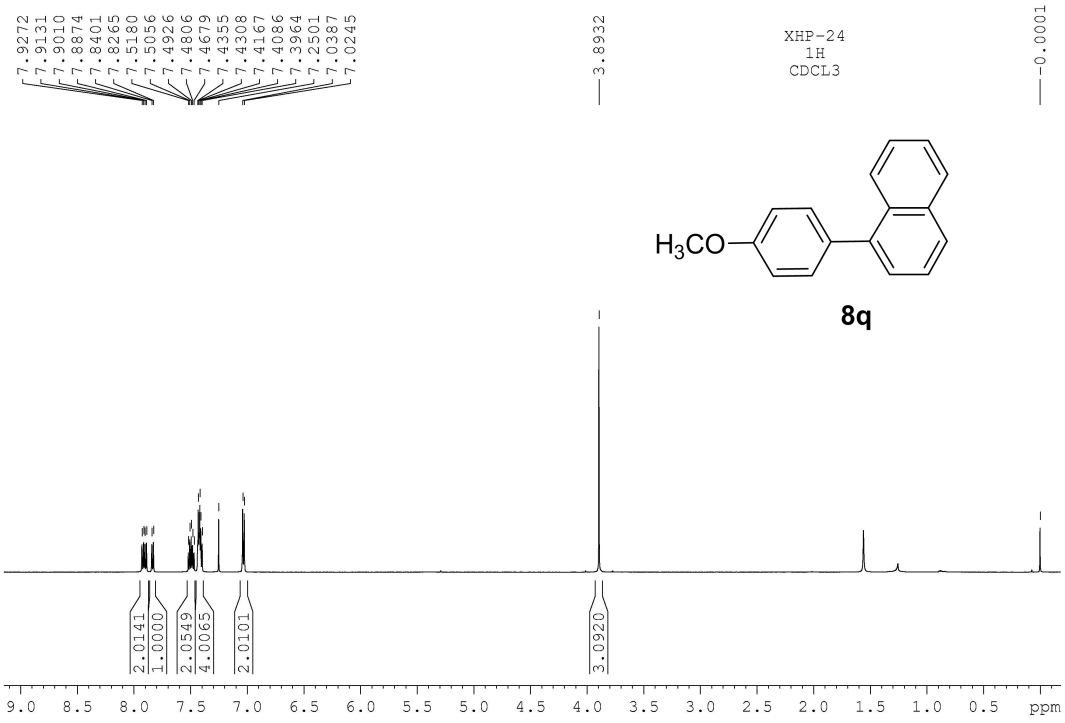

157.2141
140.4764
135.4967
132.2770
129.0262
126.1989
125.8437
112.7617
wt-8n
76.2994
75.9820
75.6645
54.1782
19.8717
H3C
H3CO
H3C
8n
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

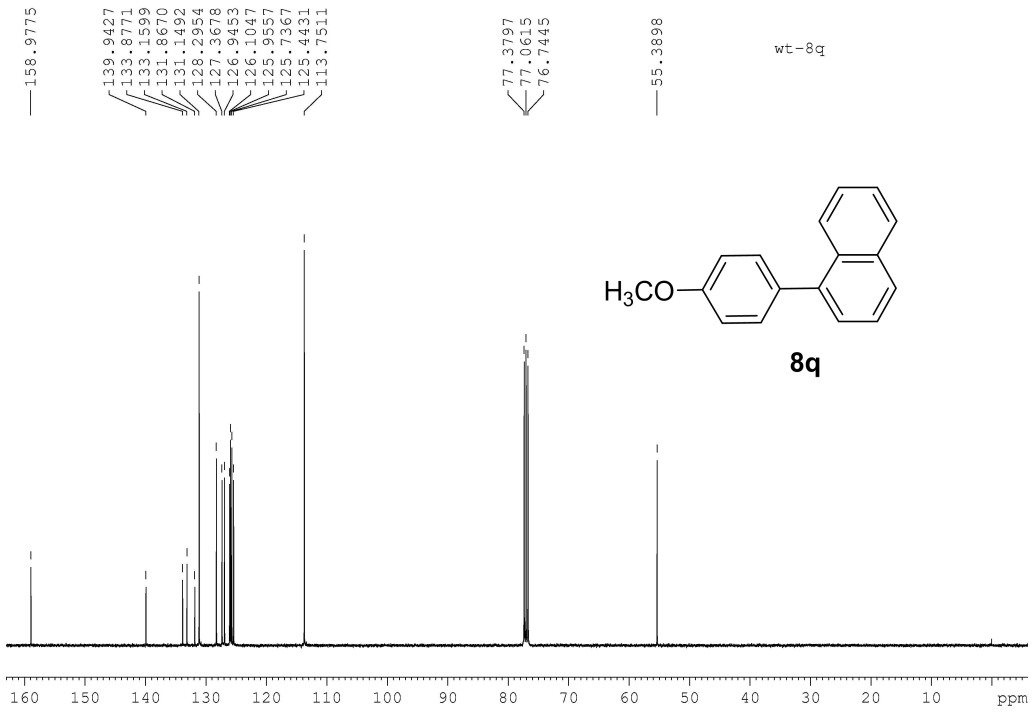

7.5008
7.4916
7.4868
7.4772
7.4738
7.4595
7.2558
7.1100
7.0957
7.0814
6.9751
6.9608
3.8475
0.0000
XHP-20
1H
CDCL3
H3CO
F
8o
4.0127
2.0038
2.0000
3.0549
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

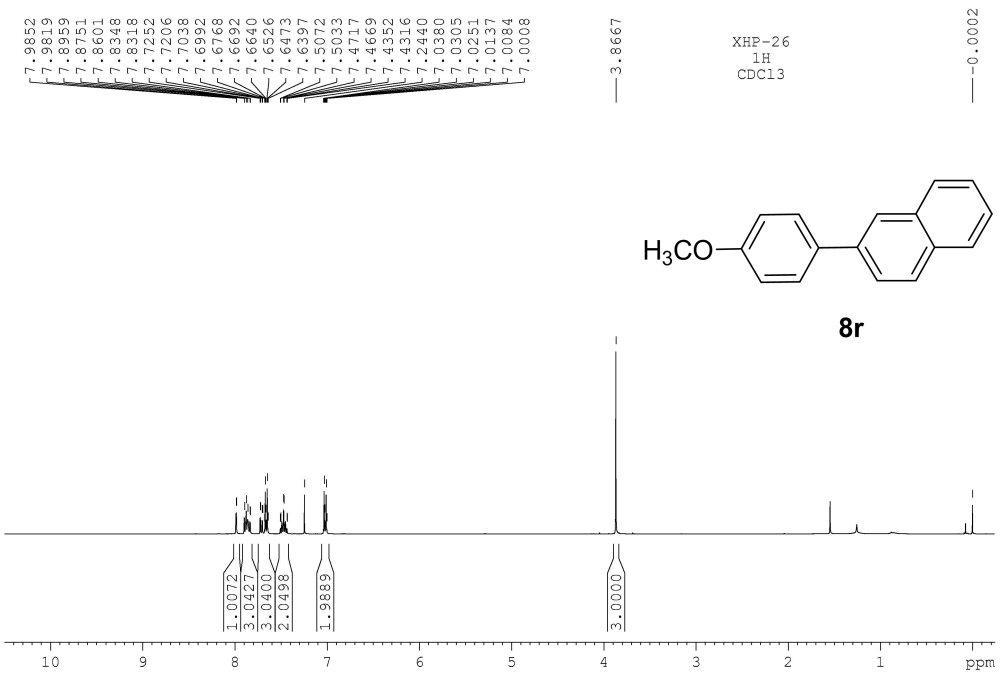

163.3257
160.8875
159.1214
136.9952
136.9651
132.8539
128.2647
128.1861
128.0425
115.6429
115.4290
114.2593
77.3425
77.0245
76.7074
55.3703
wt-8o
H3CO
F
8o
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

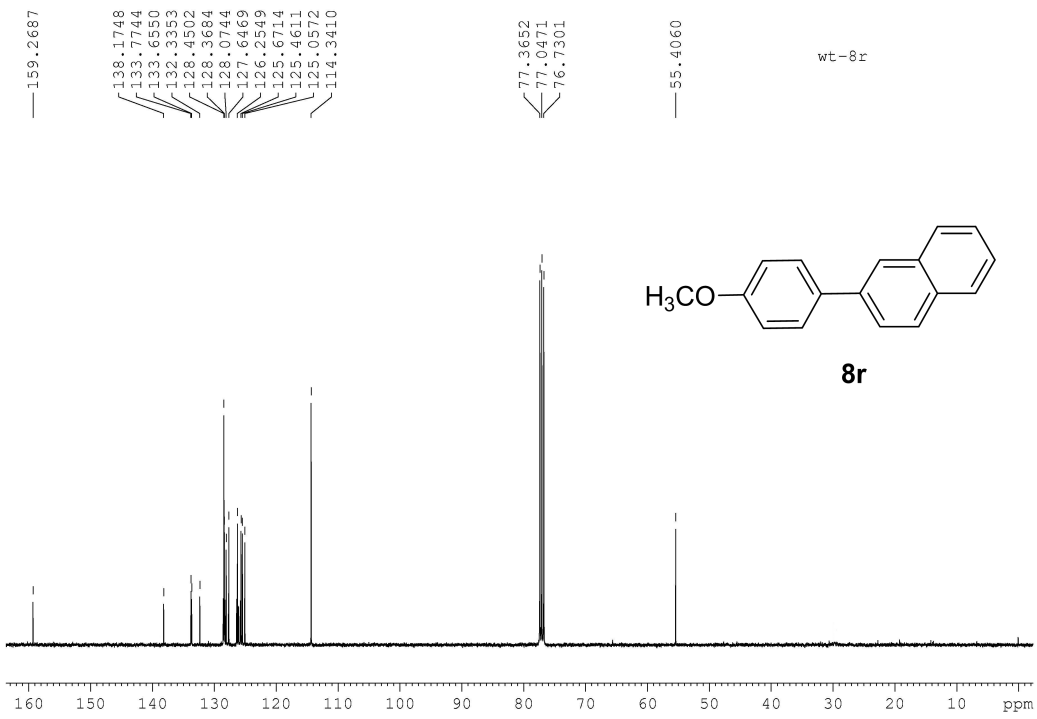

7.6756
7.6688
7.6525
7.6338
7.6272
7.5512
7.5292
7.2532
7.0110
6.9891
3.8607
XHP-36
1H
CDCl3
0.0002
H3CO
CF3
8p
4.0014
2.0065
2.0000
3.0733
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

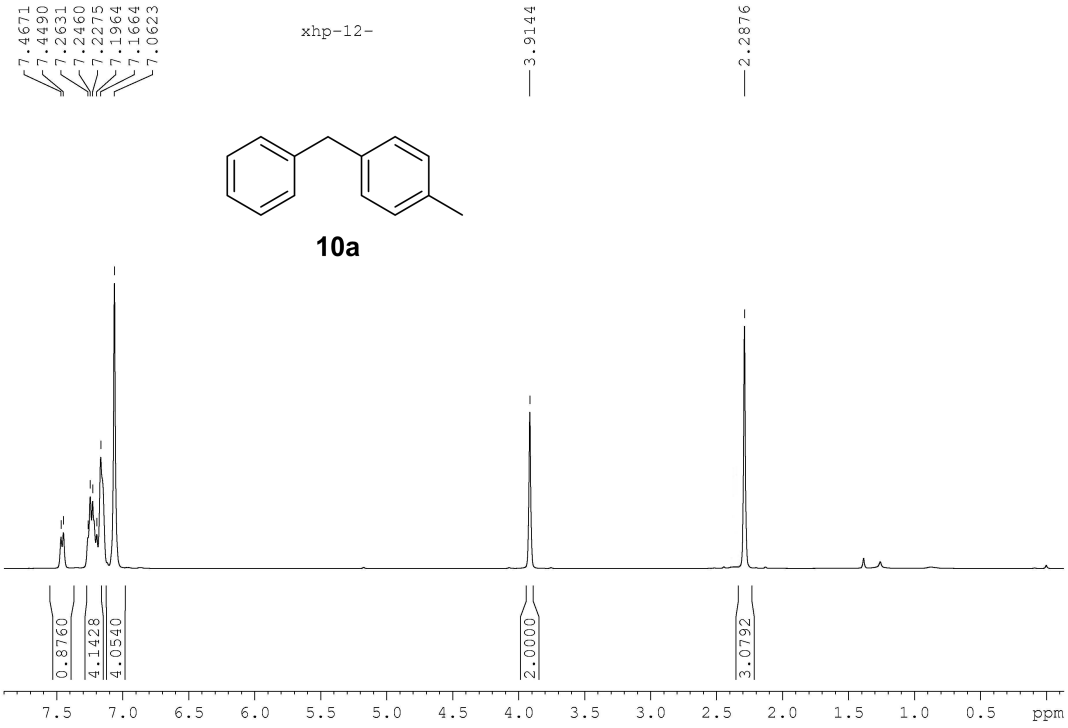

159.8533
144.2948
132.1922
128.3618
126.8755
125.7003
125.6633
114.4356
77.3437
77.0256
76.7087
55.3912
wt-8p
H3CO
CF3
8p
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.9272
7.9131
7.9010
7.8874
7.8401
7.8265
7.5180
7.5056
7.4926
7.4806
7.4679
7.4355
7.4308
7.4167
7.4086
7.3964
7.2501
7.0387
7.0245
3.8932
0.0001
XHP-24
1H
CDCL3
H3CO
8q
2.0141
1.0000
2.0549
4.0065
2.0101
3.0920
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

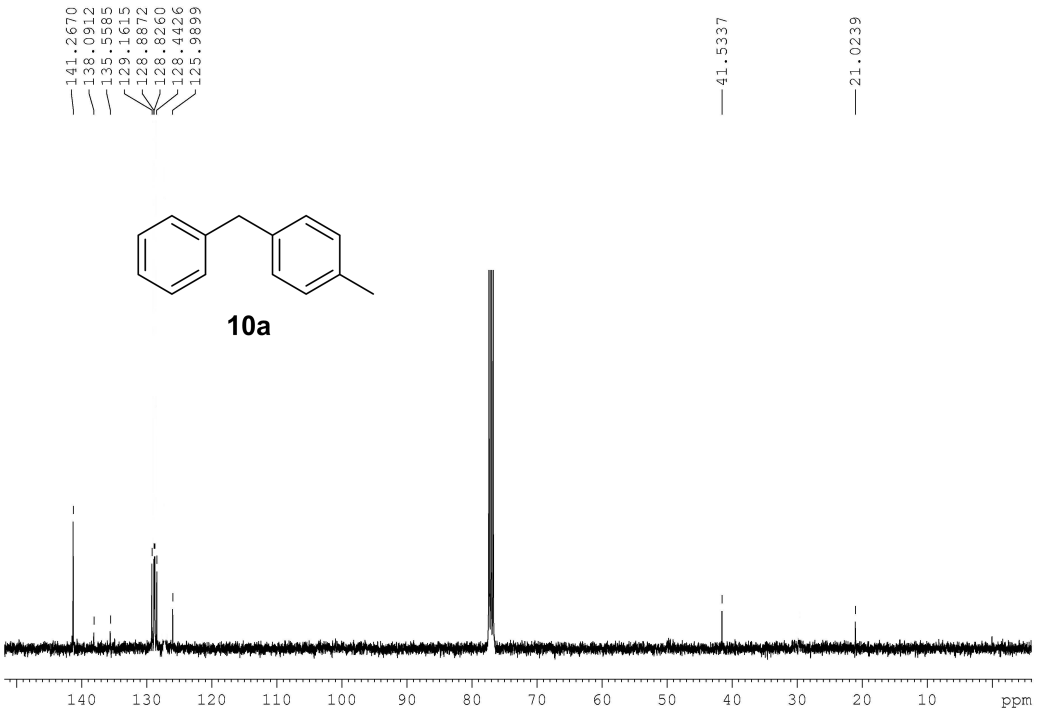

158.9775
139.9427
133.8771
133.1599
131.8670
131.1492
128.2954
127.3678
126.9453
126.1047
125.9557
125.7367
125.4431
113.7511
77.3797
77.0615
76.7445
55.3898
wt-8q
H3CO
8q
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.9852
7.9819
7.8959
7.8751
7.8601
7.8348
7.8318
7.7252
7.7206
7.7038
7.6992
7.6768
7.6692
7.6640
7.6526
7.6473
7.6397
7.5072
7.5033
7.4717
7.4669
7.4352
7.4316
7.2440
7.0380
7.0305
7.0251
7.0137
7.0084
7.0008
3.8667
XHP-26
1H
CDCl3
0.0002
H3CO
8r
1.0072
3.0427
3.0400
2.0498
1.9889
3.0000
10
9
8
7
6
5
4
3
2
1
ppm

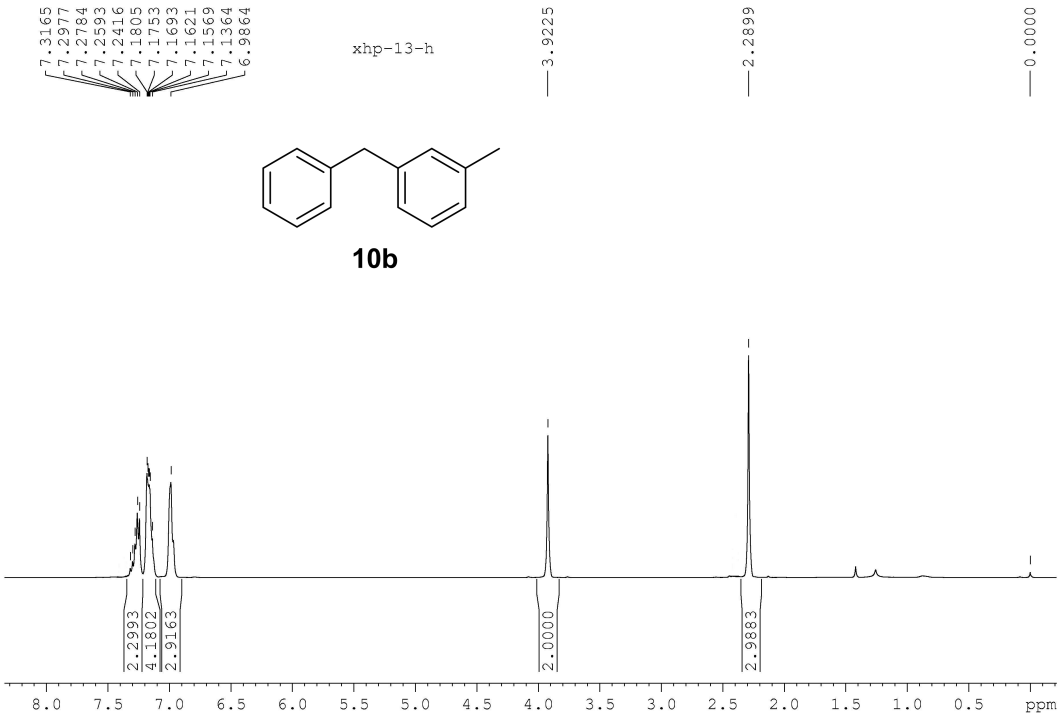

159.2687
138.1748
133.7744
133.6550
132.3353
128.4502
128.3684
128.0744
127.6469
126.2549
125.6714
125.4611
125.0572
114.3410
77.3652
77.0471
76.7301
55.4060
wt-8r
H3CO
8r
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

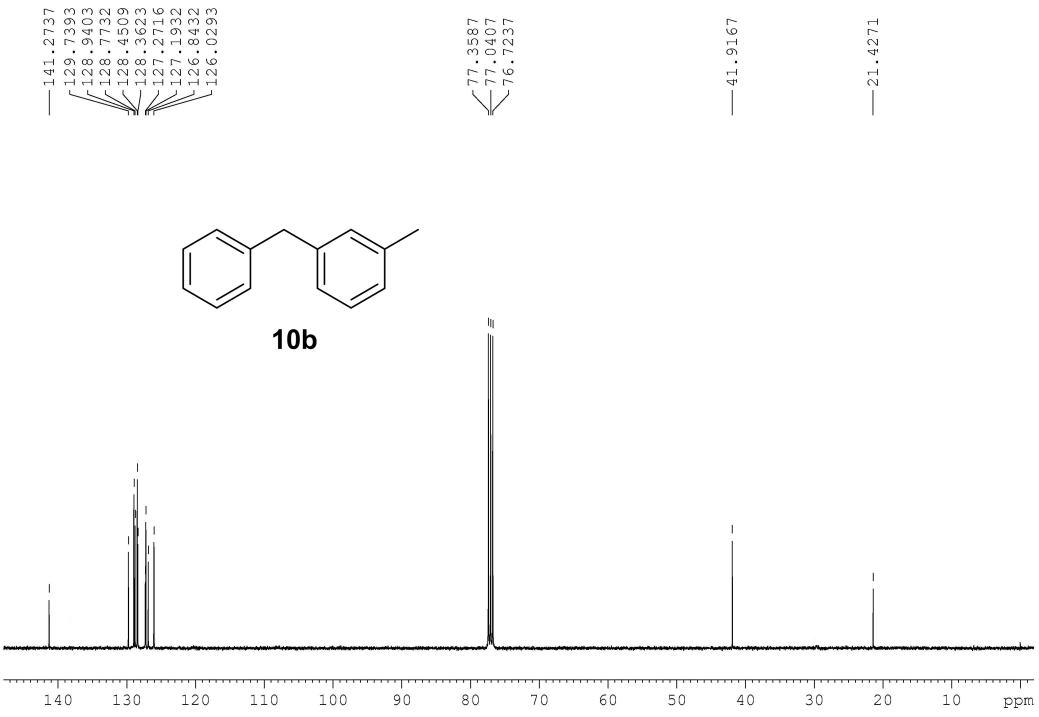

7.4671
7.4490
7.2631
7.2460
7.2275
7.1964
7.1664
7.0623
xhp-12-
3.9144
2.2876
0.8760
4.1428
4.0540
2.0000
3.0792
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

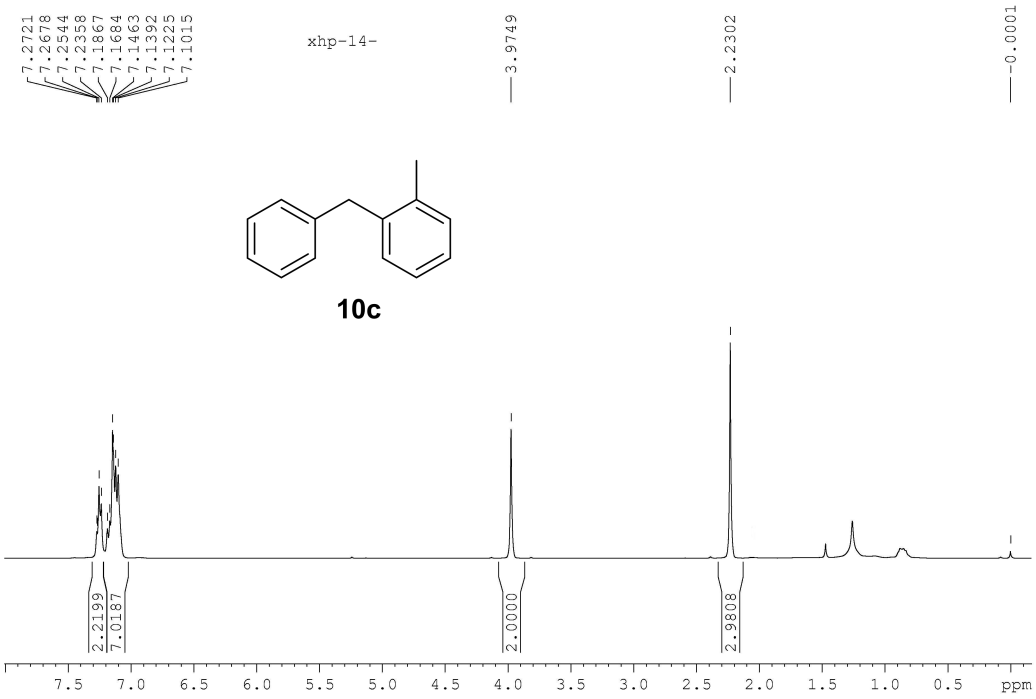
10a


141.2670
138.0912
135.5585
129.1615
128.8872
128.8260
128.4426
125.9899
41.5337
21.0239
140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

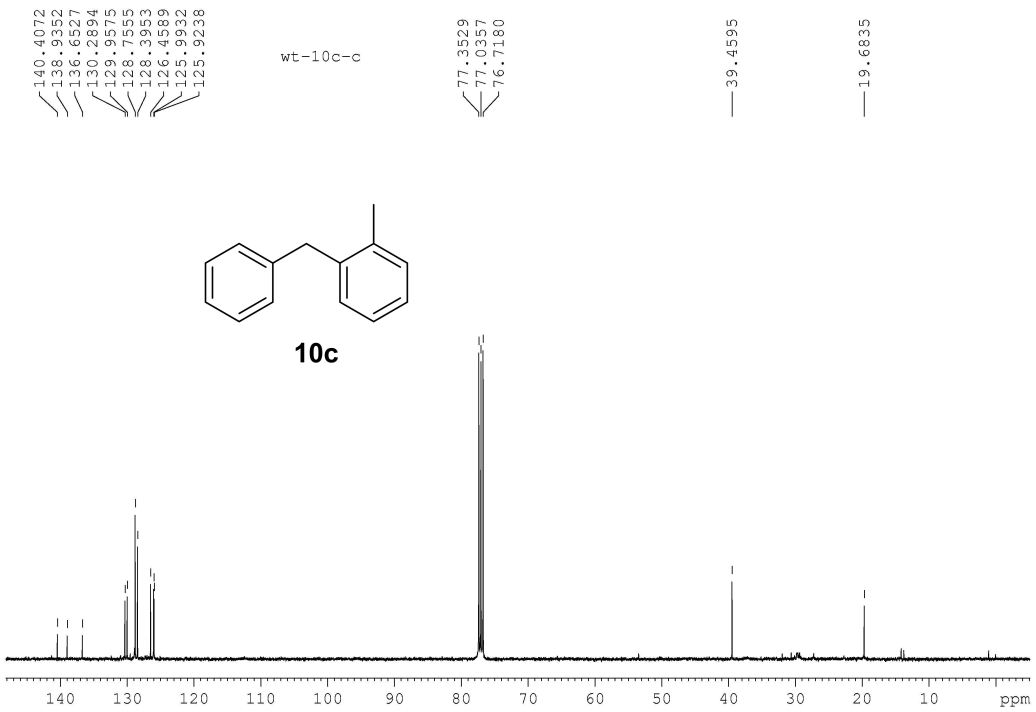
10a


7.3165
7.2977
7.2784
7.2593
7.2416
7.1805
7.1753
7.1693
7.1621
7.1569
7.1364
6.9864
xhp-13-h
3.9225
2.2899
0.0000
10b
2.2993
4.1802
2.9163
2.0000
2.9883
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

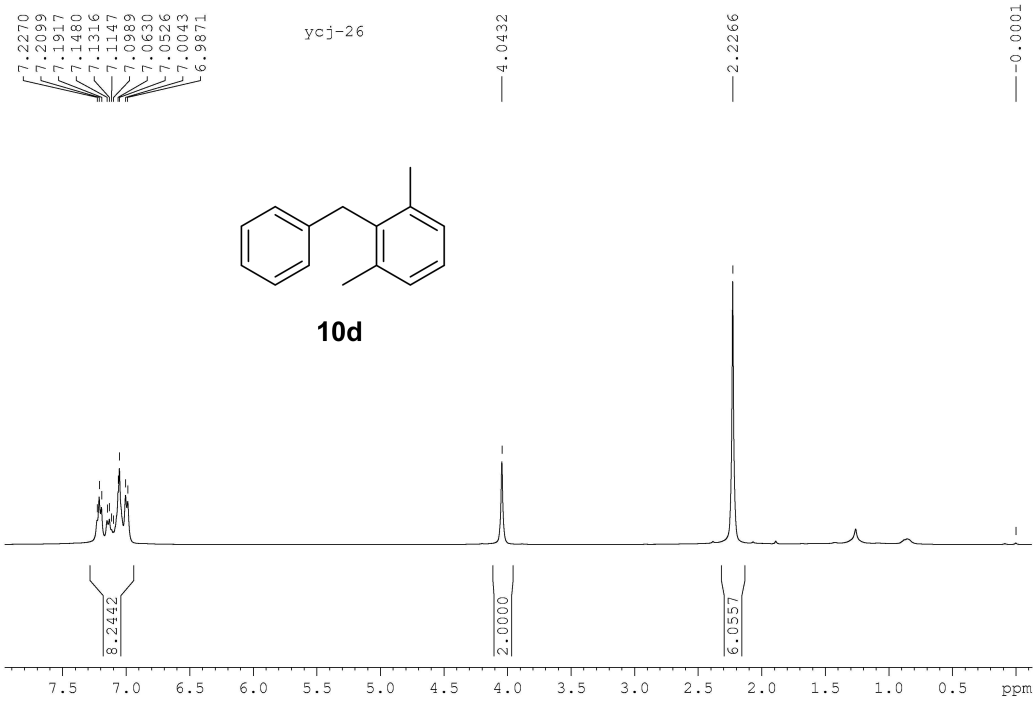

141.2737
129.7393
128.9403
128.7732
128.4509
128.3623
127.2716
127.1932
126.8432
126.0293
77.3587
77.0407
76.7237
41.9167
21.4271
10b
140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

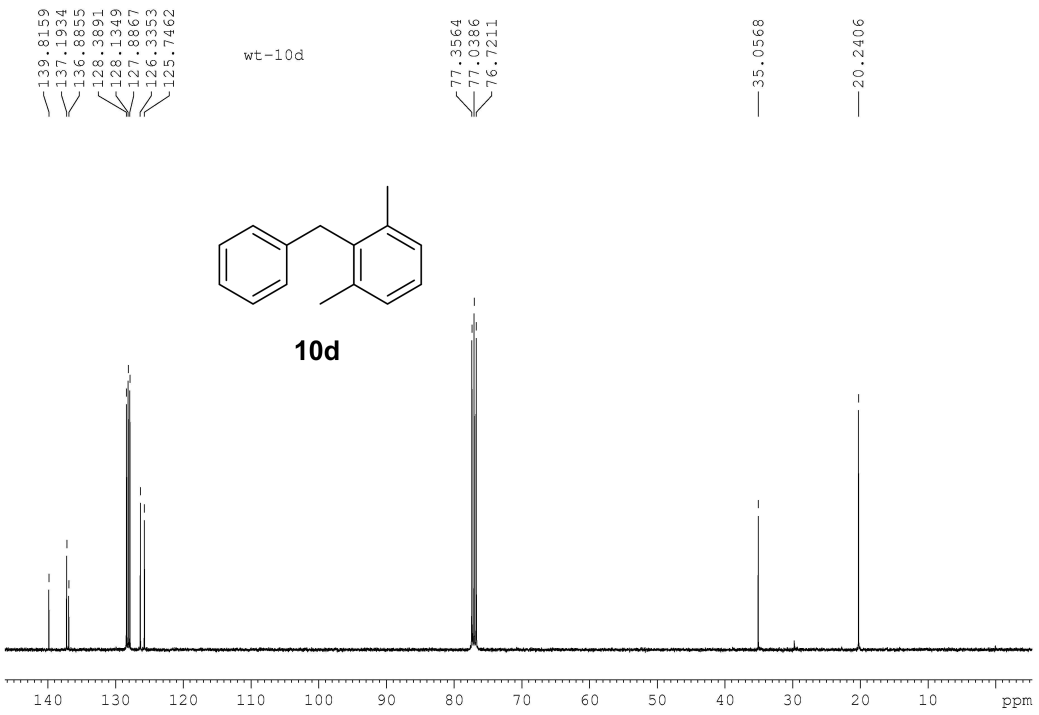

7.2721
7.2678
7.2544
7.2358
7.1867
7.1684
7.1463
7.1392
7.1225
7.1015
xhp-14-
3.9749
2.2302
-0.0001
2.2199
7.0187
2.0000
2.9808
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

10c


140.4072
138.9352
136.6527
130.2894
129.9575
128.7555
128.3953
126.4589
125.9932
125.9238
wt-10c-c
77.3529
77.0357
76.7180
39.4595
19.6835
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

10c


7.2270
7.2099
7.1917
7.1480
7.1316
7.1147
7.0989
7.0630
7.0526
7.0043
6.9871
ycj-26
4.0432
2.2266
0.0001
10d
8.2442
2.0000
6.0557
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


139.8159
137.1934
136.8855
128.3891
128.1349
127.8867
126.3353
125.7462
wt-10d
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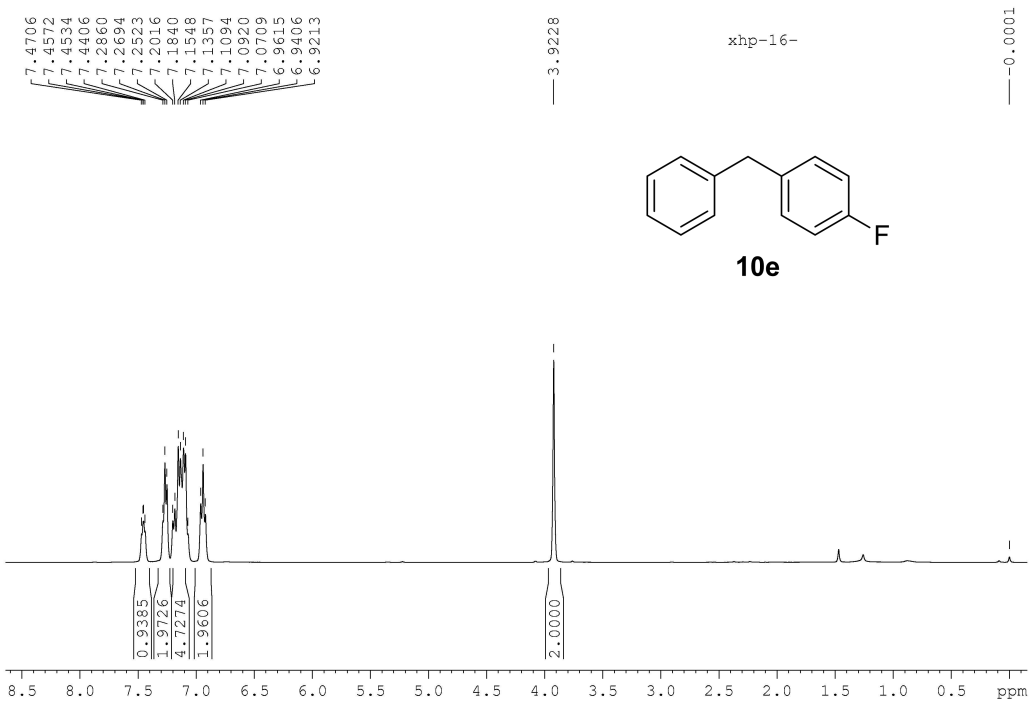
77.0386
76.7211
35.0568
20.2406
10d
140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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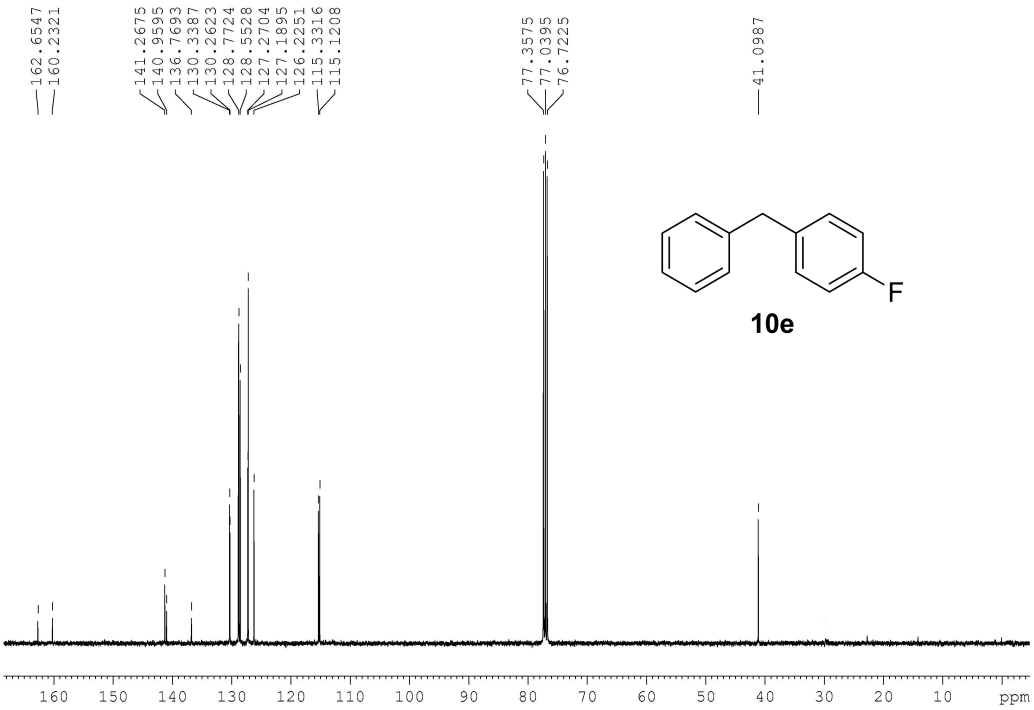
7.4572
7.4534
7.4406
7.2860
7.2694
7.2523
7.2016
7.1840
7.1548
7.1357
7.1094
7.0920
7.0709
6.9615
6.9406
6.9213
3.9228
xhp-16-
-0.0001
F
10e
0.9385
1.9726
4.7274
1.9606
2.0000
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm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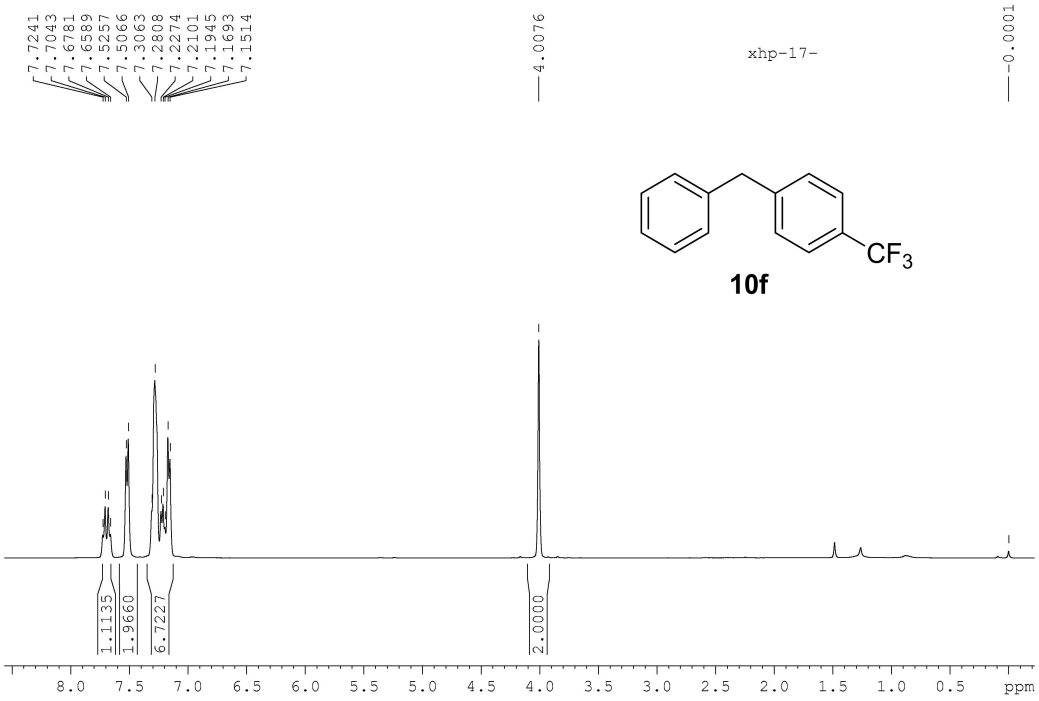
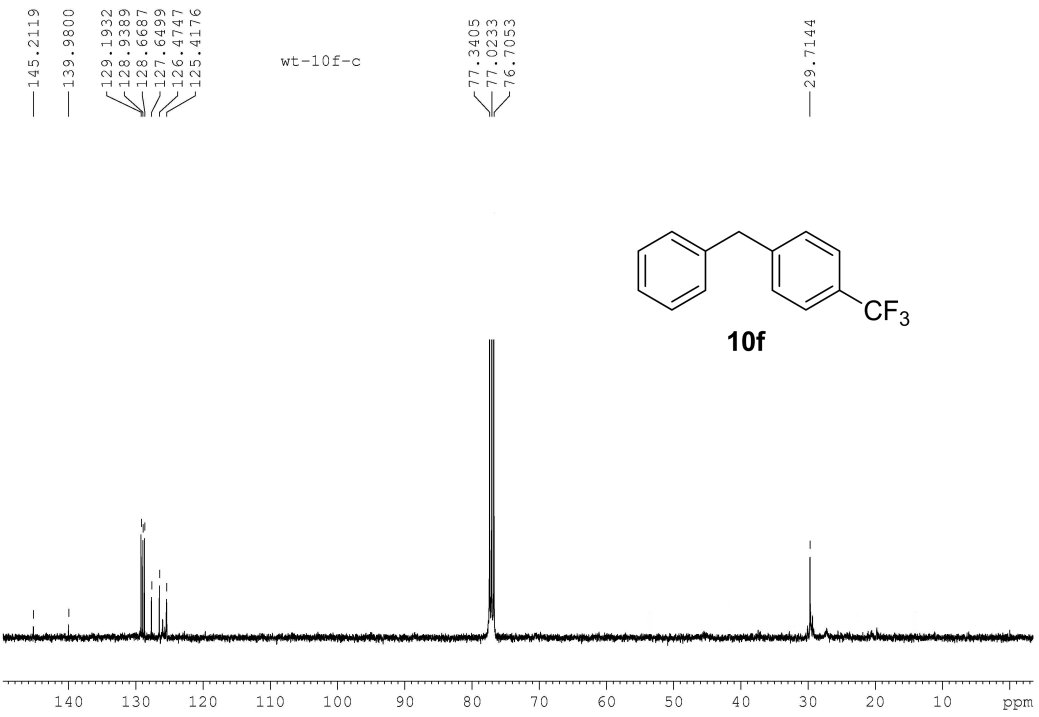
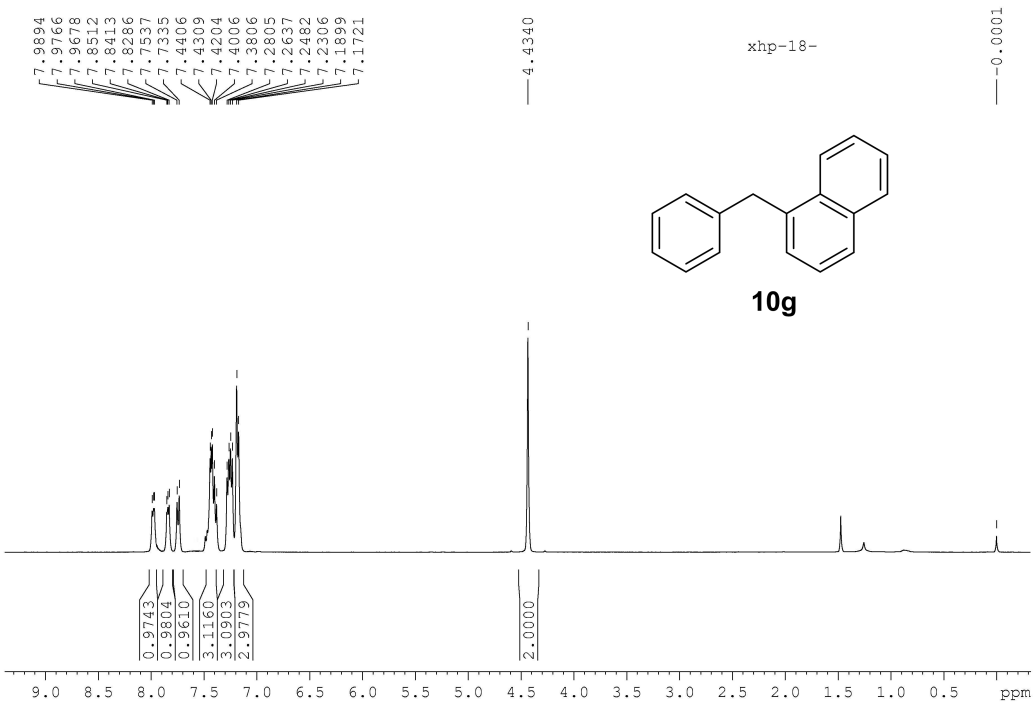
160.2321
141.2675
140.9595
136.7693
130.3387
130.2623
128.7724
128.5528
127.2704
127.1895
126.2251
115.3316
115.1208
77.3575
77.0395
76.7225
41.0987
F
10e
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.7241
7.7043
7.6781
7.6589
7.5257
7.5066
7.3063
7.2808
7.2274
7.2101
7.1945
7.1693
7.1514
4.0076
xhp-17-
-0.0001
CF3
10f
1.1135
1.9660
6.7227
2.0000
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


145.2119
139.9800
129.1932
128.9389
128.6687
127.6499
126.4747
125.4176
wt-10f-c
77.3405
77.0233
76.7053
29.7144
CF3
10f
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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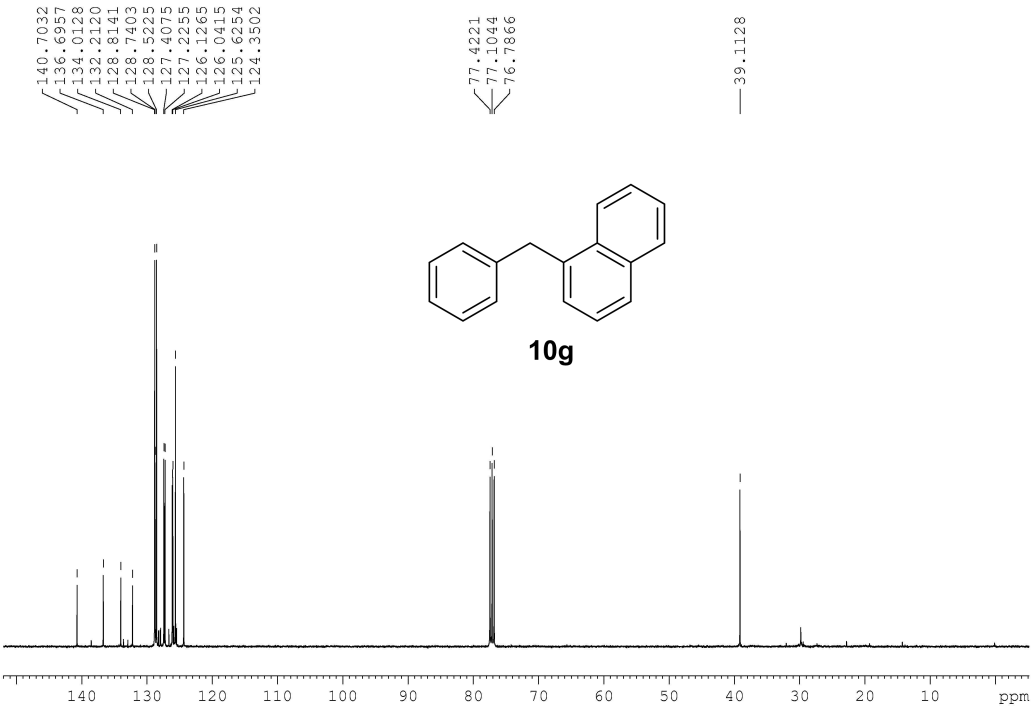
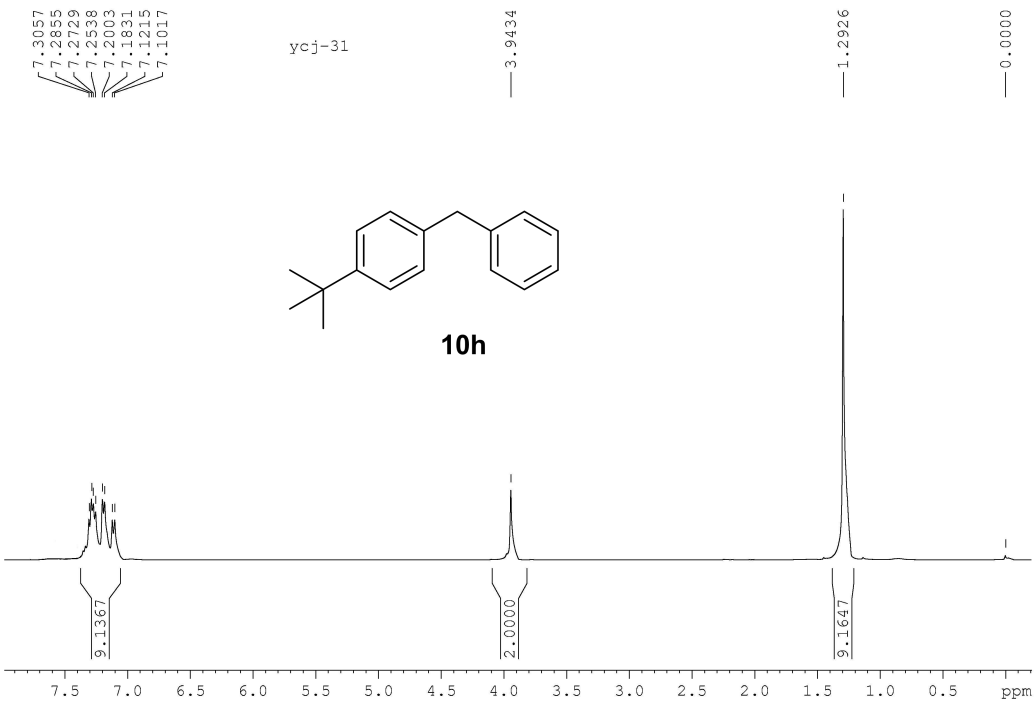
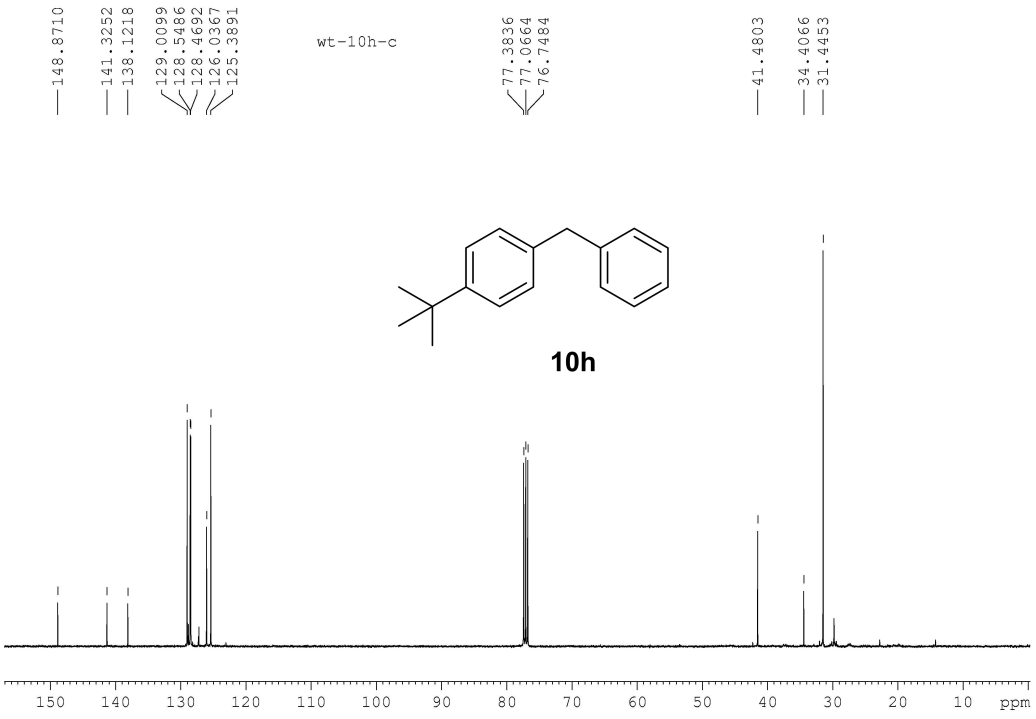
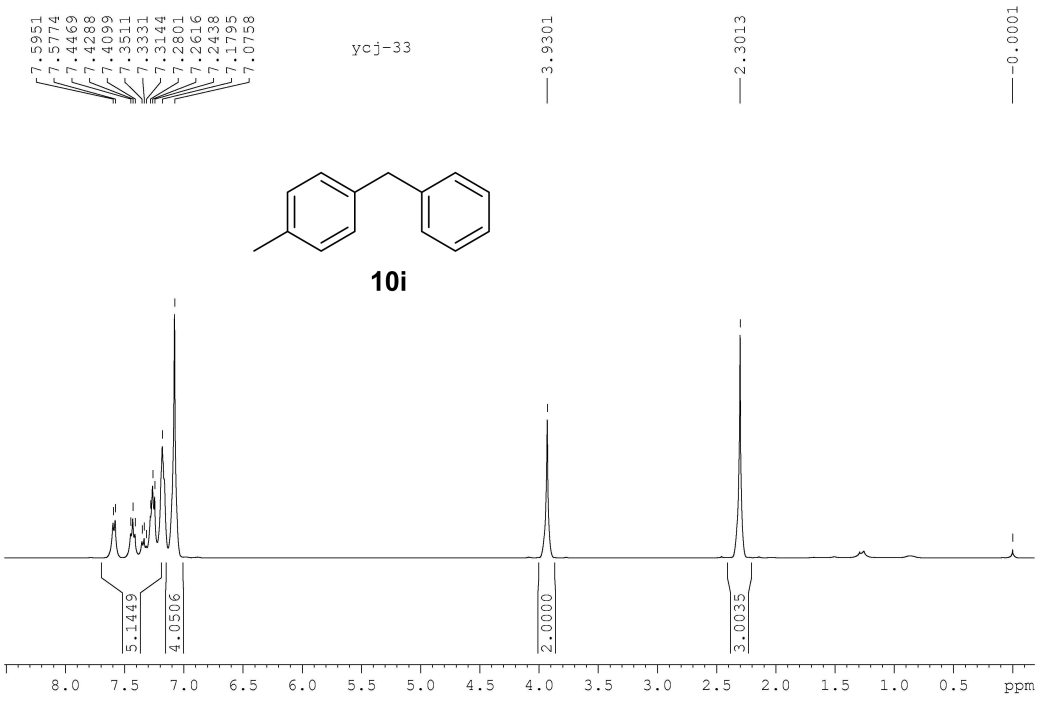
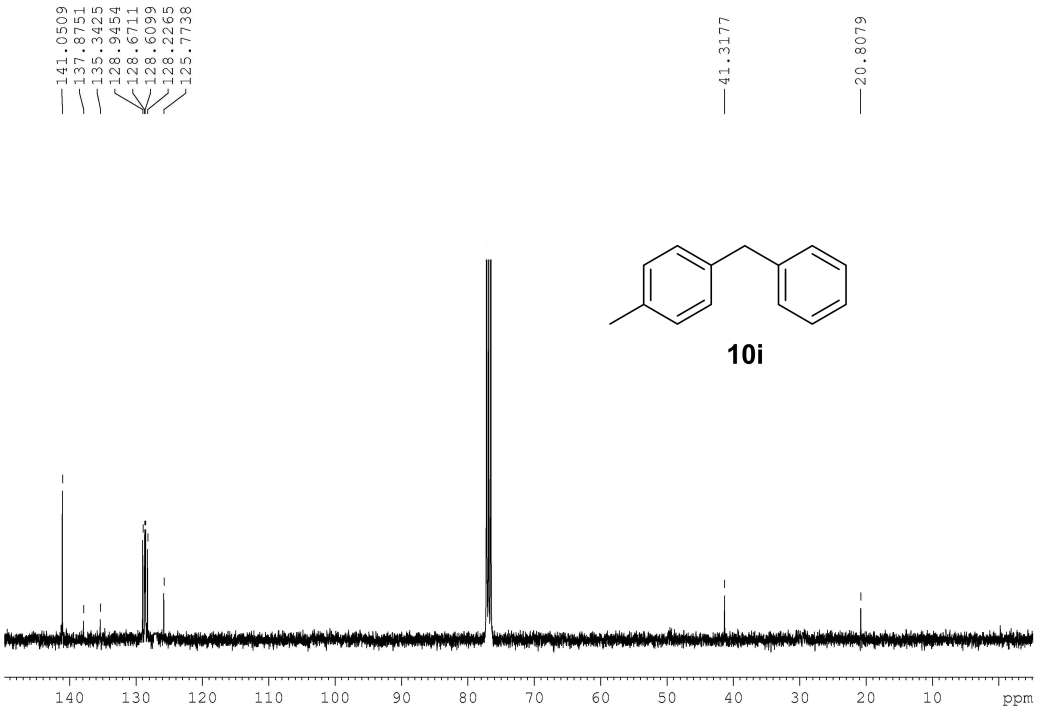
7.9766
7.9678
7.8512
7.8413
7.8286
7.7537
7.7335
7.4406
7.4309
7.4204
7.4006
7.3806
7.2805
7.2637
7.2482
7.2306
7.1899
7.1721
4.4340
xhp-18-
-0.0001
10g
0.9743
0.9804
0.9610
3.1160
3.0903
2.9779
2.0000
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

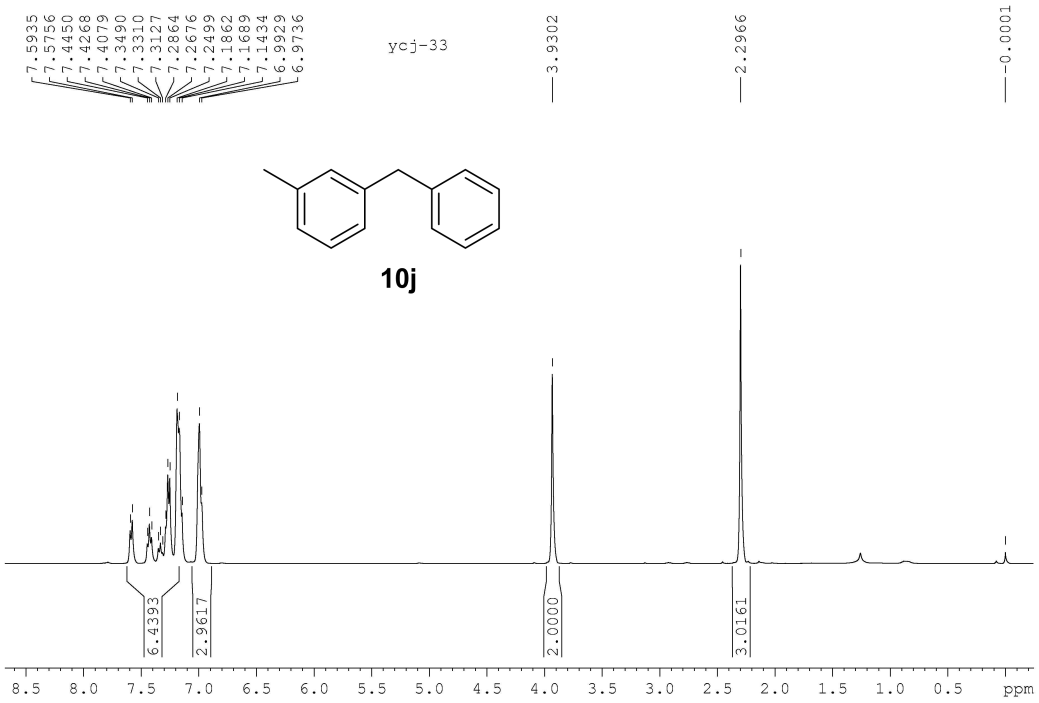

140.7032
136.6957
134.0128
132.2120
128.8141
128.7403
128.5225
127.4075
127.2255
126.1265
126.0415
125.6254
124.3502
77.4221
77.1044
76.7866
39.1128
10g
140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

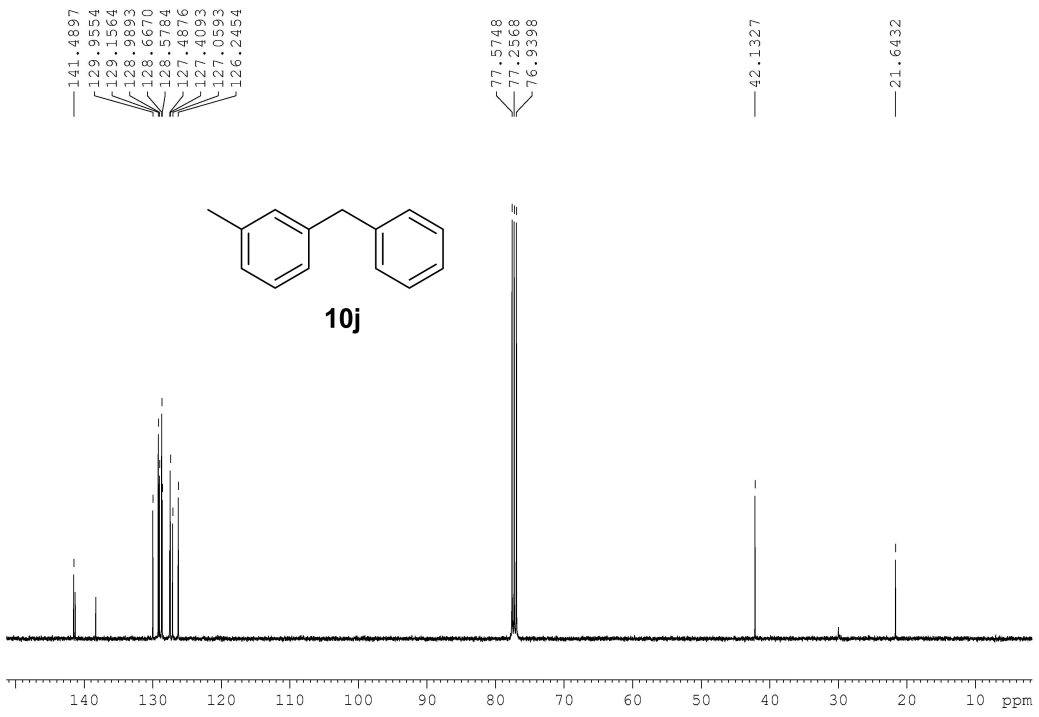

7.3057
7.2855
7.2729
7.2538
7.2003
7.1831
7.1215
7.1017
ycj-31
3.9434
1.2926
0.0000
10h
9.1367
2.0000
9.1647
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm


148.8710
141.3252
138.1218
129.0099
128.5486
128.4692
126.0367
125.3891
wt-10h-c
77.3836
77.0664
76.7484
41.4803
34.4066
31.4453
10h
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.5951
7.5774
7.4469
7.4288
7.4099
7.3511
7.3331
7.3144
7.2801
7.2616
7.2438
7.1795
7.0758
ycj-33
3.9301
2.3013
0.0001
10i
5.1449
4.0506
2.0000
3.0035
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


141.0509
137.8751
135.3425
128.9454
128.6711
128.6099
128.2265
125.7738
41.3177
20.8079
10i
140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.5935
7.5756
7.4450
7.4268
7.4079
7.3490
7.3310
7.3127
7.2864
7.2676
7.2499
7.1862
7.1689
7.1434
6.9929
6.9736
ycj-33
3.9302
2.2966
0.0001
10j
6.4393
2.9617
2.0000
3.0161
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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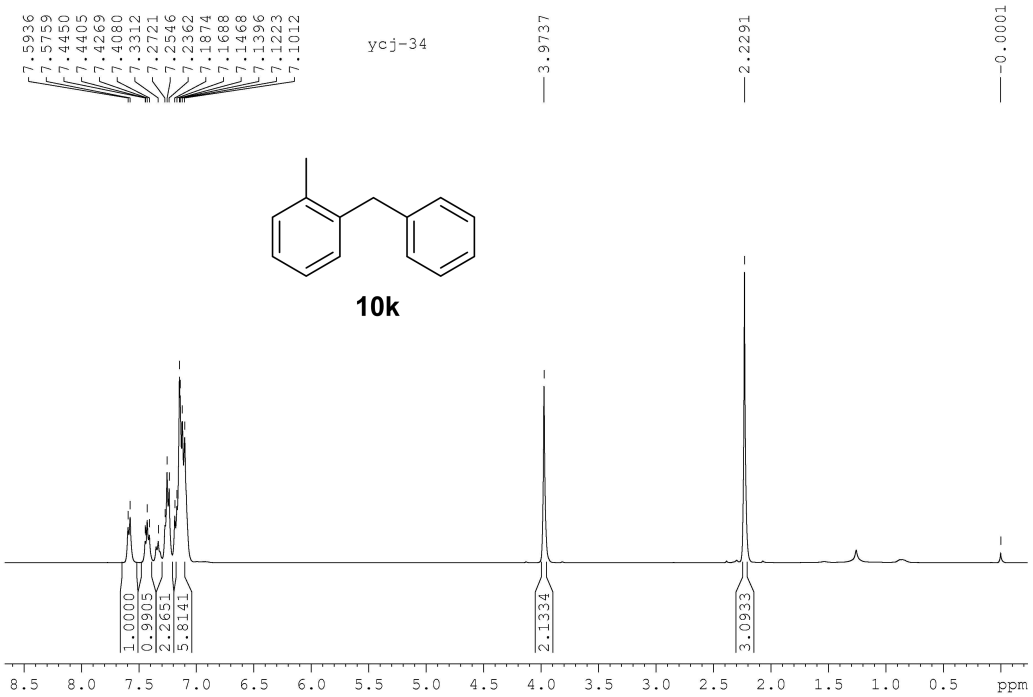
129.9554
129.1564
128.9893
128.6670
128.5784
127.4876
127.4093
127.0593
126.2454
77.5748
77.2568
76.9398
42.1327
21.6432
10j
140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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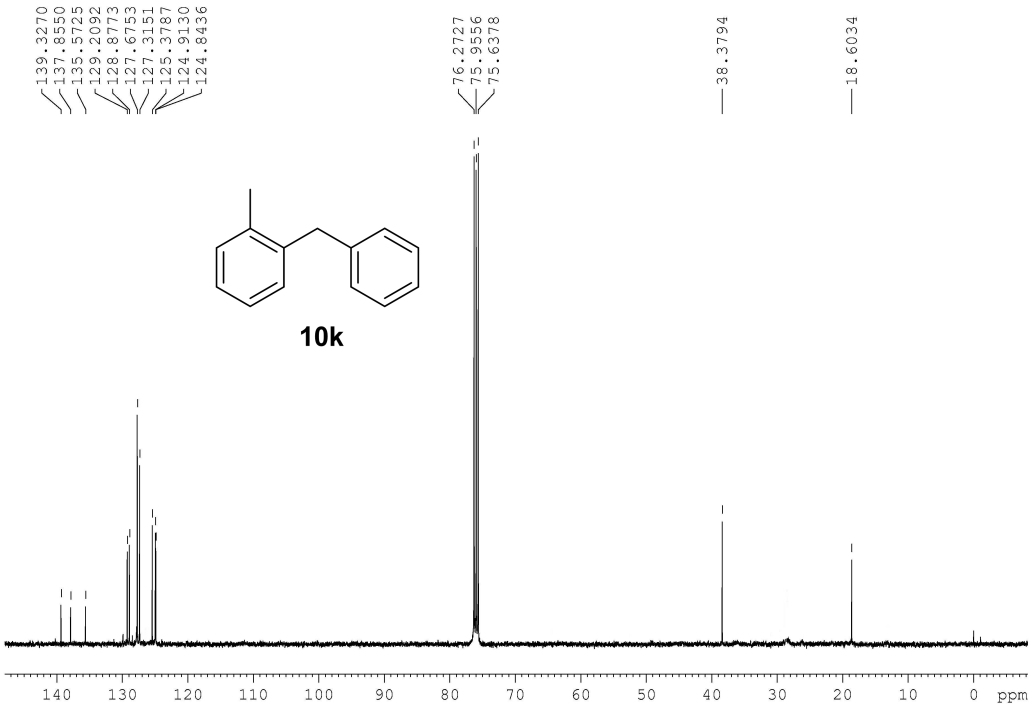
7.5759
7.4450
7.4405
7.4269
7.4080
7.3312
7.2721
7.2546
7.2362
7.1874
7.1688
7.1468
7.1396
7.1223
7.1012
ycj-34
3.9737
2.2291
0.0001
10k
1.0000
0.9905
2.2651
5.8141
2.1334
3.0933
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm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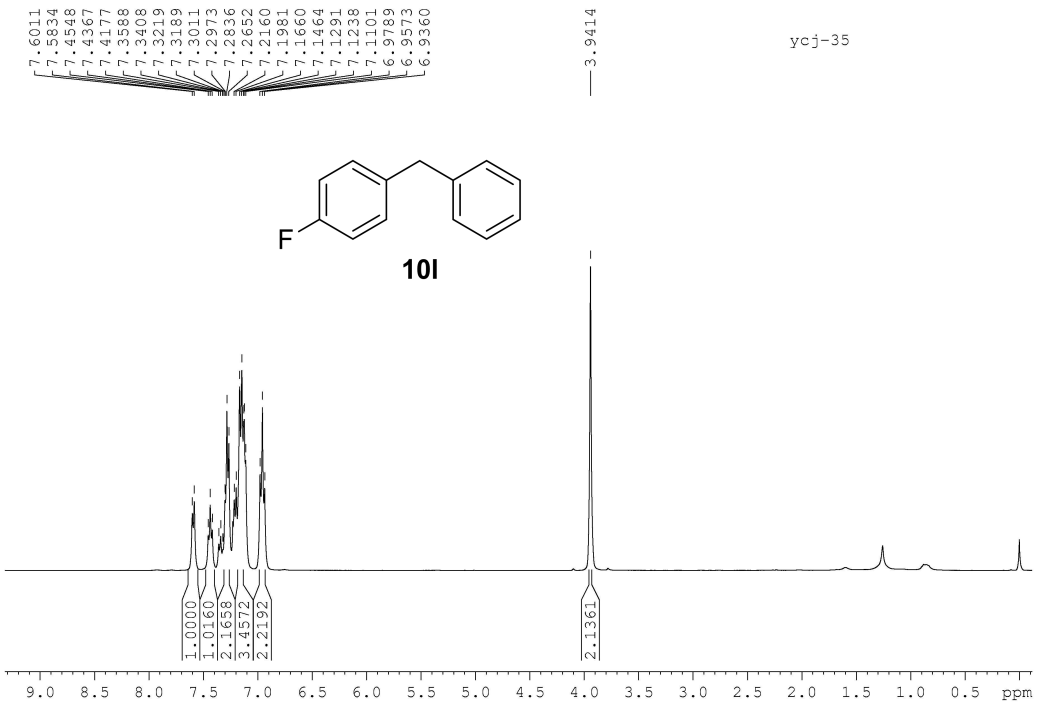
137.8550
135.5725
129.2092
128.8773
127.6753
127.3151
125.3787
124.9130
124.8436
76.2727
75.9556
75.6378
38.3794
18.6034
10k
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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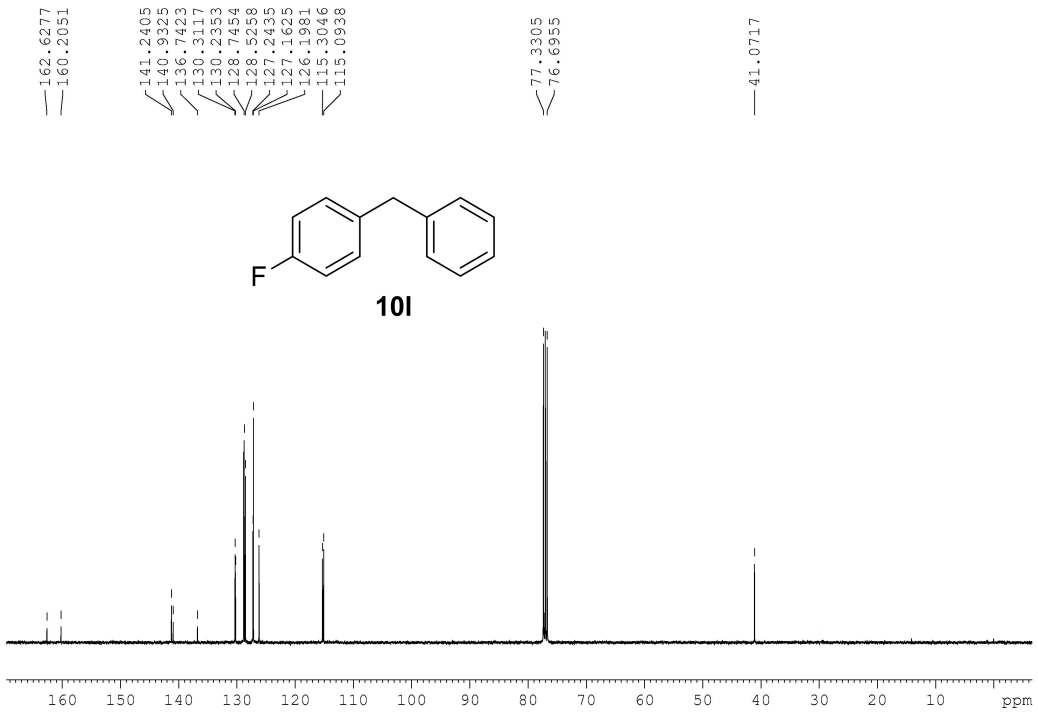
7.4548
7.4367
7.4177
7.3588
7.3408
7.3219
7.3189
7.3011
7.2973
7.2836
7.2652
7.2160
7.1981
7.1660
7.1464
7.1291
7.1238
7.1101
6.9789
6.9573
6.9360
3.9414
ycj-35
F
10l
1.0000
1.0160
2.1658
3.4572
2.2192
2.1361
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm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160.2051
141.2405
140.9325
136.7423
130.3117
130.2353
128.7454
128.5258
127.2435
127.1625
126.1981
115.3046
115.0938
77.3305
76.6955
41.0717
F
10l
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm