Supporting Information

Photolytic amino etherification reactions of aryldiazoacetates with N-heterocycles and stoichiometric amount of dioxane in aqueous medium: Synthesis of 1, 4-dioxepane/ 1, 4, 7-dioxazonan-6-one systems

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Content

1. Synthetic Procedures:

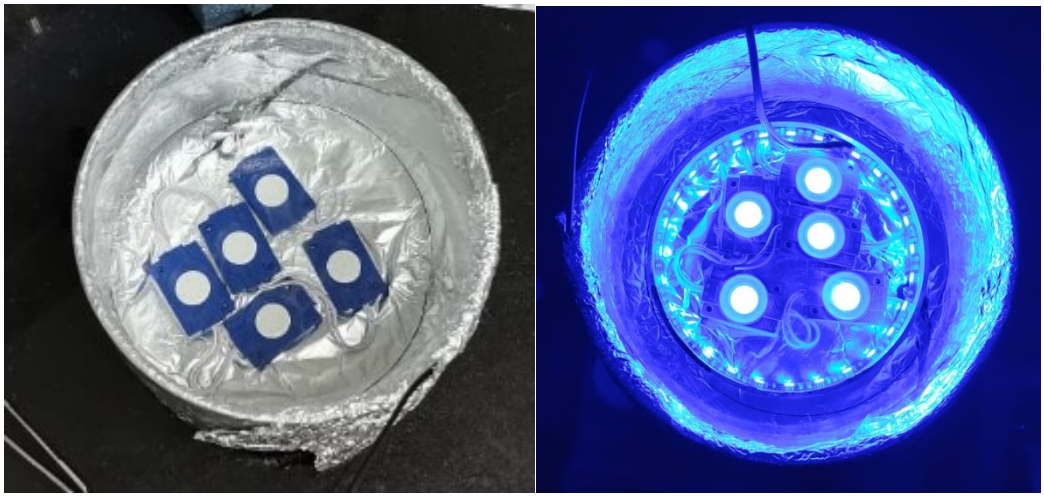
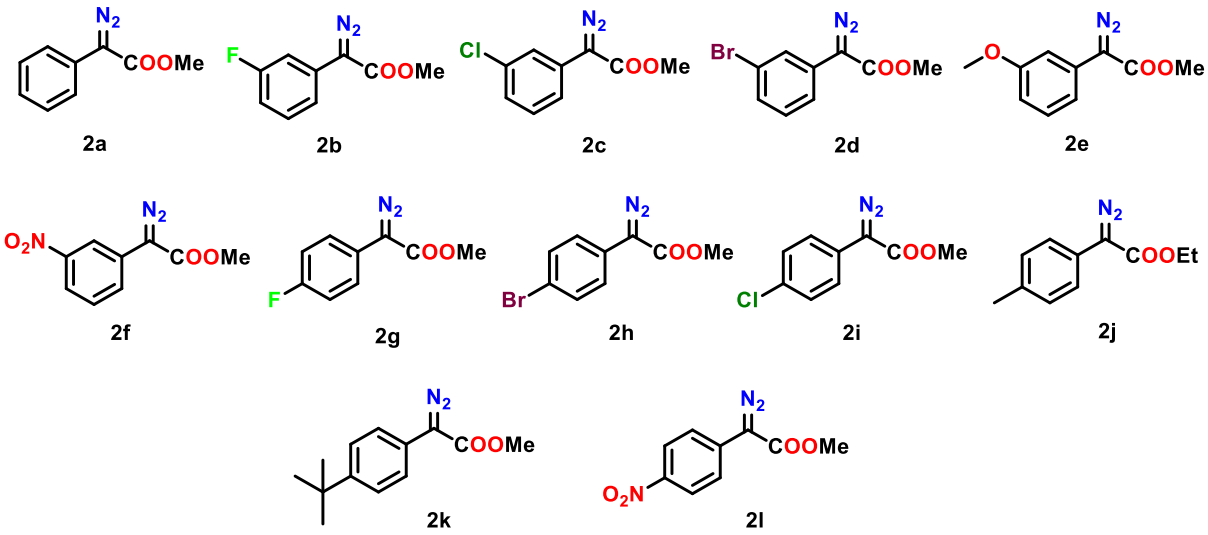
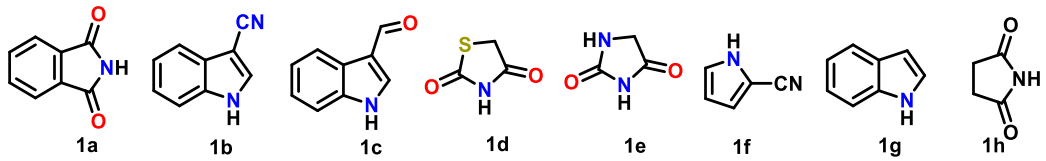


Figure SS1: Blue LED Reaction Set-up for gram scale synthesis.



Scheme S1: Structures of aryl diazoesters used in this study.



Scheme S2: Structures of various heterocycles.

1.2. General experimental Procedure

All blue light reactions were carried out under air as specified. Photochemical Reactor Aldrich® Micro Photochemical Reactor, blue LED lights (ALDKIT001-1EA). LED light is IP68 double density 12V DC water proof blue light with spectral range of 435-445 nm with wall plug power supply 500mA with 5-6 watts. The irradiation vessel material is borosilicate glass. The distance of irradiation vessel from light source is 2 cm. Reactions were monitored through TLC by visualising in UV detector. All purifications were done in silica gel (100-200 mesh size) column chromatography. All ^{1}H and ^{13}C NMR spectra were recorded taking tetramethylsilane (TMS) as an internal standard at ambient temperature unless otherwise indicated with Bruker 400 MHz instruments at 400 MHz for ^{1}H and 100 MHz for ^{13}C NMR spectroscopy. Splitting patterns are designated as singlet (s), broad singlet (br s), doublet (d), triplet (t), quartet (q), quintet (quin) doublet of doublets (dd) and triplet of doublets (td). Splitting patterns that could not be interpreted or easily visualized are designated as multiplet (m). Ultra-performance liquid chromatography (UPLC) was carried out using an Agilent 6540 accurate–mass Q-TOF LC/MS (Agilent Technologies, U.S.A.). Liquid chromatographic separations ware performed at room temperature of 25 °C, using a UPLC C18 analytical column. MS analyses were performed under the following operation parameters: dry gas temperature 350 °C, dry gas (N_2) flow rate 10 L/min, nebulizer pressure 30 psi, Vcap 4000 and fragmentor voltage 100 V. Mass spectra were acquired in the positive ion mode by scanning from 100 to 1500 in the mass to charge ratio (m/z). The mobile phase composition used for UHPLC–QTOF MS comprised of H_2O (A) and ACN (B), with optimized linear gradient elution. The injection volume was 5 µL. The flow rate was set at 0.3 mL/min. Accurate mass analysis calibration was carried out by ESI-low concentration tuning mix solution provided by Agilent technologies, U.S.A. The accuracy error threshold was set at 5 ppm. High-performance liquid chromatography (HPLC) experiments were carried out on the Agilent 1290 infinity series of LC system (Agilent Technologies, U.S.A.) with photodiode-array/ELSD detector to monitor progess of the Blue LED mediated NH-insertion reaction of Indoles. High-performance liquid chromatography (HPLC) experiments were carried out on a Waters Alliance System (Milford, MA) consisting of e2695 separation module and a 2998 photodiode-array detector. The HPLC system was controlled with EMPOWER software (Waters Corporation, Milford, MA).

1.2. Characterization data

Methyl 2-(2-(2-(1,3-dioxoisoindolin-2-yl)ethoxy)ethoxy)-2-phenylacetate, (4a): 4a was synthesised using general procedure. **2a** (63.4 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **4a,** as colourless oil, (104.7 mg, 91%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.84-7.82 (m, 2H), 7.71-7.69 (m, 2H), 7.41-7.39 (m, 2H), 7.34-7.29 (m, 3H), 4.97 (s, 1H), 3.89 (t, J = 5.8 Hz, 2H), 3.77-3.72 (m, 2H), 3.70-3.68 (m, 3H), 3.66 (s, 3H), 3.65-3.56 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.4, 168.4, 136.5, 134.0, 132.2, 128.7, 128.6, 127.4, 123.4, 81.3, 70.4, 69.0, 68.2, 52.3, 37.5. HRMS (ESI-TOF) m/z calcd for $C_{21}H_{21}NO_6$ $[M+H]^+$ 384.1442, found 384.1456. FT-IR (Neat) ν_{max} (cm^{-1}) = 3297.63, 3229.22, 2914.24, 2852.65, 1712.62, 1389.40, 1260.88, 1171.60, 1101.13, 1028.56, 715.27.

Methyl 2-(3-bromophenyl)-2-(2-(2-(1,3-dioxoisoindolin-2-yl)ethoxy)ethoxy)acetate, (**4b**): **4b** was synthesised using general procedure. **2d** (91.8 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **4b,** colourless oil, (130.4 mg, 94%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.88-7.82 (m, 2H), 7.77-7.70 (m, 2H), 7.58 (s, 1H), 7.42 (d, J = 8.0 Hz, 1H), 7.35 (d, J = 7.6 Hz, 1H), 7.19 (t, J = 7.8 Hz, 1H), 4.96 (s, 1H), 3.90 (t, J = 5.6 Hz, 2H), 3.77-3.73 (m, 2H), 3.71-3.68 (m, 2H), 3.67 (s, 3H), 3.66-3.58 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 170.9, 168.4, 138.9, 134.5, 134.1, 132.2, 131.8, 130.4, 130.2, 125.9, 123.7, 122.7, 80.6, 70.4, 69.2, 68.2, 52.5, 37.5. HRMS (ESI-TOF) m/z calcd for $C_{21}H_{20}BrNO_6$ $[M+H]^+$ 462.0547, found 462.0551. FT-IR (Neat) ν_{max} (cm^{-1}) = 3300.94, 3233.94, 2915.60, 2853.69, 1710.16, 1389.85, 1257.84, 1174.84, 1101.82, 1024.18, 877.90, 768.58, 711.85, 528.17.

Methyl 2-(4-bromophenyl)-2-(2-(2-(1,3-dioxoisoindolin-2-yl)ethoxy)ethoxy)acetate, (**4c**): **4c** was synthesised using general procedure. **2h** (91.8 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **4c,** colourless oil, (131.76 mg, 95%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.87-7.81 (m, 2H), 7.76-7.69 (m, 2H), 7.41-7.36 (m, 2H), 7.02-6.97 (m, 2H), 4.96 (s, 1H), 3.89 (t, J = 5.6 Hz, 2H), 3.76-3.71 (m, 2H), 3.70-3.67 (m, 3H), 3.66 (s, 3H), 3.64-3.56 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 170.9, 168.2, 135.0, 134.4, 133.9, 128.7, 128.6, 123.2, 80.4, 70.3, 69.0, 68.1, 52.3, 37.4. HRMS (ESI-TOF) m/z calcd for $C_{21}H_{20}BrNO_6$ $[M+H]^+$ 462.0547, found 462.0538. FT-IR (Neat) ν_{max} (cm^{-1}) = 3067.75, 2918.32, 1706.51, 1606.50, 1507.65, 1388.83, 1212.89, 1097.78, 1018.59, 828.05, 713.76, 520.47.

Methyl 2-(4-chlorophenyl)-2-(2-(2-(1,3-dioxoisoindolin-2-yl)ethoxy)ethoxy)acetate, (**4d**): **4d** was synthesised using general procedure. **2i** (75.8 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for

2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **4d,** colourless oil, (115.3 mg, 92%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.86-7.84 (m, 2H), 7.74-7.72 (m, 2H), 7.37-7.36 (m, 2H), 7.32-7.28 (m, 2H), 4.98 (s, 1H), 3.91 (t, J = 5.6 Hz, 2H), 3.78-3.70 (m, 5H), 3.68 (s, 3H), 3.63-3.59 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.1, 168.4, 135.2, 134.6, 134.0, 132.3, 128.9, 128.7, 123.4, 80.6, 70.4, 69.1, 68.2, 52.4, 37.5. HRMS (ESI-TOF) m/z calcd for $C_{21}H_{20}ClNO_6$ $[M+H]^+$ 418.1052, found 418.1066. FT-IR (Neat) ν_{max} (cm^{-1}) = 2929.98, 2873.98, 1705.45, 1388.93, 1262.33, 1092.32, 1015.00, 872.43, 820.89, 771.52, 712.77, 615.26, 517.52.

Methyl 2-(2-(2-(1,3-dioxoisoindolin-2-yl)ethoxy)ethoxy)-2-(3-methoxyphenyl)acetate, (**4e**): **4e** was synthesised using general procedure. **2e** (74.2 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **4e,** colourless oil, (106.7 mg, 86%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.83-7.81 (m, 2H), 7.71-7.68 (m, 2H), 7.22 (t, J = 8.2 Hz, 1H), 6.98-6.96 (m, 2H), 6.84-6.81 (m, 1H), 4.94 (s, 1H), 3.89-3.86 (m, 2H), 3.78 (s, 3H), 3.74-3.71 (m, 2H), 3.70-3.67 (m, 2H), 3.65 (s, 3H), 3.64-3.56 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.3, 168.3, 159.8, 137.9, 133.9, 132.2, 129.6, 123.3, 119.8, 114.6, 112.4, 81.2, 70.3, 68.9, 68.1, 55.3, 52.3, 37.4. HRMS (ESI-TOF) m/z calcd for $C_{22}H_{23}NO_7$ $[M+H]^+$ 414.1547, found 414.1536. FT-IR (Neat) ν_{max} (cm^{-1}) = 2928.18, 2876.65, 1703.15, 1378.66, 1255.16, 1089.12, 1009.68, 870.25, 819.65, 770.62, 708.67, 605.12, 507.22.

Methyl 2-(2-(2-(1,3-dioxoisoindolin-2-yl)ethoxy)ethoxy)-2-(3-fluorophenyl)acetate, (**4f**): **4f** was synthesised using general procedure. **2b** (69.9 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20 ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **4f,** colourless oil, (109.6 mg, 91%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.77-7.75 (m, 2H), 7.65-7.62 (m, 2H), 7.24-7.18 (m, 1H), 7.13-7.06 (m, 2H), 6.91 (td, J = 8.1, 2.2 Hz, 1H), 4.91 (s, 1H), 3.82 (t, J = 5.8 Hz, 2H), 3.70-3.67 (m, 1H), 3.66-3.65 (m, 2H), 3.62-3.61 (m, 2H), 3.60 (s, 3H), 3.56-3.52 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 170.9, 168.4, 162.8 (d, J = 245.0Hz), 139.0 (d, J = 8.0Hz), 134.0, 132.2, 130.1 (d, J = 9.0Hz), 123.3, 122.9 (d, J = 3.0Hz), 115.6 (d, J = 21.0 Hz), 114.3 (d, J = 22.0 Hz), 80.57, 80.56, 70.4, 69.0, 68.1, 52.4, 37.4. ^{19}F NMR (376 MHz, CDCl3) δ = −112.7 (s, 1F). HRMS (ESI-TOF) m/z calcd for $C_{21}H_{20}FNO_6$ $[M+H]^+$ 402.1347, found 402.1351. FT-IR (Neat) ν_{max} (cm^{-1}) = 3303.86, 3231.72, 3067.73, 2916.39, 1708.94, 1596.48, 1389.94, 1247.55, 1105.18, 1021.29, 879.76, 788.75, 716.28, 525.56, 435.11.

Methyl 2-(3-chlorophenyl)-2-(2-(2-(1,3-dioxoisoindolin-2-yl)ethoxy)ethoxy)acetate, (4g): 4g was synthesised using general procedure. **2c** (75.8 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After

completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **4g,** colourless oil, (112.8 mg, 90%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.86-7.84 (m, 2H), 7.73-7.71 (m, 2H), 7.44 (s, 1H), 7.33-7.24 (m, 3H), 4.98 (s, 1H), 3.91 (t, *J* = 5.6 Hz, 2H), 3.76-3.71 (m, 5H), 3.69 (s, 3H), 3.67-3.60 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 170.5, 168.3, 148.4, 138.9, 134.1, 133.2, 132.15, 129.6, 123.5, 123.3, 122.4, 80.1, 70.5, 69.5, 68.3, 52.7, 37.5. HRMS (ESI-TOF) m/z calcd for $C_{21}H_{20}ClNO_6$ $[M+H]^+$ 418.1052, found 418.1047. FT-IR (Neat) ν_{max} (cm^{-1}) = 2928.21, 2876.45, 1703.05, 1378.48, 1254.68, 1090.02, 1010.18, 872.15, 821.01, 775.46, 710.21, 605.79, 510.12.

Methyl 2-(2-(2-(1,3-dioxoisoindolin-2-yl)ethoxy)ethoxy)-2-(3-nitrophenyl)acetate, **(4h)**: **4h** was synthesised using general procedure. **2f** (79.6 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **4h,** colourless oil, (120.7 g, 94%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 8.30(t, *J* = 2.0 Hz, 1H), 8.16-8.13 (m, 1H), 7.83-7.77 (m, 3H), 7.72-7.68 (m, 2H), 7.51 (t, *J* = 8 Hz, 1H), 5.13 (s, 1H), 3.88 (t, *J* = 5.6 Hz, 2H), 3.76-3.63 (m, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 170.9, 168.4, 138.6, 134.5, 134.0, 132.2, 129.9, 128.8, 127.4, 125.4, 123.3, 80.5, 70.4, 69.1, 68.2, 52.5, 37.4. HRMS (ESI-TOF) m/z calcd for $C_{21}H_{20}N_2O_8$ $[M+H]^+$ 429.1292, found 429.1286. FT-IR (Neat) ν_{max} (cm^{-1}) = 3084.07, 2937.23, 2874.96, 1705.13, 1527.76, 1388.82, 1344.03, 1097.40, 1016.65, 879.18, 802.53, 712.17, 525.37.

Methyl 2-(2-(2-(1,3-dioxoisoindolin-2-yl)ethoxy)ethoxy)-2-(4-fluorophenyl)acetate, **(4i)**: **4i** was synthesised using general procedure. **2g** (69.9 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **4i,** colourless oil, (110.8 mg, 92%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.84-7.82 (m, 2H), 7.73-7.69 (m, 2H), 7.40-7.36 (m, 2H), 7.02-6.97 (m, 2H), 4.95 (s, 1H), 3.89 (t, *J* = 5.6 Hz, 2H), 3.74-3.67 (m, 4H), 3.65 (s, 3H), 3.64-3.55 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.3, 168.4, 162.9 (d, *J* = 245.5 Hz), 134.1, 132.4 (d, *J* = 3.0 Hz), 132.2, 129.1 (d, *J* = 8.2 Hz), 123.4, 115.6 (d, *J* = 21.4 Hz), 80.5, 70.4, 68.9, 68.2, 52.4, 37.5. ^{19}F NMR (376 MHz, $CDCl_3$) $\delta = -110.9$ (s, 1F). HRMS (ESI-TOF) m/z calcd for $C_{21}H_{20}FNO_6$ $[M+H]^+$ 402.1347, found 402.1333. FT-IR (Neat) ν_{max} (cm^{-1}) = 3063.42, 2940.17, 2876.25, 1705.67, 1590.17, 1389.38, 1259.43, 1182.06, 1096.69, 1017.65, 880.84, 785.48, 712.79, 527.26.

Ethyl 2-(2-(2-(1,3-dioxoisoindolin-2-yl)ethoxy)ethoxy)-2-(p-tolyl)acetate, (4j): **4j** was synthesised using general procedure. **2j** (73.5 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20 ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **4j**, colourless oil, (101.2 mg, 82%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.87-7.84 (m, 2H), 7.74-7.71 (m, 2H), 7.32-7.28 (m, 2H), 7.14 (d, *J* = 8.0 Hz,

2H), 4.91 (s, 1H), 4.22-4.09 (m, 2H), 3.91 (t, J = 5.8 Hz, 2H), 3.80-3.57 (m, 6H), 2.34 (s, 3H), 1.20 (t, J = 7.2 Hz), ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.1, 168.4, 138.4, 134.0, 133.7, 132.3, 129.3, 127.3, 123.4, 81.2, 70.3, 68.9, 68.2, 61.2, 37.5, 21.3, 14.2. HRMS (ESI-TOF) m/z calcd for $C_{23}H_{25}NO_6$ $[M+H]^+$ 412.1755, found 412.1741. FT-IR (Neat) ν_{max} (cm^{-1}) = 2956.93, 1707.94, 1388.20, 1258.98, 1090.69, 1021.29, 797.80, 714.88, 511.81.

Methyl 2-(4-(tert-butyl)phenyl)-2-(2-(2-(1,3-dioxoisoindolin-2-yl)ethoxy)ethoxy)acetate, (**4k**)**: 4k** was synthesised using general procedure. **2k** (83.6 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion solvent was removed *via* lyophilization, followed by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **4k**, colourless oil, (104.2 mg, 79%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.85-7.83 (m, 2H), 7.71-7.69 (m, 2H), 7.35-7.30 (m, 4H), 4.94 (s, 1H), 3.91-3.88 (m, 2H), 3.76-3.67 (m, 4H), 3.66 (s, 3H), 3.65-3.56 (m, 2H), 1.29 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.6, 168.4, 151.7, 134.0, 133.5, 132.3, 127.1, 125.6, 123.4, 81.2, 70.4, 68.9, 68.2, 52.3, 37.5, 34.7, 31.4. HRMS (ESI-TOF) m/z calcd for $C_{25}H_{29}NO_6$ $[M+H]^+$ 440.2068, found 440.2052. FT-IR (Neat) ν_{max} (cm^{-1}) = 2953.51, 2875.14, 1708.14, 1388.43, 1263.84, 1177.62, 1098.26, 1018.26, 823.76, 714.71, 533.34.

Methyl 2-(2-(2-(1,3-dioxoisoindolin-2-yl)ethoxy)ethoxy)-2-(4-nitrophenyl)acetate, (**4l**)**: 4l** was synthesised using general procedure. **2l** (79.6 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **4l**, colourless oil, (126.0 mg, 98%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 8.18-8.15 (m, 2H), 7.83-7.81 (m, 2H), 7.73-7.70 (m, 2H), 7.63-7.60 (m, 2H), 5.12 (s, 1H), 3.89 (t, J = 5.6 Hz, 2H), 3.76-3.69 (m, 5H), 3.67 (s, 3H), 3.65-3.62 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 170.4, 168.4, 148.1, 143.7, 134.1, 132.2, 128.1, 123.8, 123.7, 123.4, 80.3, 70.5, 69.5, 68.3, 52.7, 37.5. HRMS (ESI-TOF) m/z calcd for $C_{21}H_{20}N_2O_8$ $[M+H]^+$ 429.1292, found 429.1300. FT-IR (Neat) ν_{max} (cm^{-1}) = 3076.84, 2923.81, 1708.08, 1605.56, 1521.91, 1390.64, 1344.42, 1025.45, 791.49, 714.59, 435.33.

Methyl 2-(4-chlorophenyl)-2-(2-(2-(3-cyano-1H-indol-1-yl)ethoxy)ethoxy)acetate, (**5a**): **5a** was synthesised using general procedure. **2i** (75.8 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20 ml vial and stirred under blue light irradiation for 2 h, then **1b** (42.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **5a,** colourless oil (74.3 mg, 60%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.78-7.76 (m, 2H), 7.42-7.40 (m, 1H), 7.39-7.32 (m, 6H), 4.83 (s, 1H), 4.33 (t, J = 5Hz, 2H), 3.85-3.82 (m, 2H), 3.71 (s, 3H), 3.65-3.61 (m, 3H), 3.56-3.52 (m, 1H); δ_C 170.9, 136.0, 135.5, 134.9, 134.8, 129.0, 128.6, 128.0, 123.9, 122.2, 120.1, 116.1, 110.5, 80.7, 70.8, 69.6, 69.3, 52.6, 47.1. HRMS (ESI-TOF) m/z calcd for $C_{22}H_{21}ClN_2O_4$ $[M+H]^+$ 413.1263, found 413.1247. FT-IR (Neat) ν_{max} (cm^{-1}) = 2935.78, 2865.74, 2215.68, 1732.28, 1451.42, 1082.65, 1026.05, 747.54, 430.90.

Methyl 2-(2-(2-(3-cyano-1H-indol-1-yl)ethoxy)ethoxy)-2-phenylacetate, (**5b**)**: 5b** was synthesised using general procedure. **2a** (63.4 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1b** (42.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **5b,** colourless oil, (65.9 mg, 58%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.77-7.75 (m, 2H), 7.42-7.28 (m, 8H), 4.88 (s, 1H), 4.32 (t, J = 5.2 Hz, 2H), 3.85-3.82 (m, 2H), 3.71 (s, 3H), 3.66-3.61 (m, 3H), 3.57-3.54 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.1, 136.2, 135.9, 135.4, 128.9, 128.7, 127.9, 127.2, 123.7, 122.0, 119.9, 116.0, 110.4, 85.8, 81.3, 70.6, 69.4, 69.1, 52.4, 46.9; HRMS (ESI-TOF) m/z calcd for $C_{22}H_{22}N_2O_4$ $[M+H]^+$ 379.1666, found 379.1666. FT-IR (Neat) ν_{max} (cm^{-1}) = 3298.33, 2914.86, 2851.41, 2214.44, 1732.46, 1529.22, 1460.10, 1385.72, 1174.25, 1103.48, 34.50, 495.03.

Methyl 2-(2-(2-(3-formyl-1H-indol-1-yl)ethoxy)ethoxy)-2-phenylacetate, (**5c**)**: 5c** was synthesised using general procedure. **2a** (63.4 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1c** (42.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **5c,** colourless oil, (65.2 mg, 57%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 9.92 (s, 1H), 8.33-8.31 (m, 1H), 7.89 (s, 1H), 7.39-7.30 (m, 8H), 4.88 (s, 1H), 4.35 (t, J = 5.2 Hz, 2H), 3.89-3.86 (m, 2H), 3.69 (s, 3H), 3.68-3.63 (m, 3H), 3.58-3.55 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 184.7, 170.9, 139.6, 137.0, 135.9, 128.7, 128.5, 127.0, 125.1, 123.7, 122.7, 122.1, 118.1, 109.6, 81.1, 70.4, 69.1, 68.8, 52.1, 46.7; HRMS (ESI-TOF) m/z calcd for $C_{22}H_{23}NO_5$ $[M+H]^+$ 382.1649, found 382.1633. FT-IR (Neat) ν_{max} (cm^{-1}) = 3292.29, 3047.56, 2917.93, 1734.86, 1651.94, 1529.09, 1453.20, 1387.81, 1176.91, 1099.52, 913.41, 734.12, 495.31.

Methyl 2-(2-(2-(3-cyano-1H-indol-1-yl)ethoxy)ethoxy)-2-(4-fluorophenyl)acetate, (**5d**)**: 5d** was synthesised using general procedure. **2g** (69.9 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1b** (42.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **5a,** colourless oil, (77.3 mg, 57%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.78-7.75 (m, 2H), 7.42-7.40 (m, 1H), 7.36-7.29 (m, 4H), 7.05-7.01 (m, 2H), 4.84 (s, 1H), 4.33 (t, J = 5.0 Hz, 2H), 3.85-3.82 (m, 2H), 3.71 (s, 3H), 3.64-3.61 (m, 3H), 3.55-3.52 (m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.4, 163.4 (d, J = 246.0 Hz), 136.3, 135.8, 132.4 (d, J = 3.2 Hz), 129.4 (d, J = 8.3 Hz), 128.3, 124.2, 122.5, 120.4, 116.4, 116.1 (d, J = 21.5 Hz), 110.8, , 86.2, 81.0, 71.1, 69.9, 69.5, 52.8, 47.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ = −112.8 (s, 1F). HRMS (ESI-TOF) m/z calcd for $C_{22}H_{21}FN_2O_4$ $[M+H]^+$ 397.1558, found 397.1539. FT-IR (Neat) ν_{max} (cm^{-1}) = 3298.57, 2915.11, 2853.23, 2215.26, 1736.38, 1606.42, 1461.27, 1358.72, 1226.10, 1167.97, 1104.24, 827.45, 736.51, 511.65.

Methyl 2-(4-bromophenyl)-2-(2-(2-(3-formyl-1H-indol-1-yl)ethoxy)ethoxy)acetate, (**5e**): **5e** was synthesised using general procedure. **2h** (91.8 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for

2 h, then **1c** (42.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **5e,** colourless oil, (80.1 mg, 58%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 9.95 (s, 1H), 8.33-8.31 (m, 1H), 7.88 (s, 1H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.39-7.29 (m, 3H), 7.22 (d, *J* = 8.4 Hz, 2H), 4.81 (s, 1H), 4.34 (t, *J* = 5.2Hz, 2H), 3.88-3.85 (m, 2H), 3.68 (s, 3H), 3.64-3.61 (m, 3H), 3.56-3.51 (m, 1H); δ_C 184.7, 170.5, 139.5, 137.0, 134.9, 131.6, 128.6, 125.1, 123.7, 122.7, 122.0, 118.0, 109.7, 80.4, 70.4, 69.1, 68.9, 52.3, 46.8; HRMS (ESI-TOF) m/z calcd for $C_{22}H_{22}BrNO_5$ $[M+H]^+$ 462.0737, found 462.0729. FT-IR (Neat) ν_{max} (cm^{-1}) = 3109.99, 3054.75, 2922.18, 1737.74, 1650.59, 1518.23, 1454.43, 1390.76, 1174.54, 1092.69, 741.89, 510.87.

Methyl 2-(4-fluorophenyl)-2-(2-(2-(3-formyl-1H-indol-1-yl)ethoxy)ethoxy)acetate, (**5f**): **5f** was synthesised using general procedure. **2g** (69.9 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1c** (42.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **5f,** colourless oil, (71.9 mg, 60%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 9.97 (s, 1H), 8.34-8.31 (m, 1H), 7.88 (s, 1H), 7.45 (d, J = 8.4 Hz, 2H), 7.38-7.31 (m, 3H), 7.23-7.21 (m, 2H), 4.81 (s, 1H), 4.35 (t, *J* = 5.0 Hz, 2H), 3.88-3.86 (m, 2H), 3.69 (s, 3H), 3.66-3.62 (m, 3H), 3.57-3.53 (m, 1H); δ_C 185.2, 140.0, 137.7, 135.6, 132.3, 130.3, 129.2, 125.8, 124.4, 123.4, 122.7, 118.8, 110.3, 81.0, 71.1, 69.8, 69.6, 52.7, 47.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ = −113.4 (s, 1F). HRMS (ESI-TOF) m/z calcd for $C_{22}H_{22}FNO_5$ $[M+H]^+$ 400.1555, found 400.1537. FT-IR (Neat) ν_{max} (cm^{-1}) = 3111.08, 3051.55, 2921.28, 1735.61, 1642.29, 1508.16, 1451.38, 1391.25, 1^{17}1.84, 1089.19, 739.29, 509.17.

Methyl 2-(4-chlorophenyl)-2-(2-(2-(3-formyl-1H-indol-1-yl)ethoxy)ethoxy)acetate, (**5g**): **5g** was synthesised using general procedure. **2i** (75.8 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1c** (42.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **5g,** colourless oil, (78.6 mg, 63%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 9.96 (s,1H), 8.34-8.31 (m, 1H), 7.88 (s,1H), 7.39-7.36 (m, 1H), 7.33-7.31 (m, 2H), 7.29 (s, 4H), 4.83 (s, 1H), 4.35 (t, *J* =5.2, 2H), 3.87 (t, J = 4.8, 2H), 3.67 (s, 3H), 3.64-3.62 (m, 3H), 3.57-3.52 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 185.0, 170.9,139.8, 137.4,134.9, 134.8, 129.0, 128.6, 125.5, 124.0, 123.0, 122.4, 118.4, 110.0, 80.7, 70.7, 69.5, 69.2, 52.6, 47.1. HRMS (ESI-TOF) m/z calcd for $C_{22}H_{22}ClNO_5$ $[M+H]^+$ 416.1259, found 416.1248. FT-IR (Neat) ν_{max} (cm^{-1}) = 3301.28, 3106.28, 3050.08, 2918.30, 1740.56, 1651.60, 1529.47, 1457.74, 1391.40, 1173.96,1086.07, 1015.22, 742.25, 497.54.

Methyl 2-(4-bromophenyl)-2-(2-(2-(3-cyano-1H-indol-1-yl)ethoxy)ethoxy)acetate, (**5h**): **5h** was synthesised using general procedure. **2h** (91.8 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1b** (42.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate

and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **5h,** colourless oil, (82.3 mg, 60%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.78-7.76 (m, 2H), 7.42-7.40 (m, 1H), 7.36-7.29 (m, 4H), 7.05-7.01 (m, 2H), 4.84 (s, 1H), 4.33 (t, J = 5Hz, 2H), 3.85-3.82 (m, 2H), 3.714 (s, 3H), 3.65-3.61 (m, 3H), 3.56-3.52 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.1, 136.0, 129.2, 129.1, 128.0, 123.9, 122.2, 120.1, 115.9, 115.7, 110.5, 86.0, 80.1, 70.8, 69.6, 69.2, 52.6, 47.1, 29.8. HRMS (ESI-TOF) m/z calcd for $C_{22}H_{21}BrN_2O_4$ $[M+H]^+$ 459.0740, found 459.0721. FT-IR (Neat) ν_{max} (cm^{-1}) = 3386.18, 3310.24, 3190.05, 3122.78, 3057.13, 2919.07, 2860.26, 2214.73, 1738.10, 1647.68, 1513.56, 1454.79, 1347.54, 1091.74, 811.19, 741.87.

Methyl 2-(2-(2-(3-cyano-1H-indol-1-yl)ethoxy)ethoxy)-2-(3-fluorophenyl)acetate, (**5i**): **5i** was synthesised using general procedure. **2b** (69.9 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1b** (42.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **5i,** colourless oil, (73.3 mg, 62%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.78-7.75 (m, 2H), 7.42-7.40 (m, 1H), 7.42-7.40 (m, 1H), 7.35-7.26 (m, 3H), 7.17-7.11 (m, 2H), 7.06-7.01 (m, 1H), 4.86 (s, 1H), 4.33 (t, J = 5.2 Hz, 2H), 3.86-3.83 (m, 2H), 3.72 (s, 3H), 3.68-3.62 (m, 3H), 3.58-3.54 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 170.7, 162.9 (d, J = 245.3 Hz), 138.7 (d, J = 7.3 Hz), 134.0, 135.9, 135.6, 130.4 (d, J = 8.0Hz), 128.0, 123.9, 122.9 (d, J = 3.0Hz), 122.2, 116.1, 115.9 (d, J = 21.0 Hz), 114.3 (d, J = 22.5 Hz), 110.5, 86.0, 80.8 (d, J = 1.8 Hz), 70.8, 69.6, 69.4, 52.6, 47.1. HRMS (ESI-TOF) m/z calcd for $C_{22}H_{21}BrN_2O_4$ $[M+H]^+$ 459.0740, found 459.0728. FT-IR (Neat) ν_{max} (cm^{-1}) = 3368.19, 3325.78, 3128.14, 3115.26, 3078.38, 2934.39, 2878.45, 2208.4, 1731.21, 1640.04, 1412.16, 1451.49, 1307.94, 1011.48, 854.76, 705.14.

Methyl 2-(3-bromophenyl)-2-(2-(2-(3-cyano-1H-indol-1-yl)ethoxy)ethoxy)acetate, (5j): 5j was synthesised using general procedure. **2d** (91.8 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1b** (42.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **5j,** Colourless oil, (89.2 mg, 65%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.83-7.79 (m, 2H), 7.62-7.61 (m, 1H), 7.53-7.45 (m, 2H), 7.39-7.28 (m, 4H), 4.88 (s, 1H), 4.39 (t, J = 5.0 Hz, 2H), 3.90-3.88 (m, 2H), 3.78 (s, 3H), 3.71-3.59 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 170.5, 138.4, 135.8, 135.4, 131.9, 130.3, 130.1, 127.9, 125.8, 123.7, 122.7, 122.1, 119.9, 115.9, 110.4, 98.4, 85.9, 70.6, 69.5, 69.3, 52.5, 47.0. HRMS (ESI-TOF) m/z calcd for $C_{22}H_{21}BrN_2O_4$ $[M+H]^+$ 459.0740, found 459.0721. FT-IR (Neat) ν_{max} (cm^{-1}) = 3356.21, 3318.48, 3170.37, 3102.70, 3055.47, 2901.55, 2854.78, 2207.10, 1647.14, 1613.87, 1523.78, 1434.14, 1248.85, 1100.21, 799.87, 731.45.

Methyl 2-(2-(2-(3-cyano-1H-indol-1-yl)ethoxy)ethoxy)-2-(3-methoxyphenyl)acetate, (5k): **5k** was synthesised using general procedure. **2e** (74.2 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1b** (42.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **5k,** colourless oil, (73.5 mg, 60%); ^{1}H NMR ($CDCl_3$, 400

MHz) δ_H 7.78-7.76 (m, 2H), 7.42-7.36 (m, 3H), 7.34-7.28 (m, 4H), 4.85 (s, 1H), 4.34-4.32 (m, 2H), 3.86-3.83 (m, 2H), 3.72 (s, 3H), 3.65-3.55 (m, 4H), 1.31 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.1, 159.9, 137.7, 136.0, 135.6, 129.9, 128.0, 123.8, 122.2, 120.0, 119.8, 116.1, 114.5, 112.9, 110.5, 85.9, 81.3, 70.8, 69.6, 69.2, 55.4, 52.5, 47.1. HRMS (ESI-TOF) m/z calcd for $C_{23}H_{24}N_2O_5$ $[M+H]^+$ 409.1758, found 409.1748. FT-IR (Neat) ν_{max} (cm^{-1}) = 3399.21, 3308.48, 3156.15, 3111.21, 3055.89, 2923.18, 2806.21, 2224.15, 1731.18, 1638.40, 1510.50, 1451.86, 1333.38, 1091.76, 801.89, 760.25.

Methyl 2-(4-(tert-butyl)phenyl)-2-(2-(2-(3-cyano-1H-indol-1-yl)ethoxy)ethoxy)acetate, (**5l**): **5l** was synthesised using general procedure. **2k** (83.6 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1b** (42.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **5l,** colourless oil, (75.61 mg, 58%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.69-7.67 (m, 2H), 7.34-7.32 (m, 1H), 7.26-7.18 (m, 3H), 6.90-6.88 (m, 2H), 6.82-6.79 (m, 1H), 4.78 (s, 1H), 4.25 (t, J = 5.0, 2H), 3.78-3.75 (m, 2H), 3.72 (s, 3H), 3.64 (s, 3H), 3.58-3.47 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.3, 160.8, 151.9, 135.8, 135.5, 133.1, 127.9, 126.9, 125.7, 123.7, 122.0, 119.9, 110.4, 98.4, 81.2, 70.7, 69.5, 69.0, 52.3, 47.0, 34.6, 31.3. HRMS (ESI-TOF) m/z calcd for $C_{22}H_{21}BrN_2O_4$ $[M+H]^+$ 459.0740, found 459.0731. FT-IR (Neat) ν_{max} (cm^{-1}) = 3376.56, 3308.30, 3188.15, 3120.71, 3051.28, 2933.22, 2851.21, 2224.69, 1739.18, 1641.54, 1512.50, 1451.69, 1342.14, 1076.71, 801.56, 739.25.

Methyl 2-(4-chlorophenyl)-2-(2-(2-(2,4-dioxothiazolidin-3-yl)ethoxy)ethoxy)acetate, (**6a**): **6a** was synthesised using general procedure. **2i** (75.8 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1d** (35.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **6a,** colourless oil, (95.4 mg, 82%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.39 (d, J =8.4 Hz, 2H), 7.33 (d, J = 8.4Hz, 2H), 4.95 (s, 1H), 3.93 (s, 2H), 3.85-3.82 (m, 2H), 3.70 (s, 3H), 3.68-3.62 (m, 5H), 3.61-3.56 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.9, 171.6, 170.1, 135.1. 134.7, 128.9, 128.8, 80.6, 70.4, 69.1, 67.2, 52.5, 41.3, 33.8. HRMS (ESI-TOF) m/z calcd for $C_{16}H_{18}ClNO_6S$ $[M+H]^+$ 388.0616, found 388.0631. FT-IR (Neat) ν_{max} (cm^{-1}) = 3488.02, 3420.99, 2937.68, 2876.39, 1743.36, 1673.88, 1367.33, 1261.43, 1179.26, 1091.06, 1017.67, 881.44, 818.92, 770.83, 661.56, 459.87.

Methyl 2-(4-bromophenyl)-2-(2-(2-(2,4-dioxothiazolidin-3-yl)ethoxy)ethoxy)acetate, (**6b**): **6b** was synthesised using general procedure. **2h** (91.8 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1d** (35.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **6b,** colourless oil, (107.6 mg, 83%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.49 (d, J = 8.4Hz, 2H), 7.33(d, J = 8.4Hz, 2H), 4.94 (s, 1H), 3.93 (s, 2H), 3.85-3.82 (m, 2H), 3.70 (s, 3H), 3.68-3.63 (m, 5H), 3.61-3.56 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.9, 171.6, 170.1, 135.6. 131.9, 129.1, 122.9, 80.7, 70.4, 69.1, 67.2, 52.5, 41.3, 33.8 HRMS (ESI-TOF) m/z calcd for $C_{16}H_{18}BrNO_6S$ $[M+H]^+$ 434.0092, found 434.0115. FT-

IR (Neat) ν_{max} (cm^{-1}) = 3389.99, 3191.21, 2921.26, 2215.25, 1742.81, 1676.33, 1368.09, 1093.42, 883.07, 812.62, 754.62, 661.18, 458.51.

Methyl 2-(2-(2-(2,4-dioxothiazolidin-3-yl)ethoxy)ethoxy)-2-(4-fluorophenyl)acetate, (**6c**): **6c** was synthesised using general procedure. **2g** (69.9 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1d** (35.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **6c,** Colourless oil, (95.8 mg, 86%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.44-7.41(m, 2H), 7.07-7.02(m, 2H), 4.95 (s, 1H), 3.93 (s, 2H), 3.85-3.82 (m, 2H), 3.70 (s, 3H), 3.68-3.62 (m, 5H), 3.61-3.56 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.8, 171.5, 171.1, 162.9 (d, J = 245.0 Hz), 132.3 (d, J = 3.0 Hz), 129.1 (d, J = 8.0 Hz), 115.6 (d, J = 21.0 Hz), 80.6, 70.4, 69.0, 67.2, 52.5, 41.2, 33.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ = −111.3 (s, 1F). HRMS (ESI-TOF) m/z calcd for $C_{16}H_{18}FNO_6S$ $[M+H]^+$ 372.0912, found 372.0895. FT-IR (Neat) ν_{max} (cm^{-1}) = 3397.17, 3184.41, 2920.44, 1742.48, 1675.02, 1507.37, 1432.22, 1368.68, 1213.64, 1094.35, 812.50, 657.95, 513.57, 460.62.

Methyl 2-(2-(2-(2,4-dioxothiazolidin-3-yl)ethoxy)ethoxy)-2-phenylacetate, (**6d**): **6d** was synthesised using general procedure. **2a** (63.4 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1d** (35.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **6d,** colourless oil, (83.8 mg, 79%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.48-7.46 (m, 2H), 7.41-7.34 (m, 3H), 4.99 (s, 1H), 3.93 (s, 2H), 3.84-3.84 (m, 2H), 3.72 (s, 3H), 3.70-3.59 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.8, 171.5, 171.3, 136.4, 128.7, 128.6, 127.3, 81.2, 70.2, 68.8, 67.0, 52.3, 41.1, 33.7. HRMS (ESI-TOF) m/z calcd for $C_{16}H_{19}NO_6S$ $[M+H]^+$ 354.1006, found 354.0998. FT-IR (Neat) ν_{max} (cm^{-1}) = 2917.58, 2860.92, 1741.39, 1674.88, 1436.48, 1368.79, 1263.29, 1177.78, 1098.01, 886.75, 791.11, 694.97, 584.81, 467.53.

Methyl 2-(2-(2-(2,4-dioxothiazolidin-3-yl)ethoxy)ethoxy)-2-(3-fluorophenyl)acetate, (**6e**): **6e** was synthesised using general procedure. **2b** (69.9 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1d** (35.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **6e,** colourless oil, (94.7 mg, 85%); ^{1}H NMR ($CDCl_3$, 400 MHz) 7.34-7.29 (m, 1H), 7.23-7.16 (m, 2H), 7.00 (td, J = 8.3, 1.8 Hz, 1H), 4.97 (s, 1H), 3.93 (s, 2H), 3.82 (t, J = 5.4 Hz, 2H), 3.70 (s, 3H), 3.68-3.64 (m, 5H), 3.62-3.57 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.9, 171.6, 170.9, 162.9 (d, J = 245.0 Hz), 138.9 (d, J = 7.2 Hz), 130.2 (d, J = 8.1 Hz), 122.9 (d, J = 3.0 Hz), 115.7 (d, J = 20.9 Hz), 114.3 (d, J = 22.4 Hz), 80.62 (d, J = 1.7 Hz), 70.3, 69.1, 67.1, 52.5, 41.2, 33.8. HRMS (ESI-TOF) m/z calcd for $C_{16}H_{18}FNO_6S$ $[M+H]^+$ 372.0912, found 372.0924. FT-IR (Neat) ν_{max} (cm^{-1}) = 2944.34, 2878.56, 1744.17, 1674.43, 1594.92, 1438.81, 1367.81, 1190.34, 1098.40, 882.12, 788.33, 744.90, 674.15, 518.51, 459.84.

Methyl 2-(2-(2-(2,4-dioxothiazolidin-3-yl)ethoxy)ethoxy)-2-(3-methoxyphenyl)acetate, (6f): **6f** was synthesised using general procedure. **2e** (74.2 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20 ml vial and stirred under blue light irradiation for 2 h, then **1d** (35.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **6f,** Colourless oil, (93.2 mg, 81%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.28 (t, J = 8.0 Hz, 1H), 7.05-7.01 (m, 2H), 6.89-6.86 (m, 1H), 4.96 (s, 1H), 3.94 (s, 2H), 3.86-3.83 (m, 2H), 3.83 (s, 3H), 3.72 (s, 3H), 3.71-3.68 (m, 2H), 3.67-3.66 (s, 2H), 3.65-3.57 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.9, 171.6, 171.2, 159.9, 137.9, 129.7, 119.8, 114.6, 112.5, 81.2, 70.3, 68.9, 67.1, 55.4, 52.4, 41.2, 33.8. HRMS (ESI-TOF) m/z calcd for $C_{17}H_{21}NO_7S$ $[M+H]^+$ 386.1111, found 386.1109. FT-IR (Neat) ν_{max} (cm^{-1}) = 3421.76, 2941.98, 1743.28, 1674.28, 1596.00, 1438.21, 1367.38, 1254.30, 1097.94, 1031.64, 880.09, 784.70, 738.97.

Methyl 2-(2-(2-(2,5-dioxoimidazolidin-1-yl)ethoxy)ethoxy)-2-phenylacetate, (**7a**)**: 7a** was synthesised using general procedure. **2a** (63.4 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1e** (30.0 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **7a,** colourless oil, (83.8 mg, 83%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.44-7.43 (m, 2H), 7.37-7.7.31 (m, 3H), 6.36 (s, 1H), 4.98 (s, 1H), 3.90 (s, 2H), 3.73-3.70 (m, 4H), 3.68 (s, 3H), 3.67-3.63 (m, 3H), 3.62-3.57 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.7, 171.5, 158.6, 136.5, 128.8, 128.7, 127.39, 81.3, 70.2, 68.9, 67.5, 52.4, 46.5, 38.1. HRMS (ESI-TOF) m/z calcd for $C_{16}H_{20}N_2O_6$ $[M+H]^+$ 337.1394, found 337.1400. FT-IR (Neat) ν_{max} (cm^{-1}) = 3317.10, 2934.57, 2876.44, 1702.49, 1445.84, 1331.66, 1200.33, 1098.94, 995.88, 704.05, 564.52.

Methyl 2-(2-(2-(2,5-dioxoimidazolidin-1-yl)ethoxy)ethoxy)-2-(3-methoxyphenyl)acetate, (**7b**): **7b** was synthesised using general procedure. **2k** (74.2 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1e** (30.0 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **7b,** colourless oil, (91.2 mg, 83%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.21-7.17 (m, 1H), 6.95-6.93 (m, 2H), 6.80-6.77 (m, 1H), 6.37 (s, 1H), 4.89 (s, 1H), 3.84 (s, 2H), 3.73 (s, 3H), 3.65-3.63 (m, 2H), 3.62 (s, 3H), 3.61-3.58 (m, 4H), 3.56-3.51 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.7, 171.3,159.8, 159.6, 137.9, 129.7, 119.7, 114.5, 112.6, 81.1, 70.2, 68.8, 67.5, 55.4, 52.4, 46.5, 38.0. HRMS (ESI-TOF) m/z calcd for $C_{17}H_{22}N_2O_7$ $[M+H]^+$ 367.1500, found 367.1491. FT-IR (Neat) ν_{max} (cm^{-1}) = 3315.60, 2939.82, 1701.06, 1596.05, 1444.35, 1255.81, 1199.99, 1097.16, 884.69, 741.41.

Methyl 2-(2-(2-(2,5-dioxoimidazolidin-1-yl)ethoxy)ethoxy)-2-(3-fluorophenyl)acetate, (7c): **7c** was synthesised using general procedure. **2b** (69.9 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1e** (30.0 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through

TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **7c,** colourless oil, (93.5 mg, 88%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.33-7.28 (m, 1H), 7.22-7.15 (m, 2H), 7.02-6.97 (m, 1H), 6.42 (s, 1H), 4.99 (s, 1H), 3.92 (s, 2H), 3.72-3.70 (m, 2H), 3.69 (s, 3H), 3.68-3.65 (m. 4H), 3.64-3.58 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.6, 170.9, 162.9 (d, J = 245.1 Hz), 158.6, 139.0 (d, J = 7.3 Hz), 130.2 (d, J = 8.1 Hz), 122.9 (d, J = 2.9 Hz), 115.7 (d, J = 21.1 Hz), 114.3 (d, J = 22.3 Hz), 80.5 (d, J = 1.7 Hz), 70.2, 69.1, 67.5, 52.5, 46.5, 38.1. HRMS (ESI-TOF) m/z calcd for $C_{16}H_{19}FN_2O_6$ $[M+H]^+$ 355.1300, found 336.1312. FT-IR (Neat) ν_{max} (cm^{-1}) = 3317.10, 2938.78, 2878.53, 1701.07, 1594.53, 1444.65, 1200.42, 1099.24, 997.94, 888.47, 744.64, 562.50.

Methyl 2-(2-(2-(3-cyano-1H-pyrrol-1-yl)ethoxy)ethoxy)-2-(3-fluorophenyl)acetate, (**8a**): **8a** was synthesised using general procedure. **2b** (69.9 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1f** (27.6 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **8a,** colourless oil, (60.3 mg, 58%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.35-7.29 (m, 1H), 7.21-7.15 (m, 2H), 7.05-6.96 (m, 2H), 6.78-6.77 (m, 1H), 6.14-6.12 (m, 1H), 4.93 (s, 1H), 4.20 (t, J = 5.2Hz, 2H), 3.79-3.76 (m, 2H), 3.72 (s, 3H), 3.70-3.68 (m, 1H), 3.65-3.63 (m, 2H), 3.63-3.58 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 170.8, 163.0 (d, J = 245.0 Hz), 138.9 (d, J = 7Hz), 130.3 (d, J = 8Hz), 127.74, 122.9 (d, J = 3Hz), 120.2, 115.8 (d, J = 21.0 Hz), 114.3 (d, J = 23.0 Hz), 109.6, 103.7, 80.7, 80.7, 70.7, 70.4, 69.3, 52.5, 48.7. HRMS (ESI-TOF) m/z calcd for $C_{18}H_{19}FN_2O_4$ $[M+H]^+$ 347.1402, found 347.1395. FT-IR (Neat) ν_{max} (cm^{-1}) = 3123.98, 2942.88, 2878.31, 2213.38, 1742.04, 1593.03, 1443.34, 1243.62, 1102.28, 883.45, 787.13, 739.18, 685.68, 606.92, 498.16.

Methyl 2-(2-(2-(3-cyano-1H-pyrrol-1-yl)ethoxy)ethoxy)-2-(3-methoxyphenyl)acetate, (8b): 8b was synthesised using general procedure. **2e** (74.2 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1f** (27.6 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **8b,** colourless oil, (64.5 mg, 60%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.31-7.27 (m, 1H), 7.03-7.01 (m, 3H), 6.91-6.89 (m, 1H), 6.81-6.79 (m, 1H), 6.16-6.14 (m, 1H), 4.93 (s, 1H), 4.22 (t, J = 5.2Hz, 2H), 3.82 (s, 3H), 3.81-3.77 (m, 2H), 3.73 (s, 3H), 3.69-3.65 (m, 3H), 3.63-3.60 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.2, 159.9, 137.9, 129.8, 127.8, 120.2, 119.8, 114.5, 114.0, 112.7, 109.5, 103.7, 81.3, 70.7, 70.4, 69.1, 55.4, 52.4, 48.7. HRMS (ESI-TOF) m/z calcd for $C_{19}H_{22}N_2O_5$ $[M+H]^+$ 359.1601, found 359.1611. FT-IR (Neat) ν_{max} (cm^{-1}) = 3123.55, 2938.09, 2212.48, 1741.41. 1595.64, 1444.23, 1253.78, 1102.00, 1039.31, 878.59, 738.62, 690.99, 558.60, 488.01.

Methyl 2-(2-(2-(3-cyano-1H-pyrrol-1-yl)ethoxy)ethoxy)-2-phenylacetate, (**8c**): **8c** was synthesised using general procedure. **2a** (63.4 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1f** (27.6 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified

by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **8c,** colourless oil, (57.1 mg, 58%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.43-7.41 (m, 2H), 7.38-7.33 (m, 3H), 6.97 (t, *J* = 2Hz, 1H), 6.77 (dd, *J* = 4.0, 1.6Hz, 1H), 6.13-6.11 (m, 1H), 4.93 (s, 1H), 4.19 (t, *J* = 5.0Hz, 2H), 3.78-3.75 (m, 2H), 3.70 (s, 3H), 3.69-3.67 (m, 1H), 3.64 (t, *J* = 4.0 Hz, 2H), 3.61-3.58 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 171.3, 136.4, 128.8, 128.7, 128.6, 127.8, 127.3, 120.1, 109.5, 81.4, 70.7, 70.4, 69.1, 52.4, 48.7. HRMS (ESI-TOF) m/z calcd for $C_{18}H_{20}N_2O_4$ $[M+H]^+$ 329.1496, found 329.1503. FT-IR (Neat) ν_{max} (cm^{-1}) = 3124.01, 2878.49, 2213.29, 1742.11, 593.04, 1443.40, 1243.42, 1102.98, 883.59, 739.25, 685.66, 607.34.

Methyl 2-(4-(tert-butyl)phenyl)-2-(2-(2-(2,5-dioxopyrrolidin-1-yl)ethoxy)ethoxy)acetate (8d): 8d was synthesised using general procedure. **2k** (83.6 mg, 0.36 mmol) and 3 (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1h** (29.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, 8d, colourless oil, (89.3 mg, 76%); 1H NMR (CDCl3, 400 MHz) δH 7.38-7.34 (m, 4H), 4.92 (s, 1H), 3.75-3.67 (m, 6H), 3.64-3.56 (m, 5H), 2.73-2.65 (m, 4H), 1.29 (s, 9H) ; 13C NMR (CDCl3, 100 MHz) δC 177.5, 171.6, 151.8, 133.4, 127.1, 125.7, 81.1, 70.2, 68.9, 67.2, 52.3, 38.2, 34.7, 31.4, 29.7, 28.2. HRMS (ESI-TOF) m/z calcd for C17H20BrNO6 [M+H]+ 392.2068, found 392.2063. FT-IR (Neat) νmax (cm-1) = 3310.25, 2944.33, 2872.67, 1705.01, 1441.64, 1330.89, 11089.32, 1088.56, 996.18, 701.03, 560.46.

Methyl 2-(3-bromophenyl)-2-(2-(2-(2,5-dioxopyrrolidin-1-yl)ethoxy)ethoxy)acetate (**8e**): **8e** was synthesised using general procedure. **2d** (91.8 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1h** (29.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, 8e, colourless oil, (104.4 mg, 84%); 1H NMR (CDCl3, 400 MHz) δH 7.56-7.55 (m, 1H), 7.41-7.32 (m, 2H), 7.20-7.16 (m, 1H), 4.90 (s, 1H), 3.66-3.65 (m, 5H), 3.61-3.58 (m, 5H), 3.55-3.52 (m, 1H), 2.66-2.63 (m, 4H) ; 13C NMR (CDCl3, 100 MHz) δC 177.4, 170.7, 138.7, 131.7, 130.2, 125.8, 122.6, 80.3, 70.0, 69.0, 67.1, 52.4, 38.0, 29.6, 28.1. HRMS (ESI-TOF) m/z calcd for C17H20BrNO6 [M+H]+ 414.0547, found 414.0540. FT-IR (Neat) νmax (cm-1) = 2940.71, 2876.04, 1694.23, 1572.67, 1401.42, 1329.77, 1185.26, 1105.52, 900.01, 665.41, 430.83.

Methyl 2-(2-(2-(2,5-dioxopyrrolidin-1-yl)ethoxy)ethoxy)-2-phenylacetate (8f): 8f was synthesised using general procedure. **2a** (63.4 mg, 0.36 mmol) and **3** (65 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1h** (29.7 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, 8f, colourless oil, (82.5 mg, 82%); 1H NMR (CDCl3, 400 MHz) δH 7.42-7.41 (m, 2H), 7.36-7.30 (m, 3H), 4.94 (s, 1H), 3.71-3.67 (m, 5H), 3.63-3.56 (m, 6H), 2.65 (s, 4H) ; 13C NMR (CDCl3, 100 MHz) δC 178.5, 177.9, 171.7, 136.8, 129.1, 129.0, 127.7, 81.5, 70.4, 69.2, 67.5, 52.7, 38.4, 30.0, 28.5. HRMS (ESI-TOF) m/z calcd

for C17H21NO6 [M+H]+ 336.1442, found 336.1445. FT-IR (Neat) νmax (cm-1) = 3148.81, 3070.97, 2953.54, 2800.19, 1764.71, 1678.60, 1358.56, 1289.24, 1176.77, 1002.04, 929.36, 817.79, 633.97.

Methyl 5-phenyl-1,4-dioxepane-5-carboxylate, (**9a)**: **2a** (17.6 mg, 0.1 mmol) and **3** (22 ml, 0.25 mmol) was dissolved in water (5ml) in an oven dried vial, stirred and irradiated in blue light for 3 h and then continued stirring in dark for another 15 h. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate. Without any work up column chromatography was done in silica gel (100-200 mess size) with 20-40% ethyl acetate in hexane to obtain the pure compound **9a**. Colourless oil, (20.8 mg, 88%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.55 (d, J = 7.6 Hz, 2H), 7.39 (d J = 8.6 Hz, 2H), 7.32-7.30 (m, 1H), 4.00-3.77 (m, 6H), 3.74 (s, 3H), 3.13-3.07 (m, 1H), 2.59-2.53 (m, 1H); δ_C 173.4, 141.5, 128.6, 128.0, 125.8, 83.9, 71.8, 68.2, 65.7, 53.0, 41.9; HRMS (ESI) m/z calcd for $C_{13}H_{16}O_4$ $[M + H]^+$ 237.121, found 237.1129. FT-IR (Neat) ν_{max} (cm^{-1}) = 2946.64, 2863.16, 1730.67, 1444.44, 1243.92, 1141.64, 1080.89, 877.38, 698.78, 569.33, 446.12.

Methyl 5-(4-(tert-butyl)phenyl)-1,4-dioxepane-5-carboxylate, **(9b)**: **2k** (23.2 mg, 0.1 mmol) and **3** (22 ml, 0.25 mmol) was dissolved in water (5ml) in an oven dried vial, stirred and irradiated in blue light for 3 h and then continued stirring in dark for another 15 h. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate. Without any work up column chromatography was done in silica gel (100-200 mess size) with 20-40% ethyl acetate in hexane to obtain the pure compound **9b**. Colourless oil, (23.4 mg, 80%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.43 (d, J = 8.8 Hz, 2H), 7.36 (d J = 8.4 Hz, 2H), 3.94-3.75 (m, 6H), 3.71 (s, 3H), 3.09-3.03 (m, 1H), 2.57-2.50 (m, 1H), 1.31 (s, 9H); δ_C 173.6, 150.9, 138.3, 125.5, 83.8, 71.8, 68.1, 65.8, 52.9, 41.8, 34.6, 31.4; HRMS (ESI) m/z calcd for HRMS (ESI) m/z calcd for $C_{17}H_{24}O_4$ $[M + H]^+$ 293.1747, found 293.1738. FT-IR (Neat) ν_{max} (cm^{-1}) = 2951.87, 2869.53, 1732.55, 1450.41, 1249.05, 1141.02, 1084.22, 1011.92, 880.05, 832.63, 731.64, 564.43, 468.44.

Methyl 5-(3-bromophenyl)-1,4-dioxepane-5-carboxylate, **(9c)**: **2j** (25.5 mg, 0.1 mmol) and **3** (22 ml, 0.25 mmol) was dissolved in water (5ml) in an oven dried vial, stirred and irradiated in blue light for 3 h and then continued stirring in dark for another 15 h. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate. Without any work up column chromatography was done in silica gel (100-200 mess size) with 20-40% ethyl acetate in hexane to obtain the pure compound **9c**. Colourless oil, (25.2 mg, 81%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.71 (t, J = 1.8 Hz, 1H), 7.46-7.41 (m, 2H), 7.23 (t, J = 8.0 Hz, 1H), 3.98-3.73 (m, 6H), 3.73 (m, 3H), 3.05-2.99 (m, 1H), 2.52-2.46 (m, 1H); δ_C; 172.9, 143.7, 131.2, 130.1, 129.0, 124.5, 122.8, 83.4, 71.7, 68.4, 65.5, 53.2, 41.9; HRMS (ESI) m/z calcd for $C_{13}H_{15}BrO_4$ $[M + H]^+$ 315.0226, found 315.0211. FT-IR (Neat) ν_{max} (cm^{-1}) = 2947.40, 2861.48, 1732.10, 1569.08, 1439.14, 1239.88, 1143.87, 1080.09, 988.80, 881.81, 769.13, 695.96, 568.54.

Methyl 5-(3-fluorophenyl)-1,4-dioxepane-5-carboxylate, **(9d)**: **2h** (19.4 mg, 0.1 mmol) and **3** (22 ml, 0.25 mmol) was dissolved in water (5ml) in an oven dried vial, stirred and irradiated in blue light for 3 h and then continued stirring in dark for another 15 h. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate. Without any work up column chromatography was done in silica gel (100-200 mess size) with 20-40% ethyl acetate in hexane to obtain the pure compound **9d**. Colourless oil, (22.1 mg, 87%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.24-7.17 (m, 3H), 6.92-6.88 (m, 1H), 3.89-3.76 (m, 2H), 3.74-3.64 (m, 4H), 3.63 (s, 3H), 2.97-2.92 (m, 1H), 2.45-2.38 (m, 1H) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 173.0, 162.9 (d, J = 244.4 Hz), 144.1 (d, J = 7.0 Hz), 130.1 (d, J = 8.1 Hz), 121.5 (d, J =2.9 Hz), 144.9 (d, J = 21.0 Hz), 113.2 (d, J = 23.3 Hz), 83.4 (d, J = 1.9 Hz), 71.8, 68.3, 65.6, 53.2, 41.9; HRMS (ESI) m/z calcd for $C_{13}H_{15}FO_4$ $[M + H]^+$ 255.1027, found 255.1008. FT-IR (Neat) ν_{max} (cm^{-1})

= 2945.11, 2858.94, 1729.17, 1634.26, 1515.13, 1445.29, 1221.18, 1139.23, 1089.07, 1001.05, 815.58, 629.17, 563.20.

Methyl 5-(3-methoxyphenyl)-1,4-dioxepane-5-carboxylate, **(9e)**: **2e** (206 mg, 0.1 mmol) and **3** (22 ml, 0.25 mmol) was dissolved in water (5ml) in an oven dried vial, stirred and irradiated in blue light for 3 h and then continued stirring in dark for another 15 h. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate. Without any work up column chromatography was done in silica gel (100-200 mess size) with 20-40% ethyl acetate in hexane to obtain the pure compound **9e**. Colourless oil, (35.88 mg, 83%); White solid (22.6 mg, 85%), mp 246-248 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.28 (t, J = 8.0 Hz, 1H), 7.13-7.08 (m, 2H), 6.85 (dd, J = 8.2, 2.6 Hz, 1H), 3.99-3.85 (m, 2H), 3.82 (s, 3H), 3.81-3.76 (m, 4H), 3.73 (s, 3H), 3.09-3.04 (m, 1H), 2.57-2.51 (m, 1H); δ_C 173.3, 159.8, 143.1, 129.5, 118.1, 113.2, 111.8, 83.8, 71.8, 68.2, 65.7, 55.4, 53.0, 41.9; HRMS (ESI) m/z calcd for $C_{14}H_{18}O_5$ $[M + H]^+$ 267.1227, found 267.1234. FT-IR (Neat) ν_{max} (cm^{-1}) = 2946.62, 2858.23, 1731.85, 1592.92, 1440.15, 1244.16, 1144.42, 1081.61, 1041.01, 883.08, 777.29, 693.55, 563.84, 439.86.

Ethyl 5-(p-tolyl)-1,4-dioxepane-5-carboxylate, (**9f)**: **2k** (20.4 mg, 0.1 mmol) and **3** (22 ml, 0.25 mmol) was dissolved in water (5ml) in an oven dried vial, stirred and in blue light for 3 h and then continued stirring in dark for another 15 h. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate. Without any work up column chromatography was done in silica gel (100-200 mess size) with 20-40% ethyl acetate in hexane to obtain the pure compound **9f**. Colourless oil, (22.5 mg, 85%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.42 (d, J = 8.0 Hz, 2H), 7.15 (d, J = 8.0 Hz, 2H), 4.17 (q, J = 7.0 Hz, 2H), 3.96-3.74 (m, 6H), 3.05-2.99 (m, 1H), 2.55-2.49 (m, 1H), 2.33 (s, 3H), 1.19 (t, J =7.2 Hz, 3H); δ_C 173.1, 138.6, 137.6, 129.2, 125.8, 83.6, 71.8, 68.0, 65.7, 61.7, 41.8, 21.1, 14.2; HRMS (ESI) m/z calcd for $C_{15}H_{20}O_4$ $[M + H]^+$ 265.1434, found 265.1441. FT-IR (Neat) ν_{max} (cm^{-1}) = 2943.71, 2866.26, 1728.33, 1510.35, 1451.53, 1372.94, 1235.94, 1142.20, 1082.531024.43, 878.20, 791.95, 631.06, 568.96, 509.00.

Methyl 5-(3-fluorophenyl)-1,4-dioxepane-5-carboxylate, (**9g)**: **2g** (19.4 mg, 0.1 mmol) and **3** (22 ml, 0.25 mmol) was dissolved in water (5ml) in an oven dried vial, stirred and irradiated in blue light for 3 h and then continued stirring in dark for another 15 h. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate. Without any work up column chromatography was done in silica gel (100-200 mess size) with 20-40% ethyl acetate in hexane to obtain the pure compound **9g**. Colourless oil, (21.9 mg, 86%); White solid (28.8 mg, 64%), mp 246-248 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.53-7.49 (m, 2H), 7.05-7.01 (m, 2H), 3.96-3.73 (m, 6H), 3.71 (s, 3H), 3.07-3.00 (m, 1H), 2.53-2.47 (m, 1H); δ_C; 173.3, 162.5 (d, J = 245.3 Hz), 137.2 (d, J = 3.2 Hz), 127.7 (d, J = 8.1 Hz), 115.4 (d, J = 21.3 Hz), 83.4, 71.7, 68.2, 65.6, 53.1, 41.9 HRMS (ESI) m/z calcd for $C_{13}H_{15}FO_4$ $[M + H]^+$ 255.1027, found 255.1015. FT-IR (Neat) ν_{max} (cm^{-1}) = 2949.51, 2863.64, 1732.37, 1602.46, 1505.53, 1446.09, 1225.08, 1144.13, 1082.77, 999.65, 825.28, 630.67, 564.70.

Methyl 5-(4-bromophenyl)-1,4-dioxepane-5-carboxylate, **(9h)**: **2h** (25.5 mg, 0.1 mmol) and **3** (22 ml, 0.25 mmol) was dissolved in water (5ml) in an oven dried vial, stirred and irradiated in blue light for 3 h and then continued stirring in dark for another 15 h. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate. Without any work up column chromatography was done in silica gel (100-200 mess size) with 20-40% ethyl acetate in hexane to obtain the pure compound **9h**. Colourless oil, (27.7 mg, 88%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.48 (d, J = 8.8 Hz, 2H), 7.41 (d J = 8.4 Hz, 2H), 3.96-3.72 (m, 6H), 3.71 (s, 3H), 3.05-2.99 (m, 1H), 2.51-2.45 (m, 1H); δ_C 173.0, 140.5, 131.7, 127.7, 122.3, 83.5, 71.7, 68.3, 65.5, 53.1, 41.9; HRMS (ESI) m/z calcd for $C_{13}H_{15}BrO_4$ $[M + H]^+$ 315.0226, found

315.0229. FT-IR (Neat) ν_{max} (cm^{-1}) = 2946.24, 2859.79, 1731.68, 1585.99, 1446.35, 1387.07, 1241.09, 1142.15, 1078.23, 998.21, 877.54, 820.31, 779.04, 567.28, 505.48.

Methyl 5-(4-chlorophenyl)-1,4-dioxepane-5-carboxylate, (9i): 2i (21.1 mg, 0.1 mmol) and **3** (22 ml, 0.25 mmol) was dissolved in water (5ml) in an oven dried vial, stirred and irradiated in blue light for 3 h and then continued stirring in dark for another 15 h. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate. Without any work up column chromatography was done in silica gel (100-200 mess size) with 20-40% ethyl acetate in hexane to obtain the pure compound **9i**. Colourless oil, (24.4 mg, 90%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.47 (d, J = 8.8 Hz, 2H), 7.32 (d, J = 8.8 Hz, 2H), 3.96-3.70 (m, 6H), 3.70 (s, 3H), 3.05-2.99 (m, 1H), 2.51-2.45 (m, 1H); δ_C 173.1, 139.9, 134.0, 128.7, 127.4, 83.4, 71.7, 68.2, 65.5, 53.1, 41.9; HRMS (ESI) m/z calcd for $C_{13}H_{15}ClO_4$ $[M + H]^+$ 271.0732, found 271.0717. FT-IR (Neat) ν_{max} (cm^{-1}) = 2948.72, 2862.95, 1732.02, 1445.45, 1245.46, 1143.13, 1082.98, 1004.20, 875.70, 779.40, 567.57, 505.38.

5-phenyl-1,4,7-dioxazonan-6-one, (**10a**): 38.3 mg, 0.1 mmol of **4a** was dissolved in dry isopropanol (3ml) in two separate 25ml round bottom flasks, 24.3μl, 0.5 mmol of hydrazine monohydrate was added to both of the reaction mixture and reflux for 3hr with stirring. Solvent was evaporated under reduced pressure, work up in DCM (3×10ml) in water, dried over sodium sulphate and purified by column chromatography using silica gel (100-200 mesh size) with methanol (10%) in dichloromethane to afford colourless oily compound **10a** of 15.9 mg (72% yield); ^{1}H NMR (DMSO-D_6, 400 MHz) δ_H 7.41-7.39 (m, 2H), 7.36-7.29 (m, 3H), 4.81 (s, 1H), 3.58-3.53 (m, 4H), 3.39 (t, J = 5.8Hz, 2H), 2.67 (t, J = 5.6 Hz, 2H) ; ^{13}C NMR (DMSO-d_6, 100 MHz) δ_C 168.6, 134.5, 129.1, 129.0, 115.0, 114.8, 80.0, 69.4, 68.4, 40.3. HRMS (ESI-TOF) m/z calcd for $C_{12}H_{15}NO_3$ $[M+H]^+$ 222.1125, found 222.1136. FT-IR (Neat) ν_{max} (cm^{-1}) = 2948.72, 2862.95, 1732.02, 1445.45, 1245.46, 1143.13, 1082.98, 1004.20, 875.70, 779.40, 567.57, 505.38.

5-(4-bromophenyl)-1,4,7-dioxazonan-6-one, (**10b**): 46.2 mg, 0.1 mmol of **4c** was dissolved in dry isopropanol (3ml) in two separate 25ml round bottom flasks, 24.3μl, 0.5 mmol of hydrazine monohydrate was added to both of the reaction mixture and reflux for 3hr with stirring. Solvent was evaporated under reduced pressure, work up in DCM (3×10ml) in water, dried over sodium sulphate and purified by column chromatography using silica gel (100-200 mesh size) with methanol (10%) in dichloromethane to afford colourless oily compound **10b** of 20.7 mg (69% yield) respectively; ^{1}H NMR (DMSO-D_6, 400 MHz) δ_H 8.93 (s,1H), 7.44-7.41 (m, 2H), 7.19-7.15 (m, 2H), 4.82 (s, 1H), 3.56-3.50 (m, 4H), 3.42-3.38 (m, 2H), 2.50-2.49 (m, 2H) ; ^{13}C NMR (DMSO-D_6, 100 MHz) δ_C 169.0, 138.2, 128.1, 127.9, 127.0, 80.9, 72.5, 69.4, 68.4, 41.0. HRMS (ESI-TOF) m/z calcd for $C_{12}H_{14}BrNO_3$ $[M+H]^+$ 300.0230, found 300.0219. FT-IR (Neat) ν_{max} (cm^{-1}) = 2952.12, 2860.15, 1702.12, 1441.25, 1251.31, 1141.15, 1090.01, 1008.89, 871.75, 778.36, 565.61, 506.18.

5-(p-tolyl)-1,4,7-dioxazonan-6-one, (**10c**)**:** 39.9 mg, 0.1 mmol of **4j** was dissolved in dry isopropanol (3ml) in two separate 25ml round bottom flasks, 24.3μl, 0.5 mmol of hydrazine monohydrate was added to both of the reaction mixture and reflux for 3hr with stirring. Solvent was evaporated under reduced pressure, work up in DCM (3×10ml) in water, dried over sodium sulphate and purified by column chromatography using silica gel (100-200 mesh size) with methanol (10%) in dichloromethane to afford colourless oily compound **10c** of 17.7 mg (75% yield) respectively; ^{1}H NMR (CD_3OD, 400 MHz) δ_H 8.22-8.20 (m, 1H), 7.83-7.81 (m, 1H), 7.31 (d, J = 8.0 Hz, 1H) 7.16 (d, J = 8.0 Hz, 1H), 4.82 (s, 1H), 3.70-3.60 (m, 6H), 3.08-3.06 (m, 2H), 2.32 (s, 3H); 13C NMR (CD_3OD, 100 MHz) δC 171.0, 159.0, 138.2, 134.2, 131.7, 128.7, 126.9, 125.5, 81.5, 69.9, 68.6, 39.5, 19.8. HRMS (ESI-TOF) m/z calcd for $C_{12}H_{14}BrNO_3$

$[M+H]^+$ 236.1261, found 236.1255. FT-IR (Neat) ν_{max} (cm^{-1}) = 3195.50, 2875.37, 2398.25, 1638.35, 1561.70, 1439.37, 1359.63, 1248.22, 1087.45, 765.87, 696.63, 489.17.

Methyl 2-(1,3-dioxoisoindolin-2-yl)-2-phenylacetate, (**11a**)**: 11a** obtained as the N-H inserted by-product in the reaction of **1a** and **2a** with **3** in water. Colourless oil, (12 mg, 13.5%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H 7.89-7.84 (m, 2H), 7.78-7.71 (m, 2H), 7.56-7.54 (m, 2H), 7.37-7.33 (m,3H), 6.02 (s, 1H), 3.81 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ_C 168.7, 167.2, 134.5, 134.4, 132.0, 129.9, 128.8, 128.7, 123.8, 55.9, 53.2. HRMS (ESI-TOF) m/z calcd for $C_{17}H_{13}NO_4$ $[M+H]^+$ 296.0917, found 296.0904. FT-IR (Neat) ν_{max} (cm^{-1}) = 3190.21, 2865.17, 1640.15, 1660.20, 1241.02, 1078.41, 761.07, 695.28, 480.27.

Methyl 2-((5-(1,3-dioxoisoindolin-2-yl)pentyl)oxy)-2-phenylacetate (15a): 15a was synthesised using general procedure. **2a** (63.4 mg, 0.36 mmol) and tetrahydropyran **14** (74 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **15a**, colourless oil, (94.9 mg, 83%); 1H NMR (CDCl3, 400 MHz) δH 7.84-7.82 (m, 2H), 7.71-7.69 (m, 2H), 7.44-7.41 (m, 2H), 7.36-7.30 (m, 3H), 4.85 (s, 1H), 3.69 (s, 3H), 3.69-3.65 (m, 2H), 3.55-3.49 (m, 1H), 3.45-3.39 (m, 1H), 1.73-1.65 (m, 4H), 1.4-1.40 (m, 2H) ; 13C NMR (CDCl3, 100 MHz) δC 171.6, 168.6, 136.7, 134.0, 132.3, 128.7, 127.3, 123.3, 81.2, 69.7, 52.4, 38.0, 29.8, 29.2, 28.5, 23.5. HRMS (ESI-TOF) m/z calcd for C22H23NO5 [M+H]+ 382.1649, found 382.1645. FT-IR (Neat) νmax (cm-1) = 2931.17, 2864.16, 1704.27, 1442.42, 1388.84, 1268.00, 1173.57, 1108.94, 712.16, 526.94.

Ethyl 2-((5-(1,3-dioxoisoindolin-2-yl)pentyl)oxy)-2-(p-tolyl)acetate (15b): 15b was synthesised using general procedure. **2j** (73.5 mg, 0.36 mmol) and tetrahydropyran **14** (74 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **15b**, colourless oil, (92.1 mg, 75%); 1H NMR (CDCl3, 400 MHz) δH 7.88-7.86 (m, 1H), 7.84-7.82 (m, 1H), 7.77-7.75 (m, 1H), 7.71-7.69 (m, 1H), 7.32-7.29 (m, 2H), 7.18-7.13 (m, 2H), 4.78 (s, 1H), 4.18-4.12 (m, 2H) 3.69-3.65 (m, 2H), 3.53-3.47 (m, 1H), 3.43-3.39 (m, 1H), 2.33 (s, 3H), 1.70-1.67 (m, 4H), 1.45-1.40 (m, 2H), 1.23-1.18 (m, 3H); 13C NMR (CDCl3, 100 MHz) δC 171.3, 168.6, 168.1, 138.5, 134.5, 134.0, 132.8, 132.3, 129.4, 127.2, 126.6, 123.7, 123.3, 81.1, 69.5, 61.2, 38.0, 32.1, 29.8, 23.6, 21.3, 14.2. HRMS (ESI-TOF) m/z calcd for C24H27NO5 [M+H]+ 410.1962, found 410.1959. FT-IR (Neat) νmax (cm-1) = 3180.61, 3056.20, 2917.97, 2853.17, 1710.62, 1598.78, 1457.99, 1366.13, 1290.42, 1178.42, 1038.48, 799.00, 703.48, 638.40, 526.20.

Methyl 2-(4-chlorophenyl)-2-((5-(1,3-dioxoisoindolin-2-yl)pentyl)oxy)acetate (**15c**): **15c** was synthesised using general procedure. **2i** (75.8 mg, 0.36 mmol) and tetrahydropyran **14** (74 ml, 0.75 mmol) was dissolved in water (5ml) in oven dried 20ml vial and stirred under blue light irradiation for 2 h, then **1a** (44.1 mg, 0.3 mmol) was added to the reaction mixture and stirred under blue light irradiation until full consumption of starting materials monitoring through TLC. After completion of the reaction precipitate was filtered out, dissolved in ethyl acetate and purified by column chromatography in silica gel (100-200 mesh size) with ethyl acetate (15-30%) in hexane to afford the desired product, **15c**, colourless oil, (107.29 mg, 86%);

1H NMR (CDCl3, 400 MHz) δH 7.84-7.81 (m, 2H), 7.72-7.69 (m, 2H), 7.38-7.35 (m, 2H), 7.32-7.30 (m, 2H), 4.81 (s, 1H), 3.69 (s, 3H), 3.67-3.65 (m, 2H), 3.55-3.50 (m, 1H), 3.43-3.37 (m, 1H), 1.72-1.65 (m, 4H), 1.45-1.40 (2H); 13C NMR (CDCl3, 100 MHz) δC 171.2, 168.6, 135.2, 134.6, 134.0, 132.2, 128.9, 128.6, 123.3, 80.4, 69.8, 52.5, 38.0, 29.2, 28.4, 23.5. HRMS (ESI-TOF) m/z calcd for C22H22ClNO5 [M+H]+ 416.1259, found 416.1255; FT-IR (Neat) νmax (cm-1) = 2934.84, 2860.02, 1708.46, 1449.17, 1390.65, 1269.77, 1175.26, 1105.88, 706.05, 528.57.

2. HRMS studies for reaction condition optimization studies:

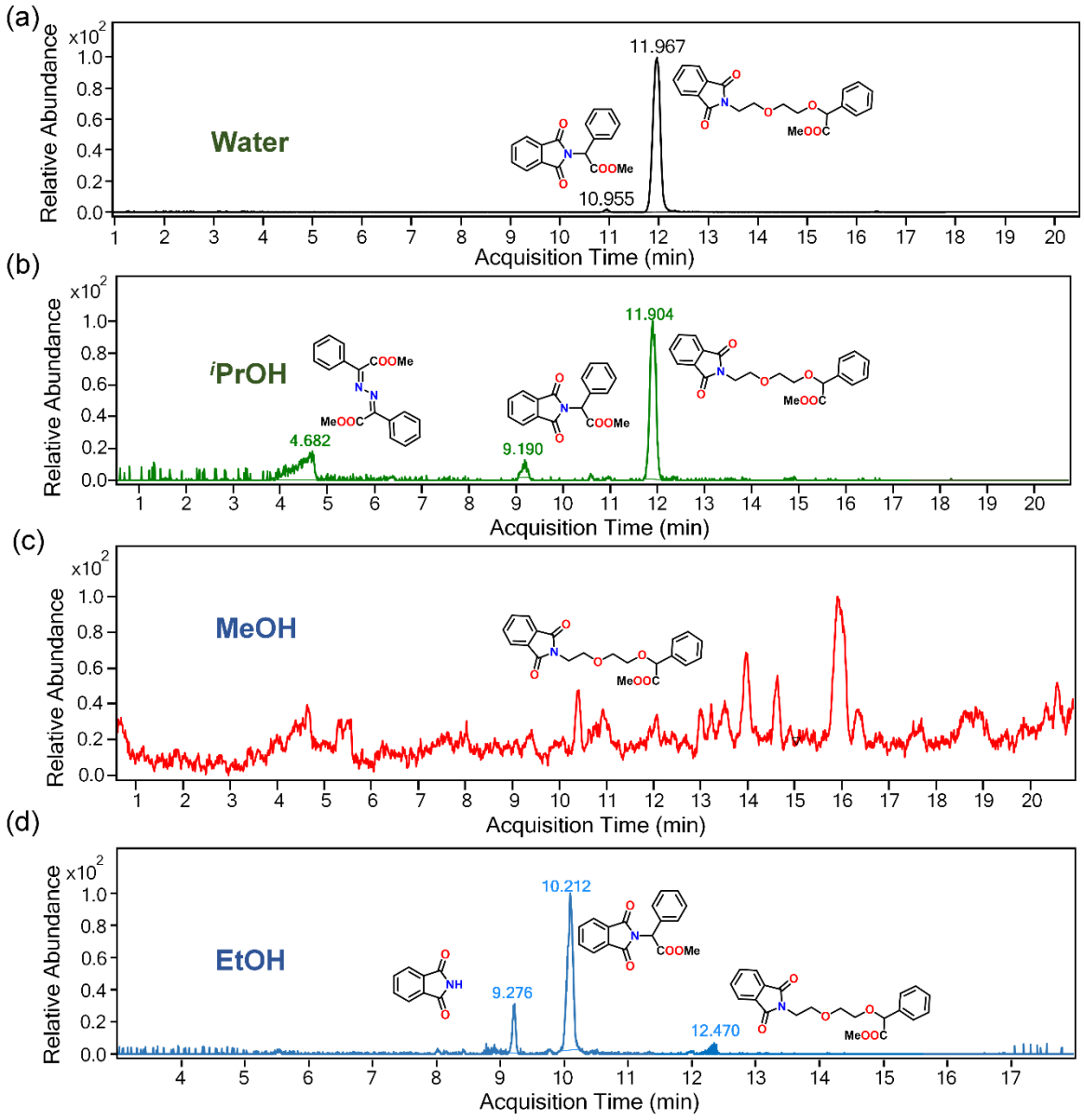


Figure S1: HRMS data of crude reactions of phthalimide **(1a)** with phenyl diazoacetate **(2a)** and 1,4-dioxane **(3)** in various solvent.

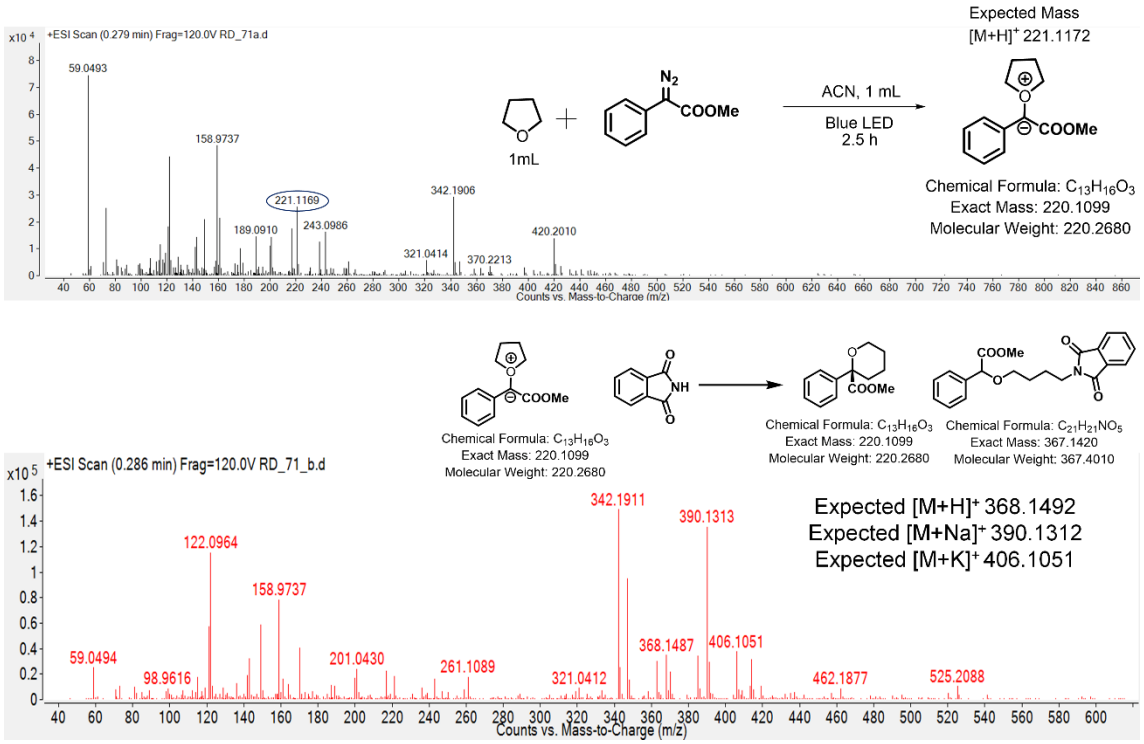


Figure S2: ESI/HRMS spectra of the crude reaction mixture obtained from the blue LED mediated reaction between phenyl diazoacetate, THF and phthalimide in water.

3. HPLC studies

Initial rate of formation of products of Blue LED mediated three-component etherification reaction between phthalimide (1a), 3CN, indole (1b) with phenyl diazoesters (2a) and 1,4 dioxane (3) in water has been calculated by HPLC based kinetic study, in which initial 0%-10% formation of various intermediated species and desired products were considered as the initial rate of formation of product.

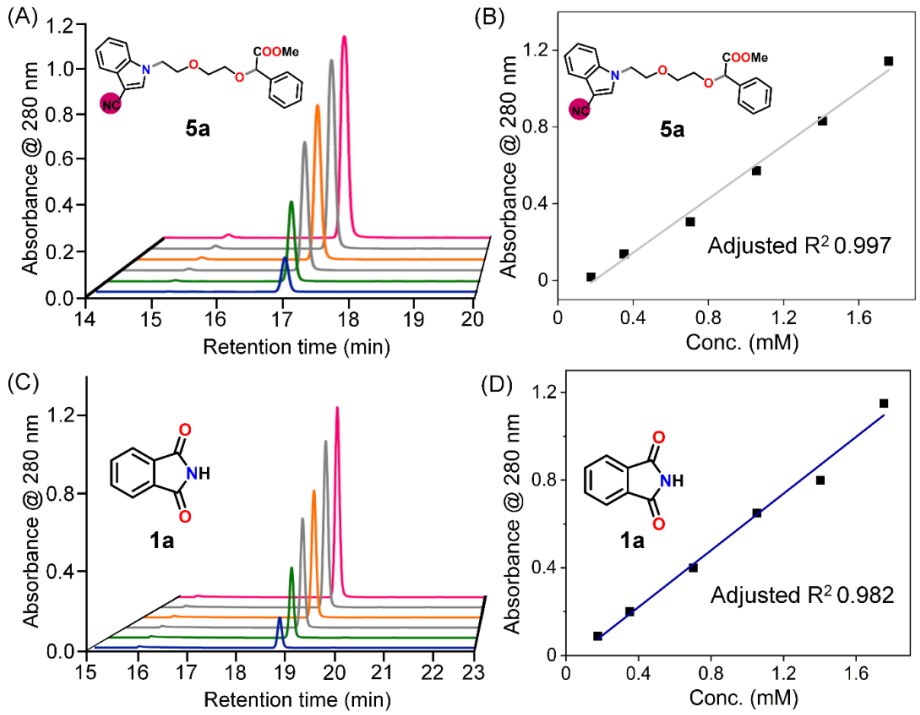


Figure S3: (A) HPLC stack chromatogram of **5a** with various concentrations at 280 nm; and (B) The corresponding standard calibration curve generated from the same. (C) HPLC stack chromatogram of **1a** with various concentrations at 280 nm; (D) The corresponding standard calibration curve generated from the same.

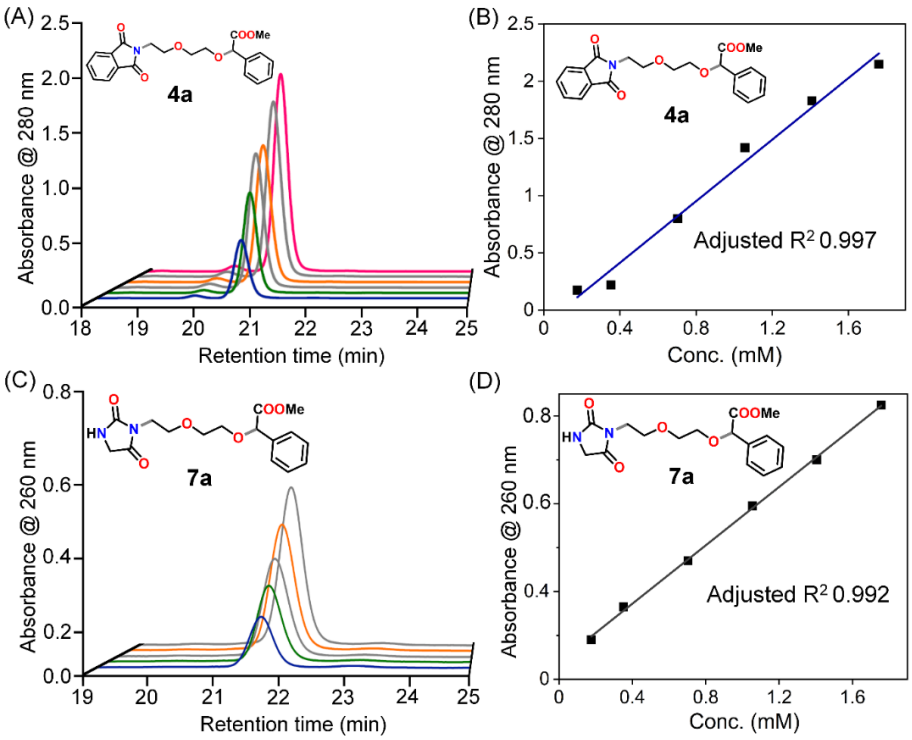


Figure S4: (A) HPLC stack chromatogram of **4a** with various concentrations at 280 nm; and (B) The corresponding standard calibration curve generated from the same. (C) HPLC stack chromatogram of **6a** with various concentrations at 260 nm; (D) The corresponding standard calibration curve generated from the same.

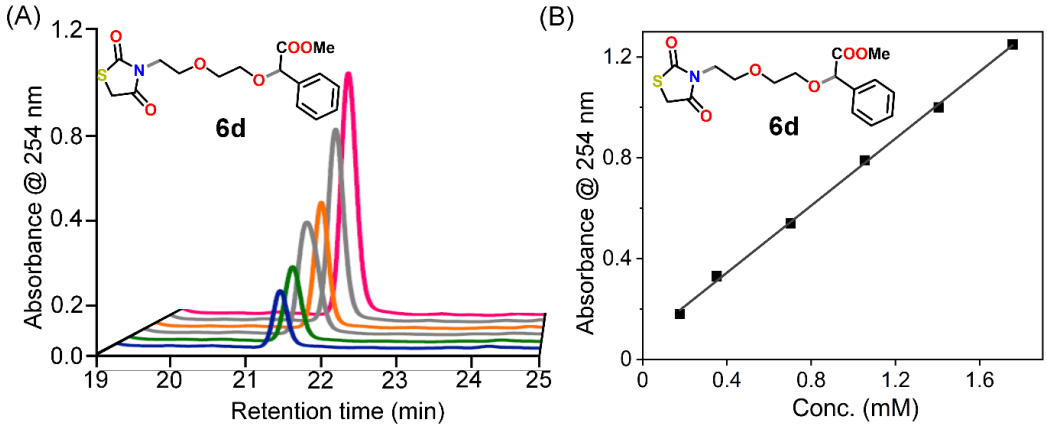


Figure S5: (A) HPLC stack chromatogram of **6d** with various concentrations at 254 nm; and (B) The corresponding standard calibration curve generated from the same.

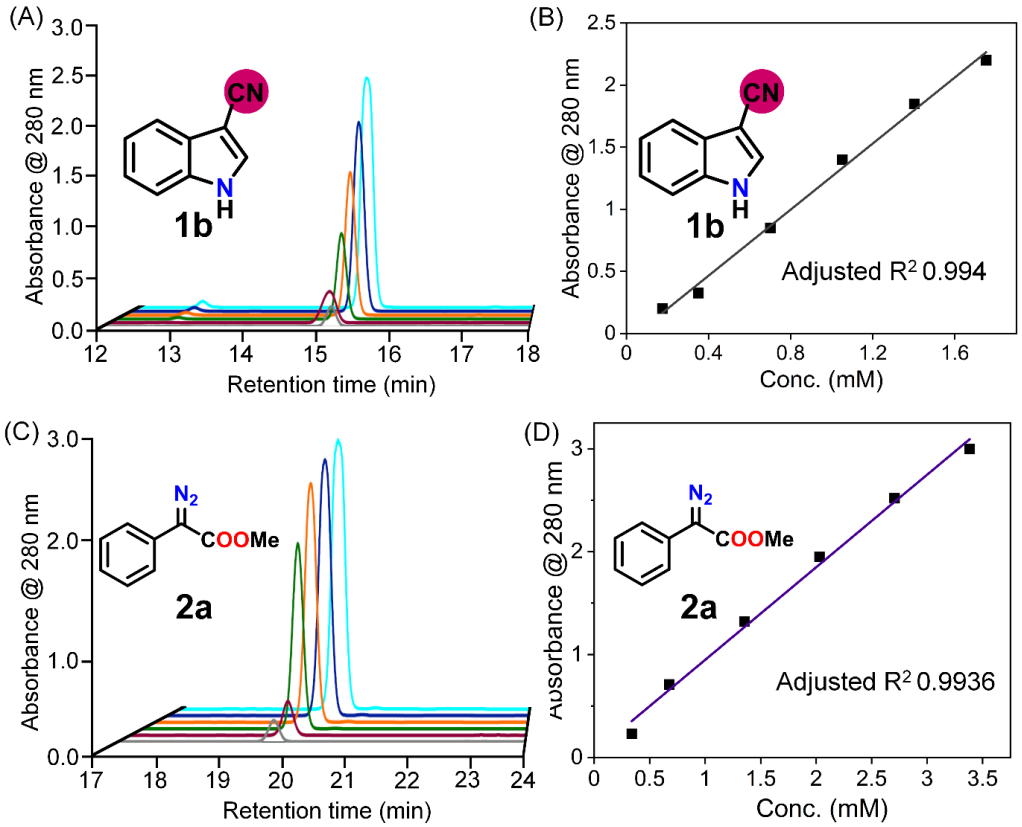


Figure S6: (A) HPLC stack chromatogram of **1b** with various concentrations at 280 nm; and (B) The corresponding standard calibration curve generated from the same. (C) HPLC stack chromatogram of **2a** with various concentrations at 280 nm; (D) The corresponding standard calibration curve generated from the same.

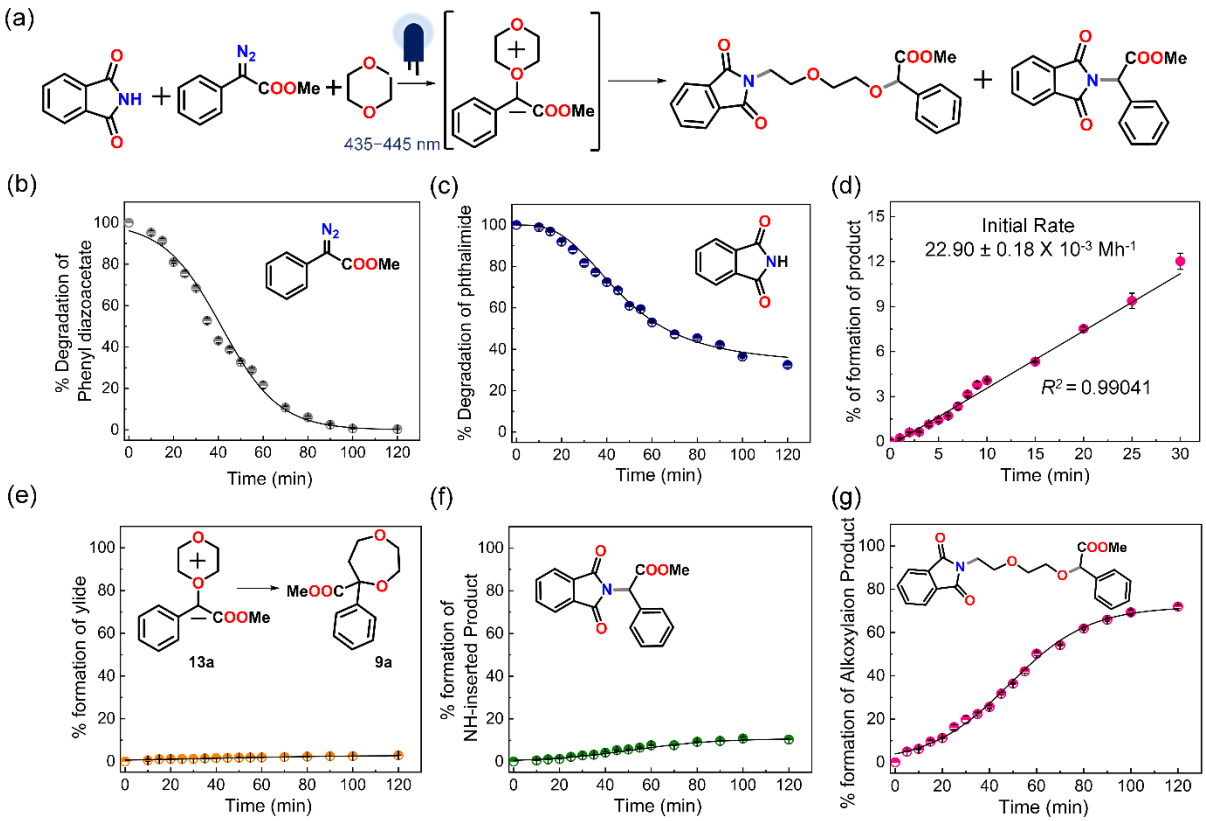


Figure S7: (a) Schematic diagram showing the Blue LED mediated three-component etherification reaction of phthalimide (**1a**) with phenyl diazoacetate (**2a**) and 1,4-dioxane (**3**) for 2 h and the production of desired product **4a** as well as the production of N-H inserted product **11a**. Diagram showing the percentage degradation of **2a** (b) and **1a** (c); (d) Showing the calculation of initial rate of formation of desired etherification product **4a** in M h^{-1}. Diagram showing the percentage formation of oxonium ylide [**13a**→**9a**] (e), N-H inserted product **11a** (f), and the desired etherified product [**4a**] (g) during the course of reaction over 2h.

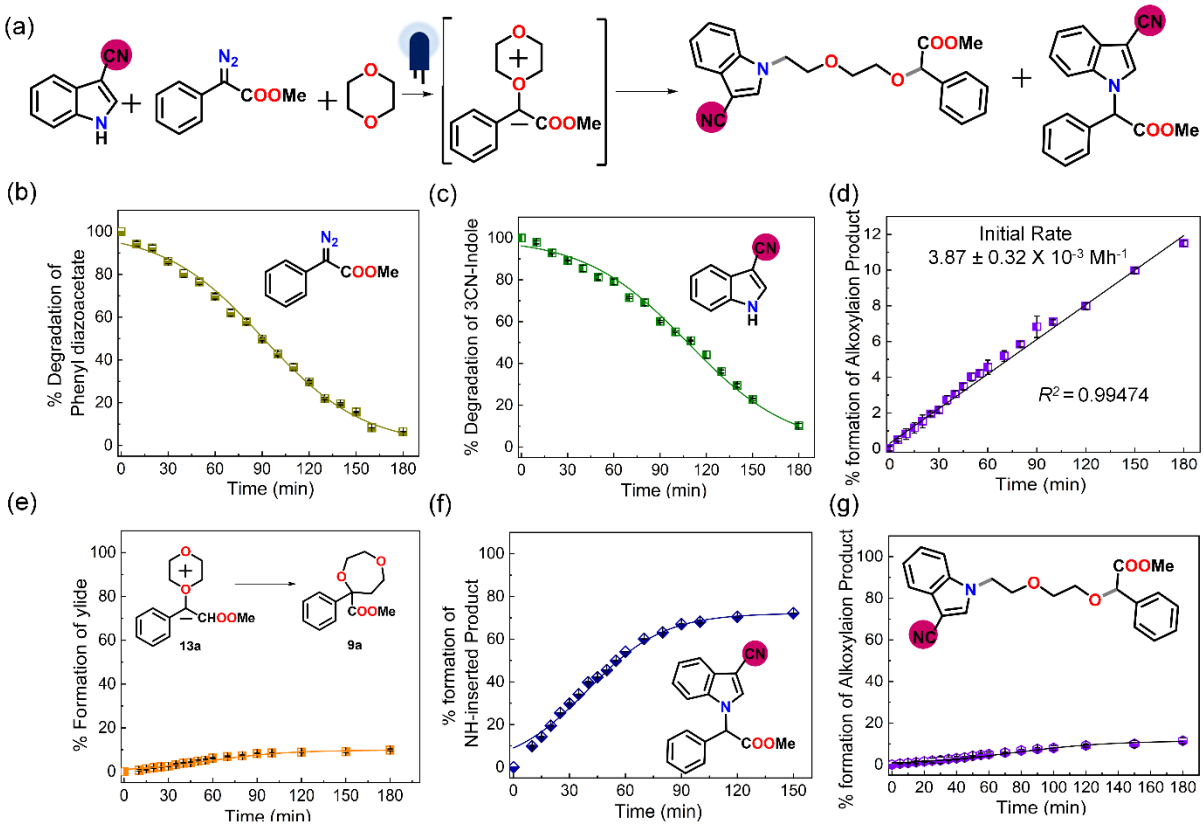


Figure S8: (a) Schematic diagram showing the Blue LED mediated three-component etherification reaction of 3CN-indole (**1b**) with phenyl diazoacetate (**2a**) and 1,4-dioxane (**3**) for 3 h and the production of desired product **5a** as well as the production of N-H inserted product **12a**. Diagram showing the percentage degradation of **2a** (b) and **1b** (c); (d) Showing the calculation of initial rate of formation of desired etherification product **5a** in M h^{-1}. Diagram showing the percentage formation of oxonium ylide [**13a→9a**] (e), N-H inserted product **12a** (f), and the desired etherified product [**5a**] (g) during the course of reaction over 3h.

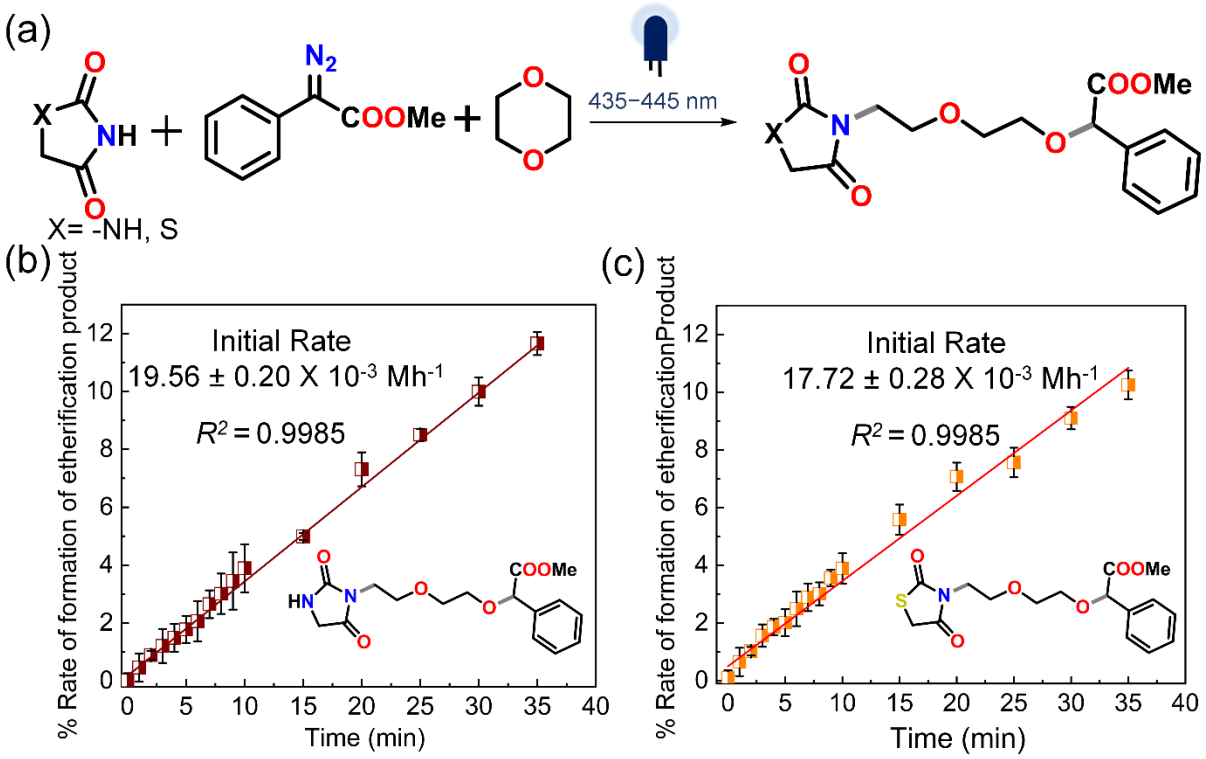


Figure S9: (a) Schematic diagram showing the Blue LED mediated three-component etherification reaction of thiazolidinedione (**1d**) and hydantoin (**1e**) with phenyl diazoacetate (**2a**) and 1,4-dioxane (**3**) for 2 h and the production of desired product **6a** and **7a**. (b) Showing the calculation of initial rate of formation of desired etherification product **6a** (b) and **7a** (c) in M h^{-1}.

4. Computational Details

All the calculations are performed by using B3LYP[S1] level of theory as implemented in the Gaussians 09 package.[S2] For geometry optimizations, 6-311++G (2d, p) basis set was used for all atoms. Frequency calculations of all the optimized structures were performed to ensure that the optimized structures were the local energy minima without any imaginary frequency, and to obtain zero-point corrections and the Gibbs free energies. Transition states were obtained using Berny optimization algorithm implemented in Gaussian 09 and were in each case verified the presence of a single imaginary vibrational frequency associated with the desired reaction coordinate, and also confirm the nature of transition states Moreover, solvent plays a crucial role on the blue LED mediated three-component amino etherification reaction. Therefore, the solvent effect has been considered in self-consistent reaction field method (SCRF) whereas natural bond orbital calculations were performed in 6-311++G (2d, p). [S3-S7] The NBO Version 3.1 program implemented in Gaussian 03 was used to perform NPA. All the HOMO and LUMO visualisation files were generated from FCHK file by the help of chemcraft software. The NBO Version 3.1 program implemented in Gaussian 09 was used to perform NPA.[S3-S7] Frequency calculations were performed at the optimization level of basis set to confirm the nature of stationary points, and to obtain zero-point corrections and the Gibbs free energies.

The reaction free energies (ΔG) (the Gibbs free energies i.e., the term of the sum of electronic and thermal free energies) are calculated using the following equation.

Where $G_{product}$ and $G_{reactant}$ are the total energies of products and reactants respectively.

$$\Delta G = G_{product} - G_{reactant}$$

Similarly, transition state energy calculated as follows

$$\Delta G^{\ddagger} = G_{transition\ state} - G_{reactant}$$

Where $G_{product}$ and $G_{reactant}$ are the total energies of products and reactants respectively.

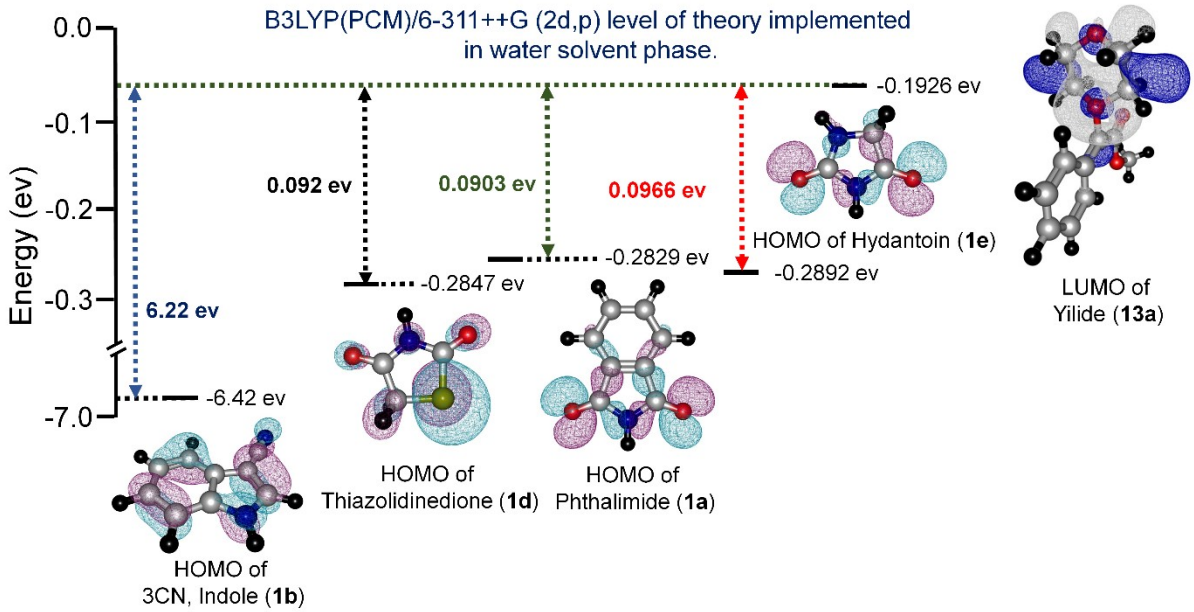


Figure S10: Representation of HOMO-LUMO energy gap between HOMO states of **1a-b** and **1d-e** LUMO of ylide **(13a)**.

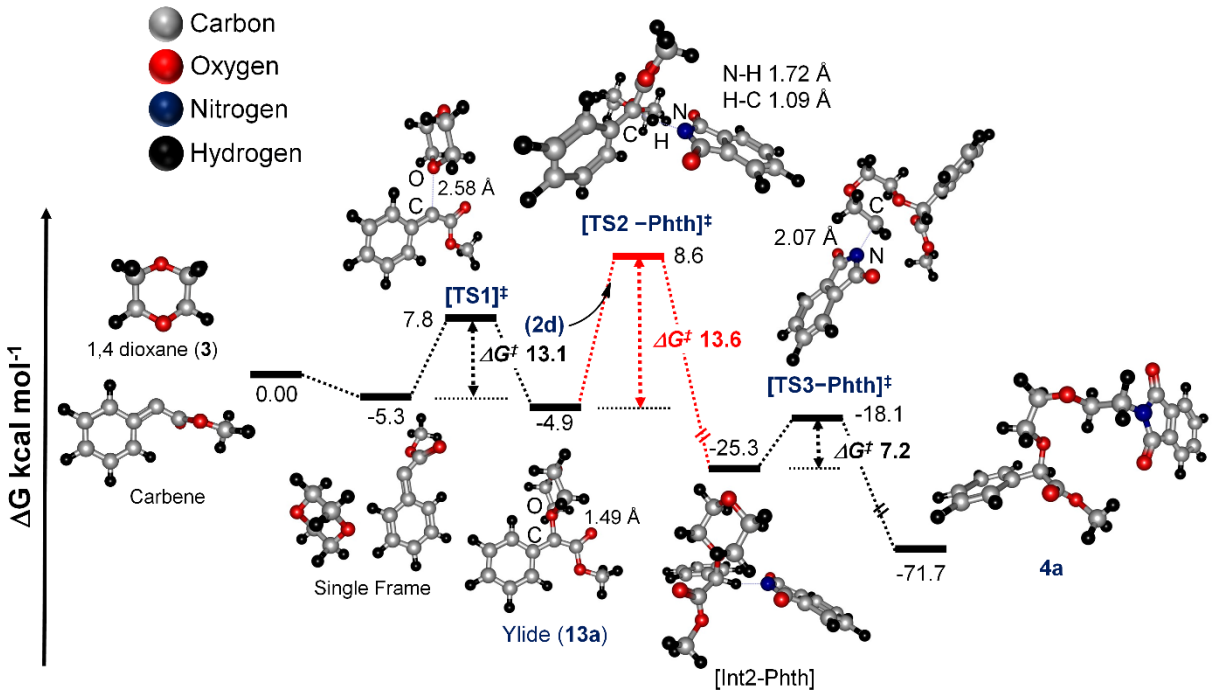


Figure S11: The total energy profile of the reactions between phthalimide (**Phth**/**1a**) and phenyl diazoacetate carbene in presence of 1,4 dioxane (**3**). All energies are in kcal mol^{-1}, relative to the free molecules. TS = transition states. **[TS1]**‡, [**TS2-Phth]**‡, and [**TS3-Phth]**‡.

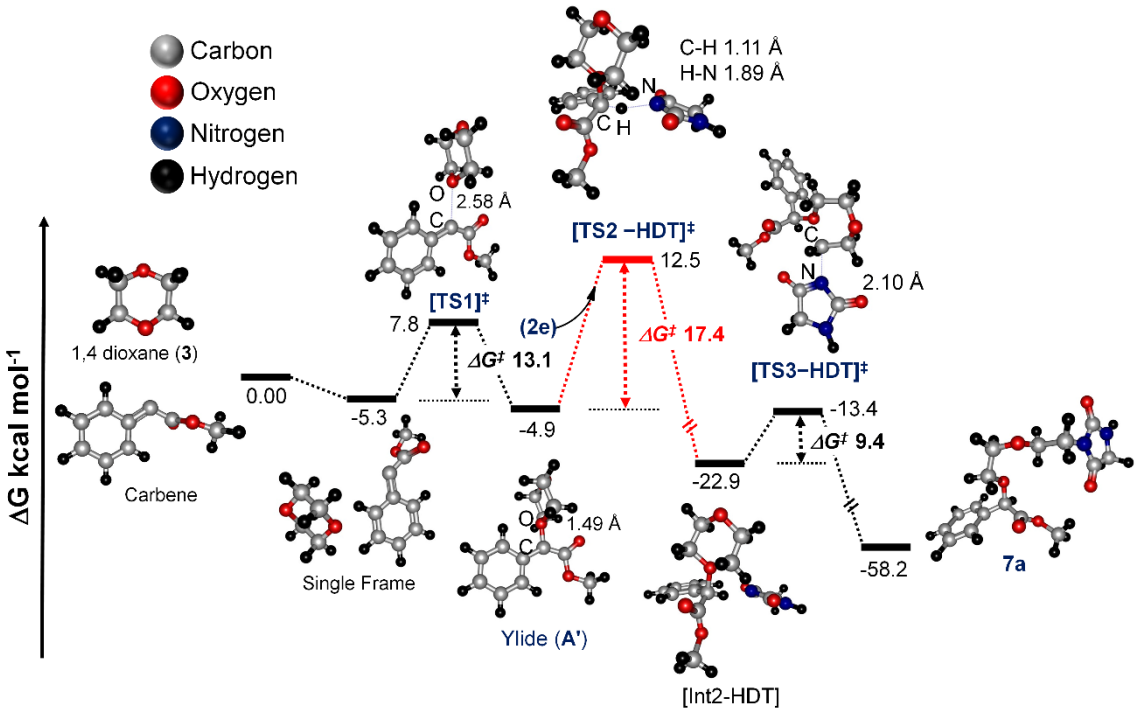


Figure S12: The total energy profile of the reactions between hydantoin (**HDT**/**1e**) and phenyl diazoacetate carbene in presence of 1,4 dioxane (**3**). All energies are in kcal mol^{-1}, relative to the free molecules. TS = transition states. **[TS1]**‡, [**TS2-HDT]**‡, and [**TS3-HDT]**‡.

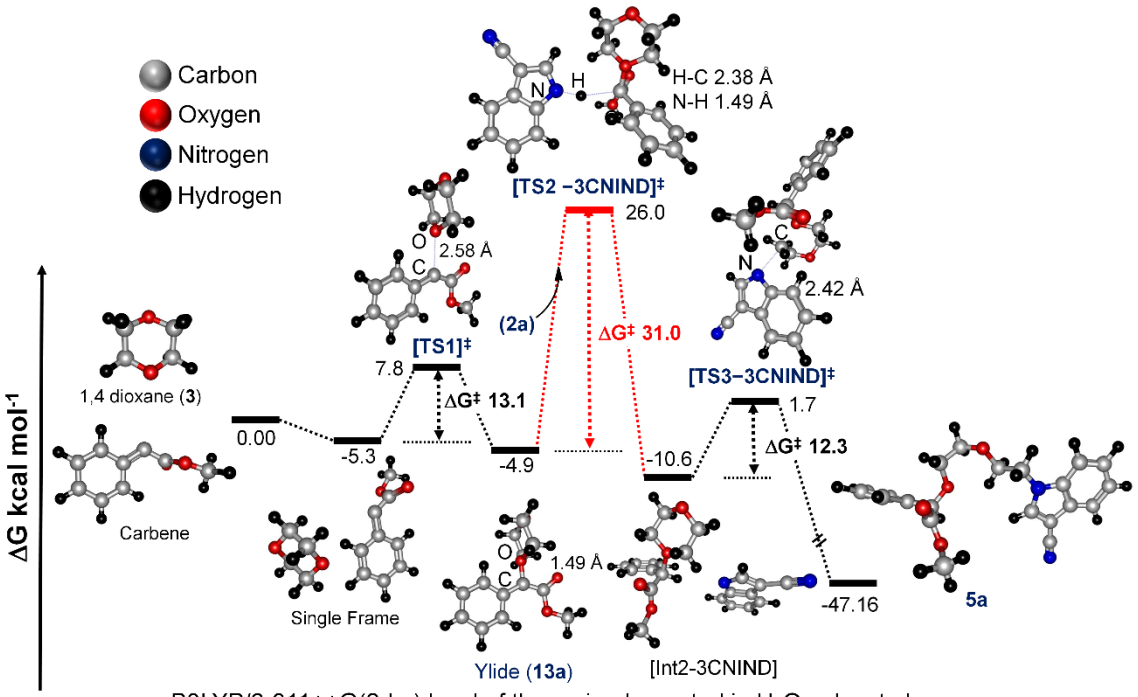


Figure S13: The total energy profile of the reactions between indole (**3CNIND**/**1b**) and phenyl diazoacetate carbene in presence of 1,4 dioxane (**3**). All energies are in kcal mol^{-1}, relative to the free molecules. TS = transition states. **[TS1]**‡, [**TS2-3CNIND]**‡, and [**TS3-3CNIND]**‡.

Table S1: Optimized Energy of the Reactants, Products, and Transition States of Blue LED mediated amino etherification reaction between phenyl diazoacetate (**2a**) with phthalimide (**1a**), hydantoin (**1e**) and 3CN-indole (**1b**).

	B3LYP(PCM)/6-311++ G (2d,p) [E^h] In water	Thermal correction to Gibbs Free Energy	Relative Energy (Kcal mol^{-1})
1,4 dioxane (**3**)	-307.6610864 A.U.	0.093075 A.U.	–
Carbene	-498.1174467 A.U.	0.108621 A.U.	–
(**3**) + Carbene	-805.7785331 A.U.	–	–
(**3**) + Carbene (single frame)	805.7869863 A.U.	0.219692 A.U.	-5.30
[TS1]‡	-805.7660213 A.U.	0.228657 A.U.	**+13.15**
Int1/Ylide (**13a**)	-805.7864384 A.U.	0.227884 A.U.	-12.81
Hydantoin (**1e**)	-376.7127128 A.U.	0.051162 A.U.	-
Int1 + (**1e**)	-1182.499151 A.U.	0.279046 A.U.	-
[TS2-HDT]‡	-1182.4712964 A.U.	0.094867 A.U.	**+17.47**
[Int2-HDT]	-1182.527785 A.U.	0.298928 A.U.	-35.44
[TS3-HDT]‡	-1182.512784 A.U.	0.027485 A.U.	**+ 9.41**
HDT Product (**7a**)	-1182.584066 A.U.	0.298165 A.U.	-44.72
3CNIndole (**1b**)	-363.8258438 A.U.	0.100102 A.U.	-
Int1 + (**1b**)	-1169.591865 A.U.	0.327986 A.U.	-
[TS2-3CNIND]‡	-1169.542348 A.U.	0.105553 A.U.	**+31.01**
[Int2-3CNIND]	-1169.600831 A.U.	0.093917 A.U.	-36.69
[TS3-3CNIND]‡	-1169.581109 A.U.	0.123722 A.U.	**+12.37**
3CNIND Product (**5a**)	-1169.660812 A.U.	0.108732 A.U.	-50.01
Phthalimide (**1a**)	-513.2672321 A.U.	0.082679 A.U.	-
Int1 + (**1a**)	-1319.033253 A.U.	0.310563 A.U.	-
[TS2-Phth]‡	-1319.011495 A.U.	0.301559 A.U.	**+13.65**
[Int2-Phth]	-1319.0657737 A.U.	0.282679 A.U.	-34.06
[TS3-Phth]‡	-1319.054284 A.U.	0.304607 A.U.	**+7.20**
Phth Product (**4a**)	-1319.139728 A.U.	0.329485 A.U.	-53.61

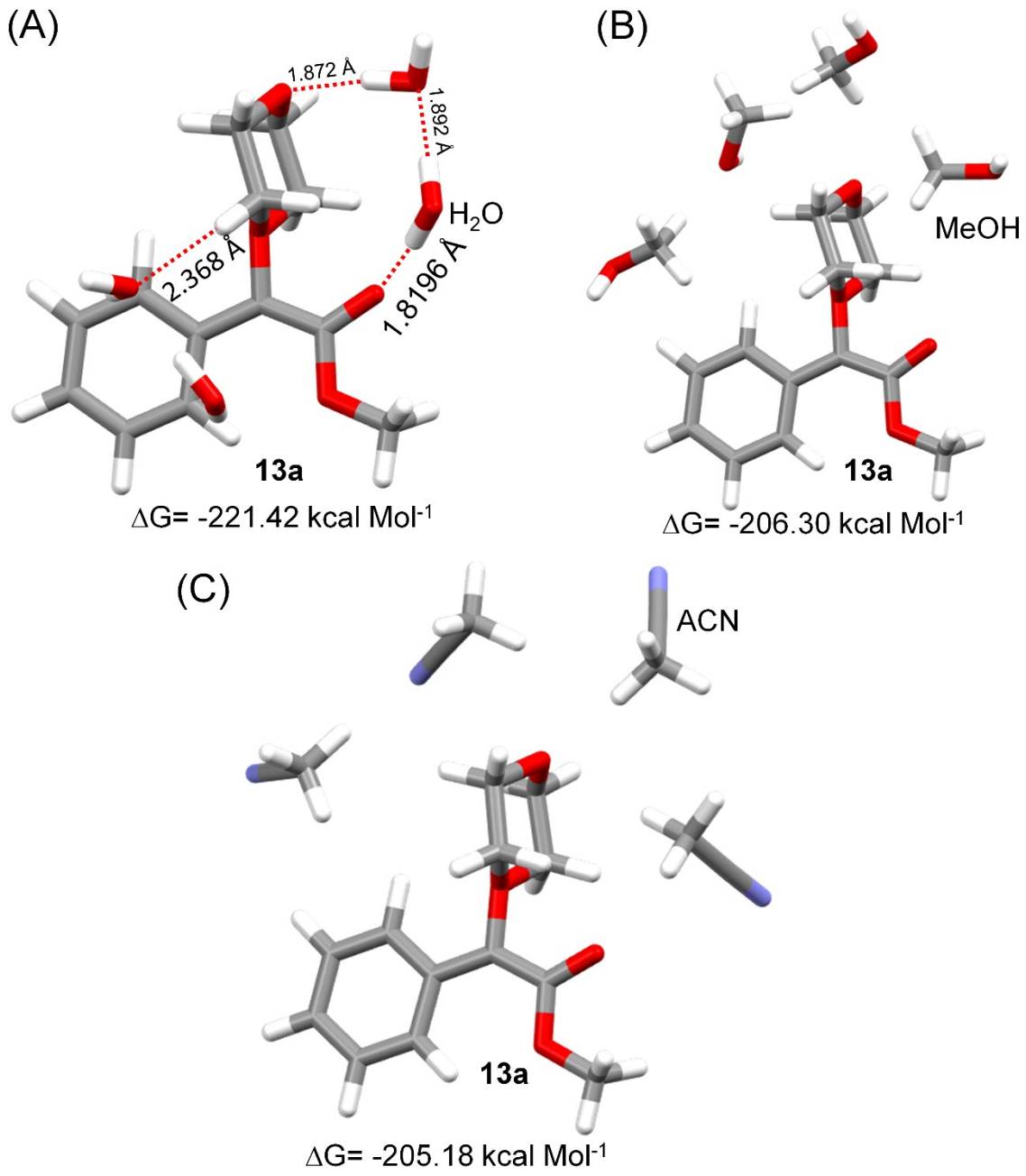


Figure S14: Optimized structure of oxonium ylide in presence of (a) water (H_2O); (b) methanol (MeOH) and (c) acetonitrile (ACN) in B3LYP(PCM)/6-311G++ (2d, p) level of theory implemented in water phase with dispersion correction D3.[a]

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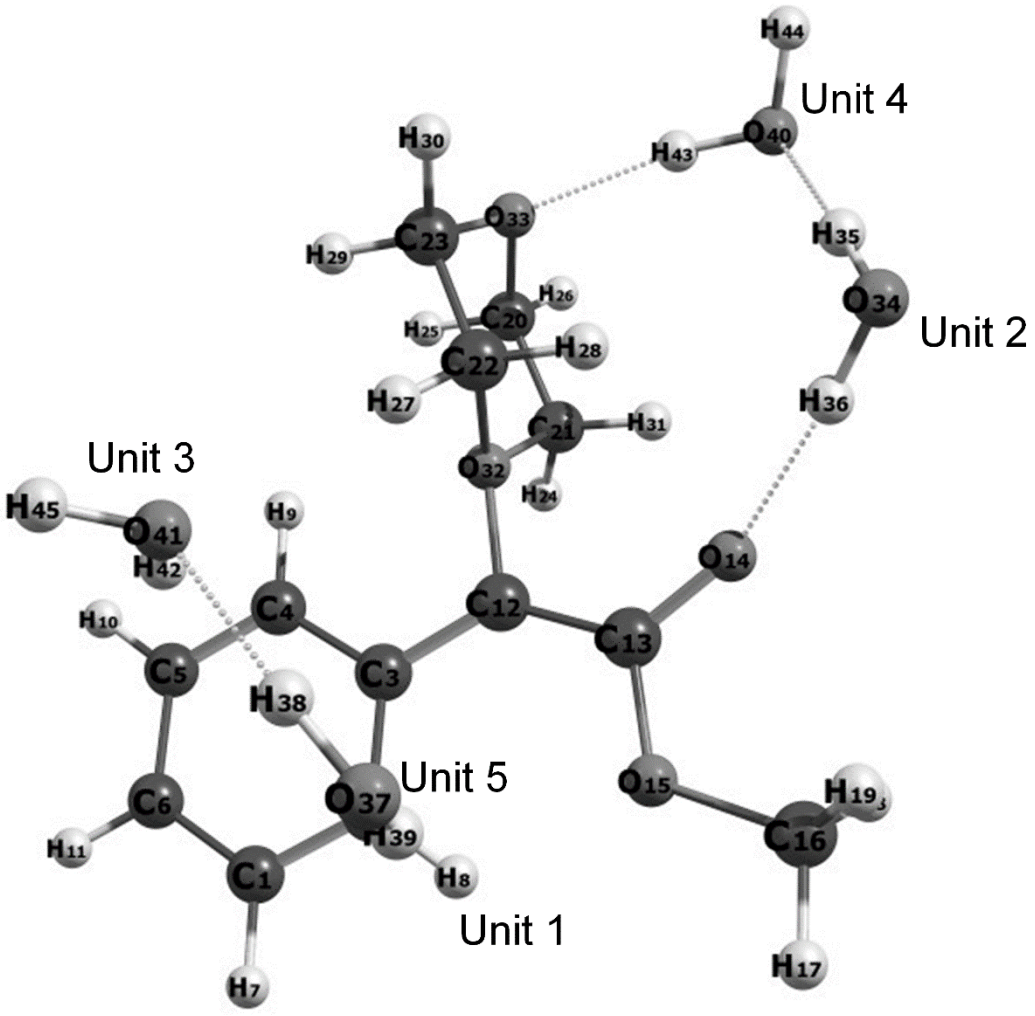
[a]Sedlak, R., Rezac, J. Empirical D3 dispersion as a replacement for ab initio dispersion terms in density functional theory-based symmetry-adapted perturbation theory. *J. Chem. Theory Comput.* **2017**, *13*,1638-1646.



Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
68. LP (1) O 14	/553. RY*(3) O 34	0.08	1.38	0.009
68. LP (1) O 14	/582. RY*(4) H 36	0.05	2.69	0.011
68. LP (1) O 14	**/726. BD*(1) O 34 - H 36**	**6.83**	**1.18**	**0.080**
from unit 1 to unit 4				
75. LP (2) O 33	/620. RY*(2) O 40	0.18	1.15	0.013
75. LP (2) O 33	/673. RY*(5) H 43	0.07	2.13	0.011
75. LP (2) O 33	**/729. BD*(1) O 40 - H 43**	**5.24**	**0.79**	**0.058**

Figure S15: Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis of oxonium ylide **13a** in presence of water by using B3LYP(PCM)/6-311G++ (2d, p) level of theory implemented in water phase with dispersion correction D3.

5. Hammett's corelations

For the Hammett's corelation parameters of the blue LED mediated three-component amino etherification reaction, phthalimide (**1a**) chosen as a model substate, and reacted with various C3(meta) and C4(para) substituted aryl diazoesters (**2a-l**) and 1,4 dioxane (**3**). Initial rate of formation of etherification product has been calculated by HPLC based kinetic study, in which initial 0%-15% formation of desired products was considered as the initial rate of formation of etherified compounds.

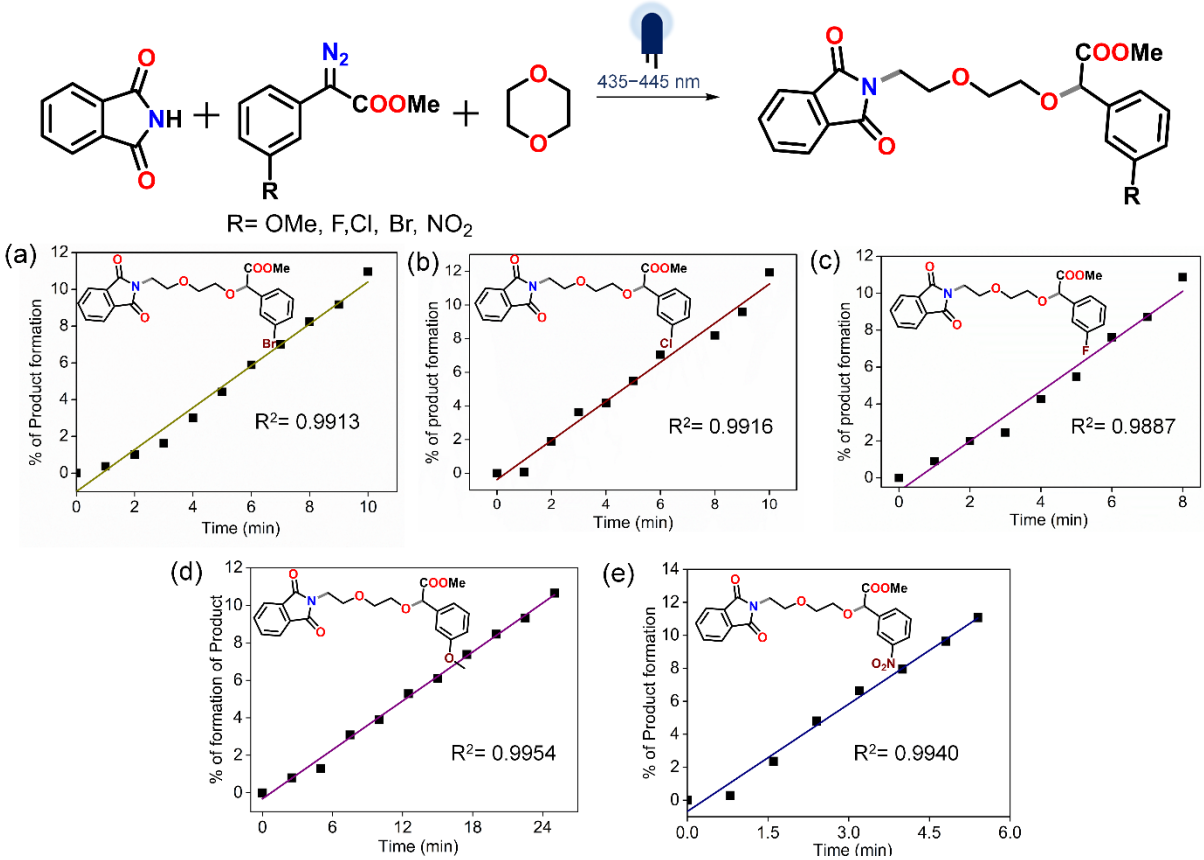


Figure S16: Schematic diagram showing the Blue LED mediated three-component etherification reaction of phthalimide (**1a**) with C3(meta) substituted aryl diazoacetate (**2a-f**) in 1,4-dioxane (**3**) for 2 h and the production of respective amino etherified products (a-e) Showing the calculation of initial rate of formation of desired etherification product in M h^{-1}.

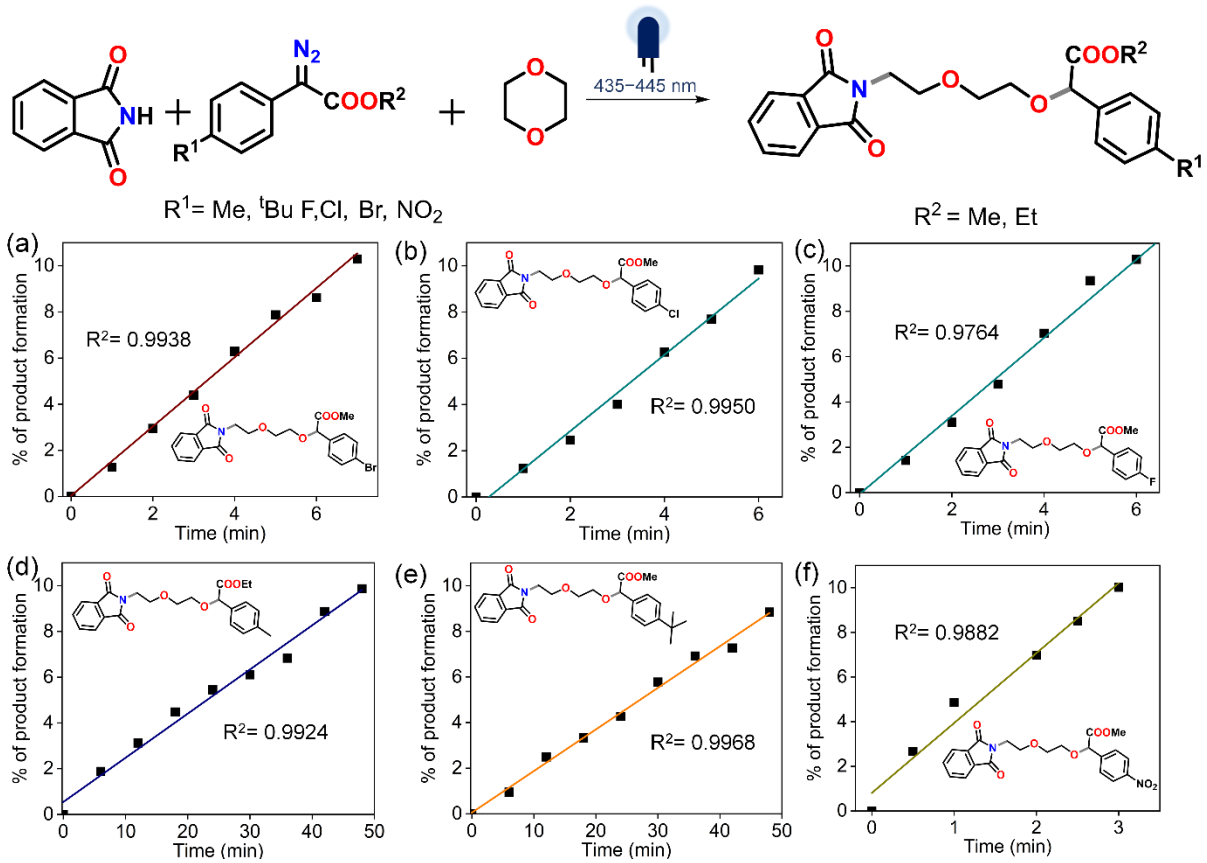


Figure S17: Schematic diagram showing the Blue LED mediated three-component etherification reaction of phthalimide (**1a**) with C4(para) substituted aryl diazoacetate (**2g-l**) in 1,4-dioxane (**3**) for 2 h and the production of respective amino etherified products. (a-e) Showing the calculation of initial rate of formation of desired etherification product in M h^{-1}.

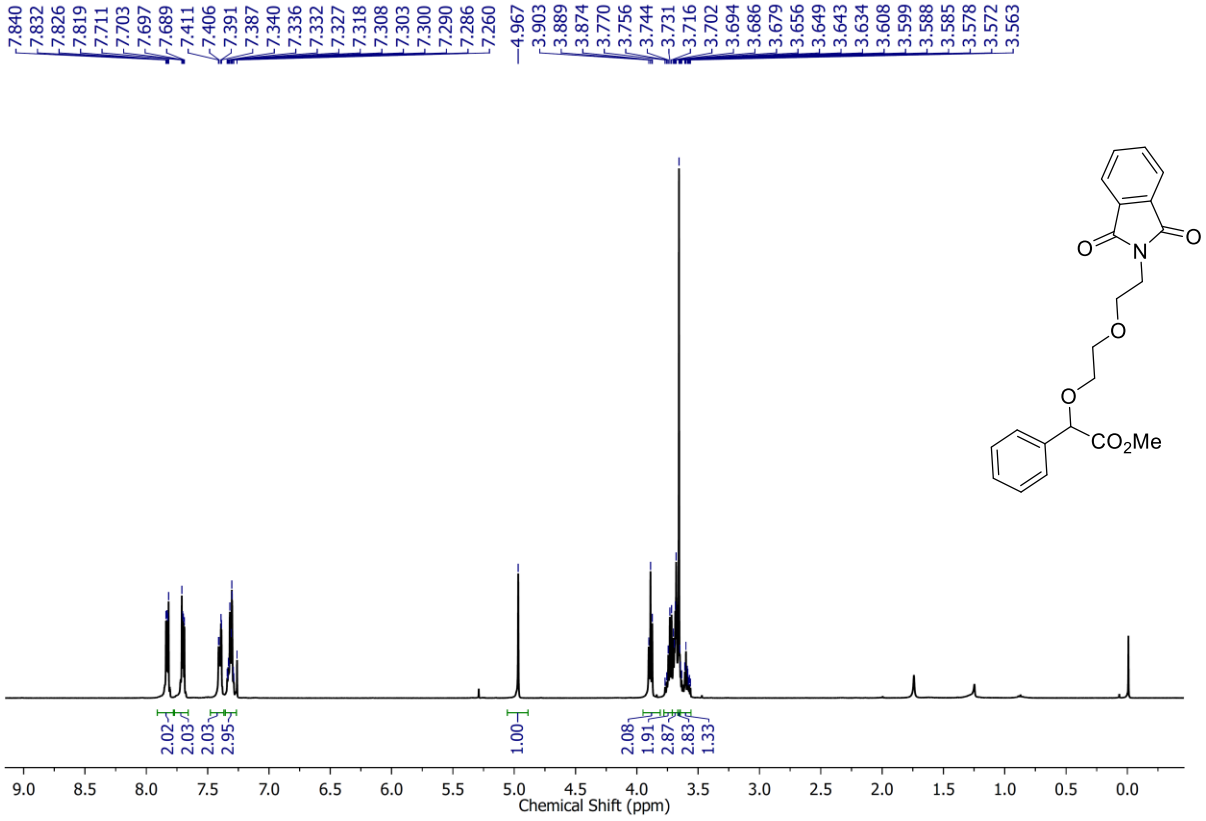
Table S2: Hammett;s corelation study: Initial rate of formation of amino etherification products from the reaction of blue LED mediated three-component reaction between phthalimide (**1a**), various aryl diazoesters (**2a-l**) and the reported σ values for the C3 and C4 substitution at the phenyl ring of the various aryl diazoesters.

Substitution	**Initial Rate of Formation of etherification products (Mh^{-1})**	σ_m [a]
─3Br	$6.84 \pm 0.29 \times 10^{-2}$	0.39
─3Cl	$6.97 \pm 0.30 \times 10^{-2}$	0.37
─3F	$8.17 \pm 0.36 \times 10^{-2}$	0.34
─3OMe	$2.61 \pm 0.13 \times 10^{-2}$	0.12
─3NO_2	$13.05 \pm 0.32 \times 10^{-2}$	0.71
Substitution	**Initial Rate of Formation of etherification products (Mh^{-1})**	σ [a]
─H	$2.29 \pm 0.26 \times 10^{-2}$	0.00
Substitution	**Initial Rate of Formation of etherification products (Mh^{-1})**	σ_p [a]
─4Br	$8.51 \pm 0.28 \times 10^{-2}$	0.23
─4Cl	$9.90 \pm 0.26 \times 10^{-2}$	0.23
─4F	$10.3 \pm 0.36 \times 10^{-2}$	0.06
─4Me	$1.15 \pm 0.25 \times 10^{-2}$	- 0.20
─4$C(Me)_3$	$1.09 \pm 0.26 \times 10^{-2}$	- 0.17
─4NO_2	$18.7 \pm 0.24 \times 10^{-2}$	0.78

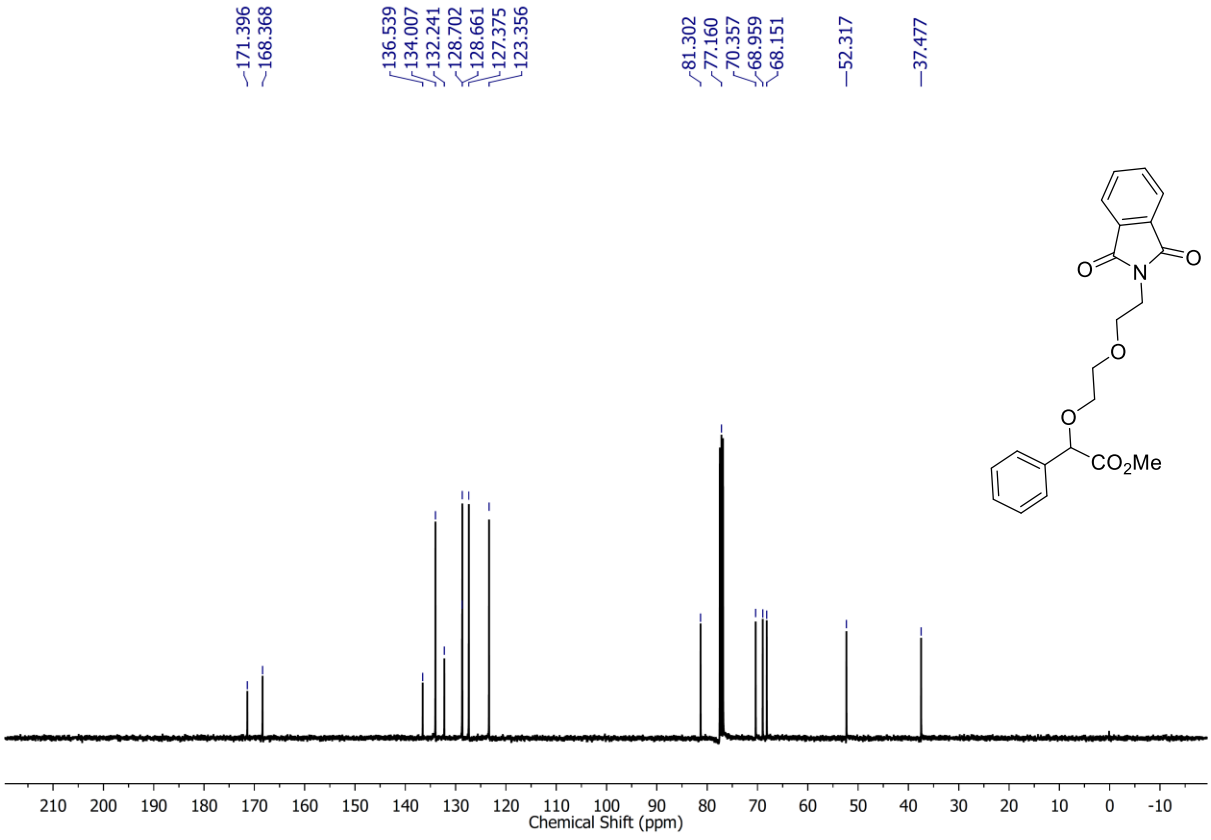
[a]Hansch, C., Leo, A., Taft, R.W. A survey of Hammett substituent constants and resonance and field parameters. Chem. Rev. **1991**, *91(2)*, 165-195.

6. ^{1}H and ^{13}C Spectra

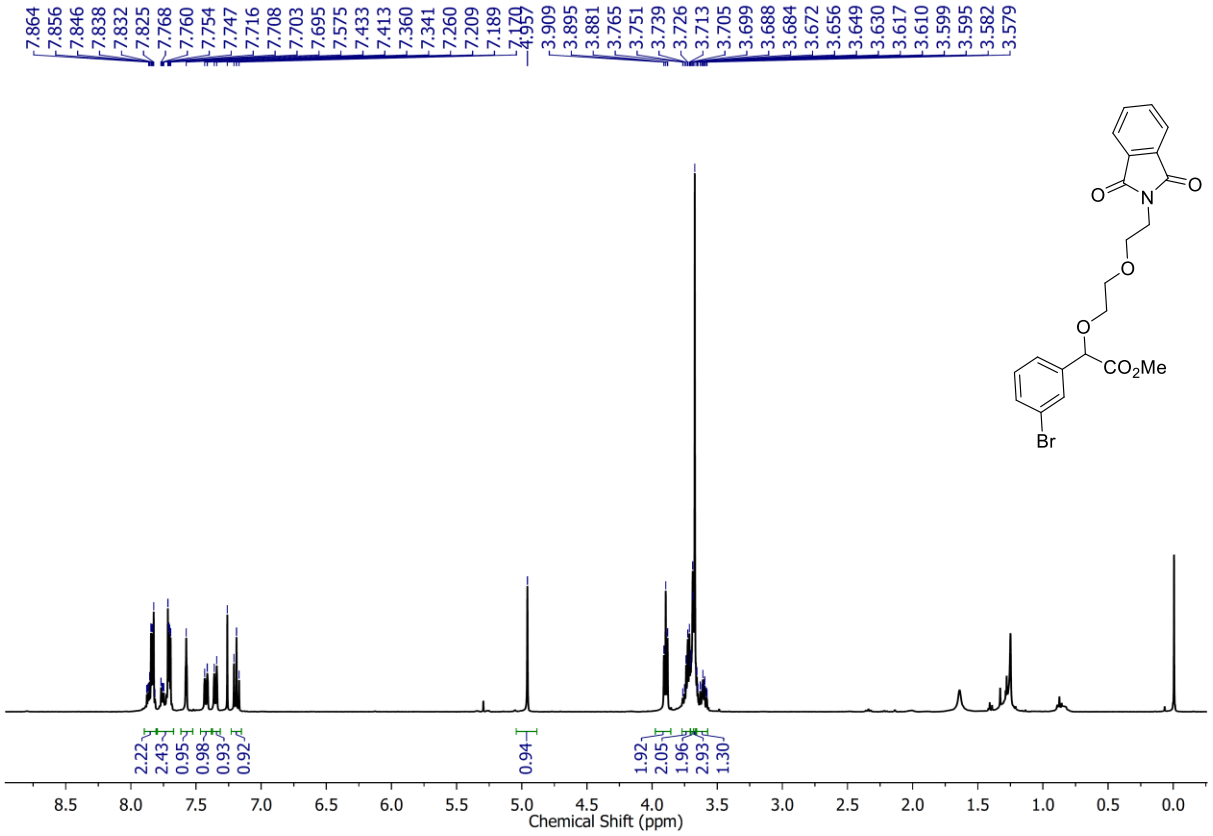
^{1}H NMR (400 MHz) of **4a** in $CDCl_3$



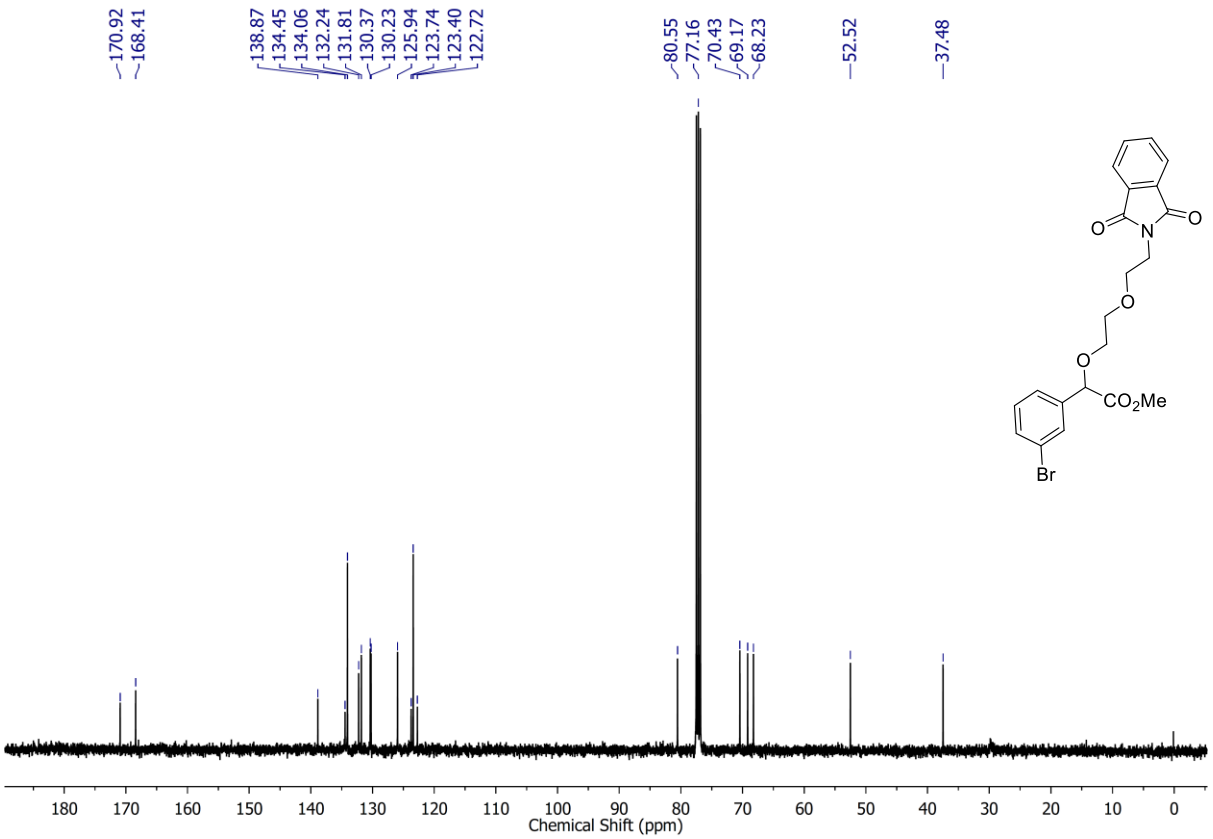
^{13}C NMR (400 MHz) of **4a** in $CDCl_3$



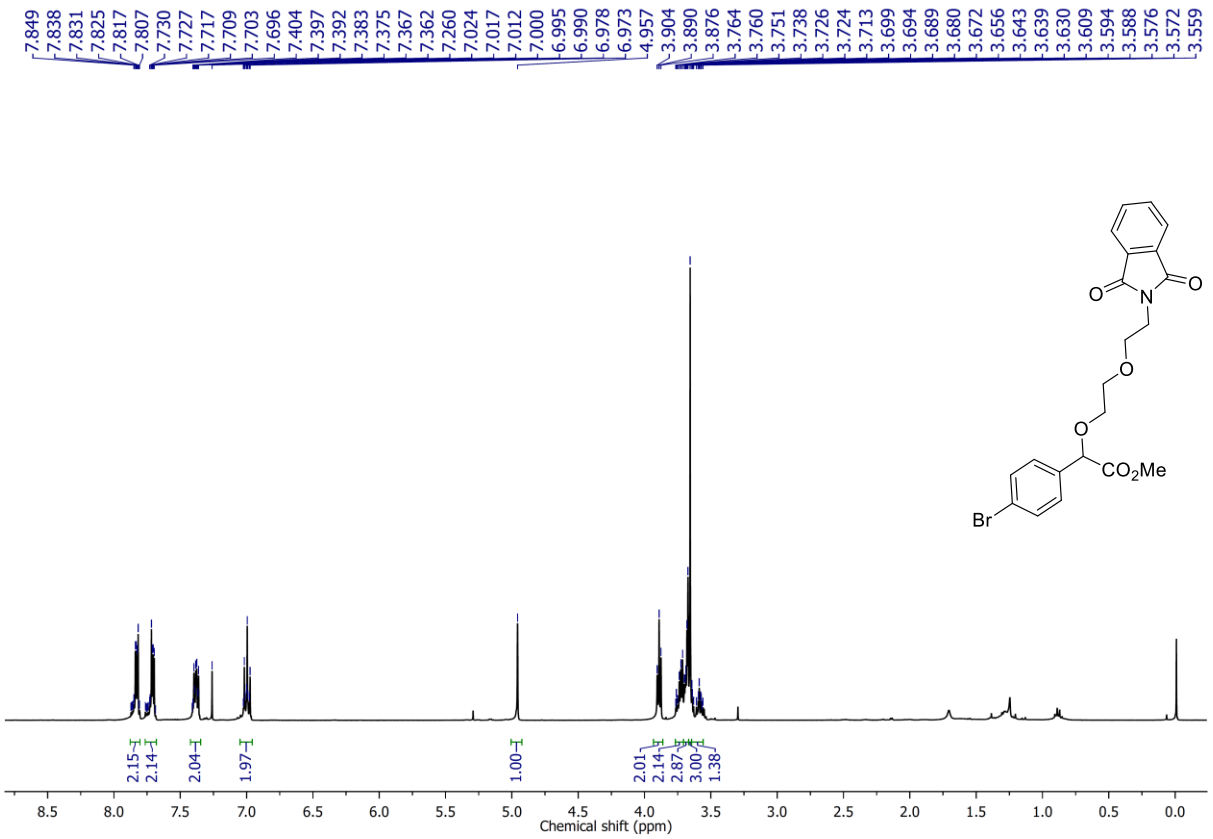
^{1}H NMR (400 MHz) of **4b** in $CDCl_3$



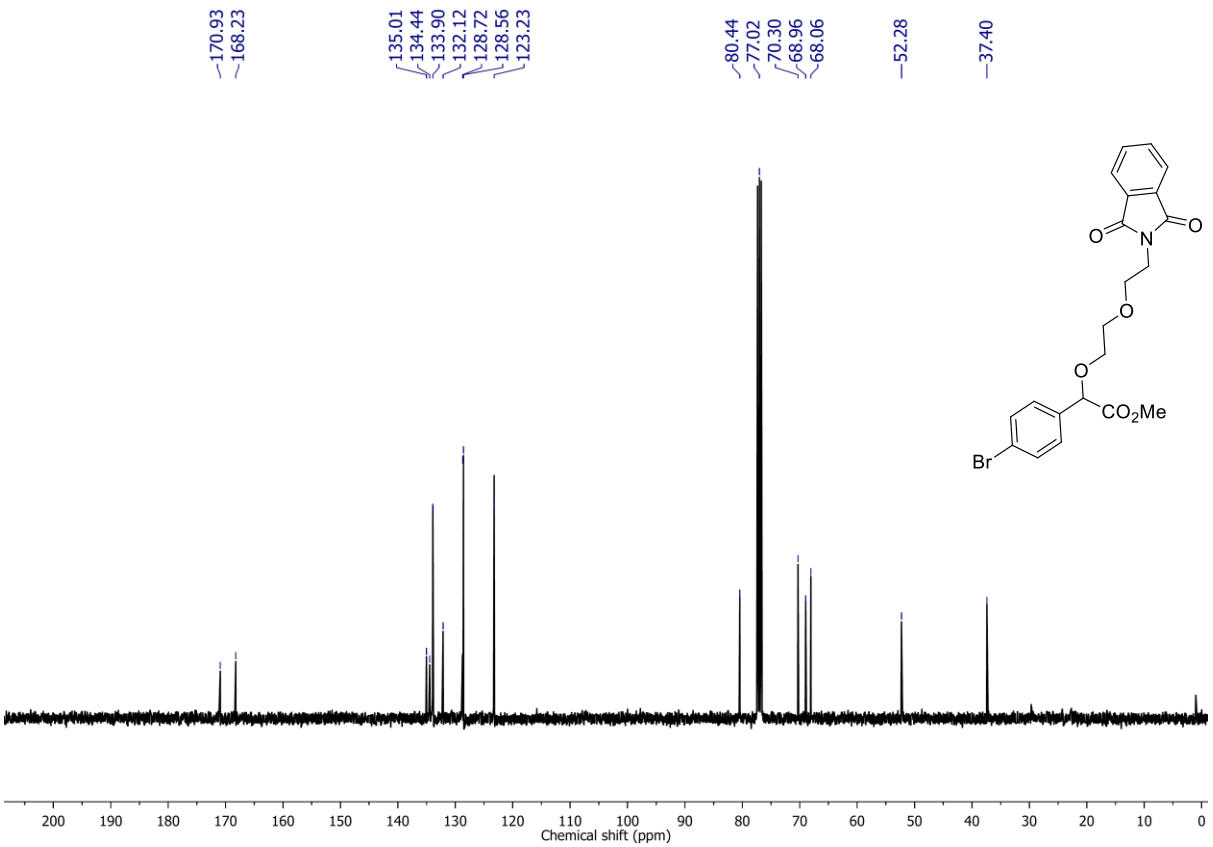
^{13}C NMR (400 MHz) of **4b** in $CDCl_3$



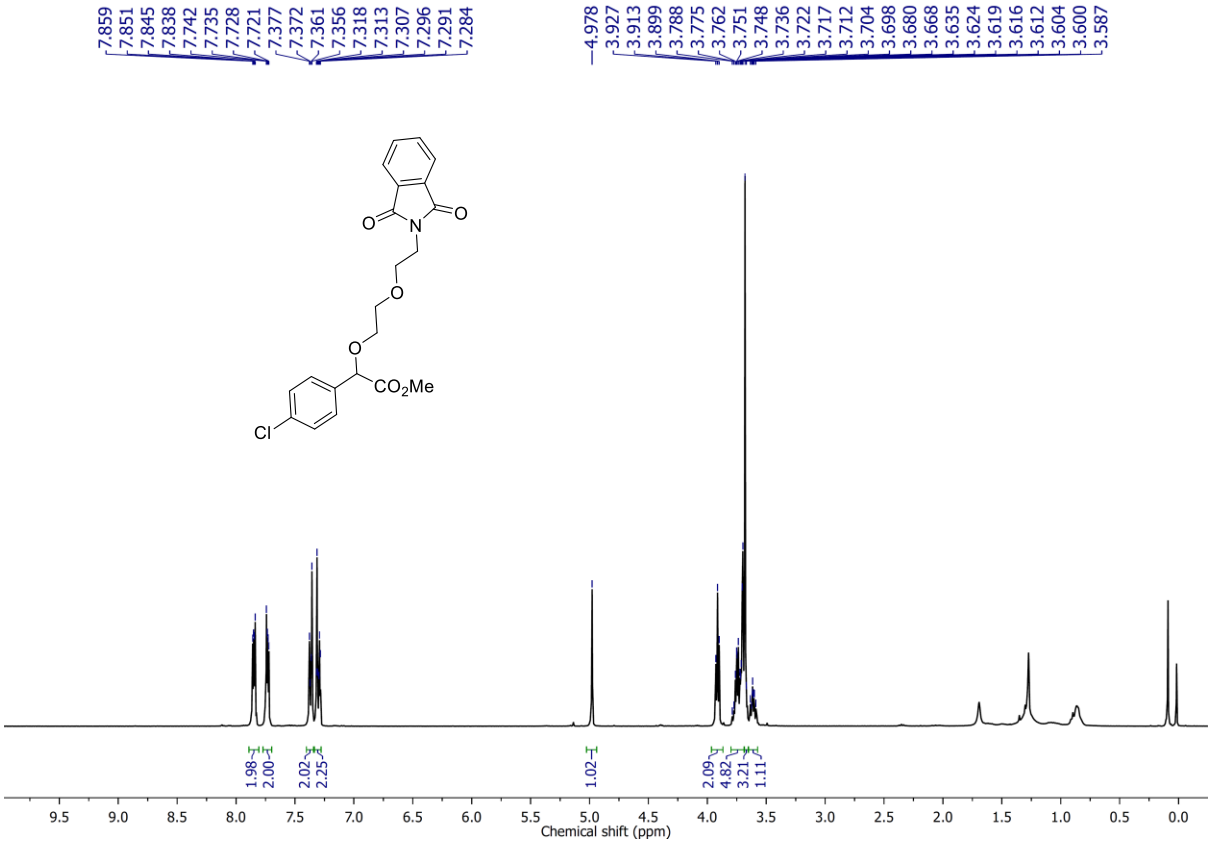
^{1}H NMR (400 MHz) of **4c** in $CDCl_3$



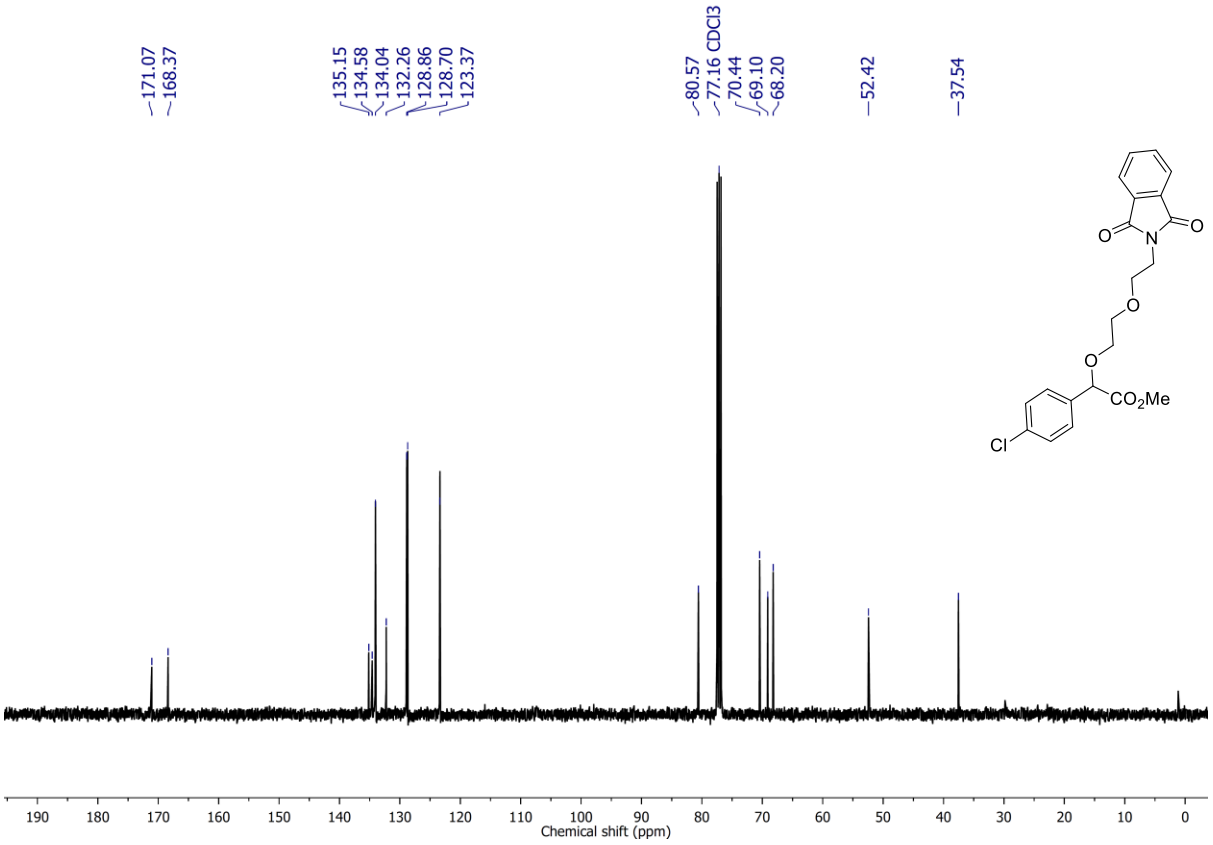
^{13}C NMR (400 MHz) of **4c** in $CDCl_3$



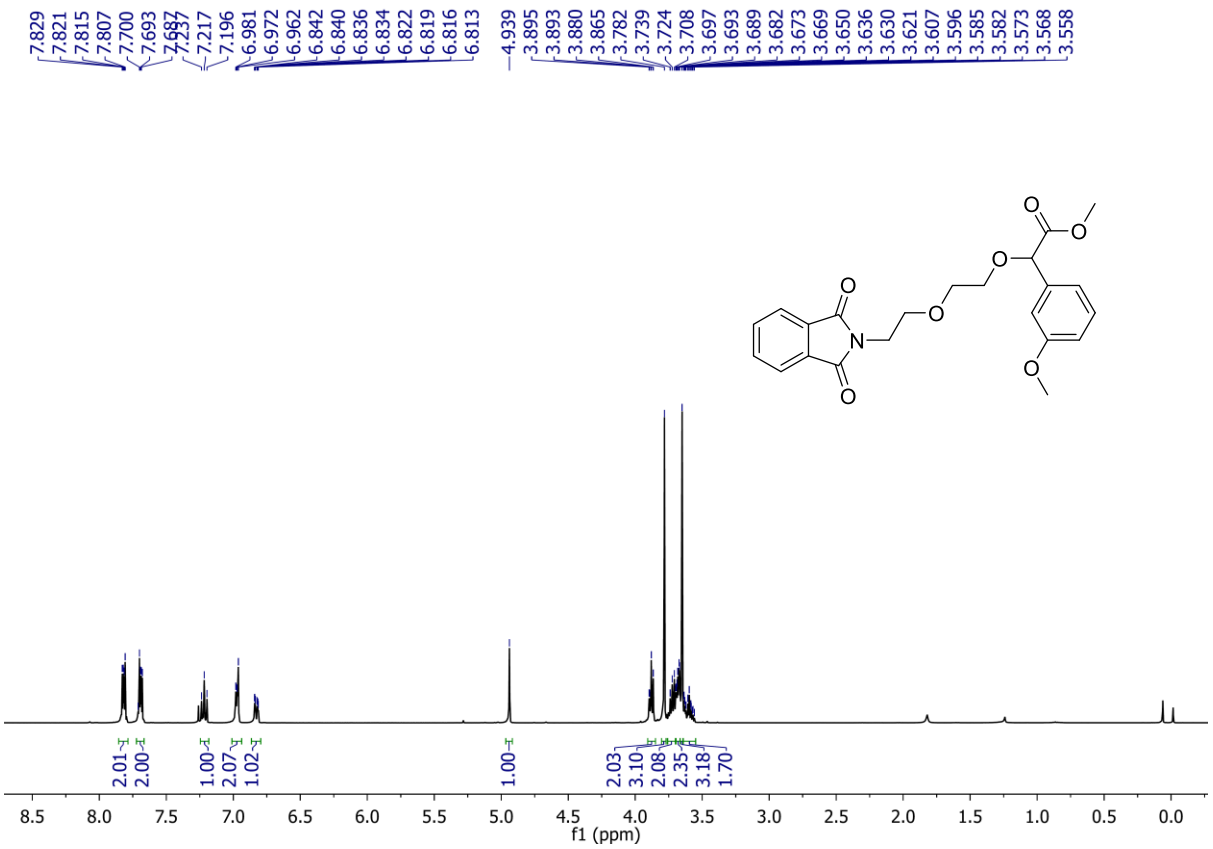
^{1}H NMR (400 MHz) of **4d** in $CDCl_3$



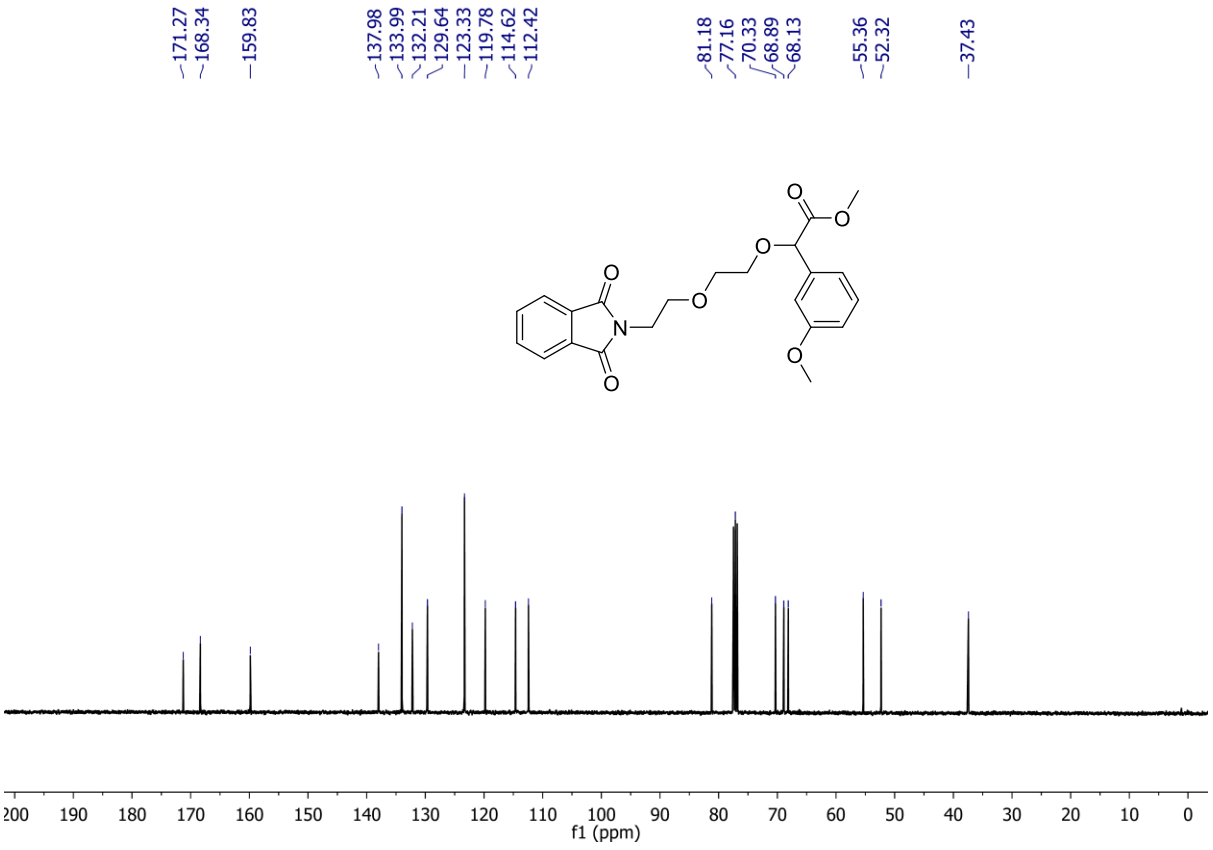
^{13}C NMR (400 MHz) of **4d** in $CDCl_3$



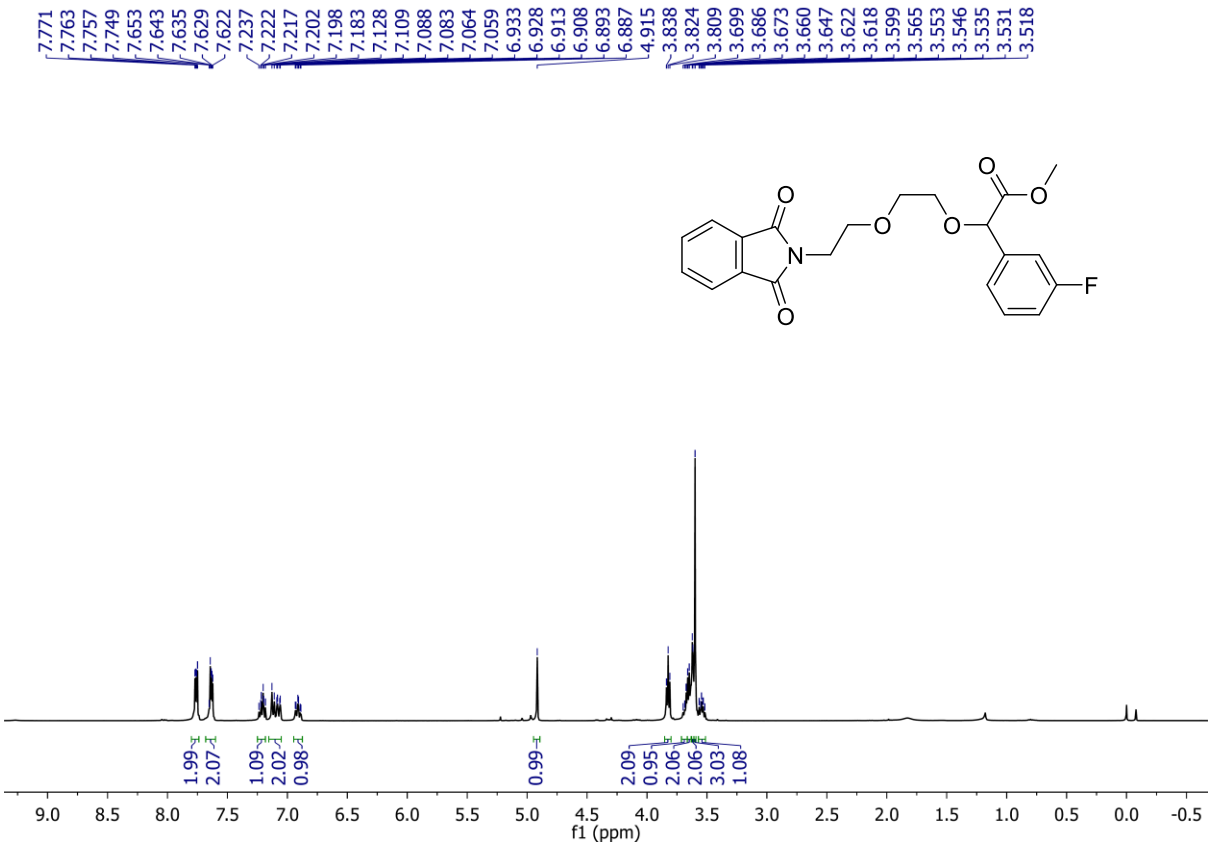
^{1}H NMR (400 MHz) of **4e** in $CDCl_3$



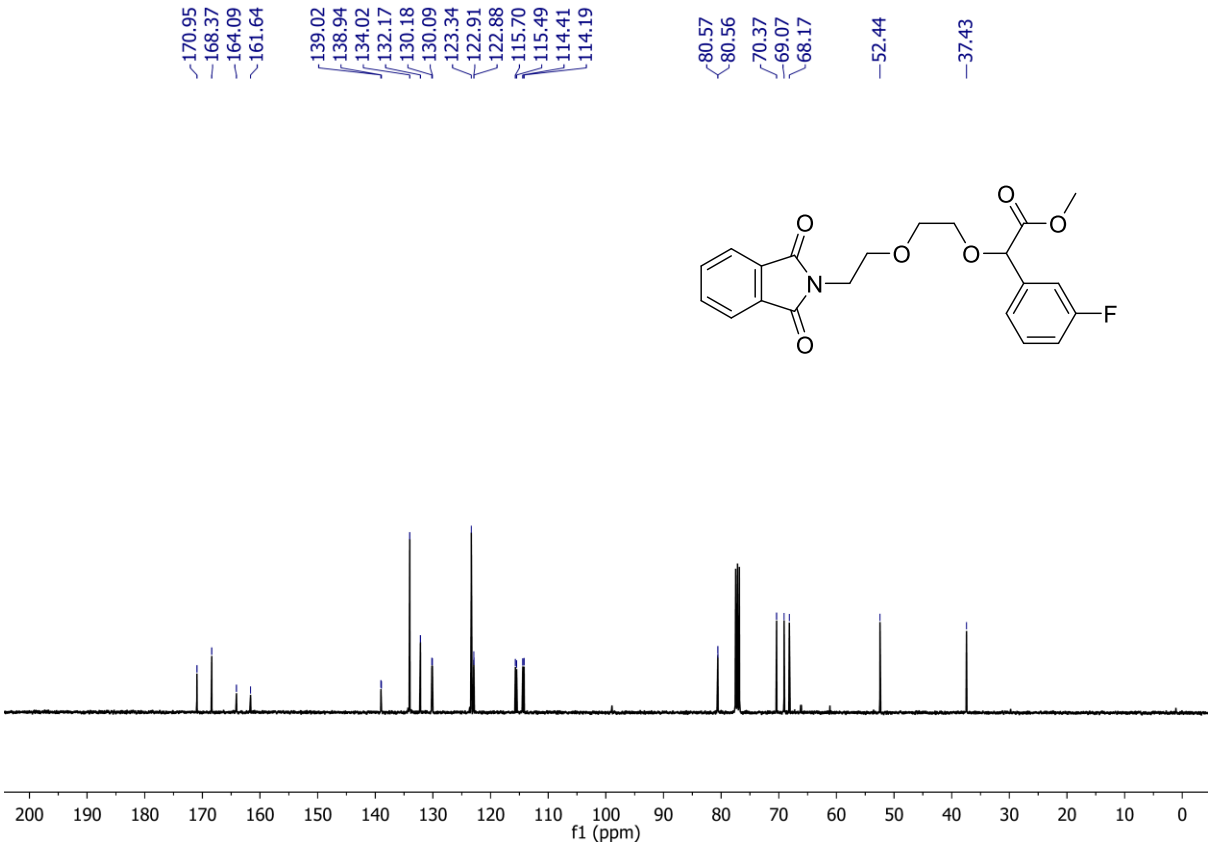
^{13}C NMR (400 MHz) of **4e** in $CDCl_3$



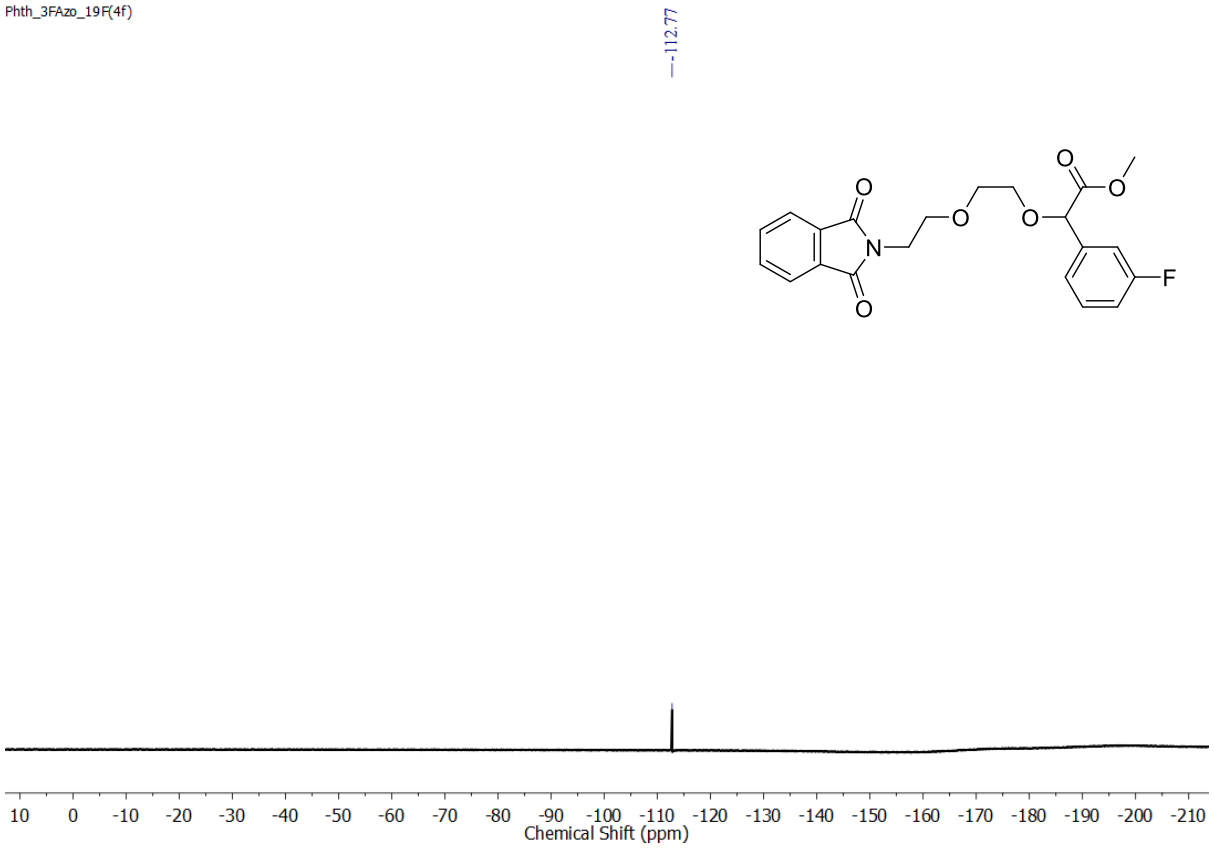
^{1}H NMR (400 MHz) of **4f** in $CDCl_3$



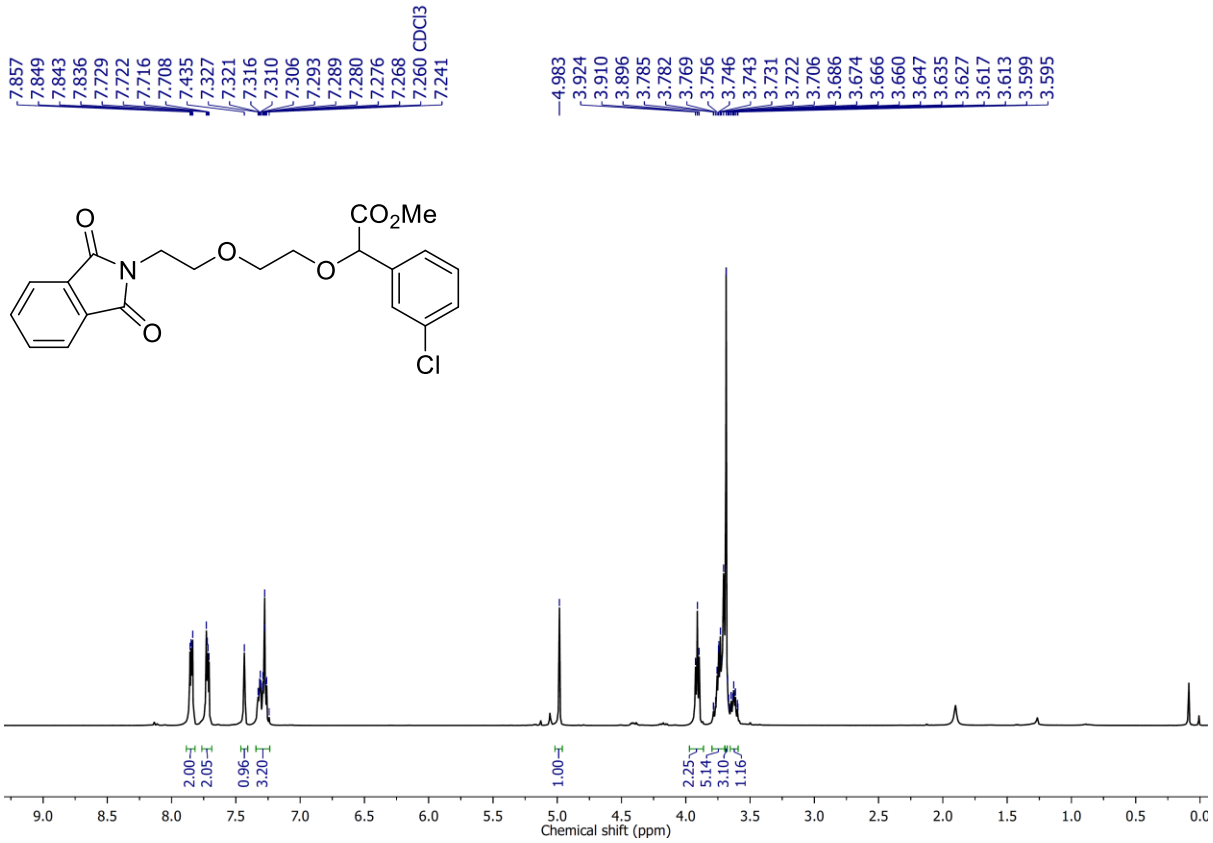
^{13}C NMR (400 MHz) of **4f** in $CDCl_3$



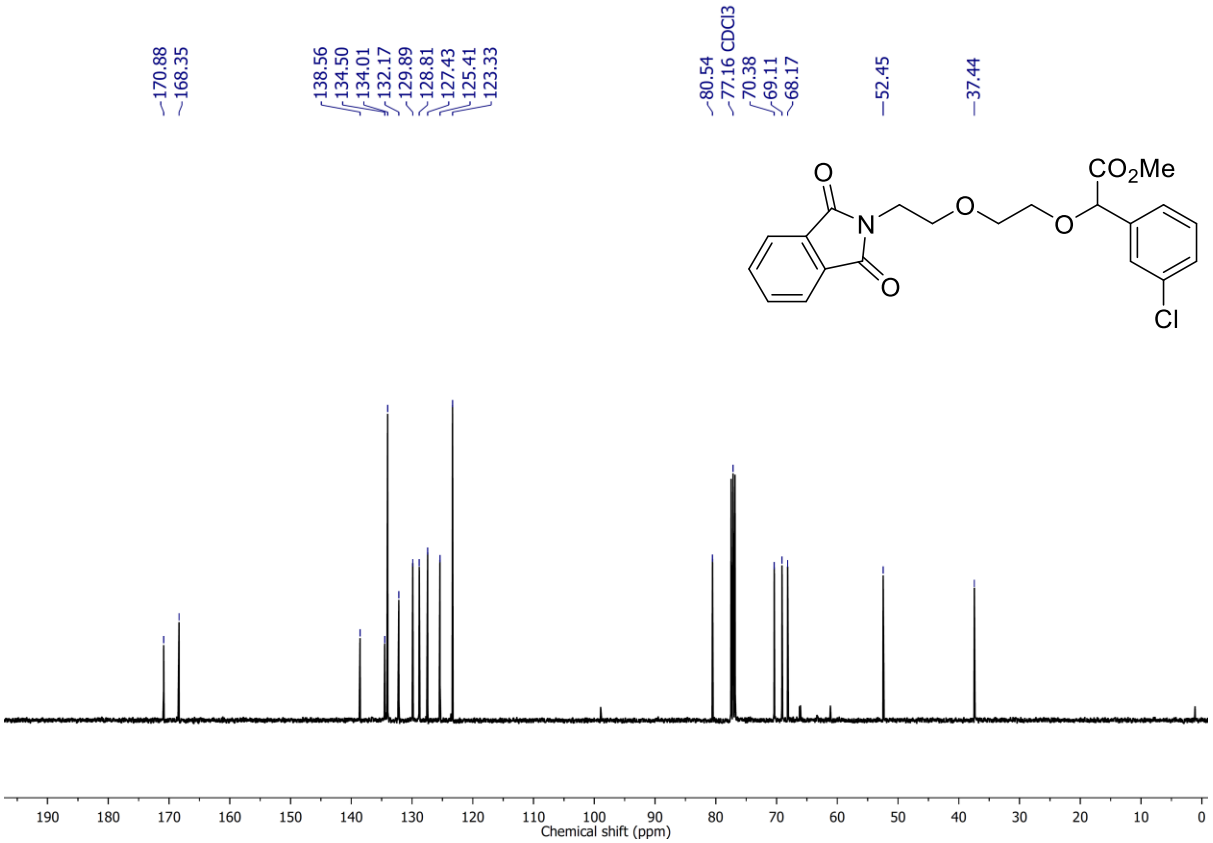
^{19}F NMR (376 MHz) of **4f** in $CDCl_3$



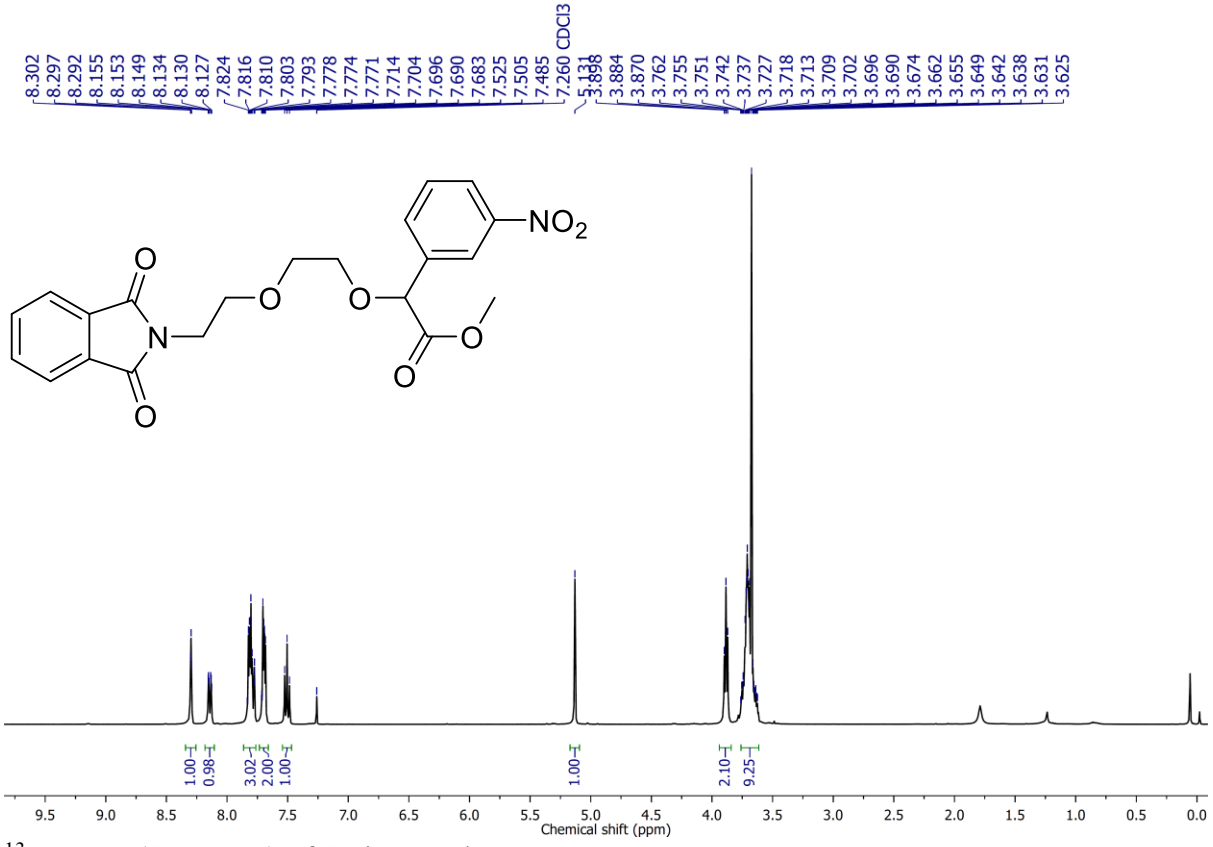
^{1}H NMR (400 MHz) of **4g** in $CDCl_3$



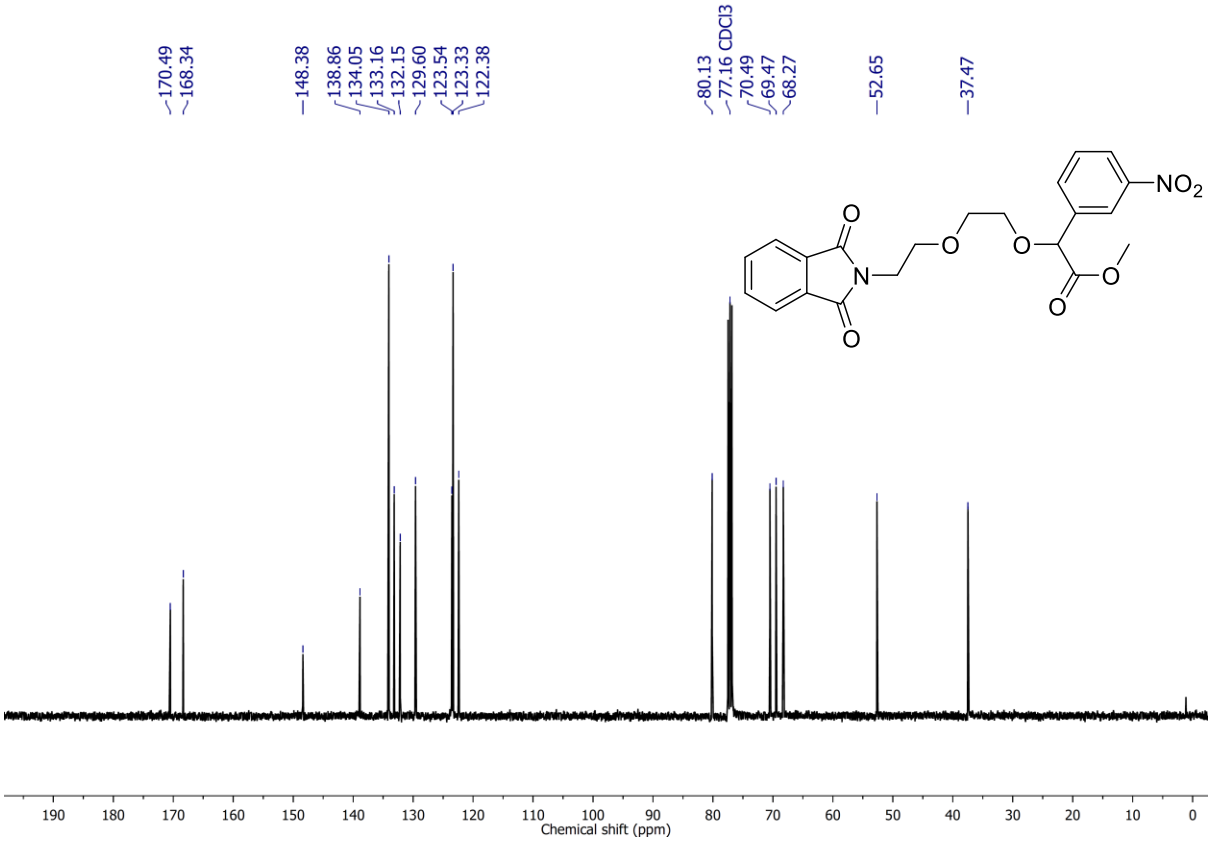
^{13}C NMR (400 MHz) of **4g** in $CDCl_3$



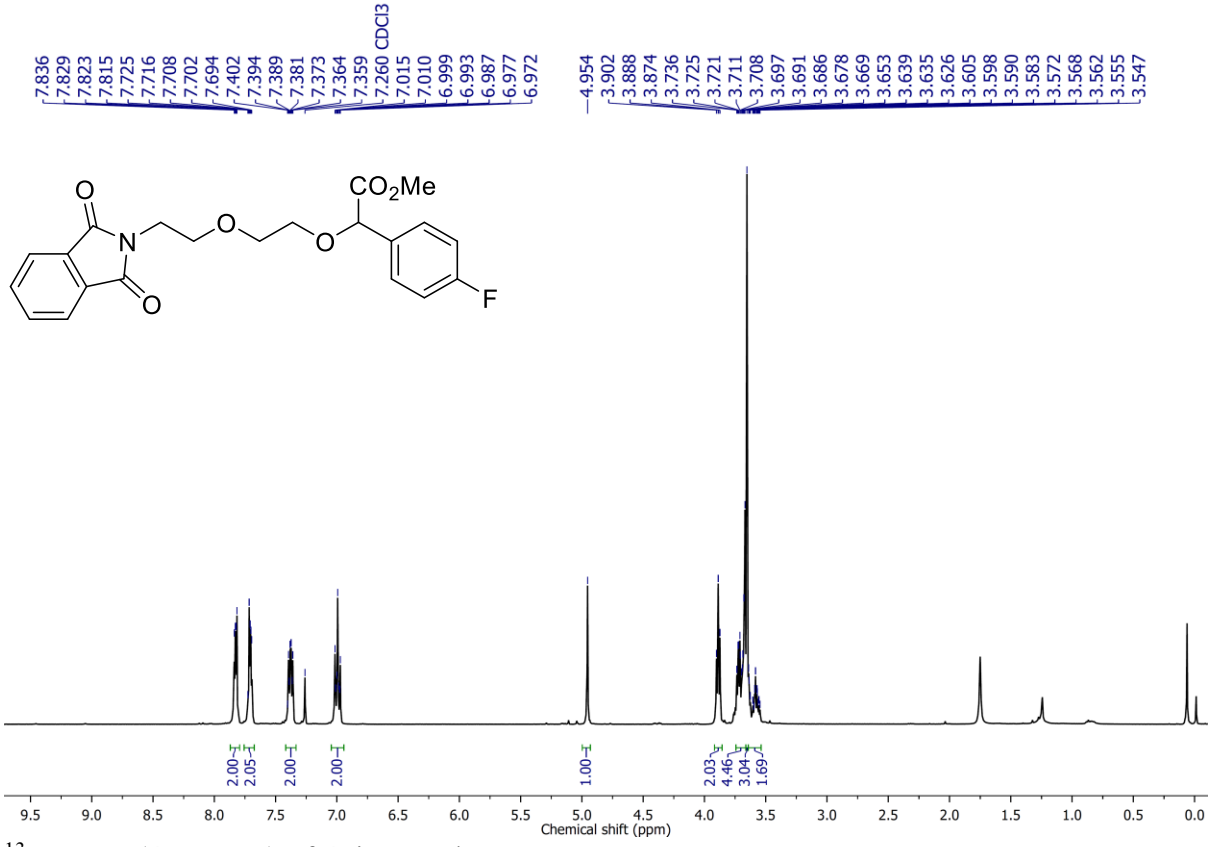
^{1}H NMR (400 MHz) of **4h** in $CDCl_3$



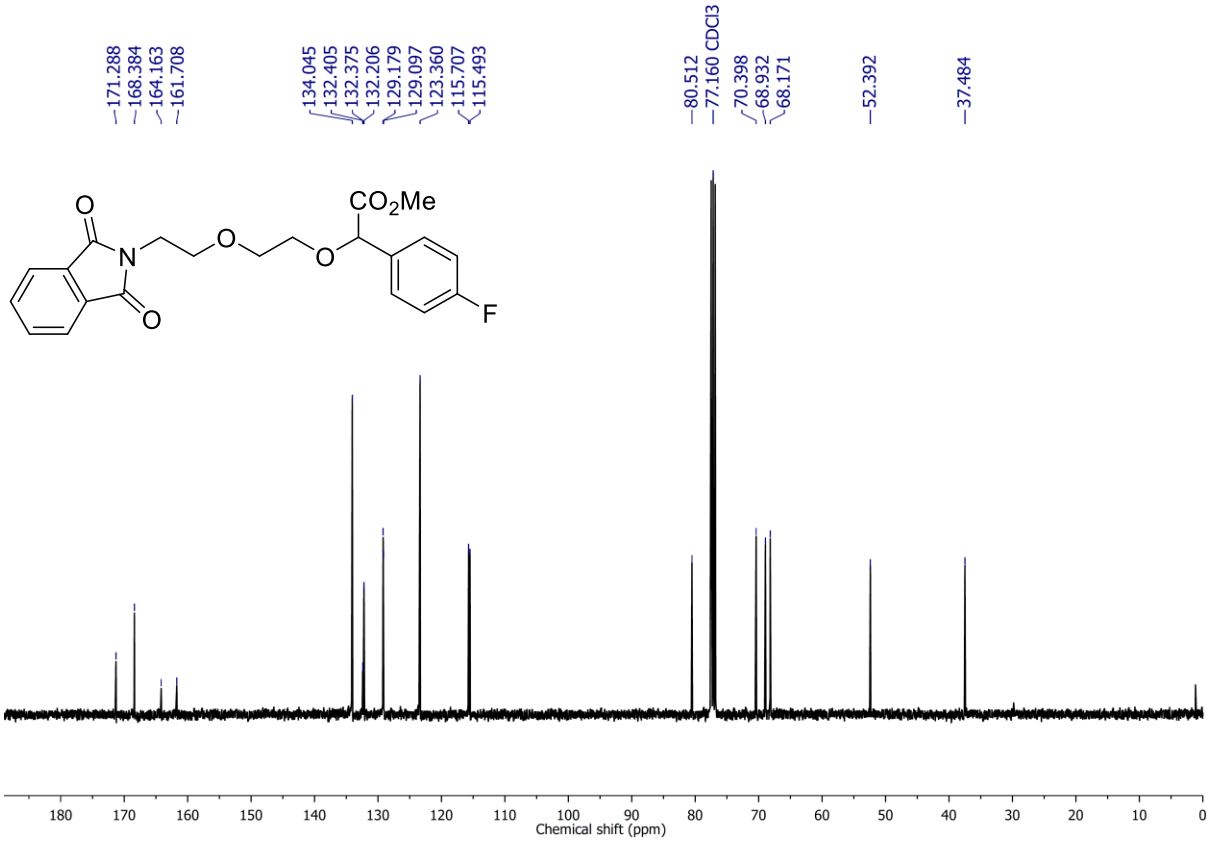
^{13}C NMR (400 MHz) of **4h** in $CDCl_3$



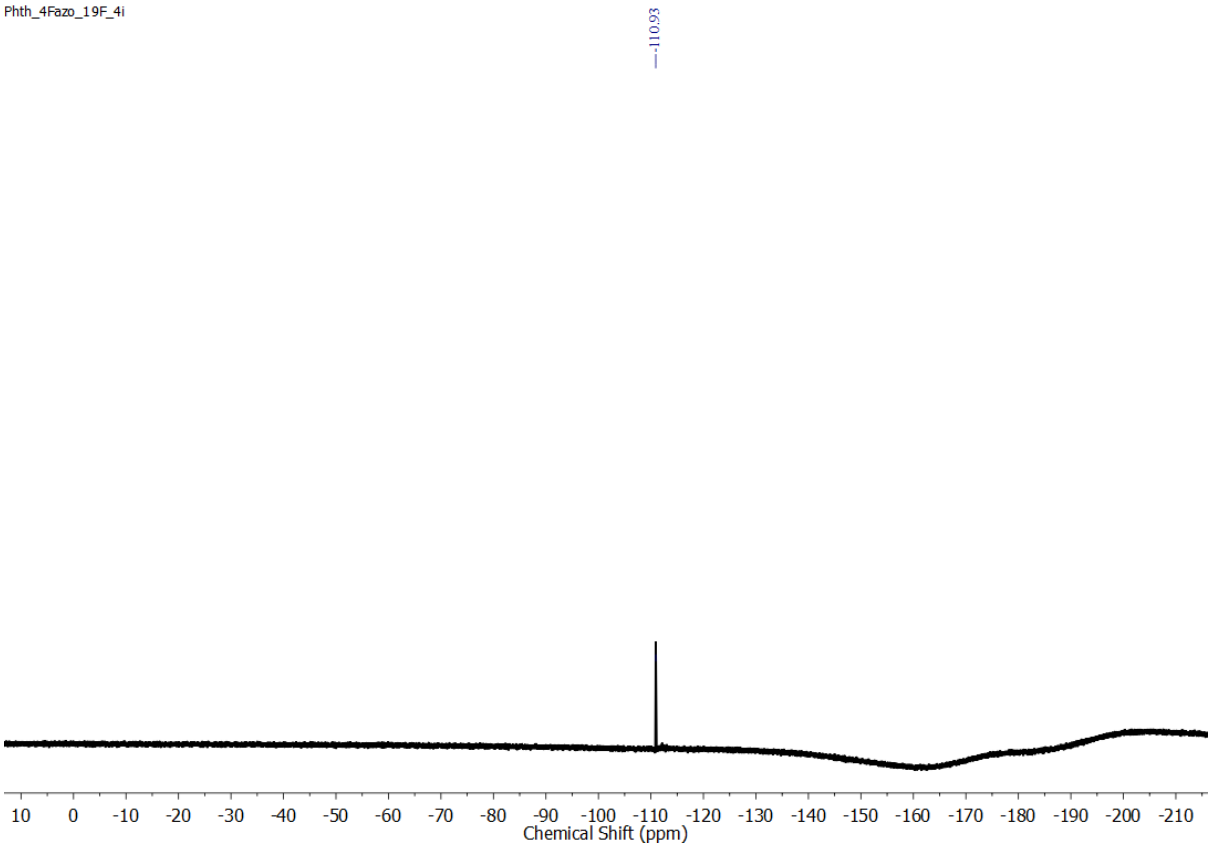
^{1}H NMR (400 MHz) of **4i** in $CDCl_3$



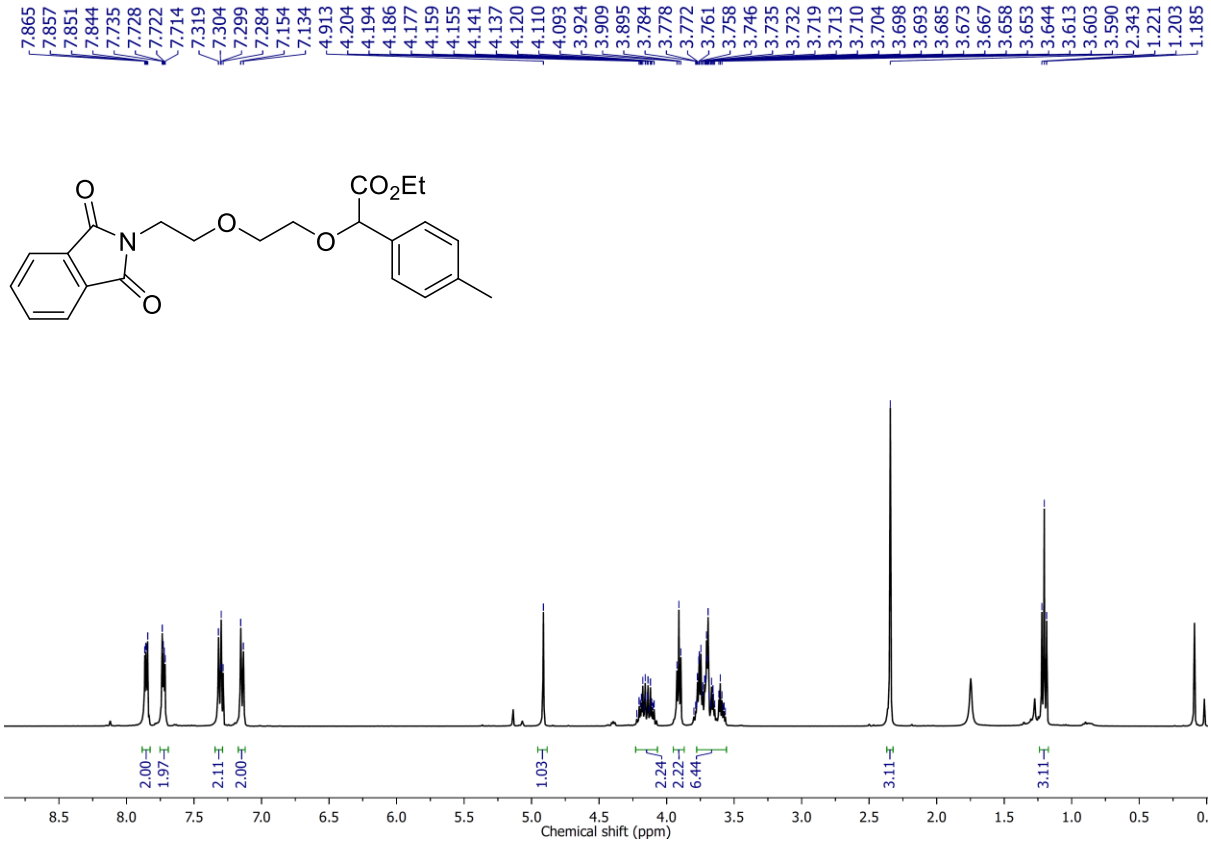
^{13}C NMR (400 MHz) of **4i** in $CDCl_3$



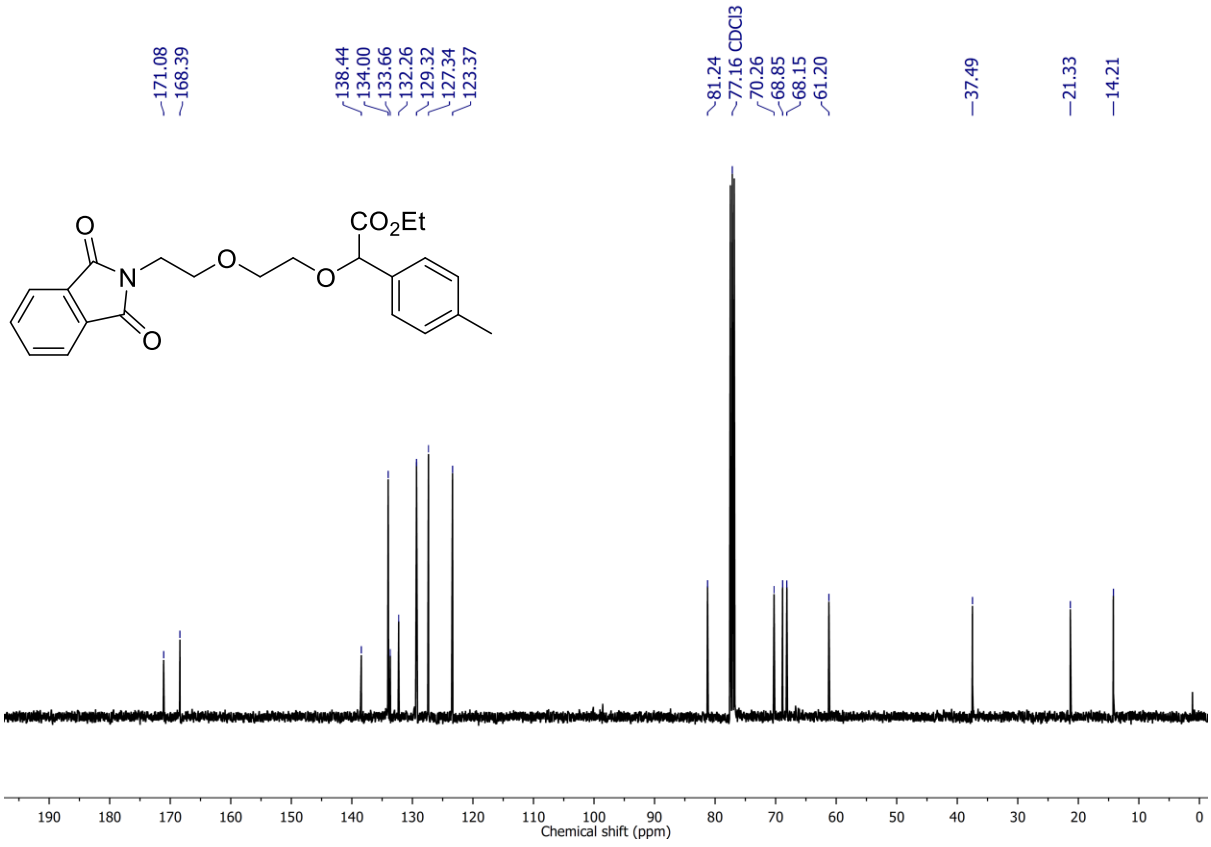
^{19}F NMR (376 MHz) of **4i** in $CDCl_3$



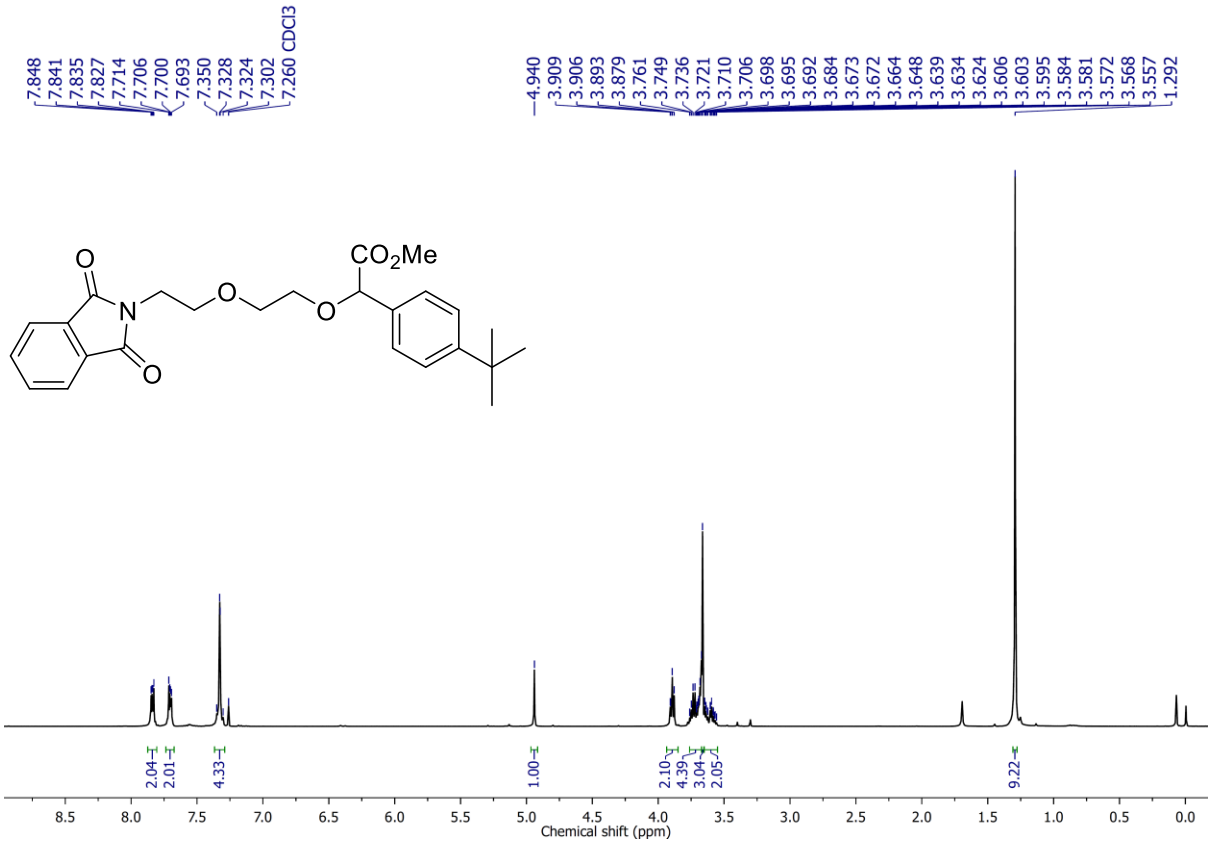
^{1}H NMR (400 MHz) of **4j** in $CDCl_3$



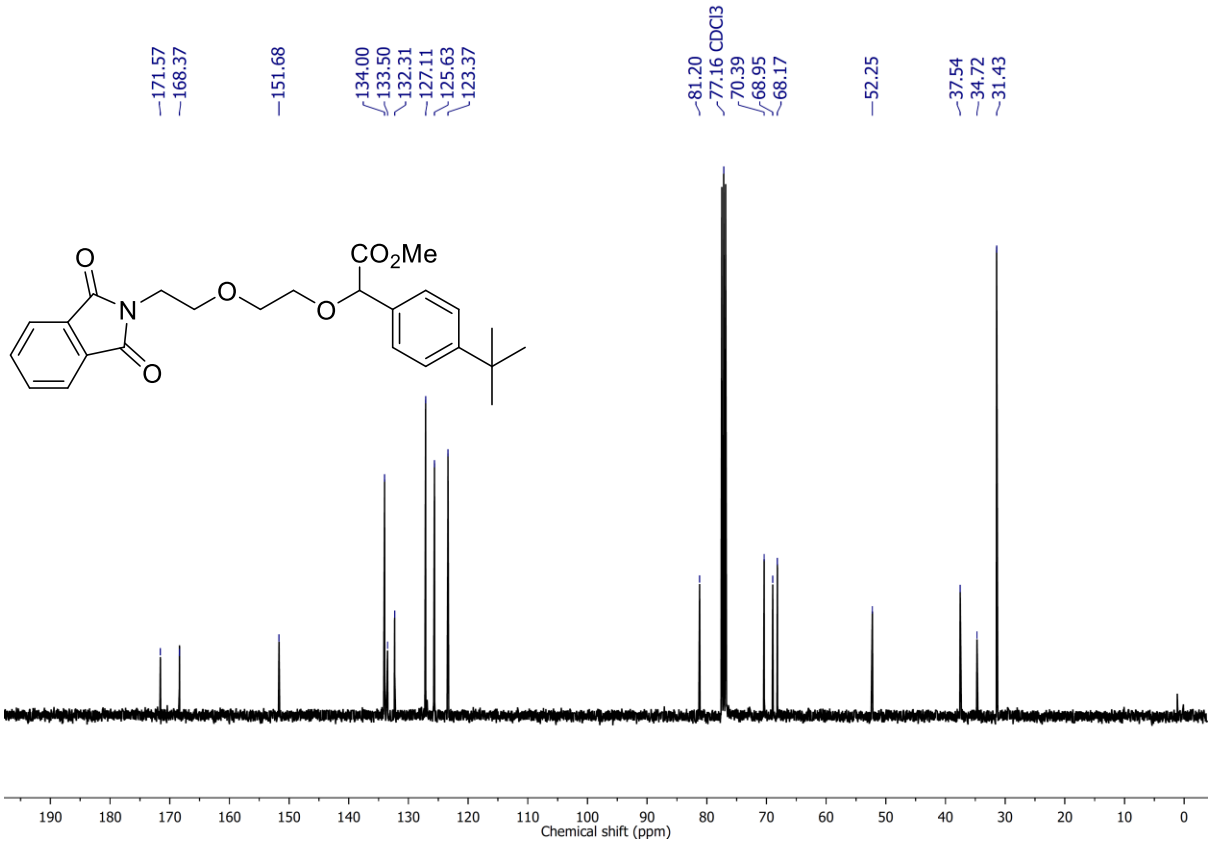
^{13}C NMR (400 MHz) of **4j** in $CDCl_3$



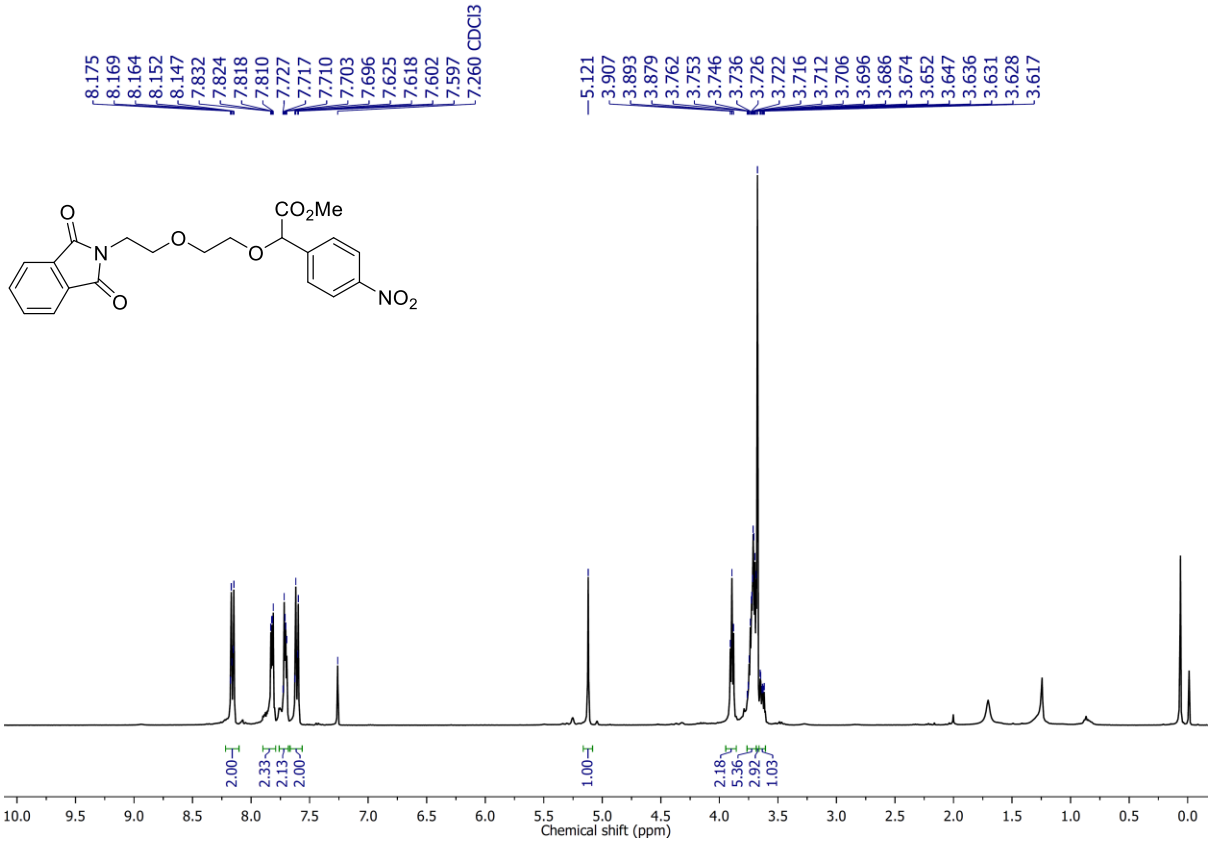
^{1}H NMR (400 MHz) of **4k** in $CDCl_3$



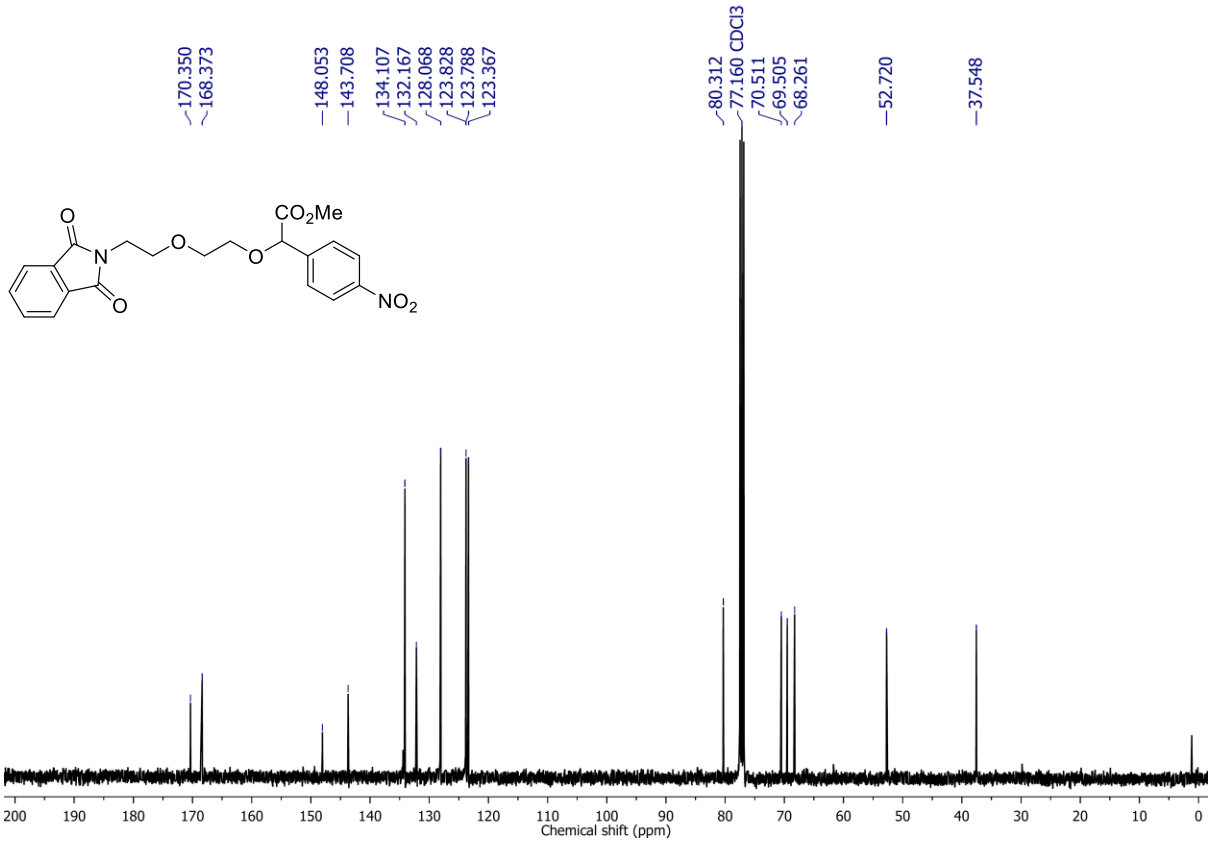
^{13}C NMR (400 MHz) of **4k** in $CDCl_3$



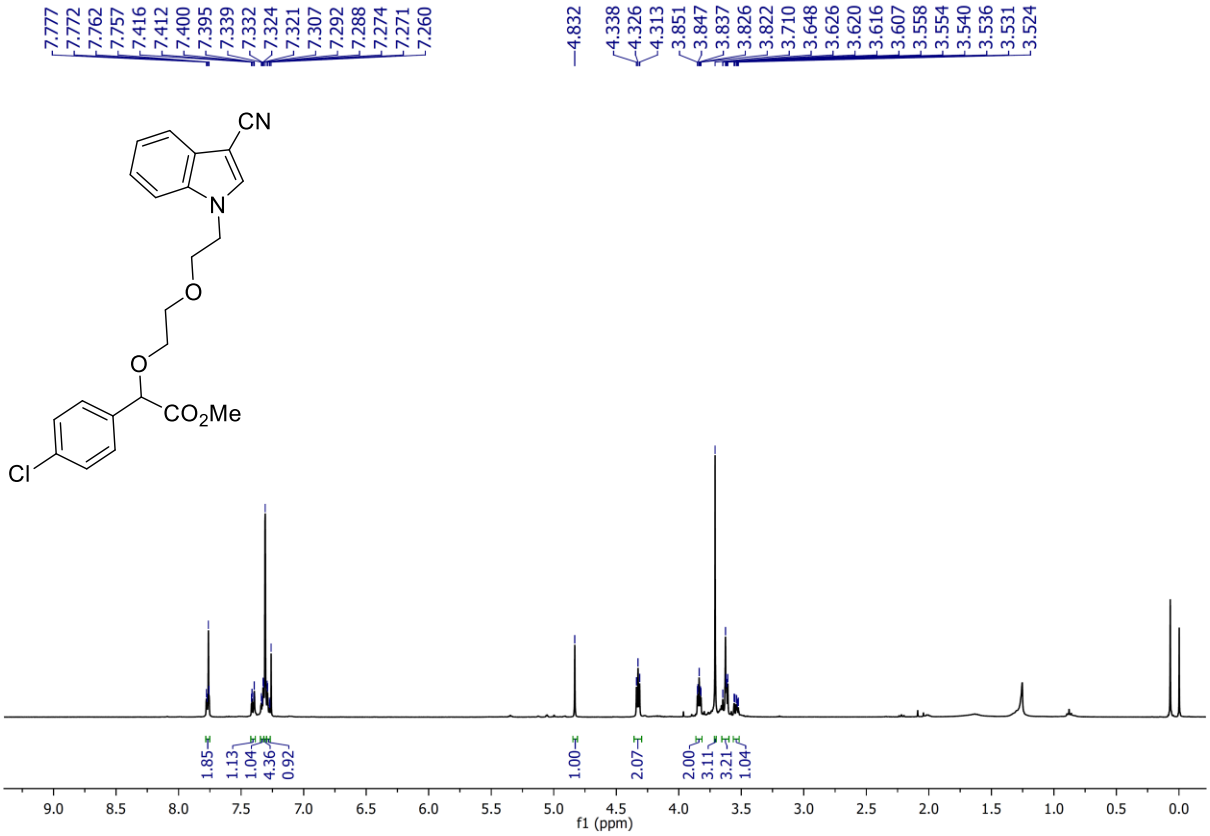
^{1}H NMR (400 MHz) of **4l** in $CDCl_3$



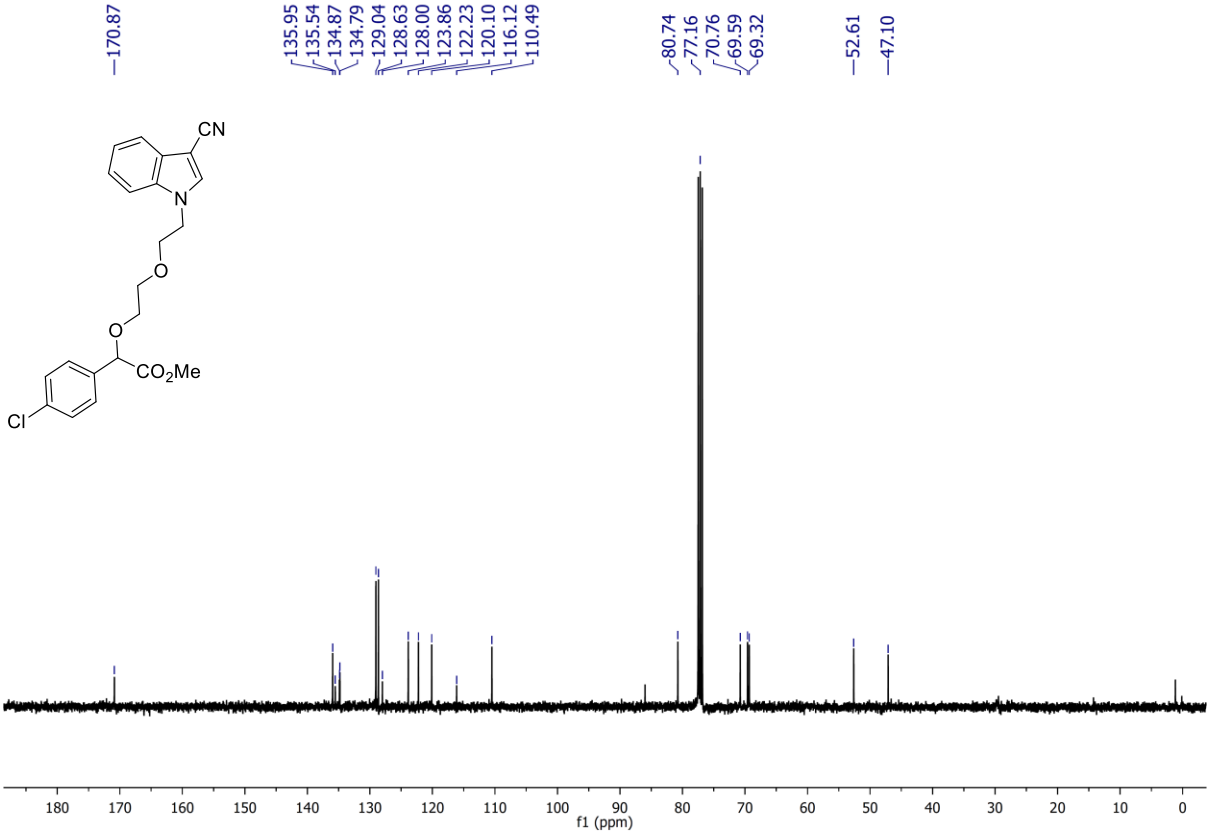
^{13}C NMR (400 MHz) of **4l** in $CDCl_3$



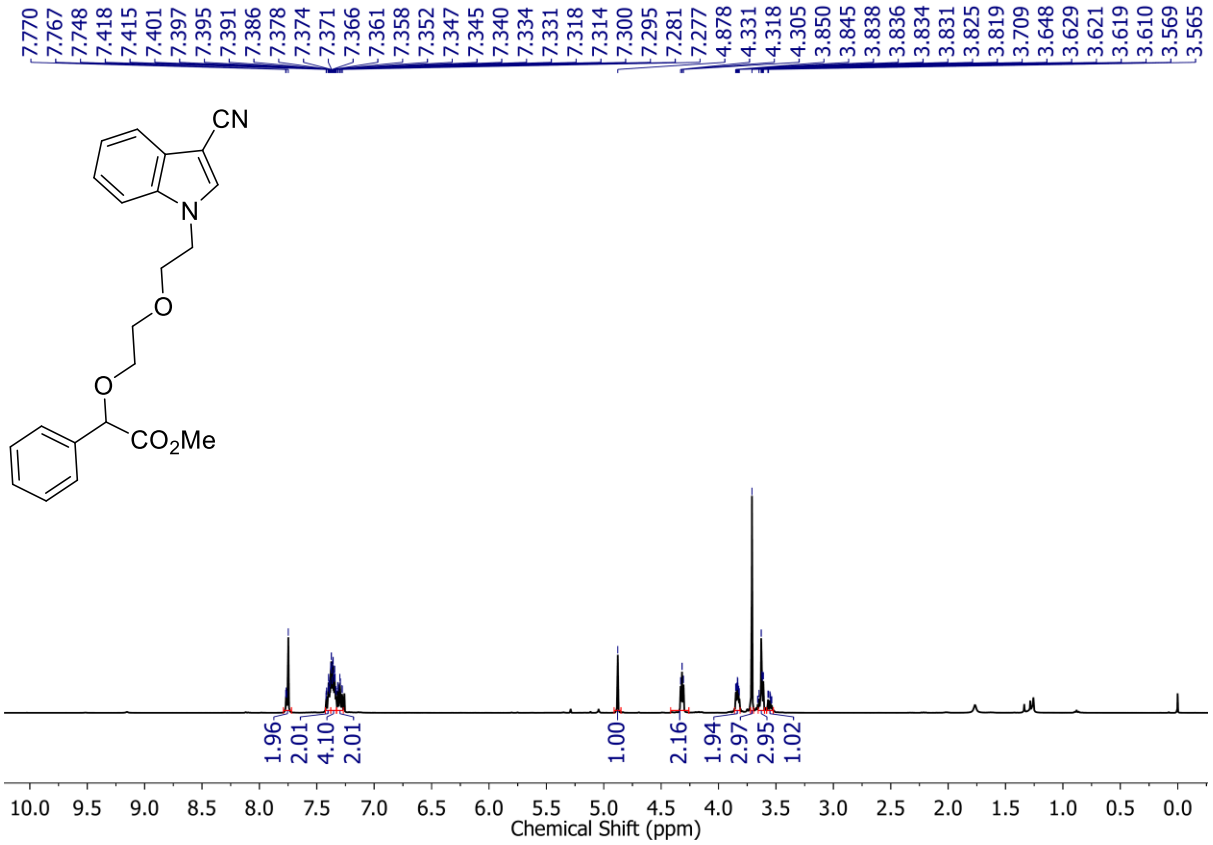
^{1}H NMR (400 MHz) of **5a** in $CDCl_3$



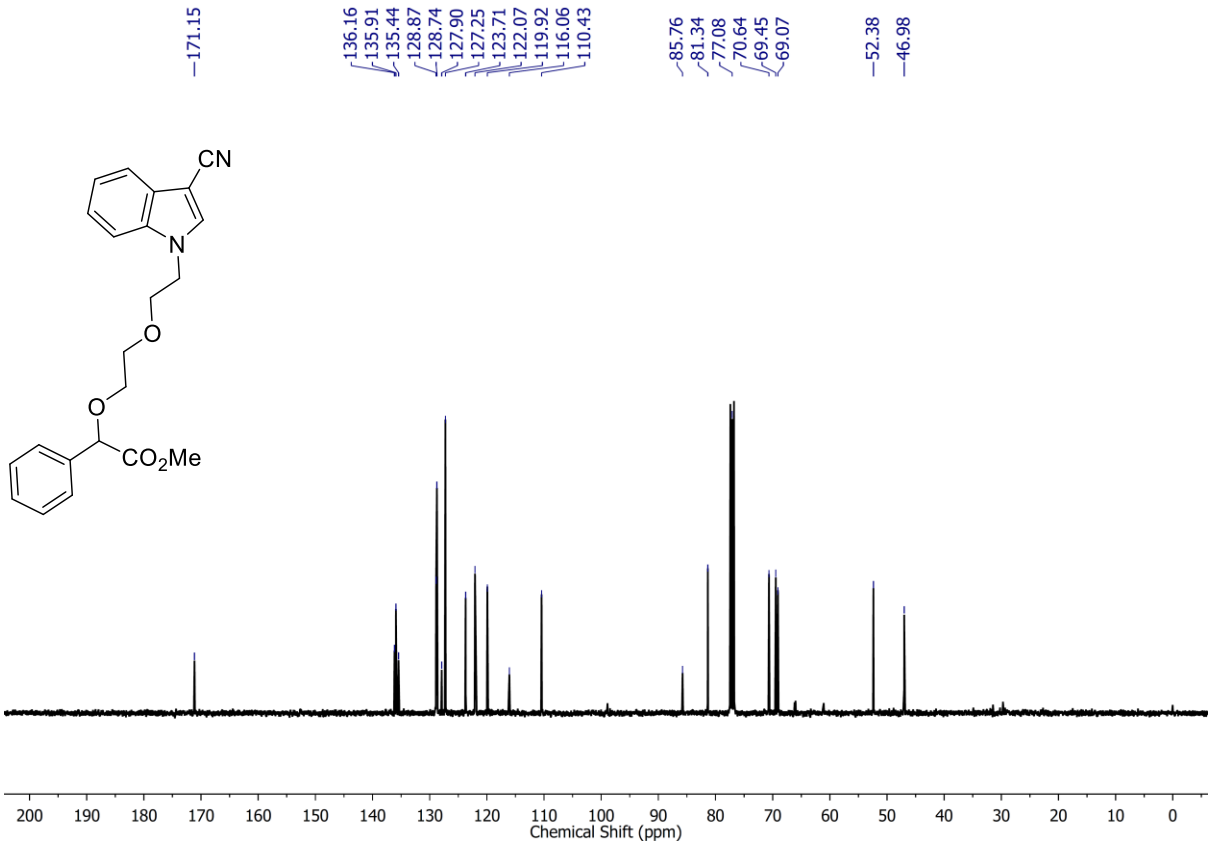
^{13}C NMR (400 MHz) of **5a** in $CDCl_3$



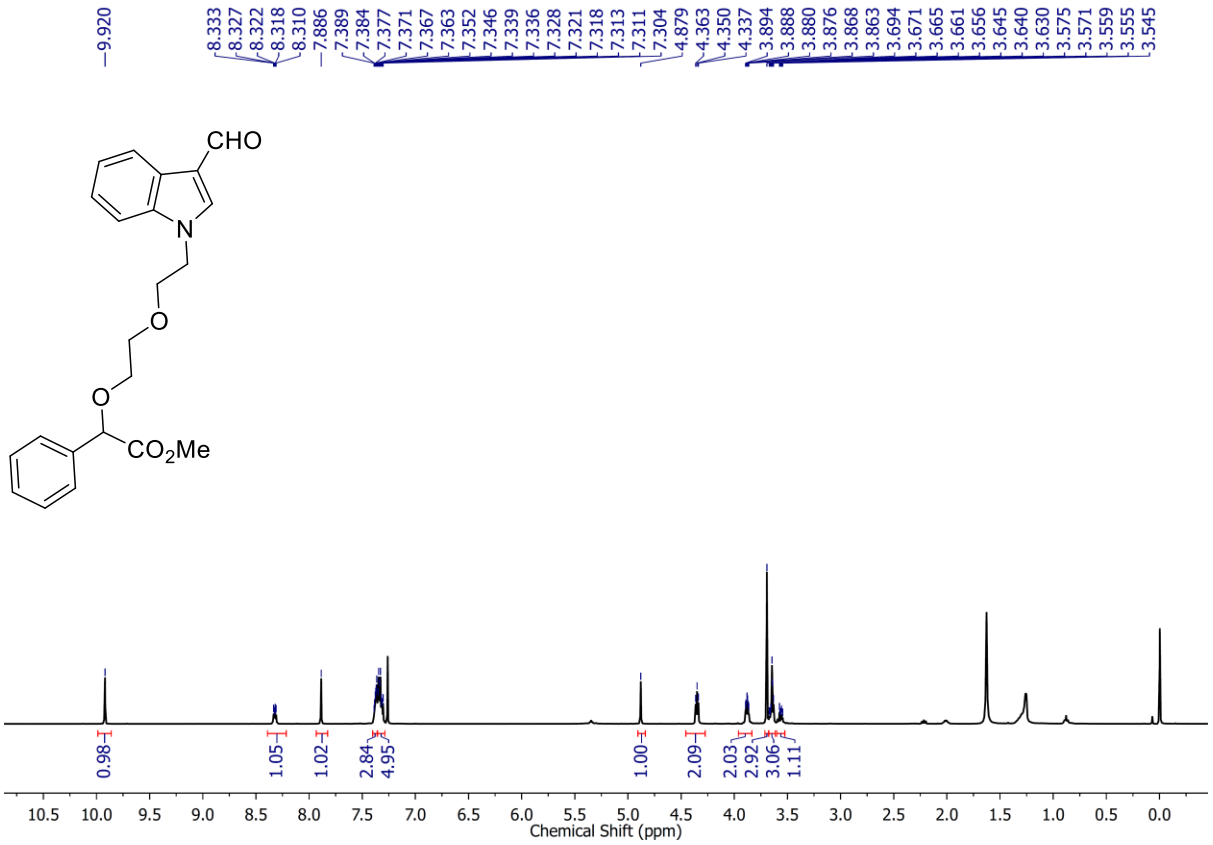
^{1}H NMR (400 MHz) of **5b** in $CDCl_3$



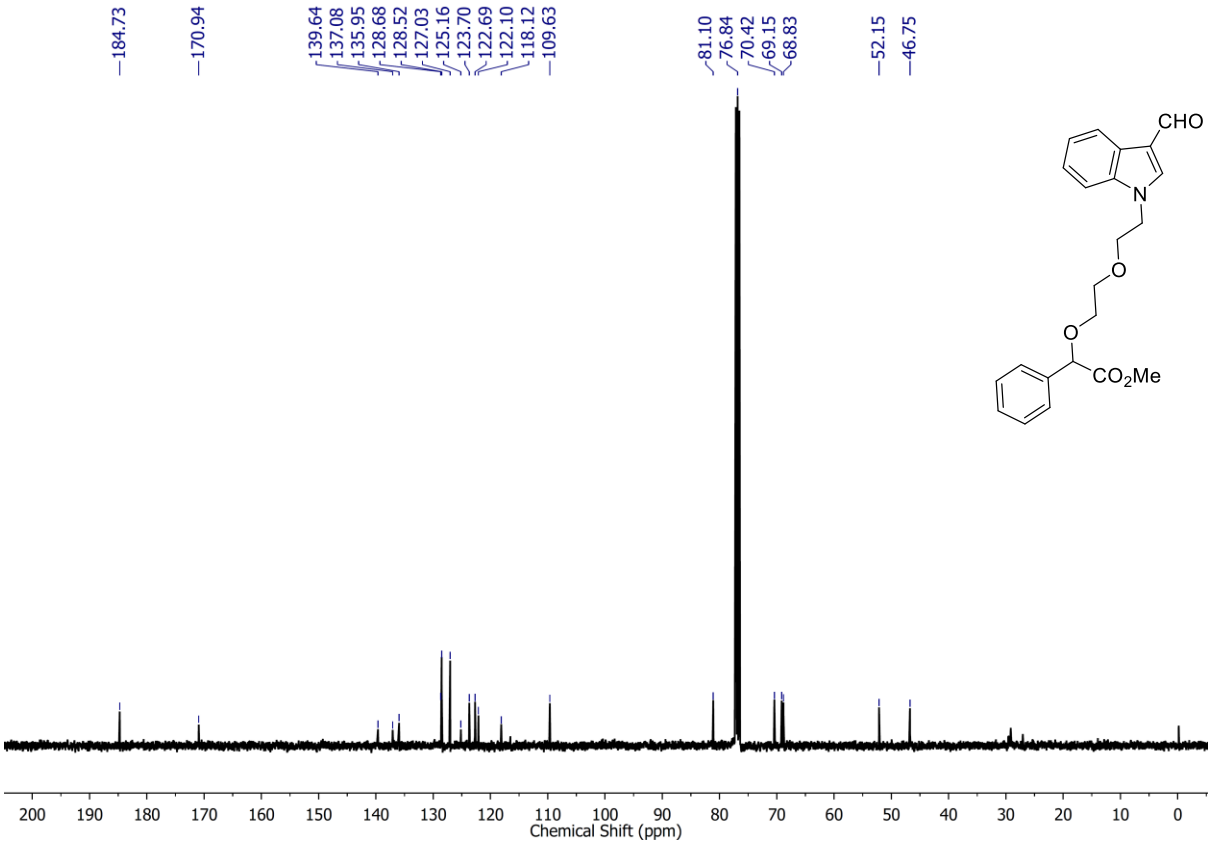
^{13}C NMR (400 MHz) of **5b** in $CDCl_3$



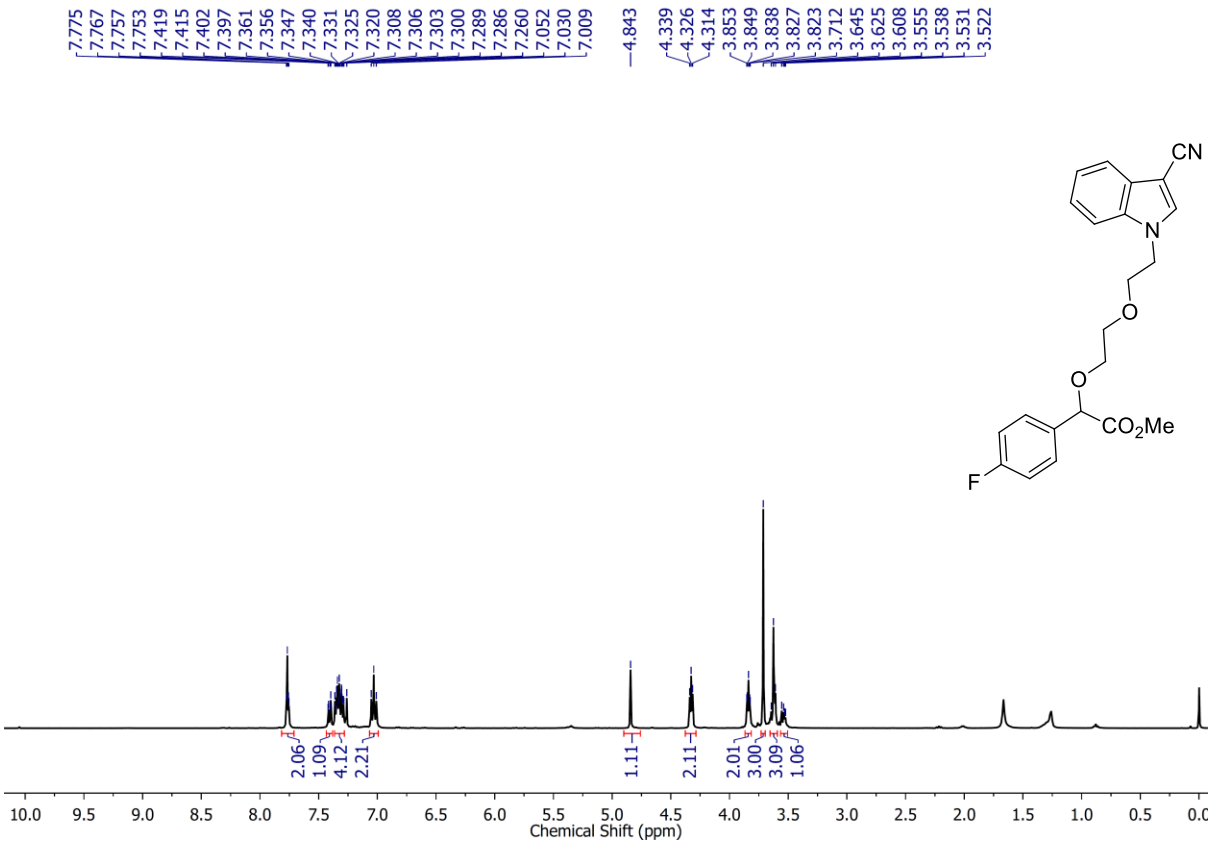
^{1}H NMR (400 MHz) of **5c** in $CDCl_3$



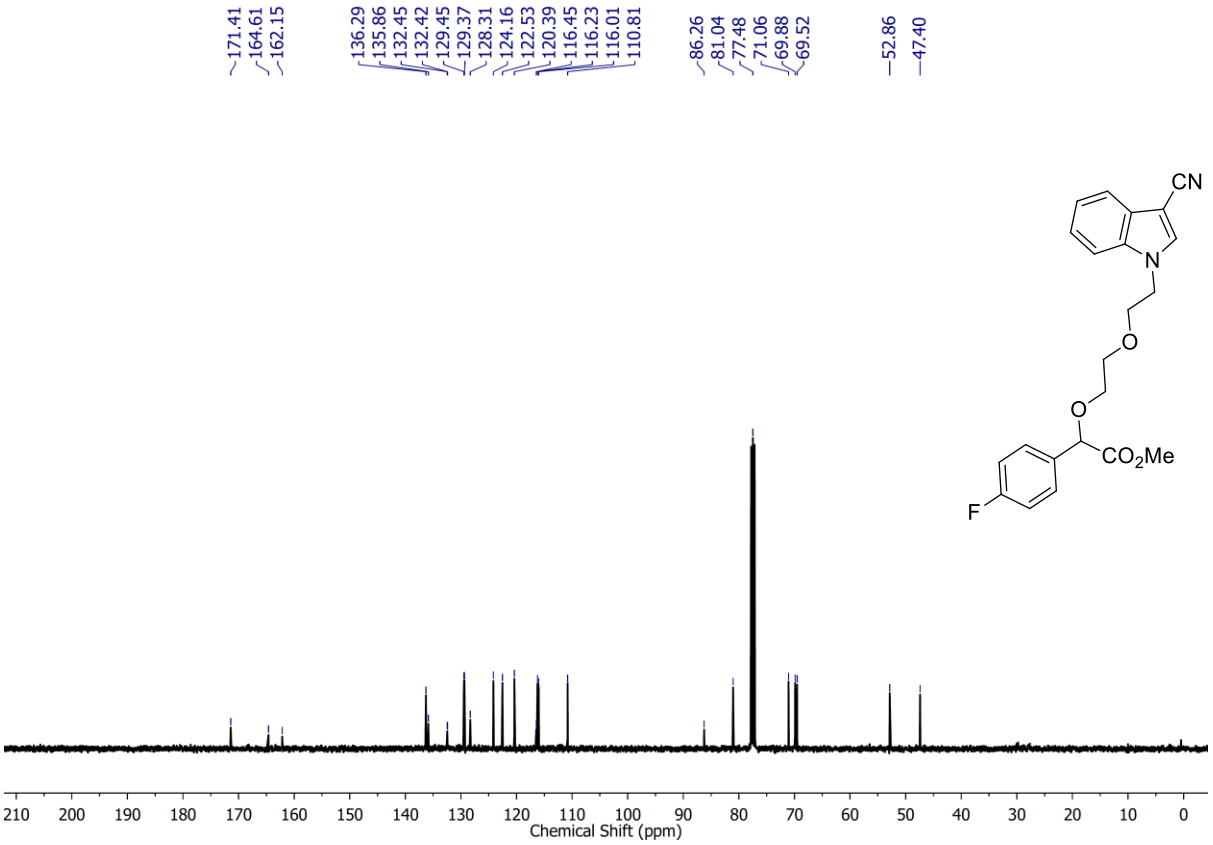
^{13}C NMR (400 MHz) of **5c** in $CDCl_3$



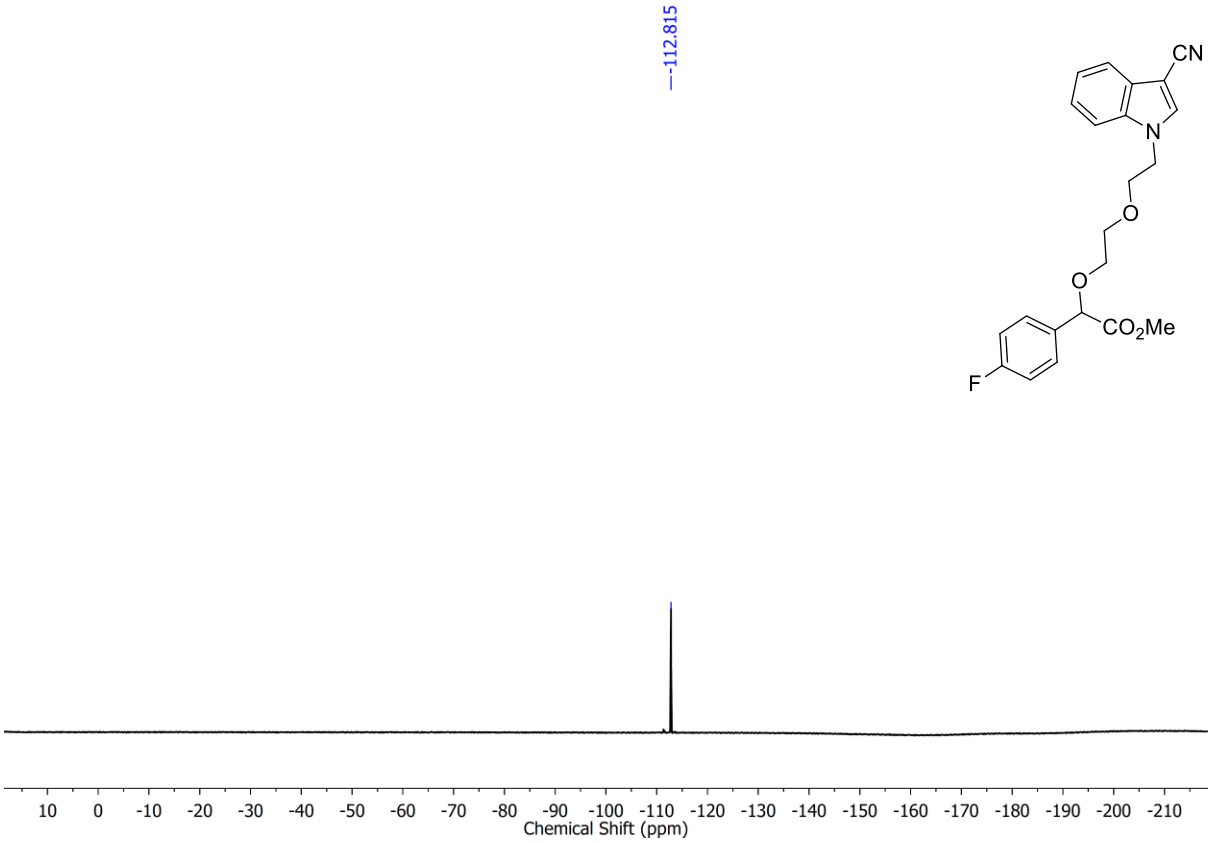
^{1}H NMR (400 MHz) of **5d** in $CDCl_3$



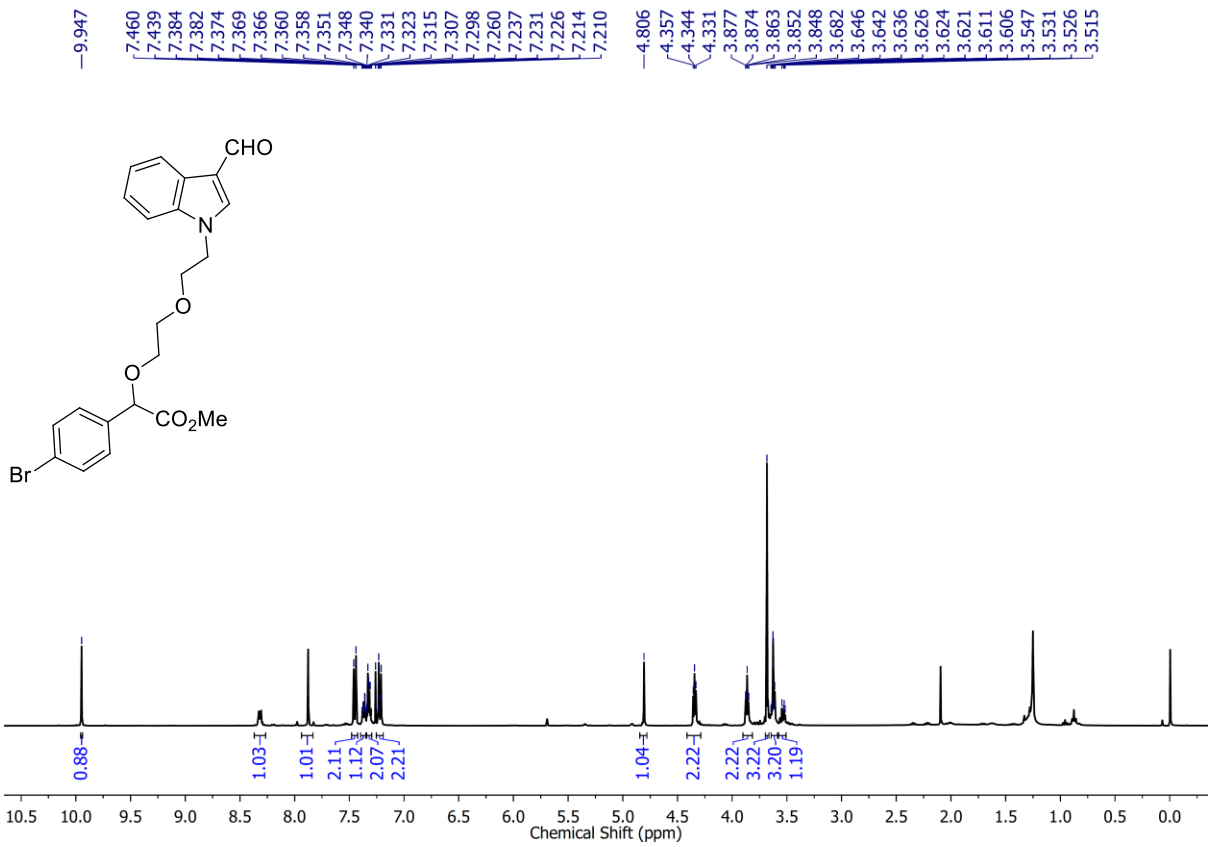
^{13}C NMR (400 MHz) of **5d** in $CDCl_3$



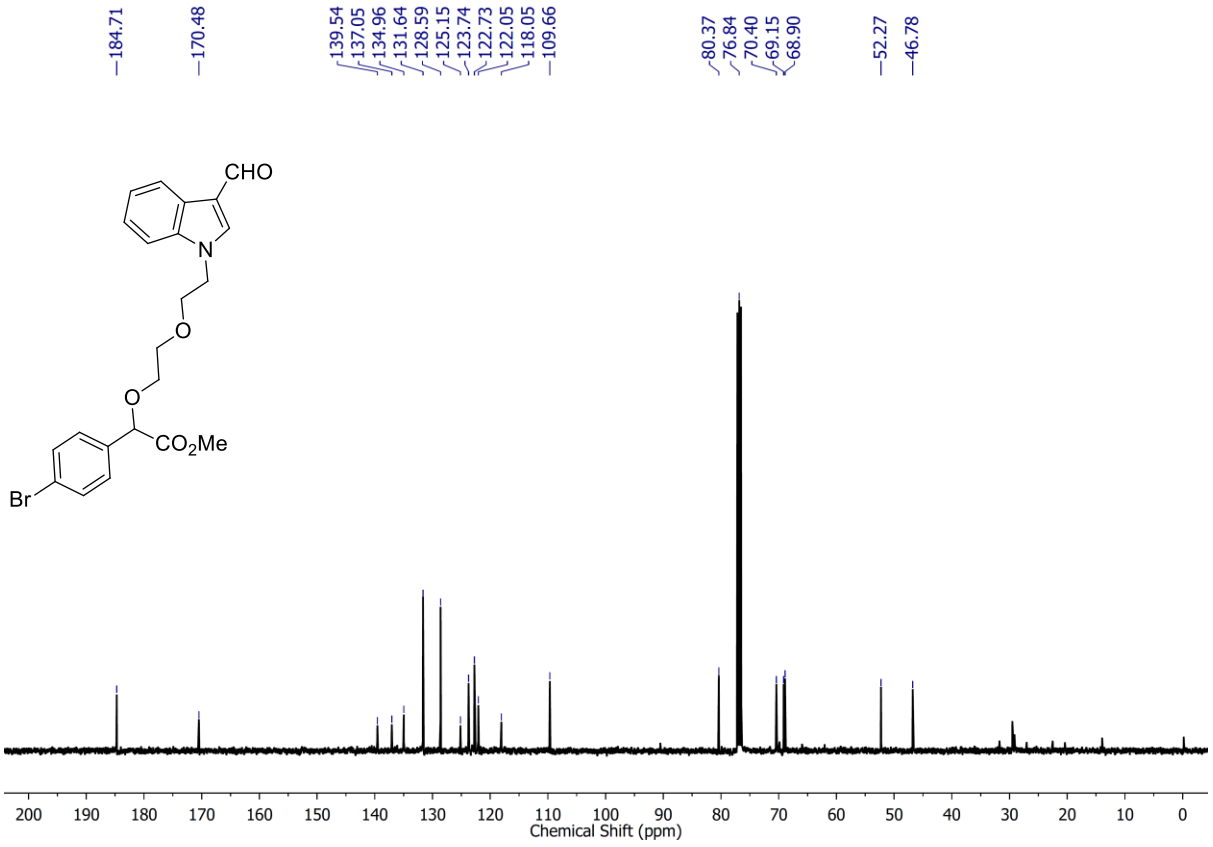
^{19}F NMR (376 MHz) of **5d** in $CDCl_3$



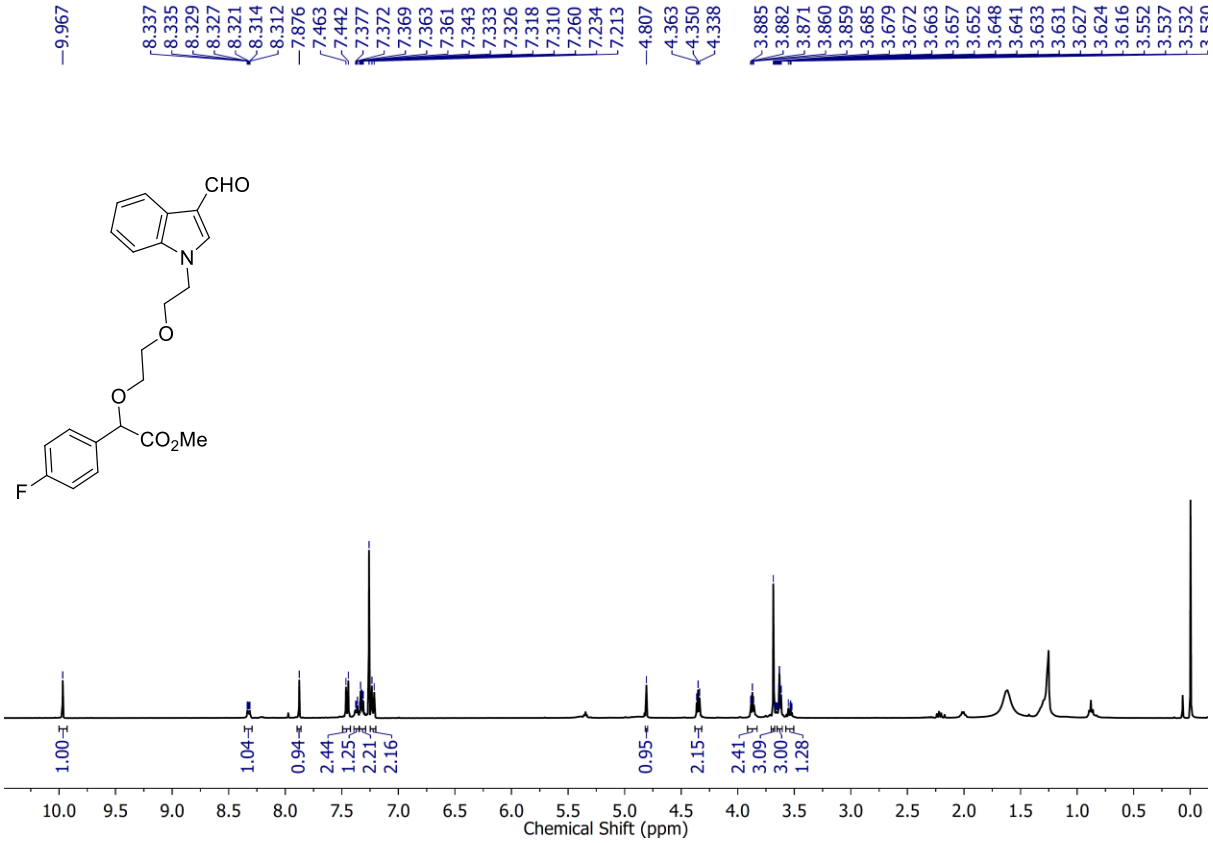
^{1}H NMR (400 MHz) of **5e** in $CDCl_3$



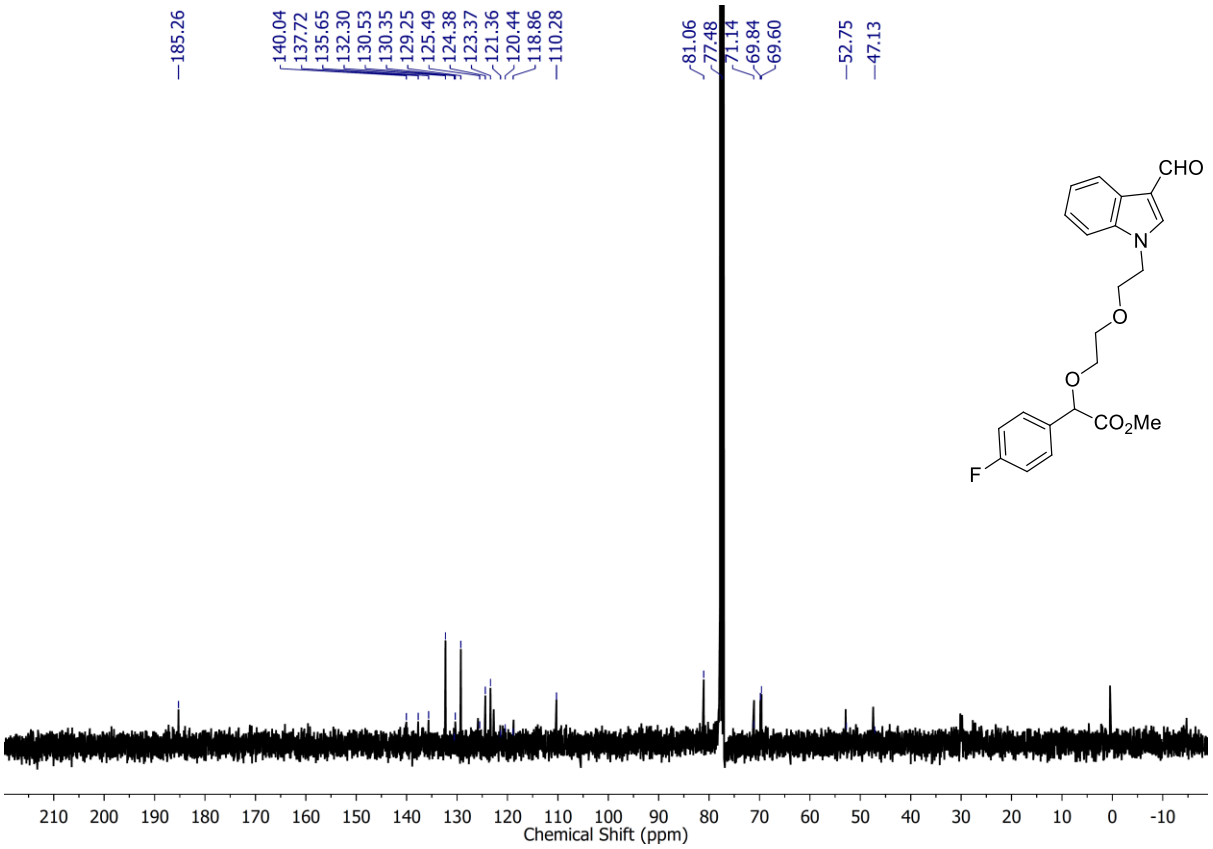
^{13}C NMR (400 MHz) of **5e** in $CDCl_3$



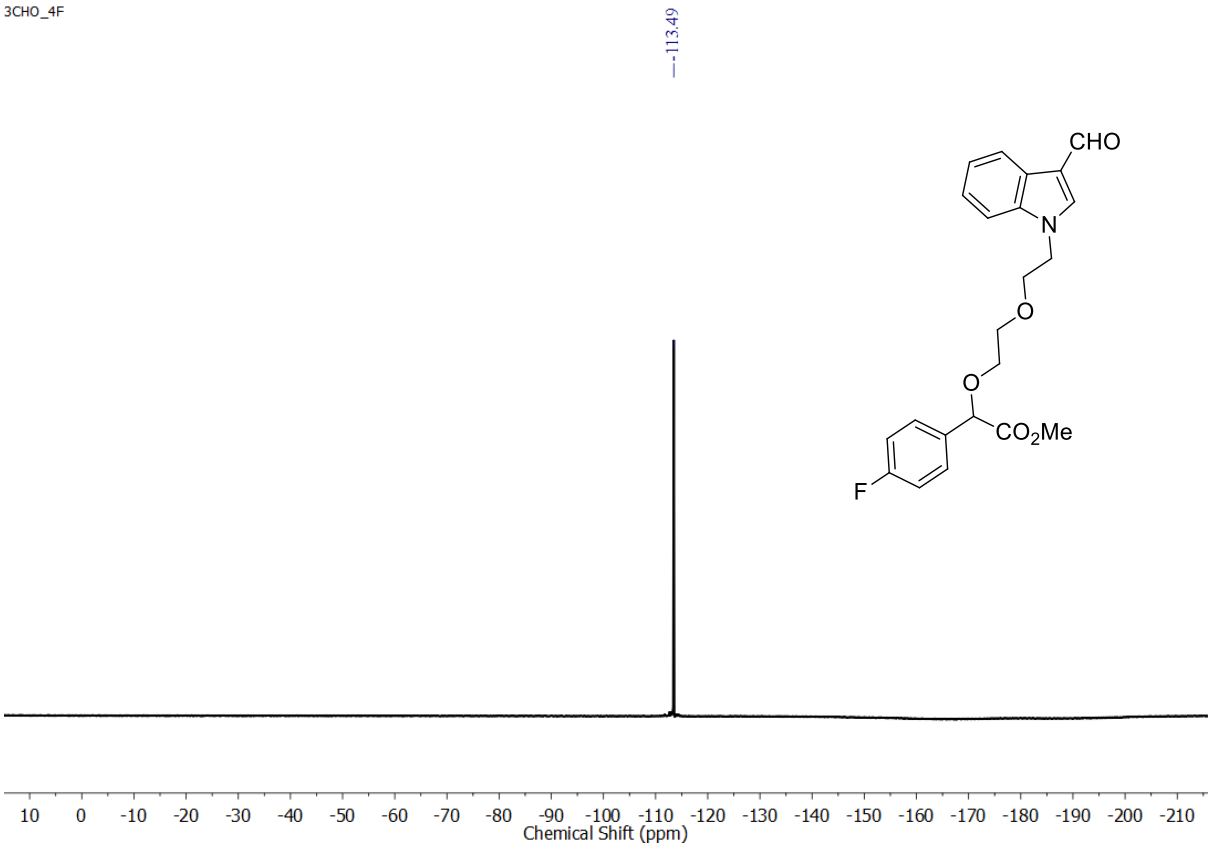
^{1}H NMR (400 MHz) of **5f** in $CDCl_3$



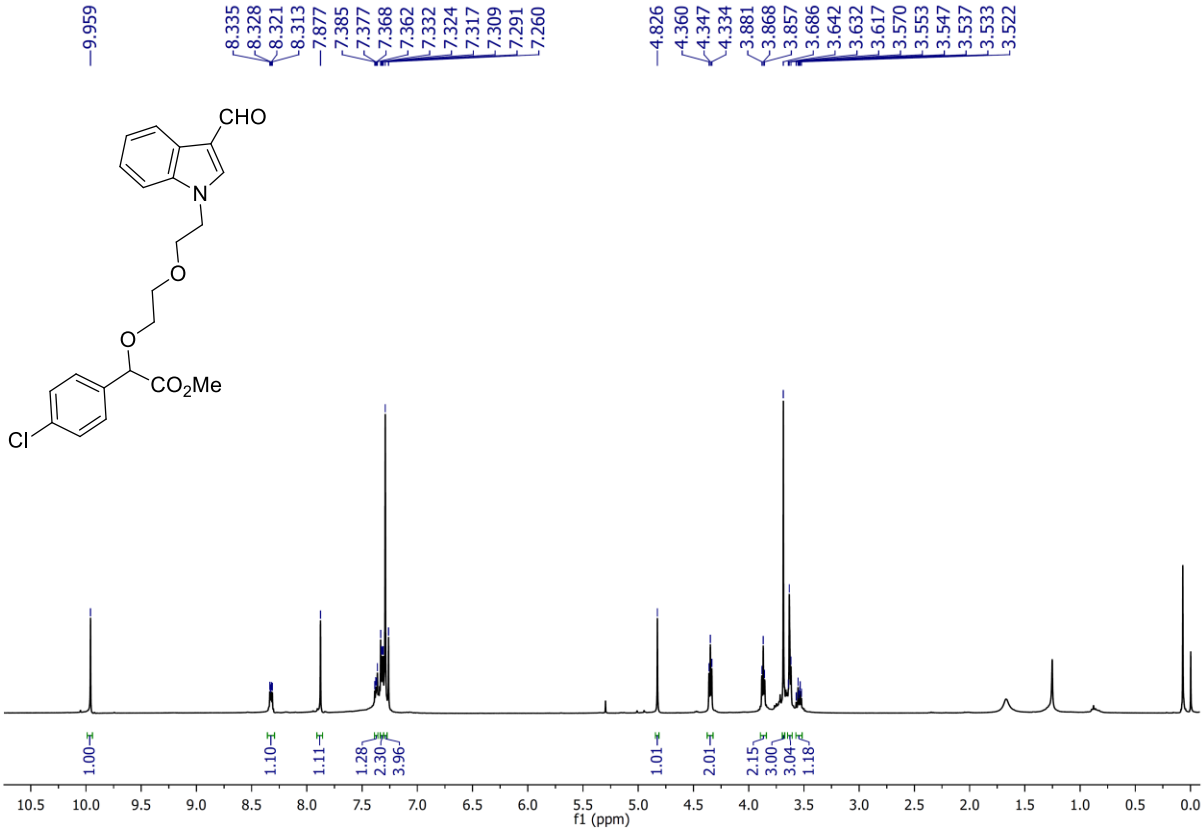
^{13}C NMR (400 MHz) of **5f** in $CDCl_3$



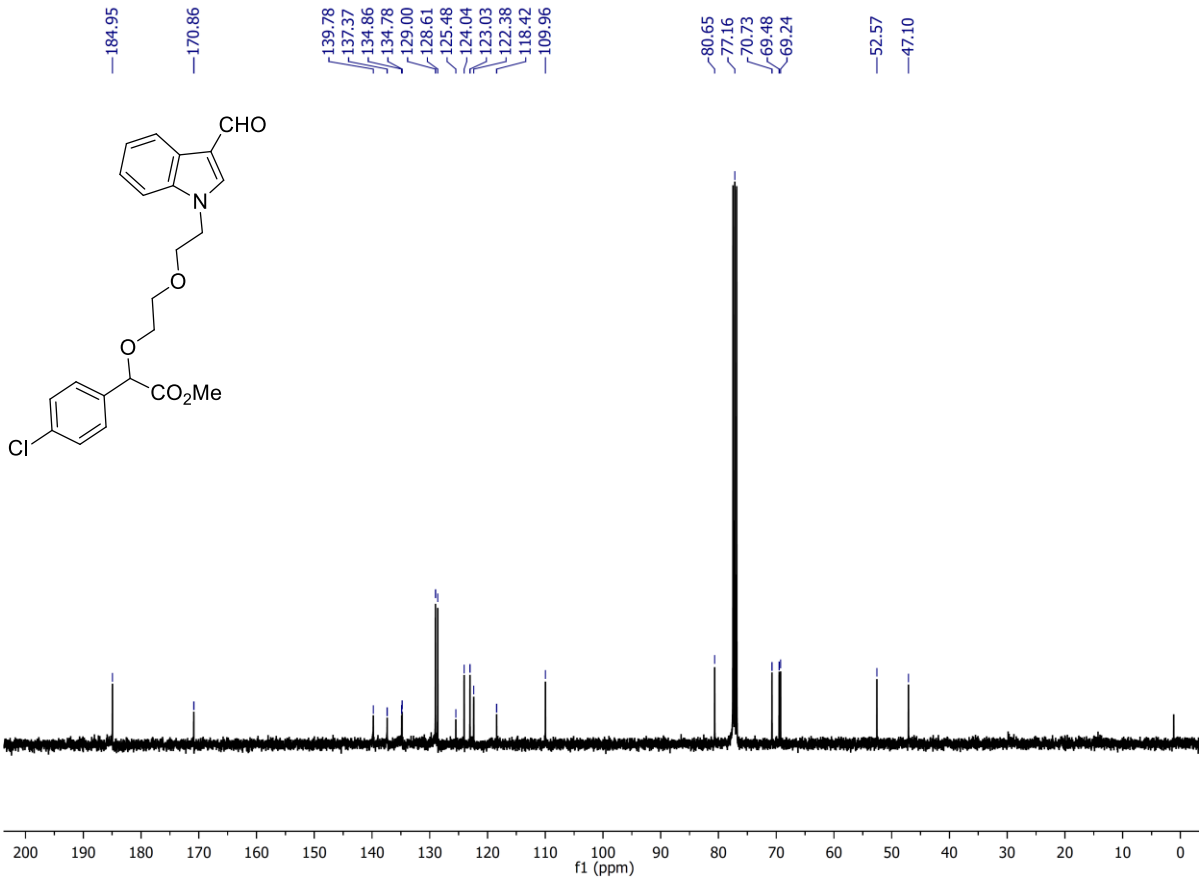
^{19}F NMR (376 MHz) of **5f** in $CDCl_3$



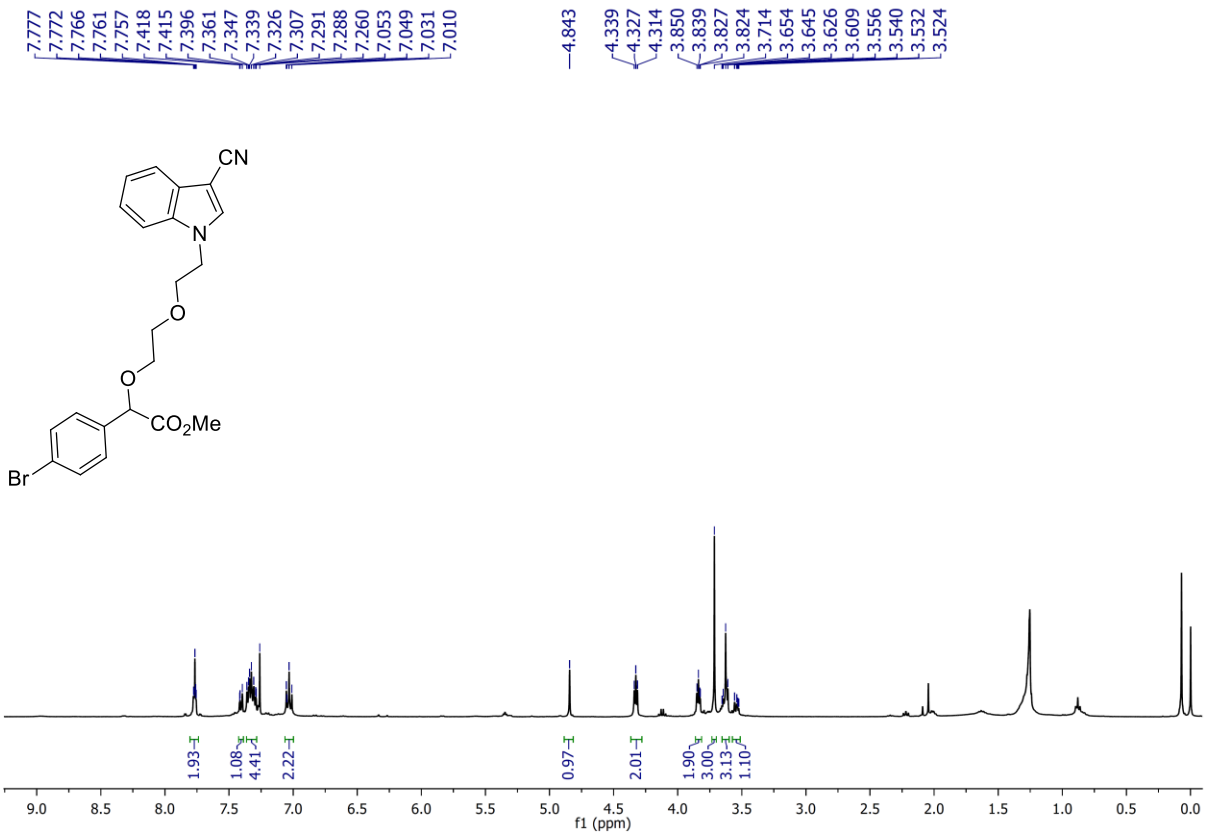
^{1}H NMR (400 MHz) of **5g** in $CDCl_3$



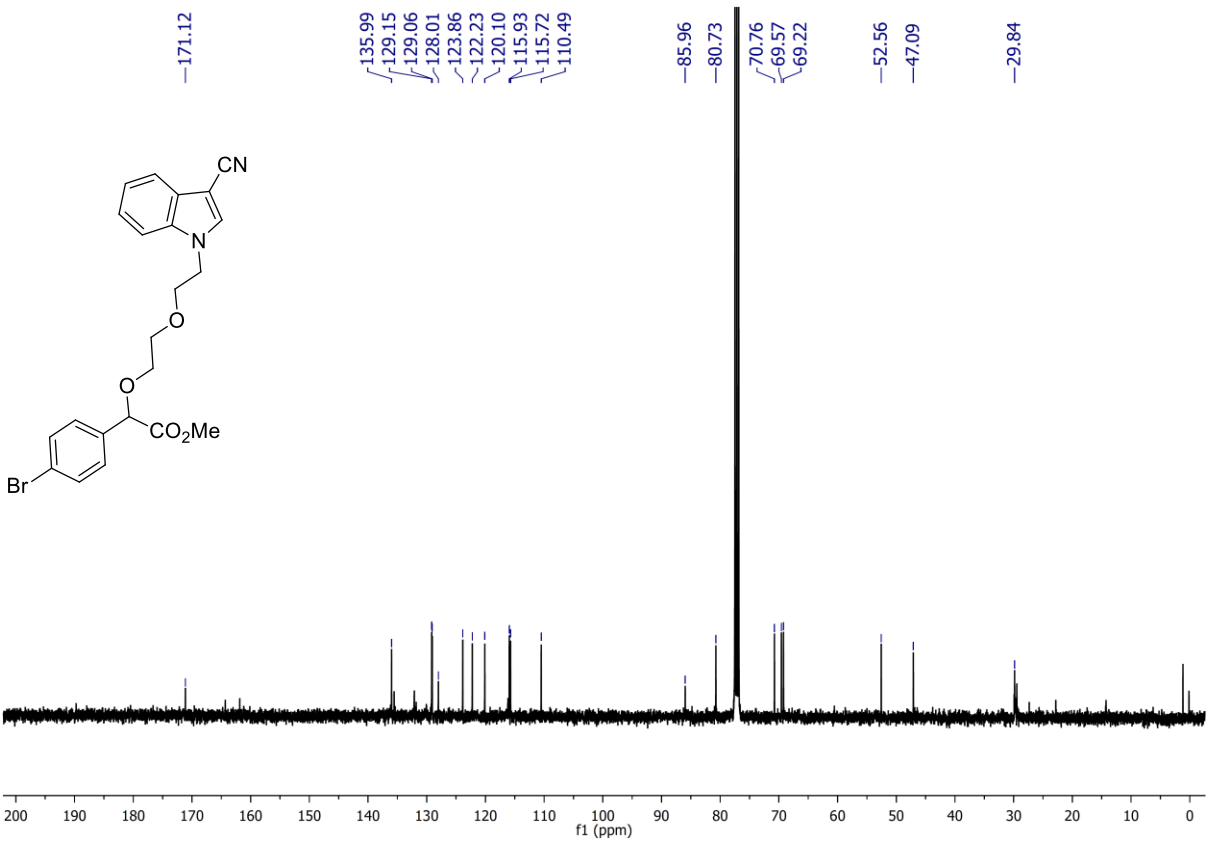
^{13}C NMR (400 MHz) of **5g** in $CDCl_3$



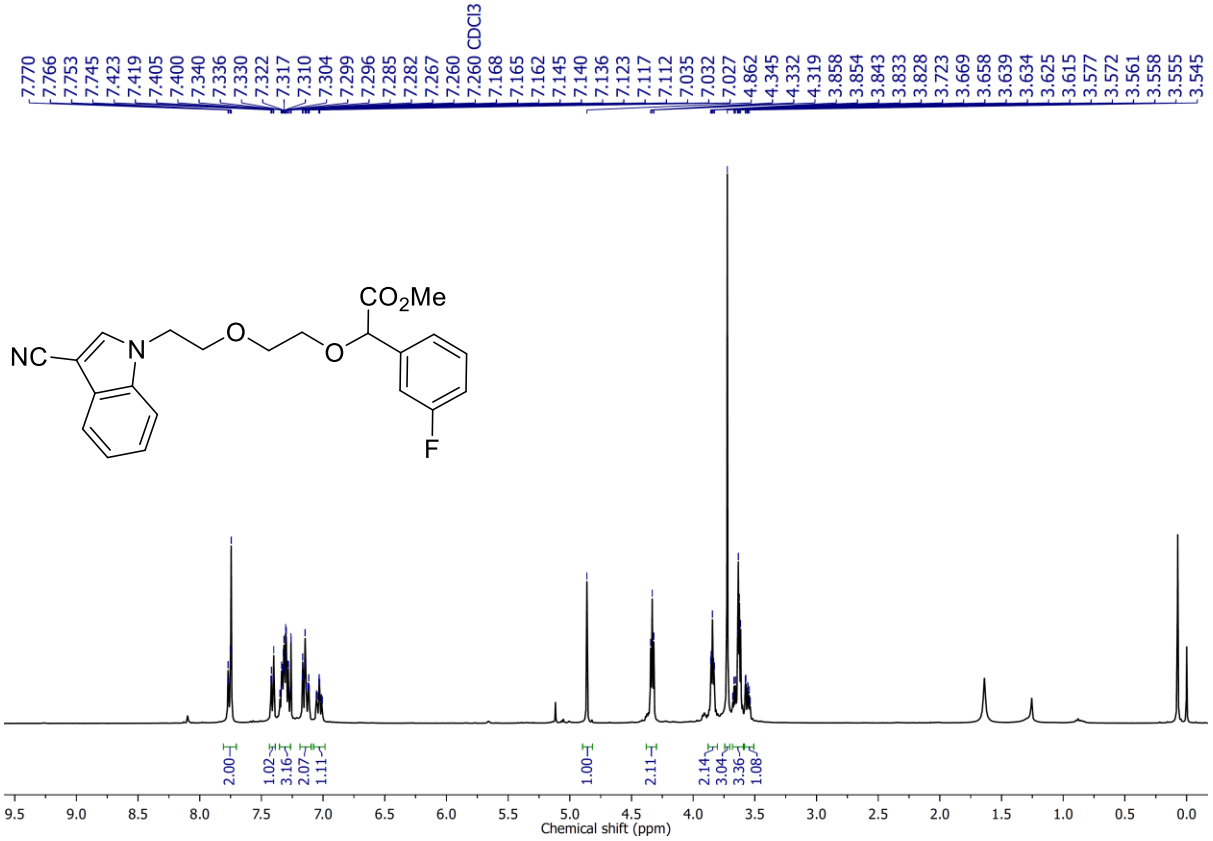
^{1}H NMR (400 MHz) of **5h** in $CDCl_3$



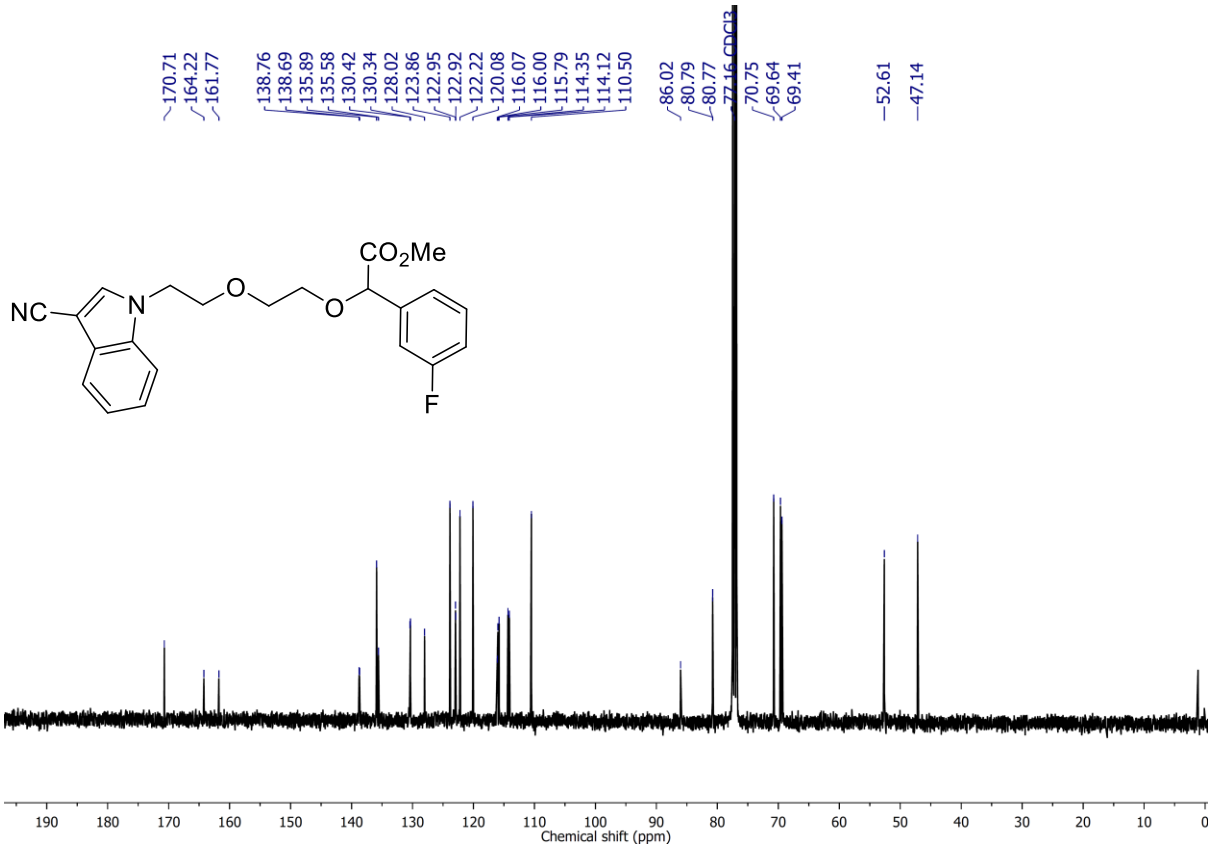
^{13}C NMR (400 MHz) of **5h** in $CDCl_3$



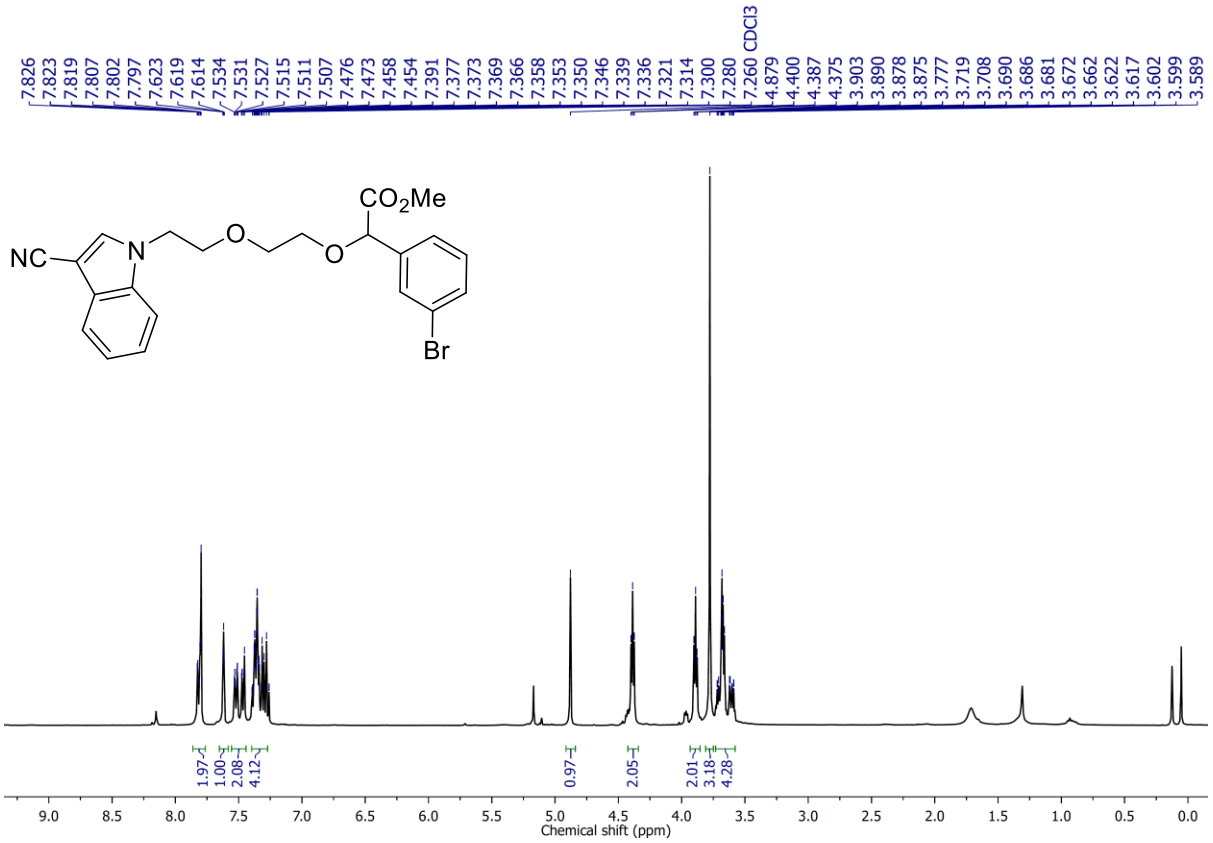
^{1}H NMR (400 MHz) of **5i** in $CDCl_3$



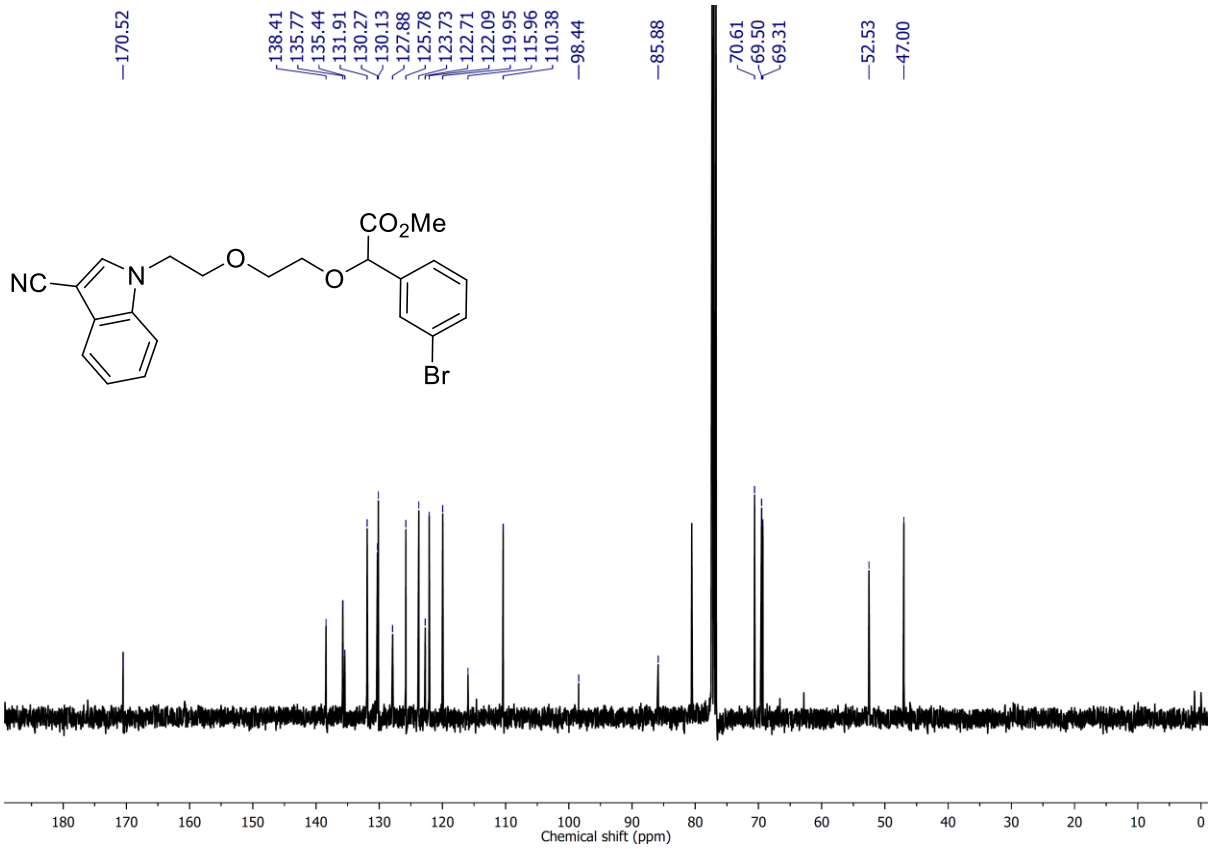
^{13}C NMR (400 MHz) of **5i** in $CDCl_3$



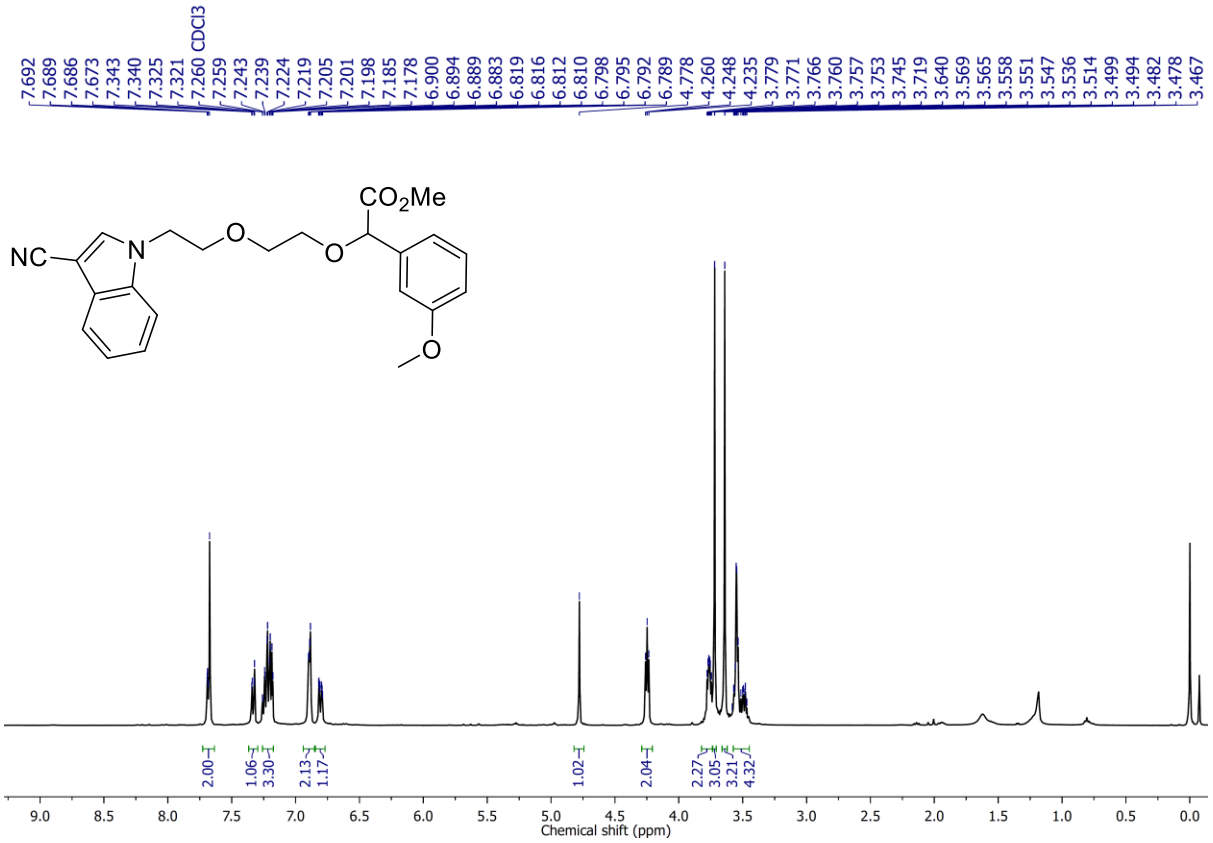
^{1}H NMR (400 MHz) of **5j** in $CDCl_3$



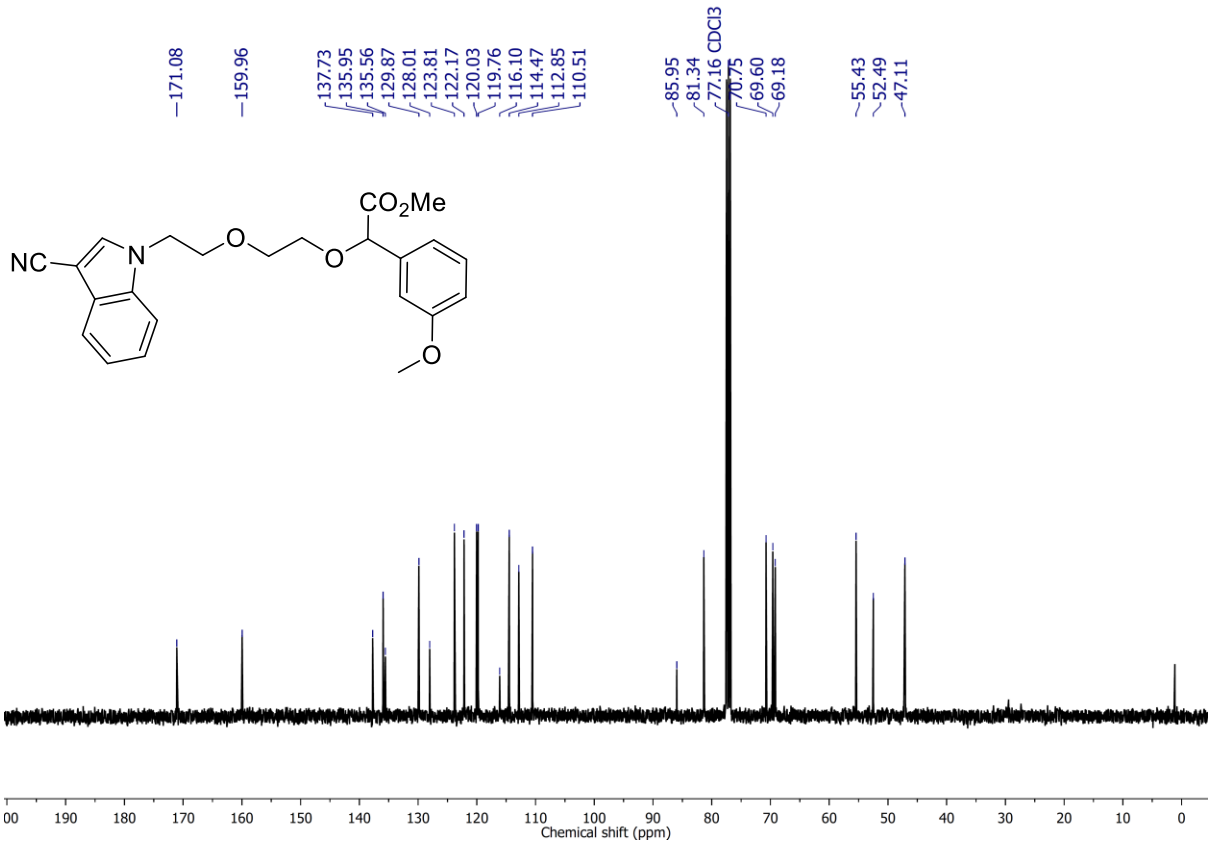
^{13}C NMR (400 MHz) of **5j** in $CDCl_3$



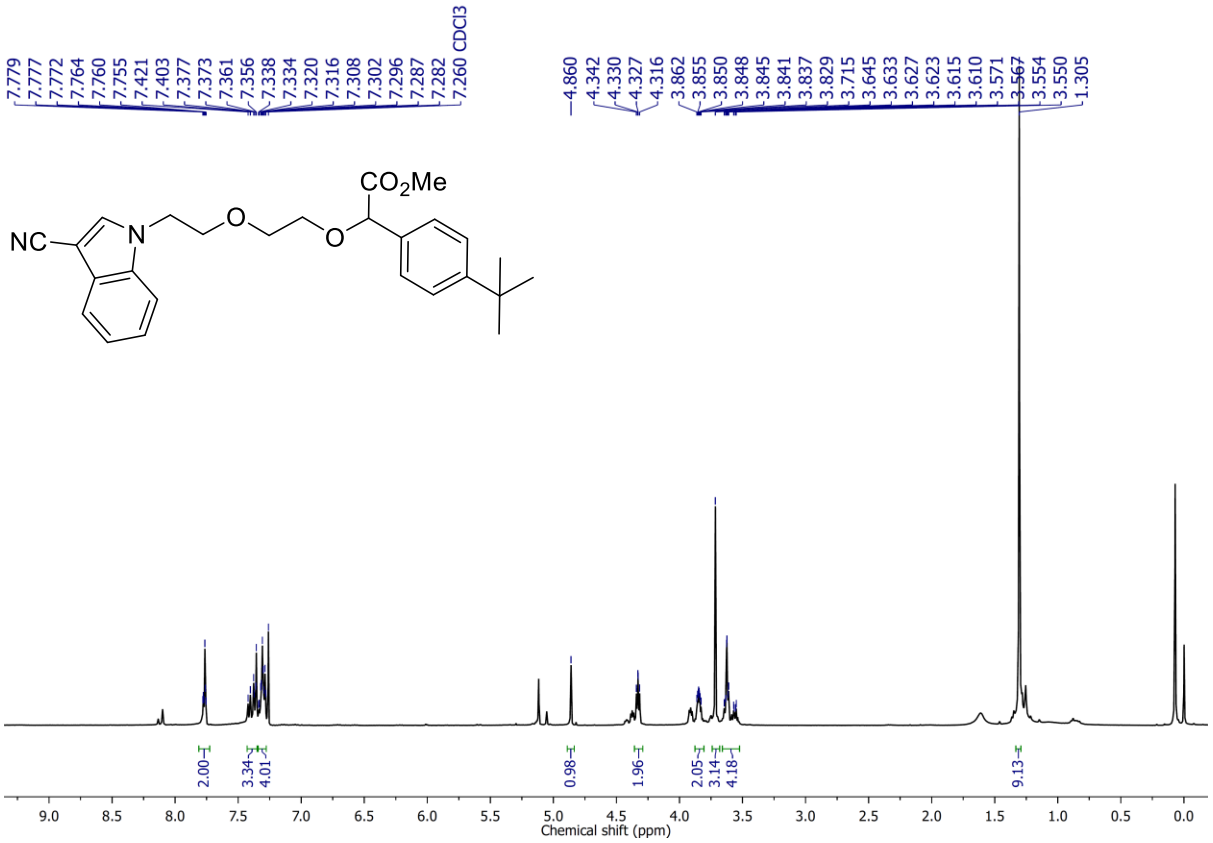
^{1}H NMR (400 MHz) of **5k** in $CDCl_3$



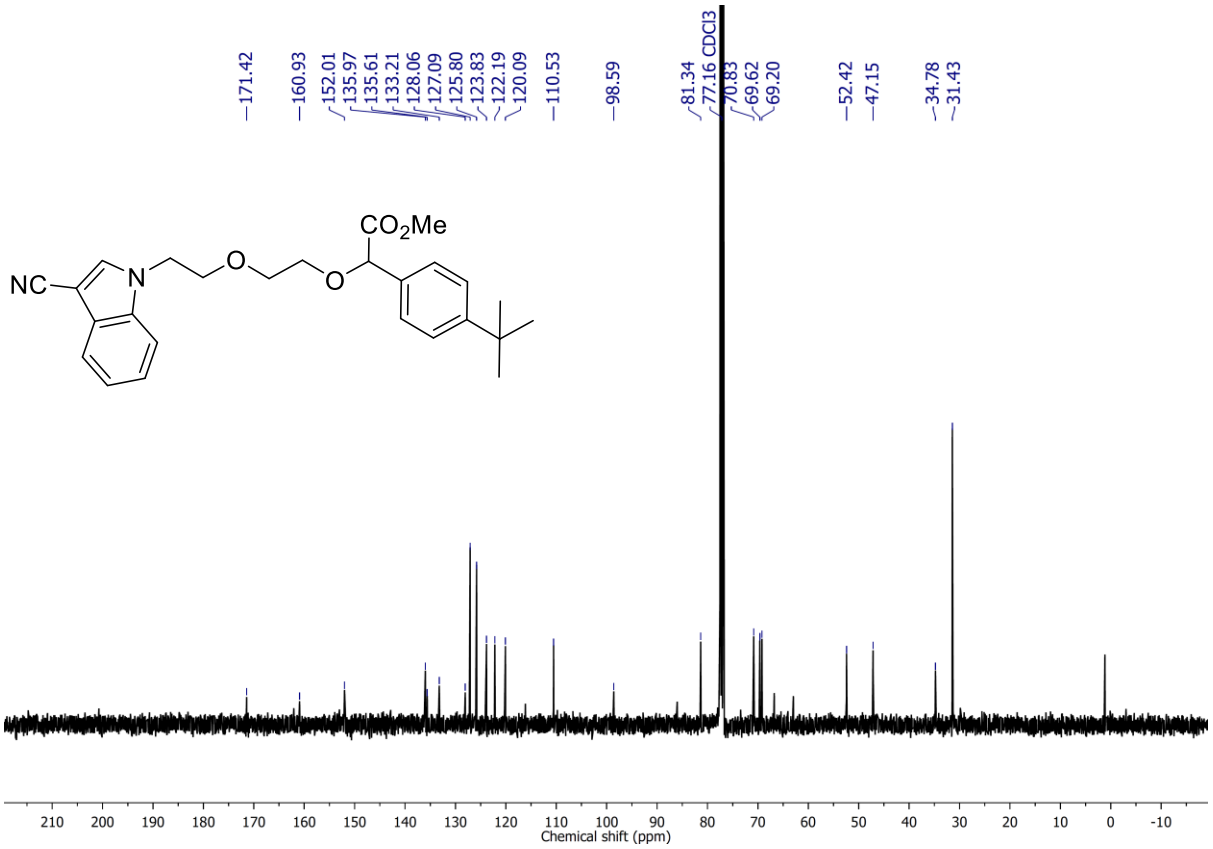
^{13}C NMR (400 MHz) of **5k** in $CDCl_3$



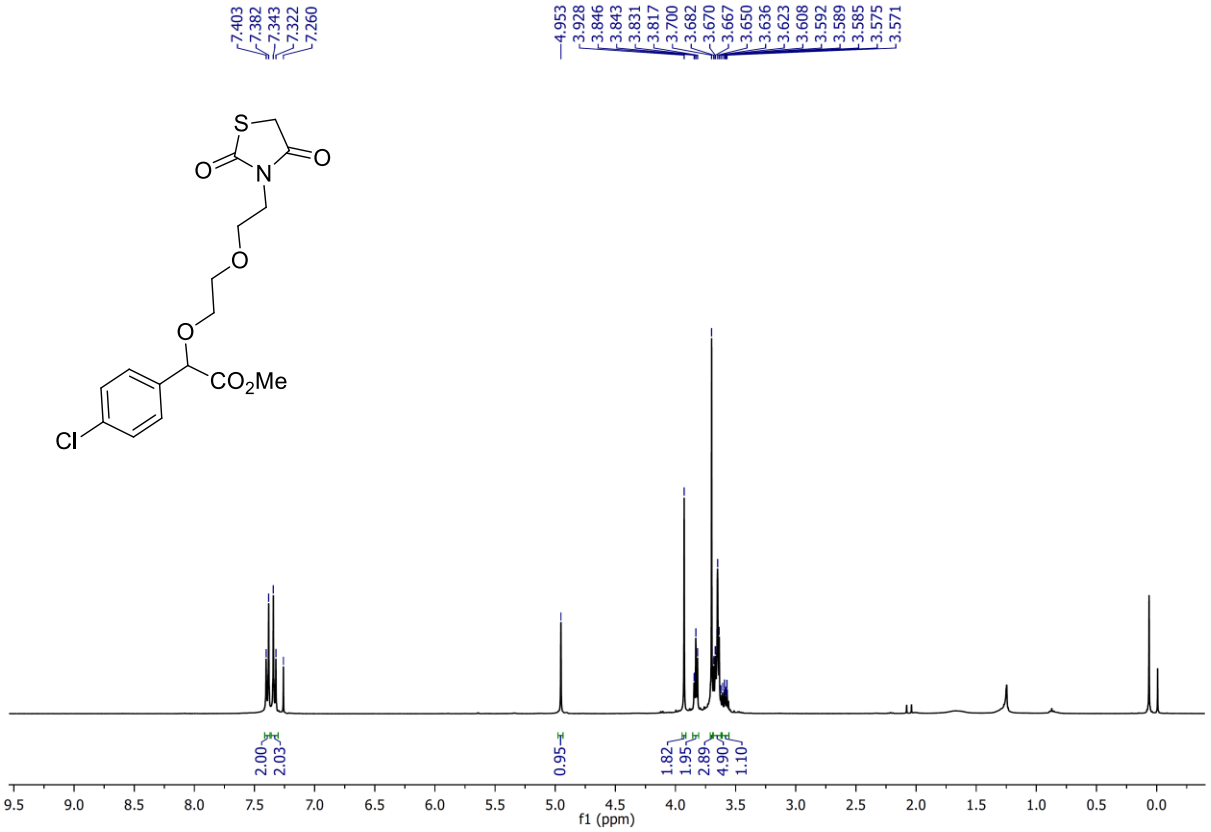
^{1}H NMR (400 MHz) of **5l** in $CDCl_3$



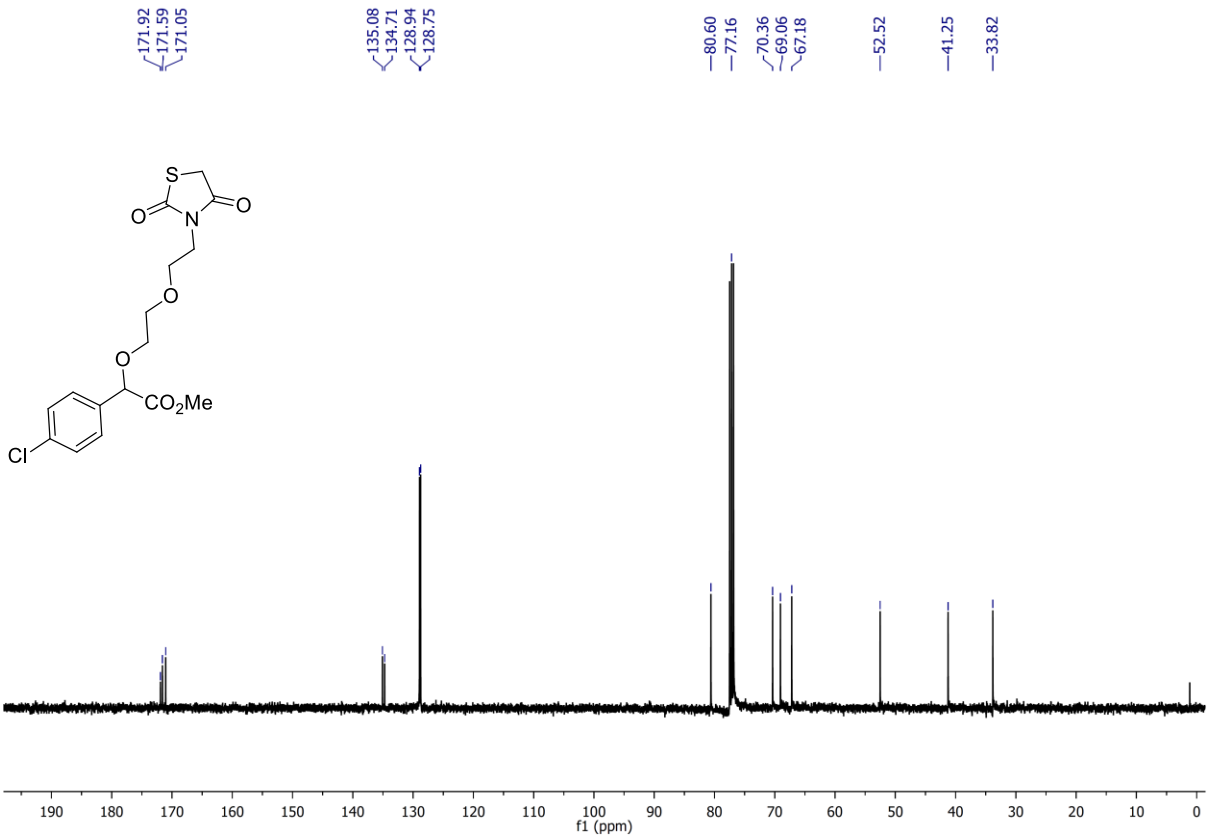
^{13}C NMR (400 MHz) of **5l** in $CDCl_3$



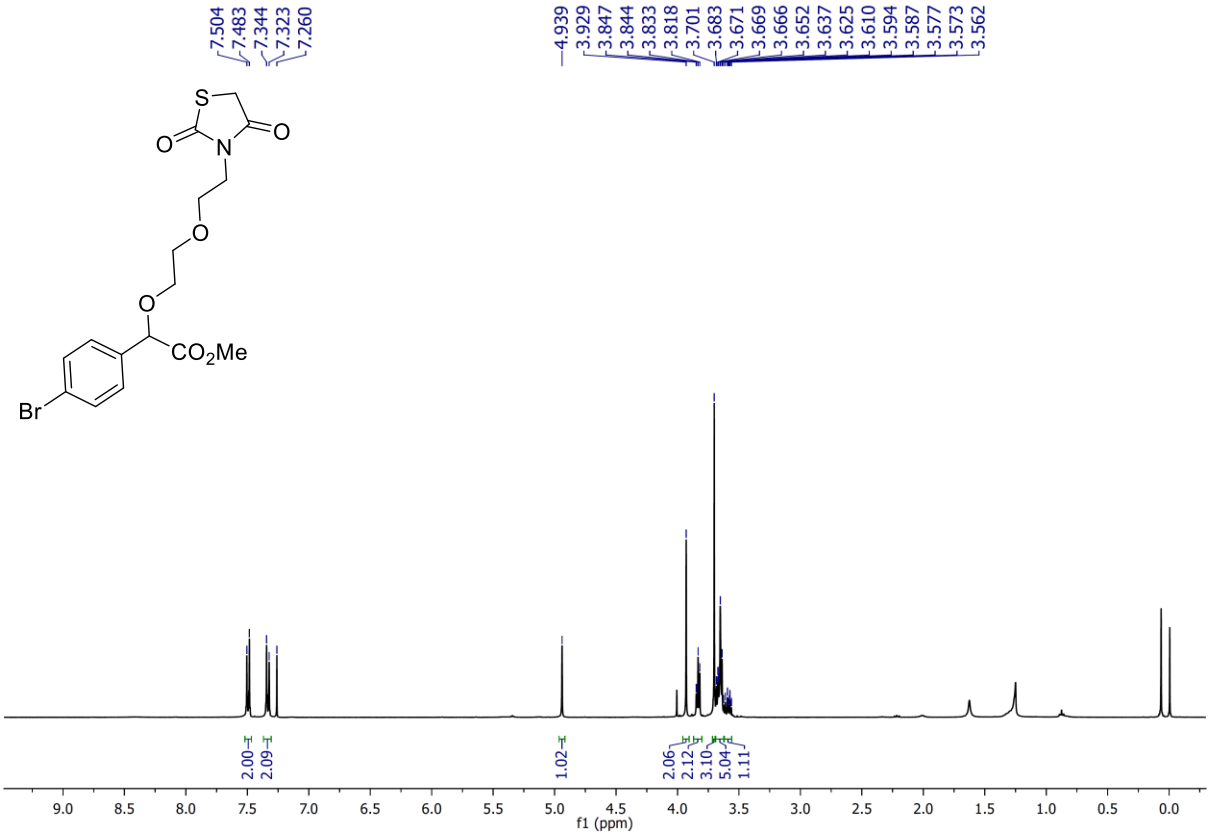
^{1}H NMR (400 MHz) of **6a** in $CDCl_3$



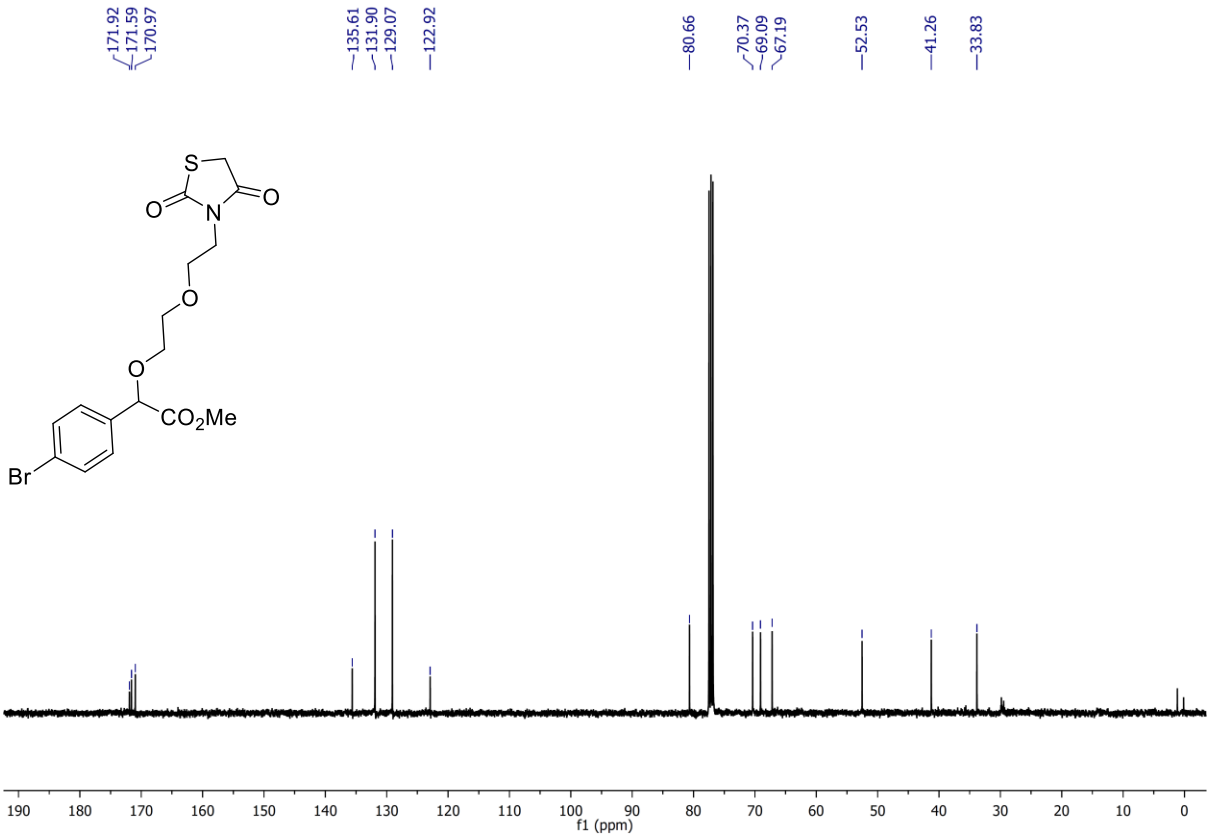
^{13}C NMR (400 MHz) of **6a** in $CDCl_3$



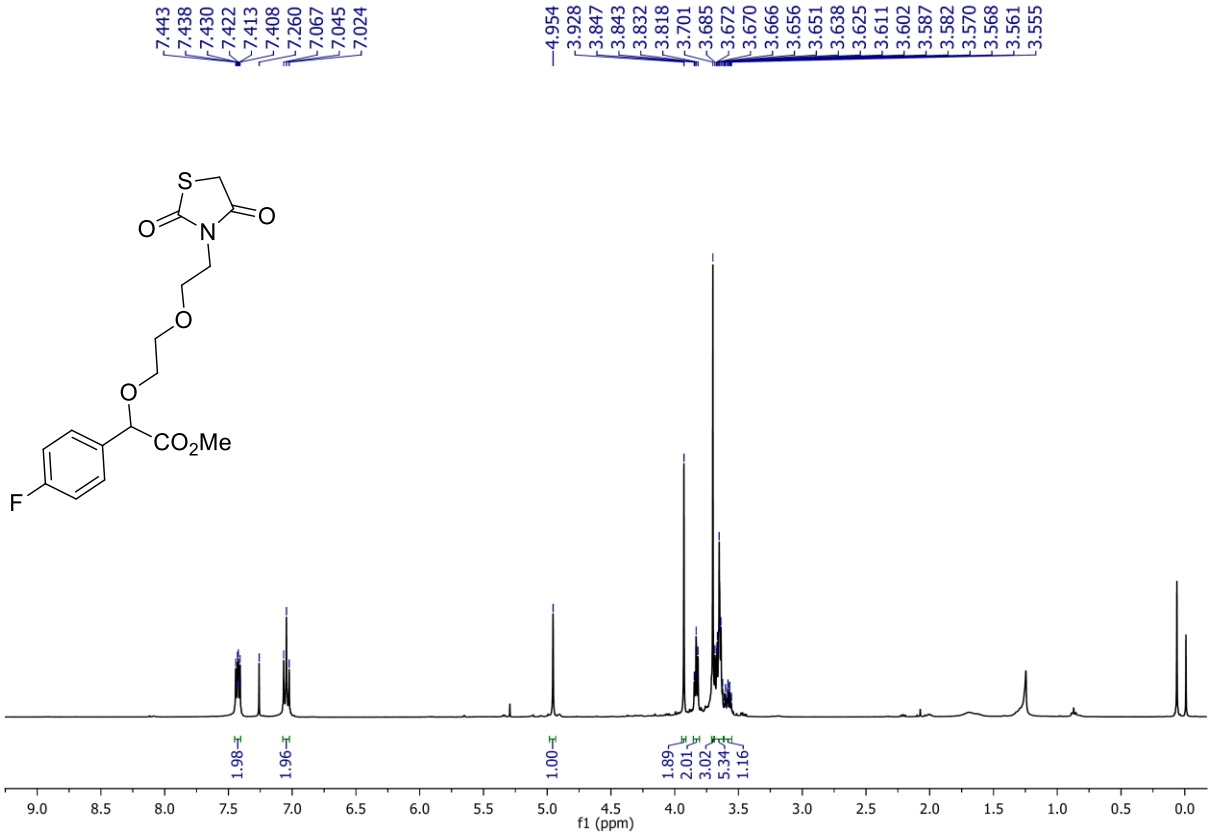
^{1}H NMR (400 MHz) of **6b** in $CDCl_3$



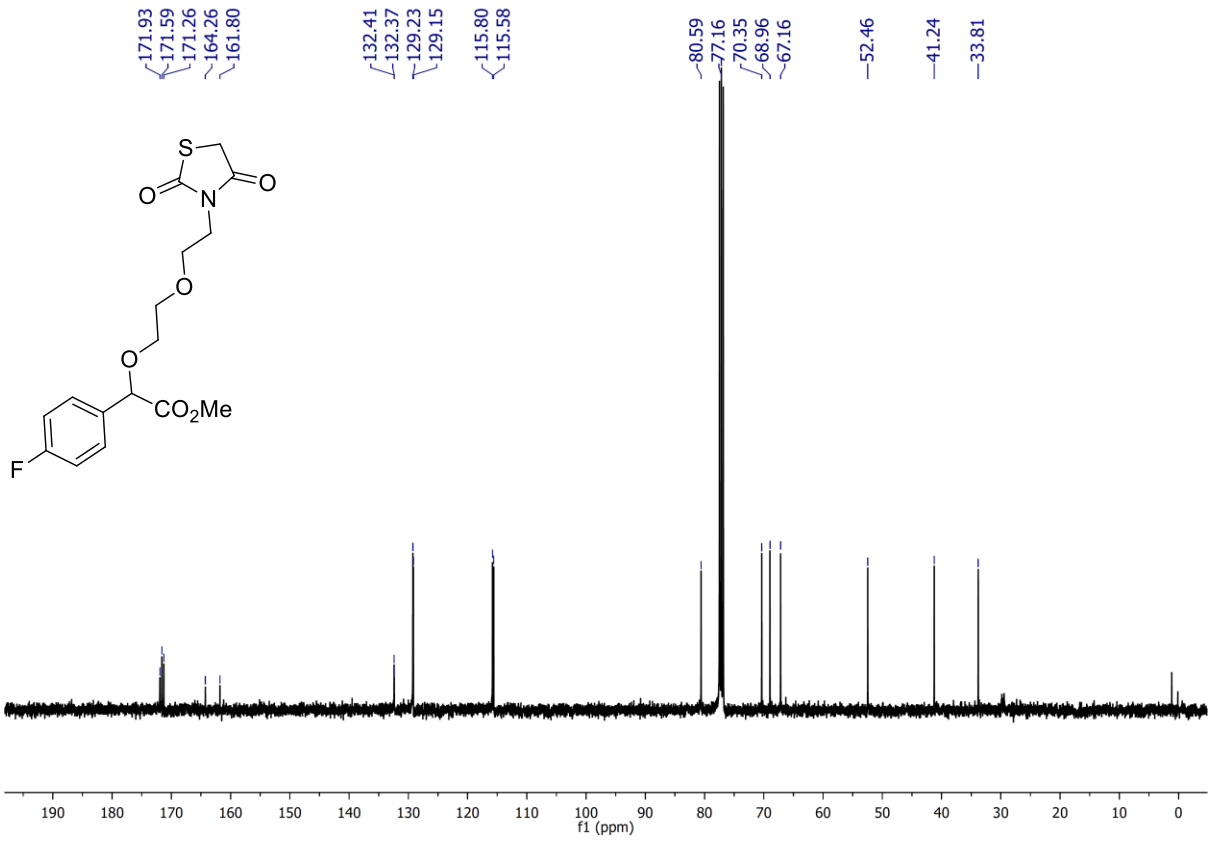
^{13}C NMR (400 MHz) of **6b** in $CDCl_3$



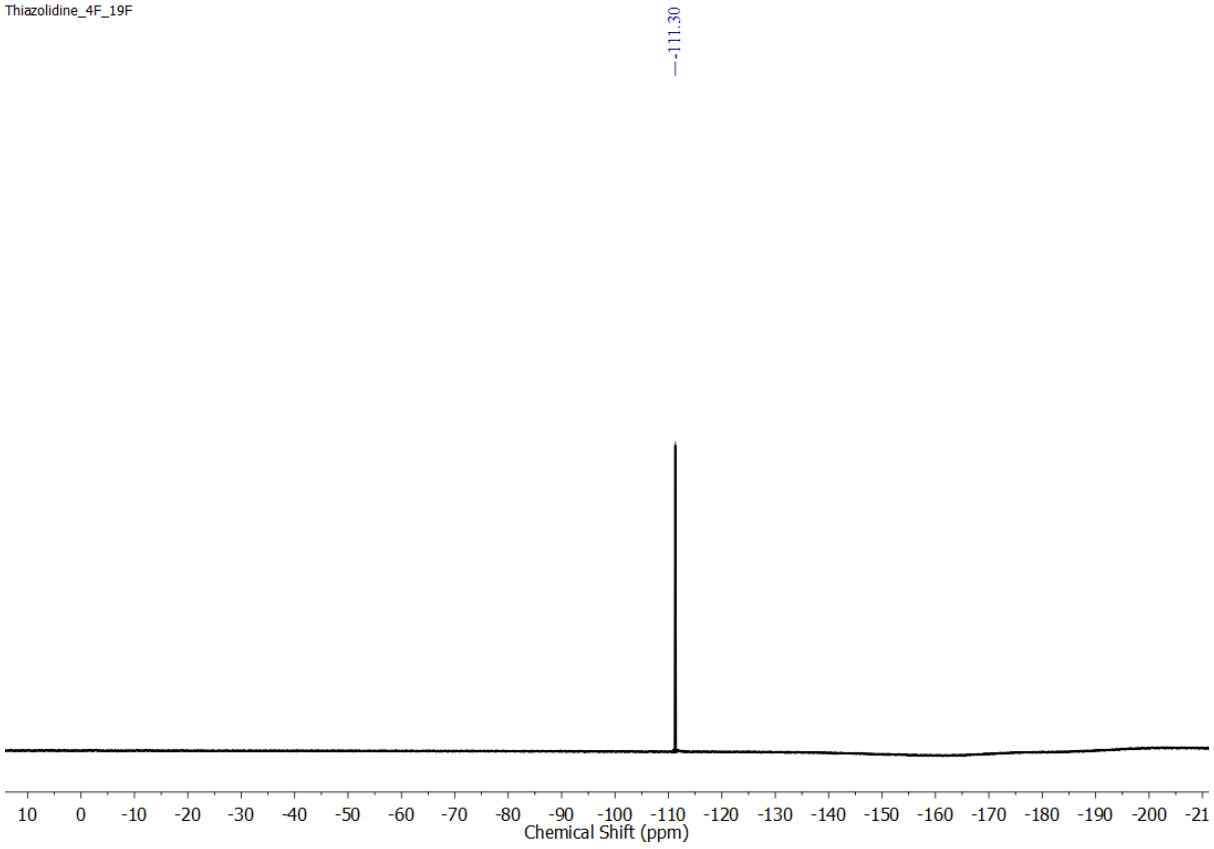
^{1}H NMR (400 MHz) of **6c** in $CDCl_3$



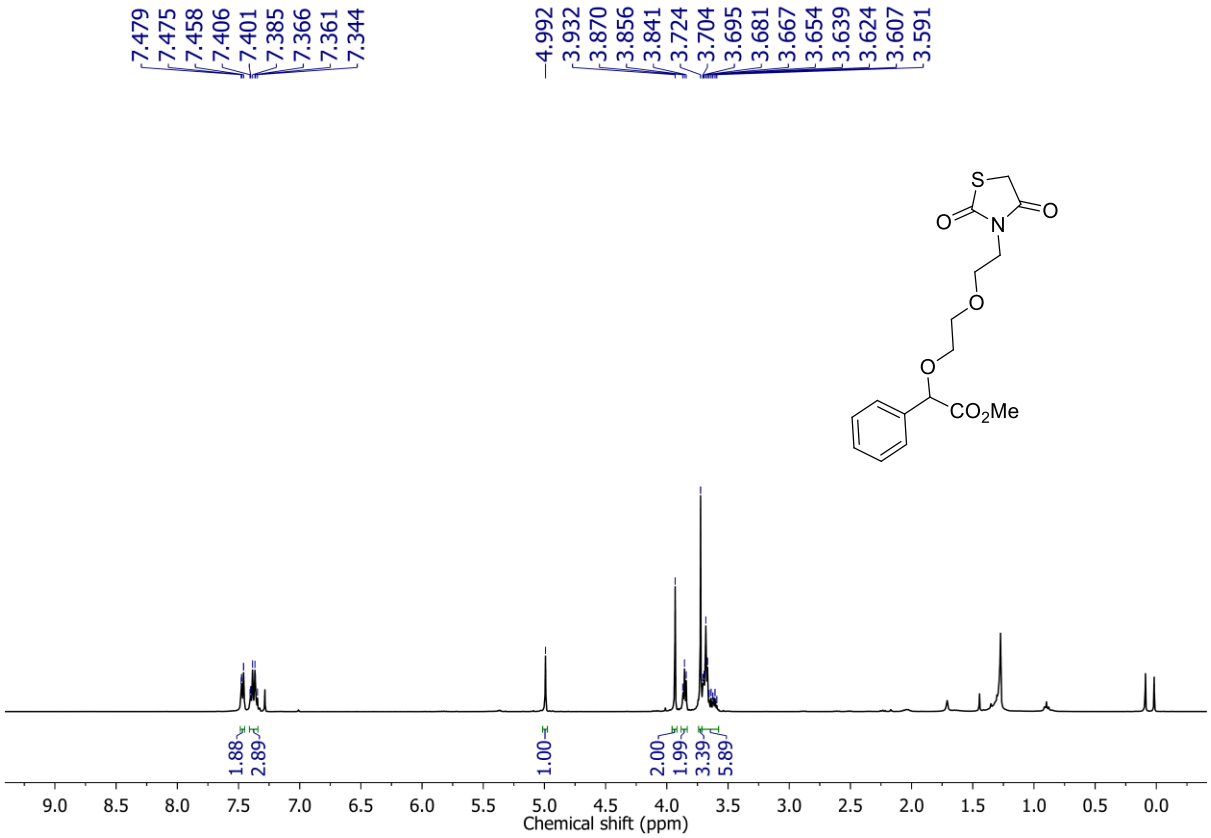
^{13}C NMR (400 MHz) of **6c** in $CDCl_3$



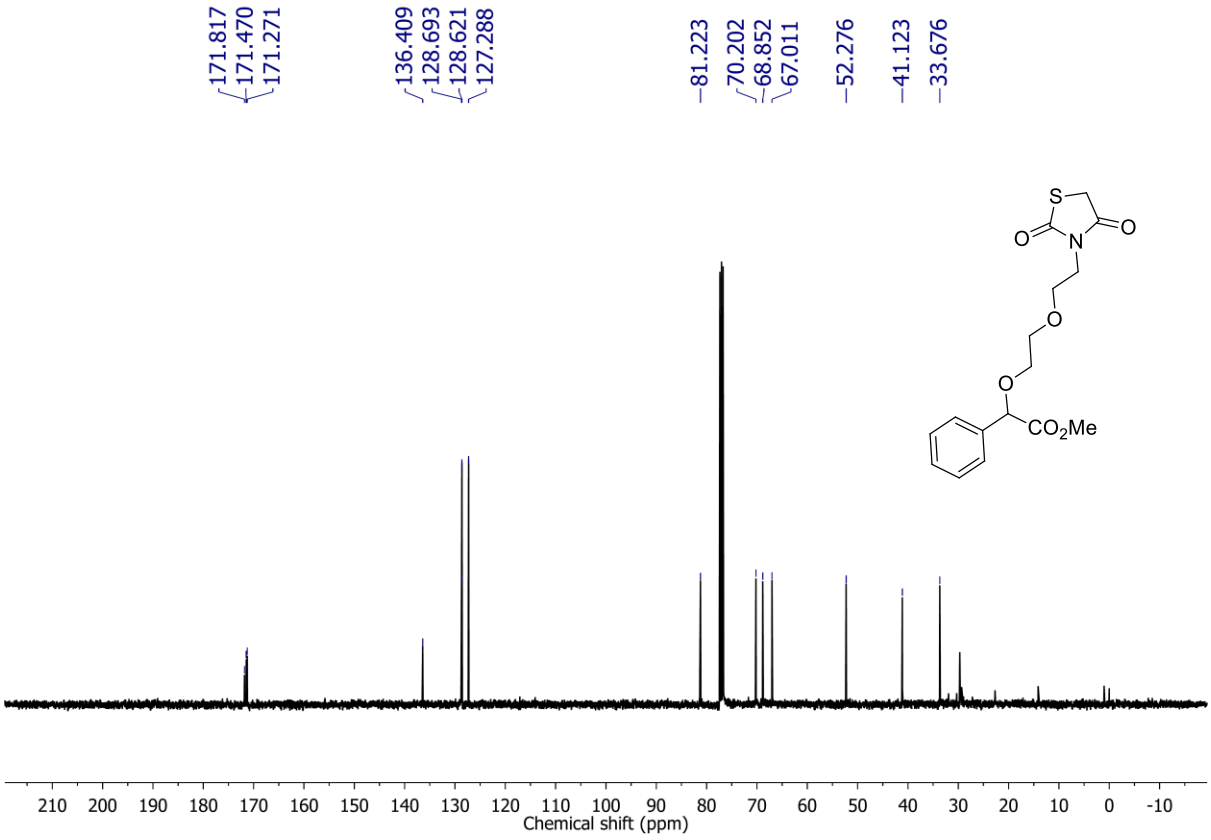
^{19}F NMR (376 MHz) of **6c** in $CDCl_3$



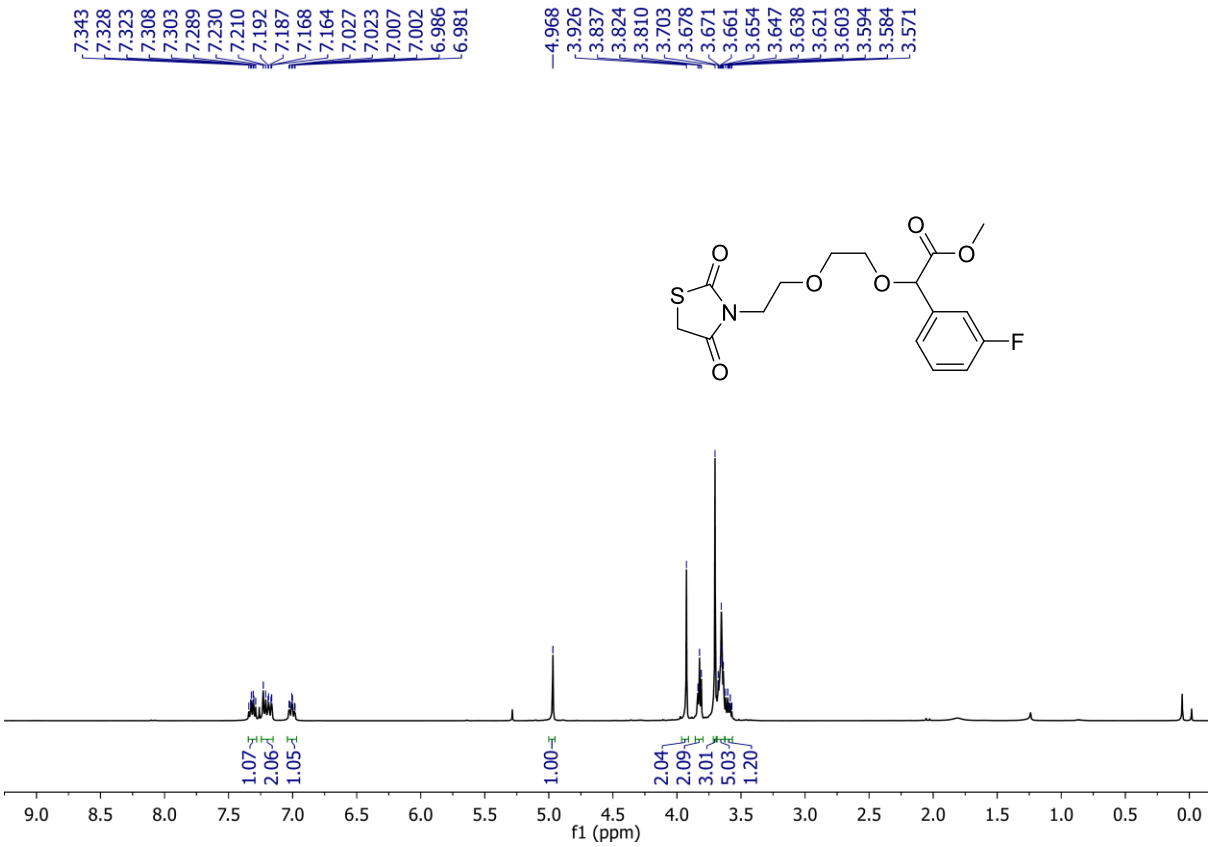
^{1}H NMR (400 MHz) of **6d** in $CDCl_3$



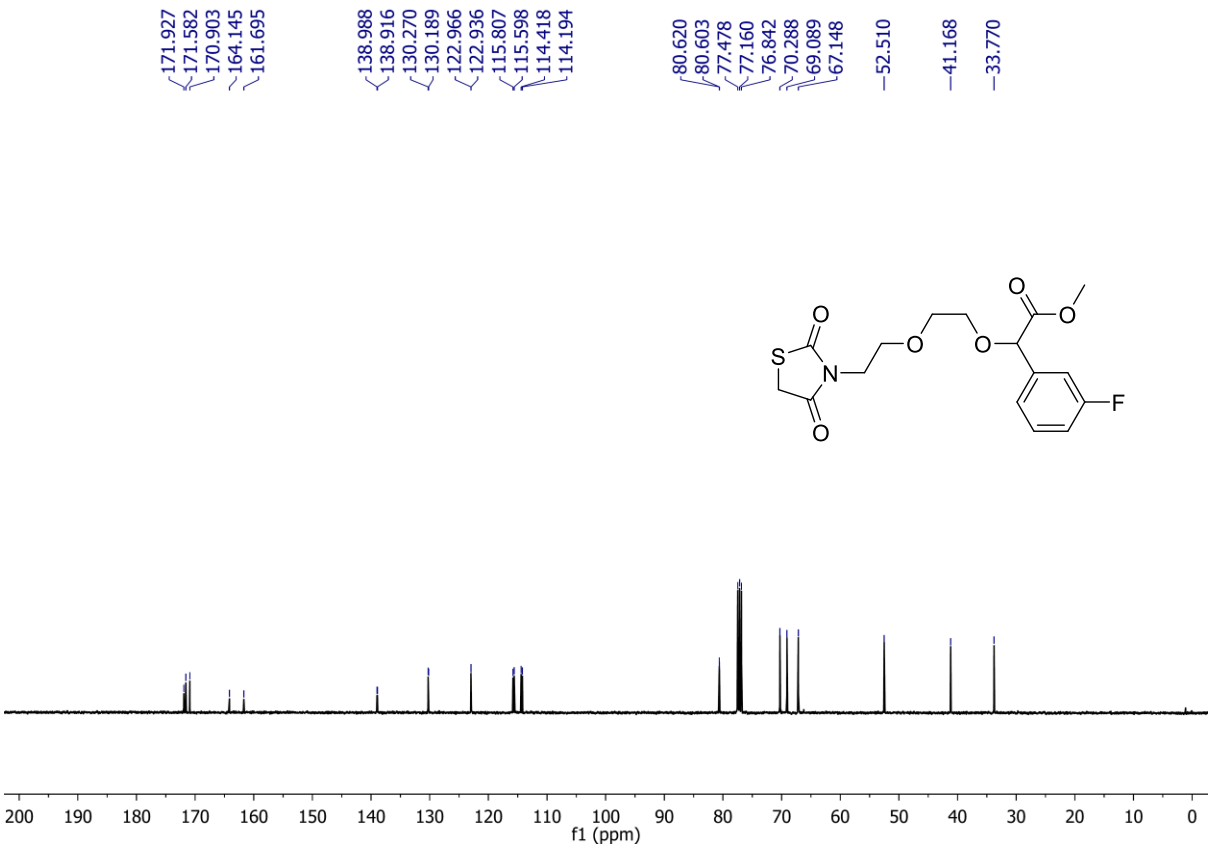
^{13}C NMR (400 MHz) of **6d** in $CDCl_3$



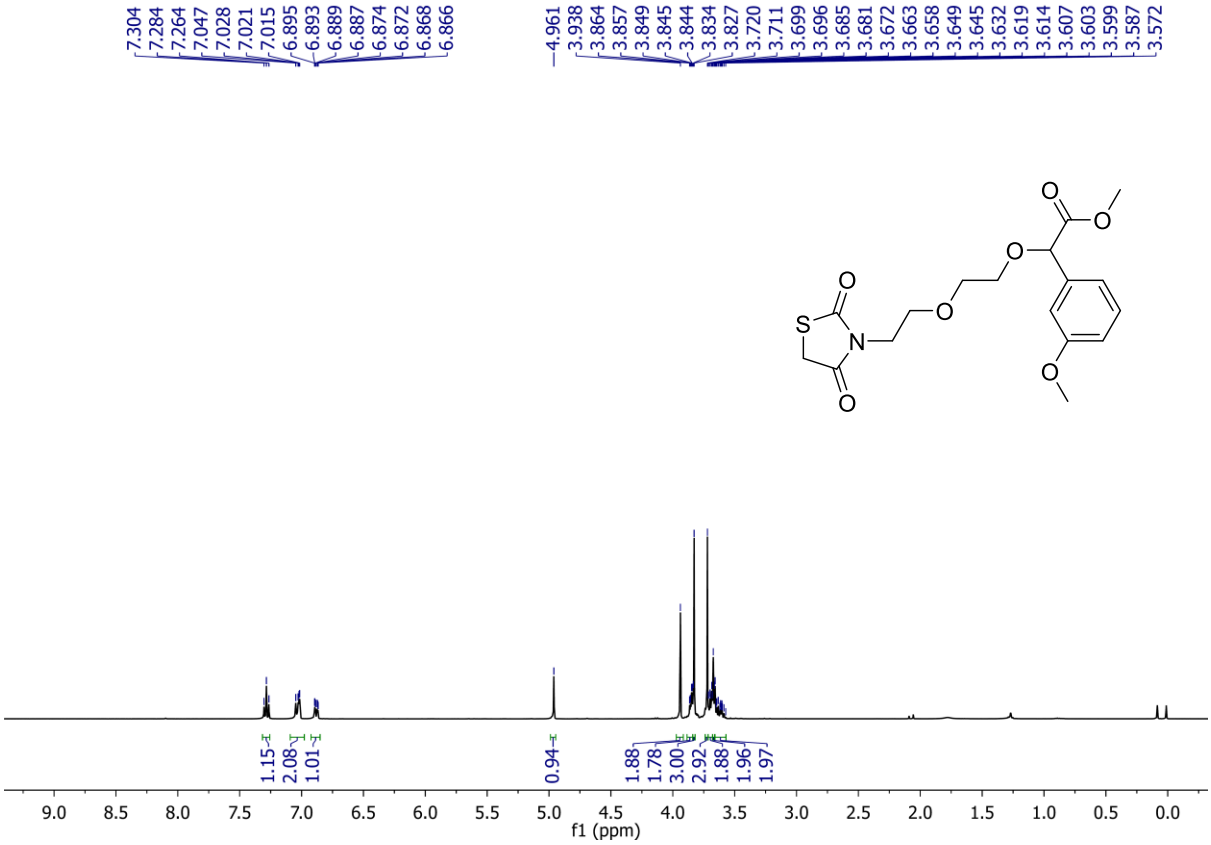
^{1}H NMR (400 MHz) of **6e** in $CDCl_3$



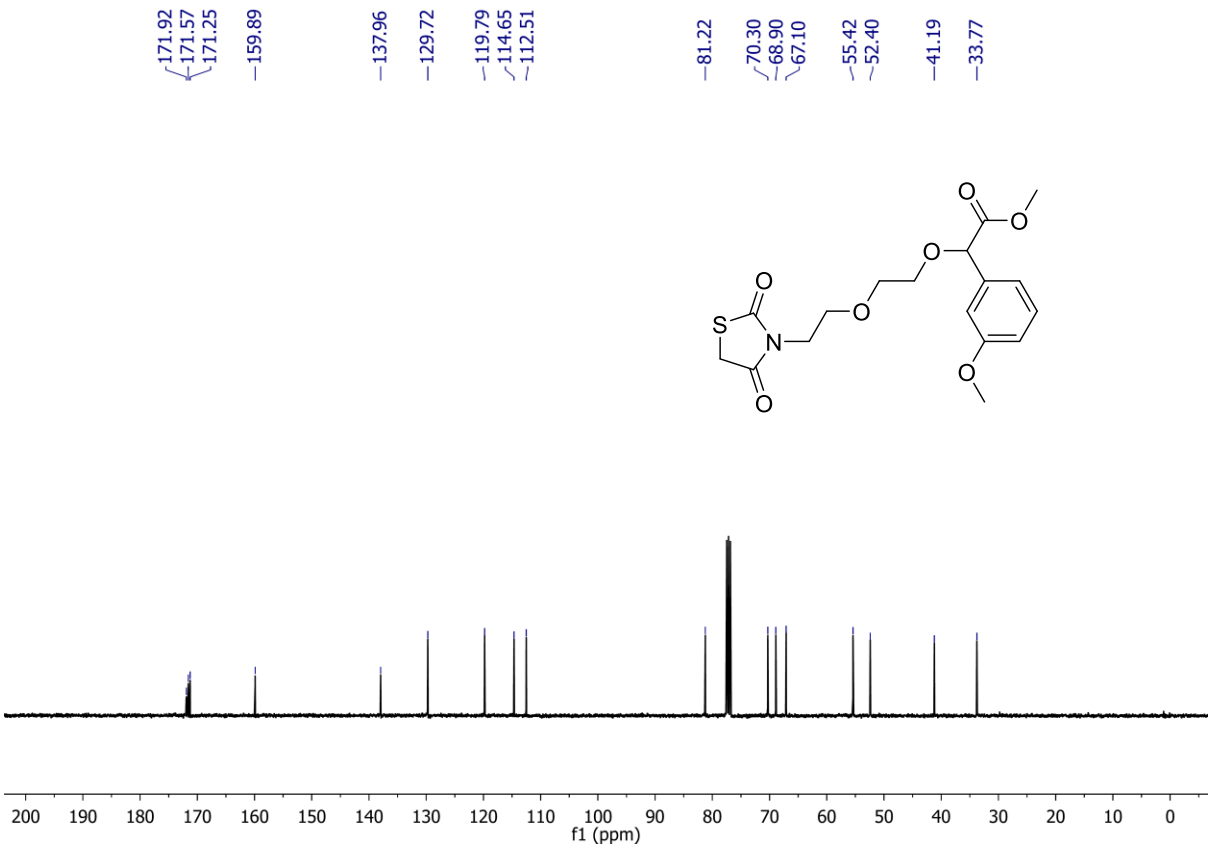
^{13}C NMR (400 MHz) of **6e** in $CDCl_3$



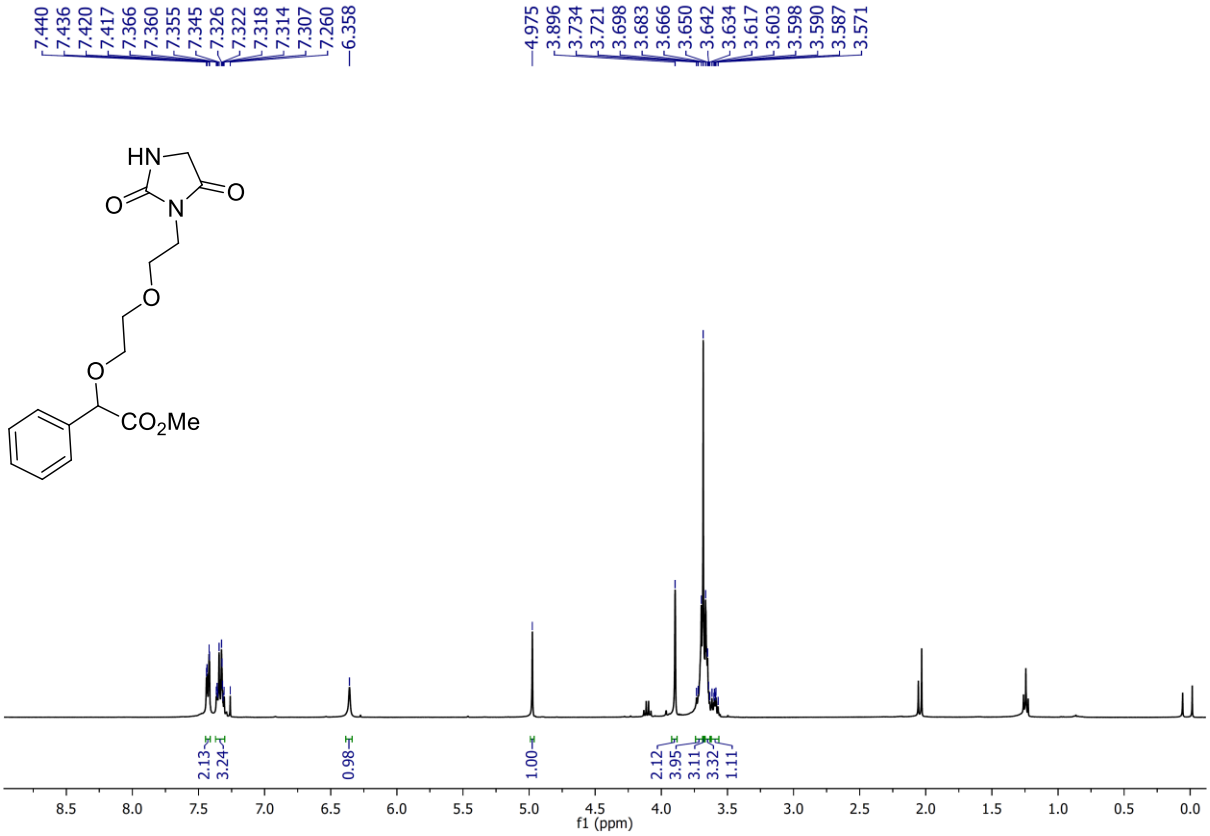
^{1}H NMR (400 MHz) of **6f** in $CDCl_3$



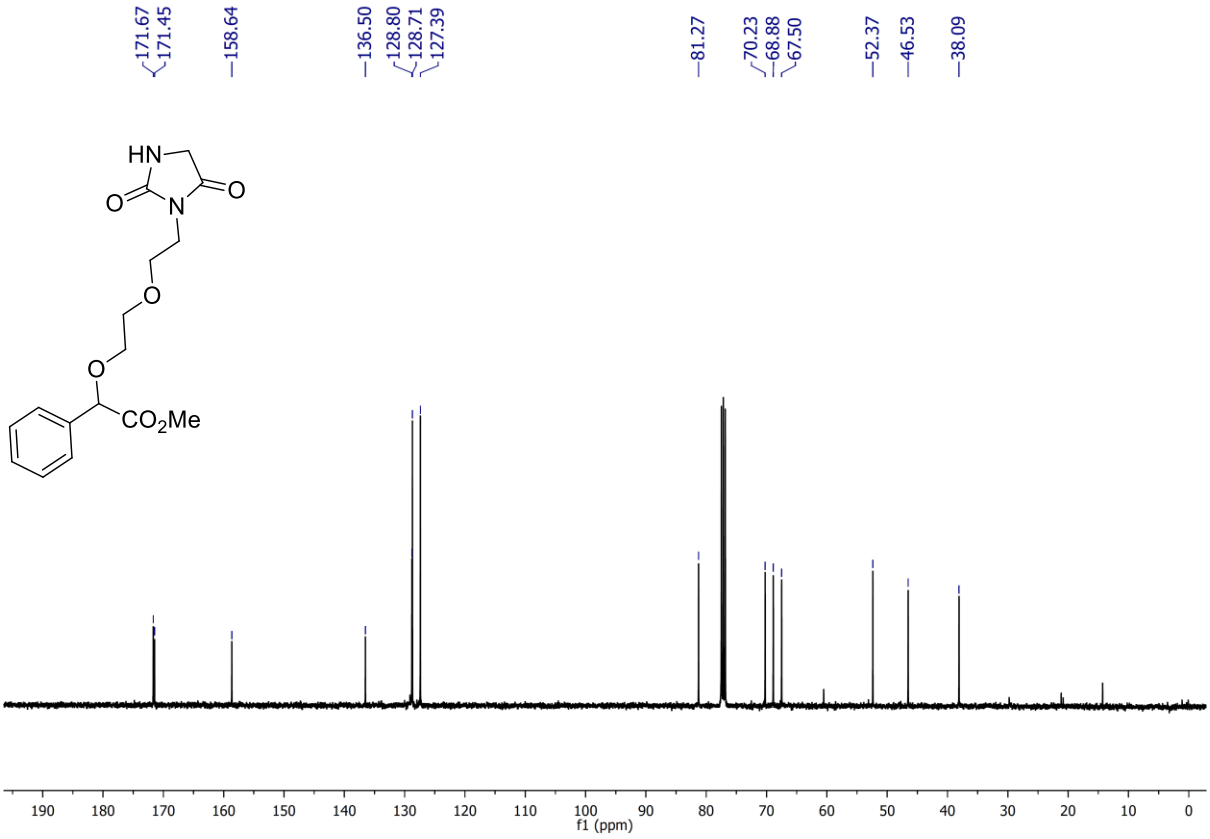
^{13}C NMR (400 MHz) of **6f** in $CDCl_3$



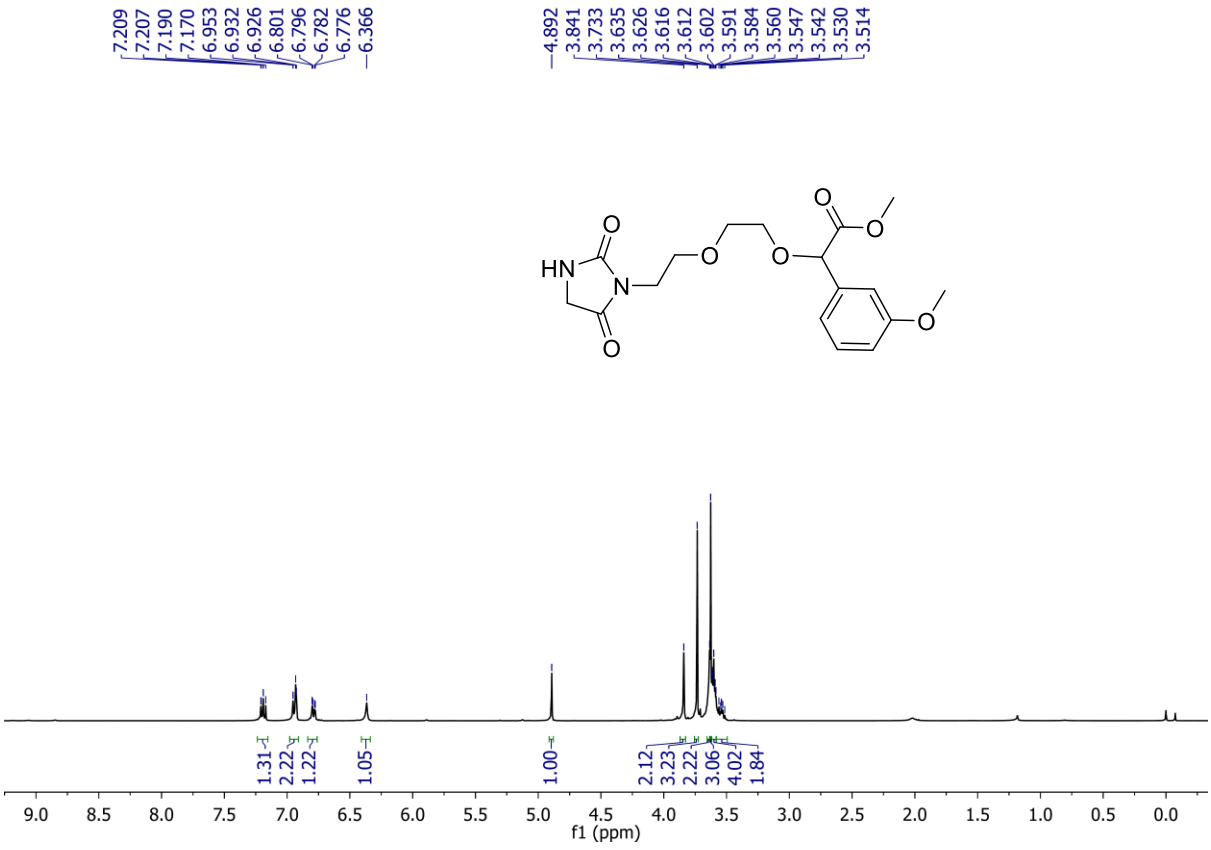
^{1}H NMR (400 MHz) of **7a** in $CDCl_3$



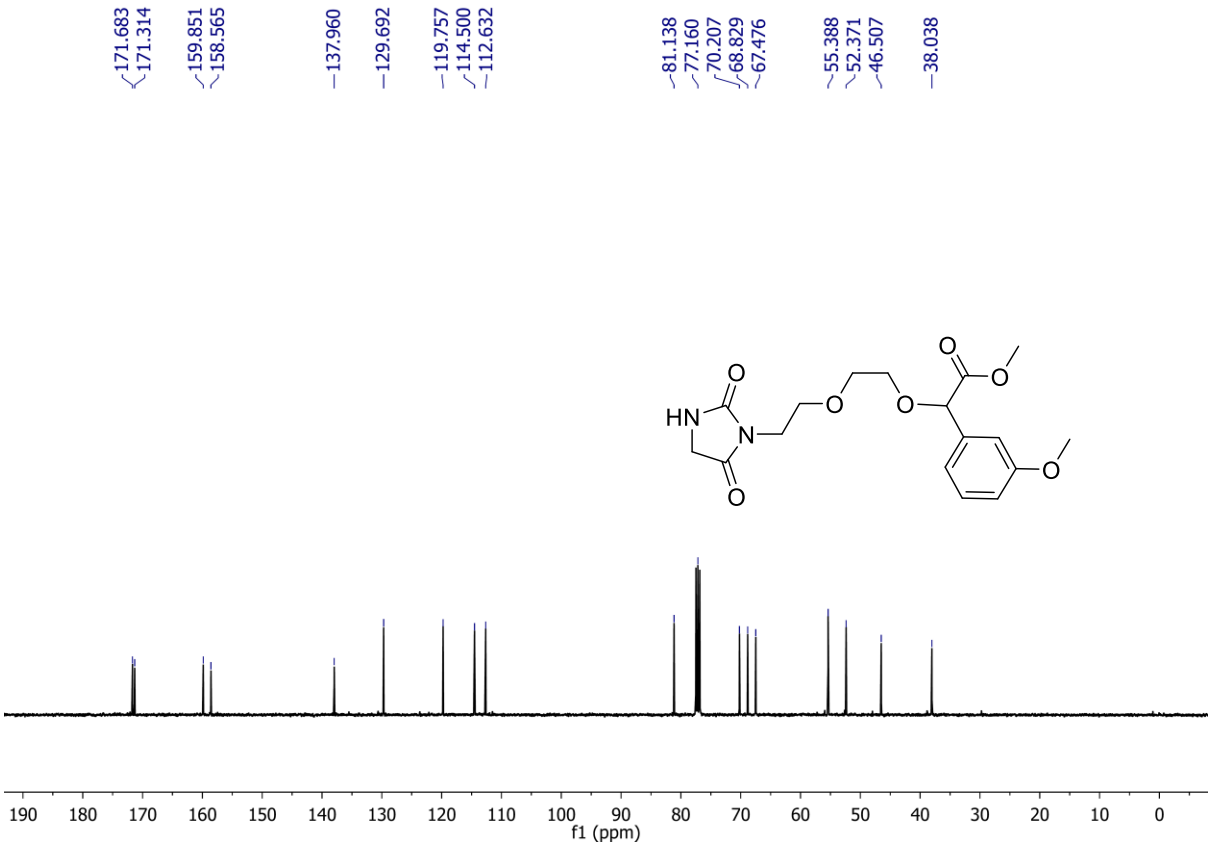
^{13}C NMR (400 MHz) of **7a** in $CDCl_3$



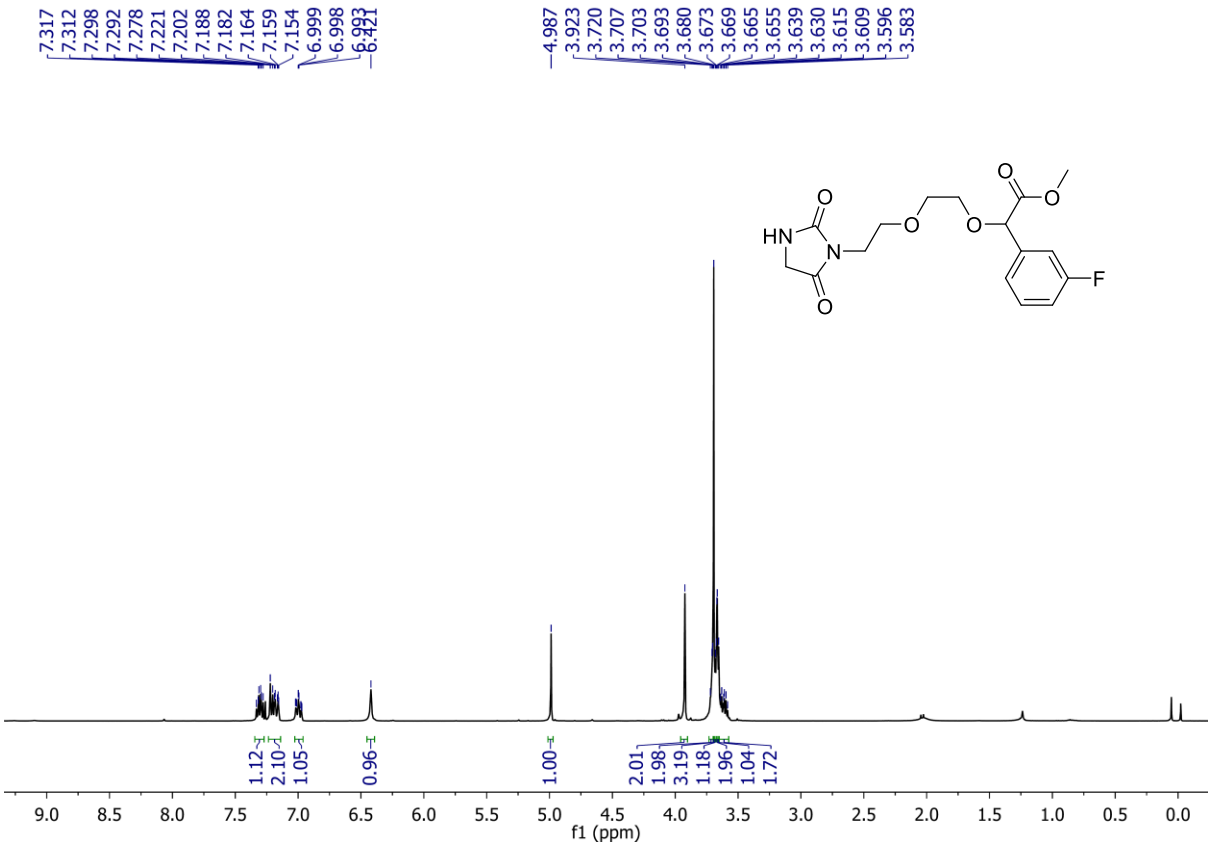
^{1}H NMR (400 MHz) of **7b** in $CDCl_3$



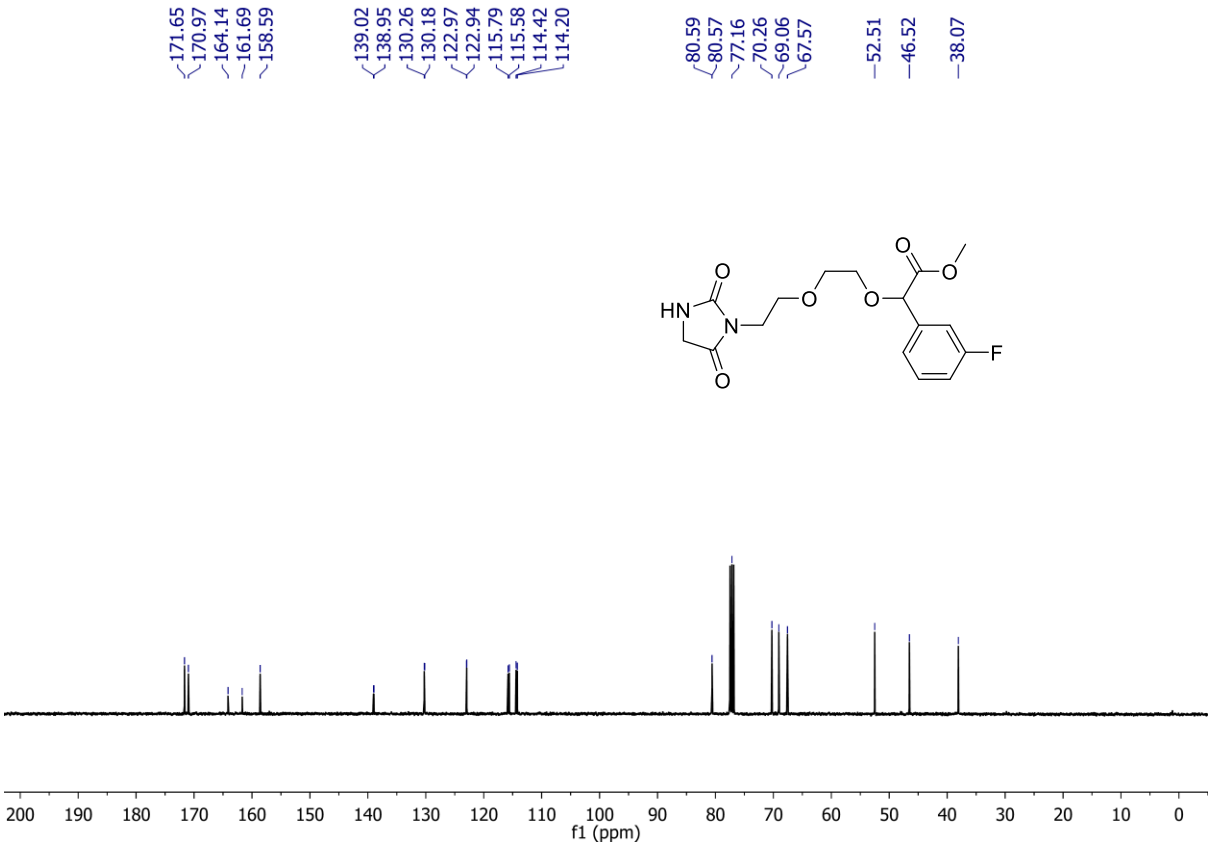
^{13}C NMR (400 MHz) of **7b** in $CDCl_3$



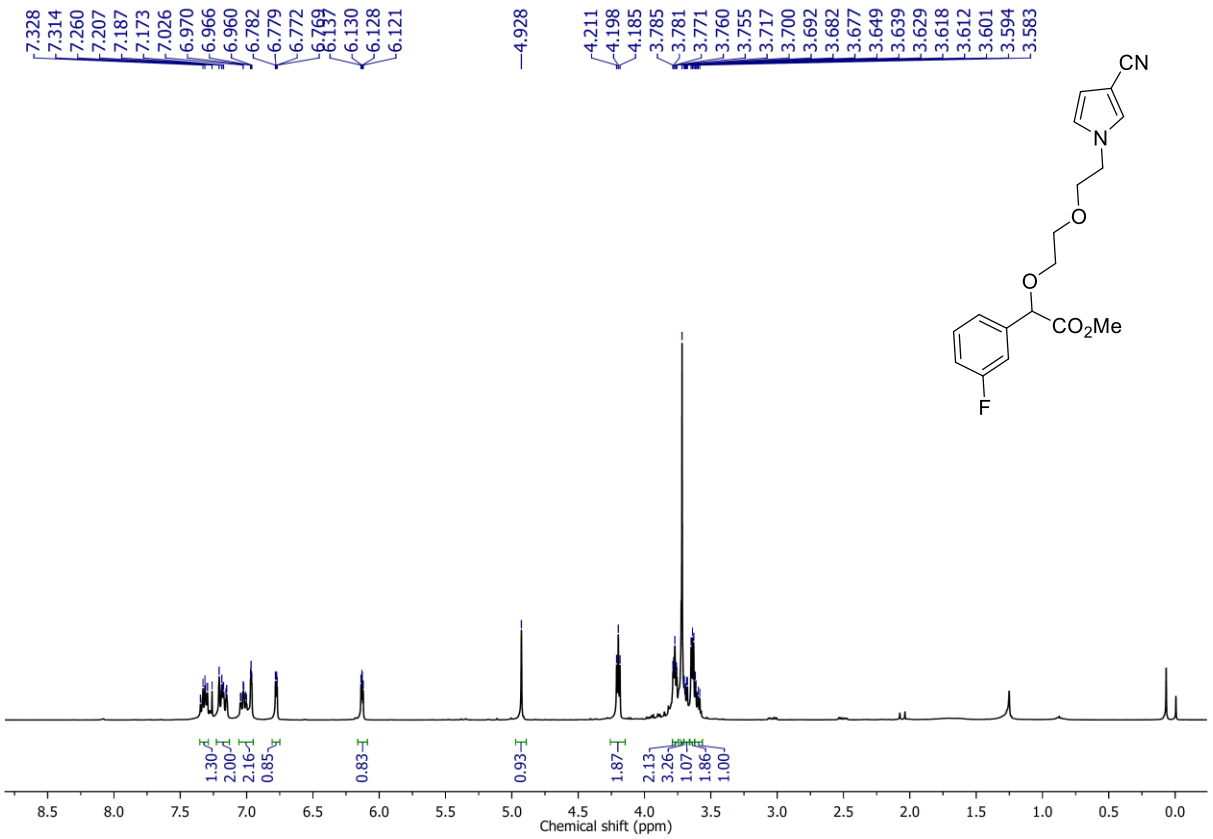
^{1}H NMR (400 MHz) of **7c** in $CDCl_3$



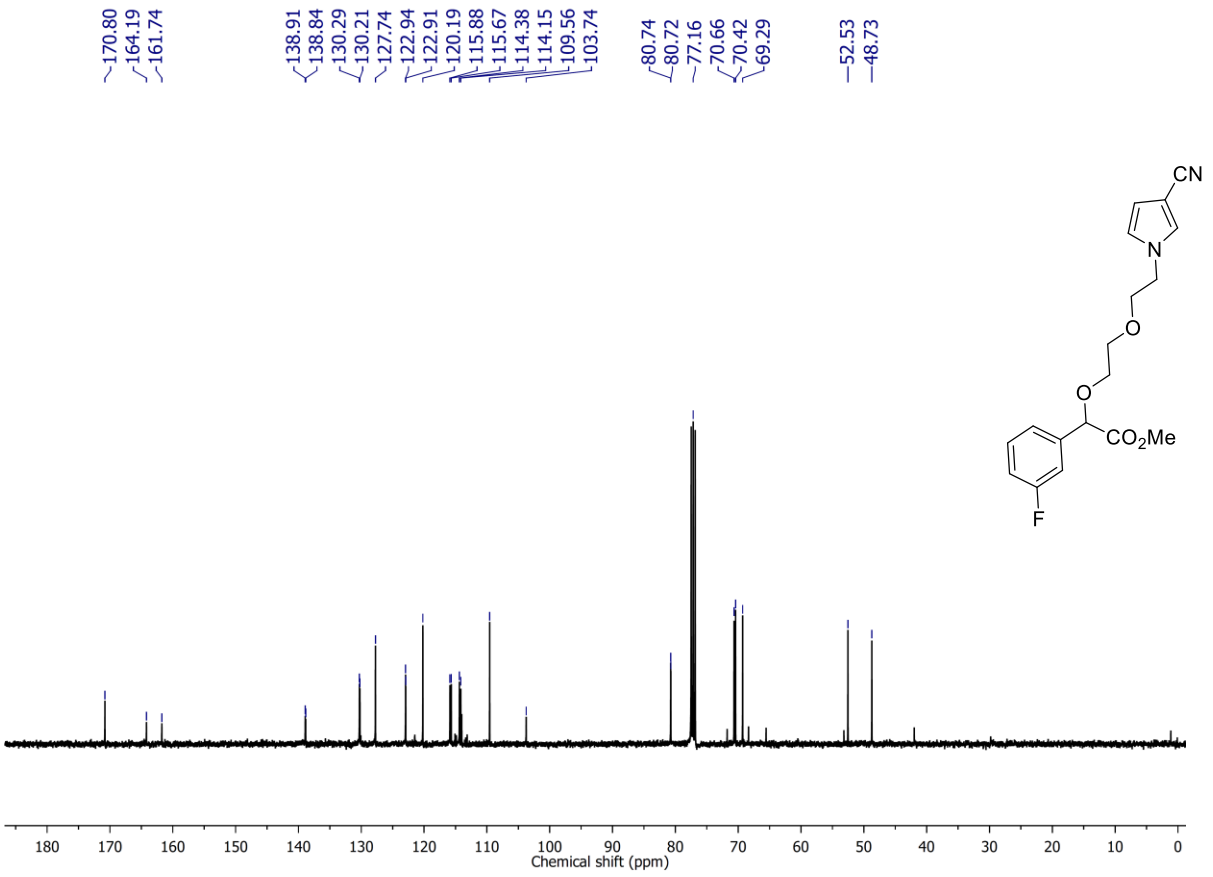
^{13}C NMR (400 MHz) of **7c** in $CDCl_3$



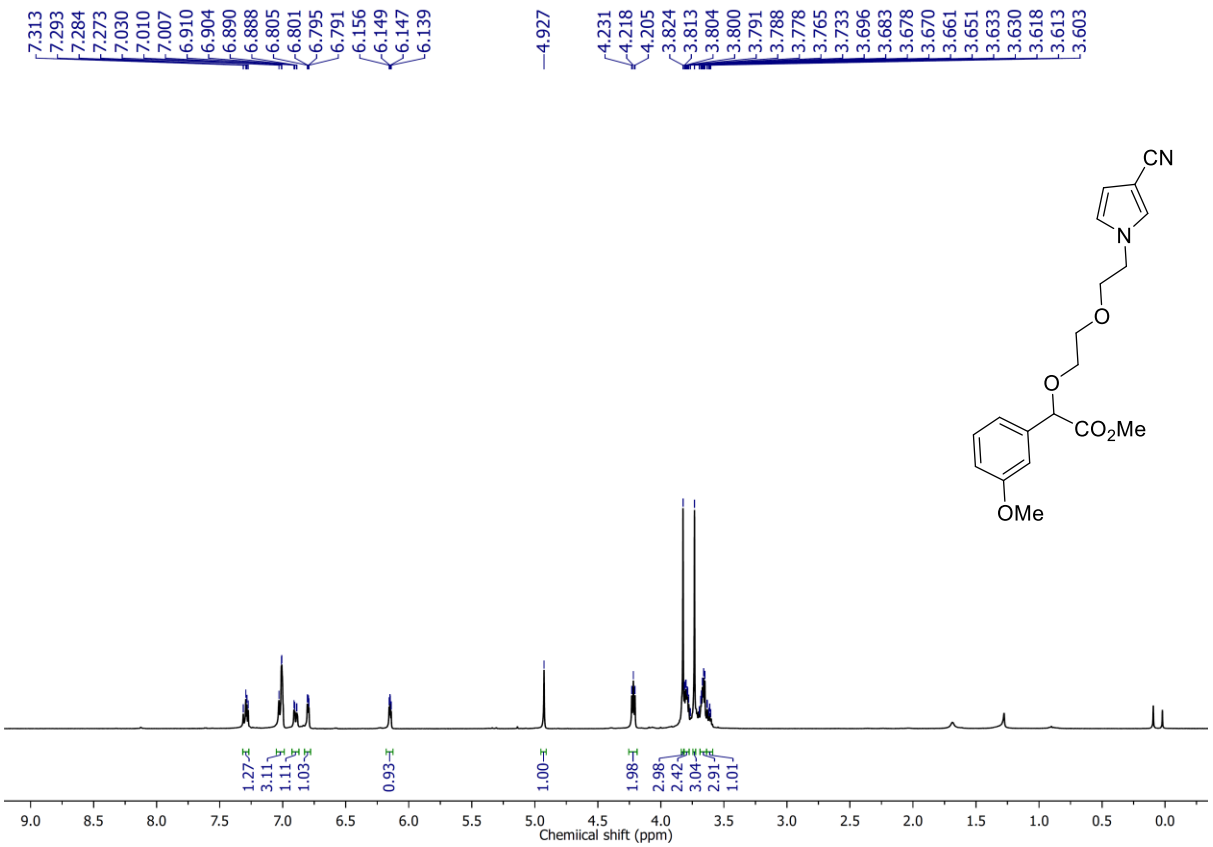
^{1}H NMR (400 MHz) of **8a** in $CDCl_3$



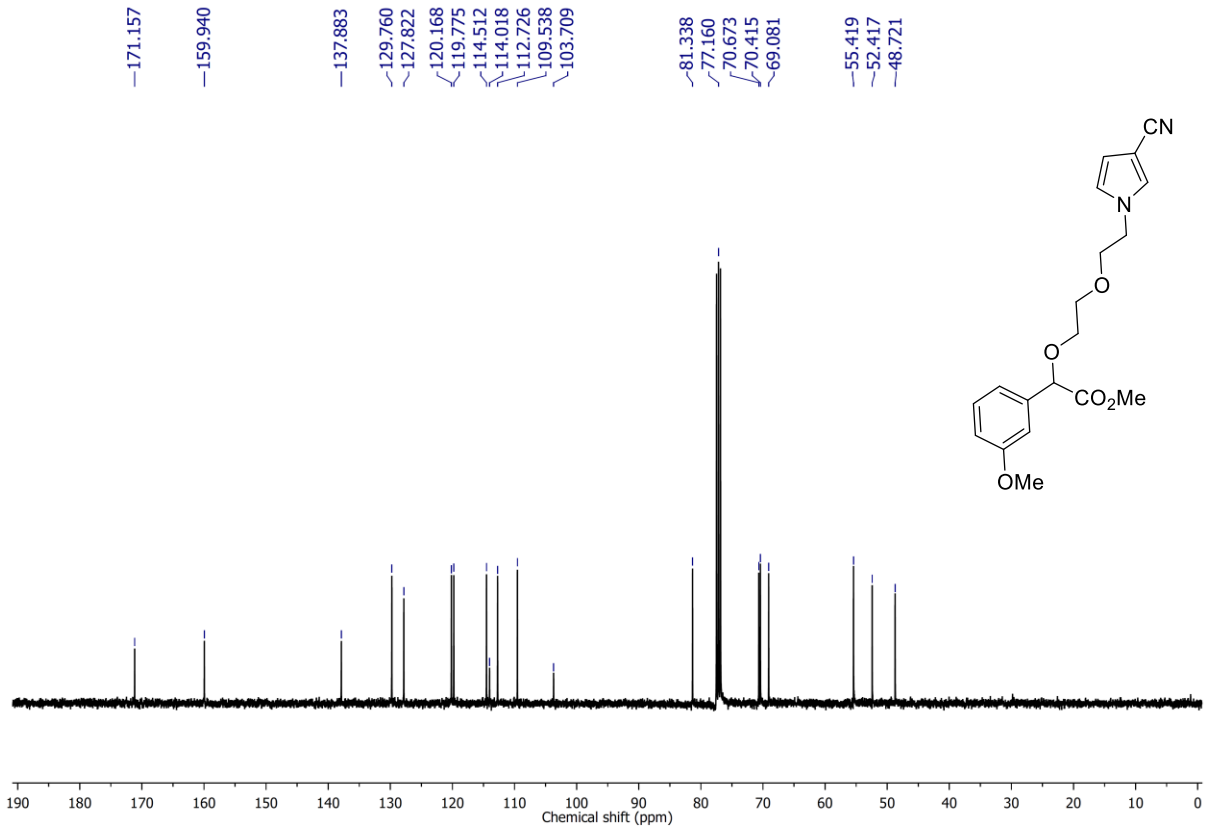
^{13}C NMR (400 MHz) of **8a** in $CDCl_3$



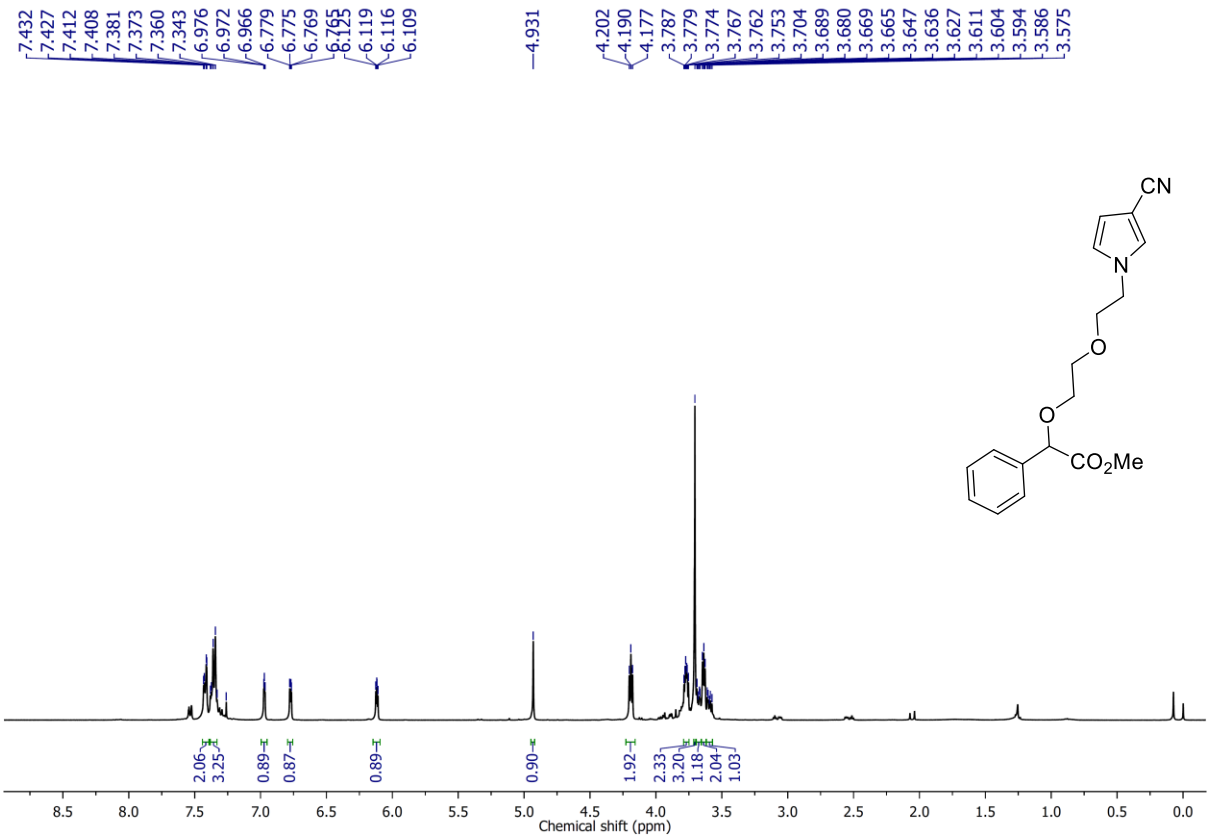
^{1}H NMR (400 MHz) of **8b** in $CDCl_3$



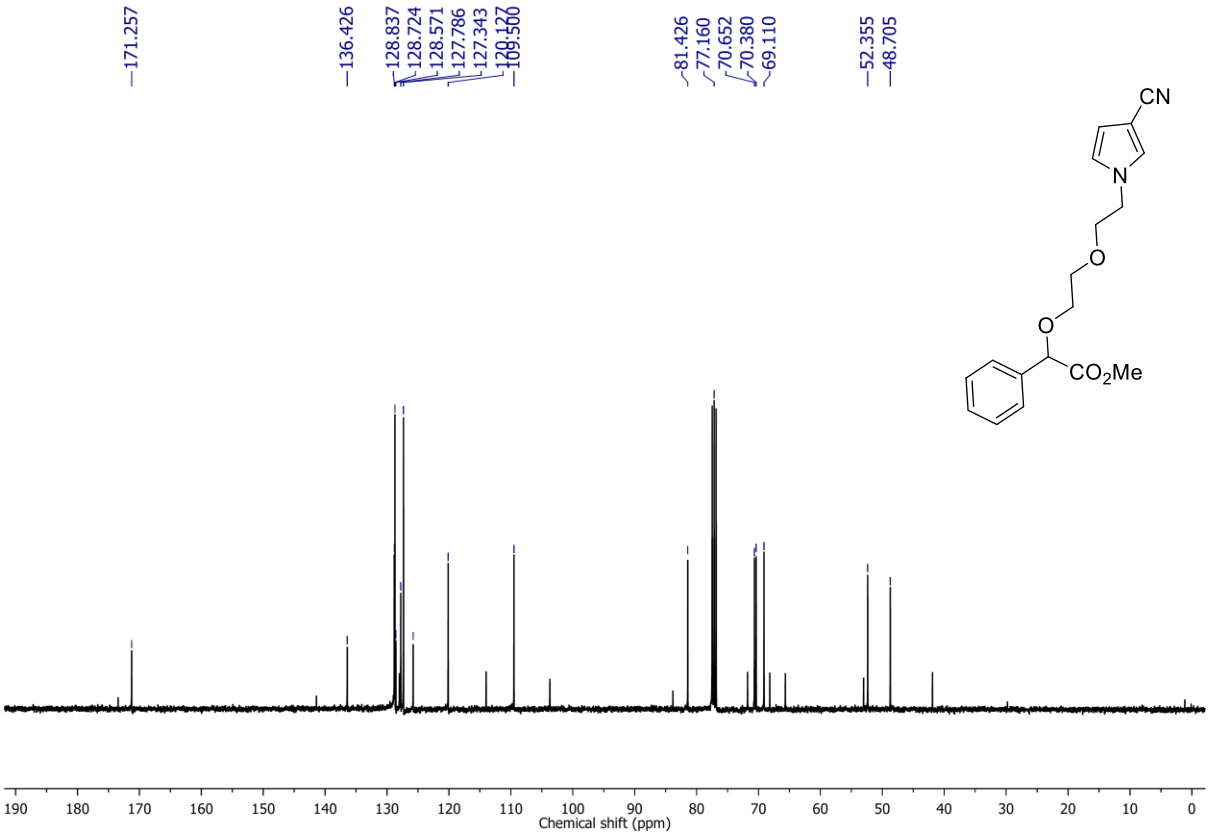
^{13}C NMR (400 MHz) of **8b** in $CDCl_3$



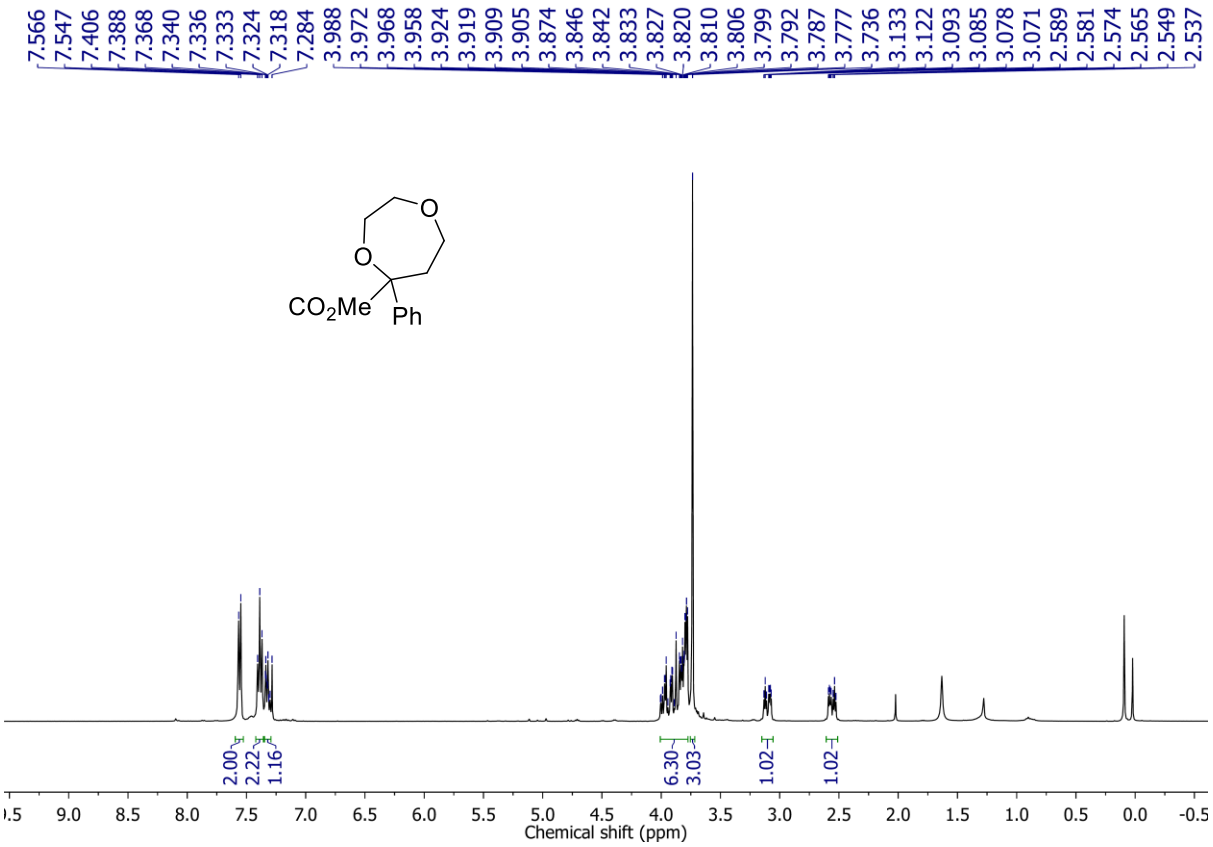
^{1}H NMR (400 MHz) of **8c** in $CDCl_3$



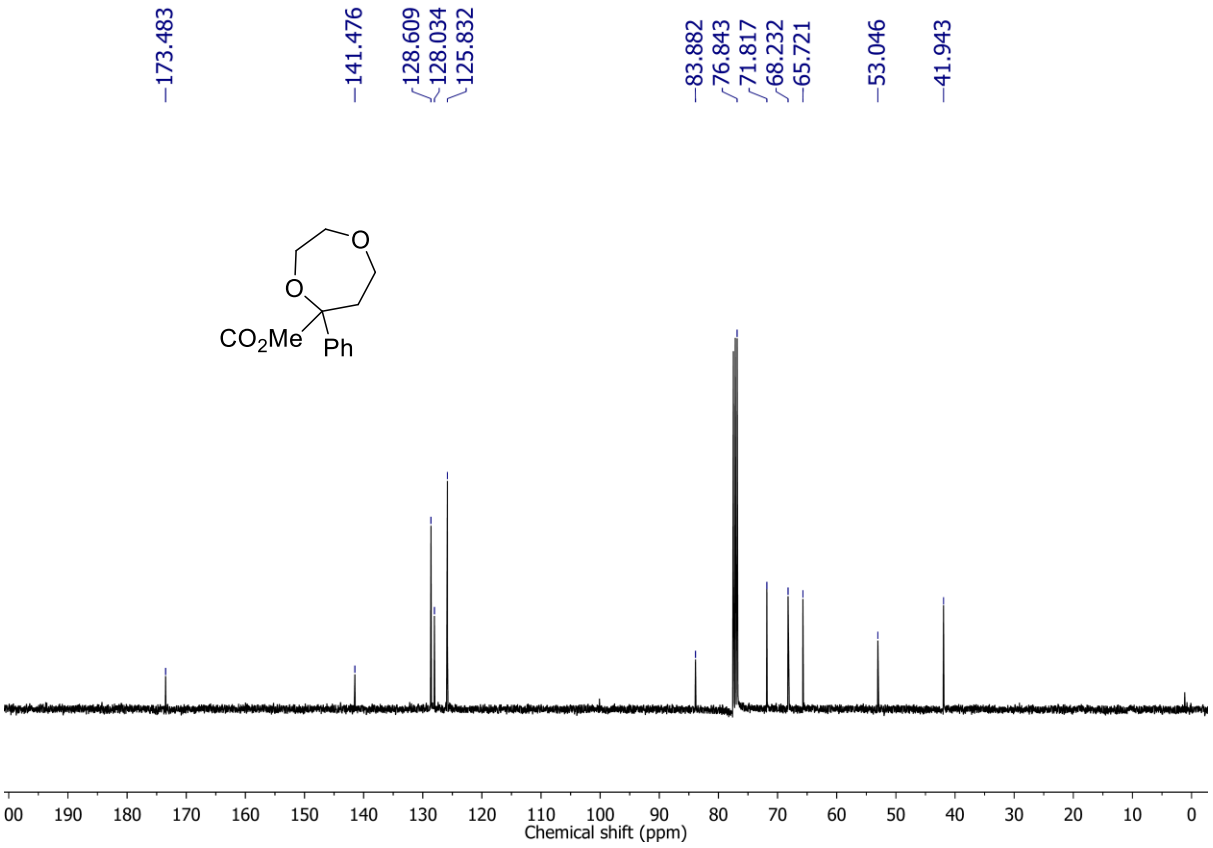
^{13}C NMR (400 MHz) of **8c** in $CDCl_3$



^{1}H NMR (400 Mz) of **9a** in $CDCl_3$



^{13}C NMR (400 MHz) of **9a** in $CDCl_3$



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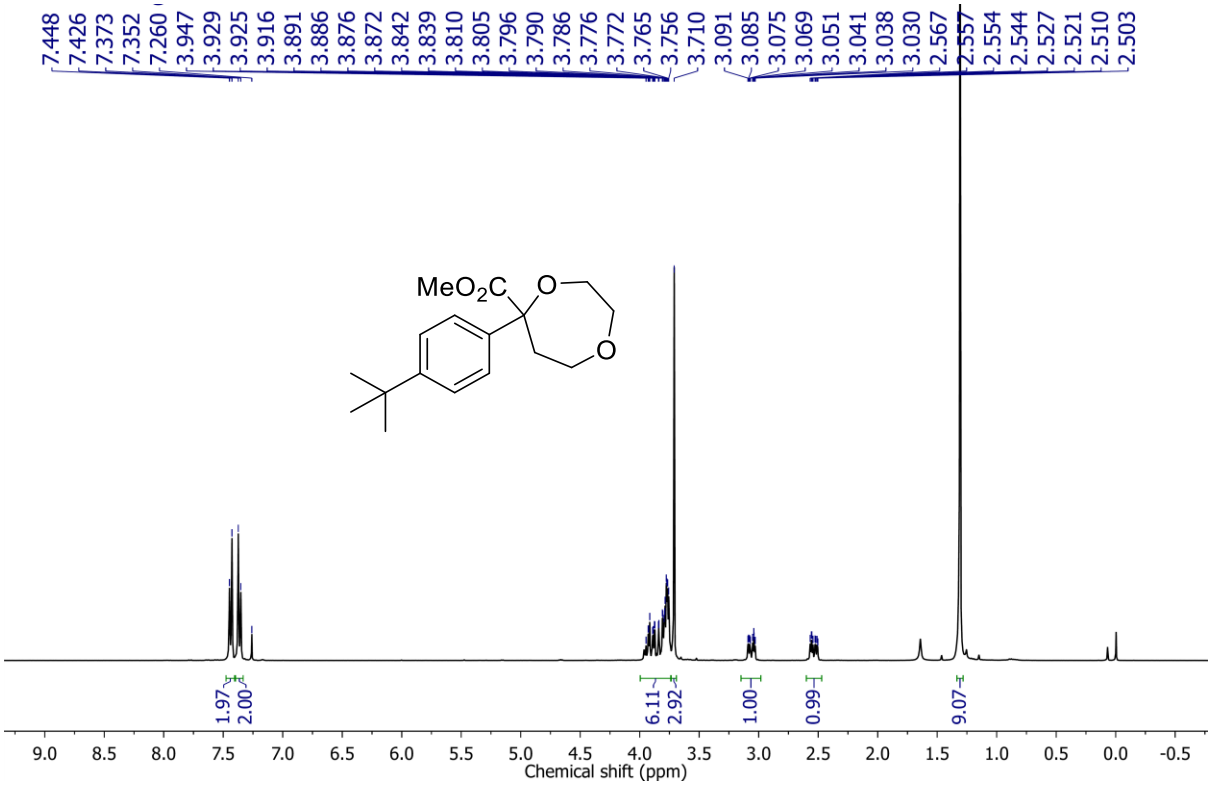
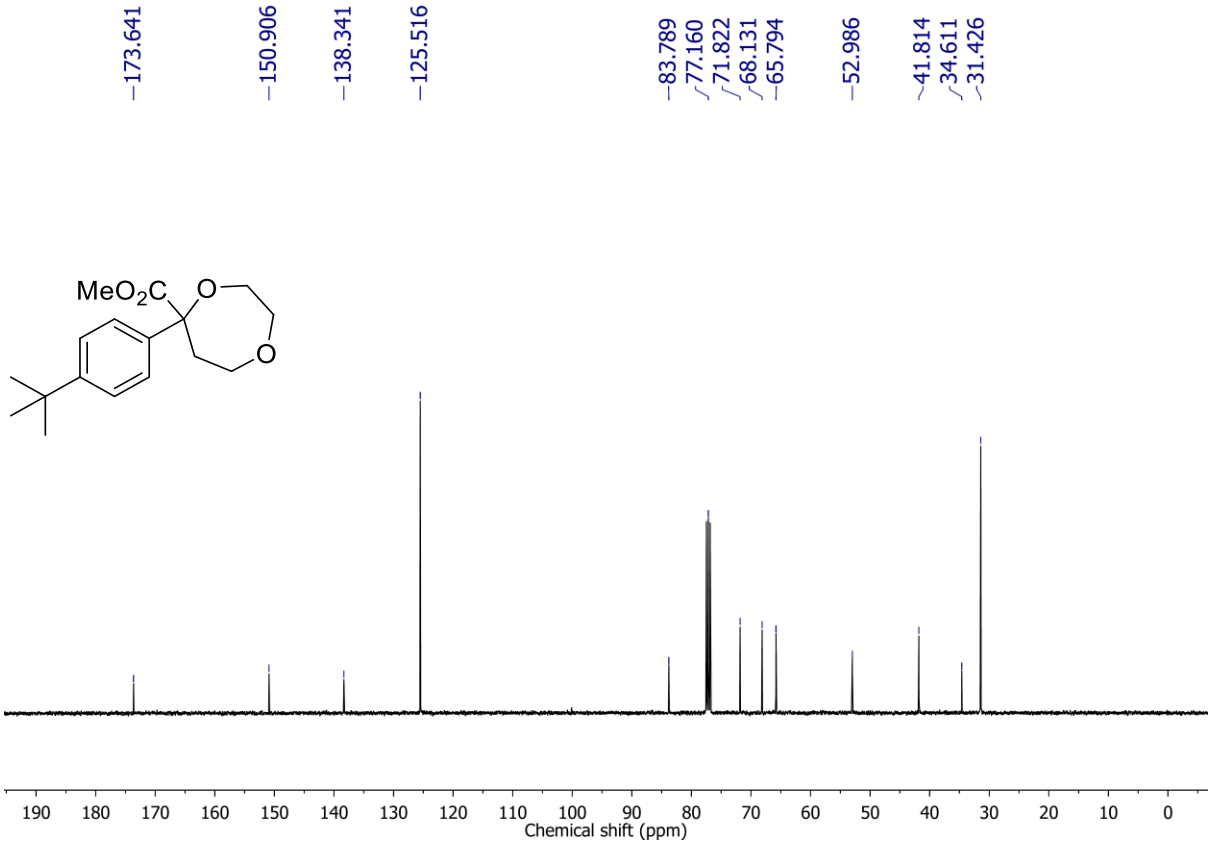
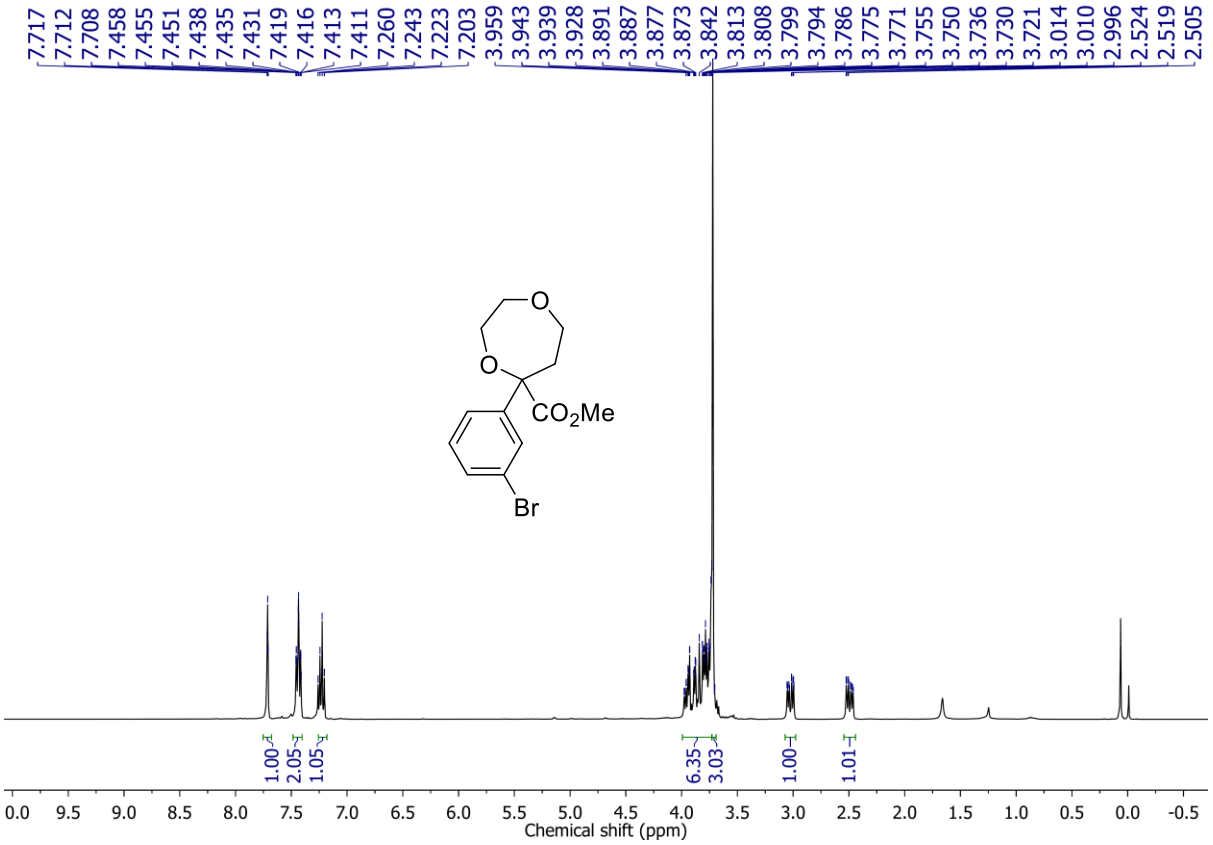


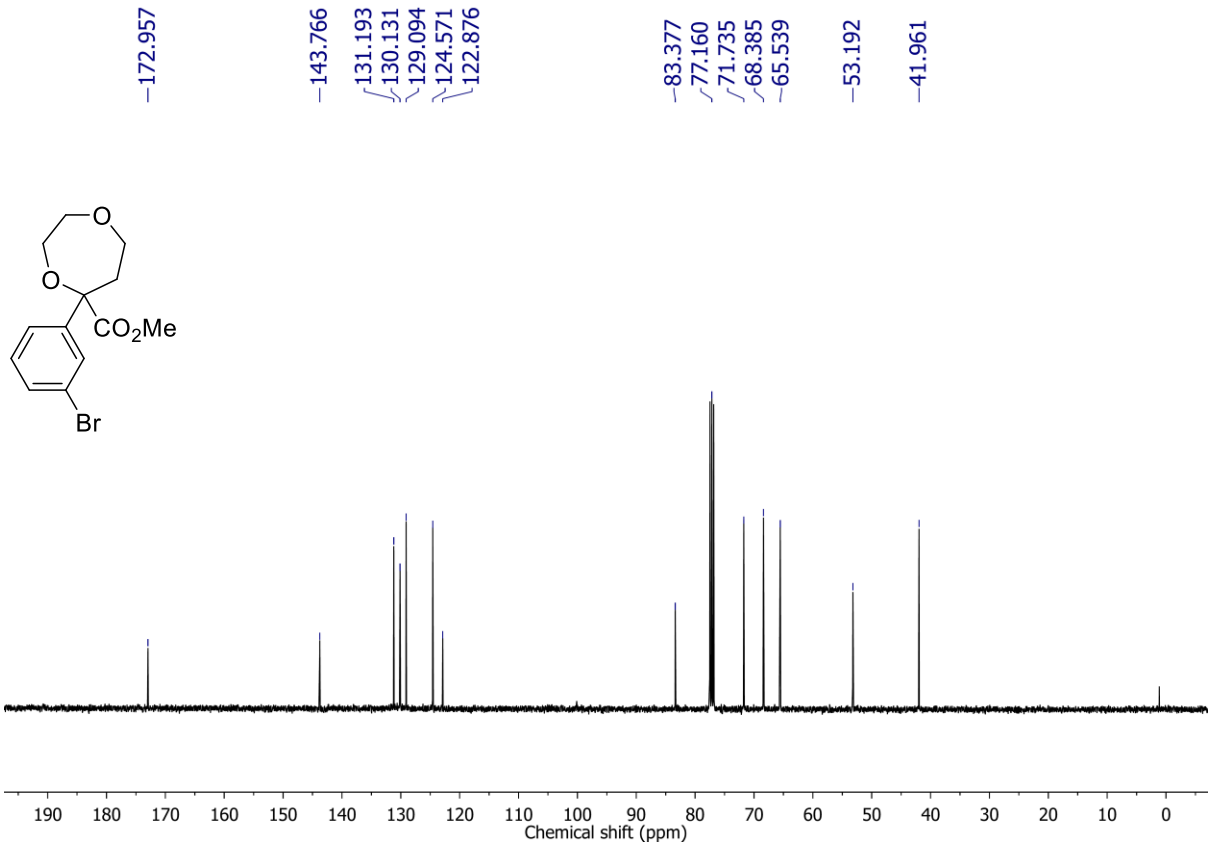
^{13}C NMR (400 MHz) of **9b** in $CDCl_3$



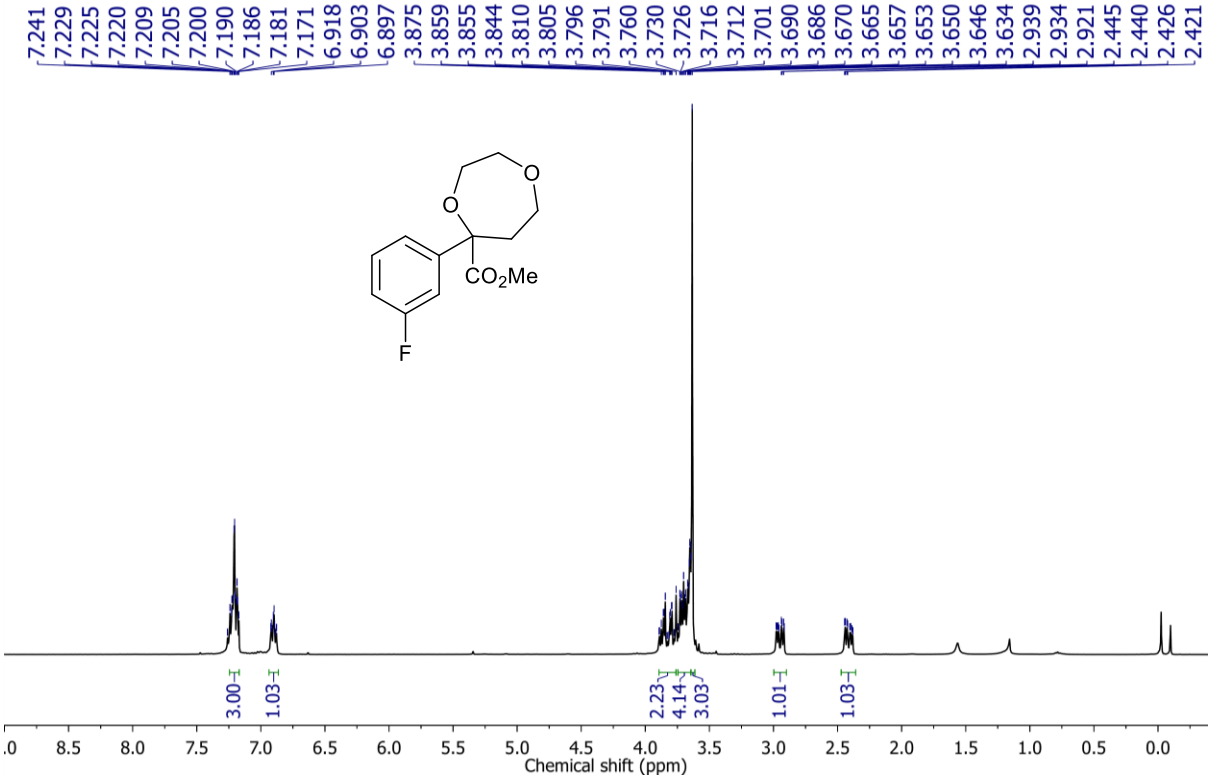
^{1}H NMR (400 MHz) of **9c** in $CDCl_3$



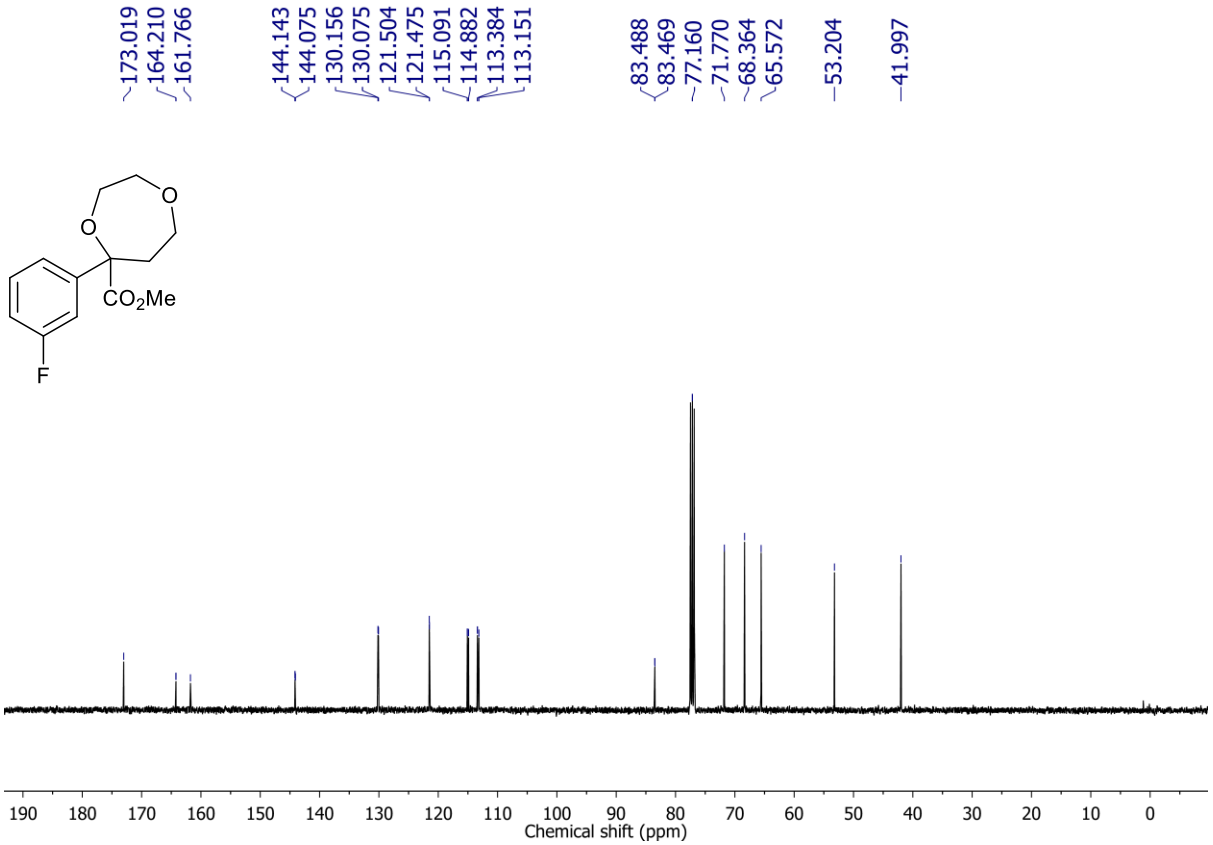
^{13}C NMR (400 MHz) of **9c** in $CDCl_3$



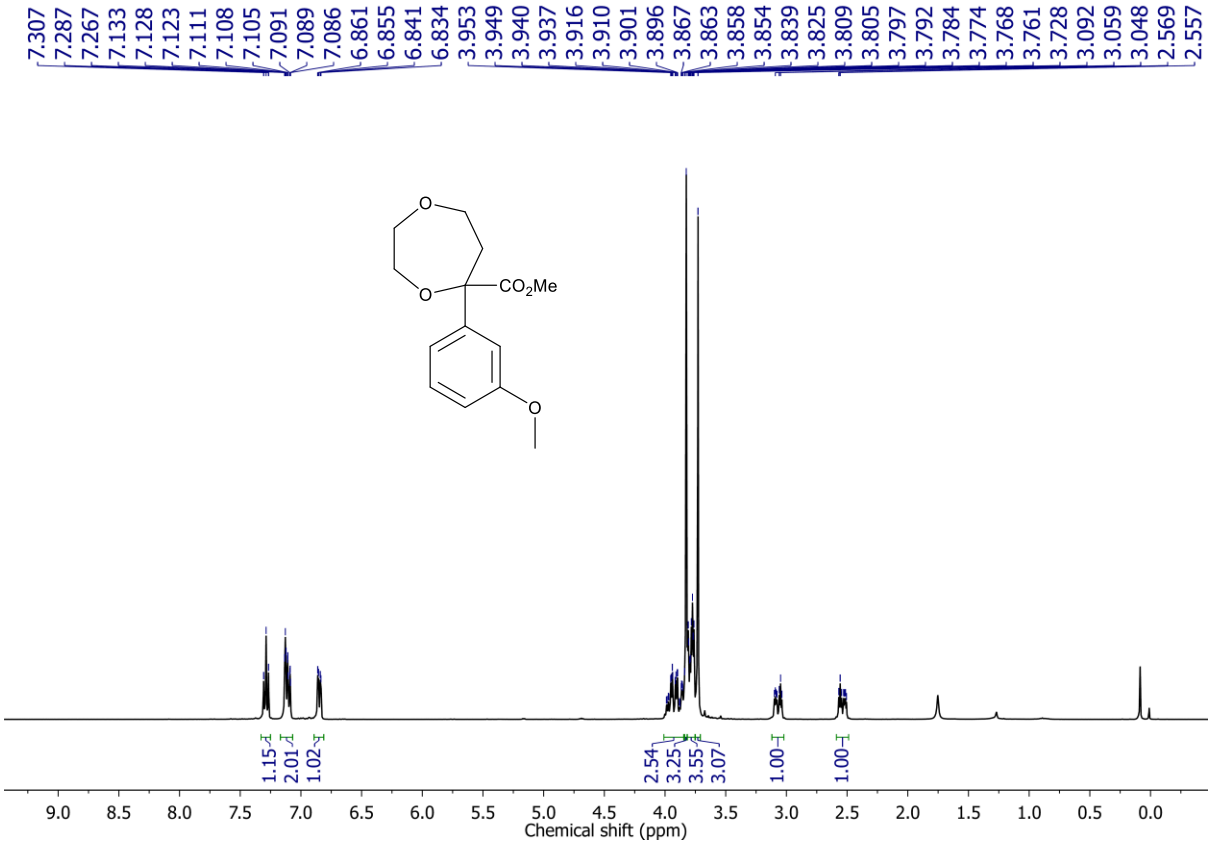
^{1}H NMR (400 MHz) of **9d** in $CDCl_3$



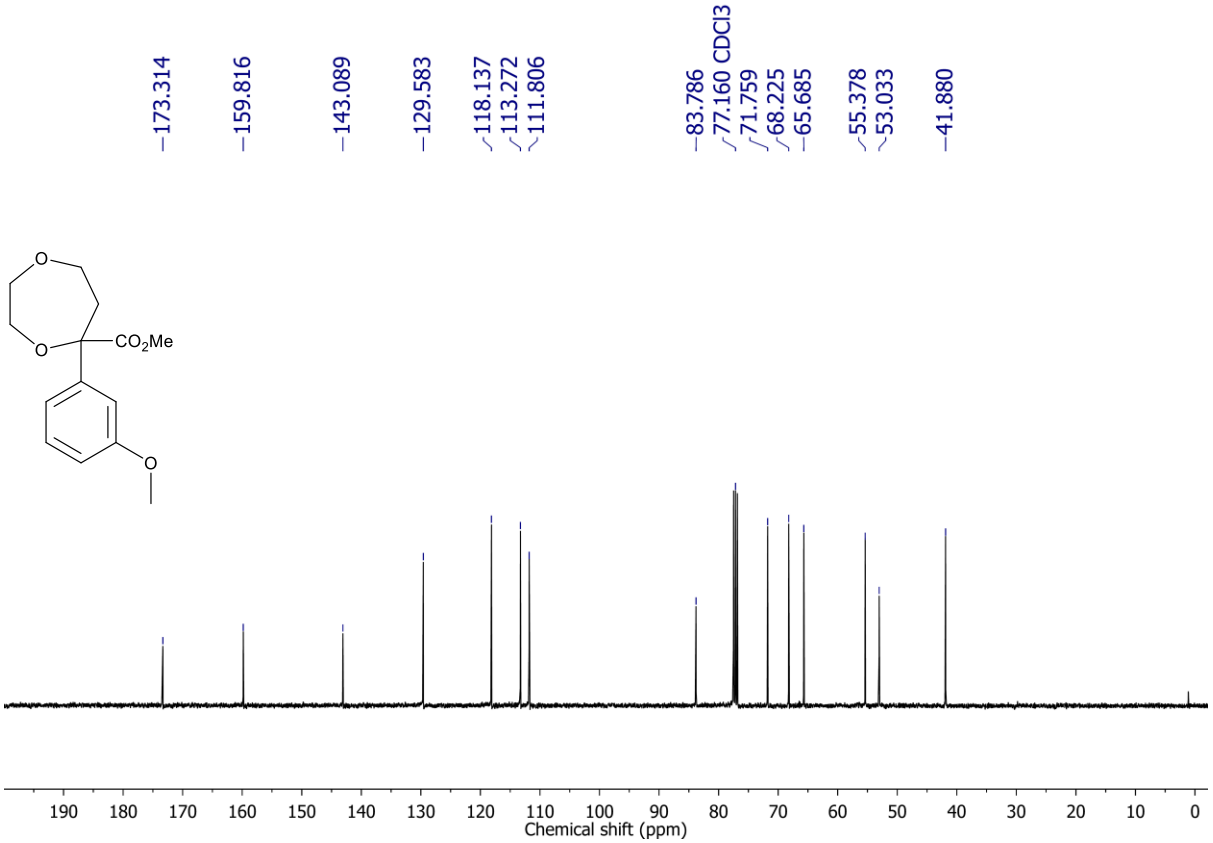
^{13}C NMR (400 MHz) of **9d** in $CDCl_3$



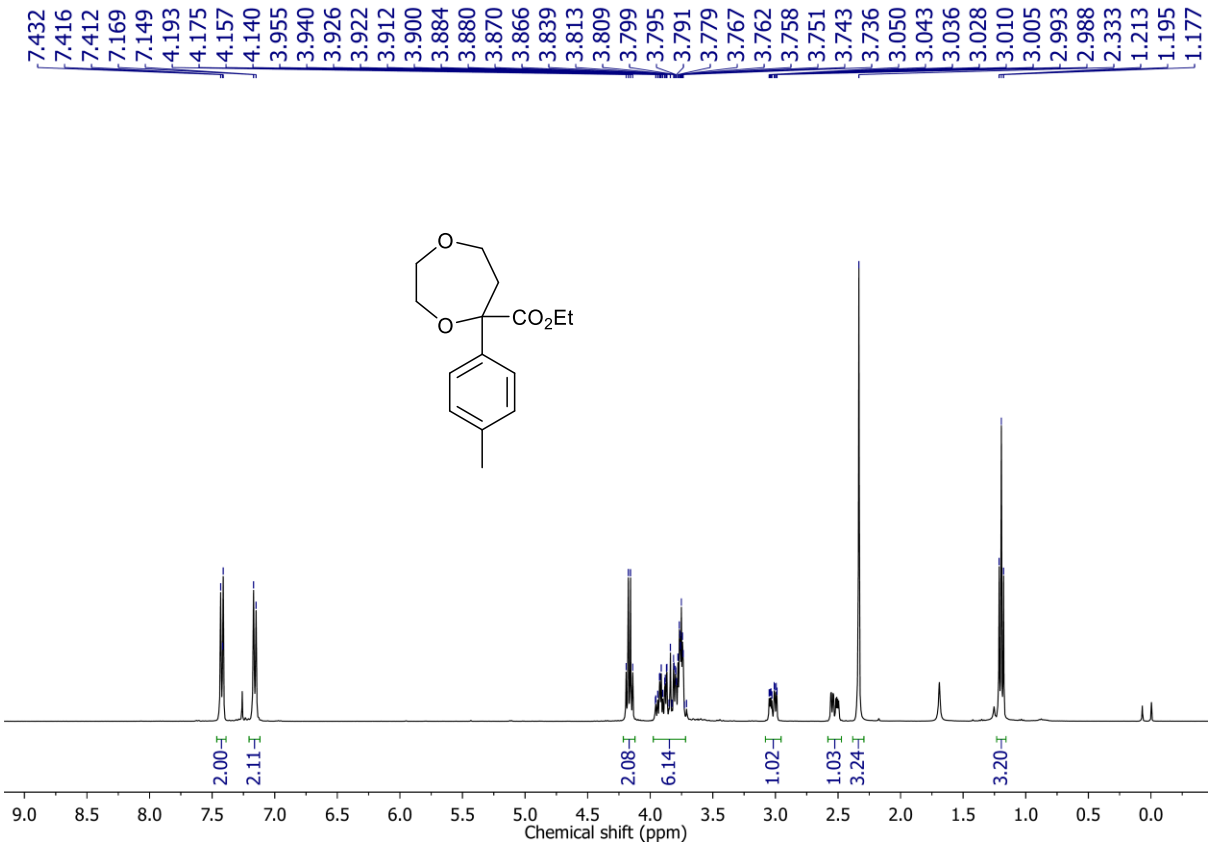
^{1}H NMR (400 MHz) of **9e** in $CDCl_3$



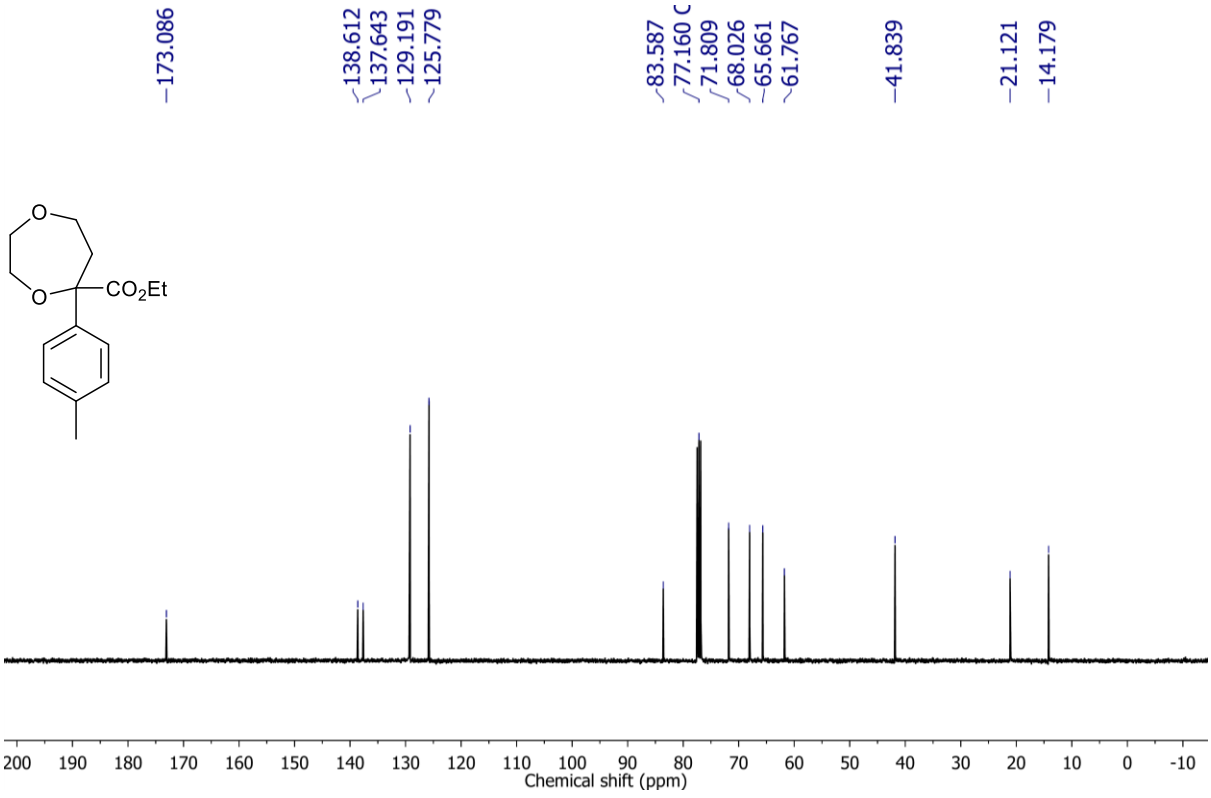
^{13}C NMR (400 MHz) of **9e** in $CDCl_3$



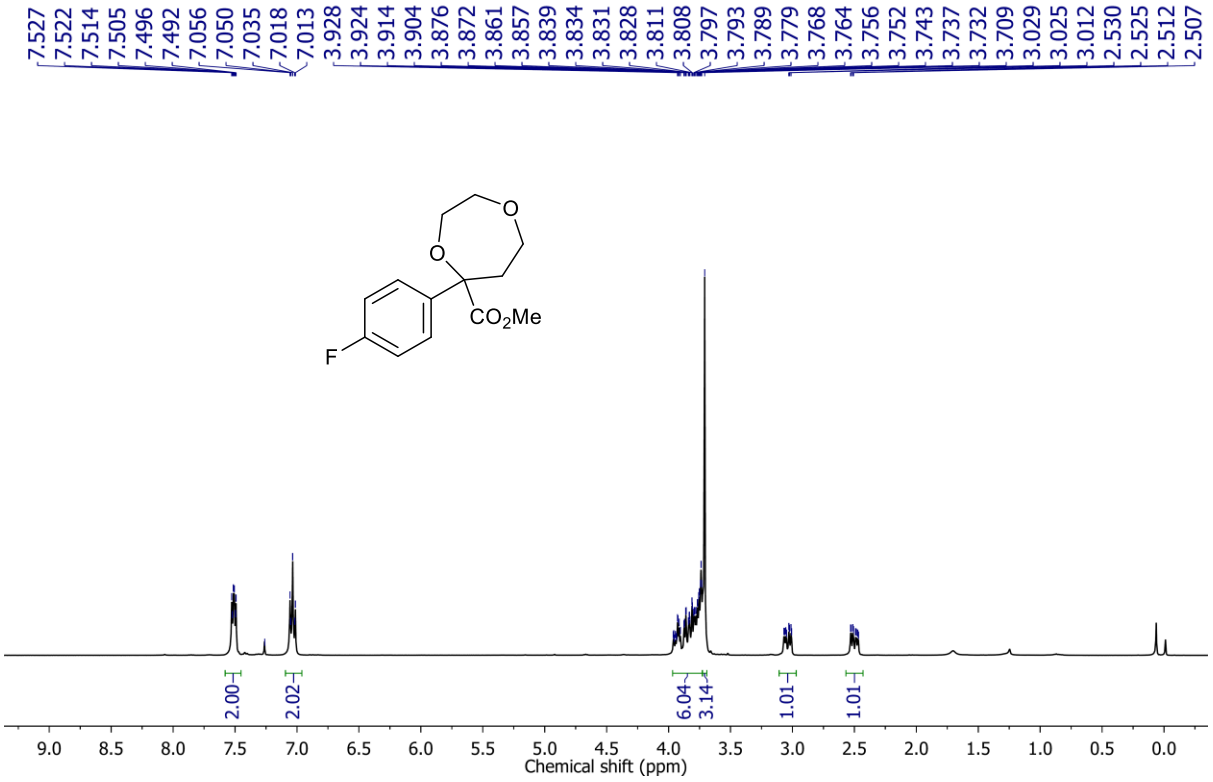
^{1}H NMR (400 MHz) of **9f** in $CDCl_3$



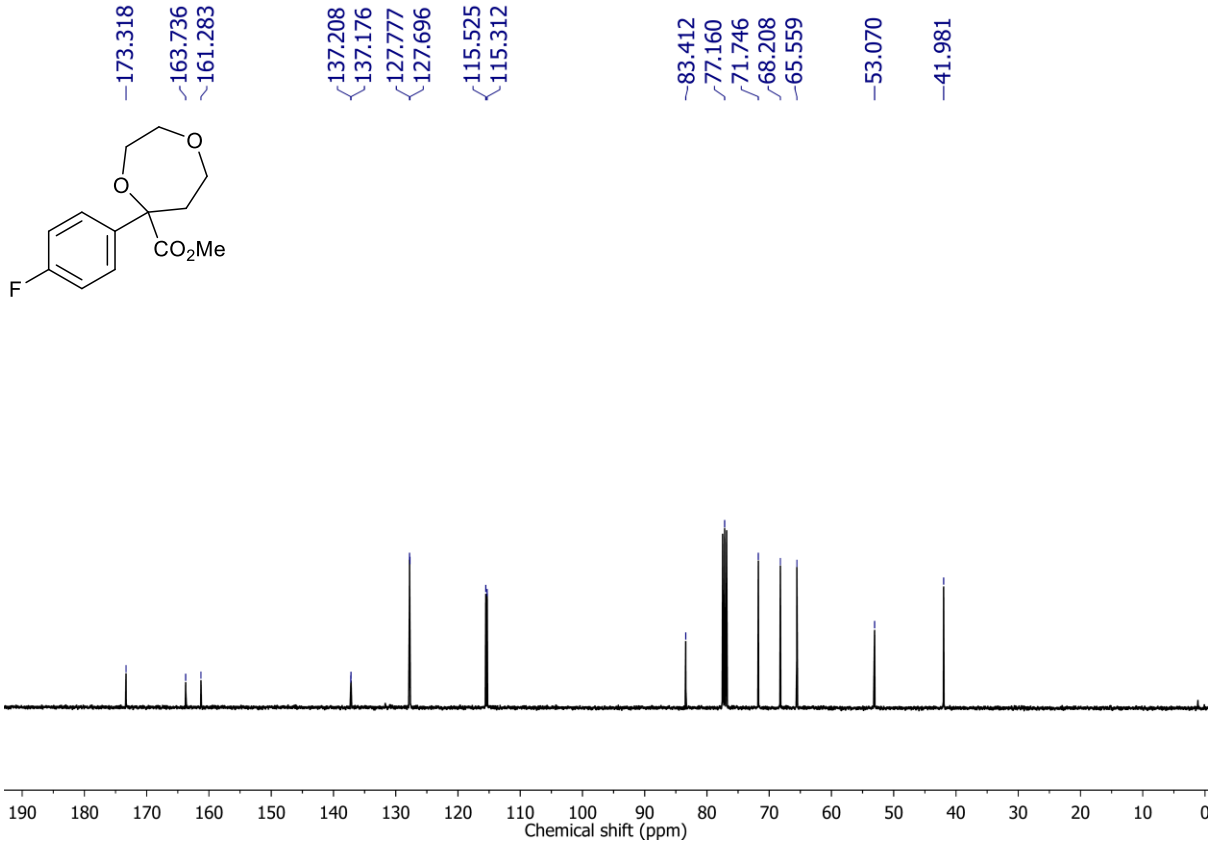
^{13}C NMR (400 MHz) of **9f** in $CDCl_3$



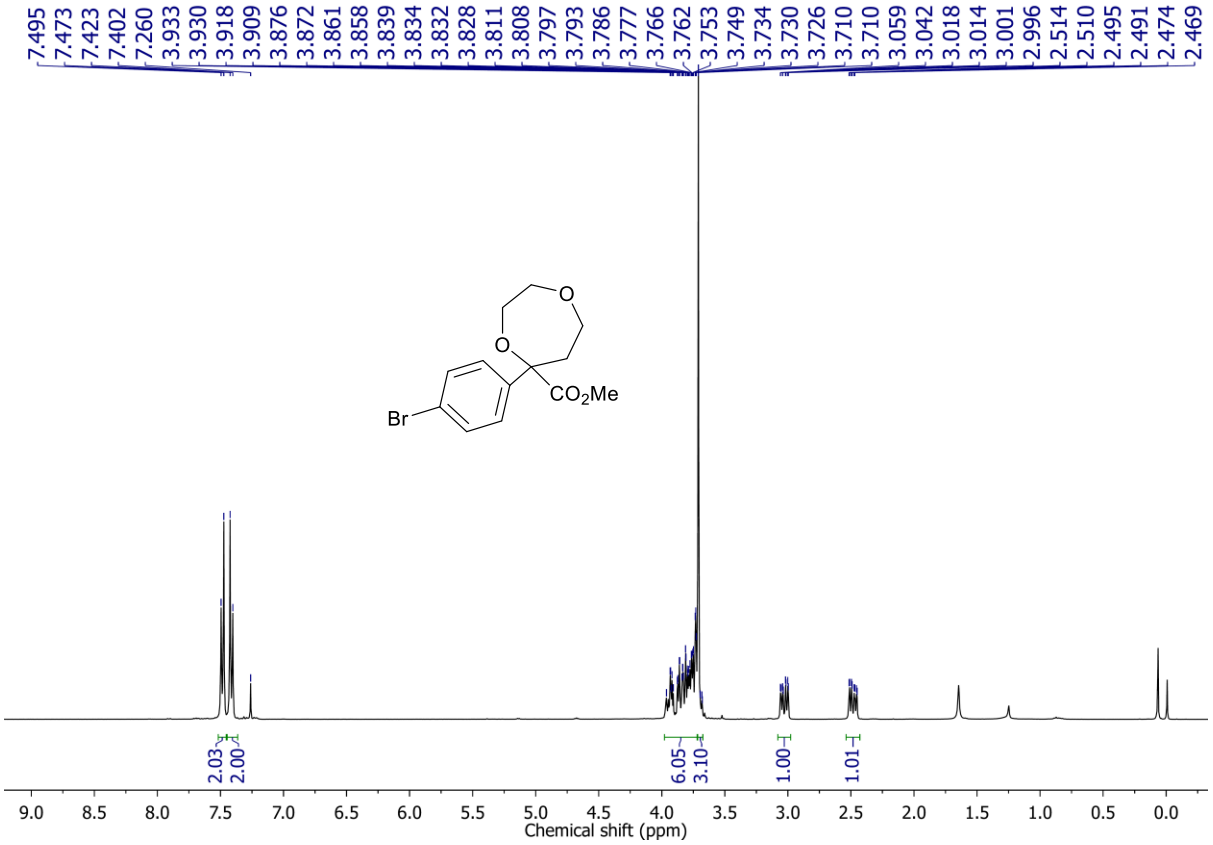
^{1}H NMR (400 MHz) of **9g** in $CDCl_3$



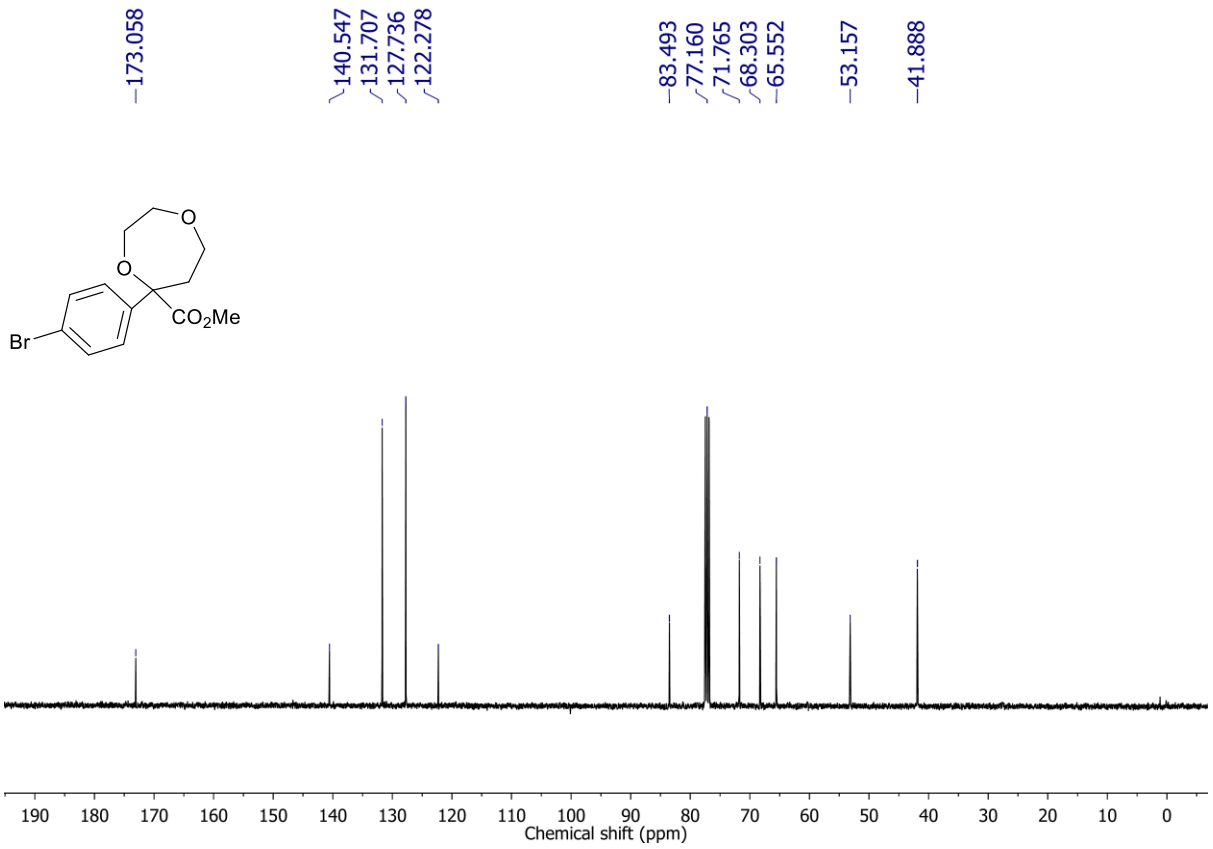
^{13}C NMR (400 MHz) of **9g** in $CDCl_3$



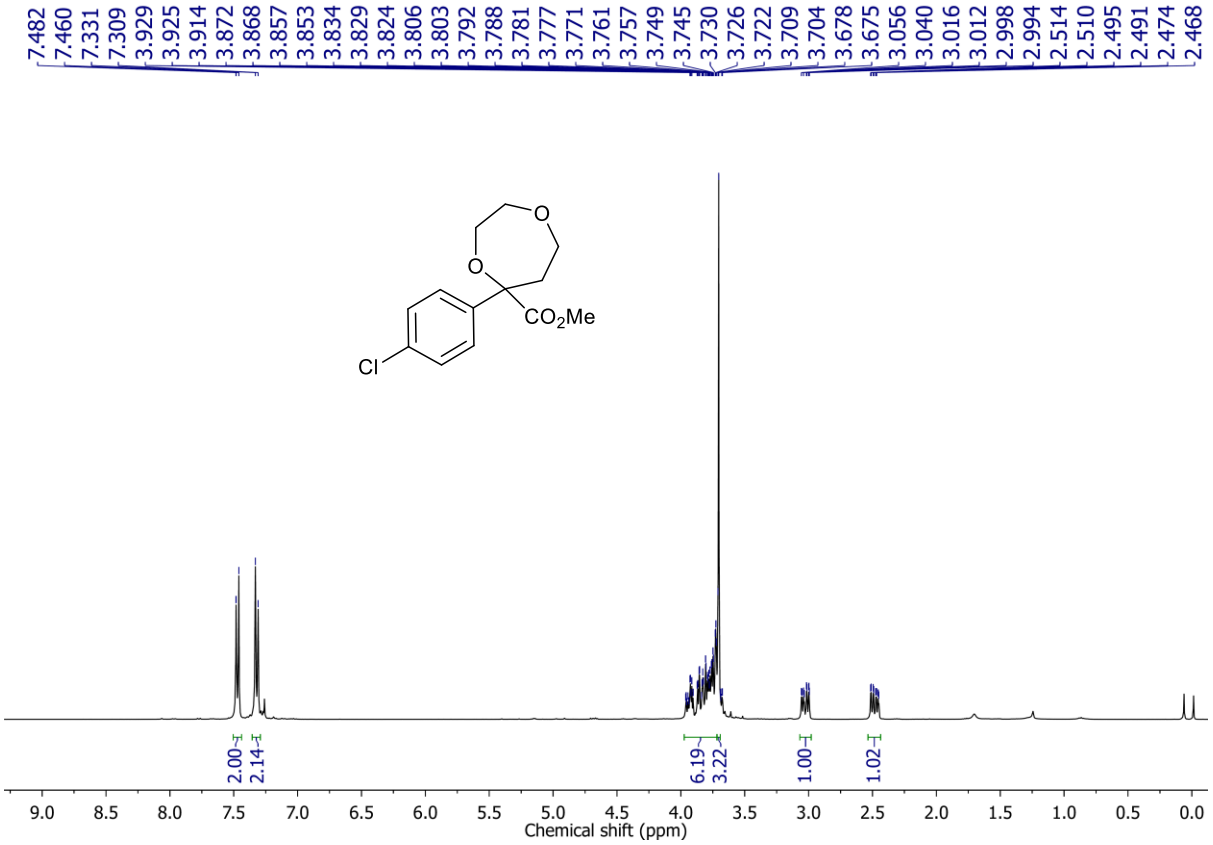
^{1}H NMR (400 MHz) of **9h** in $CDCl_3$



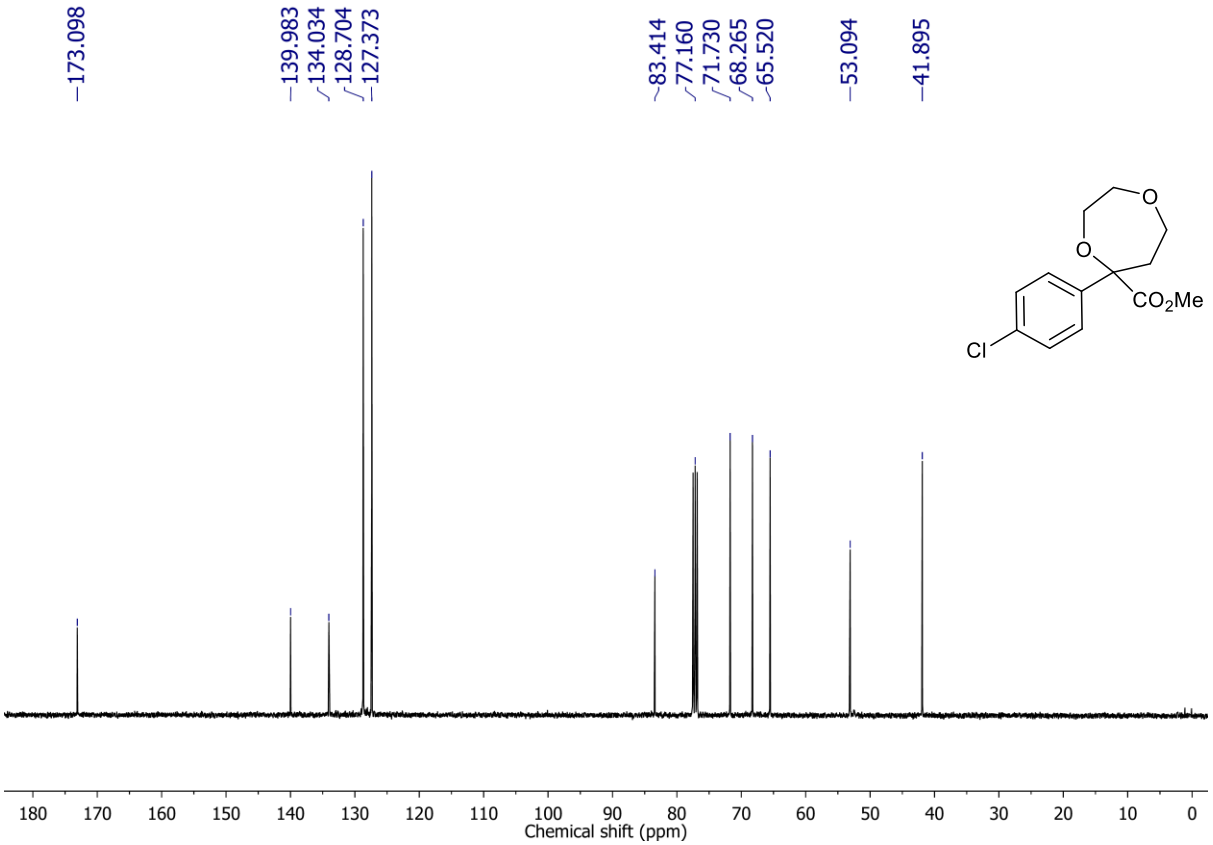
^{13}C NMR (400 MHz) of **9h** in $CDCl_3$



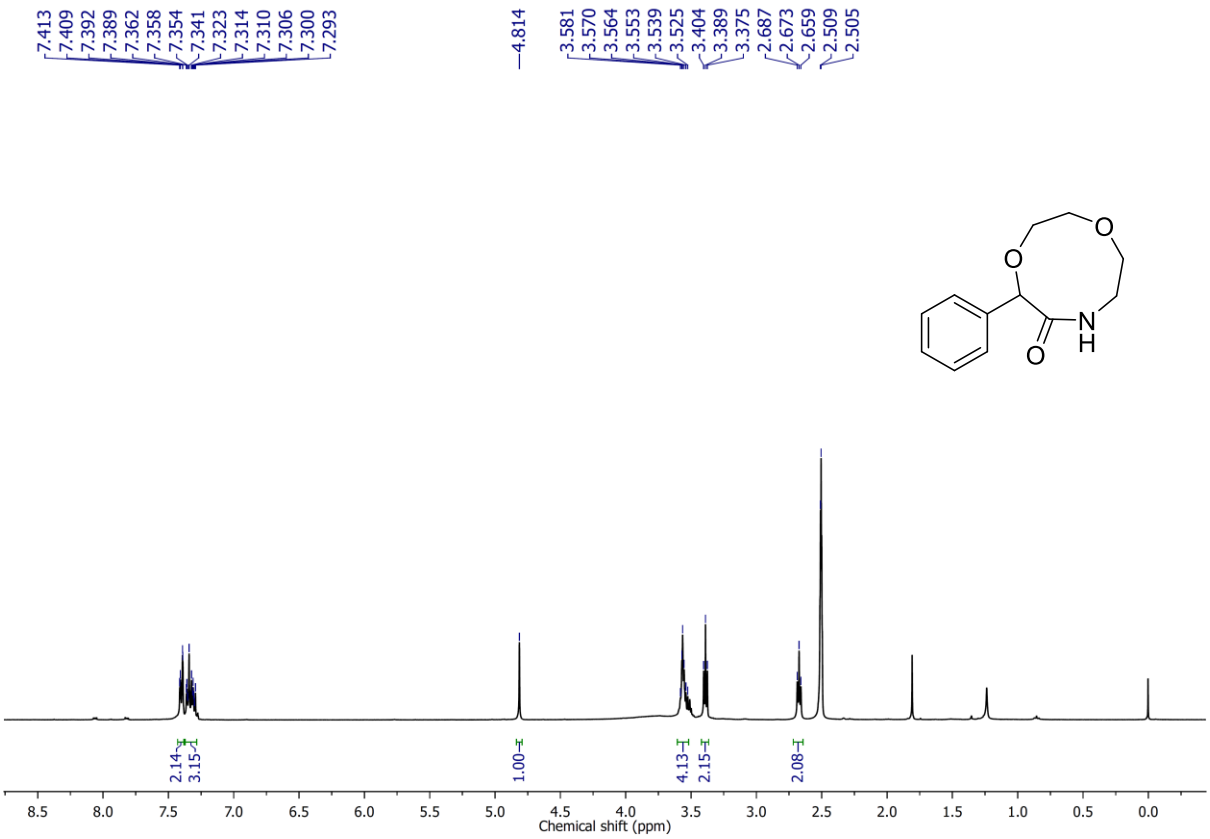
^{1}H NMR (400 MHz) of **9i** in $CDCl_3$



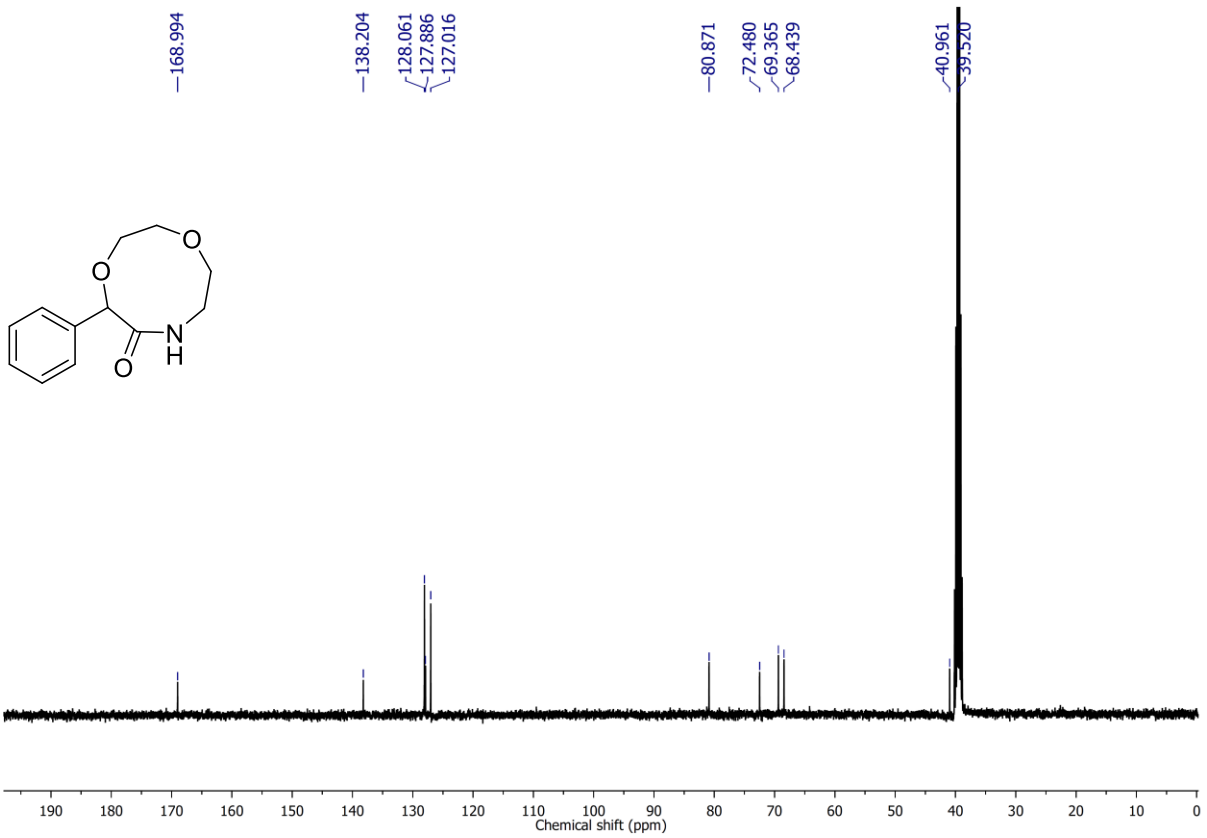
^{13}C NMR (400 MHz) of **9i** in $CDCl_3$



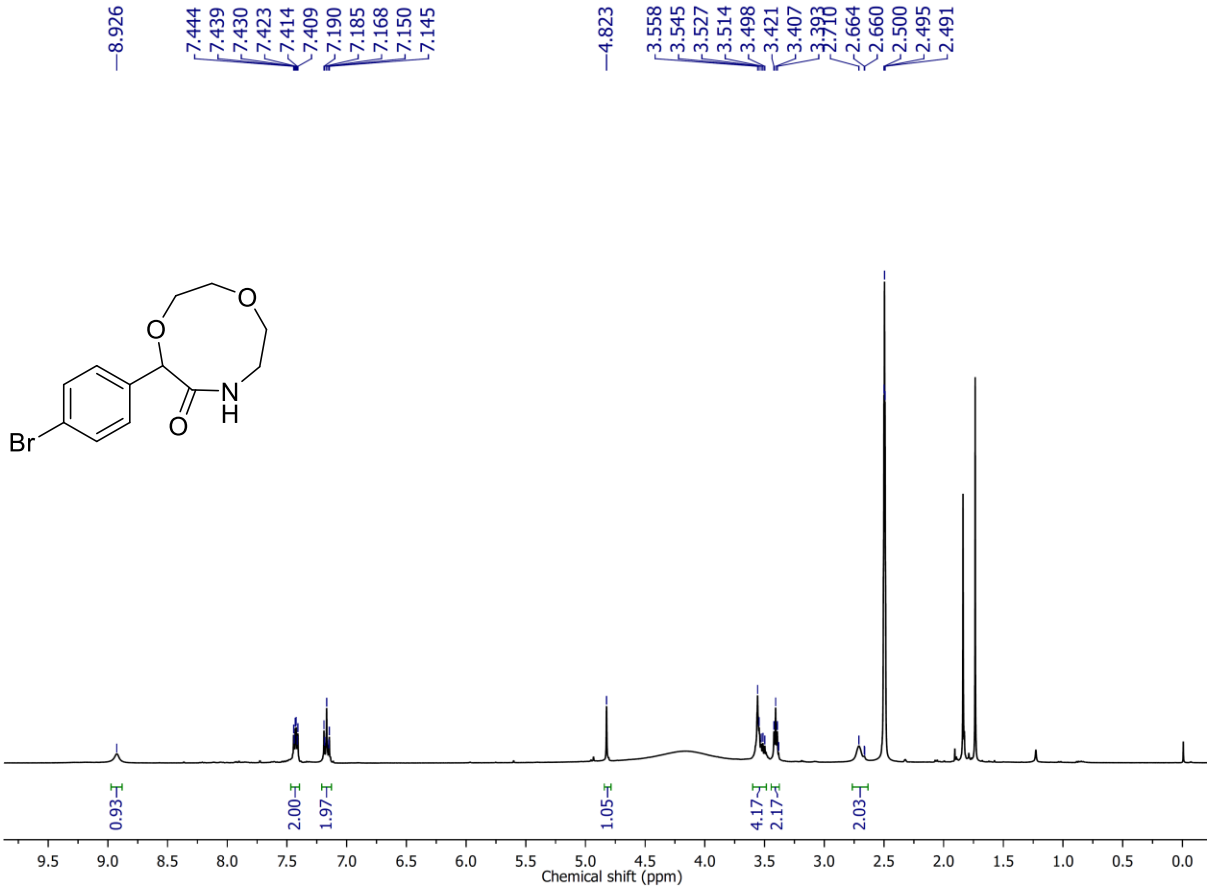
^{1}H NMR (400 MHz) of **10a** in DMSO-D_6



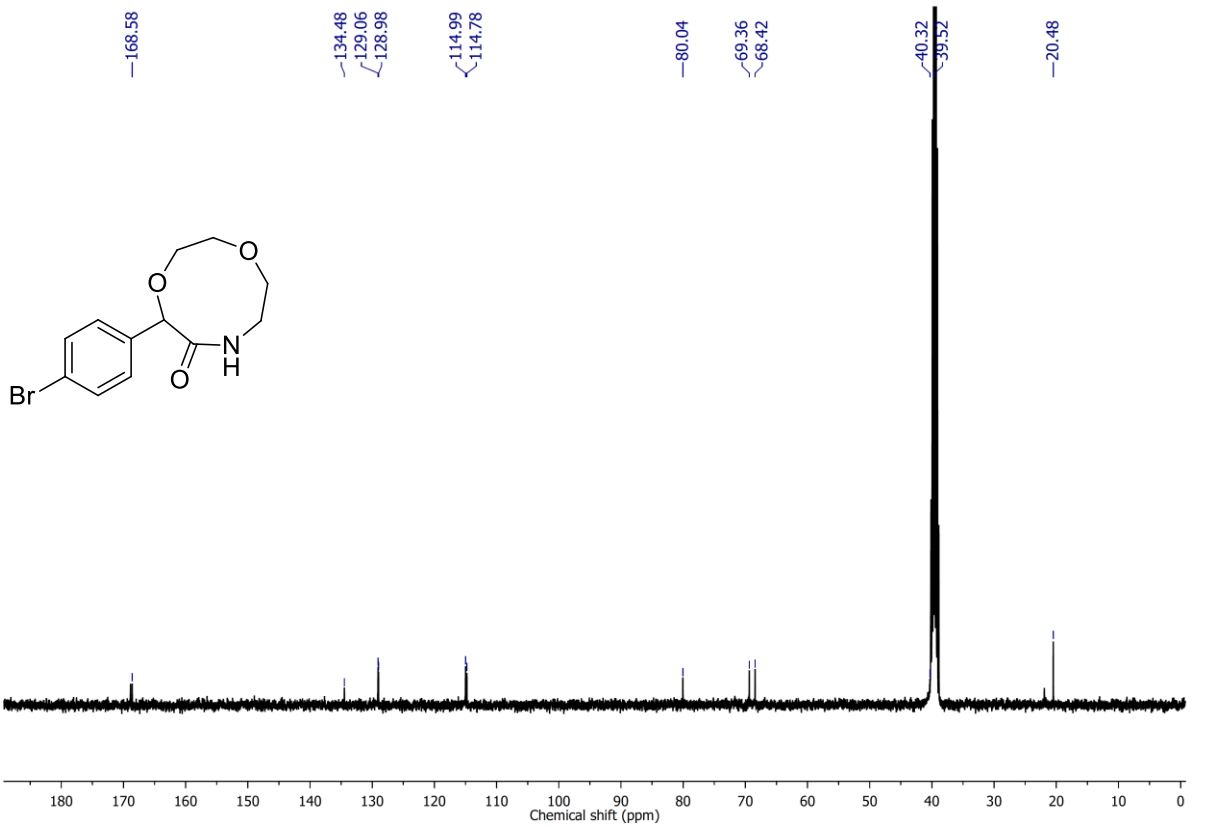
^{13}C NMR (400 MHz) of **10a** in DMSO-D_6



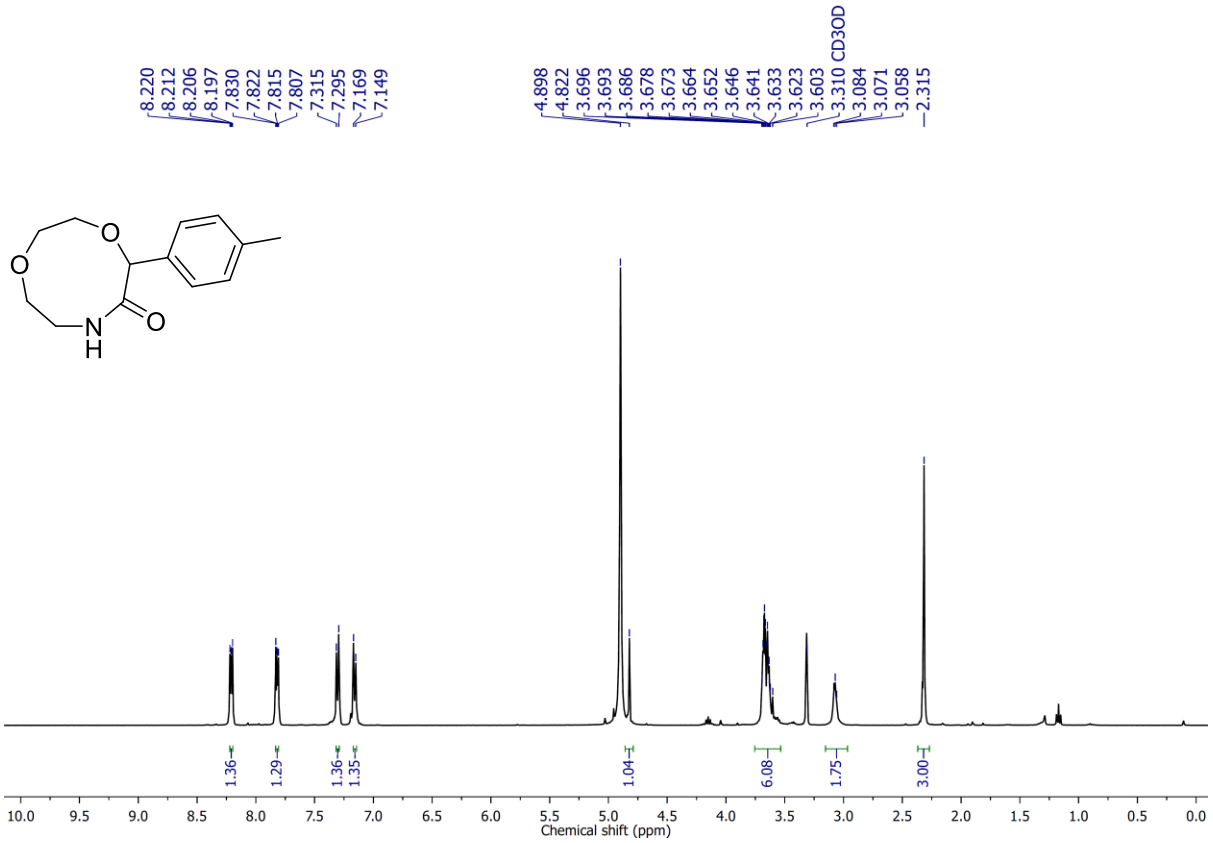
^{1}H NMR (400 MHz) of **10b** in DMSO-D_6



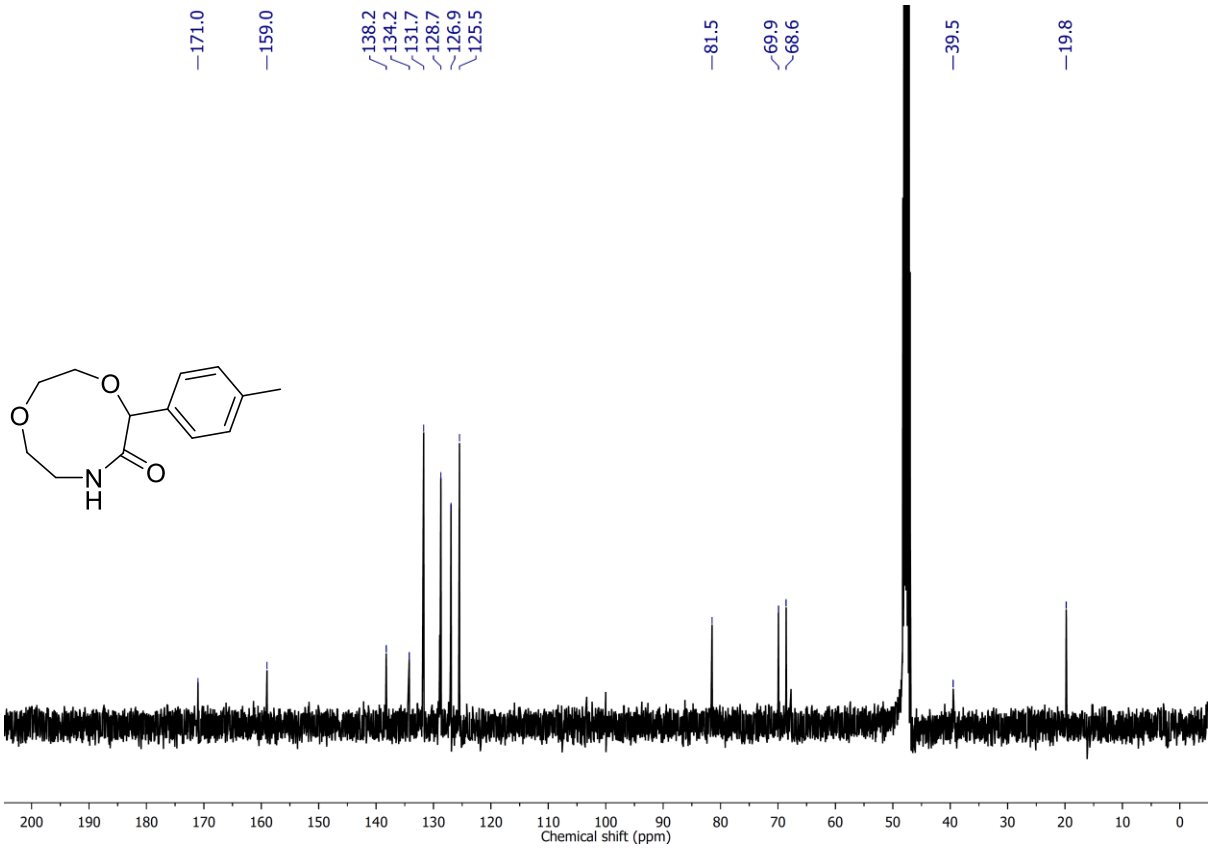
^{13}C NMR (400 MHz) of **10b** in DMSO-D_6



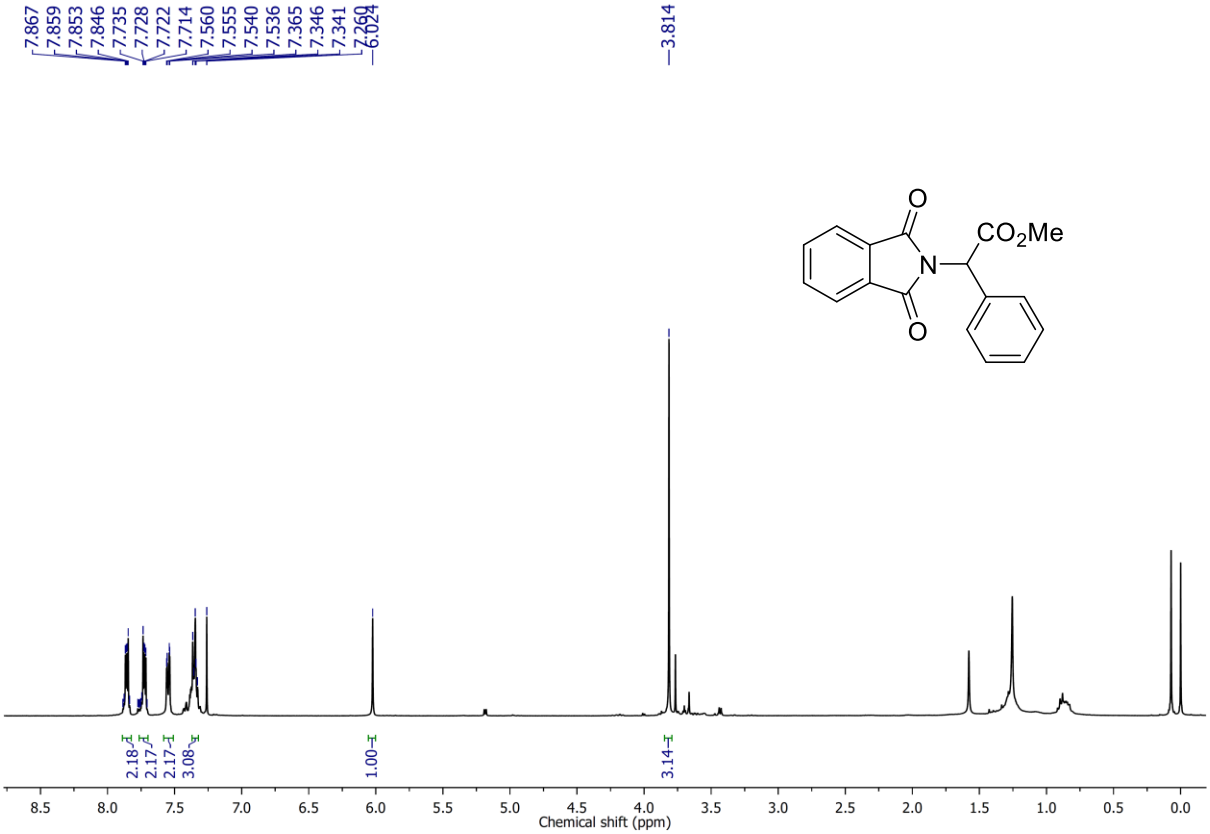
^{1}H NMR (400 MHz) of **10c** in CD_3OD



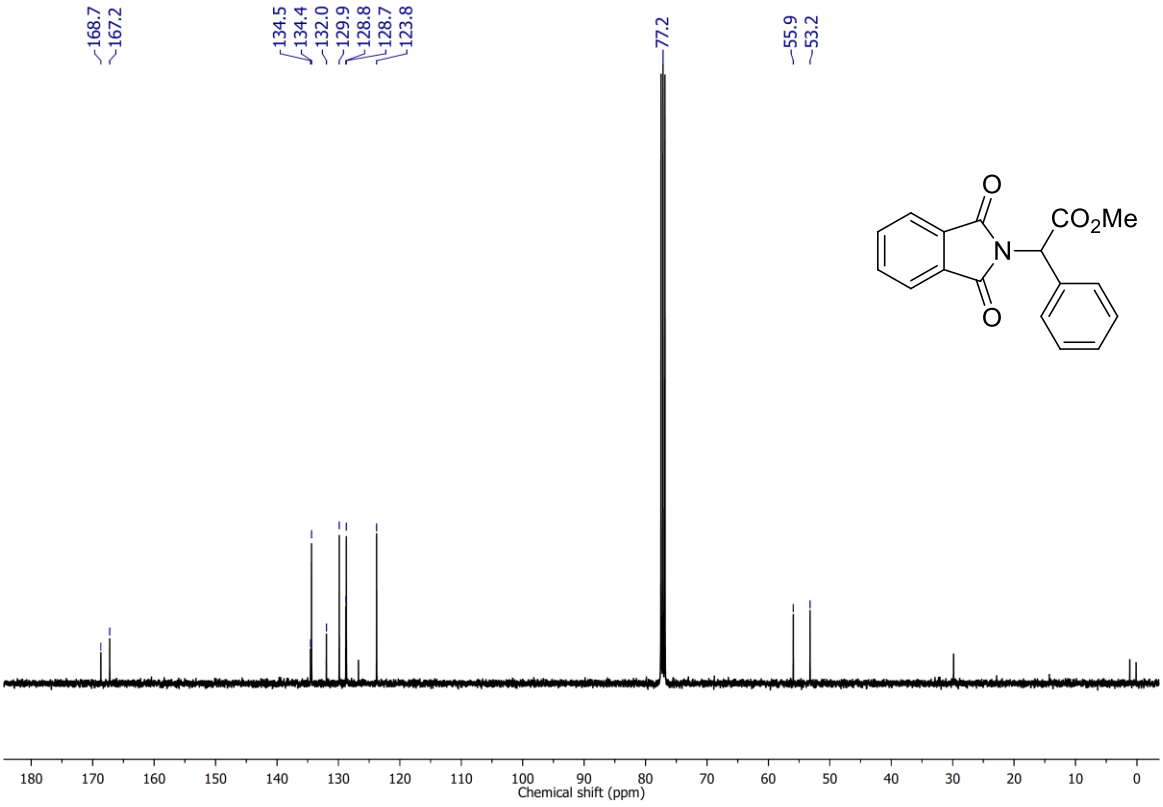
^{13}C NMR (400 MHz) of **10c** in CD_3OD



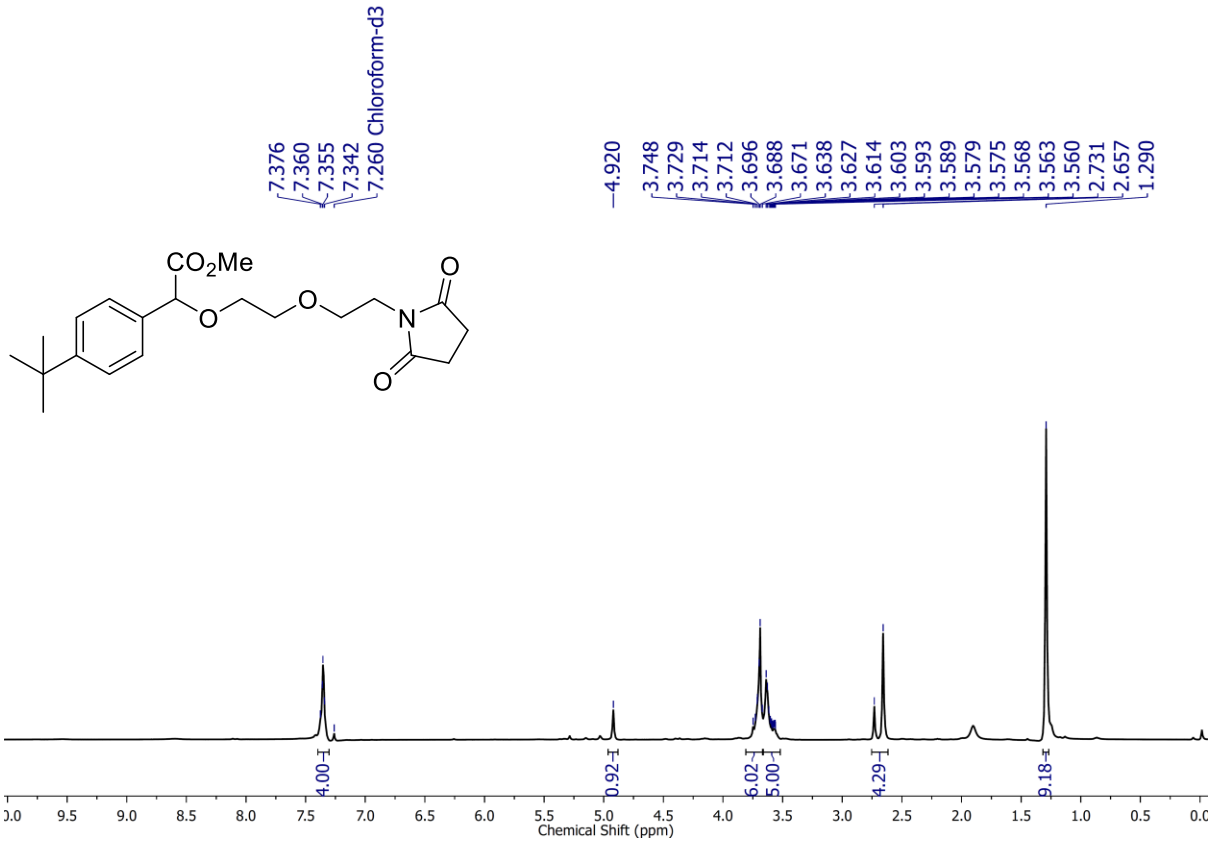
^{1}H NMR (400 MHz) of **11a** in $CDCl_3$



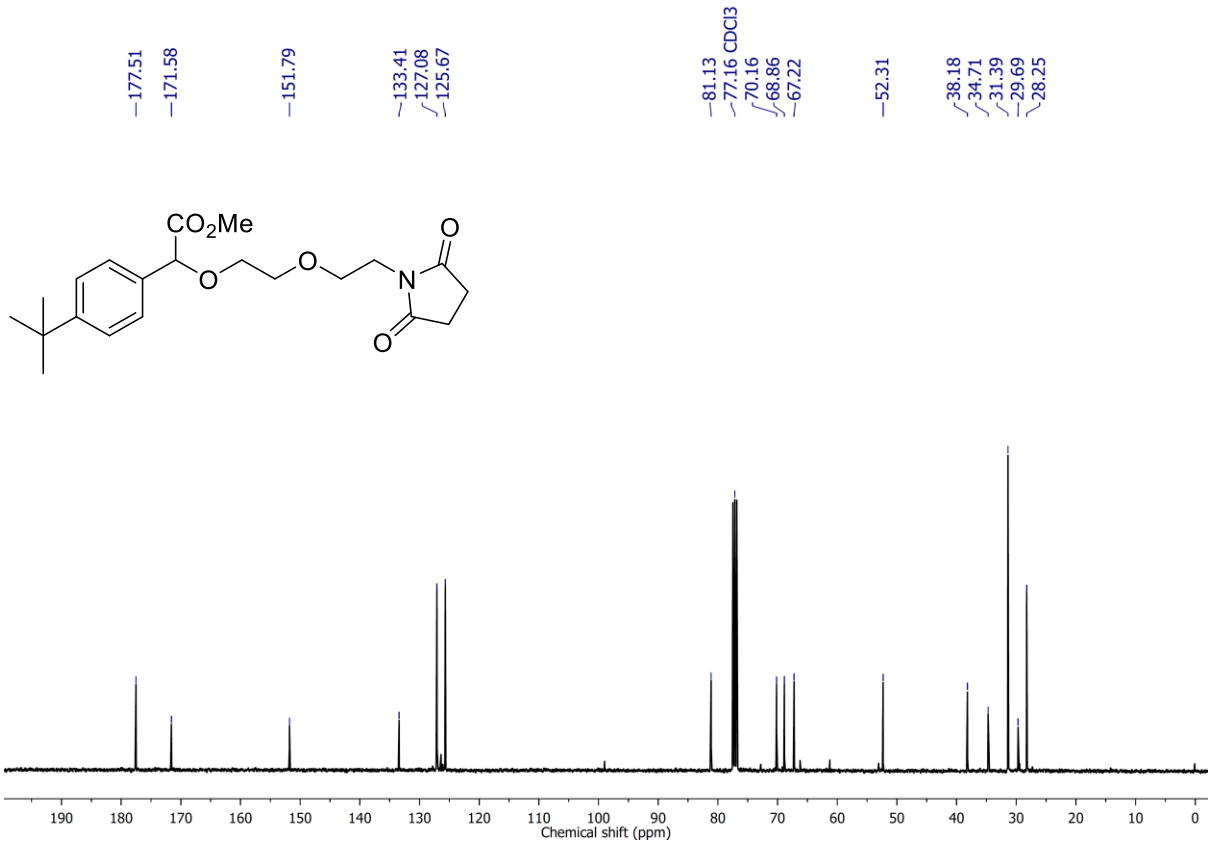
^{13}C NMR (400 MHz) of **11a** in $CDCl_3$



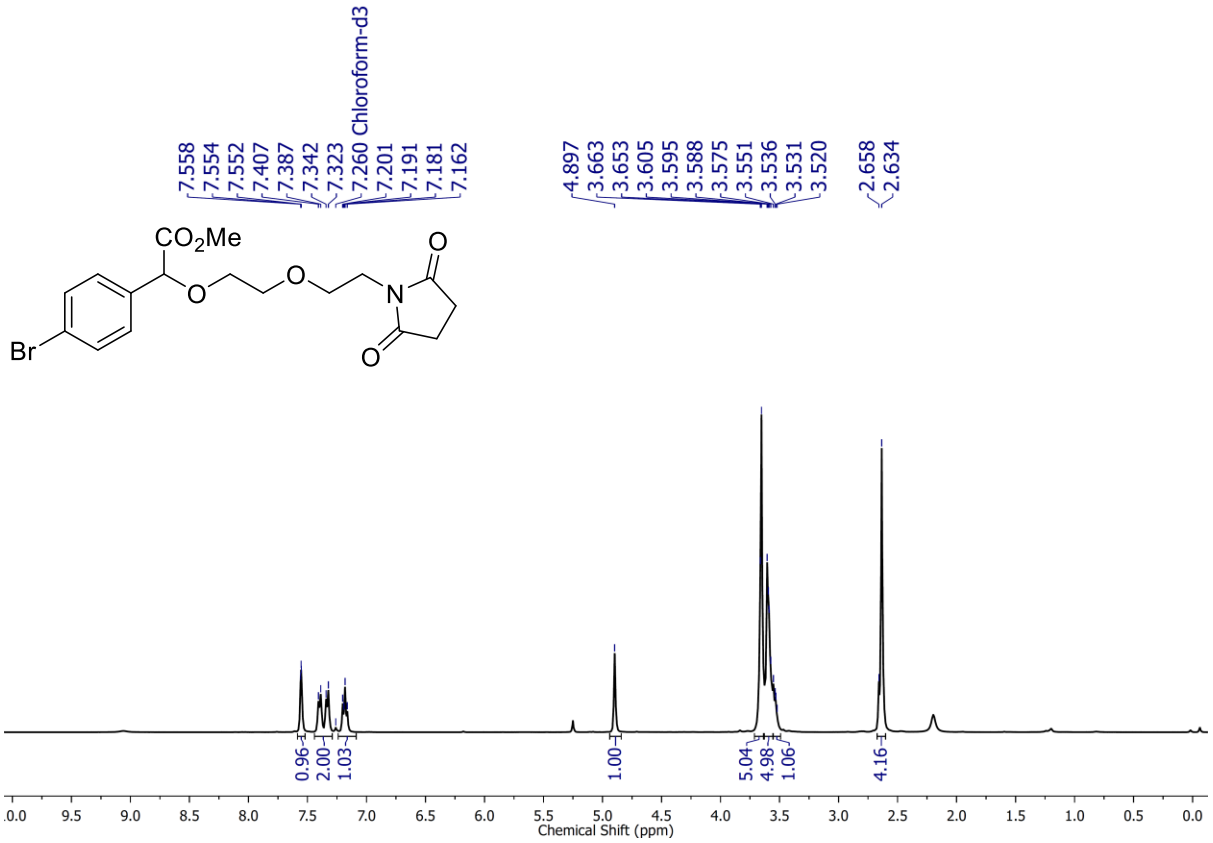
^{1}H NMR (400 MHz) of **8d** in $CDCl_3$



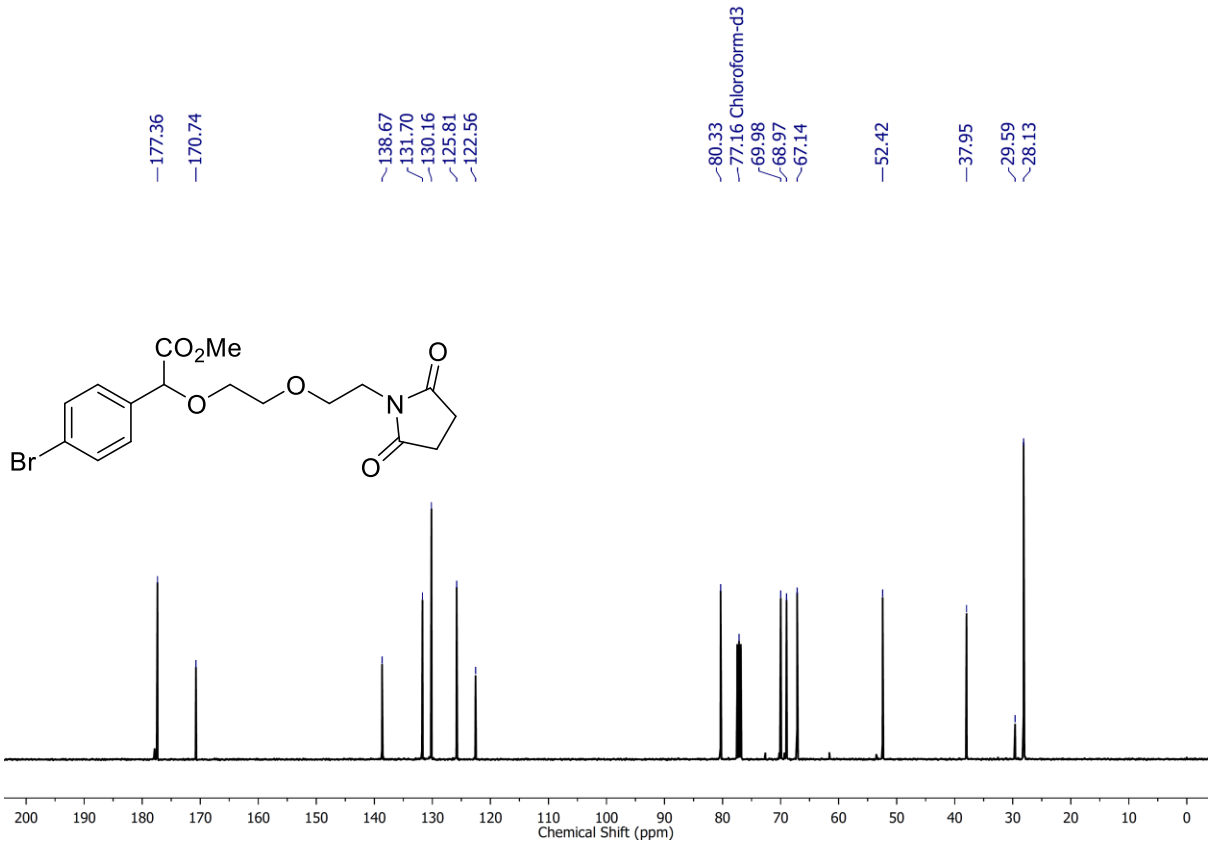
^{13}C NMR (400 MHz) of **8d** in $CDCl_3$



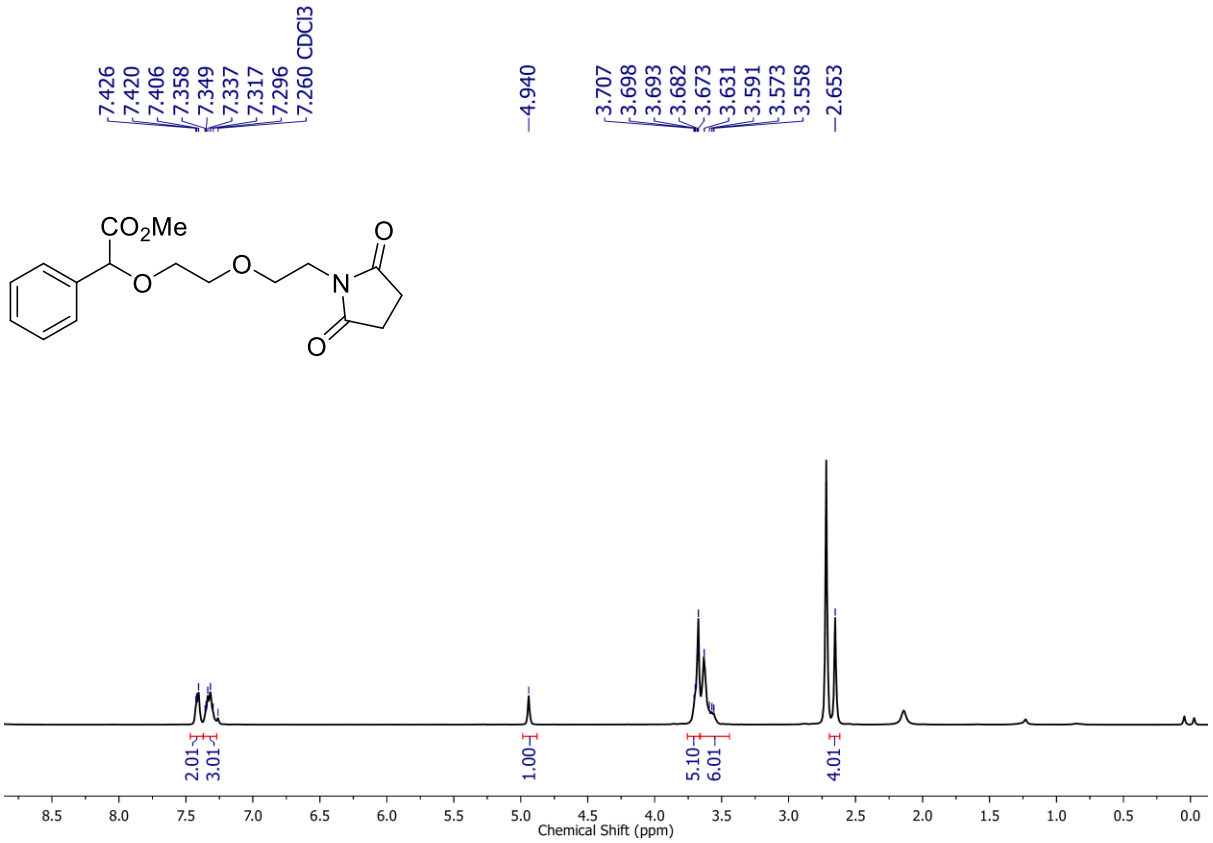
^{1}H NMR (400 MHz) of **8e** in $CDCl_3$



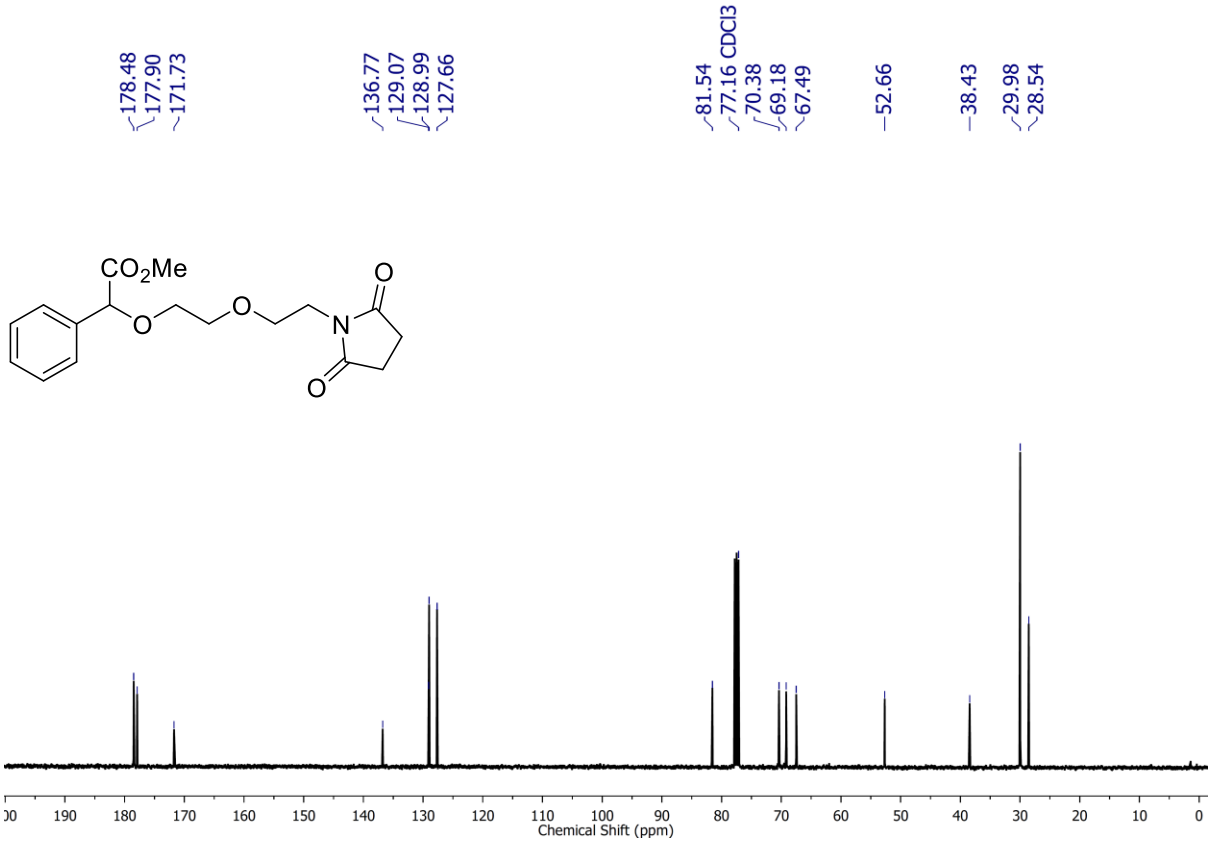
^{13}C NMR (400 MHz) of **8e** in $CDCl_3$



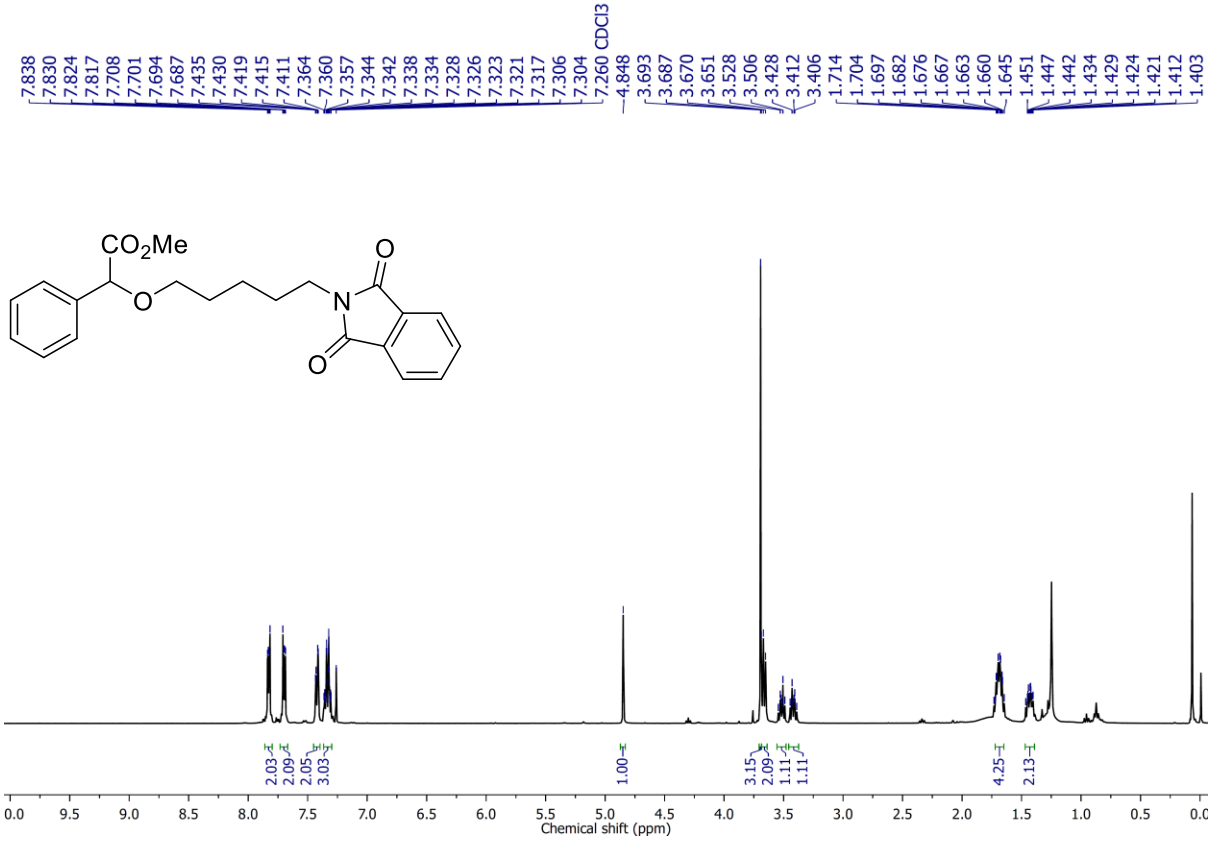
^{1}H NMR (400 MHz) of **8f** in $CDCl_3$



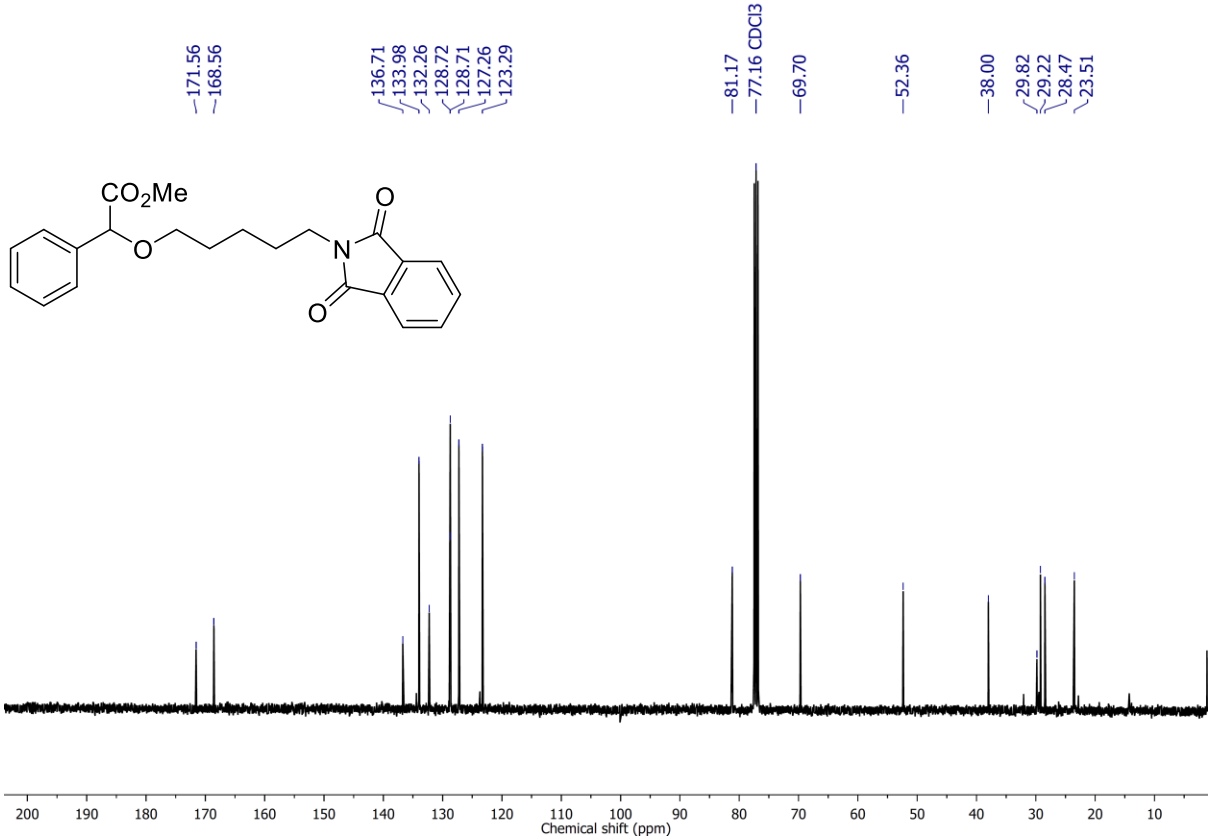
^{13}C NMR (400 MHz) of 8**f** in $CDCl_3$



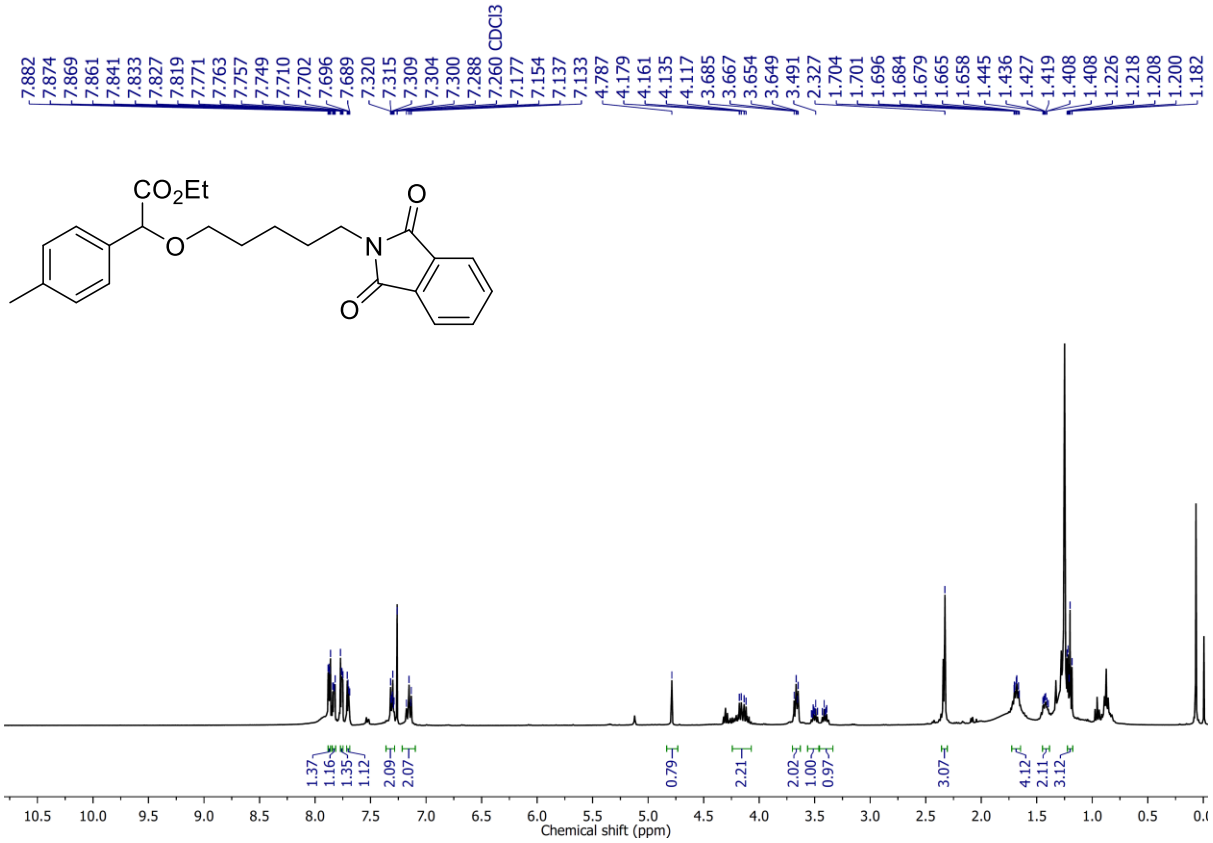
^{1}H NMR (400 MHz) of **15a** in $CDCl_3$



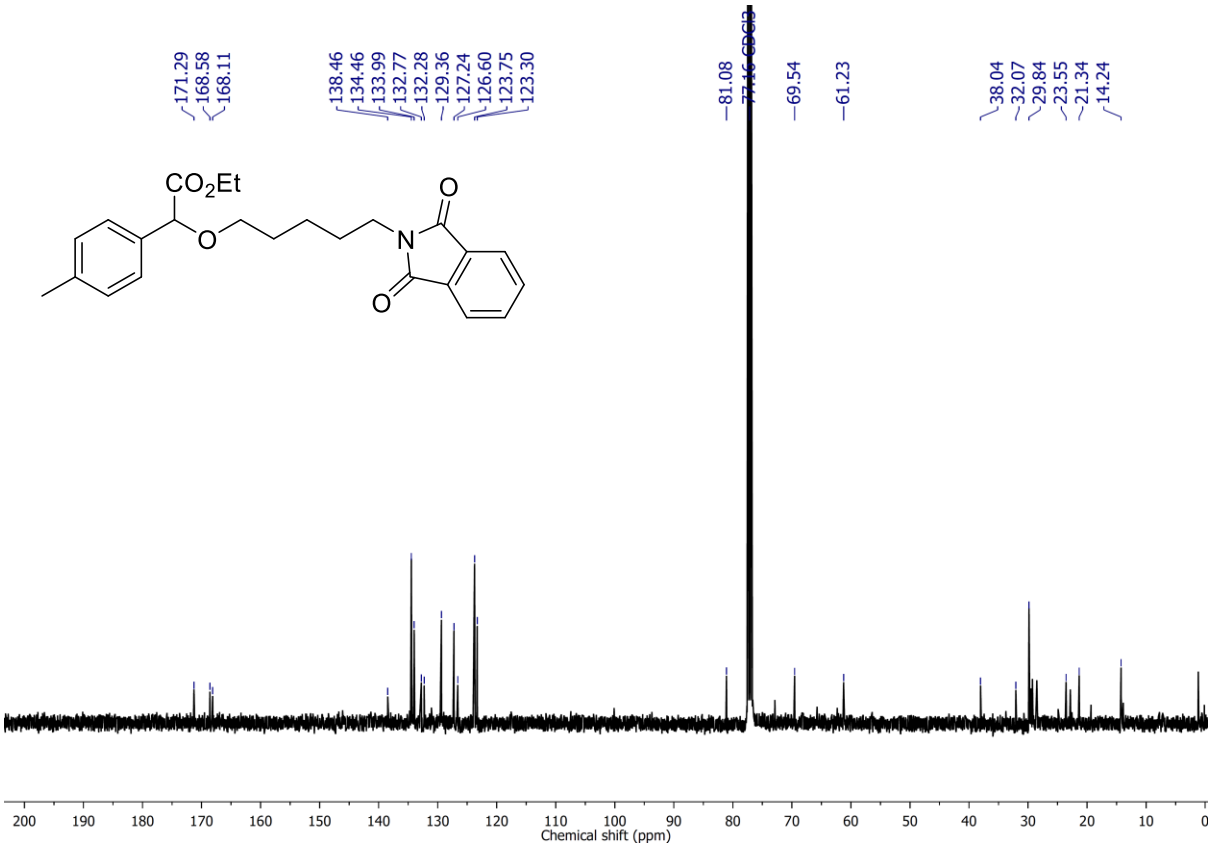
^{13}C NMR (400 MHz) of **15a** in $CDCl_3$



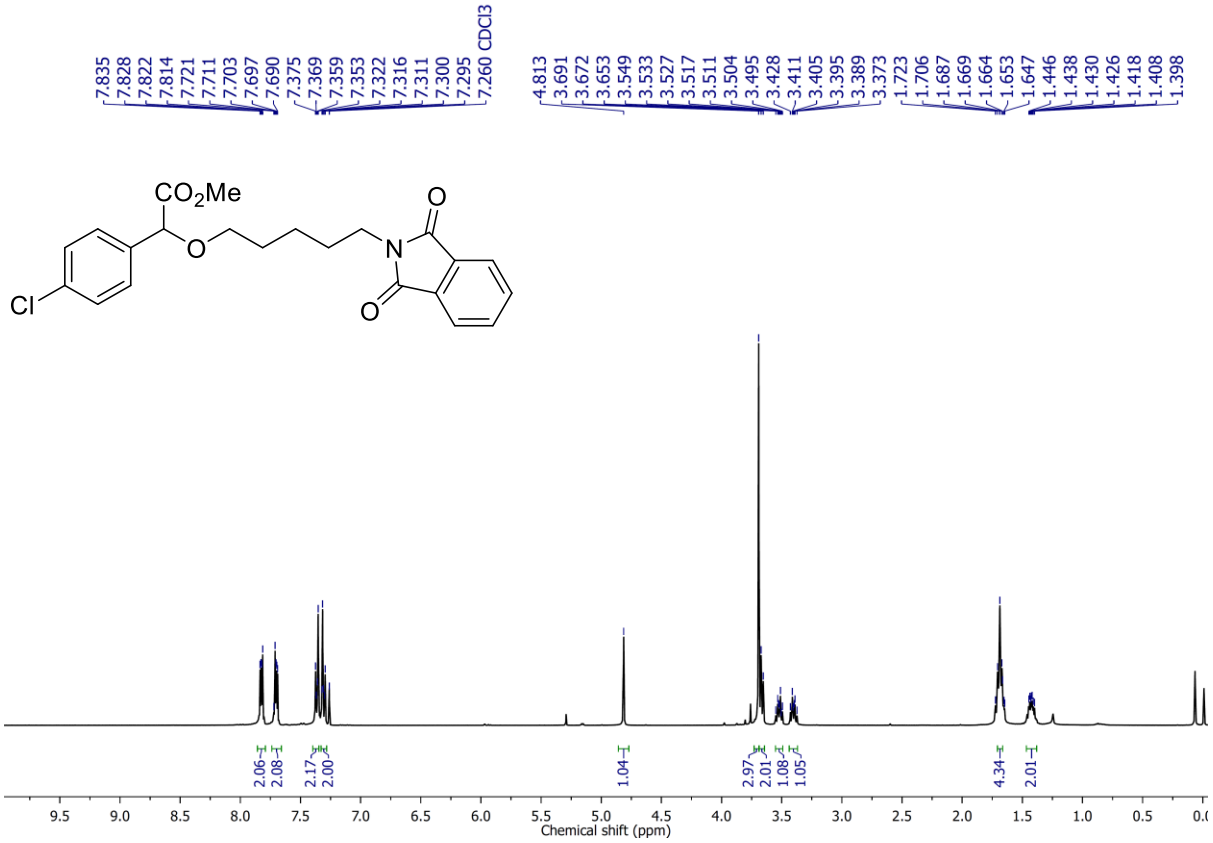
^{1}H NMR (400 MHz) of **15b** in $CDCl_3$



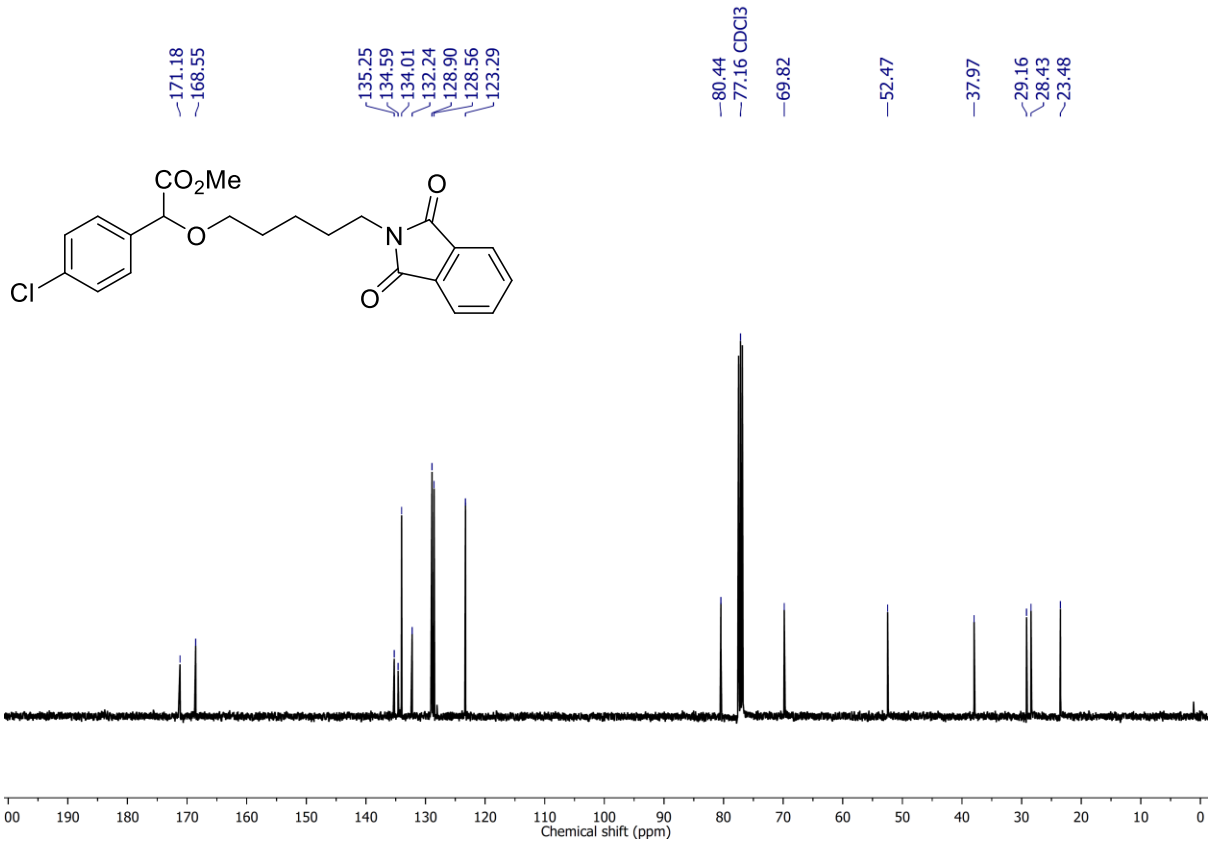
^{13}C NMR (400 MHz) of **15b** in $CDCl_3$



^{1}H NMR (400 MHz) of **15c** in $CDCl_3$



^{13}C NMR (400 MHz) of **15c** in $CDCl_3$



7. Optimized Geometries:

1,4 dioxane (3)			
6	1.211940000	0.733219000	-0.200182000
6	1.211781000	-0.733432000	0.200338000
6	-1.211940000	-0.733219000	0.200182000
6	-1.211781000	0.733432000	-0.200338000
1	2.043186000	-1.275063000	-0.246369000
1	1.254687000	0.831060000	-1.290171000
1	2.043381000	1.274699000	0.246643000
1	-2.043381000	-1.274699000	-0.246643000
1	-1.254687000	-0.831060000	1.290171000
1	-1.254382000	0.831285000	-1.290334000
1	-2.043186000	1.275063000	0.246369000
1	1.254382000	-0.831285000	1.290334000
8	-0.000104000	-1.391865000	-0.297858000
8	0.000104000	1.391865000	0.297858000

Phenyl diazo acetate carbene			
6	2.231014000	1.483947000	0.113718000
6	0.951130000	0.950040000	0.169271000
6	0.740734000	-0.451585000	0.014936000
6	1.873722000	-1.284263000	-0.193618000
6	3.153544000	-0.744766000	-0.257227000
6	3.329728000	0.636541000	-0.101414000
1	2.385987000	2.547515000	0.234284000
1	0.096807000	1.591857000	0.338416000
1	1.701557000	-2.345737000	-0.302250000
1	4.010235000	-1.384038000	-0.420007000
1	4.326279000	1.057002000	-0.146344000
6	-0.542790000	-1.065277000	0.046853000
6	-1.750034000	-0.356640000	0.303871000
8	-2.179589000	-0.197788000	1.472426000
8	-2.450703000	0.023060000	-0.822554000
6	-3.826482000	0.509283000	-0.619253000
1	-4.186242000	0.728162000	-1.618435000
1	-4.429912000	-0.264037000	-0.148025000
1	-3.825772000	1.403409000	0.000557000

(3) + Carbene [Single frame]			
6	-2.748419000	0.101205000	1.395437000
6	-2.745414000	1.394903000	0.599876000
6	-3.684316000	0.239769000	-1.307482000
6	-3.696383000	-1.061406000	-0.520371000
1	-2.948585000	2.255250000	1.234263000
1	-3.670119000	0.000327000	1.977150000
1	-1.886586000	0.042281000	2.056266000
1	-4.528474000	0.300716000	-1.992144000
1	-2.749789000	0.338158000	-1.869832000
1	-4.661644000	-1.195933000	-0.020942000
1	-3.495030000	-1.922788000	-1.155739000
1	-1.782429000	1.523793000	0.099465000
8	-3.826829000	1.375736000	-0.396825000
8	-2.631992000	-1.053273000	0.489371000
6	1.018632000	0.541708000	0.260617000
6	1.882439000	1.670138000	0.341097000
6	1.468986000	-0.795251000	0.095989000
6	0.497627000	-1.836024000	0.094726000
6	2.843387000	-1.143136000	-0.074976000
6	0.887992000	-3.161635000	-0.073744000
1	-0.545043000	-1.570921000	0.226276000
6	3.222221000	-2.466629000	-0.238667000
1	3.587146000	-0.357308000	-0.066973000
6	2.242650000	-3.474693000	-0.238881000
1	0.147074000	-3.949313000	-0.071696000
1	4.264375000	-2.726879000	-0.365332000
1	2.542320000	-4.507349000	-0.366446000
8	2.336803000	2.080224000	1.436649000
8	2.067001000	2.338613000	-0.854840000
6	2.730725000	3.651688000	-0.786626000
1	3.738441000	3.547753000	-0.389898000
1	2.750787000	3.998663000	-1.813833000
1	2.156936000	4.329329000	-0.157401000

Int1/ Ylide (13a)			
6	3.763148000	-0.928881000	0.002479000
6	2.701116000	-0.028426000	0.002586000
6	1.356780000	-0.487628000	-0.000813000
6	1.153917000	-1.891714000	-0.004250000
6	2.229822000	-2.781014000	-0.004146000
6	3.545216000	-2.312410000	-0.000801000
1	4.775606000	-0.543519000	0.005085000
1	2.886764000	1.033104000	0.005179000
1	0.148063000	-2.287330000	-0.007275000
1	2.034084000	-3.846704000	-0.006811000
1	4.377991000	-3.003119000	-0.000740000
6	0.246719000	0.437290000	-0.000918000
6	0.080823000	1.825098000	0.002409000
8	-1.047092000	2.423360000	0.005343000
8	1.279999000	2.549608000	0.002965000
6	1.185879000	4.011918000	-0.004775000
1	1.644503000	4.370371000	-0.924614000
1	0.143081000	4.314196000	0.046852000
1	1.739176000	4.377600000	0.857731000
6	-2.990291000	-1.181668000	-1.204433000
6	-1.909159000	-0.124554000	-1.265890000
6	-1.905381000	-0.132007000	1.267677000
6	-2.986564000	-1.188875000	1.203274000
1	-1.192285000	-0.291040000	-2.064308000
1	-2.560236000	-2.187647000	-1.231624000
1	-3.673075000	-1.061142000	-2.042876000
1	-1.186124000	-0.303082000	2.062974000
1	-2.277780000	0.889177000	1.278720000
1	-2.556252000	-2.194918000	1.222987000
1	-3.666766000	-1.073615000	2.044554000
1	-2.281453000	0.896722000	-1.269997000
8	-1.080531000	-0.242719000	-0.000732000
8	-3.800806000	-1.029228000	0.001146000

3CNIndole (1b)			
7	1.574126000	-1.087207000	-0.000121000
6	0.247850000	0.749400000	0.000055000
6	0.245115000	-0.677197000	0.000003000

Phthalimide (1a)			
6	0.177024000	-0.696331000	-0.000117000
6	0.177028000	0.696329000	0.000113000
6	1.356048000	1.418828000	0.000327000

6	2.401564000	0.035429000	0.000033000	1	1.345946000	2.501477000	0.000571000
6	-0.940401000	-1.420741000	-0.000060000	6	1.356011000	-1.418866000	-0.000344000
1	-0.929206000	-2.503516000	-0.000182000	1	1.345962000	-2.501511000	-0.000624000
6	-0.982929000	1.430847000	0.000029000	6	2.551426000	-0.698153000	-0.000183000
1	-1.009614000	2.513248000	-0.000073000	1	3.495815000	-1.228769000	-0.000326000
6	-2.163683000	0.694923000	0.000036000	6	2.551440000	0.698109000	0.000200000
1	-3.116188000	1.208755000	0.000075000	1	3.495847000	1.228693000	0.000412000
6	-2.142631000	-0.717662000	-0.000009000	6	-1.240099000	-1.169429000	0.000162000
1	-3.077491000	-1.262867000	0.000034000	8	-1.671075000	-2.296284000	0.000133000
1	1.891534000	-2.039328000	0.000879000	6	-1.240094000	1.169437000	-0.000009000
6	1.628004000	1.169010000	-0.000059000	8	-1.670959000	2.296294000	-0.000465000
1	1.992571000	2.181888000	-0.000100000	7	-2.008815000	0.000058000	0.000219000
1	3.472184000	-0.071789000	0.000042000	1	-3.018293000	0.000080000	0.000191000

Hydantoin (1e)

6	1.169901000	-0.174102000	-0.000058000
8	2.329454000	-0.602234000	0.000032000
6	-1.169227000	-0.209066000	0.000023000
8	-2.328892000	-0.631873000	-0.000071000
7	-0.008824000	-0.960404000	0.000161000
1	0.016307000	-1.966485000	-0.000370000
6	-0.719775000	1.254536000	0.000081000
1	-1.101602000	1.761568000	0.887733000
1	-1.101979000	1.761868000	-0.887194000
7	0.738699000	1.130636000	-0.000226000
1	1.388262000	1.896070000	0.000323000

Thiazolidinedione (1d)

6	1.028446000	-0.606194000	0.000126000
8	2.026324000	-1.270446000	-0.000139000
6	-1.338765000	-0.237167000	0.000087000
8	-2.496437000	-0.573953000	-0.000924000
7	-0.268474000	-1.108035000	0.000804000
1	-0.415259000	-2.109462000	0.000383000
16	0.972366000	1.188303000	-0.000467000
6	-0.859436000	1.207391000	0.000891000
1	-1.241125000	1.711182000	0.888067000
1	-1.242721000	1.712689000	-0.884715000

[TS1]‡

6	4.247609422	-0.680669942	0.002411108
6	3.185577422	0.219785058	0.002518108
6	1.841241422	-0.239416942	-0.000880892
6	1.638378422	-1.643502942	-0.004317892
6	2.714283422	-2.532802942	-0.004213892
6	4.029677422	-2.064198942	-0.000868892
1	5.260067422	-0.295307942	0.005017108
1	3.371225422	1.281315058	0.005111108
1	0.632524422	-2.039118942	-0.007342892
1	2.518545422	-3.598492942	-0.006878892
1	4.862452422	-2.754907942	-0.000807892
6	0.731180422	0.685501058	-0.000985892
6	0.565284422	2.073309058	0.002341108
8	-0.562630578	2.671571058	0.005275108
8	1.764460422	2.797819058	0.002897108
6	1.670340422	4.260129058	-0.004842892
1	2.128964422	4.618582058	-0.924681892
1	0.627542422	4.562407058	0.046784108
1	2.223637422	4.625811058	0.857663108
6	-3.474752422	-1.429879058	-1.204365108
6	-2.393620422	-0.372765058	-1.265822108
6	-2.389842422	-0.380218058	1.267744892
6	-3.471025422	-1.437086058	1.203341892
1	-1.676746422	-0.539251058	-2.064240108
1	-3.044697422	-2.435858058	-1.231556108
1	-4.157536422	-1.309353058	-2.042808108
1	-1.670585422	-0.551293058	2.063041892
1	-2.762241422	0.640965942	1.278787892
1	-3.040713422	-2.443129058	1.223054892
1	-4.151227422	-1.321826058	2.044621892
1	-2.765914422	0.648510942	-1.269929108
8	-1.564992422	-0.490930058	-0.000664108
8	-4.285267422	-1.277439058	0.001213892

[TS2-HDT]‡

6	3.453824000	2.108280000	-2.265607000
6	3.139729000	1.324423000	-1.155557000
6	1.861633000	0.746417000	-1.033738000
6	0.895829000	0.973324000	-2.029794000
6	1.219643000	1.760895000	-3.138206000
6	2.493000000	2.323989000	-3.260944000
1	4.435878000	2.554459000	-2.351241000
1	3.884252000	1.169977000	-0.383289000
1	-0.108944000	0.572459000	-1.933744000
1	0.466983000	1.941320000	-3.893716000

[TS2-Phth]‡

6	2.623274124	2.470883691	-1.319153896
6	2.211274124	1.634883691	-0.284153896
6	1.353274124	0.538883691	-0.537153896
6	0.937274124	0.324883691	-1.869153896
6	1.367274124	1.156883691	-2.898153896
6	2.212274124	2.237883691	-2.633153896
1	3.287274124	3.302883691	-1.096153896
1	2.548274124	1.820883691	0.729846104
1	0.245274124	-0.484116309	-2.084153896
1	1.024274124	0.969883691	-3.913153896

1	2.734503000	2.937415000	-4.119387000	1	2.543274124	2.888883691	-3.437153896
6	1.491564000	-0.096886000	0.147797000	6	0.921274124	-0.363116309	0.519846104
6	2.228999000	0.202671000	1.430351000	6	1.072274124	-0.299116309	1.943846104
8	3.125140000	-0.498077000	1.916068000	8	1.126274124	-1.278116309	2.693846104
8	1.754081000	1.348710000	1.973503000	8	1.081274124	0.981883691	2.413846104
6	2.292467000	1.818262000	3.265759000	6	0.948274124	1.106883691	3.840846104
1	2.716707000	2.802846000	3.092025000	1	1.090274124	2.166883691	4.050846104
1	1.448361000	1.878284000	3.945694000	1	-0.050725876	0.791883691	4.151846104
1	3.042834000	1.122229000	3.629725000	1	1.701274124	0.507883691	4.355846104
6	0.851124000	-3.841588000	-0.008926000	6	-0.080725876	-3.901116309	-0.458153896
6	1.211463000	-2.635571000	0.821215000	6	-0.145725876	-2.709116309	0.471846104
6	2.978530000	-2.088021000	-0.899447000	6	2.278274124	-2.432116309	0.080846104
6	2.550971000	-3.336727000	-1.648429000	6	2.210274124	-3.657116309	-0.815153896
1	0.346220000	-2.181204000	1.311626000	1	-1.058725876	-2.136116309	0.354846104
1	0.051796000	-3.599538000	-0.712461000	1	-0.316725876	-3.592116309	-1.488153896
1	0.532306000	-4.653470000	0.640309000	1	-0.826725876	-4.635116309	-0.137153896
1	3.269293000	-1.284979000	-1.568958000	1	2.971274124	-1.681116309	-0.296153896
1	3.742273000	-2.273339000	-0.147313000	1	2.470274124	-2.664116309	1.129846104
1	1.799529000	-3.086754000	-2.402925000	1	2.058274124	-3.343116309	-1.859153896
1	3.413600000	-3.789732000	-2.133324000	1	3.158274124	-4.200116309	-0.747153896
1	2.022555000	-2.821278000	1.521390000	1	0.058274124	-2.948116309	1.514846104
8	1.761478000	-1.600706000	-0.164383000	8	0.943274124	-1.768116309	0.044846104
8	2.024522000	-4.342653000	-0.736063000	8	1.187274124	-4.546116309	-0.405153896
6	-2.408400000	-0.160982000	-0.620951000	6	-2.691504667	-1.174990959	1.307586738
6	-1.992331000	-1.151922000	1.349268000	6	-2.541504667	1.092009041	0.952586738
8	-2.266105000	0.351664000	-1.761694000	6	-4.013504667	-0.614990959	1.561586738
8	-1.356976000	-1.717921000	2.285896000	6	-3.918504667	0.810009041	1.337586738
7	-3.357488000	-0.926386000	1.344410000	6	-5.211504667	-1.184990959	1.941586738
1	-3.956296000	-1.212305000	2.097895000	6	-5.026504667	1.617009041	1.503586738
6	-3.768788000	-0.285013000	0.099466000	6	-6.328504667	-0.348990959	2.104586738
1	-4.457719000	-0.893959000	-0.489950000	1	-5.298504667	-2.266990959	2.116586738
1	-4.210217000	0.702487000	0.249247000	6	-6.238504667	1.021009041	1.890586738
7	-1.422939000	-0.685266000	0.167939000	1	-4.971504667	2.702009041	1.336586738
1	0.389117000	-0.143833000	0.280464000	1	-7.288504667	-0.791990959	2.409586738
				1	-7.127504667	1.655009041	2.024586738
				8	-2.384504667	-2.455990959	1.410586738
				8	-2.071504667	2.292009041	0.666586738
				7	-1.831504667	-0.121990959	0.944586738
				1	-0.166043580	-0.292776423	0.549721054

[TS2-IND]‡				**[Int2-HDT]**			
6	5.041953272	2.218336226	2.864382881	6	-3.897553000	-1.793823000	-0.393631000
6	4.214198272	1.549660226	3.765984881	6	-3.014707000	-0.904898000	0.219309000
6	3.560456272	0.353440226	3.394545881	6	-1.651358000	-0.902940000	-0.132461000
6	3.780022272	-0.141074774	2.088985881	6	-1.178377000	-1.811089000	-1.095751000
6	4.623030272	0.524385226	1.201141881	6	-2.070563000	-2.698633000	-1.704014000
6	5.258784272	1.710648226	1.580890881	6	-3.425263000	-2.690120000	-1.360070000
1	5.532311272	3.133906226	3.175237881	1	-4.943208000	-1.794594000	-0.115341000
1	4.058756272	1.951002226	4.757258881	1	-3.384336000	-0.220942000	0.974394000
1	3.263902272	-1.036652774	1.766981881	1	-0.123448000	-1.854922000	-1.350147000
1	4.769055272	0.125262226	0.203933881	1	-1.696512000	-3.402832000	-2.434794000
1	5.909467272	2.229676226	0.887629881	1	-4.109045000	-3.384273000	-1.831380000
6	2.696500272	-0.369822774	4.323633881	6	-0.677052000	0.036295000	0.509949000
6	2.223902272	-0.041368774	5.621932881	6	-1.019738000	0.488989000	1.908544000
8	1.872334272	-0.877405774	6.491938881	8	-1.443822000	1.611367000	2.209272000
8	2.079611272	1.323418226	5.817839881	8	-0.782120000	-0.515800000	2.784856000
6	1.041947272	1.652422226	6.795833881	6	-0.997859000	-0.288193000	4.227733000
1	1.046859272	2.732533226	6.906918881	1	-1.742935000	-1.008343000	4.553048000
1	0.145891272	1.297554226	6.296621881	1	-0.045120000	-0.475424000	4.713192000
1	1.205875272	1.155338226	7.748014881	1	-1.332335000	0.731462000	4.396300000
6	2.161316272	-4.118268774	3.741748881	6	1.026571000	2.917844000	-1.291680000
6	1.718981272	-2.773582774	4.280231881	6	0.588798000	2.300389000	0.012315000

6	4.099093272	-2.401110774	4.968418881	6	-1.712813000	2.022594000	-0.991921000
6	4.414259272	-3.773548774	4.407749881	6	-1.175947000	2.674675000	-2.252767000
1	0.972028272	-2.295508774	3.655078881	1	1.374869000	1.709096000	0.489993000
1	2.428145272	-4.042251774	2.680827881	1	1.439563000	2.157614000	-1.957969000
1	1.342016272	-4.830192774	3.844989881	1	1.775167000	3.683657000	-1.103425000
1	4.895768272	-1.683214774	4.790246881	1	-2.439991000	1.246305000	-1.206989000
1	3.795560272	-2.411572774	6.013678881	1	-2.096407000	2.734728000	-0.264544000
1	4.747582272	-3.691436774	3.365806881	1	-0.825485000	1.911547000	-2.953635000
1	5.210808272	-4.229615774	4.995637881	1	-1.958393000	3.266460000	-2.723978000
1	1.422412272	-2.788684774	5.326132881	1	0.146386000	3.016498000	0.700874000
8	2.914677272	-1.851525774	4.204622881	8	-0.544450000	1.334193000	-0.343944000
8	3.272595272	-4.649590774	4.497168881	8	-0.095806000	3.602432000	-1.946172000
6	-3.061787173	1.276459607	3.089345512	6	2.583043000	-1.763699000	-0.880721000
6	-1.788481173	1.632093607	3.653824512	6	3.153058000	-0.124545000	0.542320000
6	-1.550071173	2.917878607	4.129936512	8	1.929611000	-2.502463000	-1.662777000
6	-2.575364173	3.859774607	4.053879512	8	3.062747000	0.916509000	1.256012000
6	-3.826802173	3.521939607	3.508831512	7	4.300538000	-0.883347000	0.393830000
6	-4.076021173	2.237155607	3.023830512	1	5.166601000	-0.649426000	0.844698000
6	-2.976332173	-0.106864393	2.686226512	6	4.068293000	-1.993286000	-0.525165000
6	-1.700817173	-0.548687393	3.000576512	1	4.687100000	-1.943217000	-1.423743000
1	-0.573843173	3.148764607	4.531973512	1	4.200099000	-2.972382000	-0.059935000
1	-2.401135173	4.869298607	4.419472512	7	2.119699000	-0.659577000	-0.221515000
1	-4.611028173	4.274217607	3.459947512	1	0.365294000	-0.337808000	0.417256000
1	-5.046293173	1.989271607	2.598084512				
1	-3.761890173	-0.684075393	2.220172512				
1	-1.290848173	-1.535208393	2.840257512				
7	-0.969235173	0.487186607	3.579546512				
1	0.415357629	0.295586942	4.095581726				

[Int2-Phth]				**[Int2-3CNIND]**			
6	-3.892000000	-1.744000000	-0.426000000	6	-3.898000000	-1.794000000	-0.394000000
6	-3.010000000	-0.855000000	0.187000000	6	-3.015000000	-0.905000000	0.219000000
6	-1.646000000	-0.853000000	-0.165000000	6	-1.651000000	-0.903000000	-0.132000000
6	-1.173000000	-1.761000000	-1.128000000	6	-1.178000000	-1.811000000	-1.096000000
6	-2.065000000	-2.649000000	-1.737000000	6	-2.071000000	-2.699000000	-1.704000000
6	-3.420000000	-2.640000000	-1.393000000	6	-3.425000000	-2.690000000	-1.360000000
1	-4.938000000	-1.745000000	-0.148000000	1	-4.943000000	-1.795000000	-0.115000000
1	-3.379000000	-0.171000000	0.942000000	1	-3.384000000	-0.221000000	0.974000000
1	-0.118000000	-1.805000000	-1.383000000	1	-0.123000000	-1.855000000	-1.350000000
1	-1.691000000	-3.353000000	-2.467000000	1	-1.697000000	-3.403000000	-2.435000000
1	-4.104000000	-3.335000000	-1.864000000	1	-4.109000000	-3.384000000	-1.831000000
6	-0.672000000	0.086000000	0.477000000	6	-0.677000000	0.036000000	0.510000000
6	-1.015000000	0.539000000	1.876000000	6	-1.020000000	0.489000000	1.909000000
8	-1.439000000	1.661000000	2.177000000	8	-1.444000000	1.611000000	2.209000000
8	-0.777000000	-0.466000000	2.752000000	8	-0.782000000	-0.516000000	2.785000000
6	-0.993000000	-0.239000000	4.195000000	6	-0.998000000	-0.288000000	4.228000000
1	-1.738000000	-0.959000000	4.520000000	1	-1.743000000	-1.008000000	4.553000000
1	-0.040000000	-0.426000000	4.681000000	1	-0.045000000	-0.475000000	4.713000000
1	-1.327000000	0.781000000	4.364000000	1	-1.332000000	0.731000000	4.396000000
6	1.022000000	2.868000000	-1.259000000	6	1.027000000	2.918000000	-1.292000000
6	0.584000000	2.251000000	0.045000000	6	0.589000000	2.300000000	0.012000000
6	-1.718000000	1.973000000	-0.959000000	6	-1.713000000	2.023000000	-0.992000000
6	-1.181000000	2.625000000	-2.220000000	6	-1.176000000	2.675000000	-2.253000000
1	1.370000000	1.659000000	0.523000000	1	1.375000000	1.709000000	0.490000000
1	1.434000000	2.108000000	-1.925000000	1	1.440000000	2.158000000	-1.958000000
1	1.770000000	3.634000000	-1.071000000	1	1.775000000	3.684000000	-1.103000000
1	-2.445000000	1.197000000	-1.174000000	1	-2.440000000	1.246000000	-1.207000000
1	-2.101000000	2.685000000	-0.232000000	1	-2.096000000	2.735000000	-0.265000000
1	-0.831000000	1.862000000	-2.921000000	1	-0.825000000	1.912000000	-2.954000000
1	-1.963000000	3.217000000	-2.691000000	1	-1.958000000	3.266000000	-2.724000000
1	0.141000000	2.967000000	0.734000000	1	0.146000000	3.016000000	0.701000000
8	-0.550000000	1.285000000	-0.311000000	8	-0.544000000	1.334000000	-0.344000000

8	-0.101000000	3.553000000	-1.914000000	8	-0.096000000	3.602000000	-1.946000000
6	2.583000000	-1.764000000	-0.881000000	1	0.365000000	-0.338000000	0.417000000
6	3.153000000	-0.125000000	0.542000000	6	4.420000000	-1.856000000	-0.178000000
8	1.930000000	-2.502000000	-1.663000000	6	4.438000000	0.463000000	-0.262000000
8	3.063000000	0.917000000	1.256000000	6	5.798000000	-1.417000000	-0.194000000
7	2.120000000	-0.660000000	-0.222000000	6	4.117000000	-3.202000000	-0.130000000
1	0.370000000	-0.288000000	0.385000000	6	5.780000000	0.040000000	-0.246000000
6	4.119000000	-2.032000000	-0.536000000	1	4.107000000	1.500000000	-0.299000000
6	4.301000000	-0.883000000	0.394000000	6	6.825000000	-2.338000000	-0.161000000
6	5.540000000	-0.652000000	1.023000000	6	5.175000000	-4.126000000	-0.097000000
1	5.583000000	0.195000000	1.675000000	1	3.075000000	-3.552000000	-0.118000000
6	6.391000000	-2.609000000	-0.136000000	6	6.499000000	-3.704000000	-0.112000000
1	7.259000000	-3.219000000	-0.275000000	1	7.877000000	-2.020000000	-0.172000000
6	5.175000000	-2.849000000	-0.772000000	1	4.945000000	-5.201000000	-0.058000000
1	4.921000000	-3.626000000	-1.463000000	1	7.309000000	-4.447000000	-0.085000000
6	6.598000000	-1.522000000	0.758000000	7	3.590000000	-0.660000000	-0.222000000
1	7.515000000	-1.330000000	1.275000000	6	7.036000000	0.931000000	-0.279000000
				7	7.971000000	1.594000000	-0.303000000

[TS3-HDT]‡				**[TS3-Phth]‡**			
6	-5.288966751	0.512158552	-0.372863804	6	6.500934625	1.080374796	-0.847208412
6	-3.907966751	0.665158552	-0.518863804	6	5.112934625	1.029374796	-0.988208412
6	-3.042966751	0.277158552	0.516136196	6	4.374934625	0.089374796	-0.258208412
6	-3.579966751	-0.261841448	1.696136196	6	5.033934625	-0.792625204	0.611791588
6	-4.958966751	-0.416841448	1.838136196	6	6.417934625	-0.732625204	0.748791588
6	-5.815966751	-0.028841448	0.802136196	6	7.154934625	0.204374796	0.018791588
1	-5.949966751	0.820158552	-1.172863804	1	7.068934625	1.808374796	-1.419208412
1	-3.508966751	1.087158552	-1.432863804	1	4.610934625	1.718374796	-1.657208412
1	-2.917966751	-0.554841448	2.501136196	1	4.461934625	-1.528625204	1.166791588
1	-5.362966751	-0.827841448	2.753136196	1	6.922934625	-1.420625204	1.420791588
1	-6.885966751	-0.141841448	0.915136196	1	8.234934625	0.247374796	0.122791588
6	-1.545966751	0.413158552	0.399136196	6	2.868934625	-0.031625204	-0.356208412
6	-1.063966751	1.497158552	-0.556863804	6	2.223934625	0.618374796	-1.602208412
8	-0.873966751	1.316158552	-1.763863804	8	2.275934625	1.819374796	-1.774208412
8	-0.902966751	2.657158552	0.103136196	8	1.659934625	-0.275625204	-2.389208412
6	-0.264966751	3.791158552	-0.611863804	6	0.950934625	0.248374796	-3.549208412
1	-0.732966751	3.920158552	-1.584863804	1	1.624934625	0.873374796	-4.138208412
1	-0.438966751	4.645158552	0.032136196	1	0.644934625	-0.635625204	-4.106208412
1	0.793033249	3.560158552	-0.698863804	1	0.087934625	0.816374796	-3.200208412
6	1.131033249	-2.378841448	0.127136196	6	0.242934625	0.546374796	2.408791588
6	0.839033249	-0.902841448	0.102136196	6	0.429934625	0.259374796	0.944791588
6	-1.410966751	-1.642841448	-1.210863804	6	2.530934625	1.922374796	1.234791588
6	-0.858966751	-3.047841448	-1.093863804	6	2.005934625	2.086374796	2.652791588
1	0.928033249	-0.345841448	1.018136196	1	0.447934625	-0.766625204	0.610791588
1	0.715033249	-2.842841448	1.027136196	1	0.814934625	-0.176625204	3.009791588
1	2.206033249	-2.535841448	0.112136196	1	-0.816065375	0.414374796	2.640791588
1	-2.496966751	-1.622841448	-1.176863804	1	3.612934625	2.051374796	1.186791588
1	-1.038966751	-1.110841448	-2.081863804	1	2.038934625	2.591374796	0.526791588
1	-1.253966751	-3.543841448	-0.200863804	1	2.547934625	1.403374796	3.325791588
1	-1.136966751	-3.623841448	-1.974863804	1	2.195934625	3.115374796	2.974791588
1	1.048033249	-0.353841448	-0.800863804	1	0.144934625	1.006374796	0.212791588
8	-0.918966751	-0.907841448	0.006136196	8	2.231934625	0.535374796	0.846791588
8	0.592033249	-3.042841448	-1.060863804	8	0.612934625	1.878374796	2.737791588
1	-1.104966751	0.593158552	1.375136196	1	2.589934625	-1.062625204	-0.287208412
6	4.459966751	1.505841448	0.188863804	7	-1.557934625	-0.067374796	0.469208412
1	4.680966751	2.003841448	-0.751136196	6	-2.785934625	0.822625204	0.336208412
1	4.562966751	2.209841448	1.010863804	8	-2.778934625	2.075625204	0.220208412
7	2.824966751	-0.230158552	0.274863804	8	-1.283934625	-2.531374796	0.467208412
6	4.152966751	-0.807158552	0.422863804	6	-3.984934625	-0.173374796	0.372208412
6	2.932966751	1.115841448	0.131863804	6	-3.575934625	-1.431374796	0.463208412
8	4.268966751	-2.030158552	0.557863804	6	-2.195000000	-1.543000000	0.429000000
8	1.939966751	1.884841448	-0.018136196	6	-4.569934625	-2.678374796	0.544208412

7	5.228966751	0.255841448	0.383863804	6	-5.878934625	-2.468374796	0.533208412
1	6.218966751	0.141841448	0.468863804	1	-4.129934625	-3.682374796	0.606208412
				1	-6.611934625	-3.285374796	0.586208412
				6	-6.432934625	-0.974374796	0.441208412
				1	-7.495934625	-0.855374796	0.435208412
				6	-5.645934625	0.091625204	0.372208412
				1	-5.980934625	1.004625204	0.325208412
				6	-2.026934625	-1.515374796	0.469208412

[TS3-3CNIND]‡				**HDT Product (7a)**			
6	6.669000000	1.108000000	-0.807000000	6	-5.627805000	0.031519000	-0.734394000
6	5.281000000	1.057000000	-0.948000000	6	-4.256560000	0.304295000	-0.694565000
6	4.543000000	0.117000000	-0.218000000	6	-3.539081000	0.149423000	0.501445000
6	5.202000000	-0.765000000	0.652000000	6	-4.221079000	-0.282121000	1.651532000
6	6.586000000	-0.705000000	0.789000000	6	-5.588764000	-0.556085000	1.610166000
6	7.323000000	0.232000000	0.059000000	6	-6.296871000	-0.398329000	0.414092000
1	7.237000000	1.836000000	-1.379000000	1	-6.170422000	0.157303000	-1.662332000
1	4.779000000	1.746000000	-1.617000000	1	-3.746428000	0.631757000	-1.589031000
1	4.630000000	-1.501000000	1.207000000	1	-3.673632000	-0.405880000	2.577890000
1	7.091000000	-1.393000000	1.461000000	1	-6.100181000	-0.884942000	2.505491000
1	8.403000000	0.275000000	0.163000000	1	-7.358468000	-0.605944000	0.379758000
6	3.037000000	-0.004000000	-0.316000000	6	-2.044747000	0.385719000	0.614740000
6	2.392000000	0.646000000	-1.562000000	6	-1.463070000	1.378734000	-0.376976000
8	2.444000000	1.847000000	-1.734000000	8	-1.462352000	1.248364000	-1.606663000
8	1.828000000	-0.248000000	-2.349000000	8	-0.882625000	2.430953000	0.267771000
6	1.119000000	0.276000000	-3.509000000	6	-0.172048000	3.432179000	-0.556846000
1	1.793000000	0.901000000	-4.098000000	1	0.765554000	3.003684000	-0.901039000
1	0.813000000	-0.608000000	-4.066000000	1	-0.795419000	3.728564000	-1.397070000
1	0.256000000	0.844000000	-3.160000000	1	0.004795000	4.262407000	0.117507000
6	0.411000000	0.574000000	2.449000000	6	1.731145000	-1.554316000	-0.165555000
6	0.598000000	0.287000000	0.985000000	6	2.906150000	-1.032739000	-0.990487000
6	2.699000000	1.950000000	1.275000000	6	-1.467338000	-1.745820000	-0.612985000
6	2.174000000	2.114000000	2.693000000	6	-0.369384000	-2.790897000	-0.593508000
1	0.616000000	-0.739000000	0.651000000	1	2.532737000	-0.416525000	-1.805975000
1	0.983000000	-0.149000000	3.050000000	1	1.167329000	-0.732954000	0.276056000
1	-0.648000000	0.442000000	2.681000000	1	2.081005000	-2.221474000	0.629568000
1	3.781000000	2.079000000	1.227000000	1	-2.446075000	-2.224964000	-0.514586000
1	2.207000000	2.619000000	0.567000000	1	-1.429112000	-1.178964000	-1.543317000
1	2.716000000	1.431000000	3.366000000	1	-0.242554000	-3.194173000	0.416320000
1	2.364000000	3.143000000	3.015000000	1	-0.639265000	-3.604686000	-1.266852000
1	0.313000000	1.034000000	0.253000000	1	3.474682000	-1.864293000	-1.401038000
8	2.400000000	0.563000000	0.887000000	8	-1.246072000	-0.854810000	0.536514000
8	0.781000000	1.906000000	2.778000000	8	0.901895000	-2.296433000	-1.105979000
1	2.758000000	-1.035000000	-0.247000000	1	-1.812495000	0.749269000	1.610997000
6	-3.599000000	1.299000000	0.429000000	6	3.729003000	1.155753000	-0.035447000
6	-2.153000000	1.299000000	0.429000000	6	4.932821000	-0.755554000	0.513142000
6	-1.454000000	2.489000000	0.429000000	7	3.817433000	-0.214398000	-0.186018000
6	-2.181000000	3.691000000	0.429000000	8	5.256056000	-1.949564000	0.537640000
6	-3.571000000	3.691000000	0.429000000	8	2.875313000	1.902259000	-0.536281000
6	-4.297000000	2.489000000	0.429000000	6	4.890055000	1.579290000	0.862026000
6	-4.026000000	-0.095000000	0.429000000	1	4.508296000	2.055920000	1.766650000
6	-2.876000000	-0.907000000	0.429000000	1	5.531072000	2.287509000	0.334188000
1	-0.356000000	2.506000000	0.429000000	7	5.551234000	0.304212000	1.128520000
1	-1.635000000	4.647000000	0.429000000	1	6.375651000	0.177223000	1.686995000
1	-4.117000000	4.647000000	0.430000000				
1	-5.396000000	2.506000000	0.430000000				
1	-2.876000000	-1.996000000	0.429000000				
7	-1.726000000	-0.095000000	0.429000000				
6	-5.493000000	-0.564000000	0.429000000				
7	-6.585000000	-0.913000000	0.429000000				

Phth Product (4a)				3CNIND Product (5a)			
6	-6.465612000	0.382239000	-0.443994000	6	-7.181274000	-1.646268000	-0.205433000
6	-5.074502000	0.487355000	-0.543823000	6	-5.872376000	-1.360883000	-0.609475000
6	-4.277478000	0.450364000	0.610313000	6	-5.106163000	-0.418344000	0.091610000
6	-4.900198000	0.307545000	1.861599000	6	-5.675306000	0.231486000	1.200310000
6	-6.288077000	0.200714000	1.960033000	6	-6.979237000	-0.056532000	1.604482000
6	-7.075611000	0.239026000	0.804486000	6	-7.737355000	-0.997841000	0.899395000
1	-7.069404000	0.414850000	-1.341610000	1	-7.762581000	-2.373907000	-0.755960000
1	-4.610348000	0.593335000	-1.513801000	1	-5.449705000	-1.877630000	-1.458620000
1	-4.291949000	0.276353000	2.757222000	1	-5.090362000	0.960663000	1.747084000
1	-6.753086000	0.093825000	2.931461000	1	-7.404058000	0.454195000	2.458350000
1	-8.152549000	0.161194000	0.878125000	1	-8.750801000	-1.219067000	1.206632000
6	-2.761596000	0.517931000	0.577964000	6	-3.666776000	-0.072846000	-0.257241000
6	-2.171760000	1.252505000	-0.614256000	6	-3.279312000	-0.330120000	-1.702762000
8	-2.277721000	0.904053000	-1.795979000	8	-3.111566000	-1.440802000	-2.221724000
8	-1.456146000	2.342291000	-0.213793000	8	-2.957868000	0.838093000	-2.335106000
6	-0.734489000	3.105991000	-1.254110000	6	-2.496251000	0.756611000	-3.733382000
1	0.125865000	2.529055000	-1.583178000	1	-1.524104000	0.269727000	-3.771202000
1	-1.401065000	3.316333000	-2.087123000	1	-3.212582000	0.196599000	-4.329541000
1	-0.424129000	4.017015000	-0.755156000	1	-2.429053000	1.787213000	-4.060309000
6	0.700576000	-1.913212000	-0.172883000	6	0.392445000	-1.237219000	1.102447000
6	1.830662000	-1.682268000	-1.174708000	6	1.568442000	-1.385007000	0.139737000
6	-2.529438000	-1.845664000	-0.284491000	6	-2.743336000	-2.168717000	0.810576000
6	-1.531597000	-2.981789000	-0.177910000	6	-1.599093000	-2.565602000	1.723214000
1	1.446271000	-1.151005000	-2.043144000	1	1.196865000	-1.657585000	-0.850136000
1	0.263194000	-0.968838000	0.150187000	1	-0.285036000	-0.440004000	0.797981000
1	1.065186000	-2.460316000	0.703401000	1	0.753410000	-1.030784000	2.116061000
1	-3.531266000	-2.196173000	-0.018576000	1	-3.695699000	-2.434194000	1.279129000
1	-2.537133000	-1.448202000	-1.299346000	1	-2.660936000	-2.672671000	-0.152219000
1	-1.332928000	-3.218753000	0.872336000	1	-1.595124000	-1.944337000	2.624183000
1	-1.942274000	-3.865187000	-0.667246000	1	-1.725834000	-3.607231000	2.017861000
1	2.243042000	-2.637043000	-1.495032000	1	2.201223000	-2.197877000	0.485984000
8	-2.111499000	-0.804918000	0.668026000	8	-2.677847000	-0.711329000	0.628860000
8	-0.284635000	-2.717663000	-0.883357000	8	-0.299131000	-2.517217000	1.066384000
1	-2.403893000	1.015304000	1.474310000	6	3.761113000	-0.093681000	0.283955000
6	2.999248000	0.514013000	-0.658636000	6	1.920245000	1.075912000	-0.297168000
6	4.037254000	-1.445602000	0.057586000	6	4.163336000	1.249611000	0.052216000
6	4.269717000	0.883897000	0.024297000	6	4.678481000	-1.084821000	0.655155000
6	4.893343000	-0.294998000	0.455774000	6	2.970898000	1.981714000	-0.320649000
6	4.839169000	2.127412000	0.252937000	1	0.883551000	1.243612000	-0.525673000
6	6.104918000	-0.268216000	1.129305000	6	5.511743000	1.608967000	0.203876000
6	6.066607000	2.165459000	0.934910000	6	6.012830000	-0.706082000	0.799581000
1	4.353374000	3.032961000	-0.083242000	1	4.379171000	-2.108779000	0.824041000
6	6.689410000	0.986872000	1.366149000	6	6.426696000	0.626846000	0.577763000
1	6.579056000	-1.182751000	1.457714000	1	5.830639000	2.627543000	0.032131000
1	6.538740000	3.118865000	1.130407000	1	6.745131000	-1.447887000	1.085370000
1	7.634458000	1.045098000	1.889155000	1	7.469299000	0.884111000	0.698251000
7	2.918797000	-0.888911000	-0.598968000	7	2.382230000	-0.170426000	0.068153000
8	4.226169000	-2.654912000	0.235408000	1	-3.504022000	0.985437000	-0.070188000
8	2.159580000	1.256026000	-1.188722000	6	2.888298000	3.350447000	-0.646026000
				7	2.844740000	4.488905000	-0.916959000

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