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J. Serb. Chem. Soc. 86 (3) S66–S69 (2021) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Synthesis and process optimization of Boscalid by catalyst Pd-PEPPSI-IPr$^{DtBu-An}$

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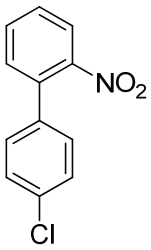
SUPPORTING DATA AND ^{1}H- AND ^{13}C-NMR SPECTRA

2-(4-chlorophenyl)nitrobenzene ***(1)***



(**1**)

Yield: 99.2 %; m.p.: 67–68 °C; ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 7.77 (1H, *dd*, J = 8.1 & 1.2 Hz, CH), 7.54 – 7.50 (1H, *m*, CH), 7.42 – 7.38 (1H, *m*, CH), 7.31–7.27 (3H, *m*, CH), 7.16–7.13 (2H, *m*, CH); ^{13}C-NMR (101 MHz, $CDCl_3$, δ / ppm): 149.0, 135.9, 135.1, 134.4, 132.4, 131.8, 129.2, 128.8, 128.5, 124.2; Mass spectrum (ESI$^+$) (*m*/*z*): 233 (M^+).

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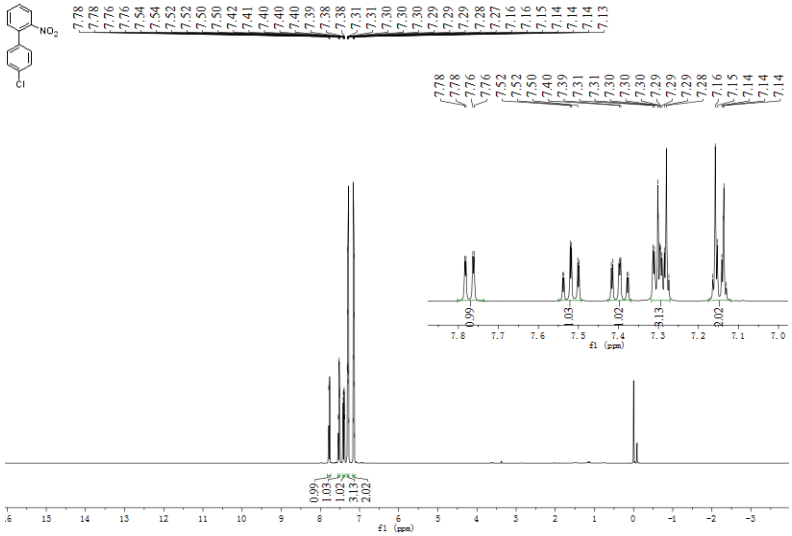

Fig. S-1. ^{1}H-NMR spectra of 2-(4-chlorophenyl)nitrobenzene (400 MHz, $CDCl_3$).

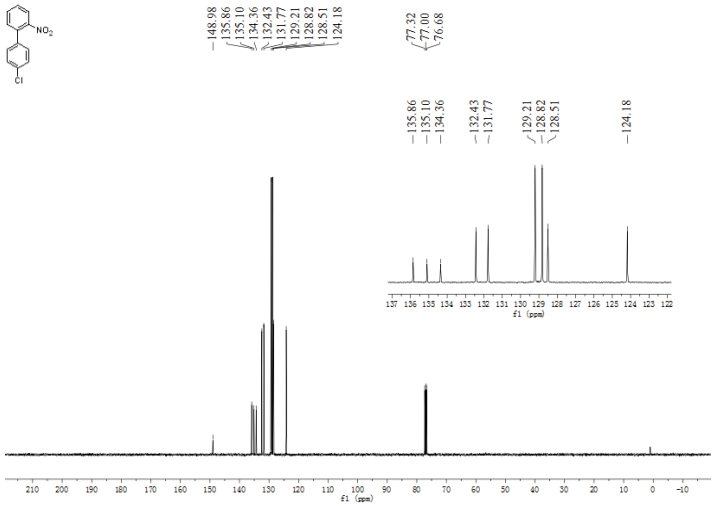

Fig. S-2. ^{13}C-NMR spectra of 2-(4-chlorophenyl)nitrobenzene (101 MHz, $CDCl_3$).

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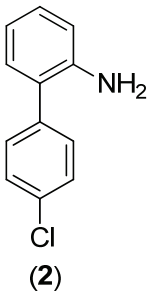
2-(4-Chlorophenyl)aniline ***(2)***



(**2**)

Yield: 98 %; ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 7.31–7.27 (4H, *m*, CH), 7.08 – 7.04 (1H, *m*, CH), 6.99 (1H, *dd*, J = 7.6 & 1.6 Hz, CH), 6.75 – 6.71 (1H, *m*, CH), 6.67 – 6.64 (1H, *m*, CH), 3.65 (2H, *s*, NH_2); ^{13}C-NMR (101 MHz, $CDCl_3$, δ / ppm): 143.2, 137.8, 133.0, 130.4, 130.3, 128.9, 126.3, 118.8, 115.7; Mass spectrum (ESI$^+$) (*m*/*z*): 204 (M^+).

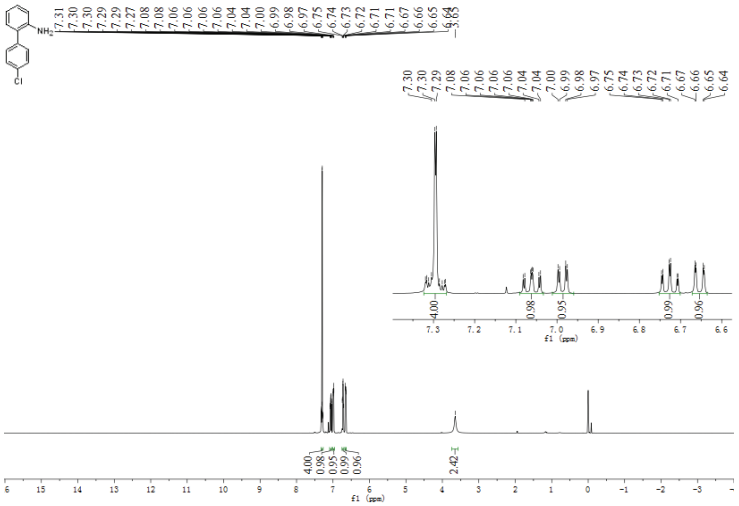


Fig. S-3. ^{1}H-NMR spectra of 2-(4-chlorophenyl)aniline (400 MHz, $CDCl_3$).

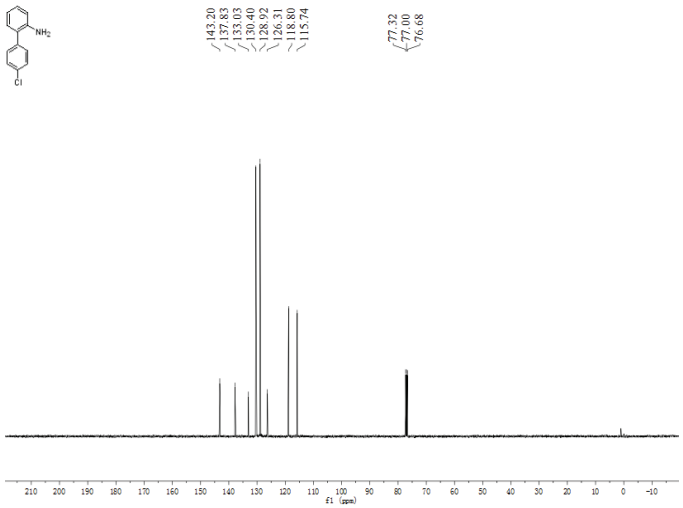


Fig. S-4. ^{13}C-NMR spectra of 2-(4-chlorophenyl)aniline (101 MHz, $CDCl_3$).

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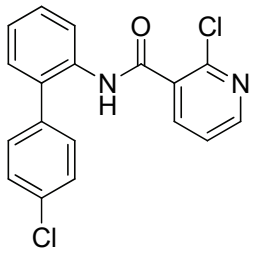
*Boscalid (**4**)*



(**4**)

Yield: 95.04 %; m.p.: 145.8 – 146.8 °C (lit. value: 141.8 – 142.8 °C[14]); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 8.40–8.35 (2H, *m*, CH), 8.20 (*s*, 1H, NH), 8.07 (*dd,* 1H, *J* = 7.6, 2.0 Hz, CH), 7.47–7.39 (*m*, 3H, CH), 7.34 – 7.30 (*m*, 3H, CH), 7.27–7.25 (*m*, 2H, CH); ^{13}C-NMR (101 MHz, $CDCl_3$, δ / ppm): 162.5, 151.1, 146.6, 139.9, 136.2, 134.3, 134.2, 132.3, 131.0, 130.7, 130.2, 129.2, 128.8, 125.3, 122.8, 122.2; (M^+) mass spectrum (ESI^+) *m*/*z*: 343.

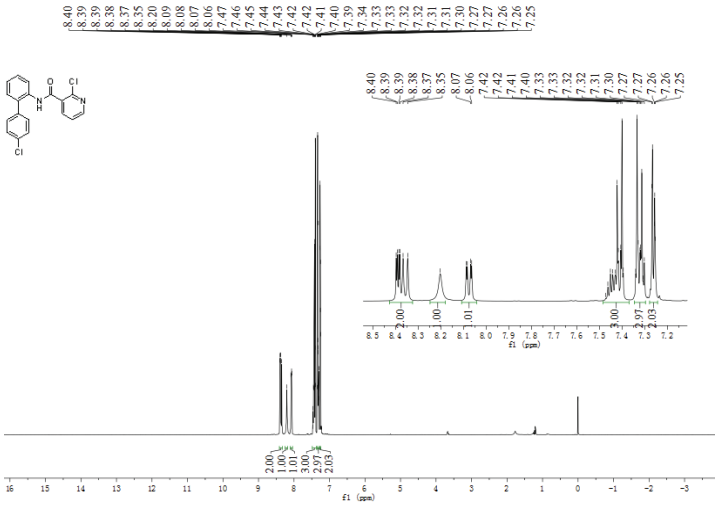


Fig. S-5. ^{1}H-NMR spectra of Boscalid (400 MHz, $CDCl_3$).

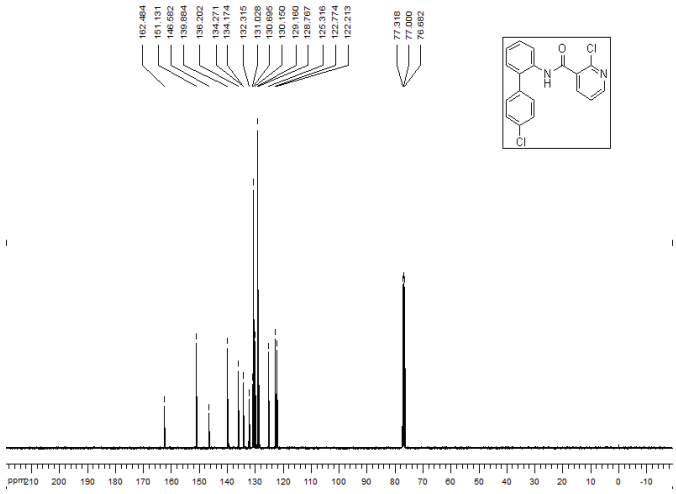


Fig. S-6. ^{13}C-NMR spectra of Boscalid (101 MHz, $CDCl_3$).

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