

**Superparamagnetic nanoparticles as a recyclable catalyst: A new access to phenol esters
via cross dehydrogenative coupling reactions**

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Supporting Information

Materials and instrumentation

All reagents and starting materials were obtained commercially from Sigma-Aldrich and Merck, and were used as received without any further purification unless otherwise noted. Nitrogen physisorption measurements were conducted using a Micromeritics 2020 volumetric adsorption analyzer system. Samples were pretreated by heating under vacuum at 150 °C for 3 h. X-ray powder diffraction (XRD) patterns were recorded using a Cu K α radiation source on a D8 Advance Bruker powder diffractometer. Elemental analysis with atomic absorption spectrometry (AAS) was performed on an AA-6800 Shimadzu. Magnetic properties were measured with a EV11 vibrating sample magnetometer (VSM) at room temperature. Scanning electron

microscopy studies were conducted on a JSM 7401F Scanning Electron Microscope (SEM). Transmission electron microscopy studies were performed using a JEOL JEM 1400 Transmission Electron Microscope (TEM) at 100 kV.

Gas chromatographic (GC) analyses were performed using a Shimadzu GC 2010-Plus equipped with a flame ionization detector (FID) and an SPB-5 column (length = 30 m, inner diameter = 0.25 mm, and film thickness = 0.25 μm). The temperature program for GC analysis held samples at 100 $^{\circ}\text{C}$ for 1 min; heated them from 100 to 280 $^{\circ}\text{C}$ at 40 $^{\circ}\text{C}/\text{min}$; held them at 280 $^{\circ}\text{C}$ for 5.5 min. Inlet and detector temperatures were set constant at 280 $^{\circ}\text{C}$. Diphenyl ether was used as an internal standard to calculate GC yield. GC-MS analyses were performed using a Shimadzu GCMS-QP2010Ultra with a ZB-5MS column (length = 30 m, inner diameter = 0.25 mm, and film thickness = 0.25 μm). The temperature program for GC-MS analysis held samples at 50 $^{\circ}\text{C}$ for 2 min; heated samples from 50 to 280 $^{\circ}\text{C}$ at 10 $^{\circ}\text{C}/\text{min}$ and held them at 280 $^{\circ}\text{C}$ for 10 min. Inlet temperature was set constant at 280 $^{\circ}\text{C}$. MS spectra were compared with the spectra gathered in the NIST library. The ^1H NMR and ^{13}C NMR were recorded on Bruker AV 500 spectrometers using residual solvent peak as a reference.

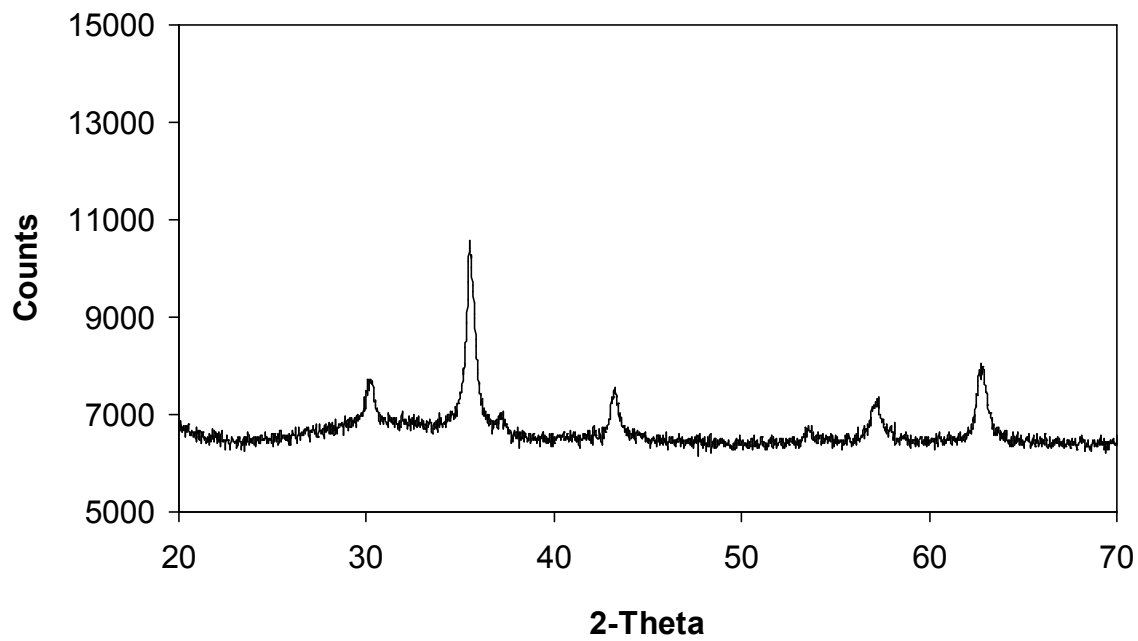


Fig. S1. X-ray powder diffractograms of the CuFe_2O_4 catalyst.

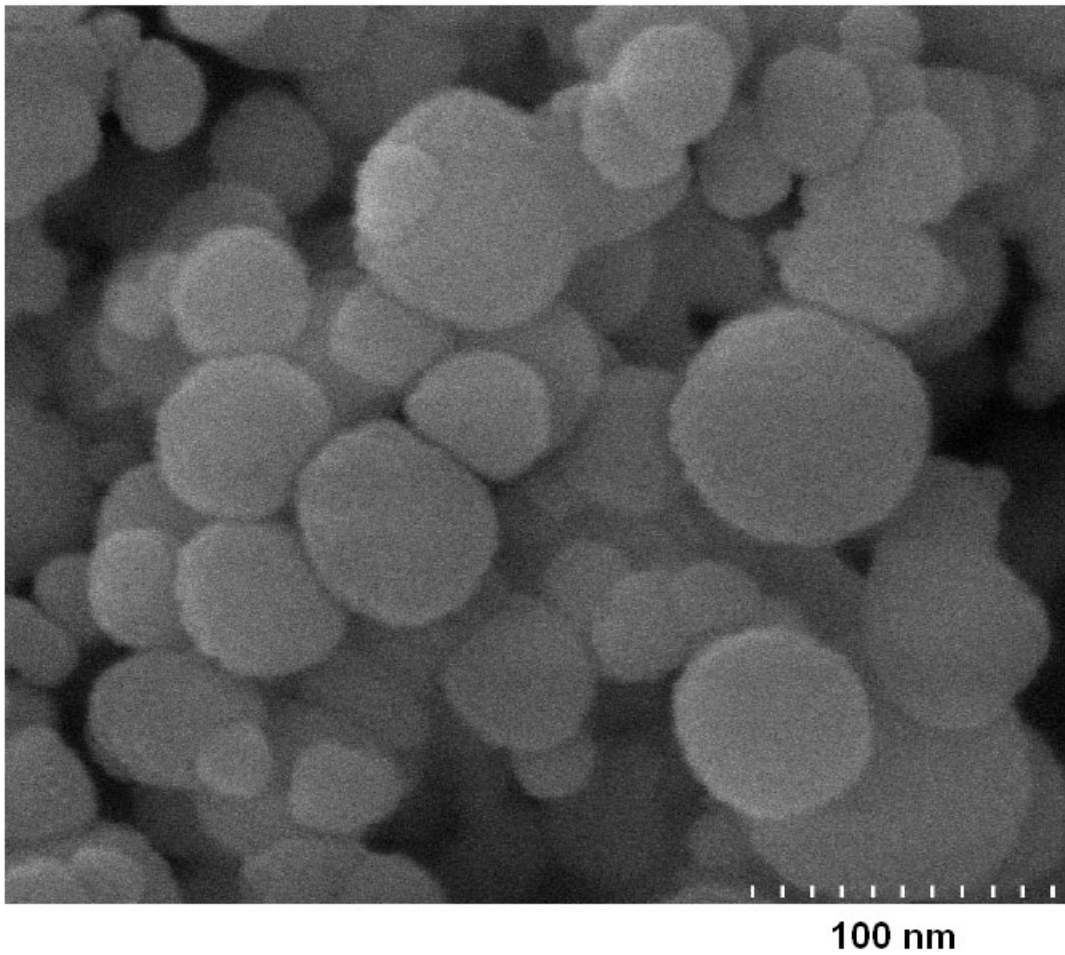
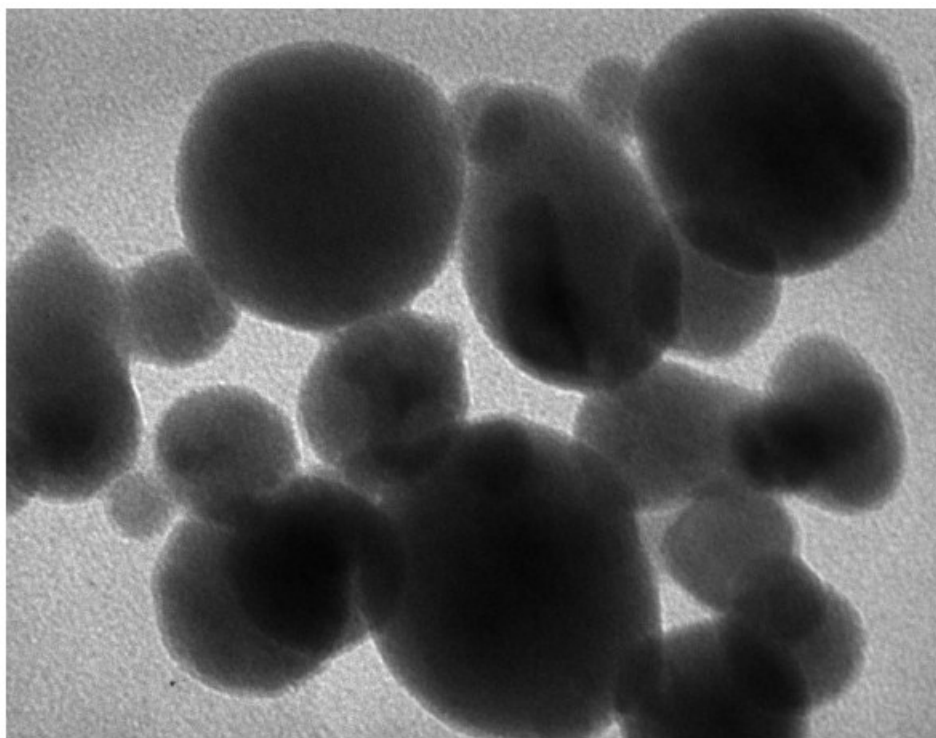


Fig. S2. SEM micrograph of the CuFe₂O₄ catalyst.



20 nm

Fig. S3. TEM micrograph of the CuFe_2O_4 catalyst.

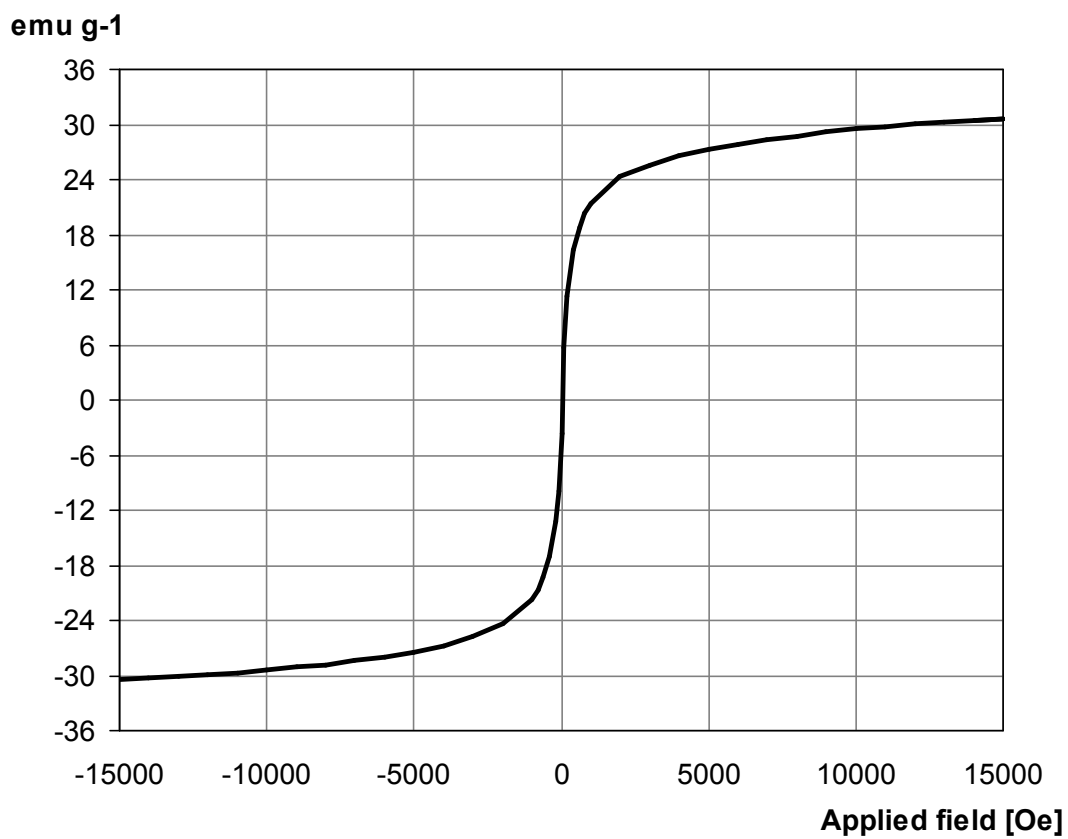


Fig. S4. Magnetization curves for the CuFe_2O_4 catalyst measured at room temperature.

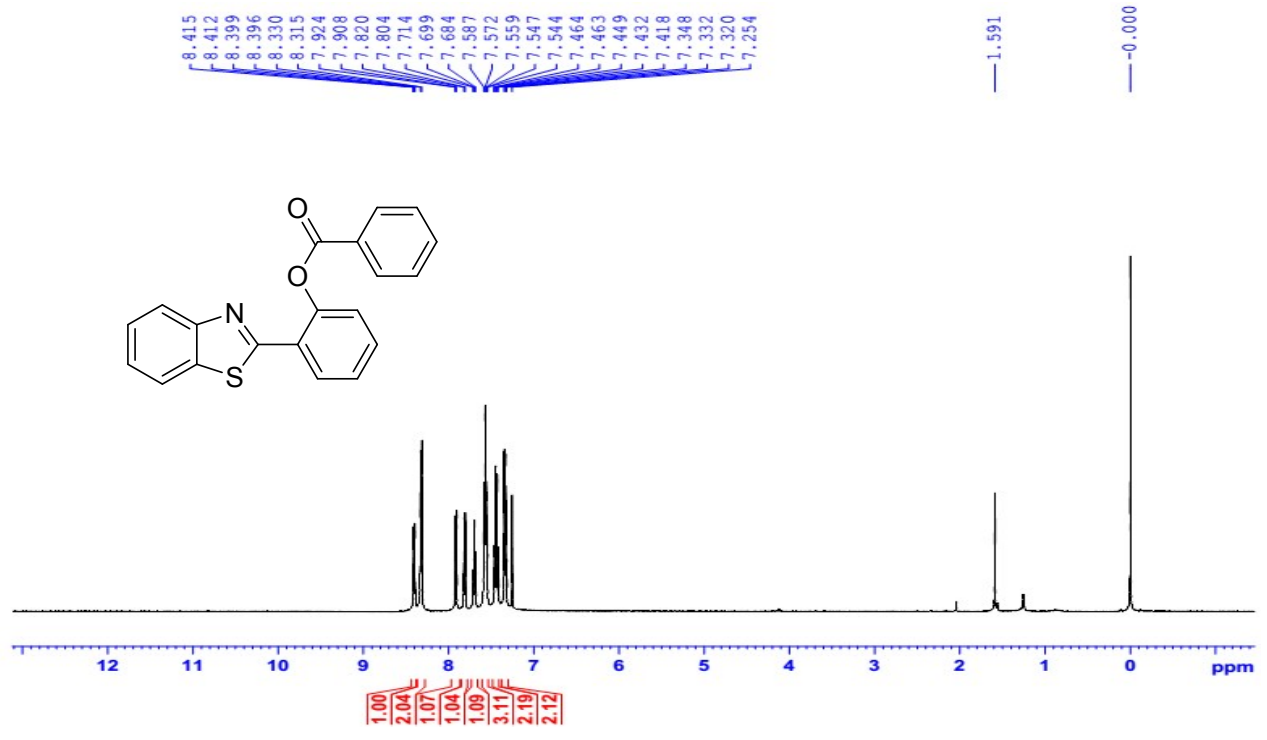


Fig. S5. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

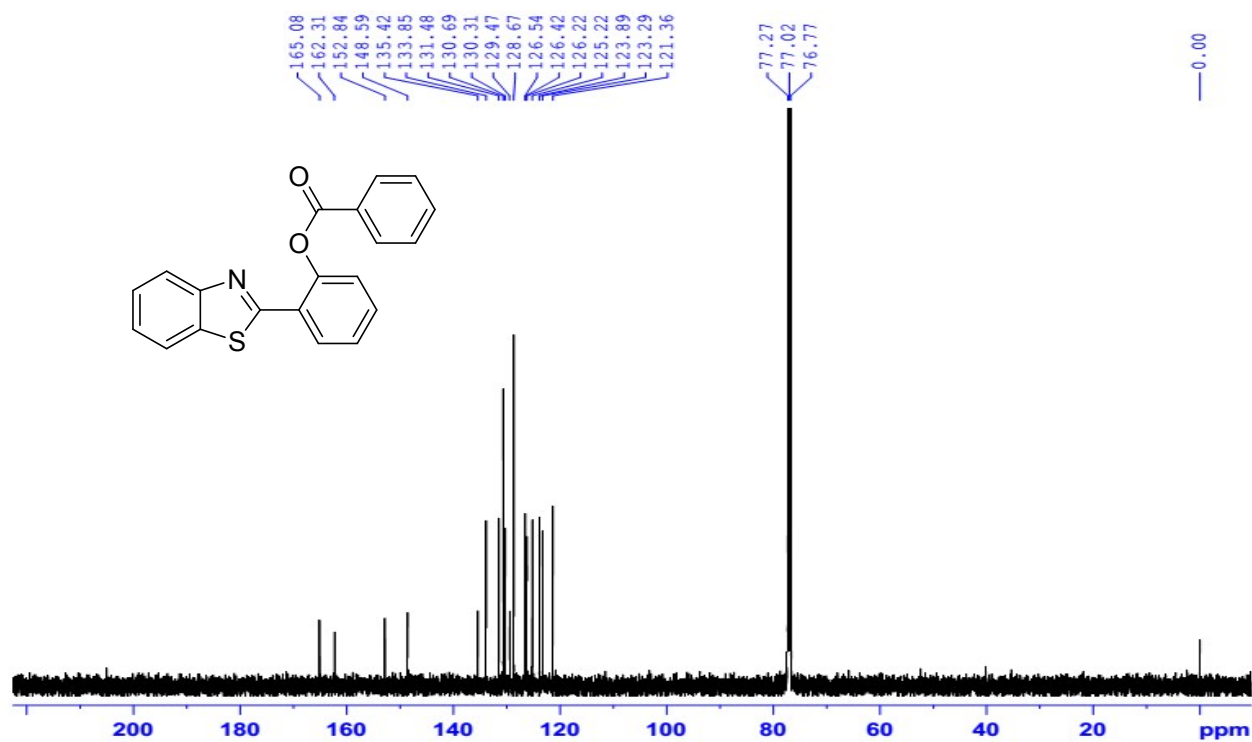


Fig. S6. ^{13}C -NMR of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): yellow solid, 83% yield. ^1H -NMR (500 MHz, CDCl_3 -*d*) δ 8.40 (dd, $J = 7.9$ Hz, $J = 1.5$ Hz, 1H, ArH), 8.32 (d, $J = 8.0$ Hz, 2H, ArH), 7.91 (d, $J = 8.0$ Hz, 1H, ArH), 7.81 (d, $J = 8.0$ Hz, 1H, ArH), 7.68 – 7.71 (m, 1H, ArH), 7.54 – 7.59 (m, 3H, ArH), 7.42 – 7.46 (m, 2H, ArH), 7.32 – 7.35 (m, 2H, ArH); ^{13}C -NMR (125 MHz, CDCl_3 -*d*) δ 165.1, 162.3, 152.8, 148.6, 135.4, 133.8, 131.5, 130.7, 130.3, 129.5, 128.7, 126.5, 126.4, 126.2, 125.2, 123.9, 123.3, 121.4.

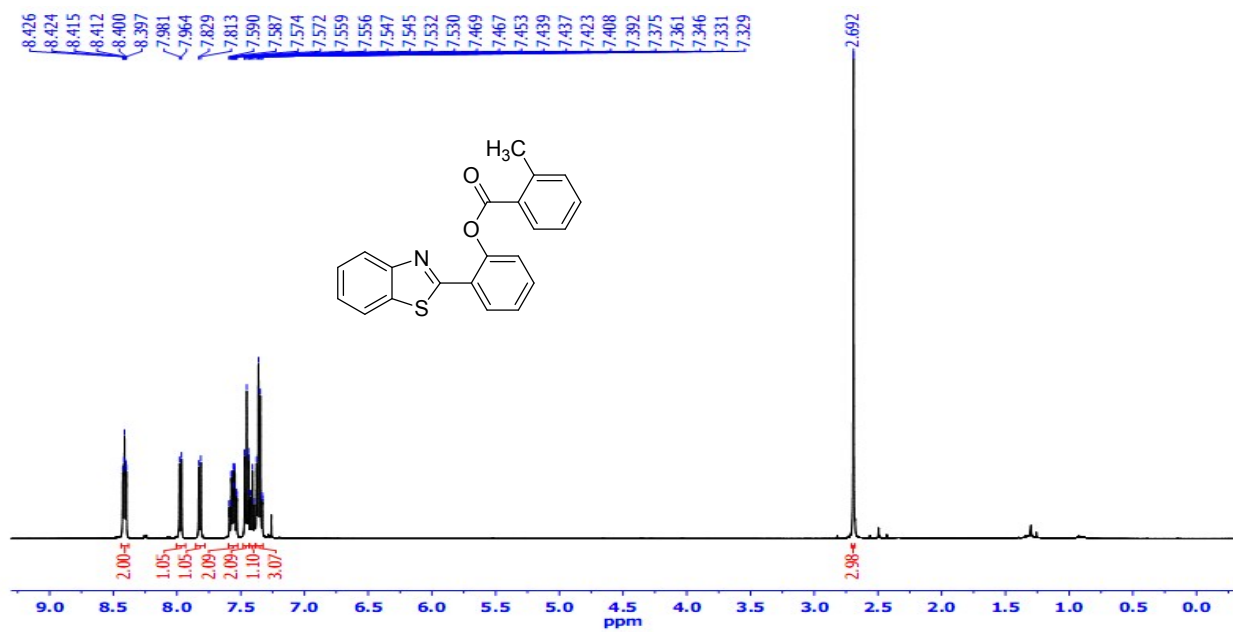


Fig. S7. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 2-methylbenzoate.

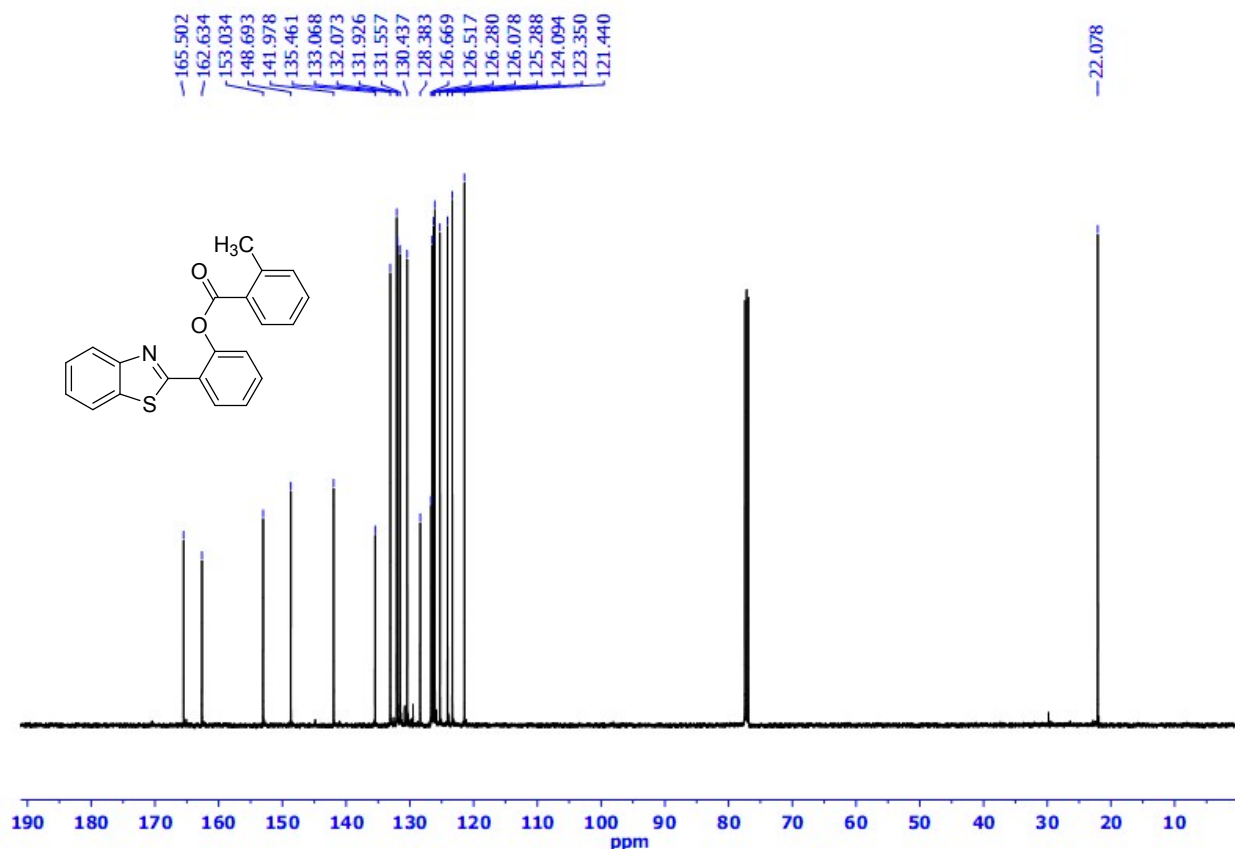


Fig. S8. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 2-methylbenzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl 2-methylbenzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): yellow gummy, 82% yield. ¹H-NMR (500 MHz, CDCl₃-d) δ 8.38 – 8.42 (m, 2H, ArH), 7.97 (d, *J* = 8.2 Hz, 1H, ArH), 7.82 (d, *J* = 8.0 Hz, 1H, ArH), 7.53 – 7.59 (m, 2H, ArH), 7.44 – 7.47 (m, 2H, ArH), 7.39 – 7.42 (m, 1H, ArH), 7.33 – 7.38 (m, 3H, ArH), 2.69 (s, 3H, CH₃); ¹³C-NMR (125 MHz, CDCl₃-d) δ 165.5, 162.6, 153.0, 153.0, 148.7, 141.9, 135.4, 133.1, 132.1, 131.9, 131.5, 130.4, 128.4, 126.7, 126.5, 126.1, 125.3, 124.1, 123.3, 121.4, 22.1.

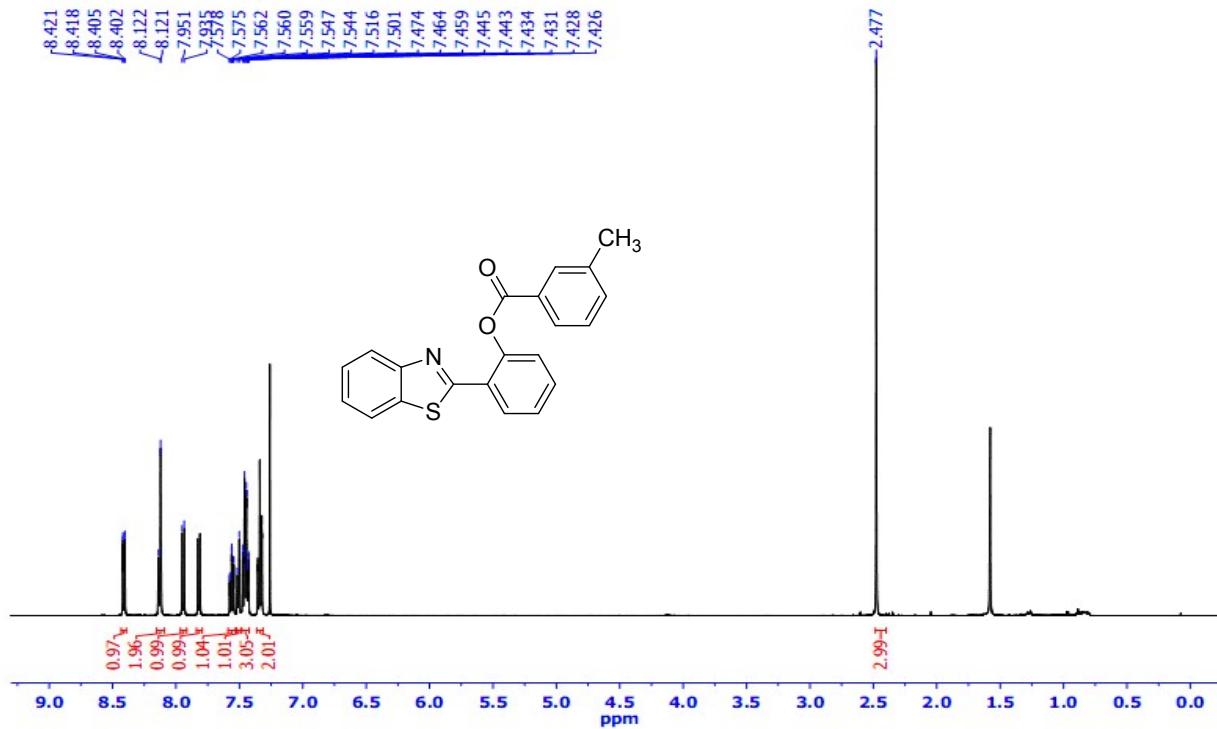


Fig. S9. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 3-methylbenzoate.

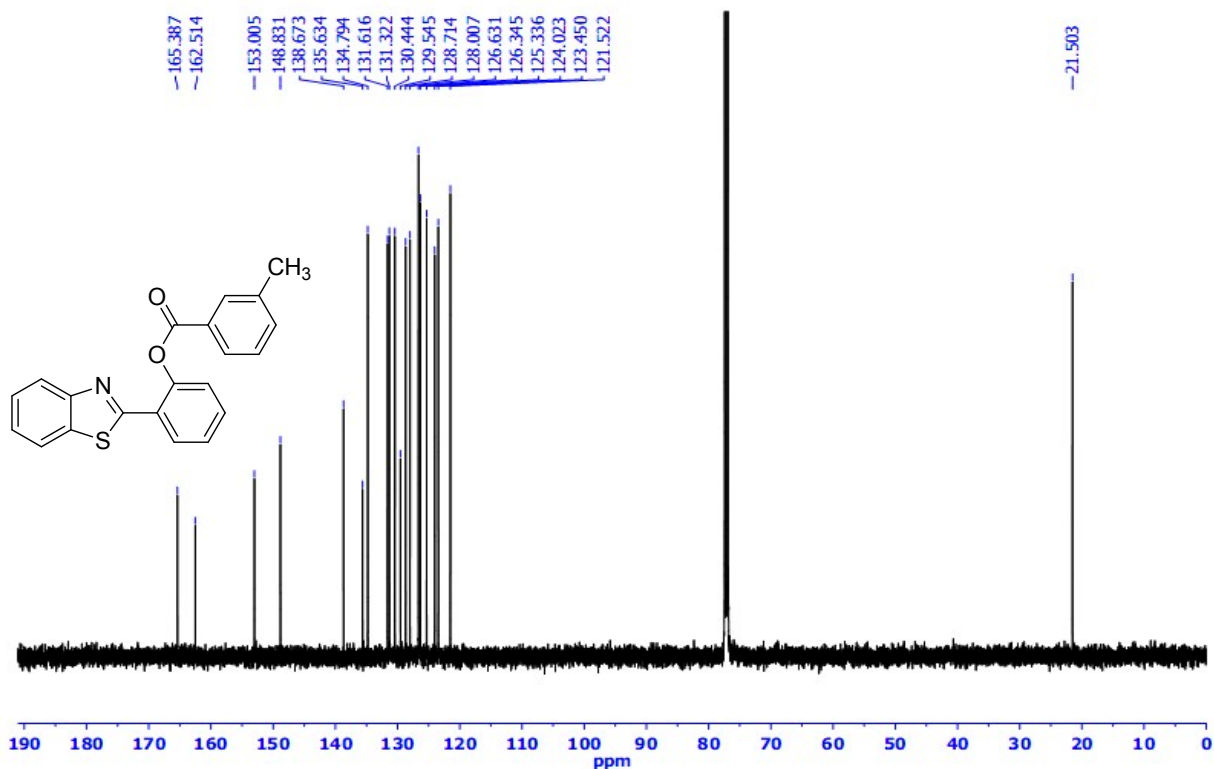


Fig. S10. ^{13}C -NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 3-methylbenzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl 3-methylbenzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 15:1): white solid, 88% yield. ^1H -NMR (500 MHz, CDCl_3 -*d*) δ 8.41 (dd, $J = 7.9$ Hz, $J = 1.6$ Hz, 1H, ArH), 8.12 – 8.14 (m, 2H, ArH), 7.94 (d, $J = 8.1$ Hz, 1H, ArH), 7.82 (d, $J = 8.1$ Hz, 1H, ArH), 7.53 – 7.59 (m, 1H, ArH), 7.50 – 7.52 (m, 1H, ArH), 7.42 – 7.48 (m, 3H, ArH), 7.31 – 7.36 (m, 2H, ArH), 2.48 (s, 3H, CH_3); ^{13}C -NMR (125 MHz, CDCl_3 -*d*) δ 165.4, 162.5, 153.0, 148.8, 138.6, 135.6, 134.8, 131.6, 131.3, 130.4, 129.5, 128.7, 128.0, 126.6, 126.3, 125.3, 124.0, 123.4, 121.5, 21.5.

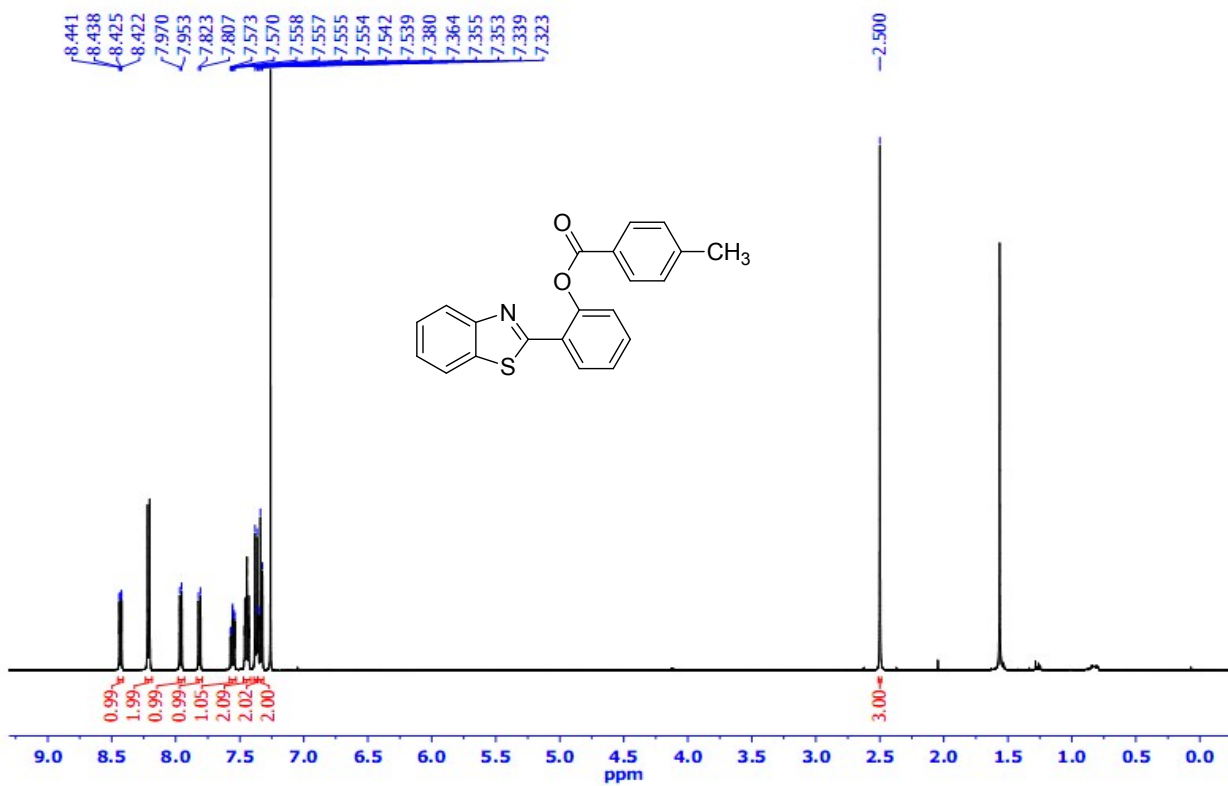


Fig. S11. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 4-methylbenzoate.

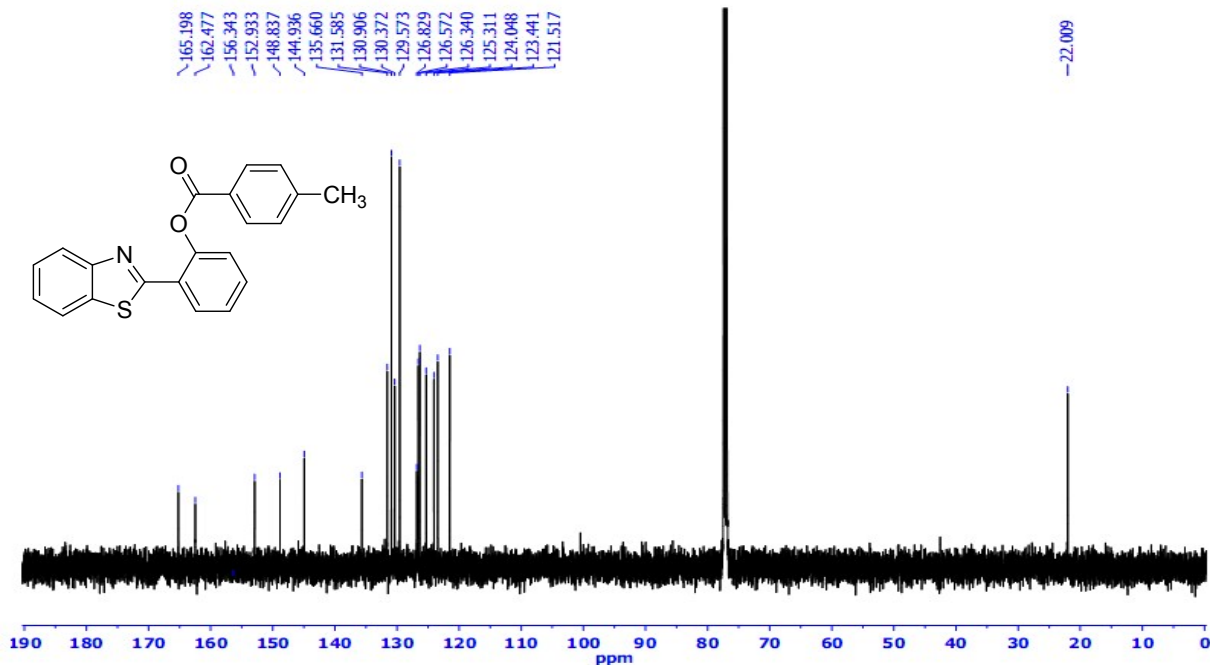


Fig. S12. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 4-methylbenzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl 4-methylbenzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): white solid, 84% yield. ¹H-NMR (500 MHz, CDCl₃-d) δ 8.43 (dd, *J* = 7.9 Hz, *J* = 1.6 Hz, 1H, ArH), 8.21 (d, *J* = 8.2 Hz, 2H, ArH), 7.96 (d, *J* = 8.2 Hz, 1H, ArH), 7.81 (d, *J* = 7.8 Hz, 1H, ArH), 7.54 – 7.57 (m, 1H, ArH), 7.42 – 7.46 (m, 2H, ArH), 7.35 – 7.38 (m, 2H, ArH), 7.32 – 7.34 (m, 2H, ArH), 2.50 (s, 3H, CH₃); ¹³C-NMR (125 MHz, CDCl₃-d) δ 165.2, 162.5, 156.3, 152.3, 148.8, 144.4, 135.6, 131.6, 130.1, 130.4, 129.6, 126.8, 126.6, 126.3, 125.3, 124.0, 123.4, 121.5, 22.0.

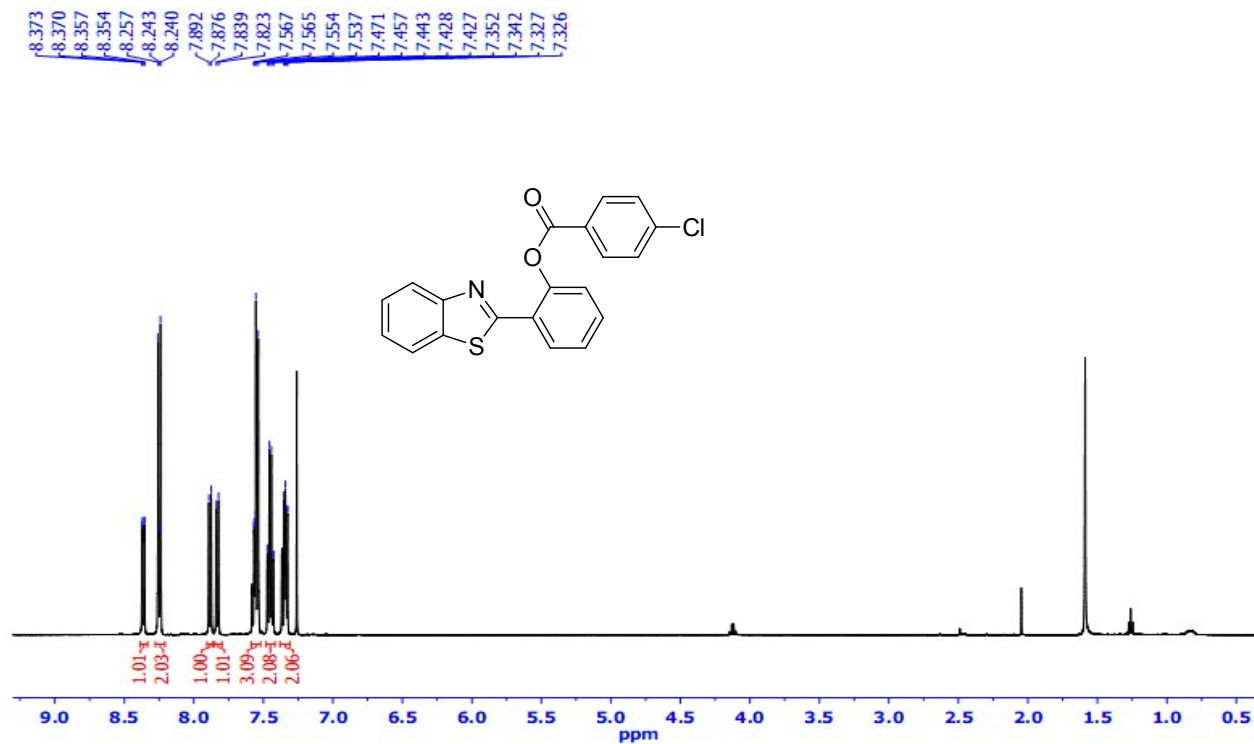


Fig. S13. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 4-chlorobenzoate.

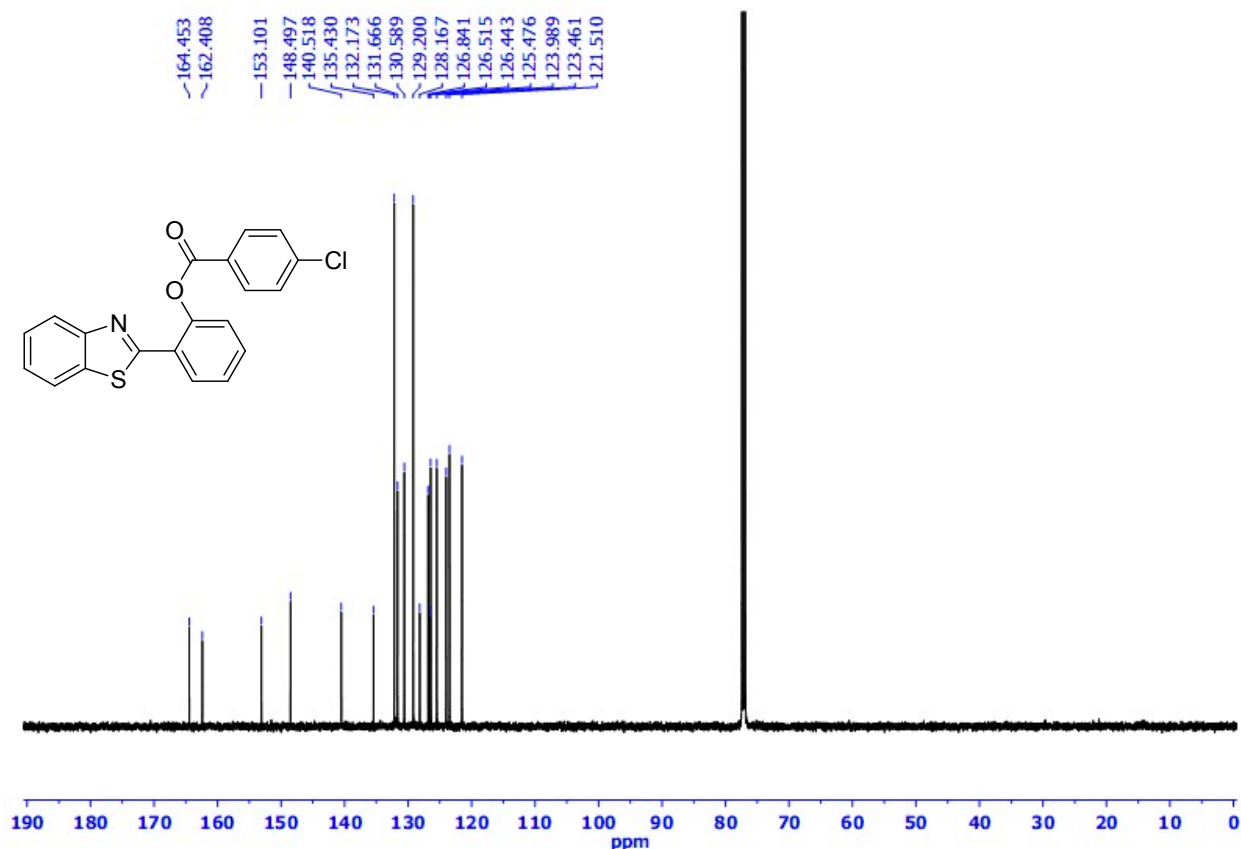


Fig. S14. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 4-chlorobenzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl 4-chlorobenzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): white solid, 70% yield. ¹H-NMR (500 MHz, CDCl₃-*d*) δ 8.36 (dd, *J* = 7.9 Hz, *J* = 1.5 Hz, 1H, Ar*H*), 8.28 – 8.21 (m, 2H, Ar*H*), 7.88 (d, *J* = 8.1 Hz, 1H, Ar*H*), 7.83 (d, *J* = 8.0 Hz, 1H, Ar*H*), 7.54 – 7.57 (m, 3H, Ar*H*), 7.43 – 7.47 (m, 2H, Ar*H*), 7.33 – 7.35 (m, 2H, Ar*H*); ¹³C-NMR (125 MHz, CDCl₃-*d*) δ 164.4, 162.4, 153.1, 148.5, 140.2, 135.4, 132.2, 131.6, 130.6, 129.2, 128.2, 126.8, 126.5, 126.4, 125.5, 124.0, 123.5, 121.5.

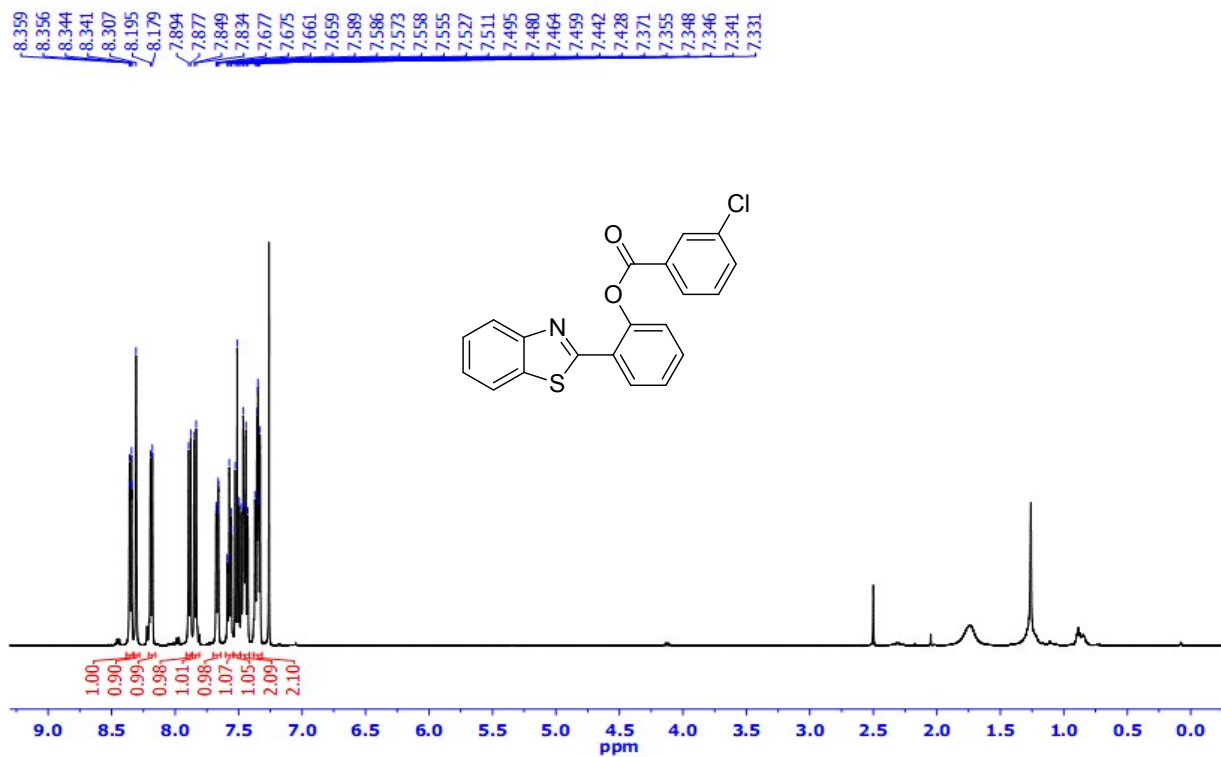


Fig. S15. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 3-chlorobenzoate.

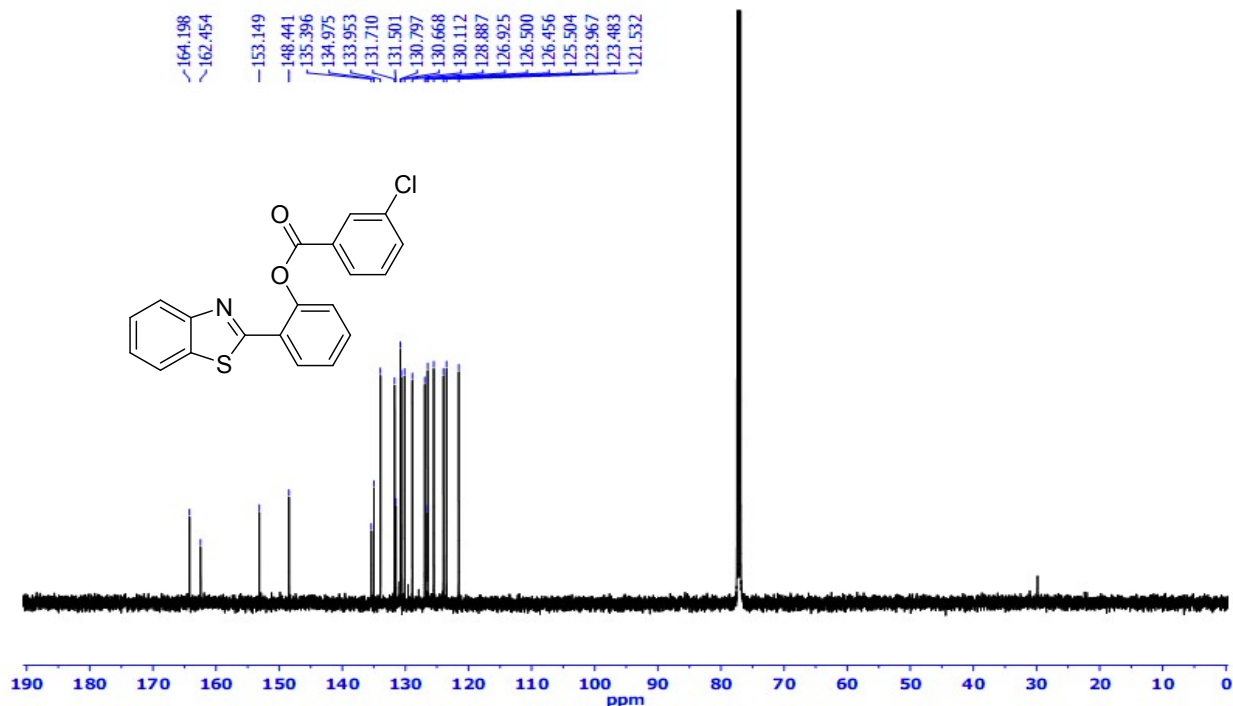


Fig. S16. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 3-chlorobenzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl 3-chlorobenzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): white solid, 74% yield. ¹H-NMR (500 MHz, CDCl₃-d) δ 8.35 (dd, *J* = 7.9 Hz, *J* = 1.5 Hz, 1H, Ar*H*), 8.31 (s, br, 1H, Ar*H*), 7.19 (d, *J* = 7.8 Hz, 1H, Ar*H*), 7.88 (d, *J* = 8.2 Hz, 1H, Ar*H*), 7.84 (d, *J* = 8.1 Hz, 1H, Ar*H*), 7.66 – 7.68 (m, 1H, Ar*H*), 7.56 – 7.59 (m, 1H, Ar*H*), 7.50 – 7.53 (m, 1H, Ar*H*), 7.43 – 7.48 (m, 2H, Ar*H*), 7.33 – 7.37 (m, 2H, Ar*H*); ¹³C-NMR (125 MHz, CDCl₃-d) δ 164.2, 162.4, 153.2, 148.4, 135.4, 134.9, 133.9, 131.7, 131.5, 130.8, 130.6, 130.1, 128.9, 126.9, 126.5, 126.5, 125.5, 123.9, 123.5, 121.5.

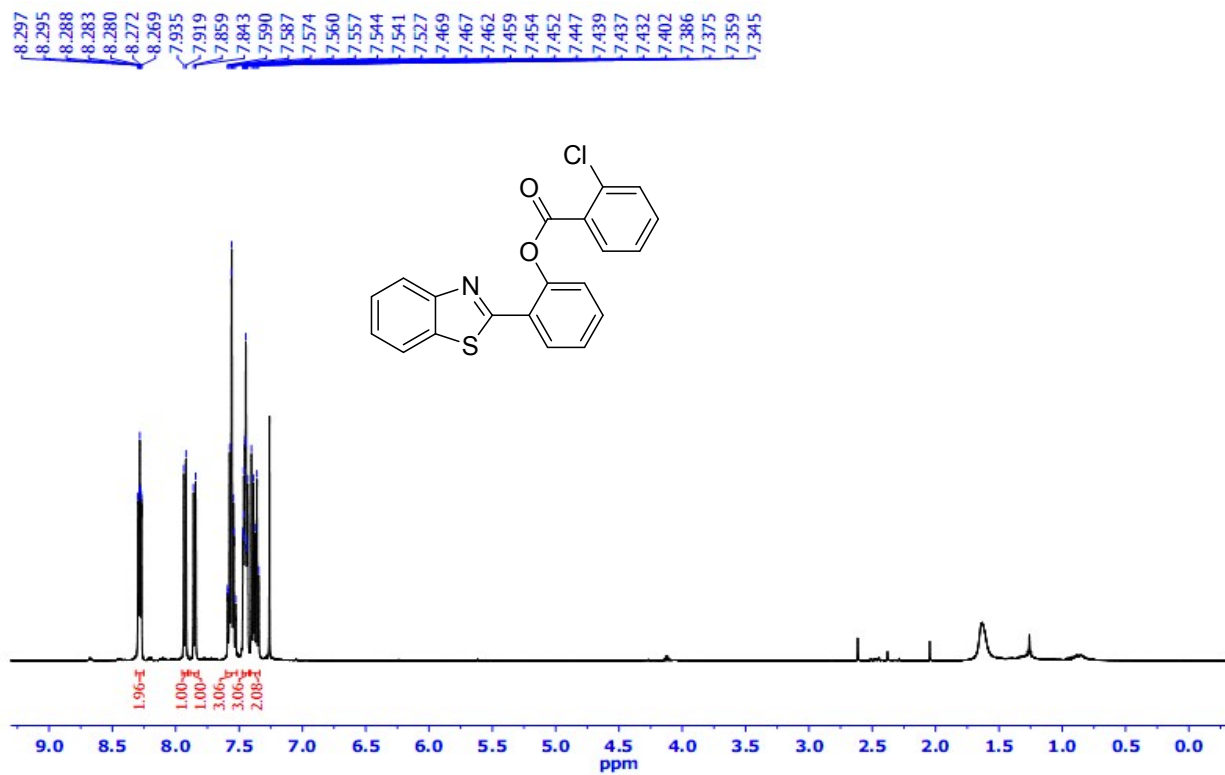


Fig. S17. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 2-chlorobenzoate.

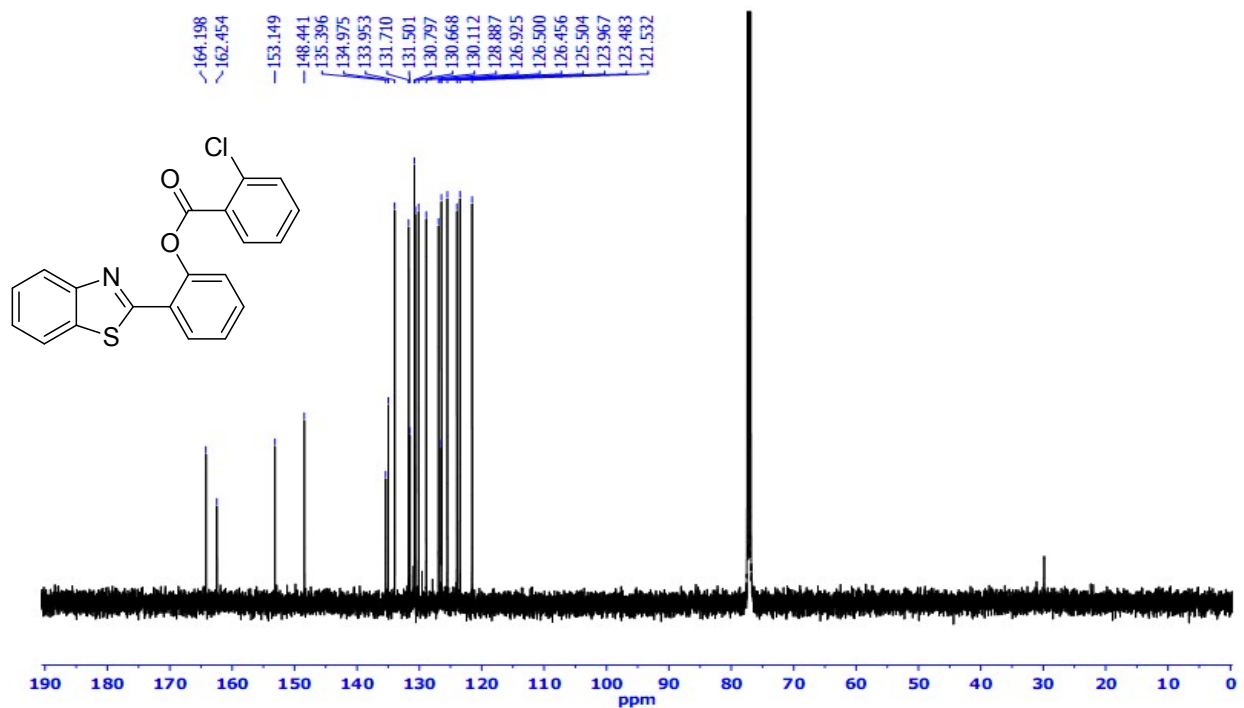


Fig. S18. ^{13}C -NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 2-chlorobenzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl 2-chlorobenzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): white solid, 71% yield. ^1H -NMR (500 MHz, CDCl_3 -*d*) δ 8.27 – 8.29 (m, 2H, ArH), 7.93 (d, J = 8.2 Hz, 1H, ArH), 7.85 (d, J = 8.0 Hz, 1H, ArH), 7.53 – 7.59 (m, 3H, ArH), 7.49 – 7.47 (m, 3H, ArH), 7.35 – 7.40 (m, 2H, ArH); ^{13}C -NMR (125 MHz, CDCl_3 -*d*) δ 164.2, 162.4, 153.2, 148.4, 135.4, 134.9, 133.9, 131.7, 131.5, 130.8, 130.6, 130.1, 128.9, 126.9, 126.5, 126.5, 125.5, 123.9, 123.5, 121.5.

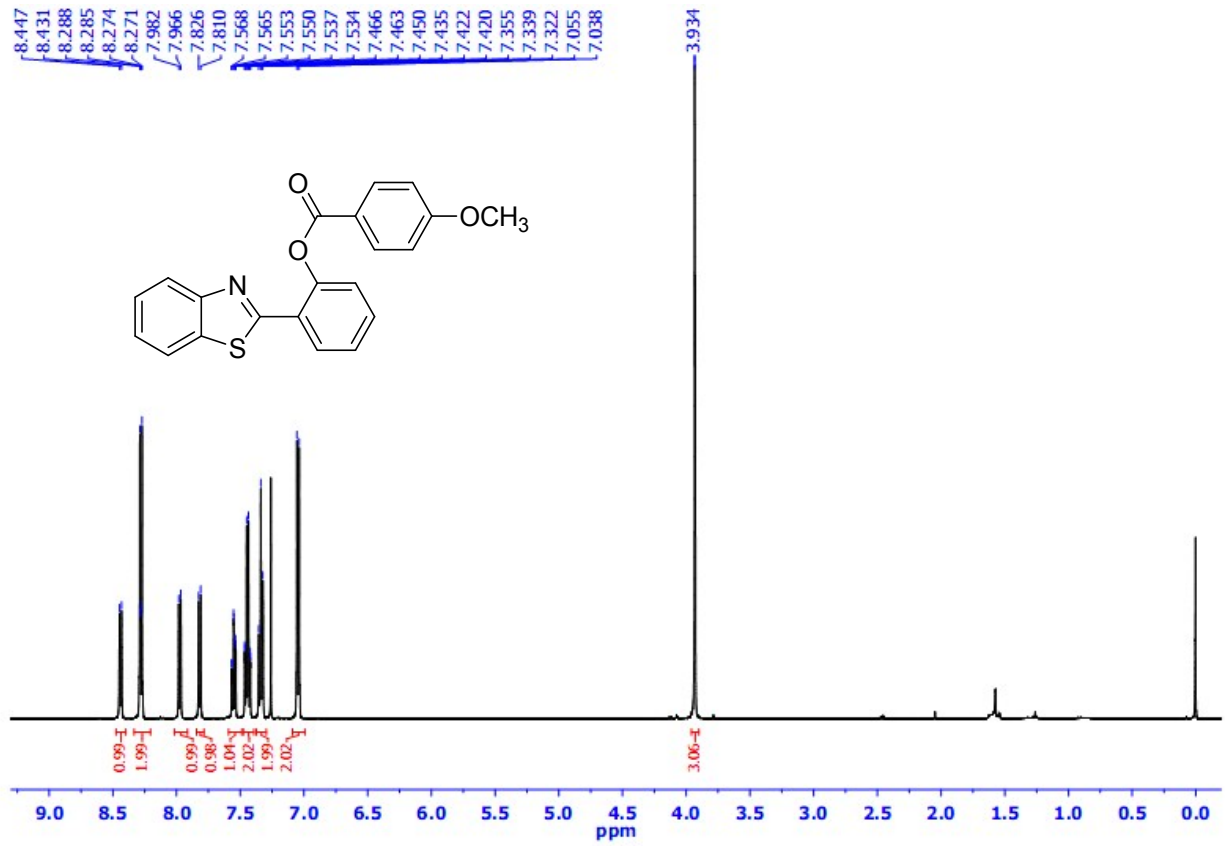


Fig. S19. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 4-methoxybenzoate.

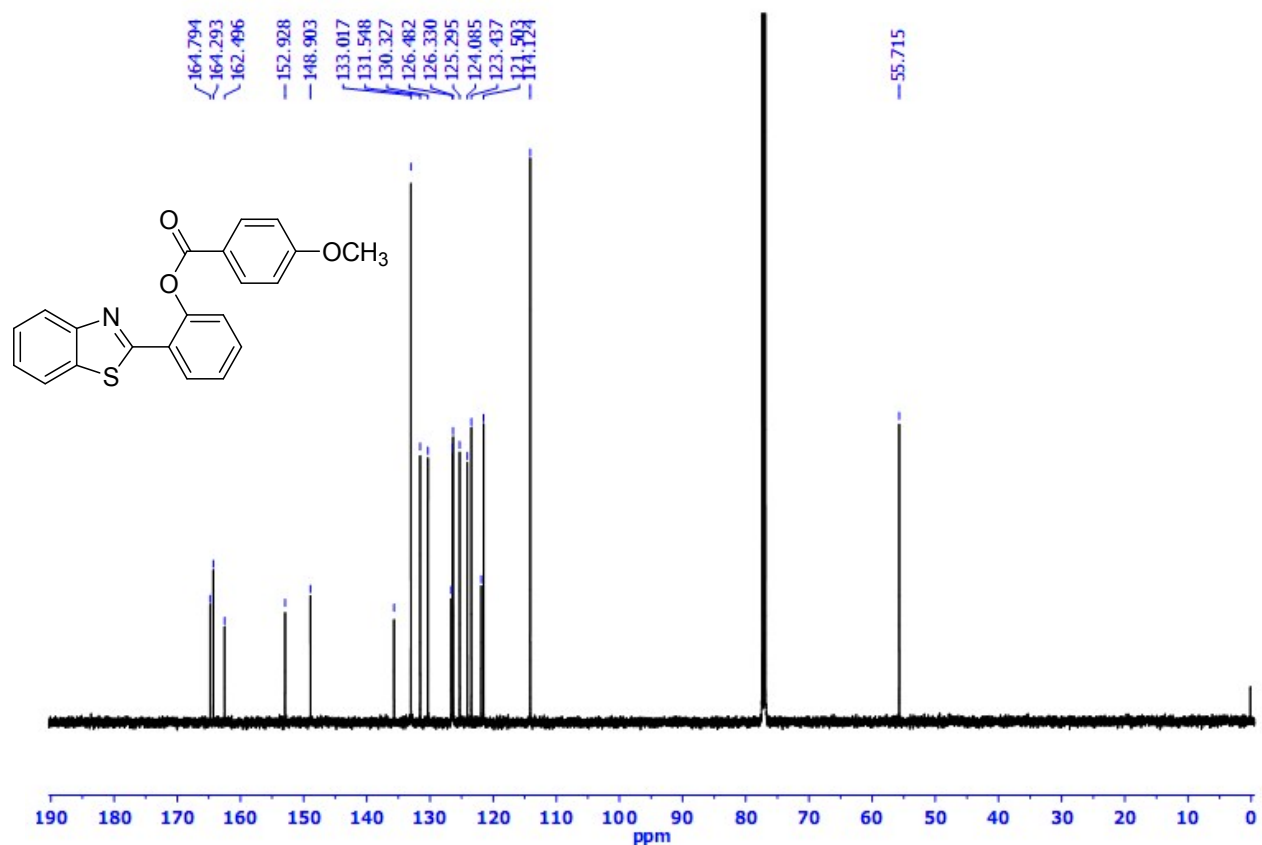


Fig. S20. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 4-methoxybenzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl 4-methoxybenzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 9:1): white solid, 83% yield. ¹H NMR (500 MHz, CDCl₃) δ 8.44 (d, *J* = 7.9 Hz, 1H, ArH), 8.33 – 8.20 (m, 2H, ArH), 7.97 (d, *J* = 8.2 Hz, 1H, ArH), 7.82 (d, *J* = 8.0 Hz, 1H, ArH), 7.55 (td, *J* = 7.8, 1.6 Hz, 1H, ArH), 7.44 (td, *J* = 7.8, 1.1 Hz, 2H, ArH), 7.34 (t, *J* = 8.2 Hz, 2H, ArH), 7.05 (d, *J* = 8.8 Hz, 2H, ArH), 3.93 (s, 3H, CH₃); ¹³C-NMR (125 MHz, CDCl₃-*d*) δ 164.8, 164.3, 162.5, 152.9, 148.9, 135.7, 133.0, 131.6, 130.3, 126.6, 126.5, 126.3, 125.3, 124.1, 123.4, 121.9, 121.5, 114.1, 55.7.

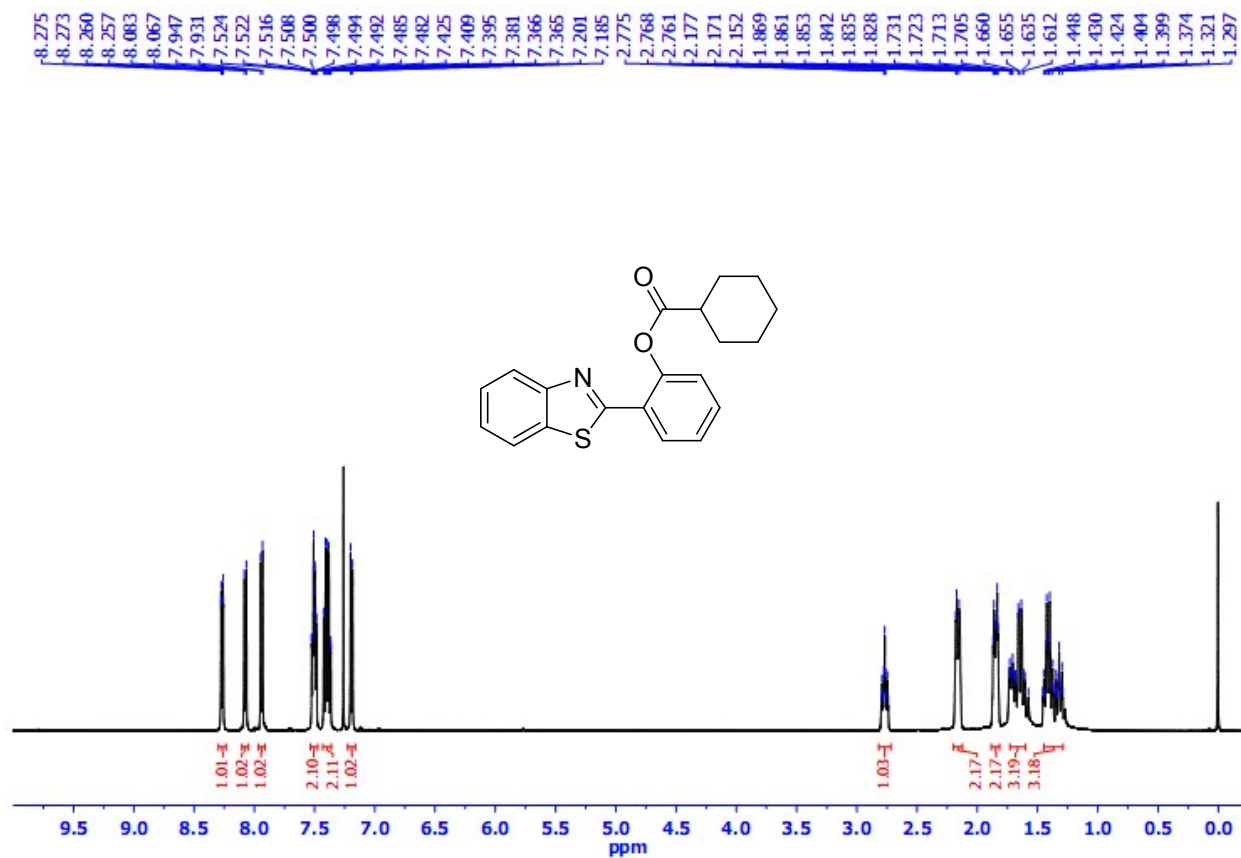


Fig. S21. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl cyclohexanecarboxylate.

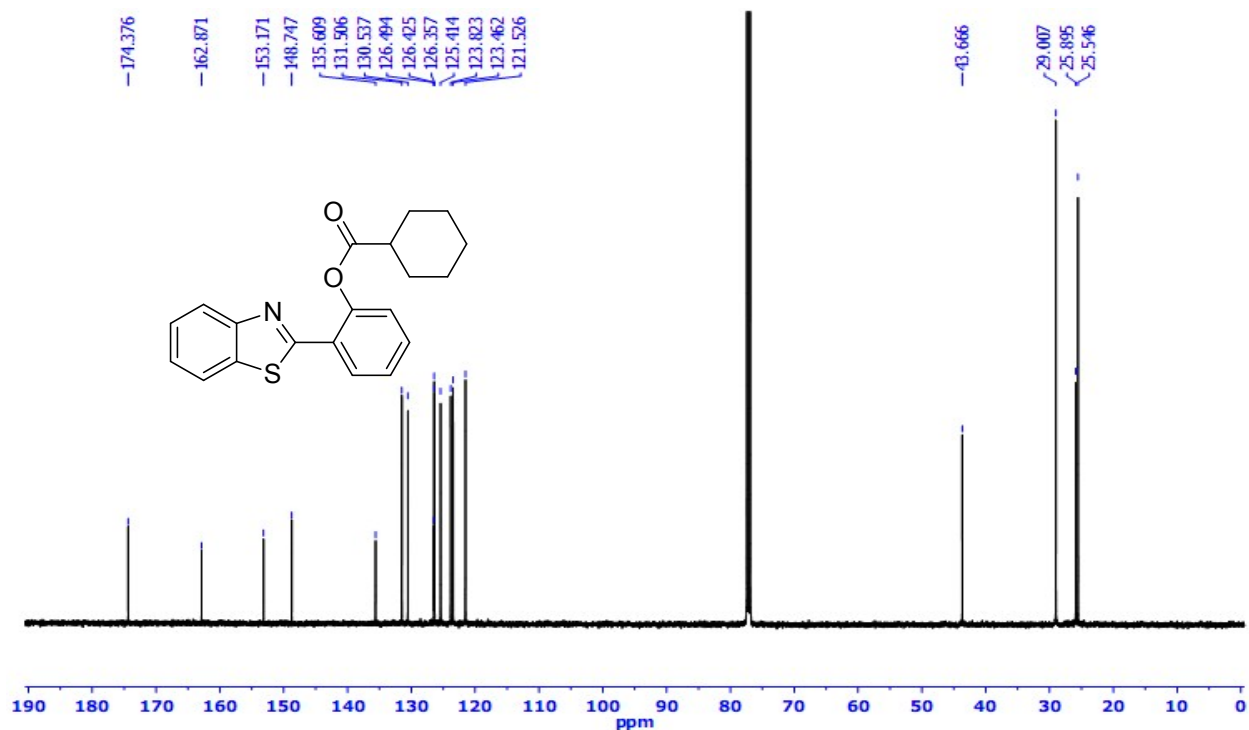


Fig. S22. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl cyclohexanecarboxylate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl cyclohexanecarboxylate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 9:1): yellow solid, 73% yield. ¹H NMR (500 MHz, CDCl₃) δ 8.27 (dd, *J* = 7.8, 1.4 Hz, 1H, ArH), 8.07 (d, *J* = 8.2 Hz, 1H, ArH), 7.94 (d, *J* = 8.0 Hz, 1H, ArH), 7.48 – 7.52 (m, 2H, ArH), 7.43 – 7.36 (m, 2H, ArH), 7.19 (d, *J* = 8.1 Hz, 1H, ArH), 2.74– 2.80 (m, 1H, >CH-), 2.20 – 2.12 (m, 2H, CH₂), 1.88 – 1.82 (m, 2H, CH₂), 1.73 – 1.60 (m, 3H, CH₂), 1.45 – 1.29 (m, 3H, CH₂). ¹³C-NMR (125 MHz, CDCl₃-*d*) δ 174.3, 162.8, 153.1, 148.7, 135.6, 131.5, 130.5, 126.4, 126.4, 126.3, 125.4, 123.8, 123.4, 121.5, 43.6, 29.0, 25.8, 25.5.

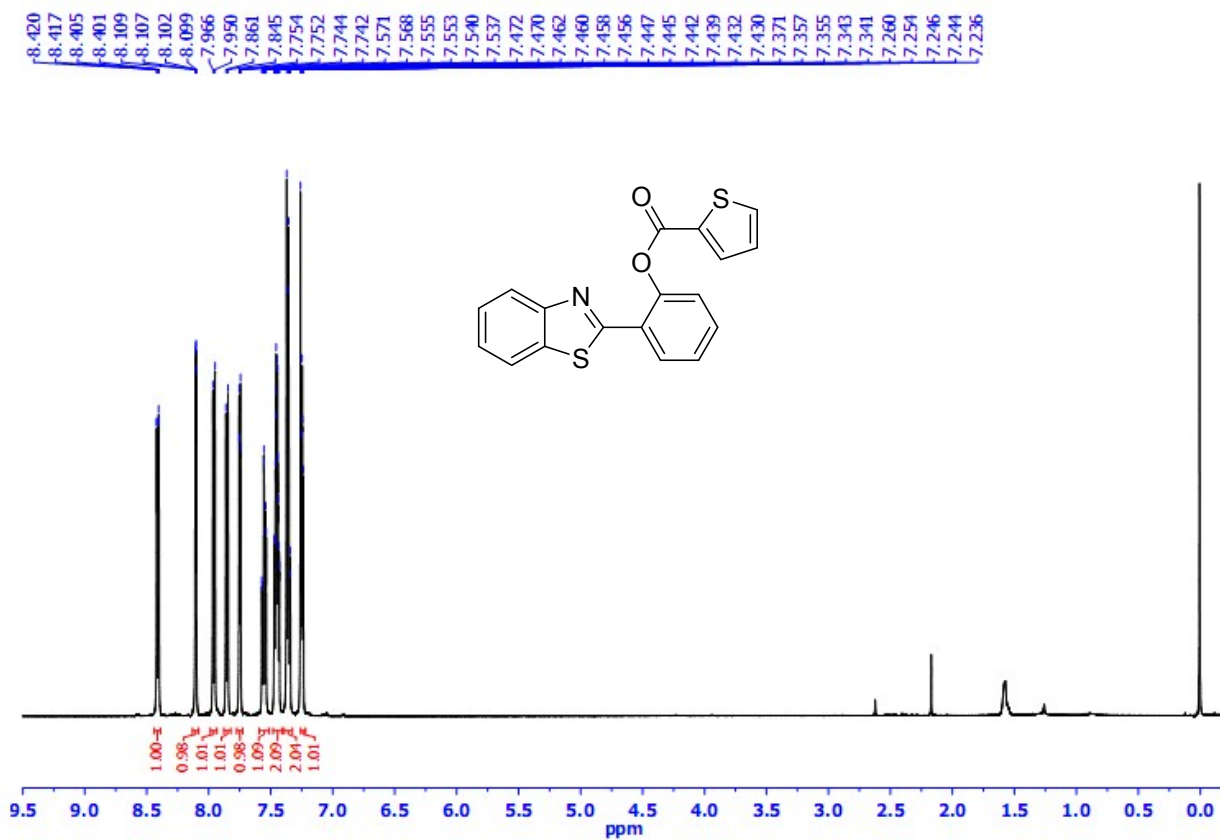


Fig. S23. $^1\text{H-NMR}$ spectra of 2-(benzo[d]thiazol-2-yl)phenyl thiophene-2-carboxylate.

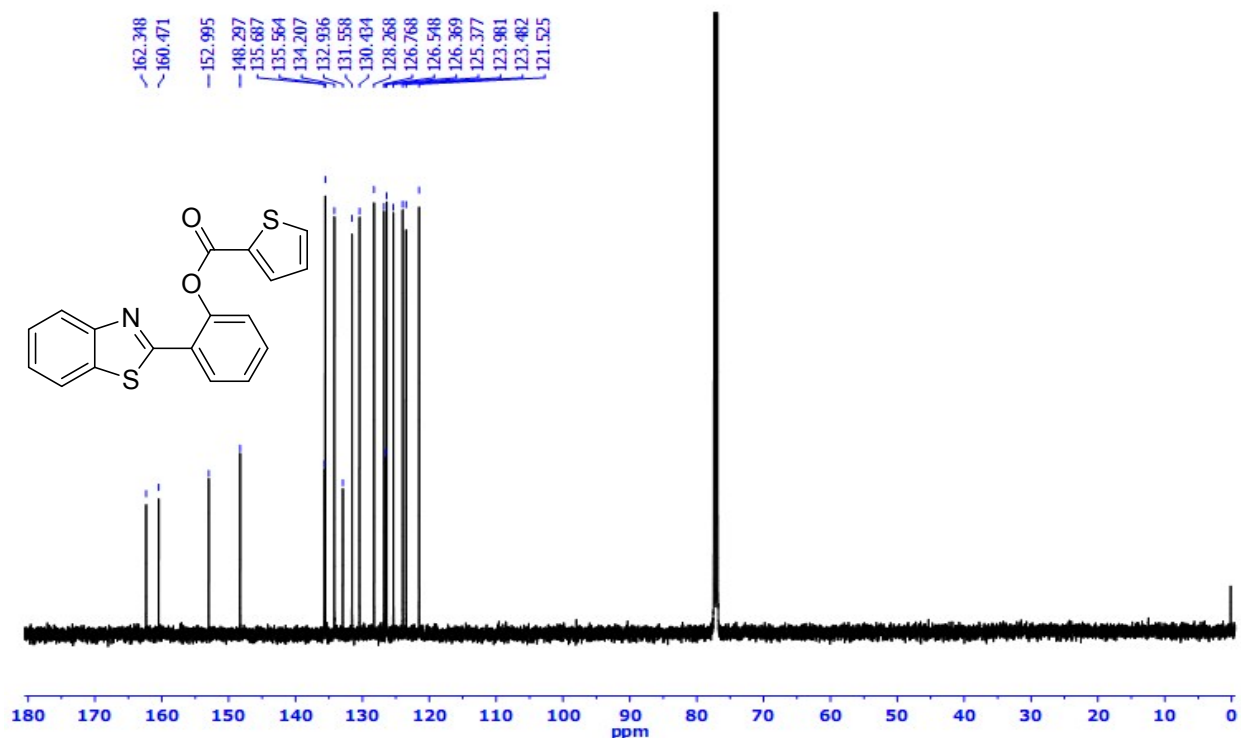


Fig. S24. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl thiophene-2-carboxylate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl thiophene-2-carboxylate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 9:1): yellow solid, 56% yield. ¹H NMR (500 MHz, CDCl₃) δ 8.41 (dd, *J* = 7.9, 1.6 Hz, 1H, *ArH*), 8.10 (dd, *J* = 3.8, 1.2 Hz, 1H, *ArH*), 7.96 (d, *J* = 8.1 Hz, 1H, *ArH*), 7.85 (d, *J* = 8.0 Hz, 1H, *ArH*), 7.75 (dd, *J* = 5.0, 1.1 Hz, 1H, *ArH*), 7.55 (td, *J* = 8.0, 1.6 Hz, 1H, *ArH*), 7.43 - 7.47 (m, 2H, *ArH*), 7.39 - 7.32 (m, 2H, *ArH*), 7.24 (dd, *J* = 4.9, 3.8 Hz, 1H, *ArH*); ¹³C-NMR (125 MHz, CDCl₃-*d*) δ 162.3, 160.4, 153.0, 148.30, 135.7, 135.5, 134.2, 132.9, 131.6, 130.4, 128.3, 126.8, 126.5, 126.4, 125.4, 123.9, 123.5, 121.5.

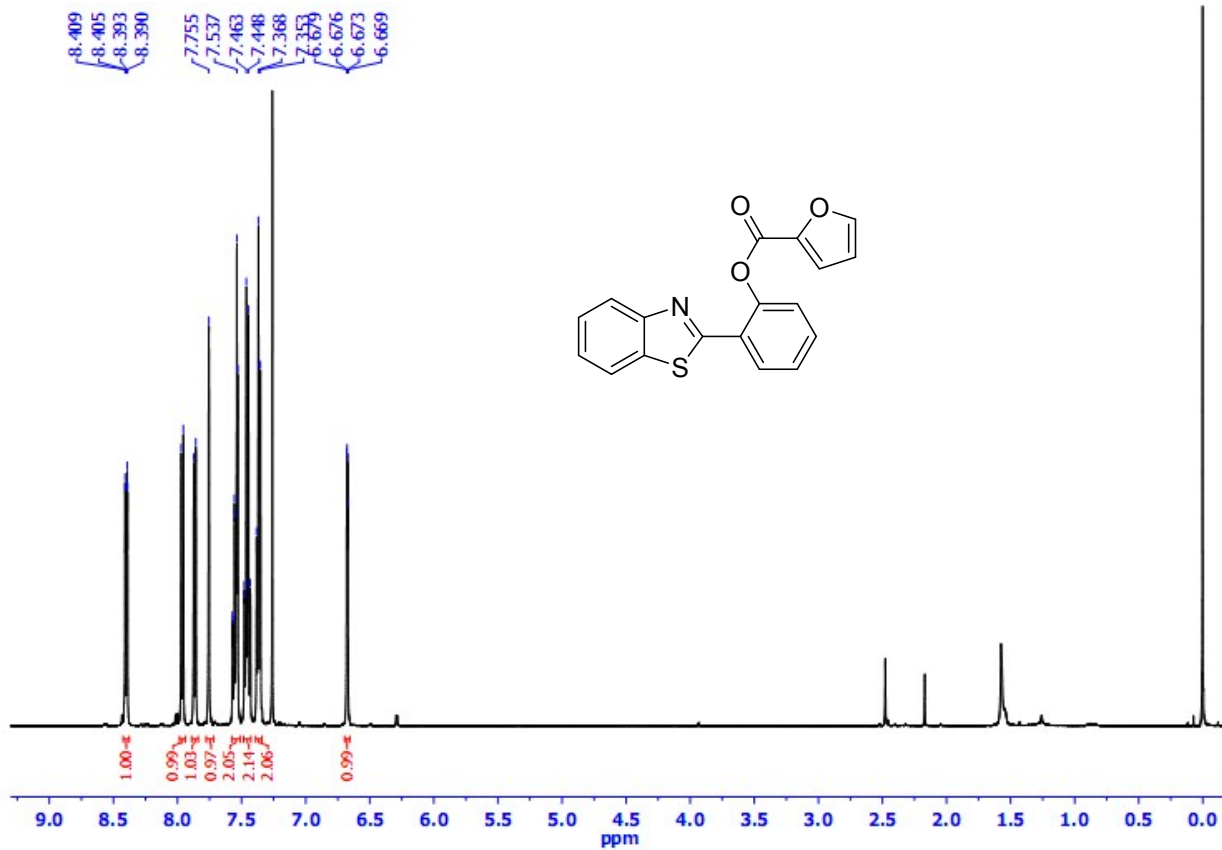


Fig. S25. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl furan-2-carboxylate.

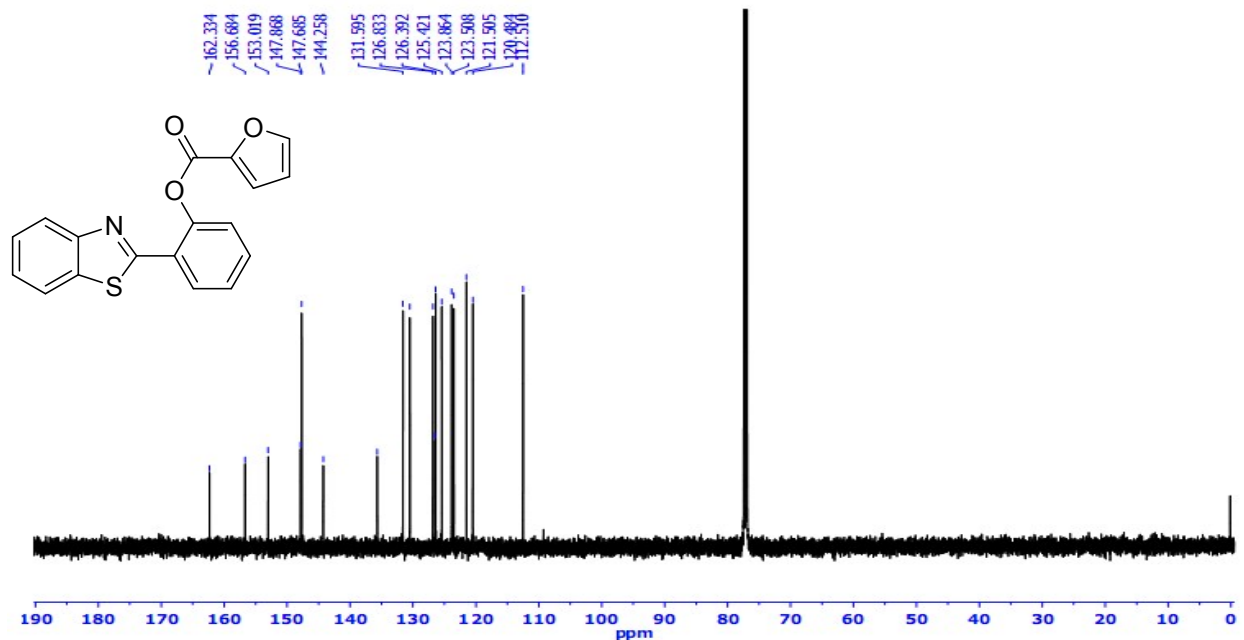


Fig. S26. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl furan-2-carboxylate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl furan-2-carboxylate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): yellow solid, 59% yield. ¹H NMR (500 MHz, CDCl₃-*d*) δ 8.40 (dd, *J* = 7.9, 1.6 Hz, 1H, Ar*H*), 7.96 (d, *J* = 8.2 Hz, 1H, Ar*H*), 7.86 (d, *J* = 8.0 Hz, 1H, Ar*H*), 7.76 (s, 1H, Ar*H*), 7.58 – 7.51 (m, 2H, Ar*H*), 7.48 – 7.43 (m, 2H, Ar*H*), 7.37 (t, *J* = 7.6 Hz, 2H, Ar*H*), 6.67 (dd, *J* = 3.5, 1.7 Hz, 1H, Ar*H*); ¹³C-NMR (125 MHz, CDCl₃-*d*) δ 162.3, 156.7, 153.0, 147.9, 147.7, 144.3, 135.7, 131.6, 130.5, 126.8, 126.5, 126.4, 125.4, 123.9, 123.5, 121.5, 120.5, 112.5.

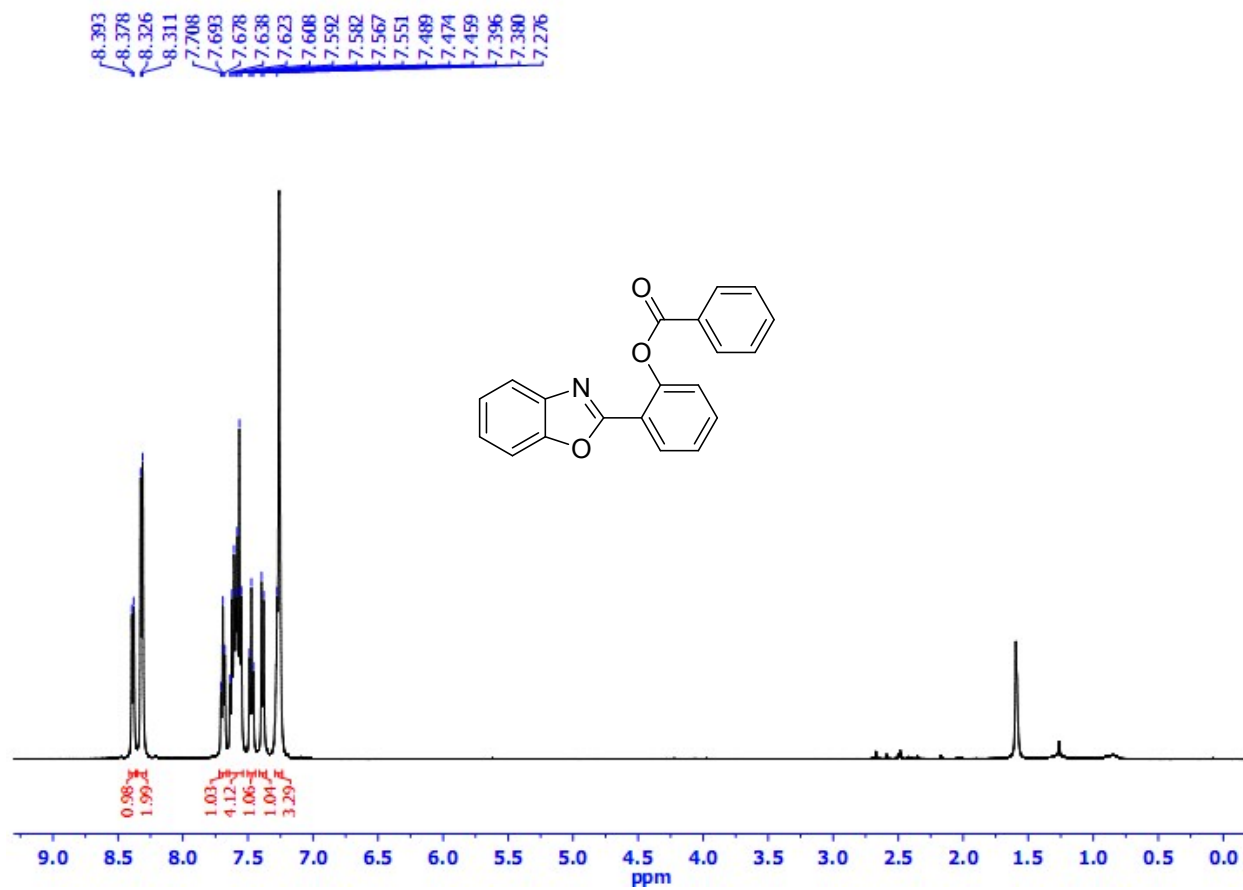


Fig. S27. ¹H-NMR spectra of 2-(benzo[d]oxazol-2-yl)phenyl benzoate.

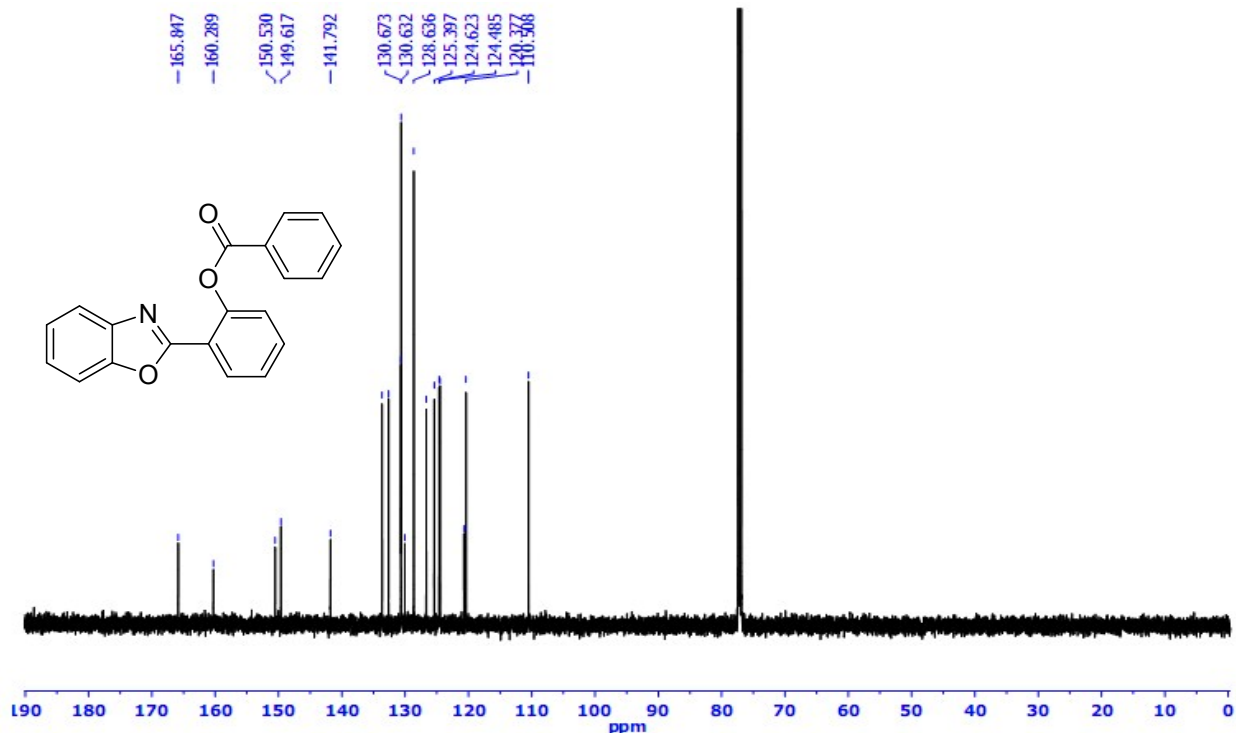


Fig. S28. ¹³C-NMR spectra of 2-(benzo[d]oxazol-2-yl)phenyl benzoate.

Characterization Data for 2-(benzo[d]oxazol-2-yl)phenyl benzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): white solid, 55% yield. ¹H NMR (500 MHz, CDCl₃-*d*) δ 8.39 (d, *J* = 7.4 Hz, 1H, Ar*H*), 8.32 (d, *J* = 7.5 Hz, 2H, Ar*H*), 7.69 (t, *J* = 7.4 Hz, 1H, Ar*H*), 7.65 – 7.54 (m, 4H, Ar*H*), 7.47 (t, *J* = 7.5 Hz, 1H, Ar*H*), 7.39 (d, *J* = 8.0 Hz, 1H, Ar*H*), 7.28 (s, 3H, Ar*H*); ¹³C-NMR (125 MHz, CDCl₃-*d*) δ 165.8, 160.3, 150.5, 149.6, 141.8, 133.6, 132.6, 130.7, 130.6, 130.0, 128.6, 126.7, 125.4, 124.6, 124.5, 120.7, 120.4, 110.5.

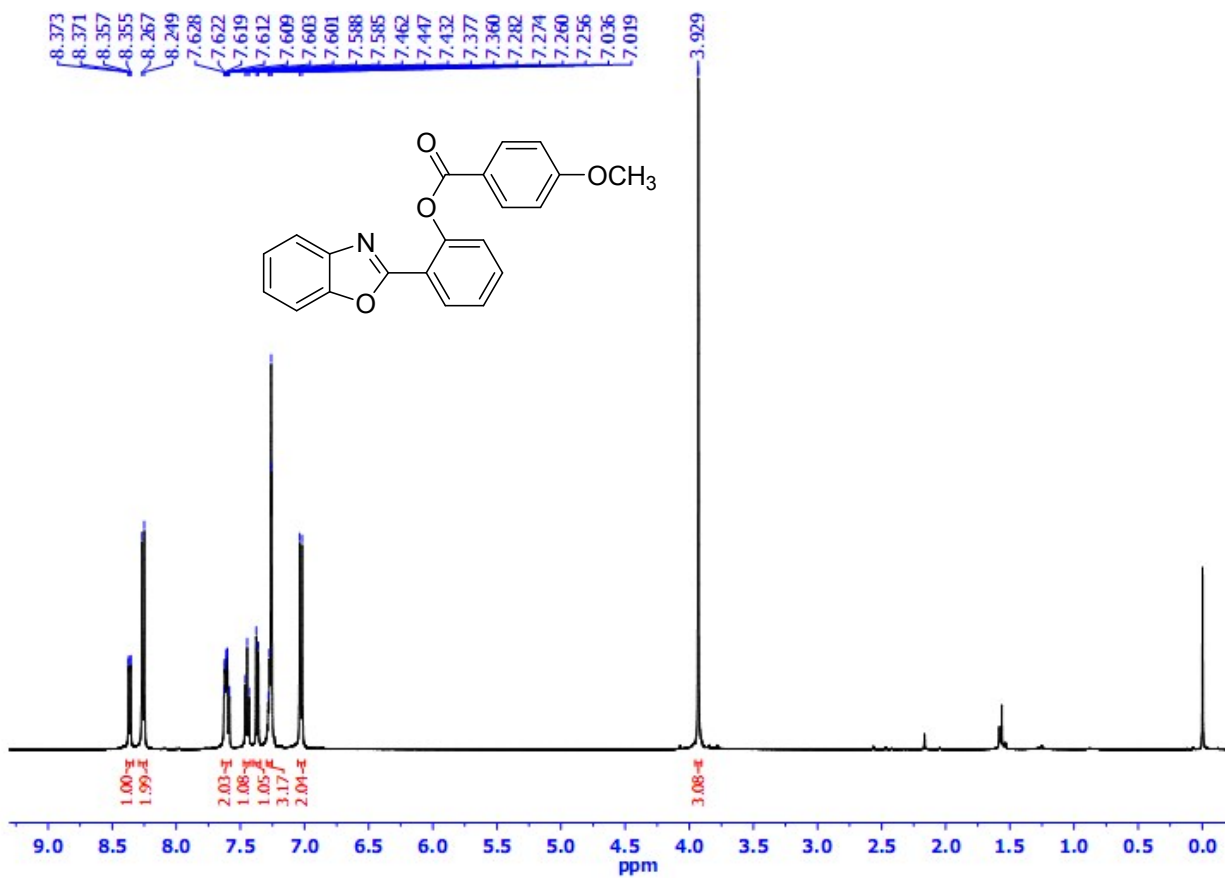


Fig. S29. ¹H-NMR spectra of 2-(benzo[d]oxazol-2-yl)phenyl 4-methoxybenzoate

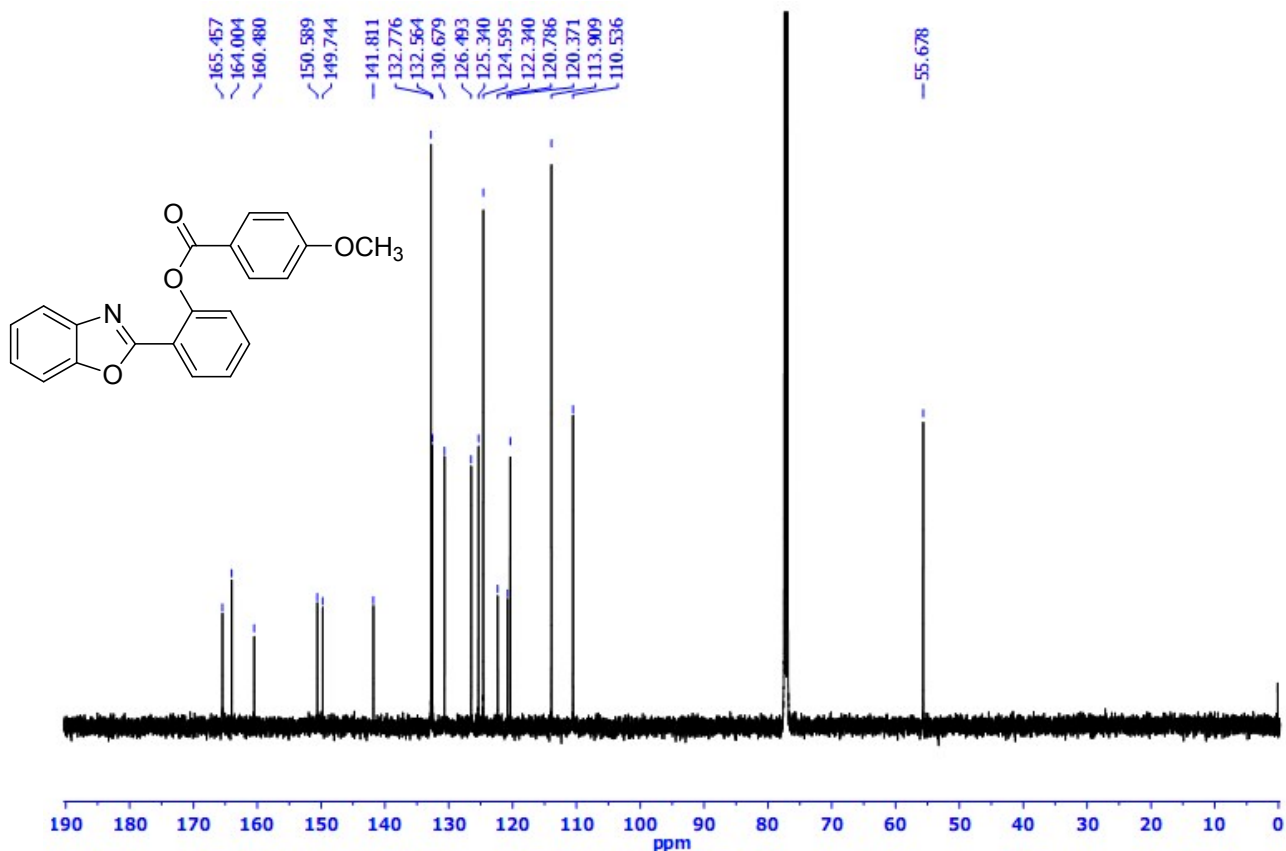


Fig. S30. ¹³C-NMR spectra of 2-(benzo[d]oxazol-2-yl)phenyl 4-methoxybenzoate.

Characterization Data for 2-(benzo[d]oxazol-2-yl)phenyl 4-methoxybenzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): white solid, 75% yield. ¹H NMR (500 MHz, CDCl₃-d) δ 8.36 (dd, *J* = 7.9, 1.3 Hz, 1H, ArH), 8.26 (d, *J* = 8.7 Hz, 2H, ArH), 7.64 – 7.57 (m, 2H, ArH), 7.45 (t, *J* = 7.6 Hz, 1H, ArH), 7.37 (d, *J* = 8.1 Hz, 1H, ArH), 7.27 (dd, *J* = 10.0, 3.1 Hz, 3H, ArH), 7.03 (d, *J* = 8.8 Hz, 2H, ArH), 3.93 (s, 3H, CH₃); ¹³C-NMR (125 MHz, CDCl₃-d) δ 165.4, 164.0, 160.5, 150.6, 149.7, 141.8, 132.8, 132.5, 130.7, 126.5, 125.3, 124.6, 122.3, 120.8, 120.4, 113.9, 110.5, 55.6

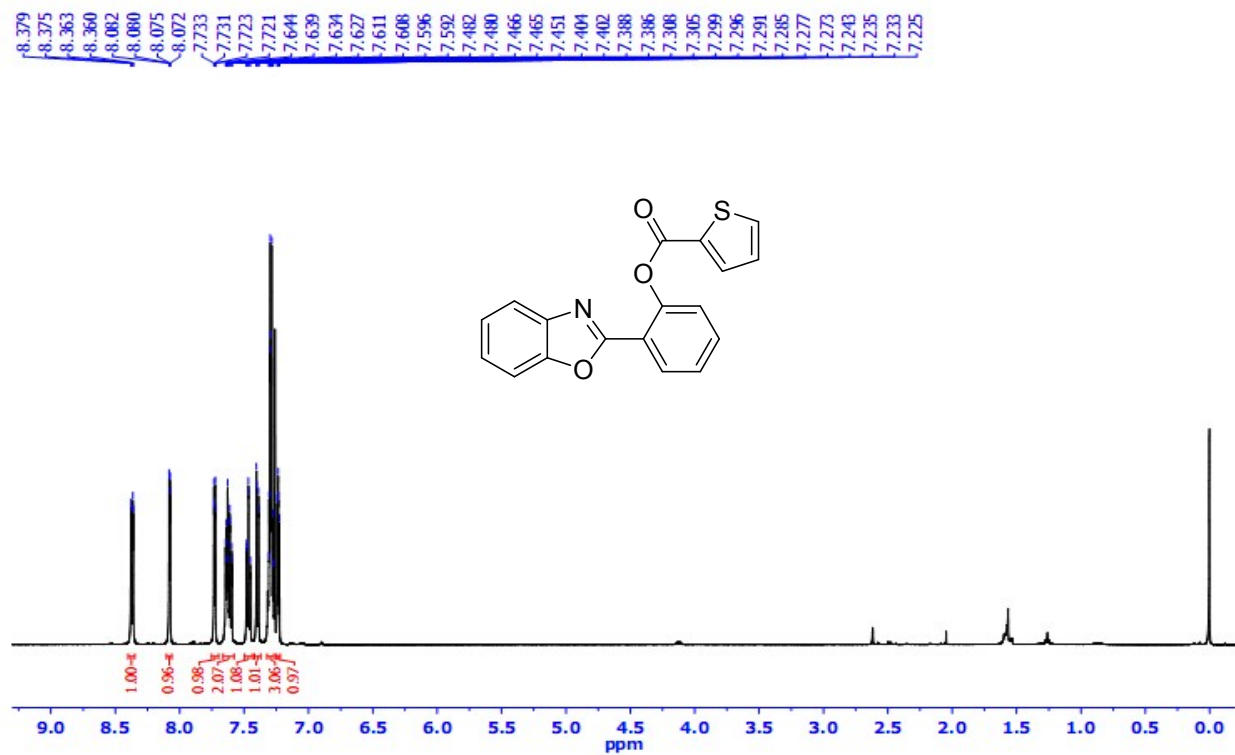
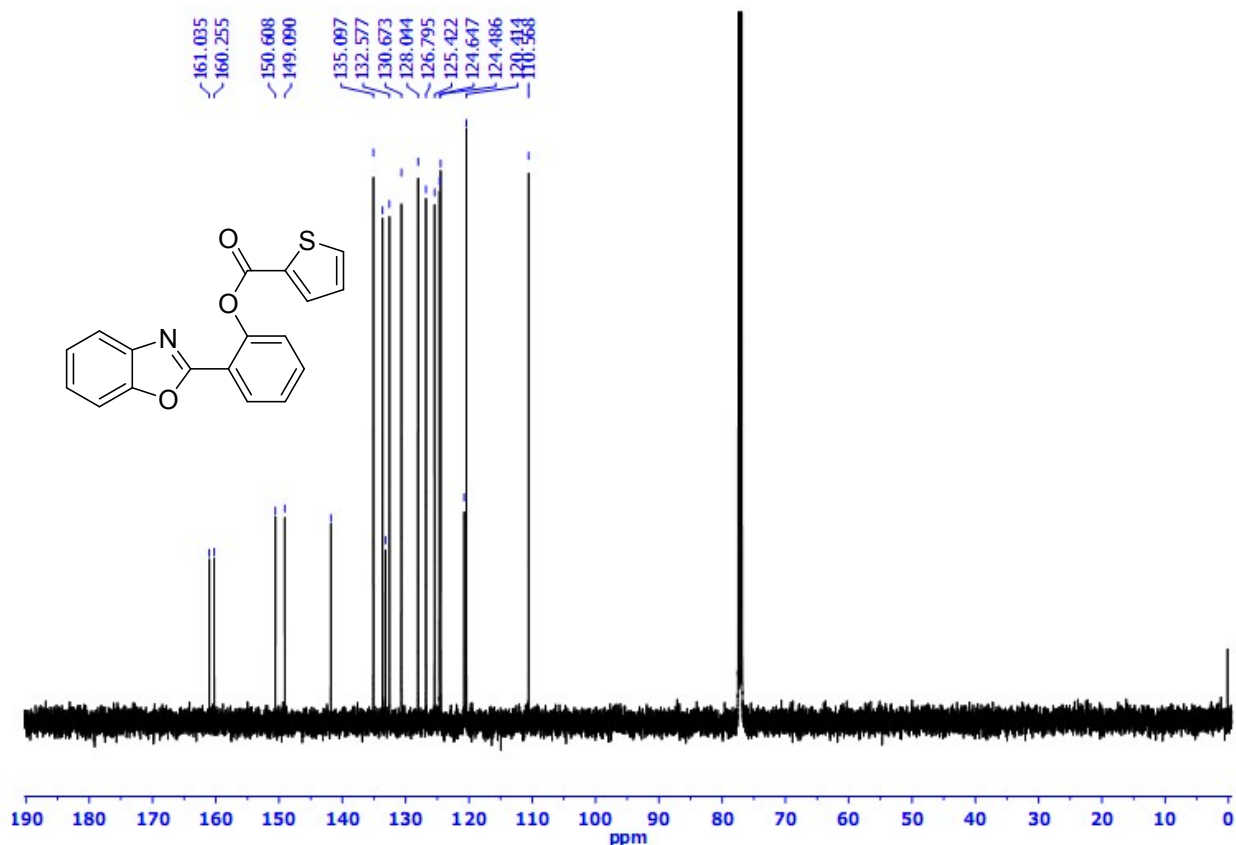


Fig. S31. ¹H-NMR spectra of 2-(benzo[d]oxazol-2-yl)phenyl thiophene-2-carboxylate.



. Fig. S32. ¹³C-NMR spectra of 2-(benzo[d]oxazol-2-yl)phenyl thiophene-2-carboxylate.

Characterization Data for 2-(benzo[d]oxazol-2-yl)phenyl thiophene-2-carboxylate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 9:1): yellow solid, 59 % yield. ¹H NMR (500 MHz, CDCl₃-*d*) δ 8.37 (dd, *J* = 7.9, 1.6 Hz, 1H, *ArH*), 8.08 (dd, *J* = 3.7, 1.2 Hz, 1H, *ArH*), 7.73 (dd, *J* = 5.0, 1.0 Hz, 1H, *ArH*), 7.62 (ddd, *J* = 9.5, 6.5, 2.1 Hz, 2H, *ArH*), 7.49 – 7.44 (m, 1H, *ArH*), 7.39 (dd, *J* = 8.1, 0.9 Hz, 1H, *ArH*), 7.32 – 7.27 (m, 3H, *ArH*), 7.23 (dd, *J* = 4.9, 3.9 Hz, 1H, *ArH*); ¹³C-NMR (125 MHz, CDCl₃-*d*) δ 161.0, 160.2, 150.6, 149.1, 141.8, 135.1, 133.6, 133.2, 132.6, 130.7, 128.0, 126.8, 125.4, 124.6, 124.5, 120.7, 120.4, 110.6.

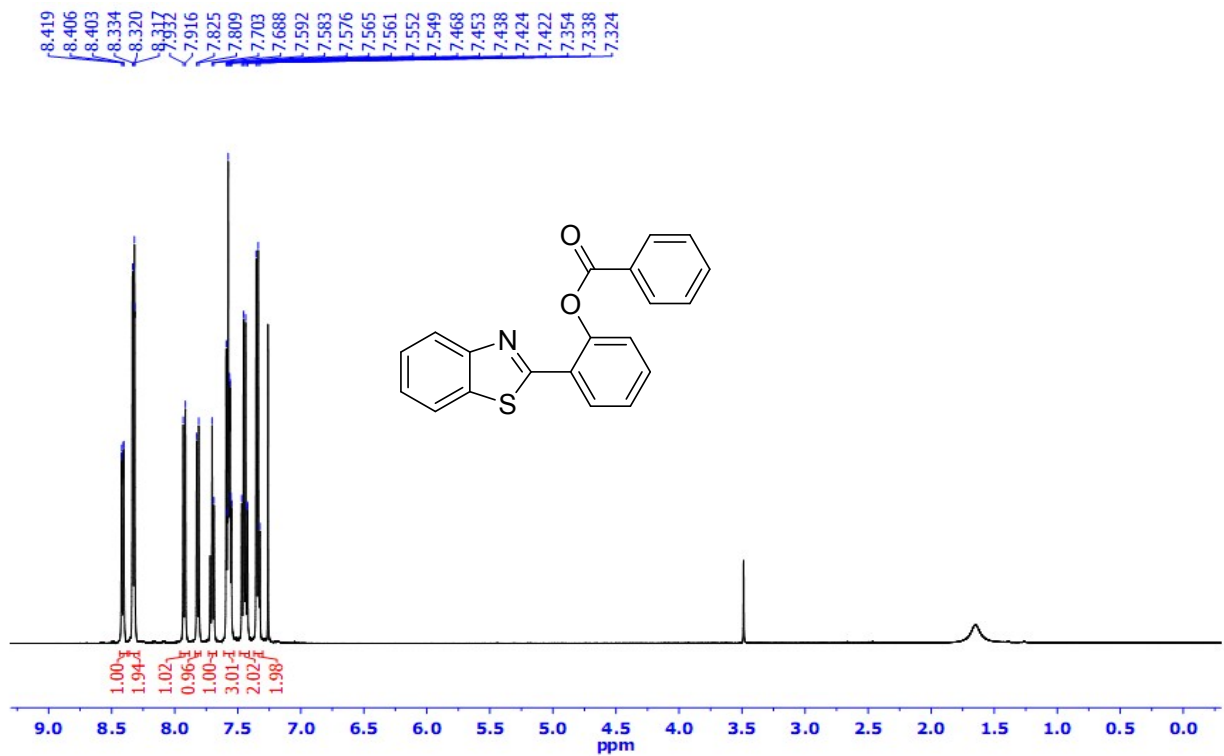


Fig. S33. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

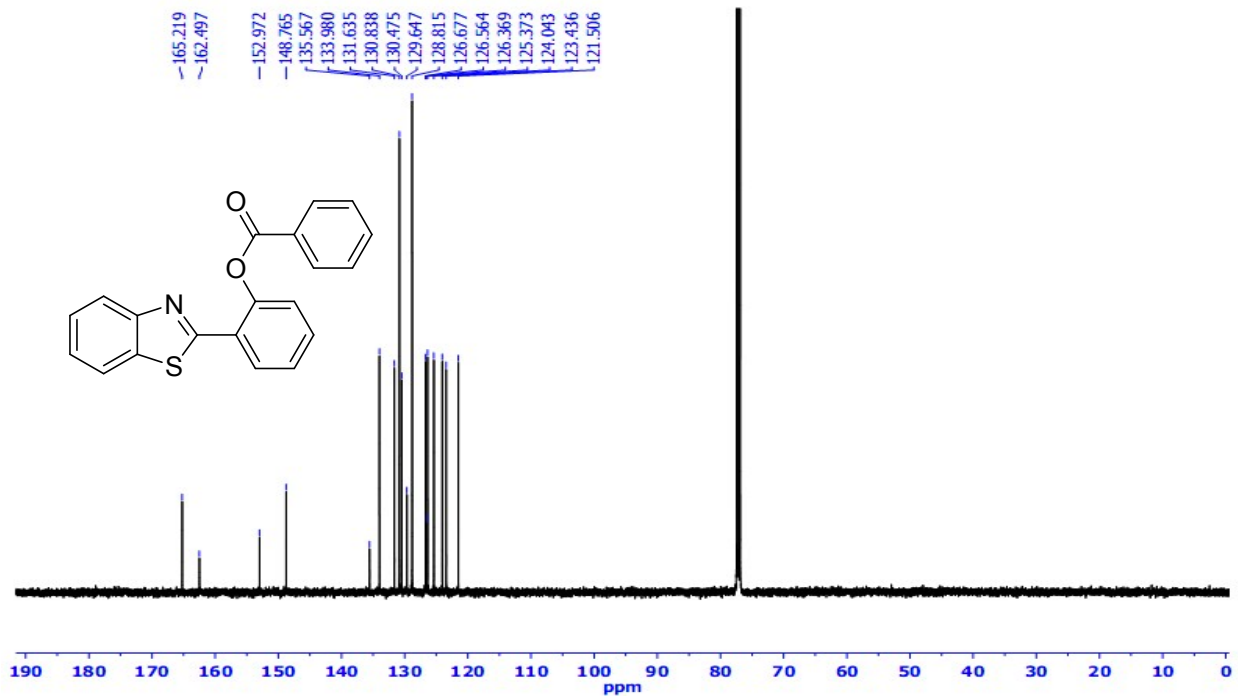


Fig. S34. ¹³C-NMR of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): yellow solid, 60% yield. ¹H-NMR (500 MHz, CDCl₃-*d*) δ 8.41 (dd, *J* = 7.9 Hz, *J* = 1.5 Hz, 1H, Ar*H*), 8.31 – 8.33 (m, 2H, Ar*H*), 7.92 (d, *J* = 8.2 Hz, 1H, Ar*H*), 7.82 (d, *J* = 8.0 Hz, 1H, Ar*H*), 7.69 – 7.70 (m, 1H, Ar*H*), 7.53 – 7.61 (m, 3H, Ar*H*), 7.41 – 7.48 (m, 2H, Ar*H*), 7.32 – 7.35 (m, 2H, Ar*H*); ¹³C-NMR (125 MHz, CDCl₃-*d*) δ 165.2, 162.5, 152.9, 148.8, 135.6, 133.9, 131.6, 130.8, 130.5, 129.7, 128.8, 126.7, 126.6, 126.4, 125.4, 124.0, 123.4, 121.5.

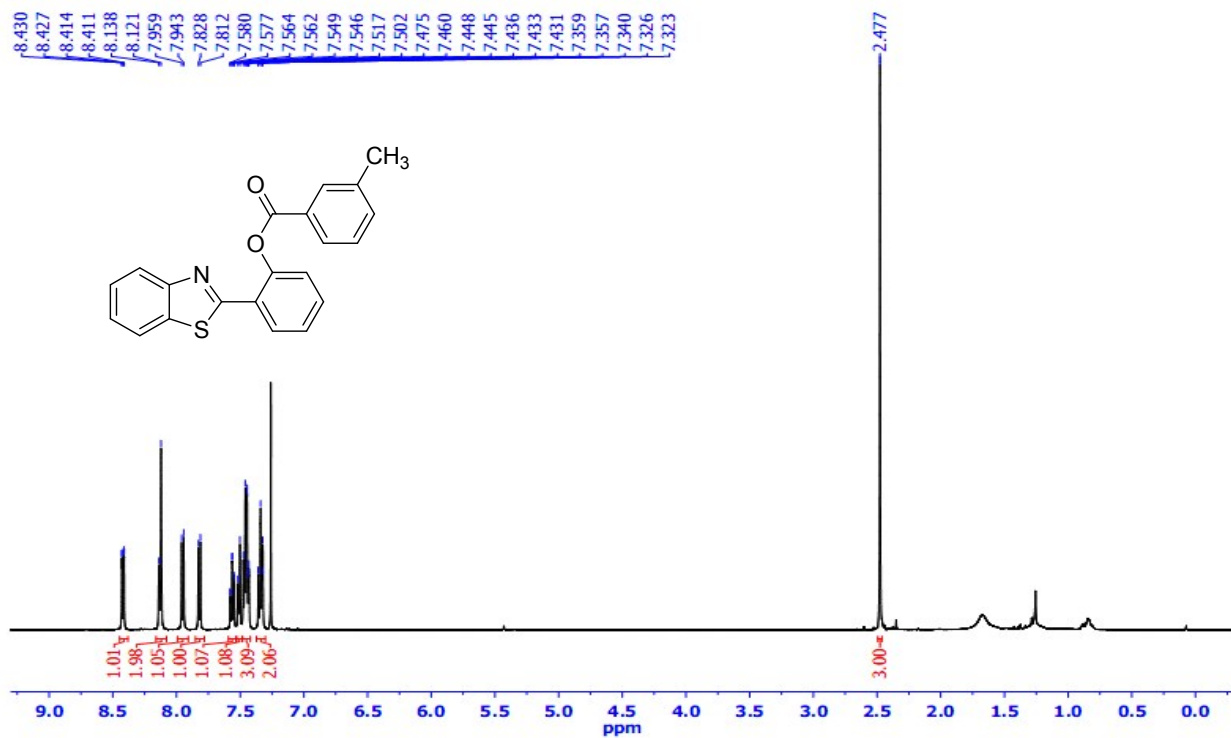


Fig. S35. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 3-methylbenzoate.

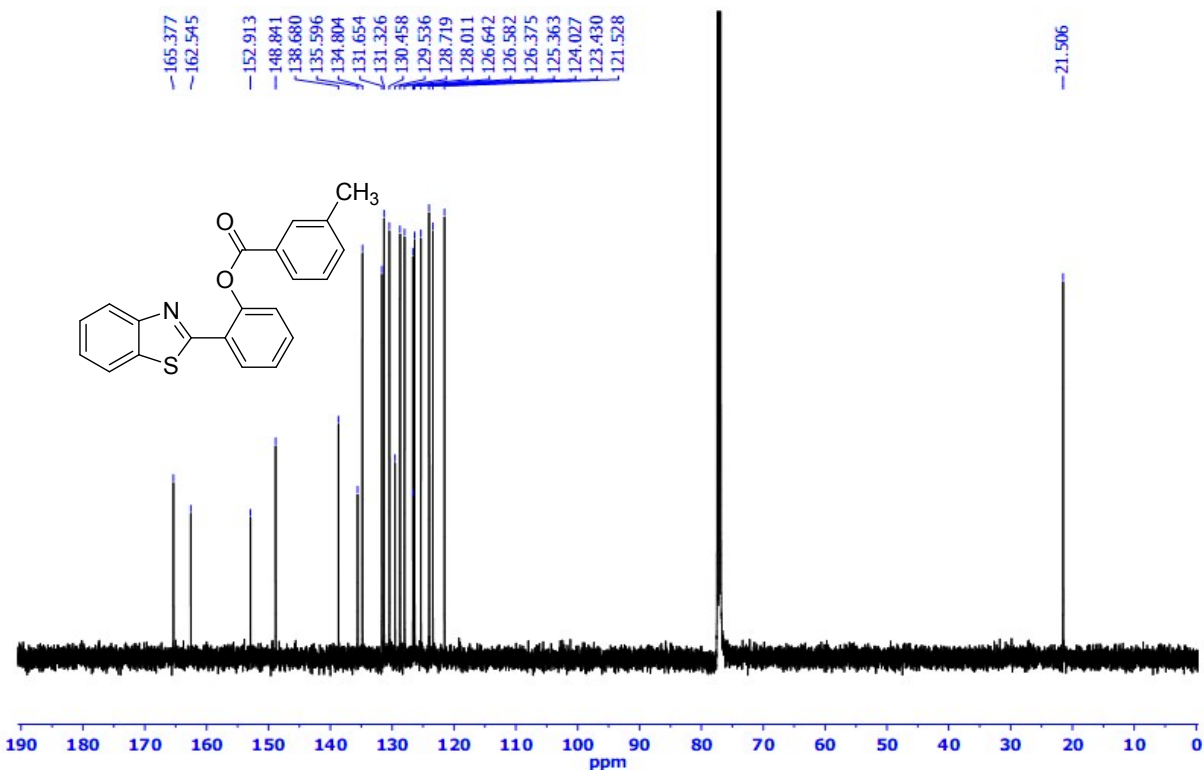


Fig. S36. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 3-methylbenzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl 3-methylbenzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 15:1): white solid, 65% yield. ¹H-NMR (500 MHz, CDCl₃-d) δ 8.42 (dd, *J* = 7.9 Hz, *J* = 1.5 Hz, 1H, ArH), 8.12 – 8.14 (m, 2H, ArH), 7.95 (d, *J* = 8.1 Hz, 1H, ArH), 7.82 (d, *J* = 8.0 Hz, 1H, ArH), 7.55 – 7.58 (m, 1H, ArH), 7.50 – 7.51 (m, 1H, ArH), 7.43 – 7.46 (m, 3H, ArH), 7.32 – 7.36 (m, 2H, ArH), 2.48 (s, 3H, CH₃); ¹³C-NMR (125 MHz, CDCl₃-d) δ 165.4, 162.5, 152.9, 148.8, 138.7, 135.6, 134.8, 131.6, 131.3, 130.5, 129.5, 128.7, 128.0, 126.6, 126.58, 126.4, 125.4, 124.0, 123.4, 121.5, 21.5.

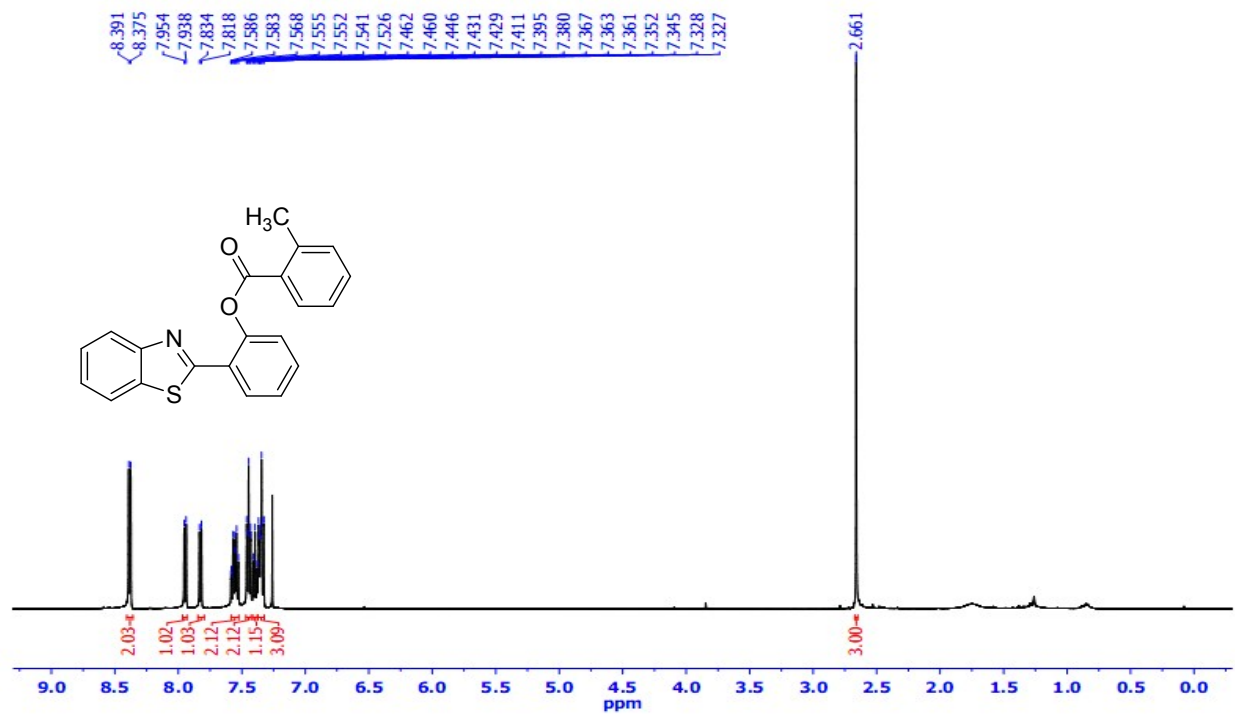


Fig. S37. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 2-methylbenzoate.

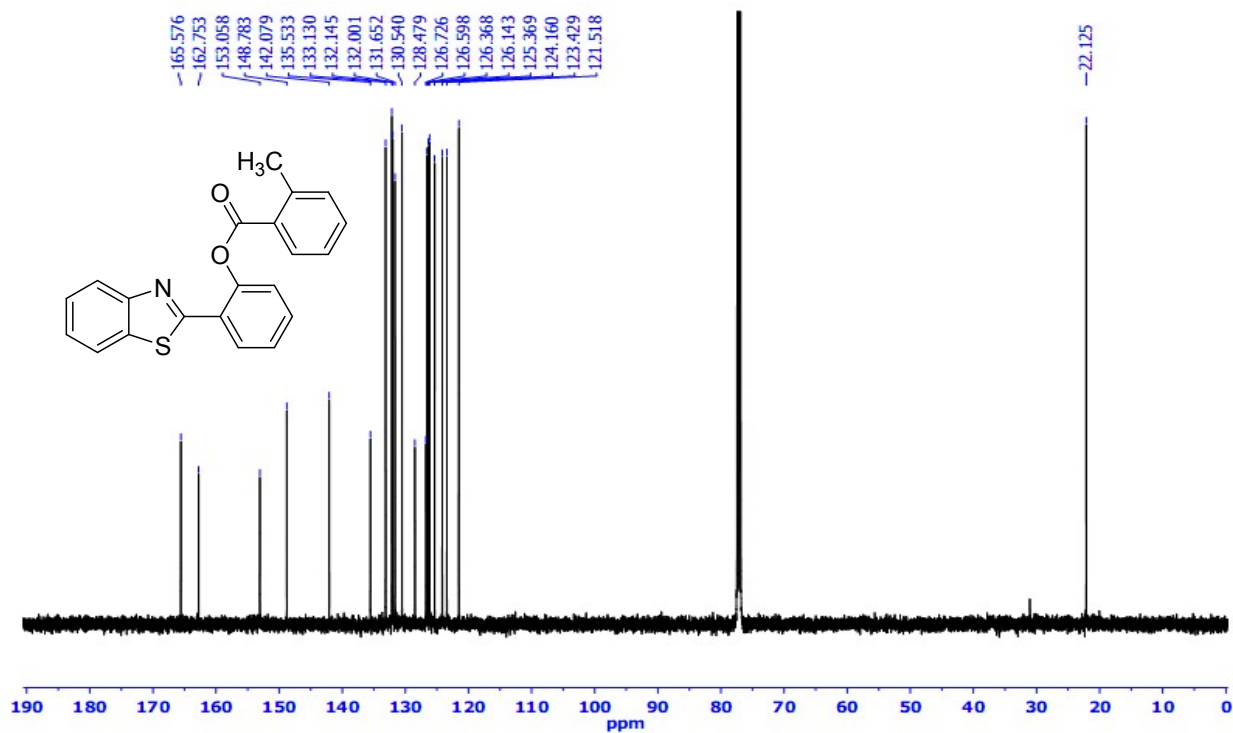


Fig. S38. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 2-methylbenzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl 2-methylbenzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): yellow gummy, 63% yield. ¹H-NMR (500 MHz, CDCl₃-d) δ 8.38 (d, *J* = 7.9 Hz, 2H, Ar*H*), 7.95 (d, *J* = 8.2 Hz, 1H, Ar*H*), 7.82 (d, *J* = 8.0 Hz, 1H, Ar*H*), 7.53 – 7.59 (m, 2H, Ar*H*), 7.43 – 7.46 (m, 2H, Ar*H*), 7.38 – 7.41 (m, 1H, Ar*H*), 7.33 – 7.37 (m, 3H, Ar*H*), 2.66 (s, 3H, CH₃); ¹³C-NMR (125 MHz, CDCl₃-d) δ 165.5, 162.7, 153.1, 148.8, 142.1, 135.5, 133.1, 132.1, 132.00, 131.6, 130.5, 128.5, 126.7, 126.6, 126.4, 126.1, 125.4, 124.2, 123.4, 121.5, 22.1.

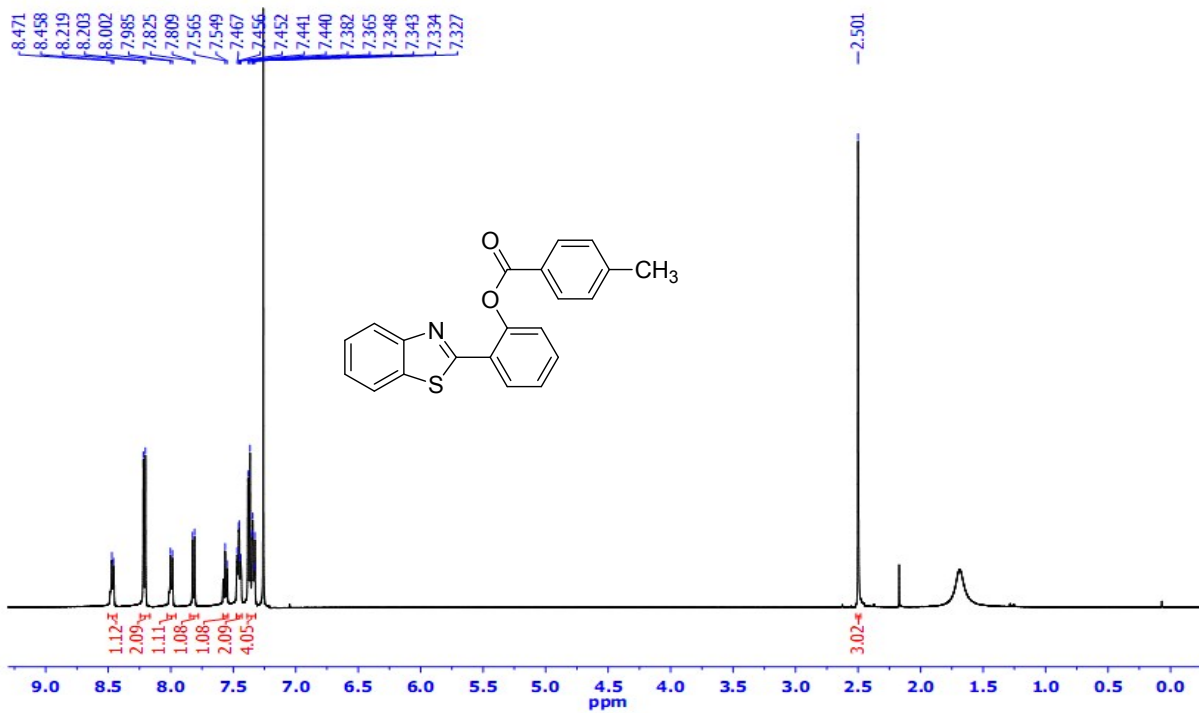


Fig. S39. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 4-methylbenzoate.

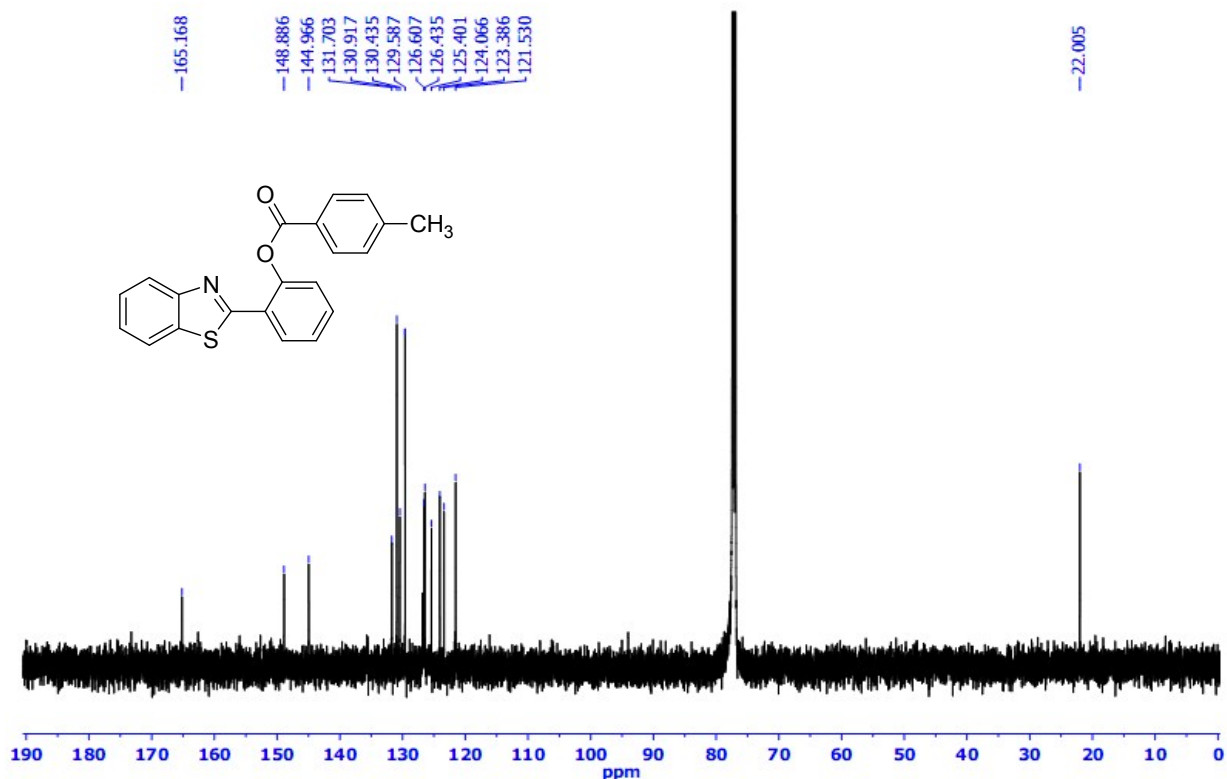


Fig. S40. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 4-methylbenzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl 4-methylbenzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): white solid, 75% yield. ¹H-NMR (500 MHz, CDCl₃-*d*) δ 8.46 – 8.47 (m, 1H, ArH), 8.21 (d, *J* = 8.2 Hz, 2H, ArH), 7.99 (d, *J* = 8.0 Hz, 1H, ArH), 7.82 (d, *J* = 8.0 Hz, 1H, ArH), 7.55 – 7.57 (m, 1H, ArH), 7.44 – 7.47 (m, 2H, ArH), 7.33 – 7.38 (m, 4H, ArH), 2.50 (s, 3H, CH₃); ¹³C-NMR (125 MHz, CDCl₃-*d*) δ 165.2, 148.9, 144.9, 131.7, 130.9, 130.4, 129.6, 126.6, 126.4, 125.4, 124.2, 123.4, 121.5, 22.0.

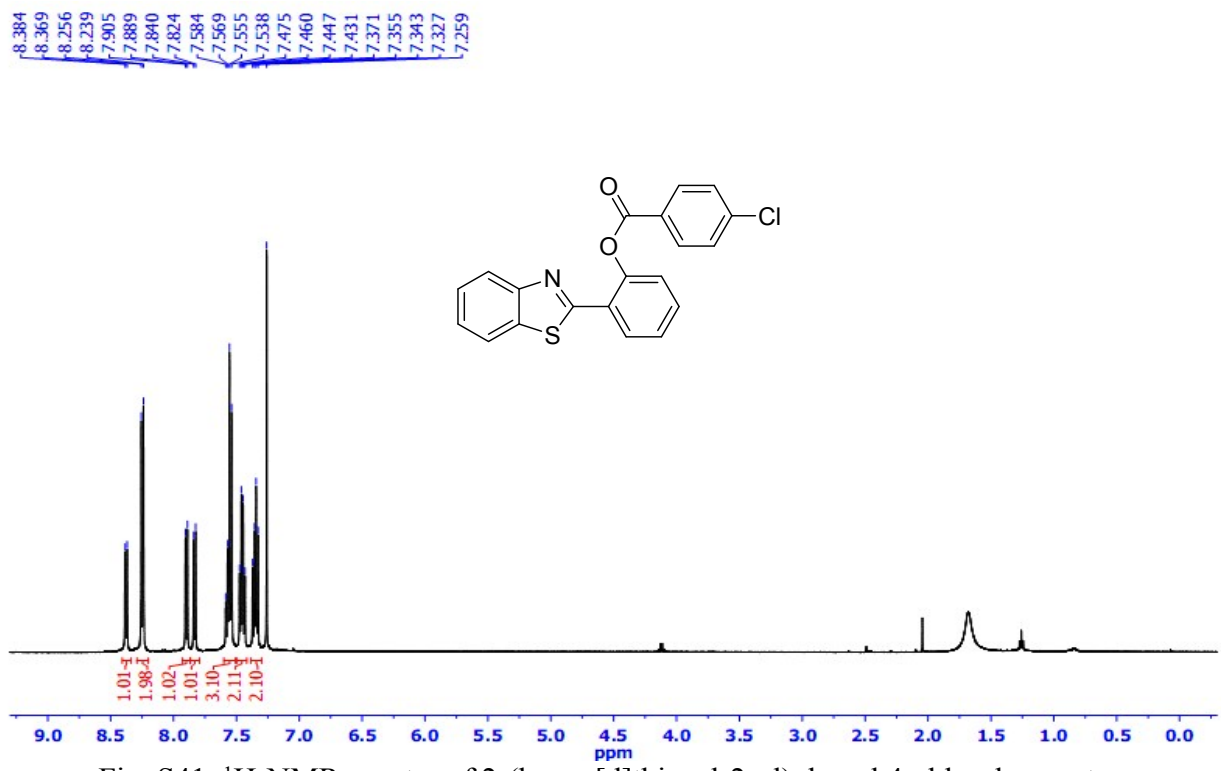


Fig. S41. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 4-chlorobenzoate.

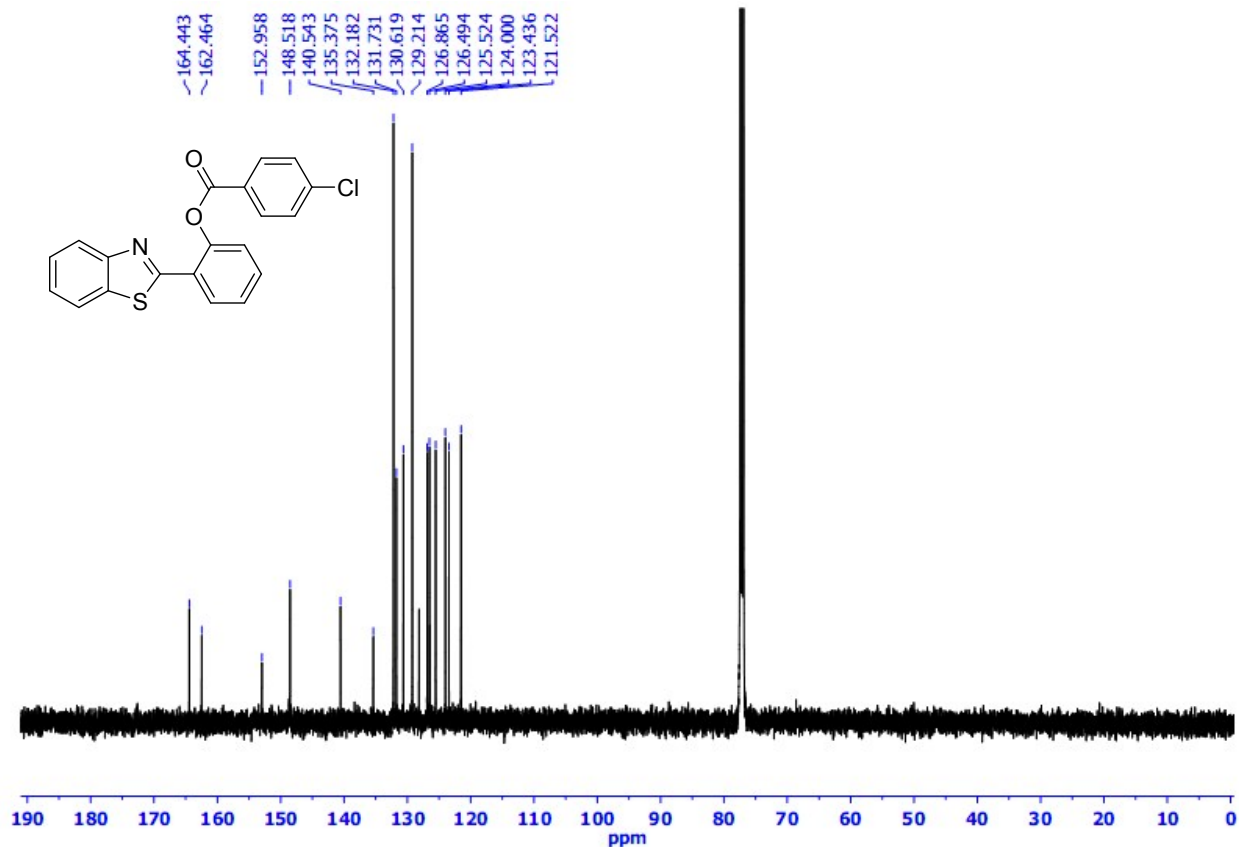


Fig. S42. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl 4-chlorobenzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl 4-chlorobenzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): white solid, 66% yield. ¹H-NMR (500 MHz, CDCl₃-*d*) δ 8.38 (d, *J* = 7.9 Hz, 1H, ArH), 8.25 (d, *J* = 8.4 Hz, 2H, ArH), 7.90 (d, *J* = 8.2 Hz, 1H, ArH), 7.83 (d, *J* = 8.0 Hz, 1H), 7.54 – 7.58 (m, 3H, ArH), 7.43 – 7.48 (m, 2H, ArH), 7.33- 7.37 (m, 2H, ArH).; ¹³C-NMR (125 MHz, CDCl₃-*d*) δ 164.4, 162.5, 152.9, 148.5, 140.5, 135.4, 132.2, 131.7, 130.6, 129.2, 126.9, 126.5, 125.5, 124.0, 123.4, 121.5.

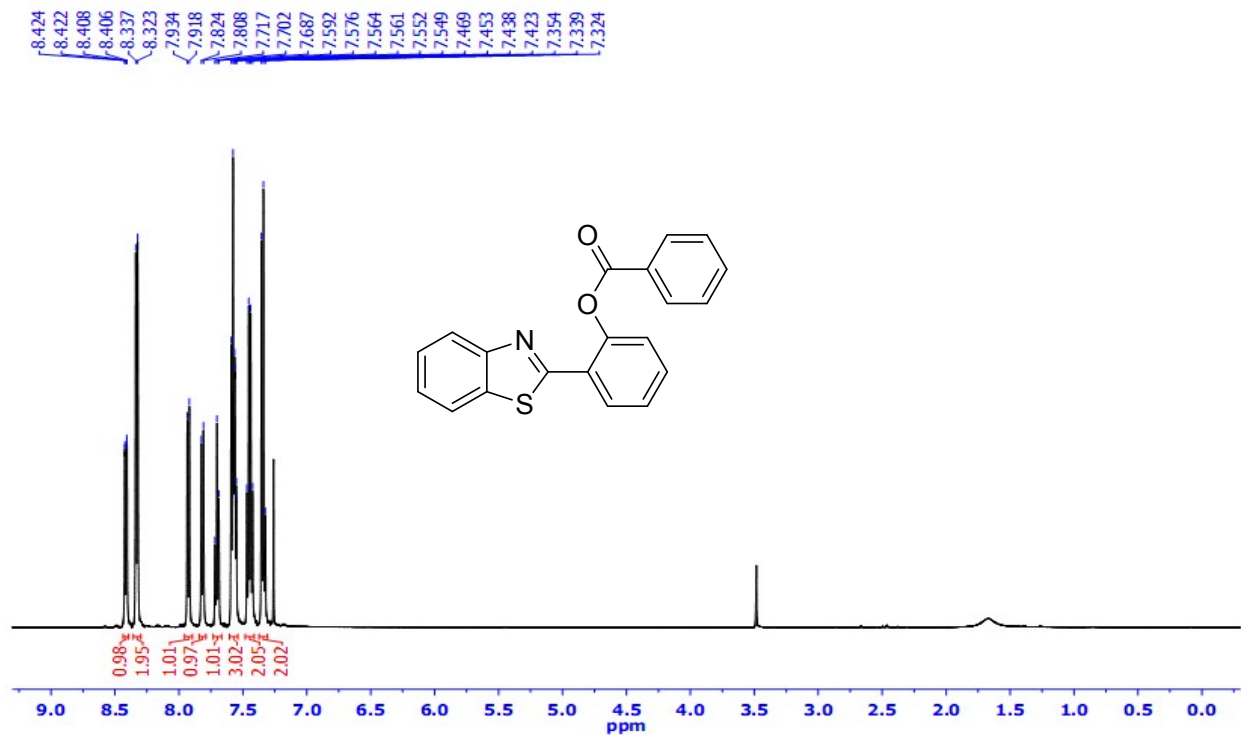


Fig. S43. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

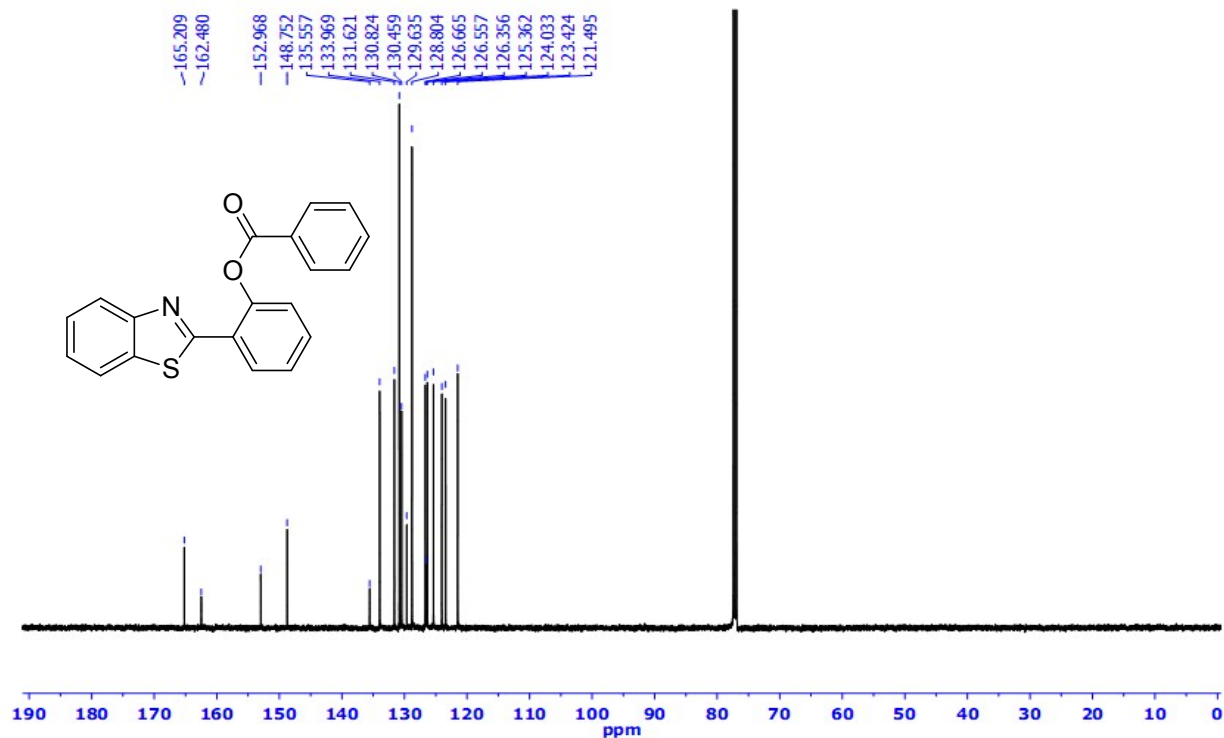


Fig. S44. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl benzoate

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): yellow solid, 60% yield. ¹H-NMR (500 MHz, CDCl₃-*d*) δ 8.41 (dd, *J* = 7.9 Hz, *J* = 1.2 Hz, 1H, ArH), 8.33 (d, *J* = 7.4 Hz, 2H, ArH), 7.93 (d, *J* = 8.2 Hz, 1H, ArH), 7.82 (d, *J* = 8.0 Hz, 1H, ArH), 7.69 – 7.71 (m, 1H, ArH), 7.55 – 7.59 (m, 3H, ArH), 7.42 – 7.47 (m, 2H, ArH), 7.32 – 7.35 (m, 2H, ArH); ¹³C-NMR (125 MHz, CDCl₃-*d*) δ 165.2, 162.5, 152.9, 148.8, 135.6, 133.9, 131.6, 130.8, 130.5, 129.3, 128.8, 126.7, 126.6, 126.4, 125.4, 124.0, 123.4, 121.5.

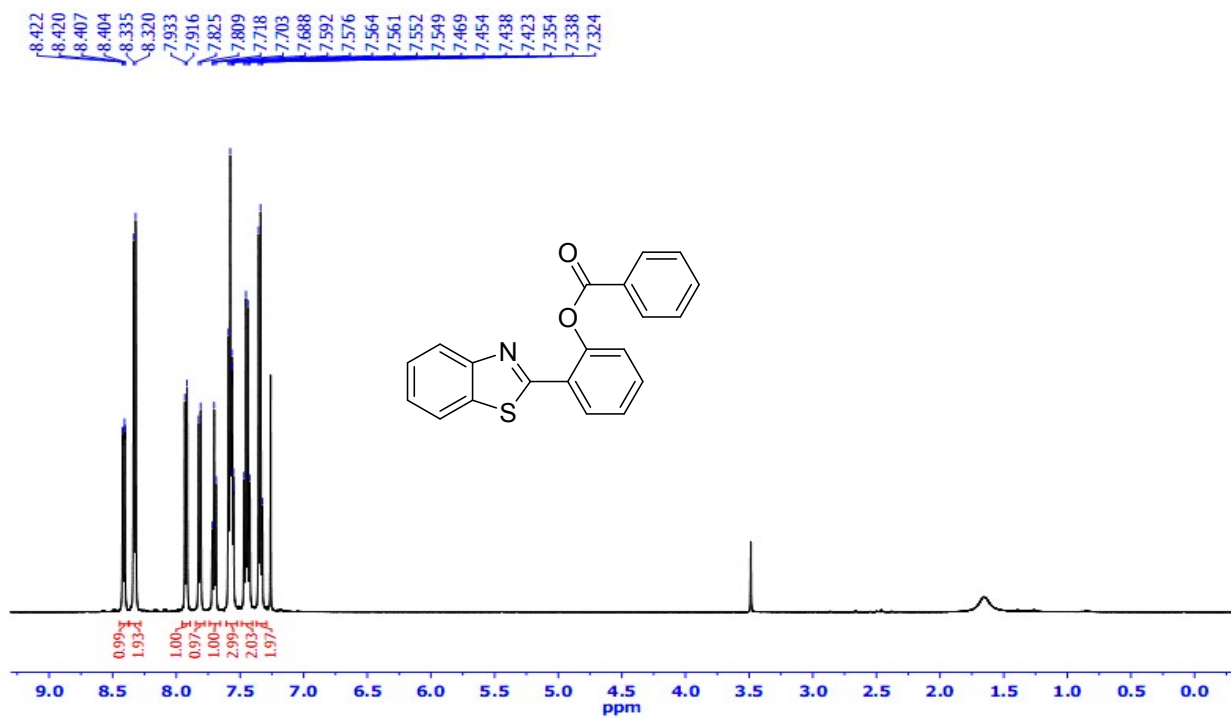


Fig. S45. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

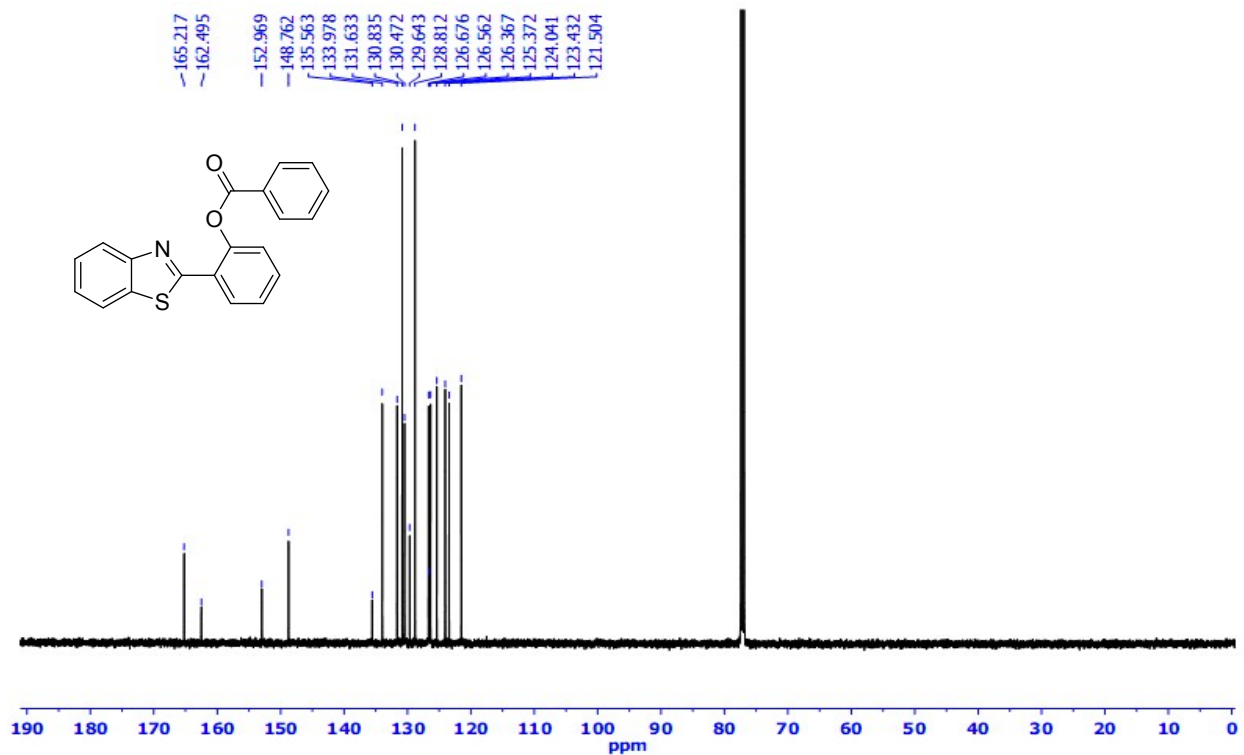


Fig. S46. ¹³C-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl benzoate

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): yellow solid, 73% yield. ¹H-NMR (500 MHz, CDCl₃-*d*) δ 8.41 (dd, *J* = 7.9 Hz, *J* = 1.3 Hz, 1H, ArH), 8.33 (d, *J* = 7.4 Hz, 2H, ArH), 7.92 (d, *J* = 8.2 Hz, 1H, ArH), 7.82 (d, *J* = 8.0 Hz, 1H, ArH), 7.69 – 7.72 (m, 1H, ArH), 7.55 – 7.59 (m, 3H, ArH), 7.42 – 7.47 (m, 2H, ArH), 7.32 – 7.35 (m, 2H, ArH); ¹³C-NMR (125 MHz, CDCl₃-*d*) δ 165.2, 162.5, 152.9, 148.8, 135.6, 133.9, 131.6, 130.8, 130.5, 129.6, 128.8, 126.7, 126.6, 126.4, 125.4, 124.0, 123.4, 121.5.

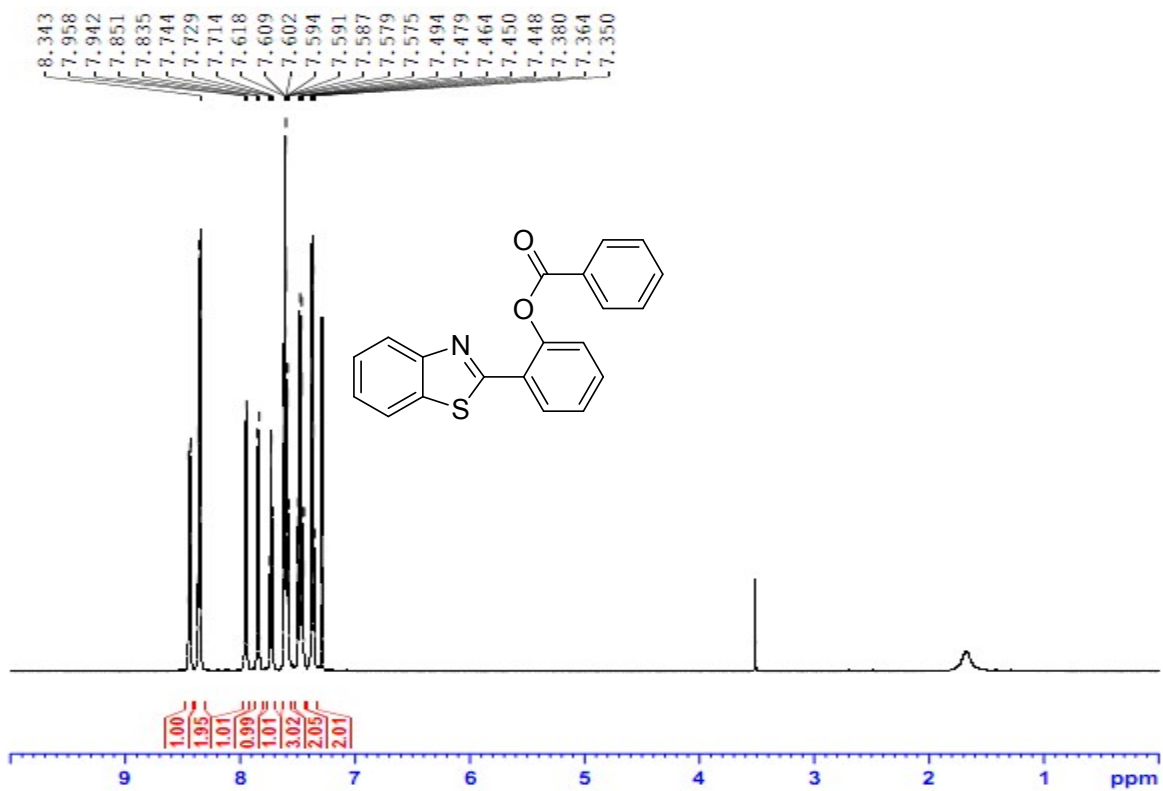


Fig. S47. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

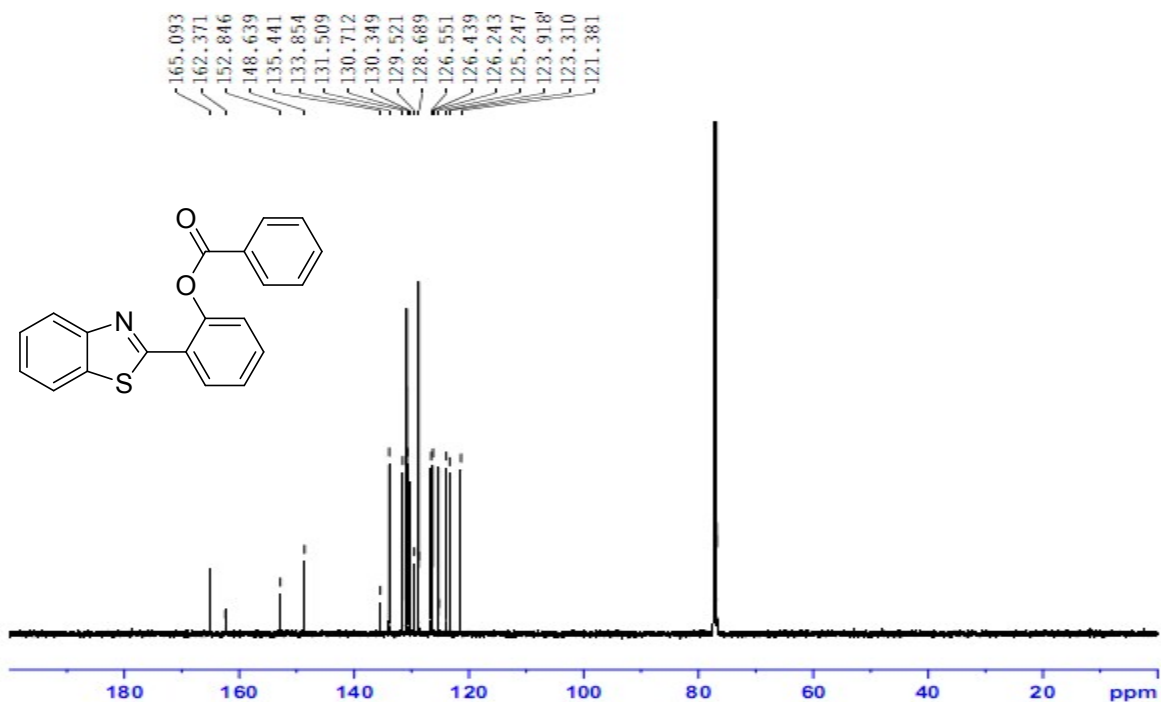


Fig. S48. ^{13}C -NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): yellow solid, 75% yield. ^1H -NMR (500 MHz, CDCl_3 -*d*) δ 8.43 (dd, $J = 8.0$ Hz, $J = 1.5$ Hz, 1H, ArH), 8.34 – 8.36 (m, 2H, ArH), 7.94 (d, $J = 8.2$ Hz, 1H, ArH), 7.84 (d, $J = 8.0$ Hz, 1H, ArH), 7.71 – 7.74 (m, 1H, ArH), 7.57 – 7.62 (m, 3H, ArH), 7.45 – 7.49 (m, 2H, ArH), 7.35 – 7.38 (m, 2H, ArH); ^{13}C -NMR (125 MHz, CDCl_3 -*d*) δ 165.2, 162.5, 152.9, 148.8, 135.6, 133.9, 131.6, 130.8, 130.5, 129.7, 128.8, 126.7, 126.6, 126.4, 125.4, 124.0, 123.4, 121.5.

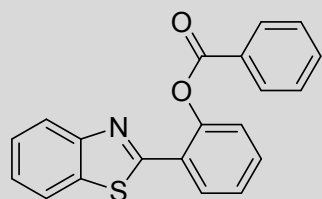


Fig. S49. ¹H-NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

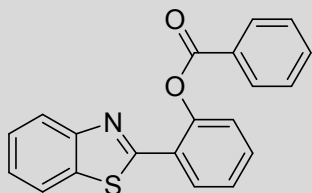


Fig. S50. ^{13}C -NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl benzoate

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): yellow solid, 69% yield. ^1H -NMR (500 MHz, CDCl_3 -*d*) δ 8.41 (dd, $J = 7.9$ Hz, $J = 1.2$ Hz, 1H, ArH), 8.33 (d, $J = 7.4$ Hz, 2H, ArH), 7.93 (d, $J = 8.2$ Hz, 1H, ArH), 7.82 (d, $J = 8.0$ Hz, 1H, ArH), 7.69 – 7.71 (m, 1H, ArH), 7.55 – 7.59 (m, 3H, ArH), 7.42 – 7.47 (m, 2H, ArH), 7.32 – 7.35 (m, 2H, ArH); ^{13}C -NMR (125 MHz, CDCl_3 -*d*) δ 165.2, 162.5, 152.9, 148.8, 135.6, 133.9, 131.6, 130.8, 130.5, 129.3, 128.8, 126.7, 126.6, 126.4, 125.4, 124.0, 123.4, 121.5.

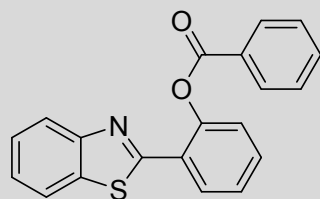


Fig. S51. $^1\text{H-NMR}$ spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

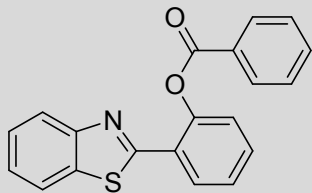


Fig. S52. ^{13}C -NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl benzoate

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): yellow solid, 80% yield. ^1H -NMR (500 MHz, CDCl_3 -*d*) δ 8.41 (dd, $J = 7.9$ Hz, $J = 1.2$ Hz, 1H, *ArH*), 8.33 (d, $J = 7.4$ Hz, 2H, *ArH*), 7.93 (d, $J = 8.2$ Hz, 1H, *ArH*), 7.82 (d, $J = 8.0$ Hz, 1H, *ArH*), 7.69 – 7.71 (m, 1H, *ArH*), 7.55 – 7.59 (m, 3H, *ArH*), 7.42 – 7.47 (m, 2H, *ArH*), 7.32 – 7.35 (m, 2H, *ArH*); ^{13}C -NMR (125 MHz, CDCl_3 -*d*) δ 165.2, 162.5, 152.9, 148.8, 135.6, 133.9, 131.6, 130.8, 130.5, 129.3, 128.8, 126.7, 126.6, 126.4, 125.4, 124.0, 123.4, 121.5.

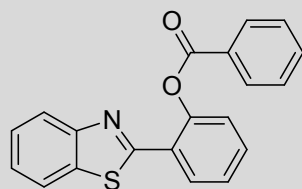


Fig. S53. $^1\text{H-NMR}$ spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

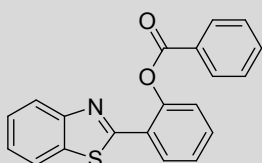


Fig. S54. ^{13}C -NMR spectra of 2-(benzo[d]thiazol-2-yl)phenyl benzoate.

Characterization Data for 2-(benzo[d]thiazol-2-yl)phenyl benzoate

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): yellow solid, 68% yield. ^1H -NMR (500 MHz, CDCl_3 -*d*) δ 8.41 (dd, $J = 7.9$ Hz, $J = 1.3$ Hz, 1H, ArH), 8.33 (d, $J = 7.4$ Hz, 2H, ArH), 7.92 (d, $J = 8.2$ Hz, 1H, ArH), 7.82 (d, $J = 8.0$ Hz, 1H, ArH), 7.69 – 7.72 (m, 1H, ArH), 7.55 – 7.59 (m, 3H, ArH), 7.42 – 7.47 (m, 2H, ArH), 7.32 – 7.35 (m, 2H, ArH); ^{13}C -NMR (125 MHz, CDCl_3 -*d*) δ 165.2, 162.5, 152.9, 148.8, 135.6, 133.9, 131.6, 130.8, 130.5, 129.6, 128.8, 126.7, 126.6, 126.4, 125.4, 124.0, 123.4, 121.5.

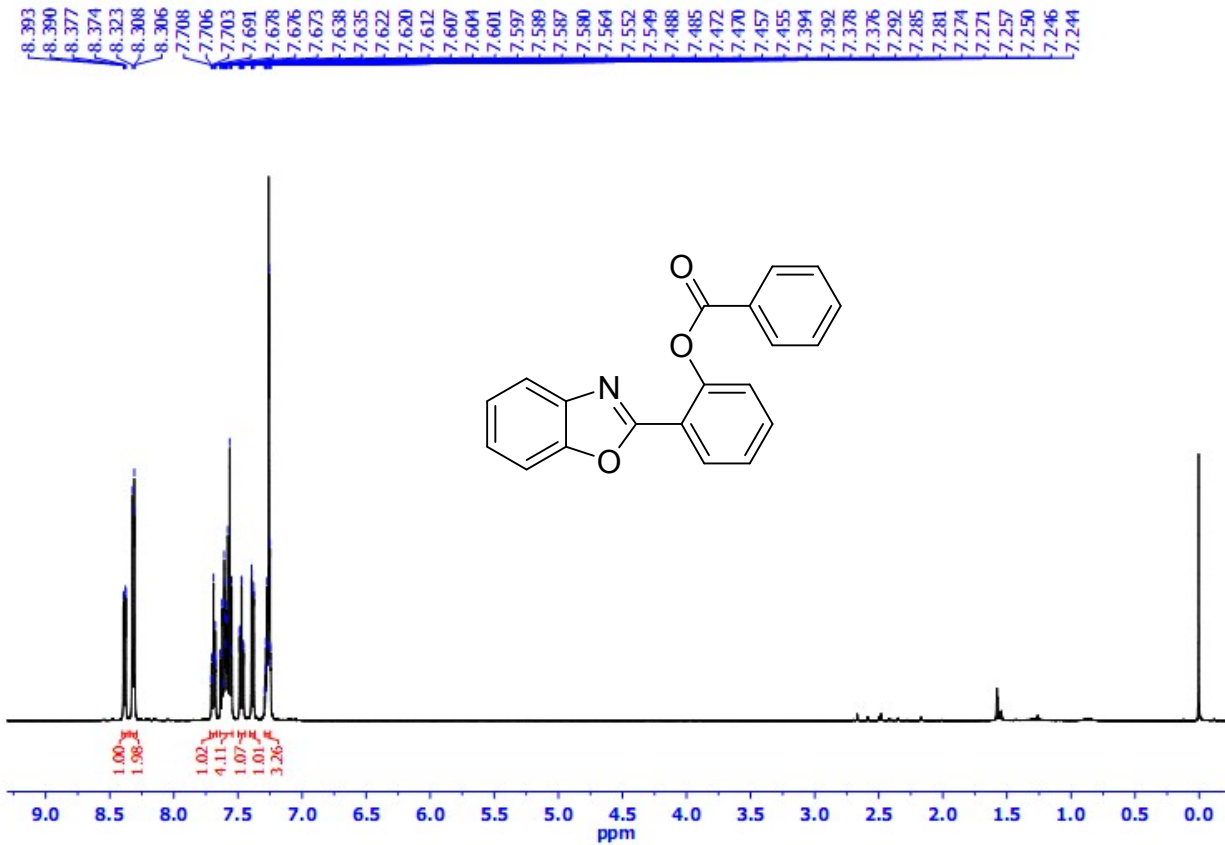


Fig. S55. ¹H-NMR spectra of 2-(benzo[d]oxazol-2-yl)phenyl benzoate.

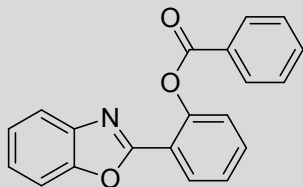
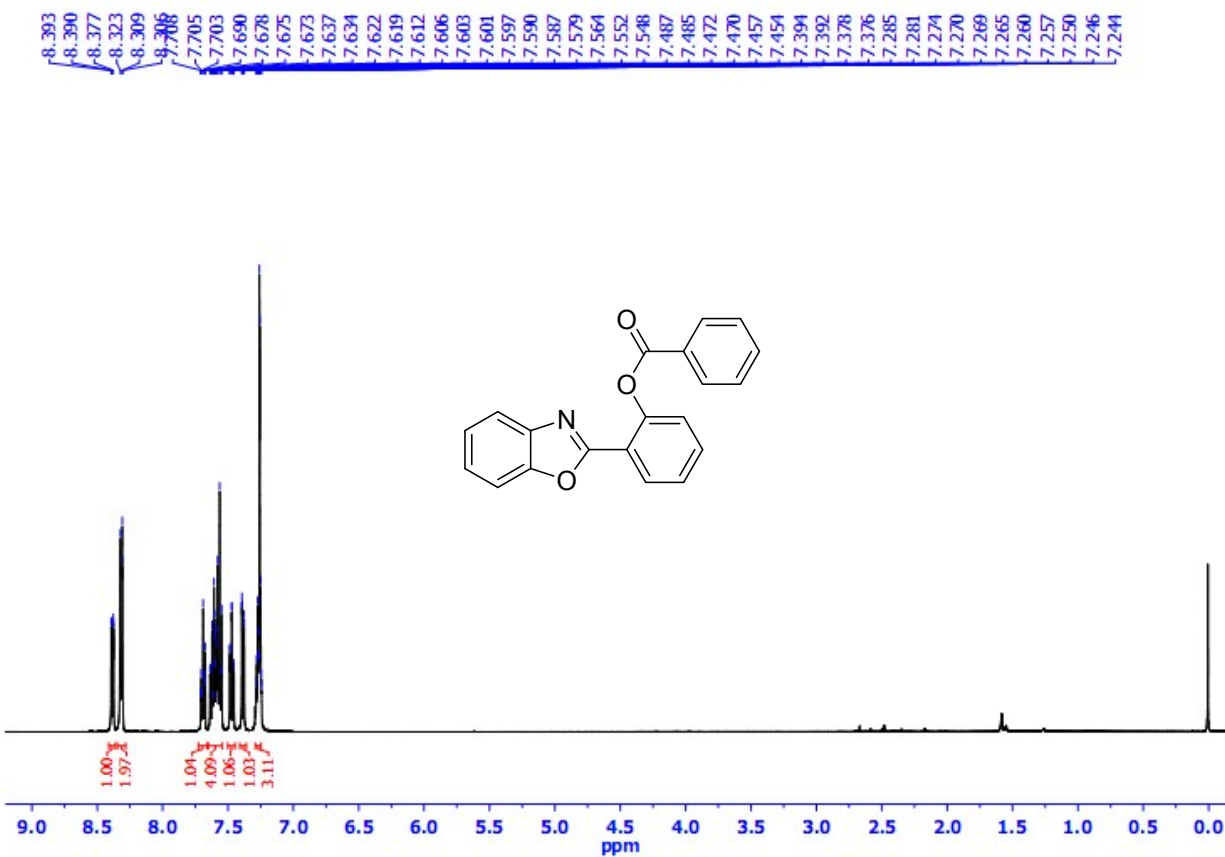


Fig. S56. ^{13}C -NMR spectra of 2-(benzo[d]oxazol-2-yl)phenyl benzoate.

Characterization Data for 2-(benzo[d]oxazol-2-yl)phenyl benzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): white solid, 51% yield. ^1H NMR (500 MHz, CDCl_3 -*d*) δ 8.38 (dd, $J = 7.9, 1.6$ Hz, 1H, ArH), 8.34 – 8.29 (m, 2H, ArH), 7.72 – 7.67 (m, 1H, ArH), 7.64 – 7.54 (m, 4H, ArH), 7.47 (td, $J = 7.7, 1.1$ Hz, 1H, ArH), 7.39 (dd, $J = 8.1, 0.9$ Hz, 1H, ArH), 7.29 – 7.25 (m, 3H, ArH); ^{13}C -NMR (125 MHz, CDCl_3 -*d*) δ 165.8, 160.3, 150.5, 149.6, 141.8, 133.6, 132.6, 130.7, 130.6, 130.0, 128.6, 126.7, 125.4, 124.6, 124.5, 120.7, 120.4, 110.5.



S57. ¹H-NMR spectra of 2-(benzo[d]oxazol-2-yl)phenyl benzoate

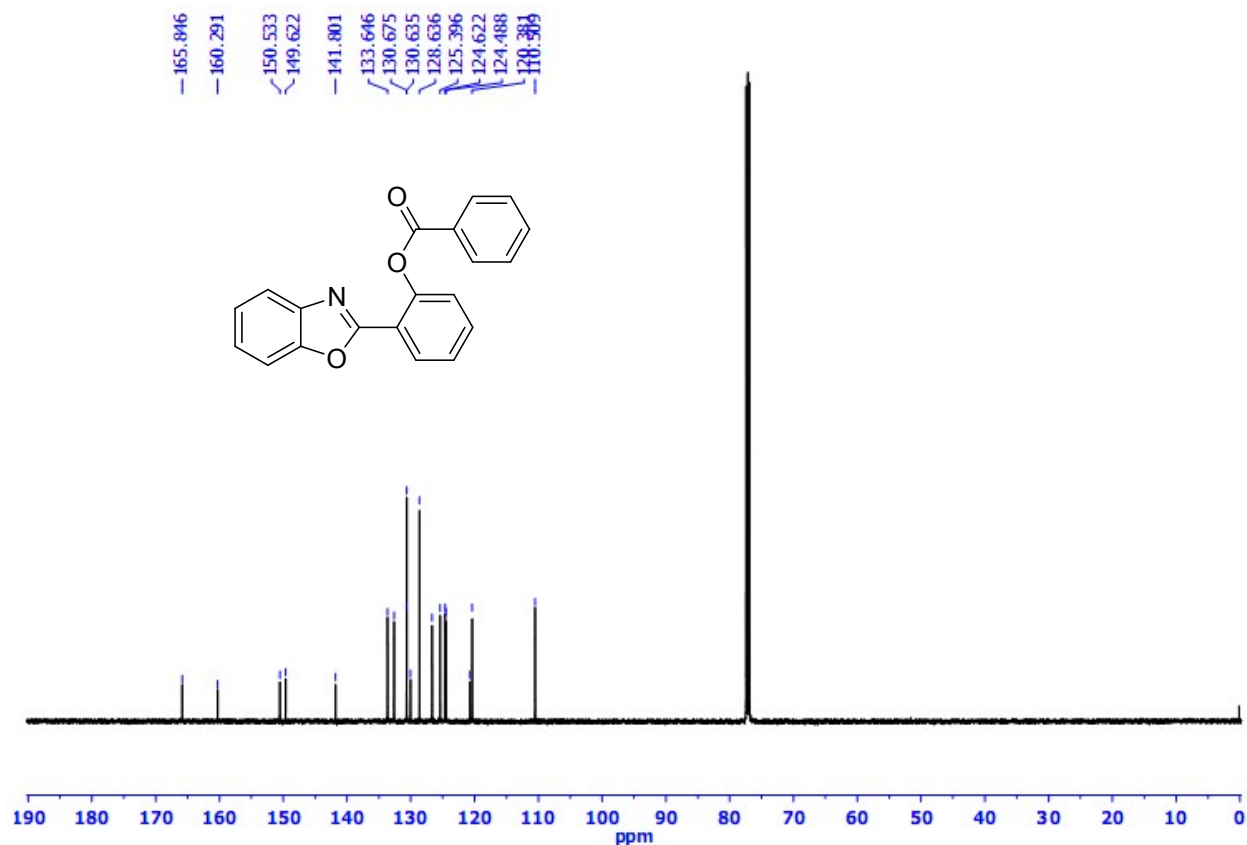


Fig. S58. ¹³C-NMR spectra of 2-(benzo[d]oxazol-2-yl)phenyl benzoate.

Characterization Data for 2-(benzo[d]oxazol-2-yl)phenyl benzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): white solid, 52% yield. ¹H NMR (500 MHz, CDCl₃-d) 8.38 (dd, *J* = 7.9, 1.6 Hz, 1H, ArH), 8.35 – 8.28 (m, 2H, ArH), 7.73 – 7.66 (m, 1H, ArH), 7.65 – 7.54 (m, 4H, ArH), 7.47 (td, *J* = 7.7, 1.1 Hz, 1H, ArH), 7.39 (dd, *J* = 8.1, 0.9 Hz, 1H, ArH), 7.27 (m, 3H, ArH).; ¹³C-NMR (125 MHz, CDCl₃-d) δ 165.8, 160.3, 150.5, 149.6, 141.8, 133.6, 132.6, 130.7, 130.6, 130.0, 128.6, 126.7, 125.4, 124.6, 124.5, 120.7, 120.4, 110.5.

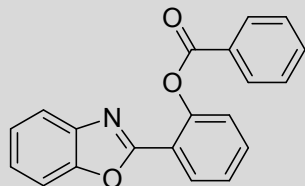


Fig. S59. ¹H-NMR spectra of 2-(benzo[d]oxazol-2-yl)phenyl benzoate.

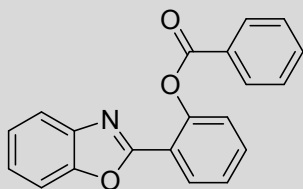


Fig. S60. ^{13}C -NMR spectra of 2-(benzo[d]oxazol-2-yl)phenyl benzoate.

Characterization Data for 2-(benzo[d]oxazol-2-yl)phenyl benzoate.

Prepared as shown in the general experimental procedure and purified on silica gel (hexane/ethyl acetate = 10:1): white solid, 60% yield. ^1H NMR (500 MHz, CDCl_3-d) δ 8.39 (d, $J = 7.4$ Hz, 1H, ArH), 8.32 (d, $J = 7.5$ Hz, 2H, ArH), 7.69 (t, $J = 7.4$ Hz, 1H, ArH), 7.65 – 7.54 (m, 4H, ArH), 7.47 (t, $J = 7.5$ Hz, 1H, ArH), 7.39 (d, $J = 8.0$ Hz, 1H, ArH), 7.28 (s, 3H, ArH); ^{13}C -NMR (125 MHz, CDCl_3-d) δ 165.8, 160.3, 150.5, 149.6, 141.8, 133.6, 132.6, 130.7, 130.6, 130.0, 128.6, 126.7, 125.4, 124.6, 124.5, 120.7, 120.4, 110.5.

