Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Copper-Catalyzed Oxidative Coupling of Arylboronic Acids with Aryl Carboxylic Acids: $Cu_3(BTC)_2$ MOF as a Sustainable Catalyst to Access Aryl Esters

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1. Characterization of $Cu_3(BTC)_2$ MOF Catalysts:[1]

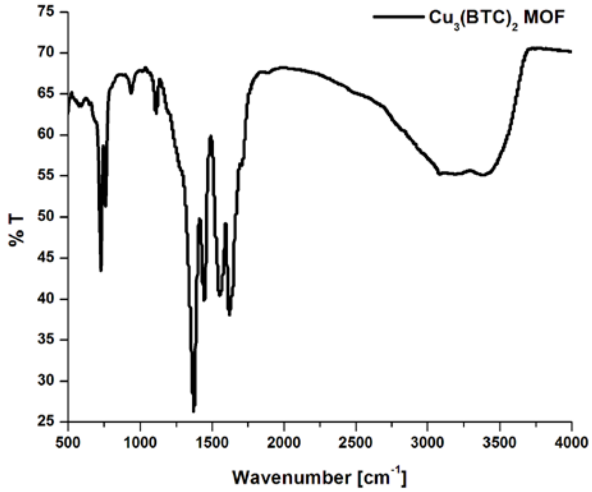


Figure S1 FT-IR spectrum of $Cu_3(BTC)_2$ MOF

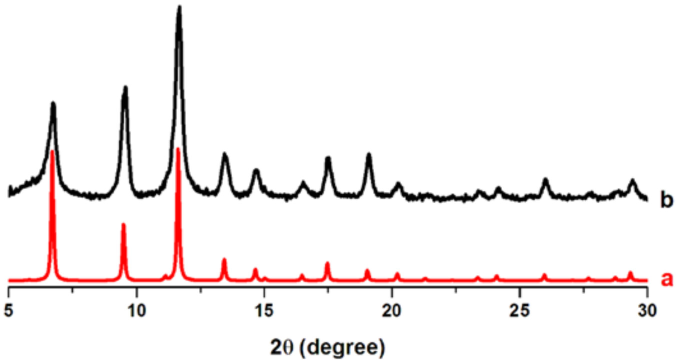


Figure S2 Powder XRD pattern of simulated (a) and as-synthesized $Cu_3(BTC)_2$ MOF (b)

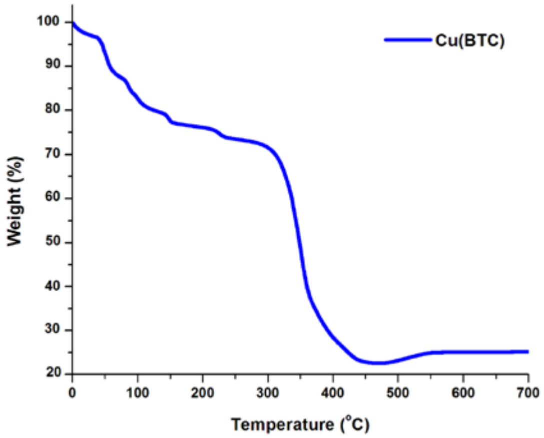


Figure S3 TGA analysis of $Cu_3(BTC)_2$ MOF

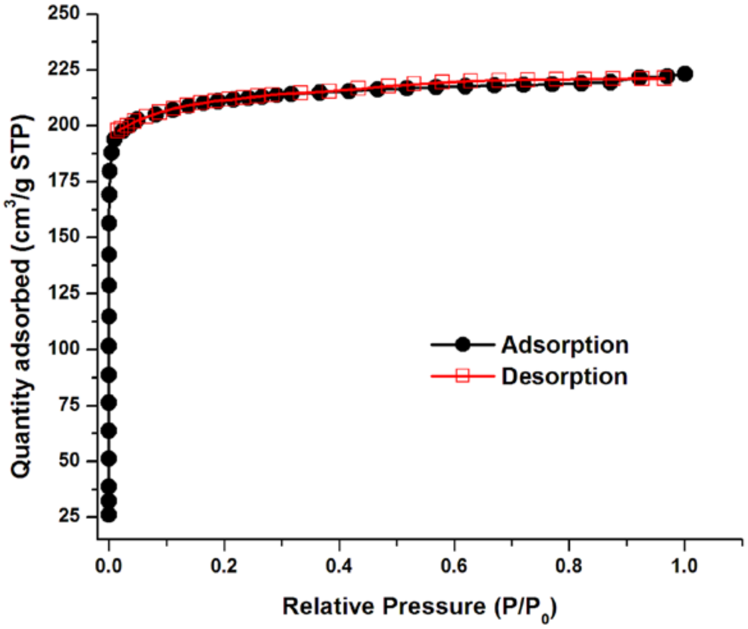


Figure S4 Nitrogen adsorption/desorption isotherm of the $Cu_3(BTC)_2$ MOF

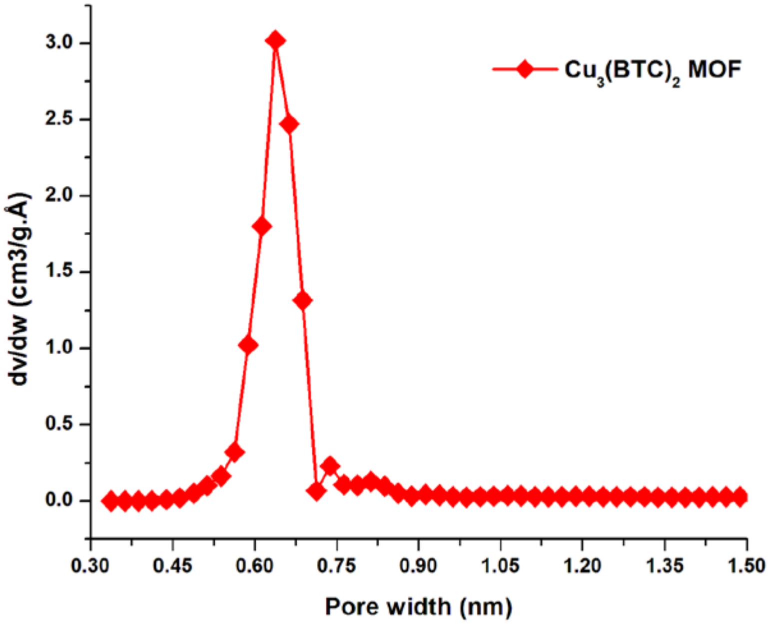


Figure S5 Pore size distribution of the $Cu_3(BTC)_2$ MOF

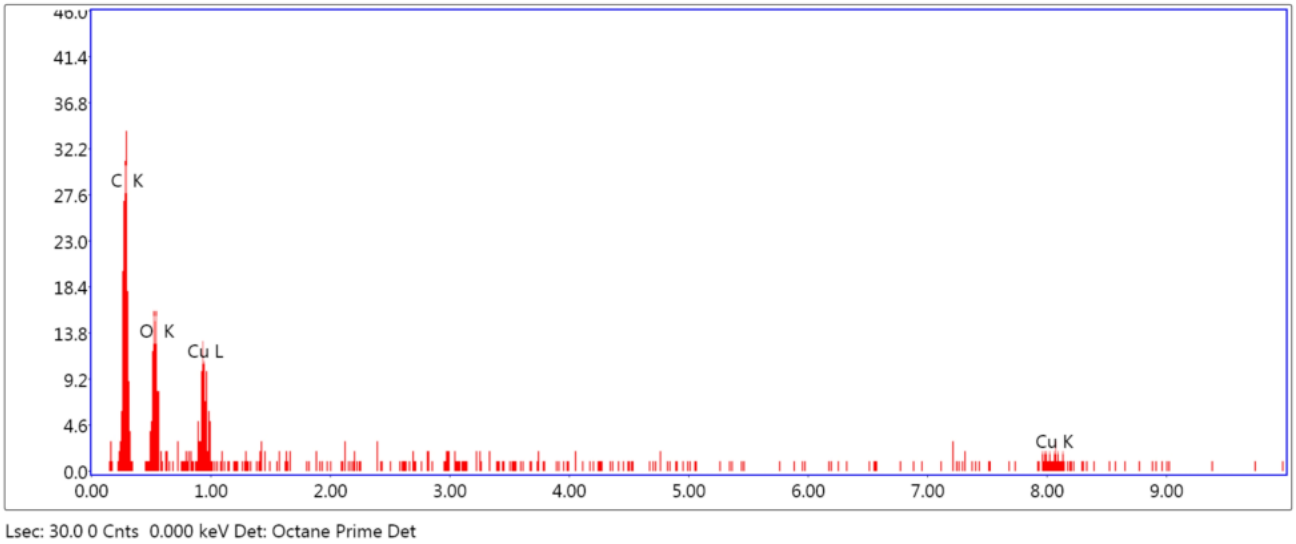


Figure S6 EDAX analysis of $Cu_3(BTC)_2$ MOF

Element	Weight %	Atomic %	Error %	Net Int.	K Ratio	Z	R	A	F
C K	48.18	67.18	15.78	5.35	1.0943	0.2208	1.0000	0.9486	0.4188
O K	24.46	25.61	20.21	3.14	1.0435	0.0663	1.0000	0.9702	0.2599
Cu K	27.36	7.21	32.09	1.21	0.7406	0.2165	1.0601	1.0491	1.0081

1.1 Characterization of Cu(BDC) MOF

Cu(BDC) was synthesized by solvothermal process as reported in literature.[2] Copper nitrate trihydrate (8.45 g) and terephthalic acid (5.80 g) was taken in equimolar quantities of 34.9 mmol in 780 mL of DMF in 1L RB flask, then the mixture was stirred for 30 min. After it was transferred to Teflon lined autoclave and heated in an air-oven up to 110 °C for 36 h. After the reaction was over, the autoclave was cooled slowly to room temperature and small fine blue crystals were found inside the autoclave. Then the mother liquor was simply decanted and washed with DMF to remove unreacted copper nitrate trihydrate and terephthalic acid. The solid was filtered through the Whatman filter paper (No. 3). Then repeatedly washed with excess of DMF and dried in a hot air oven at 220 °C for 24 h. In FT-IR spectrum of Cu(BDC) MOF exhibits the peaks at 1666 cm^{-1} indicates that DMF molecule was coordinated to Cu^{II} center and absence of strong absorption bands at 1760–1690 cm^{-1} confirmed the deprotonation of carboxylic acid groups in 1,4-benzene dicarboxylic acid. In Powder XRD, the presence of a very sharp peak nearly at 10.37° indicates that MOF was highly crystalline in nature and the observed pattern exactly matches with reported and simulated patterns. Cu(BDC) MOF was dissolved in dil. HNO_3 and the quantitative analysis by ICP-OES showed 19.93 % of copper was present. These characterization results and powder XRD pattern were in good agreement with literature.

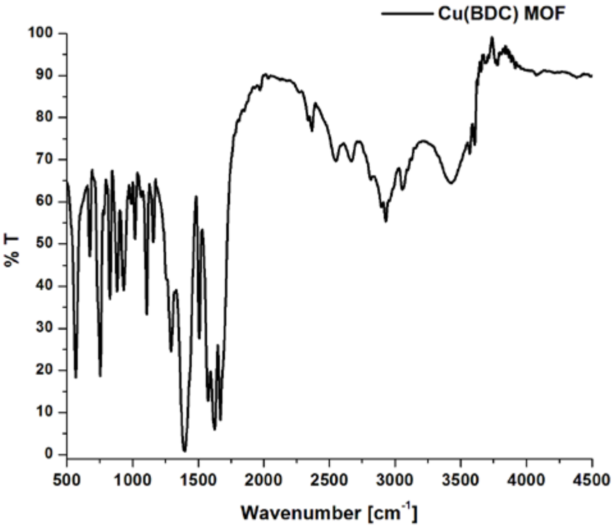


Figure S7 FT-IR spectrum of Cu(BDC) MOF

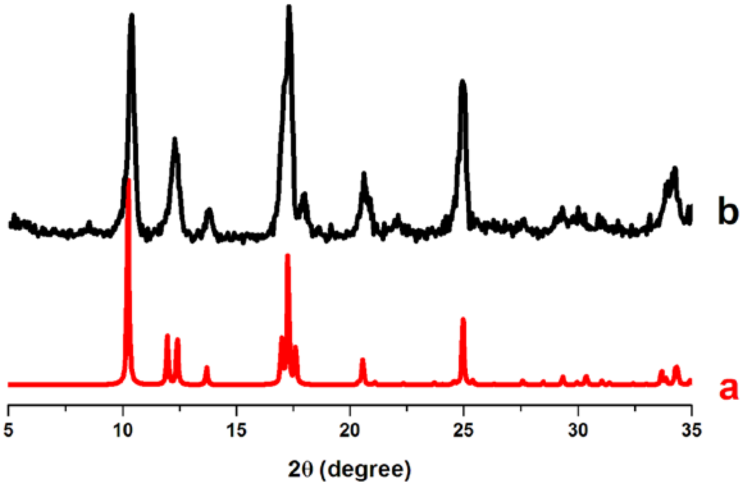


Figure S8 Powder XRD pattern of simulated (a) and as-synthesized Cu(BDC) MOF (b)

1.2 Synthesis and Characterization of Cu(BDC)(DABCO) MOF:

Cu(BDC)(DABCO) MOF was synthesized by solvothermal process as reported in literature.[3] A mixture of terephthalic acid (0.506 g, 3.1 mmol), 1,4 Diazabicyclo[2.2.2]octane [DABCO (0.188 g, 1.67 mmol)] and Copper nitrate trihydrate (0.8 g, 3.3 mmol) was dissolved in equimolar quantities of 80 mL of DMF in 250 mL RB flask, and then the mixture was stirred for 30 min. After it was transferred to Teflon lined autoclave and heated in an air-oven up to 120 °C for 48 h. After the reaction was over, the autoclave was cooled slowly to room temperature and blue crystals were found inside the autoclave. Then the mother liquor was simply decanted and washed with DMF to remove unreacted copper nitrate trihydrate and terephthalic acid. The solid was filtered through the Whatman filter paper (No.3). Then repeatedly washed with excess of DMF and dried at 140 °C for 6 h under vacuum to yield $Cu_2(BDC)_2(DABCO)$ as light blue crystals. In FT-IR spectrum of Cu(BDC)(DABCO) MOF exhibits the peaks at 1622 cm^{-1} indicates that DMF molecule was coordinated to Cu^{II} center and absence of strong absorption bands at 1760–1690 cm^{-1} confirmed the deprotonation of carboxylic acid groups in 1,4-benzene dicarboxylic acid. In Powder XRD, the presence of a very sharp peak nearly at 10.24° indicates that MOF was highly crystalline in nature and the observed pattern exactly matches with reported and simulated patterns. Cu(BDC)(DABCO) MOF was dissolved in dil. HNO_3 and the quantitative analysis by ICP-MS showed 19.93 % of copper was present. These characterization results and powder XRD pattern were in good agreement with literature.

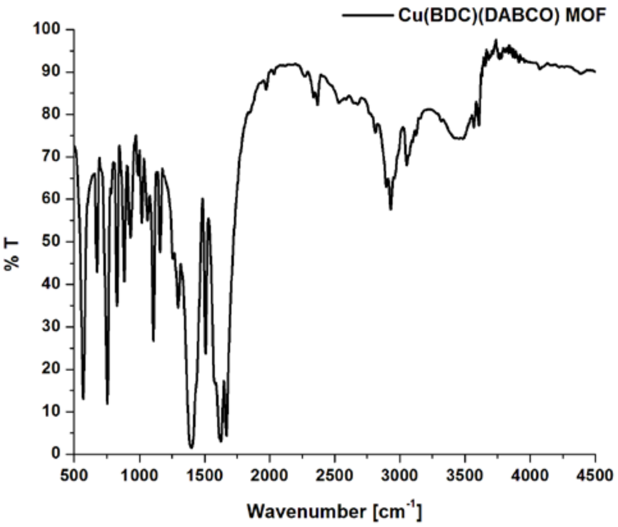


Figure S9 FT-IR spectrum of Cu(BDC)(DABCO) MOF

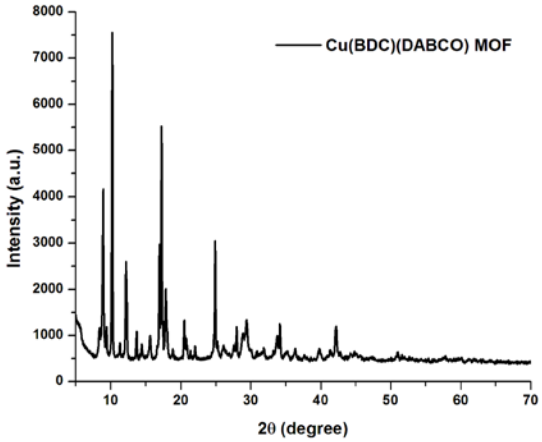


Figure S10 Powder XRD pattern of Cu(BDC)(DABCO) MOF

1.2 Synthesis and Characterization of Cu(bpy)(H_2O)$_2$(BF_4)$_2$(bpy):

Cu(bpy)(H_2O)$_2$(BF_4)$_2$(bpy) MOF was synthesized according to the reported literature procedure.[4] First, 4,4’-bipyridine (0.624 g, 2 mmol) in 4 mL of ethanol was slowly added to an 16 mL aqueous solution of Cu(BF_4)$_2$·H_2O (0.618 g, 1 mmol) at room temperature and the blue precipitate was formed gradually. The mixture was stirred for 4 h at room temperature, after the solid was filtered off, washed with water and ethanol, dried in air at room temperature and then in vacuum at 100 °C for 2 h and stored under argon. It was characterized using FT-IR, PXRD and elemental analysis. In FT-IR spectrum of $Cu(bpy)(H_2O)_2(BF_4)_2(bpy)$ MOF peaks were present at 3323 and 1301 cm^{-1} due to the bond formation between 4,4'-bipyridine and water molecule in copper salt. Peaks at 1599 and 1666 cm^{-1} were indicated the presence of uncoordinated bipyridine molecules in framework. Elemental analysis by ICP-OES showed the presence of 6.99 $mmolg^{-1}$ of copper. These characterization results and powder XRD pattern were in good agreement with literature.

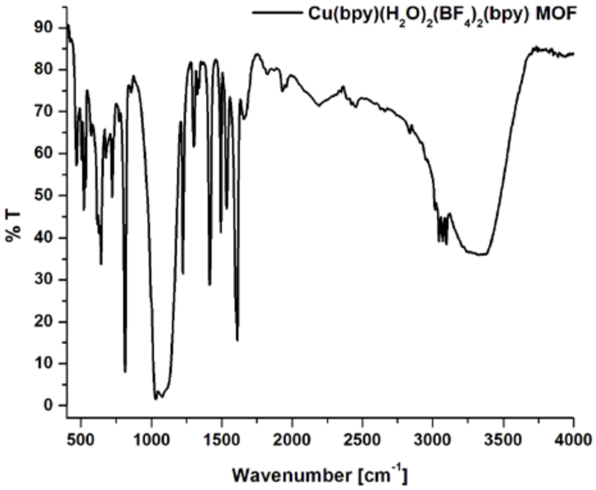


Figure S11 FT-IR spectrum of $Cu(bpy)(H_2O)_2(BF_4)_2(bpy)$ MOF

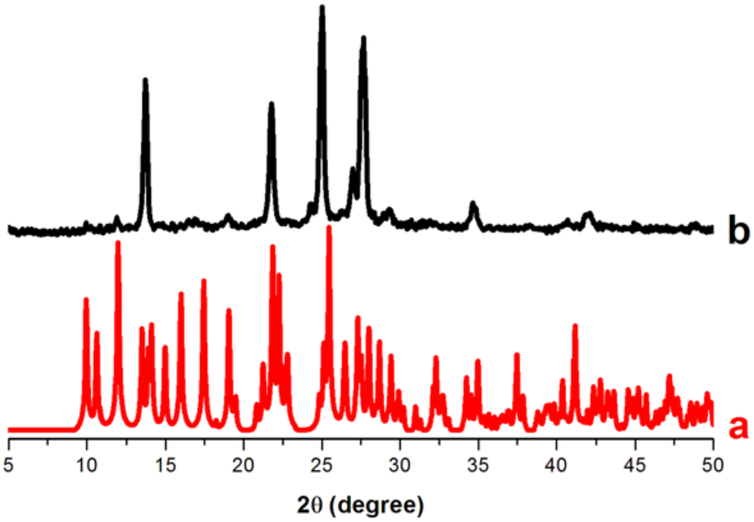


Figure S12 Powder XRD pattern of simulated (a) and as-synthesized $Cu(bpy)(H_2O)_2(BF_4)_2(bpy)$ MOF (b)

1.4 Synthesis and Characterization of Fe(BTC) MOF:

Fe(BTC) MOF was prepared according to the reported literature.[5] The reactants $Fe(NO_3)_3 \cdot 9H_2O$ (2.5 mmol) and 1,3,5-benzenetricarboxylicacid (H_3BTC, 3.1 mmol) with a 1:1 molar ratio were dissolved in 40 mL of DMF. The mixture was heated at 150 °C for 24 h in a Teflon lined stainless steel autoclave. After cooled to room temperature, the solid was filtered off and washed with DMF and ethanol for several times, then dried at 60 °C in vacuum for 6 h. The dried Fe(BTC) MOF powder was obtained and characterized. In FT-IR, the absence of strong absorption bands at 1760–1690 cm^{-1} and the presence of strong peak at 1620 cm^{-1} were due to the deprotonation of –COOH groups in benzene tricarboxylic acid, which is lower than the C=O stretching vibrations of carboxylic acids and confirmed the formation of Fe(BTC) MOF. Elemental analysis by ICP-OES showed the iron loading was 2.675 $mmolg^{-1}$. Observed results and PXRD pattern were good agreement reported values.

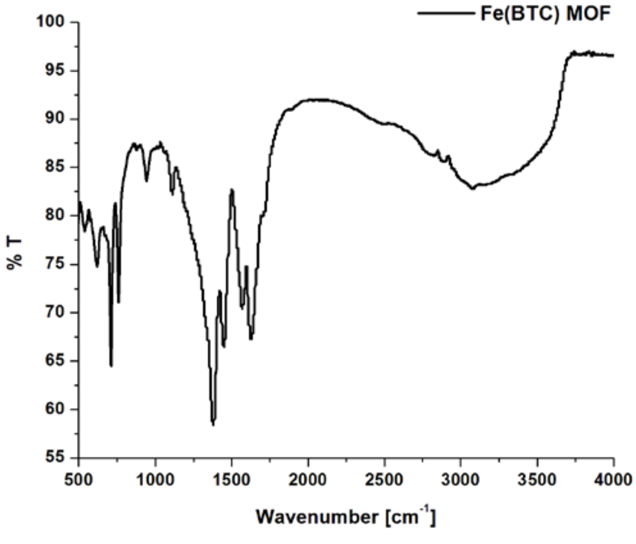


Figure S13 FT-IR spectrum of Fe(BTC) MOF

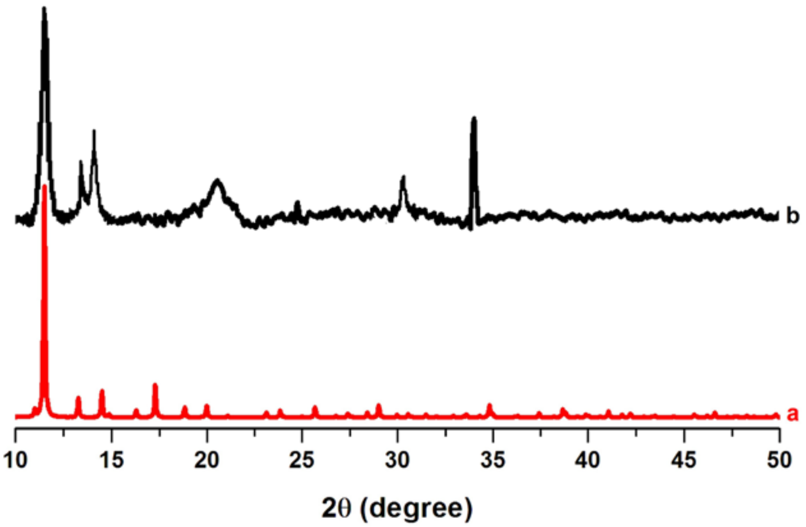


Figure S14 Powder XRD pattern of simulated (a) and as-synthesized Fe(BTC) MOF (b)

1.5 Synthesis and Characterization of Fe-MIL-53:

Fe-MIL-53 was prepared according to the reported literature.[6] 4.04 g (10 mmol) of terephthalic acid, 1.66 g (10 mmol) of iron(III) nitrate nonahydrate and 100 mL of DMF were placed in a stainless steel autoclave and heated for 48 h. Crude MIL-53(Fe)-$(H_2\text{-BDC})_x$ was recovered as an orange solid by filtration, washed with DMF, acetone and dried in air. Then the solid was dried at 100 °C under vacuum for 8 h. The PXRD pattern and FT-IR analysis were good agreement with reported. The absence of strong absorption bands at 1760–1690 cm^{-1} was due to the deprotonation of –COOH groups in benzene dicarboxylic acid and the presence of strong peak at 1625 cm^{-1}, which was lower than the C=O stretching vibrations of carboxylic acids revealed the formation of Fe-MIL-53 MOF.

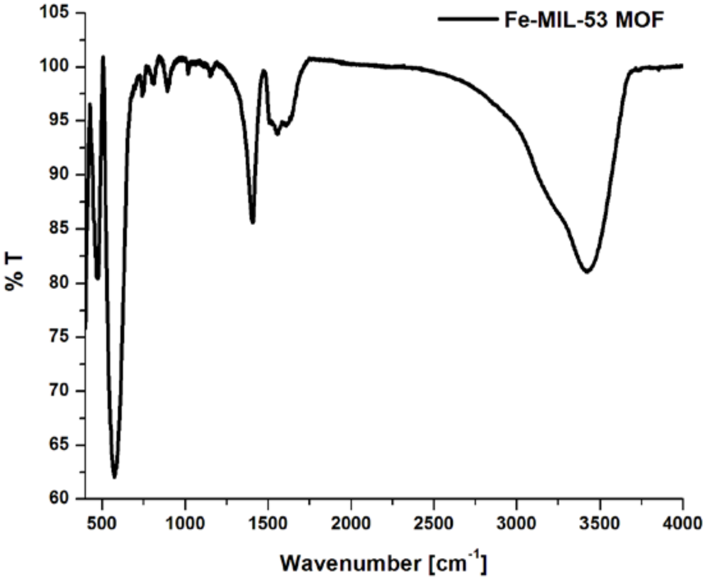


Figure S15 FT-IR spectrum of Fe-MIL-53 MOF

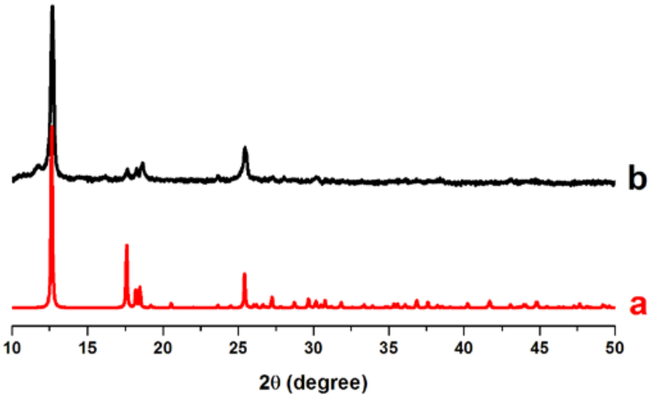


Figure S16 Powder XRD pattern of simulated (a) and as-synthesized Fe-MIL-53 MOF (b)

1.6 Synthesis and Characterization of the Ni(HBTC)BPY MOF:

Ni(HBTC)BPY MOF was prepared according to the reported literature.[7] In a typical preparation, a mixture of H_3BTC (H_3BTC = 1,3,5- benzenetricarboxylic acid; 0.63 g, 2.99 mmol), 4,4-bipy (4,4-bipy = 4,4-bipyridine; 0.705 g, 3 mmol), and $Ni(NO_3)_2 \cdot 6H_2O$ (1.74 g, 5.98 mmol) was dissolved in DMF (DMF = N,N-dimethylformamide; 60 mL) in a 100 mL RB flask. Then the mixture was transferred to Teflon-lined autoclave and was heated at 100 °C in an isothermal oven for 24 h. After cooling the vial to room temperature, the solid product was removed by decanting with mother liquor and washed with DMF (3× 10 mL). Solvent exchange was then carried out with DCM (3× 10 mL) at room temperature. The product was then dried at 140 °C for 6 h under vacuum, yielding to get Ni(HBTC)BPY as green crystals. In FT-IR spectrum of Ni(HBTC)BPY showed the absence of strong absorption band at 1760–1690 cm^{-1} the strong peak at 1610 cm^{-1}, which was lower than the C=O stretching vibrations of carboxylic acids were confirmed the deprotonation of carboxylic acid groups in 1,3,5-benzene tricarboxylic acid. SEM images shows well defined cyclohexyl structure. EDAX analysis of this MOF shows 3.4 wt % of Ni was present. These characterization results and powder XRD pattern were in good agreement with literature.

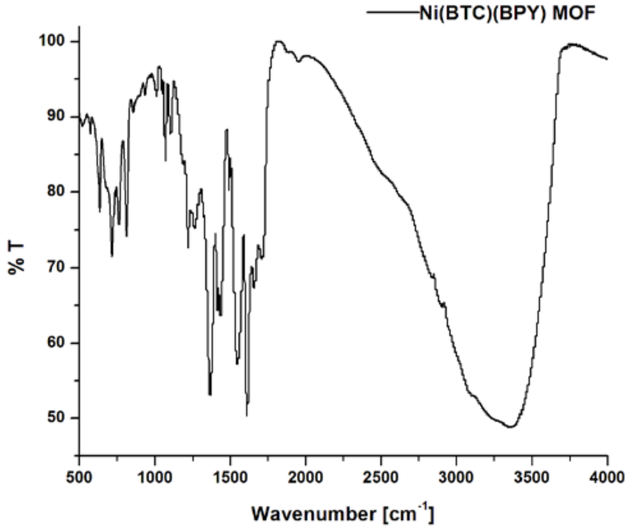


Figure S17 FT-IR spectrum of Ni(HBTC)BPY MOF

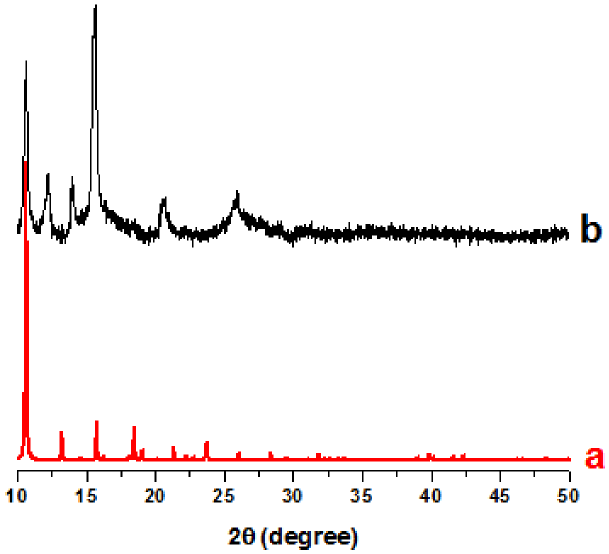


Figure S18 Powder XRD pattern of simulated (a) and as-synthesized Ni(HBTC)(BPY) MOF (b)

1.7 Synthesis and Characterization of the $Ni_2(BDC)_2(DABCO)$ MOF:

$Ni_2(BDC)_2(DABCO)$ MOF was synthesized according to the reported literature procedure,[8] a solid mixture of H_2BDC (H_2BDC = 1,4 benzenedicarboxylic acid; 2.075 g, 12.49 mmol), DABCO (DABCO = 1,4-diazabicyclo[2.2.2]octane; 0.84 g, 7.49 mmol), and $Ni(NO_3)_2.6H_2O$ (2.9 g, 9.975 mmol) was dissolved in DMF (DMF = N,N'-dimethylformamide; 75 mL). The resulting solution was transferred to Teflon-lined autoclave. Then it was heated at 100 °C in an isothermal oven for 48 h. After cooling the vials to room temperature, the solid product was removed by decanting with mother liquor and washed in DMF (3 x 10 mL) for 3 days. Solvent exchange was carried out with methanol (3 x 10 mL) at room temperature for 3 days. The material was then evacuated under vacuum at 140 °C for 6 h, yielding 0.425 g of $Ni_2(BDC)_2(DABCO)$ in the form of green crystals (72 % yield). In FT-IR spectrum of $Ni_2(BDC)_2(DABCO)$ showed the absence of strong absorption band at 1760–1690 cm^{-1} confirmed the deprotonation of carboxylic acid groups in 1,4-benzene dicarboxylic acid. EDAX analysis of this MOF shows 9.97 wt % of Ni was present. These characterization results and powder XRD pattern were in good agreement with literature.

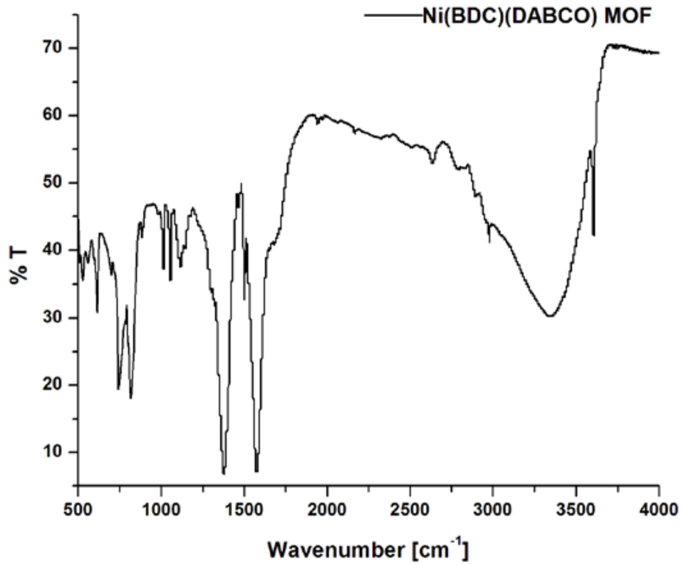


Figure S19 FT-IR spectrum of $Ni_2(BDC)_2(DABCO)$ MOF

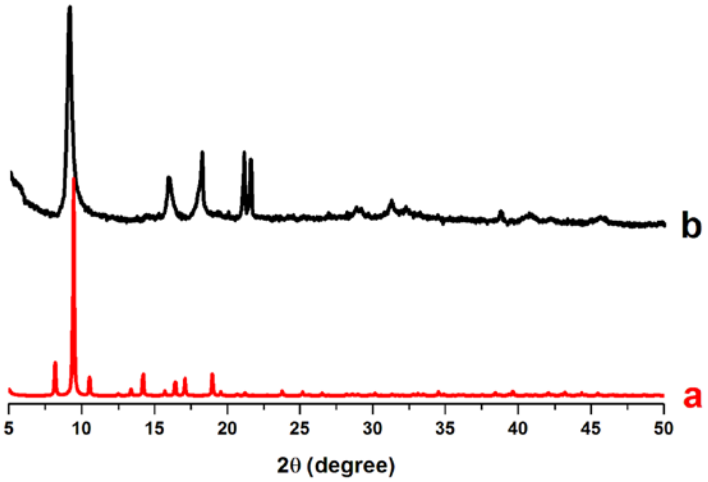
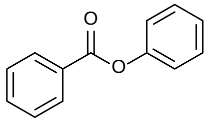
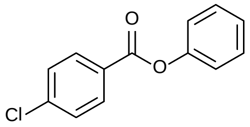
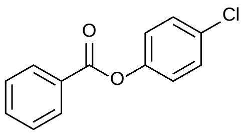
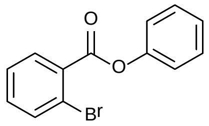
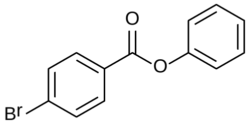
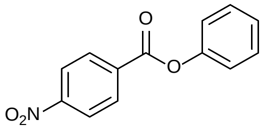
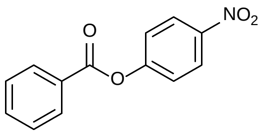
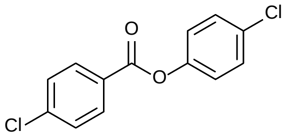
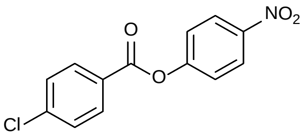
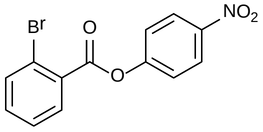
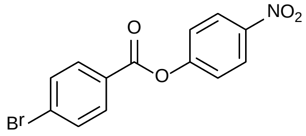
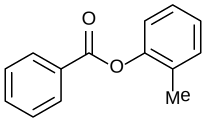
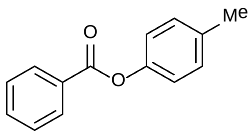
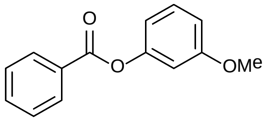


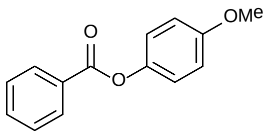
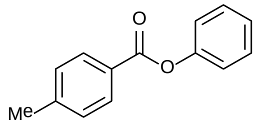
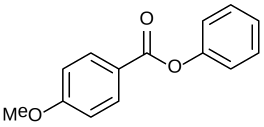
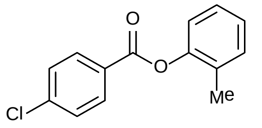
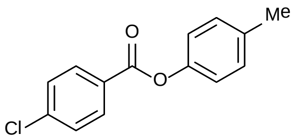
Figure S20 Powder XRD pattern of simulated (a) and as-synthesized $Ni_2(BDC)_2(DABCO)$ MOF (b)

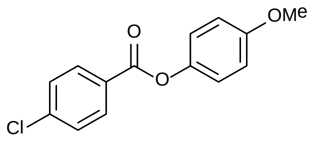
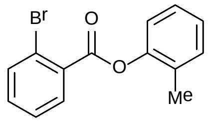
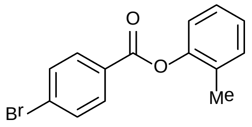
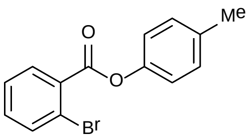
2. NMR data:

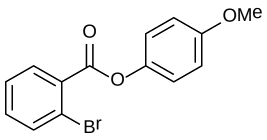
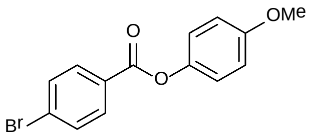
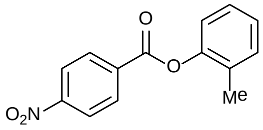
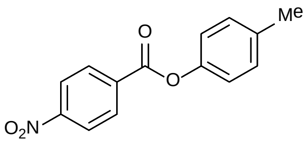
Phenyl benzoate (4a) ^{1}H NMR (300 MHz, CDCl$_3$) δ: 7.17–7.31 (m, 3H), 7.37–7.47 (m, 2H), 7.51 (t, 2H, J = 6.0 Hz), 7.59–7.67 (m, 1H), 8.19–8.23 (m, 2H). **(Fig. S21)** ^{13}C NMR (75 MHz, CDCl$_3$) δ: 121.67, 125.81, 128.52, 129.43, 129.67, 130.12, 133.49, 151.02, 165.09. **(Fig. S22)**	
phenyl 4-chlorobenzoate (4b) ^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.21 (d, 2H, J = 8.0 Hz), 7.28 (t, 1H, J = 8.0 Hz), 7.44 (t, 2H, J = 8.0 Hz), 7.49 (d, 2H, J = 8.0 Hz), 8.14 (d, 2H, J = 8.0 Hz). **(Fig. S23)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 121.60, 126.03, 128.00, 128.94, 129.53, 131.53, 140.11, 150.75, 164.34. **(Fig. S24)**	
4-chlorophenyl benzoate (4c) ^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.18 (d, 2H, J = 8.0 Hz), 7.40 (d, 2H, J = 8.0 Hz), 7.52 (t, 2H, J = 8.0 Hz), 7.66 (t, 1H, J = 8.0 Hz), 8.20 (d, 2H, J = 8.0 Hz). **(Fig. S25)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 123.06, 128.58, 129.11, 129.48, 130.14, 131.20, 133.74, 149.36, 164.88. **(Fig. S26)**	
phenyl 2-bromobenzoate (4d) ^{1}H NMR (300 MHz, CDCl$_3$) δ: 7.29 (dd, 3H, J = 9.0, 17.9 Hz), 7.41 (ddd, 4H, J = 4.2, 8.0, 12.8 Hz), 7.72 (dd, 1H, J = 1.4, 7.6 Hz), 8.00 (dd, 1H, J = 2.0, 7.4 Hz). **(Fig. S27)** ^{13}C NMR (75 MHz, CDCl$_3$) δ: 121.29, 121.85, 125.84, 127.08, 129.25, 130.97, 131.46, 132.91, 134.24, 150.36, 164.24. **(Fig. S28)**	
phenyl 4-bromobenzoate (4e) ^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.20 (d, 2H, J = 7.7 Hz), 7.29 (d, 1H, J = 7.3 Hz), 7.43 (t, 2H, J = 7.8 Hz), 7.65 (d, 2H, J = 8.4 Hz), 8.06 (d, 2H, J = 8.4 Hz). **(Fig. S29)**	

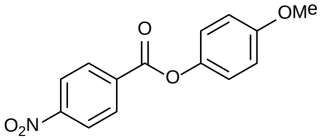
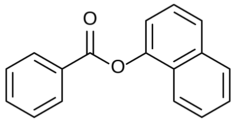
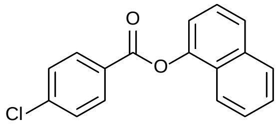
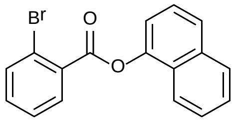
^{13}C NMR (100 MHz, CDCl$_3$) δ: 121.58, 126.04, 128.49, 128.81, 129.53, 131.64, 131.94, 150.75, 164.47. **(Fig. S30)**	
phenyl 4-nitrobenzoate (4f) ^{1}H NMR (300 MHz, CDCl$_3$) δ: 7.23–7.28 (m, 2H), 7.34 (d, 1H, J = 7.5 Hz), 7.43–7.51 (m, 2H), 8.38 (d, 4H, J = 1.7 Hz). **(Fig. S31)** ^{13}C NMR (75 MHz, CDCl$_3$) δ: 121.35, 123.64, 126.34, 129.61, 131.21, 134.87, 150.43, 150.79, 163.26. **(Fig. S32)**	
4-nitrophenyl benzoate (4g) ^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.42 (d, 2H, J = 9.1 Hz), 7.54 (t, 2H, J = 7.8 Hz), 7.68 (t, 1H, J = 7.5 Hz), 8.20 (d, 2H, J = 7.2 Hz), 8.32 (d, 2H, J = 9.1 Hz). **(Fig. S33)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 122.60, 125.23, 128.51, 128.76, 130.29, 134.22, 145.38, 155.71, 164.20. **(Fig. S34)**	
4-chlorophenyl 4-chlorobenzoate (4h) ^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.16 (d, 2H, J = 8.9 Hz), 7.39 (d, 2H, J = 8.9 Hz), 7.49 (d, 2H, J = 8.7 Hz), 8.12 (d, 2H, J = 8.7 Hz). **(Fig. S35)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 123.04, 127.62, 129.05, 129.63, 131.47, 131.59, 140.40, 149.21, 164.14. **(Fig. S36)**	
4-nitrophenyl 4-chlorobenzoate (4i) ^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.50 (d, 2H, J = 8.6 Hz), 7.56 (d, 2H, J = 8.5 Hz), 8.07 (d, 2H, J = 8.6 Hz), 8.27 (d, 2H, J = 8.6 Hz). **(Fig. S37)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 122.55, 125.30, 126.93, 129.18, 131.65, 140.88, 145.47, 155.43, 163.39. **(Fig. S38)**	
4-nitrophenyl 2-bromobenzoate (4j) ^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.44–7.49 (m, 4H), 7.75–7.79 (m, 1H), 8.02–8.05 (m, 1H), 8.33 (m, 2H, J= 9.1 Hz). **(Fig. S39)**	

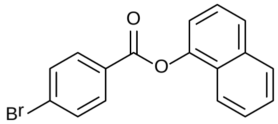
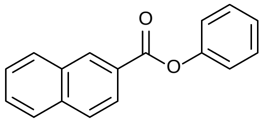
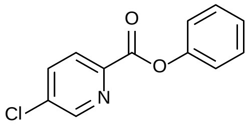
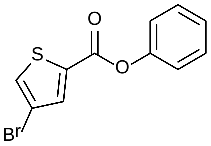
^{13}C NMR (100 MHz, CDCl$_3$) δ: 121.09, 122.50, 125.28, 127.47, 130.17, 132.03, 133.79, 134.88, 145.54, 155.29, 163.41. **(Fig. S40)**	
4-nitrophenyl 4-bromobenzoate (4k) ^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.42 (d, 2H, *J* = 9.0 Hz), 8.00 (d, 2H, *J* = 8.5 Hz), 8.06 (d, 2H, *J* = 8.5 Hz), 8.34 (d, 2H, *J* = 9.0 Hz). **(Fig. S41)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 122.60, 125.36, 127.49, 130.24, 131.17, 131.95, 132.23, 132.40, 161.47. **(Fig. S42)**	
***o*-tolyl benzoate (4l)** ^{1}H NMR (300 MHz, CDCl$_3$) δ: 2.24 (s, 4H), 7.15–7.29 (m, 3H), 7.49–7.54 (m, 2H), 7.62–7.66 (m, 2H), 8.23 (d, 2H, *J* = 7.9 Hz). **(Fig. S43)** ^{13}C NMR (75 MHz, CDCl$_3$) δ: 16.17, 121.97, 126.02, 126.93, 128.56, 130.12, 131.12, 133.03, 133.50, 134.63, 149.51, 164.81. **(Fig. S44)**	
***p*-tolyl benzoate (4m)** ^{1}H NMR (400 MHz, CDCl$_3$) δ: 2.37 (s, 3H), 7.09 (d, 2H, *J* = 8.5 Hz), 7.22 (d, 2H, *J* = 8.2 Hz), 7.50 (t, 2H, *J* = 7.7 Hz), 7.59–7.66 (m, 1H), 8.20 (dd, 2H, *J* = 1.3, 8.3 Hz). **(Fig. S45)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 20.88, 121.34, 128.51, 129.67, 129.97, 130.12, 133.47, 135.49, 148.69, 165.37. **(Fig. S46)**	
3-methoxyphenyl benzoate (4n) ^{1}H NMR (300 MHz, CDCl$_3$) δ: 3.90 (s, 3H), 6.89 (s, 1H), 7.47–7.60 (m, 4H), 7.62–7.73 (m, 2H), 8.23 (d, 2H, *J* = 7.1 Hz). **(Fig. S47)** ^{13}C NMR (75 MHz, CDCl$_3$) δ: 56.48, 107.77, 118.29, 120.32, 128.41, 128.64, 130.30, 130.34, 134.00, 146.27, 154.29, 163.98. **(Fig. S48)**	

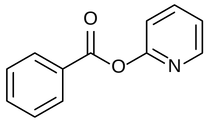
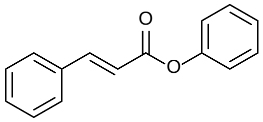
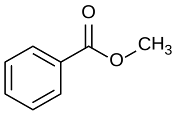
4-methoxyphenyl benzoate (4o) ^{1}H NMR (400 MHz, CDCl$_3$) δ: 3.80 (s, 3H), 6.93 (d, 2H, *J* = 9.0 Hz), 7.13 (d, 2H, *J* = 9.0 Hz), 7.49 (t, 2H, *J* = 7.7 Hz), 7.62 (t, 1H, *J* = 7.4 Hz), 8.19 (d, 2H, *J* = 7.3 Hz). **(Fig. S49)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 55.53, 114.47, 122.39, 128.49, 129.51, 130.07, 133.49, 144.33, 157.24, 165.61. **(Fig. S50)**	
***p*-tolyl benzoate (4p)** ^{1}H NMR (300 MHz, CDCl$_3$) δ: 2.46 (s, 3H), 7.23 (dd, 2H, *J* = 6.6, 7.8 Hz), 7.27 (s, 1H), 7.32 (d, 2H, *J* = 8.5 Hz), 7.40–7.48 (m, 2H), 8.10 (d, 2H, *J* = 8.2 Hz). **(Fig. S51)** ^{13}C NMR (75 MHz, CDCl$_3$) δ: 21.63, 121.65, 125.67, 126.68, 129.33, 129.18, 130.09, 144.28, 150.90, 165.13. **(Fig. S52)**	
4-methoxyphenyl benzoate (4q) ^{1}H NMR (300 MHz, CDCl$_3$) δ: 2.46 (s, 3H), 7.23 (dd, 2H, *J* = 6.6, 7.8 Hz), 7.27 (s, 1H), 7.32 (d, 2H, *J* = 8.5 Hz), 7.40–7.48 (m, 2H), 8.10 (d, 2H, *J* = 8.2 Hz). **(Fig. S53)** ^{13}C NMR (75 MHz, CDCl$_3$) δ: 21.63, 121.65, 125.67, 126.68, 129.33, 129.18, 130.09, 144.28, 150.90, 165.13. **(Fig. S54)**	
***o*-tolyl 4-chlorobenzoate (4r)** ^{1}H NMR (300 MHz, CDCl$_3$) δ: 2.36 (s, 3H), 7.18 (d, 4H, *J* = 20.1 Hz), 7.39 (s, 2H), 7.71 (s, 1H), 7.98 (s, 1H). **(Fig. S55)** ^{13}C NMR (75 MHz, CDCl$_3$) δ: 16.13, 121.81, 126.18, 126.96, 127.76, 128.91, 130.10, 131.15, 131.45, 140.08, 149.25, 164.06. **(Fig. S56)**	
***p*-tolyl 4-chlorobenzoate (4s)** ^{1}H NMR (400 MHz, CDCl$_3$) δ: 2.37 (s, 3H), 7.08 (d, 2H, *J* = 8.5 Hz), 7.22 (d, 2H, *J* = 8.2 Hz), 7.47 (d, 2H, *J* = 8.6 Hz),	

8.12 (d, 2H, *J* = 8.6 Hz). **(Fig. S57)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 20.86, 121.23, 128.10, 128.87, 130.01, 131.48, 135.65, 139.98, 148.50, 164.49. **(Fig. S58)**	
4-methoxyphenyl 4-chlorobenzoate (4t) ^{1}H NMR (400 MHz, CDCl$_3$) δ: 3.81 (s, 3H), 6.93 (d, 2H, *J* = 8.8 Hz), 7.12 (d, 2H, *J* = 8.9 Hz), 7.47 (d, 2H, *J* = 8.4 Hz), 8.12 (d, 2H, *J* = 8.4 Hz). **(Fig. S59)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 55.57, 114.53, 122.32, 128.06, 128.88, 131.47, 140.00, 144.20, 157.38, 164.69. **(Fig. S60)**	
***o*-tolyl 2-bromobenzoate (4u)** ^{1}H NMR (400 MHz, CDCl$_3$) δ: 2.27 (s, 3H), 7.17 (t, 2H, *J* = 7.5 Hz), 7.25 (dd, 2H, *J* = 7.5, 10.8 Hz), 7.38 (ddd, 2H, *J* = 4.6, 9.2, 10.6, Hz), 7.71 (d, 1H, *J* = 7.9 Hz), 8.02 (dd, 1H, *J* = 1.7, 7.5 Hz). **(Fig. S61)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 16.36, 121.76, 122.14, 126.23, 126.96, 127.25, 130.13, 131.18, 131.22, 131.63, 133.07, 134.57, 149.21, 164.18. **(Fig. S62)**	
***o*-tolyl 4-bromobenzoate (4v)** ^{1}H NMR (300 MHz, CDCl$_3$) δ: 2.22 (s, 3H), 7.09–7.34 (m, 4H), 7.66 (d, 2H, *J* = 8.6 Hz), 8.08 (d, 2H, *J* = 8.6 Hz). **(Fig. S63)** ^{13}C NMR (75 MHz, CDCl$_3$) δ: 16.11, 121.77, 126.12, 126.92, 128.20, 128.71, 130.03, 131.10, 131.50, 131.85, 149.21, 164.03. **(Fig. S64)**	
***p*-tolyl 2-bromobenzoate (4w)** ^{1}H NMR (300 MHz, CDCl$_3$) δ: 7.25 (ddd, 3H, *J* = 1.1, 7.4, 14.5 Hz), 7.39–7.48 (m, 2H), 7.48–7.56 (m, 2H), 7.61–7.68 (m, 1H), 8.21 (dd, 2H, *J* = 1.3, 8.4 Hz). **(Fig. S65)**	

^{13}C NMR (75 MHz, $CDCl_3$) δ: 20.65, 120.97, 121.83, 127.07, 129.77, 131.21, 131.44, 132.83, 134.24, 135.45, 148.20, 164.46. **(Fig. S66)**	
4-methoxyphenyl 2-bromobenzoate (4x) ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.72 (s, 3H), 6.85 (d, 2H, *J* = 8.2 Hz), 7.08 (d, 2H, *J* = 9.0 Hz), 7.28–7.35 (m, 2H), 7.62 (d, 1H, *J* = 7.7 Hz), 7.89 (d, 1H, *J* = 8.0 Hz). **(Fig. S67)** ^{13}C NMR (100 MHz, $CDCl_3$) δ: 55.55, 114.48, 122.08, 122.25, 127.24, 131.48, 131.64, 132.99, 134.48, 144.10, 157.41, 164.89. **(Fig. S68)**	
4-methoxyphenyl 4-bromobenzoate (4y) ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.82 (s, 3H), 6.94 (d, 2H, *J* = 9.0 Hz), 7.12 (d, 2H, *J* = 9.0 Hz), 7.64 (d, 2H, *J* = 8.5 Hz), 8.05 (d, 2H, *J* = 8.5 Hz). **(Fig. S69)** ^{13}C NMR (100 MHz, $CDCl_3$) δ: 55.64, 114.57, 122.38, 128.54, 128.77, 131.65, 131.94, 144.20, 157.42, 164.89. **(Fig. S70)**	
***o*-tolyl 4-nitrobenzoate (4z)** ^{1}H NMR (300 MHz, $CDCl_3$) δ: 2.25 (s, 3H), 6.75–6.87 (m, 1H), 7.06–7.17 (m, 1H), 7.21–7.23 (m, 2H), 8.40 (d, 4H, *J* = 2.5 Hz). **(Fig. S71)** ^{13}C NMR (75 MHz, $CDCl_3$) δ: 15.99, 120.20, 121.52, 123.56, 126.40, 126.99, 131.06, 131.19, 134.51, 148.94, 150.65, 163.00. **(Fig. S72)**	
***p*-tolyl 4-nitrobenzoate (4aa)** ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.10 (d, 2H, *J* = 8.4 Hz), 7.23 (d, 2H, *J* = 8.2 Hz), 8.32 (d, 2H, *J* = 9.0 Hz), 8.36 (d, 2H, *J* = 9.0 Hz). **(Fig. S73)** ^{13}C NMR (100 MHz, $CDCl_3$) δ: 20.80, 120.96, 123.57, 130.06, 131.15, 134.94, 136.02, 148.19, 150.71, 163.42.	

(Fig. S74)	
4-methoxyphenyl 4-nitrobenzoate (4ab) ^{1}H NMR (400 MHz, CDCl$_3$) δ: 3.84 (s, 3H), 6.96 (d, 2H, *J* = 9.0 Hz), 7.15 (d, 2H, *J* = 9.1 Hz), 8.36 (d, 4H, *J* = 2.2 Hz). **(Fig. S75)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 55.62, 114.64, 122.15, 123.67, 131.23, 135.05, 143.95, 150.84, 157.65, 163.65. **(Fig. S76)**	
naphthalen-1-yl benzoate (4ac) ^{1}H NMR (300 MHz, CDCl$_3$) δ: 7.30–7.39 (m, 2H), 7.51–7.74 (m, 7H), 7.96 (d, 1H, *J* = 8.2 Hz), 8.18 (s, 1H), 8.33 (d, 1H, *J* = 7.0 Hz). **(Fig. S77)** ^{13}C NMR (75 MHz, CDCl$_3$) δ: 118.29, 121.75, 124.91, 125.59, 127.23, 127.56, 128.77, 130.32, 133.91, 145.84, 164.98. **(Fig. S78)**	
naphthalen-1-yl 4-chlorobenzoate (4ad) ^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.51 (dt, 2H, *J* = 2.3, 4.1 Hz), 7.55–7.58 (m, 1H), 7. 58–7.61 (m, 1H), 7.62–7.65 (m, 1H), 7.68 (s, 1H), 7.84 (d, 1H, *J* = 8.0 Hz), 8.07 (d, 2H, *J* = 8.7 Hz), 8.27 (d, 2H, *J* = 8.6 Hz). **(Fig. S79)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 121.52, 123.36, 125.04, 126.71, 127.04, 127.75, 128.32, 128.61, 129.23, 129.34, 130.35, 131.84, 140.86, 141.39, 161.26. **(Fig. S80)**	
naphthalen-1-yl 2-bromobenzoate (4ae) ^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.16 (s, 1H), 7.29 (s, 1H), 7.39 (d, 1H, *J* = 6.0 Hz), 7.42 (d, 1H, *J* = 7.6 Hz), 7.49 (d, 1H, *J* = 7.0 Hz), 7.51 (s, 1H), 7.55 (d, 1H, *J* = 10.2 Hz), 7.70 (d, 1H, *J* = 9.1 Hz), 7.93 (d, 1H, *J* = 8.0 Hz), 8.10 (dd, 1H, *J* = 1.9, 7.5 Hz), 8.22 (d, 1H, *J* = 8.6 Hz). **(Fig. S81)** ^{13}C NMR (100 MHz, CDCl$_3$) δ: 118.25, 121.86, 122.67,	

124.99, 125.63, 127.44, 127.55, 127.73, 127.84, 129.74, 130.80, 131.73, 132.11, 133.61, 134.98, 145.61, 164.38. **(Fig. S82)**	
naphthalen-1-yl 4-bromobenzoate (4af) ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.35 (s, 1H), 7.48 (s, 4H), 7.68 (d, 2H, *J* = 6.9 Hz), 7.77 (s, 1H), 7.87 (d, 1H, *J* = 5.4 Hz), 8.16 (d, 2H, *J* = 6.7 Hz). **(Fig. S83)** ^{13}C NMR (100 MHz, $CDCl_3$) δ: 118.16, 121.03, 121.53, 125.15, 125.41, 126.27, 126.52, 126.58, 127.60, 128.09, 131.75, 132.11, 149.40, 164.65. **(Fig. S84)**	
phenyl 2-naphthoate (4ag) ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.26–7.29 (m, 3H), 7.41–7.48 (m, 2H), 7.50–7.57 (m, 2H), 7.59–7.65 (m, 1H), 7.88 (d, 1H, *J* = 8.1 Hz), 8.05 (d, 1H, *J* = 8.2 Hz), 8.45 (d, 1H, *J* = 7.3 Hz), 9.04 (d, 1H, *J* = 8.7 Hz). **(Fig. S85)** 13C NMR (100 MHz, $CDCl_3$) δ: 121.83, 124.45, 125.66, 125.76, 125.87, 126.33, 128.10, 128.62, 129.49, 131.15, 131.61, 133.83, 134.25, 150.90, 165.75. **(Fig. S86)**	
phenyl 5-chloropicolinate (4ah) ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.24 (s, 1H), 7.32 (d, 1H, *J* = 7.3 Hz), 7.45 (t, 3H, *J* = 7.6 Hz), 7.90 (d, 1H, *J* = 8.3 Hz), 8.25 (d, 1H, *J* = 8.3 Hz), 8.79 (s, 1H). **(Fig. S87)** ^{13}C NMR (75 MHz, $CDCl_3$) δ: 121.50, 126.25, 126.60, 129.54, 136.41, 136.91, 145.35, 149.10, 150.65, 163.02. **(Fig. S88)**	
phenyl 4-bromothiophene-2-carboxylate (4ai) ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.20 (d, 2H, *J* = 8.0 Hz), 7.29 (d, 1H, *J* = 7.4 Hz), 7.42 (t, 2H, *J* = 7.9 Hz), 7.54 (d, 1H, *J* = 1.5 Hz), 7.87 (d, 1H, *J* = 1.5 Hz). **(Fig. S89)** ^{13}C NMR (100 MHz, $CDCl_3$) δ: 110.96, 121.51, 126.26,	

129.59, 130.65, 133.89, 136.58, 150.36, 159.41. **(Fig. S90)**	
<u>pyridin-2-yl benzoate (4aj)</u> ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.54 (d, 2H, *J* = 7.8 Hz), 7.64 –7.71 (m, 3H), 8.16 (d, 3H, *J* = 7.1 Hz), 8.23 (d, 2H, *J* = 7.1 Hz). **(Fig. S91)** ^{13}C NMR (75 MHz, $CDCl_3$) δ: 116.47, 121.97, 128.66, 130.27, 133.67, 134.36, 139.48, 148.29, 162.12, 164.53. **(Fig. S92)**	
<u>phenyl cinnamate (4ak)</u> ^{1}H NMR (300 MHz, $CDCl_3$) δ: 6.64 (d, 1H, *J* = 16.0 Hz), 7.18 (d, 2H, *J* = 7.6 Hz), 7.26 (s, 2H), 7.42 (dd, 4H, *J* = 5.5, 8.8 Hz), 7.59 (s, 2H), 7.88 (d, 1H, *J* = 16.0 Hz). **(Fig. S93)** ^{13}C NMR (75 MHz, $CDCl_3$) δ: 117.16, 121.53, 125.66, 128.18, 128.86, 129.32, 130.58, 134.01, 146.43, 150.68, 165.24. **(Fig. S94)**	
<u>methyl benzoate (4al)</u> ^{1}H NMR (300 MHz, $CDCl_3$) δ: 3.91 (s, 3H), 7.44 (m, 2H), 7.55 (d, 1H, *J* = 7.2 Hz), 8.04 (d, 2H, *J* = 7.2 Hz). **(Fig. S95)** ^{13}C NMR (75 MHz, $CDCl_3$) δ: 51.52, 127.92, 129.06, 129.81, 132.47, 165.84. **(Fig. S96)**	

3. References:

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4. NMR Spectra of isolated Compounds from 4a – 4al:

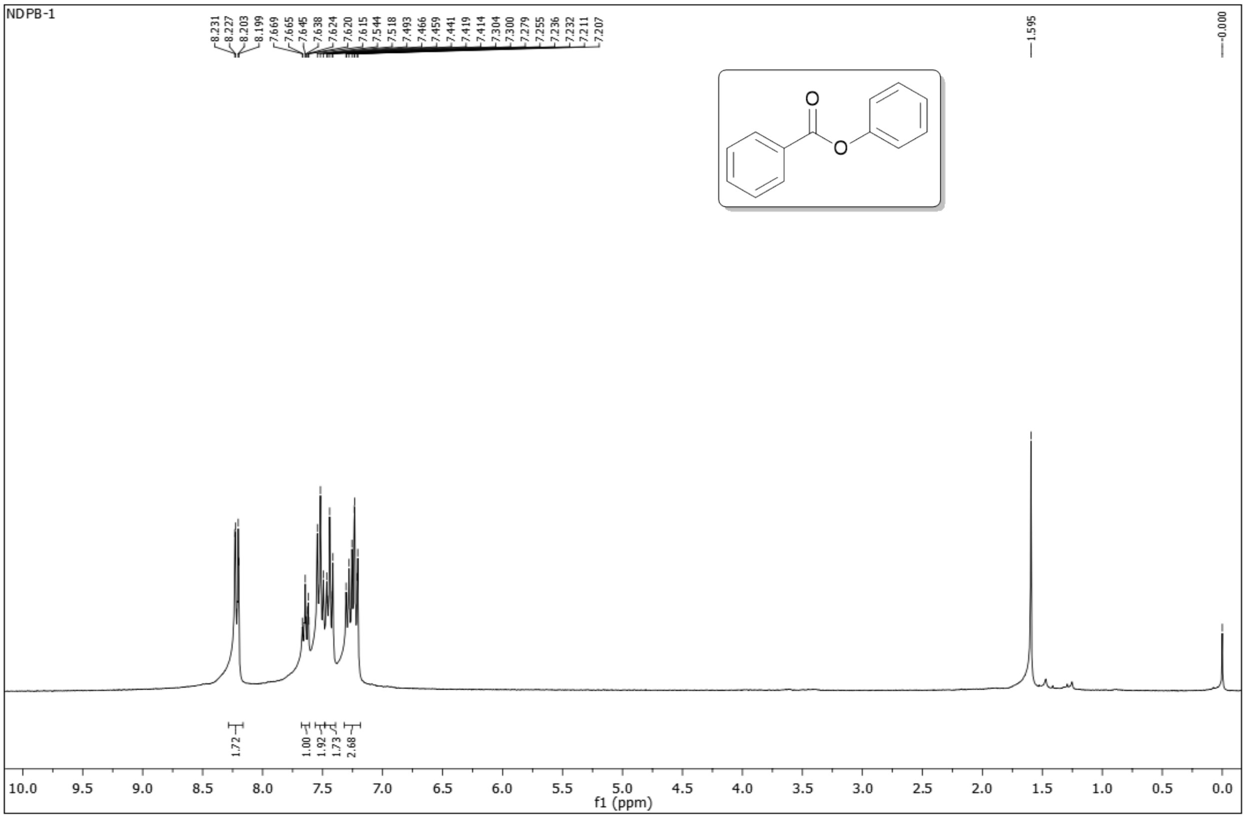

Fig. S21 ^{1}H NMR spectrum of phenyl benzoate **4a** (300 MHz, $CDCl_3$)

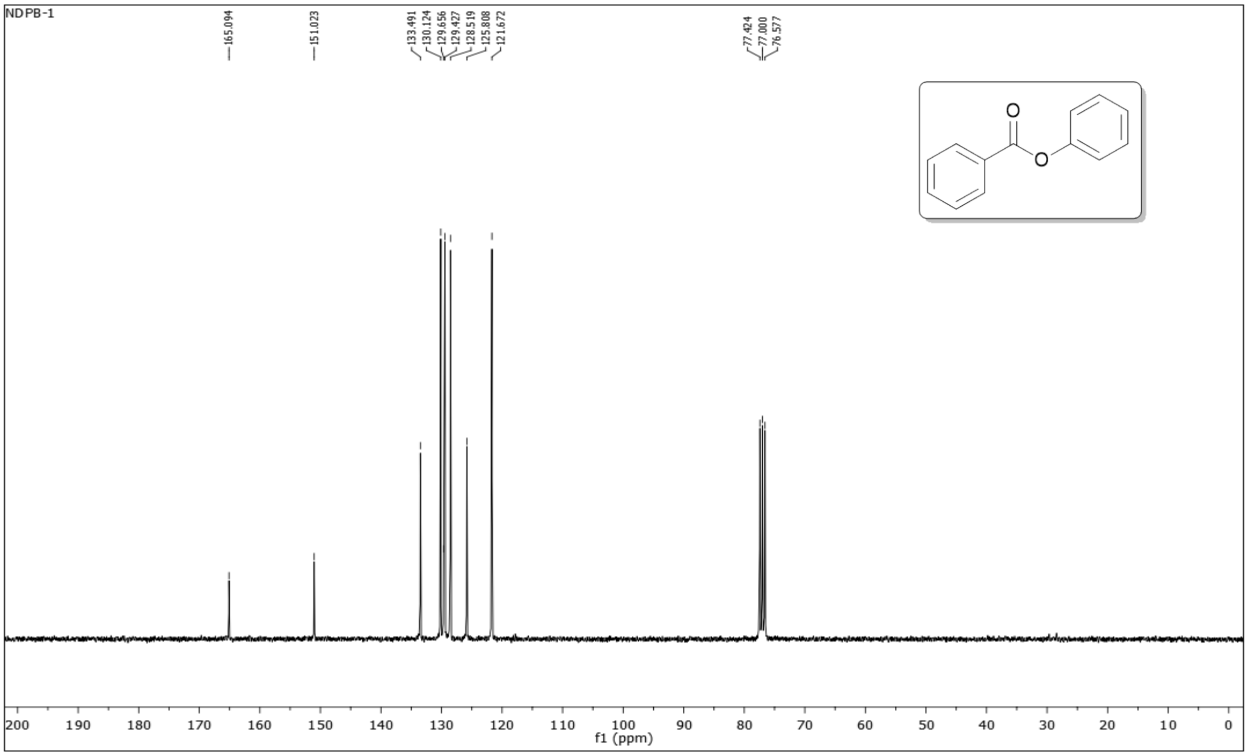

Fig. S22 ^{13}C NMR spectrum of phenyl benzoate **4a** (75 MHz, $CDCl_3$)

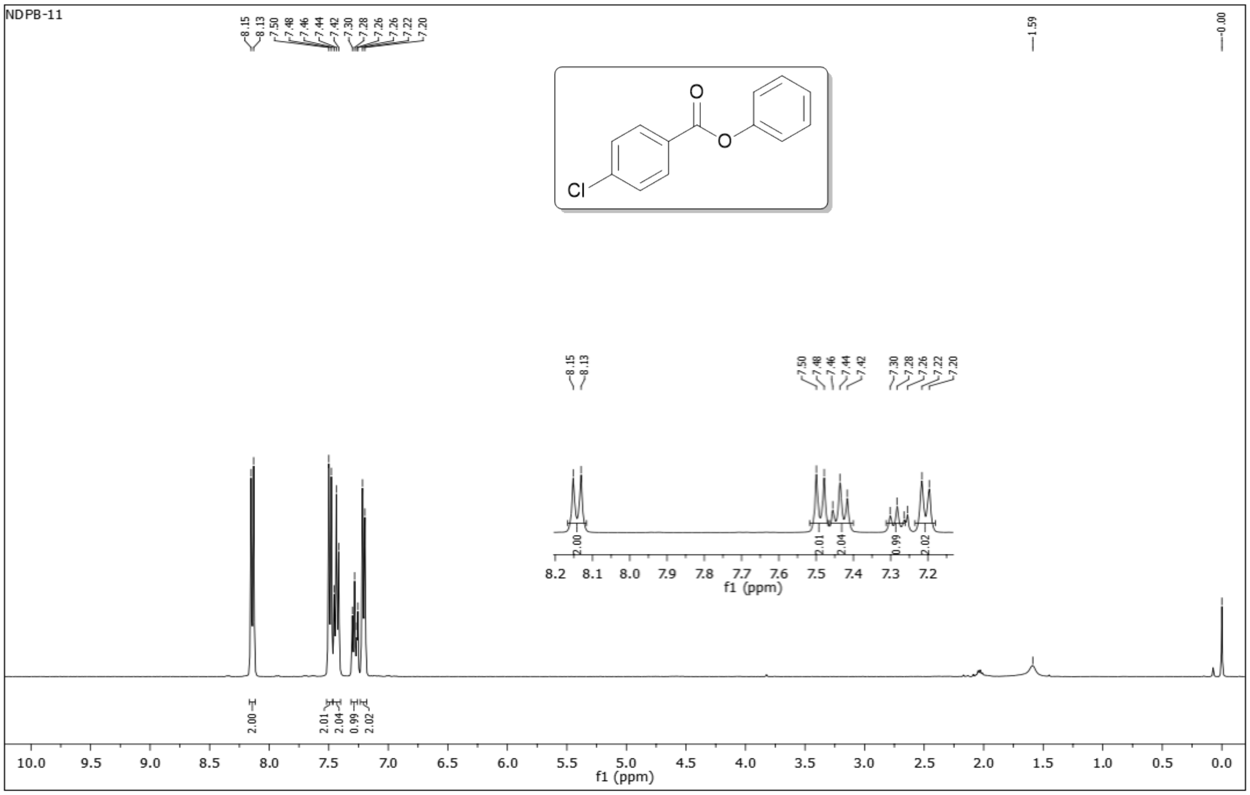

Fig. S23 ^{1}H NMR spectrum of phenyl 4-chlorobenzoate **4b** (400 MHz, $CDCl_3$)

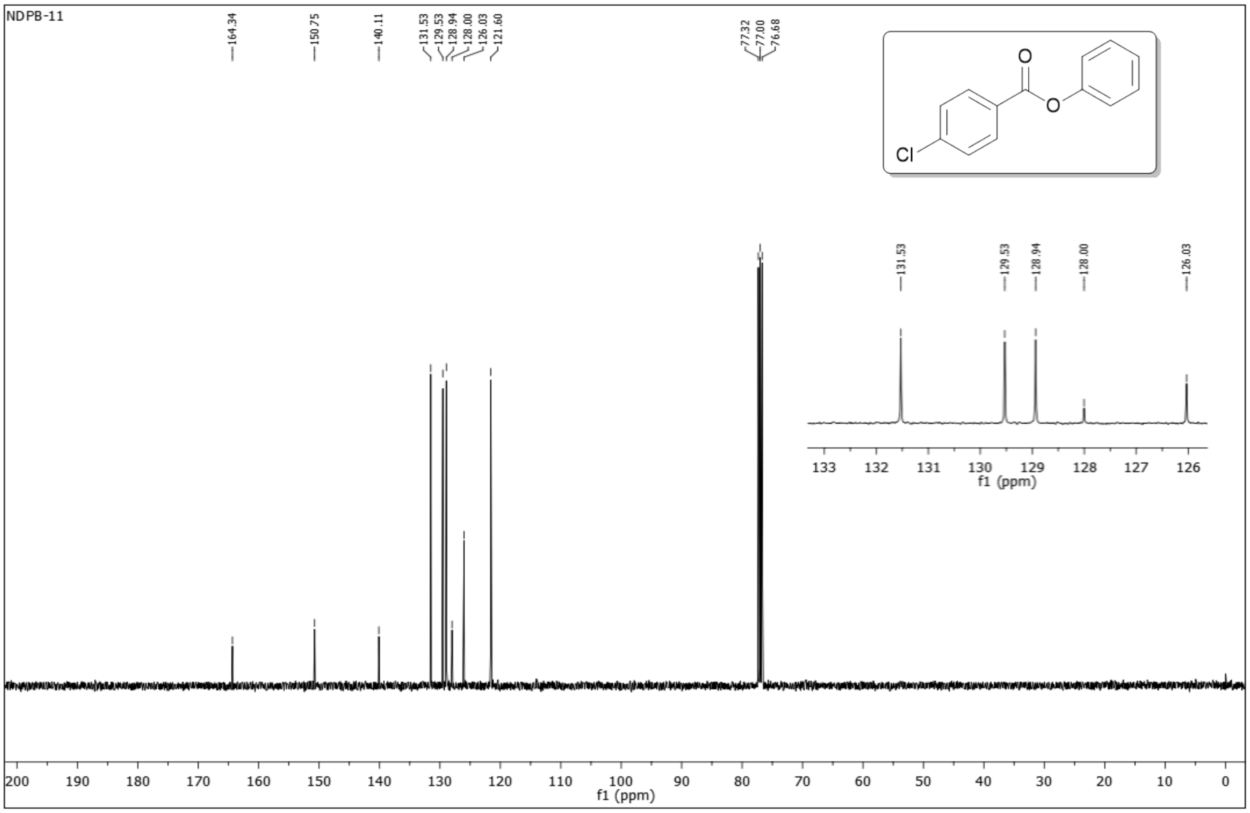

Fig. S24 ^{13}C NMR spectrum of Phenyl 4-chlorobenzoate **4b** (100 MHz, $CDCl_3$)

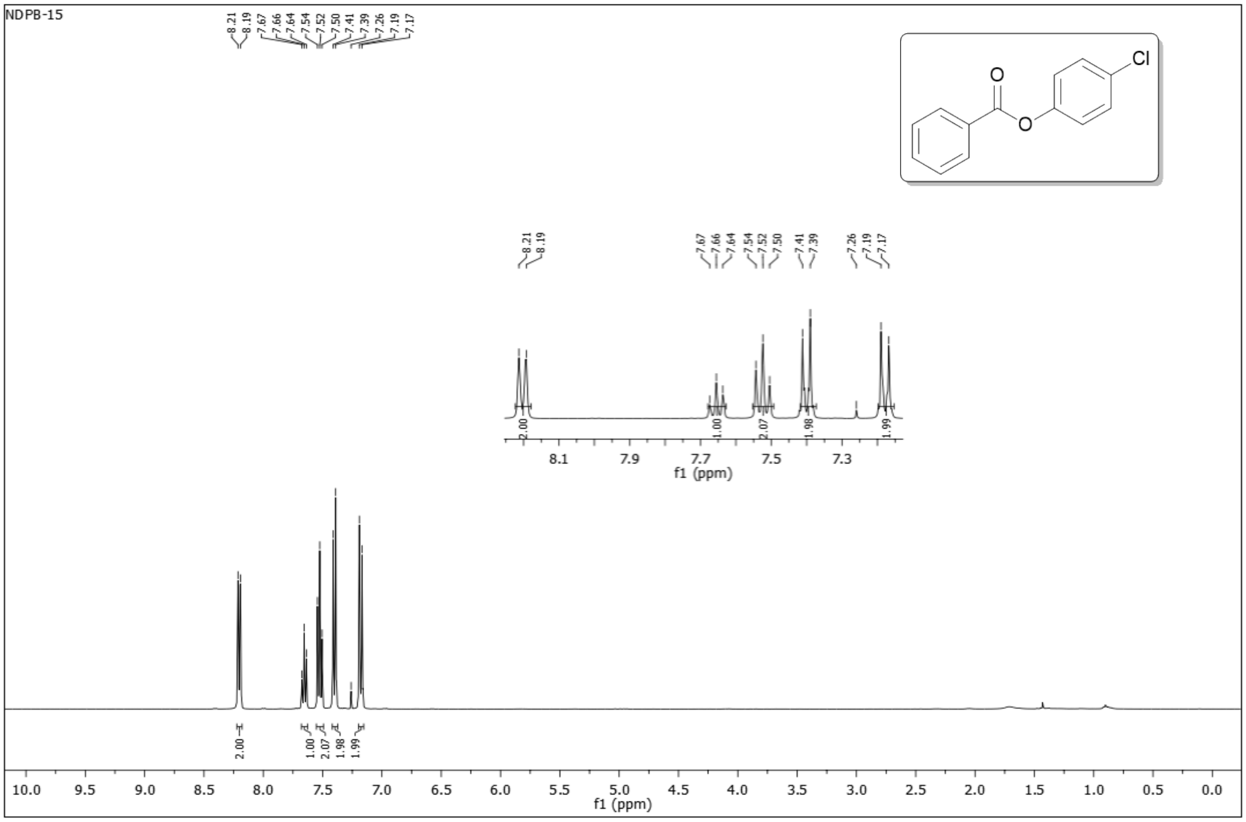

Fig. S25 ^{1}H NMR spectrum of phenyl 4-nitrobenzoate **4c** (400 MHz, CDCl$_3$)

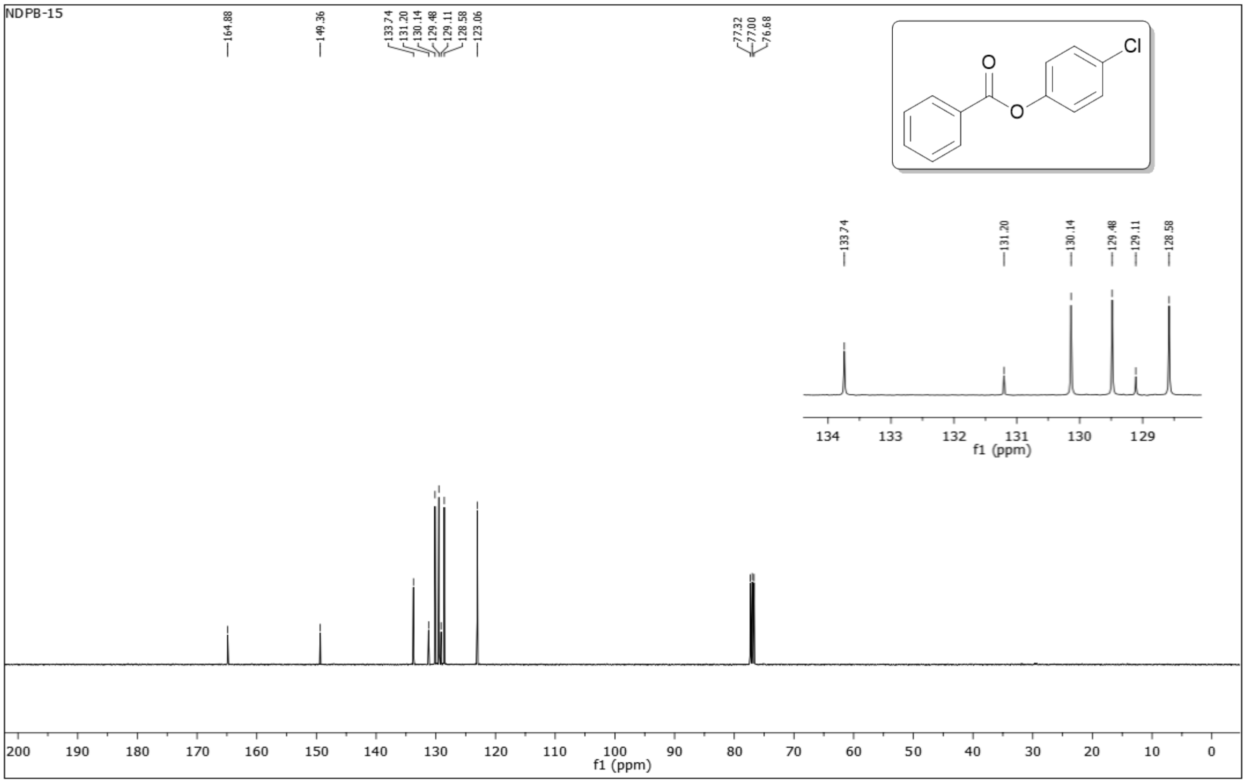

Fig. S26 ^{13}C NMR spectrum of phenyl 4-nitrobenzoate **4c** (100 MHz, CDCl$_3$)

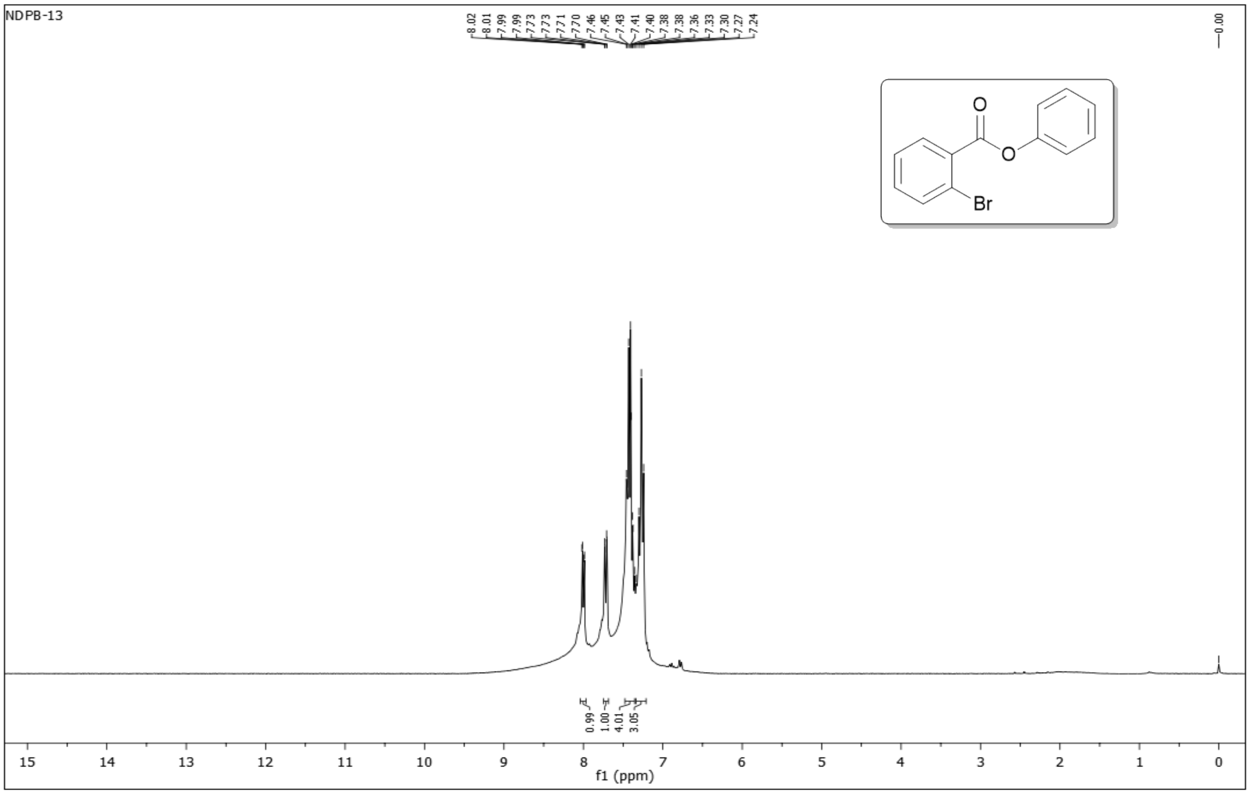

Fig. S27 ^{1}H NMR spectrum of phenyl 2-bromobenzoate **4d** (300 MHz, $CDCl_3$)

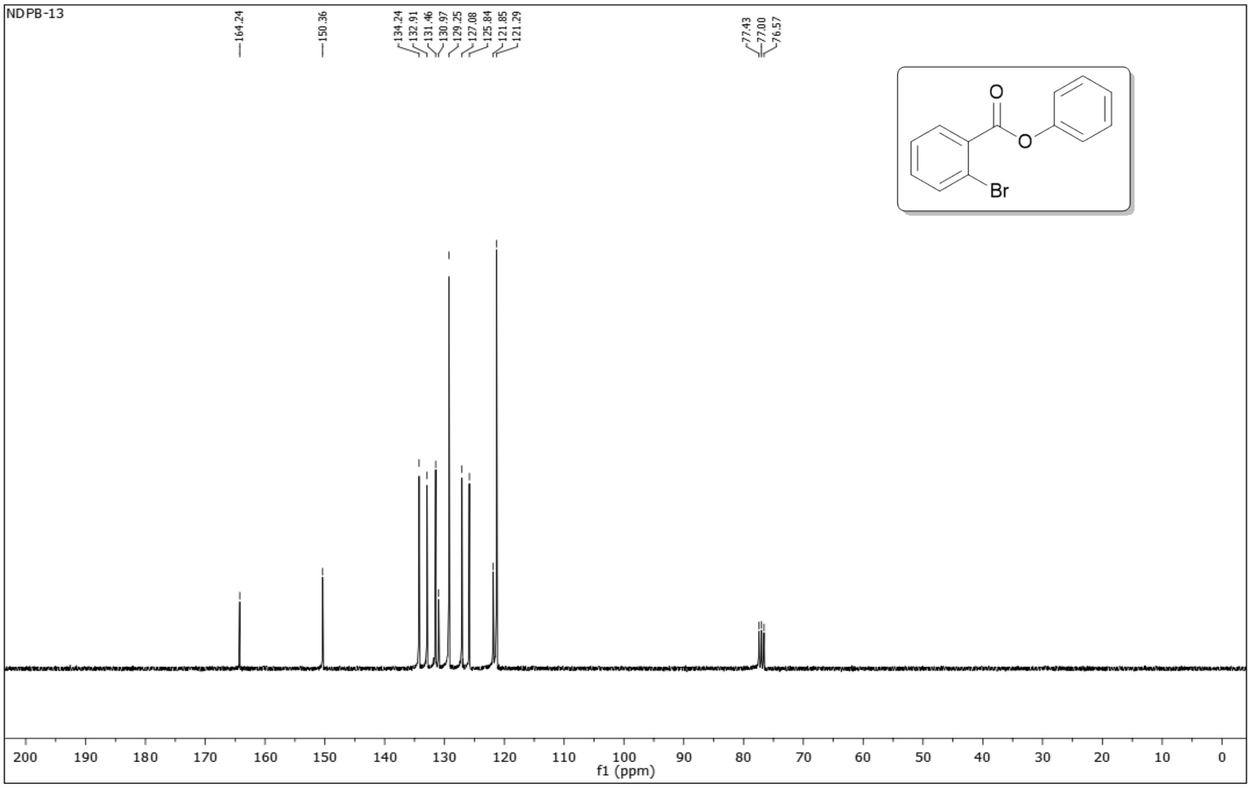

Fig. S28 ^{13}C NMR spectrum of phenyl 2-bromobenzoate **4d** (75 MHz, $CDCl_3$)

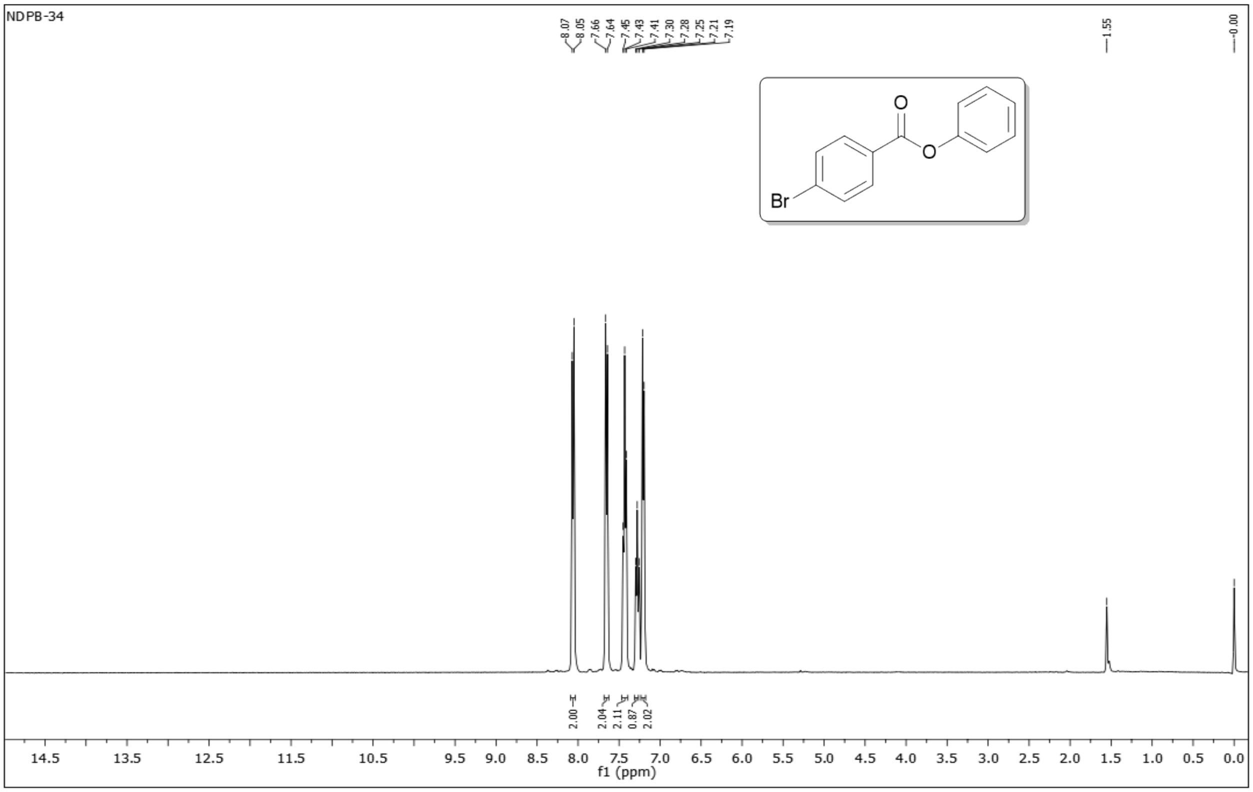

Fig. S29 ^{1}H NMR spectrum of phenyl 4-bromobenzoate **4e** (400 MHz, $CDCl_3$)

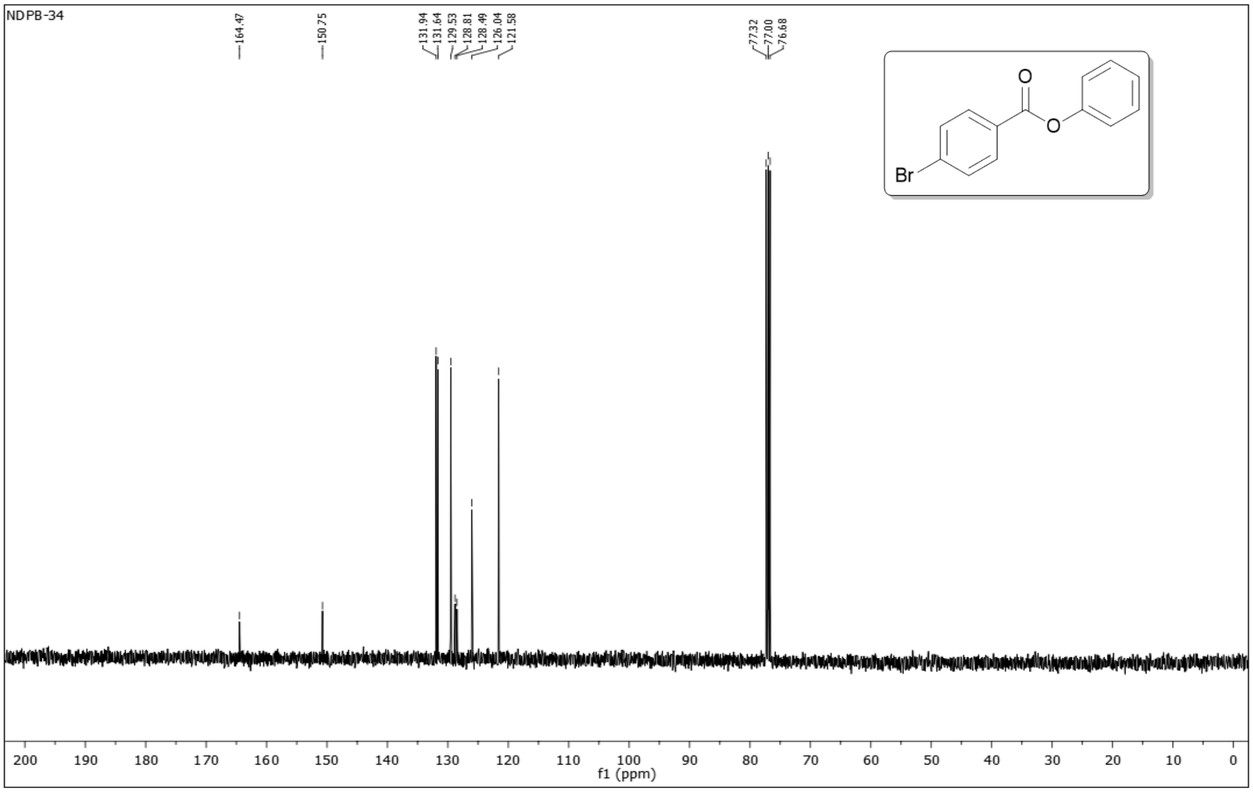

Fig. S30 ^{13}C NMR spectrum of phenyl 4-bromobenzoate **4e** (100 MHz, $CDCl_3$)

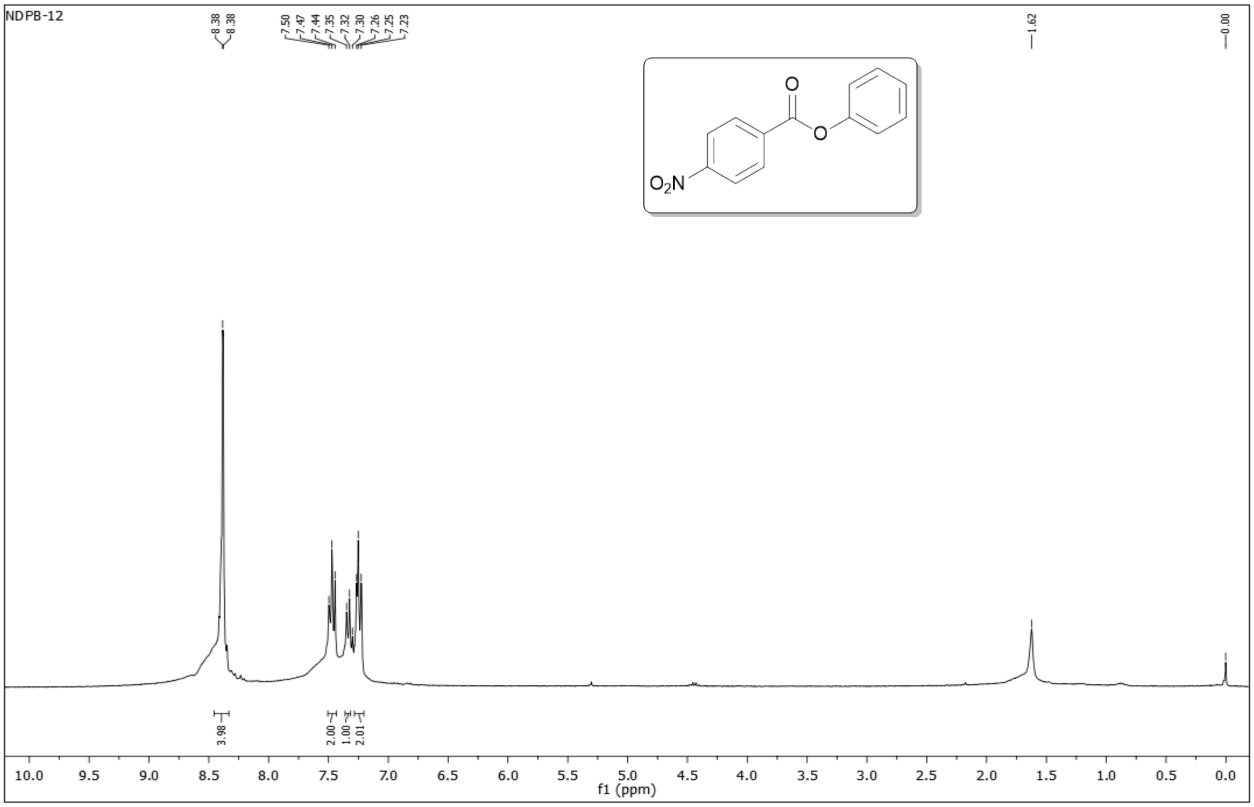

Fig. S31 ^{1}H NMR spectrum of phenyl 4-nitrobenzoate **4f** (300 MHz, $CDCl_3$)

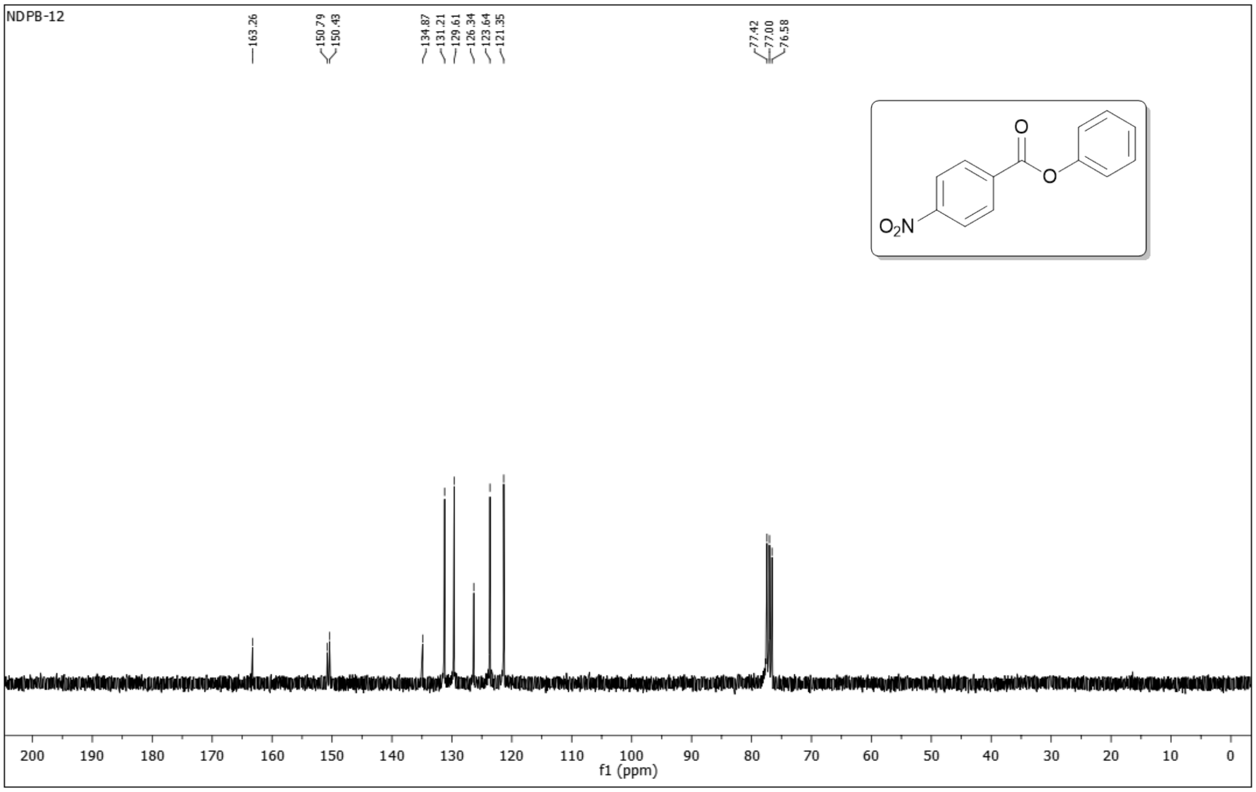

Fig. S32 ^{13}C NMR spectrum of phenyl 4-nitrobenzoate **4f** (75 MHz, $CDCl_3$)

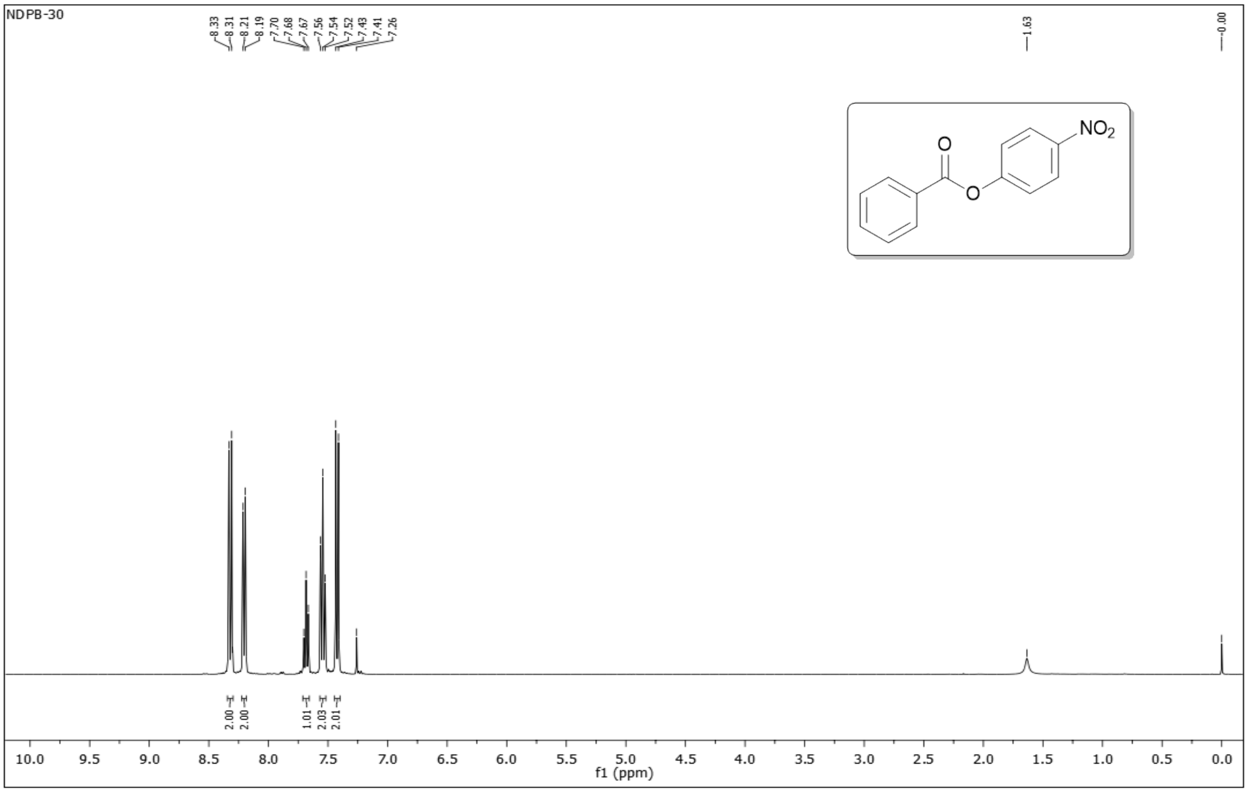

Fig. S33 ^{1}H NMR spectrum of 4-nitrophenyl benzoate **4g** (400 MHz, $CDCl_3$)

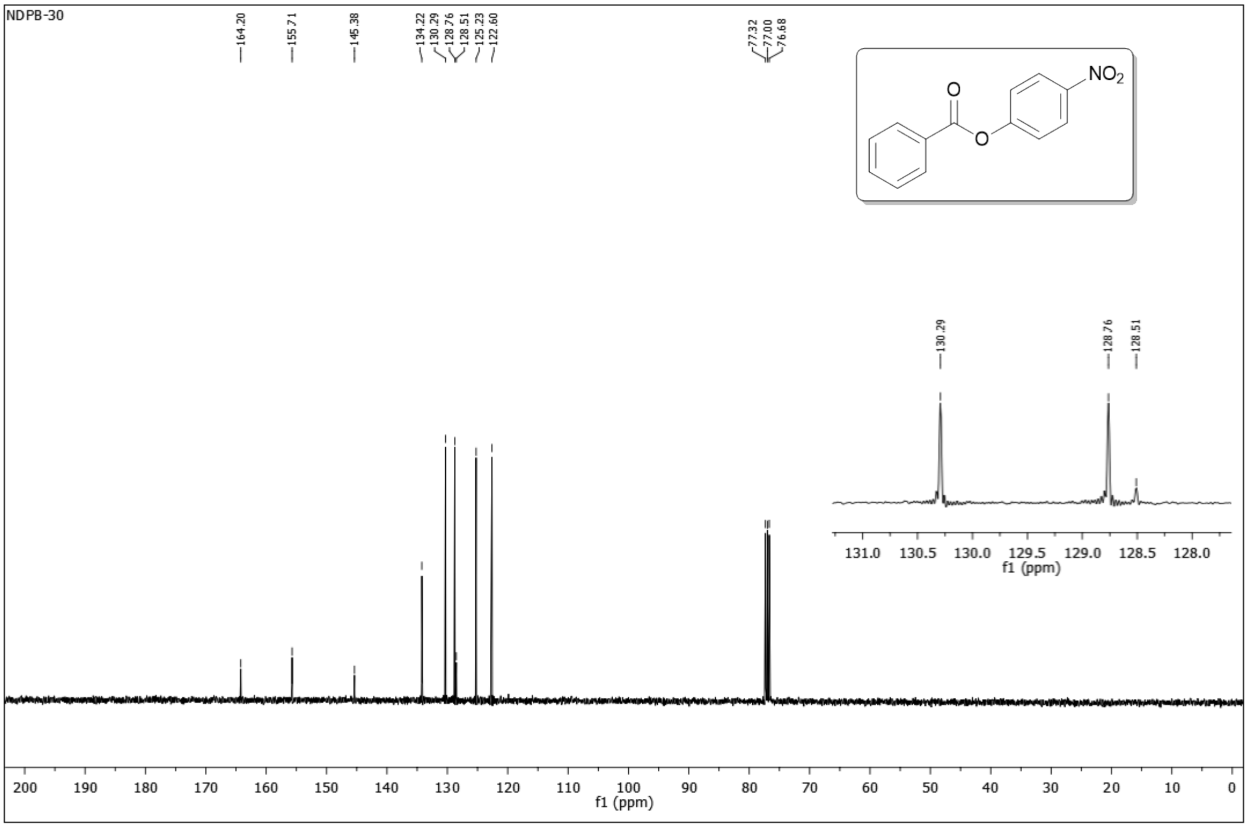

Fig. S34 ^{13}C NMR spectrum of 4-nitrophenyl benzoate **4g** (100 MHz, $CDCl_3$)

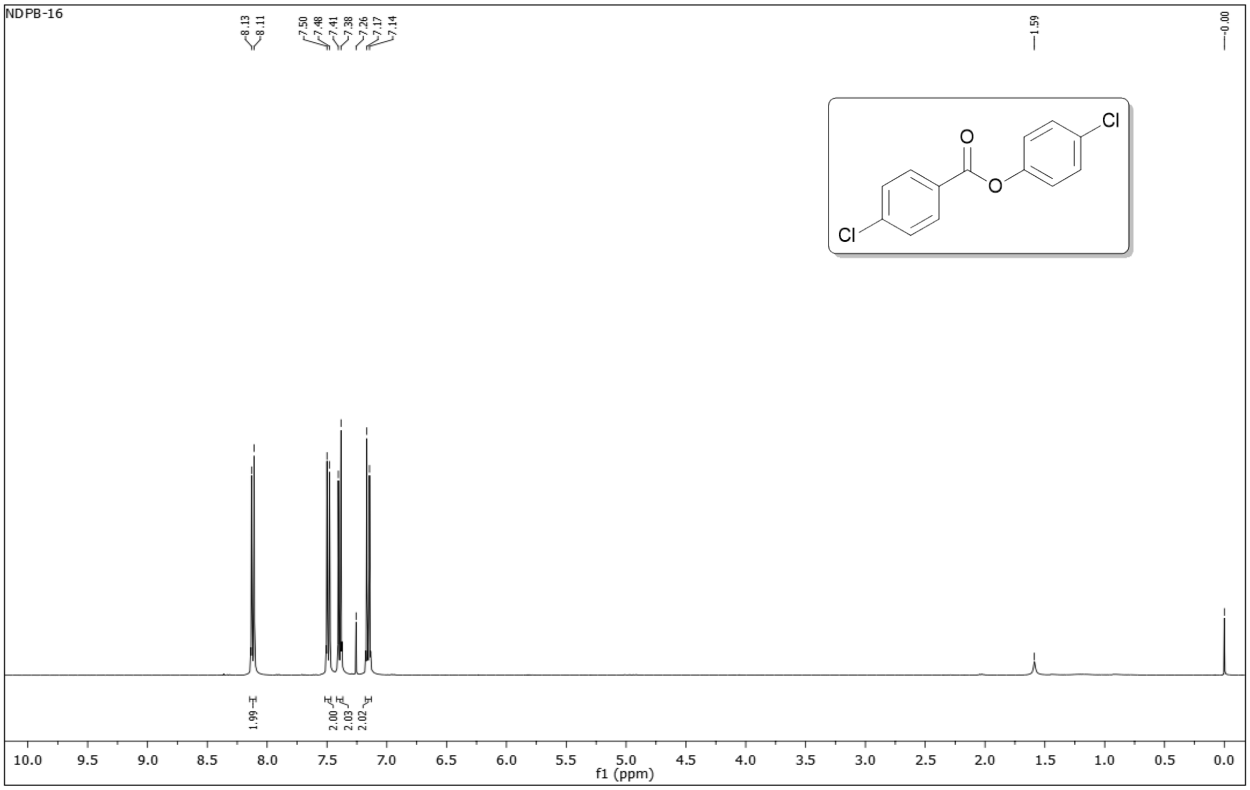

Fig. S35 ^{1}H NMR spectrum of 4-chlorophenyl 4-chlorobenzoate **4h** (400 MHz, $CDCl_3$)

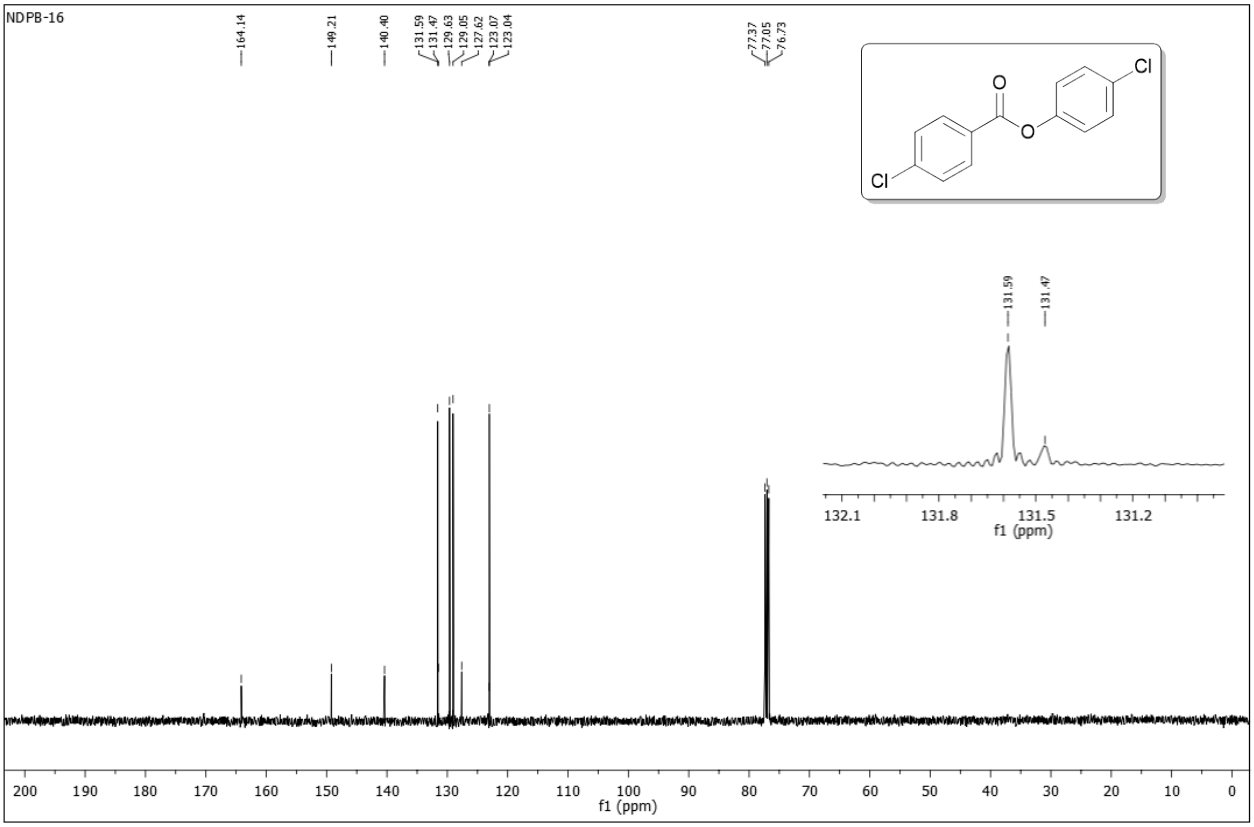

Fig. S36 ^{13}C NMR spectrum of 4-chlorophenyl 4-chlorobenzoate **4h** (100 MHz, $CDCl_3$)

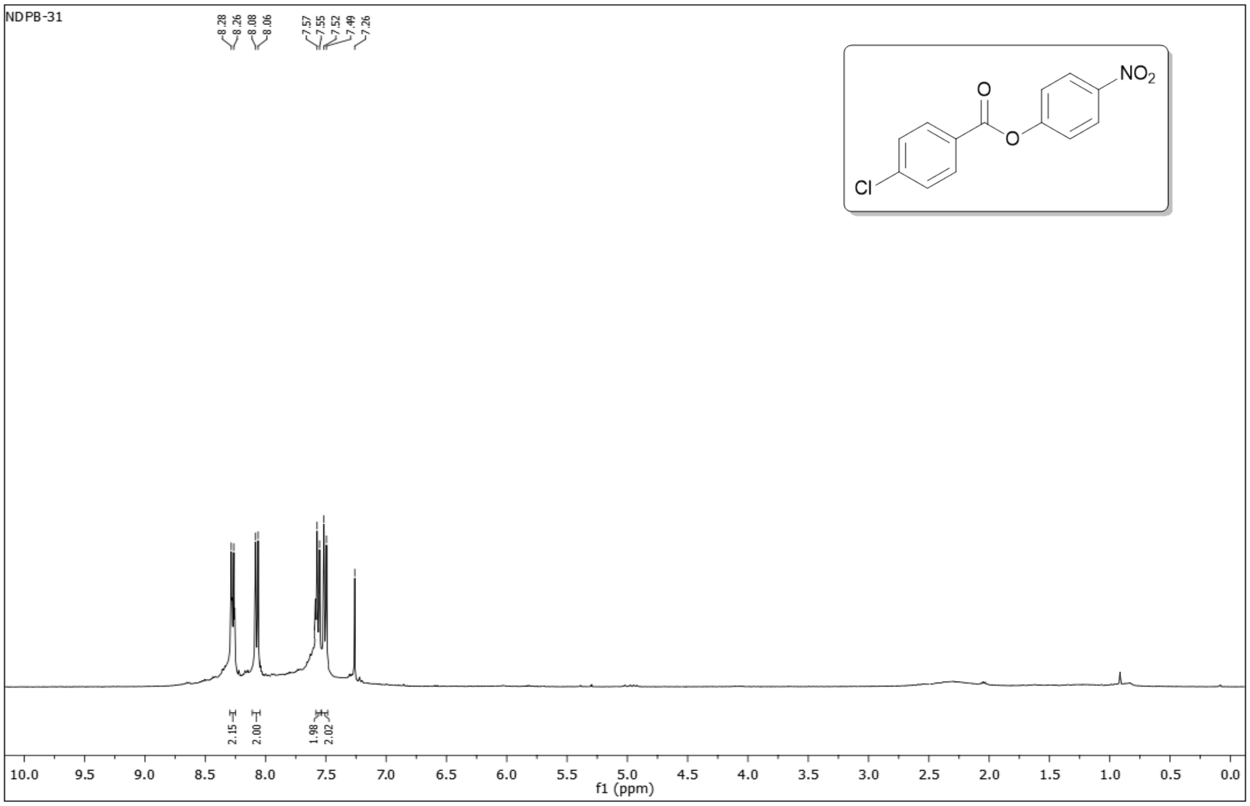

Fig. S37 ^{1}H NMR spectrum of 4-nitrophenyl 4-chlorobenzoate **4i** (400 MHz, $CDCl_3$)

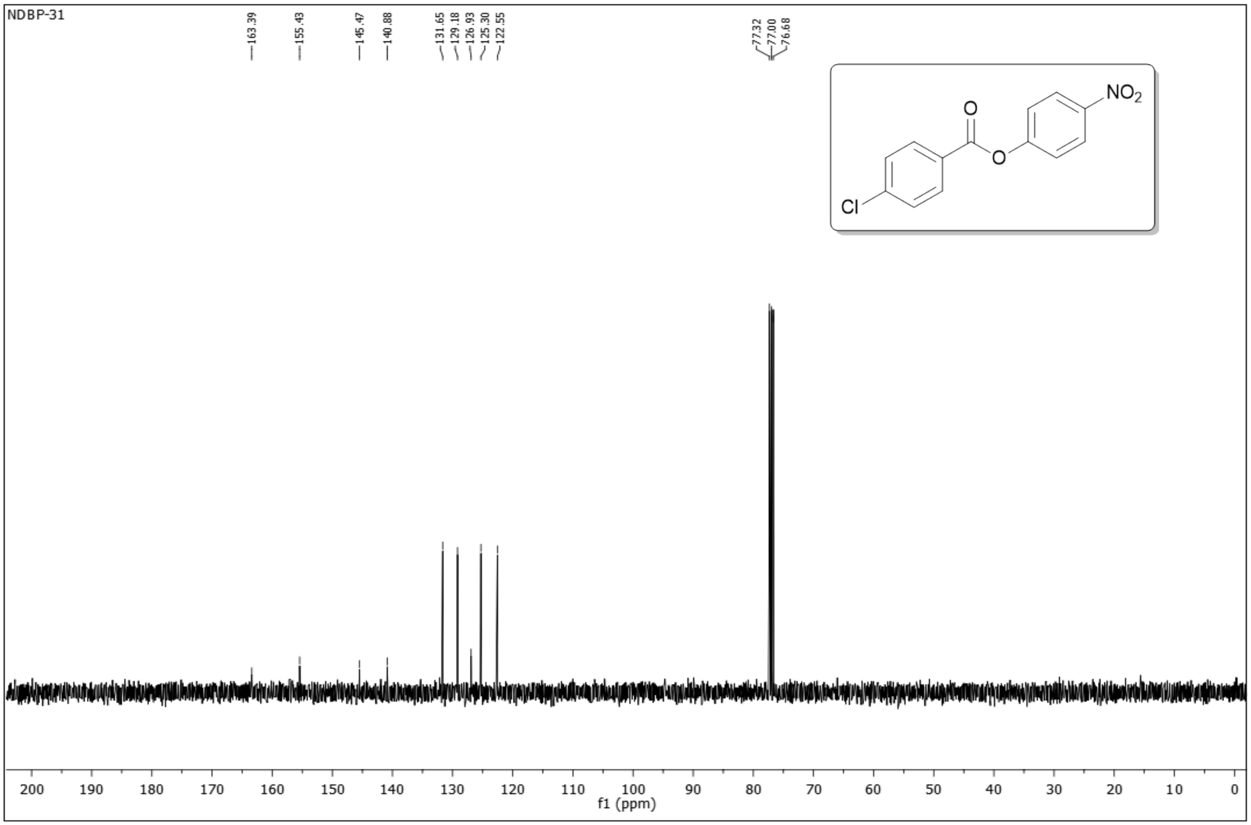

Fig. S38 ^{13}C NMR spectrum of 4-nitrophenyl 4-chlorobenzoate **4i** (100 MHz, $CDCl_3$)

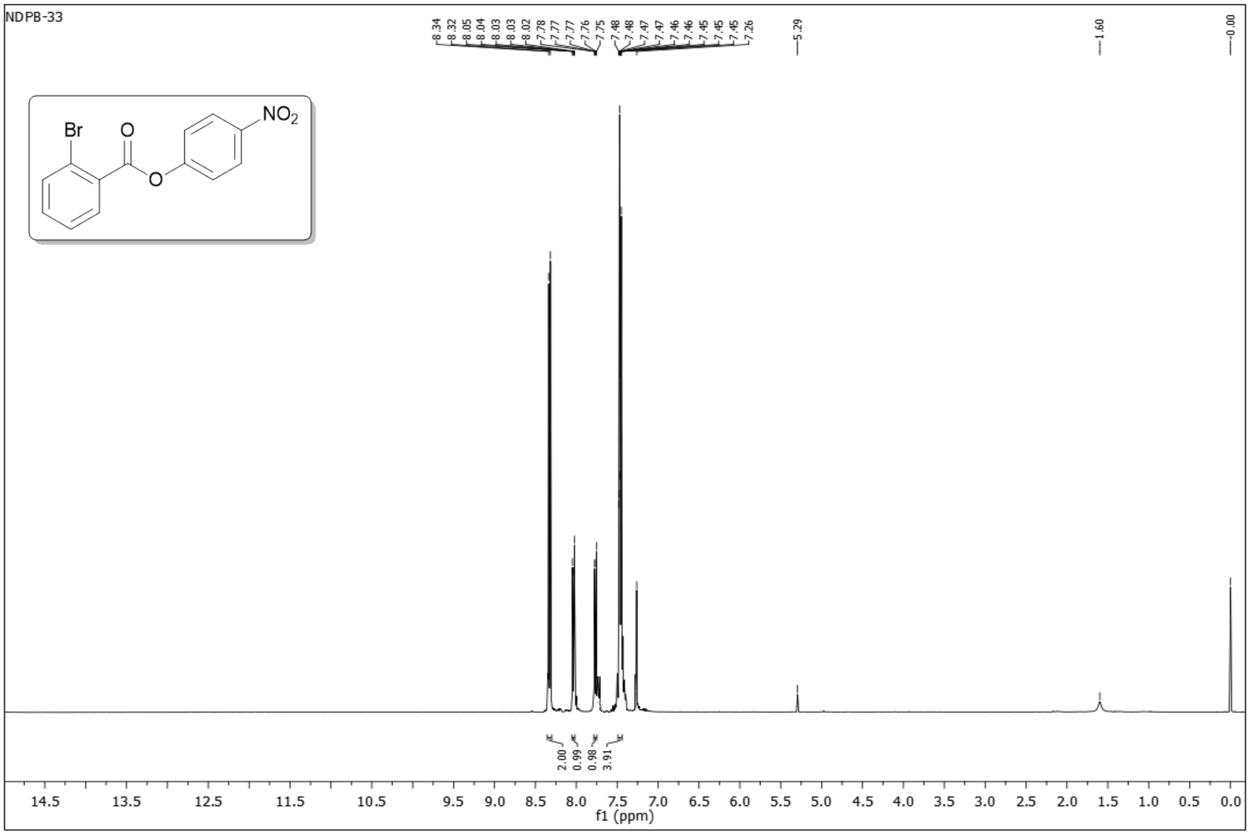

Fig. S39 ^{1}H NMR spectrum of 4-nitrophenyl 2-bromobenzoate **4j** (400 MHz, $CDCl_3$)

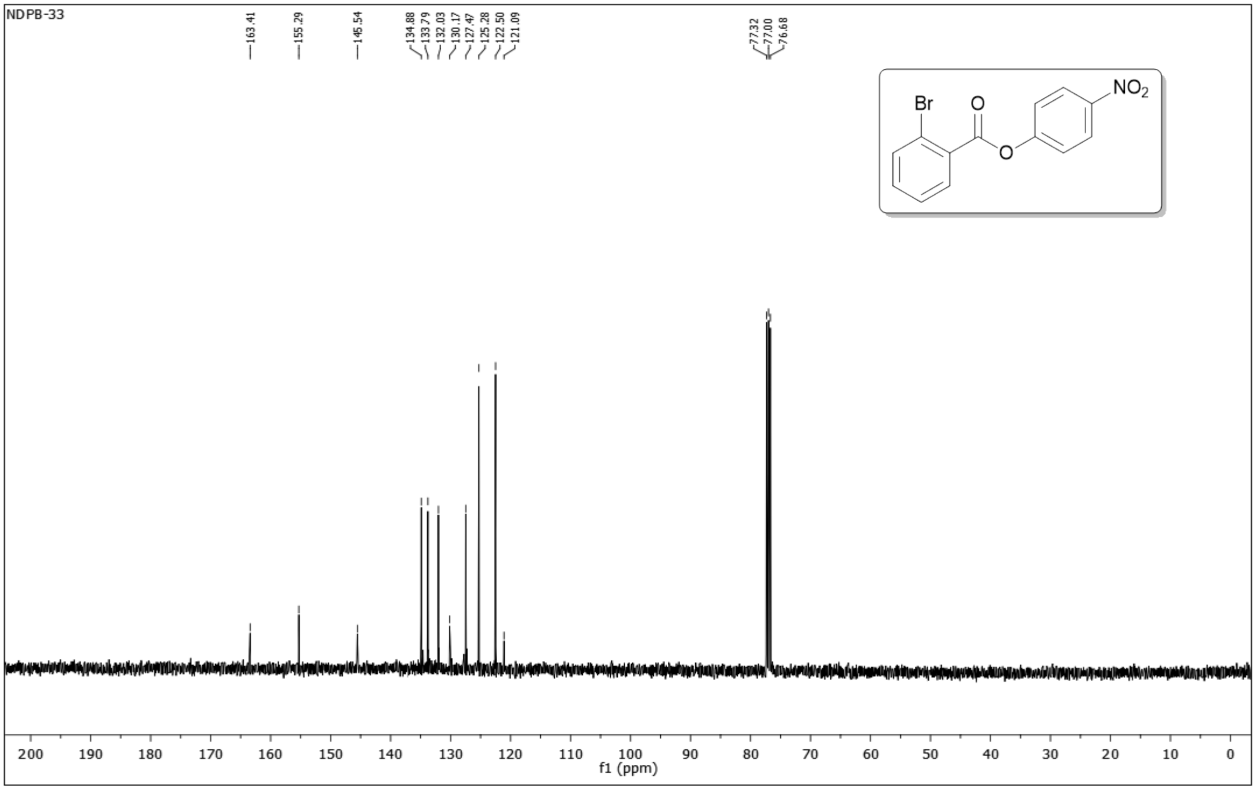

Fig. S40 ^{13}C NMR spectrum of 4-nitrophenyl 2-bromobenzoate **4j** (100 MHz, $CDCl_3$)

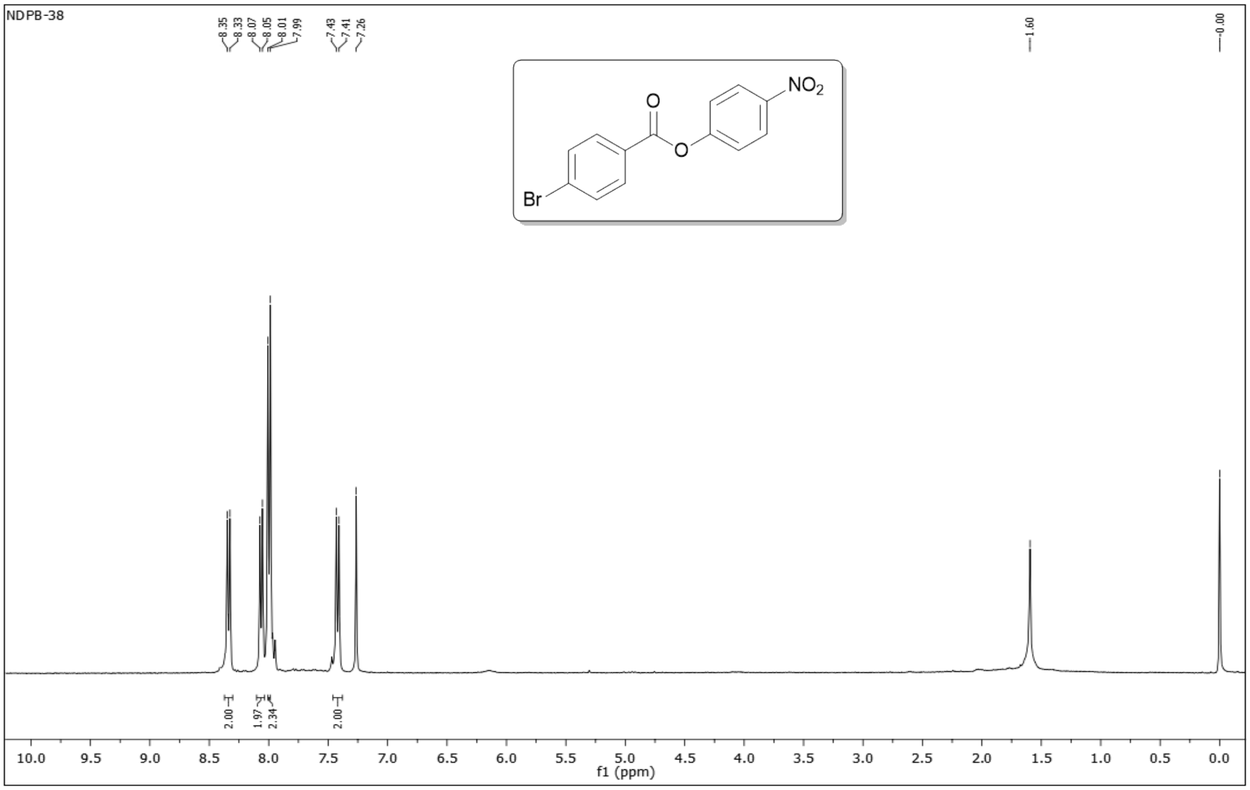

Fig. S41 ^{1}H NMR spectrum of 4-nitrophenyl 4-bromobenzoate **4k** (400 MHz, CDCl$_3$)

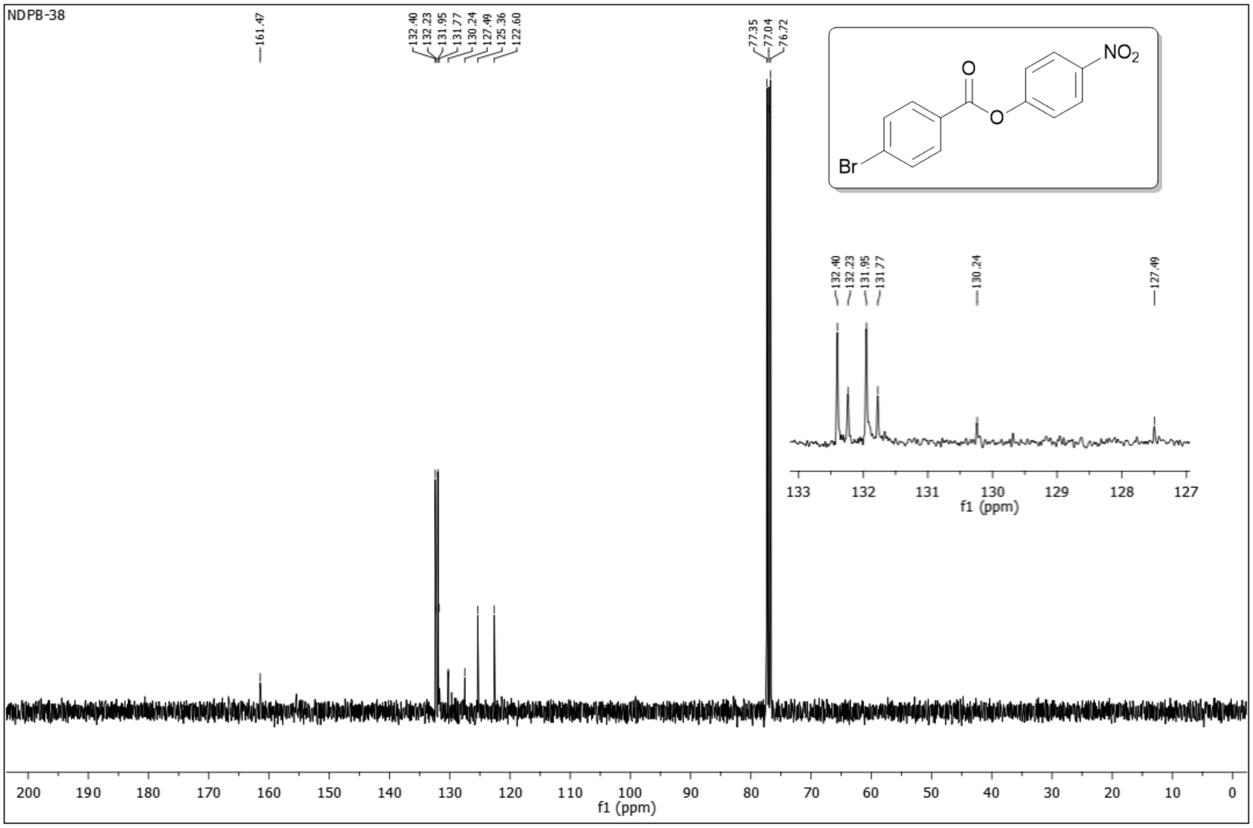

Fig. S42 ^{13}C NMR spectrum of 4-nitrophenyl 4-bromobenzoate **4k** (100 MHz, CDCl$_3$)

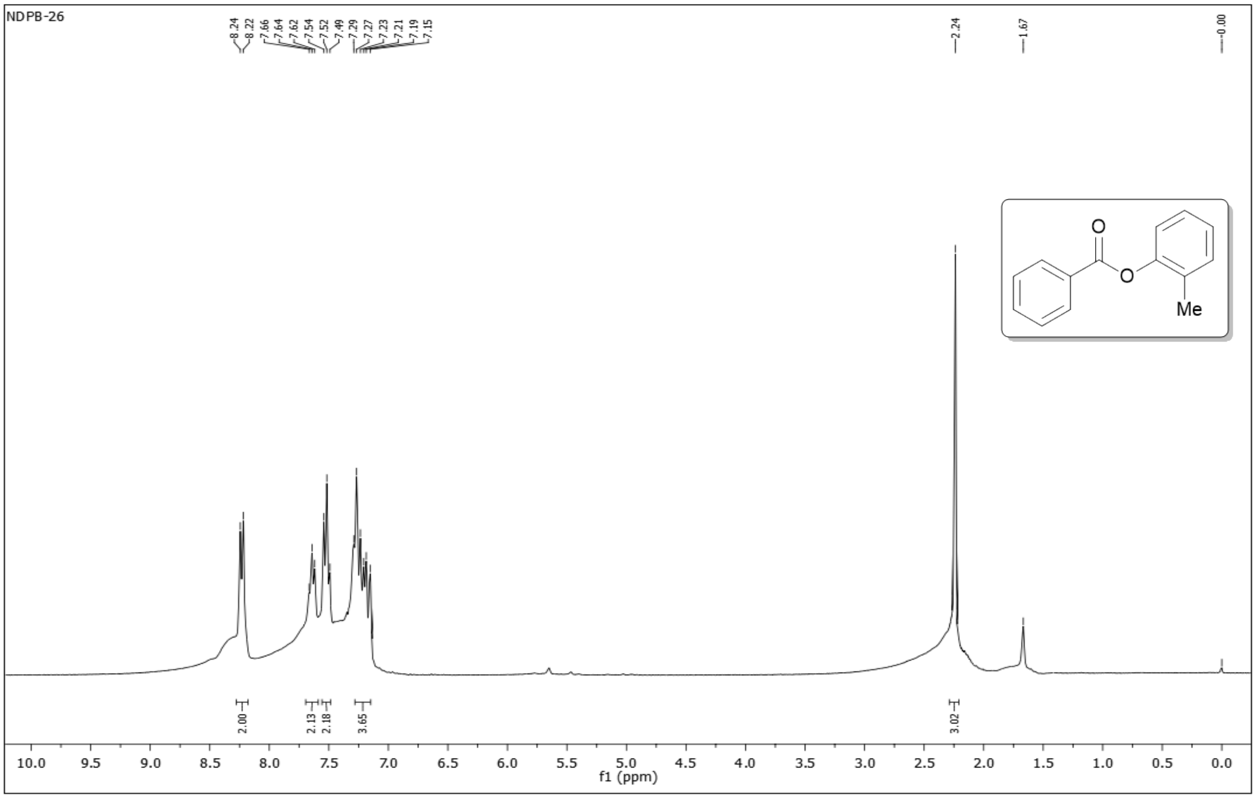

Fig. S43 ^{1}H NMR spectrum of *o*-tolyl benzoate **4l** (300 MHz, $CDCl_3$)

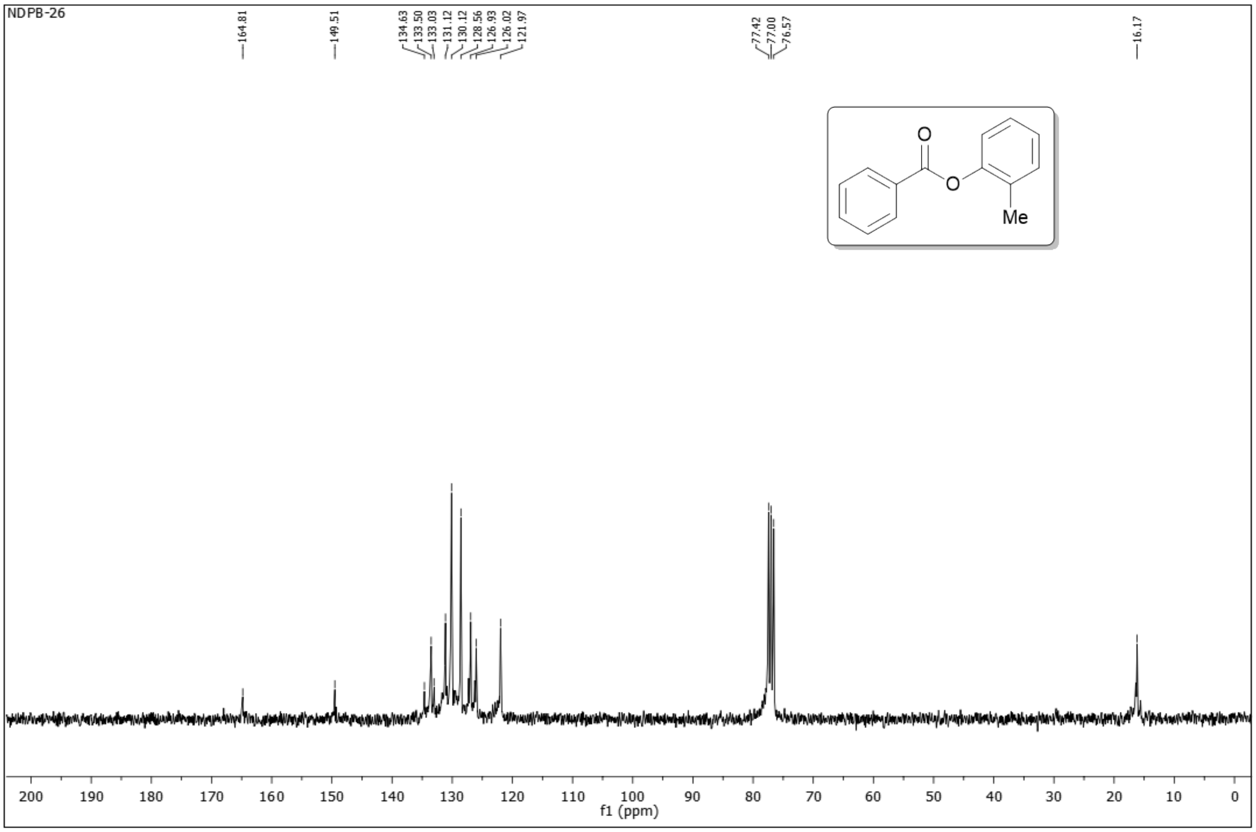

Fig. S44 ^{13}C NMR spectrum of *o*-tolyl benzoate **4l** (75 MHz, $CDCl_3$)

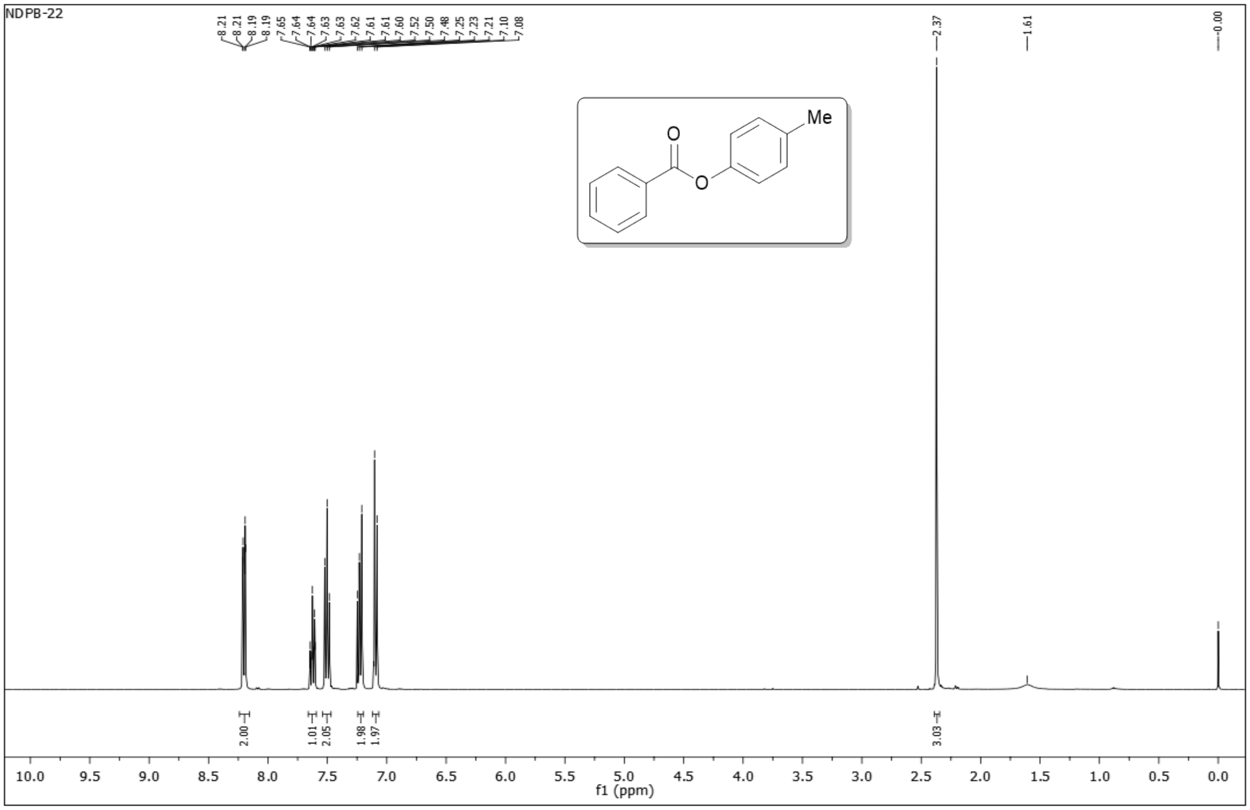

Fig. S45 ^{1}H NMR spectrum of *p*-tolyl benzoate **4m** (400 MHz, $CDCl_3$)

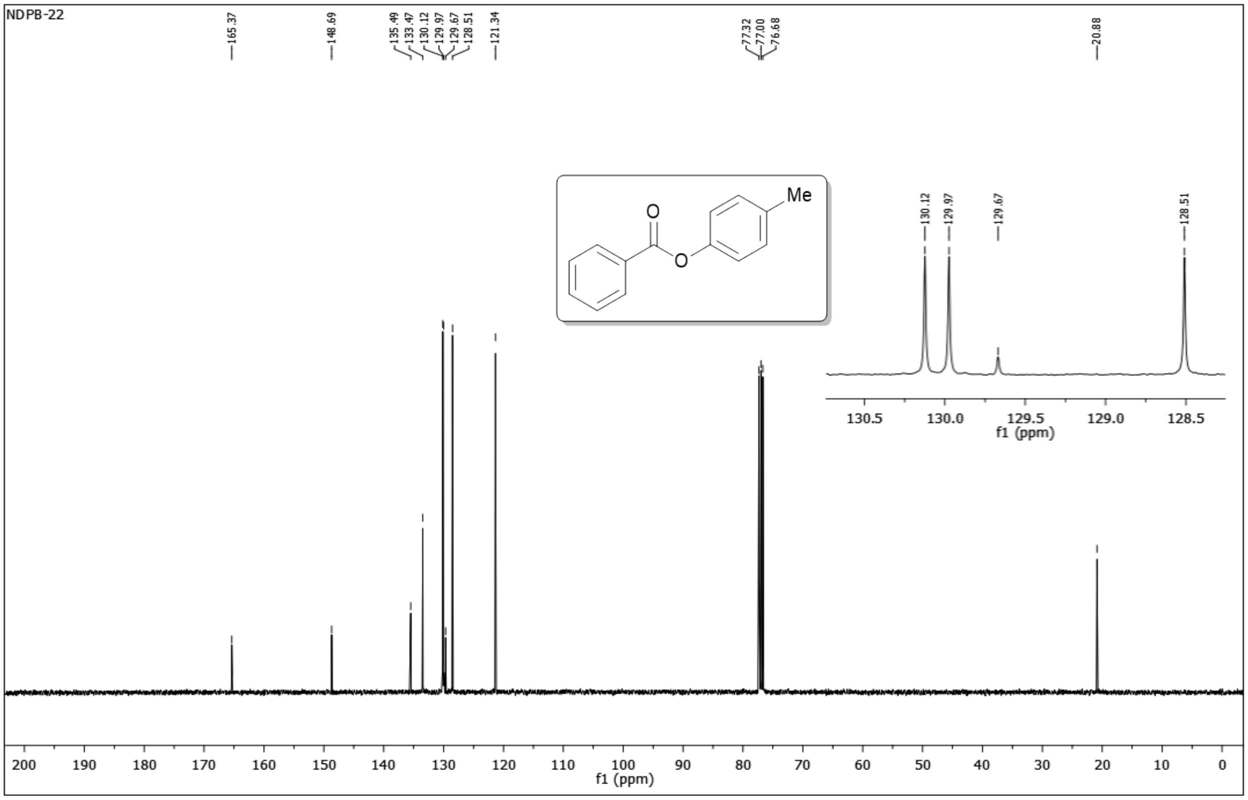

Fig. S46 ^{13}C NMR spectrum of *p*-tolyl benzoate **4m** (100 MHz, $CDCl_3$)

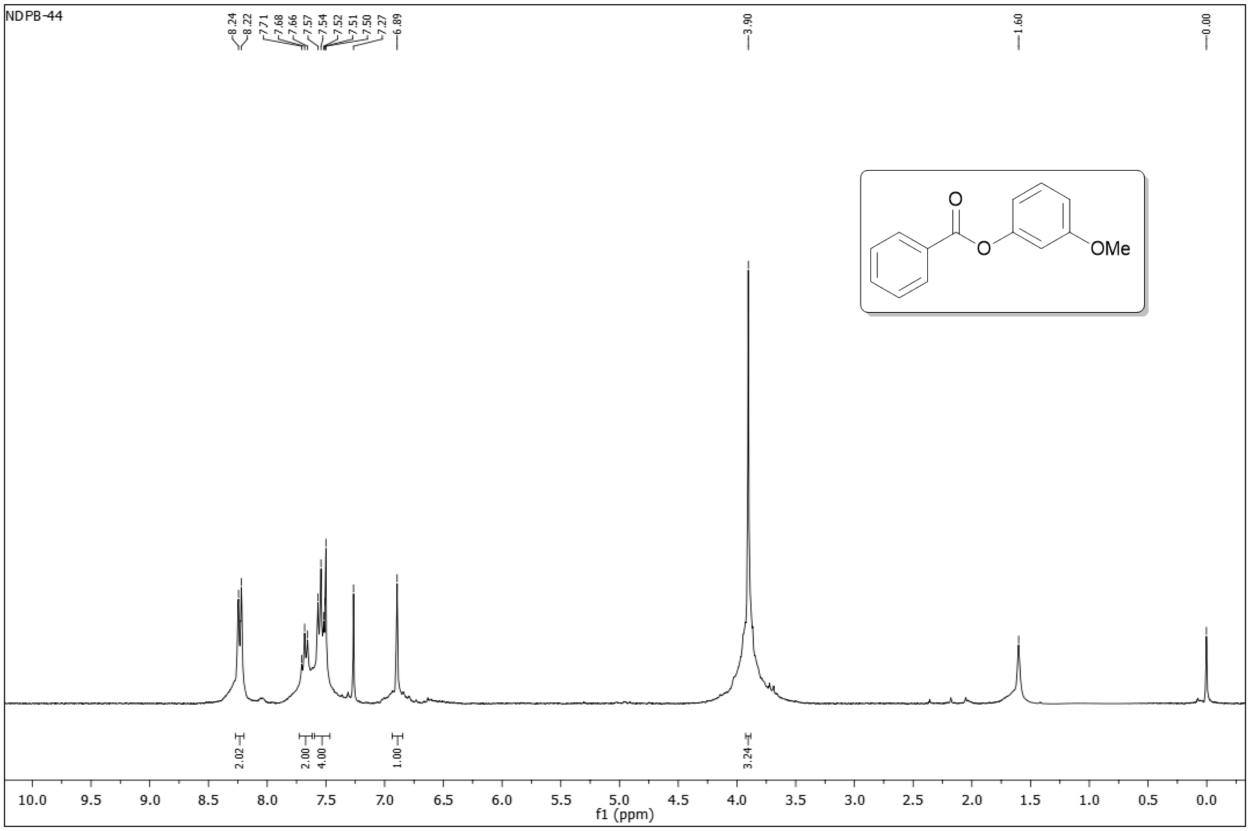

Fig. S47 ^{1}H NMR spectrum of 3-methoxyphenyl benzoate **4n** (300 MHz, $CDCl_3$)

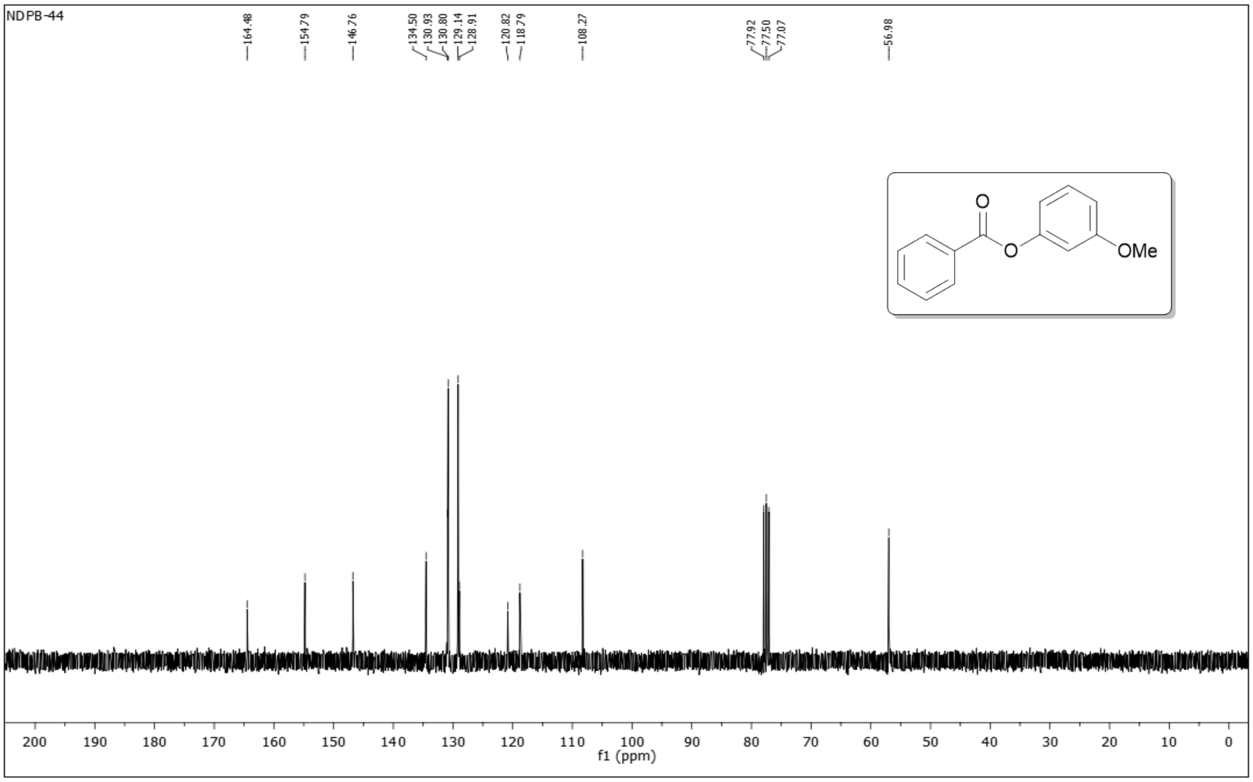

Fig. S48 ^{13}C NMR spectrum of 3-methoxyphenyl benzoate **4n** (75 MHz, $CDCl_3$)

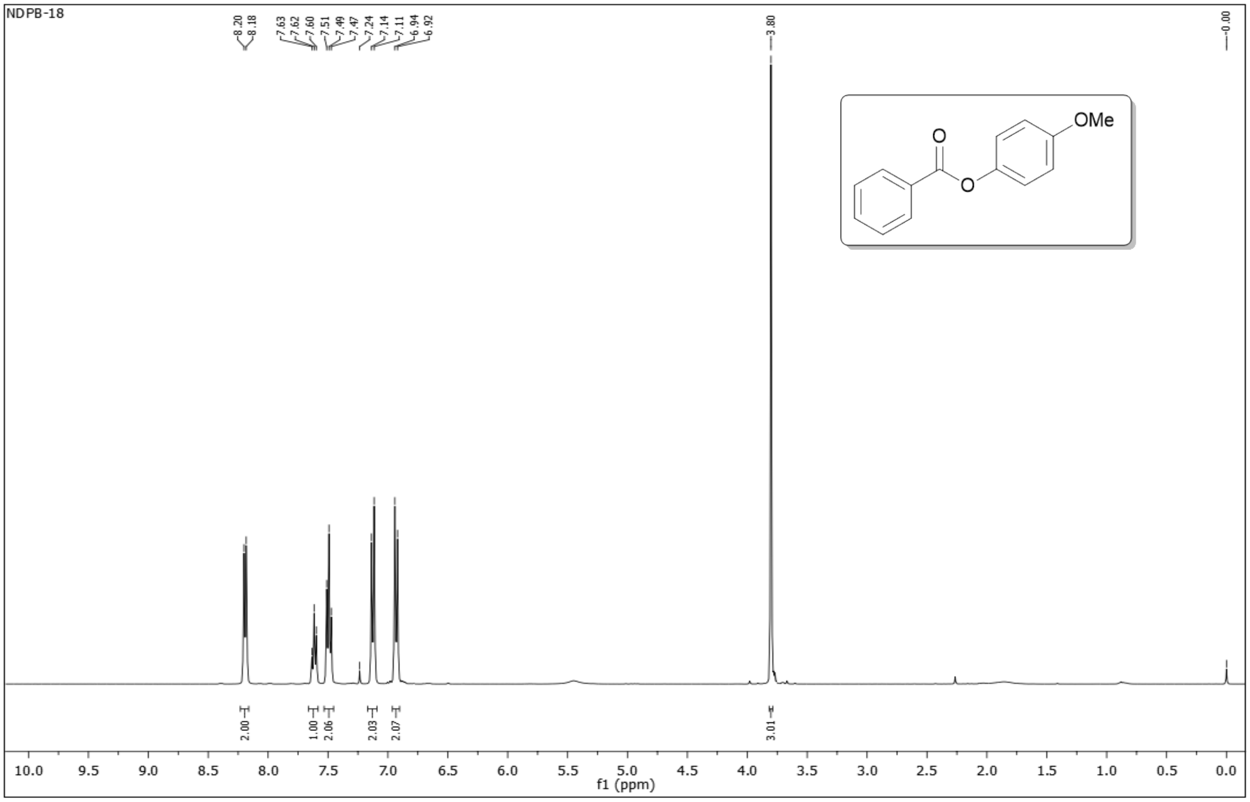

Fig. S49 ^{1}H NMR spectrum of 4-methoxyphenyl benzoate **4o** (400 MHz, CDCl$_3$)

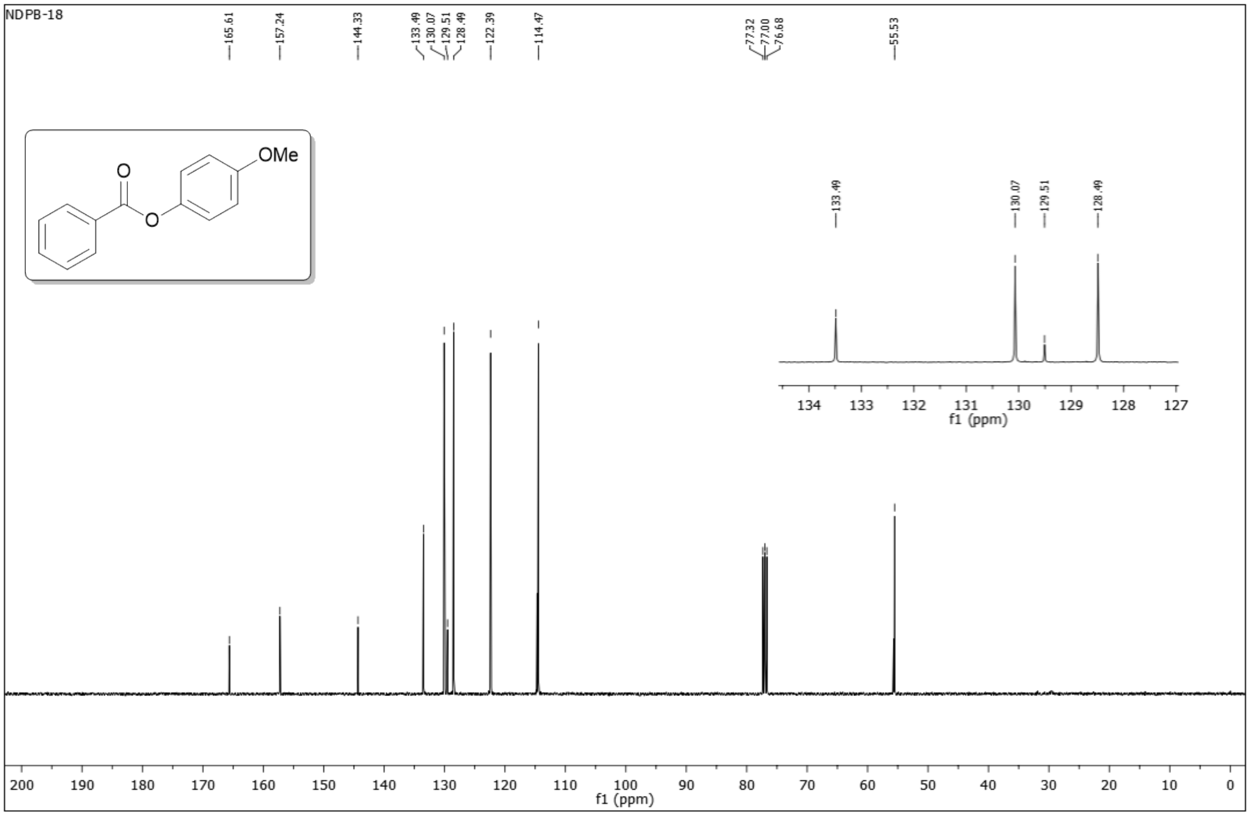

Fig. S50 ^{13}C NMR spectrum of 4-methoxyphenyl benzoate **4o** (100 MHz, CDCl$_3$)

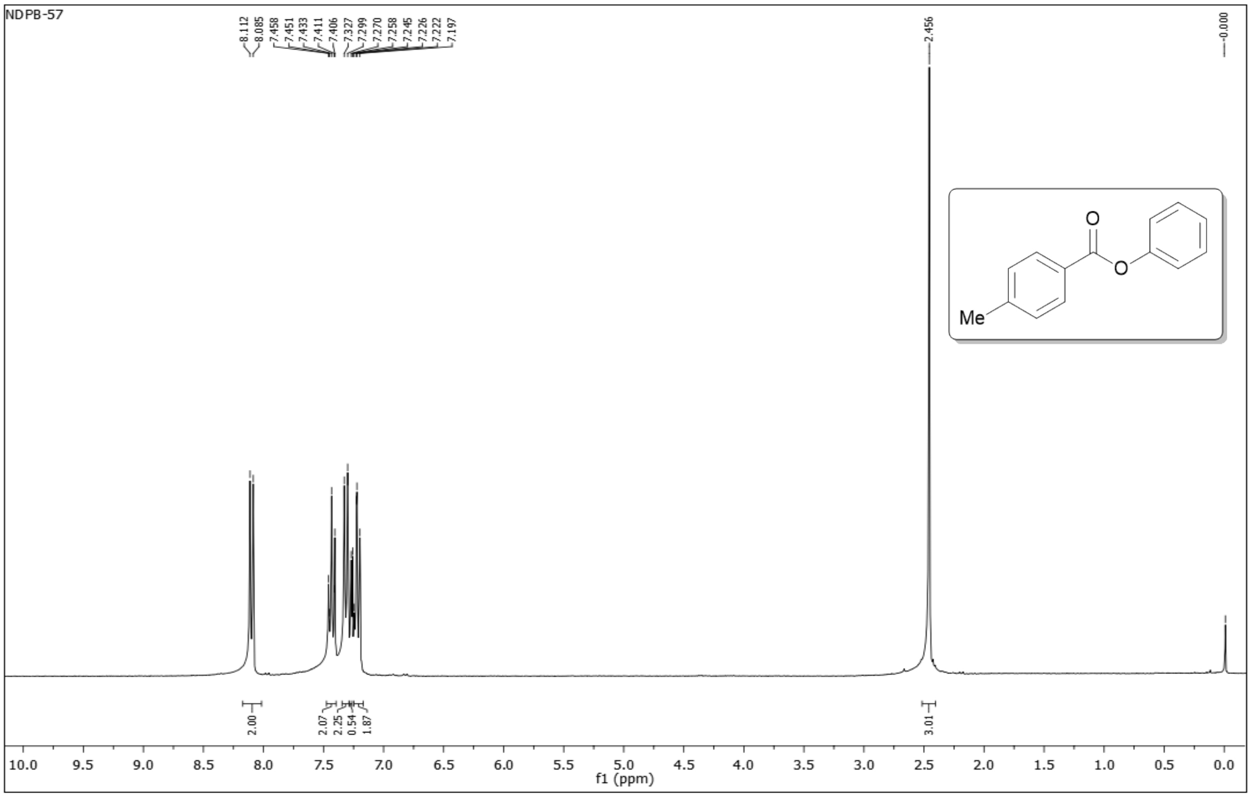

Fig. S51 ^{1}H NMR spectrum of phenyl 4-methylbenzoate **4p** (300 MHz, $CDCl_3$)

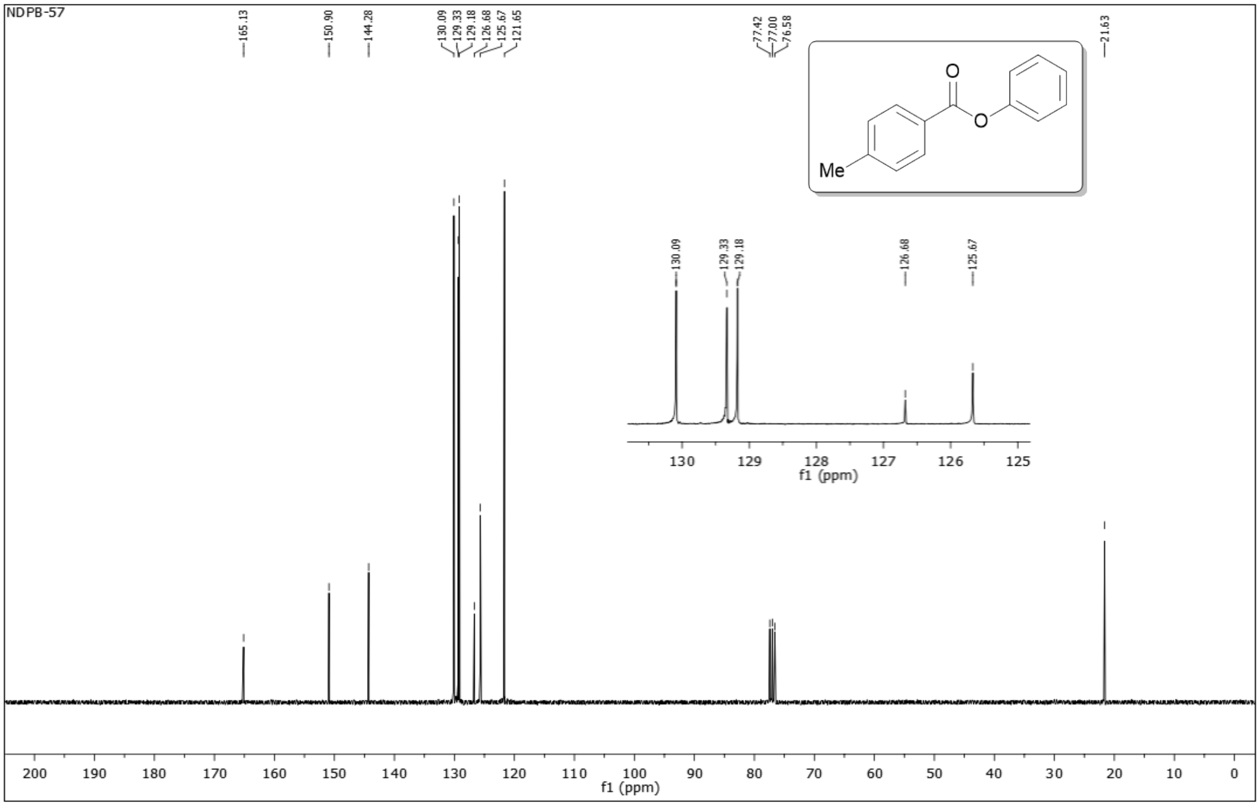

Fig. S52 ^{13}C NMR spectrum of phenyl 4-methylbenzoate **4p** (75 MHz, $CDCl_3$)

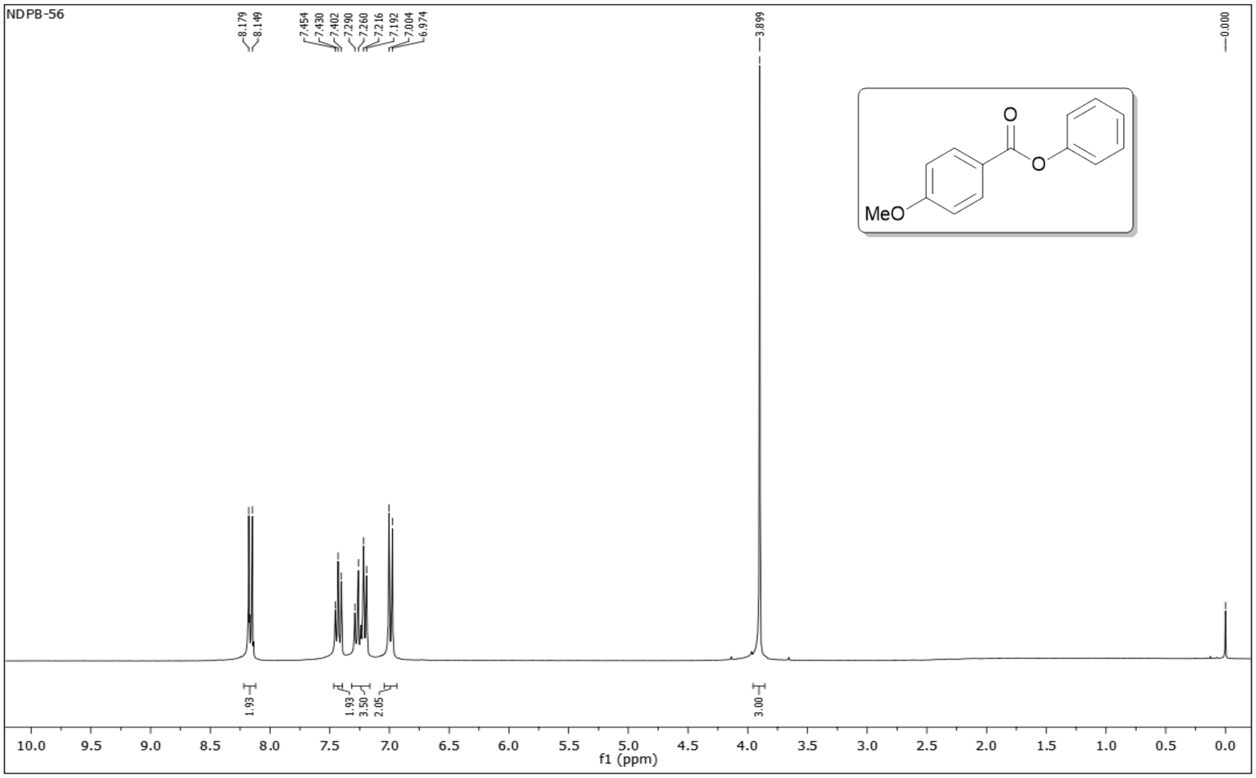

Fig. S53 ^{1}H NMR spectrum of phenyl 4-methoxybenzoate **4q** (300 MHz, $CDCl_3$)

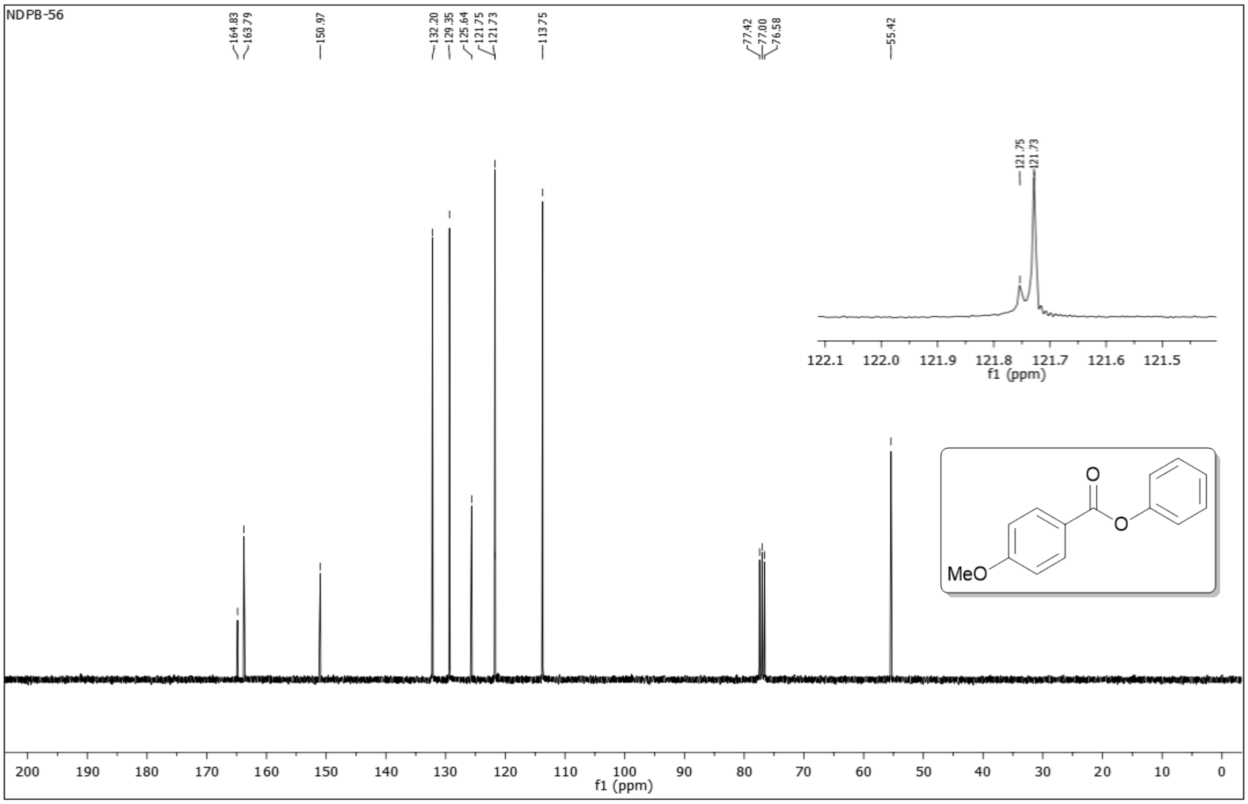

Fig. S54 ^{13}C NMR spectrum of phenyl 4-methoxybenzoate **4q** (75 MHz, $CDCl_3$)

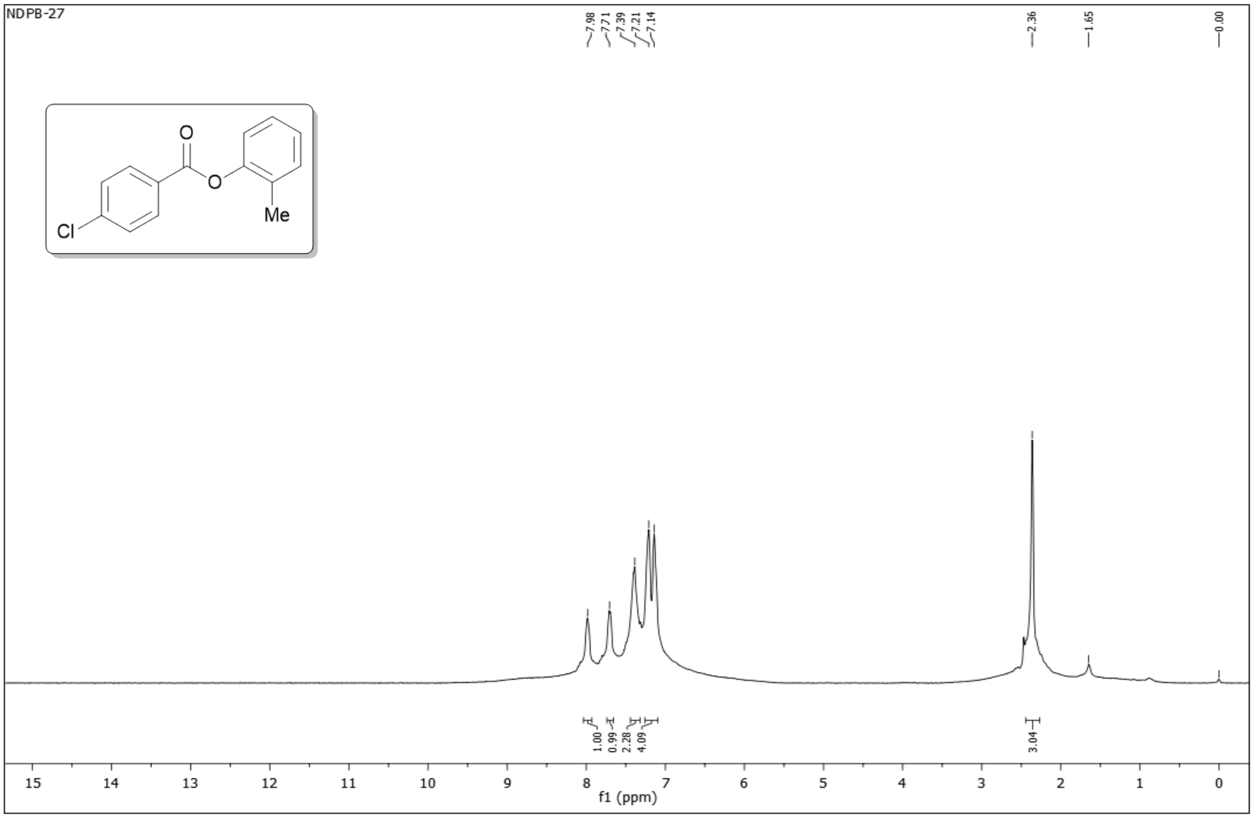

Fig. S55 ^{1}H NMR spectrum of *o*-tolyl 4-chlorobenzoate **4r** (300 MHz, $CDCl_3$)

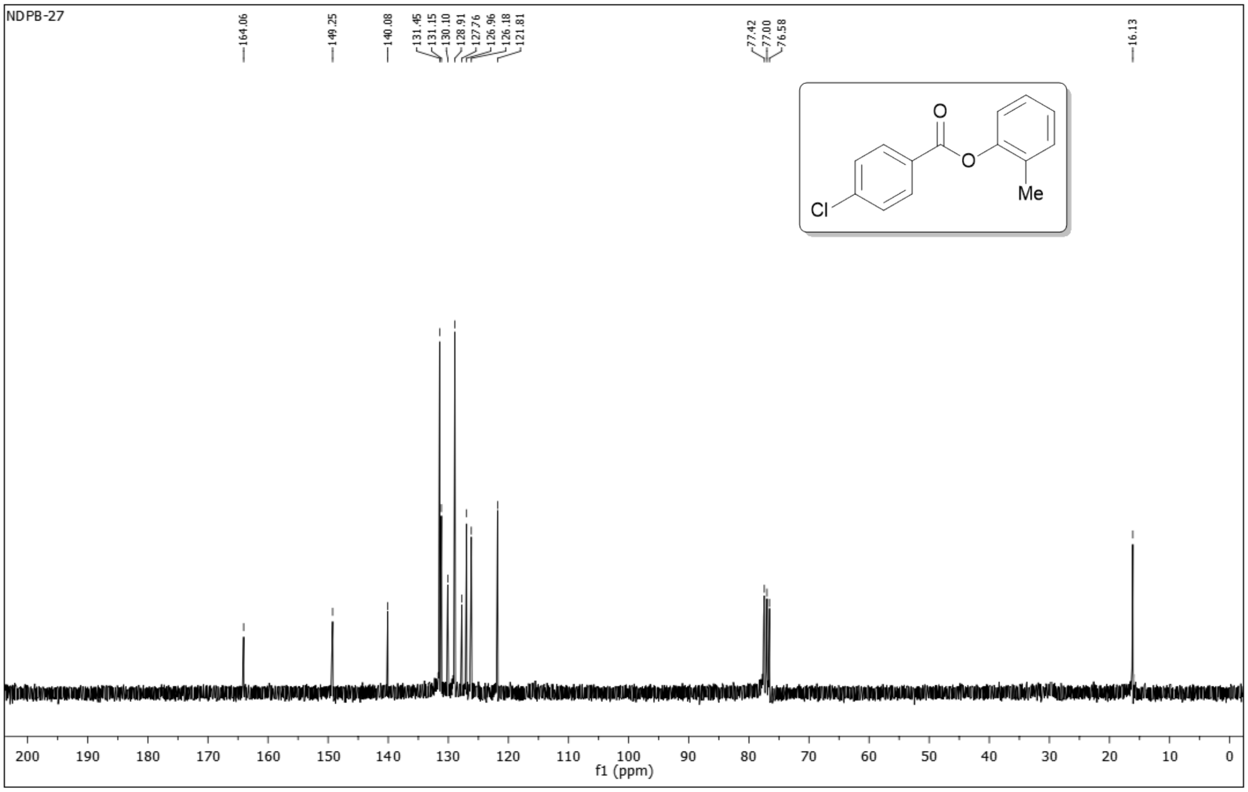

Fig. S56 ^{13}C NMR spectrum of *o*-tolyl 4-chlorobenzoate **4r** (75 MHz, $CDCl_3$)

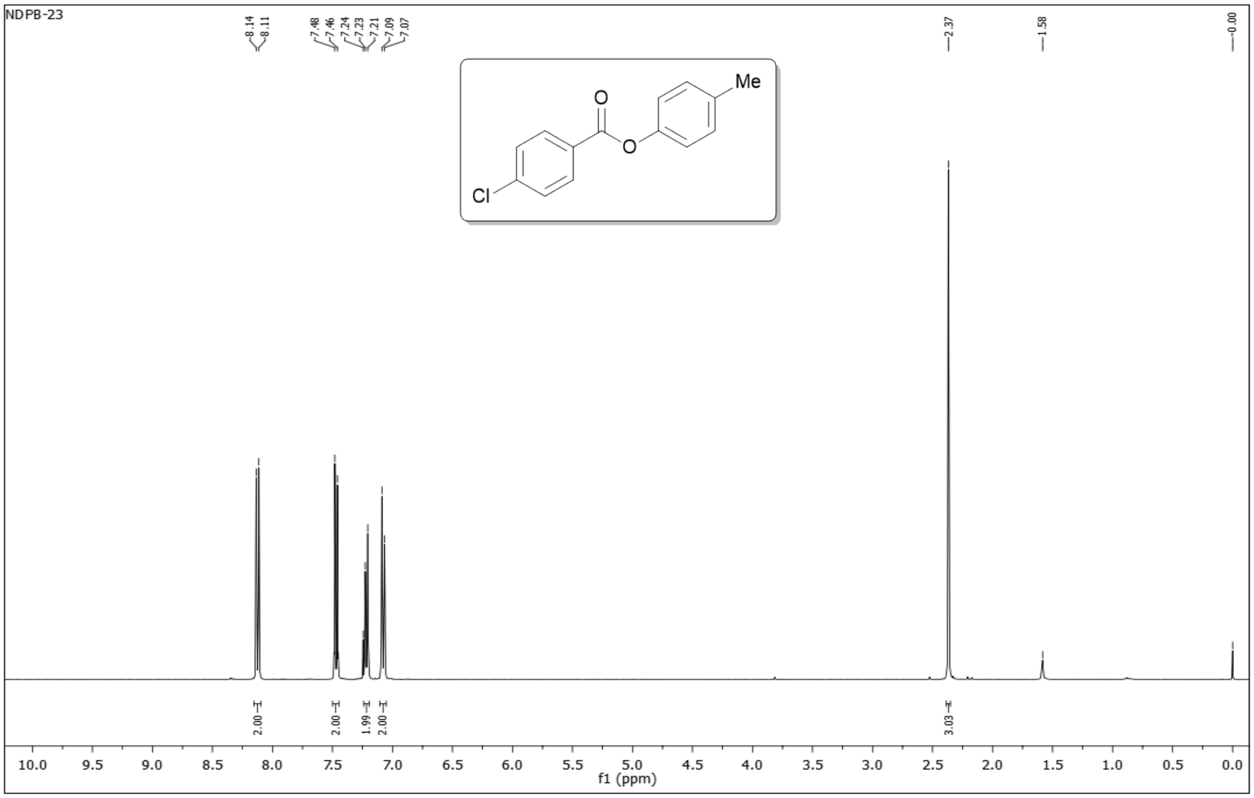

Fig. S57 ^{1}H NMR spectrum of *p*-tolyl 4-chlorobenzoate **4s** (400 MHz, $CDCl_3$)

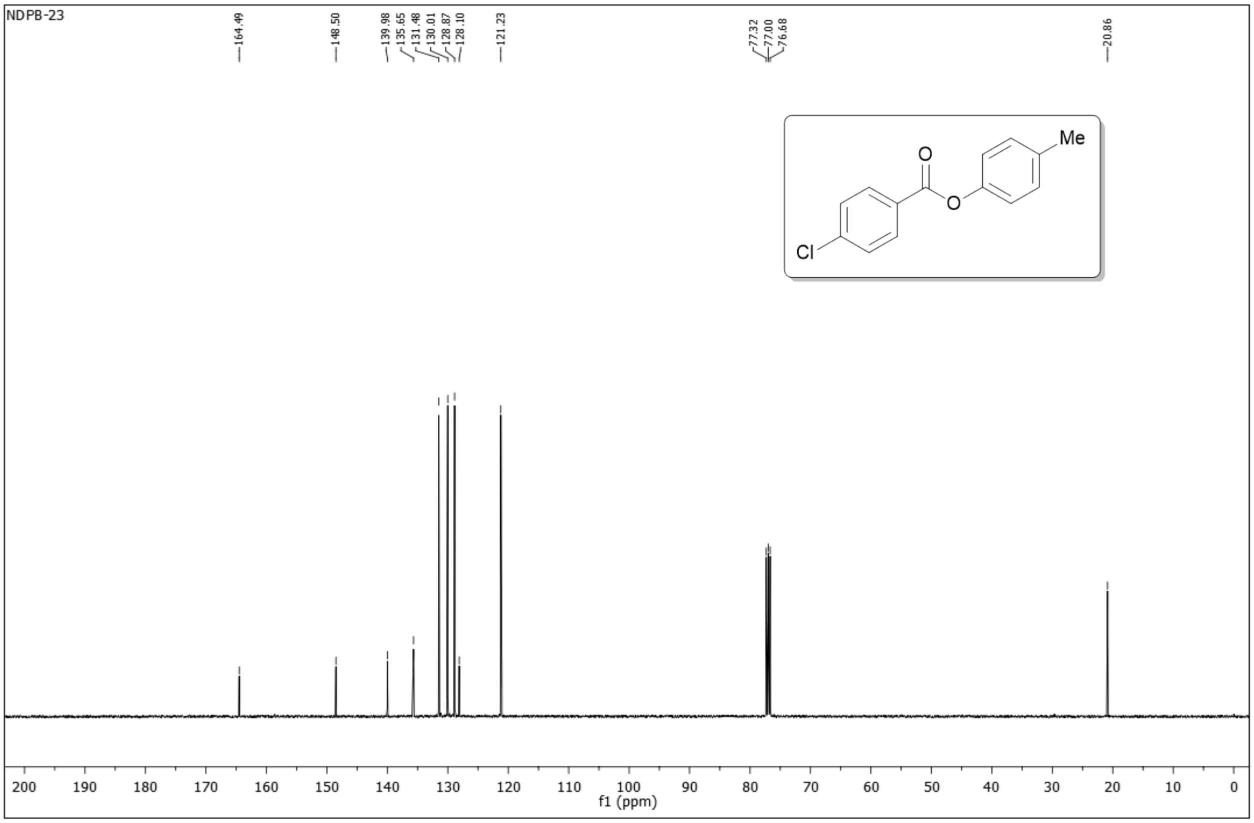

Fig. S58 ^{13}C NMR spectrum of *p*-tolyl 4-chlorobenzoate **4s** (100 MHz, $CDCl_3$)

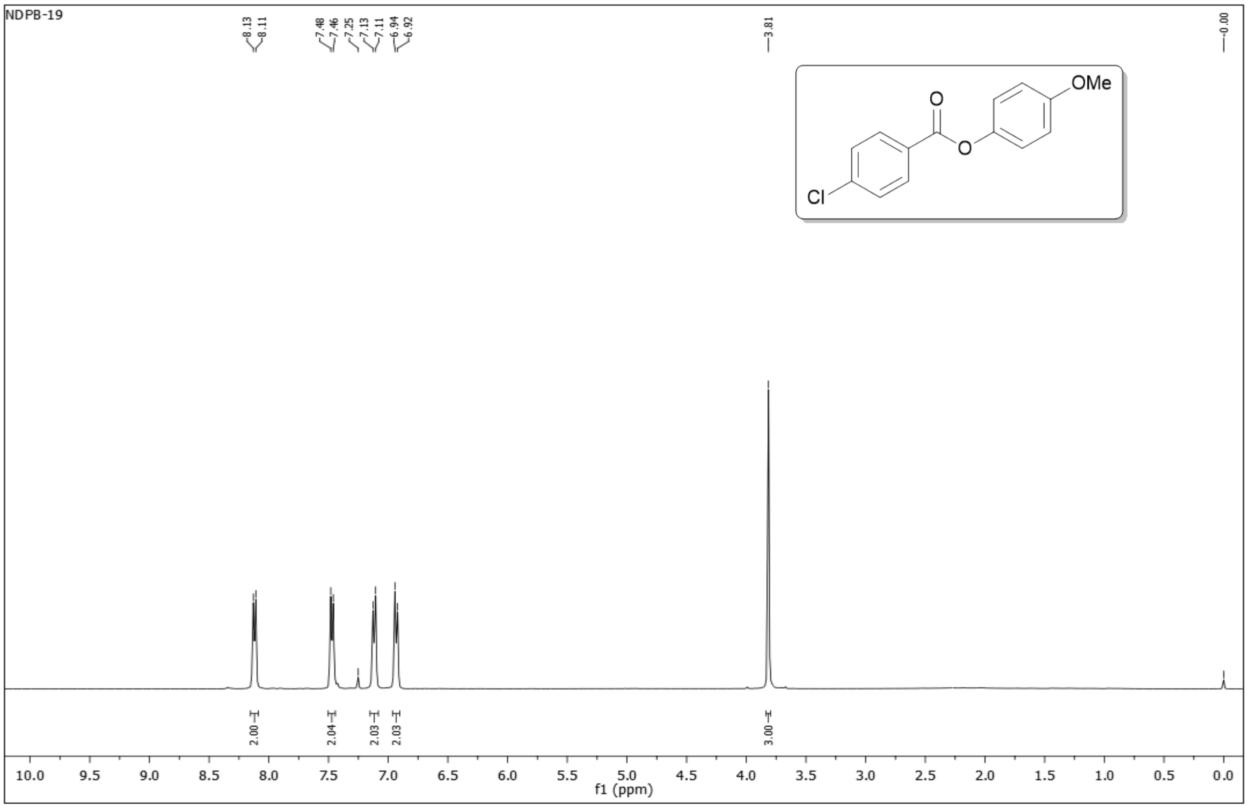

Fig. S59 ^{1}H NMR spectrum of 4-methoxyphenyl 4-chlorobenzoate **4t** (400 MHz, $CDCl_3$)

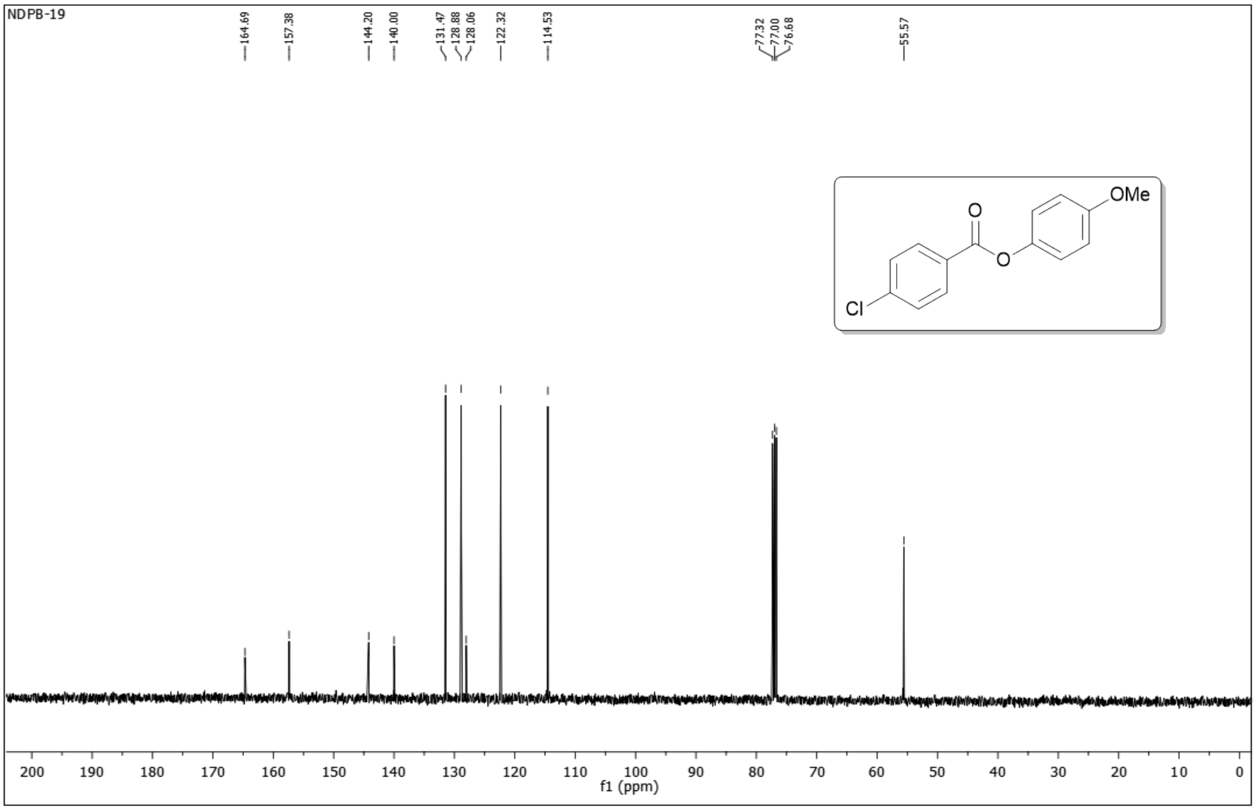

Fig. S60 ^{13}C NMR spectrum of 4-methoxyphenyl 4-chlorobenzoate **4t** (100 MHz, $CDCl_3$)

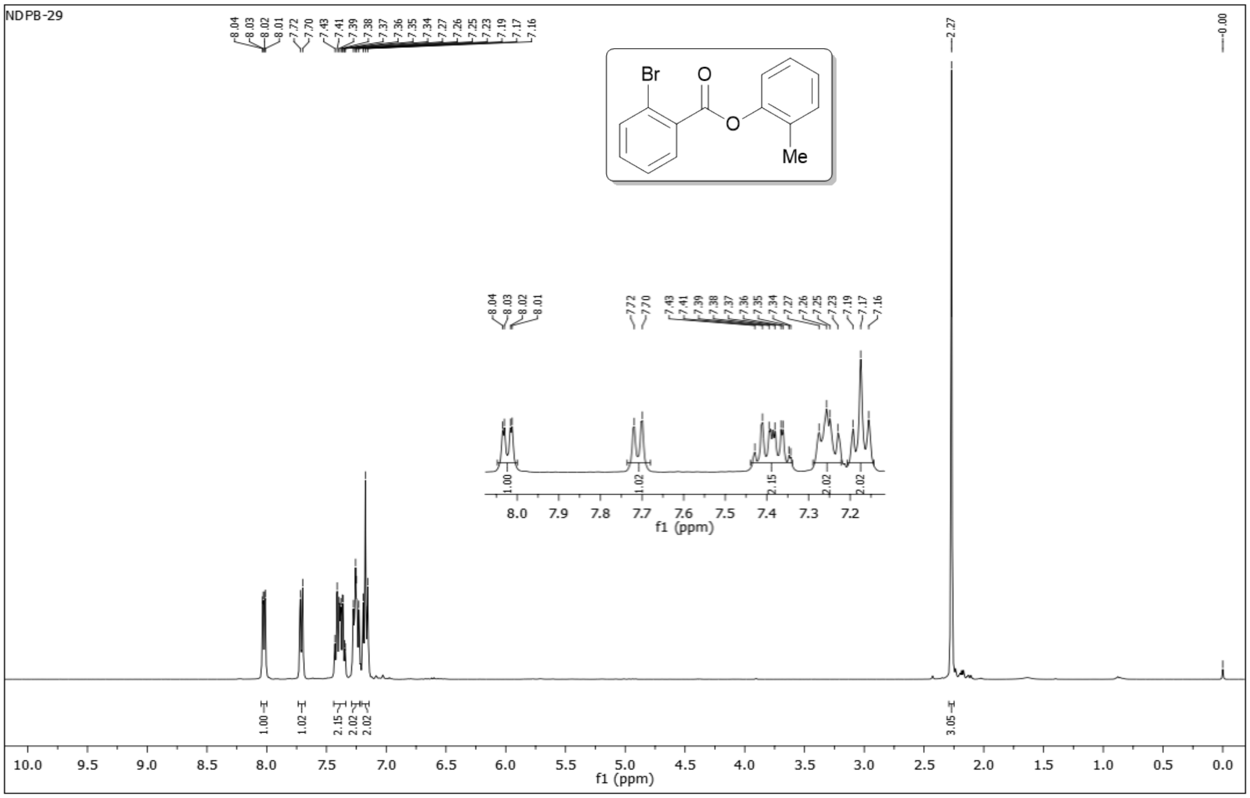

Fig. S61 ^{1}H NMR spectrum of *o*-tolyl 2-bromobenzoate **4u** (400 MHz, $CDCl_3$)

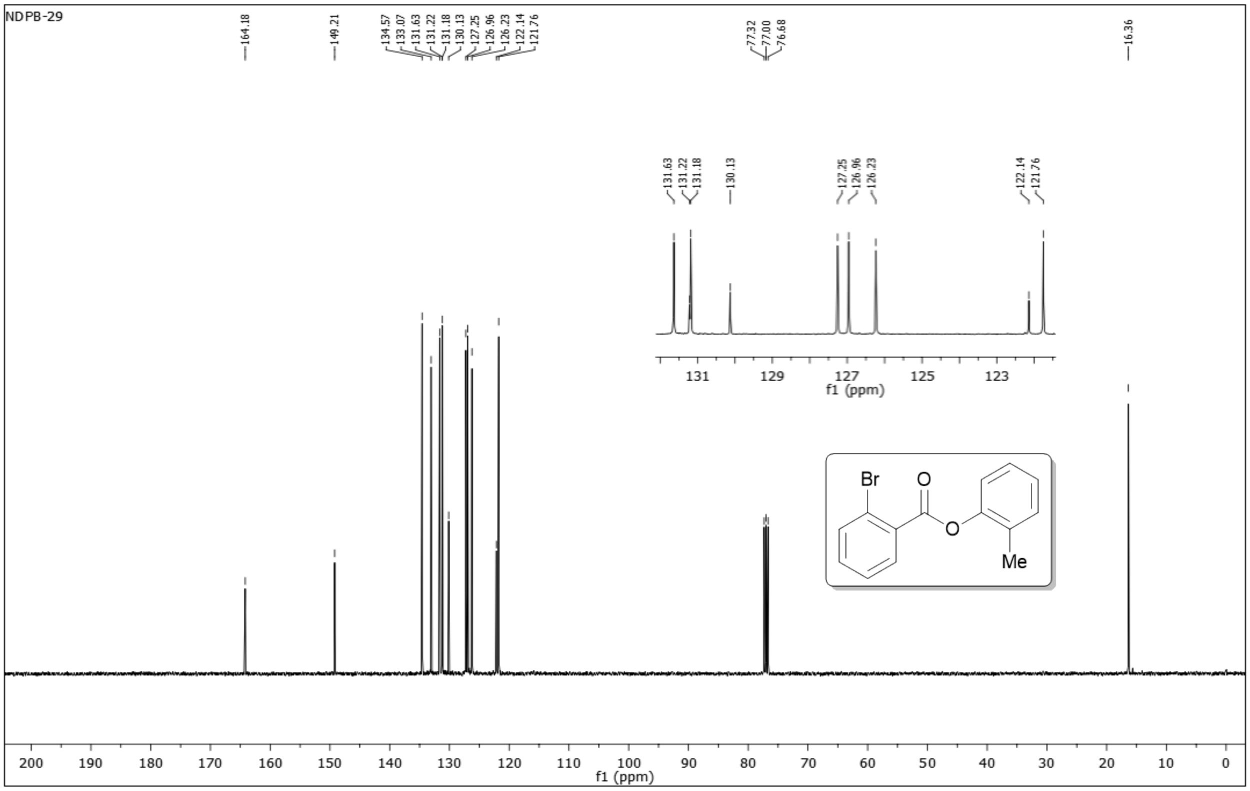

Fig. S62 ^{13}C NMR spectrum of *o*-tolyl 2-bromobenzoate **4u** (100 MHz, $CDCl_3$)

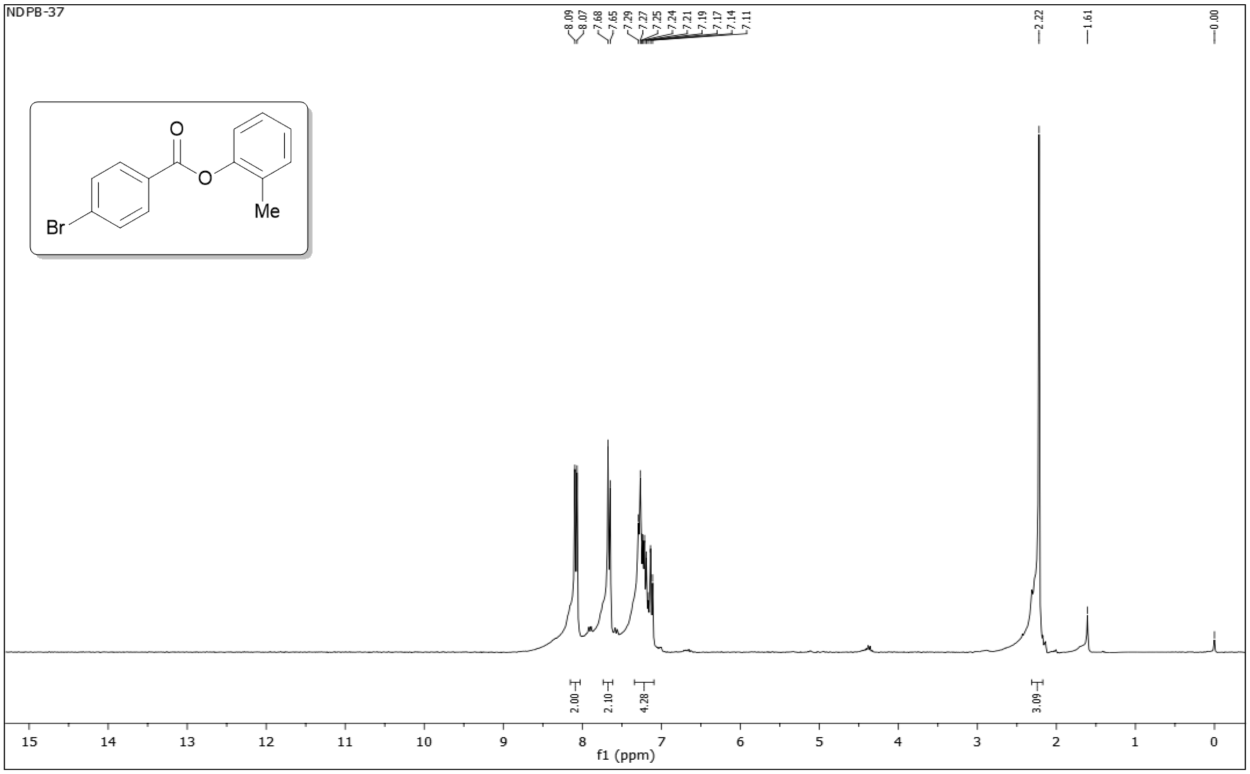

Fig. S63 ^{1}H NMR spectrum of *o*-tolyl 4-bromobenzoate **4v** (300 MHz, $CDCl_3$)

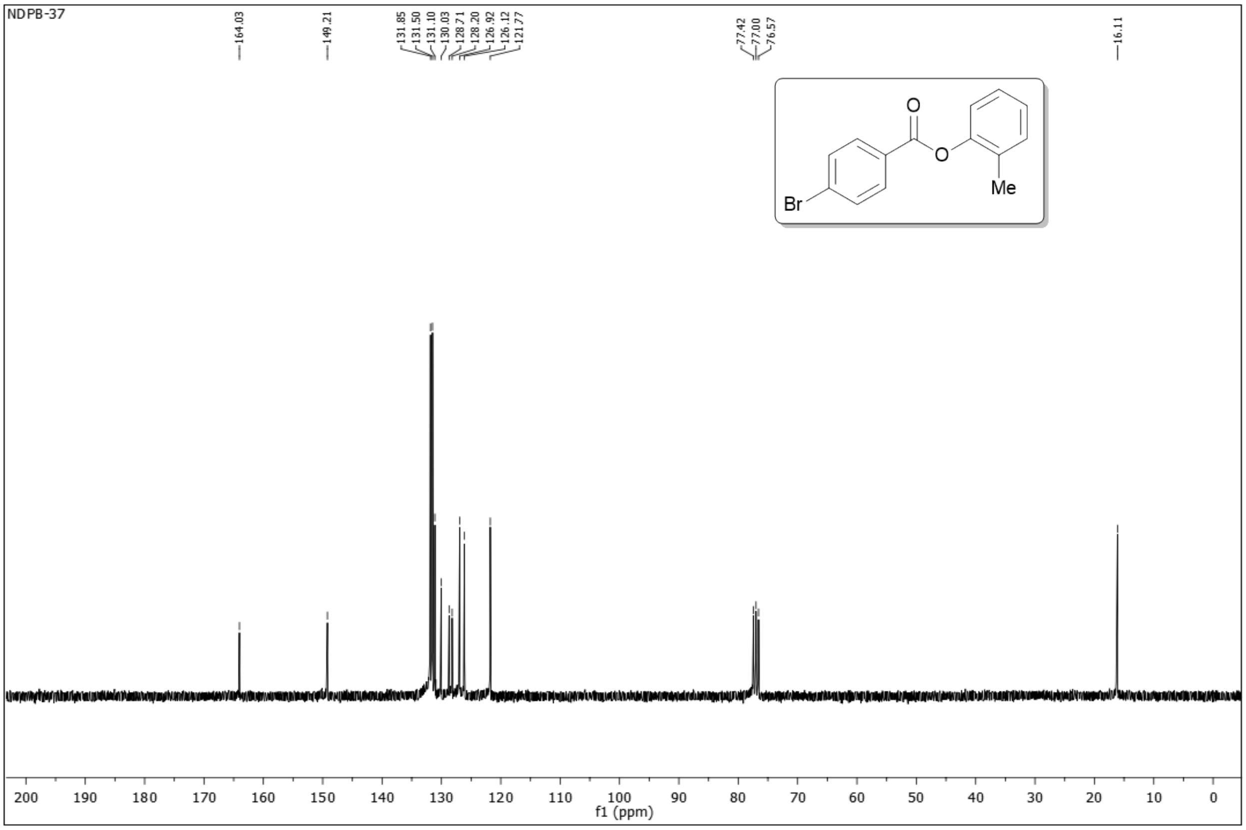

Fig. S64 ^{13}C NMR spectrum of *o*-tolyl 4-bromobenzoate **4v** (75 MHz, $CDCl_3$)

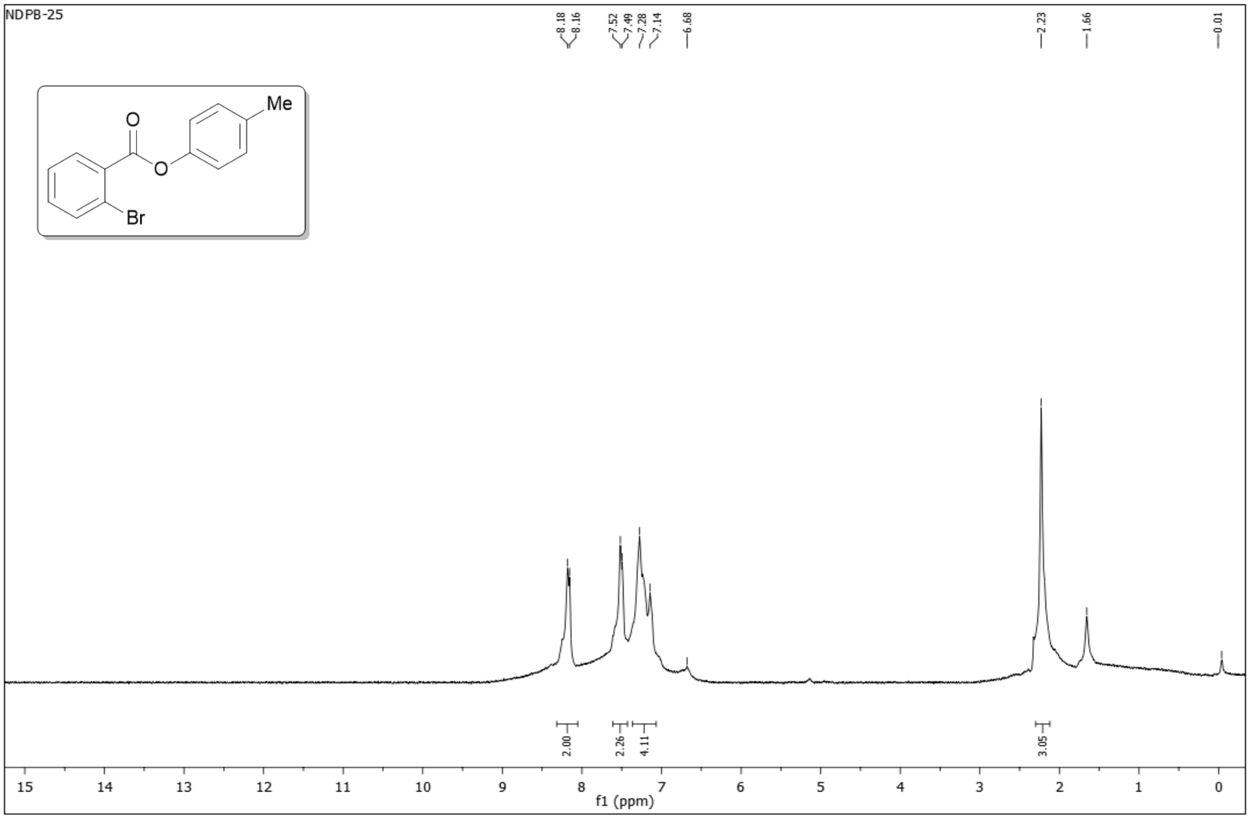

Fig. S65 ^{1}H NMR spectrum of *p*-tolyl 2-bromobenzoate **4w** (300 MHz, $CDCl_3$)

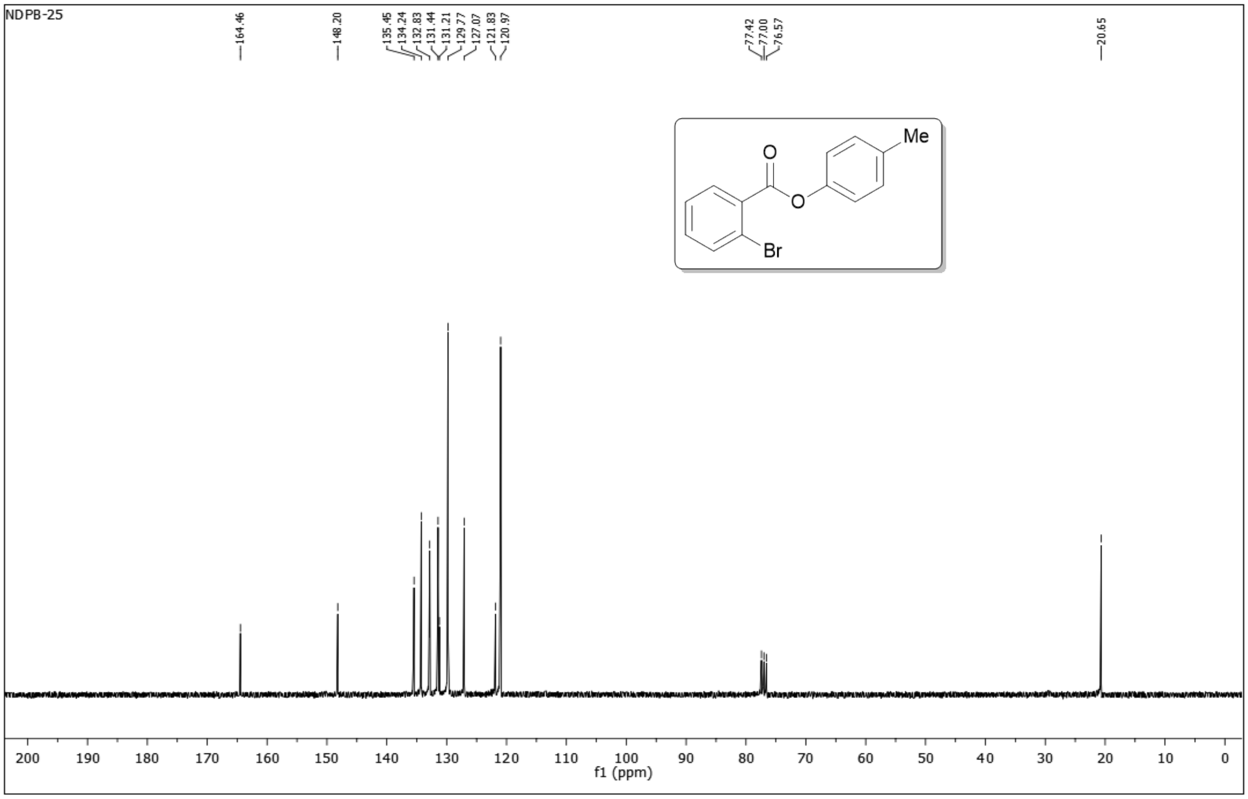

Fig. S66 ^{13}C NMR spectrum of *p*-tolyl 2-bromobenzoate **4w** (75 MHz, $CDCl_3$)

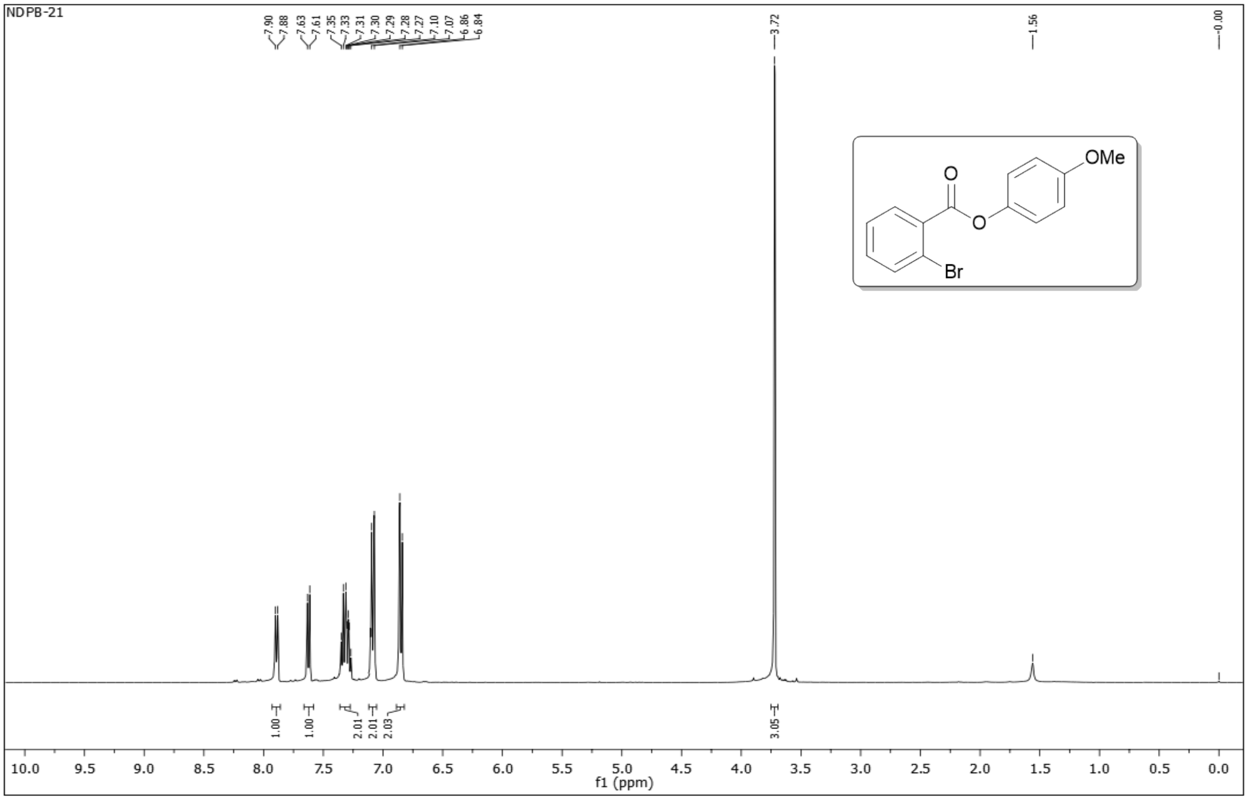

Fig. S67 ^{1}H NMR spectrum of 4-methoxyphenyl 2-bromobenzoate **4x** (400 MHz, $CDCl_3$)

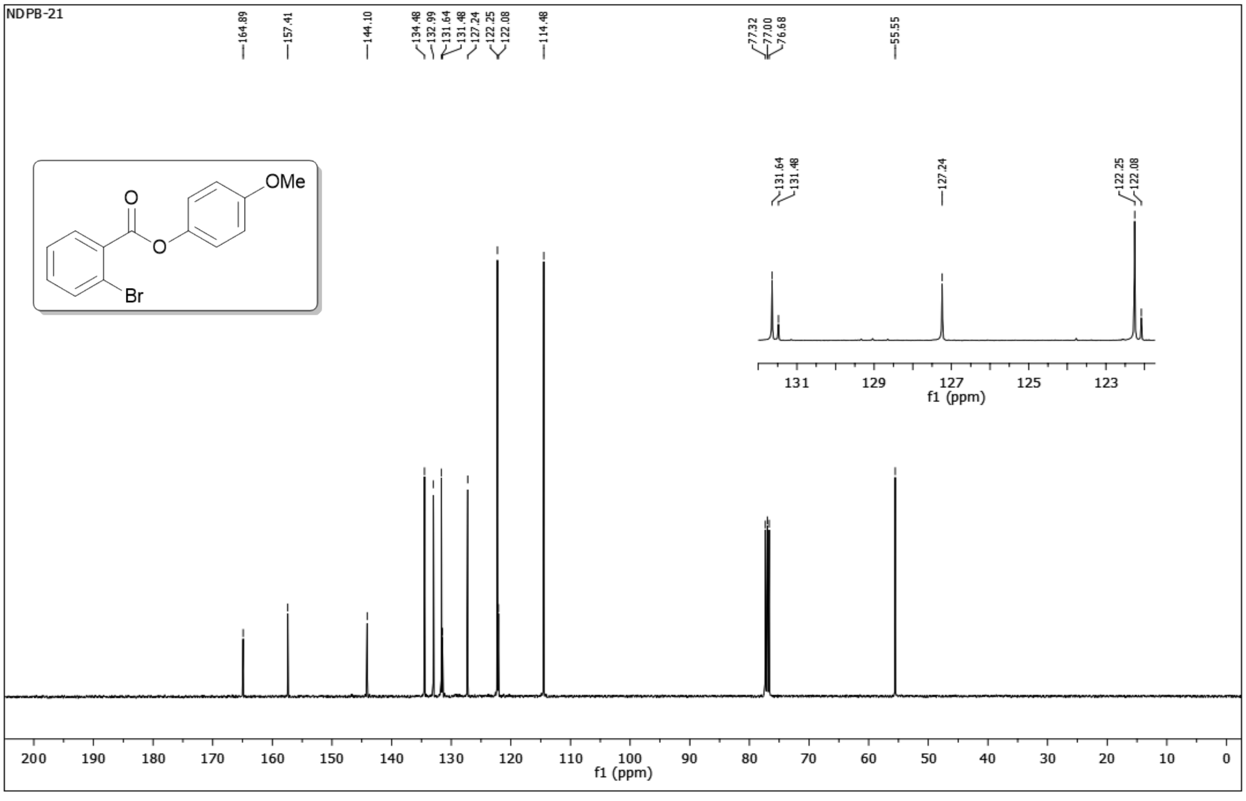

Fig. S68 ^{13}C NMR spectrum of 4-methoxyphenyl 2-bromobenzoate **4x** (100 MHz, $CDCl_3$)

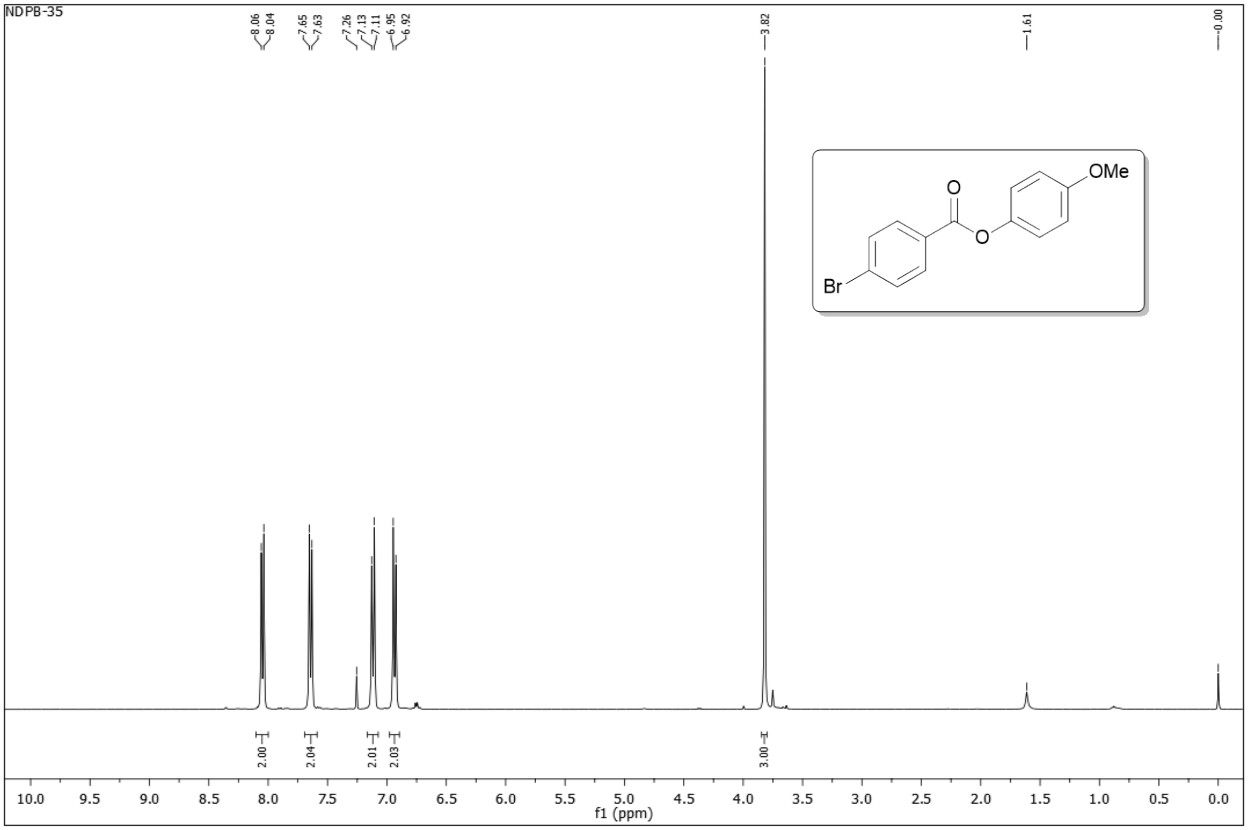

Fig. S69 ^{1}H NMR spectrum of 4-methoxyphenyl 4-bromobenzoate **4y** (400 MHz, $CDCl_3$)

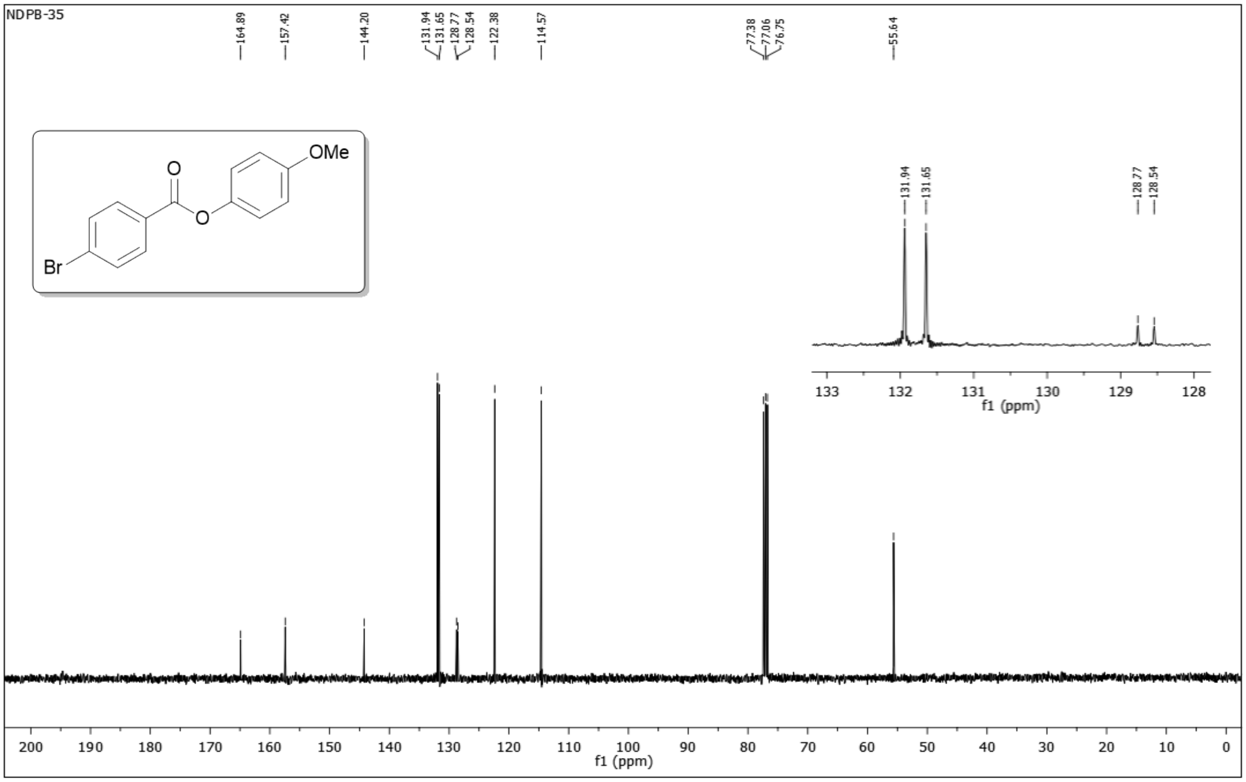

Fig. S70 ^{13}C NMR spectrum of 4-methoxyphenyl 4-bromobenzoate **4y** (100 MHz, $CDCl_3$)

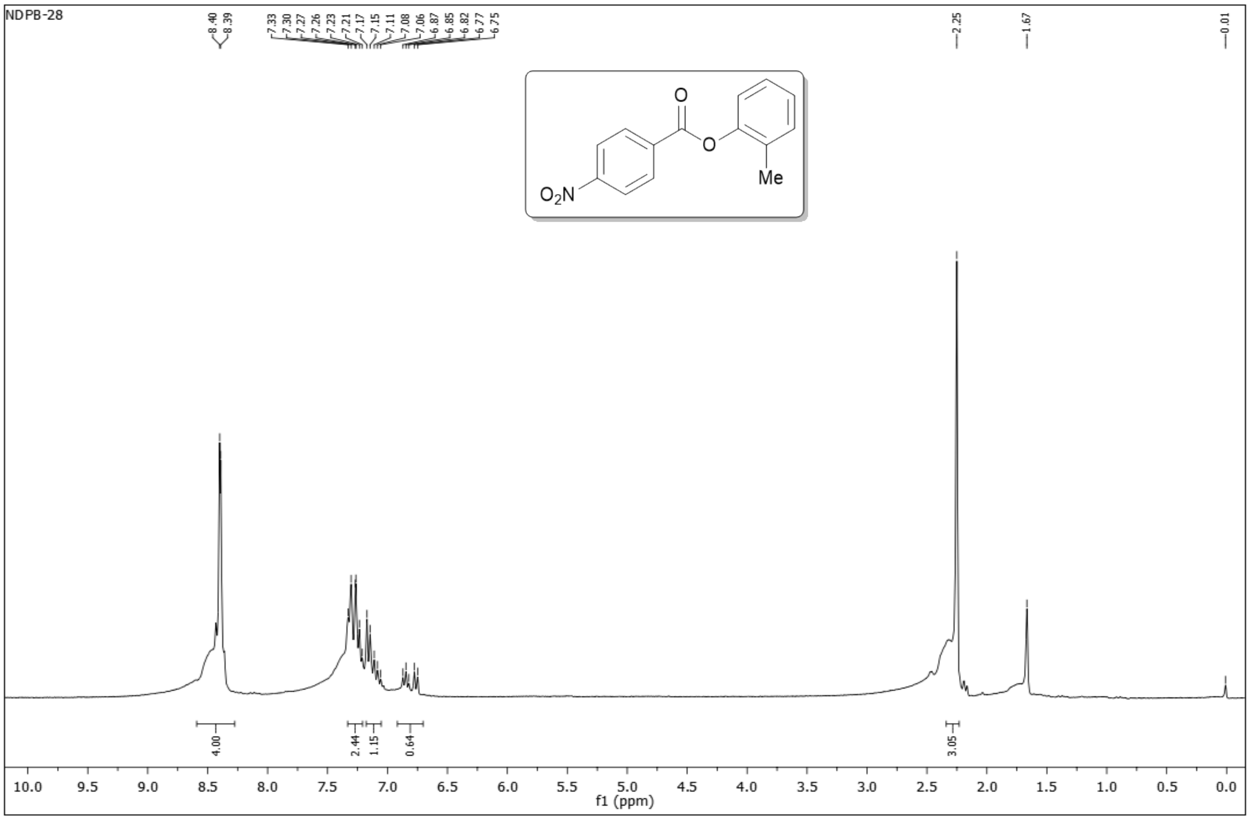

Fig. S71 ^{1}H NMR spectrum of *o*-tolyl 4-nitrobenzoate **4z** (300 MHz, $CDCl_3$)

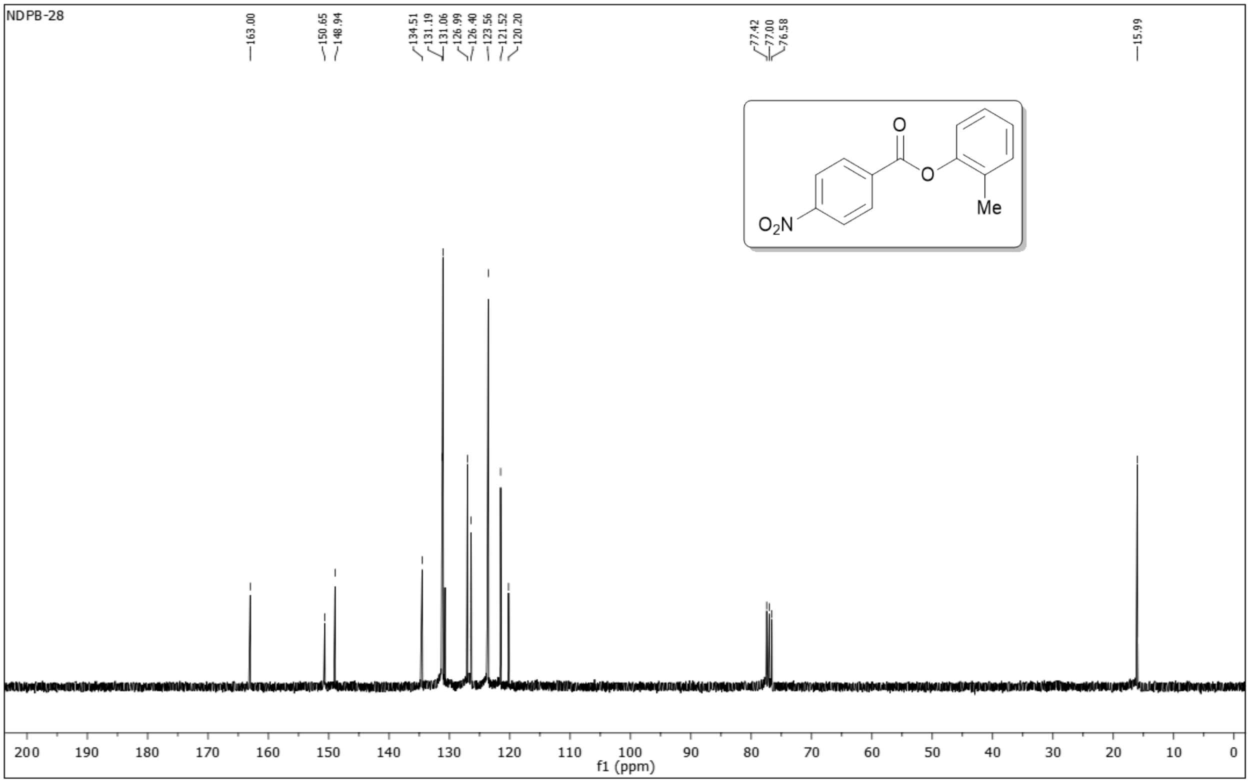

Fig. S72 ^{13}C NMR spectrum of *o*-tolyl 4-nitrobenzoate **4z** (75 MHz, $CDCl_3$)

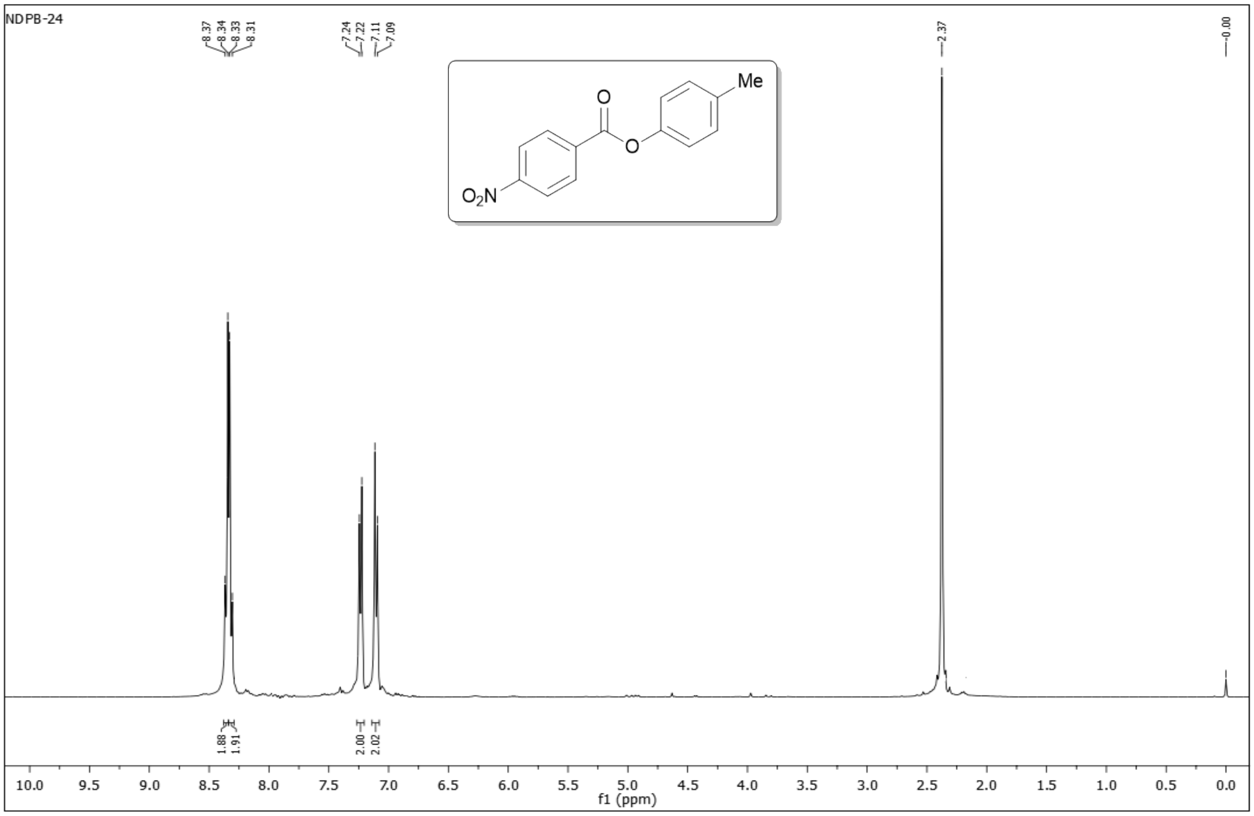

Fig. S73 ^{1}H NMR spectrum of *p*-tolyl 4-nitrobenzoate **4aa** (400 MHz, $CDCl_3$)

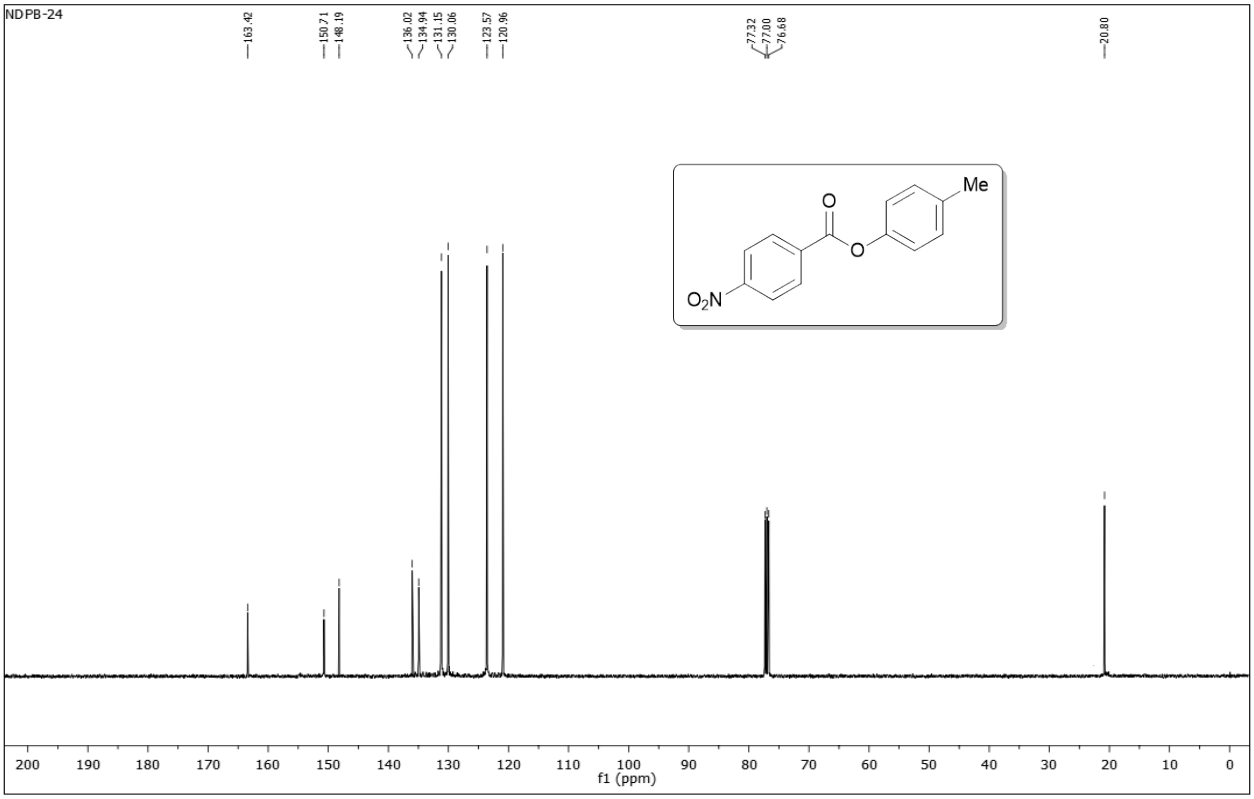

Fig. S74 ^{13}C NMR spectrum of *p*-tolyl 4-nitrobenzoate **4aa** (100 MHz, $CDCl_3$)

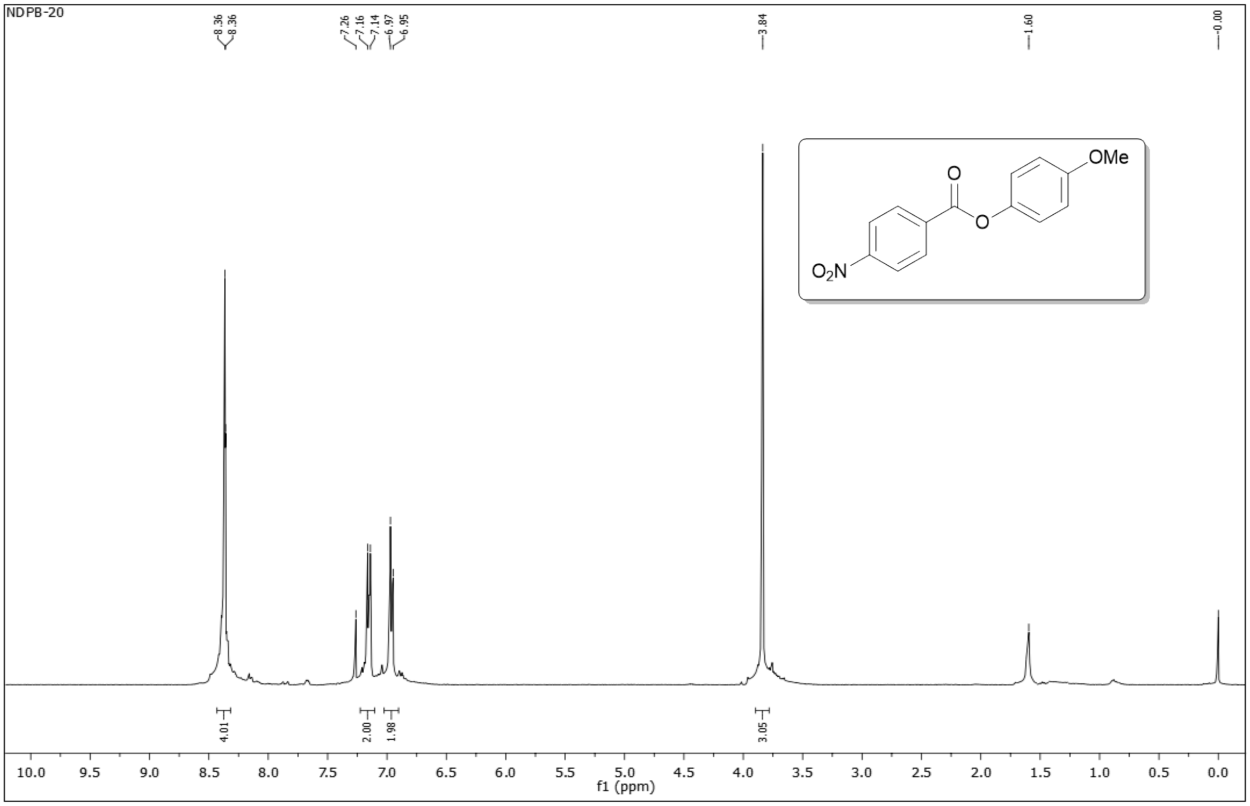

Fig. S75 ^{1}H NMR spectrum of 4-methoxyphenyl 4-nitrobenzoate **4ab** (400 MHz, $CDCl_3$)

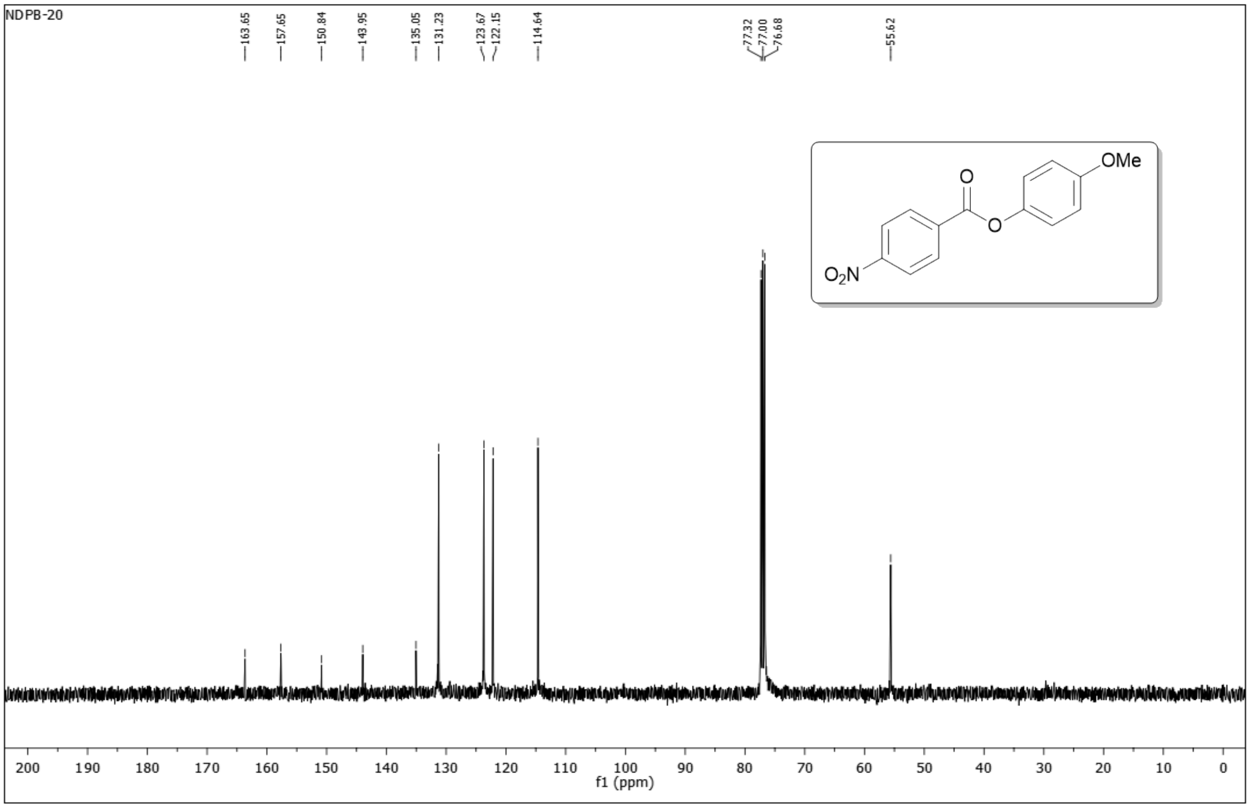

Fig. S76^{13}C NMR spectrum of 4-methoxyphenyl 4-nitrobenzoate **4ab** (100 MHz, $CDCl_3$)

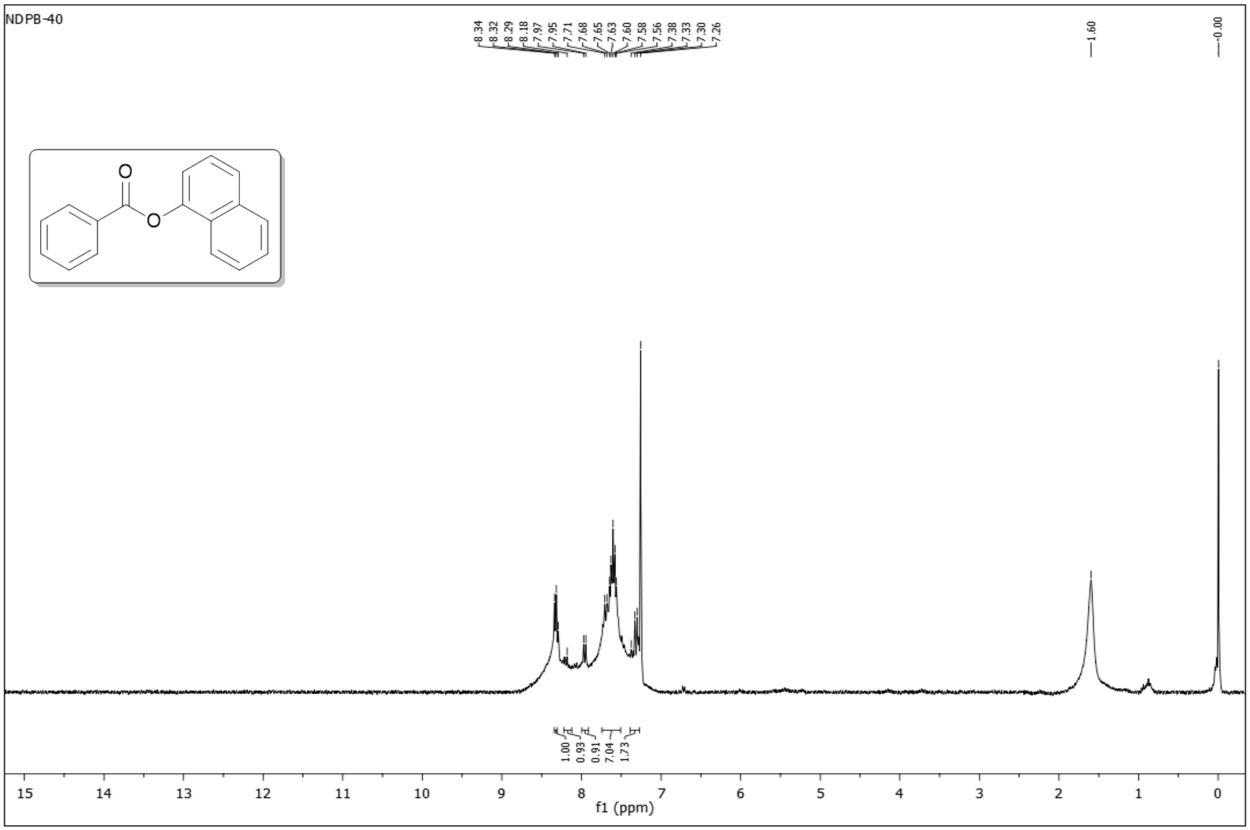

Fig. S77 ^{1}H NMR spectrum of naphthalen-1-yl benzoate **4ac** (300 MHz, CDCl$_3$)

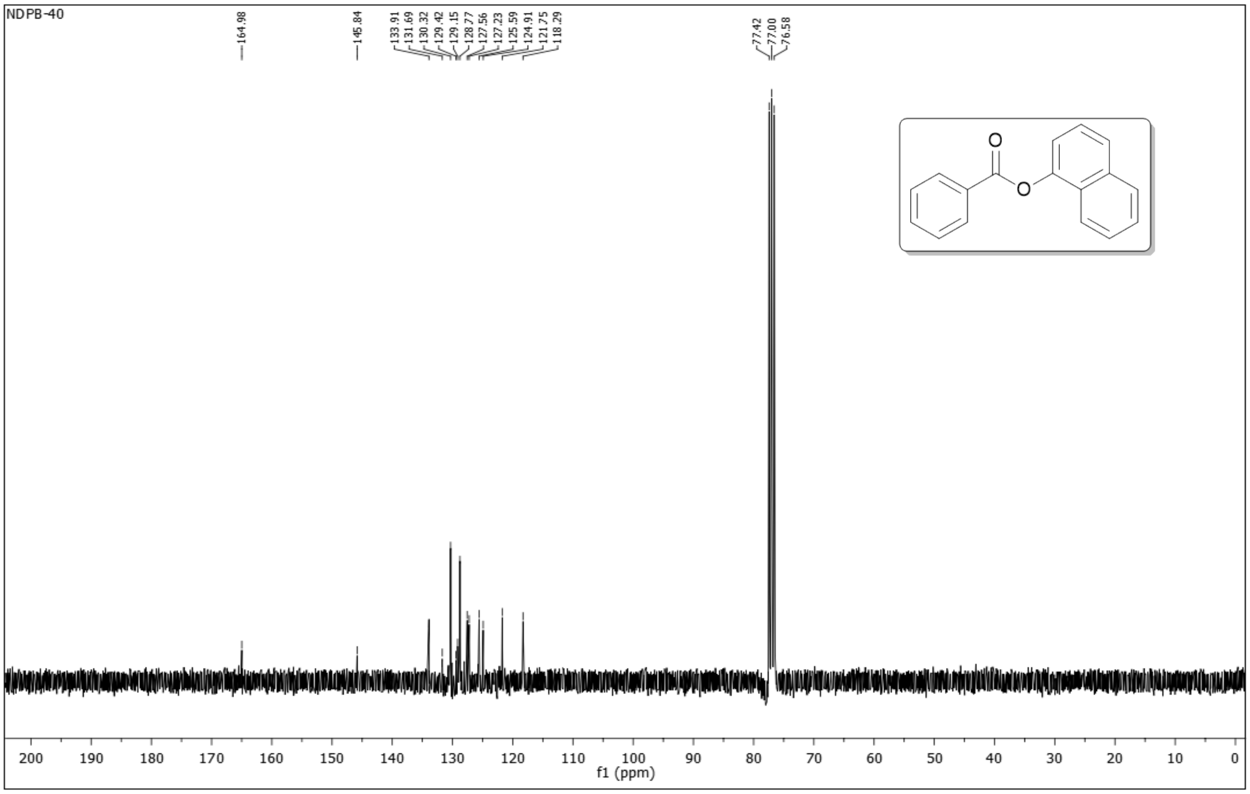

Fig. S78 ^{13}C NMR spectrum of naphthalen-1-yl benzoate **4ac** (75 MHz, CDCl$_3$)

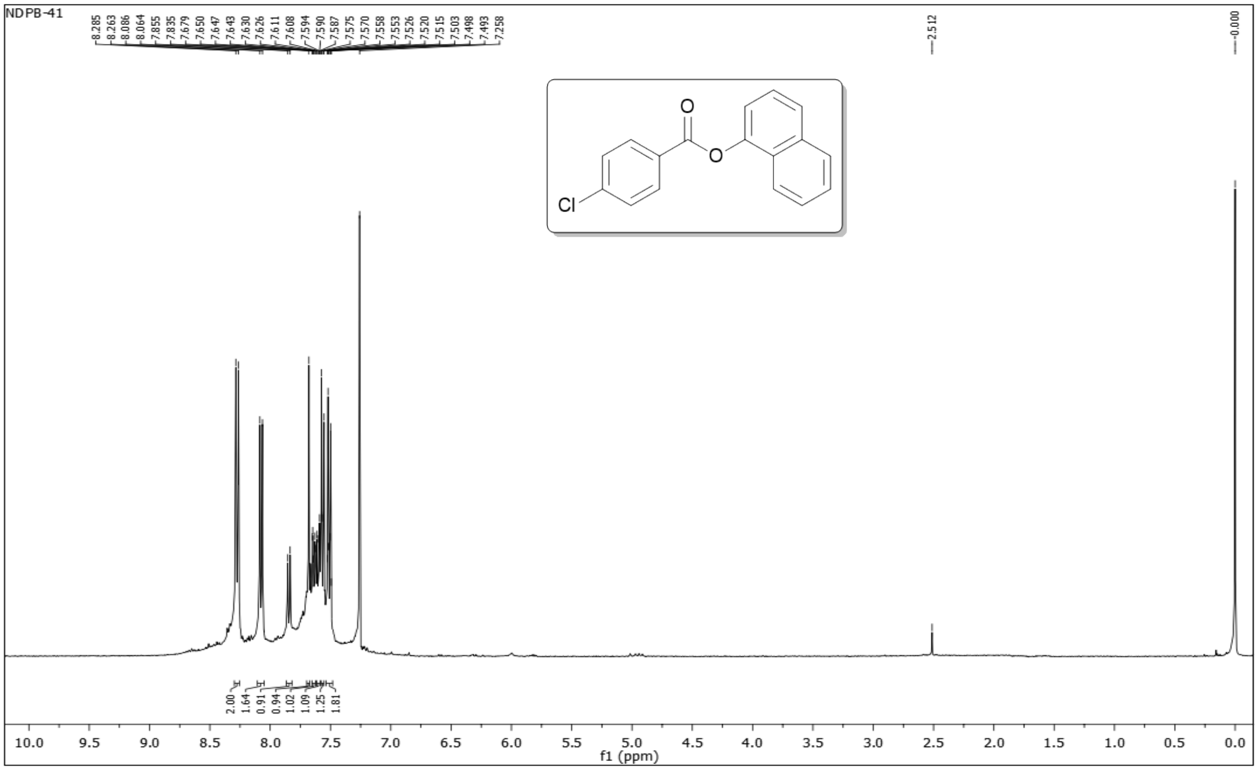

Fig. S79 ^{1}H NMR spectrum of naphthalen-1-yl 4-chlorobenzoate **4ad** (400 MHz, $CDCl_3$)

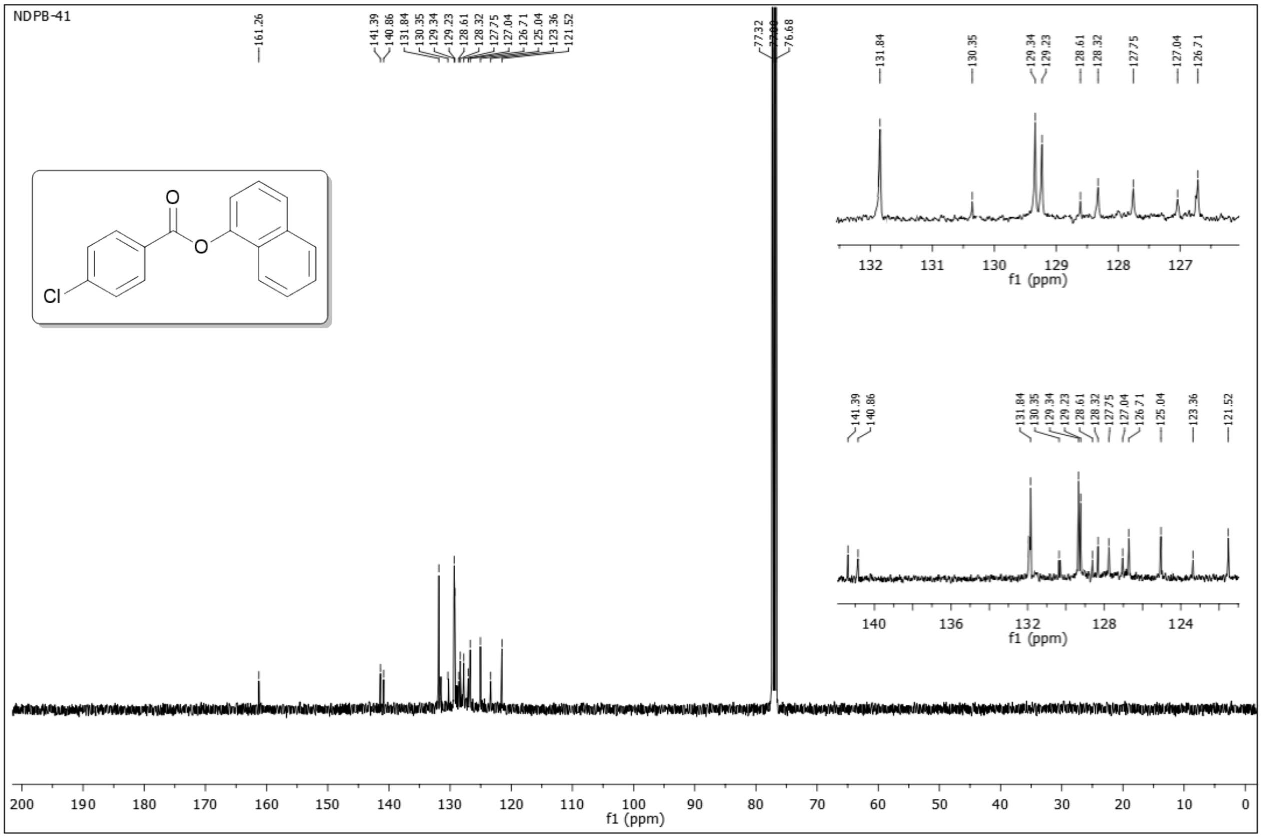

Fig. S80^{13}C NMR spectrum of naphthalen-1-yl 4-chlorobenzoate **4ad** (100 MHz, $CDCl_3$)

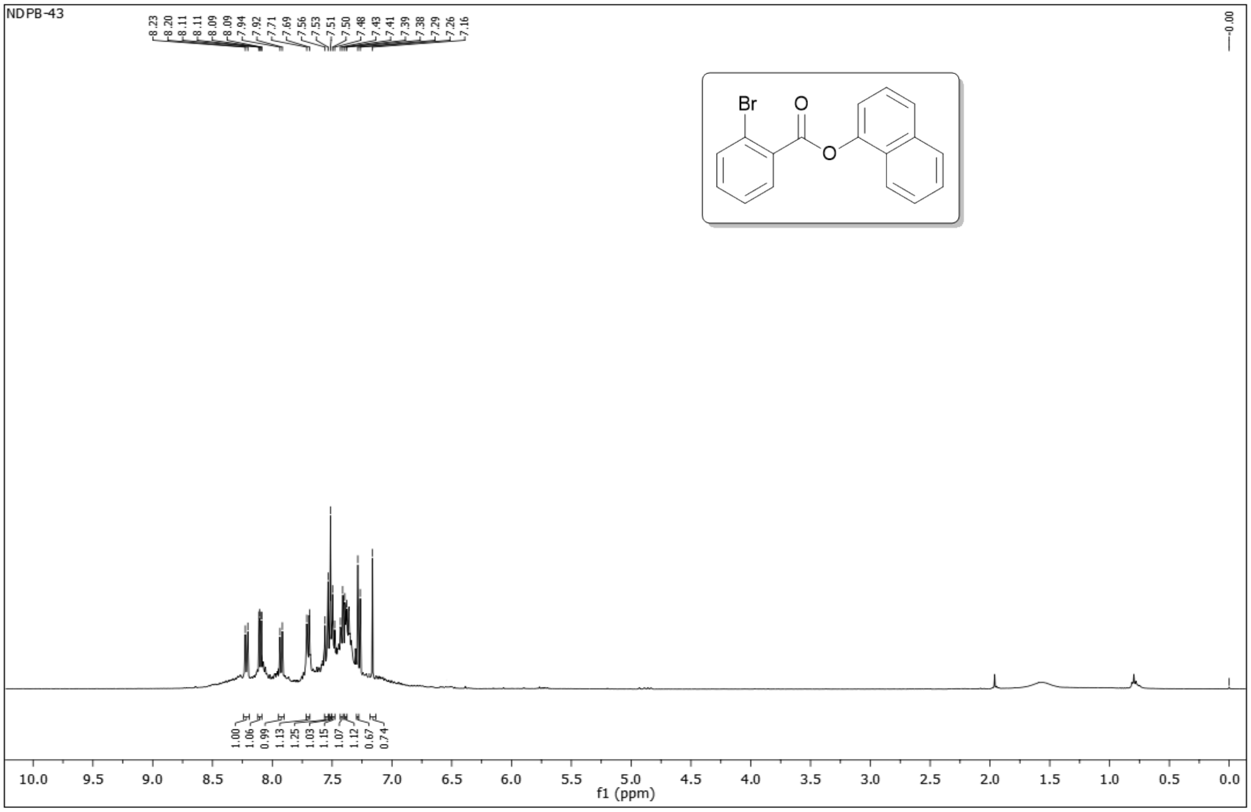

Fig. S81 ^{1}H NMR spectrum of naphthalen-1-yl 2-bromobenzoate **4ae** (400 MHz, $CDCl_3$)

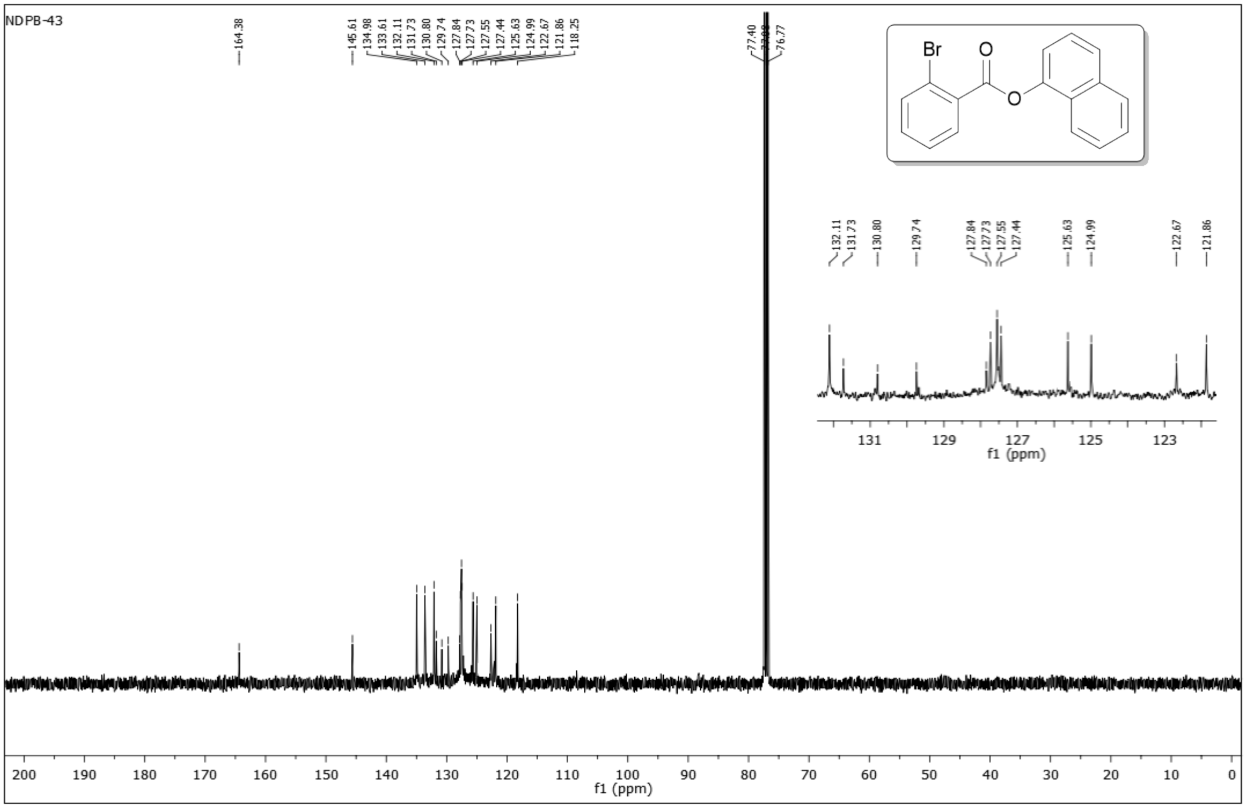

Fig. S82 ^{13}C NMR spectrum of naphthalen-1-yl 2-bromobenzoate **4ae** (100 MHz, $CDCl_3$)

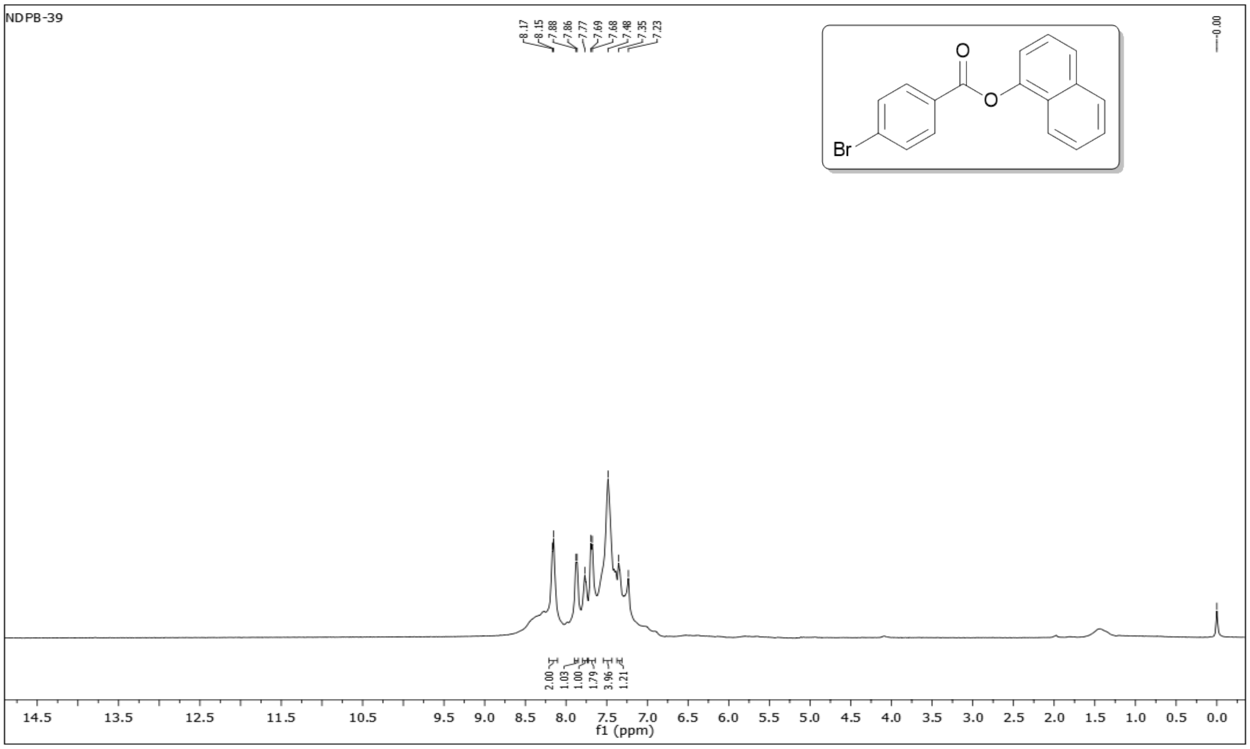

Fig. S83 ^{1}H NMR spectrum of naphthalen-1-yl 4-bromobenzoate **4af** (400 MHz, $CDCl_3$)

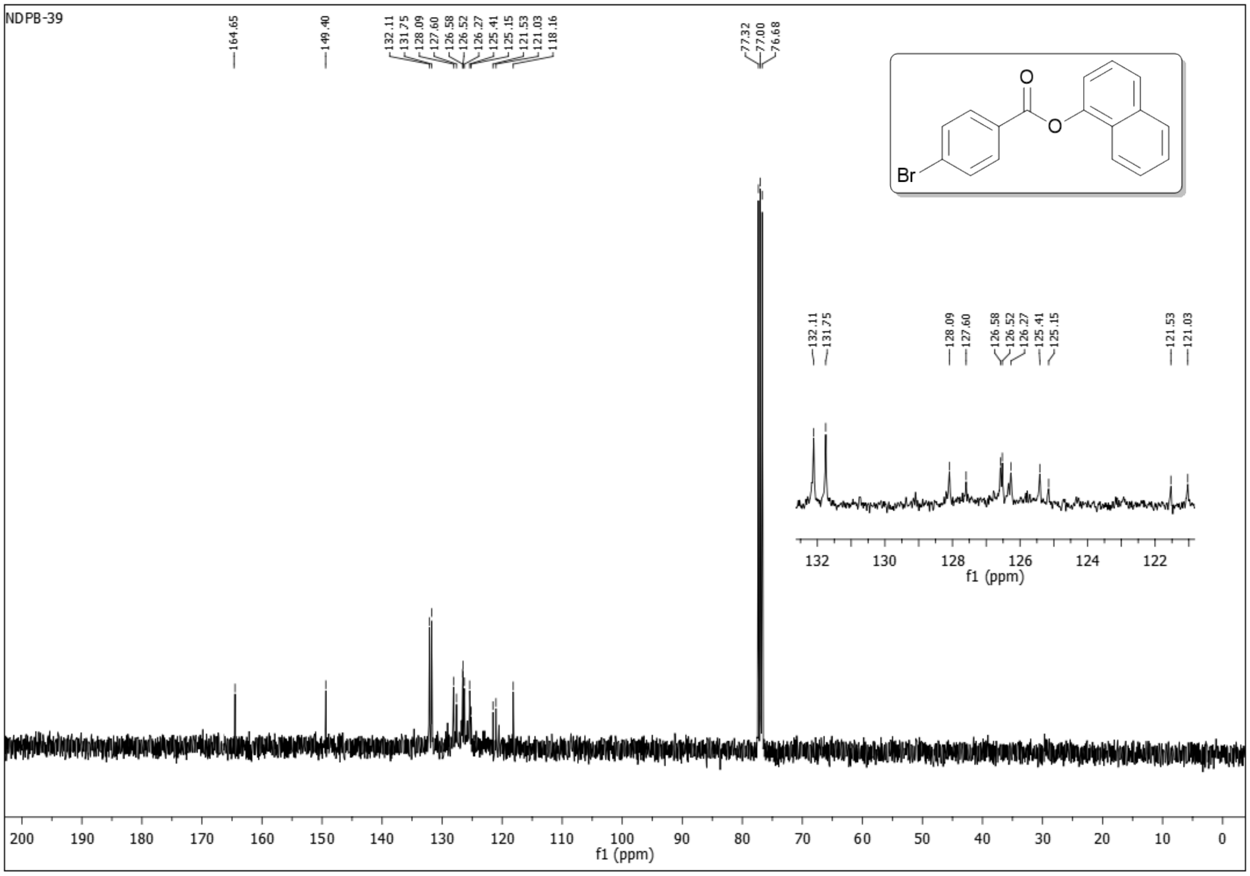

Fig. S84 ^{13}C NMR spectrum of naphthalen-1-yl 4-bromobenzoate **4af** (100 MHz, $CDCl_3$)

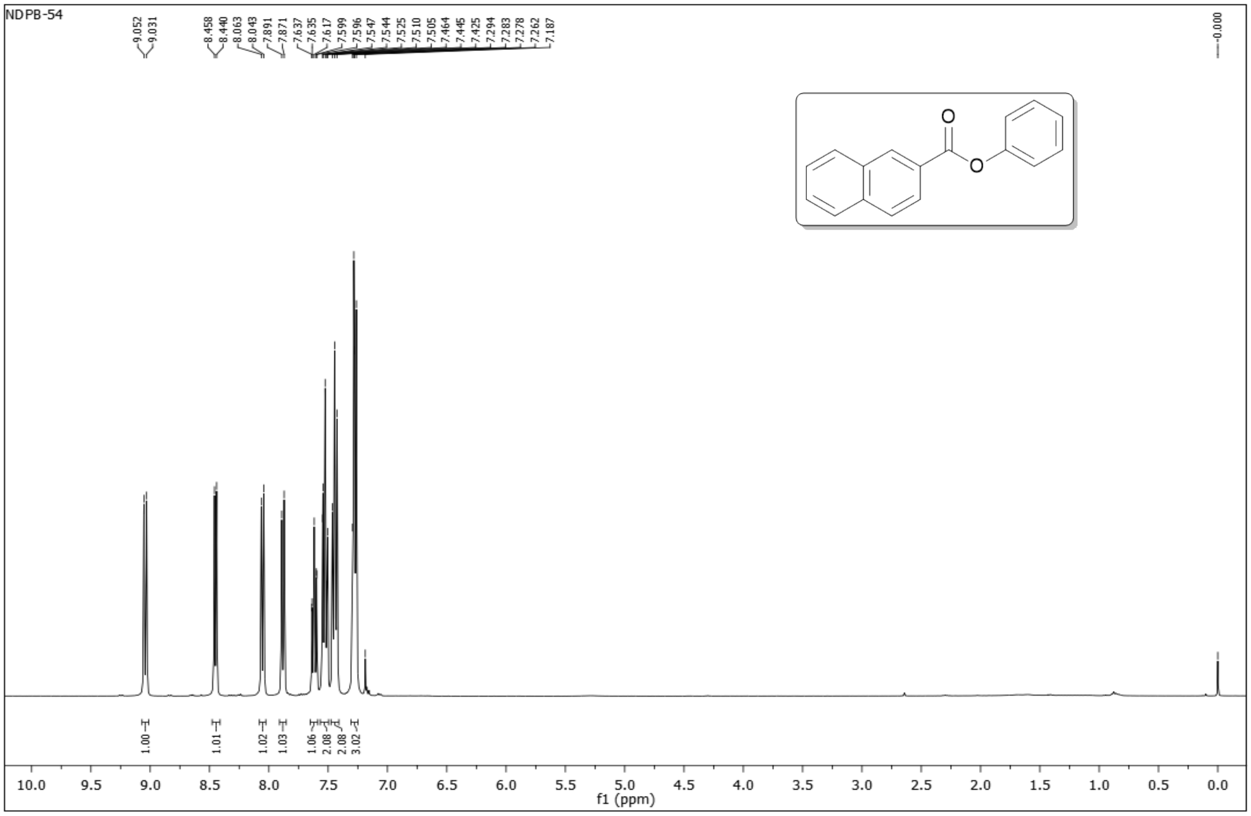

Fig. S85 ^{1}H NMR spectrum of phenyl 2-naphthoate **4ag** (400 MHz, $CDCl_3$)

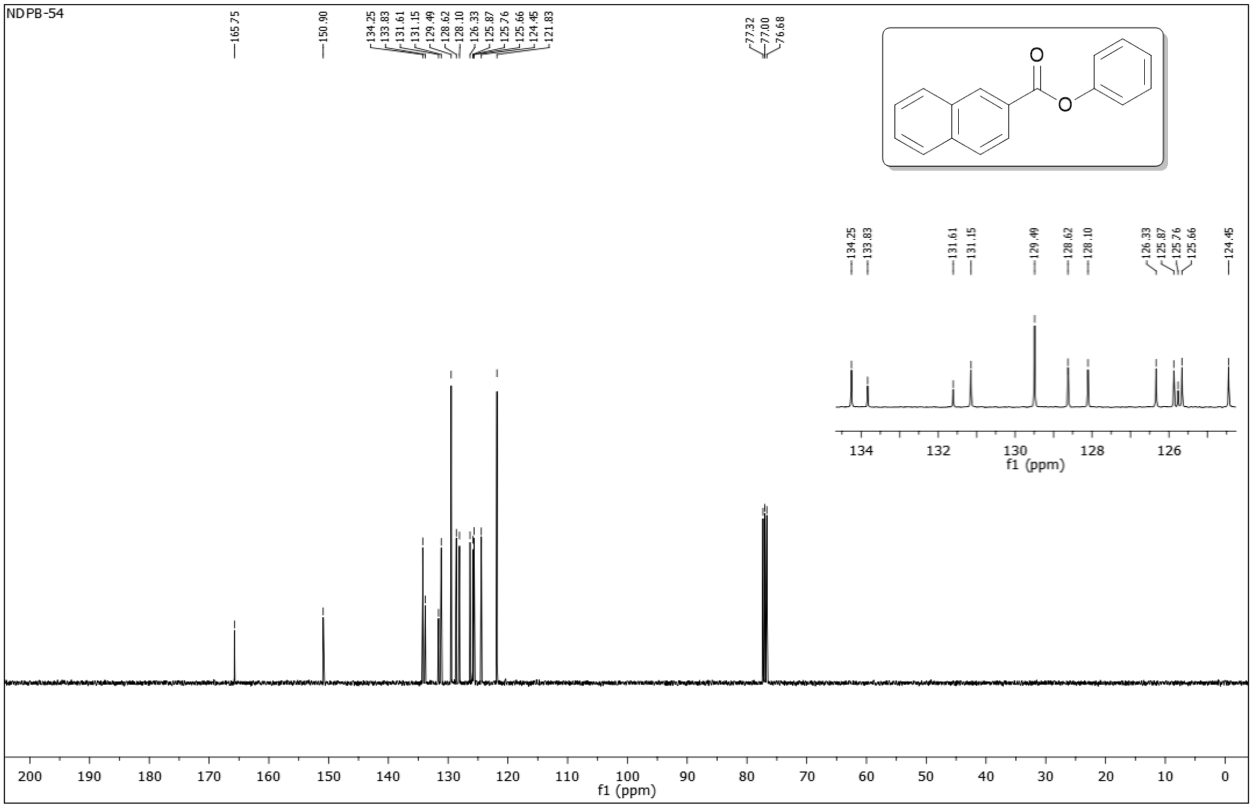

Fig. S86 ^{13}C NMR spectrum of phenyl 2-naphthoate **4ag** (100 MHz, $CDCl_3$)

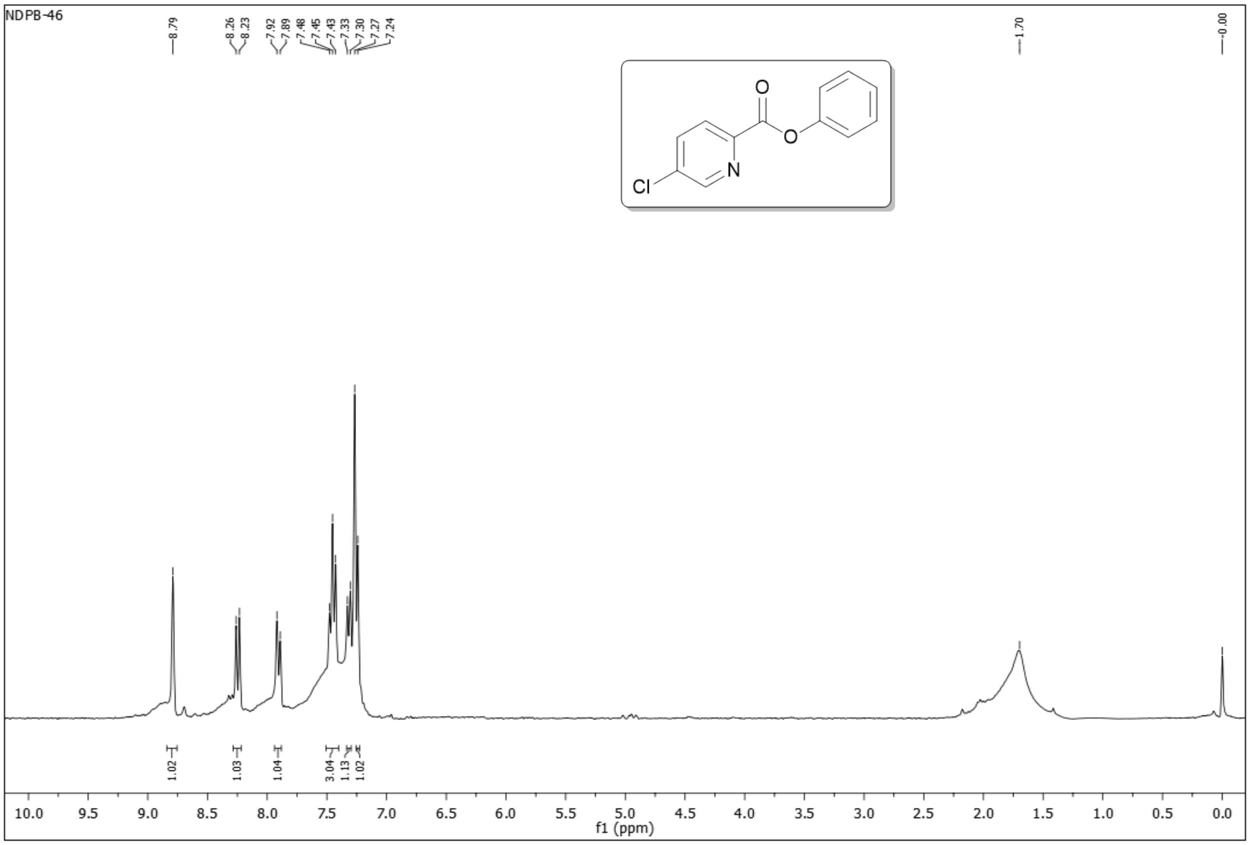

Fig. S87 ^{1}H NMR spectrum of phenyl 5-chloropicolinate **4ah** (300 MHz, $CDCl_3$)

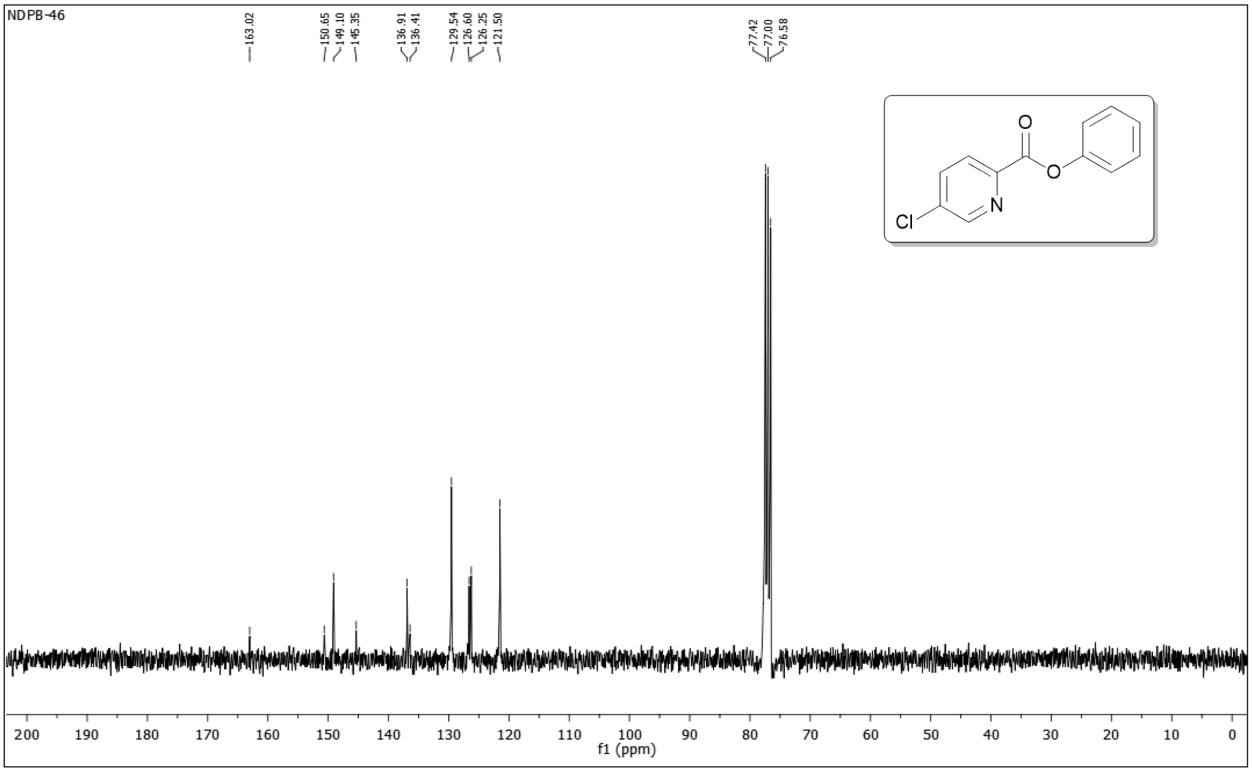

Fig. S88 ^{13}C NMR spectrum of phenyl 5-chloropicolinate **4ah** (75 MHz, $CDCl_3$)

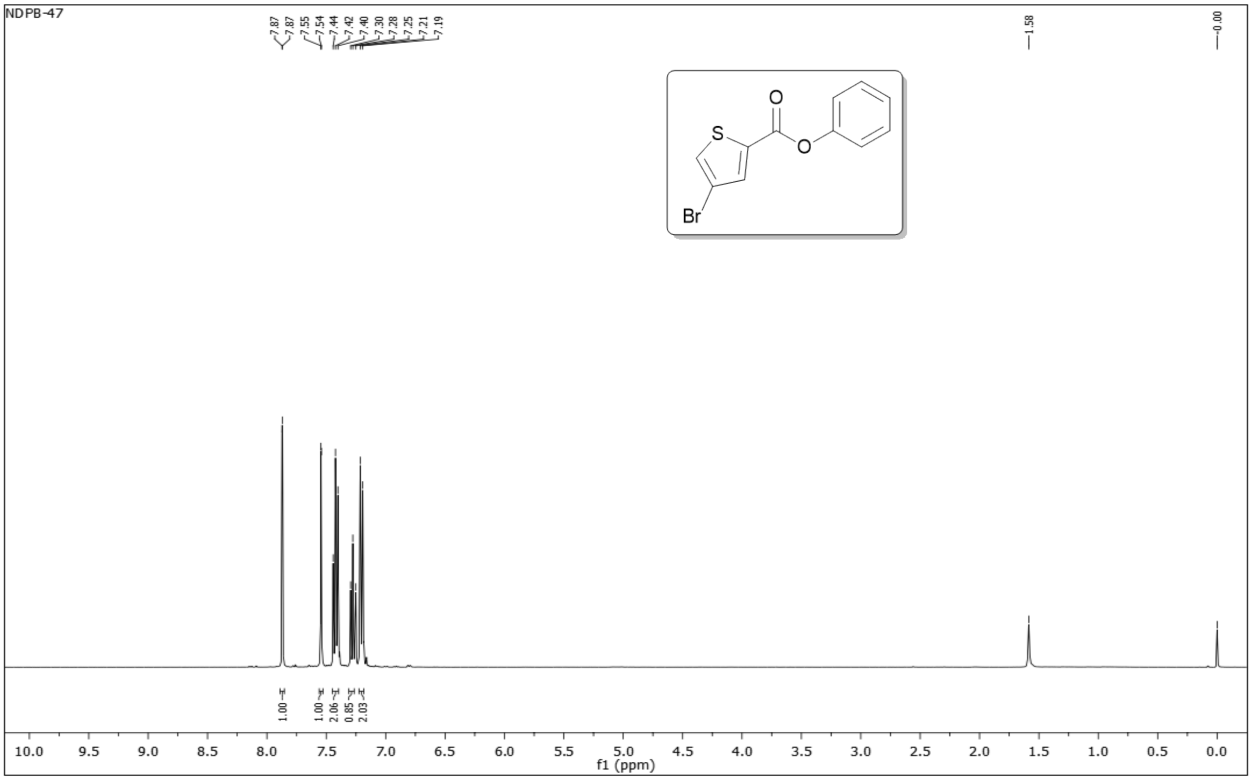

Fig. S89 ^{1}H NMR spectrum of phenyl 4-bromothiophene-2-carboxylate **4ai** (400 MHz, $CDCl_3$)

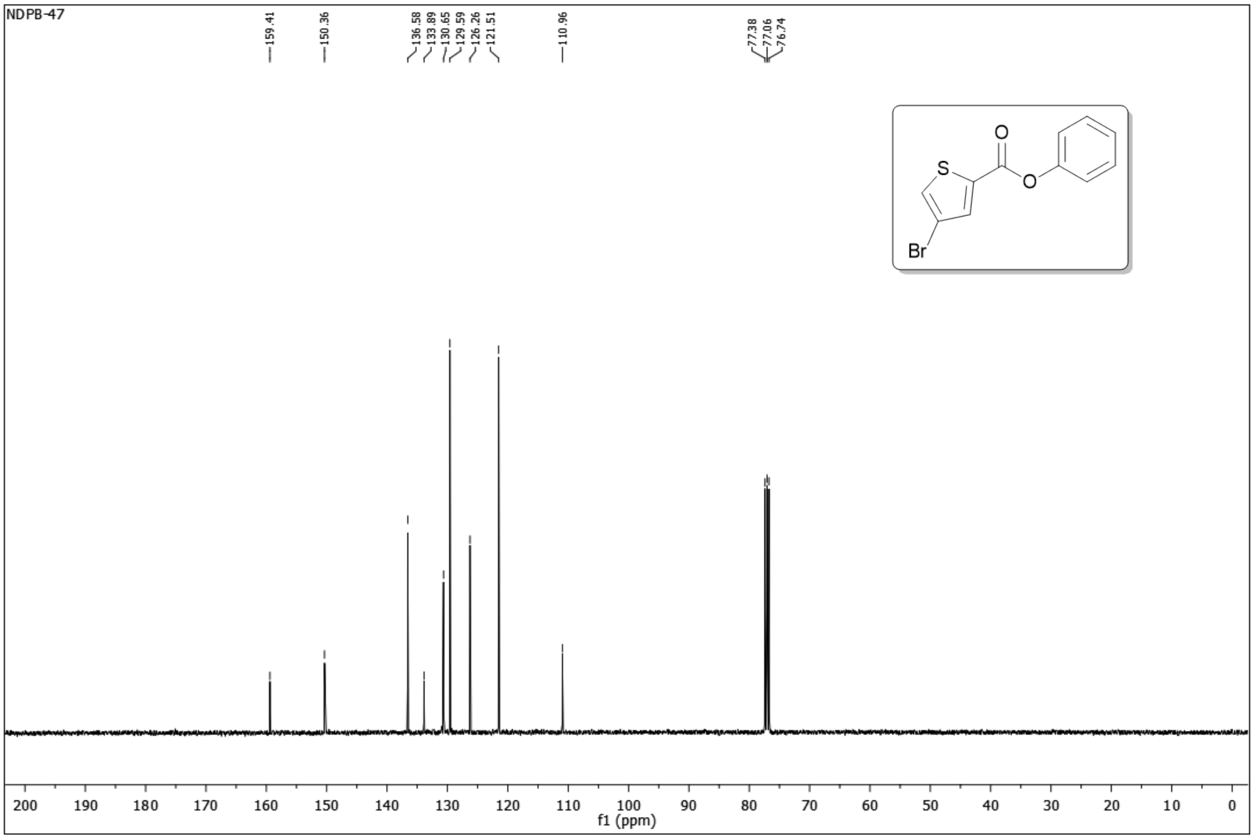

Fig. S90 ^{13}C NMR spectrum of phenyl 4-bromothiophene-2-carboxylate **4ai** (100 MHz, $CDCl_3$)

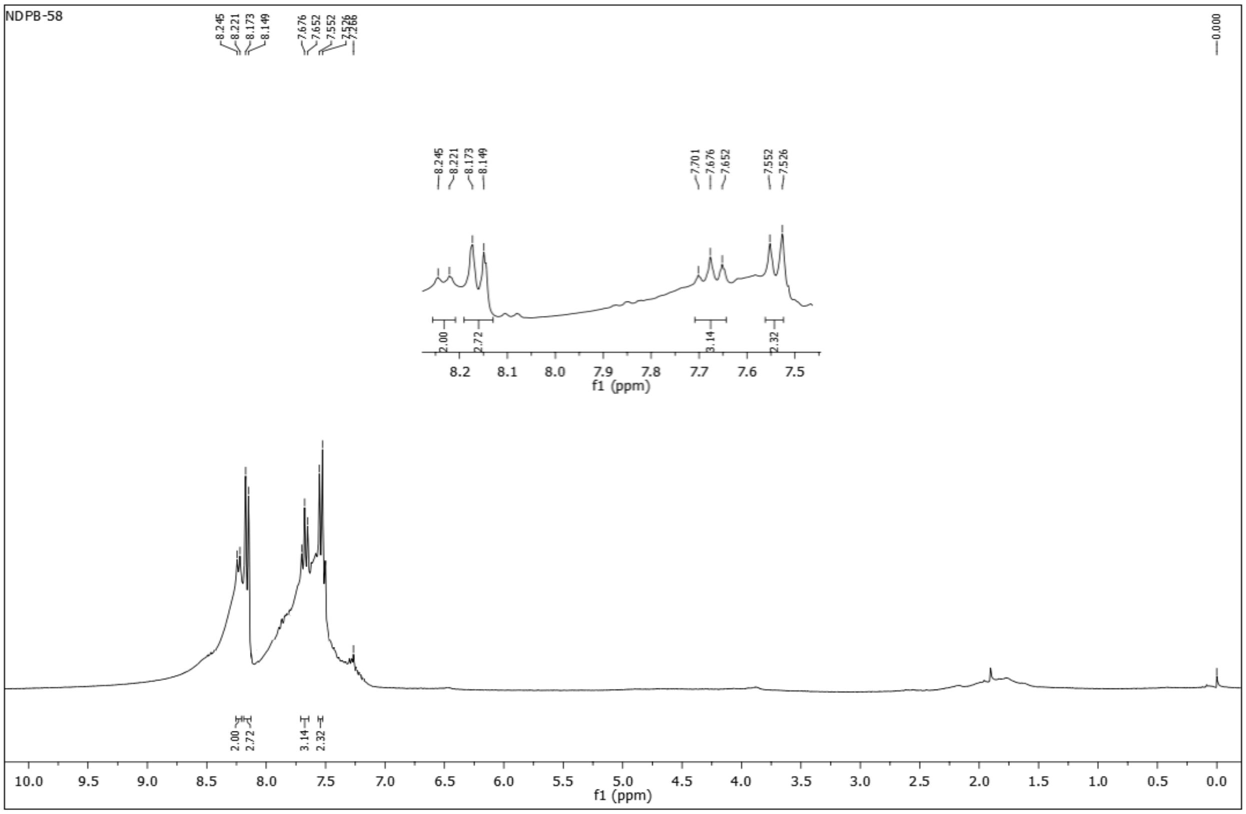

Fig. S91 ^{1}H NMR spectrum of pyridin-2-yl benzoate **4aj** (300 MHz, $CDCl_3$)

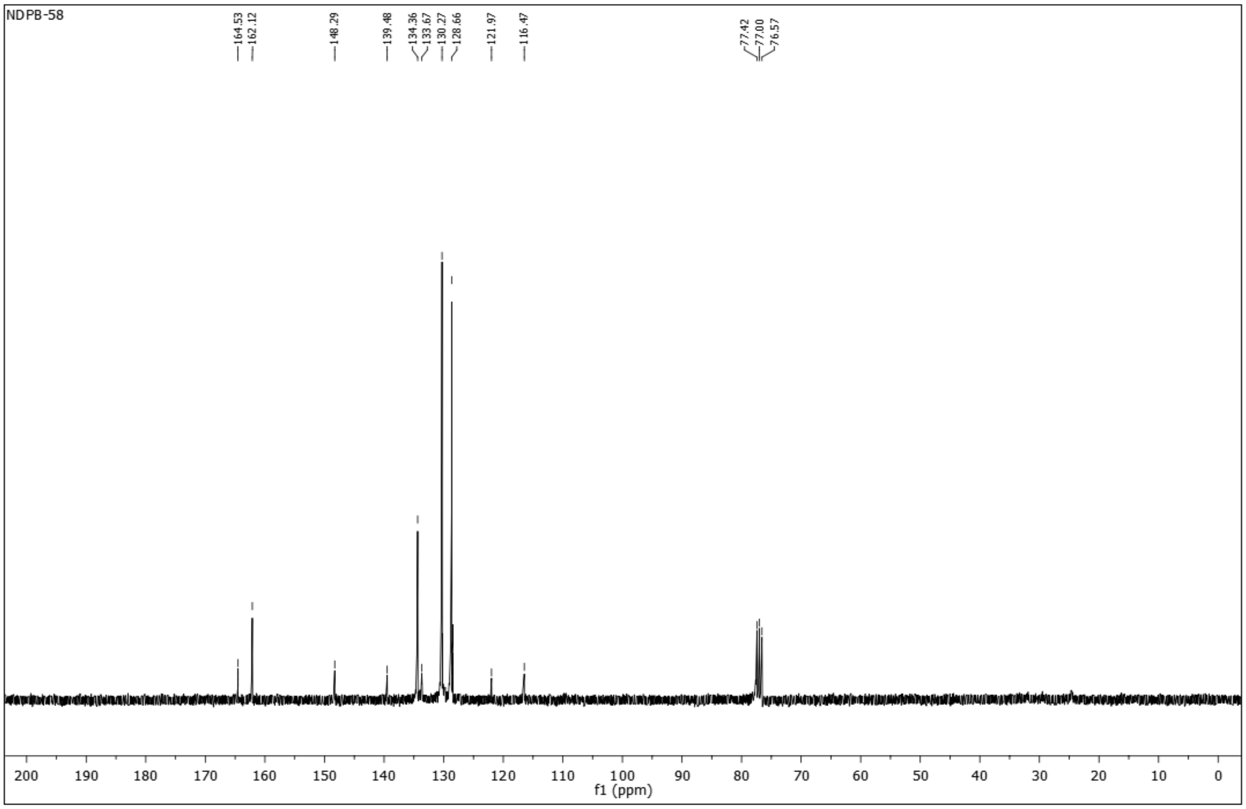

Fig. S92 ^{1}H NMR spectrum of pyridin-2-yl benzoate **4aj** (75 MHz, $CDCl_3$)

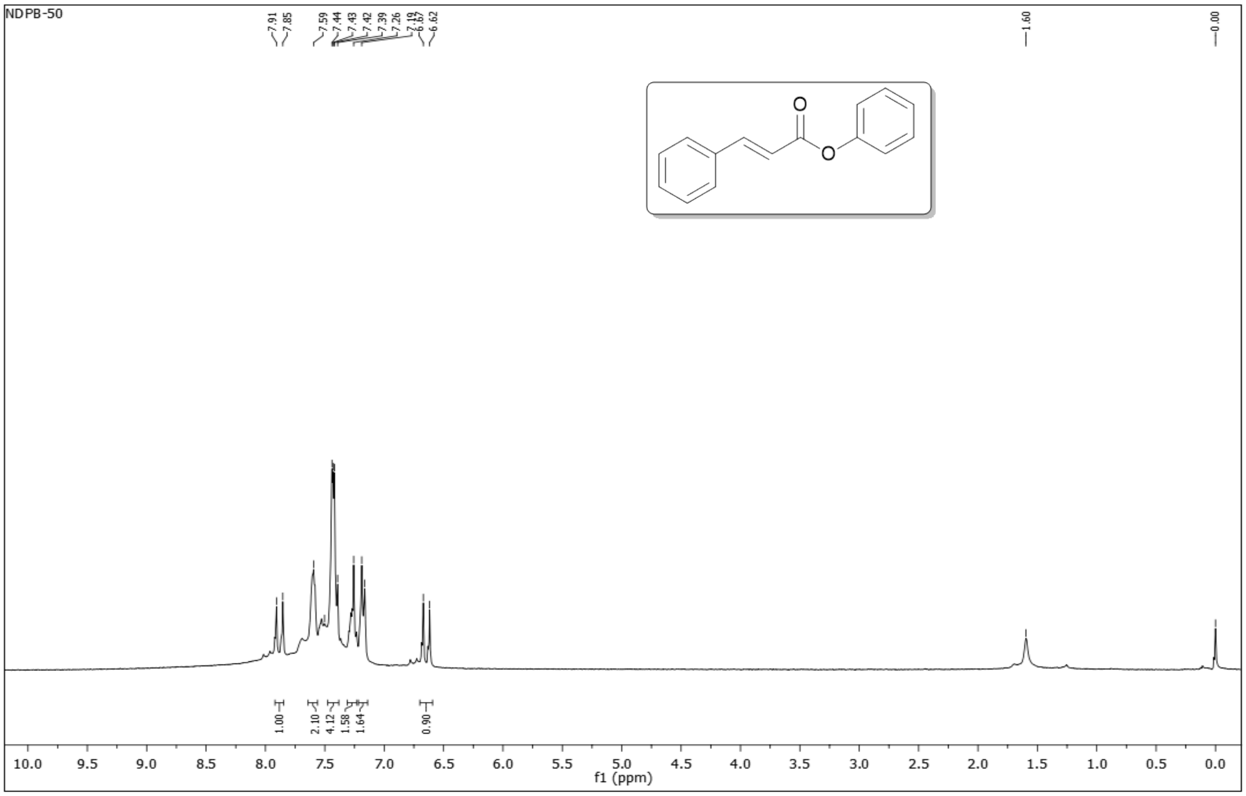

Fig. S93 ^{1}H NMR spectrum of phenyl cinnamate **4ak** (300 MHz, $CDCl_3$)

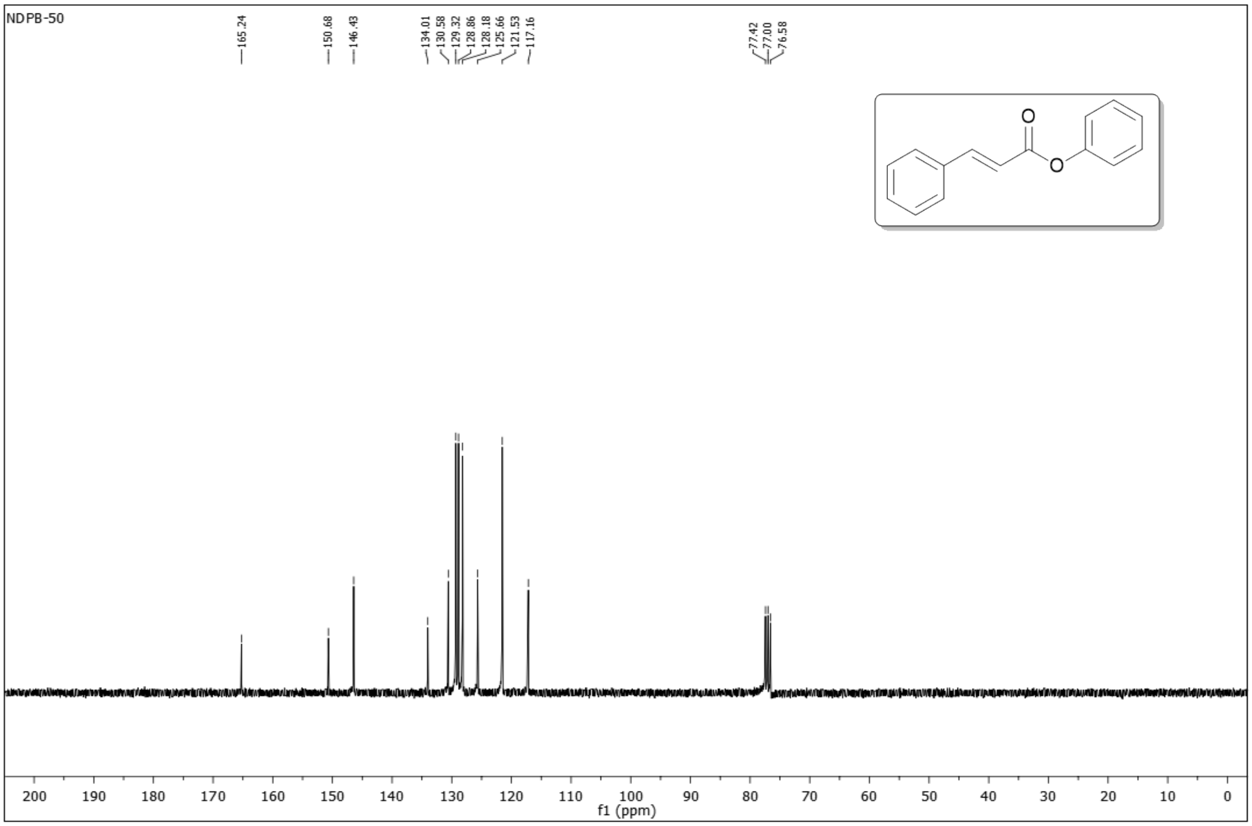

Fig. S94 ^{13}C NMR spectrum of phenyl cinnamate **4ak**(75 MHz, $CDCl_3$)

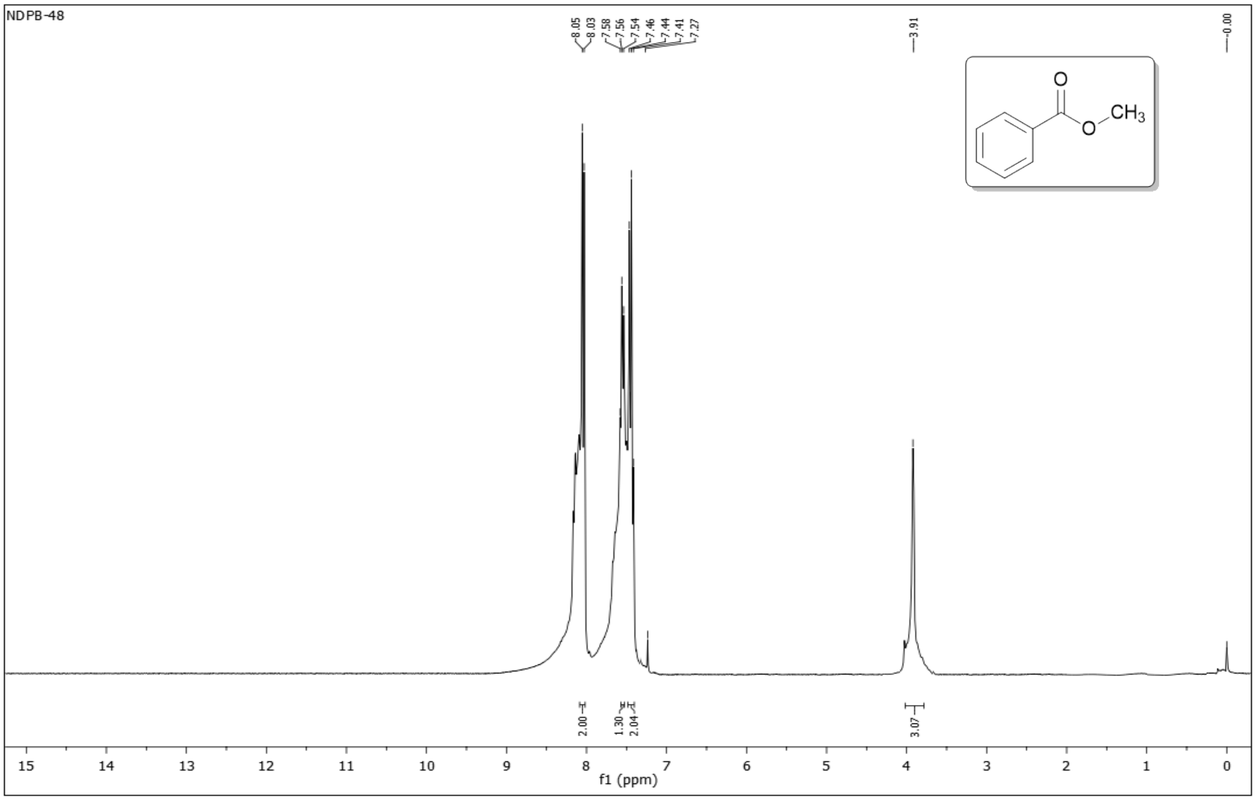

Fig. S95 ^{1}H NMR spectrum of methyl benzoate **4al** (300 MHz, $CDCl_3$)

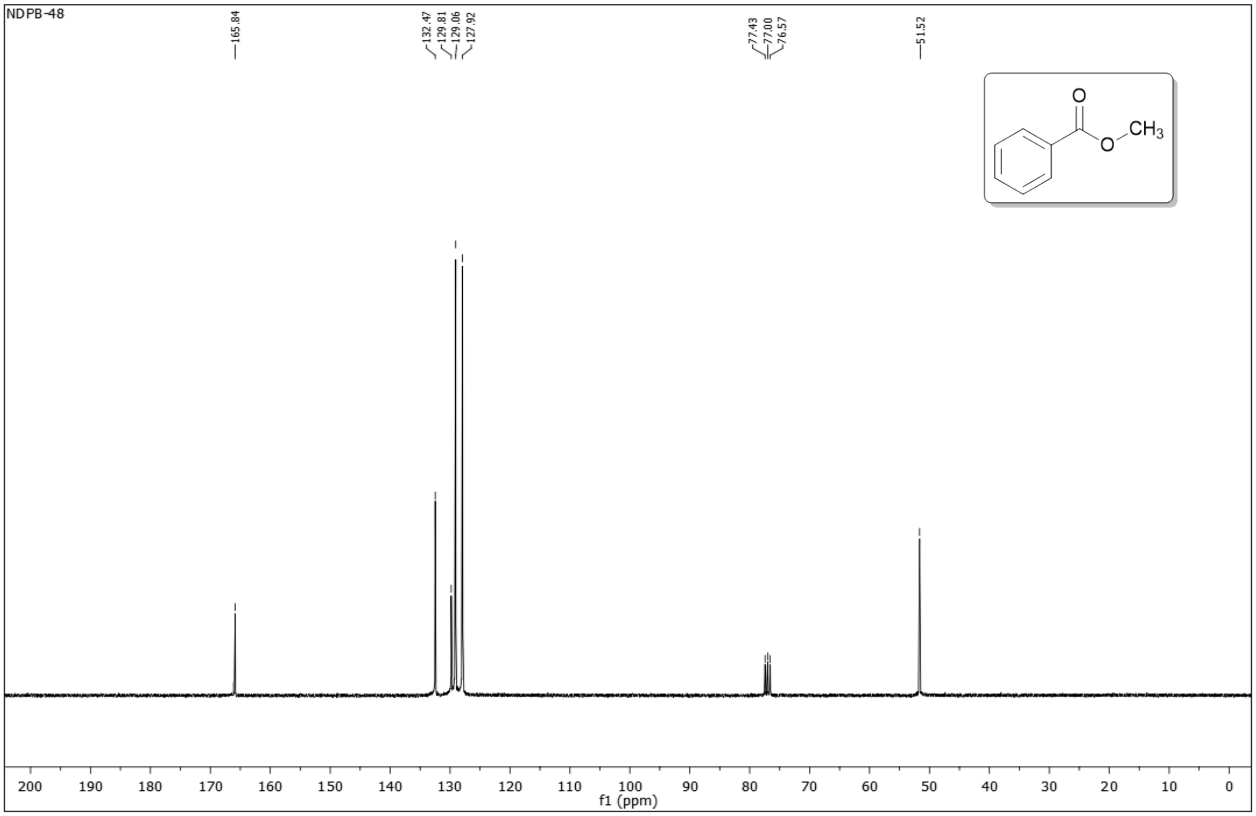

Fig. S96 ^{13}C NMR spectrum of methyl benzoate **4al** (75 MHz, $CDCl_3$)