Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supporting information for

Preparation and Characterization of PdCu@Ti_3C_2 Catalyst for Suzuki-Miyaura Coupling Reaction

Table S1. The content of Pd and Cu elements in the PdCu@Ti_3C_2, Pd^1@Ti_3C_2, Pd^2@Ti_3C_2

Sample	Element	Mass fraction（%)
PdCu@Ti_3C_2	Cu	9.16%
	Pd	3.59%
Pd^1@Ti_3C_2	Pd	1.40%
Pd^2@Ti_3C_2	Pd	1.02%
Cu@Ti_3C_2	Cu	11.43%

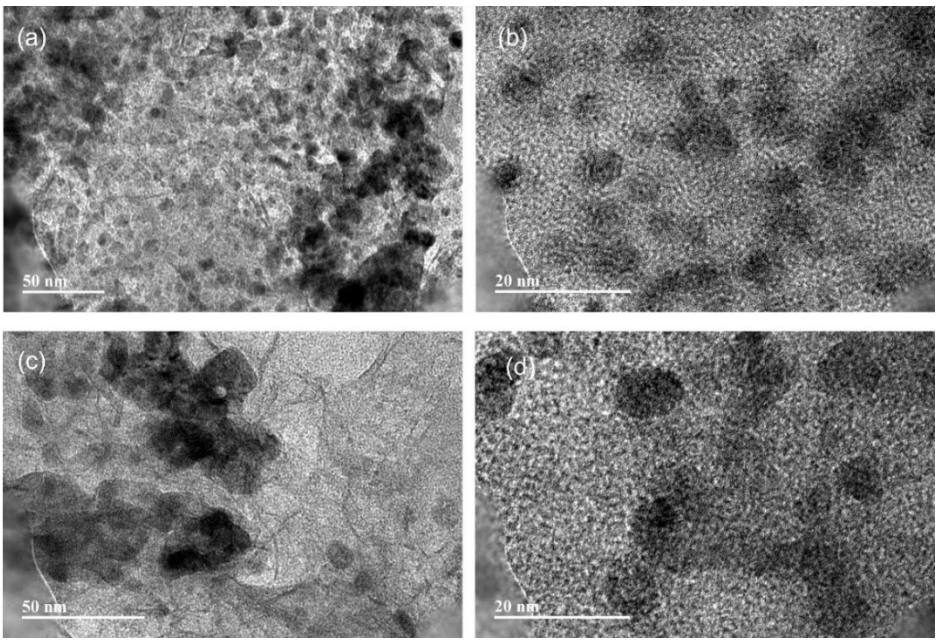


Figure S1. (a) Low magnification TEM image of PdCu@Ti_3C_2 after first cycle (b) HRTEM image of PdCu nanoparticles after first cycle. (c) Low magnification TEM image of PdCu@Ti_3C_2 after tenth cycle (d) HRTEM image of PdCu nanoparticles

after fifth cycle.

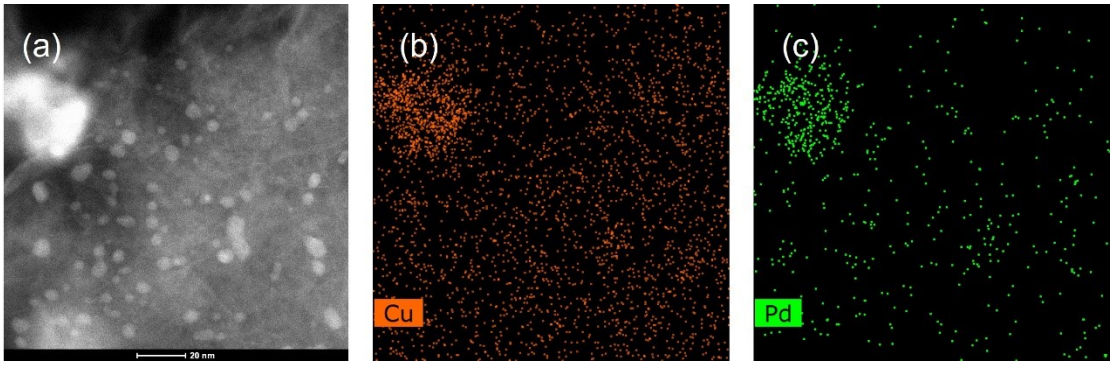
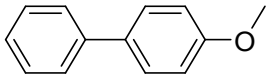


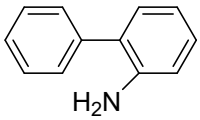
Figure S2. (a)STEM image of PdCu@Ti_3C_2 after tenth cycle. (b-f) EDS mapping of PdCu@Ti_3C_2 after cycle.

^{1}H and ^{13}C NMR spectra of the product

4-Methoxybiphenyl 3a:

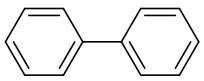


^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.5 Hz, 2H), 7.52 (d, *J* = 8.8 Hz, 2H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 6.97 (d, *J* = 8.7 Hz, 2H), 3.83 (s, 3H). **2-Aminebiphenyl 3b:**



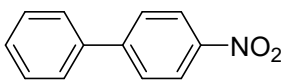
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.2 Hz, 4H), 7.33 (t, *J* = 6.8 Hz, 1H), 7.15 – 7.11 (m, 2H), 6.82 (t, *J* = 7.4 Hz, 1H), 6.75 (d, *J* = 8.0 Hz, 1H), 3.63 (s, 2H).

Biphenyl 3c:



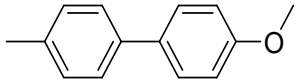
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.1 Hz, 4H), 7.40 (t, *J* = 7.7 Hz, 4H), 7.31 (t, *J* = 7.4 Hz, 2H).

4-Nitrobiphenyl 3d:



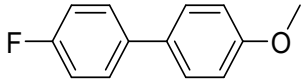
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.9 Hz, 2H), 7.74 (d, *J* = 8.9 Hz, 2H), 7.62 (d, *J* = 7.1 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.44 (t, *J* = 7.3 Hz, 1H).

1-Methoxy-4-(4-methylphenyl)benzene 3e:



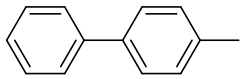
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.8 Hz, 2H), 7.46 (d, *J* = 8.1 Hz, 2H), 7.24 (d, *J* = 7.9 Hz, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H), 2.39 (s, 3H).

1-Fluoro-4-(4-methylphenyl)benzene 3f:



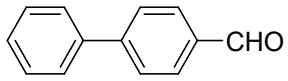
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 4H), 7.14 – 7.08 (m, 2H), 7.00 – 6.96 (m, 2H), 3.86 (s, 3H).

4-Methylbiphenyl 3g:



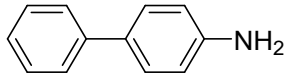
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.5 Hz, 2H), 7.48 (d, *J* = 8.1 Hz, 2H), 7.41 (d, *J* = 7.9 Hz, 2H), 7.32 (d, *J* = 4.8 Hz, 1H), 7.22 (d, *J* = 7.9 Hz, 2H), 2.37 (s, 3H).

4-Phenylbenzaldehyde 3h:



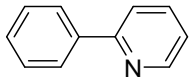
^{1}H NMR (600 MHz, $CDCl_3$) δ 10.06 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 2H), 7.75 (d, *J* = 7.9 Hz, 2H), 7.64 (d, *J* = 7.4 Hz, 2H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.3 Hz, 1H).

Biphenyl-4-amine 3i:



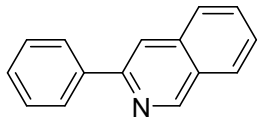
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.1 Hz, 2H), 7.42 – 7.37 (m, 4H), 7.26 (d, *J* = 6.9 Hz, 1H), 6.73 (d, *J* = 7.6 Hz, 2H), 3.69 (s, 2H).

2-Phenylpyridine 3j:



^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.6 Hz, 1H), 7.99 (d, *J* = 7.7 Hz, 2H), 7.72 (d, *J* = 6.9 Hz, 2H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.41 (t, *J* = 7.3 Hz, 1H), 7.21 (t, *J* = 5.6 Hz, 1H).

3-Phenylquinoline 3k:

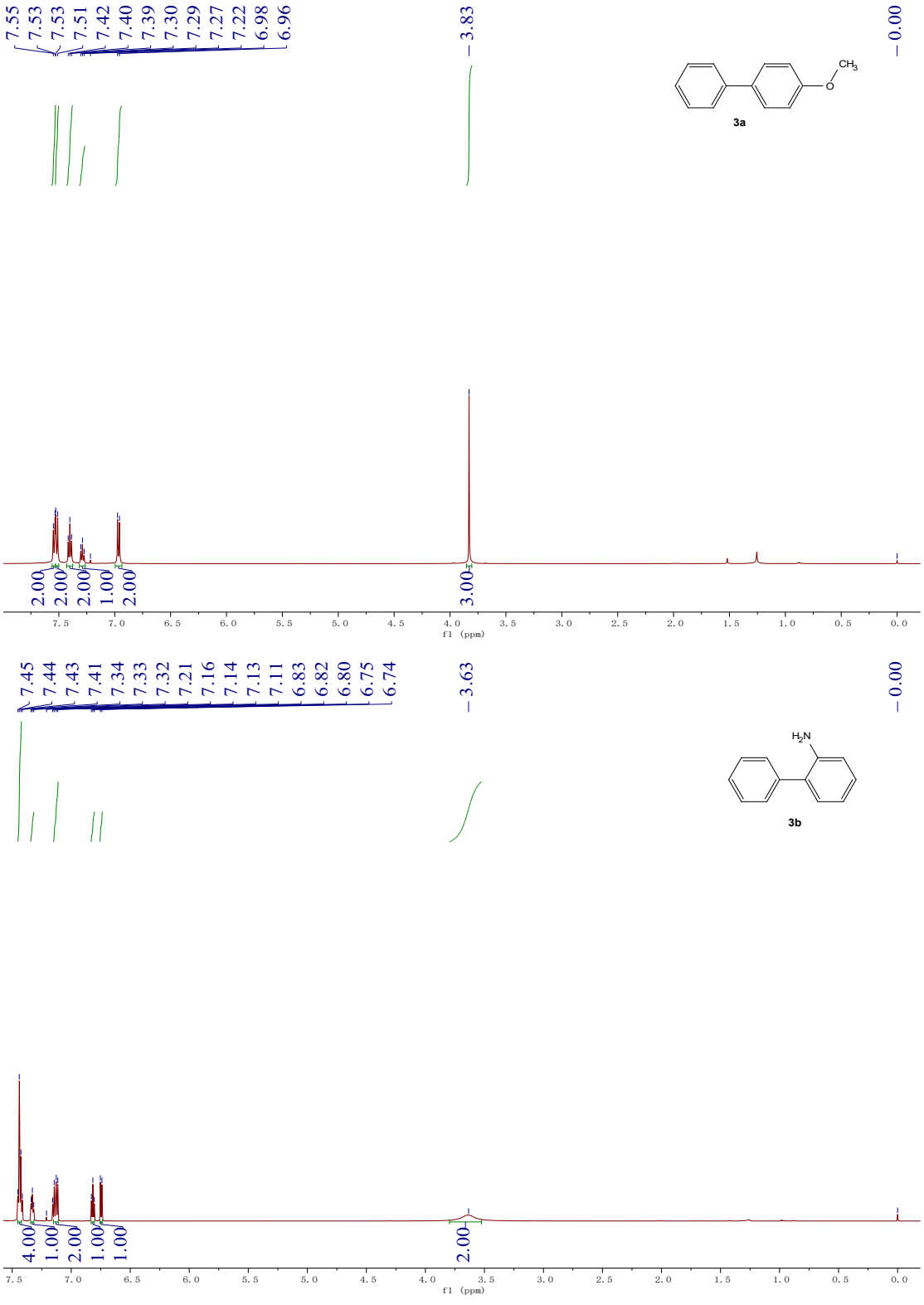


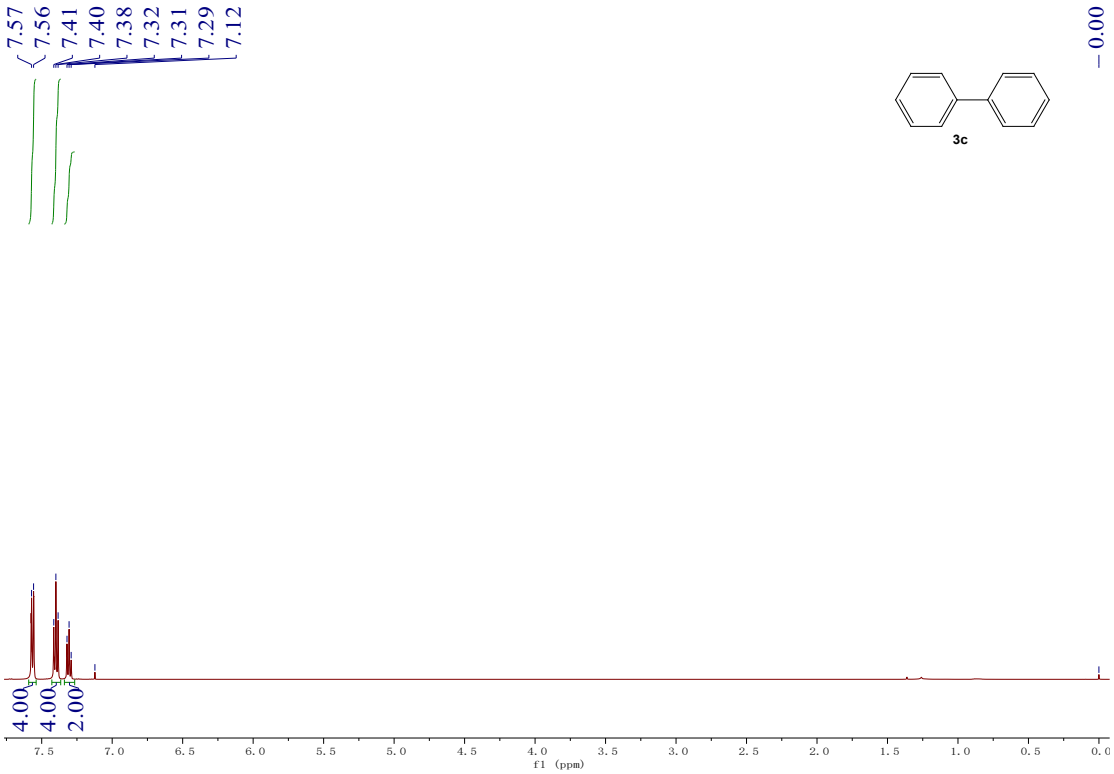
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.25 (s, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.83 (d, *J* = 8.1 Hz, 1H), 7.70 – 7.66 (m, 3H), 7.54 (t, *J* = 7.5 Hz, 1H), 7.49 (t, *J* = 7.5 Hz,

2H), 7.41 (t, J = 7.4 Hz, 1H).

Key Intermediates for the Synthesis of Abemaciclib

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.97 (d, J = 3.4 Hz, 1H), 8.16 (s, 1H), 7.63 (d, J = 11.8 Hz, 1H), 4.89 – 4.84 (m, 1H), 2.65 (s, 3H), 1.60 (d, J = 6.9 Hz, 6H).

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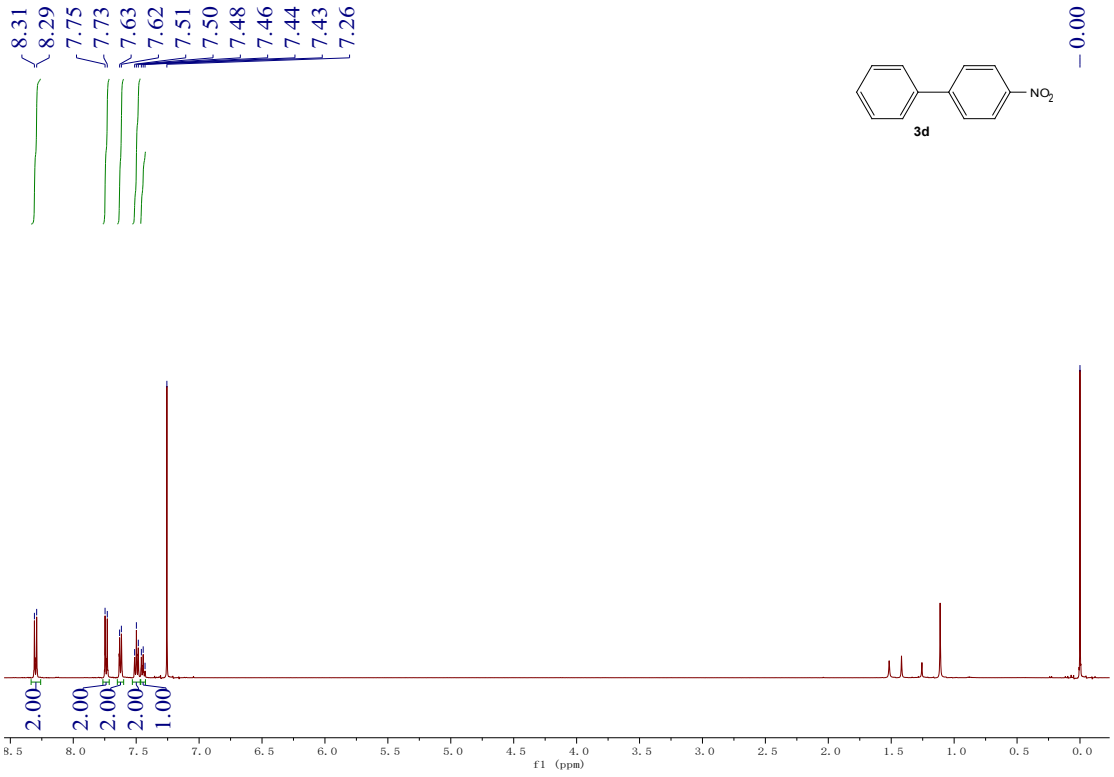
f1 (ppm)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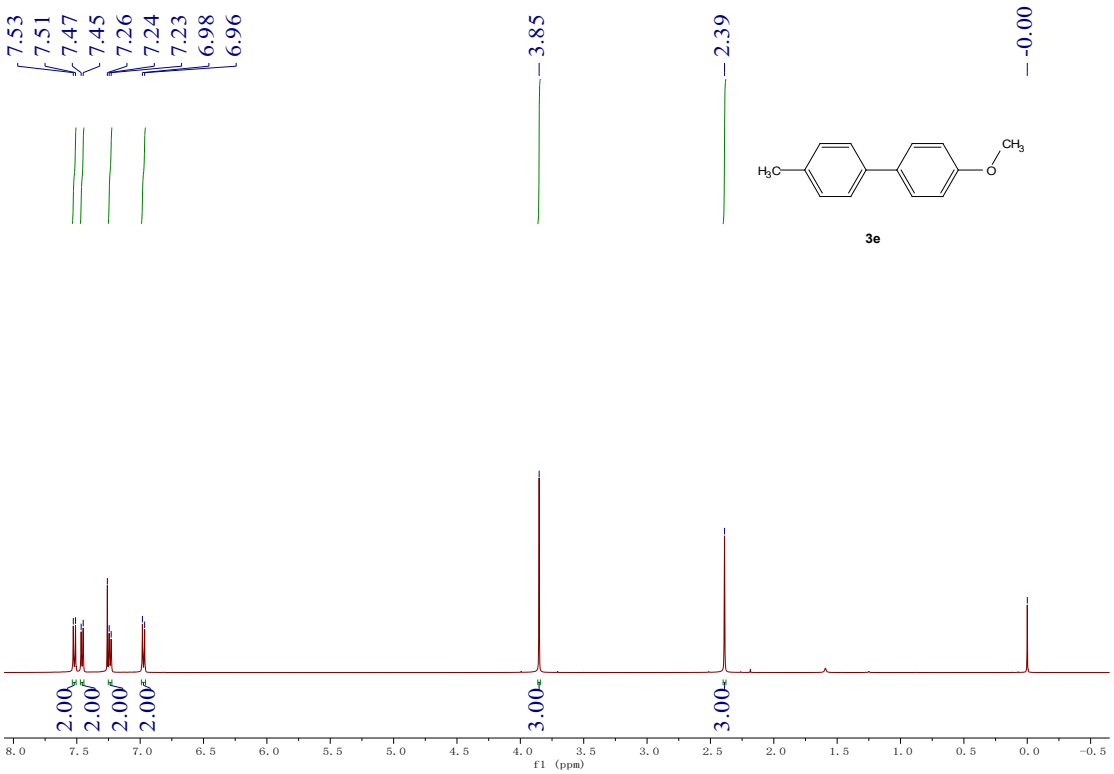
f1 (ppm)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O
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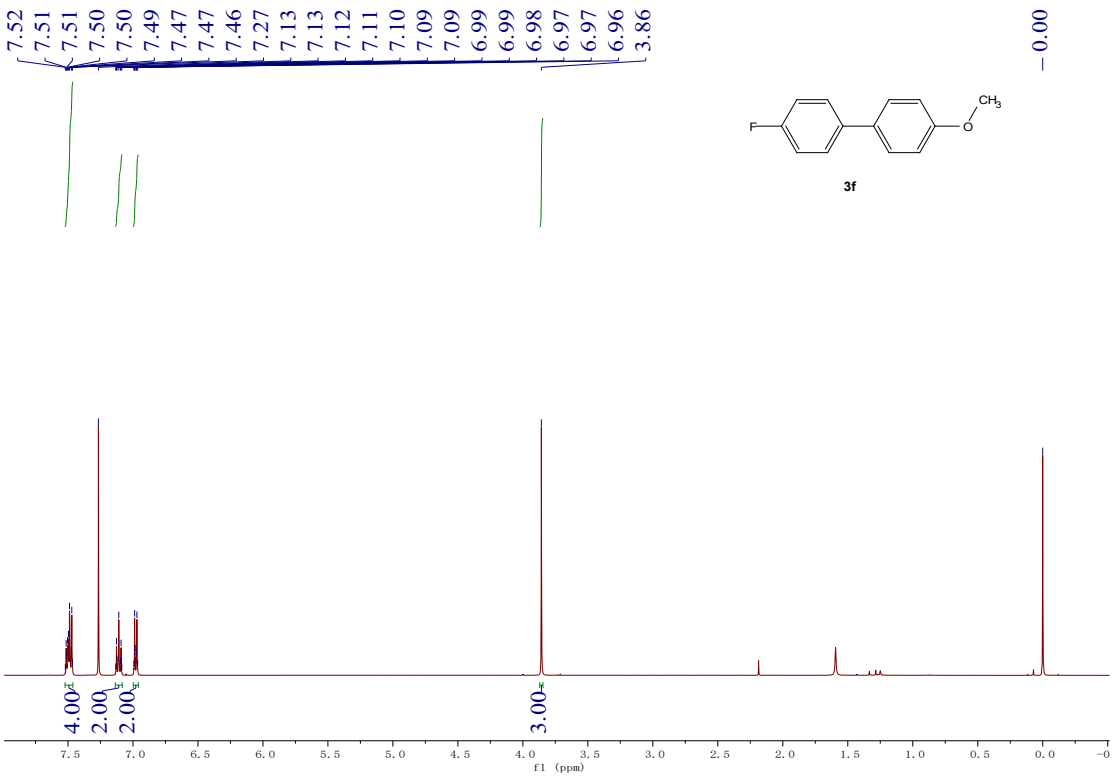
2.00
2.00
3.00
3.00
f1 (ppm)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7.12
7.11
7.10
7.09
7.09
6.99
6.99
6.98
6.97
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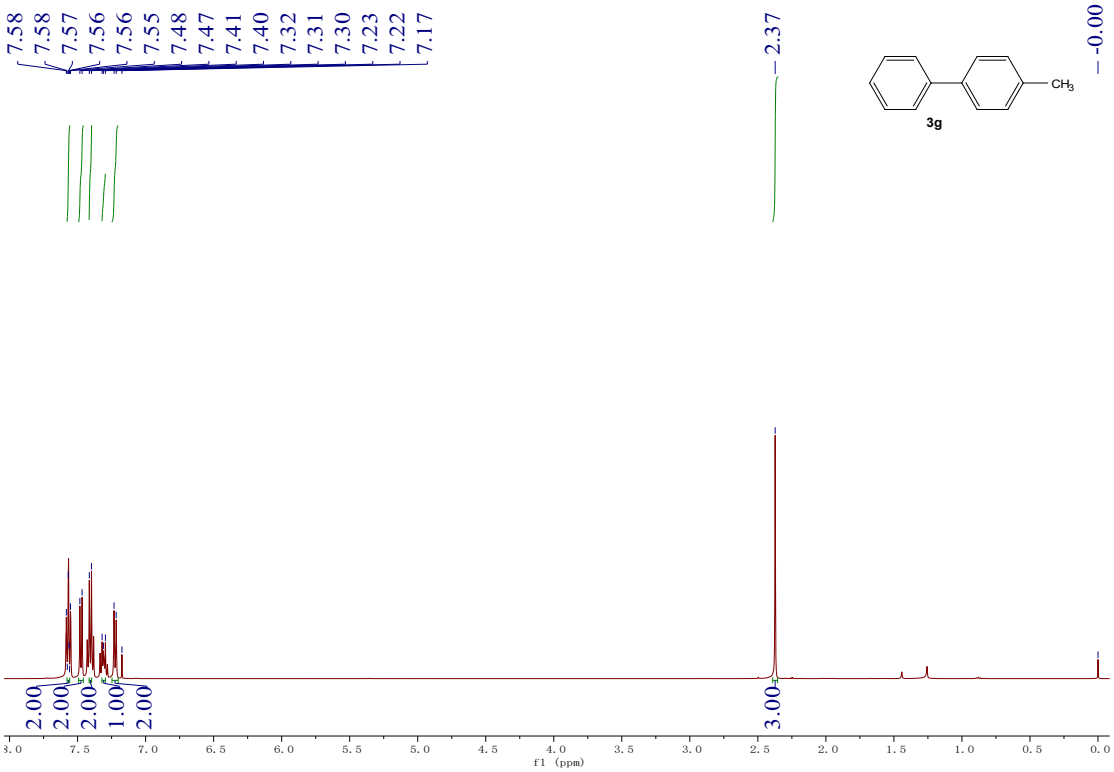
3.00
f1 (ppm)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7.23
7.22
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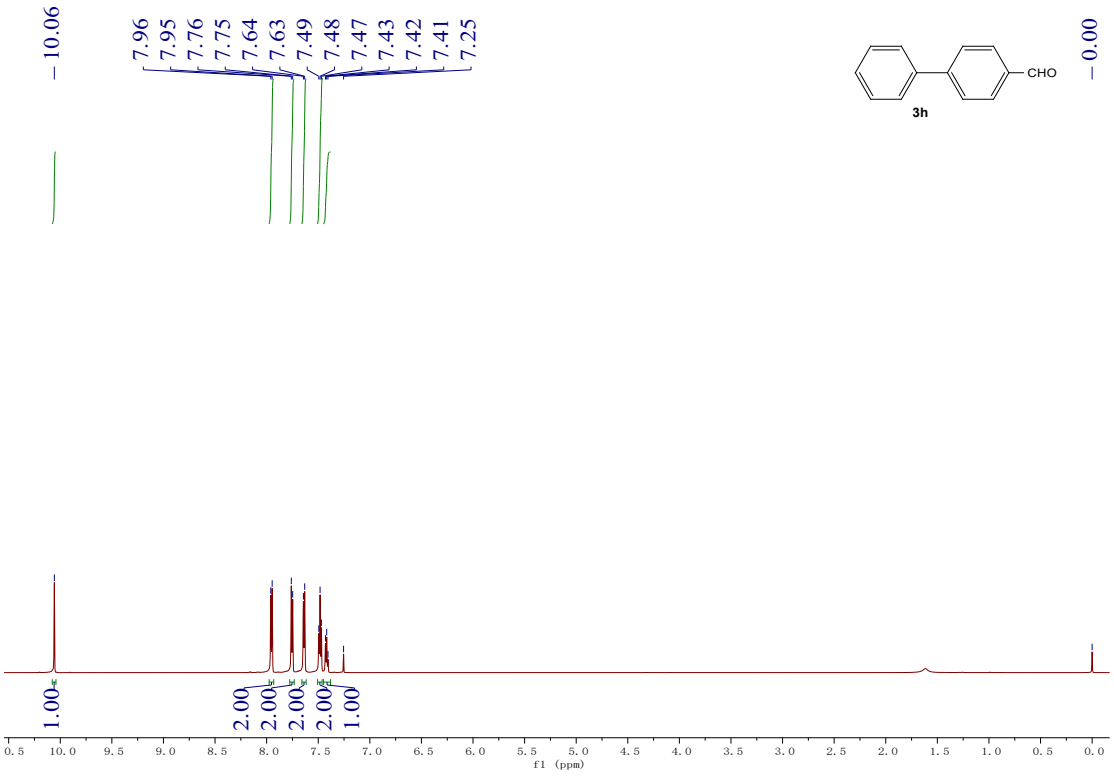
1.00
2.00
3.00
f1 (ppm)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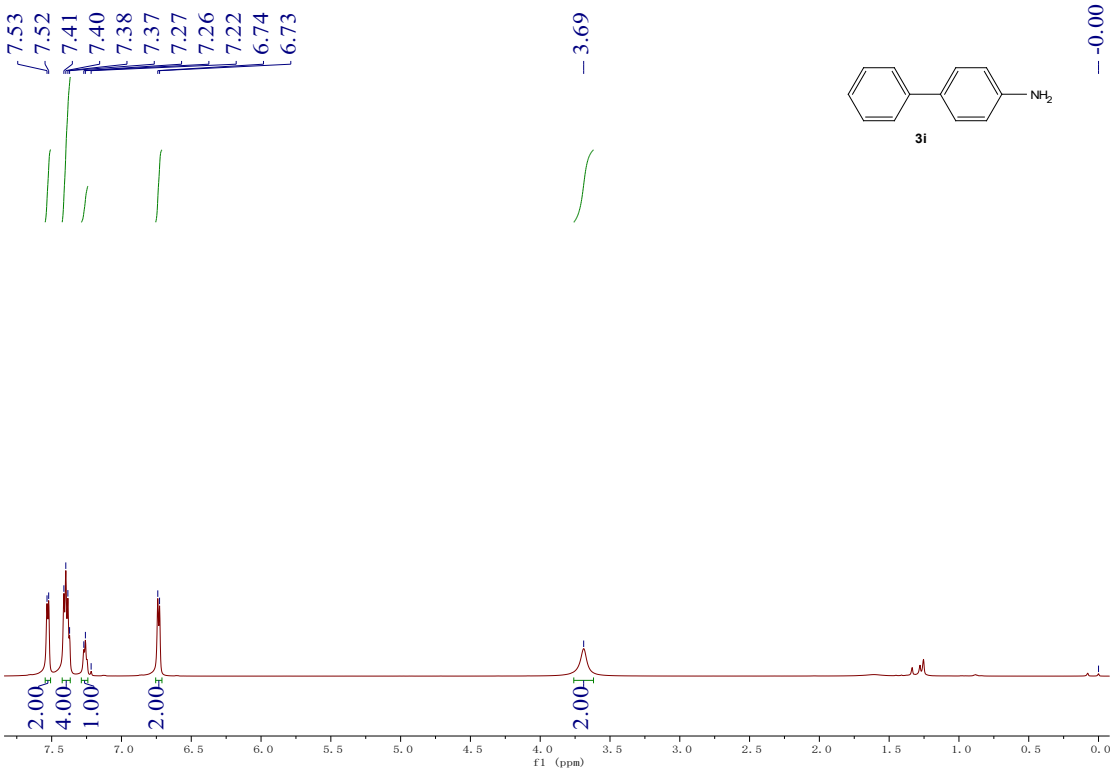
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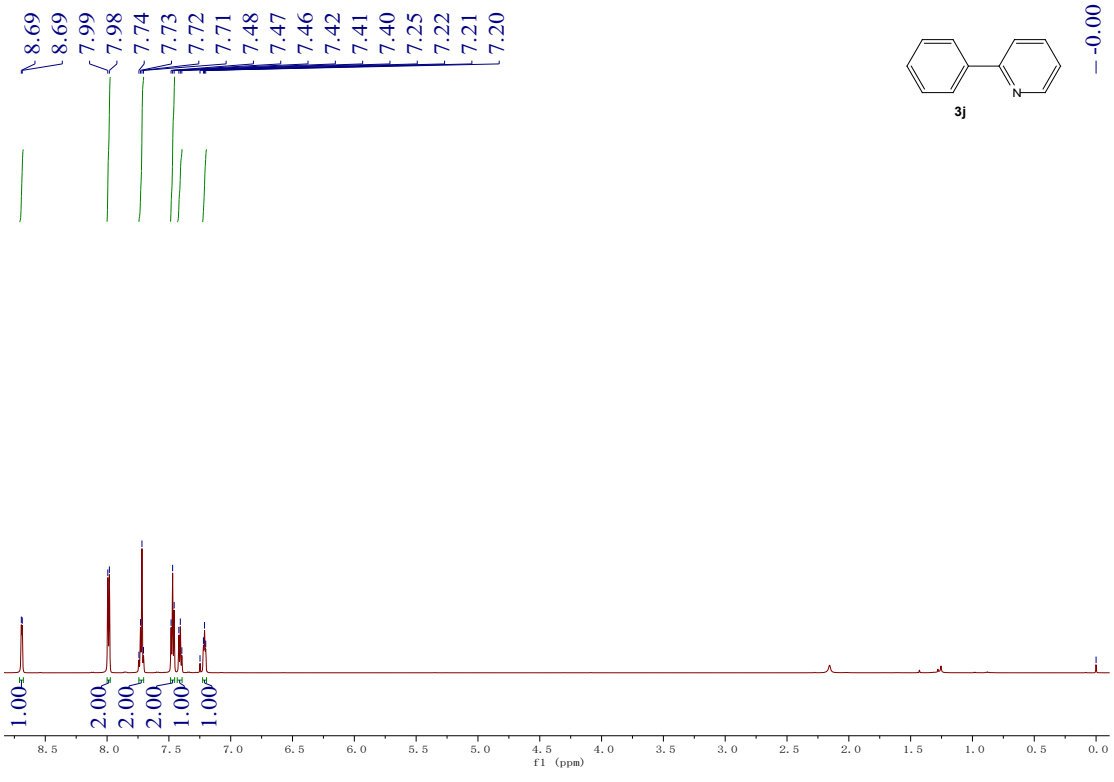
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7.40
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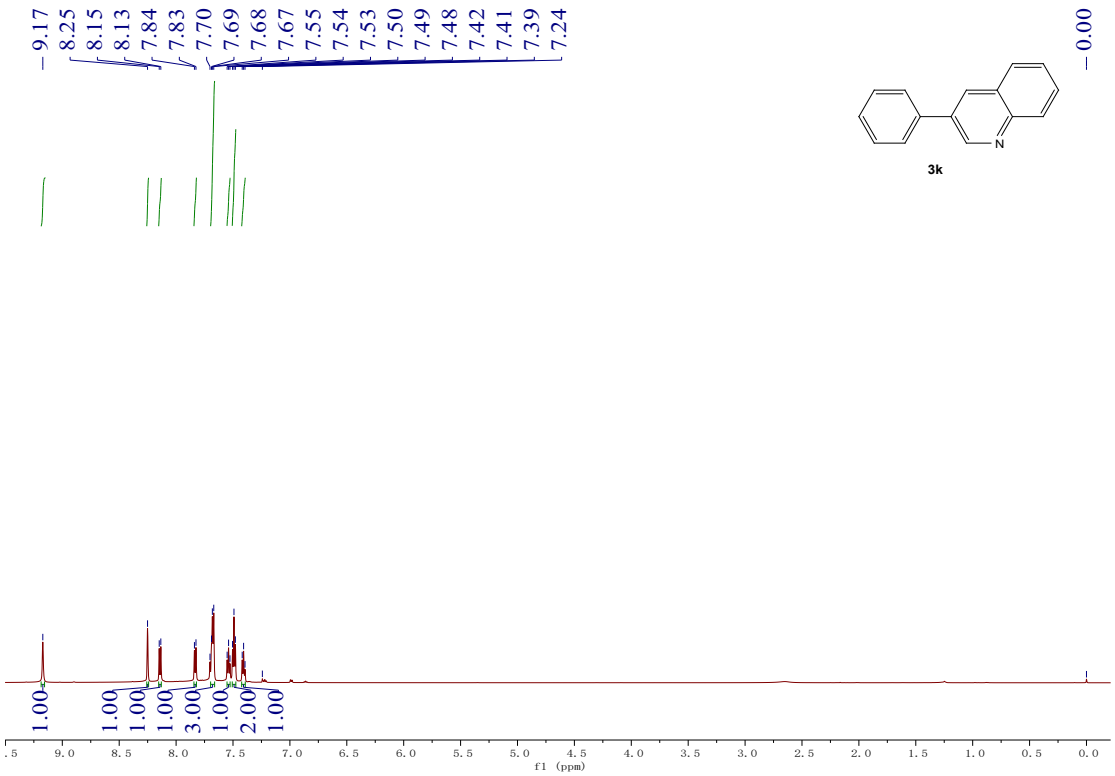
1.00
f1 (ppm)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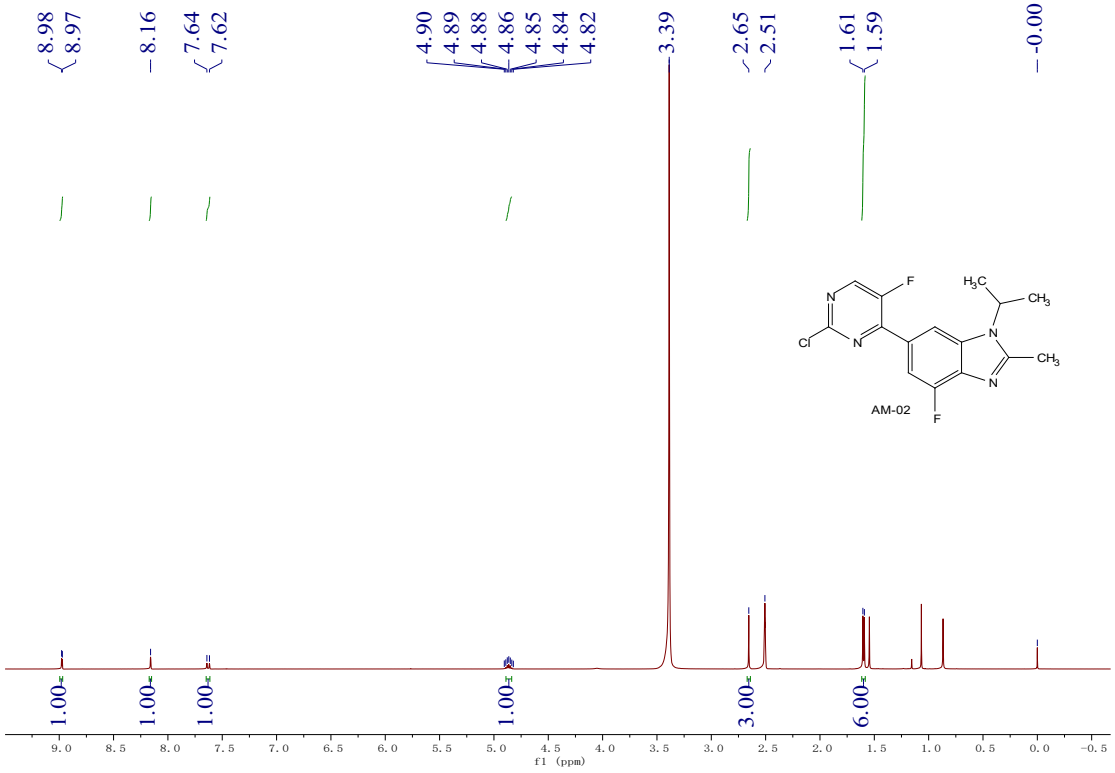
f1 (ppm)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1.00
1.00
1.00
3.00
6.00
f1 (ppm)