

Electronic Supporting Information

Positional effects of electron-donating and withdrawing groups on the photophysical properties of single benzene fluorophores

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General methods and materials

All chemicals in this study were purchased from chemical company. All commercial reagents and solvents were directly used without additional purification. evaporation and removal of organic solvents during the synthesis was carried out using a rotary evaporator with a diaphragm pump, and residual solvents were removed on a vacuum line held at 0.1–1 torr. TLC (thin layer chromatography) was performed on pre-coated plate with silica gel 60 F254. Visualization on TLC was achieved using UV light (254 nm). For the separation of organic compounds, the flash column chromatography was performed on silica gel (400–630 mesh) with proper organic eluents. Proton nuclear magnetic resonance spectra (¹H NMR) were recorded on Bruker AVANCE 400 (400 MHz) and 500 (500 MHz). ¹³C NMR was recorded on Bruker AVANCE 400 (100 MHz) and 500 (125 MHz) and was fully decoupled by broad band decoupling. Infrared (IR) spectra were recorded on Bruker Alpha FT-IR spectrometer. HPLC were recorded on Waters ACQUOTY ultra performance lc system with UV detector. UV–Vis absorption and photoluminescence (PL) spectra were obtained using Agilent Cary 8454 and HORIBA FluoroMax Plus spectrophotometers, respectively. The PL spectra of the solutions were measured using quartz cuvettes with a path length of 1 cm in oxygen-free solvents (20 μM in toluene, THF and MeCN). The absolute PLQYs of the solutions were measured using a FluoroMax Plus spectrophotometer (HORIBA) equipped with a 3.2-inch integrating sphere (FL-QM-sphere, HORIBA). The fluorescence decay lifetime was measured using a FluoroMax Plus spectrophotometer equipped with a DeltaTime TCSPC accessory. The data collection for single crystal structure analysis was performed on a Bruker D8 QUEST diffractometer equipped with I μ s 3.0 Mo x-ray tube ($\lambda = 0.71073\text{\AA}$) and Photon II detector. The selected crystal was coated with Parabar oil for mounting on goniometer under a stream of N₂ (g) at 220 K. The diffraction data were integrated, scaled, and reduced by using the Bruker APEX4 software. The crystal structure was solved by SHELX structure solution program and refined by full-matrix least-squares calculations with the SHELXL.

General procedures for nitration, reduction, acetylation, deacetylation and esterification

General procedure for nitration (Method A-1, A-2, A-3 and A-4):

Method A-1^{S1}: SBBF (5 mmol) was dissolved in conc. sulfuric acid (5 mL), and the mixture was stirred at 0 °C. Then 60% nitric acid (0.5 mL, 6.5 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 solid were formed. The mixture was extracted with ethyl acetate (EA), organic layer was dried by treatment with MgSO₄. The organic solvents were removed under reduced pressure, and the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent to obtain the desired product.

Method A-2^{S1}: SBBF (1 mmol) were dissolved in Ac₂O (5 mL). To mixture solution was added 60% nitric acid (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 H₂O (20 mL). Saturated NaHCO₃ solution was added to the mixture until neutral by pH paper. The organic phase was extracted with 25 mL of EA and then the organic solution was dried with MgSO₄, filtered, and evaporated. The solid mixture was separated by silica gel column chromatography and the desired compound was obtained.

Method A-3: SBBF (1 mmol) were dissolved in Ac₂O (5 mL). To mixture solution was added 60% nitric acid (1 mL) at 0 °C and stirred at 40 °C for 24 h. Once conversion was complete (monitored by TLC), the solution was poured into H₂O (20 mL). Saturated NaHCO₃ solution was added to the mixture until neutral by pH paper. The organic phase was extracted with 25 mL of EA and then the organic solution was dried with MgSO₄, filtered, and evaporated. The solid mixture was separated by silica gel column chromatography and the desired compound was obtained.

Method A-4: SBBF (5 mmol) was dissolved in conc. sulfuric acid (5 mL), and the mixture was stirred at 0 °C. Then 60% nitric acid (0.5 mL, 6.5 mmol) was slowly added to the cooled mixture solution, and the solution was continuously stirred at room temperature for 4 h. The reaction was quenched by addition of ice, and solid were formed. The mixture was extracted with EA, organic layer was dried by treatment with MgSO₄. The organic solvents were removed under reduced pressure, and the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent to obtain the desired product.

General procedure for reduction of nitro group (Method B)^{S1}: SBBF (1 mmol) was dissolved in ethanol (4 mL) and EA (1 ml), and hydrogenation was performed using 10% Pd/C (35 mg, 10 wt.%) under H₂ (1 atm) at 50 °C for 18 h. The resulting suspension filtered through celite with EA and ethanol and evaporated to remove volatile solvents. The solid mixture was separated by silica gel column chromatography and the desired compound, and the desired compound was obtained.

General procedure for acetylation of Ar-NH₂ (Method C): SBBF (1 mmol) was added to DCM (5 mL), followed by the addition of Et₃N (0.278 mL, 2 mmol). Subsequently, acid anhydride of acid chloride was slowly added dropwise. The mixture was stirred at room temperature overnight. After the completion of the reaction, water was added to react with the remaining acid anhydride for 10 minutes. The mixture was extracted with EA, and the organic layer was dried by treatment with MgSO₄. The organic solvents were removed under reduced pressure, and the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent to obtain the desired acetylation product.

General procedure for deacetylation of acetamide (or esterification) (Method D): Acetamide SBBF (1 mmol) was added to MeOH (10 mL), followed by the slow dropwise addition of sulfuric acid (1 mL). The mixture was then allowed to react overnight at 80 °C. After the completion of the reaction, water (5 mL) was added, and neutralization was carried out using saturated NaHCO₃. The mixture was extracted with EA, and the organic layer was dried by treatment with MgSO₄. The organic solvents were removed under reduced pressure, and the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent to obtain the desired deacetylation product.

General procedure for oxidation of benzylic position (Method E-1 and E-2):

Method E-1: Target SBBF (1 mmol) was dissolved in *t*-BuOH (5 mL), and water (5 ml) followed by the addition KMnO₄ (2 mmol). The mixture was stirred at 100 °C 1 h, additional KMnO₄ was added. After the completion of the reaction monitored by TLC, evaporation under reduced pressure to remove *t*-BuOH, and solution was acidified by 2M HCl. 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.

Method E-2^{S2}: Target SBBF (1 mmol) was dissolved in water (10 ml) followed by the addition KMnO₄ (6 mmol) and MgSO₄ (6 mmol). The mixture was stirred at 90 °C for 24h. After the completion of the reaction monitored by TLC, the resulting brown solution was filtered using hot water. After cooling to room temperature, and solution was acidified by 2M HCl. 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.

General procedure for methylation of carboxylic acid (Method F): Target SBBF (1 mmol) was dissolved in DMF (15 mL), followed by the addition MeI (2.7 mmol) and NaHCO₃ (3.5 mmol). The mixture was stirred at 60 °C for 24 h. After the completion of the reaction, the mixture was extracted with EA, and the organic layer was dried by treatment with MgSO₄. The organic solvents were removed under reduced pressure and using with DCM (5 mL) and *n*-hexane (50 mL) for recrystallized overnight in a refrigerator. The precipitate was collected by filtration and washed with Hexane. The desired compound was obtained by air drying.

Synthetic Procedures for SBBFs

The obtained substrates, **1E2A3A**,^{S3} **1E3A4A**,^{S3} **1E3A4A**,^{S4} **1E3A5A**,^{S5} **1E2E4A**,^{S6} **1E2E4A5A**,^{S7} **1E2A4A5E**,^{S8} **1E2A3A4E**,^{S1} and **1E2A4E5A**^{S9} were identified with reported spectra in the literature.

Methyl 2,3-diaminobenzoate (1E2A3A), methyl 2,5-diaminobenzoate (1E2A5A) and methyl 3,4-diaminobenzoate (1E3A4A): The compound **1E2A3A**, **1E2A5A** and **1E3A4A** was synthesized through a four-step process. First, methyl 3-amino-benzoate (**1E3A**) (10 mmol) reacted follow method C using AcCl (1.1 equiv.) without additional purification and following reaction using method A-2 The nitrated compound was reduction with method B without additional purification. Finally, reaction using Method D, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent.

Methyl 2,3-diaminobenzoate (1E2A3A)^{S3}: White solid; overall yield 14%; ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.10 (dd, *J* = 8.1, 1.5 Hz, 1H), 6.70 (dd, *J* = 7.5, 1.5 Hz, 1H), 6.39 (dd, *J* = 8.1, 7.5 Hz, 1H), 6.20 (s, 2H), 4.76 (s, 2H), 3.76 (s, 3H); ¹³C{¹H} NMR (126 MHz, DMSO-*d*₆) δ 168.7, 139.6, 135.9, 118.7, 117.3, 115.3, 108.9, 51.3; IR (cm⁻¹) 3448, 3426, 3365, 3077, 2947, 1879, 1690, 1639, 1610, 1558, 1468, 1432, 1282.

Methyl 2,5-diaminobenzoate (1E2A5A)^{S10}: White solid; overall yield 25%; ¹H NMR (500 MHz, DMSO-*d*₆) δ 6.99 (d, *J* = 2.8 Hz, 1H), 6.69 (dd, *J* = 8.7, 2.7 Hz, 1H), 6.56 (d, *J* = 8.7 Hz, 1H), 5.86 (s, 2H), 4.41 (s, 2H), 3.75 (s, 3H); ¹³C{¹H} NMR (126 MHz, DMSO-*d*₆) δ 168.0, 143.2, 137.8, 123.4, 117.7, 113.8, 109.3, 51.2; IR (cm⁻¹) 3448, 3418, 3397, 3350, 3264, 3032, 2957, 1679, 1633, 1592, 1566, 1497, 1435.

Methyl 3,4-diaminobenzoate (1E3A4A)^{S3}: White solid; overall yield 3%; ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.16 (d, *J* = 2.0 Hz, 1H), 7.09 (dd, *J* = 8.1, 2.0 Hz, 1H), 6.51 (d, *J* = 8.1 Hz, 1H), 5.28 (s, 2H), 4.66 (s, 2H), 3.71 (s, 3H); ¹³C{¹H} NMR (126 MHz, DMSO-*d*₆) δ 166.8, 140.5, 133.8, 120.2, 117.1, 114.8, 112.6, 51.0; IR (cm⁻¹) 3434, 3361, 3195, 2923, 2851, 1688, 1662, 1625, 1584, 1511, 1449, 1426.

Methyl 2,4-diaminobenzoate (1E2A4A)^{S11}: The compound **1E2A4A** was synthesized through a two-step process. First, 2-amino-4-nitrobenzoic acid (10 mmol) reacted follow method D without additional purification and following reaction using Method B, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent. The desired white product was obtained in overall yield 20%; ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.39 (d, *J* = 8.5 Hz, 1H), 6.40 (s, 2H), 5.82 (dd, *J* = 8.5, 2.2 Hz, 1H) 5.79 (d, *J* = 2.2 Hz, 1H), 5.61 (s, 2H), 3.66 (s, 3H); ¹³C{¹H} NMR (126 MHz, DMSO-*d*₆) δ 167.6, 153.9, 153.1, 132.0, 104.0, 98.4, 97.3, 50.5; IR (cm⁻¹) 3423, 3333, 3231, 2942, 1650, 1622, 1579, 1549, 1509, 1450.

Methyl 2,6-diaminobenzoate (1E2A6A)^{S12}: Compound **1E2A6A** was synthesized through

two-steps was 2,6-diaminobenzoic acid reacted follow method D, ester was synthesized without purification. And next reduction follows method B, and crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent. The desired product was obtained as a brown solid in yield 80%; ¹H NMR (400 MHz, DMSO-*d*₆) δ 6.80 (t, *J* = 8.0 Hz, 1H), 6.19 (s, 4H), 5.85 (d, *J* = 8.0 Hz, 2H), 3.78 (s, 3H); ¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 169.6, 152.6, 134.2, 103.2, 96.4, 51.6; IR (cm⁻¹) 3479, 3365, 2924, 2852, 1677, 1582, 1463, 1433, 1350.

Methyl 3,5-diaminobenzoate (1E3A5A)^{S4}: Compound **1E3A5A** was synthesized through method D. 3,5-diaminobenzoic acid reacted follow method D; Yellow solid; yield 80%; ¹H NMR (500 MHz, DMSO-*d*₆) δ 6.43 (d, *J* = 2.1 Hz, 2H), 6.02 (t, *J* = 2.1 Hz, 1H), 4.99 (s, 4H), 3.74 (s, 3H); ¹³C{¹H} NMR (126 MHz, DMSO-D6) δ 167.27, 149.38, 130.54, 103.67, 103.64, 51.53; IR (cm⁻¹) 3381, 3308, 3212, 3021, 2946, 2842, 1703, 1598, 1463, 1434, 1352, 1293.

Dimethyl 3-aminophthalate (1E2E3A)^{S5}: Compound **1E2E3A** was synthesized through a two-step process. First, Dimethyl 3-Nitrophthalic acid (10 mmol) reacted follow method F without additional purification. And reduction using method B, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent. The desired product was obtained as a yellow oil in overall yield 25%; ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.24 (dd, *J* = 8.4, 7.3 Hz, 1H), 6.92 (dd, *J* = 8.4, 1.2 Hz, 1H), 6.75 (dd, *J* = 7.3, 1.1 Hz, 1H), 6.09 (s, 2H), 3.75 (s, 3H), 3.74 (s, 3H); ¹³C{¹H} NMR (126 MHz, DMSO-*d*₆) δ 168.6, 167.6, 148.8, 133.6, 131.8, 119.1, 115.6, 111.0, 52.3; IR (cm⁻¹) 3479, 3376, 2951, 1702, 1608, 1462, 1432, 1311.

Dimethyl 4-aminophthalate (1E2E4A)^{S6}: Compound **1E2E4A** was synthesized through a two-step process. First, Dimethyl phthalate (10 mmol) reacted follow method A-1 without additional purification. And reduction using method B, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent. The desired product was obtained as white solid in overall yield 25%; ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.57 (d, *J* = 8.5 Hz, 1H), 6.63 (dd, *J* = 8.5, 2.4 Hz, 1H), 6.59 (d, *J* = 2.4 Hz, 1H), 6.16 (s, 2H), 3.75 (s, 3H), 3.70 (s, 3H); ¹³C{¹H} NMR (126 MHz DMSO-*d*₆) δ 169.4, 165.9, 152.7, 136.5, 131.5, 113.9, 113.6, 111.8, 52.2, 51.6; IR (cm⁻¹) 3438, 3354, 3246, 2949, 1727, 1692, 1648, 1598, 1563, 1433, 1345.

Dimethyl 2-aminoisophthalate (1E2A3E) and **Dimethyl 4-aminoisophthalate (1E2A5E)**: **1E2A3E** and **1E2A5E** compounds were synthesized through a four-step process. First, *m*-xylene (10 mmol) reacted according to method A-2. The mono-nitrated *m*-xylene was oxidized with method E without additional purification and esterified with method D. Finally, after reduction using method B, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent.

Dimethyl 2-aminoisophthalate (1E2A3E)^{S13}: Yellow solid; overall yield 7%; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.04 (d, *J* = 7.8 Hz, 2H), 8.01 (s, 2H), 6.63 (t, *J* = 7.8 Hz, 1H), 3.82 (s, 6H); ¹³C{¹H} NMR (101 MHz, DMSO) δ 167.4, 152.1, 137.2, 113.8, 111.2, 51.9; IR (cm⁻¹) 3446, 3335, 2958, 2851, 1691, 1605, 1572, 1464, 1435, 1381.

Dimethyl 4-aminoisophthalate (1E2A5E)^{S14}: Yellow solid; overall yield 4%; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.37 (d, *J* = 2.1 Hz, 1H), 7.77 (dd, *J* = 8.8, 2.2 Hz, 1H), 7.35 (s, 2H), 6.83 (d, *J* = 8.9 Hz, 1H), 3.82 (s, 3H), 3.77 (s, 3H); ¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 167.2, 165.6, 154.6, 134.2, 133.5, 116.4, 115.5, 108.0, 51.7, 51.5; IR (cm⁻¹) 3448, 3341, 2950, 1684, 1617, 1595, 1561, 1456, 1433, 1361, 1327.

Dimethyl 3,4-diaminophthalate (1E2E3A4A): Compound **1E2E3A4A** was synthesized through a five-step process. First, 3-amino-*o*-xylene (10 mmol) reacted followed method C, reacted follow method A-1 without additional purification. And following reaction using method E-2. The oxidation compound was esterification using method D without additional purification. The crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent to dimethyl 3-amino, 4-nitrophthalate was separated. Finally, after reduction using method B, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent. The desired product was obtained as an orange solid in overall yield 4%; ¹H NMR (500 MHz, DMSO-*d*₆) δ 6.98 (d, *J* = 8.2 Hz, 1H), 6.56 (d, *J* = 8.2 Hz, 1H), 5.56 (s, 2H), 4.88 (s, 2H), 3.68 (s, 6H); ¹³C{¹H} NMR (126 MHz, DMSO-*d*₆) δ 169.1, 166.9, 140.5, 132.4, 120.1, 116.9, 116.6, 112.5, 52.0, 51.6; IR (cm⁻¹) 3364, 2950, 1696, 1617, 1587, 1493, 1453, 1432.

Dimethyl 3,5-diaminophthalate (1E2E3A5A): Compound **1E2E3A5A** was synthesized through a four-step process. First 3-nitro phthalic acid (10 mmol) reacted followed method F, following reaction using method B. The Reduction compound was nitration with method A-4 without additional purification. The crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent to dimethyl 3-Amino,5-nitrophthalate was separated. Finally, after reduction using method B, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent. The desired product was obtained as a brown oil, in overall yield 9%; ¹H NMR (500 MHz, CDCl₃) δ 6.08 (d, *J* = 2.1 Hz, 1H), 5.93 (d, *J* = 2.1 Hz, 1H), 4.68 (s, 4H), 3.81 (s, 3H), 3.75 (s, 3H); ¹³C{¹H} NMR (126 MHz, CDCl₃) δ 170.4, 167.3, 151.3, 149.8, 138.0, 105.6, 101.3, 100.6, 52.2, 51.5; IR (cm⁻¹) 3485, 3470, 3364, 2948, 1692, 1600, 1455, 1430, 1397, 1346; HR-MS (ESI) : Calculated for C₁₀H₁₂N₂O₄ [M+Na]⁺: 247.0689, found: 247.0689.

Dimethyl 3,6-diaminophthalate (1E2E3A6A): Compound **1E2E3A6A** was synthesized through a six-step process. First 3-nitro phthalic acid (10 mmol) reacted followed Method F, without additional purification and following reaction using method B. The crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent to dimethyl 3-aminophthalate was separated. The Reduction compound was Acetylation with

method C without additional purification and following nitration with method A-3. The crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent to dimethyl 3-acetamino, 6-nitrophthalate was separated. The nitrated compound was esterification with method D without additional purification. Finally, reduction using Method B, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent. The desired product was obtained as a yellow solid in overall yield 7%; ¹H NMR (500 MHz, DMSO-*d*₆) δ 6.77 (s, 2H), 5.21 (s, 4H), 3.70 (s, 6H); ¹³C{¹H} NMR (126 MHz, DMSO-*d*₆) δ 168.3, 139.4, 122.3, 111.6, 51.8; IR (cm⁻¹) 3470, 3445, 3361, 2922, 2851, 2105, 1692, 1602, 1480, 1444, 1312; HR-MS (ESI) : Calculated for C₁₀H₁₂N₂O₄ [M+Na]⁺: 247.0689, found: 247.0689.

Dimethyl 4,5-diaminophthalate (1E2E4A5A)^{S7}: Compound **1E2E3A4A** was synthesized through a five-step process. First 4-amino-*o*-xylene (10 mmol) reacted followed Method C, without additional purification and reacted follow method A-1 without additional purification. And following reaction using method E-1. The oxidation compound was esterification with method D without additional purification. The crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent to dimethyl 4-amino-5-nitrophthalate was separated. Finally, reduction using Method B, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent. The desired product was obtained as an orange solid in overall yield 10%; ¹H NMR (500 MHz, DMSO-*d*₆) δ 6.80 (s, 2H), 5.22 (s, 4H), 3.69 (s, 6H); ¹³C{¹H} NMR (126 MHz, DMSO-*d*₆) δ 168.2, 137.0, 120.6, 113.5, 51.7; IR (cm⁻¹) 3415, 3359, 3299, 2948, 1715, 1688, 1625, 1574, 1520, 1437, 1372, 1327.

Dimethyl 2,4-diaminoisophthalate (1E2A3E4A): Compound **1E2A3E4A** was synthesized through a four-step process. First, methyl 3-methyl benzoate (5 mmol) reacted follow method A-1, di-nitrated compound was synthesized, purified by chromatography on silica gel using *n*-hexane/EA as the eluent to methyl 3-methyl-2,6-dinitrobenzoate was separated. The nitrated compound was oxidation with method E-1 without additional purification and following esterification with method D. Finally, reduction using Method B, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent. The desired product was obtained as a white solid in overall yield 2%; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.27 (s, 2H), 7.59 (d, *J* = 9.0 Hz, 1H), 7.16 (s, 2H), 5.95 (d, *J* = 9.1 Hz, 1H), 3.81 (s, 3H), 3.69 (s, 3H); ¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 168.6, 167.7, 156.5, 155.5, 135.8, 104.0, 96.7, 93.4, 51.4, 50.8; IR (cm⁻¹) 3502, 3434, 3368, 2950, 2922, 2851, 1679, 1572, 1534, 1491, 1433, 1383, 1345; HR-MS (ESI) : Calculated for C₁₀H₁₂N₂O₄ [M+H]⁺: 225.0870, found: 225.0872.

Dimethyl 2,5-diaminoisophthalate (1E2A3E5A) and Dimethyl 4,5-diaminoisophthalate (1E2A3A5E): Compound **1E2A3E5A** and **1E2A3A5E** was synthesized through a four-step process. First, dimethyl 5-amino-isophthalate (**1E3E5A**) (10 mmol) reacted follow method C using AcCl (1.1 equiv.) without additional purification

and following reaction using method A-2 The nitrated compound was reduction with method B without additional purification. Finally, reaction using Method D, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent.

Dimethyl 2,5-diaminoisophthalate (1E2A3E5A): Yellow solid; overall yield 16%; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.46 (s, 2H), 7.34 (broad, 2H), 4.75 (s, 2H), 3.79 (s, 6H); ¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 167.5, 144.9, 136.7, 123.2, 111.6, 51.7; IR (cm⁻¹) 3458, 3396, 3350, 3001, 2950, 1693, 1661, 1574, 1548, 1432; HR-MS (ESI) : Calculated for C₁₀H₁₂N₂O₄ [M+Na]⁺: 247.0689, found: 247.0689.

Dimethyl 4,5-diaminoisophthalate (1E2A3A5E): White solid; overall yield 51%; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.85 (d, *J* = 2.0 Hz, 1H), 7.27 (d, *J* = 2.0 Hz, 1H), 6.89 (s, 2H), 5.08 (s, 2H), 3.81 (s, 3H), 3.75 (s, 3H); ¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 168.1, 166.2, 143.5, 135.7, 121.9, 115.9, 115.8, 107.5, 51.6, 51.4; IR (cm⁻¹) 3442, 3397, 3342, 2951, 1680, 1621, 1572, 1483, 1437, 1333, 1307; HR-MS (ESI) : Calculated for C₁₀H₁₂N₂O₄ [M+Na]⁺: 247.0689, found: 247.0689.

Dimethyl 4,6-diaminoisophthalate (1E2A4A5E)^{S8}: Compound **1E2A4A5E** was synthesized through a three-step process. First, *m*-xylene (10 mmol) reacted follow method A-1. The nitrated compound was oxidation with method E-1 without additional purification and following esterification with method D. Finally, reaction using Method B, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent. The desired product was obtained as a white solid in yield 6%; ¹H NMR (500 MHz, DMSO-*d*₆) δ 8.33 (s, 1H), 6.92 (s, 4H), 5.91 (s, 1H), 3.74 (s, 6H); ¹³C{¹H} NMR (126 MHz, DMSO-*d*₆) δ 167.0, 154.6, 136.9, 100.3, 97.2, 51.0; IR (cm⁻¹) 3430, 3318, 2953, 1672, 1629, 1586, 1543, 1434, 1307.

Dimethyl 2,3-diaminoterephthalate (1E2A3A4E)^{S1}: Compound **1E2A3A4E** was synthesized through a four-step process. First, dimethyl 2-amino-terephthalate (**1E2A4E**) (2 mmol) reacted follow method C using AcCl (1.1 equiv.) without additional purification and following reaction using method A-1. The nitrated compound was reduction with method B without additional purification. Finally, reaction using Method D, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent. The desired product was obtained as a yellow solid in overall yield 2%; ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.02 (s, 2H), 6.70 (s, 4H), 3.80 (s, 6H); ¹³C{¹H} NMR (126 MHz, DMSO-*d*₆) δ 168.2, 140.6, 115.6, 109.8, 51.7, 39.5; IR (cm⁻¹) 3441, 3366, 3013, 2957, 2921, 2849, 1689, 1624, 1605, 1532, 1433, 1312.

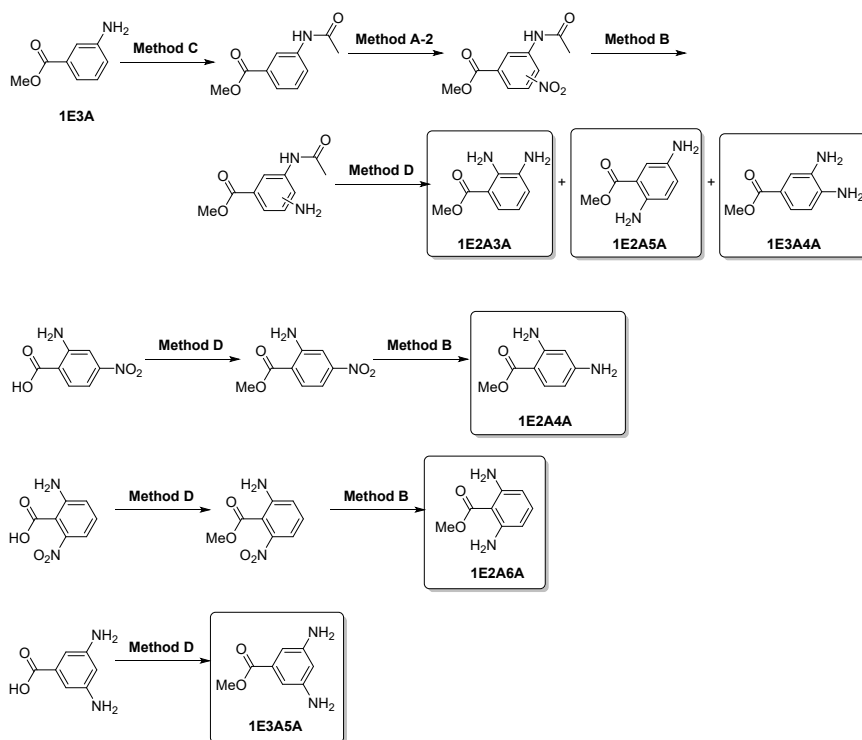
Dimethyl 2,5-diaminoterephthalate (1E2A4E5A)^{S1}: Dimethyl 1,4-cyclohexanedione-2,5-dicarboxylate (1 g, 4.3 mmol) was dissolved in 50 mL acetic acid solution, followed by the addition of phenyl hydrazine (1 mL, 1.01 mmol). The mixture was stirred at room temperature under atmospheric conditions for 2 hours. Subsequently, water (50 mL) was

added, and the mixture was neutralized with a saturated K_2CO_3 solution. The mixture was extracted with EA, organic layer was dried by treatment with $MgSO_4$. The organic solvents were removed under reduced pressure, and the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent. The desired product was obtained as a yellow solid in yield 32%; 1H NMR (500 MHz, $CDCl_3$) δ 7.27 (s, 2H), 5.07 (s, 2H), 3.86 (s, 6H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 167.7, 140.7, 119.0, 117.6, 52.0; IR (cm^{-1}) 3467, 3365, 2954, 1679, 1573, 1502.

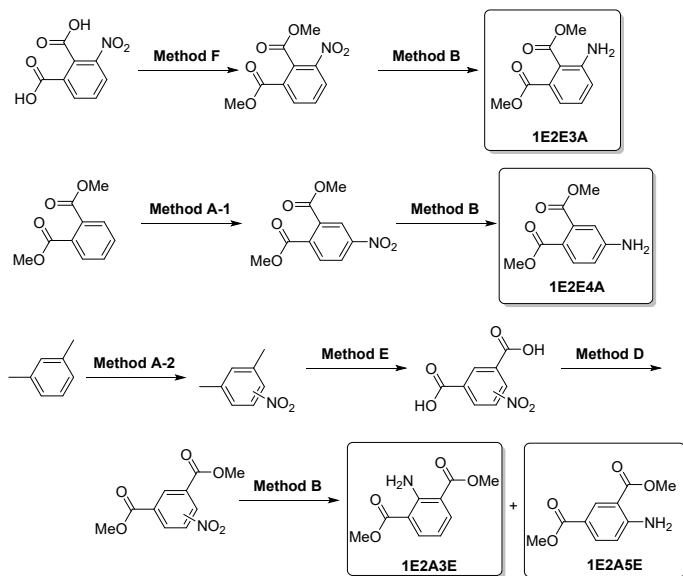
Dimethyl 2,6-diaminoterephthalate (1E2A4E6A): Compound **1E2A4E6A** was synthesized through a two-step process. First, Dimethyl 2-amino-terephthalate (**1E2A4E**) (2 mmol) reacted follow method A-1. The nitrated compound was reduction with method B, the crude reaction mixture was purified by chromatography on silica gel using *n*-hexane/EA as the eluent. The desired product was obtained as a brown solid in overall yield 1.5%; 1H NMR (500 MHz, $DMSO-d_6$) δ 6.47 (s, 2H), 6.43 (broad, 2H), 3.80 - 3.77 (m, 6H); $^{13}C\{^1H\}$ NMR (126 MHz, $DMSO-d_6$) δ 169.0, 166.9, 152.4, 134.0, 103.3, 102.8, 98.5, 52.4, 51.8, 40.5; IR (cm^{-1}) 3508, 3373, 2918, 2849, 1716, 1669, 1583, 1477, 1439, 1385, 1319; HR-MS (ESI) : Calculated for $C_{10}H_{12}N_2O_4$ $[M+H]^+$: 225.0870, found: 225.0872.

Computational details

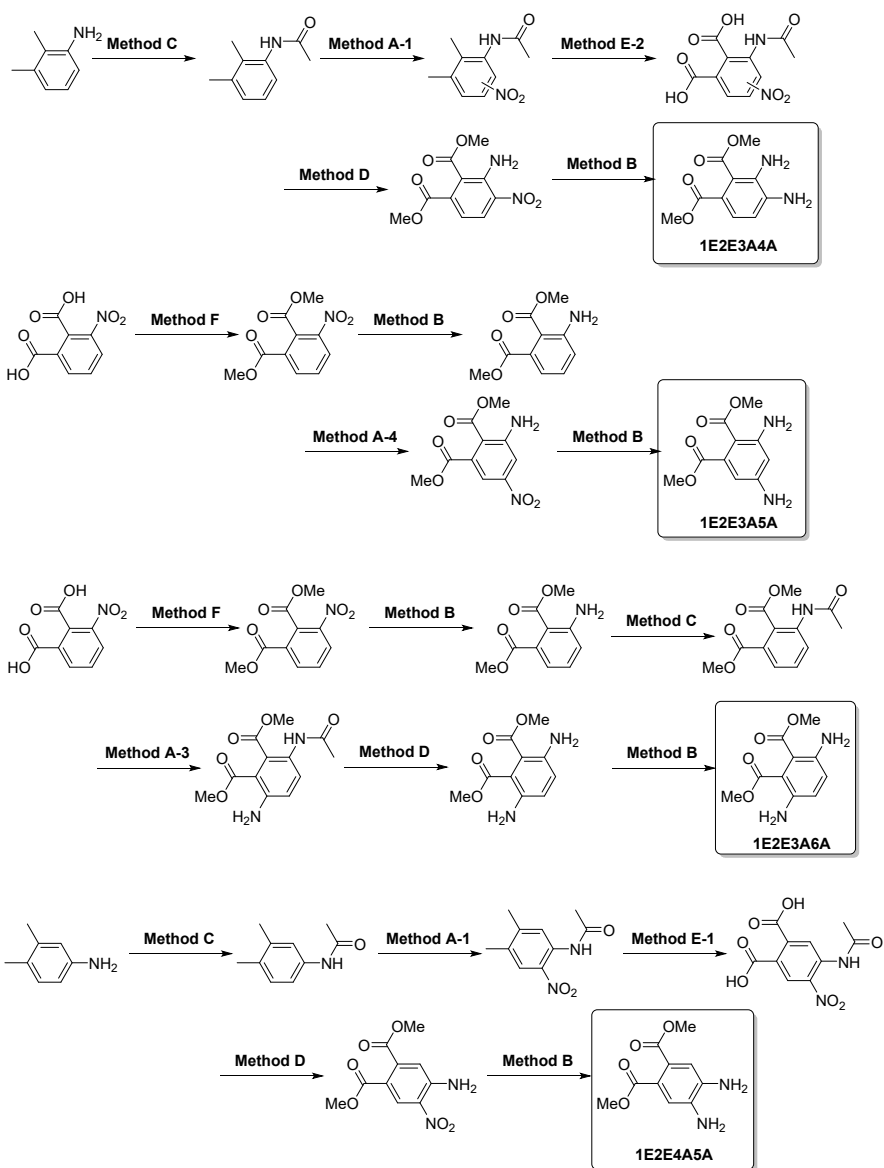
All calculations were conducted using the Gaussian 09 package.^{S15} Ground state calculation DFT/cam-B3LYP, 6-31g(d) level of theory and excited state calculations doing TD-DFT/cam-B3LYP, 6-31g(d) level of theory. The cam-B3LYP functional was used to achieve improved accuracy for molecules exhibiting electronic transitions with charge-transfer characteristics.^{S16}



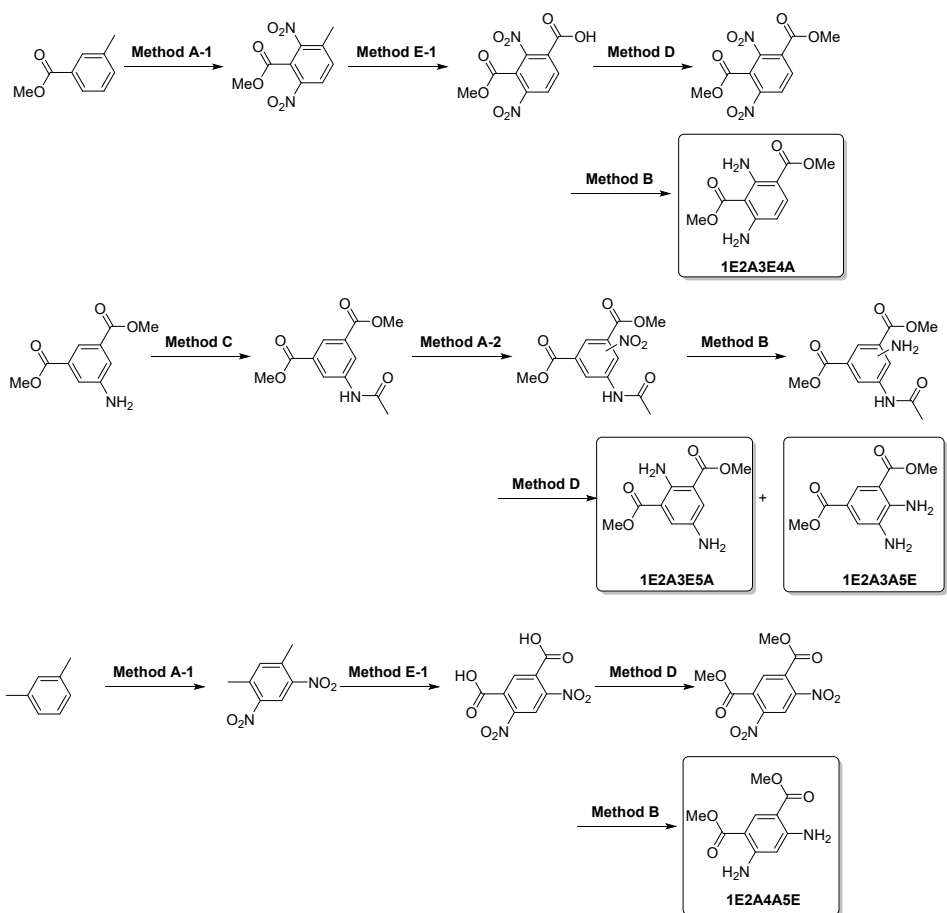
Scheme S1. Synthetic scheme for **1E2A3A**, **1E2A4A**, **1E2A5A**, **1E2A4A**, **1E2A6A**, and **1E3A5A**.



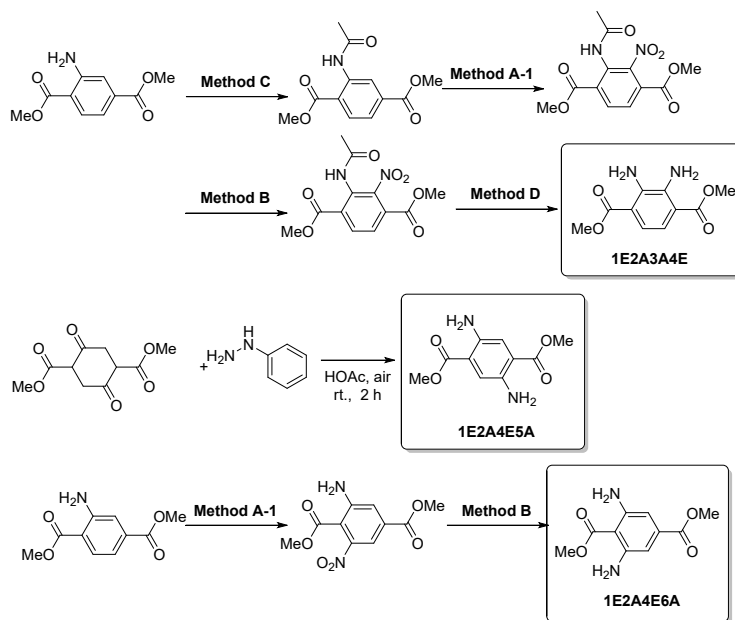
Scheme S2. Synthetic scheme for **1E2E3A**, **1E2E4A**, **1E2A3E**, and **1E2A5E**.



Scheme S3. Synthetic scheme for **1E2E3A4A**, **1E2E3A5A**, **1E2E3A6A**, and **1E2E4A5A**.



Scheme S4. Synthetic scheme for **1E2A3E4A**, **1E2A3E5A**, **1E2A3A5E**, and **1E2A4A5E**.



Scheme S5. Synthetic scheme for **1E2A3A4E**, **1E2A4E5A** and **1E2A4E6A**.

Table S1 Photophysical data of mono-amino & mono-ester and di-amino & mono-ester SBBFs in toluene, THF and MeCN.

Compound	Solvent	λ_{abs} [nm] ($\epsilon \times 10^{-3} \text{ M}^{-1} \text{ cm}^{-1}$)	λ_{ex} [nm]	λ_{em} [nm]	Stokes shift [cm^{-1}]	ϕ_{PL} [%] ^a	τ [ns] ^b	K_r [$\times 10^7 \text{ s}^{-1}$]	K_{nr} [$\times 10^8 \text{ s}^{-1}$]
Mono-amino & mono-ester									
1E2A	Tol	336 (6.91)	335	388	4078	48	6.29	7.65	0.82
	THF	339 (8.75)	337	392	4163	59	7.20	8.16	0.57
	MeCN	335 (5.45)	334	395	4624	60	7.26	8.22	0.55
1E3A	Tol	321 (6.32)	321	373	4343	31	0.54	57.54	12.76
	THF	322 (5.06)	326	390	5034	51	9.90	5.19	0.49
	MeCN	323 (3.99)	322	395	5739	42	12.22	3.41	0.48
1E4A	Tol	286 (50.21)	294	322	2958	62	0.65	95.55	5.83
	THF	288 (28.32)	285	328	4600	N.A.	0.63	N.A.	N.A.
	MeCN	285 (24.40)	283	329	4941	N.A.	3.45	N.A.	N.A.
Di-amino & mono-ester									
1E2A3A	Tol	346 (6.82)	344	429	5760	55	8.18	6.70	0.55
	THF	352 (6.89)	352	442	5785	47	9.43	4.93	0.57
	MeCN	348 (6.22)	348	450	6513	33	8.00	4.08	0.84
1E2A4A	Tol	322 (6.07)	321	367	3905	19	0.62	29.89	13.14
	THF	321 (10.01)	322	369	3956	14	0.63	21.49	13.72
	MeCN	320 (9.72)	321	372	4271	16	0.67	23.19	12.61
1E2A5A	Tol	375 (2.58)	376	465	5090	47	9.51	4.97	0.55
	THF	386 (5.66)	385	480	5141	43	11.14	3.87	0.51
	MeCN	379 (5.25)	379	483	5681	54	10.26	5.28	0.45
1E2A6A	Tol	358 (12.59)	356	414	3935	42	7.07	6.00	0.81
	THF	371 (3.30)	365	427	3978	32	6.89	4.61	0.99
	MeCN	368 (2.68)	370	445	4555	6	11.97	0.51	0.78
1E3A4A	Tol	308 (18.19)	313	368	4775	28	0.62	44.71	11.66
	THF	308 (18.19)	319	383	5238	50	0.57	88.35	8.71
	MeCN	316 (9.40)	317	390	5905	53	0.40	131.38	11.86
1E3A5A	Tol	336 (2.99)	336	390	4121	11	2.94	3.60	3.04
	THF	343 (5.03)	343	404	4402	12	3.73	3.13	2.37
	MeCN	341 (4.65)	340	411	5081	19	4.06	4.74	1.99

^a Absolute photoluminescence quantum yield (PLQY). ^b Emission lifetime.

Table S2 Photophysical data of mono-amino & di-ester SBBFs in toluene, THF and MeCN.

Compound	Solvent	λ_{abs} [nm] ($\epsilon \times 10^{-3} \text{ M}^{-1} \text{ cm}^{-1}$)	λ_{ex} [nm]	λ_{em} [nm]	Stokes shift [cm^{-1}]	ϕ_{PL} [%] ^a	T [ns] ^b	K_r [$\times 10^7 \text{ s}^{-1}$]	K_{nr} [$\times 10^8 \text{ s}^{-1}$]
Mono-amino & di-ester									
1E2E3A	Tol	340 (4.66)	339	426	6024	39	7.63	5.16	0.79
	THF	343 (5.71)	341	435	6337	53	9.54	5.54	0.49
	MeCN	341 (6.14)	337	435	6685	66	9.40	6.98	0.37
1E2E4A	Tol	285 (15.33)	300	400	8333	66	0.74	88.69	4.64
	THF	283 (19.63)	283	412	11064	N.A.	3.34	N.A.	N.A.
	MeCN	282 (19.63)	279	417	11861	N.A.	0.63	N.A.	N.A.
1E2A3E	Tol	373 (10.36)	366	407	2752	53	6.08	8.65	0.78
	THF	369 (9.02)	364	405	2781	34	6.26	5.41	1.06
	MeCN	363 (7.09)	362	406	2994	50	6.27	7.94	0.80
1E2A5E	Tol	331 (5.88)	329	378	3940	32	0.58	55.69	11.67
	THF	332 (7.50)	333	383	3920	28	0.43	66.21	16.63
	MeCN	331 (6.19)	330	383	4193	23	0.47	48.13	16.46
1E3E5A	Tol	337 (6.54)	337	384	3632	9	2.33	3.69	3.92
	THF	337 (3.87)	346	402	4026	13	3.69	3.44	2.37
	MeCN	340 (7.38)	340	401	4474	14	3.59	3.97	2.39
1E2A4E	Tol	366 (7.00)	363	420	3739	64	10.19	6.29	0.35
	THF	371 (6.36)	368	425	3645	50	11.33	4.38	0.44
	MeCN	365 (6.91)	363	428	4184	58	14.58	3.98	0.29

^a Absolute photoluminescence quantum yield (PLQY). ^b Emission lifetime.

Table S3 Photophysical data of di-amino & di-ester SBBFs in toluene, THF and MeCN.

Compound	Solvent	λ_{abs} [nm] ($\epsilon \times 10^{-3} \text{ M}^{-1} \text{ cm}^{-1}$)	λ_{ex} [nm]	λ_{em} [nm]	Stokes shift [cm^{-1}]	ϕ_{PL} [%] ^a	τ [ns] ^b	K_{f} [$\times 10^7 \text{ s}^{-1}$]	K_{nr} [$\times 10^8 \text{ s}^{-1}$]
Di-amino & di-ester									
1E2E3A4A	Tol	324 (14.06)	332	452	7997	23	4.43	5.29	1.73
	THF	333 (8.37)	338	457	7704	31	4.75	6.50	1.45
	MeCN	329 (13.18)	331	461	8520	21	4.16	4.94	1.91
1E2E3A5A	Tol	329 (9.11)	331	429	6901	6	0.86	7.38	10.89
	THF	330 (6.55)	332	439	7341	4	0.85	4.78	11.29
	MeCN	330 (8.54)	340	440	6684	1	0.82	1.52	12.04
1E2E3A6A	Tol	391 (4.31)	392	498	5430	39	8.50	4.58	0.72
	THF	398 (7.42)	400	503	5119	38	9.04	4.22	0.68
	MeCN	391 (6.73)	391	499	5535	34	9.02	3.79	0.73
1E2E4A5A	Tol	310 (10.3)	308	396	7215	34	0.48	70.00	13.88
	THF	291 (14.26)	316	422	7949	28	0.59	46.78	12.27
	MeCN	316 (9.85)	316	436	8710	28	3.57	7.92	2.01
1E2A3E4A	Tol	360 (7.08)	360	390	2137	7	2.83	2.60	3.27
	THF	358 (9.24)	357	389	2304	24	2.74	8.92	2.76
	MeCN	356 (8.62)	354	394	2868	25	3.31	7.51	2.27
1E2A3E5A	Tol	423 (7.25)	422	494	3454	45	9.67	4.63	0.57
	THF	428 (8.13)	428	511	3795	65	11.09	5.84	0.32
	MeCN	420 (8.41)	422	510	4089	52	10.45	5.00	0.46
1E2A3A5E	Tol	344 (5.63)	344	418	5146	24	3.59	6.81	2.11
	THF	351 (10.18)	350	431	5370	21	3.78	5.65	2.08
	MeCN	347 (7.90)	347	436	5883	17	13.05	1.28	0.64
1E2A4A5E	Tol	331 (14.74)	331	357	2200	0.4	0.52	0.85	19.15
	THF	333 (7.96)	331	362	2587	0.8	0.53	1.45	18.72
	MeCN	331 (6.19)	329	365	2998	1	3.54	0.31	2.79
1E2A3A4E	Tol	391 (4.62)	389	471	4476	67	10.03	6.64	0.33
	THF	399 (6.33)	400	476	3992	63	11.04	5.75	0.33
	MeCN	392 (7.33)	391	478	4655	47	10.77	4.38	0.49
1E2A4E5A	Tol	443 (3.91)	443	539	4020	53	11.36	4.70	0.41
	THF	451 (6.64)	447	553	4288	47	11.26	4.16	0.47
	MeCN	440 (6.01)	440	553	4644	32	10.95	2.94	0.62
1E2A4E6A	Tol	394 (5.55)	394	450	3158	39	9.57	4.05	0.64
	THF	392 (4.82)	396	453	3177	35	8.12	4.33	0.80
	MeCN	387 (5.65)	391	455	3597	19	0.38	50.21	21.29

^a Absolute photoluminescence quantum yield (PLQY). ^b Emission lifetime.

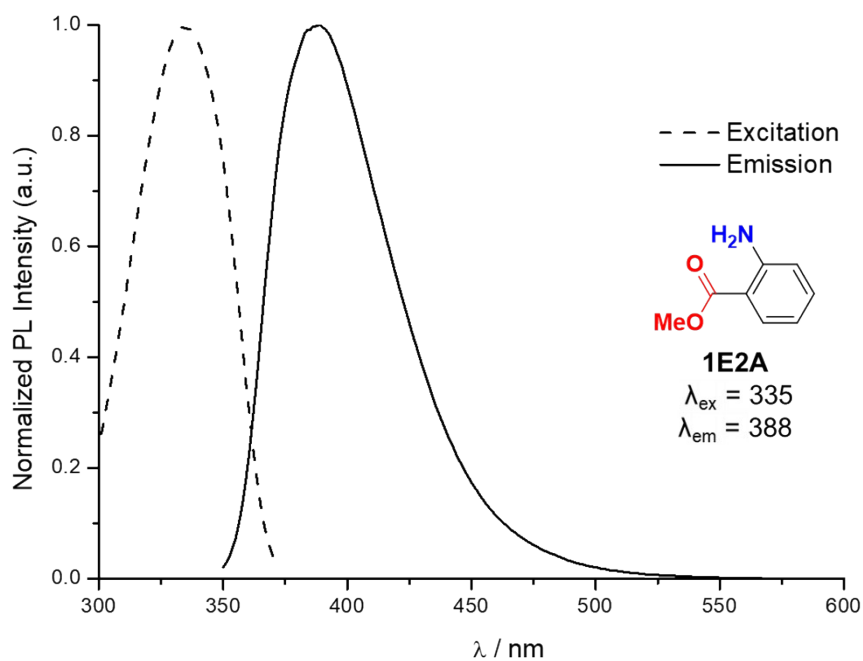


Fig. S1 Emission and excitation spectra of **1E2A** in toluene.

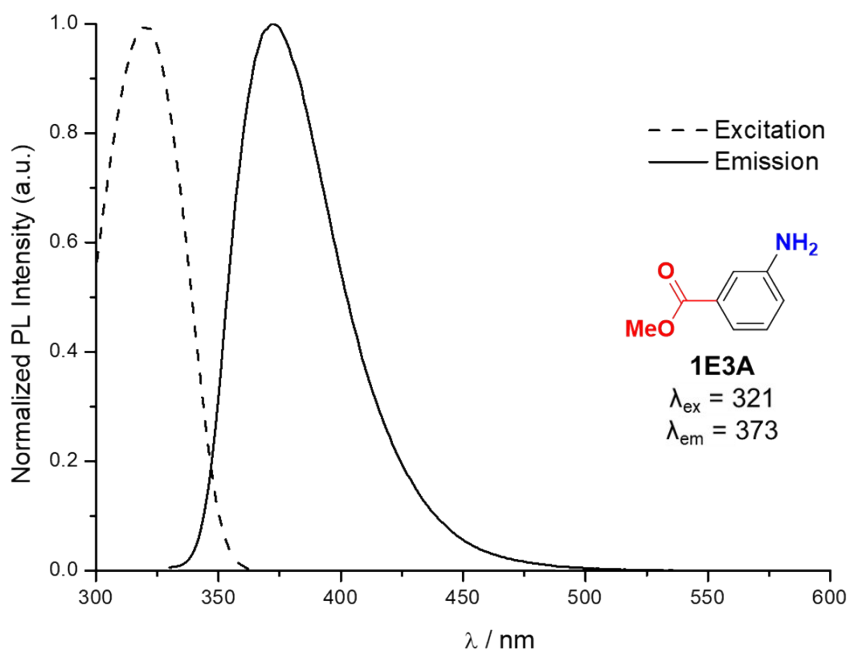


Fig. S2 Emission and excitation spectra of **1E3A** in toluene.

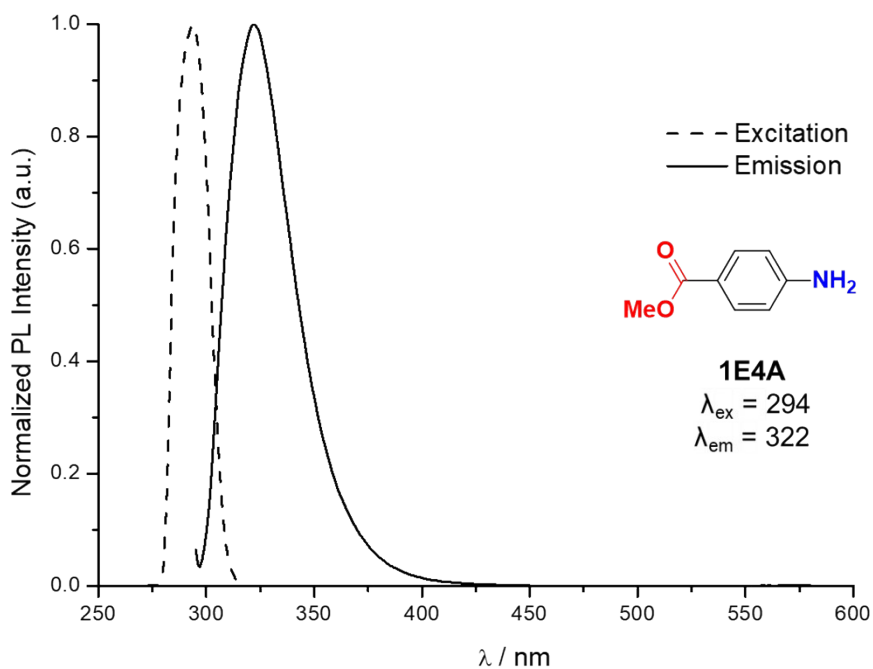


Fig. S3 Emission and excitation spectra of **1E4A** in toluene.

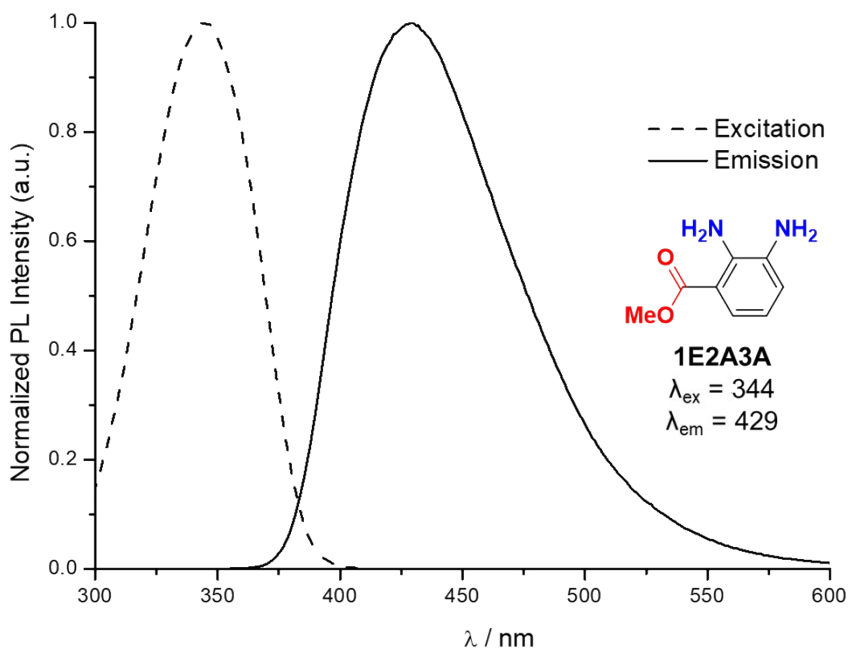


Fig. S4 Emission and excitation spectra of **1E2A3A** in toluene.

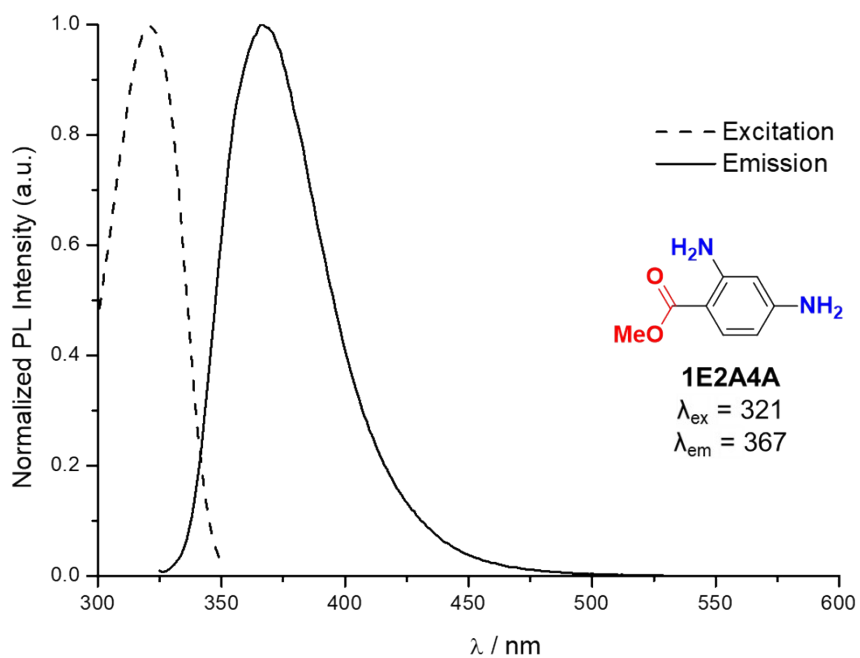


Fig. S5 Emission and excitation spectra of **1E2A4A** in toluene.

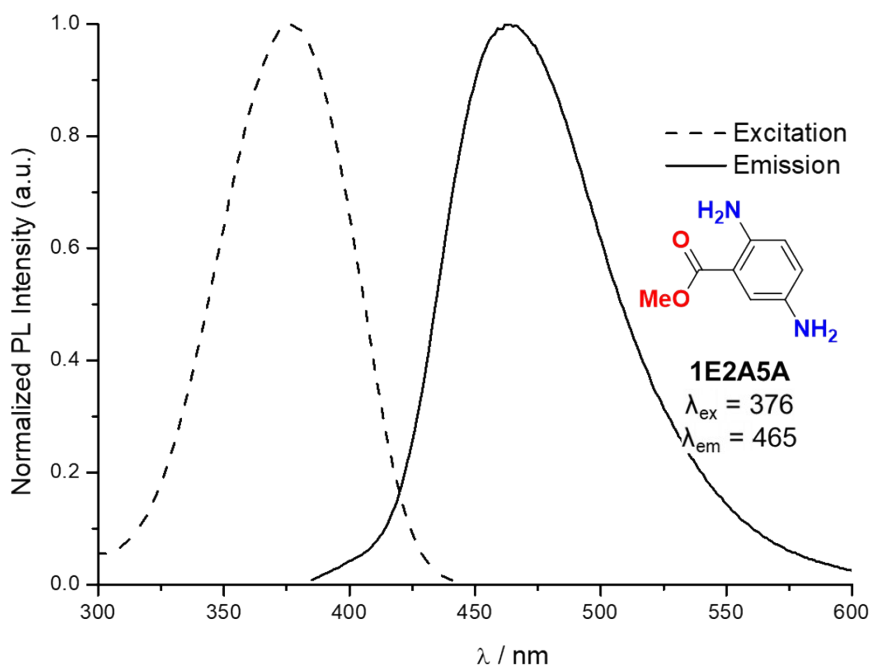


Fig. S6 Emission and excitation spectra of **1E2A5A** in toluene.

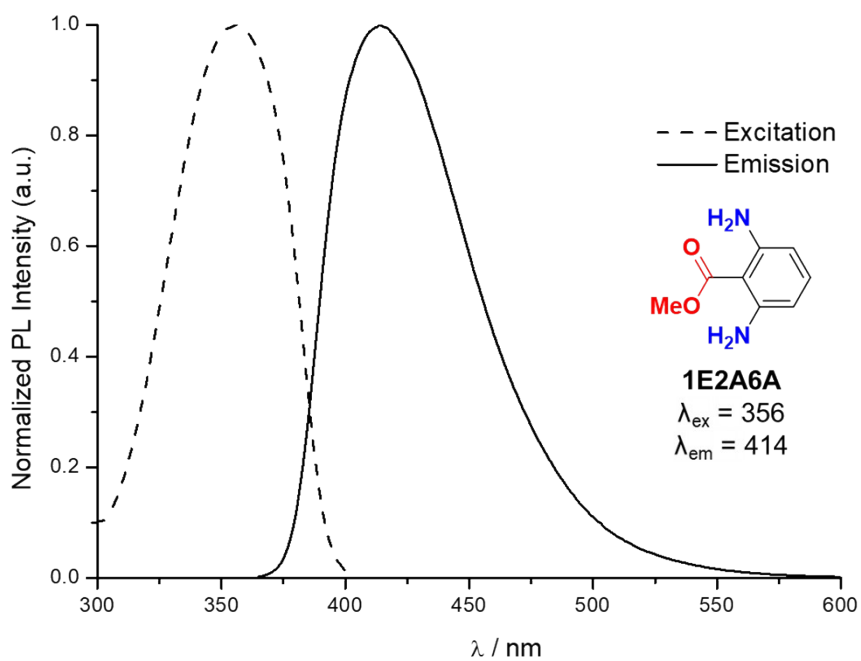


Fig. S7 Emission and excitation spectra of **1E2A6A** in toluene.

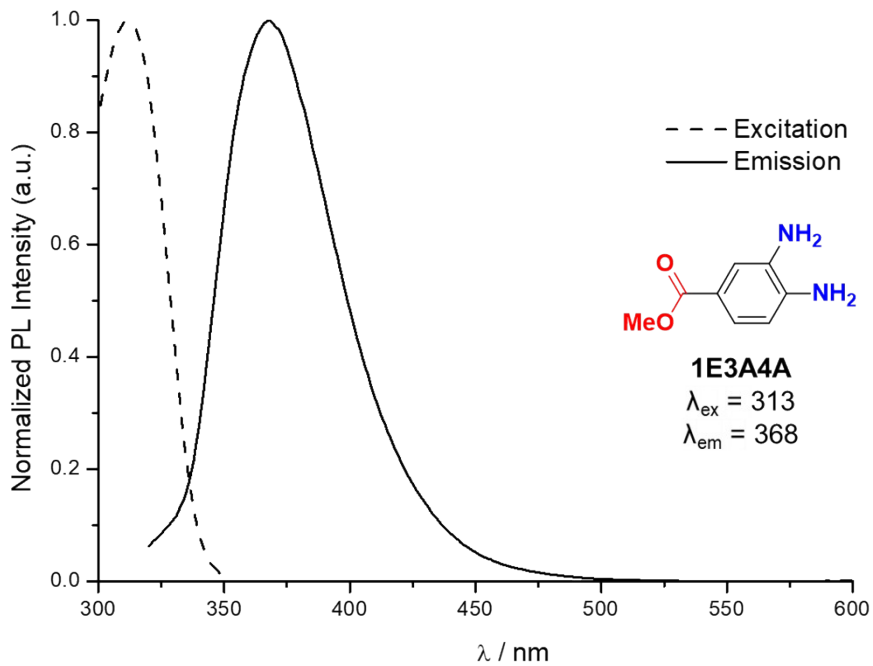


Fig. S8 Emission and excitation spectra of **1E3A4A** in toluene.

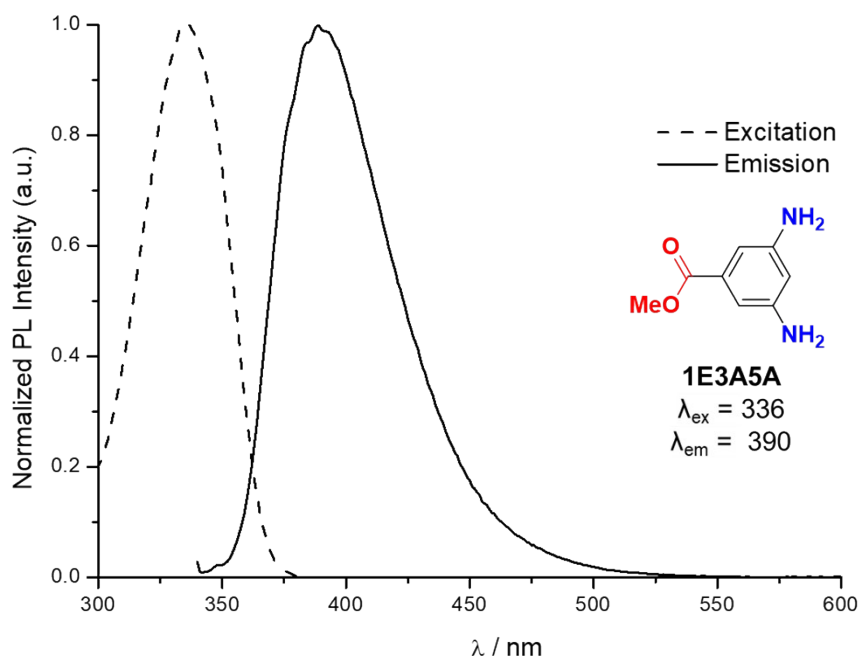


Fig. S9 Emission and excitation spectra of **1E3A5A** in toluene.

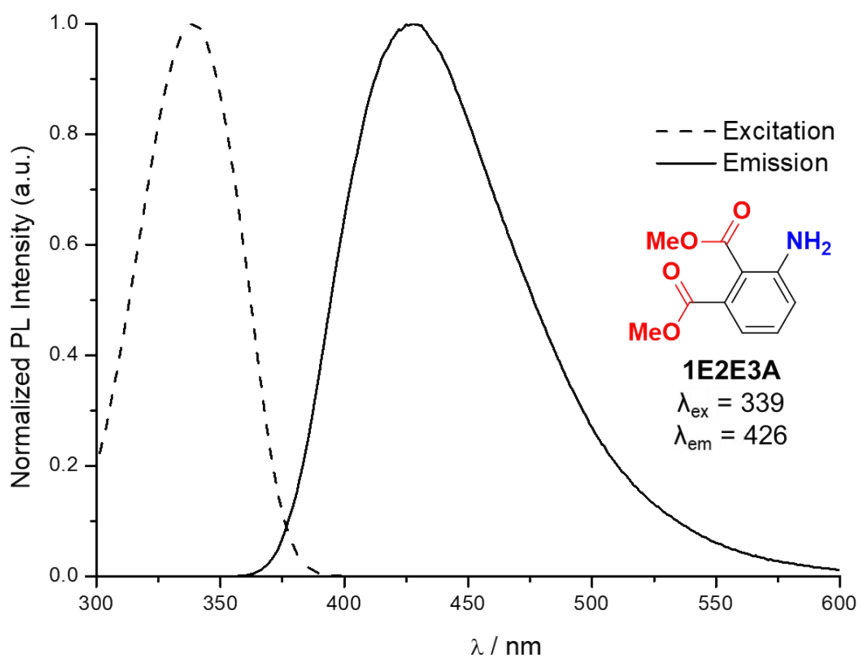


Fig. S10 Emission and excitation spectra of **1E2E3A** in toluene.

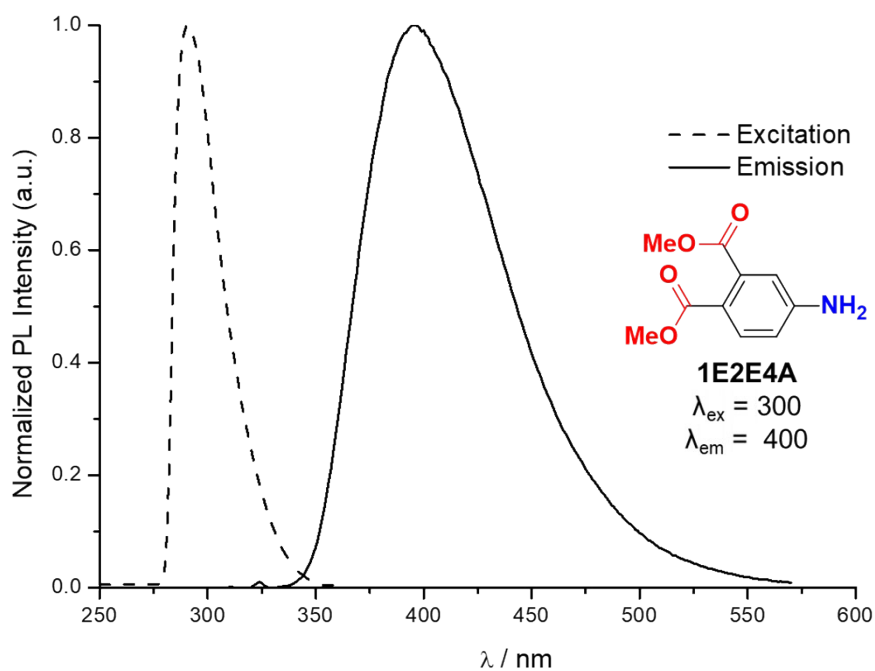


Fig. S11 Emission and excitation spectra of **1E2E4A** in toluene.

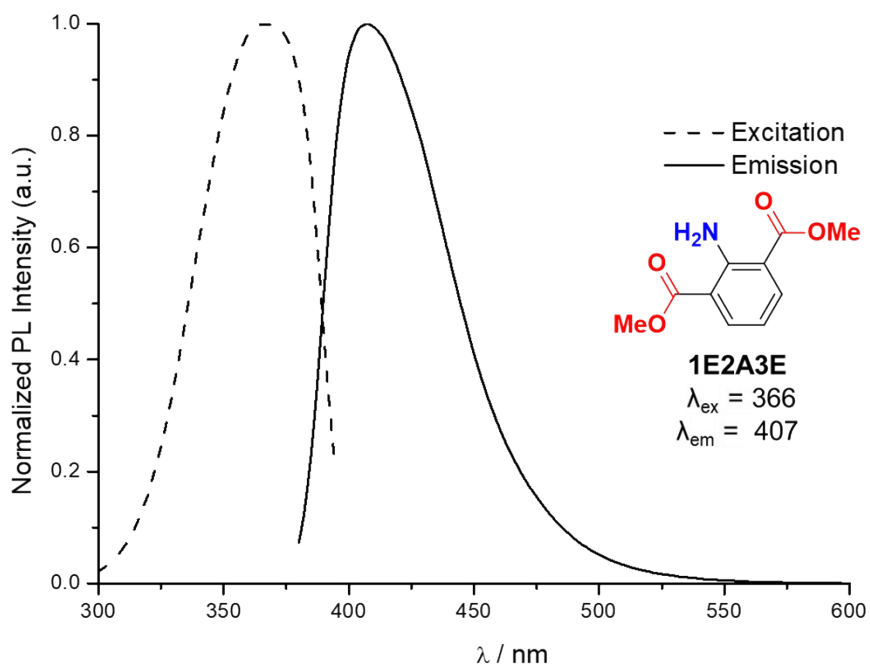


Fig. S12 Emission and excitation spectra of **1E2A3E** in toluene.

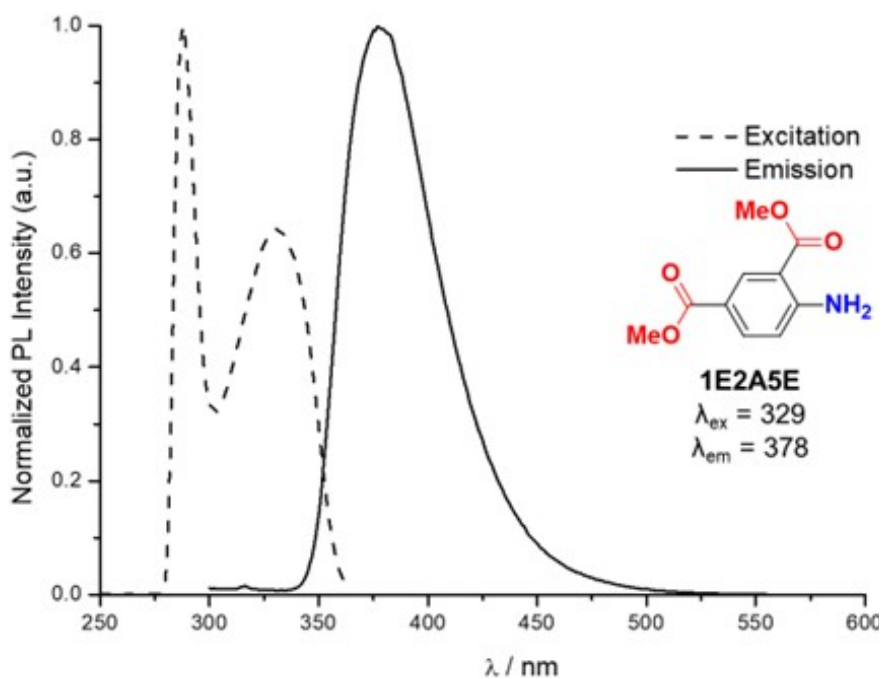


Fig. S13 Emission and excitation spectra of **1E2A5E** in toluene.

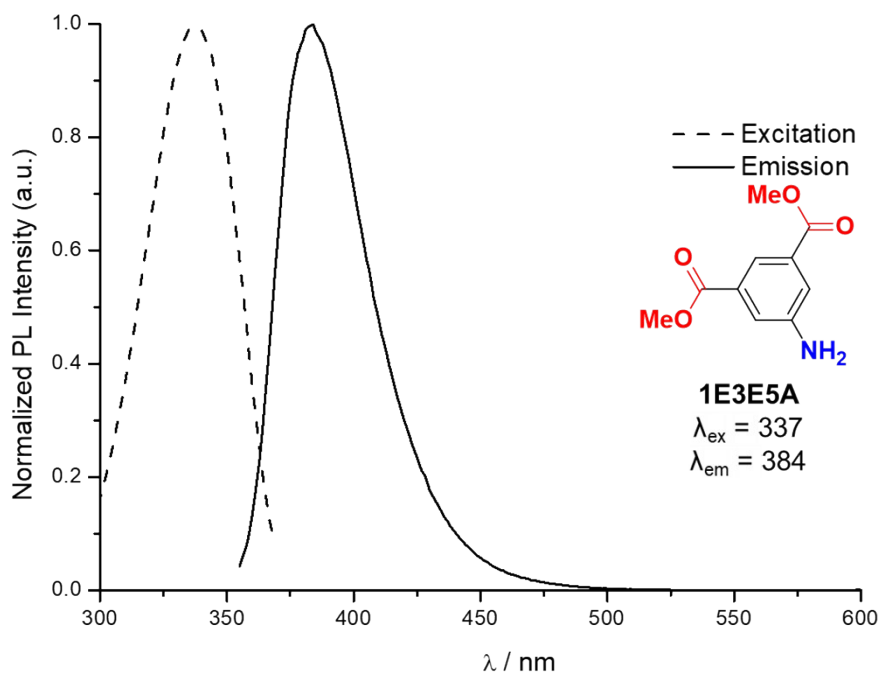


Fig. S14 Emission and excitation spectra of **1E3E5A** in toluene.

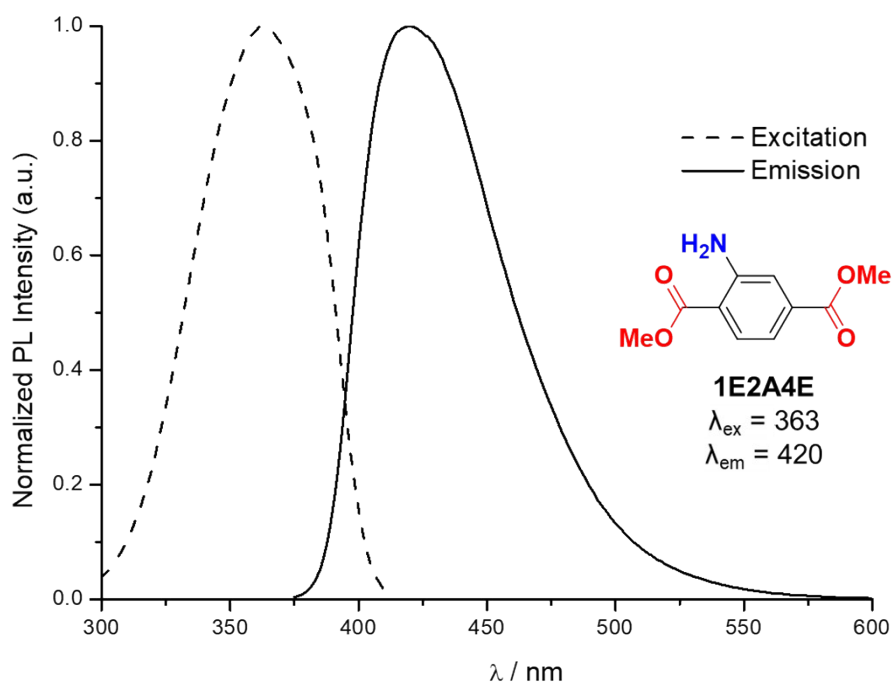


Fig. S15 Emission and excitation spectra of **1E2A4E** in toluene.

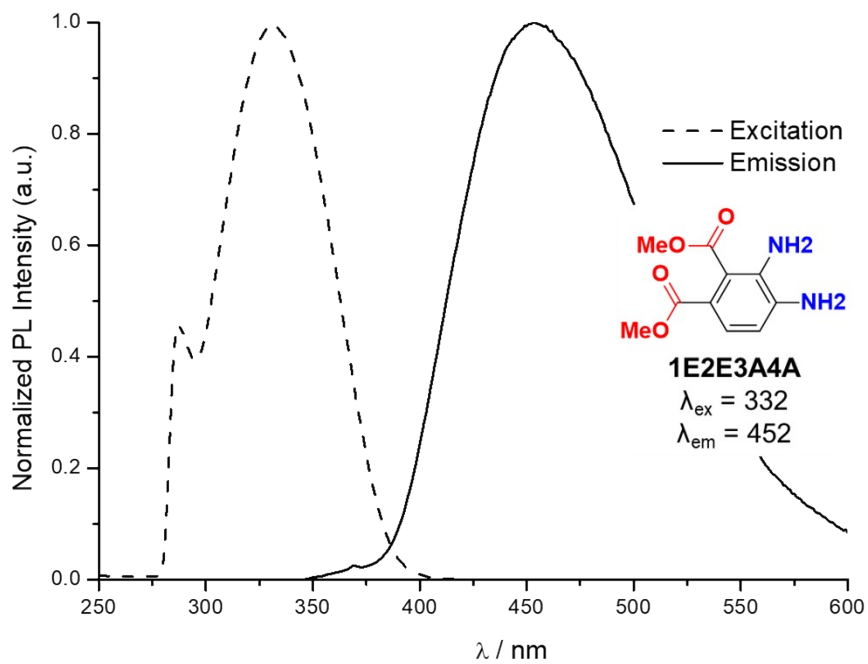


Fig. S16 Emission and excitation spectra of **1E2E3A4A** in toluene.

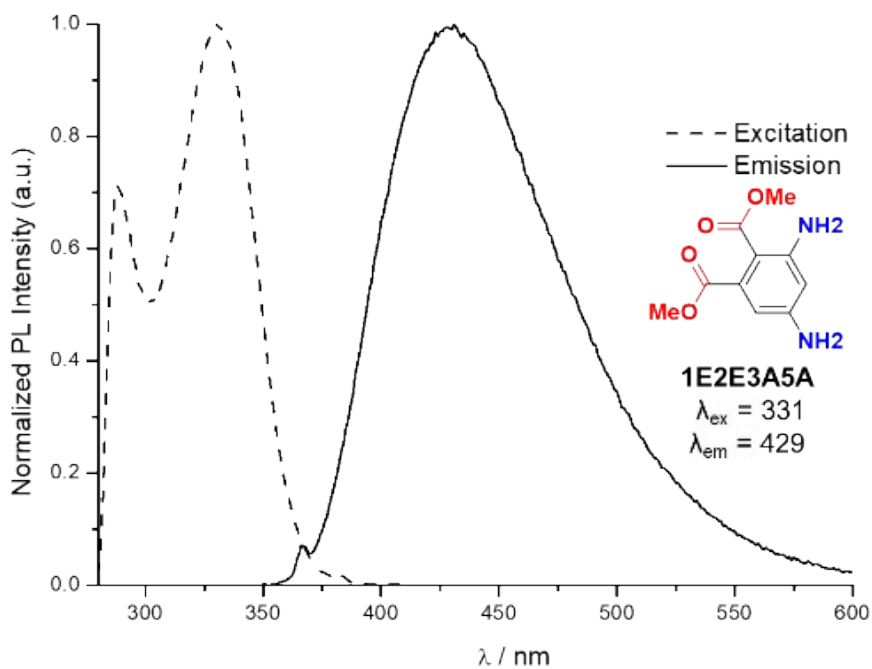


Fig. S17 Emission and excitation spectra of **1E2E3A5A** in toluene.

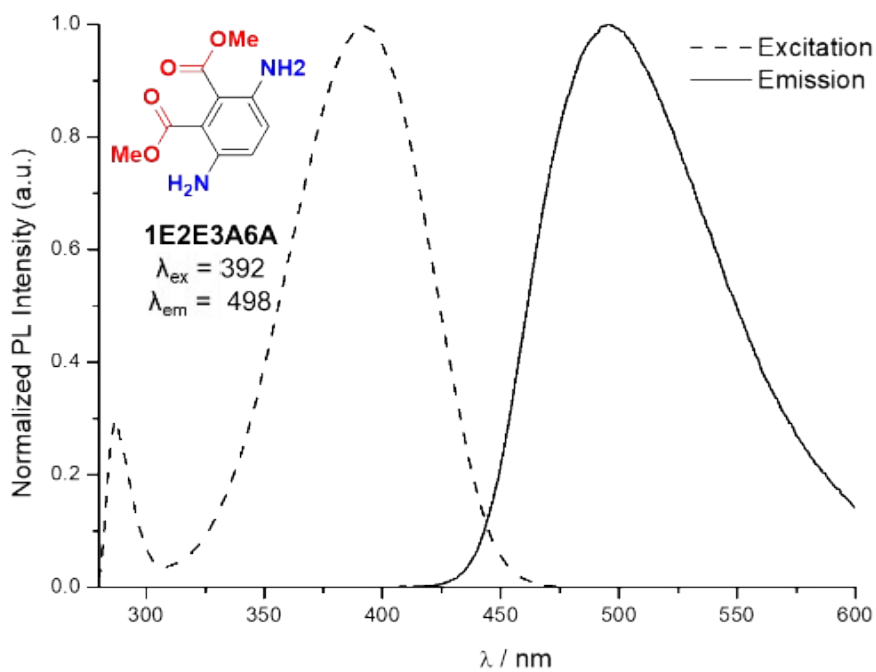


Fig. S18 Emission and excitation spectra of **1E2E3A6A** in toluene.

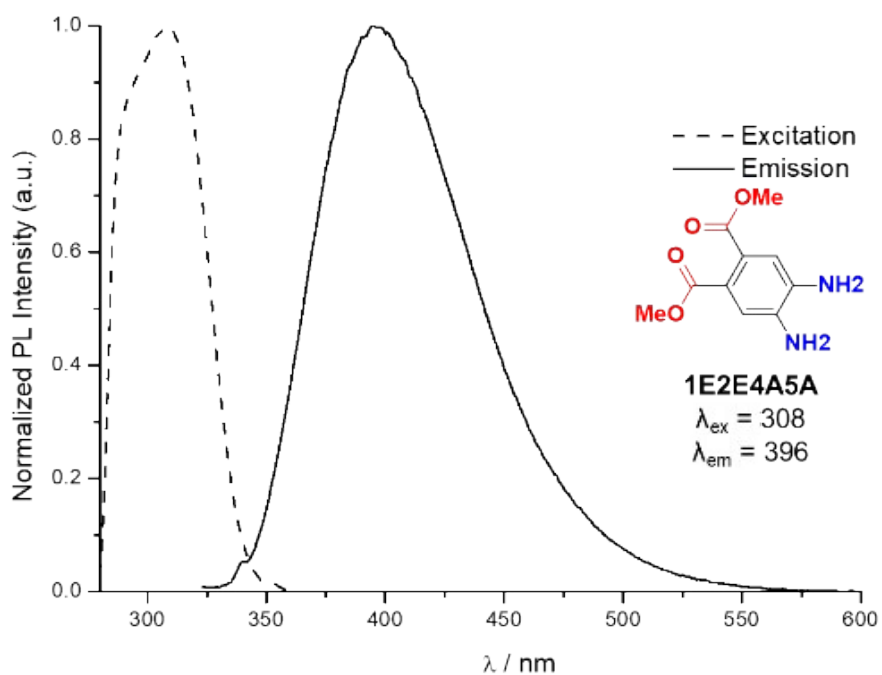


Fig. S19 Emission and excitation spectra of **1E2E4A5A** in toluene.

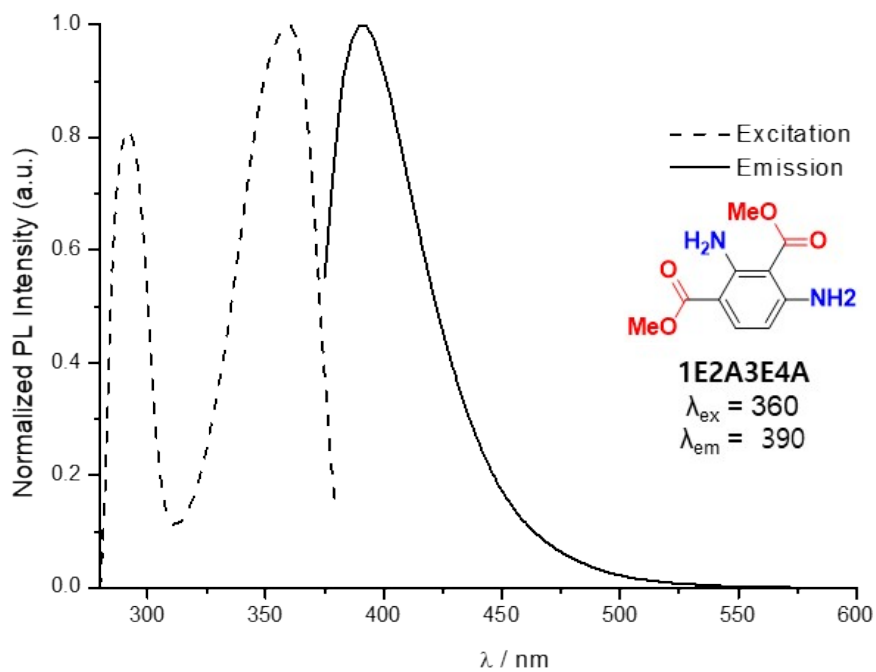


Fig. S20 Emission and excitation spectra of **1E2A3E4A** in toluene.

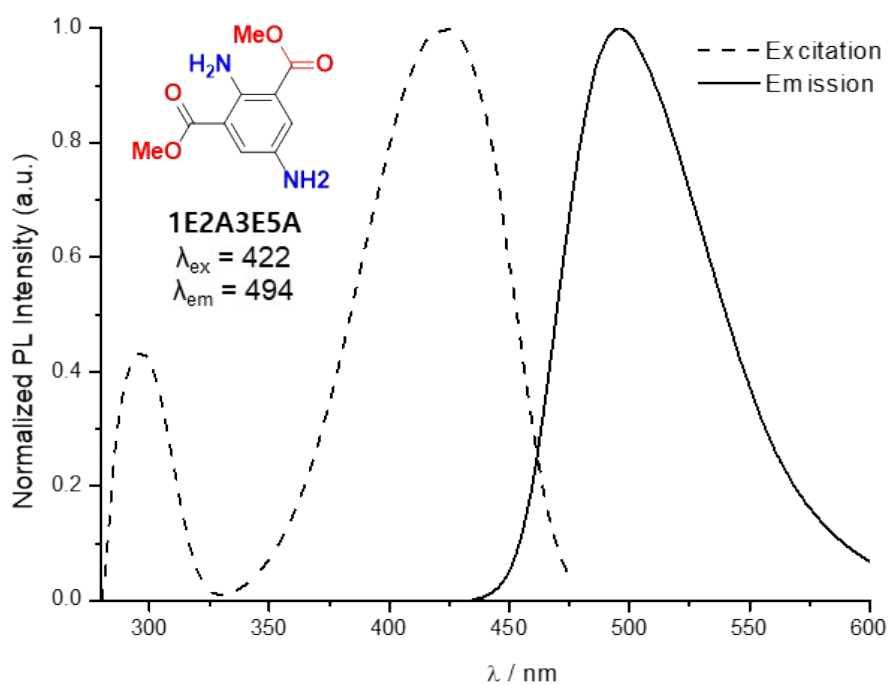


Fig. S21 Emission and excitation spectra of **1E2A3E5A** in toluene.

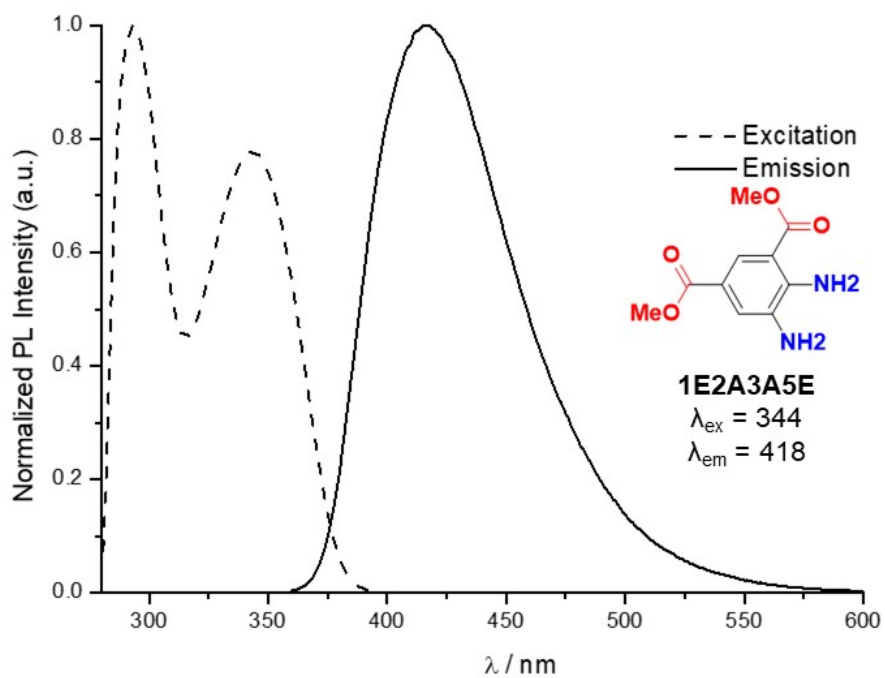


Fig. S22 Emission and excitation spectra of **1E2A3A5E** in toluene.

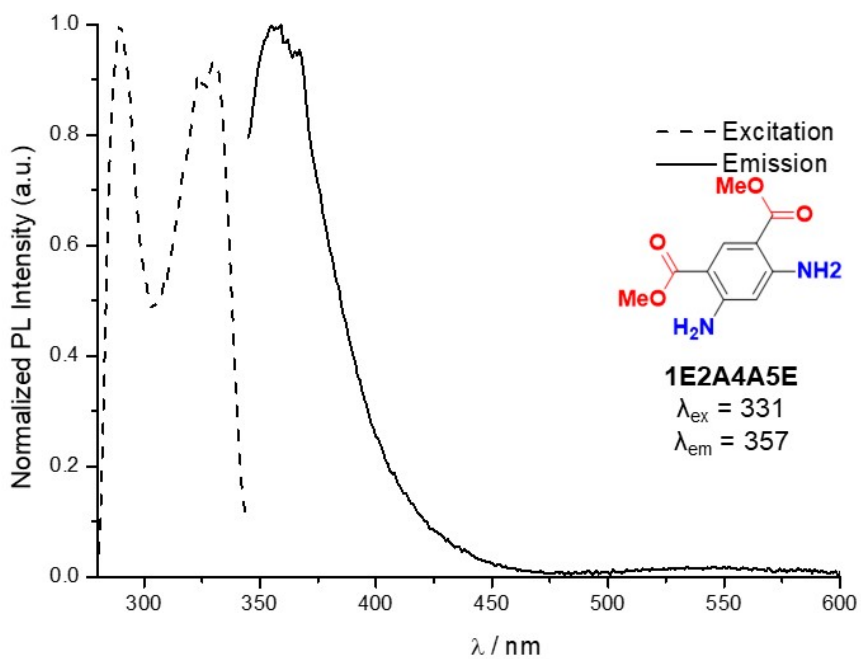


Fig. S23 Emission and excitation spectra of **1E2A4A5E** in toluene.

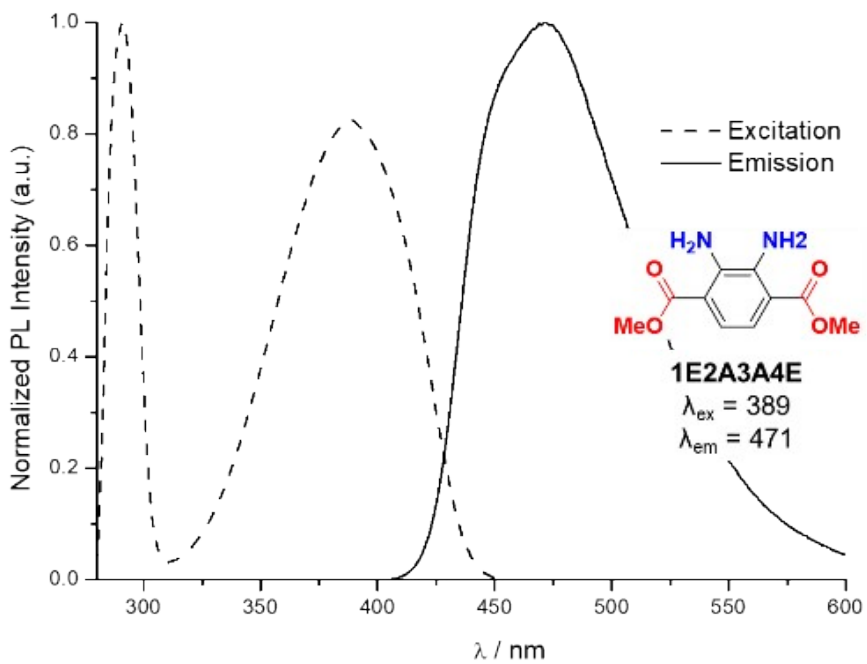


Fig. S24 Emission and excitation spectra of **1E2A3A4E** in toluene.

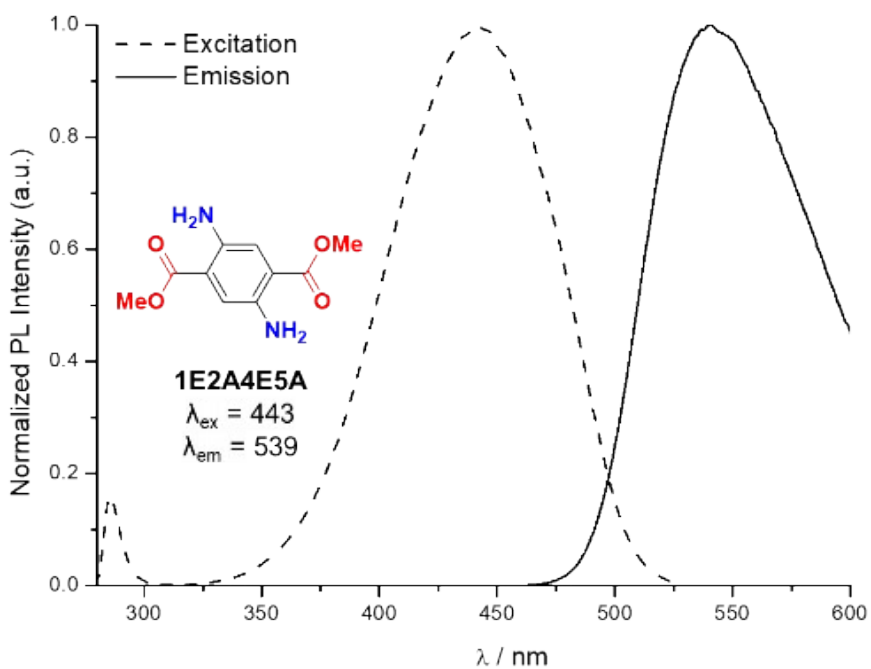


Fig. S25 Emission and excitation spectra of **1E2A4E5A** in toluene.

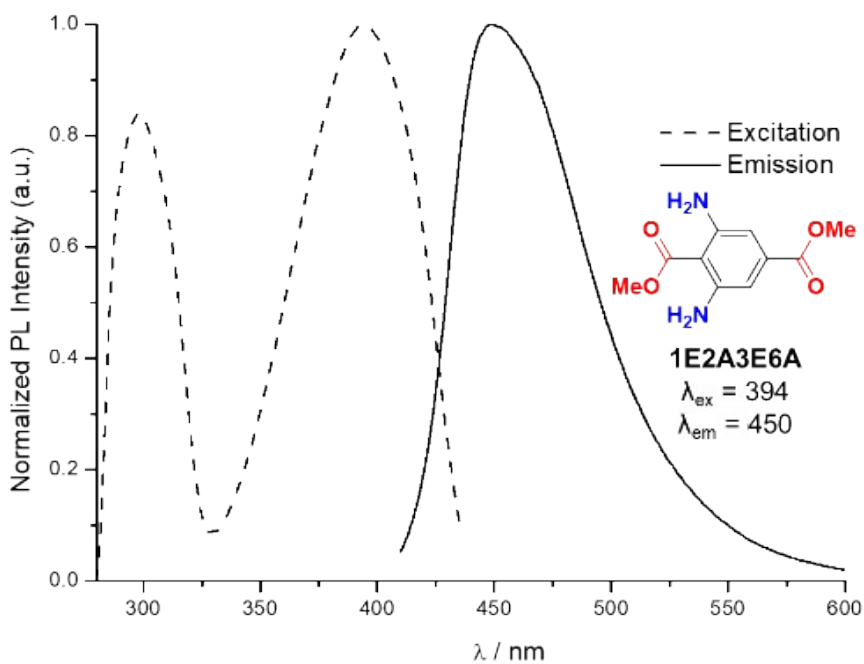


Fig. S26 Emission and excitation spectra of **1E2A4E6A** in toluene.

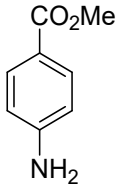
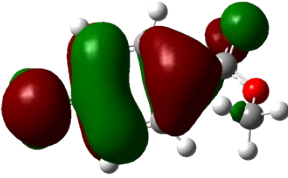
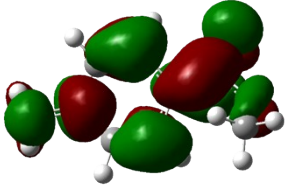
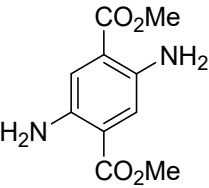
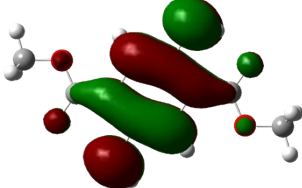
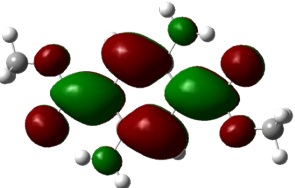
 1E4A	HOMO	LUMO
		
	-7.21 ev	0.51 ev
 1E2A4E5A	HOMO	LUMO
		
	-6.72 ev	-0.56 ev

Fig. S27 HOMOs and LUMOs for **1E4A** and **1E2A4E5A**.

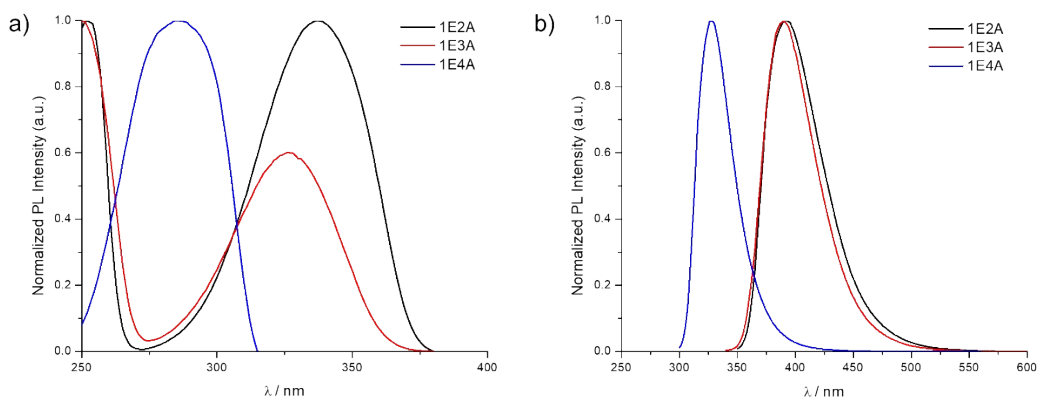


Fig. S28 a) Excitation and b) emission spectra of mono-amino & mono-ester series in THF.

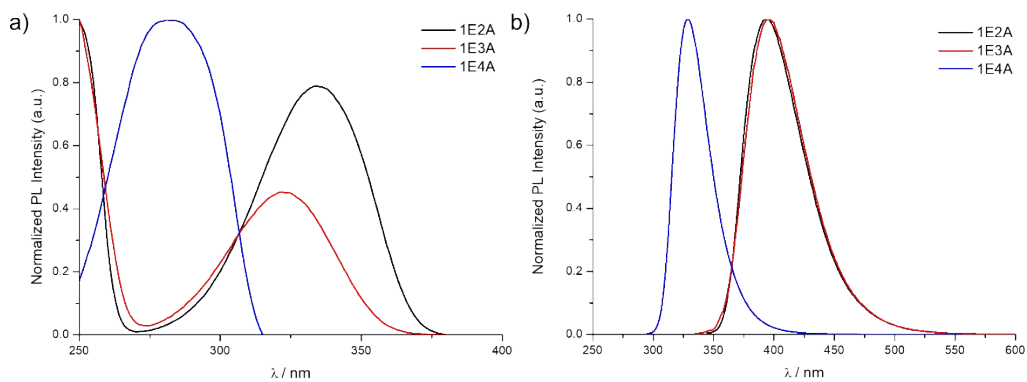


Fig. S29 a) Excitation and b) emission spectra of mono-amino & mono-ester series in MeCN.

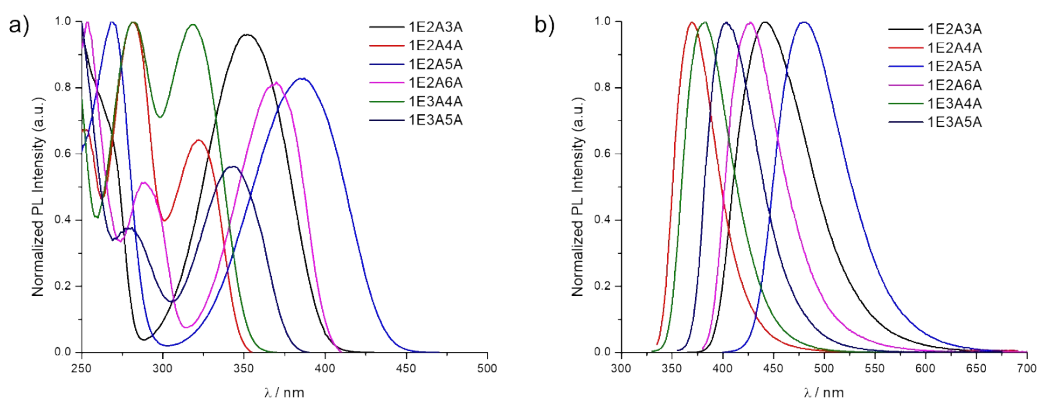


Fig. S30 a) Excitation and b) emission spectra of di-amino & mono-ester series in THF.

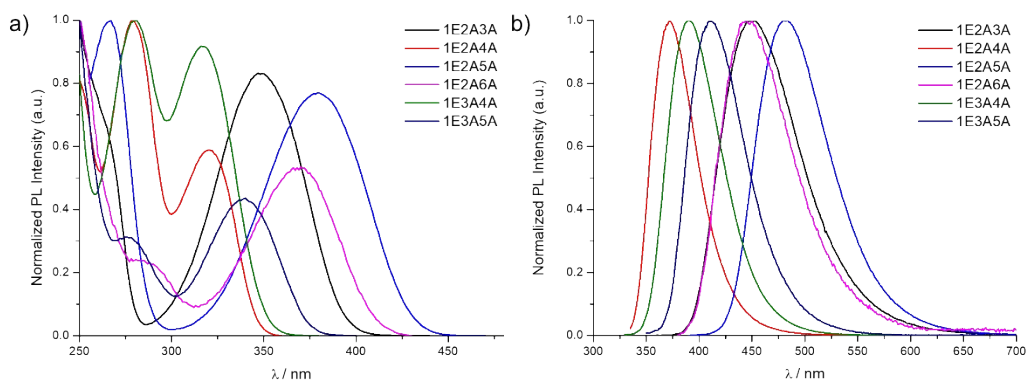


Fig. S31 a) Excitation and b) emission spectra of di-amino & mono-ester series in MeCN.

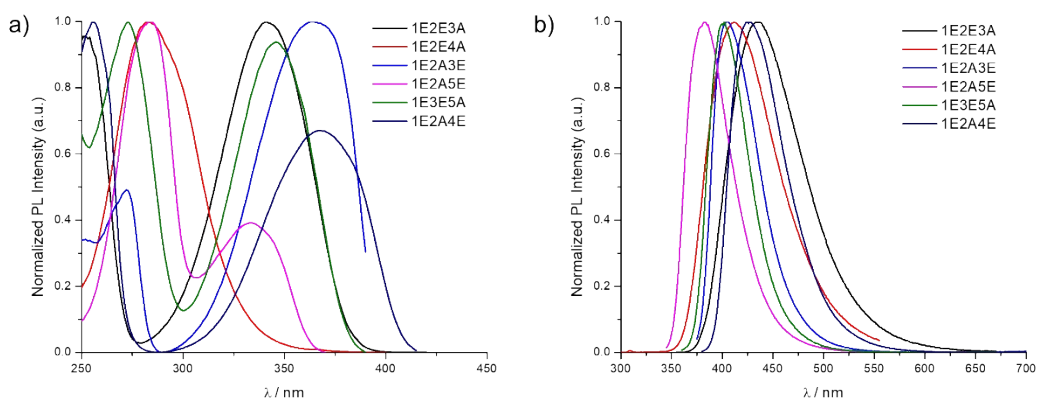


Fig. S32 a) Excitation and b) emission spectra of mono-amino & di-ester series in THF.

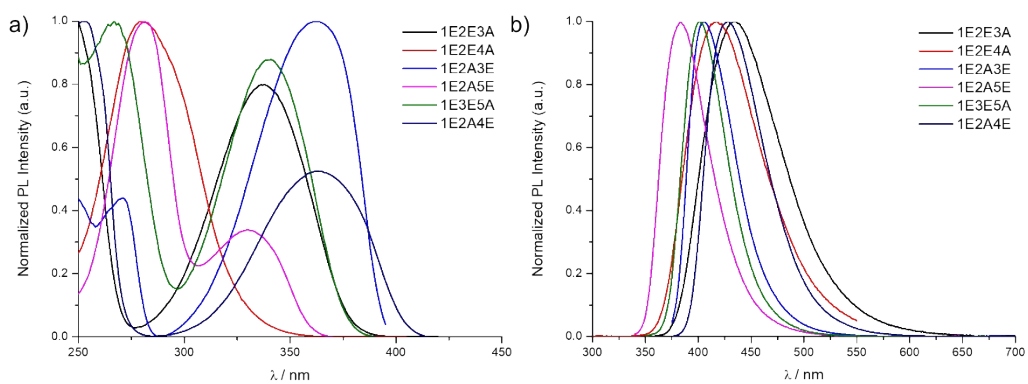


Fig. S33 a) Excitation and b) emission spectra of mono-amino & di-ester series in MeCN.

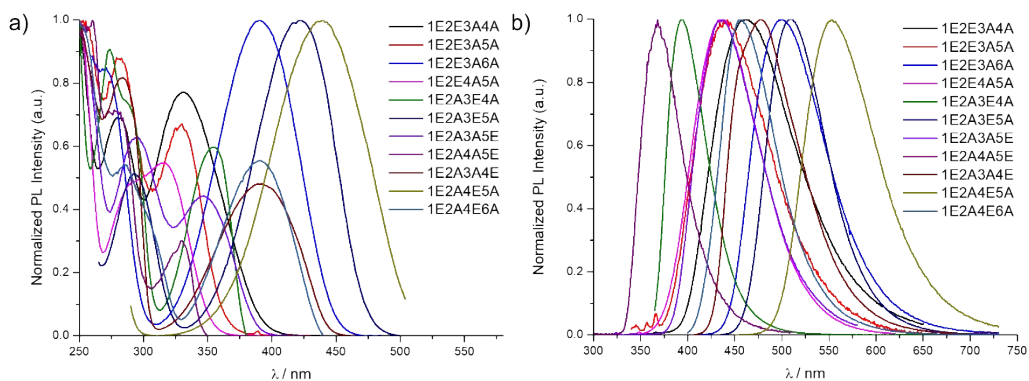


Fig. S34 a) Excitation and b) emission spectra of di-amino & di-ester series in THF.

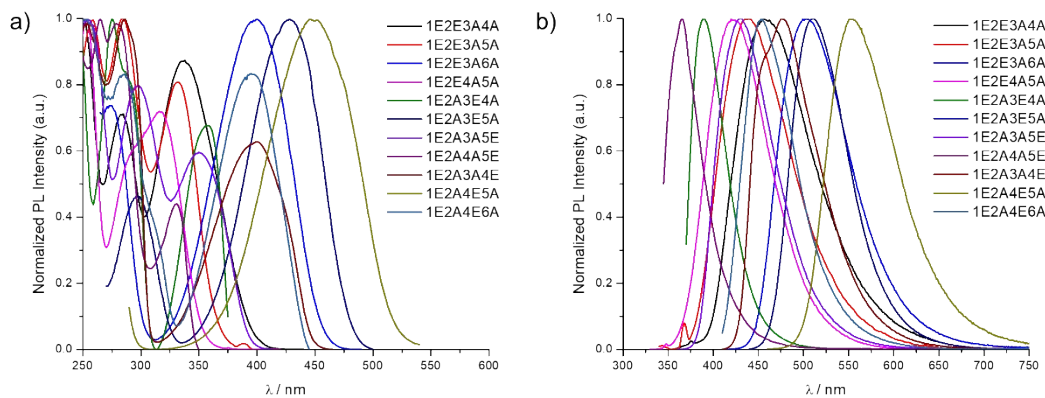


Fig. S35 a) Excitation and b) emission spectra of di-amino & di-ester series in MeCN.

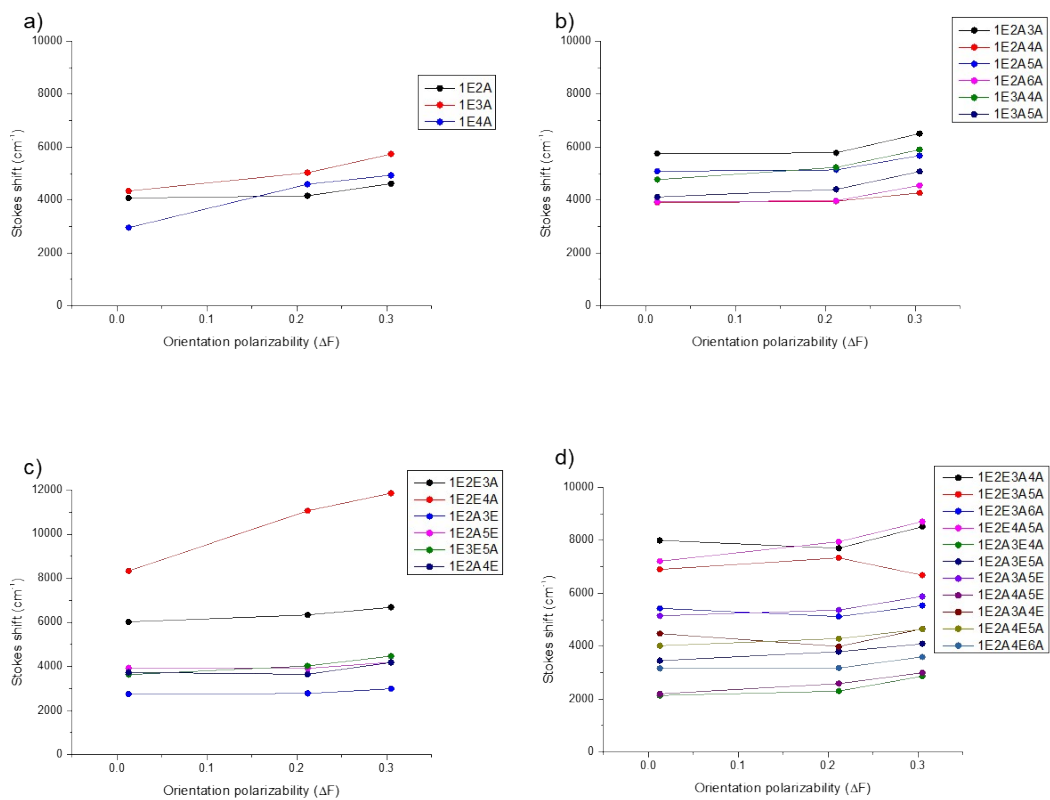


Fig. S36 Lippert–Mataga plot of (a) mono-ester mono-amino SBBF, (b) mono-ester di-amino SBBF, (c) di-ester mono-amino SBBF and (d) di-ester di-amino SBBF series.

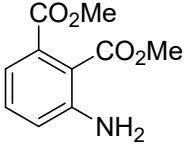
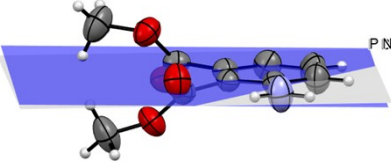
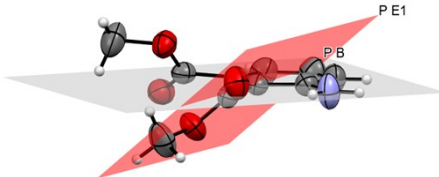
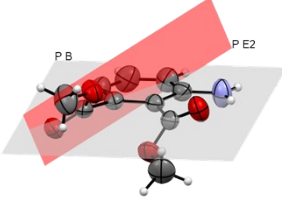
 <p>1E2E3A</p>	N	
	 <p>1.8°</p>	
E-1	E-2	
 <p>44.8°</p>	 <p>40.7°</p>	

Fig. S37 Angular distortions between benzene plane and functional groups (E-1: ester at C1; E-2: ester at C2; N: amine at C3) of **1E2E3A** from crystal structural analysis.^{S17}

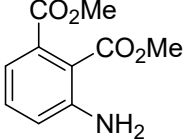
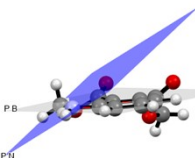
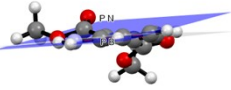
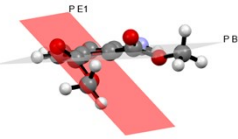
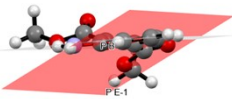
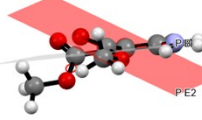
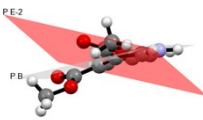
 <p>1E2E3A</p>	N		
	GS	ES	
 <p>31.5°</p>		 <p>8.8°</p>	
E-1		E-2	
GS	ES	GS	ES
 <p>49.6°</p>	 <p>22.8°</p>	 <p>31.1°</p>	 <p>31.2°</p>

Fig. S38 Planar angles between functional group and benzene plane based on DFT calculated structure in ground state and excited state of **1E2E3A**.

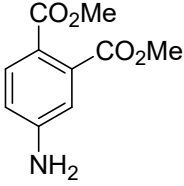
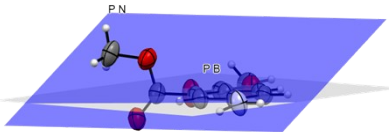
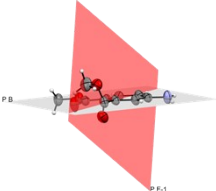
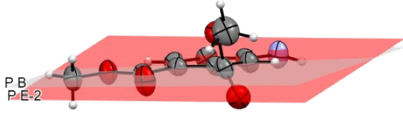
 <p>1E2E4A</p>	N	
	 <p>17.3°</p>	
E-1	E-2	
 <p>75.9°</p>	 <p>4.7°</p>	

Fig. S39 Angular distortions between benzene plane and functional groups (E-1: ester at C1; E-2: ester at C2; N: amine at C4) of **1E2E4A** from crystal structural analysis.

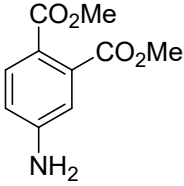
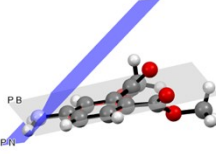
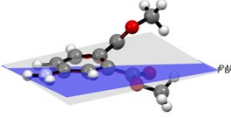
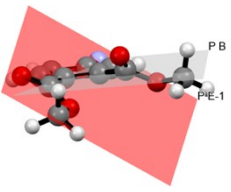
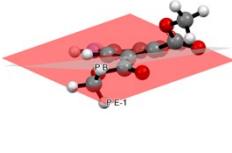
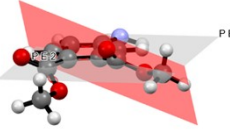
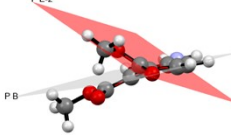
 <p>1E2E4A</p>	N			
	GS		ES	
	 <p>35.8°</p>		 <p>4.35°</p>	
E-1		E-2		
GS	ES	GS	ES	
 <p>37.2°</p>	 <p>16.33°</p>	 <p>36.3°</p>	 <p>40.6°</p>	

Fig. S40 Planar angles between functional group and benzene plane based on DFT calculated structure in ground state and excited state of **1E2E4A**

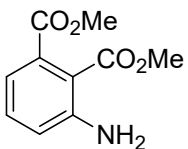
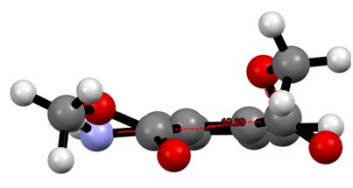
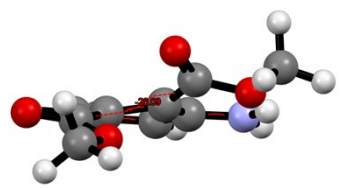
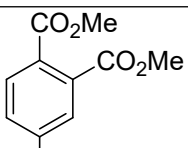
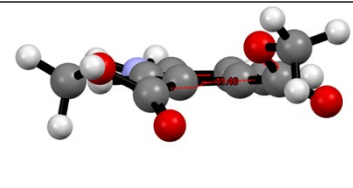
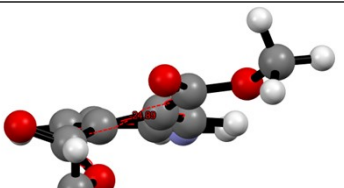
	N	
	GS	ES
 1E2E3A	 <i>10.4°</i>	 <i>26.1°</i>
 1E2E4A	 <i>11.5°</i>	 <i>24.9°</i>

Fig. S41 Torsion angles between functional group and benzene plane based on DFT calculated structure in ground state and excited state of **1E2E3A** and **1E2E4A**.

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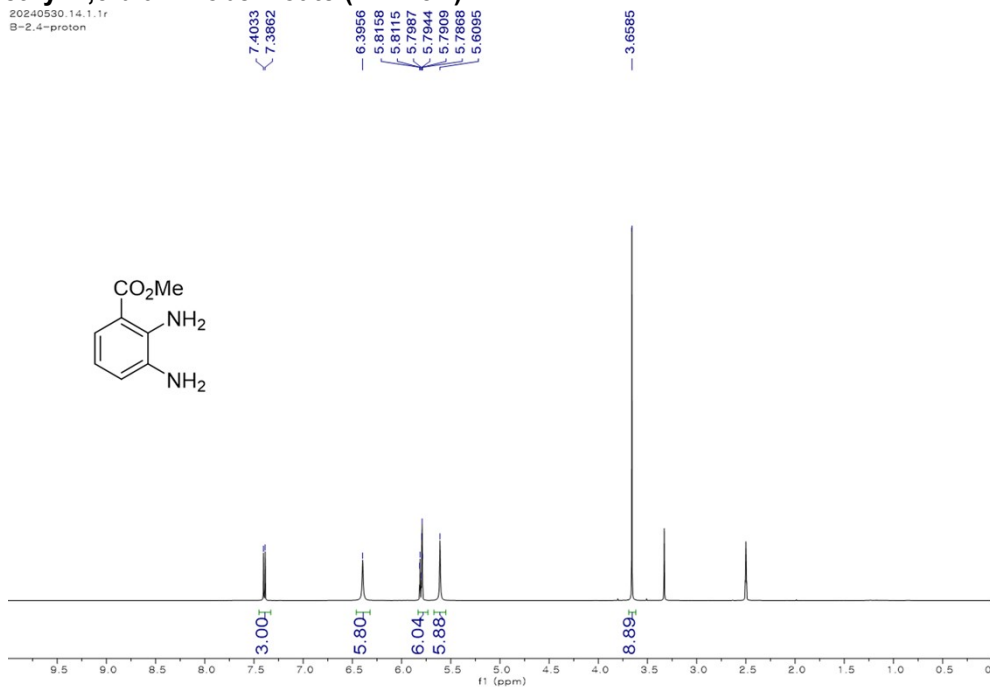
S17 R. G. Lavanya, G. N. Anil Kuma, *CCDC 1903412*; DOI: 10.5517/ccdc.csd.cc21wnd0

Appendix I

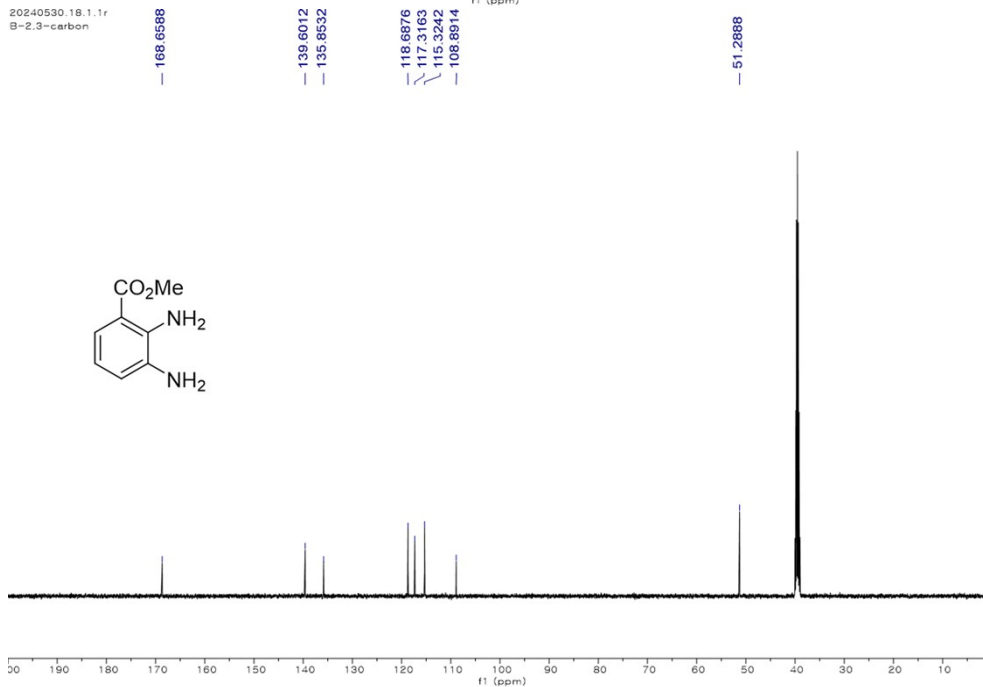
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NMR and IR for the obtained
compounds
(including HPLC data for
1E2A3E4A and 1E2A4E6A)**

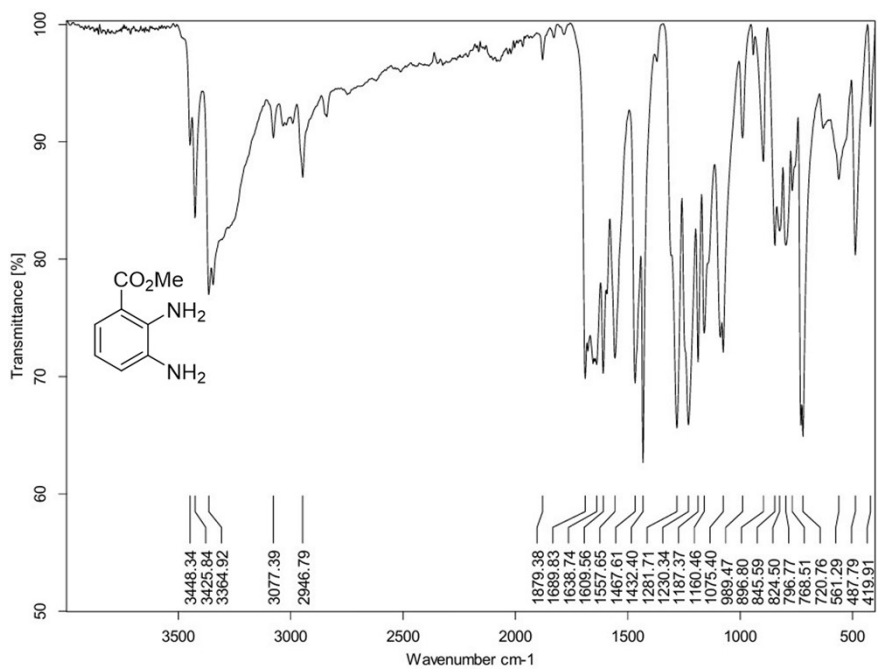
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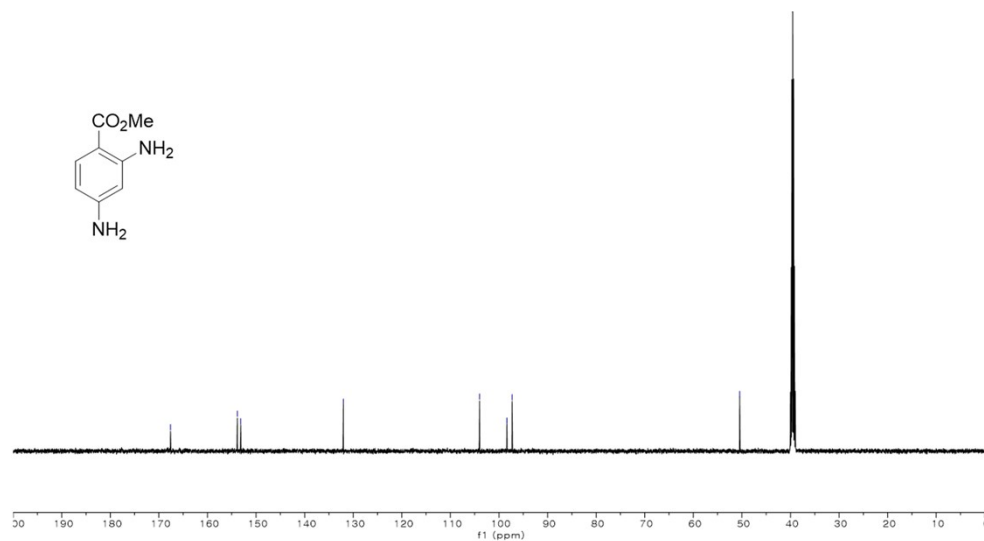
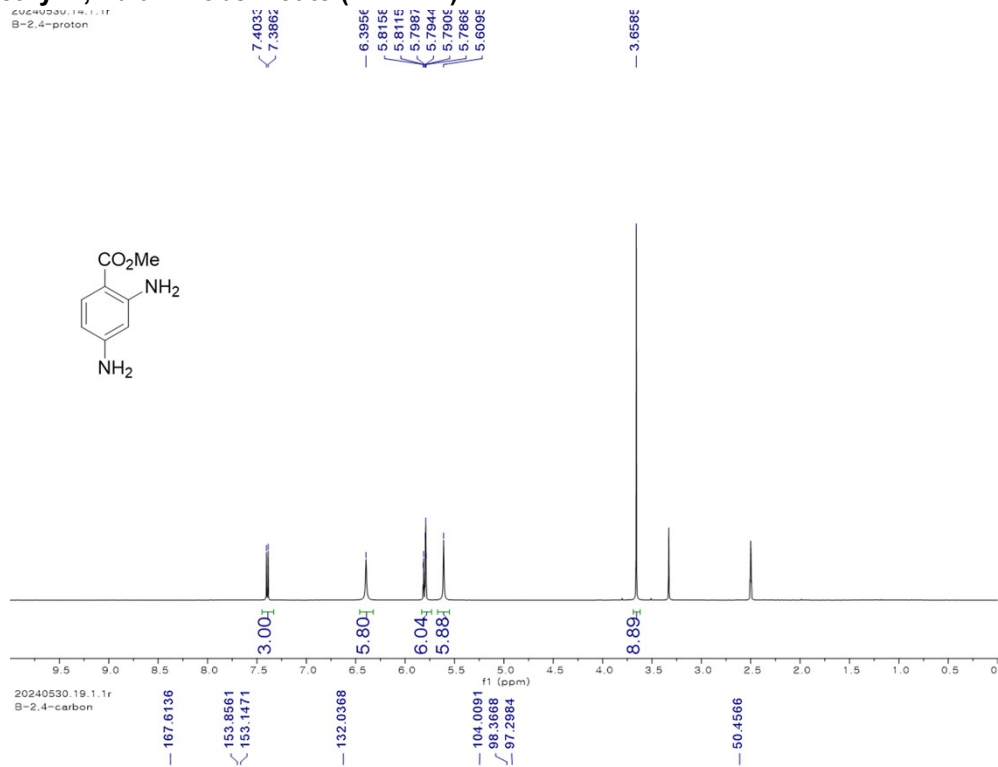
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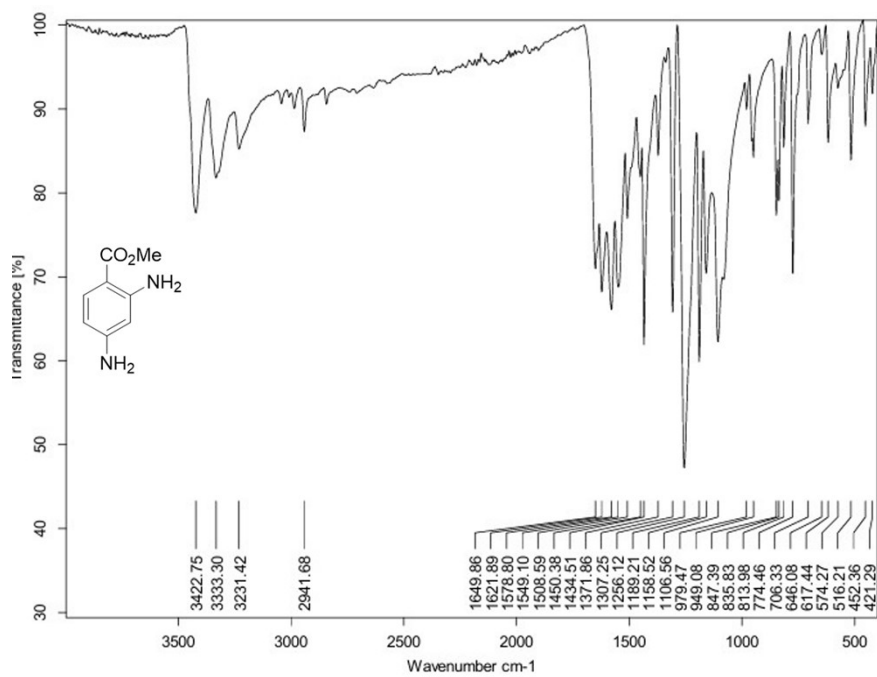




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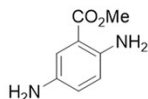
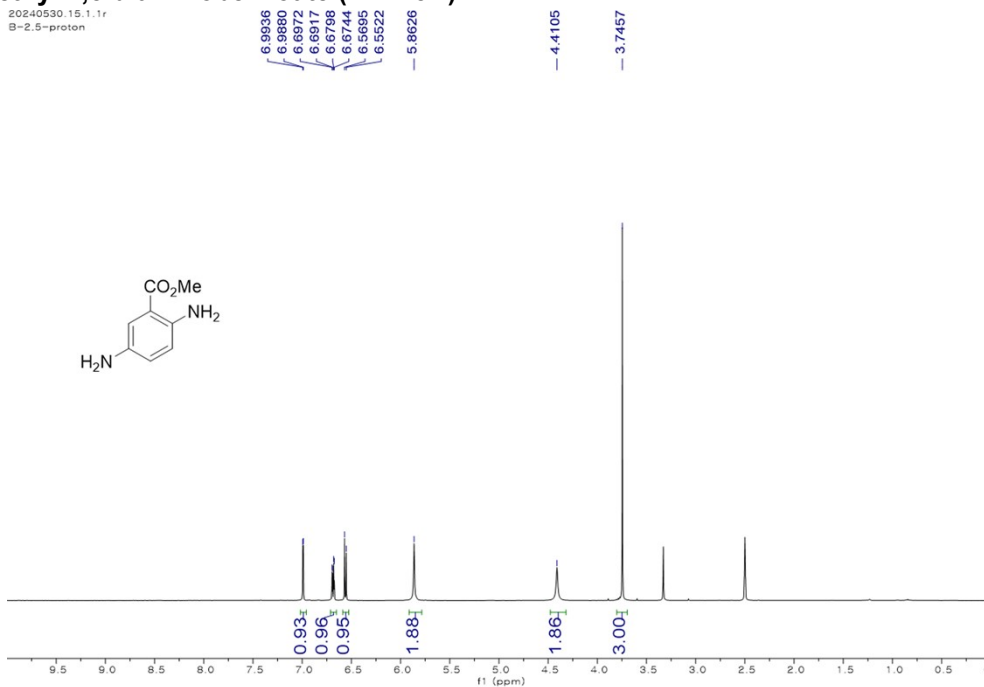
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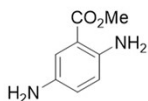
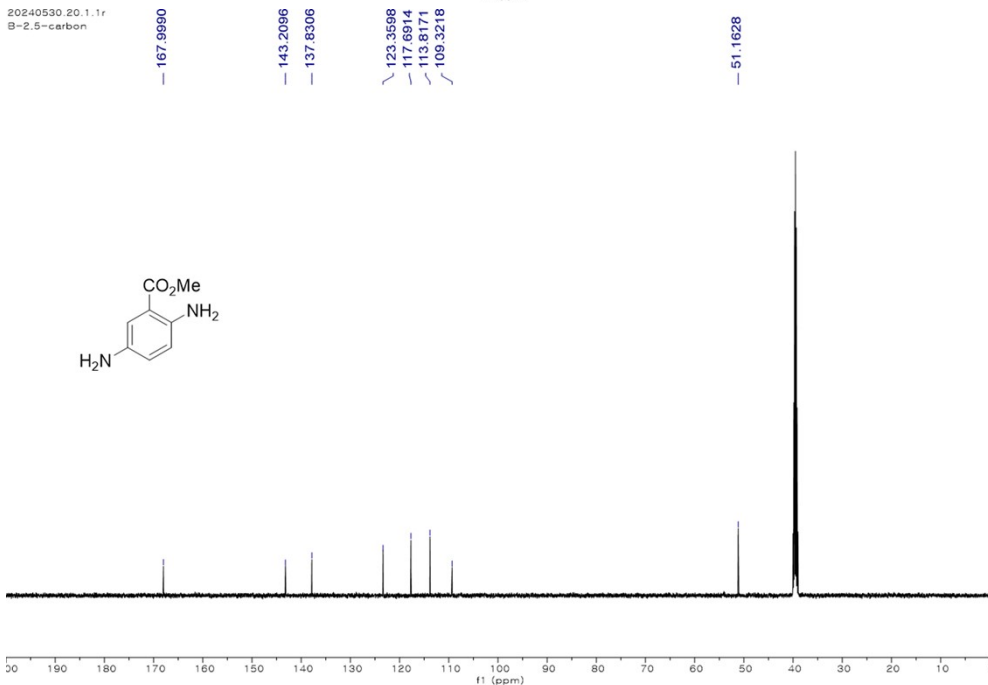


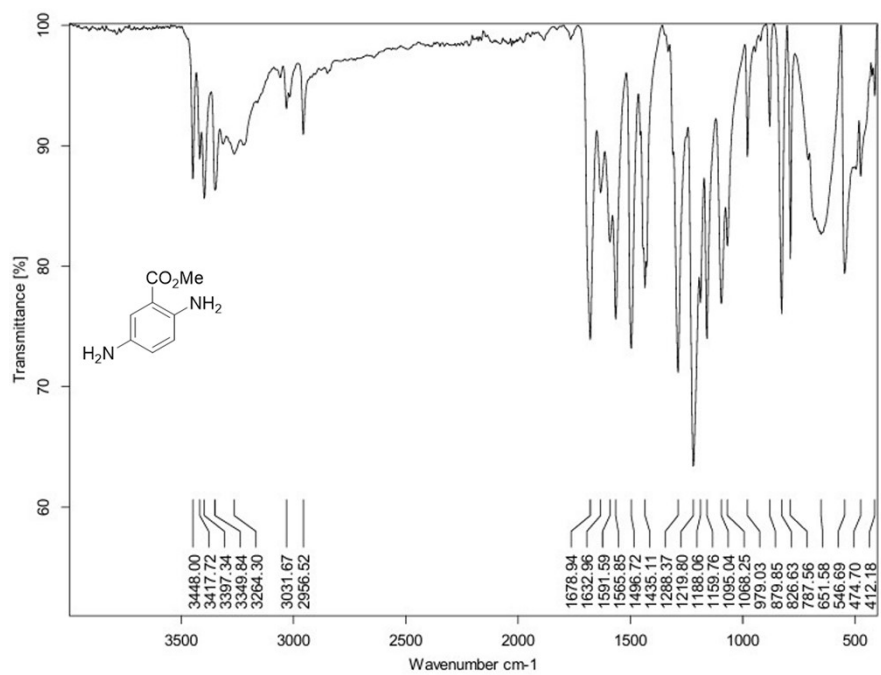
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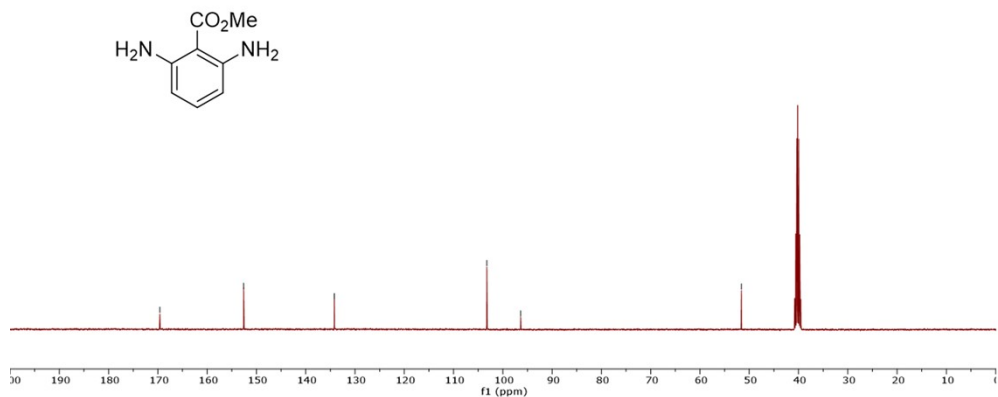
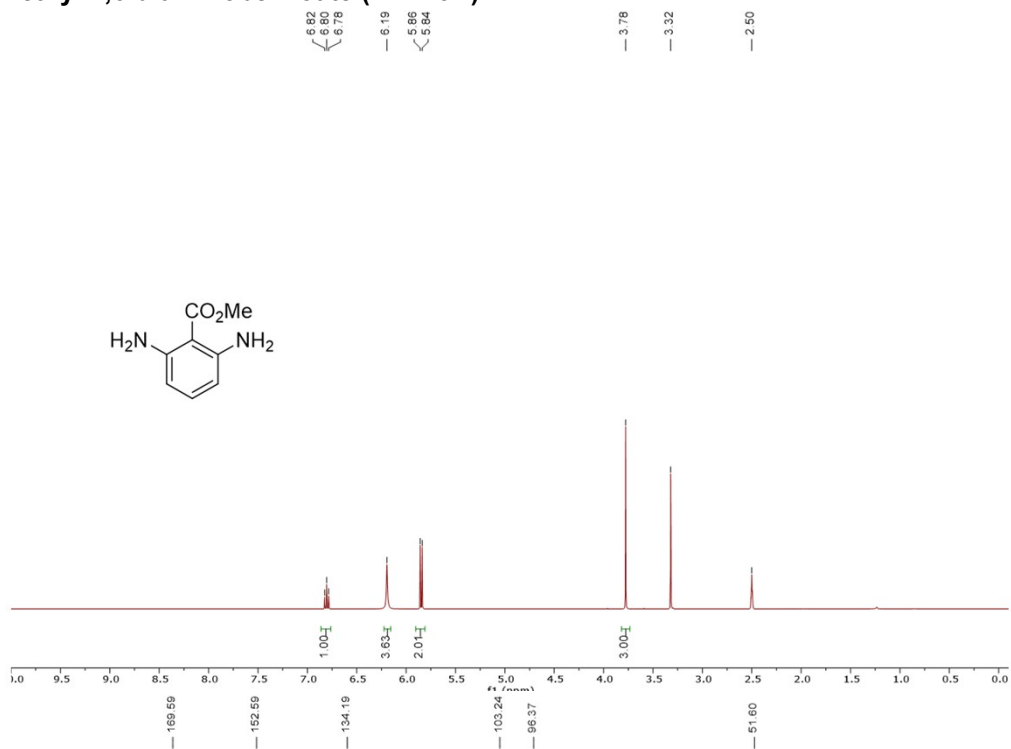


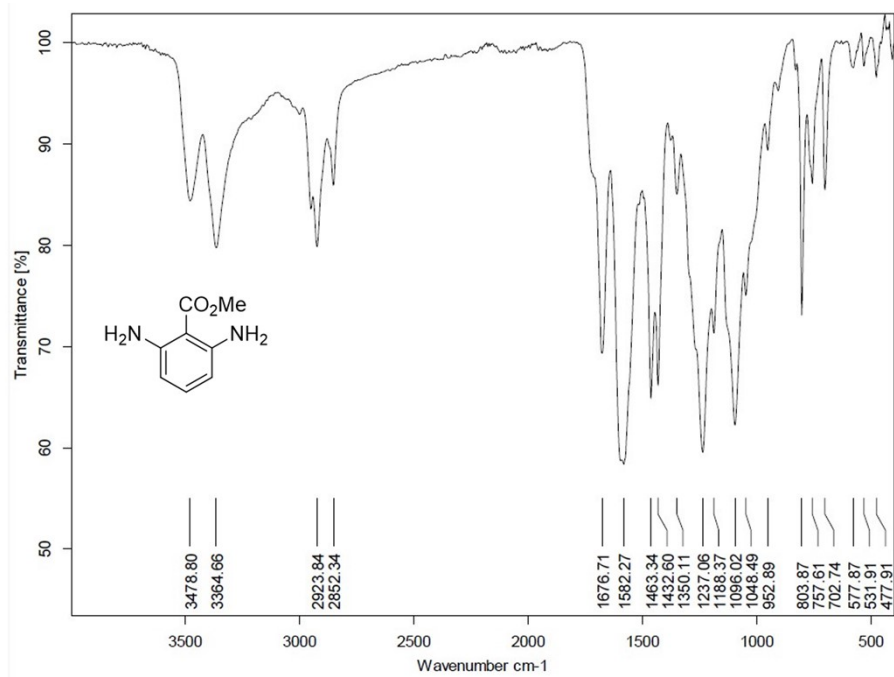
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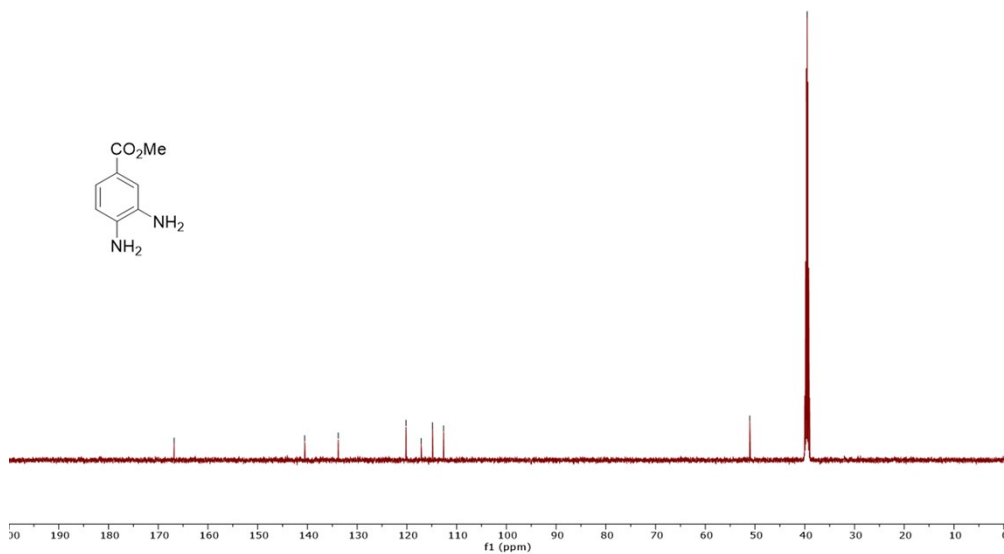
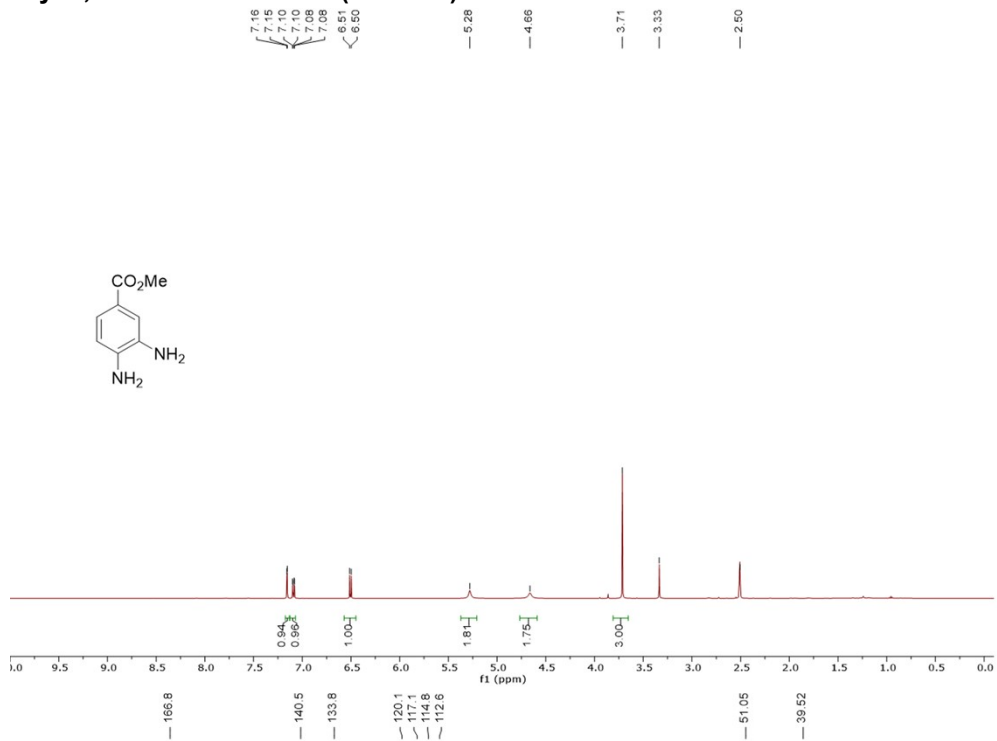


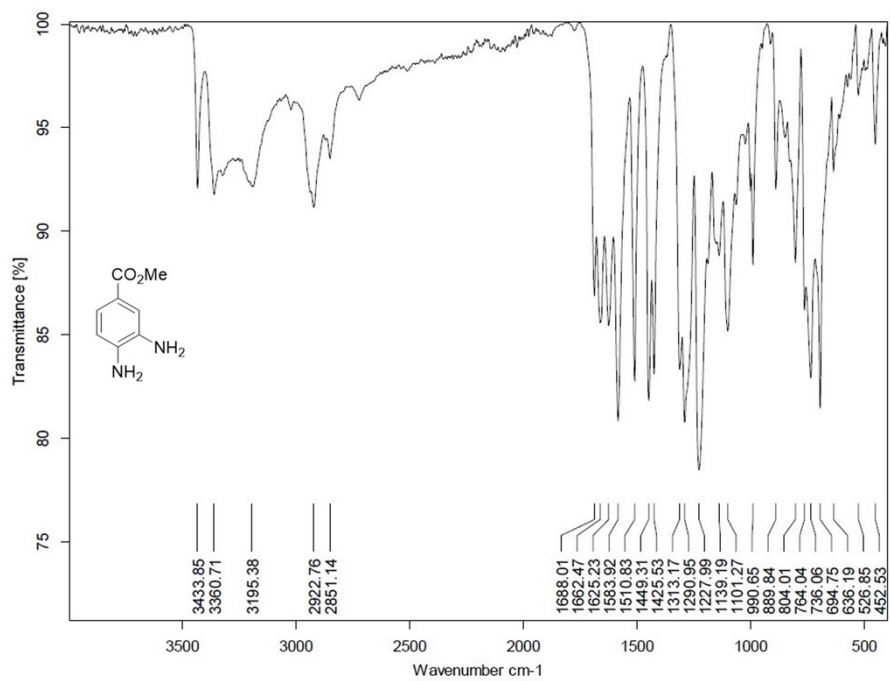
Methyl 2,6-diaminobenzoate (1E2A6A)





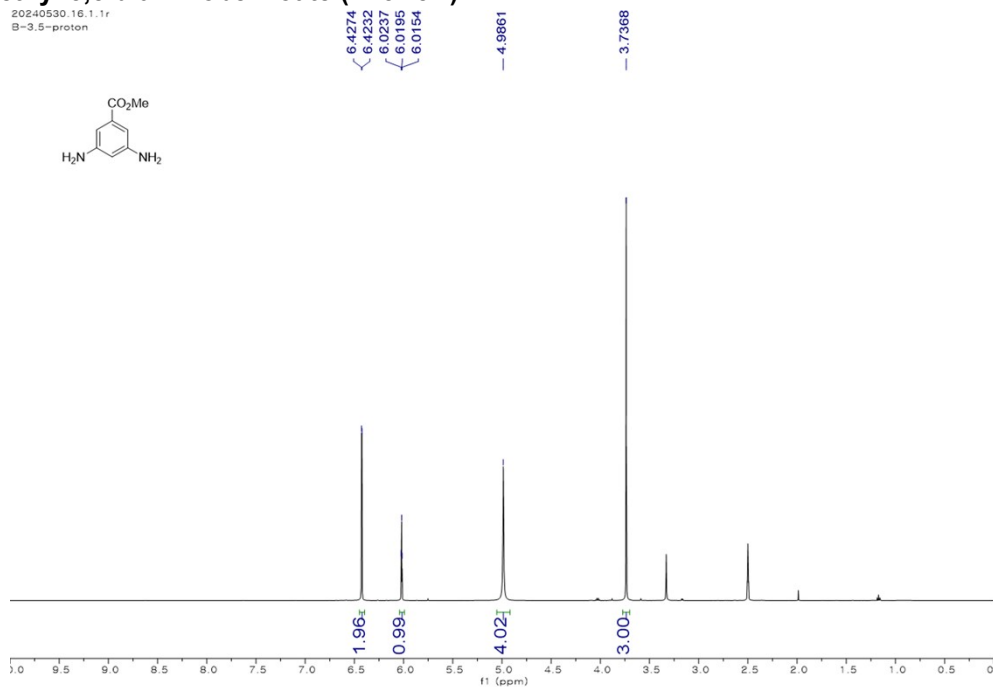
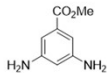
Methyl 3,4-diaminobenzoate (1E3A4A)



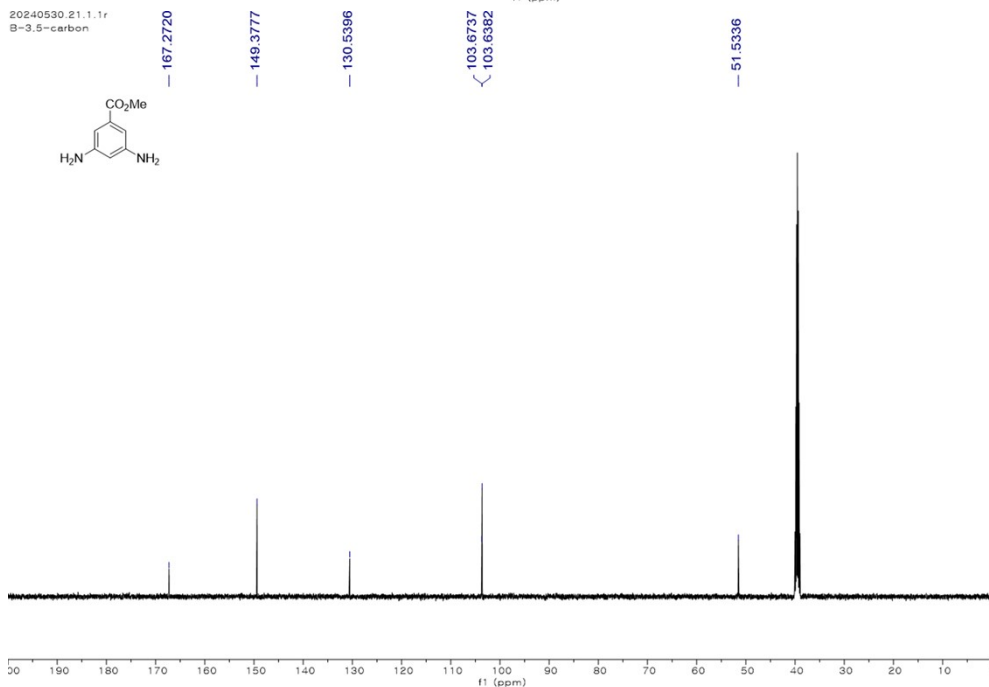
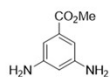


Methyl 3,5-diaminobenzoate (1E3A5A)

20240530.16.1.1r
B-3.5-proton

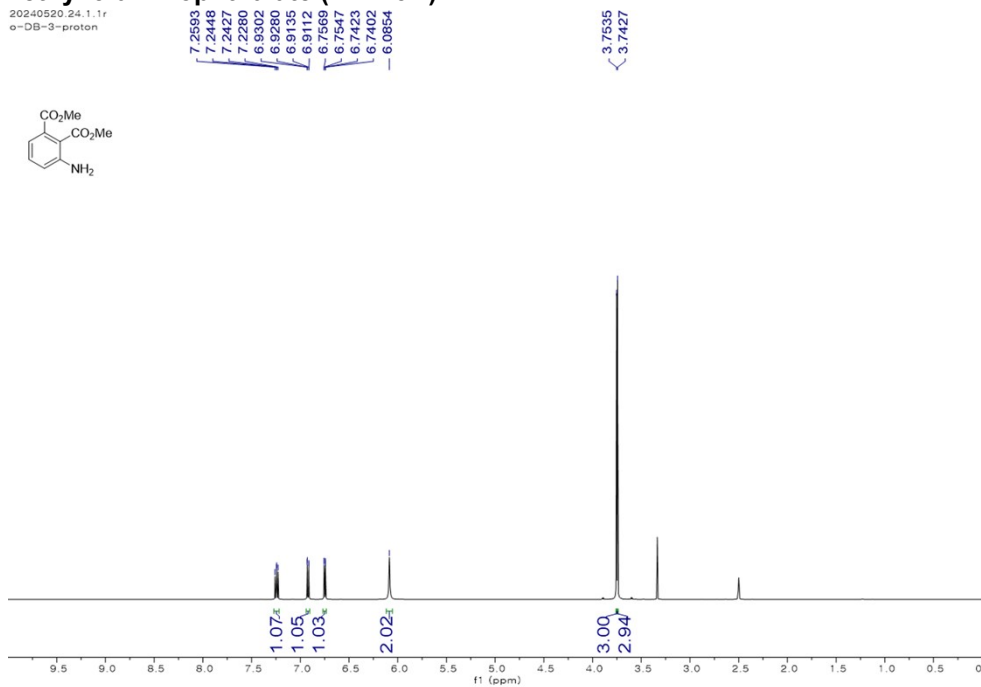


20240530.21.1.1r
B-3.5-carbon

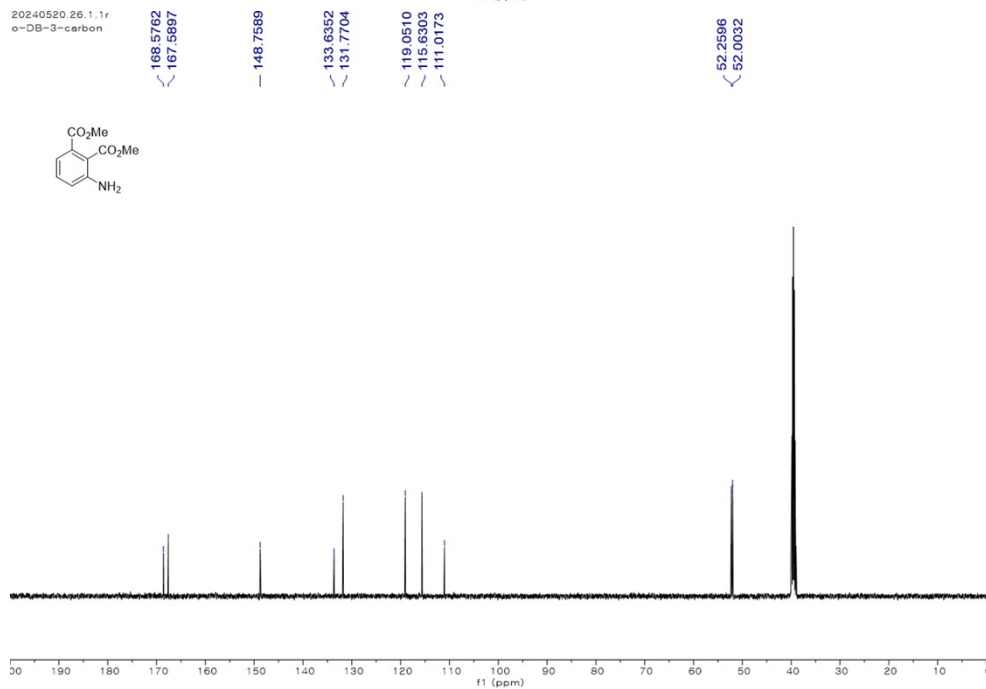


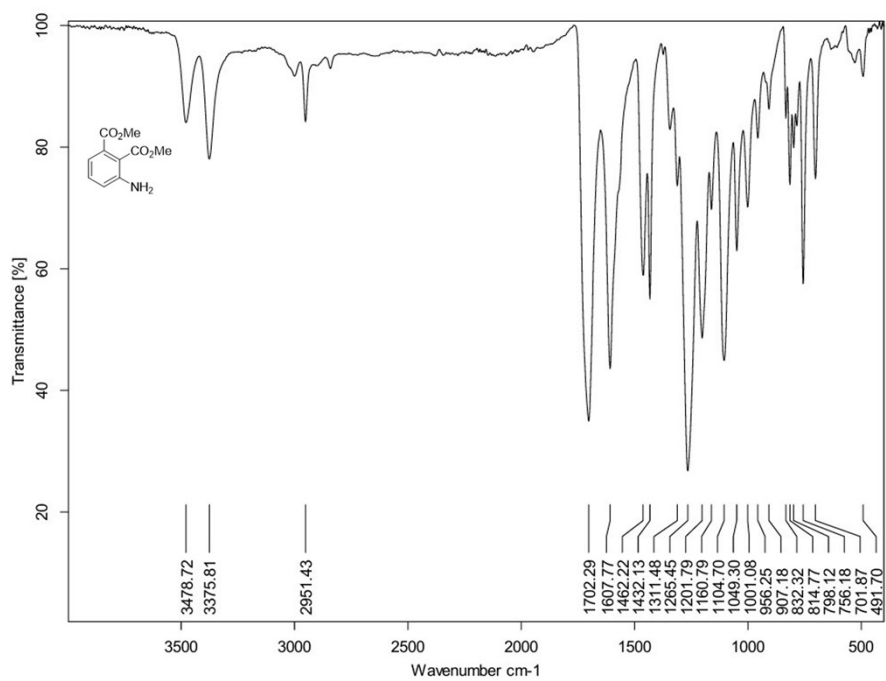
Dimethyl 3-aminophthalate (1E2E3A)

20240520_24.1.1r
o-DB-3-proton



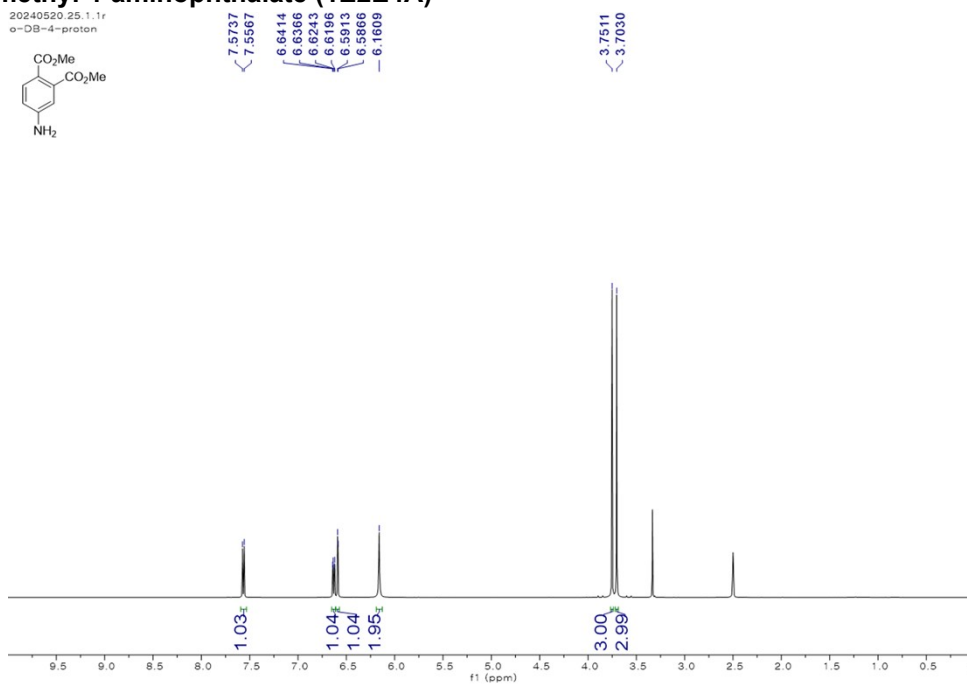
20240520_26.1.1r
o-DB-3-carbon



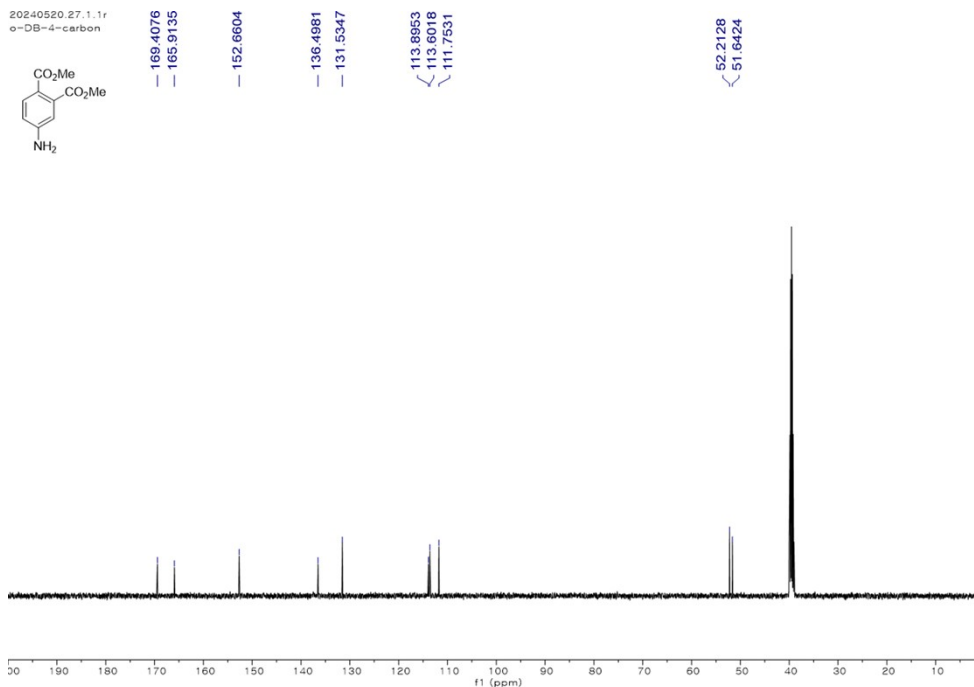


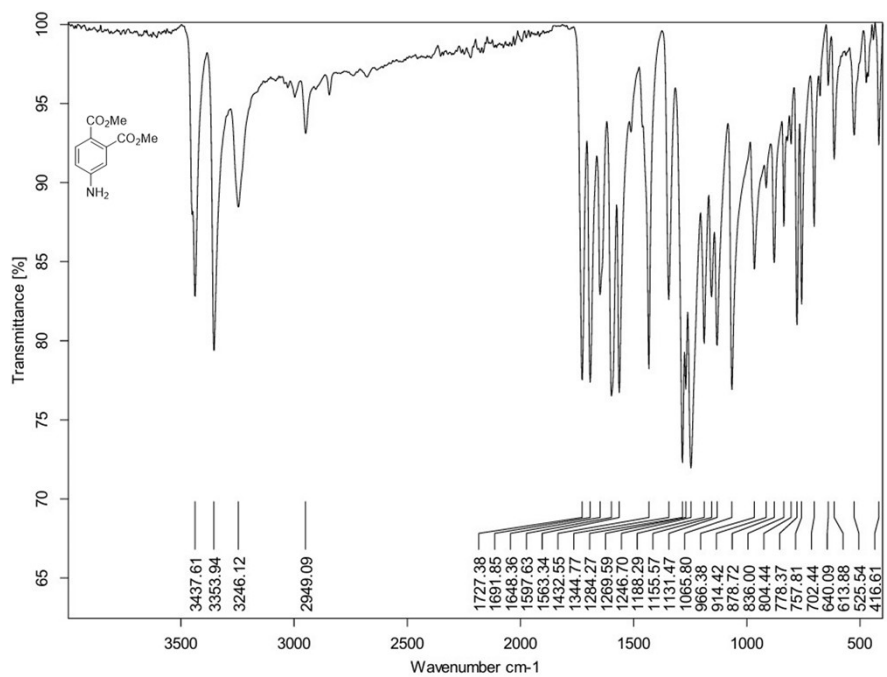
Dimethyl 4-aminophthalate (1E2E4A)

20240520.25.1.1r
o-DB-4-proton

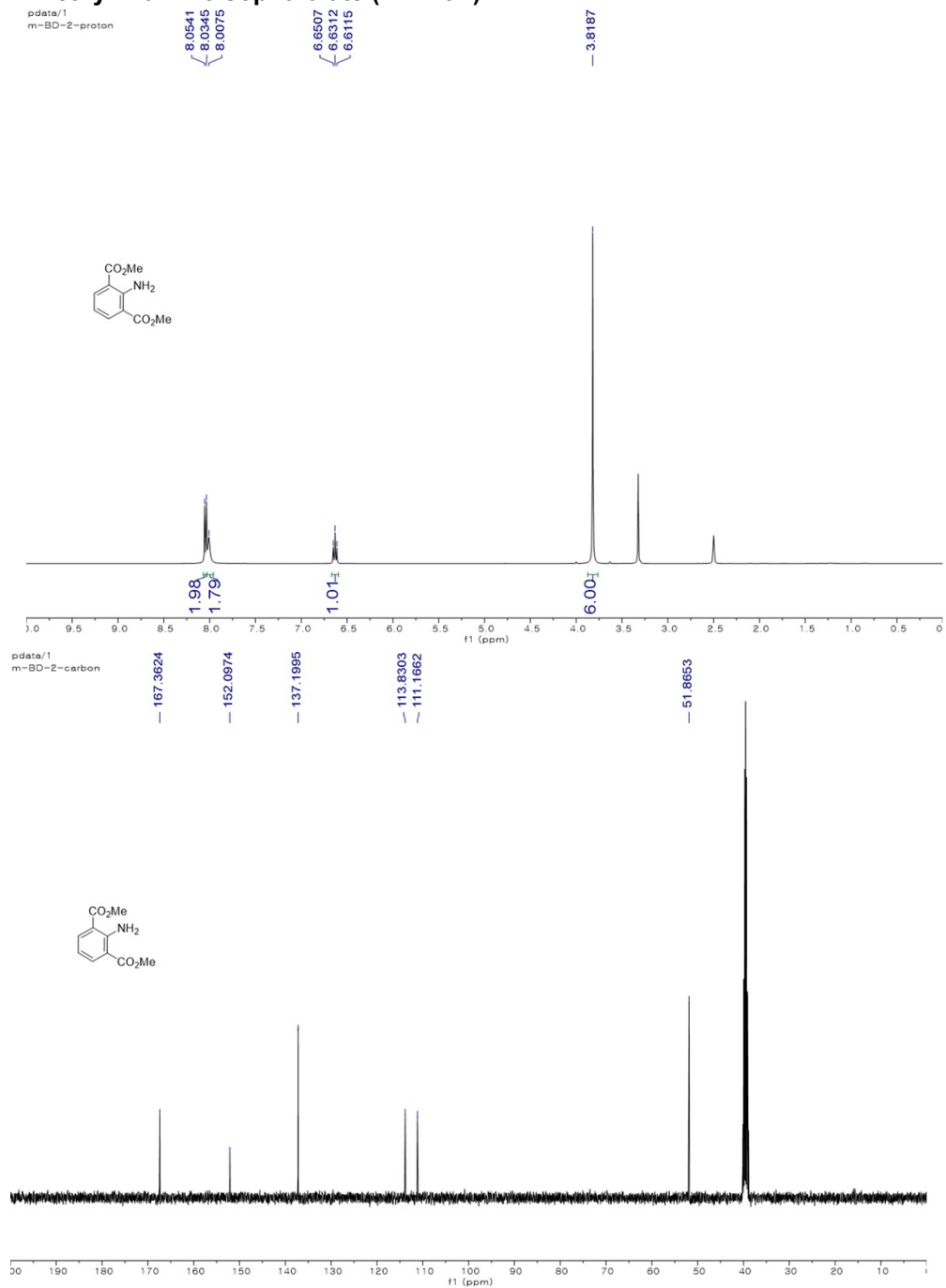


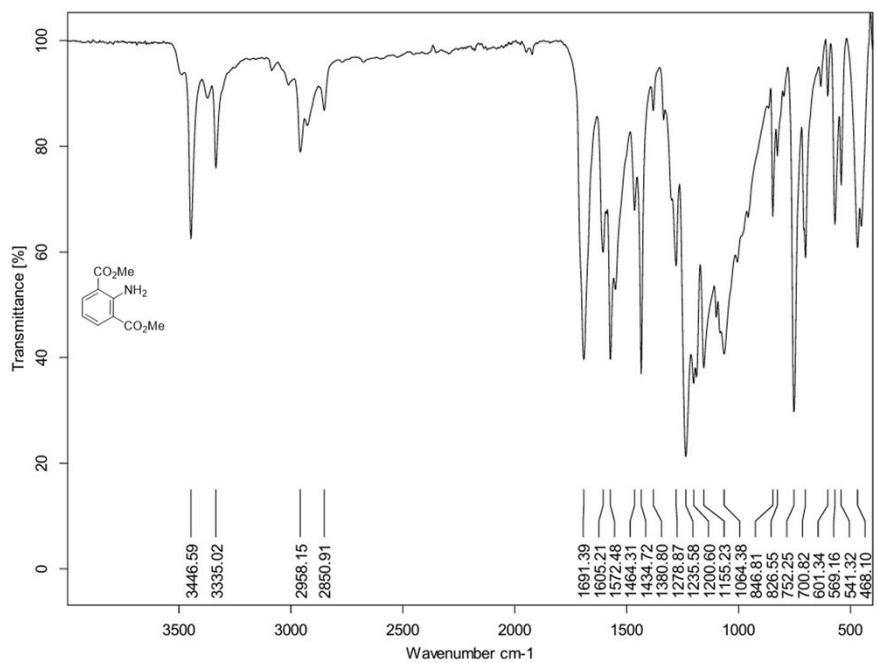
20240520.27.1.1r
o-DB-4-carbon





Dimethyl 2-aminoisophthalate (1E2A3E)



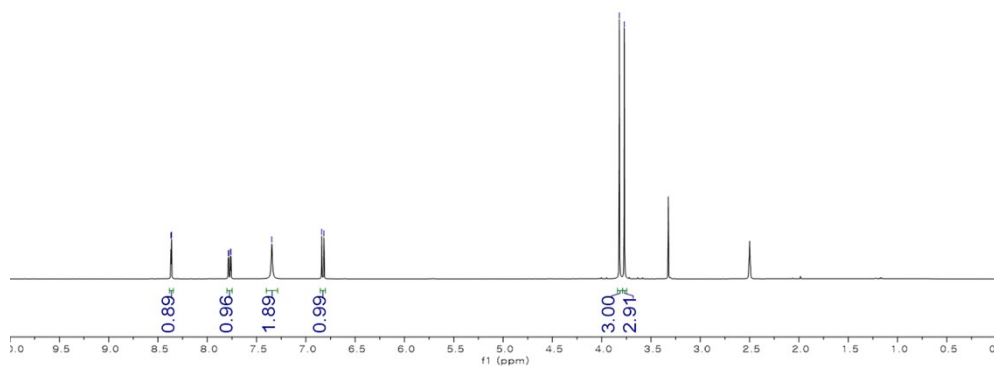


Dimethyl 4-aminoisophthalate (1E2A5E)

pdate/1
m-DB-4-proton



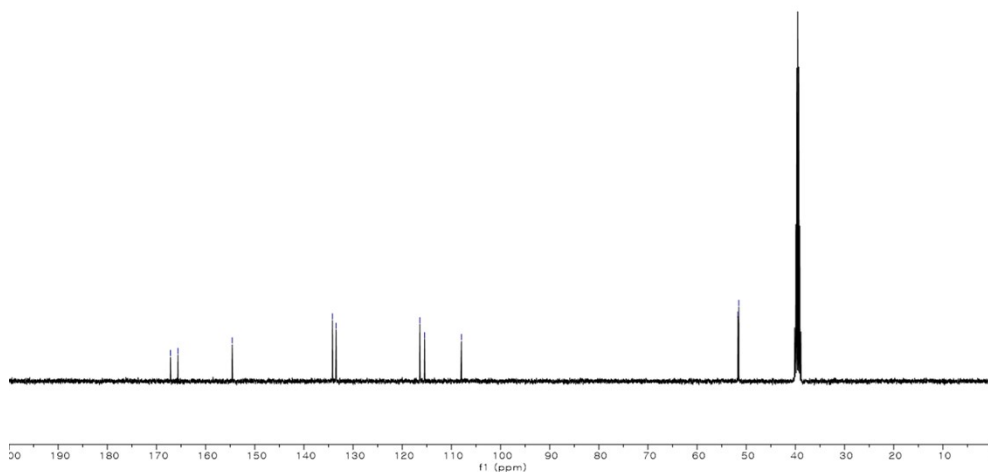
8.3661
8.3628
7.7874
7.7818
7.7653
7.7599
7.3455
6.8390
6.8169
3.8211
3.7703

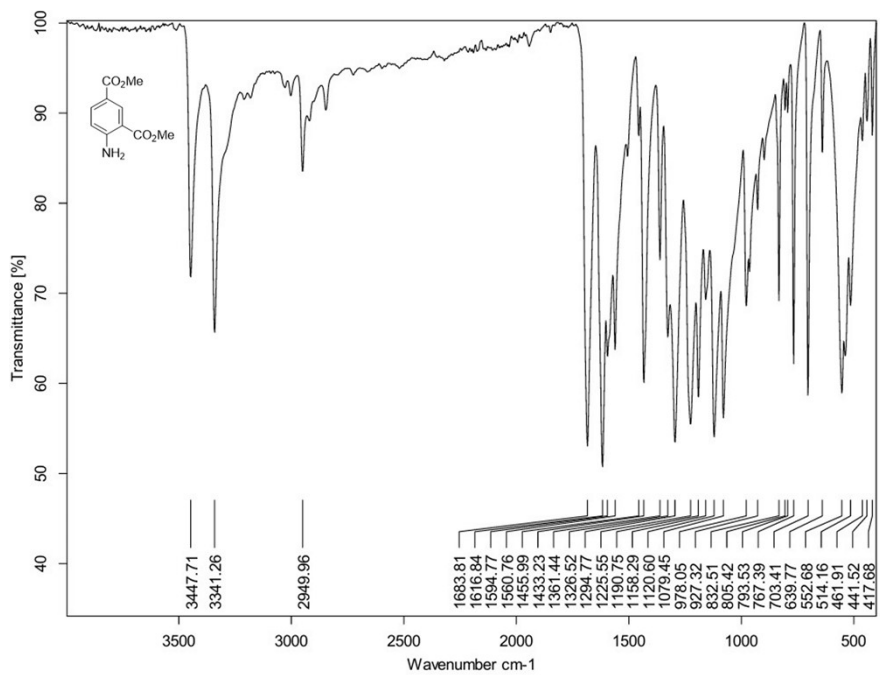


pdate/1
m-DB-4-carbon



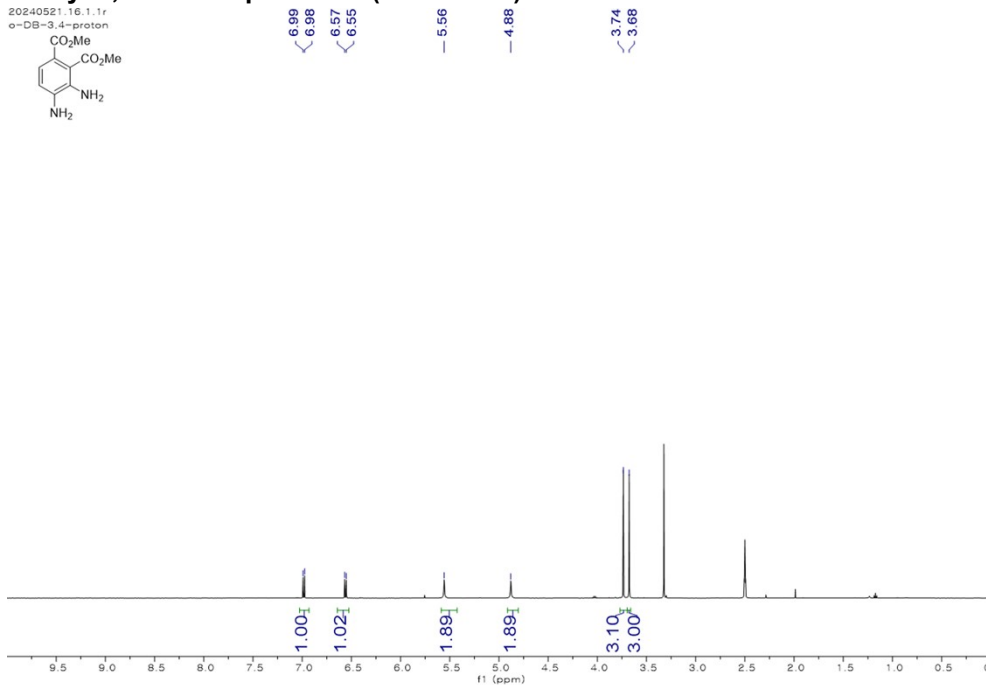
167.1618
165.6470
154.5894
134.1922
133.4544
116.4203
115.4526
107.9643
51.6889
51.5226



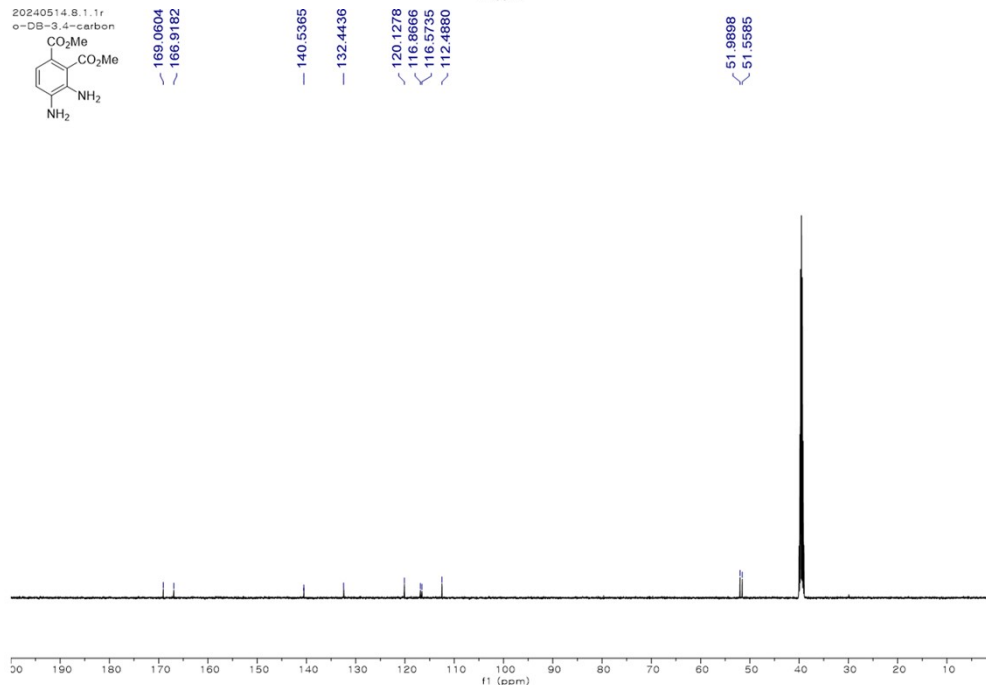


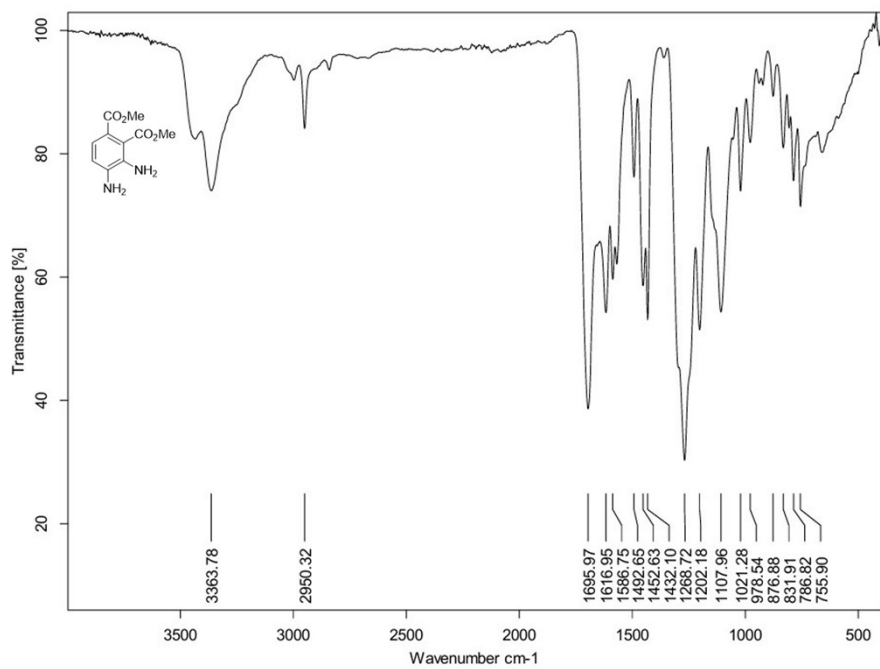
Dimethyl 3,4-diaminophthalate (1E2E3A4A)

20240521.16.1.1r
o-DB-3,4-proton



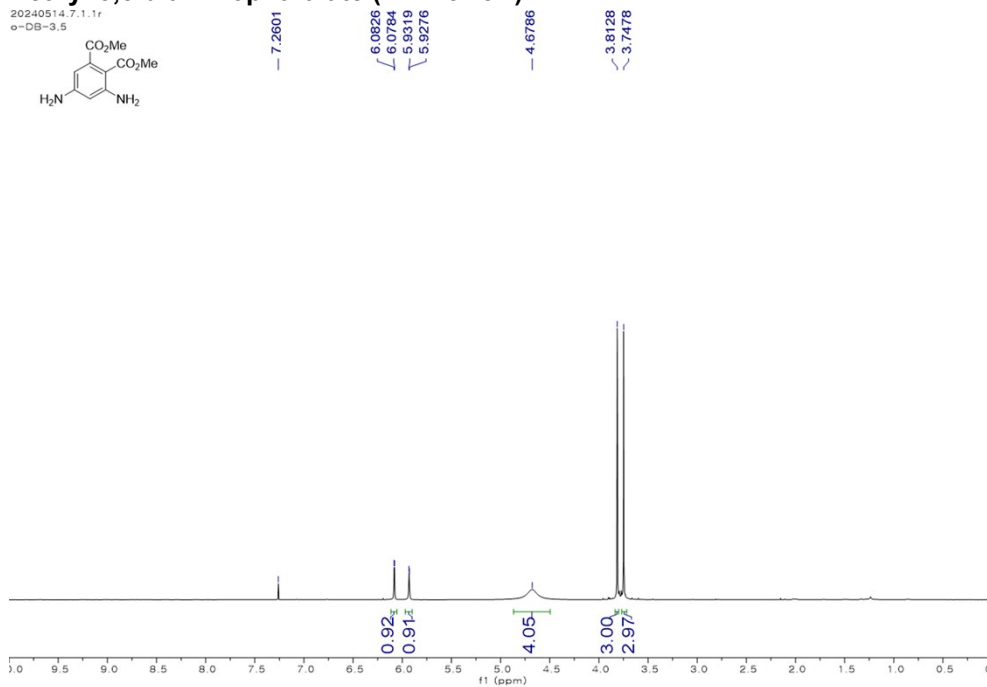
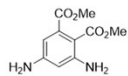
20240514.8.1.1r
o-DB-3,4-carbon



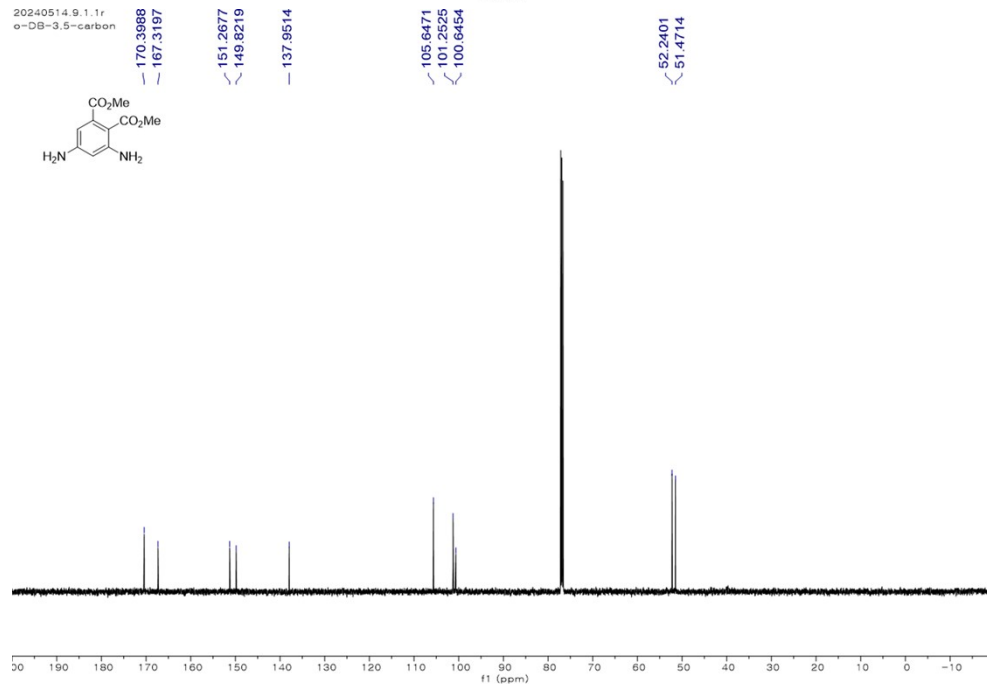
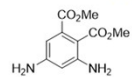


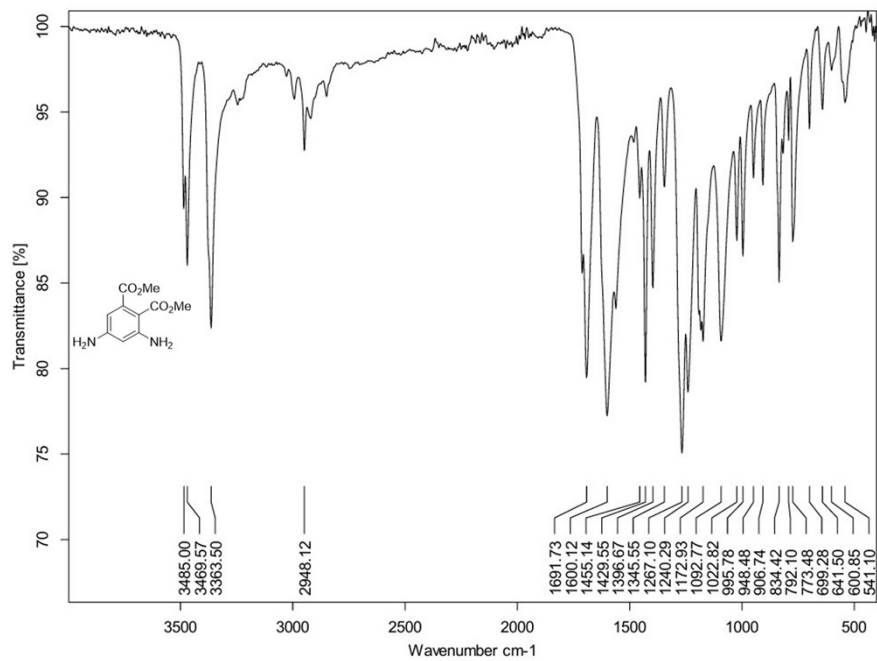
Dimethyl 3,5-diaminophthalate (1E2E3A5A)

20240514.7.1.1r
o-DB-3.5



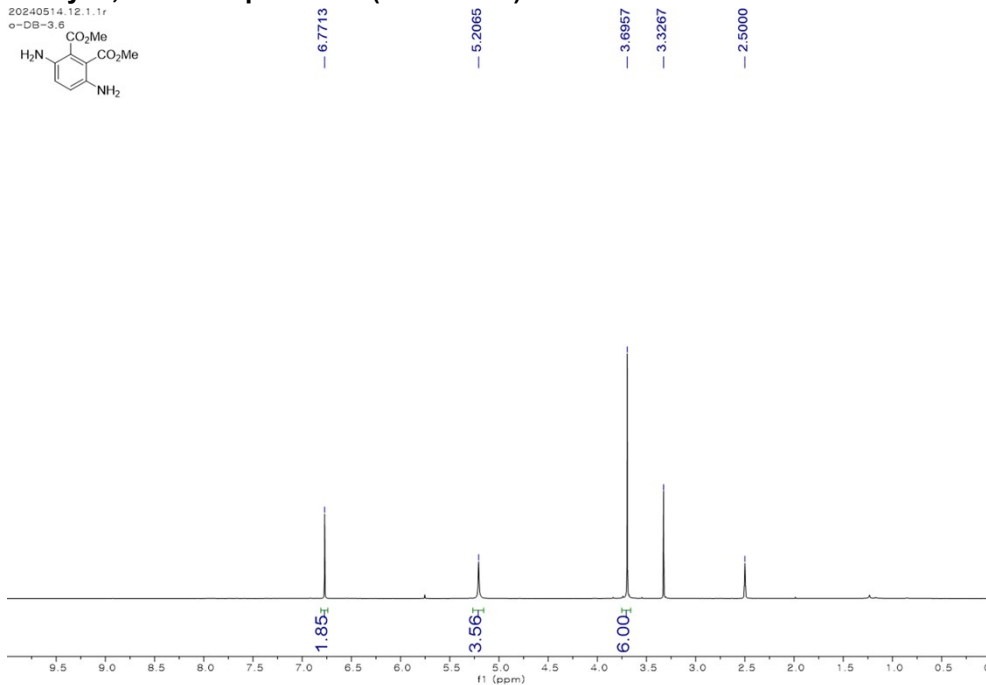
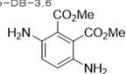
20240514.9.1.1r
o-DB-3.5-carbon



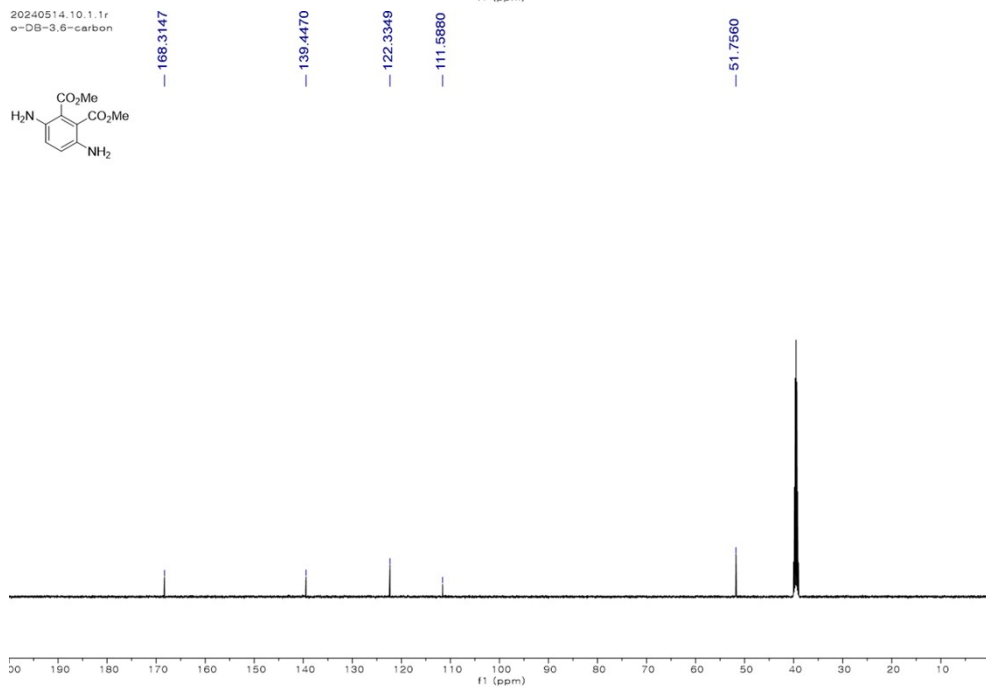
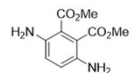


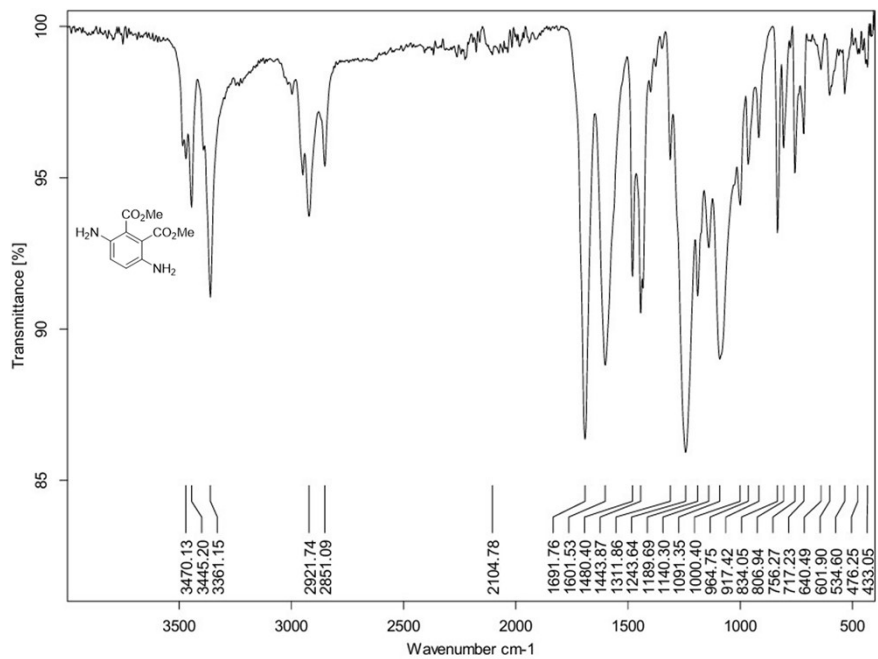
Dimethyl 3,6-diaminophthalate (1E2E3A6A)

20240514.12.1.1.r
o-DB-3.6



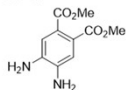
20240514.10.1.1.r
o-DB-3.6-carbon





Dimethyl 4,5-diaminophthalate (1E2E4A5A)

20240514.9.1.1.r
o-DB-4.5



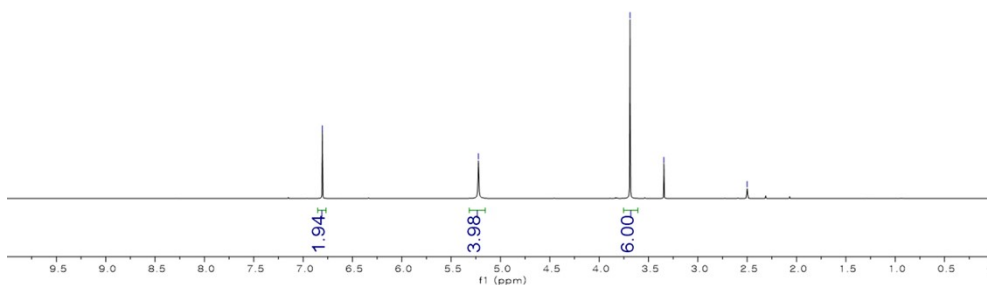
6.8050

5.2233

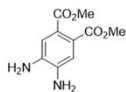
3.6871

3.3440

2.5000



20240514.11.1.1.r
o-DB-4.5-carbon



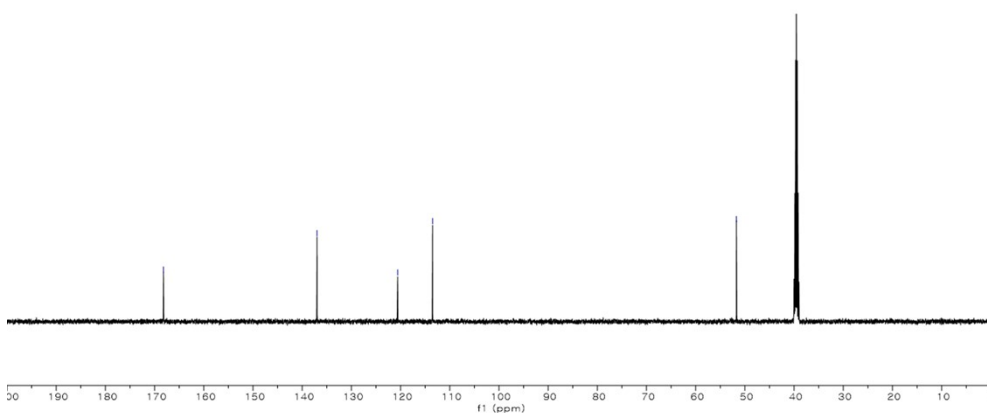
168.1921

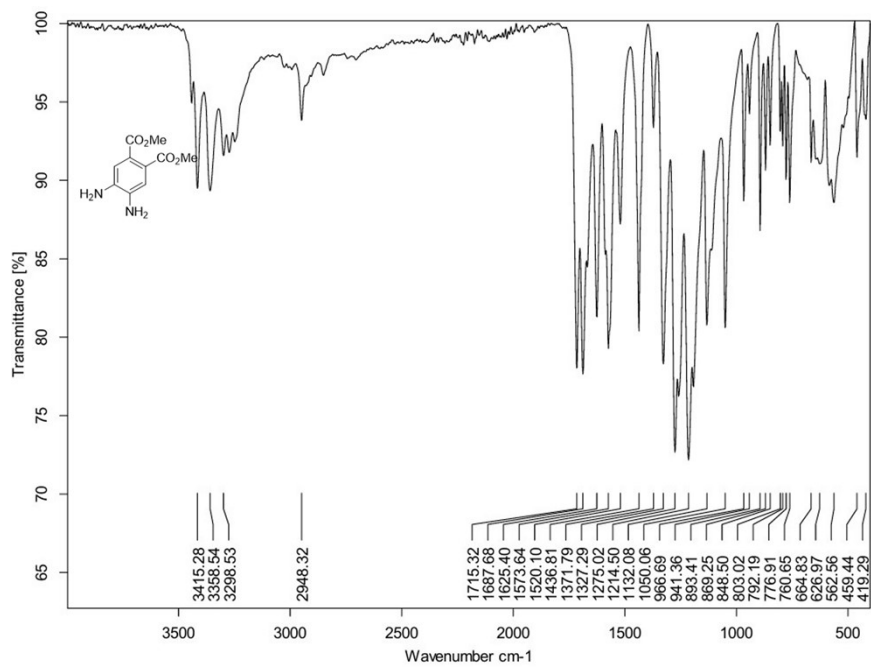
136.9774

120.6015

113.5048

51.7196

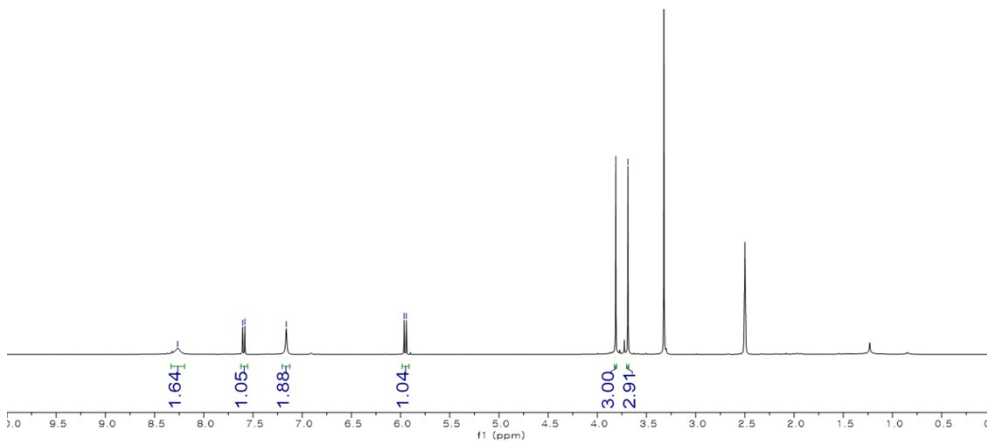




Dimethyl 2,4-diaminoisophthalate (1E2A3E4A)

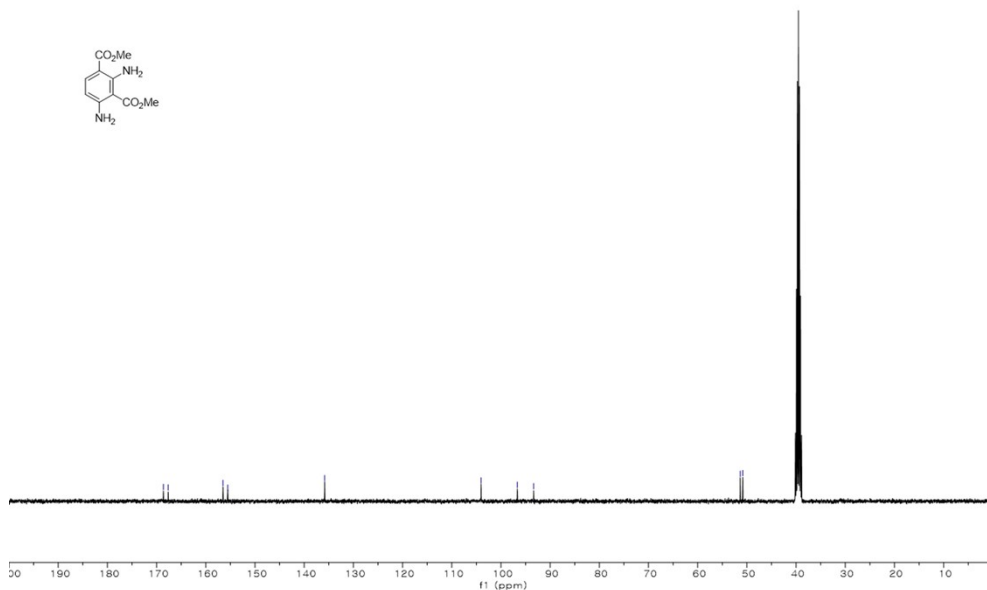
pdate/1
m-DB-2,4-proton

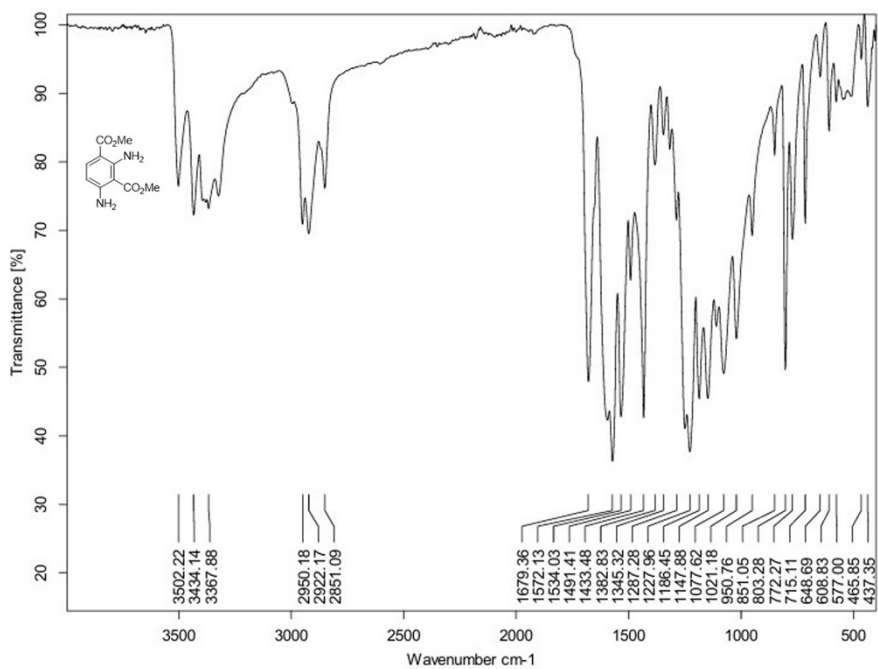
8.2654
7.6052
7.5826
7.1620
5.8637
5.8409
3.8125
3.6889



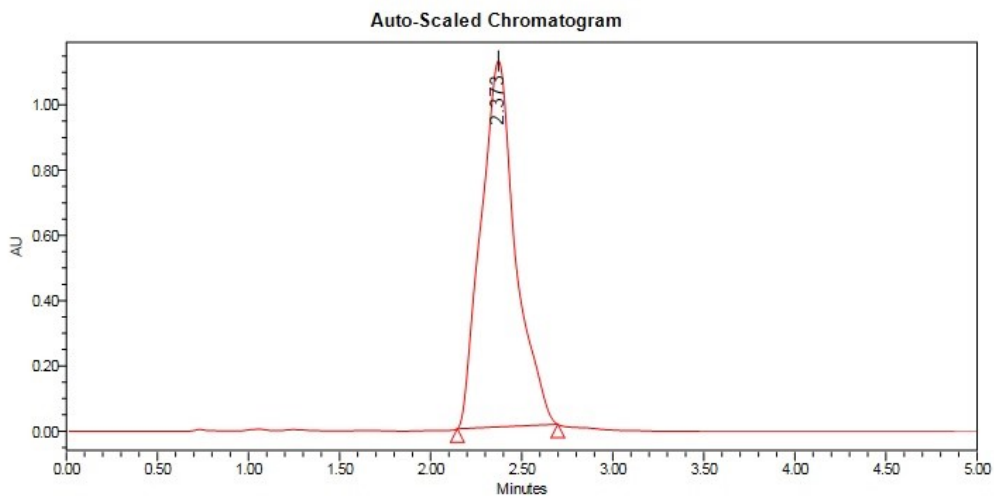
pdate/1
m-DB-2,4-carbon

168.6219
167.6535
156.4874
155.5356
135.8445
104.0358
96.6685
93.3609
51.3614
50.8274





[Additional HPLC data to check purity of **1E2A3E4A**]



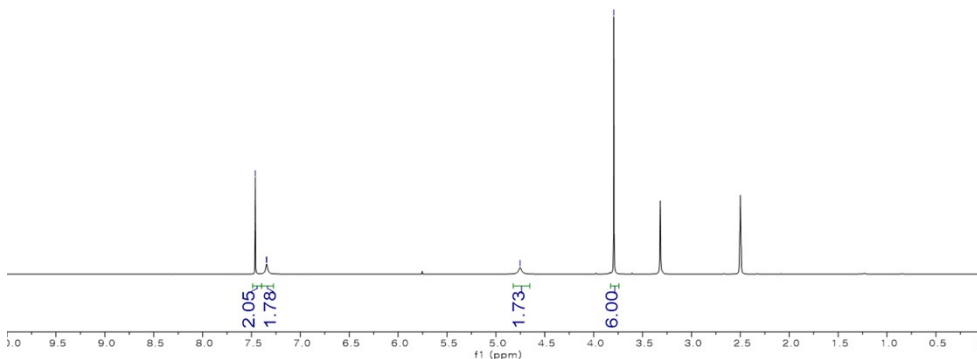
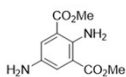
Dimethyl 2,5-diaminoisophthalate (1E2A3E5A)

pdata/1
m-DB-2.5-proton

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7.3457
7.3451

4.7526

3.7842



pdata/1
m-DB-2.5-carbon

167.4789

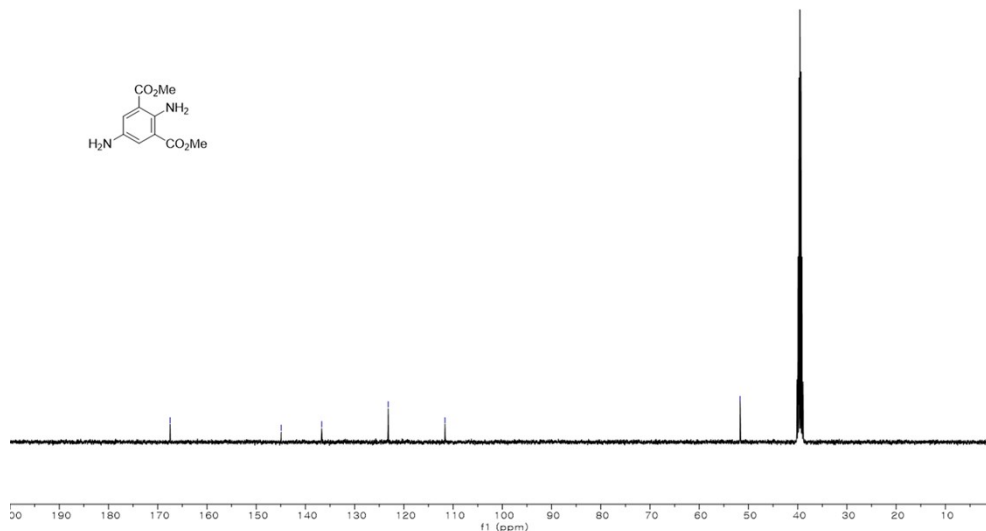
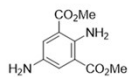
144.9300

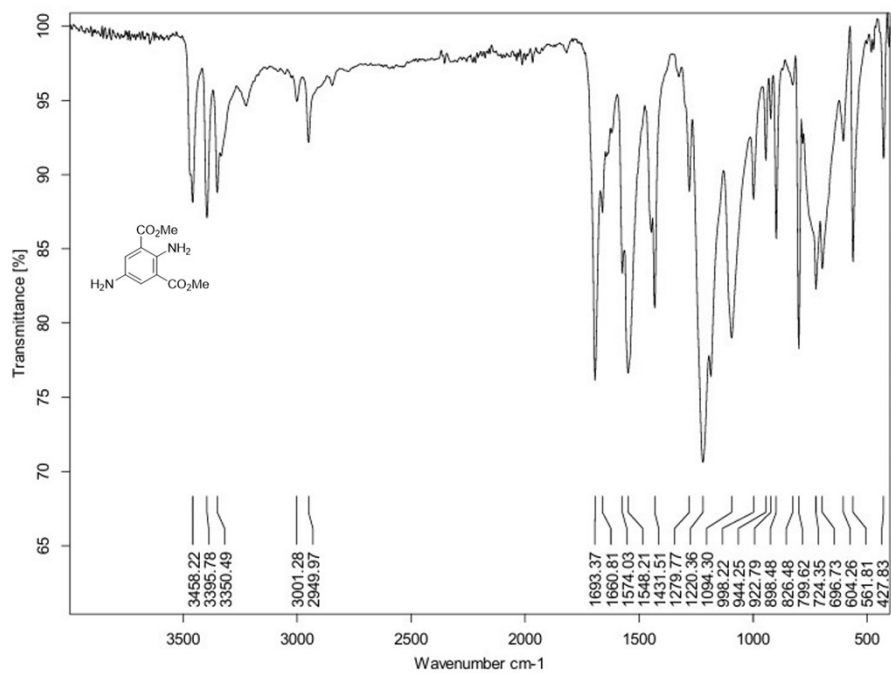
136.6834

123.1794

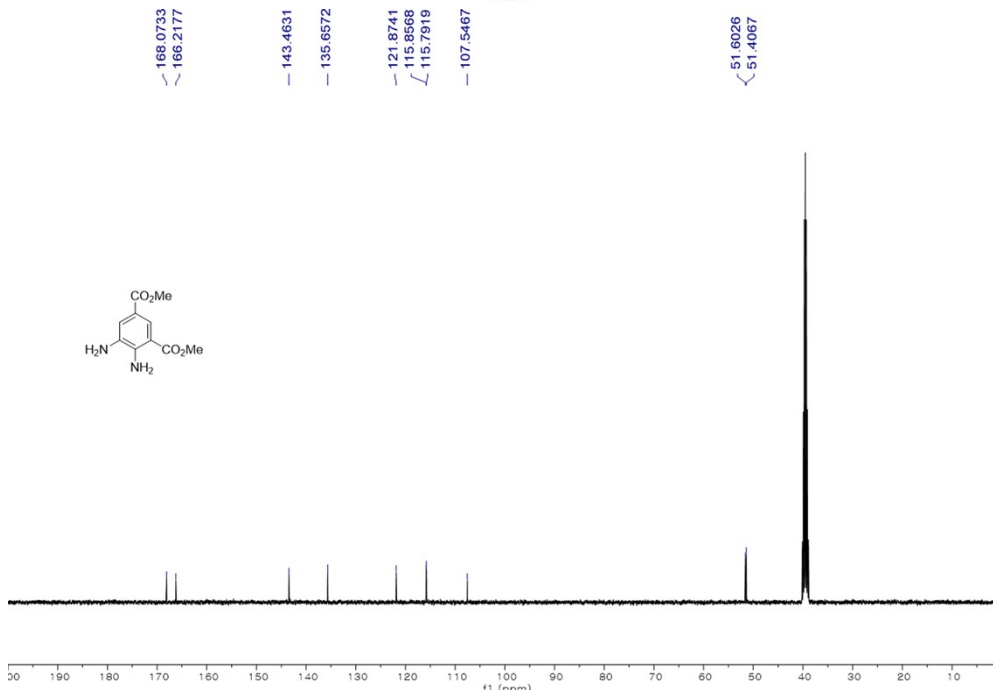
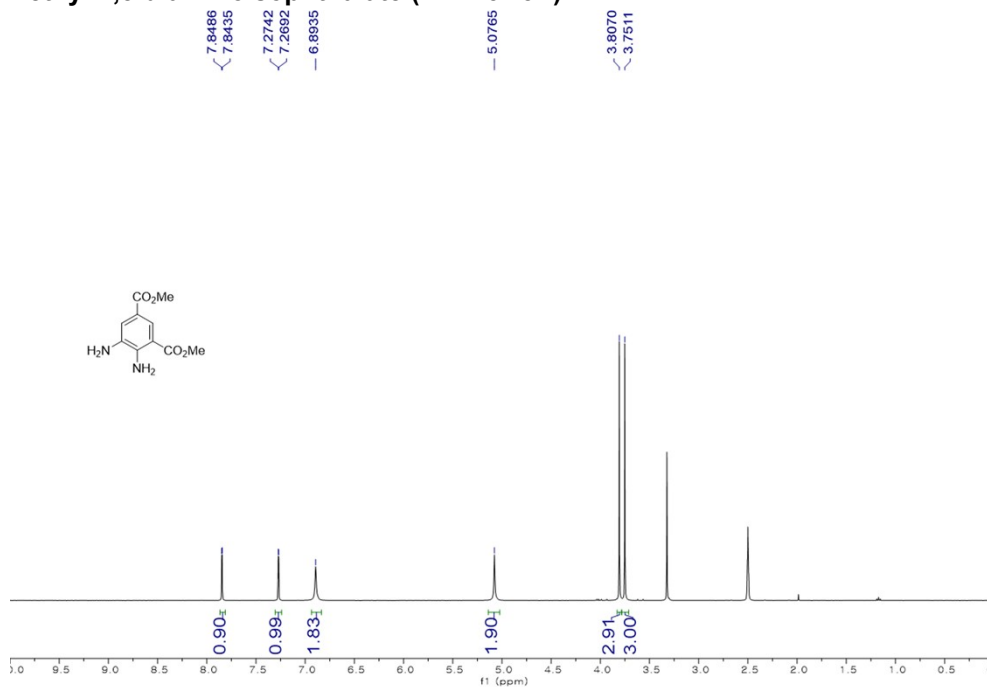
111.6357

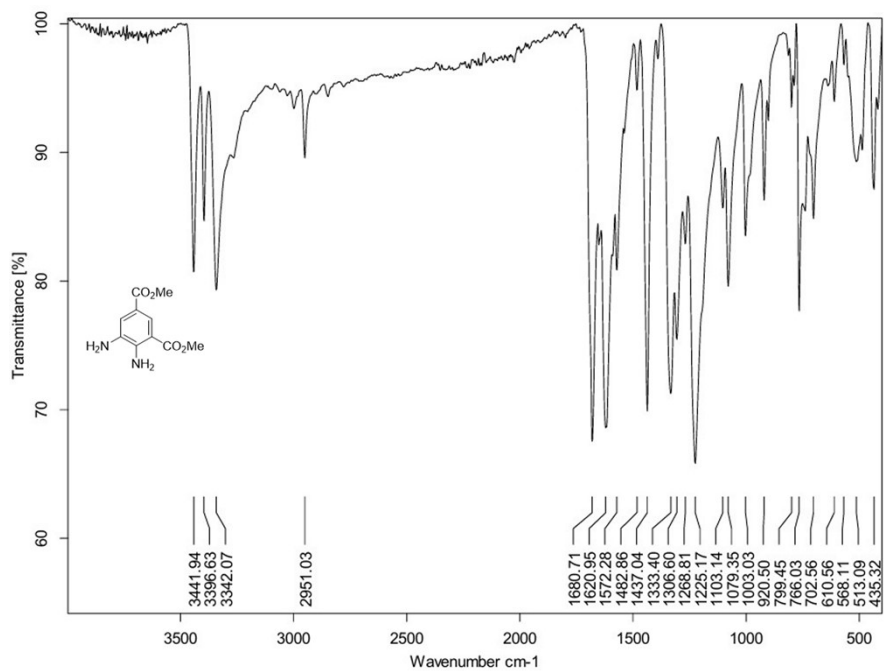
51.6970



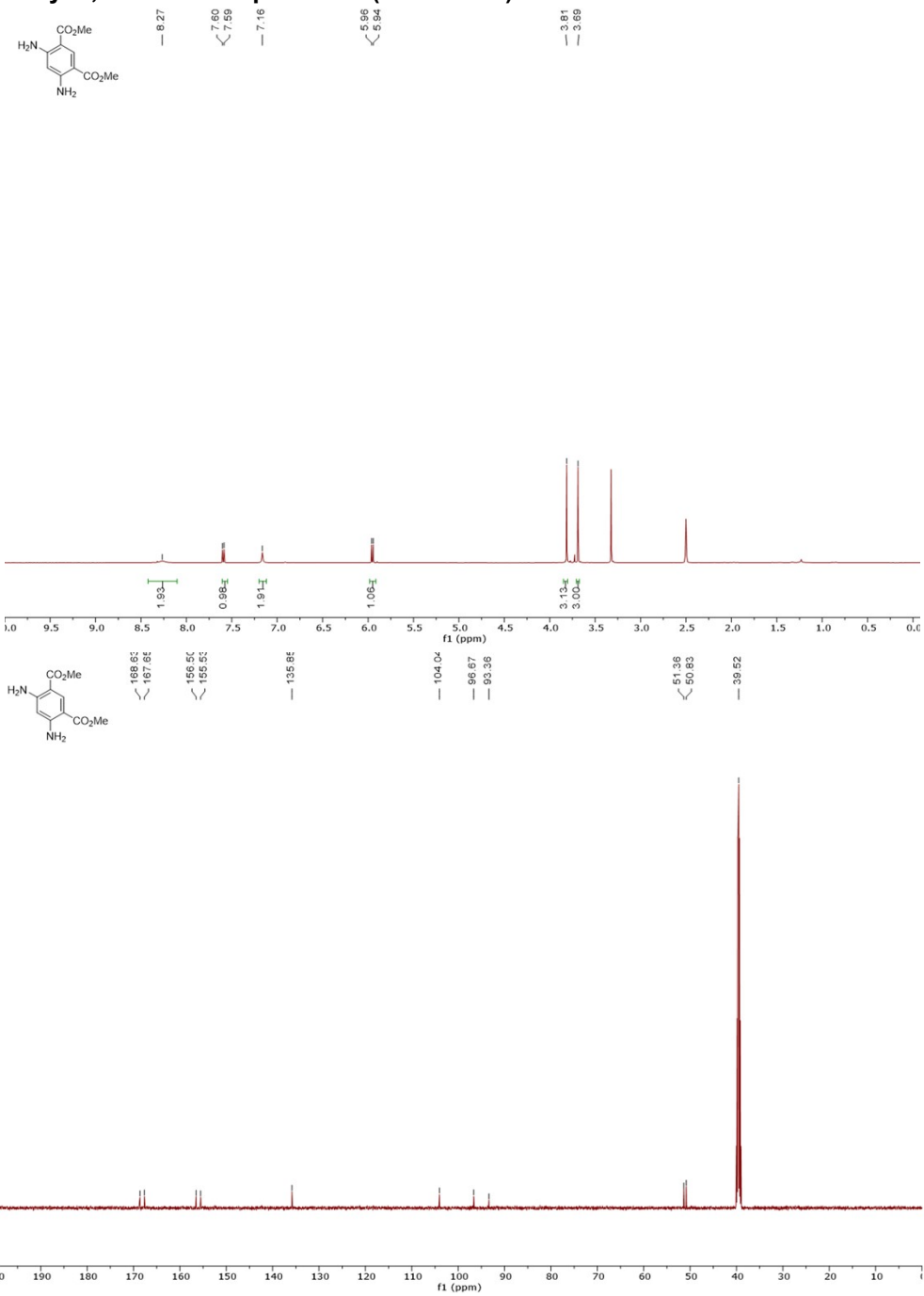


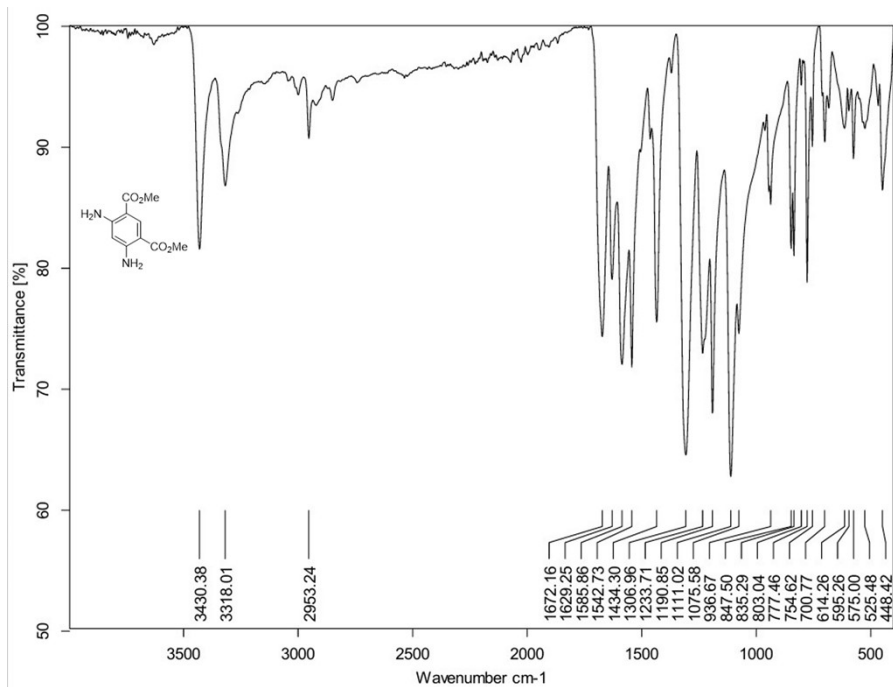
Dimethyl 4,5-diaminoisophthalate (1E2A3A5E)



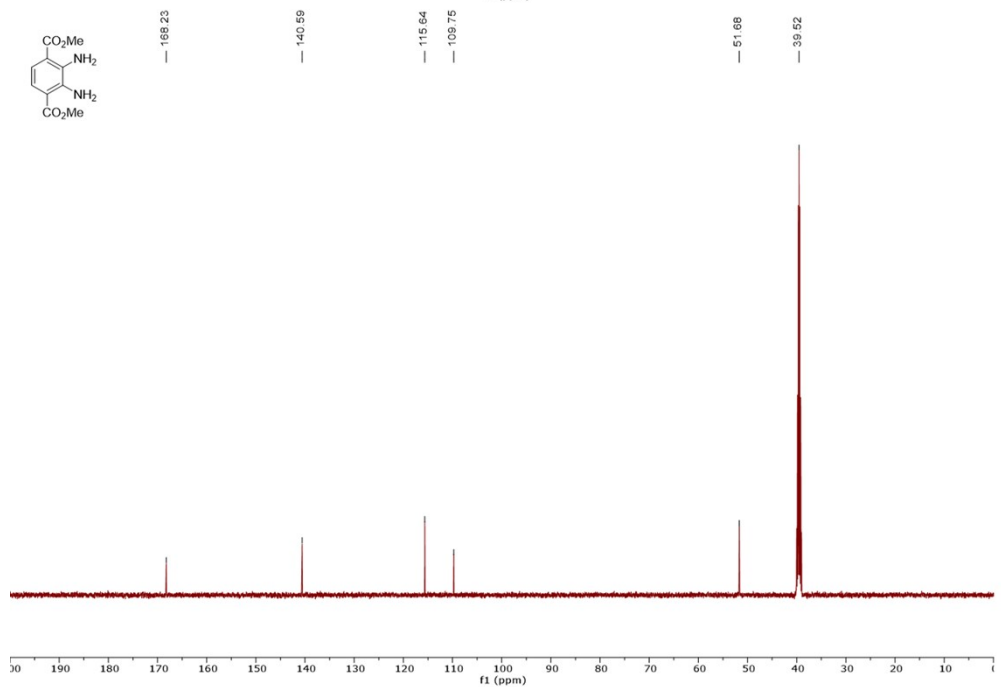
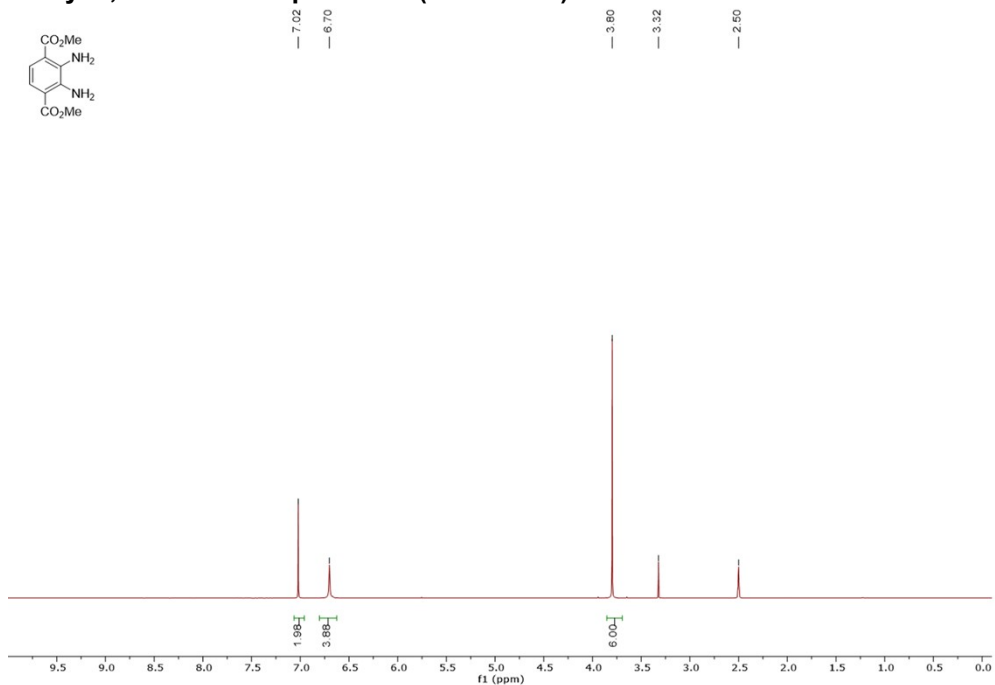


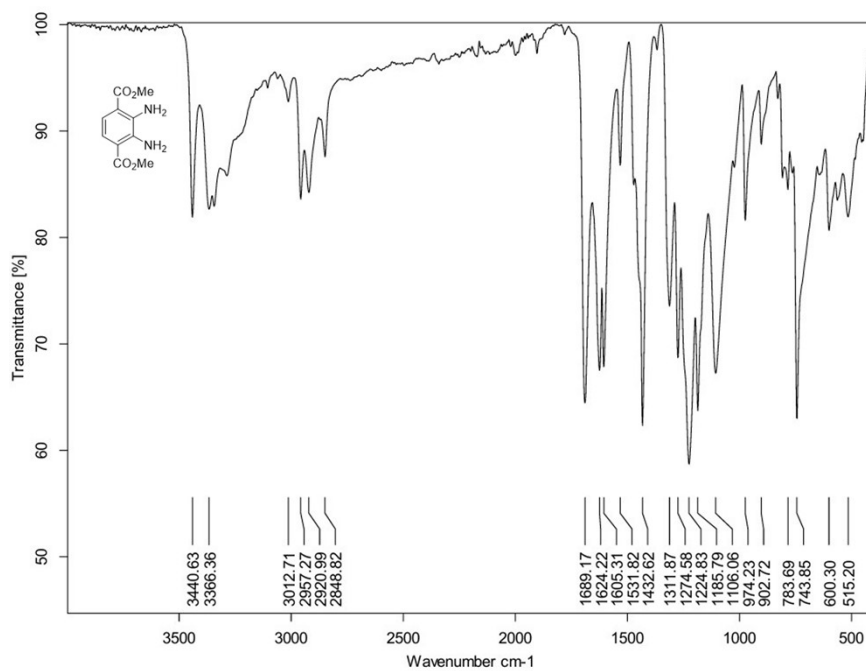
Dimethyl 4,6-diaminoisophthalate (1E2A4A5E)



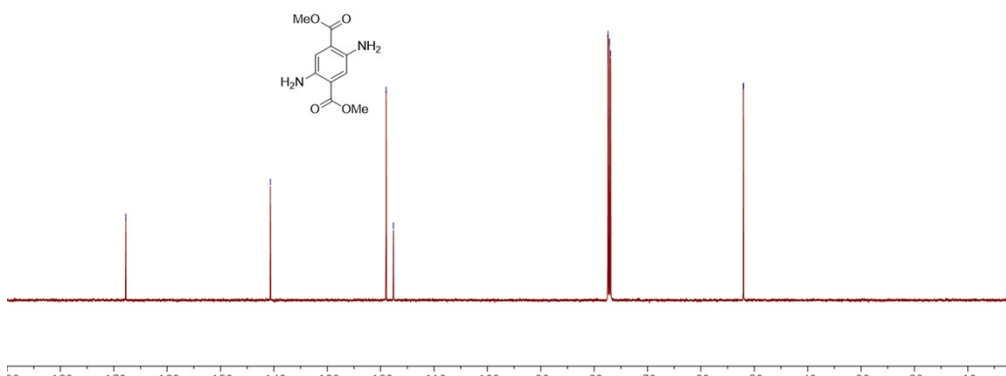
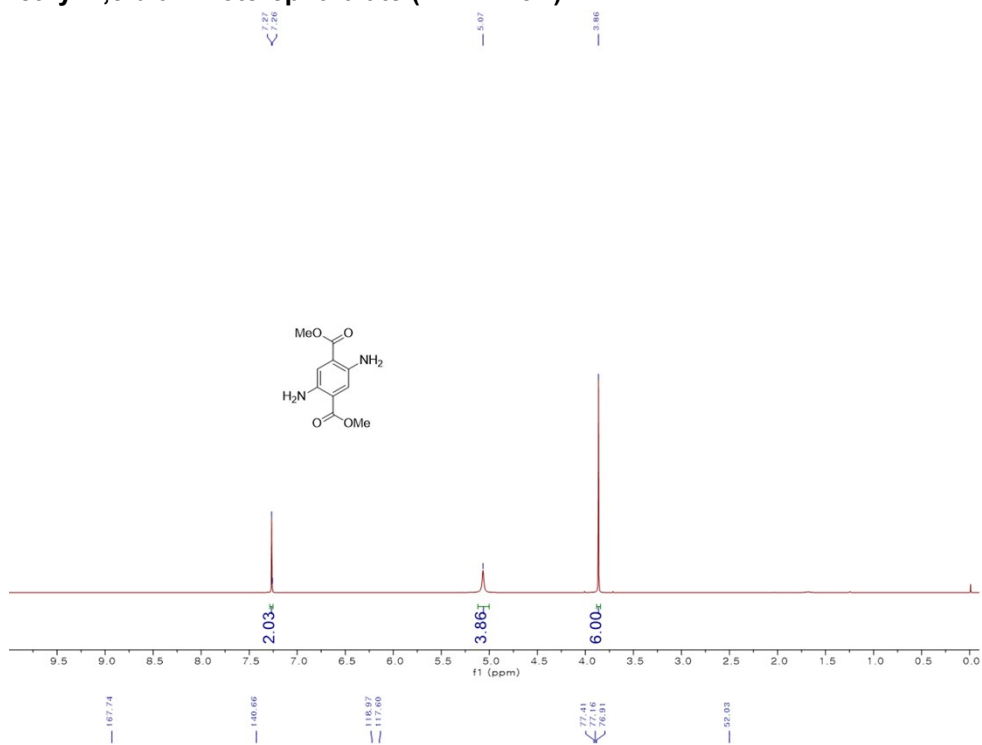


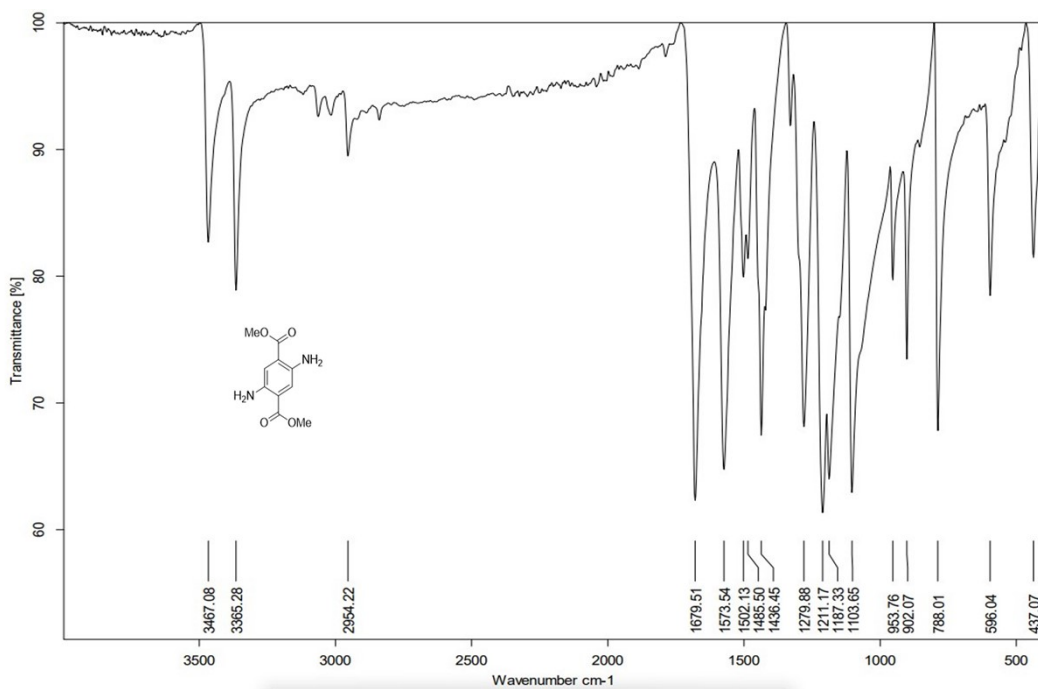
Dimethyl 2,3-diaminoterephthalate (1E2A3A4E)



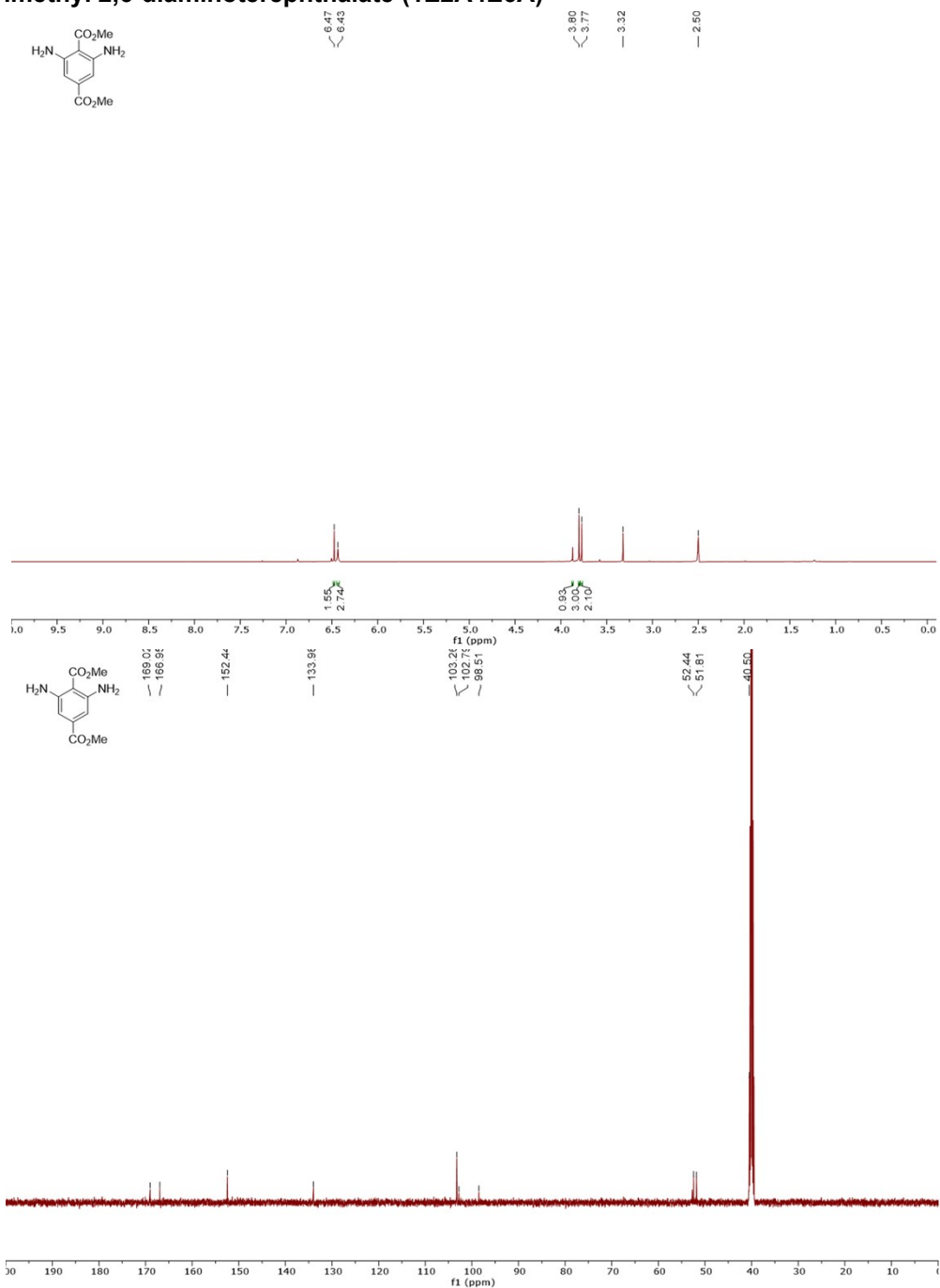
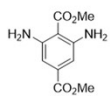


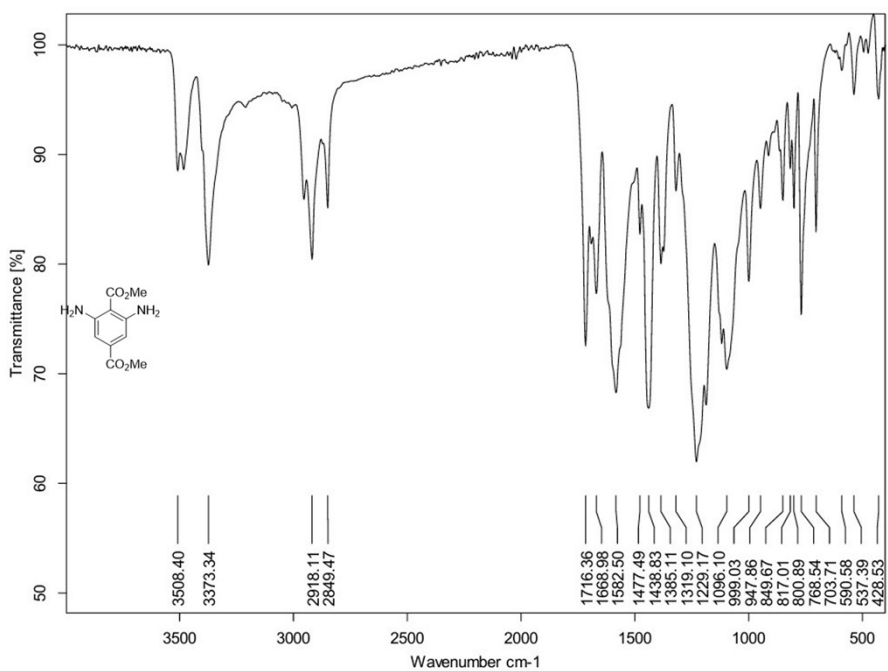
Dimethyl 2,5-diaminoterephthalate (1E2A4E5A)



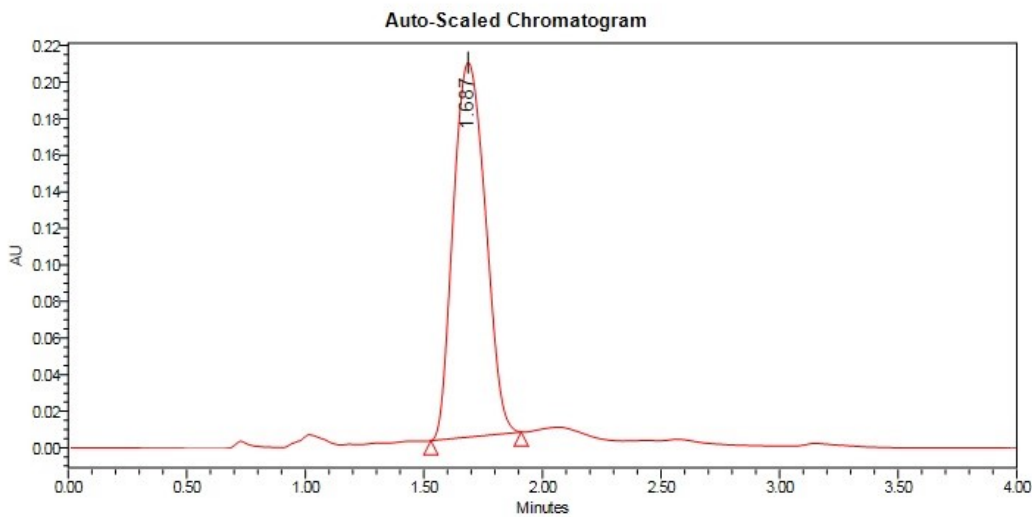


Dimethyl 2,6-diaminoterephthalate (1E2A4E6A)





[Additional HPLC data to check purity of **1E2A4E6A**]



Appendix II

Crystal data for 1E2E4A

Table AP1. Crystal data and structure refinement for **1E2E4A**

_Empirical formula	C ₁₀ H ₁₁ N O ₄
Formula weight	209.20
Temperature	253(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	<i>P</i> -1
Unit cell dimensions	<i>a</i> = 8.831(6) Å, α = 73.42(2)° <i>b</i> = 9.067(6) Å, β = 81.83(2)° <i>c</i> = 13.811(9) Å, γ = 86.68(2)°
Volume	1049.0(12) Å ³
Z	4
Density (calculated)	1.325 Mg/m ³
Absorption coefficient	0.104 mm ⁻¹
F(000)	440
Crystal size	0.116 x 0.053 x 0.048 mm ³
Theta range for data collection	2.421 to 26.000°.
Index ranges	-10 ≤ <i>h</i> ≤ 10, -11 ≤ <i>k</i> ≤ 11, -16 ≤ <i>l</i> ≤ 16
Reflections collected	28678
Independent reflections	4081 [R(int) = 0.0880]
Completeness to theta = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7453 and 0.6624
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4081 / 0 / 287
Goodness-of-fit on F ²	1.039
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	R1 = 0.0491, wR2 = 0.1293
R indices (all data)	R1 = 0.0828, wR2 = 0.1530
Largest diff. peak and hole	0.217 and -0.212 e·Å ⁻³

Table AP2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1E2E4A** U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(1)	226(2)	7870(2)	1520(1)	61(1)
C(2)	807(2)	7269(2)	2422(1)	45(1)
C(3)	709(2)	5690(2)	2942(1)	48(1)
C(4)	1322(2)	5102(2)	3841(1)	45(1)
C(5)	2037(2)	6052(2)	4277(1)	42(1)
C(6)	2093(2)	7644(2)	3778(1)	43(1)
C(7)	1496(2)	8236(2)	2863(1)	47(1)
C(8)	2781(2)	5428(2)	5208(1)	45(1)
O(9)	3507(2)	6189(2)	5567(1)	69(1)
O(10)	2592(2)	3909(2)	5614(1)	54(1)
C(11)	3268(3)	3223(3)	6540(2)	61(1)
C(12)	2738(2)	8801(2)	4194(2)	49(1)
O(13)	3938(2)	9450(2)	3845(1)	63(1)
O(14)	1750(2)	9117(2)	4939(1)	64(1)
C(15)	2225(3)	10266(3)	5379(2)	77(1)
N(21)	5295(3)	7138(3)	6937(2)	66(1)
C(22)	5868(2)	6525(2)	7841(1)	48(1)
C(23)	5950(2)	4937(2)	8299(2)	51(1)
C(24)	6575(2)	4362(2)	9194(2)	49(1)
C(25)	7127(2)	5338(2)	9690(1)	43(1)
C(26)	6983(2)	6940(2)	9251(1)	43(1)
C(27)	6390(2)	7517(2)	8340(1)	47(1)
C(28)	7851(2)	4739(2)	10625(2)	46(1)
O(29)	8416(2)	5534(2)	11047(1)	65(1)
O(30)	7844(2)	3197(2)	10975(1)	62(1)
C(31)	8566(3)	2534(3)	11885(2)	70(1)
C(32)	7398(2)	8117(2)	9745(2)	48(1)
O(33)	8527(2)	8898(2)	9466(1)	70(1)
O(34)	6288(2)	8286(2)	10476(1)	59(1)
C(35)	6517(3)	9465(3)	10960(2)	73(1)

Table AP3. Bond lengths [Å] and angles [°] for **1E2E4A**

N(1)-C(2)	1.368(2)	N(21)-C(22)	1.369(3)
N(1)-H(1A)	0.89(3)	N(21)-H(21A)	0.82(3)
N(1)-H(1B)	0.85(3)	N(21)-H(21B)	0.91(3)
C(2)-C(7)	1.408(3)	C(22)-C(23)	1.400(3)
C(2)-C(3)	1.409(3)	C(22)-C(27)	1.410(3)
C(3)-C(4)	1.378(3)	C(23)-C(24)	1.377(3)
C(3)-H(3)	0.9400	C(23)-H(23)	0.9400
C(4)-C(5)	1.404(2)	C(24)-C(25)	1.408(2)
C(4)-H(4)	0.9400	C(24)-H(24)	0.9400
C(5)-C(6)	1.411(3)	C(25)-C(26)	1.411(3)
C(5)-C(8)	1.479(2)	C(25)-C(28)	1.471(3)
C(6)-C(7)	1.390(3)	C(26)-C(27)	1.382(3)
C(6)-C(12)	1.505(3)	C(26)-C(32)	1.506(3)
C(7)-H(7)	0.9400	C(27)-H(27)	0.9400
C(8)-O(9)	1.212(2)	C(28)-O(29)	1.214(2)
C(8)-O(10)	1.341(2)	C(28)-O(30)	1.342(2)
O(10)-C(11)	1.448(2)	O(30)-C(31)	1.449(3)
C(11)-H(11A)	0.9700	C(31)-H(31A)	0.9700
C(11)-H(11B)	0.9700	C(31)-H(31B)	0.9700
C(11)-H(11C)	0.9700	C(31)-H(31C)	0.9700
C(12)-O(13)	1.211(3)	C(32)-O(33)	1.209(2)
C(12)-O(14)	1.337(3)	C(32)-O(34)	1.339(3)
O(14)-C(15)	1.454(2)	O(34)-C(35)	1.449(2)
C(15)-H(15A)	0.9700	C(35)-H(35A)	0.9700
C(15)-H(15B)	0.9700	C(35)-H(35B)	0.9700
C(15)-H(15C)	0.9700	C(35)-H(35C)	0.9700
C(2)-N(1)-H(1A)	116.9(18)	C(7)-C(6)-C(5)	120.48(17)
C(2)-N(1)-H(1B)	116.5(18)	C(7)-C(6)-C(12)	115.86(17)
H(1A)-N(1)-H(1B)	125(3)	C(5)-C(6)-C(12)	123.64(16)
N(1)-C(2)-C(7)	120.23(19)	C(6)-C(7)-C(2)	120.89(19)
N(1)-C(2)-C(3)	121.47(17)	C(6)-C(7)-H(7)	119.6
C(7)-C(2)-C(3)	118.29(17)	C(2)-C(7)-H(7)	119.6
C(4)-C(3)-C(2)	120.66(17)	O(9)-C(8)-O(10)	122.88(18)
C(4)-C(3)-H(3)	119.7	O(9)-C(8)-C(5)	124.30(19)
C(2)-C(3)-H(3)	119.7	O(10)-C(8)-C(5)	112.81(16)
C(3)-C(4)-C(5)	121.45(19)	C(8)-O(10)-C(11)	115.88(16)
C(3)-C(4)-H(4)	119.3	O(10)-C(11)-H(11A)	109.5
C(5)-C(4)-H(4)	119.3	O(10)-C(11)-H(11B)	109.5
C(4)-C(5)-C(6)	118.17(17)	H(11A)-C(11)-H(11B)	109.5
C(4)-C(5)-C(8)	122.17(18)	O(10)-C(11)-H(11C)	109.5

C(6)-C(5)-C(8)	119.60(16)	H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5	O(30)-C(31)-H(31B)	109.5
O(13)-C(12)-O(14)	124.44(19)	H(31A)-C(31)-H(31B)	109.5
O(13)-C(12)-C(6)	124.4(2)	O(30)-C(31)-H(31C)	109.5
O(14)-C(12)-C(6)	110.94(19)	H(31A)-C(31)-H(31C)	109.5
C(12)-O(14)-C(15)	116.02(19)	H(31B)-C(31)-H(31C)	109.5
O(14)-C(15)-H(15A)	109.5	O(33)-C(32)-O(34)	123.90(19)
O(14)-C(15)-H(15B)	109.5	O(33)-C(32)-C(26)	124.6(2)
H(15A)-C(15)-H(15B)	109.5	O(34)-C(32)-C(26)	111.26(18)
O(14)-C(15)-H(15C)	109.5	C(32)-O(34)-C(35)	116.16(19)
H(15A)-C(15)-H(15C)	109.5	O(34)-C(35)-H(35A)	109.5
H(15B)-C(15)-H(15C)	109.5	O(34)-C(35)-H(35B)	109.5
C(22)-N(21)-H(21A)	121(2)	H(35A)-C(35)-H(35B)	109.5
C(22)-N(21)-H(21B)	120.7(18)	O(34)-C(35)-H(35C)	109.5
H(21A)-N(21)-H(21B)	118(3)	H(35A)-C(35)-H(35C)	109.5
N(21)-C(22)-C(23)	122.36(19)	H(35B)-C(35)-H(35C)	109.5
N(21)-C(22)-C(27)	119.4(2)		
C(23)-C(22)-C(27)	118.23(18)		
C(24)-C(23)-C(22)	120.68(18)		
C(24)-C(23)-H(23)	119.7		
C(22)-C(23)-H(23)	119.7		
C(23)-C(24)-C(25)	121.67(19)		
C(23)-C(24)-H(24)	119.2		
C(25)-C(24)-H(24)	119.2		
C(24)-C(25)-C(26)	117.52(18)		
C(24)-C(25)-C(28)	122.20(18)		
C(26)-C(25)-C(28)	120.27(16)		
C(27)-C(26)-C(25)	120.79(17)		
C(27)-C(26)-C(32)	115.93(17)		
C(25)-C(26)-C(32)	123.24(16)		
C(26)-C(27)-C(22)	121.01(19)		
C(26)-C(27)-H(27)	119.5		
C(22)-C(27)-H(27)	119.5		
O(29)-C(28)-O(30)	122.21(19)		
O(29)-C(28)-C(25)	124.47(19)		
O(30)-C(28)-C(25)	113.32(16)		
C(28)-O(30)-C(31)	115.97(17)		
O(30)-C(31)-H(31A)	109.5		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1 #2 x-1,y,z-

Table AP4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1E2E4A** The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*U^{11} + \dots + 2hk a^* b^* U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
N(1)	72(1)	58(1)	56(1)	-9(1)	-30(1)	-14(1)
C(2)	44(1)	50(1)	44(1)	-14(1)	-12(1)	-3(1)
C(3)	47(1)	54(1)	48(1)	-20(1)	-12(1)	-8(1)
C(4)	47(1)	43(1)	45(1)	-13(1)	-7(1)	-6(1)
C(5)	40(1)	47(1)	41(1)	-16(1)	-8(1)	0(1)
C(6)	42(1)	45(1)	47(1)	-18(1)	-12(1)	-1(1)
C(7)	48(1)	46(1)	50(1)	-12(1)	-15(1)	-2(1)
C(8)	47(1)	46(1)	45(1)	-16(1)	-10(1)	0(1)
O(9)	91(1)	58(1)	67(1)	-15(1)	-43(1)	-7(1)
O(10)	66(1)	49(1)	48(1)	-10(1)	-20(1)	0(1)
C(11)	73(2)	57(1)	51(1)	-6(1)	-20(1)	5(1)
C(12)	56(1)	43(1)	52(1)	-16(1)	-22(1)	4(1)
O(13)	62(1)	58(1)	77(1)	-24(1)	-20(1)	-10(1)
O(14)	71(1)	66(1)	67(1)	-36(1)	-14(1)	-1(1)
C(15)	102(2)	71(2)	77(2)	-45(1)	-26(1)	2(1)
N(21)	85(2)	63(1)	58(1)	-20(1)	-29(1)	-11(1)
C(22)	45(1)	58(1)	45(1)	-19(1)	-8(1)	-5(1)
C(23)	54(1)	54(1)	52(1)	-25(1)	-3(1)	-14(1)
C(24)	53(1)	45(1)	52(1)	-18(1)	-2(1)	-10(1)
C(25)	43(1)	42(1)	47(1)	-16(1)	-3(1)	-7(1)
C(26)	42(1)	45(1)	45(1)	-16(1)	-7(1)	-6(1)
C(27)	50(1)	44(1)	50(1)	-15(1)	-12(1)	-4(1)
C(28)	46(1)	44(1)	51(1)	-15(1)	-6(1)	-4(1)
O(29)	82(1)	51(1)	70(1)	-16(1)	-34(1)	-8(1)
O(30)	83(1)	43(1)	63(1)	-12(1)	-23(1)	-5(1)
C(31)	87(2)	56(1)	66(1)	-9(1)	-25(1)	6(1)
C(32)	59(1)	39(1)	47(1)	-9(1)	-20(1)	-5(1)
O(33)	84(1)	65(1)	64(1)	-18(1)	-13(1)	-33(1)
O(34)	66(1)	59(1)	65(1)	-33(1)	-14(1)	2(1)
C(35)	101(2)	60(1)	78(2)	-41(1)	-42(2)	23(1)

Table AP5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1E2E4A**.

	x	y	z	U(eq)
H(1A)	520(30)	8810(30)	1150(20)	91
H(1B)	-190(30)	7230(30)	1290(20)	91
H(3)	2215030	267357		
H(4)	12614041	416954		
H(7)	15549297	253457		
H(11A)	30062144	679792		
H(11B)	28783750	704792		
H(11C)	43713315	639592		
H(15A)	142510423	5900115		
H(15B)	241211228	4849115		
H(15C)	31569914	5679115		
H(21A)	4990(30)	6580(30)	6630(20)	98
H(21B)	5290(30)	8170(30)	6640(20)	98
H(23)	55754255	799261		
H(24)	66343290	948159		
H(27)	63358588	804856		
H(31A)	84851422	12080105		
H(31B)	80612927	12434105		
H(31C)	96372807	11750105		
H(35A)	56769460	11495110		
H(35B)	655710464	10457110		
H(35C)	74719260	11250110		

Table AP6. Hydrogen bonds for **1E2E4A** [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	\angle (DHA)
N(1)-H(1A)...O(33)#1	0.89(3)	2.17(3)	3.054(3)	168(2)
N(1)-H(1B)...O(29)#2	0.85(3)	2.15(3)	2.991(3)	166(3)
N(21)-H(21A)...O(9)	0.82(3)	2.21(3)	2.958(3)	151(3)
N(21)-H(21B)...O(13)#1	0.91(3)	2.18(3)	3.053(3)	159(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1 #2 x-1,y,z-1

Appendix III

**Cartesian coordinates for the
optimized structures (1E4A,
1E2A4E5A, 1E2E3A, and 1E2E4A)**

1E4A (GS)

C	-0.449354	1.293427	0.361146
C	-1.813681	0.092587	0.437956
C	-2.377748	-0.124167	0.023158
C	-1.52608	-1.124053	-0.469096
C	-0.158635	-0.920185	-0.521497
C	0.404974	0.286709	-0.099101
C	1.849756	0.604658	-0.225527
O	2.248116	1.719939	-0.473738
O	2.764623	-0.385595	-0.103242
C	2.552855	-1.530303	0.722627
N	-3.736238	-0.347248	0.138197
H	-0.021211	2.244588	0.658486
H	-2.460003	1.88006	0.814676
H	-1.947913	-2.063877	-0.813294
H	0.471612	-1.703864	-0.927472
H	3.472495	-1.676268	1.292165
H	1.718219	-1.385825	1.410102
H	2.370982	-2.414221	0.106559
H	-4.122643	-1.071691	-0.45105
H	-4.322314	0.47504	0.180305

1E4A (ES)

C	0.581058	1.334282	0.080461
C	1.943324	1.133224	0.174376
C	2.499565	-0.145299	0.046038
C	1.63363	-1.225693	-0.186473
C	0.271867	-1.044234	-0.280903
C	-0.298345	0.246594	-0.145477
C	-1.680109	0.441575	-0.23876
O	-2.347565	1.566885	-0.129345
O	-2.58064	-0.559265	-0.476324
C	-3.323852	-1.010396	0.669332
N	3.882838	-0.335387	0.085677
H	0.178981	2.33628	0.183651
H	2.59903	1.98338	0.344969
H	2.049681	-2.22343	-0.301897
H	-0.37507	-1.893594	-0.470115
H	-3.839463	-1.915418	0.346819
H	-2.642037	-1.233506	1.494509
H	-4.053465	-0.259843	0.977922
H	4.173697	-1.263060	0.364185
H	4.391589	0.375623	0.593995

1E2A4E5A (GS)

C	1.38751	-0.15423	0.0728
C	0.83852	1.14627	0.23898
N	1.61291	2.24952	0.49798
C	-0.55574	1.25219	0.15341
H	-1.0239	2.2194	0.27463
C	-1.38922	0.15468	-0.0741
C	-2.85416	0.36627	-0.12492
O	-3.68779	-0.51976	-0.25201
O	-3.21007	1.65266	-0.0112
C	-4.61391	1.92429	-0.04056
C	-0.84023	-1.14582	-0.24027
N	-1.61462	-2.24908	-0.49927
C	0.55403	-1.25175	-0.1547
H	1.02219	-2.21896	-0.27593
O	3.20835	-1.65223	0.00991
C	4.61219	-1.92387	0.03926
O	3.68608	0.52019	0.25069
H	4.69929	-3.004	-0.06465
H	5.04491	-1.59363	0.98573
H	5.11641	-1.41731	-0.7862
H	-4.70102	3.00442	0.06338
H	-5.11813	1.41772	0.78489
H	-5.04662	1.59407	-0.98703
C	-1.08574	-3.59049	-0.49451
H	-0.36516	-3.74361	-1.3074
H	-1.91178	-4.28642	-0.64672
H	-0.5906	-3.8447	0.45405
H	-2.61071	-2.11468	-0.41096
C	1.08402	3.59094	0.49318
H	0.36342	3.74407	1.30606
H	0.58889	3.84512	-0.45539
H	1.91006	4.28687	0.64539
H	2.60899	2.11513	0.40964

1E2A4E5A (ES)

C 2.869259429 -0.3440283917 0.1287134247
C 1.43429463 -0.1720048823 0.0638828802
C 0.8218380826 1.133789635 0.1837100747
N 1.615897337 2.210316663 0.3599754439
C -0.5764052294 1.267366467 0.116452108
H -1.016557807 2.25136825 0.2072919182
C -1.436011677 0.1724425452 -0.0651897601
C -2.870976498 0.3444659678 -0.1300198125
O -3.712704771 -0.5550425459 -0.2886163785
O -3.258029486 1.634697701 0.0023578769
C -4.661918707 1.876512456 -0.0531079997
C -0.8235551002 -1.133351908 -0.1850175466
N -1.617614312 -2.209878854 -0.361283588
C 0.5746881931 -1.266928776 -0.1177592233
H 1.014840786 -2.250930546 -0.2085991002
O 3.256312316 -1.634260249 -0.0036633206
C 4.66020149 -1.876075132 0.0518031697
O 3.710987738 0.555480138 0.2873096959
H 4.774666225 -2.952447436 -0.0715768345
H 5.070442873 -1.558524124 1.013374766
H 5.177309918 -1.344780411 -0.750795054
H -4.776383542 2.952884639 0.0702729658
H -5.179026836 1.34521697 0.7494899101
H -5.072160329 1.558962228 -1.014679752
C -1.151393415 -3.568001989 -0.4985929618
H -0.4978526488 -3.676790739 -1.371814832
H -2.016223508 -4.218244921 -0.6263028977
H -0.5982979437 -3.88963703 0.3913809392
H -2.616565895 -2.001089165 -0.3963947198
C 1.149676476 3.568439914 0.4972837248
H 0.4961356909 3.677229387 1.370505492
H 0.5965810281 3.890074245 -0.3926904501
H 2.014506579 4.218682929 0.6249931678
H 2.614848912 2.001526965 0.3950866734

1E2E3A (GS)

C	-2.9823	0.474278		-0.89786
C	-1.604980	0.382325		-0.62676
C	-0.886841	0.573829		-0.38471
C	-1.572382	0.802917		-0.40333
C	-2.924172	0.870334		-0.69062
C	-3.625811	0.692451		-0.93803
H	-3.53355	-0.44108	-1.095	
H	-3.416343	0.835234		-0.71129
H	-4.688111	0.729929		-1.15849
C	-0.907744	0.102688		-0.06724
O	-1.028845	0.11223	-0.71676	
O	-0.251574	0.041751		1.101369
C	0.479857		5.21925	1.439842
H	0.917589		5.024812	2.418369
H	1.262291		5.397324	0.698783
H	-0.181766	0.086705		1.479514
C	0.592216		1.611226	-0.24836
O	1.293264		2.522629	-0.61943
O	1.114883		0.506724	0.335825
C	2.540468		0.505307	0.453075
H	2.796576		-0.442110	0.925788
H	3.005873		0.585101	-0.5311
H	2.8694	1.343349		1.069743
N	-1.00219	-0.85544	-0.68316	
H	-0.13274	-0.95607	-0.18188	
H	-1.6217	-1.65012	-0.63393	

1E2E3A (ES)

C	-2.9823	0.474278		-0.89786
C	-1.604980	0.382325		-0.62676
C	-0.886841	0.573829		-0.38471
C	-1.572382	0.802917		-0.40333
C	-2.924172	0.870334		-0.69062
C	-3.625811	0.692451		-0.93803
H	-3.53355	-0.44108	-1.095	
H	-3.416343	0.835234		-0.71129
H	-4.688111	0.729929		-1.15849
C	-0.907744	0.102688		-0.06724
O	-1.028845	0.11223	-0.71676	
O	-0.251574	0.041751		1.101369
C	0.479857		5.21925	1.439842
H	0.917589		5.024812	2.418369
H	1.262291		5.397324	0.698783
H	-0.181766	0.086705		1.479514
C	0.592216		1.611226	-0.24836
O	1.293264		2.522629	-0.61943
O	1.114883		0.506724	0.335825
C	2.540468		0.505307	0.453075
H	2.796576		-0.442110	0.925788
H	3.005873		0.585101	-0.5311
H	2.8694	1.343349		1.069743
N	-1.00219	-0.85544	-0.68316	
H	-0.13274	-0.95607	-0.18188	
H	-1.6217	-1.65012	-0.63393	

1E2E4A (GS)

C	2.831719	-0	0.209312	0.090983
C	1.798849		0.733164	0.022415
C	0.471892		0.337578	-0.076835
C	0.142975		-1.025326	-0.09062
C	1.175981		-1.958366	-0.052539
C	2.50008	-1.567183	0.039143	
H	0.918212		-3.011358	-0.084619
H	3.287616		-2.314776	0.071022
C	-1.245313	-1.559898	-0.094195	
O	-1.580097	-2.572182	-0.665386	
O	-2.072485	-0.843821	0.682237	
C	-3.439234	-1.249707	0.645402	
H	-3.963431	-0.58524	1.33129	
H	-3.837014	-1.144235	-0.366214	
H	-3.540728	-2.289367	0.963111	
C	-0.565544	1.386172	-0.318418	
O	-1.513069	1.262314	-1.055654	
O	-0.290432	2.526776	0.33918	
C	-1.202973	3.596845	0.091292	
H	-0.843869	4.435316	0.686745	
H	-1.214235	3.854481	-0.969964	
H	-2.212801	3.314352	0.395422	
H	2.035837	1.791555	0.022492	
N	4.153695	0.200833	0.14422	
H	4.317047	1.130934	0.502325	
H	4.815558	-0.475989	0.496065	

1E2E4A (ES)

C	-2.762257	-0.24039	-0.180917
C	-1.739505	0.709447	-0.361301
C	-0.424776	0.419713	0.054281
C	-0.143823	-0.986311	0.239738
C	-1.177079	-1.906645	0.488716
C	-2.49875	-1.552782	0.322791
H	-0.896598	-2.921613	0.748671
H	-3.311184	-2.250733	0.489973
C	1.223401	-1.539996	0.126354
O	1.646377	-2.387353	0.88807
O	1.904697	-1.053187	-0.912741
C	3.292052	-1.383589	-0.93671
H	3.683976	-0.943065	-1.852668
H	3.78617	-0.950097	-0.064797
H	3.43498	-2.466283	-0.938472
C	0.594458	1.408009	0.275747
O	1.724063	1.187872	0.705306
O	0.167425	2.670662	-0.038521
C	1.128154	3.689239	0.192657
H	0.646358	4.626203	-0.08986
H	1.4243	3.718014	1.244619
H	2.024599	3.527605	-0.411877
H	-1.96896	1.673154	-0.804781
N	-4.036733	0.077093	-0.505588
H	-4.272941	0.991702	-0.861025
H	-4.785319	-0.588663	-0.385699