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Supporting Information

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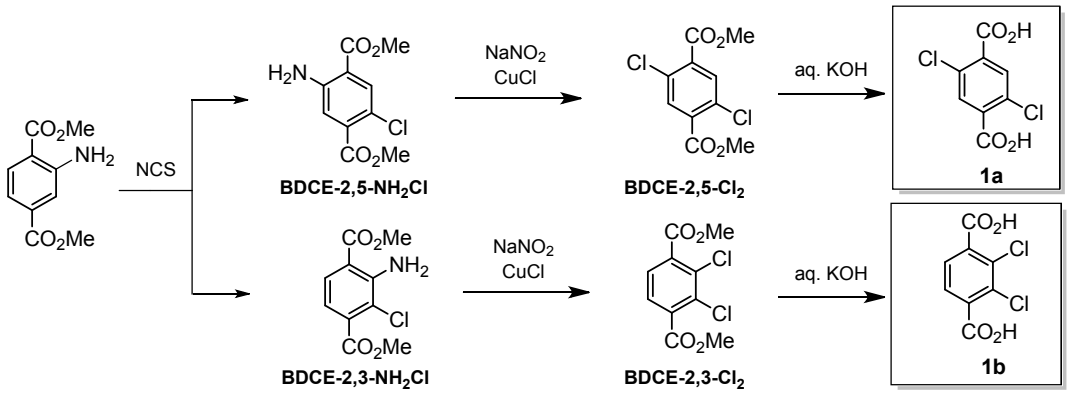
General Methods.

Evaporation of organic solvents was carried out by using a rotary evaporator with an aspirator or diaphragm, and residual solvents were removed on a vacuum line held at 0.1–1 torr. Analytical thin layer chromatography (TLC) was performed on pre-coated silica gel 60 F_{254} plates. Visualization on TLC was achieved by the use of UV light (254 nm). Flash column chromatography was undertaken on silica gel (400-630 mesh). Proton nuclear magnetic resonance spectra (^{1}H NMR) were recorded on FT AM 400 or 500 (400 MHz or 500 MHz). Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0 ppm for TMS. The following abbreviations were used to describe peak patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, and m = multiplet. Coupling constants, *J*, were reported in Hertz unit (Hz). Carbon 13 nuclear magnetic resonance spectroscopy (^{13}C NMR) was recorded on FT AM 400 or 500 (100 MHz or 125 MHz) and was fully decoupled by broad band decoupling. Chemical shifts were reported in ppm referenced to the center line of a triplet at 77.0 ppm of chloroform-*d* and a septet at 39.52 ppm of DMSO-d_6.

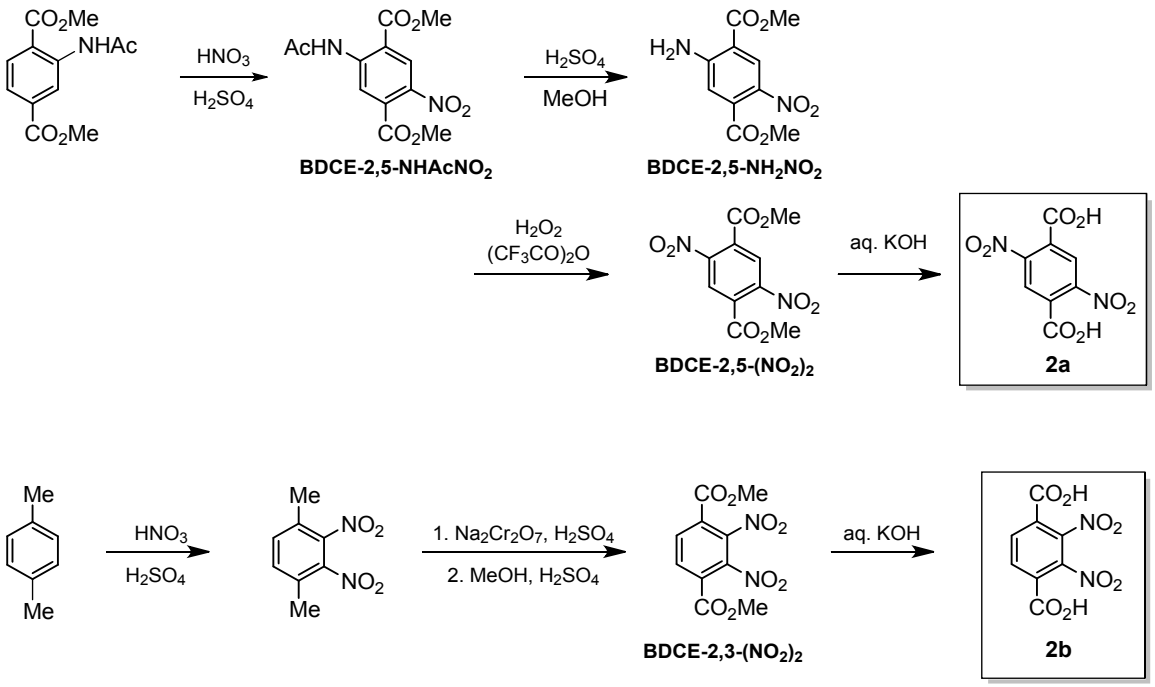
Materials

Tetrahydrofuran (THF), iodomethane, ethanol were purchased from Deajung Chemical and ethyl acetate (EtOAc), dimethylformamide (DMF), methanol, sodium dichromate were purchased from Samchun Chemical. 2,5-diaminoterephthalic acid (**4a,** Aldrich), dimethyl-2-aminoterephthalate (Alfa Aesar), *N*-chlorosuccinimide (NCS, Alfa Aesar), *N,N*-diethylformamide (DEF, TCI) and all chemical reagents were used without further purification unless otherwise stated. Dimethy-2-amino-3-chlorterephthalate, dimethyl-2-amino-5-chloroterephthalate and dimethyl-2-acetamido-5-nitroterephthalate were prepared following literature procedures.[S1, S2]

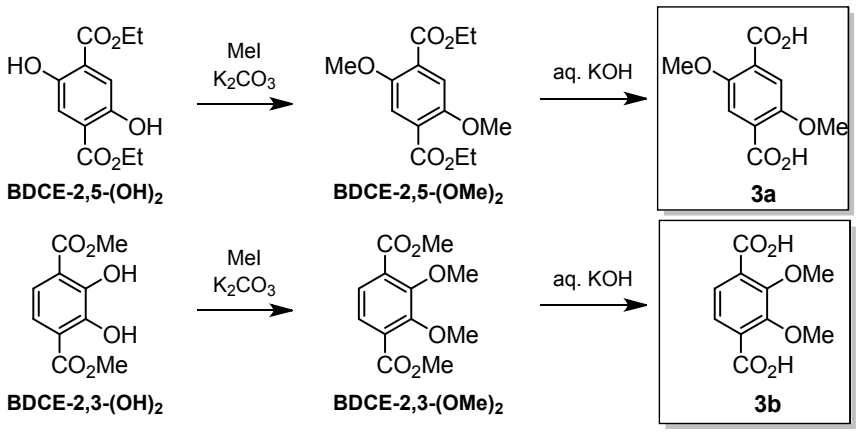
Overall Schemes for Ligand Synthesis



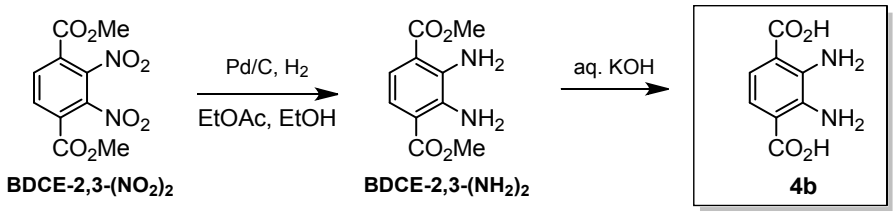
Scheme S1 Synthesis of BDC-2,5/2,3-Cl_2 (**1a** and **1b**).



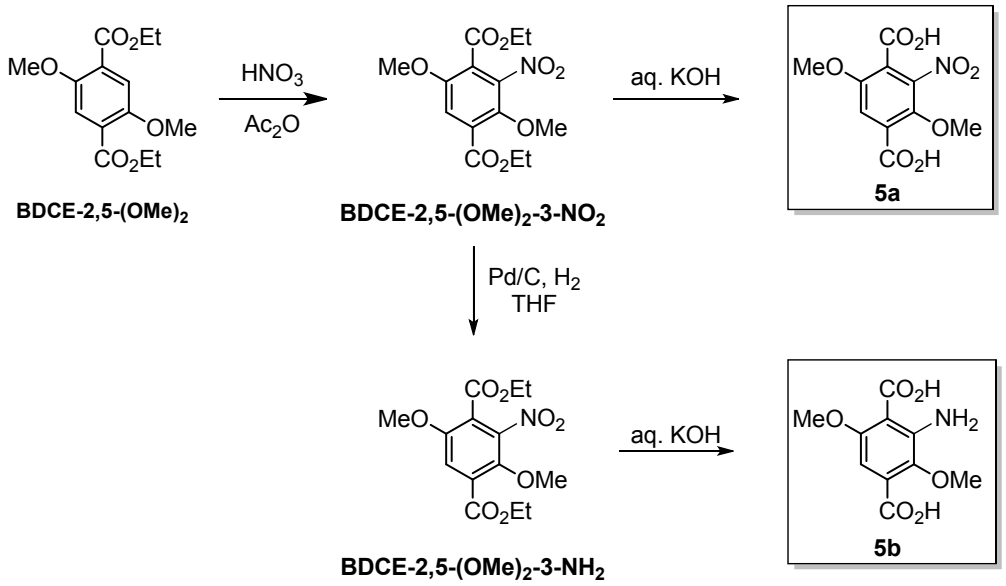
Scheme S2 Synthesis of BDC-2,5/2,3-$(NO_2)_2$ (**2a** and **2b**).



Scheme S3 Synthesis of BDC-2,5/2,3-$(OMe)_2$ (**3a** and **3b**).

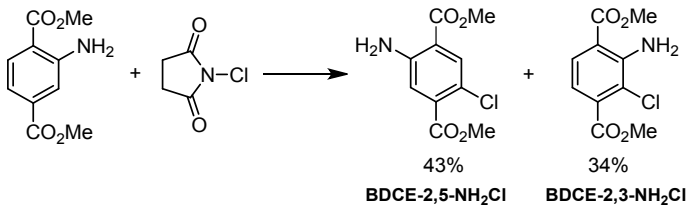


Scheme S4 Synthesis of BDC-2,3-$(NH_2)_2$ (**4b**).



Scheme S5 Synthesis of BDC-2,5-$(OMe)_2$-3-NO_2/NH_2 (**5a** and **5b**).

Detailed Procedures of Ligand Synthesis

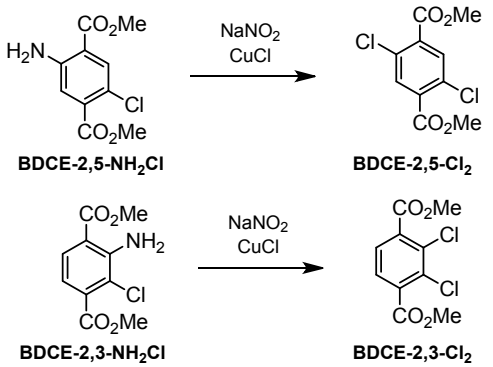


Dimethyl-2-amino-5-chloroterephthalate and Dimethyl-2-amino-3-chloroterephthalate.[S1]

Dimethyl-2-aminoterephtalate (2.0 g, 10 mmol) and *N*-chlorosuccinimide (1.4 g, 10.5 mmol) were dissolved in isopropanol (200 mL). The mixture was stirred at 60 °C for 24 h. Once conversion was complete (monitored by TLC), the, solvent was evaporated. The solid mixture was separated by silica gel column chromatography (10% EtOAc/*n*-Hexane) and the desired compounds, dimethyl-2-amino-5-chloroterephthalate (1.05 g, 43%) and dimethyl-2-amino-3-chloroterephthalate (827 mg, 34%), were obtained

Dimethyl-2-amino-5-chloroterephthalate: ^{1}H NMR ($CDCl_3$, 400MHz, ppm.): δ 7.89 (1H, s), 7.07 (1H, s), 5.79 (2H, br), 3.91 (3H, s), 3.88 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 167.1, 165.9, 148.5, 135.0, 133.1, 119.4, 119.0, 113.6, 52.7, 52.2.

Dimethyl-2-amino-3-chloroterephthalate: ^{1}H NMR ($CDCl_3$, 400 MHz, ppm.): δ 7.84 (1H, d, J = 8.4 Hz), 6.94 (1H, d, J = 8.4 Hz), 3.93 (3H, s), 3.90 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 167.8, 166.6, 147.4, 135.3, 129.5, 118.7, 116.2, 113.3, 52.8, 52.3.



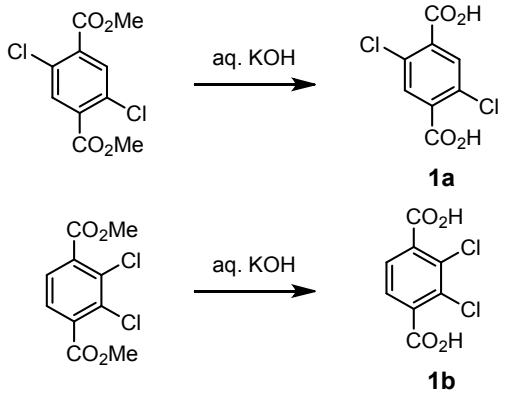
Dimethyl-2,5-dichloroterephthalate and Dimethyl-2,3-dichloroterephthalate.

Dimethyl-2-amino-5-chloroterephthalate (244 mg, 1 mmol) was dissolved in 500 µL of water and 600 µL of 36% HCl solution at 0 °C. The solution was stirred at 0 °C, and $NaNO_2$ aqueous solution (90 mg of $NaNO_2$ in 1 mL of H_2O) was added dropwise to the solution for 1 hour at 0 °C. Then the mixture was slowly transferred into a CuCl/HCl solution (119 mg of CuCl in 500 µL of 36% HCl). The mixture was stirred for 1 h at 0 °C and an additional 2 h at room temperature. The resultant was extracted with EtOAc, the organic layer was dried using $MgSO_4$, and the ethyl acetate was evaporated under reduced pressure. The obtained solid mixture was separated by silica gel column chromatography (10% EtOAc/*n*-Hexane) and the desired compound, dimethyl-2,5-dichloroterephthalate (90 mg, 34 %), was obtained as a colorless solid.

Dimethyl-2,5-dichloroterephthalate : ^{1}H NMR (DMSO, 400 MHz, ppm.): δ 8.00 (2H, s), 3.89 (s, 6H) ^{13}C NMR (DMOS,400 MHz, ppm): δ 163.8, 133.8, 132.6, 130.4, 53.1. ESI-MS(+) *m/z* calcd. For $C_{10}H_8Cl_2NaO_4$ $[M+Na]^+$: 284.9692, found $[M+Na]^+$: 284.9691.

Dimethyl-2,3-dichloroterephthalate was obtained in comparable yield from a similar procedure using dimethyl-2-amino-3-chloroterephthalate as the starting material.

Dimethyl-2,3-dichloroterephthalate : ^{1}H NMR ($CDCl_3$, 400 MHz, ppm.): δ 7.64 (2H, s), 3.95 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 165.5 135.2 133.4 128.2 53.1. ESI-MS(+) *m/z* calcd. For $C_{10}H_8Cl_2NaO_4$ $[M+Na]^+$: 284.9692, found $[M+Na]^+$: 284.9492.



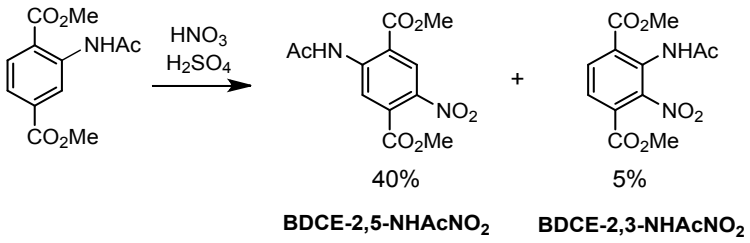
*2,5-Dichloroterephthalic acid (**1a**) and 2,3-Dichloroterephthalic acid (**1b**).*

Dimethyl-2,5-dichloroterephthalate (263 mg, 1 mmol) was dissolved in 5 mL of THF, and 5 mL of a 4% KOH aqueous solution was slowly added to the THF solution. The mixture was stirred under reflux condition (66 °C) overnight. Once conversion was complete (monitored by TLC), THF was removed by evaporation and the mixture was acidified with a 1.0 M HCl aqueous solution. The precipitate was collected by filtration, and washed with water. The desired compound was obtained by air drying (**1a**, 161 mg, 69%) as a colorless solid.

2,5-Dichloroterephthalic acid (**1a**): ^{1}H NMR (DMSO-d_6, 400 MHz, ppm.): δ 7.90 (2H, s), ^{13}C NMR (DMSO-d_6, 100 MHz, ppm): δ 163.7, 133.7, 132.6, 130.4, 53.1. ESI-MS(-) *m/z* calcd. For $C_8H_3Cl_2O_4$ $[M-H]^-$: 232.9414, found $[M-H]^-$: 232.9415.

2,3-Dichloroterephthalic acid (**1b**) was obtained in comparable yield from a similar procedure using dimethyl-2,3-dichloroterephthalate as the starting material.

2,3-Dichloroterephthalic acid (**1b**): ^{1}H NMR (DMSO-d_6, 400 MHz, ppm.): δ 7.73 (2H, s); ^{13}C NMR (DMSO-d_6, 100 MHz, ppm): δ 166.1, 136.2, 130.5, 128.2. ESI-MS(-) *m/z* calcd. For $C_8H_3Cl_2O_4$ $[M-H]^-$: 232.9414, found $[M-H]^-$: 232.9412.



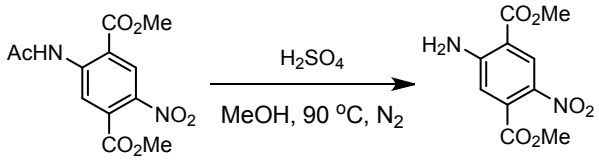
Dimethyl-2-acetamido-5-nitroterephthalte and Dimethyl-2-acetamido-3-nitroterephthalte.[S2]

Dimethyl-2-acetamidoterephthalate (3.8 g, 15 mmol) was dissolved in conc. sulfuric acid (30 mL), and the mixture was stirred at 0 °C. Then 60% nitric acid (8.6 mL, 21 mmol) was slowly added to the cooled mixture solution, and the solution was continuously stirred for 2 h at 0 °C. The reaction was quenched by addition of ice, and yellow precipitants were formed. The yellow solid mixture was separated by silica gel column chromatography (25% EtOAc/*n*-Hexane) and the desired compound, dimethyl-2-acetamido-5-nitroterephthalte (1.8 g, 40%) and

dimethyl-2-acetamido-3-nitroterephthalate (220 mg, 5%), were obtained as a pale yellow solid.

Dimethyl 2-acetamido-5-nitroterephthalate: ^{1}H NMR ($CDCl_3$, 400 MHz, ppm.): δ 11.35 (1H, s, br), 9.03 (1H, s), 8.76 (1H, s), 4.01 (3H, s), 3.96 (3H, s), 2.29 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 169.4, 166.7, 165.7, 145.8, 139.7, 134.6, 127.7, 119.9, 115.2, 53.6, 53.3, 25.6.

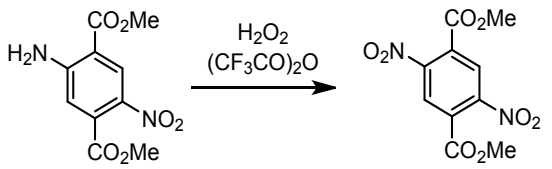
Dimethy-2-acetamido-3-nitroterephthalate: ^{1}H NMR ($CDCl_3$, 400 MHz, ppm.): δ 9.21 (1H, s, br), 8.12 (1H, d, J = 8.2), 7.63 (1H, d, J = 8.2 Hz), 3.95 (3H, s), 3.91 (3H, s), 2.19 (3H, s); ^{13}C NMR ($CDCl_3$, 150 MHz, ppm): δ 169.2, 165.7, 164.3, 145.0, 133.0, 131.1, 130.7, 128.0, 125.9, 53.7, 53.3, 24.0.



Dimethyl-2-Amino-5-nitroterephthate

Dimethyl-2-acetamido-5-nitroterephthalte (296 mg, 1 mmol) was dissolved in 3 mL of MeOH. To this, 0.7 mL of a conc. H_2SO_4 was added. The mixture was stirred under reflux condition (90 °C) for 4 h in N_2 atmosphere. Once conversion was complete (monitored by TLC), MeOH was removed by evaporation and ethyl acetate was added to the mixture. The organic layer was washing with saturated $NaHCO_3$ solution, brine and dried using $MgSO_4$. The yellow solid mixture was separated by silica gel column chromatography (10% EtOAc/*n*-Hexane) and the desired compound, dimethyl-2-amino-5-nitroterephthalte (221 mg, 87%) were obtained as an ivory solid.

Dimethyl 2-amino-5-nitroterephthalate : ^{1}H NMR (DMSO-d_6, 500 MHz, ppm.): δ 8.51 (1H, s), 7.97 (2H, s, br), 6.94 (1H, s), 3.86 (3H, s), 3.84 (3H, s); ^{13}C NMR (DMSO-d_6, 125 MHz, ppm): δ 166.2, 165.7, 154.8, 134.0, 132.3, 129.8, 116.0, 108.3, 53.1, 52.3. ESI-MS(+) *m/z* calcd. For $C_{10}H_{10}N_2NaO_6$ $[M+Na]^+$: 277.0431, found $[M+Na]^+$: 277.0435.

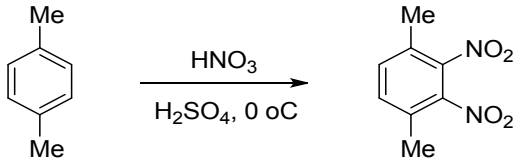


BDCE-2,5-(NO_2)$_2$

Dimethyl-2,5-dinitroterephthalate

Trifluoroacetic anhydride (4.3 mL, 31.1 mmol) was slowly added to the solution mixture of 30% H_2O_2 (2.7 mL, 26.6mmol) and CH_2Cl_2 (15 mL) at 0 °C. The solution mixture was warmed to room temperature, and dimethyl-2-amino-5-nitroterephthalate solution (428 mg, 1.68 mmol in CH_2Cl_2 4.5 mL) was slowly added to the mixture. After stirring for 3 h at 45 °C, the mixture was cooled to 0 °C and Na_2SO_3 was slowly added for quenching the reaction. The resulting mixture was extracted with CH_2Cl_2. The organic phase was washed with brine. The solution was then dried using $MgSO_4$, filtered, and evaporated for CH_2Cl_2. The solid mixture was recrystallized from EtOAc, and the desired compound, dimethyl-2,5-dinitroterephthalate (267 mg, 23%), was obtained as a greenish solid.

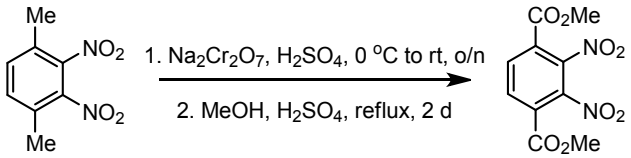
Dimethyl-2,5-dinitroterephthalate : ^{1}H NMR (DMSO-d_6, 400 MHz, ppm.): δ 8.61 (2H, s), 3.92 (6H, s); ^{13}C NMR (DMSO-d_6, 100 MHz, ppm): δ 162.5 149.0 129.3 126.5 54.0. ESI-MS(+) *m/z* calcd. For $C_{10}H_8N_2NaO_8$ $[M+Na]^+$: 307.0173, found $[M+Na]^+$: 307.0173.



2,3-Dinitro-p-xylene.

p-Xylene (3.2 g, 30 mmol) was dissolved in conc. sulfuric acid (20 mL), and the mixture was stirred at 0 °C. Then 60% nitric acid (4.6 mL, 60 mmol) was slowly added to cooled mixture, and the mixture was continuously stirred for 2 h at 0 °C. The crashed ice was added to the reaction flask, and the resulting yellow solid was filtered. The yellow solid mixture was separated by silica gel column chromatography (10% EtOAc/*n*-Hexane) and the desired compound, 2,3-dinitro-*p*-xylene (1.8g, 40%) were obtained as a pale yellow solid.

2,3-Dinitro-*p*-xylene : ^{1}H NMR ($CDCl_3$, 400 MHz, ppm.): δ 7.39 (2H, s), 2.43 (6H, s); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 143.6 133.9, 130.6, 17.8. ESI-MS(+) *m/z* calcd. For $C_8H_8N_2NaO_4$ $[M+Na]^+$: 219.0376, found $[M+Na]^+$: 219.0375.

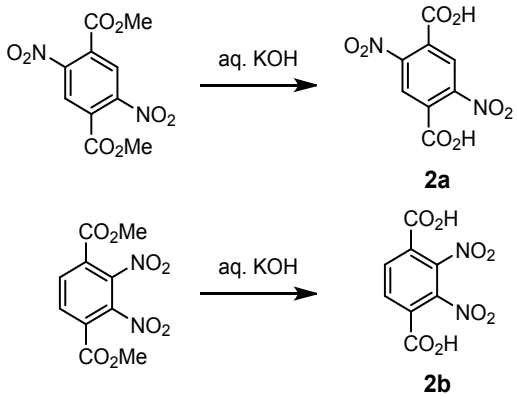


BDCE-2,3-$(NO_2)_2$

Dimethyl-2,3-dinitroterephthalate.[S3]

2,3-Dinitro-*p*-xylene (1,5 g, 7.65 mmol) was dissolved in conc. sulfuric acid (45 mL) and the mixture was cooled to 0 °C. Sodium dichromate (13.7 g, 46 mmol) was added to the mixture for a small quantity (1 g) every 0.5 h. After adding the mixture was warmed to room temperature and stirred overnight. The crashed ice was added to the reaction flask, and the reaction was quenched with sodium sulfide. And then it was extracted with EtOAc (30 mL X 8). The organic phase was dried using $MgSO_4$, after filtration the solvent was evaporated *in vaccuo*. Methanol (80 mL) and conc. sulfuric acid (8 mL) was added to the resulting solid, the mixture was stirred for 2 d at 70 °C. The methanol was evaporated in *vaccuo*, the mixture was extracted with EtOAc/water. The organic solution was dried with $MgSO_4$, and after filtration, the solution was evaporated in *vaccuo*. The resulting solid was purified by silica gel column chromatography (25% EtOAc/*n*-Hexane), and the desired compound, dimethy-2,3-dinitroterephthalate (798 mg, 37%) was obtained as an ivory solid.

Dimethyl-2,3-dinitroterephthalate : ^{1}H NMR ($CDCl_3$, 400 MHz, ppm.): δ 8.17 (2H, s), 3.96 (6H, s); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 161.9, 142.7, 133.0, 128.8, 54.1. ESI-MS(+) *m/z* calcd. For $C_{10}H_8N_2NaO_8$ $[M+Na]^+$: 307.0173, found $[M+Na]^+$: 307.0171.



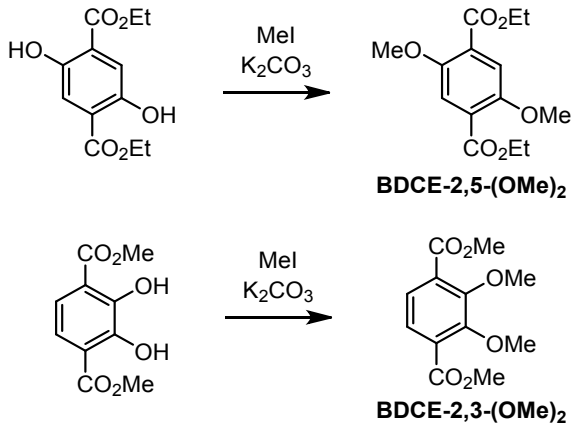
*2,5-Dinitroterephthalic acid (**2a**) and 2,3-Dinitroterephthalic acid (**2b**).*

Dimethyl-2,5-dinitroterephthalate (284 mg, 1 mmol) was dissolved in 5 mL of THF. And 5 mL of a 4% KOH aqueous solution was slowly added to the THF solution. The mixture was stirred under room temperature for 2 h. Once conversion was complete (monitored by TLC), THF was removed by evaporation and the mixture was acidified with a 1.0 M HCl aqueous solution. The solution was stored overnight in a refrigerator. The precipitate was collected by filtration, and washed with water. The desired compound was obtained by air drying (**2a**, 249 mg, 98%) as a yellow solid.

2,5-Dinitroterephthalic acid (**2a**): ^{1}H NMR (DMSO-d_6, 400 MHz, ppm.): δ 8.12 (2H, s); ^{13}C NMR (DMSO-d_6, 100 MHz, ppm): δ 163.3, 149.3, 124.9. ESI-MS(-) *m/z* calcd. For $C_8H_3N_2O_8$ $[M\text{-}H]^-$: 254.9895, found $[M\text{-}H]^-$: 254.9897.

2,3-Dinitroterephthalic acid (**2b**) was obtained in comparable yield from a similar procedure using dimethyl-2,3-dichloroterephthalate as a starting material.

2,3-Dinitroterephthalic acid (**2b**): ^{1}H NMR (DMSO-d_6, 400 MHz, ppm.): δ 8.04 (2H, s); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 163.3, 141.5, 132.9, 132.8. ESI-MS(-) *m/z* calcd. For $C_8H_3N_2O_8$ $[M\text{-}H]^-$: 254.9895, found $[M\text{-}H]^-$: 254.9898.



Diethyl-2,5-dimethoxyterephthalate and Dimethyl-2,3-dimethoxyterephthalate.

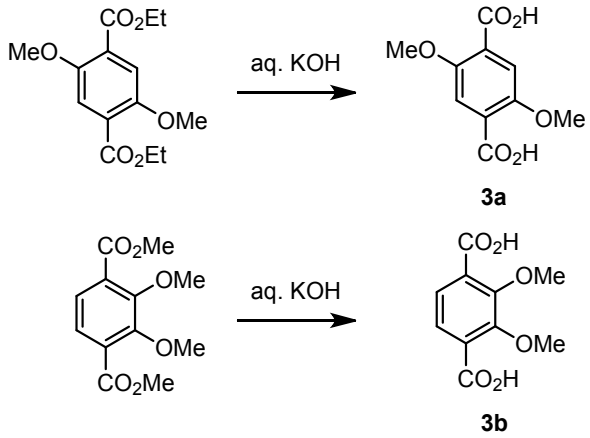
Diethyl-2,5-dihydroxyterephthalate (1.27 g, 5 mmol), potassium carbonate (830 mg, 16 mmol), and iodomethane (1 mL, 16 mmol) were dissolved in acetone (15 mL). The mixture was stirred under reflux condition (60°C) for overnight. Once conversion was complete (monitored by TLC), the solvent was evaporated. And then water was

added to dissolve all of the inorganic salts. The solution was three times extracted with ethyl acetate. The solution was then dried using $MgSO_4$, and after filtration the solution was evaporated *in vaccuo*. Then the desired compound, dimethyl 2,5-dimethoxyterephthalate (1.11 g, 79%), were obtained as a colorless solid.

Diethyl-2,5-dimethoxyterephthalate : ^{1}H NMR ($CDCl_3$, 500 MHz, ppm.): δ 7.35 (2H, s), 4.35 (4H, q, J = 7.1 Hz), 3.87 (6H, s), 1.38 (6H, t, J = 7.1 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 165.5, 152.3, 124.4, 115.4, 67.3, 58.8, 14.2. ESI-MS(+) *m/z* calcd. For $C_{14}H_{18}LiO_6$ $[M+Li]^+$: 289.1258, found $[M+Li]^+$: 289.1258.

Dimethyl-2,3-dimethoxyterephthalate was obtained in comparable yield from a similar procedure using dimethyl-2,3-dihydroxyterephthalate as a starting material.

Dimethyl-2,3-dimethoxyterephthalate : ^{1}H NMR ($CDCl_3$, 500 MHz, ppm.): δ 7.47 (2H, s), 3.92 (3H, s), 3.90 (3H, s); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 165.8, 153.8, 129.5, 125.1, 61.7, 52.4. ESI-MS(+) *m/z* calcd. For $C_{12}H_{14}NaO_6$ $[M+Na]^+$: 277.0683, found $[M+Na]^+$: 277.0682.



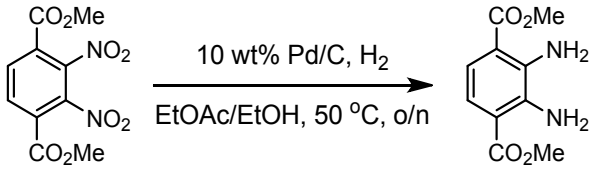
*2,5-Dimethoxyterephthalic acid (**3a**) and 2,3-Dimethoxyterephthalic acid (**3b**).*

Diethyl-2,5-dihydroxyterephthalate (1.11 g, 3.94 mmol) was dissolved in 20 mL of THF. To this, 20 mL of a 4% KOH aqueous solution was added. The mixture was stirred under reflux condition (66 ^{o}C) for overnight. Once conversion was complete (monitored by TLC), THF was removed by evaporation and the mixture was acidified with a 1.0 M HCl aqueous solution. The precipitate was collected by filtration, and washed with water. The desired compound was obtained by air drying (**3a**, 840 mg, 94%) as a colorless solid.

2,5-Dimethoxyterephthalic acid (**3a**): ^{1}H NMR (DMSO-d_6, 500 MHz, ppm.): δ 7.29 (2H, s), 3.78 (6H, s); ^{13}C NMR (DMSO-d_6, 125 MHz, ppm): δ 166.8, 151.1, 125.0, 114.5, 56.4. ESI-MS(-) *m/z* calcd. For $C_{10}H_9O_6$ $[M-H]^-$: 225.0405, found $[M-H]^-$: 225.0405.

2,3-Dimethoxyterephthalic acid (**3b**) was obtained in comparable yield from a similar procedure using Dimethyl-2,3-dihydroxyterephthalate as a starting material.

2,3-Dimethoxyterephthalic acid (**3b**): ^{1}H NMR (DMSO-d_6, 500 MHz, ppm.): δ 7.39 (2H, s), 3.82 (6H, s); ^{13}C NMR (DMSO-d_6, 125 MHz, ppm): δ 166.8, 152.5, 130.5, 124.5, 61.5. ESI-MS(-) *m/z* calcd. For $C_{10}H_9O_6$ $[M-H]^-$: 225.0405, found $[M-H]^-$: 225.0405.



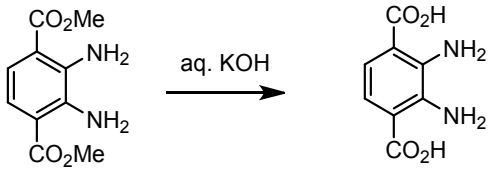
BDCE-2,3-$(NH_2)_2$

Dimethyl-2,3-Diaminterephthalate.

A suspention of dimethyl-2,3-dinitroterephthalate (284 mg, 1 mmol) and 10 wt% Pd/C (27 mg, 10 mmol%) in EtOH/EtOAc (EtOAc: EtOH = 1mL: 4mL) was stirred under H_2 atmosphere at 50 °C for overnight. Once converstion was complete (monitored by TLC), the mixture was filtered through celite and evaporated of EtOH/EtOAc. The crude product was separated by silica gel column chromatography (10% EtOAc/*n*-Hexane) and the desired compound, dimethyl 2,3-diaminoterephthalate (186 mg, 84%), was obtained as a yellow solid.

Before confirm the product, chloroform-*d* (590 μL) must shake with 40% NaOD/D_2O solution (10 μL) and carefully decant the chloroform-*d* to NMR cell.

Dimethyl-2,3-diaminoterephthalate: ^{1}H NMR ($CDCl_3$, 400 MHz, ppm.): δ 7.30 (2H, s), 5.55 (4H, br) 3.89 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 168.8, 141.0, 118.5, 114.3, 52.0. ESI-MS(+) *m/z* calcd. For $C_{10}H_{10}N_2O_4$ $[M\text{-}H]^-$: 225.0870, found $[M\text{-}H]^-$: 225.0867.

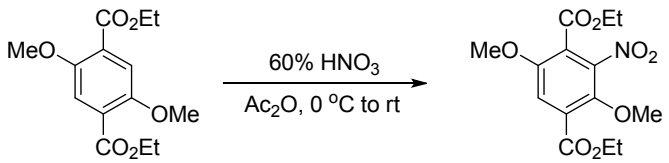


4b

*2,3-Diaminoterephthalic acid (4**b**).*

Dimethyl-2,3-diaminoterephthalate (168 mg, 0.75 mmol) was dissolved in 5 mL of THF. To this, 5 mL of a 4% KOH aqueous solution was added. The mixture was stirred under reflux condition (66 °C) for overnight. Once conversion was complete (monitored by TLC), THF was removed by evaporation and the mixture was acidified with a 1.0 M HCl aqueous solution. The precipitate was collected by filtration, and washed with water. The desired compound was obtained by air drying (**4a**, 120 mg, 82%) as a brown solid.

2,3-Diaminoterephthalic acid (**4a**): ^{1}H NMR (DMSO-d_6, 400 MHz, ppm.): δ 7.00 (2H, s); ^{13}C NMR (DMSO-d_6, 100 MHz, ppm): δ 170.0, 140.8, 116.2, 110.7. ESI-MS(-) *m/z* calcd. For $C_8H_7N_2O_4$ $[M\text{-}H]^-$: 225.0411, found $[M\text{-}H]^-$: 225.0412.



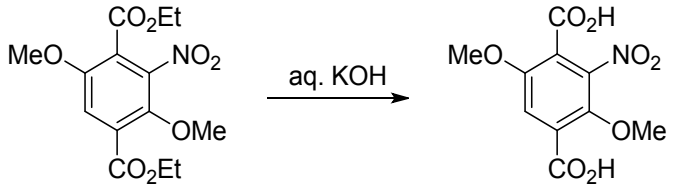
BDCE-2,5-$(OMe)_2$-3-(NO_2)

Diethyl 2,5-dimethoxy-3-nitroterephthalate

Diethyl 2,5-dimethoxyterephthalate (500 mg, 1.77 mmol) were dissolved in Ac_2O (5 mL). To mixture solution was added 60% HNO_3 (1 mL) at 0 °C and stirred at room temperature for 24 h. Once conversion was complete (monitored by TLC), the solution was poured into H_2O (20 mL). Saturated $NaHCO_3$ solution was added to the

mixture until neutral by pH paper. The organic phase was extracted with 25 mL of $CHCl_3$ and then the organic solution was dried with $MgSO_4$, filtered, and evaporated. The solid mixture was separated by silica gel column chromatography (10% EtOAc/*n*-Hexane) and the desired compound was obtained as a yellow solid (350 mg, 60%).

Diethyl 2,5-dimethoxy-3-nitroterephthalate : ^{1}H NMR ($CDCl_3$, 500 MHz, ppm.): δ 7.54 (s, 1H), 4.44 (q, 2H, J = 7 Hz), 4.34 (q, 2H, J = 7 Hz), 3.92 (s, 6H), 1.43 (t, 3H, J = 7 Hz), 1.33 (t, 3H, J = 7 Hz) ; ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 163.82, 161.93, 152.48, 145.66, 145.39, 128.73, 120.90, 116.67, 64.84, 62.73, 62.33, 57.02, 14.15, 13.70. ESI-MS(+) *m/z* calcd. For $C_{14}H_{17}NNaO_8$ $[M+Na]^+$: 350.0852 found $[M+Na]^+$: 350.0856

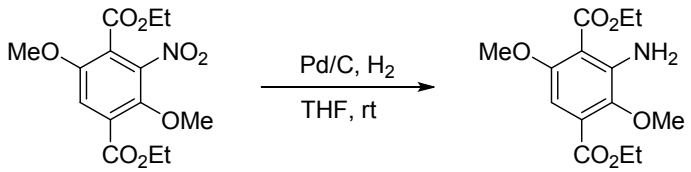


5a

*2,5-Dimethoxy-3-nitroterephthalic acid (**5a**)*

Diethyl 2,5-dimethoxy-3-nitroterephthalate (330 mg, 1.01 mmol) was dissolved in 4 mL of THF. To this, 4 mL of a 4% KOH aqueous solution was added dropwise. The mixture was stirred at room temperature overnight. Once conversion was complete (monitored by TLC), THF and H_2O was removed by evaporation and the mixture was acidified with a small amount of H_2O and concentrated HCl at 0 °C. The precipitate was collected by filtration, and washed with 1M HCl solution. The desired compound was obtained by air drying as a pale yellow solid (**5a**, 232 mg, 86%).

2,5-Dimethoxy 3-aminoterephthalic acid (**5a**) : ^{1}H NMR (DMSO-d_6, 500 MHz, ppm.): δ 7.63 (s, 1H), 3.89 (s, 3H), 3.81 (s, 3H) ; ^{13}C NMR (DMSO-d_6, 125 MHz, ppm): δ 165.40, 163.76, 152.02, 144.64, 144.19, 129.74, 121.35, 117.33, 64.73, 57.47. ESI-MS(-) *m/z* calcd. For $C_{10}H_8NO_8$ $[M-H]^-$: 270.0255, found $[M-H]^-$: 270.0256.

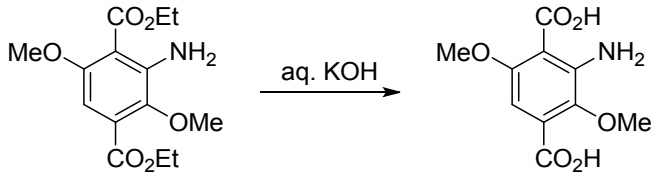


BDCE-2,5-(OMe)$_2$-3-NH$_2$

Diethyl 3-amino-2,5-dimethoxyterephthalate

Diethyl 2,5-dimethoxy-3-nitroterephthalate (350 mg, 1.07 mmol) was dissolved in THF (5 mL), and hydrogenation was performed using 10% Pd/C (35 mg, 10 wt%) under H_2 (1 atm) at room temperature for 18 h. The resulting suspension filtered through celite and evaporated to remove volatile solvents. The solid mixture was separated by silica gel column chromatography (7% EtOAc/*n*-Hexane) and the desired compound, diethyl 3-amino-2,5-dimethoxyterephthalate (300 mg, 95%), was obtained as a pale yellow oil.

Diethyl 3-amino-2,5-dimethoxyterephthalate : ^{1}H NMR ($CDCl_3$, 500 MHz, ppm.): δ 6.60 (s, 1H), 4.39 (q, 2H, J = 7 Hz), 4.38 (q, 2H, J = 7 Hz), 3.82 (s, 3H), 3.80 (s, 3H), 1.41 (t, 3H, J = 7 Hz), 1.38 (t, 3H, J = 7 Hz) ; ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 167.43, 165.94, 155.27, 143.91, 141.42, 126.49, 108.64, 100.41, 61.50, 61.29, 61.18, 56.38, 14.38, 14.33. ESI-MS(+) *m/z* calcd. For $C_{14}H_{19}LiNO_6$ $[M+Li]^+$: 304.1367 found $[M+Li]^+$: 304.1368.



5b

*3-Amino-2,5-dimethoxyterephthalic acid (**5b**)*

Diethyl 3-amino-2,5-dimethoxyterephthalate (300 mg, 1.01 mmol) was dissolved in 4 mL of THF. To this, 4 mL of a 4% KOH aqueous solution was added dropwise. The mixture was stirred at room temperature overnight. Once conversion was complete (monitored by TLC), THF and H_2O was removed by evaporation and the mixture was acidified with a small amount of H_2O and concentrated HCl at 0 °C. The precipitate was collected by filtration, and washed with 1M HCl solution. The desired compound was obtained by air drying as a pale yellow solid (**5b**, 219 mg, 90%).

3-Amino-2,5-dimethoxyterephthalic acid (**5b**) : ^{1}H NMR (DMSO-d_6, 500 MHz, ppm.): δ 7.63 (s, 1H), 3.89 (s, 3H), 3.81 (s, 3H) ; ^{13}C NMR (DMSO-d_6, 125 MHz, ppm): δ 165.40, 163.76, 152.02, 144.64, 144.19, 129.74, 121.35, 117.33, 64.73, 57.47. ESI-MS(-) *m/z* calcd. For $C_{10}H_8NO_8$ $[M-H]^-$: 270.0255, found $[M-H]^-$: 270.0256.

MOF Synthesis

DMOF Synthesis

The DMOF series was prepared and activated using a modified method from what has been previously described.[S4]

DMOF-2,5-Cl_2

3a (117 mg, 0.5 mmol) and $Zn(NO_3)_2{\cdot}6H_2O$ (149 mg, 0.5 mmol) were dissolved in 12.5 mL of DMF. To this mixture, dabco (1,4-diazabicyclo[2.2.2]octane, 90 mg, 0.8 mmol) was added. Upon adding, a yellow gel formed. This gel was filtered using a filter with a fritted disc of fine porosity. The solution was then transferred to a scintillation vial and heated at a rate of 2.5 ^{o}C/min from room temperature to 120 ^{o}C. The temperature was then held for 24 h and then cooled to room temperature at a rate of 2.5 ^{o}C/min. The resulting crystals were then washed three times with 5 mL of DMF. The solvent was then exchanged with chloroform (5 mL) over three days, replacing the old chloroform with fresh chloroform every 24 h.

DMOF-2,3-Cl_2

3b (94 mg, 0.4 mmol) and $Zn(NO_3)_2{\cdot}6H_2O$ (119 mg, 0.4 mmol) were dissolved in 10 mL of DMF. To this mixture, dabco (72 mg, 0.64 mmol) was added. Upon adding, a yellow precipitate formed. This precipitate was filtered using a filter with a fritted disc of fine porosity. The solution was then transferred to a scintillation vial and heated at a rate of 1 ^{o}C/min from room temperature to 120 ^{o}C. The temperature was then held for 48 h and then cooled to room temperature at a rate of 1 ^{o}C/min. The resulting crystals were then washed three times with 5 mL of DMF. The solvent was then exchanged with chloroform (5 mL) over three days, replacing the old chloroform with fresh chloroform every 24 h.

DMOF-2,5-$(NO_2)_2$

2a (51 mg, 0.2 mmol) and $Zn(NO_3)_2{\cdot}6H_2O$ (60 mg, 0.2 mmol) were dissolved in 2.5 mL of DEF. To this mixture, dabco (11 mg, 0.1 mmol) was added. The solution was heated in an autoclave at a rate of 1 ^{o}C/min from room temperature to 105 ^{o}C. The temperature was then held for 24 h and then cooled to room temperature at a rate of 1 ^{o}C/min. The resulting crystals were then washed three times with 5 mL of DMF. The solvent was then exchanged with chloroform (5 mL) over three days, replacing the old chloroform with fresh chloroform every 24 h.

DMOF-2,3-$(NO_2)_2$

2b (51 mg, 0.2 mmol) and $Zn(NO_3)_2{\cdot}6H_2O$ (59 mg, 0.2 mmol) were dissolved in 2.5 mL of DMF. To this mixture, dabco (11. mg, 0.1 mmol) was added. The solution was heated in an autoclave at a rate of 1 ^{o}C/min from room temperature to 105 ^{o}C. The temperature was then held for 48 h and then cooled to room temperature at a rate of 1 ^{o}C/min. The resulting crystals were then washed three times with 5 mL of DMF. The solvent was then exchanged with chloroform (5 mL) over three days, replacing the old chloroform with fresh chloroform every 24 h.

DMOF-2,5-$(OMe)_2$

4a (113 mg, 0.5 mmol) and $Zn(NO_3)_2{\cdot}6H_2O$ (149 mg, 0.5 mmol) were dissolved in 12.5 mL of DMF. To this mixture, dabco (90 mg, 0.8 mmol) was added. Upon adding, a white precipitate formed. This precipitate was filtered using a filter with a fritted disc of fine porosity. The solution was then transferred to a scintillation vial and heated at a rate of 2.5 ^{o}C/min from room temperature to 100 ^{o}C. The temperature was then held for 24 h and then cooled to room temperature at a rate of 2.5 ^{o}C/min. The resulting crystals were then washed three times with 5 mL of DMF. The solvent was then exchanged with chloroform (5 mL) over three days, replacing the old

chloroform with fresh chloroform every 24 h.

DMOF-2,3-(OMe)$_2$

4b (113 mg, 0.5 mmol) and $Zn(NO_3)_2{\cdot}6H_2O$ (149 mg, 0.5 mmol) were dissolved in 12.5 mL of DMF. To this mixture, dabco (90 mg, 0.8 mmol) was added. Upon adding, a white precipitate formed. This precipitate was filtered using a filter with a fritted disc of fine porosity. The solution was then transferred to a scintillation vial and heated at a rate of 1 ^{o}C/min from room temperature to 100 ^{o}C. The temperature was then held for 48 h and then cooled to room temperature at a rate of 1 ^{o}C/min. The resulting crystals were then washed three times with 5 mL of DMF. The solvent was then exchanged with chloroform (5 mL) over three days, replacing the old chloroform with fresh chloroform every 24 h.

DMOF-2,5-(OMe)$_2$-3-NO$_2$

5a (163 mg, 0.5 mmol) and $Zn(NO_3)_2{\cdot}6H_2O$ (149 mg, 0.5 mmol) were dissolved in 10 mL of DMF. To this mixture, dabco (90 mg, 0.8 mmol) was added. Upon adding, a white precipitate formed. This precipitate was filtered using a filter with a fritted disc of fine porosity. The solution was then transferred to a scintillation vial and heated at a rate of 2.5 ^{o}C/min from room temperature to 100 ^{o}C. The temperature was then held for 48 h and then cooled to room temperature at a rate of 2.5 ^{o}C/min. The resulting crystals were then washed three times with 5 mL of DMF. The solvent was then exchanged with chloroform (5 mL) over three days, replacing the old chloroform with fresh chloroform every 24 h.

DMOF-2,3-(OMe)$_2$-3-NH$_2$

5b (149 mg, 0.5 mmol) and $Zn(NO_3)_2{\cdot}6H_2O$ (149 mg, 0.5 mmol) were dissolved in 10 mL of DMF. To this mixture, dabco (90 mg, 0.8 mmol) was added. Upon adding, a white precipitate formed. This precipitate was filtered using a filter with a fritted disc of fine porosity. The solution was then transferred to a scintillation vial and heated at a rate of 1 ^{o}C/min from room temperature to 100 ^{o}C. The temperature was then held for 48 h and then cooled to room temperature at a rate of 1 ^{o}C/min. The resulting crystals were then washed three times with 5 mL of DMF. The solvent was then exchanged with chloroform (5 mL) over three days, replacing the old chloroform with fresh chloroform every 24 h.

MOF characterization

Digestion and Analysis by ^1H NMR of DMOF Series

Approximately 10 mg of DMOF material was dried under vacuum and digested with sonication in 590 µL of DMSO-d_6 and 10 µL of 35% DCl/D_2O solution).

Thermal Analysis

Approximately 10 mg of DMOF was used for TGA measurements, after BET analysis (activated). Sample was analyzed under a stream of N_2 using a TGA/DSC 1 running from room temperature to 800 ^oC with a scan rate of 10 ^oC/min.

Powder X-ray Diffraction

Approximately 10 mg of DMOF was air-dried for 1 min prior to PXRD analysis. PXRD data was collected at ambient temperature on a Bruker D8 Discover at 40 kV, 40 mA for CuKa (1 = 1.5406 Å), with a scan speed of 1 sec/step, a step size of 0.02° in 2θ, and a 2θ range of 5-55°.

Powder X-ray Diffraction Refinement

For the analysis of unit cell parameter of the DMOFs, we have measured diffraction the frameworks using a strong synchrotron X-ray source (0.9000 Å) in Pohang Accelerator Laboratory (2D SMC beamline) equipped with 2D area CCD detector. The framework sample was prepared in a 0.5 mm borosilicate capillary and mounted on a goniometer head. The diffraction data was collected using a Debye-Scherrer mode with a detector distance of 180 mm. The collected 2D diffraction image was merged and processed using a fit2d program. The merged PXRD data was used for the determination of unit-cell parameters. The PXRD data was indexed using Conograph GUI (developed by J-PARC neutron diffraction group, Japan). The indexed parameter was selected based on Wolff figure of merit[S5,S6] and unit cell parameter of the frameworks was determined.

BET Surface Area Analysis

Approximately 20-50 mg of DMOF sample was evacuated under vacuum for a moment at room temperature. Samples were then transferred to a pre-weighed sample tube and degassed at 100 ^oC on a Micromeritics ASAP 2020 Adsorption Analyzer for a minimum of 12 h or until the outgas rate was <5 µmHg/min. The sample tube was re-weighted to obtain a consistent mass for the degassed MOF materials. BET surface area (m^2/g) measurements were collected at 77 K by N_2 on a Micromeritics ASAP 2020 Adsorption Analyzer using a volumetric technique.

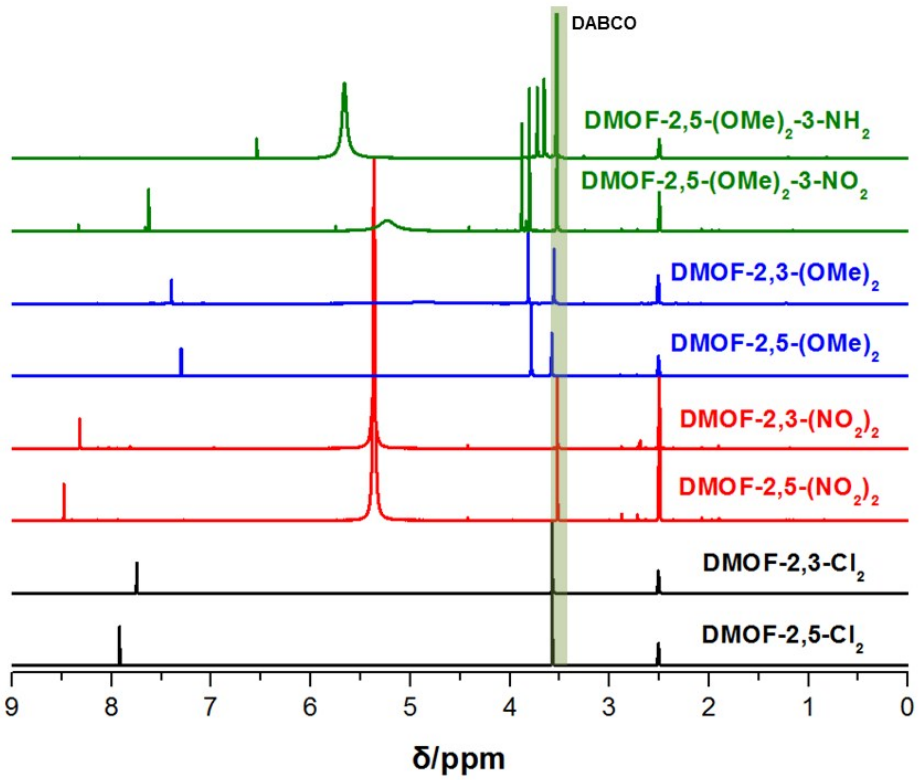


Fig. S1 ^{1}H NMR of regioisomeric DMOFs after acid digestion.

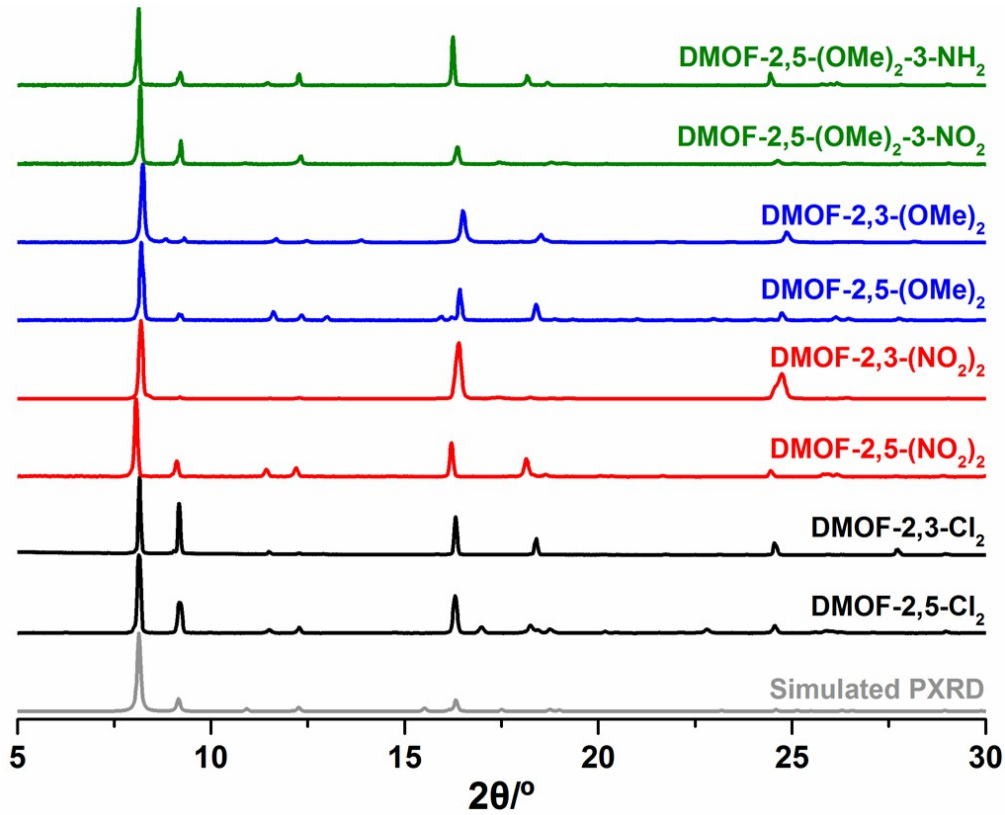


Fig. S2 PXRD patterns of simulated and synthesized DMOFs.

Table S1 The unit cell parameter of the obtained DMOFs after PXRD data refinement

DMOF	Suggested space group #	a=b=c (Å)	α=β=γ (°)
DMOF-1 (ref. 16)	**123** (determined in single crystal structure)	10.929	9.608
DMOF-2,3-Cl_2	75, 81, 83, 89, 99, 111, 115, **123**	10.899	9.661
DMOF-2,3-$(OMe)_2$	75, 81, 83, 89, 99, 111, 115, **123**	10.948	9.636
DMOF-2,5-Cl_2	75, 81, 83, 89, 99, 111, 115, **123**	10.917	9.639
DMOF-2,5-$(NO_2)_2$	75, 81, 83, 89, 99, 111, 115, **123**	10.914	9.699
DMOF-2,5-(OMe)-3-(NO_2)	75, 81, 83, 89, 99, 111, 115, **123**	10.880	9.607

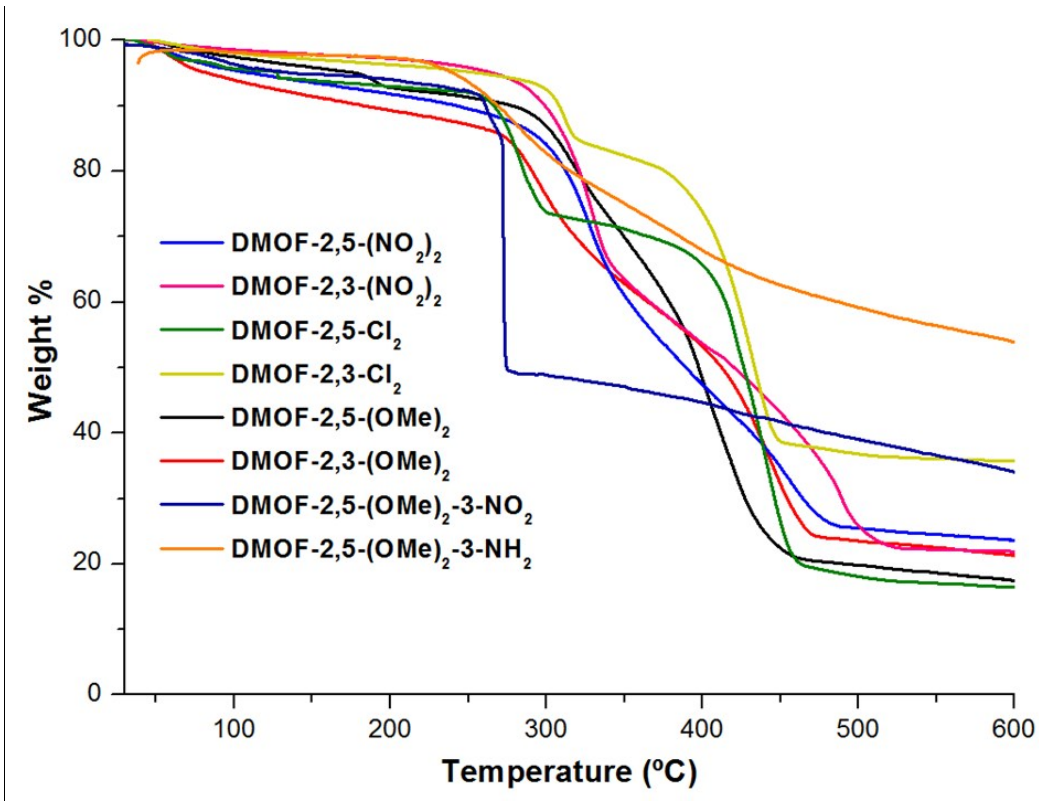


Fig. S3 TGA of regioisomeric DMOFs.

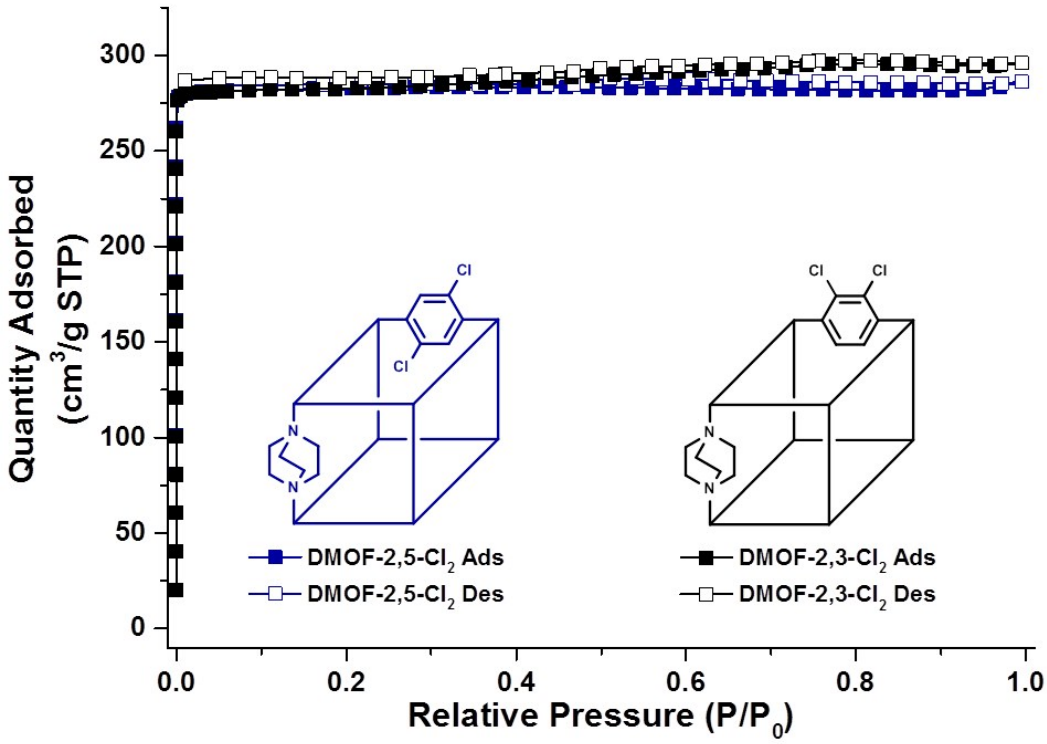


Fig. S4 N_2 isotherm (77 K) of DMOF-2,5-Cl_2 and DMOF-2,3-Cl_2. Adsorption and desorption traces are indicated by filled and open symbols, respectively.

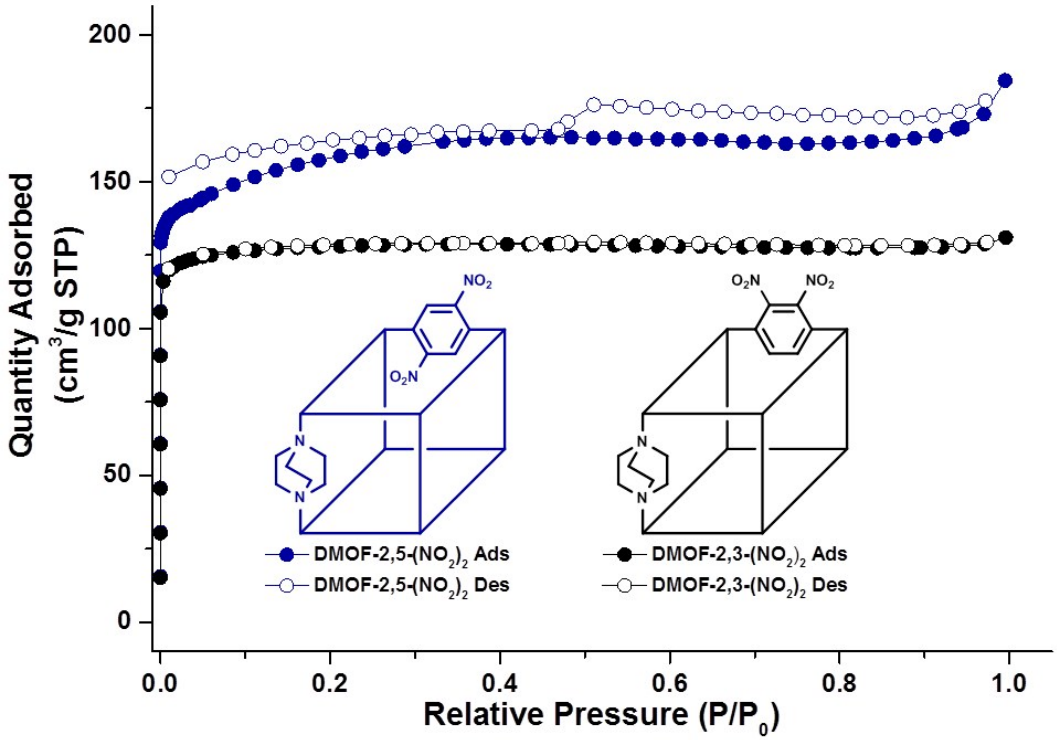


Fig. S5 N_2 isotherm (77 K) of DMOF-2,5-$(NO_2)_2$ and DMOF-2,3-$(NO_2)_2$. Adsorption and desorption traces are indicated by filled and open symbols, respectively.

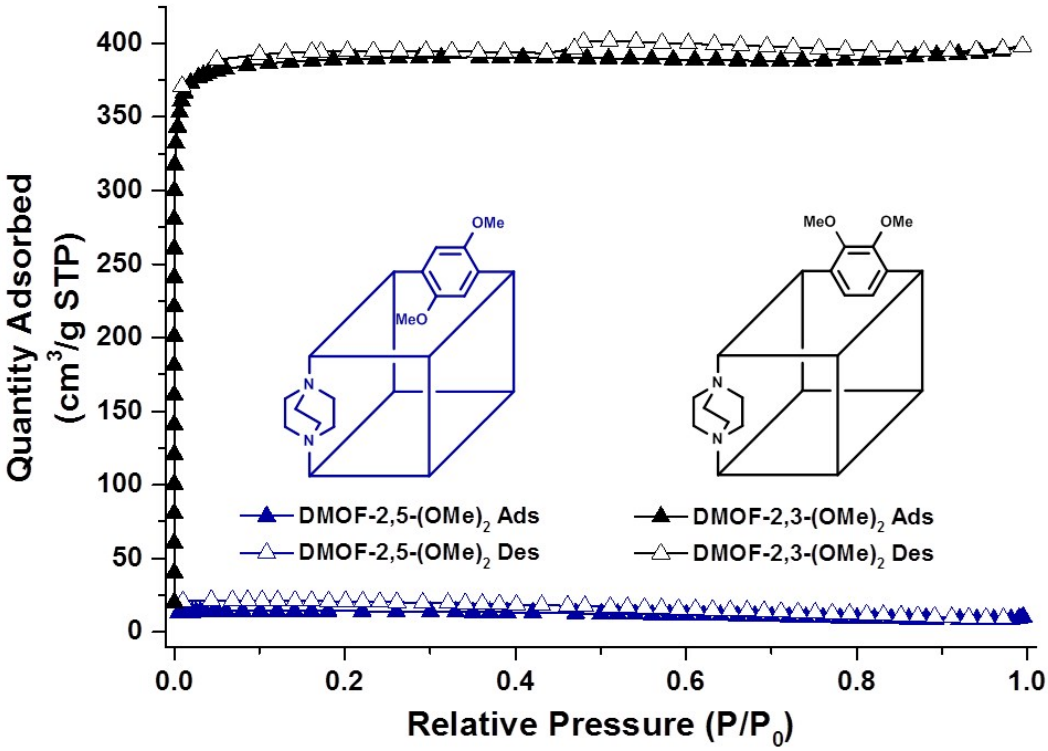


Fig. S6 N_2 isotherm (77 K) of DMOF-2,5-$(OMe)_2$ and DMOF-2,3-$(OMe)_2$. Adsorption and desorption traces are indicated by filled and open symbols, respectively.

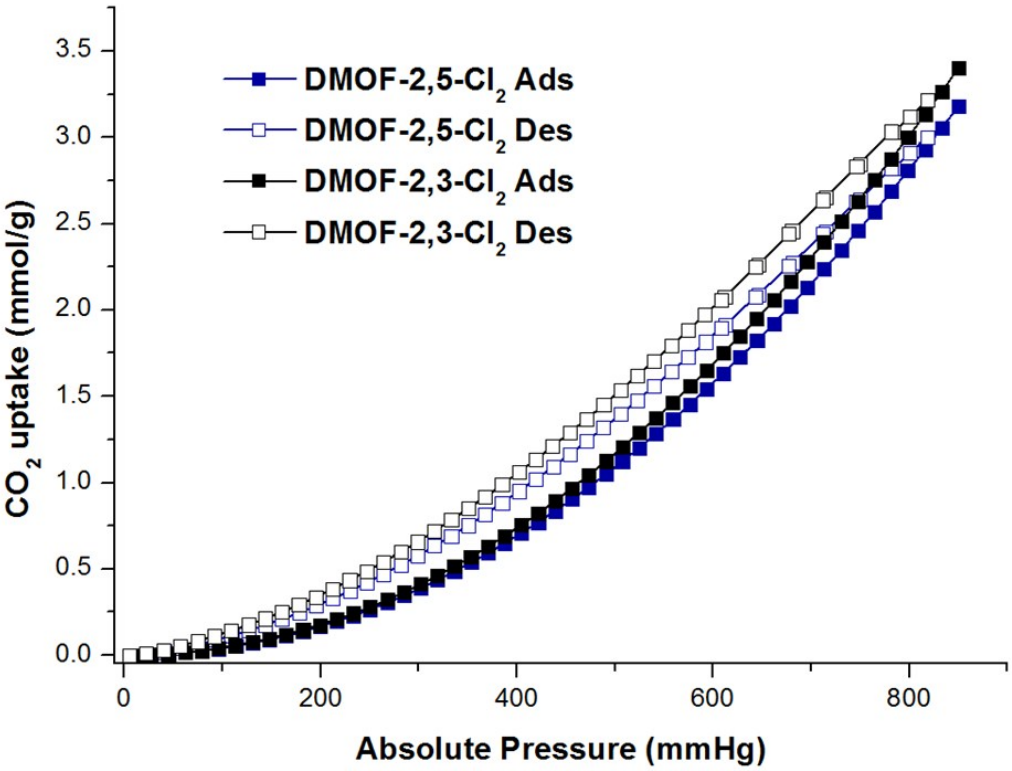


Fig. S7 CO_2 isotherm (298 K) of DMOF-2,5-Cl_2 and DMOF-2,3-Cl_2. Adsorption and desorption traces are indicated by filled and open symbols, respectively.

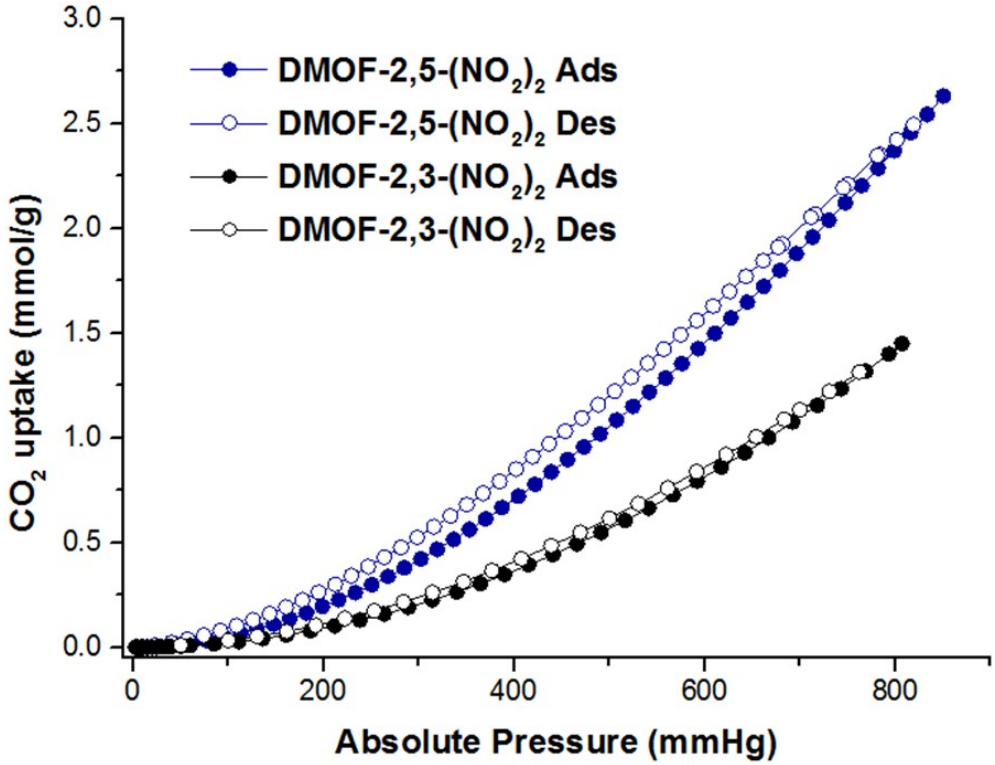


Fig. S7 CO_2 isotherm (298 K) of DMOF-2,5-$(NO_2)_2$ and DMOF-2,3-$(NO_2)_2$. Adsorption and desorption traces are indicated by filled and open symbols, respectively.

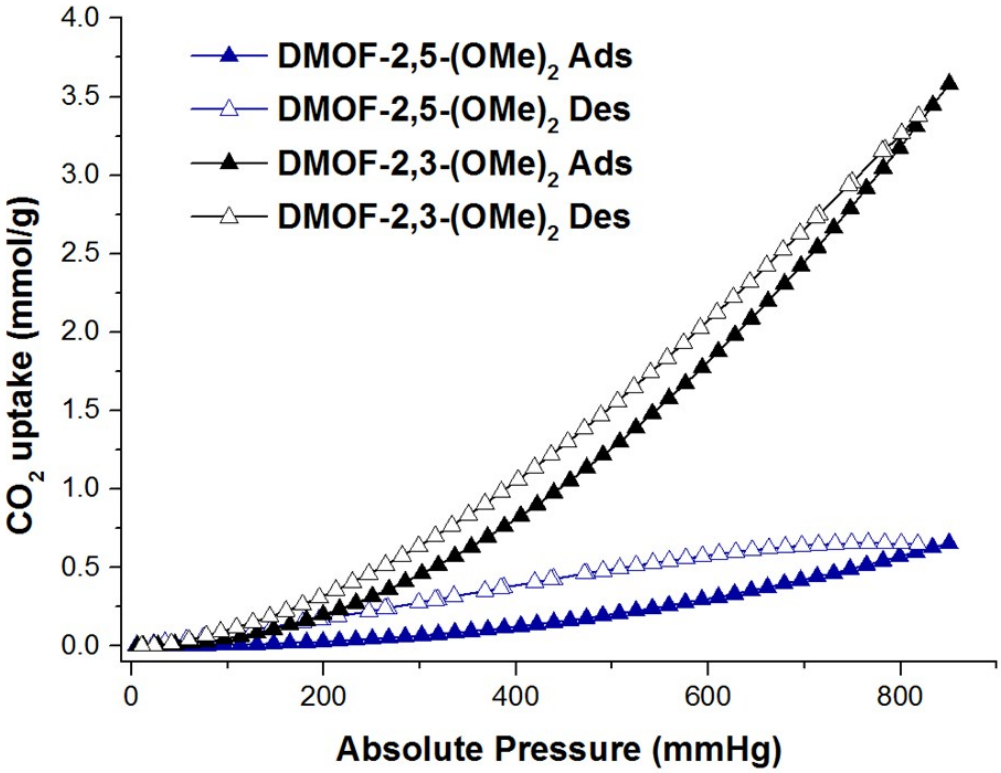


Fig. S9 CO_2 isotherm (298 K) of DMOF-2,5-$(OMe)_2$ and DMOF-2,3-$(OMe)_2$. Adsorption and desorption traces are indicated by filled and open symbols, respectively.

Table S2 CO_2 uptake (mmol/g, 298 K) for DMOFs at near 760 torr

DMOF	CO_2 uptake at 760 torr
DMOF-2,5-Cl_2	2.569
DMOF-2,3-Cl_2	2.752
DMOF-2,5-$(NO_2)_2$	2.206
DMOF-2,3-$(NO_2)_2$	1.435
DMOF-2,5-$(OMe)_2$	0.516
DMOF-2,3-$(OMe)_2$	2.916
DMOF-2,5-$(OMe)_2$-NO_2	2.116
DMOF-3-NH_2-2,5-$(OMe)_2$	1.567

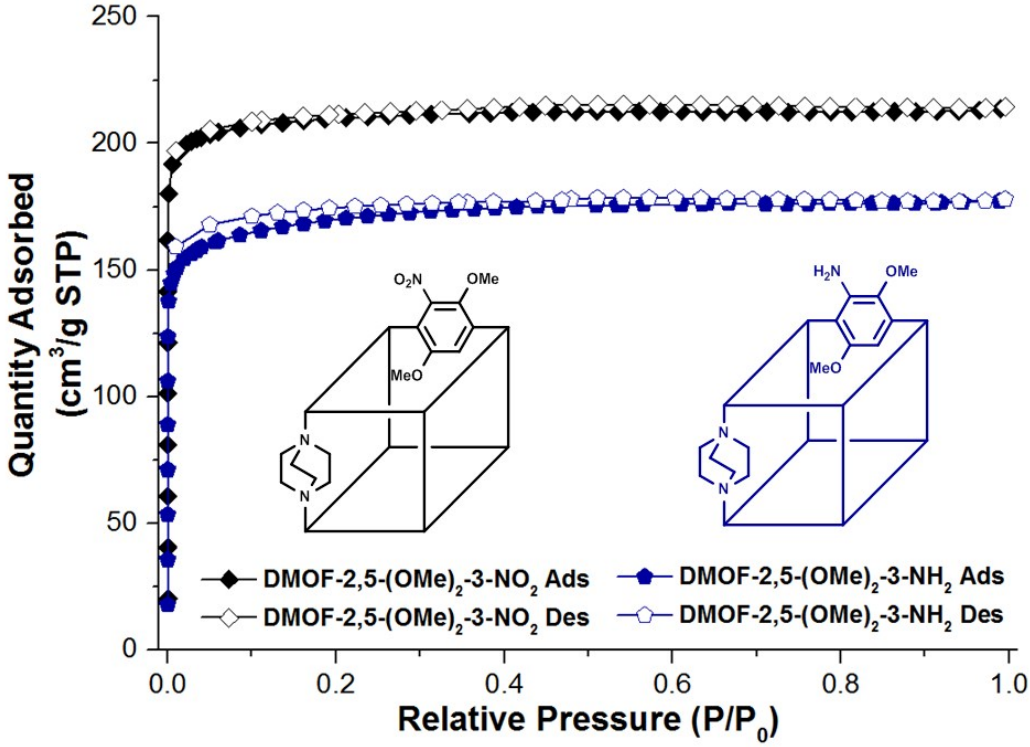


Fig. S10 N_2 isotherm (77 K) of DMOF-2,5-$(OMe)_2$-3-NO_2 and of DMOF-2,5-$(OMe)_2$-3-NH_2. Adsorption and desorption traces are indicated by filled and open symbols, respectively.

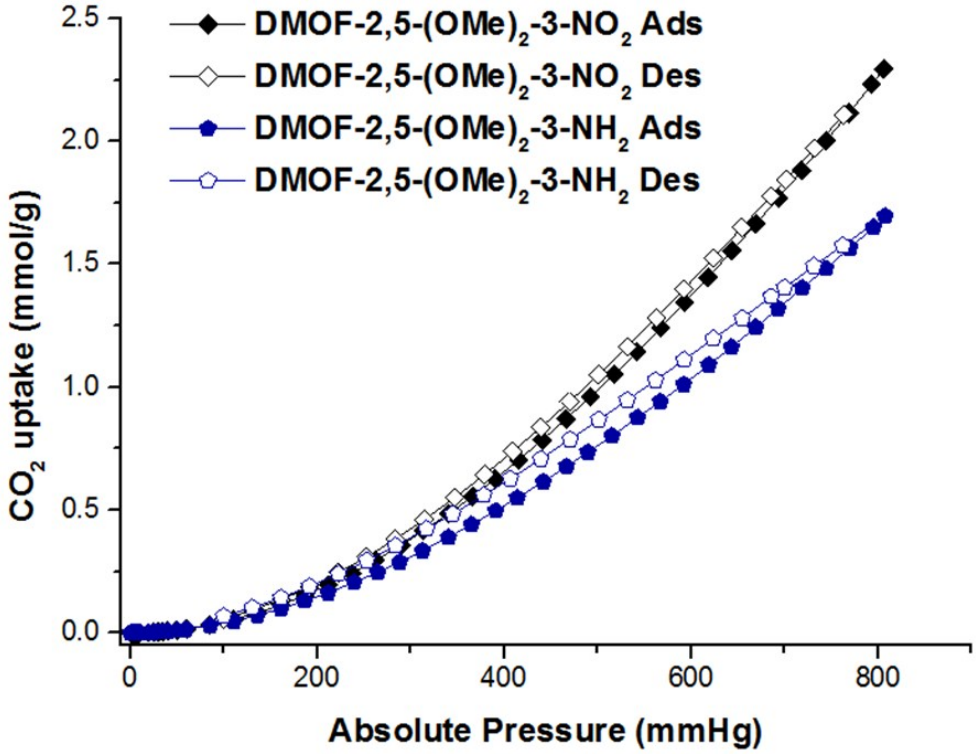


Fig. S11 CO_2 isotherm (298 K) of DMOF-2,5-$(OMe)_2$-3-NO_2 and DMOF-2,3-$(OMe)_2$-3-NH_2. Adsorption and desorption traces are indicated by filled and open symbols, respectively.

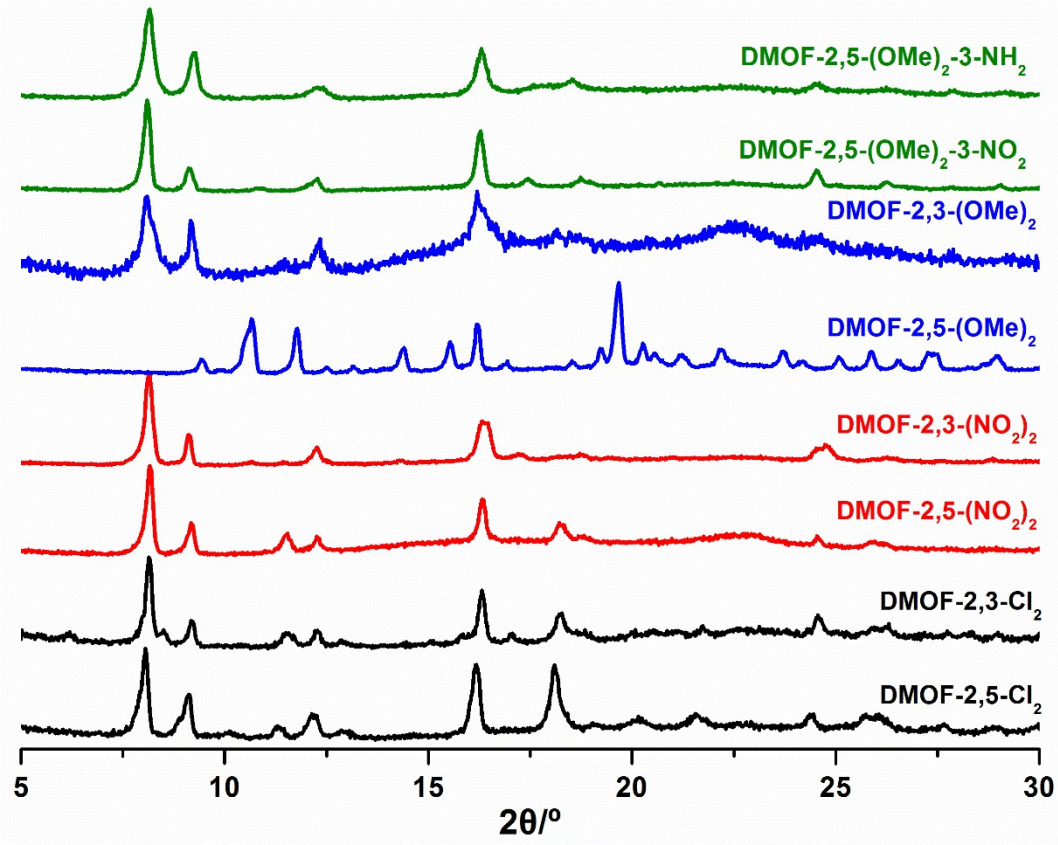


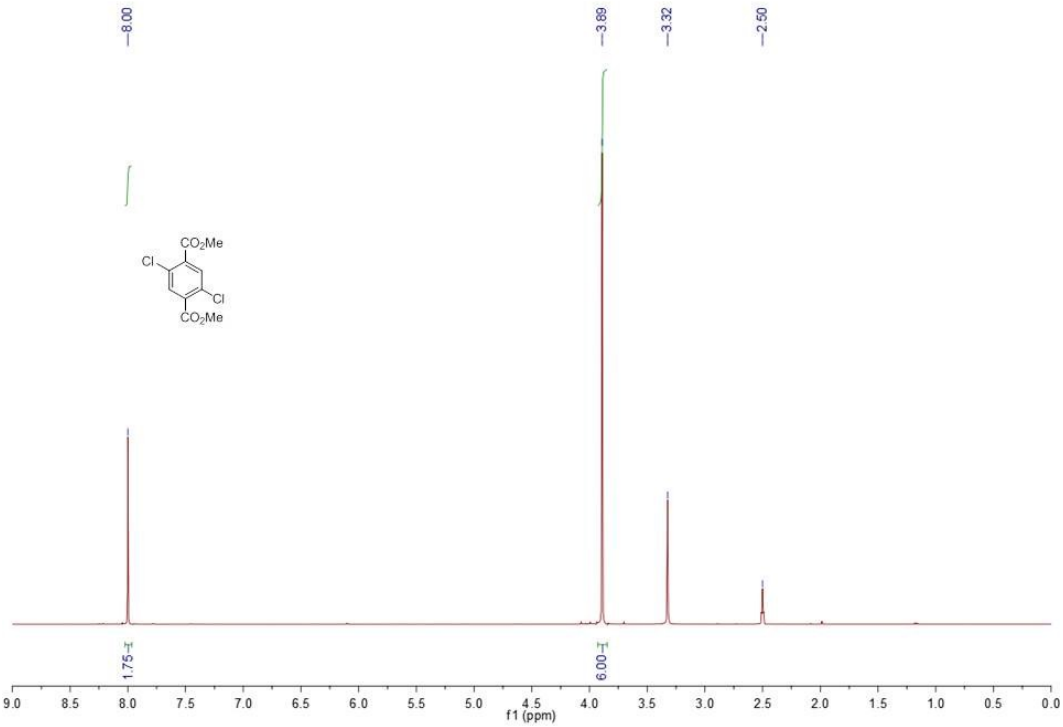
Fig. S12 PXRD patterns of the obtained DMOFs after evacuation under vacuum (and re-exposed to air for measurement).

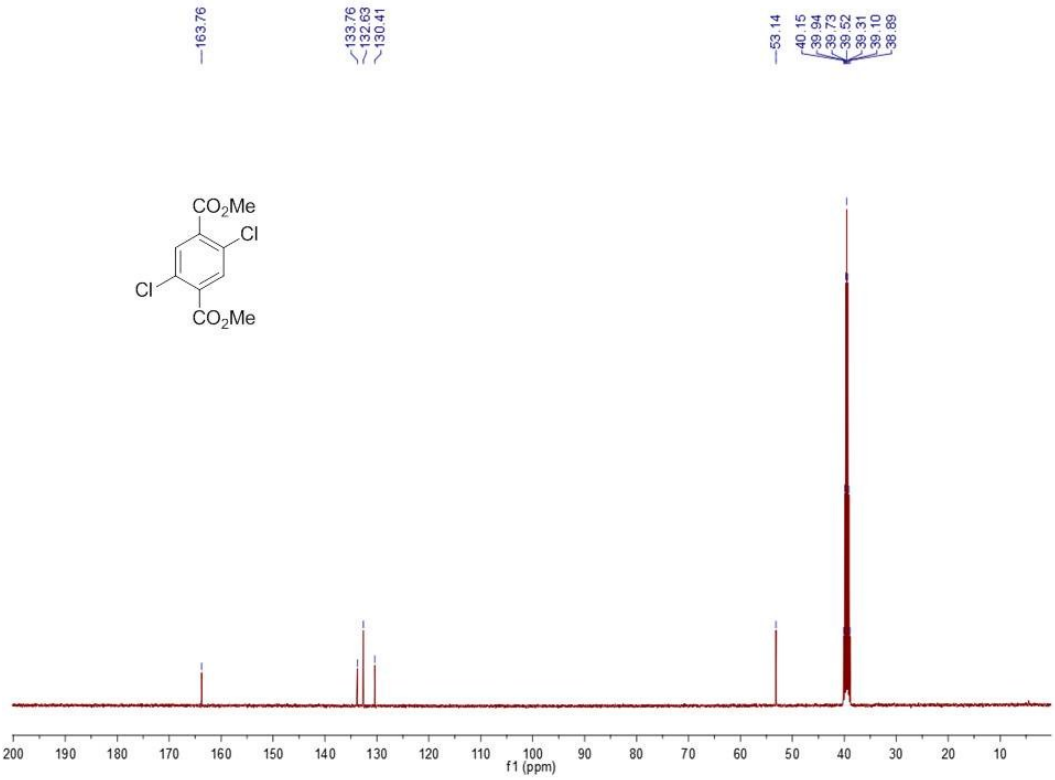
References for ESI

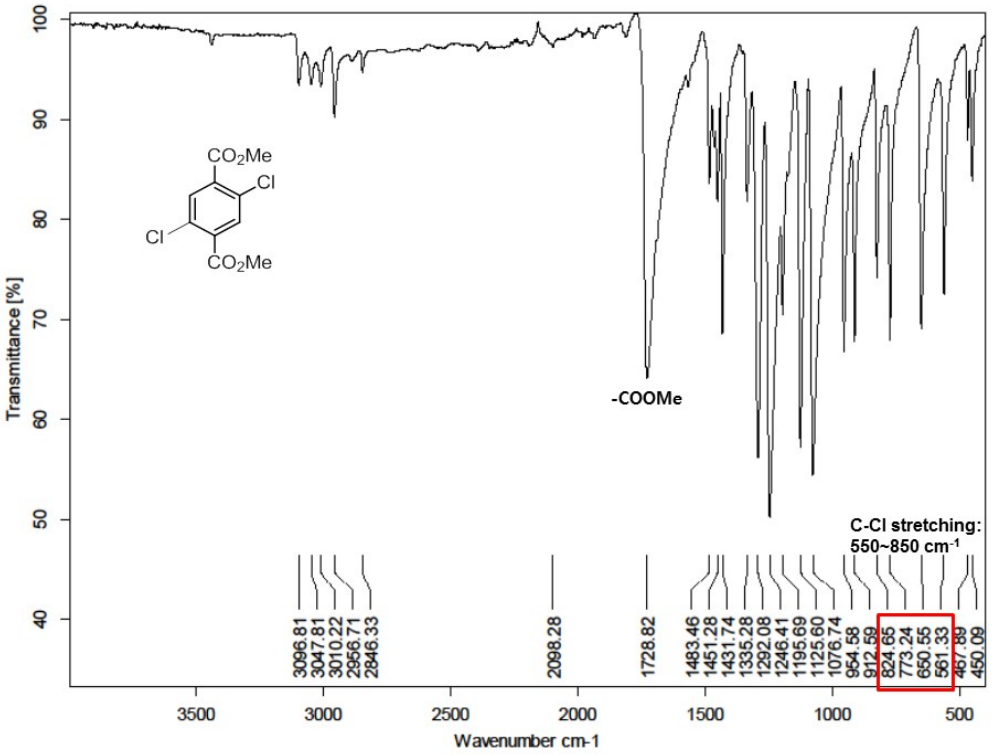
S1 Kim, M.; Boissonnault, J. A.; Dau, P. V.; Cohen, S. M. *Angew. Chem. Int. Ed.* **2011**, *50*, 12193.
S2 Heldmann, C.; Shulze, M.; Wegner, G. *Macromolecules*, **1996**, *29*, 4686.
S3 Pound, G. J.; Pletnev, A. A.; Fanga, X.; Pletneva, E. V. *Chem. Commun*. **2011**, *47*, 5714.
S4 Wang, Z.; Tanabe, K. K.; Cohen, S. M. *Inorg. Chem*. **2009**, *48*, 296.
S5 P. M. de Wolff, *J. Appl. Cryst.*, **1968**, *1*, 108.
S6 R. Oishi-Tomiyasu, *J. Appl. Cryst.*, **2013**, *46*, 1277.
S7 Uemura, K.; Yamasaki, Y.; Onishi, F.; Kita, H.; Ebihara, M. *Inorg. Chem*. **2010**, *49*, 10133.

Spectral Copies of ^{1}H, ^{13}C NMR and IR of Obtained Compounds

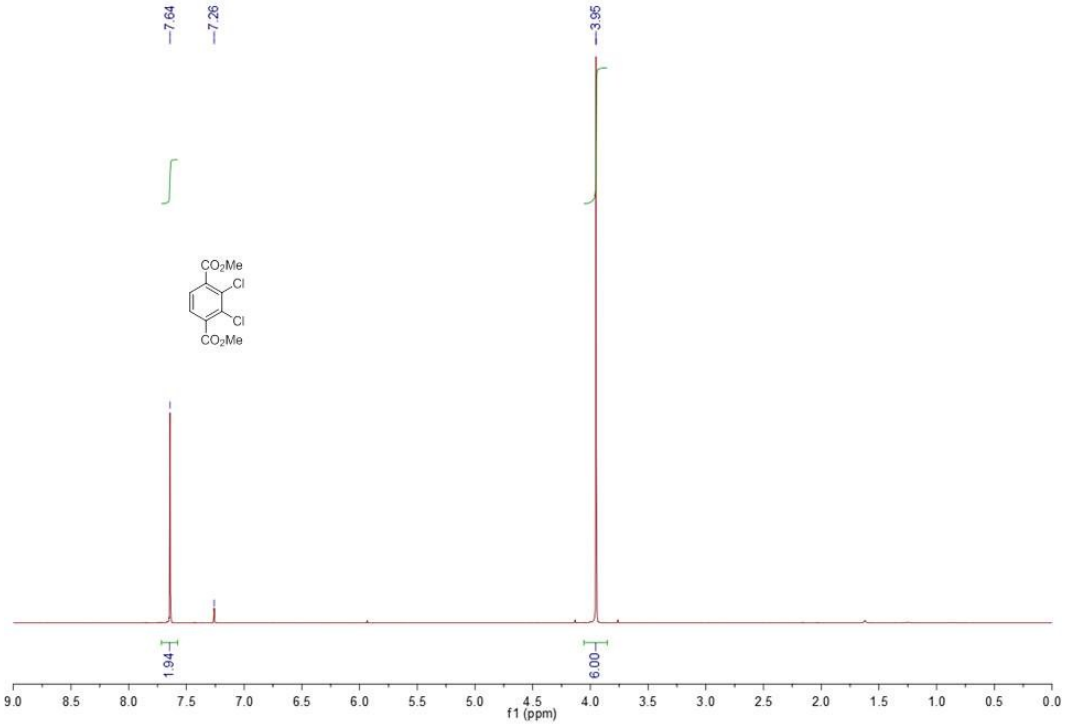
Dimethyl-2,5-dichloroterephthalate (**BDCE-2,5-Cl$_2$**)

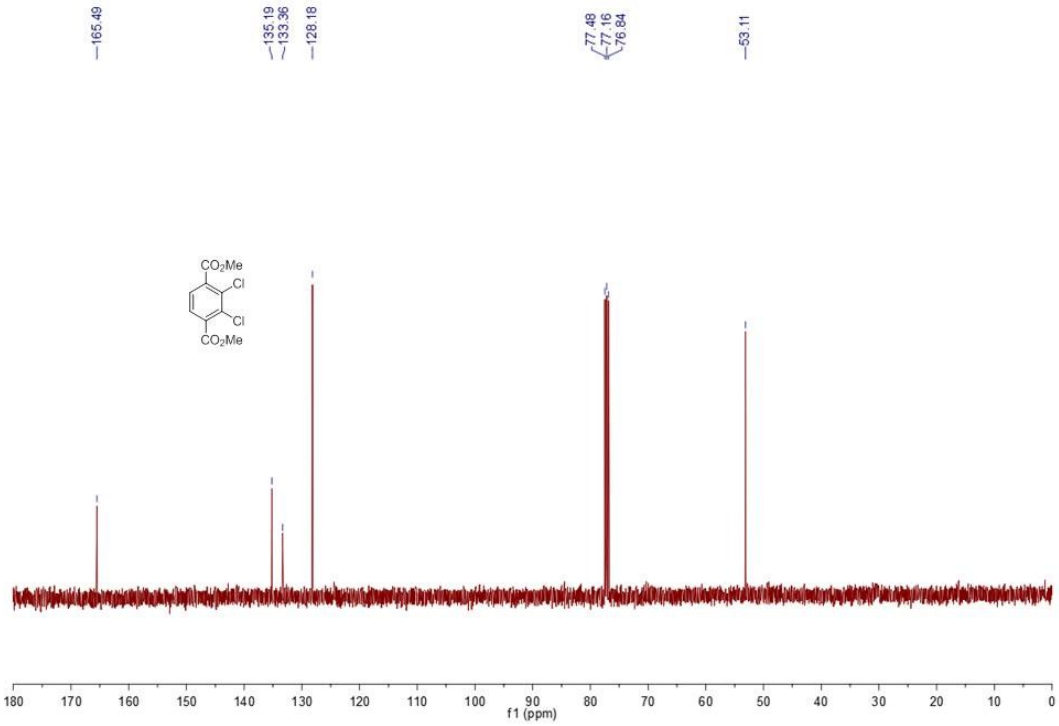


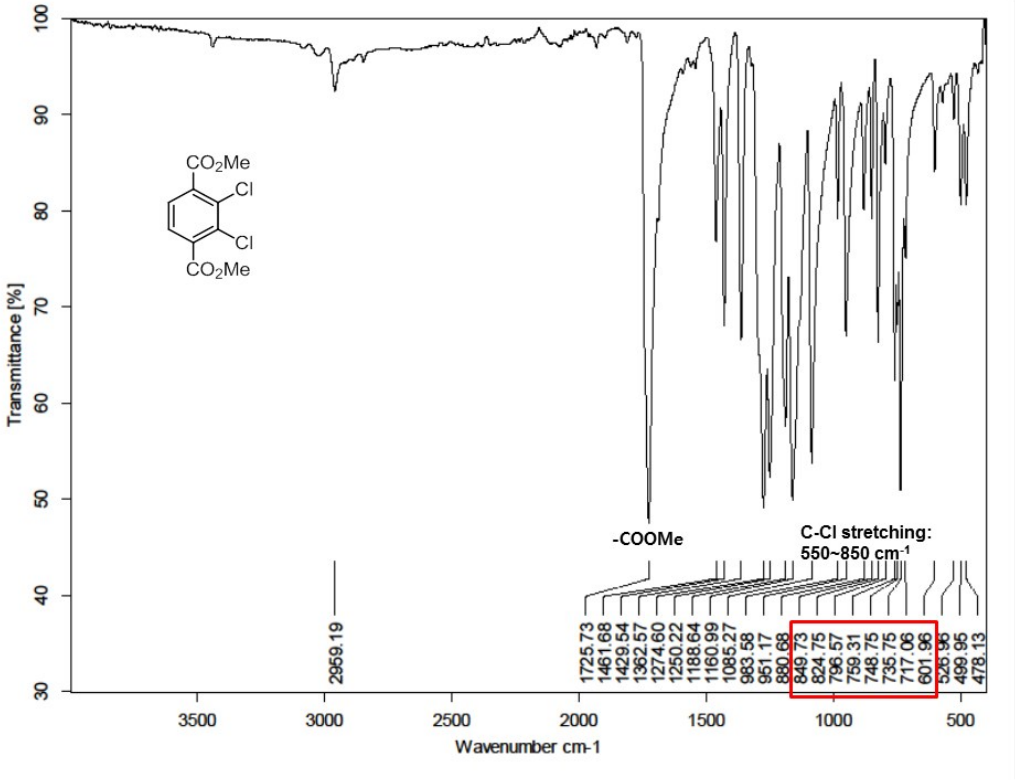



Transmittance [%]
Wavenumber cm-1
CO2Me
Cl
Cl
CO2Me
-COOMe
C-Cl stretching:
550~850 cm-1
3096.81
3047.81
3010.22
2956.71
2846.33
2098.28
1728.82
1483.46
1451.28
1431.74
1335.28
1292.08
1246.41
1195.69
1125.60
1076.74
954.58
912.59
824.65
773.24
650.55
561.33
467.89
450.09

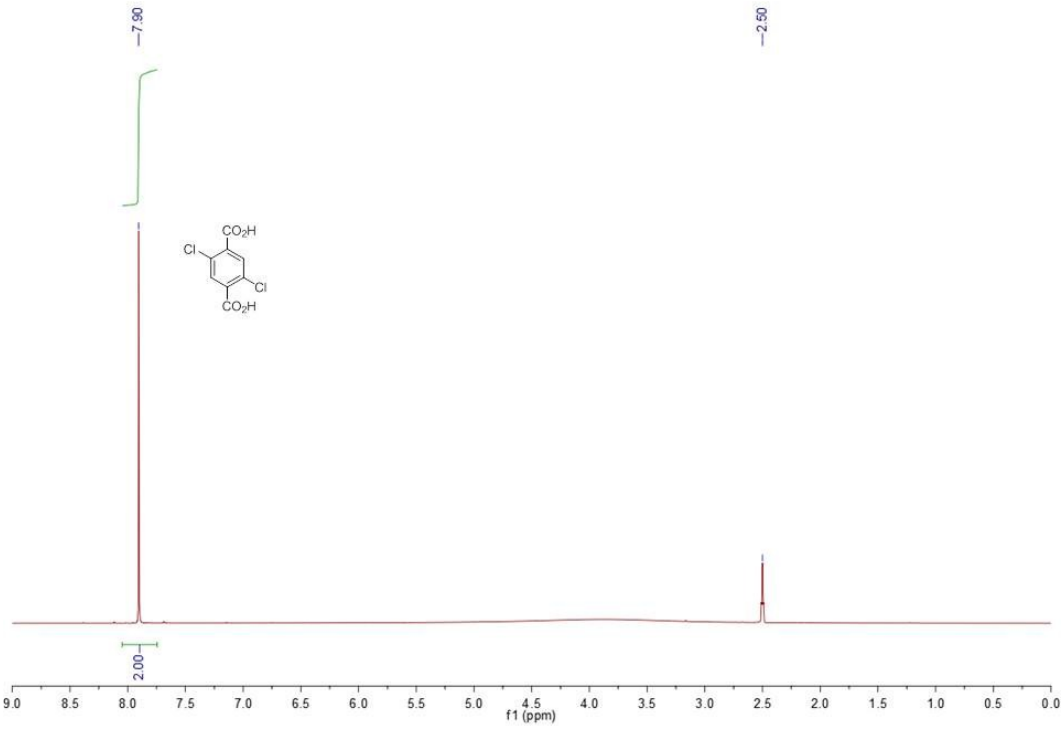
Dimethyl-2,3-dichloroterephthalate (**BDCE-2,3-Cl_2**)

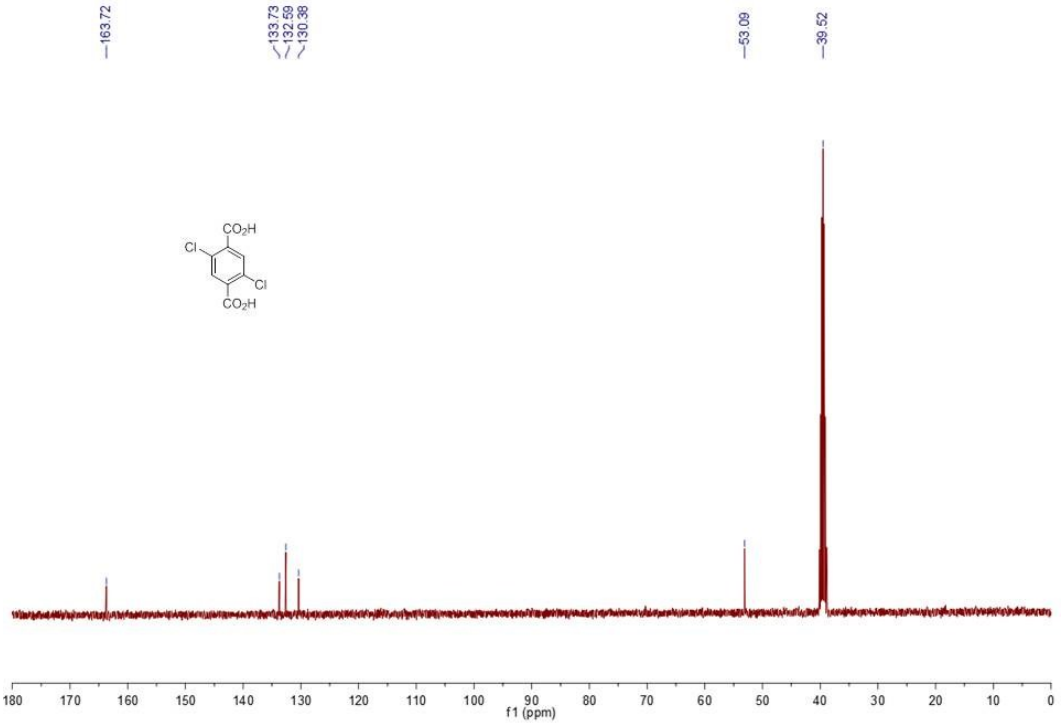


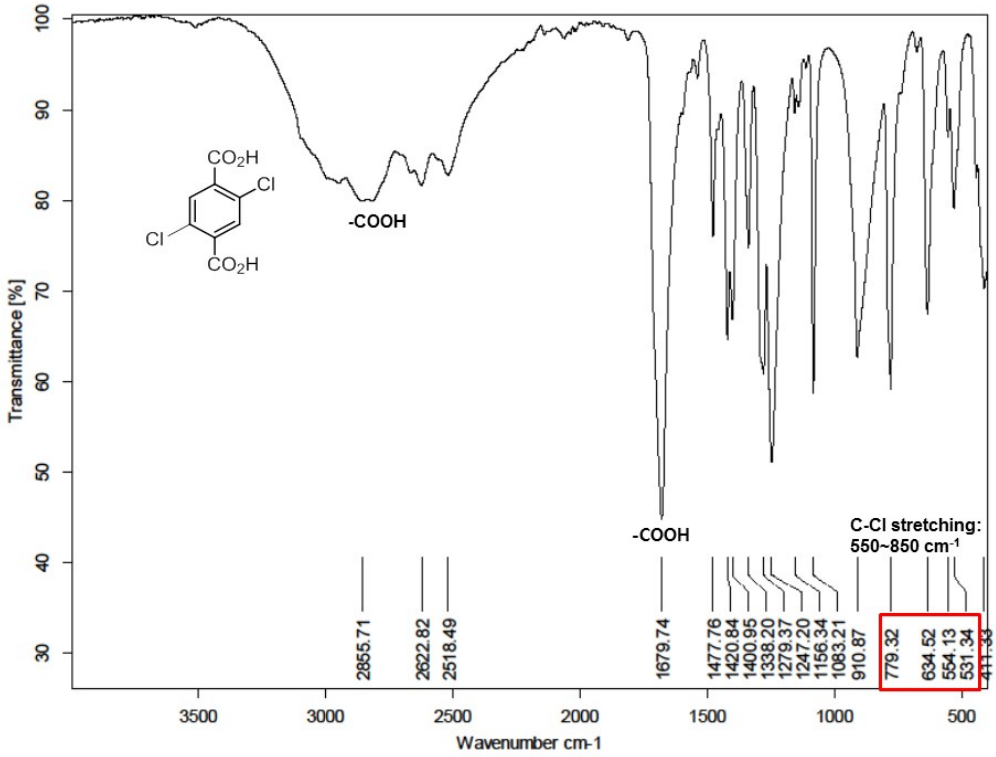



Transmittance [%]
Wavenumber cm-1
CO2Me
Cl
Cl
CO2Me
-COOMe
C-Cl stretching:
550~850 cm-1
2959.19
1725.73
1461.68
1429.54
1362.57
1274.60
1250.22
1188.64
1160.99
1085.27
983.58
951.17
880.68
849.73
824.75
796.57
759.31
748.75
735.75
717.06
601.96
526.96
499.95
478.13

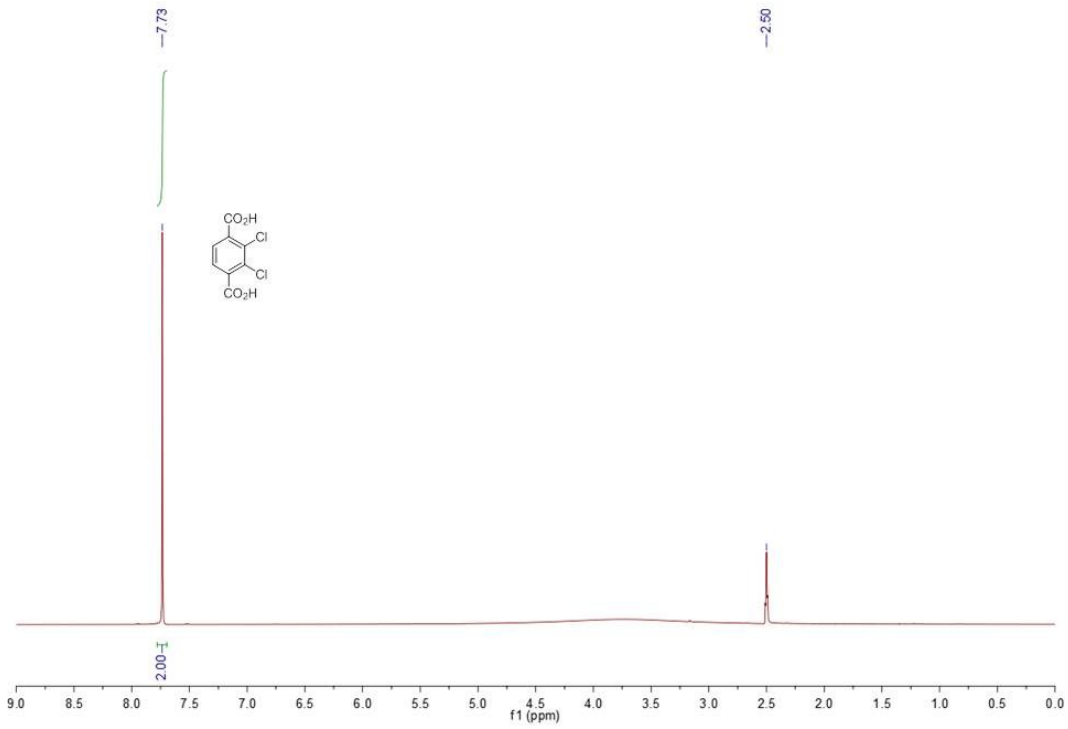
2,5-Dichloroterephthalic acid (**1a**)

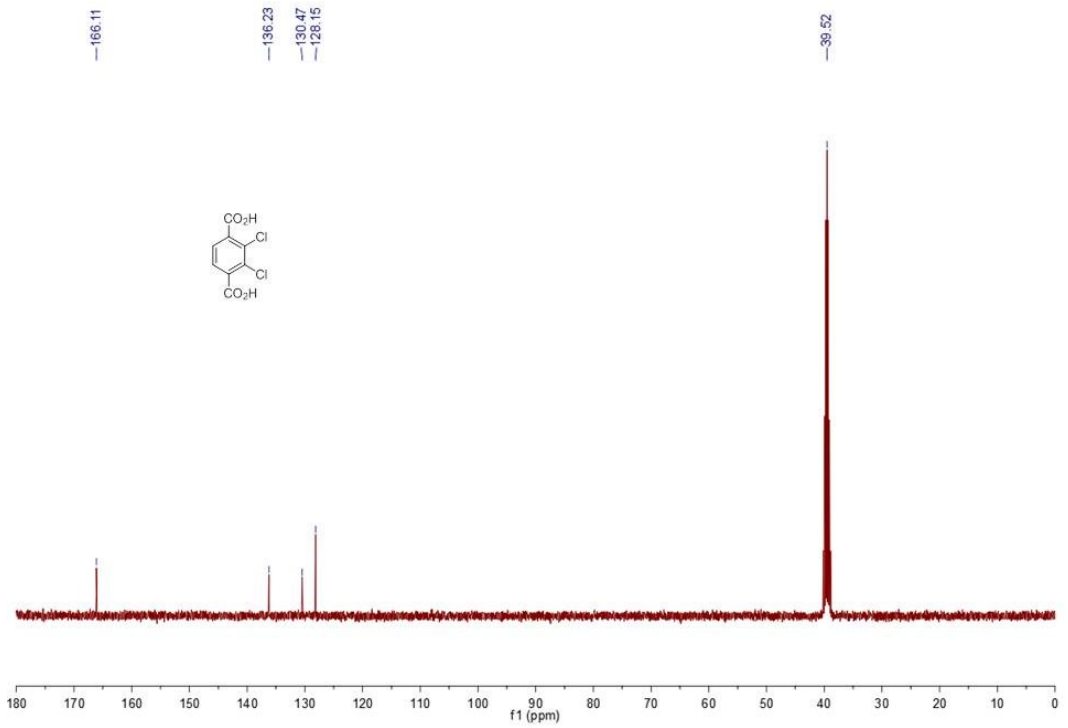


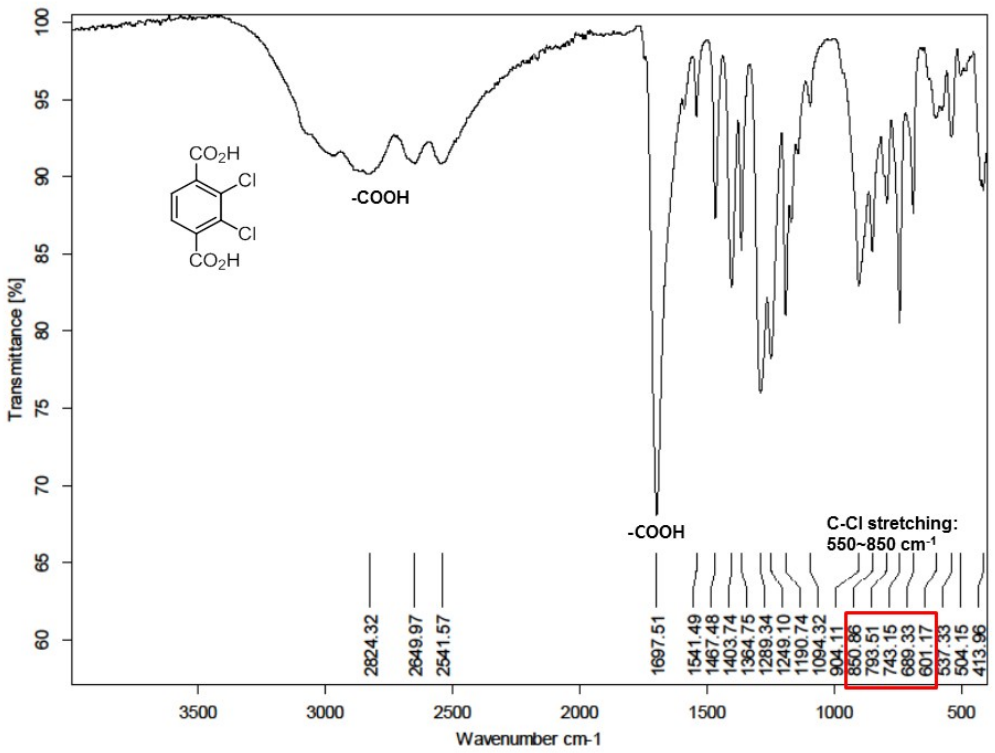



Transmittance [%]
Wavenumber cm-1
-COOH
-COOH
C-Cl stretching:
550~850 cm-1
2855.71
2622.82
2518.49
1679.74
1477.76
1420.84
1400.95
1338.20
1279.37
1247.20
1156.34
1083.21
910.87
779.32
634.52
554.13
531.34
411.33

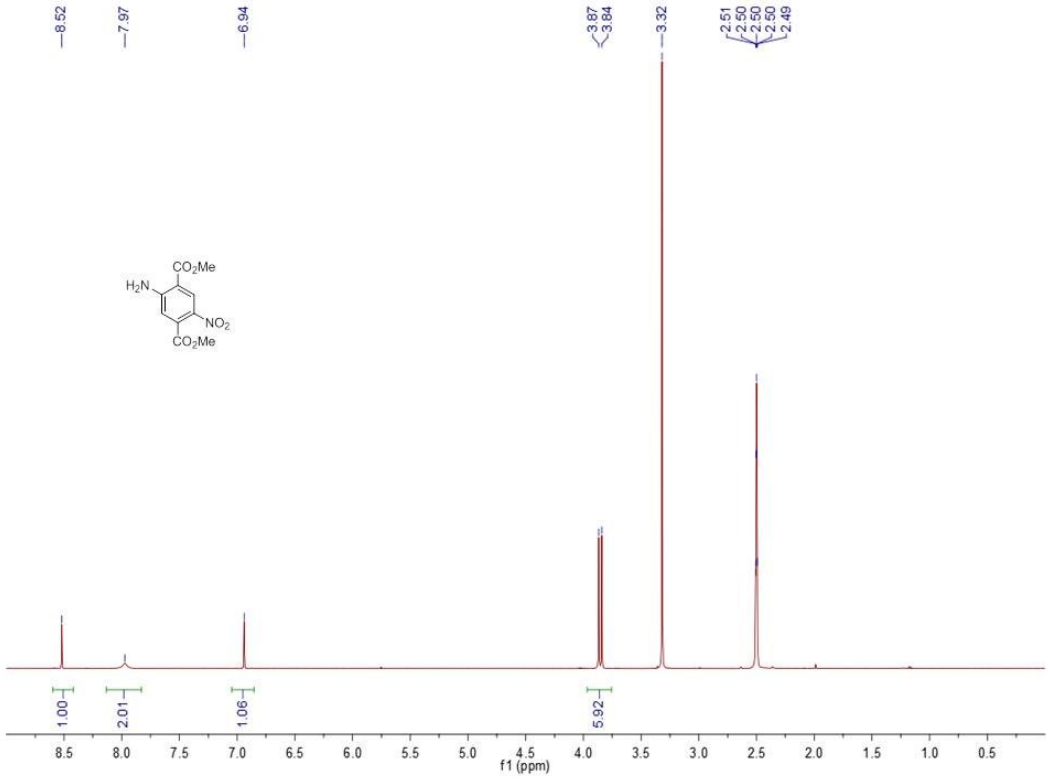
2,3-Dichloroterephthalic acid (**1b**)

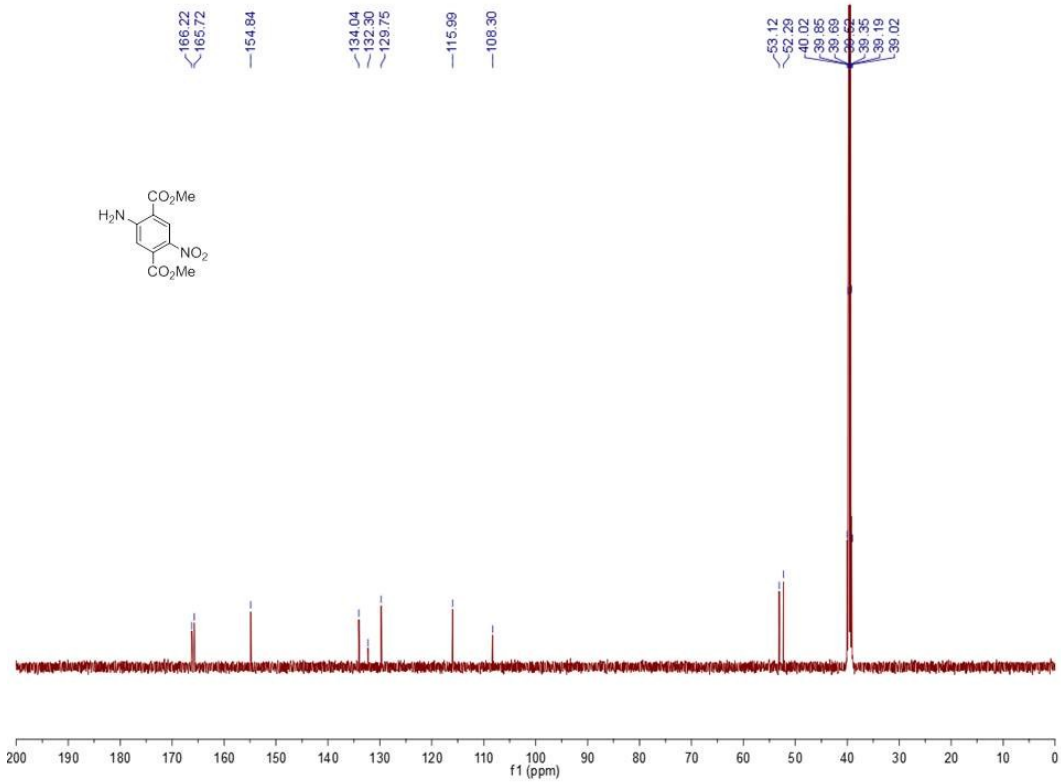


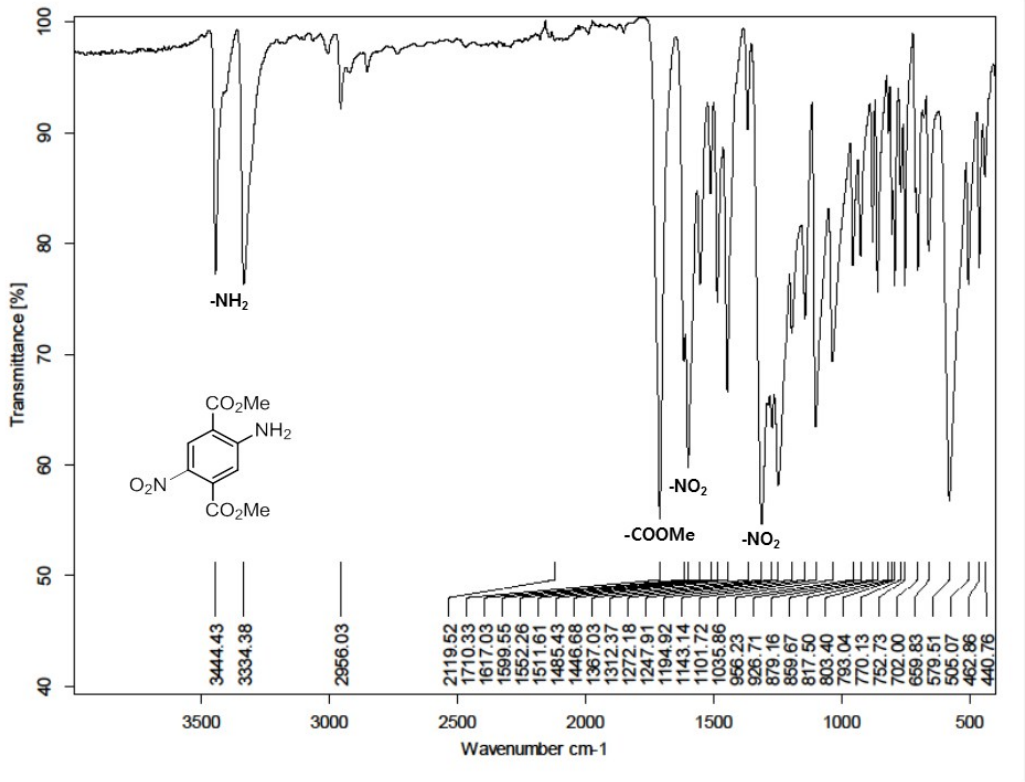



Transmittance [%]
Wavenumber cm-1
-COOH
-COOH
C-Cl stretching:
550~850 cm-1
2824.32
2649.97
2541.57
1697.51
1541.49
1467.48
1403.74
1364.75
1289.34
1249.10
1190.74
1094.32
904.11
850.86
793.51
743.15
689.33
601.17
537.33
504.15
413.96

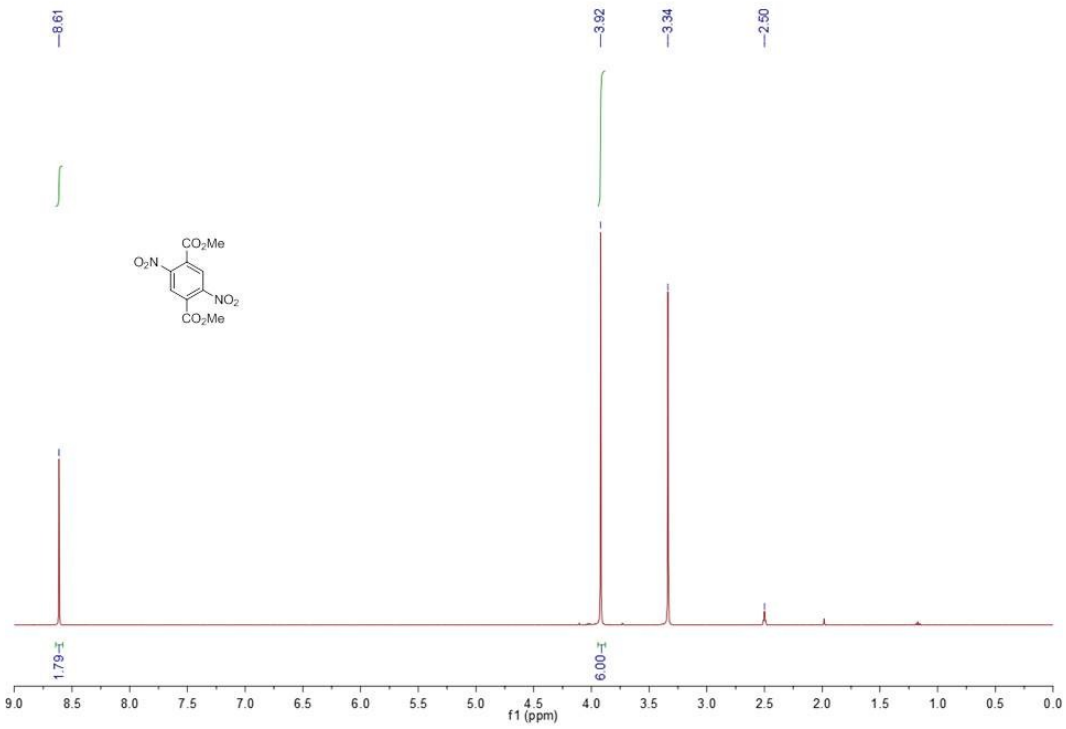
Dimethyl-2,5-dinitroterephthalate (**BDCE-2,5-NH_2NO_2**)

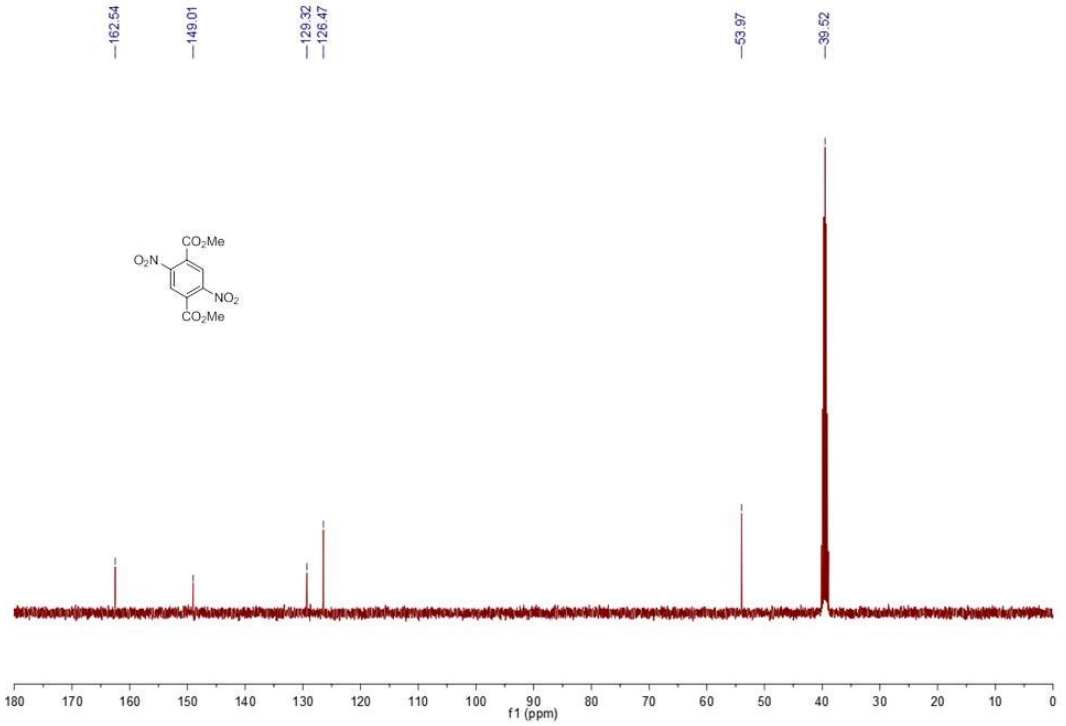


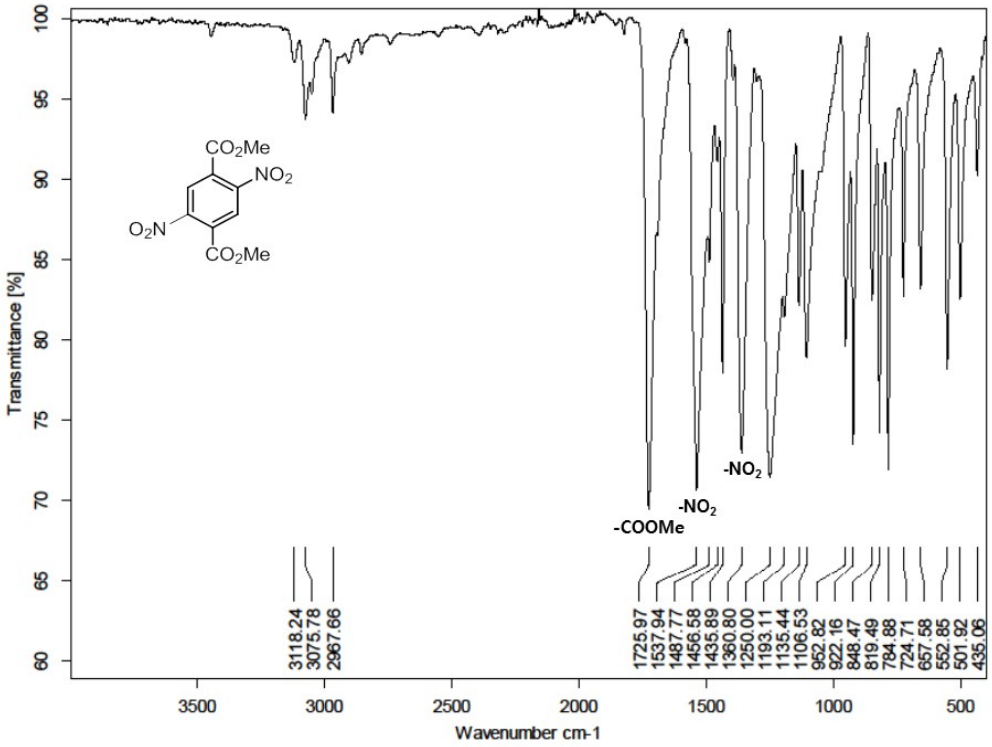



Transmittance [%]
Wavenumber cm-1
-NH2
-NO2
-COOMe
-NO2
CO2Me
NH2
O2N
CO2Me
3444.43
3334.38
2956.03
2119.52
1710.33
1617.03
1599.55
1552.26
1511.61
1485.43
1446.68
1367.03
1312.37
1272.18
1247.91
1194.92
1143.14
1101.72
1035.86
956.23
926.71
879.16
859.67
817.50
803.40
793.04
770.13
752.73
702.00
659.83
579.51
505.07
462.86
440.76

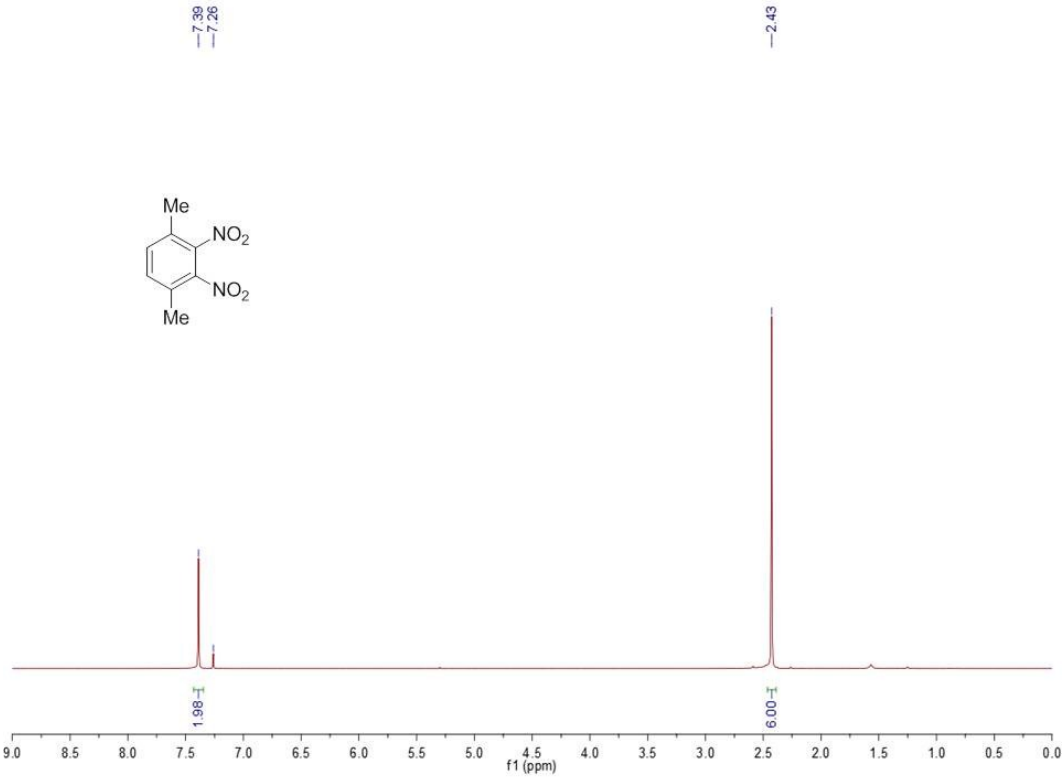
Dimethyl-2,5-dinitroterephthalate (**BDCE-2,5-$(NO_2)_2$**)

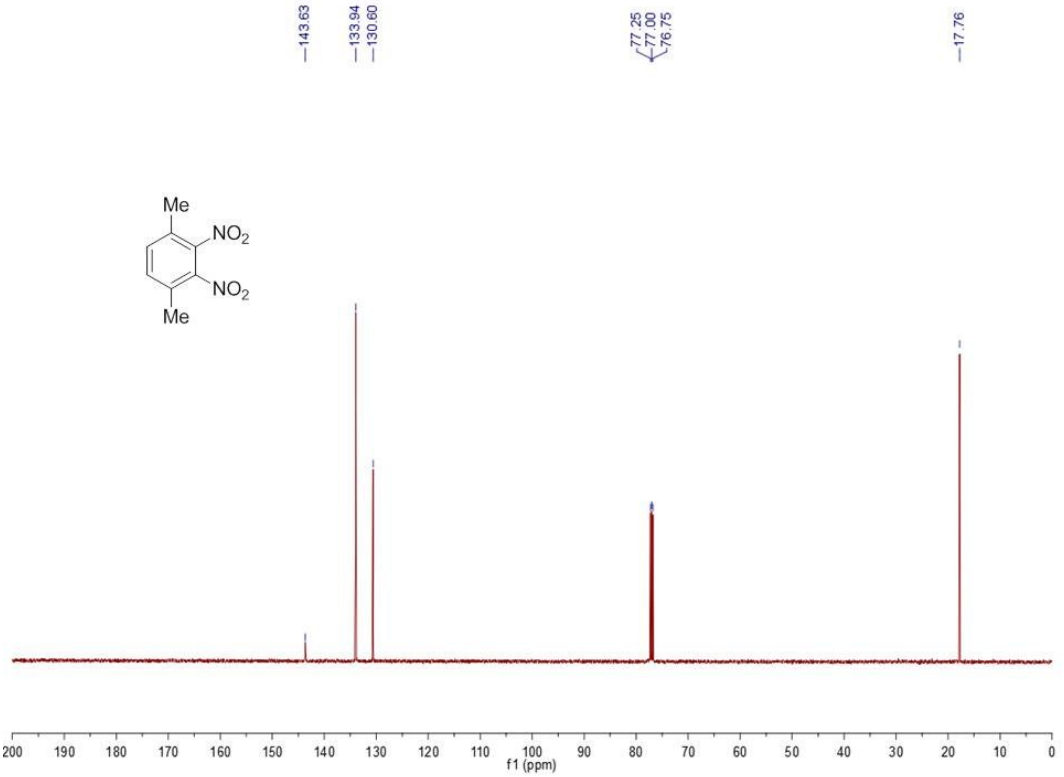


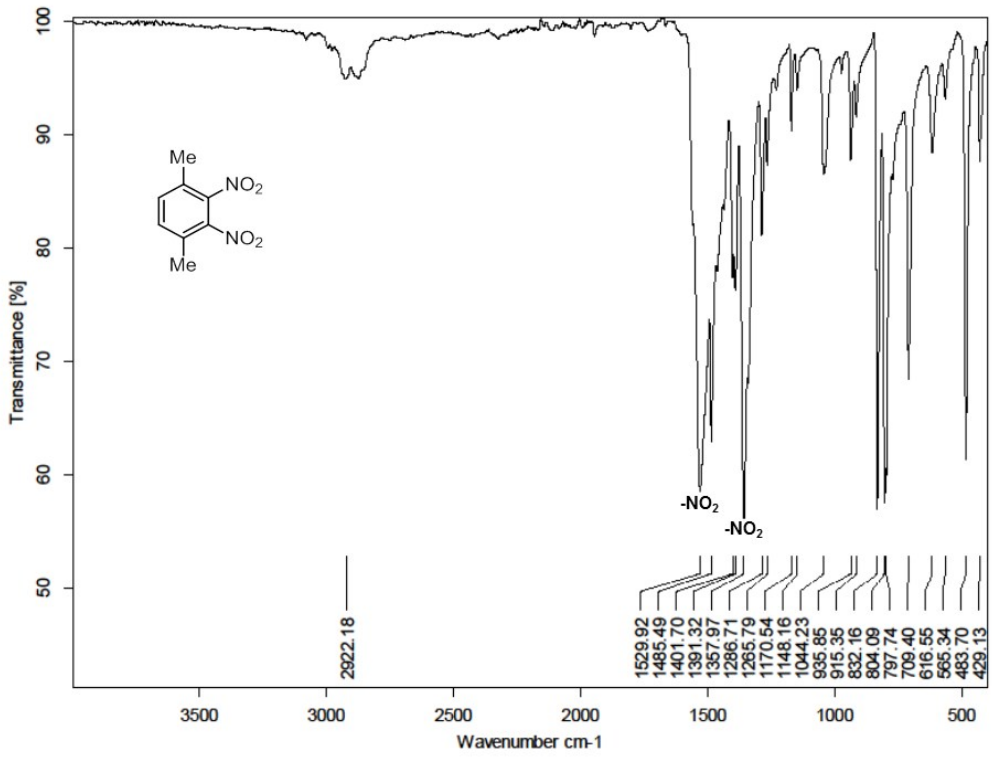



Transmittance [%]
Wavenumber cm-1
CO2Me
NO2
O2N
CO2Me
-COOMe
-NO2
-NO2
3118.24
3075.78
2987.66
1725.97
1537.94
1487.77
1456.58
1435.89
1360.80
1250.00
1193.11
1135.44
1106.53
952.82
922.16
848.47
819.49
784.88
724.71
657.58
552.85
501.92
435.06

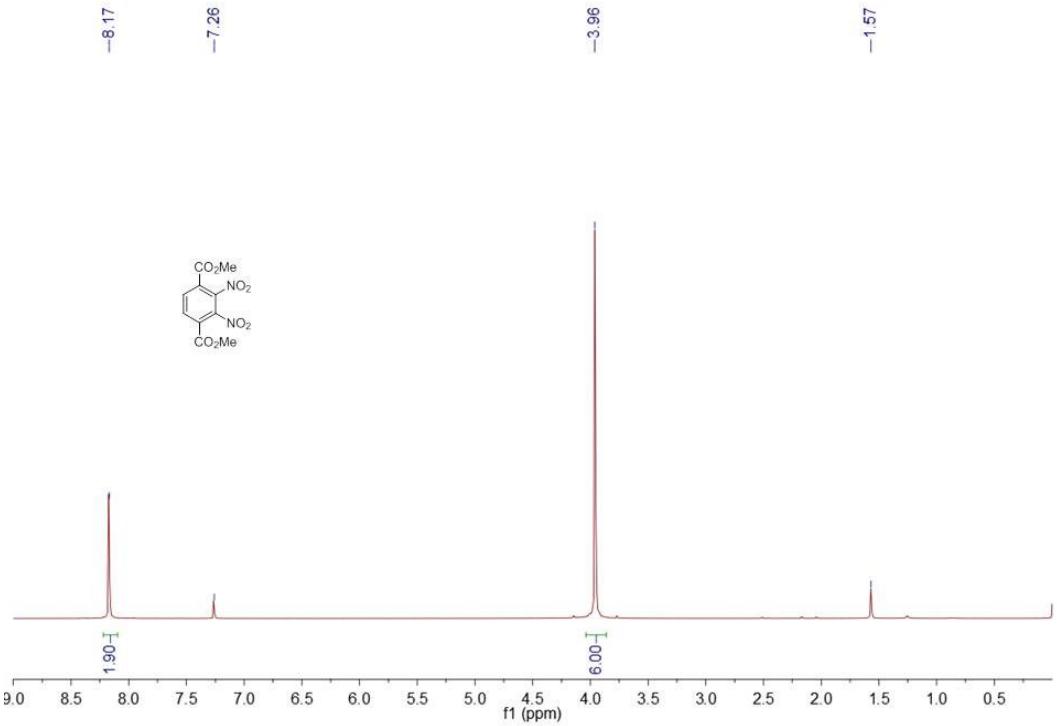
2,3-Dinitro-*p*-xylene

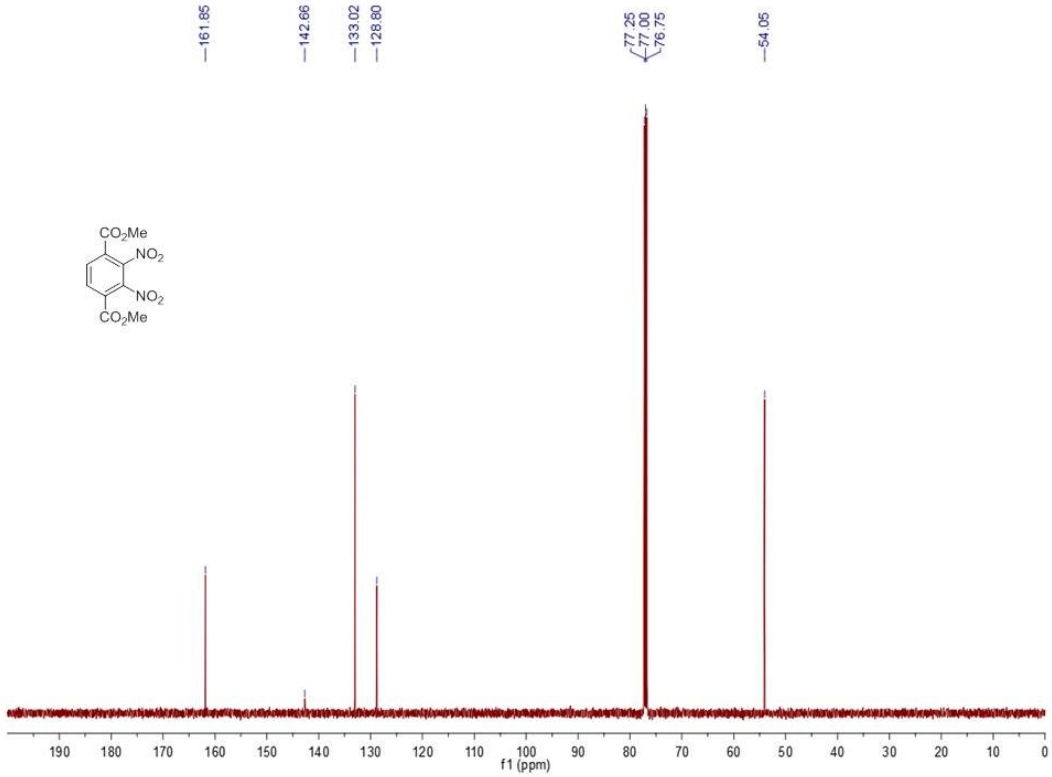


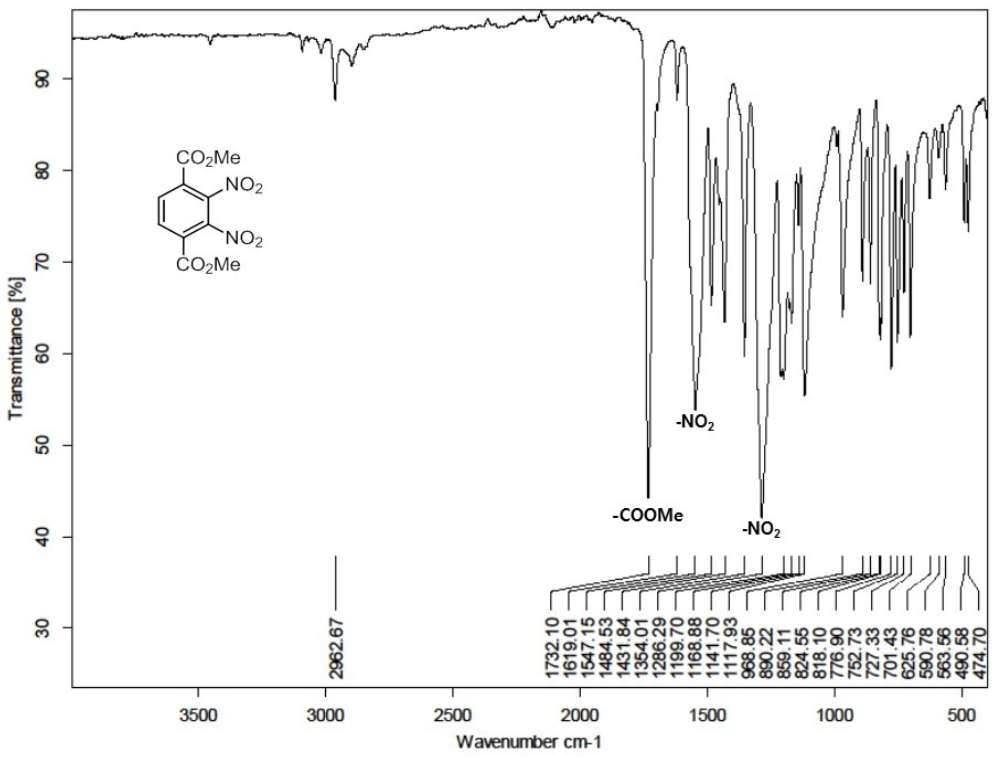



Me
NO2
NO2
Me
-NO2
-NO2
2922.18
1529.92
1485.49
1401.70
1391.32
1357.97
1286.71
1265.79
1170.54
1148.16
1044.23
935.85
915.35
832.16
804.09
797.74
709.40
616.55
565.34
483.70
429.13
Transmittance [%]
Wavenumber cm-1

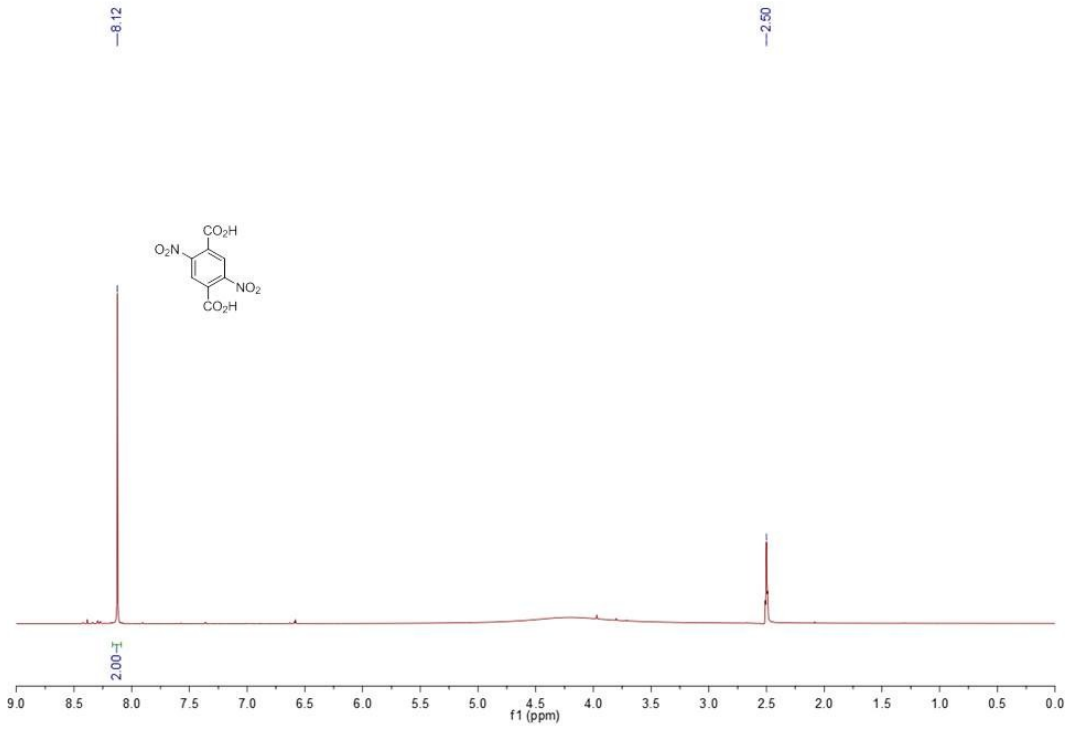
Dimethyl-2,3-dinitroterephthalate (**BDCE-2,3-$(NO_2)_2$**)

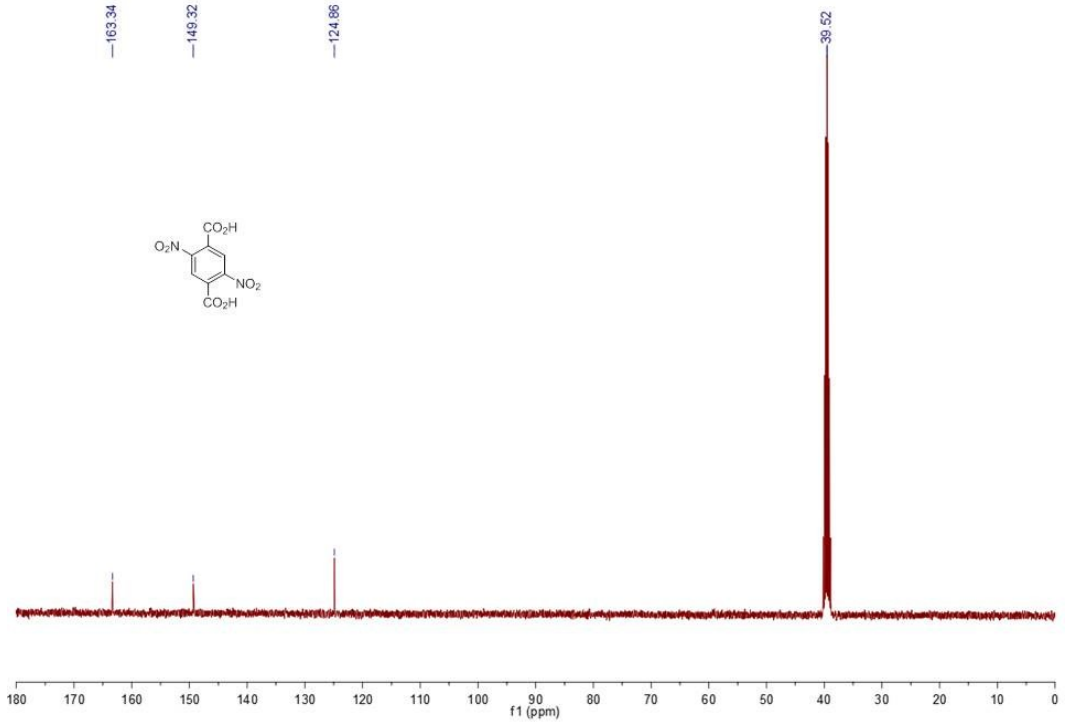


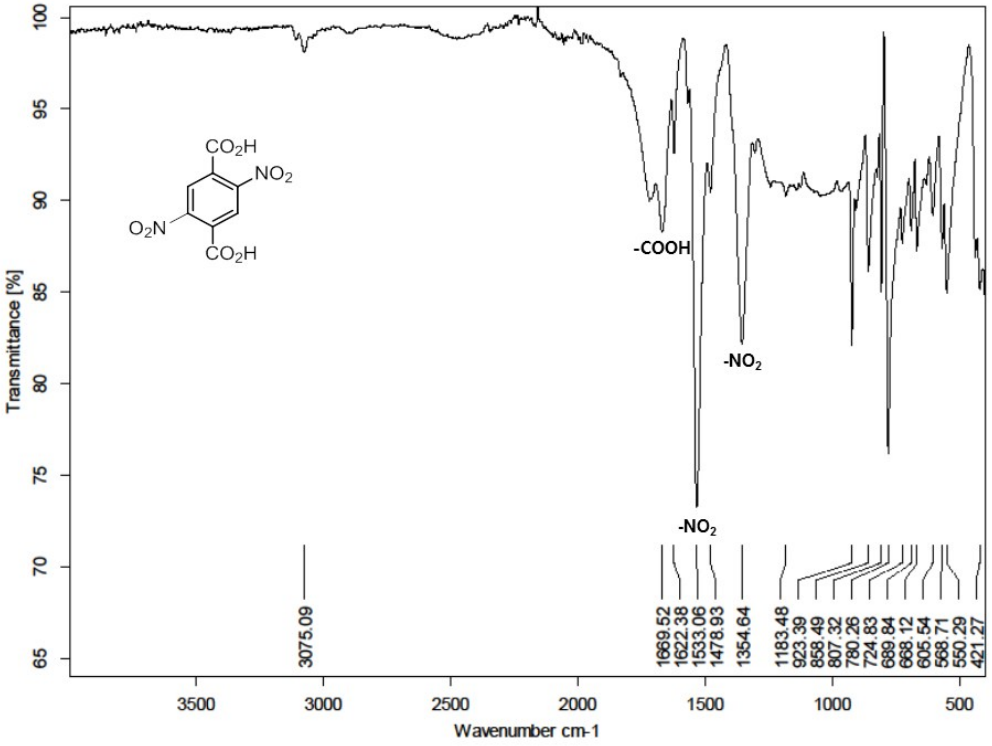



CO2Me
NO2
NO2
CO2Me
Transmittance [%]
Wavenumber cm-1
-COOMe
-NO2
-NO2
2962.67
1732.10
1619.01
1547.15
1484.53
1431.84
1354.01
1286.29
1199.70
1168.88
1141.70
1117.93
968.85
890.22
859.11
824.55
818.10
776.90
752.73
727.33
701.43
625.76
590.78
563.56
490.58
474.70

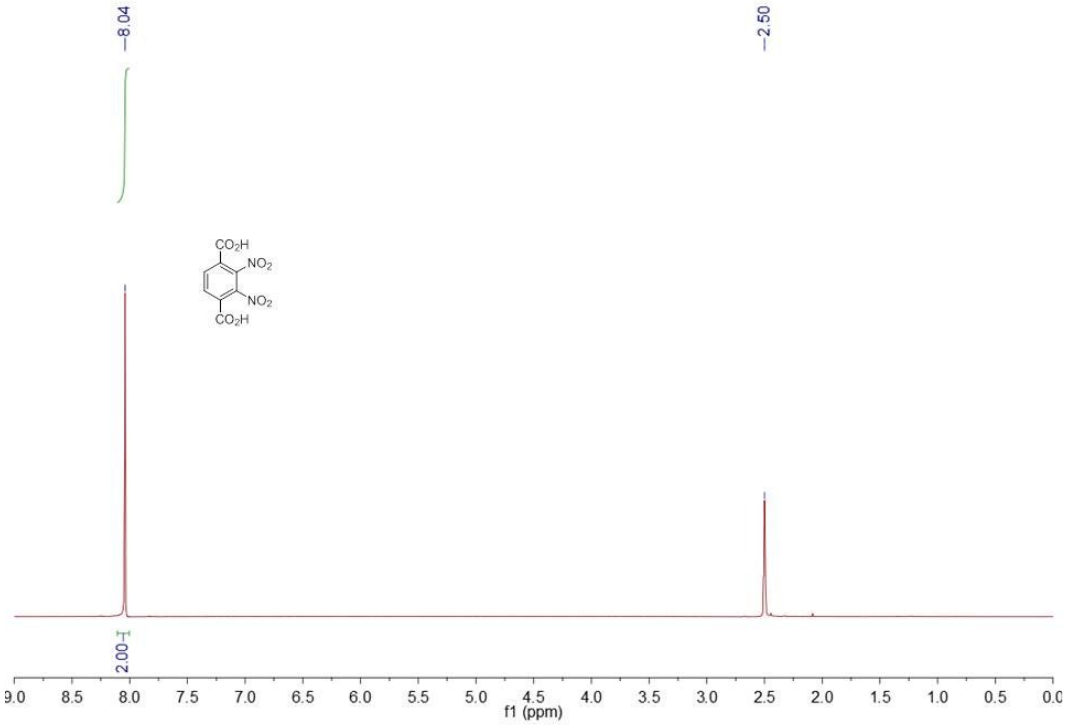
2,5-Dinitroterephthalic acid (**2a**)

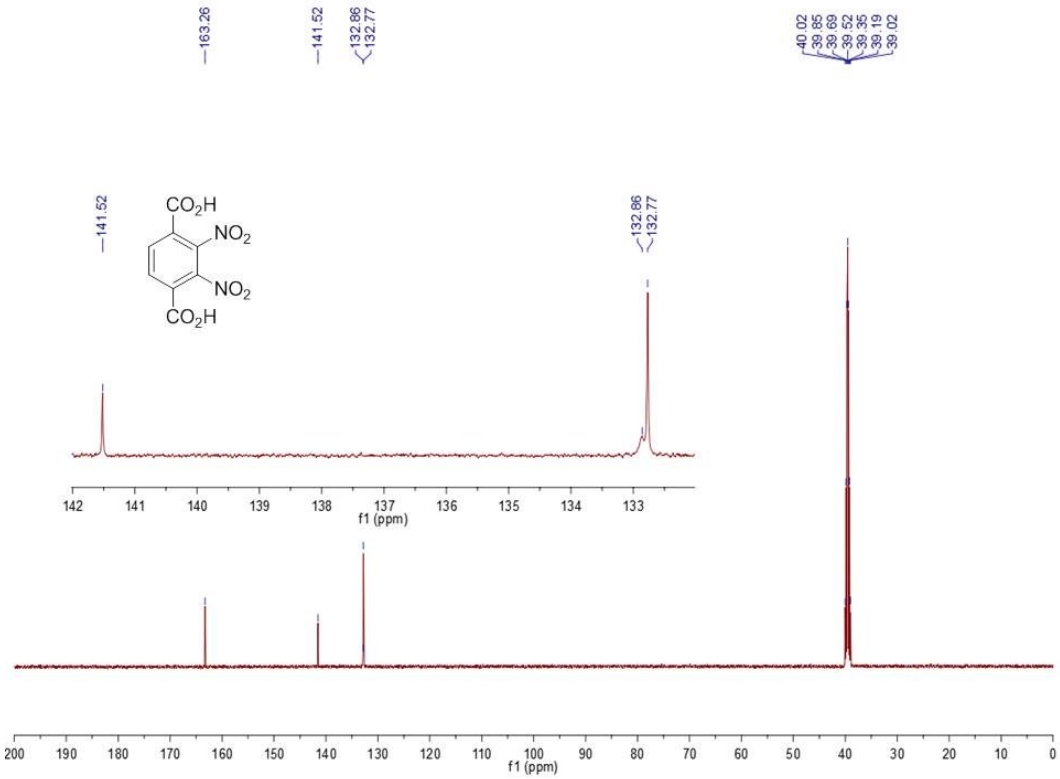


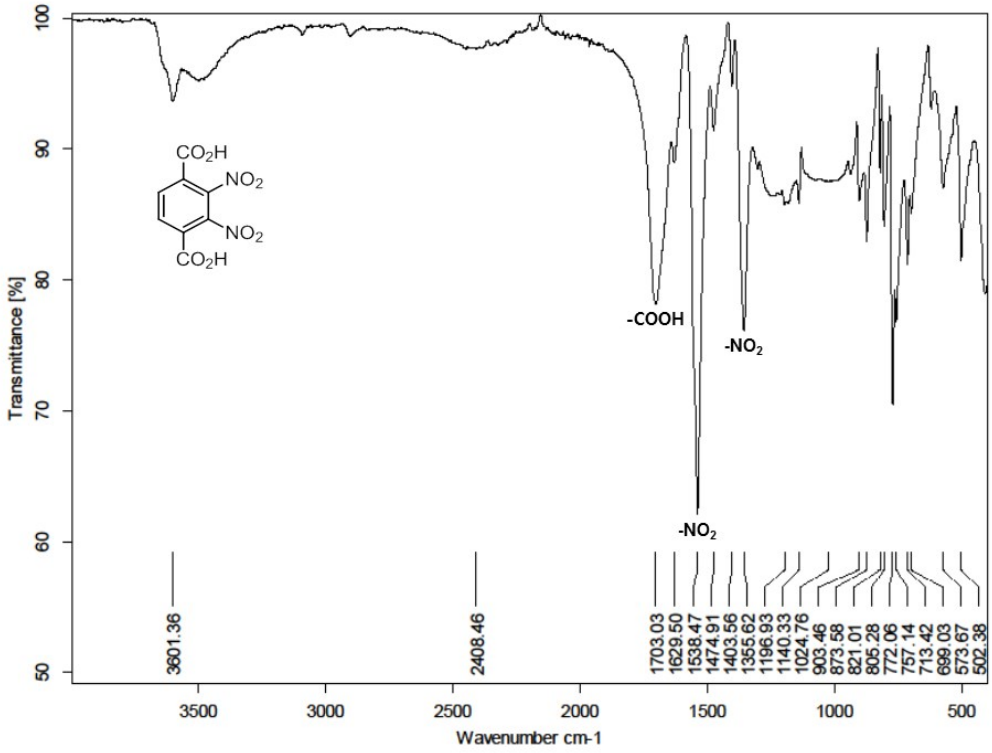



Transmittance [%]
Wavenumber cm-1
-COOH
-NO2
-NO2
3075.09
1669.52
1622.38
1533.06
1478.93
1354.64
1183.48
923.39
858.49
807.32
780.26
724.83
689.84
668.12
605.54
568.71
550.29
421.27

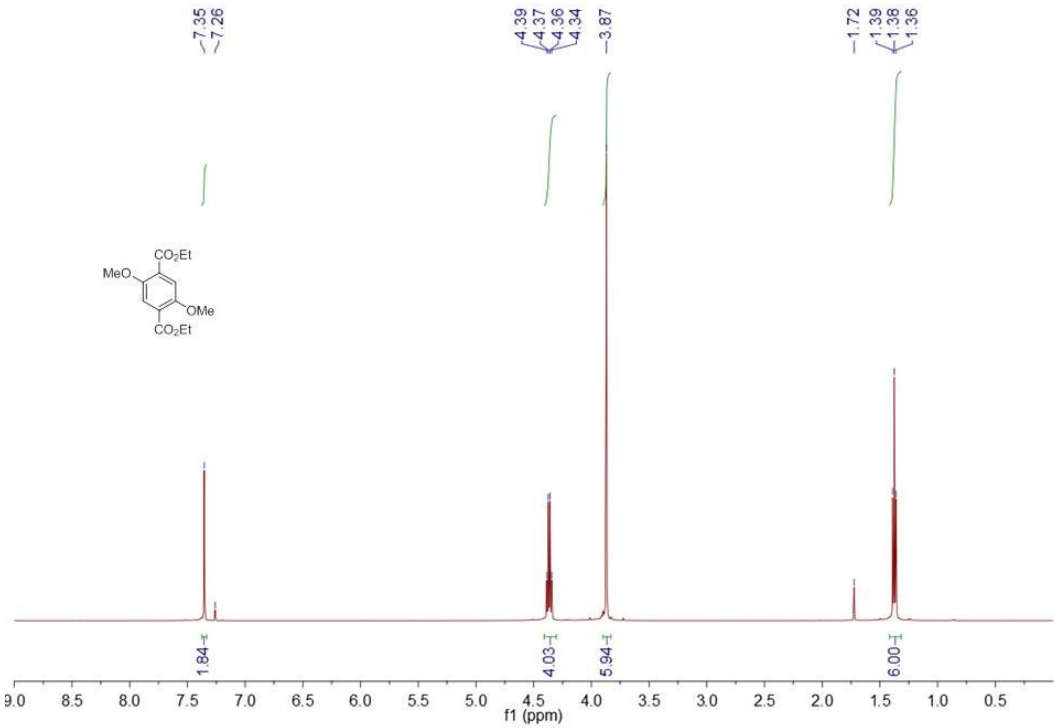
2,3-Dinitroterephthalic acid (**2b**)

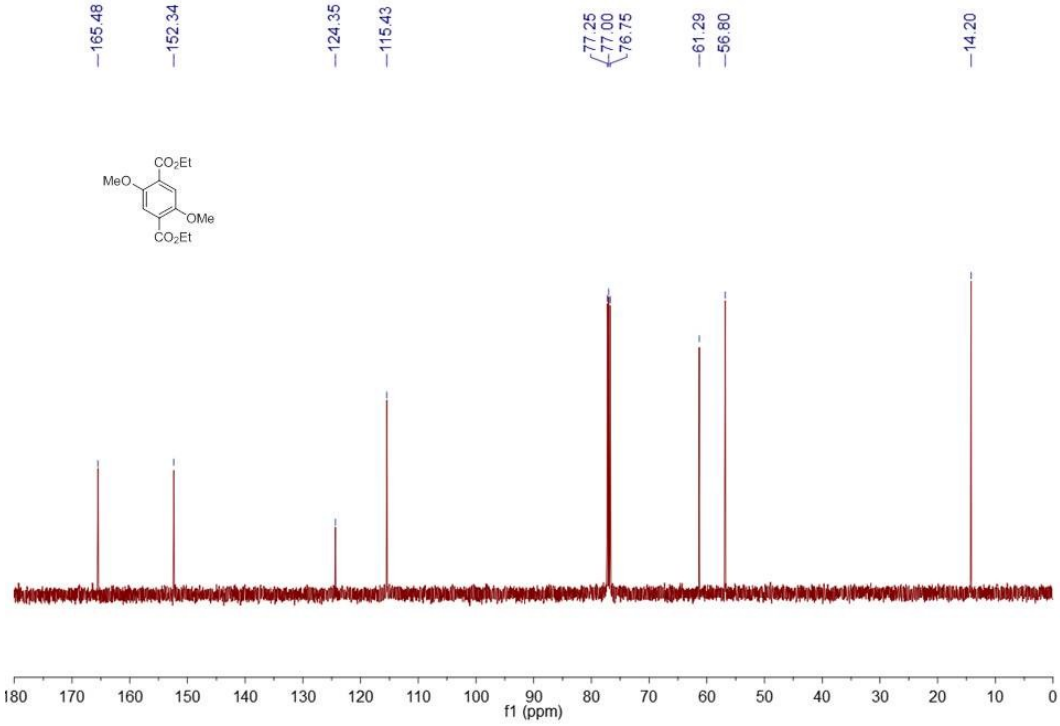


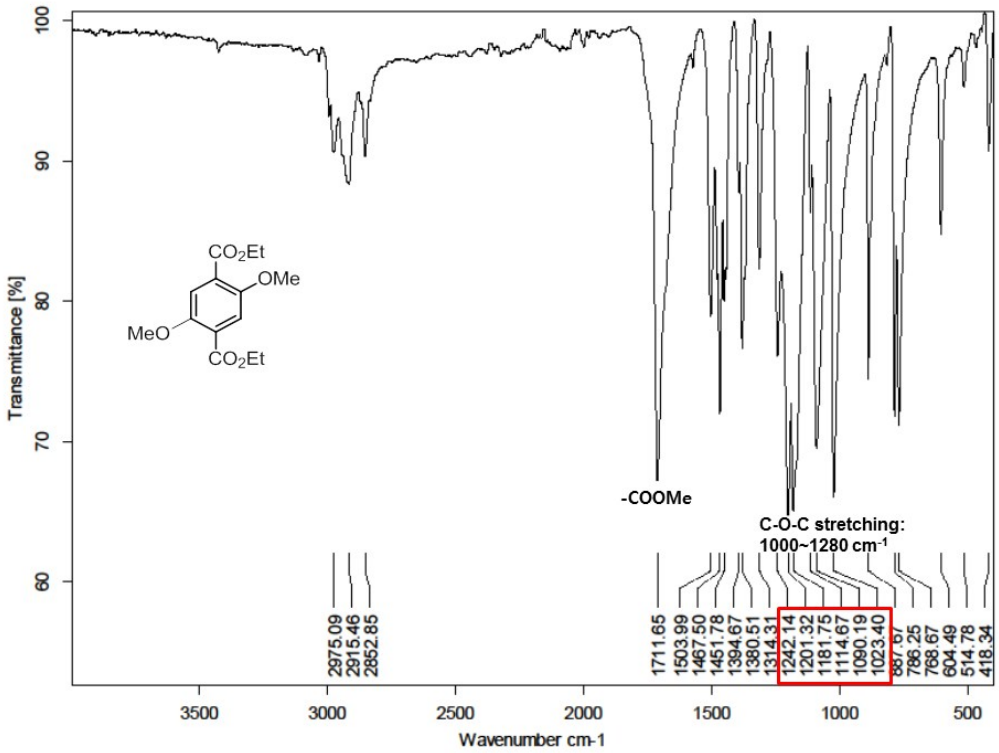



Transmittance [%]
Wavenumber cm-1
-COOH
-NO2
-NO2
3601.36
2408.46
1703.03
1629.50
1538.47
1474.91
1403.56
1355.62
1196.93
1140.33
1024.76
903.46
873.58
821.01
805.28
772.06
757.14
713.42
699.03
573.67
502.38

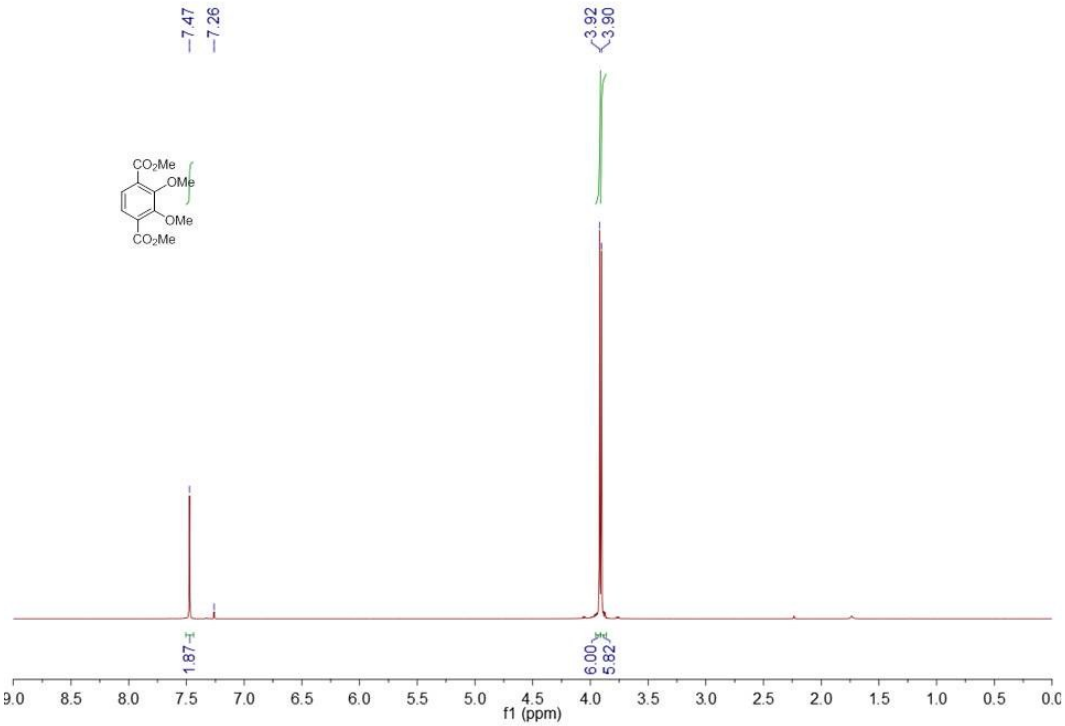
Diethyl-2,5-dimethoxyterephthalate (**BDCE-2,5-(OMe)$_2$**)

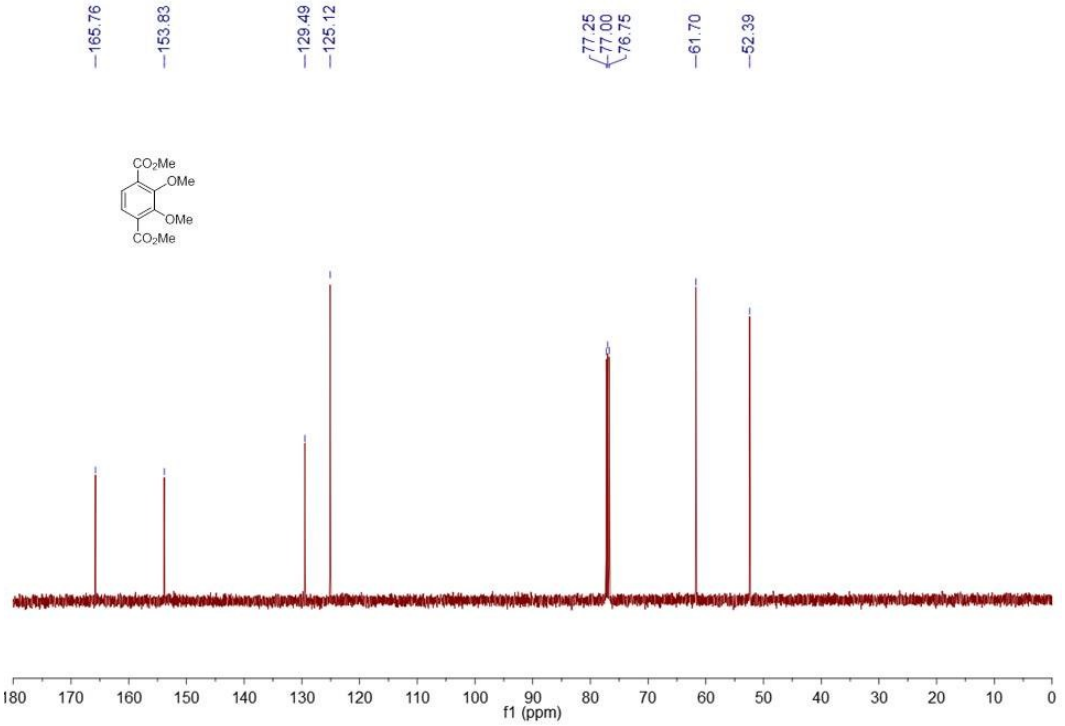


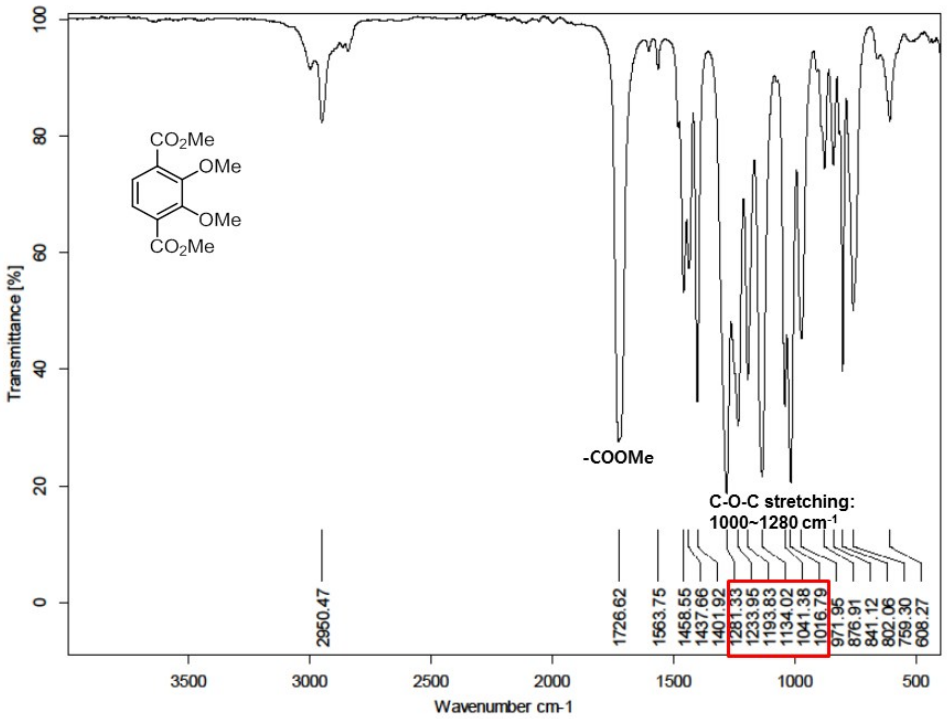



Transmittance [%]
Wavenumber cm-1
CO2Et
OMe
MeO
CO2Et
-COOMe
C-O-C stretching:
1000~1280 cm-1
2975.09
2915.46
2852.85
1711.65
1503.99
1467.50
1451.78
1394.67
1380.51
1314.31
1242.14
1201.32
1181.75
1114.67
1090.19
1023.40
887.57
786.25
768.67
604.49
514.78
418.34

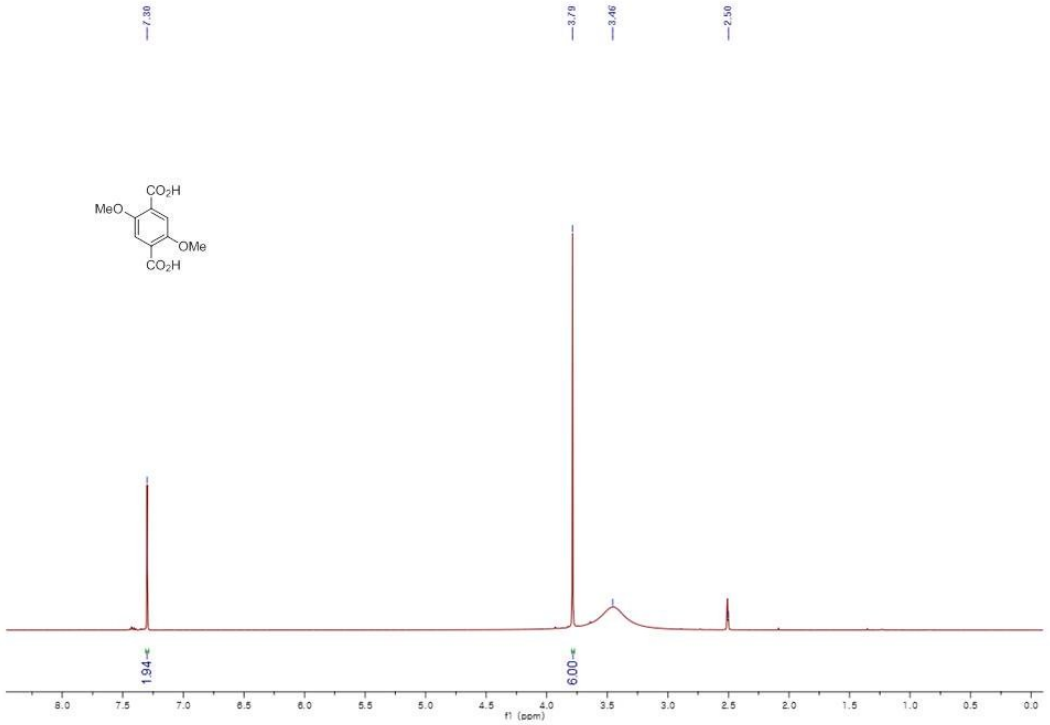
Dimethyl-2,3-dimethoxyterephthalate (**BDCE-2,3-(OMe)$_2$**)

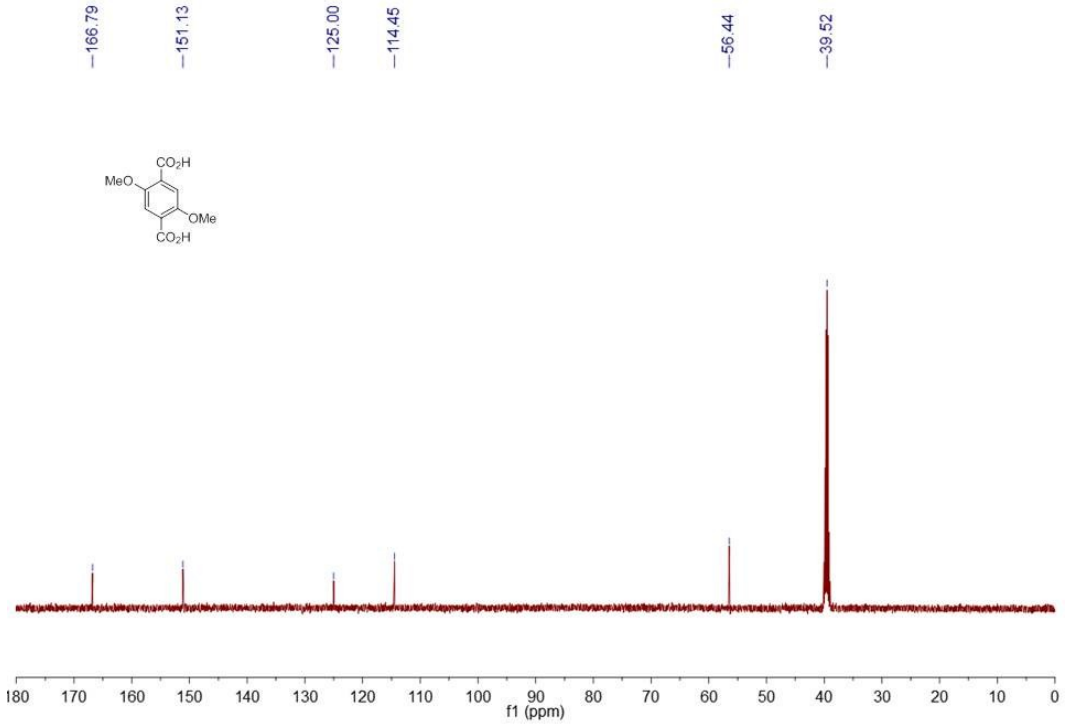


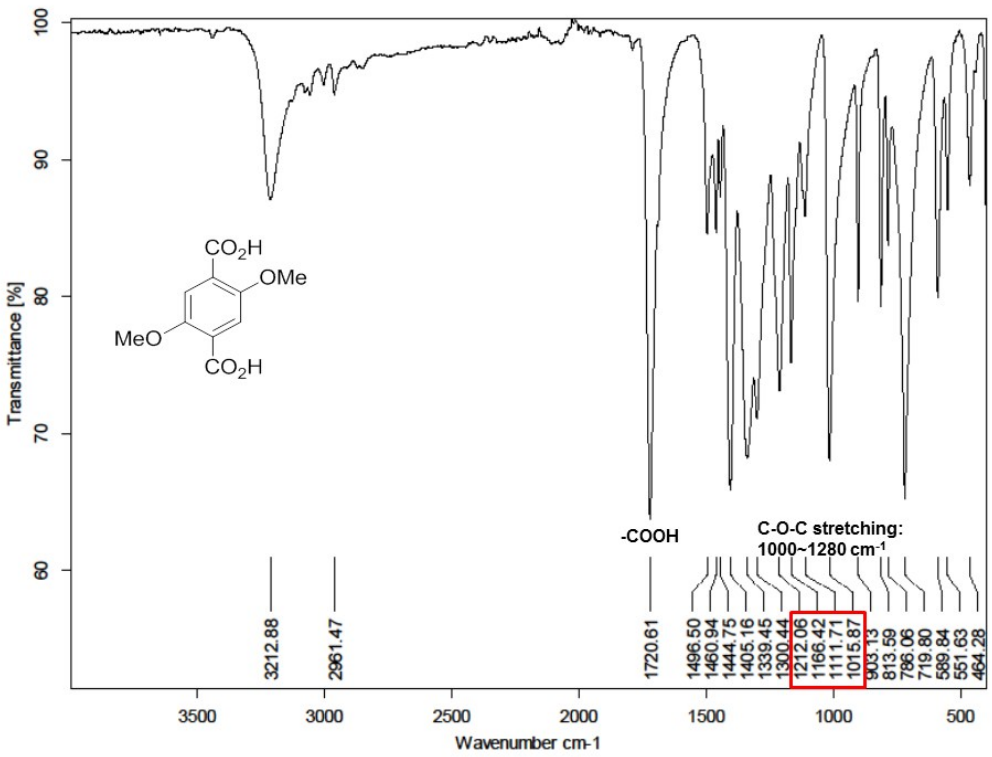



CO2Me
OMe
OMe
CO2Me
-COOMe
C-O-C stretching:
1000~1280 cm-1
2950.47
1726.62
1563.75
1458.55
1437.66
1401.92
1281.33
1233.95
1193.83
1134.02
1041.38
1016.79
971.95
876.91
841.12
802.06
759.30
608.27
Transmittance [%]
Wavenumber cm-1

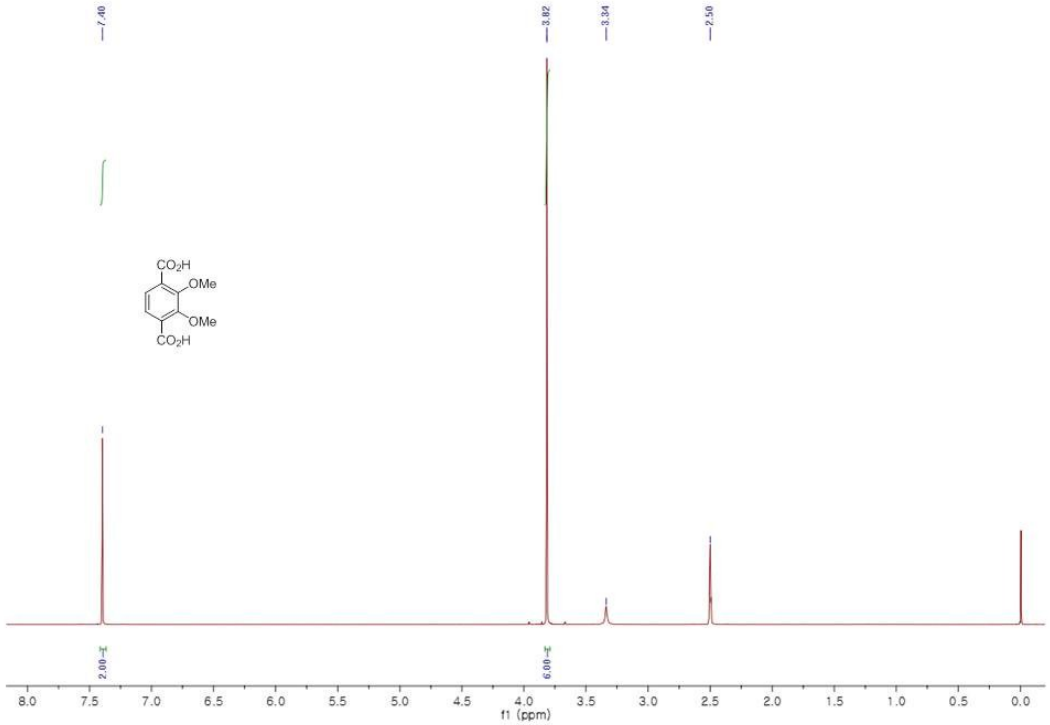
2,5-Dimethoxyterephthalic acid (**3a**)

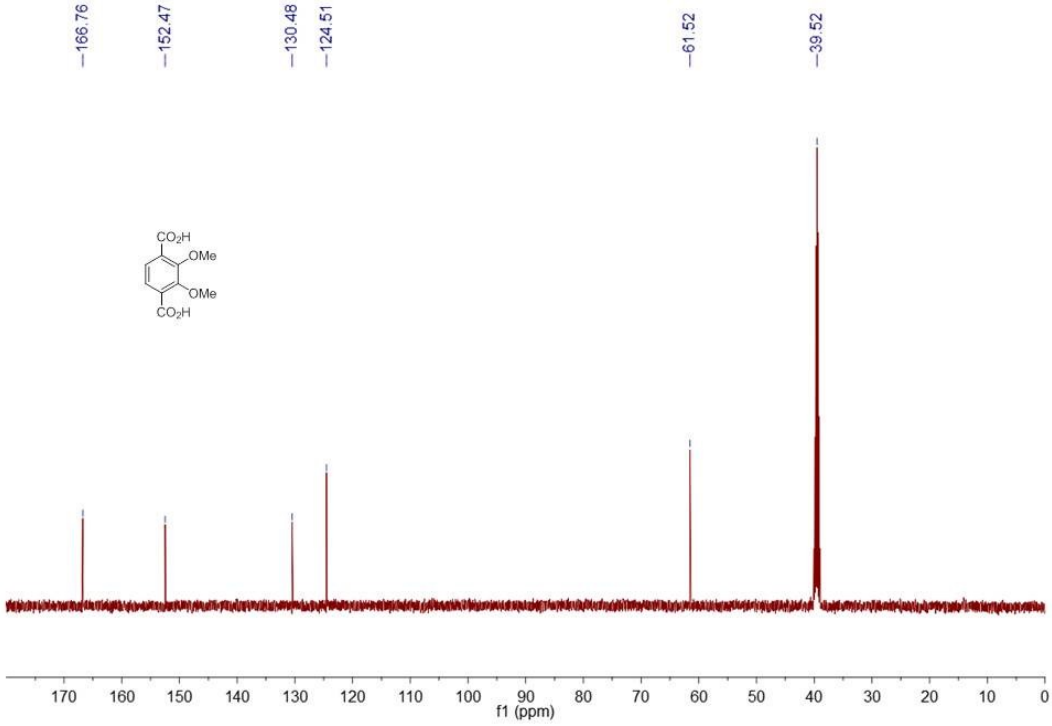


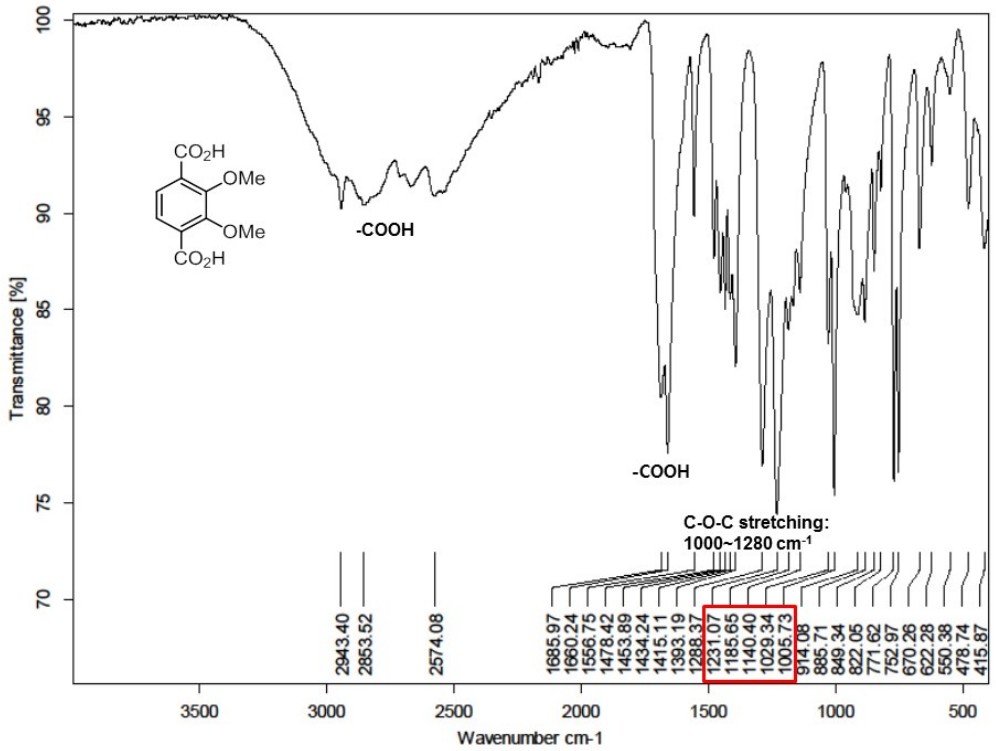



Transmittance [%]
Wavenumber cm-1
CO2H
OMe
MeO
CO2H
-COOH
C-O-C stretching:
1000~1280 cm-1
3212.88
2961.47
1720.61
1496.50
1460.94
1444.75
1405.16
1339.45
1300.44
1212.06
1166.42
1111.71
1015.87
903.13
813.59
786.06
719.80
589.84
551.63
464.28

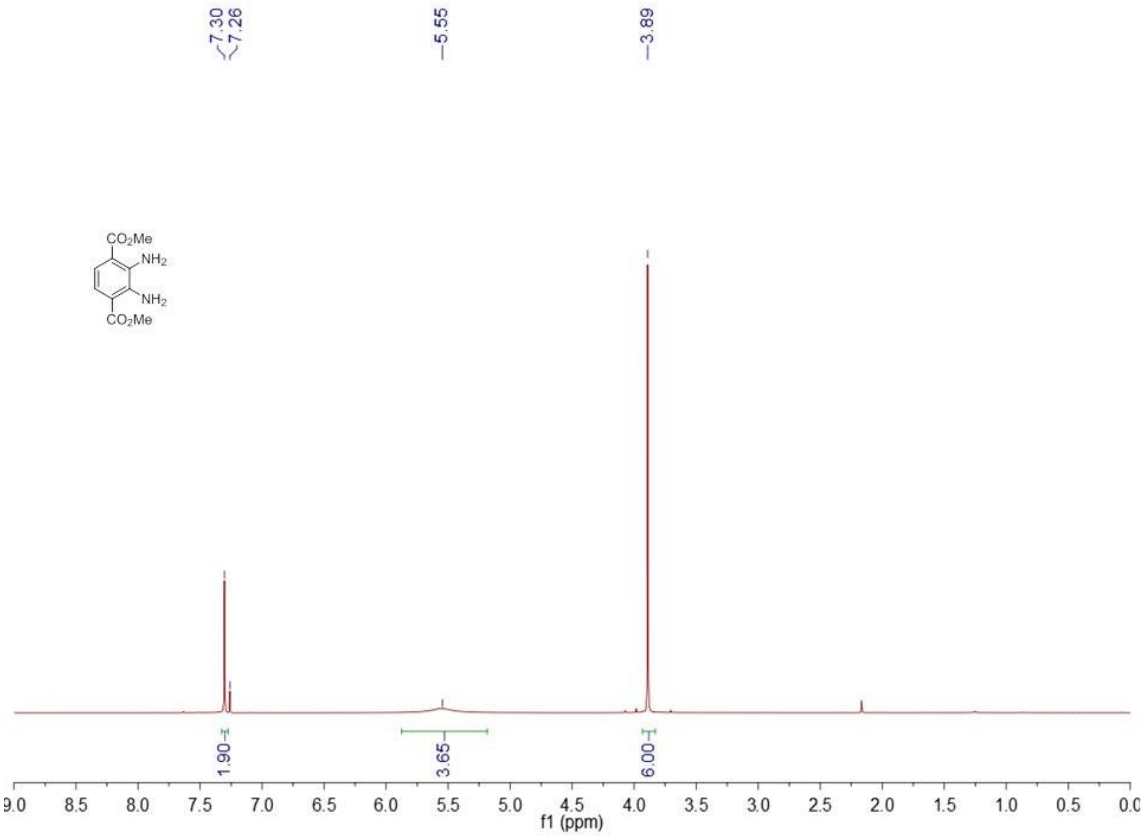
2,3-Dimethoxyterephthalic acid (**3b**)

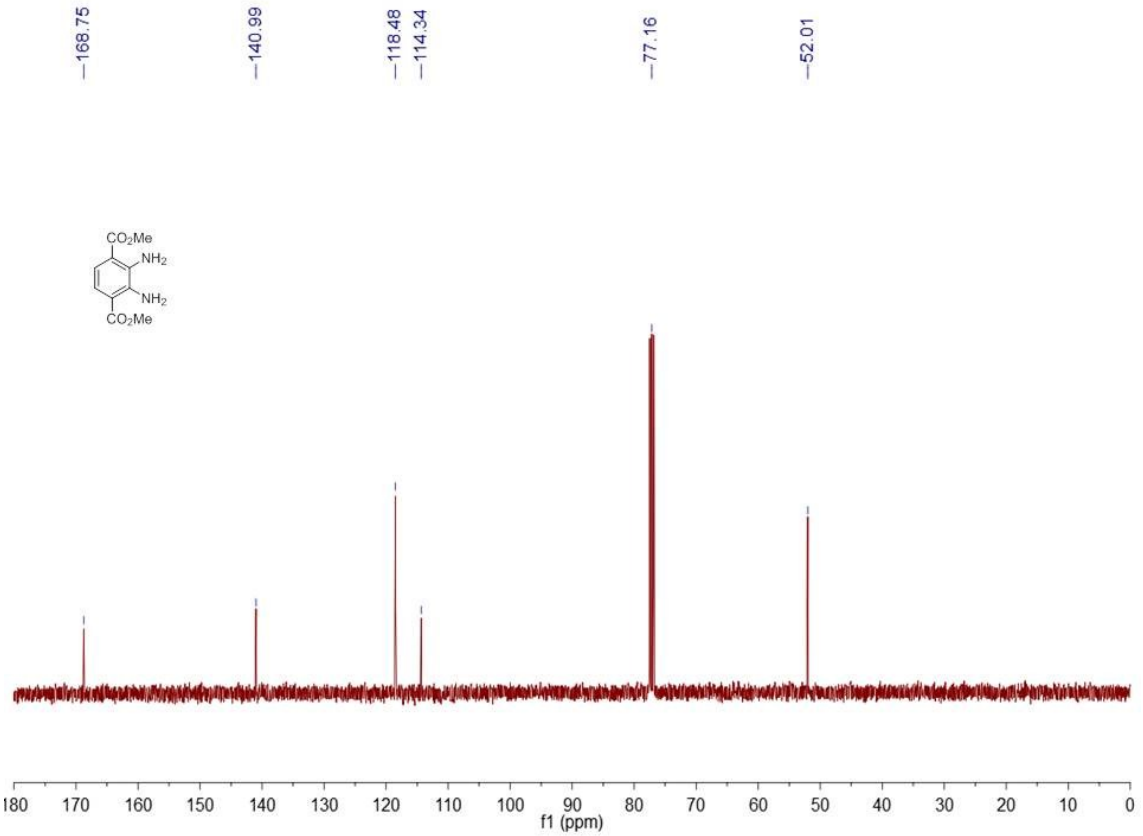


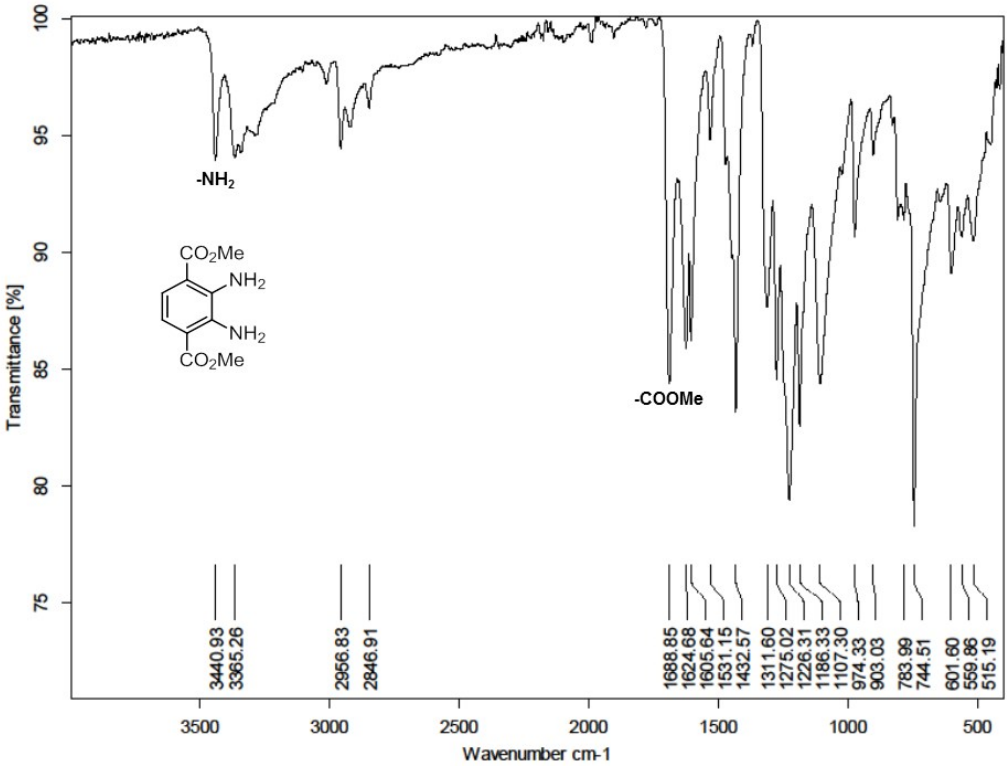



Transmittance [%]
Wavenumber cm-1
-COOH
-COOH
C-O-C stretching:
1000~1280 cm-1
2943.40
2853.52
2574.08
1685.97
1660.24
1556.75
1478.42
1453.89
1434.24
1415.11
1393.19
1288.37
1231.07
1185.65
1140.40
1029.34
1005.73
914.08
885.71
849.34
822.05
771.62
752.97
670.26
622.28
550.38
478.74
415.87

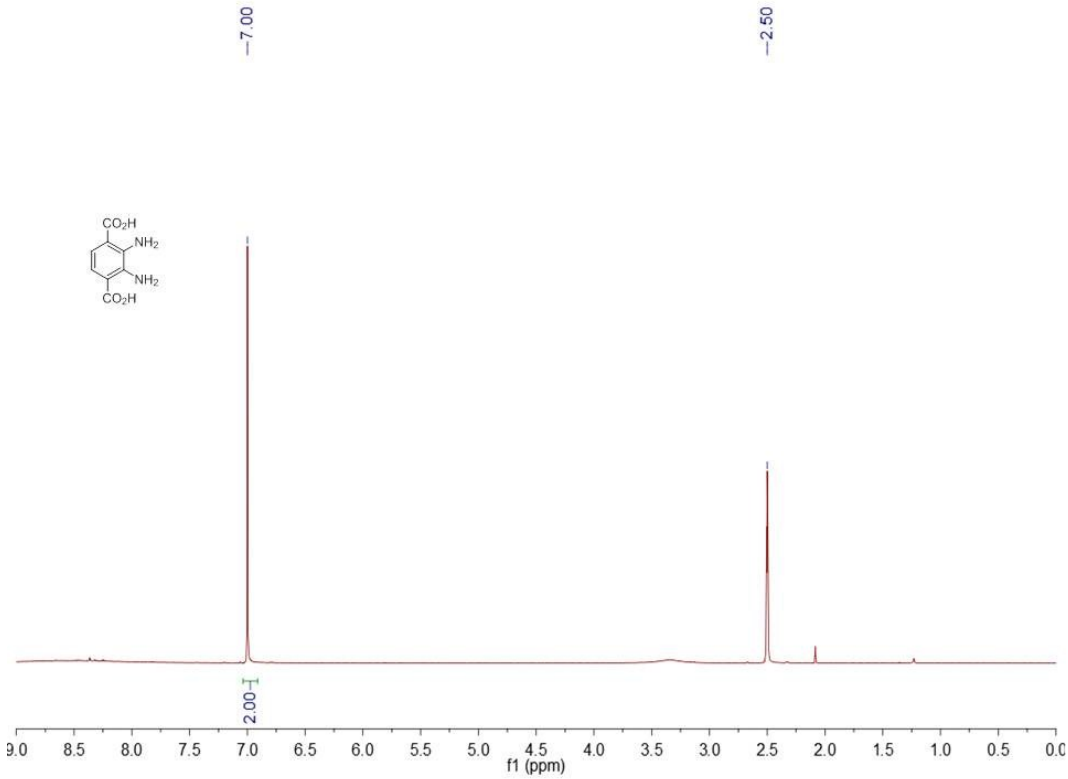
Dimethyl-2,3-diaminoterephthalate (**BDCE-2,3(NH_2)$_2$**)

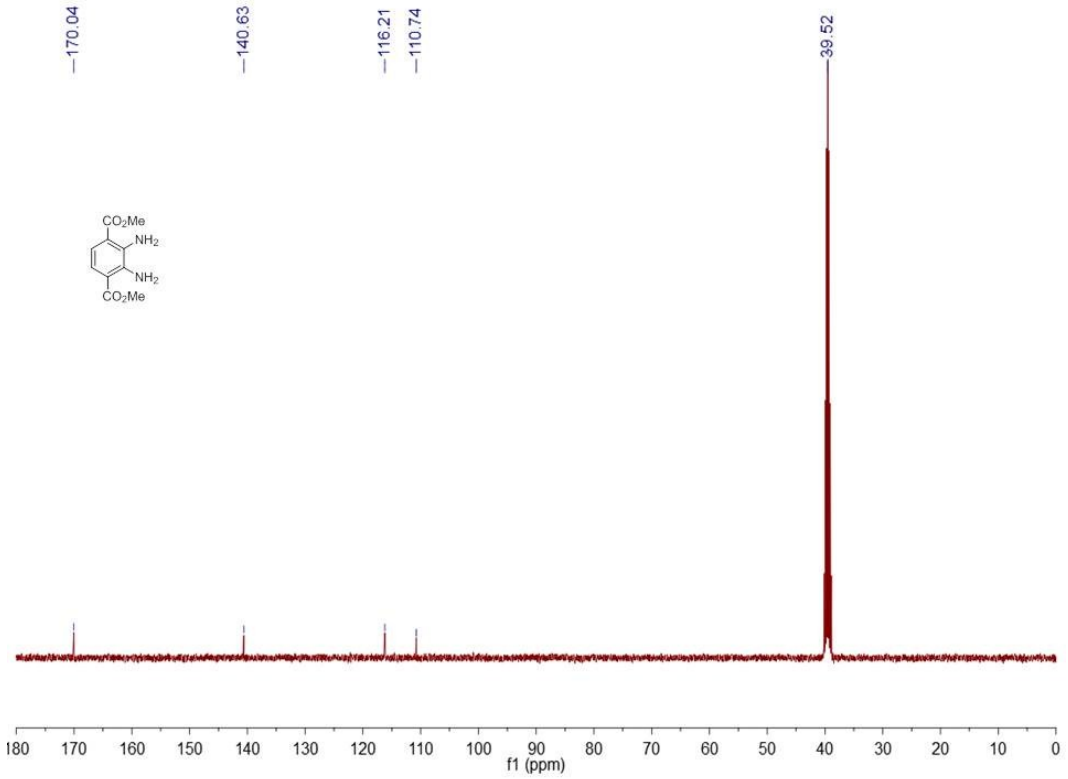


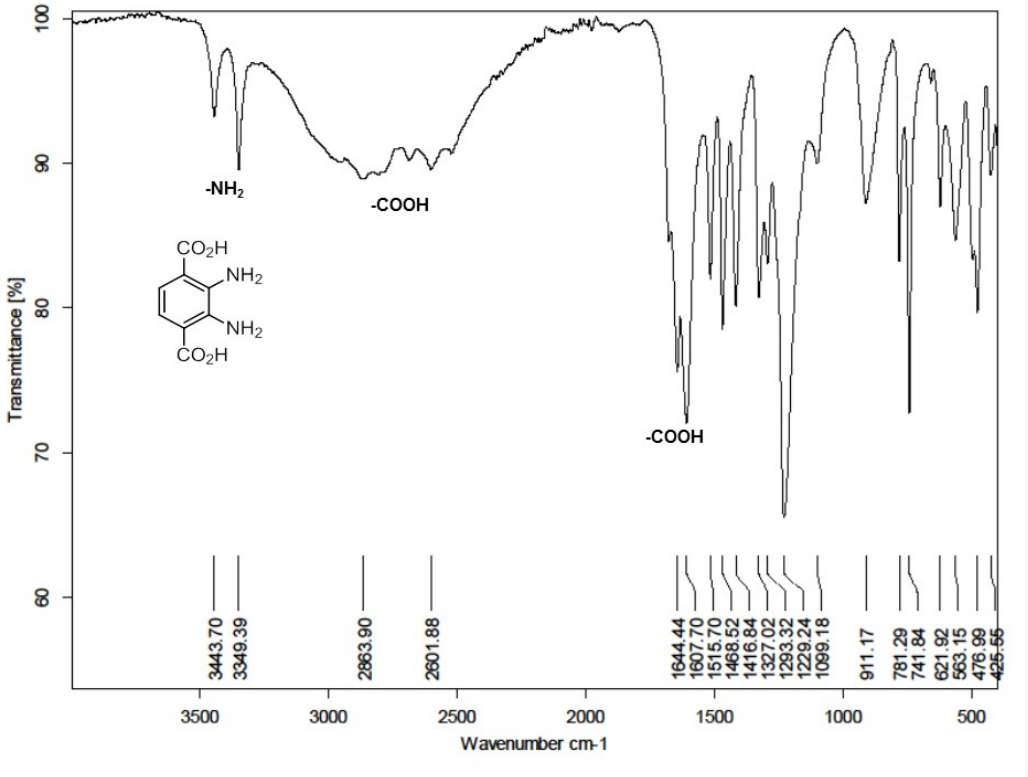



Transmittance [%]
Wavenumber cm-1
-NH2
-COOMe
CO2Me
NH2
NH2
CO2Me
3440.93
3365.26
2956.83
2846.91
1688.85
1624.68
1605.64
1531.15
1432.57
1311.60
1275.02
1226.31
1186.33
1107.30
974.33
903.03
783.99
744.51
601.60
559.86
515.19

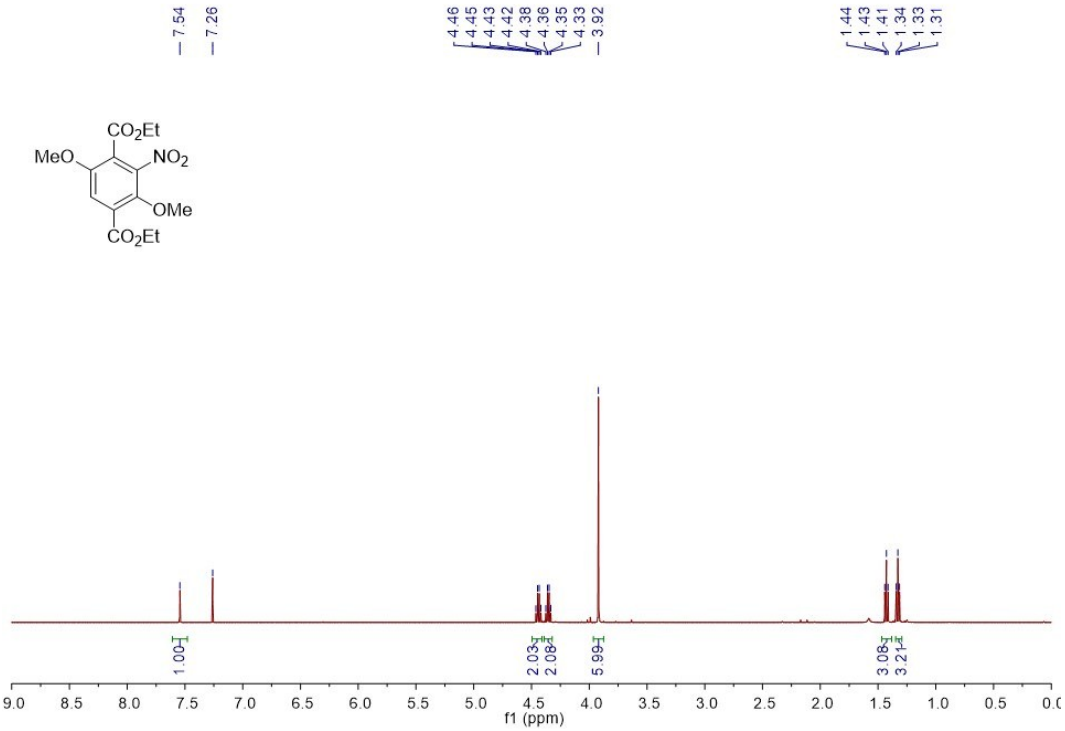
2,3-Diaminoterephthalic acid (**4b**)

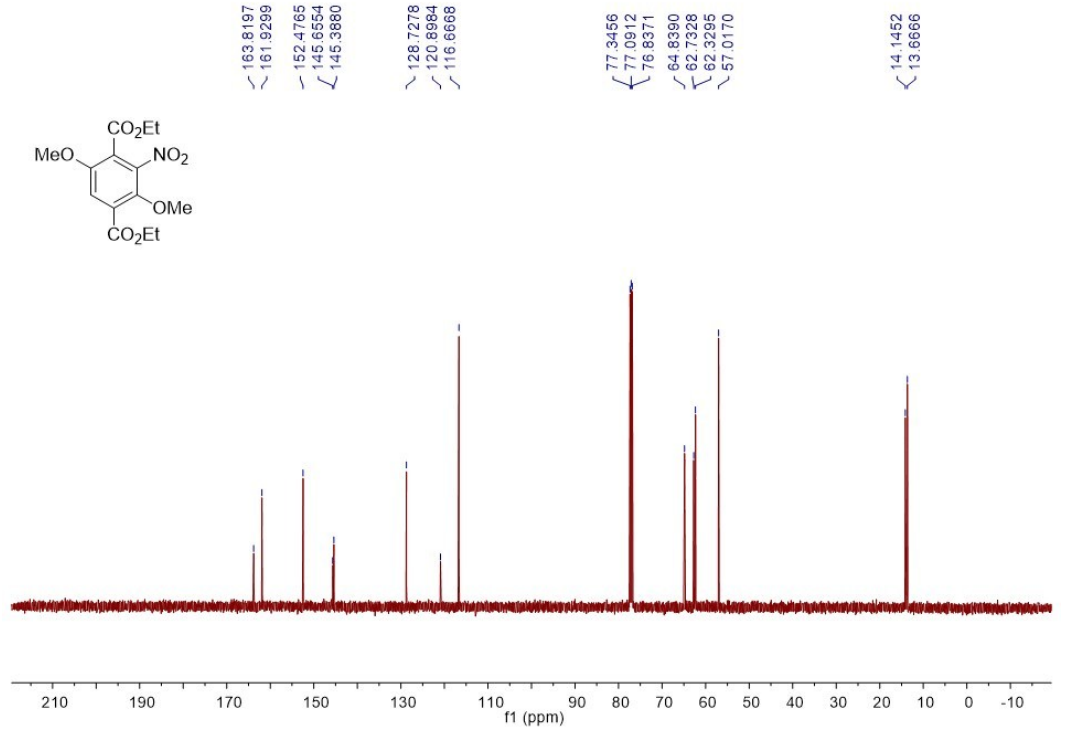


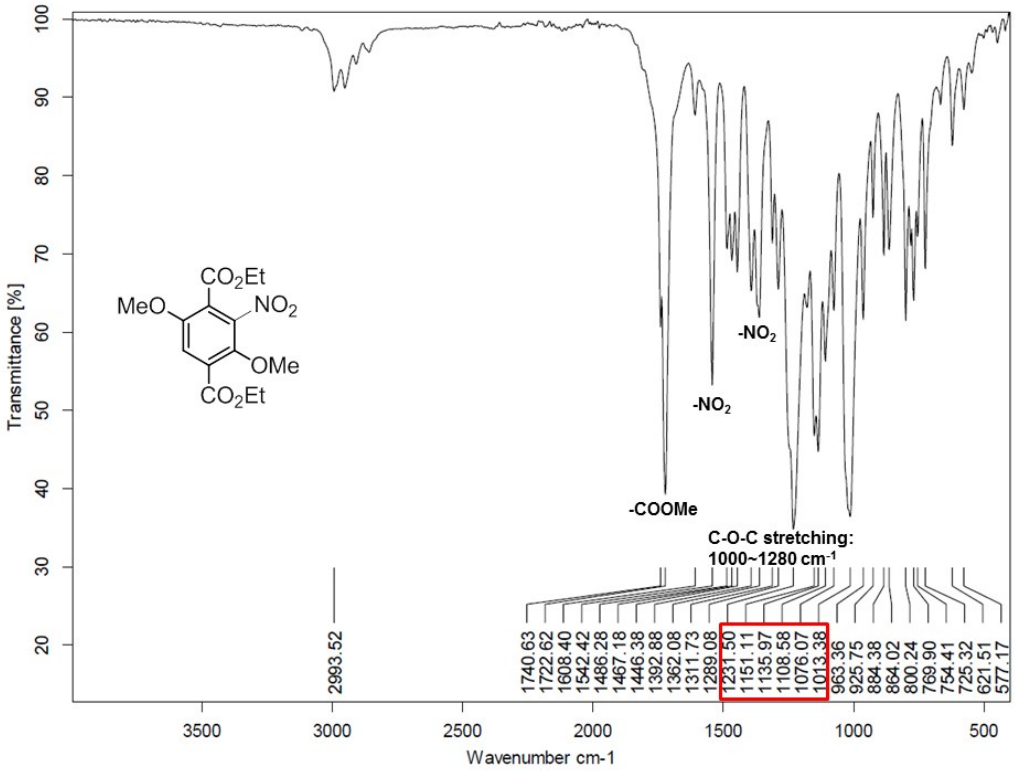



Transmittance [%]
Wavenumber cm-1
-NH2
-COOH
-COOH
CO2H
NH2
NH2
CO2H
3443.70
3349.39
2863.90
2601.88
1644.44
1607.70
1515.70
1468.52
1416.84
1327.02
1293.32
1229.24
1099.18
911.17
781.29
741.84
621.92
563.15
476.99
425.55

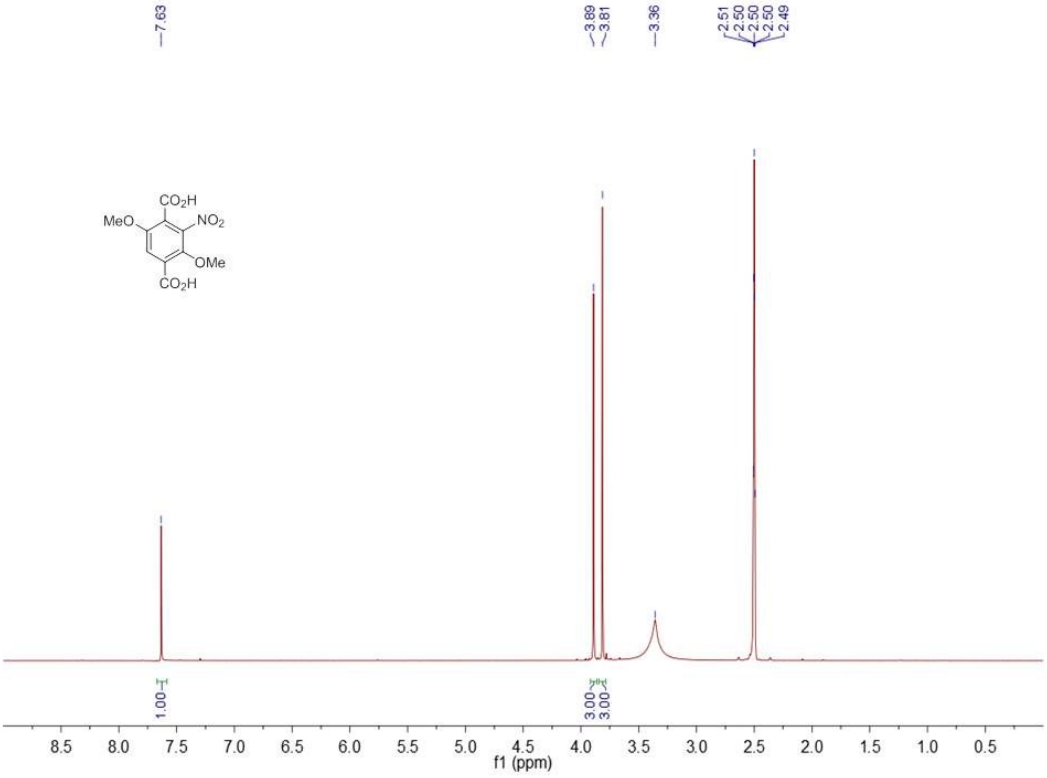
Diethyl 2,5-dimethoxy-3-nitroterephthalate(**BDCE-2,5-(OMe)$_2$-3-NO$_2$**)

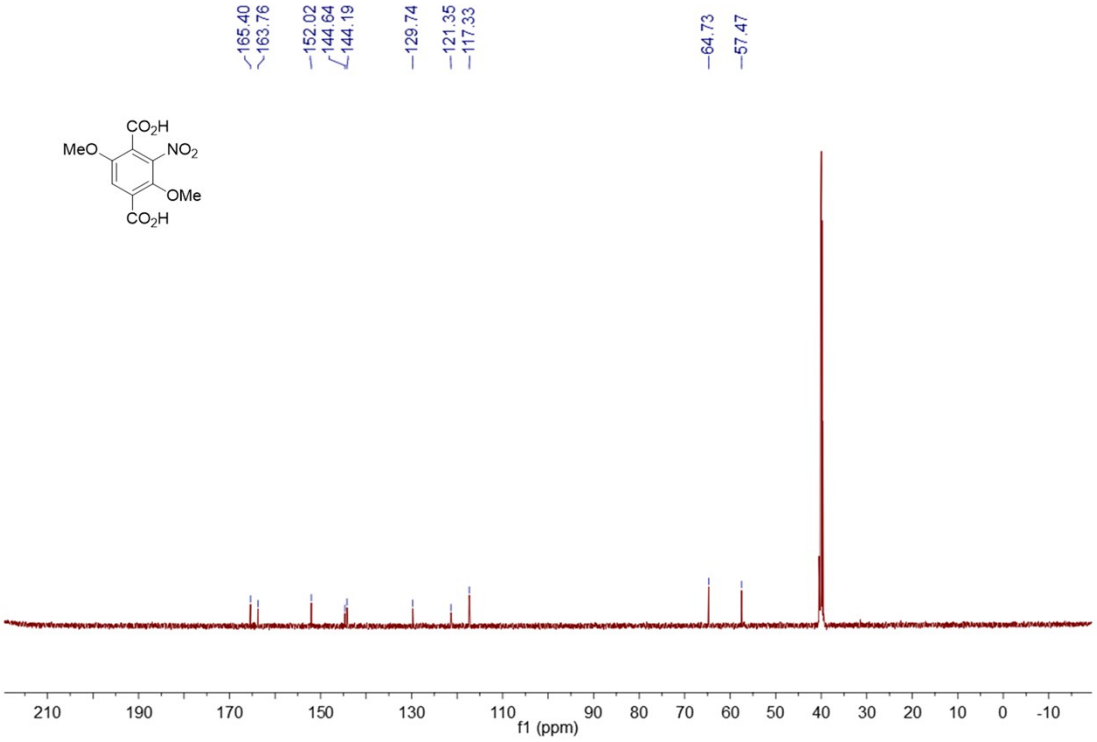


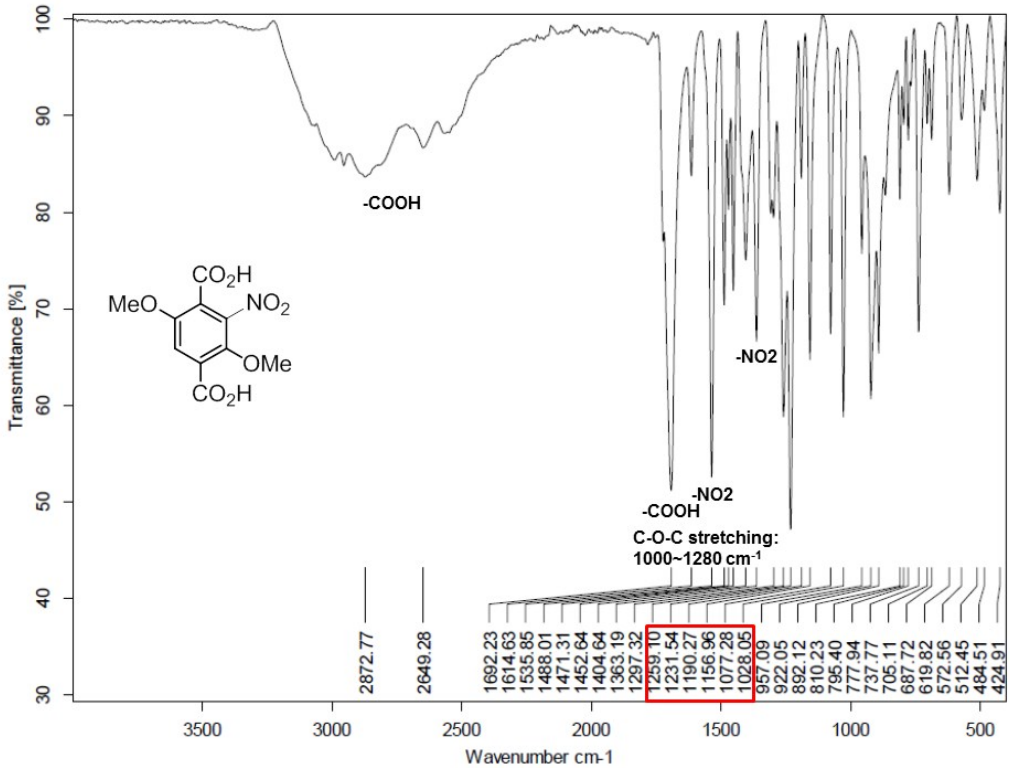



Transmittance [%]
Wavenumber cm-1
CO2Et
MeO
NO2
OMe
CO2Et
-COOMe
-NO2
-NO2
C-O-C stretching:
1000~1280 cm-1
2993.52
1740.63
1722.62
1608.40
1542.42
1486.28
1467.18
1446.38
1392.88
1362.08
1311.73
1289.08
1231.50
1151.11
1135.97
1108.58
1076.07
1013.38
963.36
925.75
884.38
864.02
800.24
769.90
754.41
725.32
621.51
577.17

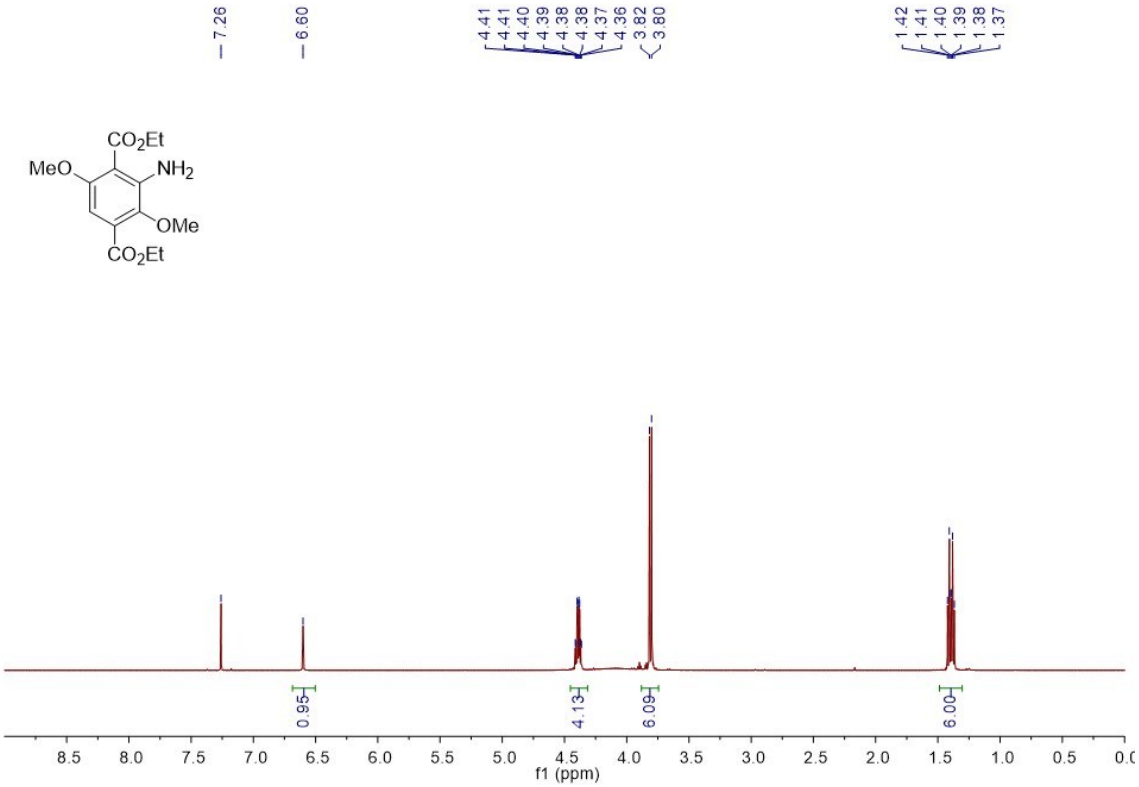
2,5-dimethoxy-3-nitroterephthalic acid(**5a**) 13C

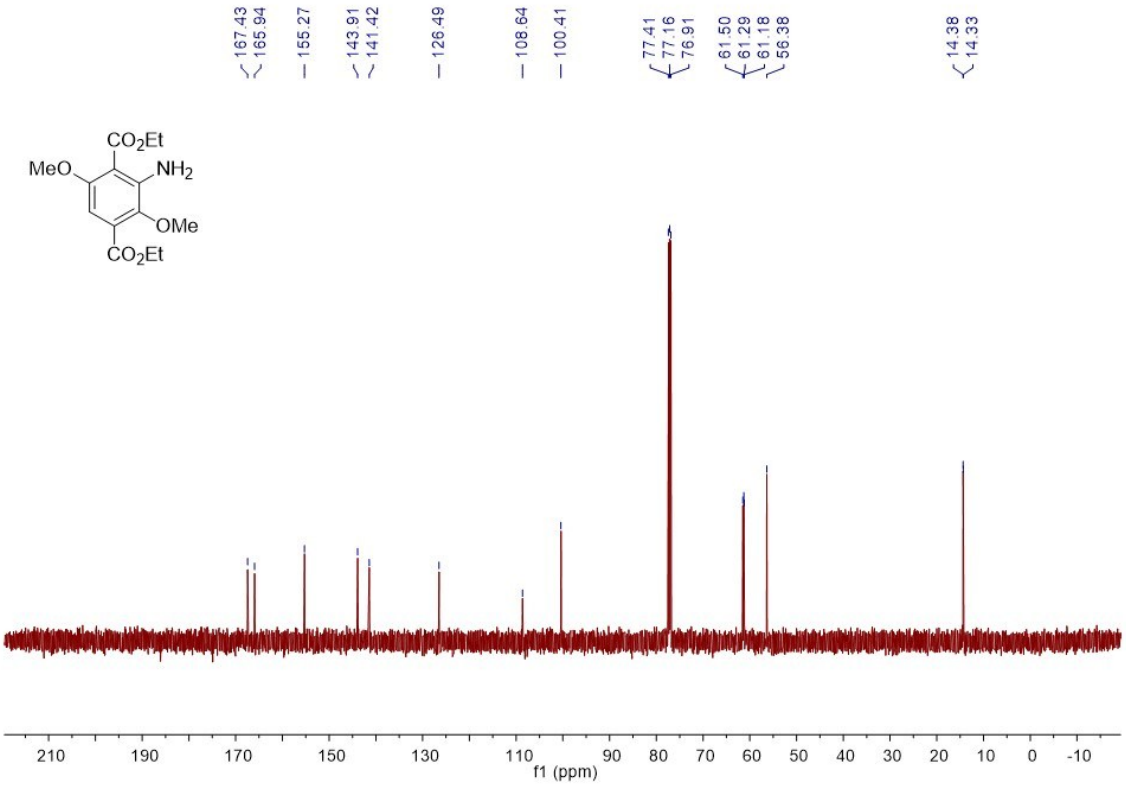


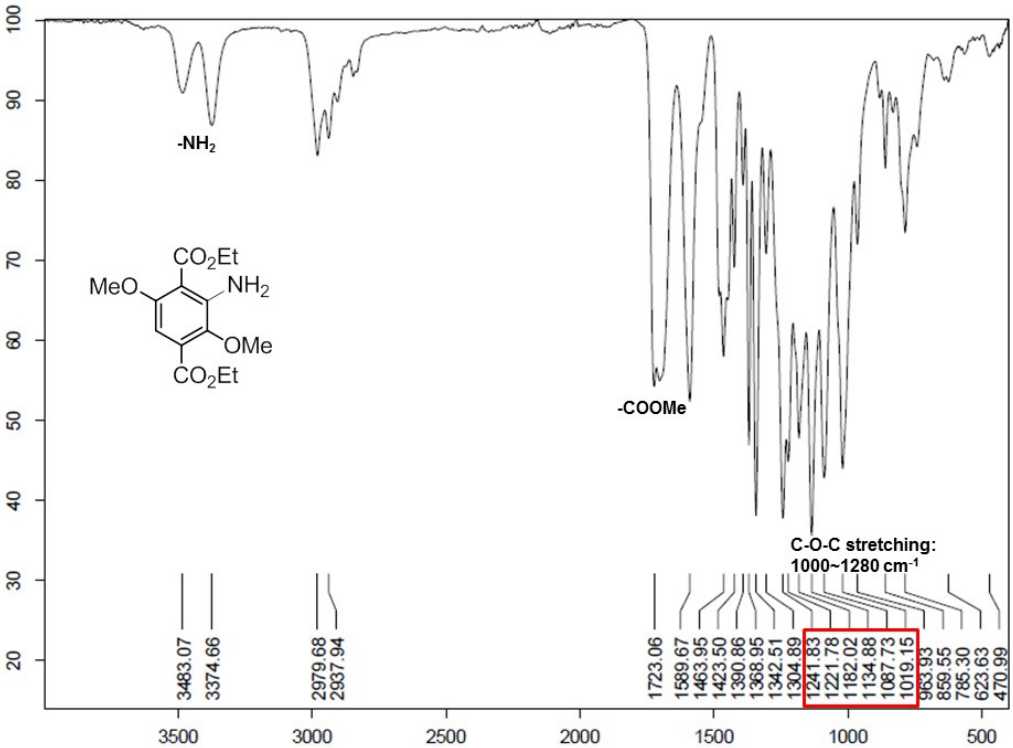



Transmittance [%]
Wavenumber cm-1
-COOH
-NO2
-NO2
-COOH
C-O-C stretching:
1000~1280 cm-1
CO2H
MeO
NO2
OMe
CO2H
2872.77
2649.28
1692.23
1614.63
1535.85
1488.01
1471.31
1452.64
1404.64
1363.19
1297.32
1259.10
1231.54
1190.27
1156.96
1077.28
1028.05
957.09
922.05
892.12
810.23
795.40
777.94
737.77
705.11
687.72
619.82
572.56
512.45
484.51
424.91

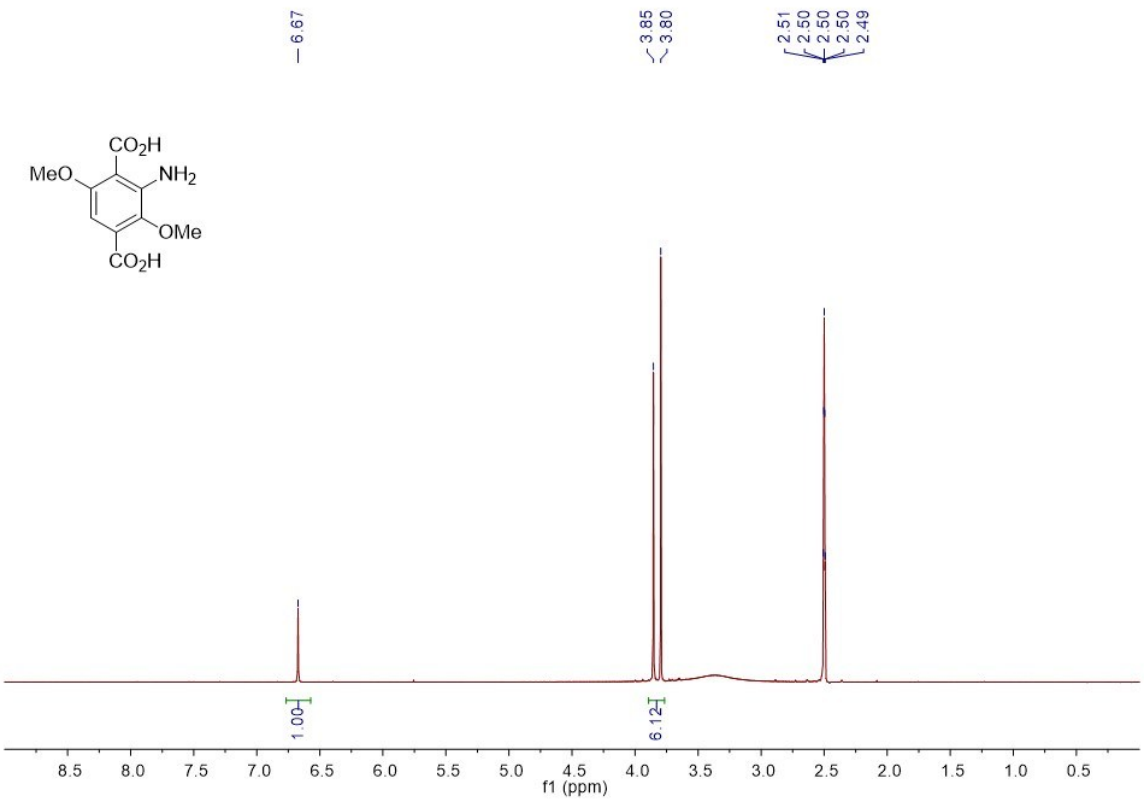
Diethyl 3-amino-2,5-dimethoxyterephthalate(**BDCE-2,5-(OMe)$_2$-3-NH$_2$**)

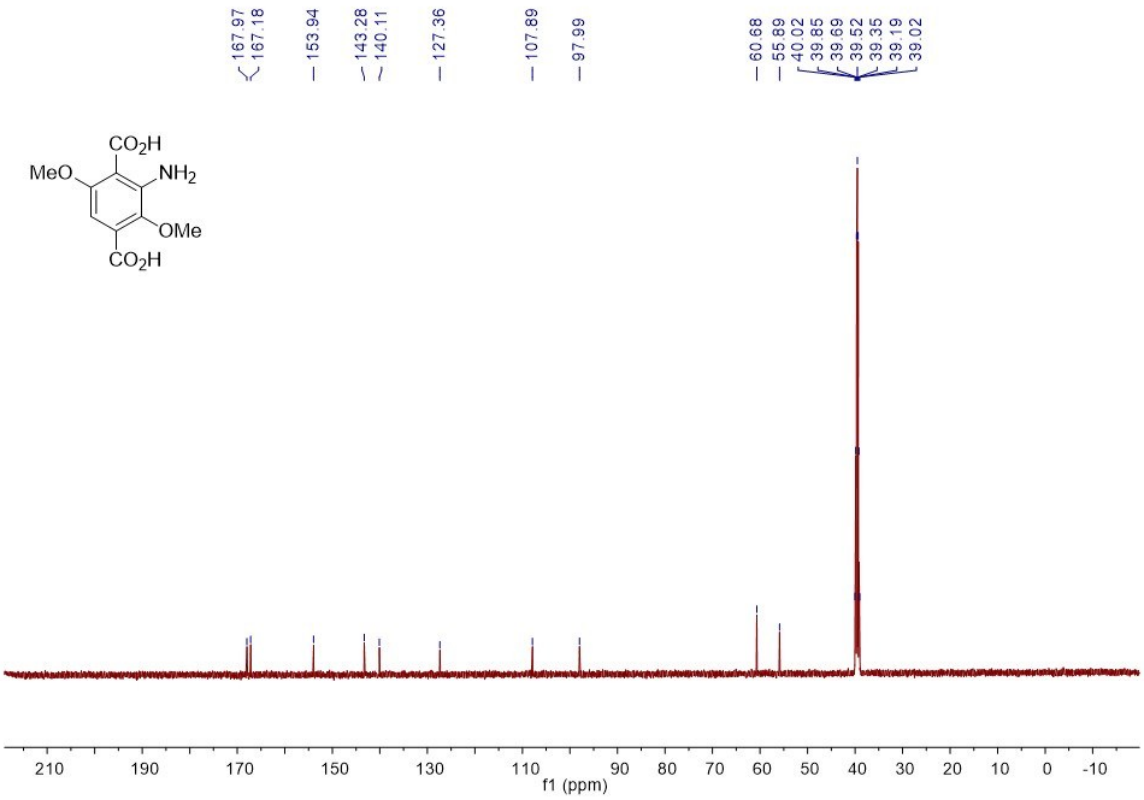


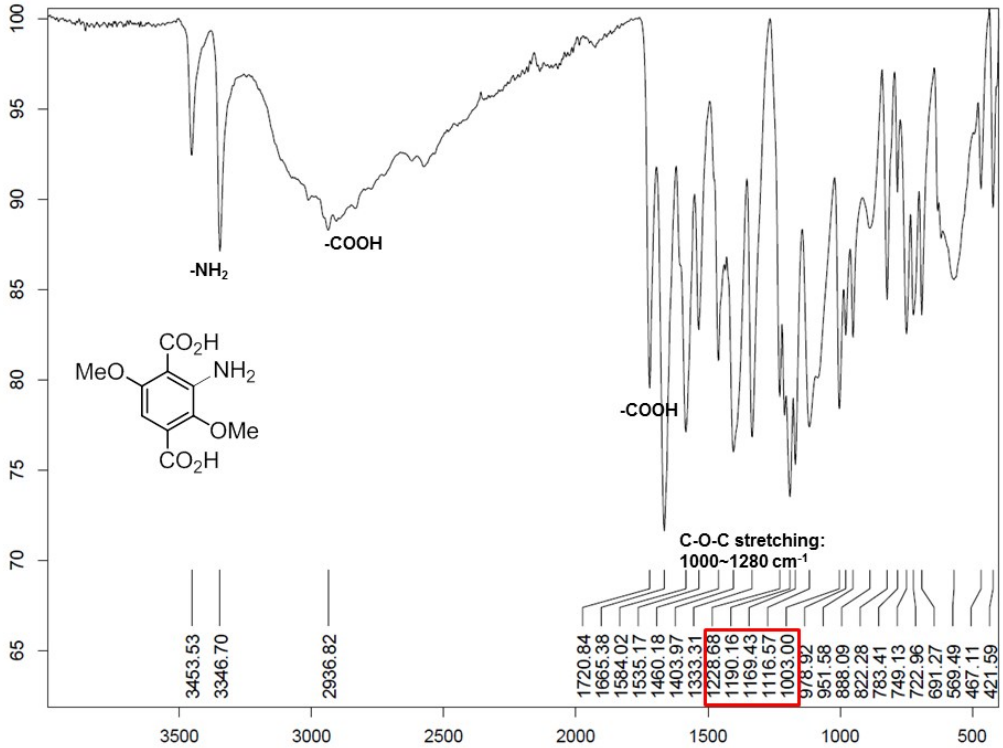



-NH2
CO2Et
MeO
NH2
OMe
CO2Et
-COOMe
C-O-C stretching:
1000~1280 cm-1
3483.07
3374.66
2979.68
2937.94
1723.06
1589.67
1463.95
1423.50
1390.86
1368.95
1342.51
1304.89
1241.83
1221.78
1182.02
1134.88
1087.73
1019.15
963.93
859.55
785.30
623.63
470.99
100
90
80
70
60
50
40
30
20
3500
3000
2500
2000
1500
1000
500

3-Amino-2,5-dimethoxyterephthalic acid(**5b**)






-NH2
-COOH
-COOH
C-O-C stretching:
1000~1280 cm-1
CO2H
NH2
MeO
OMe
CO2H
3453.53
3346.70
2936.82
1720.84
1665.38
1584.02
1535.17
1460.18
1403.97
1333.31
1228.68
1190.16
1169.43
1116.57
1003.00
978.92
951.58
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783.41
749.13
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691.27
569.49
467.11
421.59
100
95
90
85
80
75
70
65
3500
3000
2500
2000
1500
1000
500