

Visible-Light-Induced Dual Catalysis for *N*- α C(*sp*³)-H Amination and Alkenylation of *N*-alkyl Benzamides

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(A) General Information

Melting points were determined on a digital melting point apparatus and temperatures were uncorrected. Proton nuclear magnetic resonance (^1H NMR) spectra and carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded at 400 and 100 MHz, respectively. ^1H NMR spectrum uses TMS ($\delta = 0.00$ ppm) as internal standard, ^{13}C NMR spectrum uses CDCl_3 ($\delta = 77.00$ ppm) as internal standard. Data are presented as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz) and integration. IR spectra were recorded on a Perkin-Elmer PE-983 spectrometer with absorption in cm^{-1} . High Resolution Mass Spectra (HRMS) were recorded by ESI method. The employed solvents were dry up by standard methods when necessary. Commercially obtained reagents were used without further purification. For thin-layer chromatography (TLC), silica gel plates (Huanghai GF254) were used. Column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

Substrates **3**, quinuclidine and photocatalysts are commercially available. Except for **1d**, **1j~1n**, **1r**, **1ac~1ae** and **1ah**, substrates **1** were available in our previous work¹.

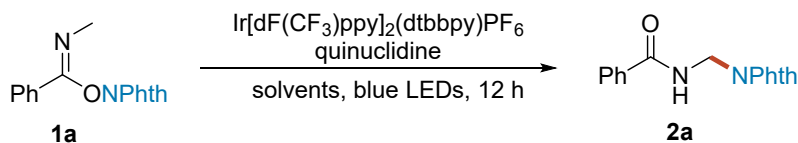
(B) Reaction Setup

8W LED strip (1 meter, NVC[®] Lighting) was purchased from <https://nvc.tmall.com/>. The strip was wound in two circles and equipped with a fan. The 5 mL sealed tubes used in this report are made by Shanghai Institute of Organic Chemistry.



Fig. S1 8 W LEDs Strip and Reaction Setup

(C) Reaction Optimization and Controls

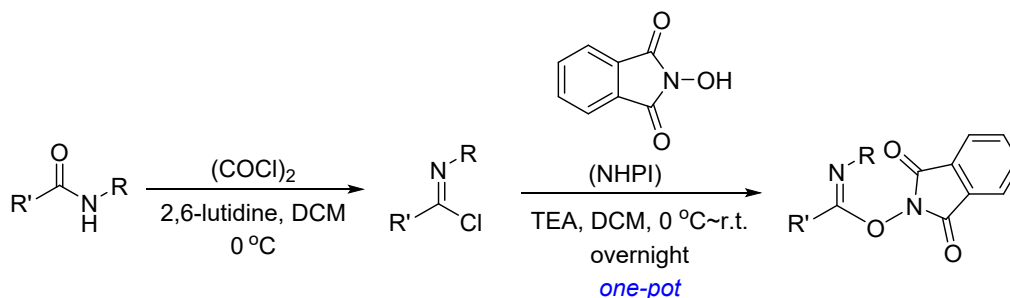


entry	solvent	cond./(mol/L)	[Ir]/(mol%)	quinuclidine/(mol%)	yield/(%) ^a
1	CH ₃ CN	0.1	2	20	82 ^b
2	CH ₃ CN	0.1	2	20	86
3	DCM	0.1	2	20	70
4	THF	0.1	2	20	17
5	Toluene	0.1	2	20	48
6	CDCl ₃	0.1	2	20	0
7	DCE	0.1	2	20	71
8	EA	0.1	2	20	56
9	DMF	0.1	2	20	73
10	Acetone- <i>d</i> ₆	0.1	2	20	87
11	DMSO- <i>d</i> ₆	0.1	2	20	97
12	DMSO- <i>d</i> ₆	0.2	2	20	97
13	DMSO- <i>d</i> ₆	0.2	1	10	99/97 ^c
14	DMSO- <i>d</i> ₆	0.2	w/o	w/o	0
15	DMSO- <i>d</i> ₆	0.2	1	w/o	0
16	DMSO- <i>d</i> ₆	0.2	w/o	10	0
17	DMSO	0.2	1	10	97^{c,d}

Reaction conditions: unless otherwise noted, a solution of **1a** (0.2 mmol), Ir[dF(CF₃)ppy]₂(dtbbpy)PF₆ (2 mol%) and quinuclidine (20 mol%) in solvent (2.0 mL) was irradiated by 8 W blue LED strip at room temperature for 12h. ^aYields were determined via ¹H-NMR analysis of the crude reaction mixture relative to benzyl methyl ether as an internal standard. ^b Ir(ppy)₂(dtbbpy)PF₆ as photocatalyst. ^c Isolated yield. ^d 0.5 h.

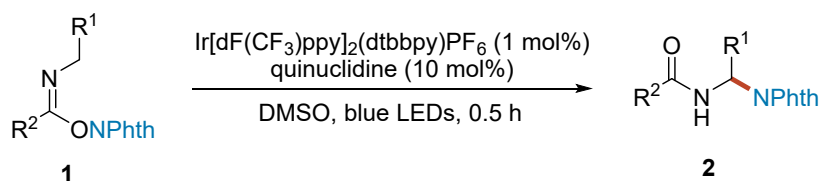
(D) General Procedure for the Preparation of NHPI Imidate Esters 1d, 1j~1n, 1r, 1ac~1ae and 1ah¹

1ah¹



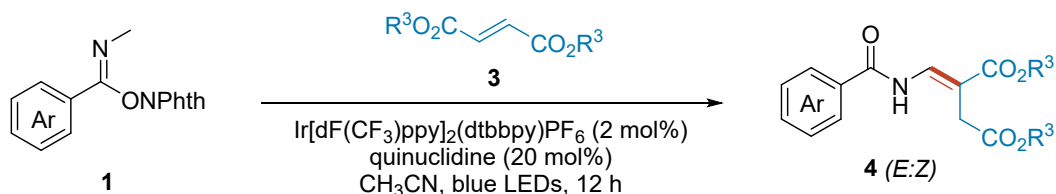
To a solution of 1.0 equiv of amide in CH₂Cl₂ (0.2 M) was added 1.5 equiv of 2,6-lutidine then 1.0 equiv of oxalyl chloride dropwise at 0 °C under an argon atmosphere resulting in the evolution of gas. After stirring for 20-45 min, 1.0 equiv of NHPI was added all at once and 2.5 equiv of triethylamine was added dropwise. Upon finishing the addition of triethylamine, the cooling bath was removed. After the reaction mixture was stirred overnight at room temperature, and CH₂Cl₂ was removed. The residue was diluted with 20 mL of ethyl acetate, filtered, and concentrated under reduced pressure, then the corresponding residue was purified by a column chromatography (SiO₂) using pure DCM or EtOAc/petroleum ether solvent mixtures as eluent to give the target NHPI imidate esters.

(E) General Procedure for the Photoredox Catalysis Enabled Amination Reaction



A dry 10 mL sealed tube equipped with a Teflon cap and a magnetic stirrer was charged with the photocatalyst Ir[dF(CF₃)ppy]₂(dtbbpy)PF₆ (0.002 mmol, 0.01 equiv), NHPI imidate ester **1** (0.2 mmol, 1.0 equiv) and quinuclidine (0.02 mmol, 0.1 equiv), then injected 1.0 mL of dry dimethyl sulfoxide through a syringe. The above mixture was degassed by bubbling argon for 10 minutes, and then the reaction tube was sealed with a Teflon cap under argon and placed in the blue light of an 8 W blue LED strip at room temperature (using a fan to maintain the temperature). After half an hour of reaction, the reaction mixture was directly purified by a column chromatography (SiO₂) using PE/EA = 1/1 as eluent to obtain the desired amidation product **2**.

(F) General Procedure for the Photoredox Catalysis Enabled Alkenylation Reaction

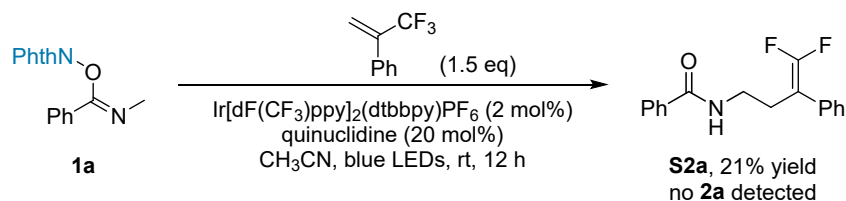
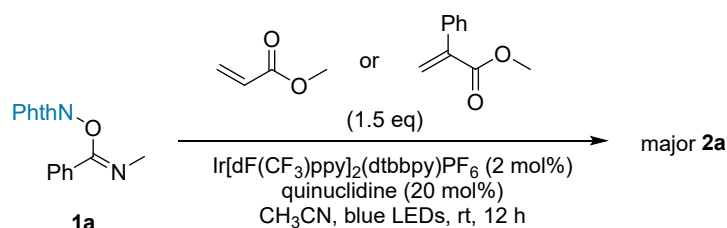


A dry 10 mL sealed tube equipped with a Teflon cap and a magnetic stirrer was charged with the photocatalyst $Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$ (0.004 mmol, 0.01 equiv), NHPI imidate ester **1** (0.2 mmol, 1.0 equiv), fumarate ester **3** (0.3 mmol, 1.5 equiv) and quinuclidine (0.04 mmol, 0.2 equiv), then injected 2.0 mL of dry acetonitrile through a syringe. The above mixture was degassed by bubbling argon for 10 minutes, and then the reaction tube was sealed with a Teflon cap under argon atmosphere and placed in the blue light of an 8 W blue LED strip at room temperature (using a fan to maintain the temperature). After 12 hours of reaction, the reaction solvent was removed, and the residue was analyzed by 1H NMR to determine the E/Z selectivity. After that, the reaction mixture was directly purified by a column chromatography (SiO_2) with PE/EA = 1/1 as the eluent to obtain the desired amidation product **4**.

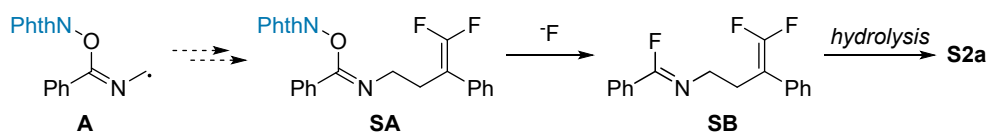
(G) Other Attempts

Besides dimethyl fumarate, other alkenes such as benzyl acrylate and methyl 2-benzyl acrylate were also used to react with **1a** in an attempt to capture the radical intermediate **A**, but both mainly gave rearranged product **2a**. As for (3,3,3-trifluoroprop-1-en-2-yl)benzene, the rearranged product is not obtained at this time, and an additional product **S2a** was isolated, as show below.

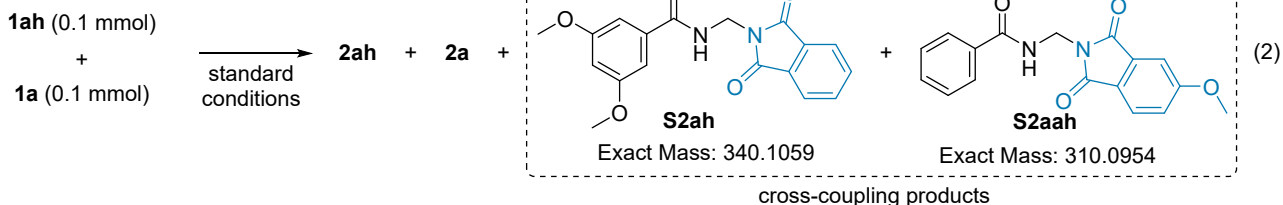
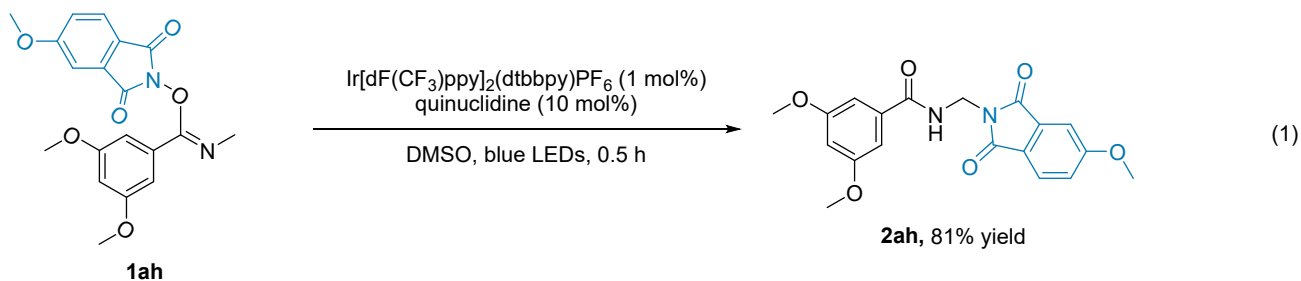
A possible process was given, the radical intermediate **A** was captured by (3,3,3-trifluoroprop-1-en-2-yl)benzene and subsequently substituted by F^- to give SB, which was hydrolyzed to give **S2a**.



Possible process:

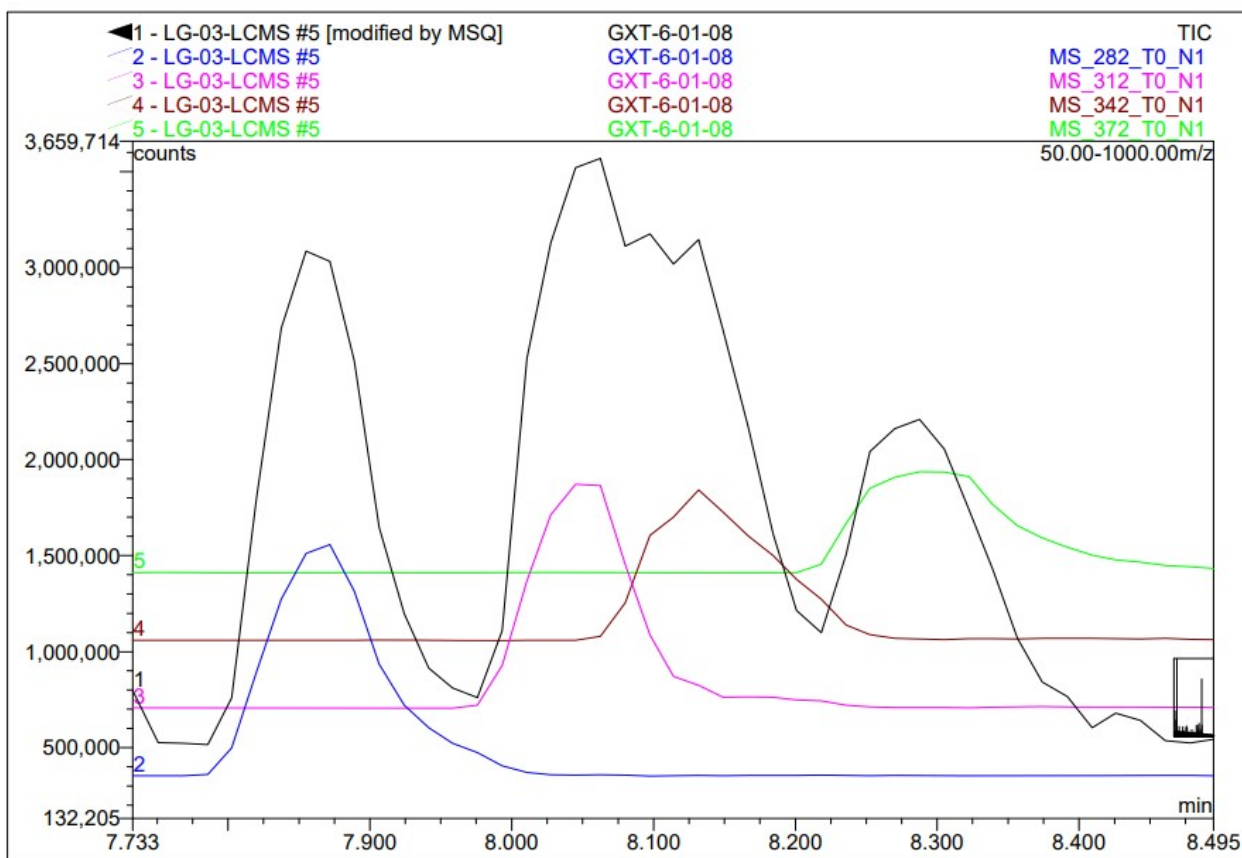


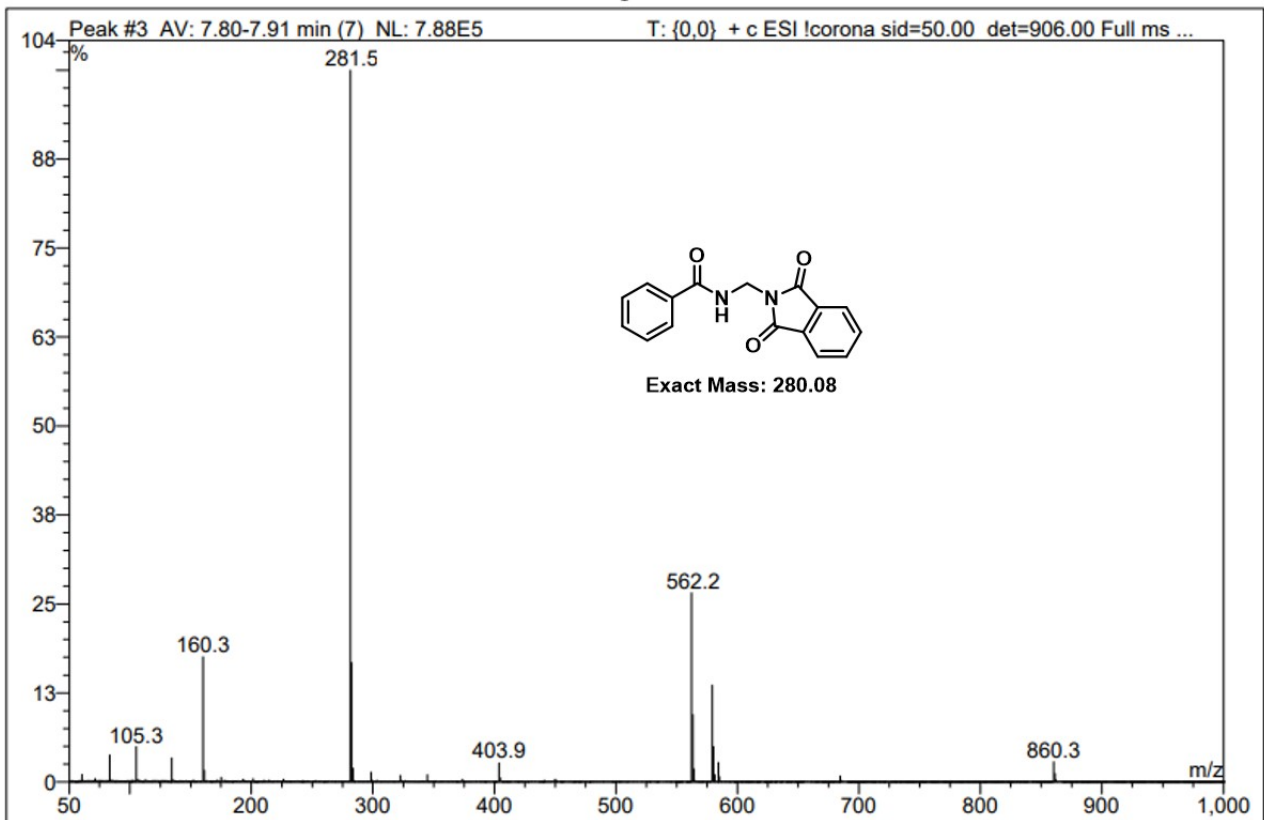
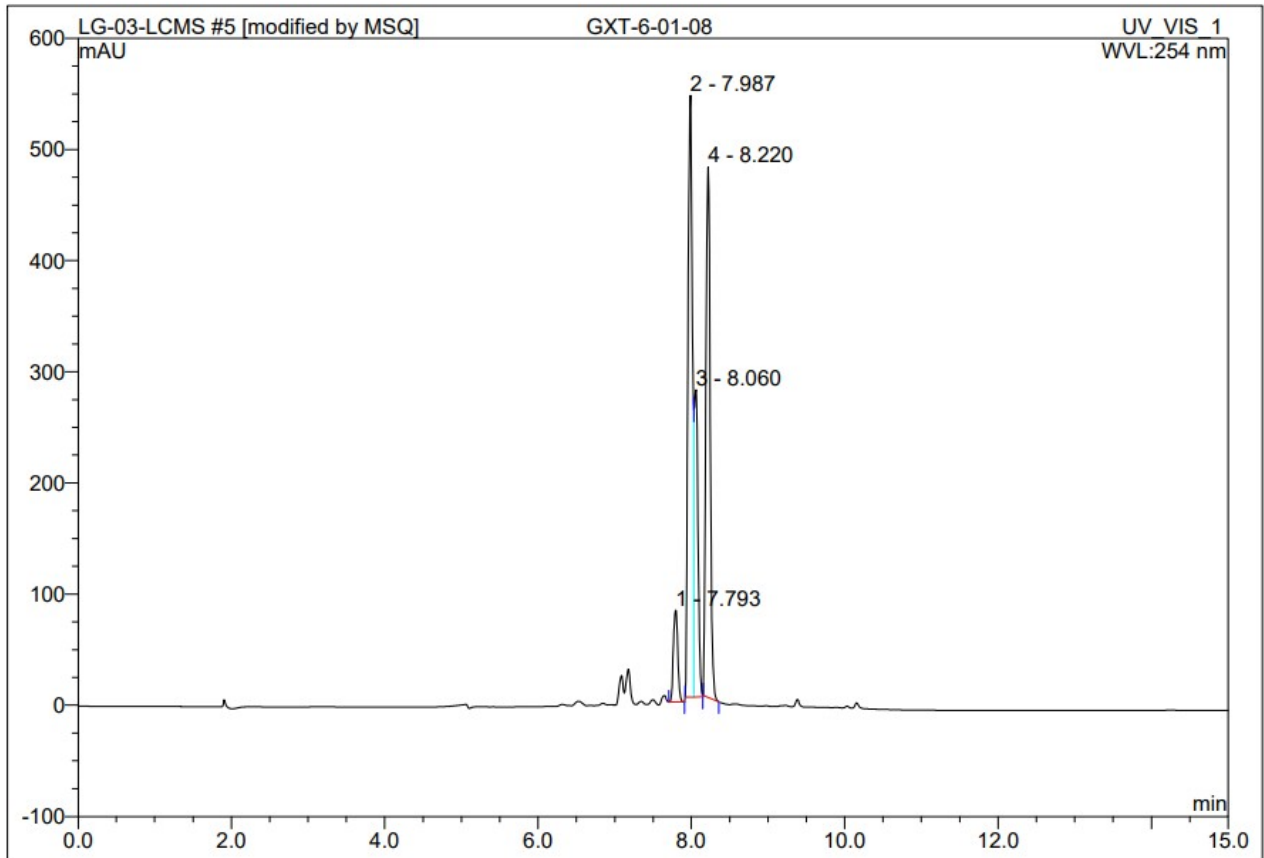
(H) Crossover Experiment

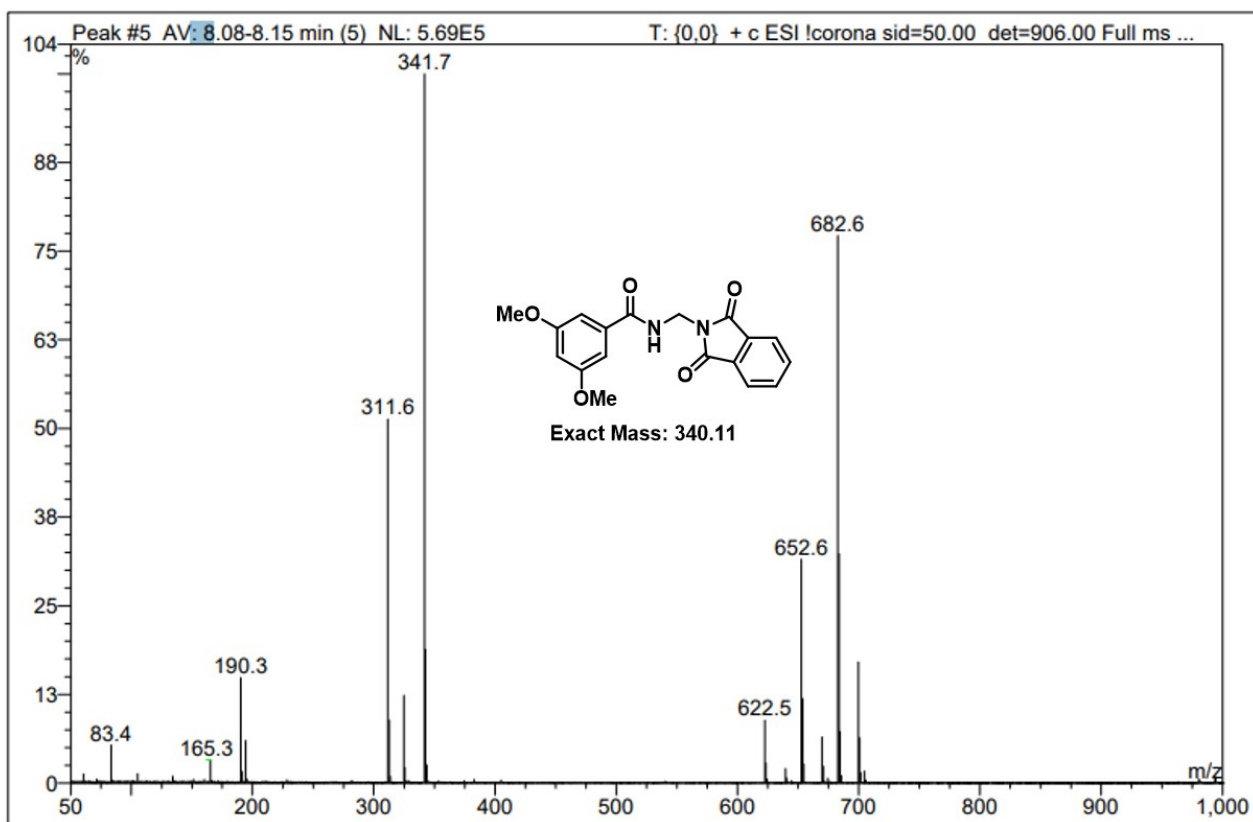
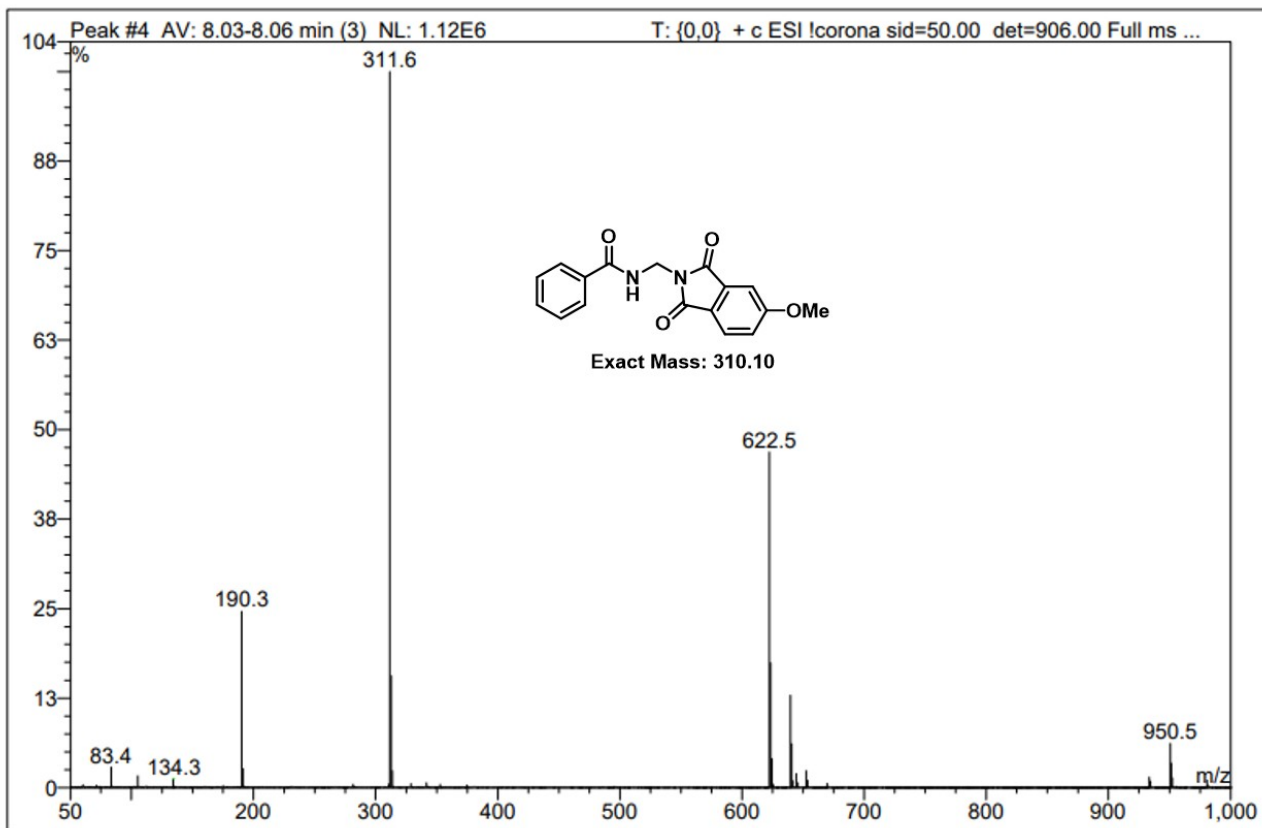


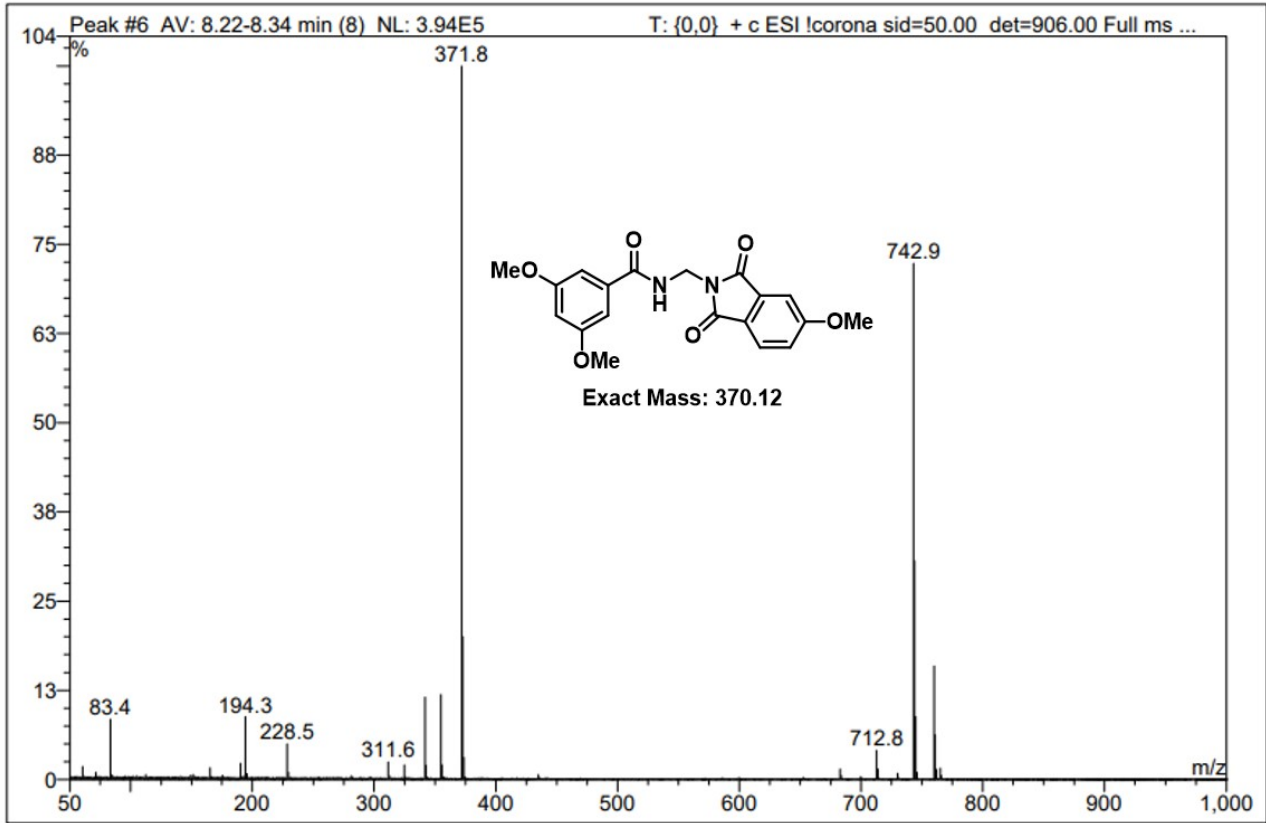
Firstly, **1ah** was demonstrated could undergo amination reaction smoothly to give **2ah** in 81% yield under standard conditions. Then a crossover experiment was performed with a mixture **1ah** (0.1 mmol) and **1a** (0.1 mmol) under the general procedure for the photoredox catalysis enabled amination reaction. The results was determined by LCMS. Except for usual products **2ah** and **2a**,

cross-over products **S2ah** and **S2aah** were also detected, revealing that the ⁻NPhth rebound process is intermolecular.

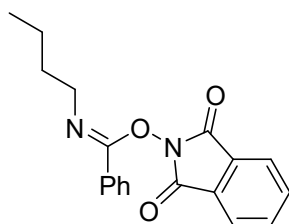




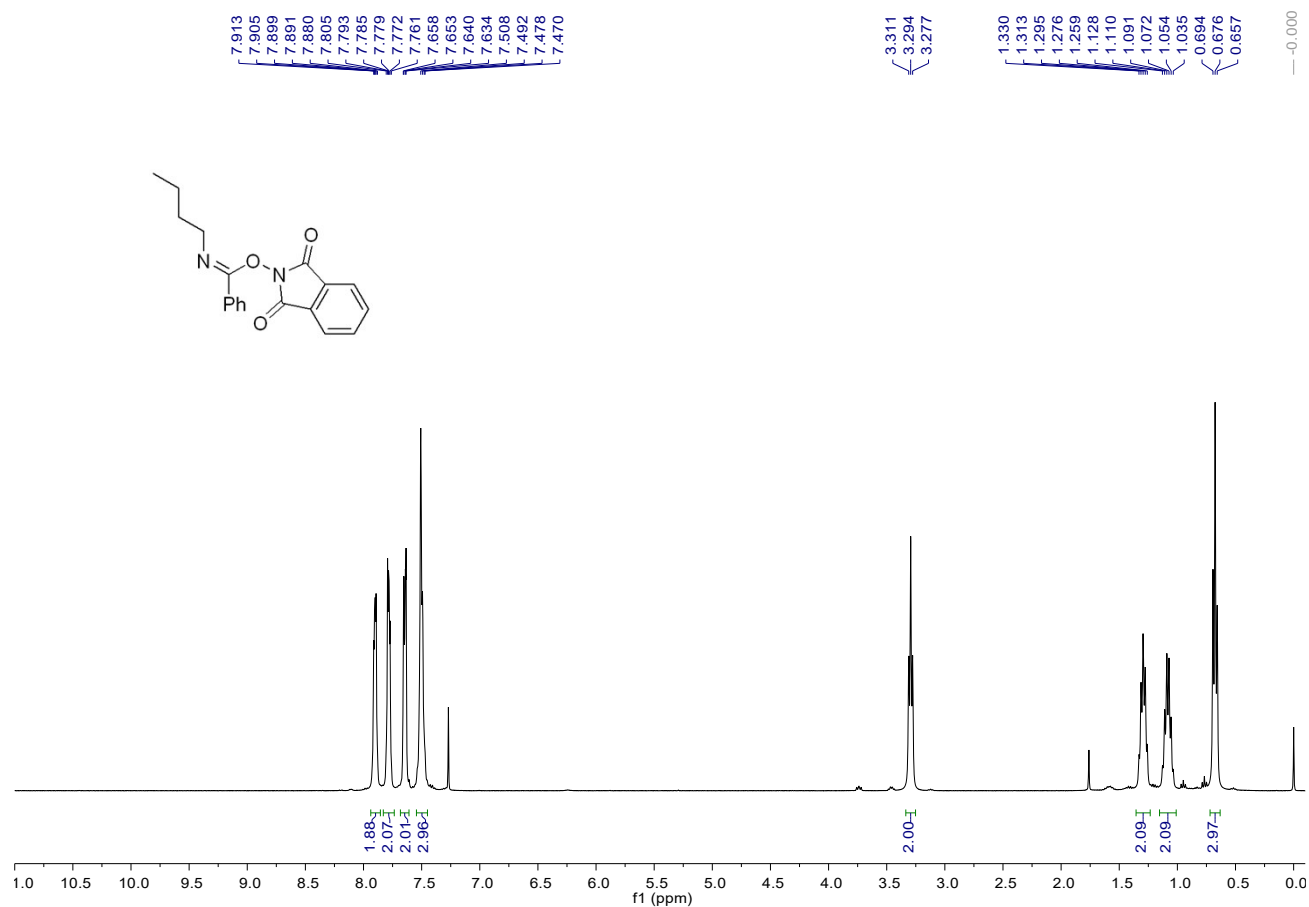


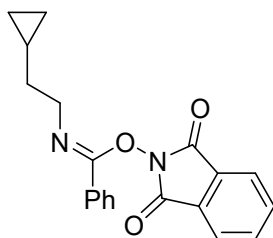
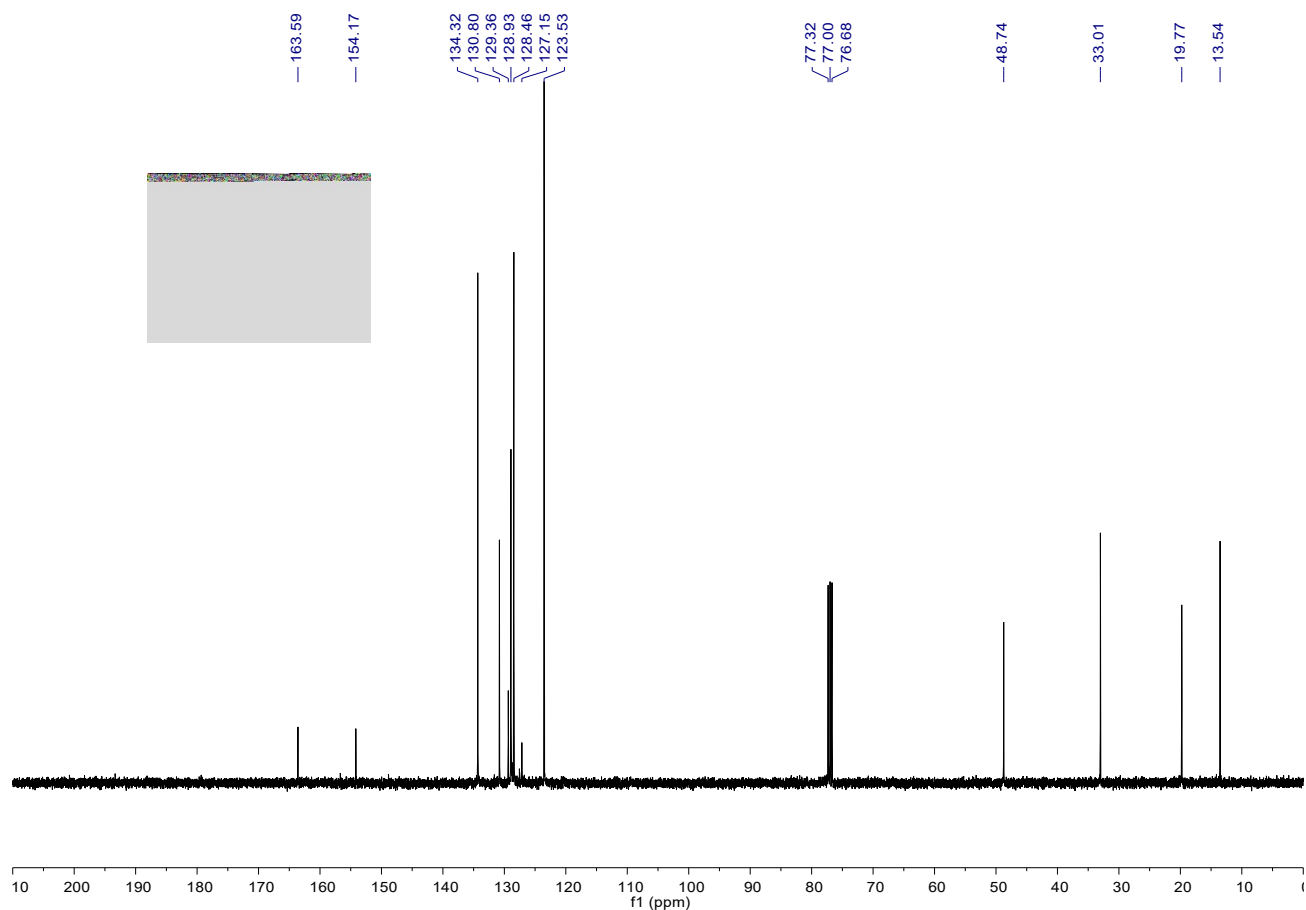


(I) Spectroscopic Data of Substrates and Products

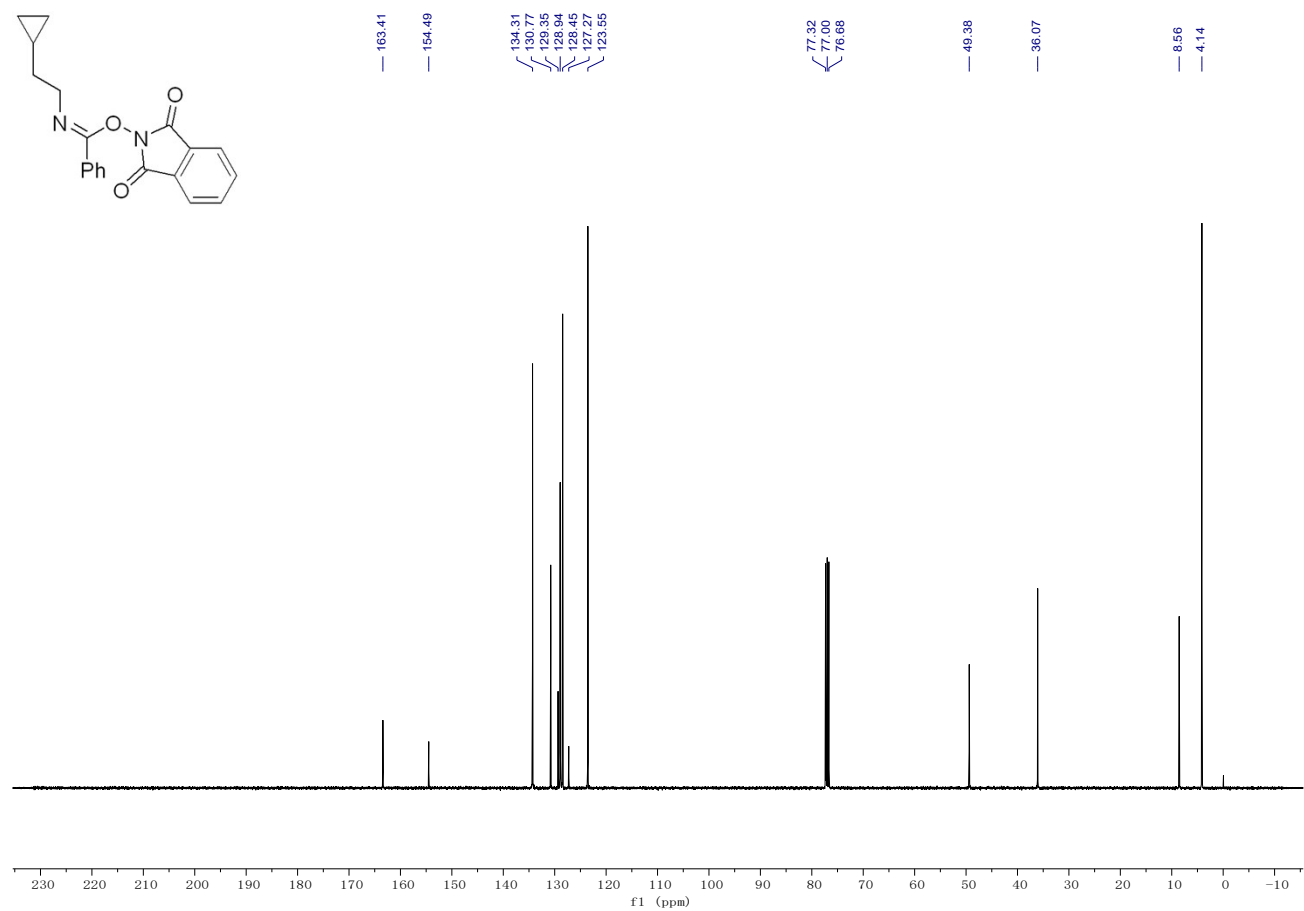
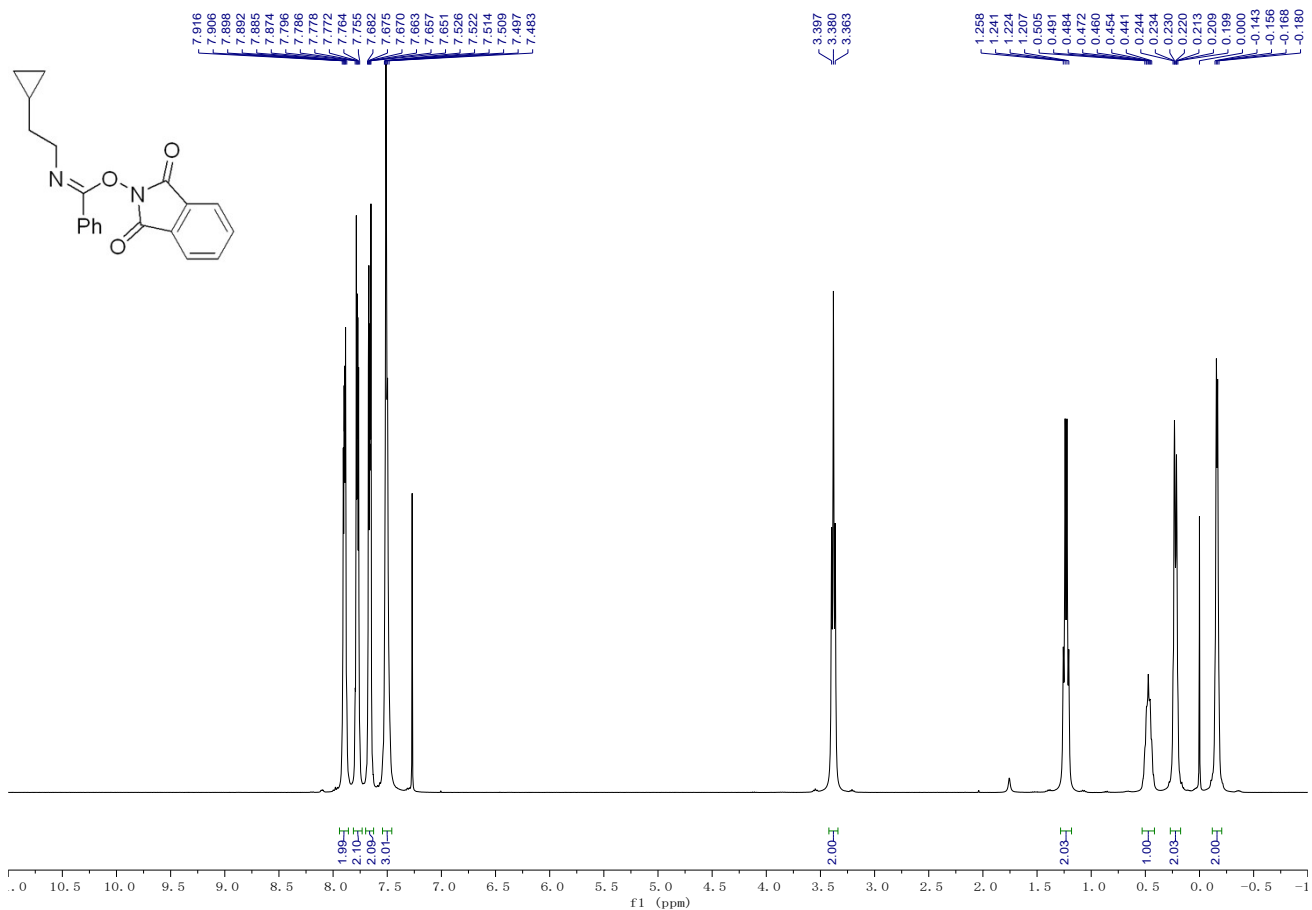


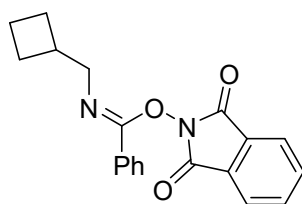
1,3-dioxoisindolin-2-yl (Z)-N-butylbenzimidate (1d). A white solid, 2.26 g, 77% yield; M.p.: 41-43 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.94-7.85 (m, 2H), 7.78 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.68-7.61 (m, 2H), 7.54-7.45 (m, 3H), 3.29 (t, $J = 6.7$ Hz, 2H), 1.36-1.23 (m, 2H), 1.08 (h, $J = 7.4$ Hz, 2H), 0.68 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 163.6, 154.2, 134.3, 130.8, 129.4, 128.9, 128.5, 127.2, 123.5, 48.7, 33.0, 19.8, 13.5; IR (neat) ν 2951, 2867, 1739, 1705, 1465, 1362, 1182, 1017, 878, 762, 717 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{19}\text{H}_{19}\text{N}_2\text{O}_3^+$ Requires: 323.1390, Found: 323.1383.



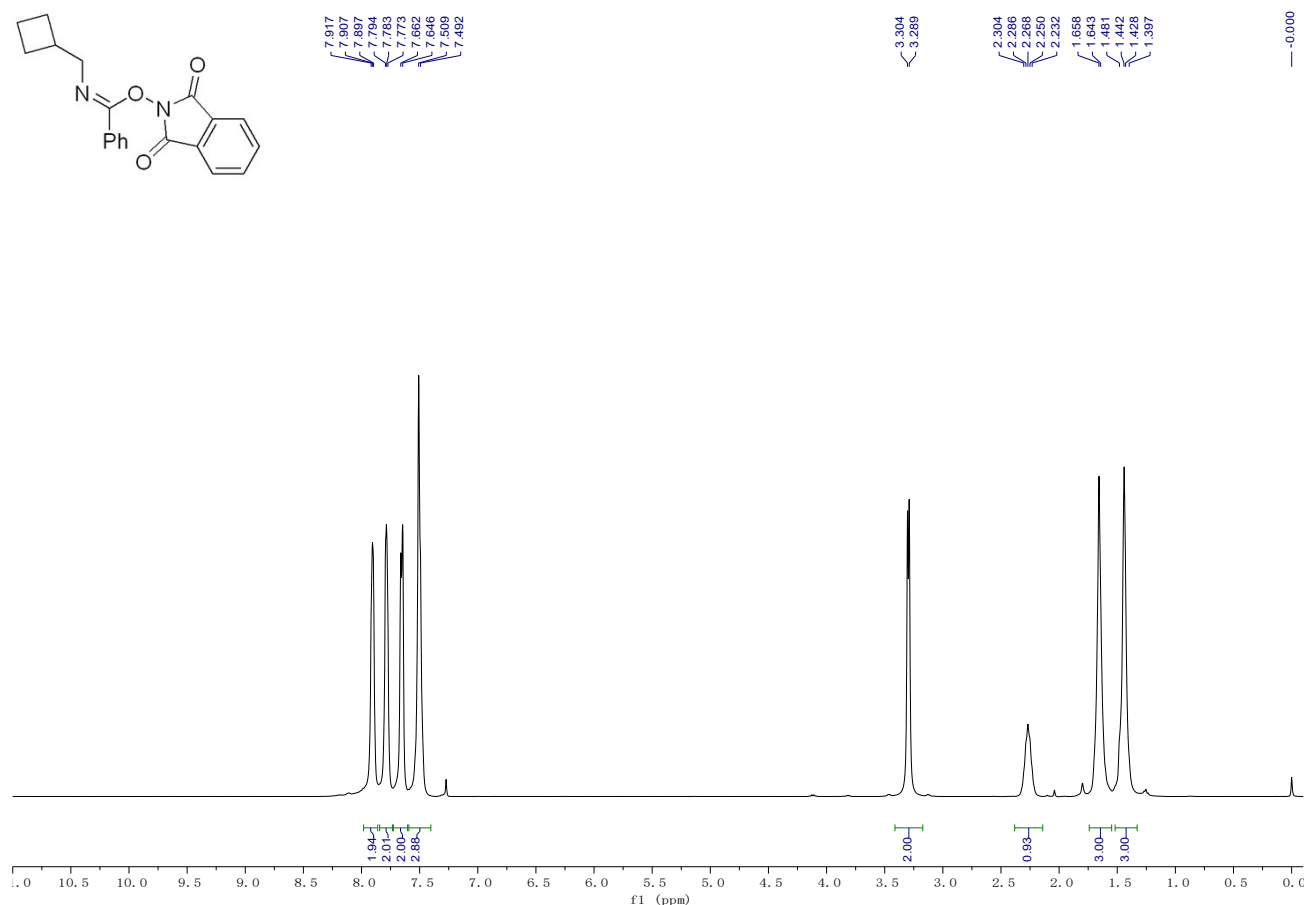


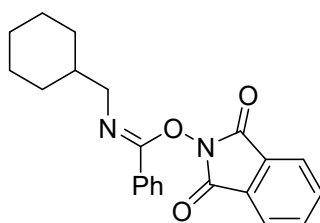
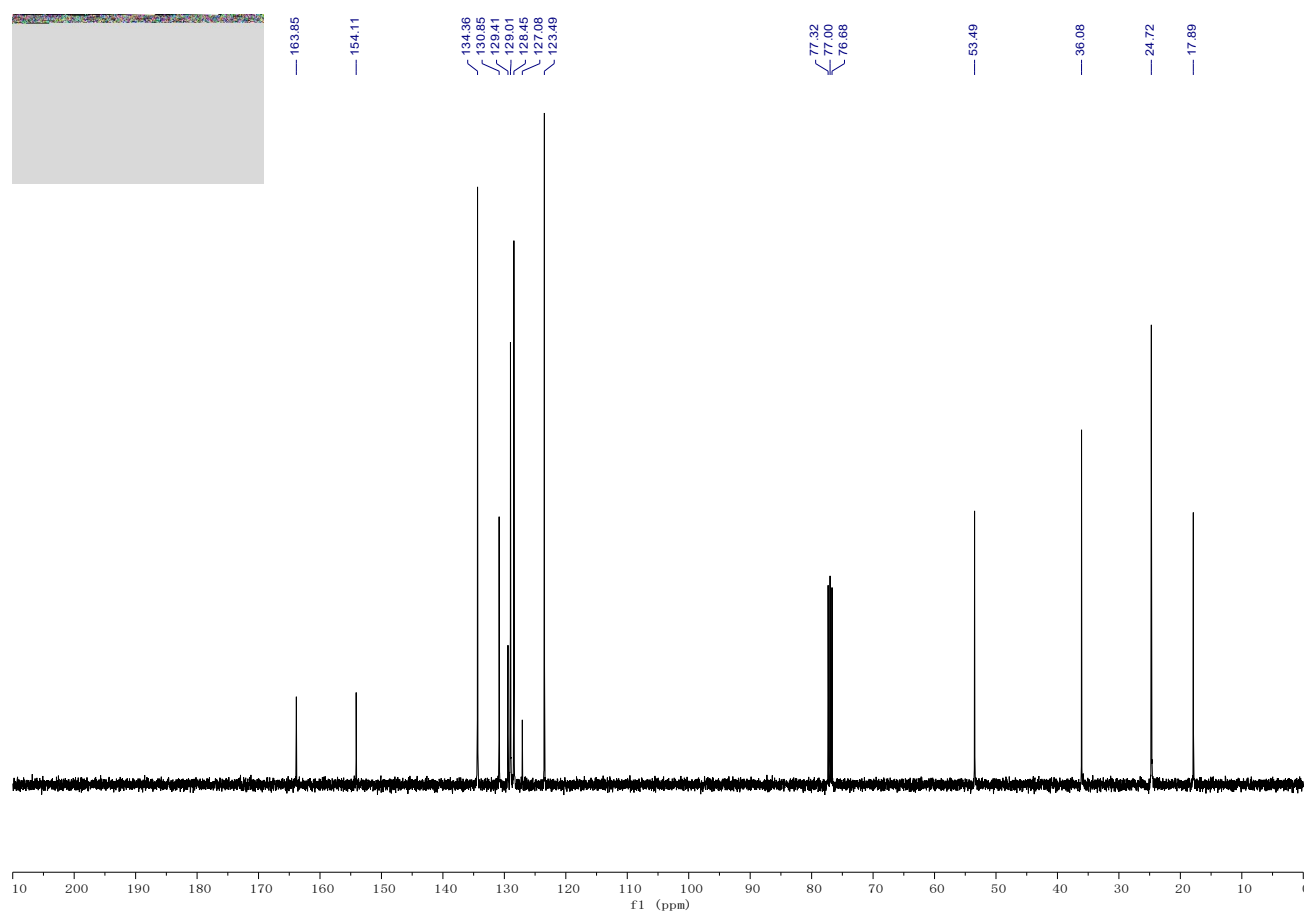
1,3-dioxoisindolin-2-yl (Z)-N-(2-cyclopropylethyl)benzimidate (1j). A white solid, 962 mg, 58% yield; M.p.: 81-82 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.94-7.86 (m, 2H), 7.78 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.70-7.63 (m, 2H), 7.54-7.46 (m, 3H), 3.38 (t, $J = 6.8$ Hz, 2H), 1.23 (q, $J = 6.8$ Hz, 2H), 0.53-0.42 (m, 1H), 0.27-0.17 (m, 2H), -0.12--0.21 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 163.4, 154.5, 134.3, 130.8, 129.3, 128.9, 128.5, 127.3, 123.5, 49.4, 36.1, 8.6, 4.1; IR (neat) ν 2941, 2889, 1793, 1736, 1709, 1601, 1466, 1362, 1319, 1241, 1185, 1052, 1005, 878 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{20}\text{H}_{19}\text{N}_2\text{O}_3^+$ Requires: 335.1390, Found: 335.1384.



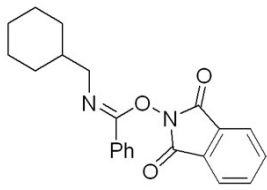


1,3-dioxoisindolin-2-yl (Z)-N-(cyclobutylmethyl)benzimidate (1k). A white solid, 1.10 g, 66% yield; M.p.: 97-99 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.91 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.78 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.69-7.62 (m, 2H), 7.55-7.45 (m, 3H), 3.29 (d, $J = 6.1$ Hz, 2H), 2.33-2.21 (m, 1H), 1.73-1.60 (m, 3H), 1.50-1.37 (m, 3H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 163.9, 154.2, 134.4, 130.9, 129.5, 129.1, 128.5, 127.2, 123.5, 53.6, 36.2, 24.8, 17.9; IR (neat) ν 2976, 2928, 2863, 1794, 1736, 1602, 1465, 1317, 1238, 1183, 1113, 1077, 1019, 878, 780 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{20}\text{H}_{19}\text{N}_2\text{O}_3^+$ Requires: 335.1390, Found: 335.1389.

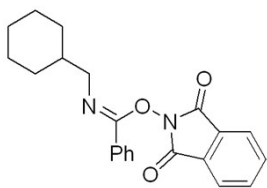
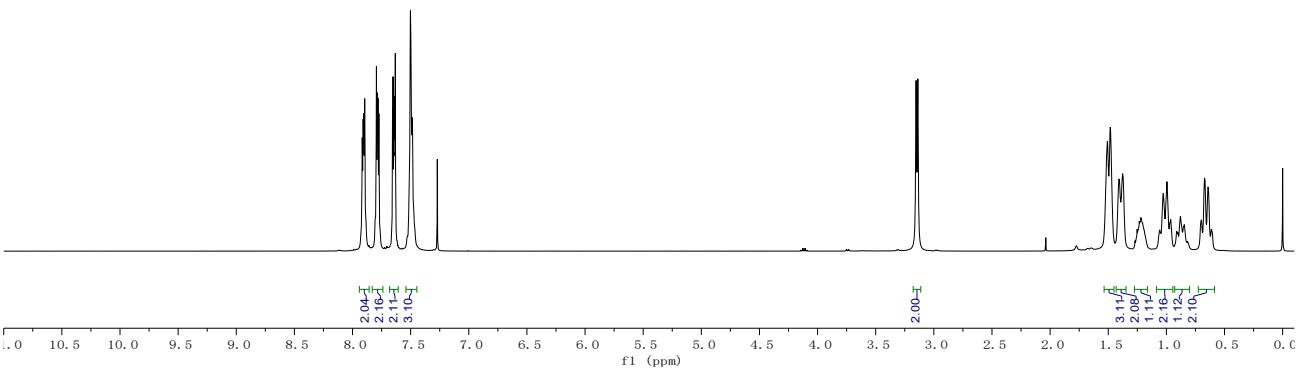




1,3-dioxoisindolin-2-yl (Z)-N-(cyclohexylmethyl)benzimidate (11). A white solid, 1.57 g, 87% yield; M.p.: 115-117 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.94-7.86 (m, 2H), 7.78 (dd, $J = 5.5$, 3.1 Hz, 2H), 7.68-7.61 (m, 2H), 7.54-7.45 (m, 3H), 3.15 (d, $J = 6.0$ Hz, 2H), 1.54-1.45 (m, 3H), 1.43-1.35 (m, 2H), 1.27-1.16 (m, 1H), 1.09-0.94 (m, 2H), 0.93-0.80 (m, 1H), 0.73-0.59 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 163.8, 153.9, 134.3, 130.8, 129.5, 129.0, 128.4, 127.2, 123.5, 55.4, 39.1, 30.5, 26.3, 25.8; IR (neat) ν 2919, 2852, 1797, 1733, 1599, 1465, 1373, 1241, 1184, 1060, 1037, 922, 878 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{22}\text{H}_{23}\text{N}_2\text{O}_3^+$ Requires: 363.1703, Found: 363.1697.

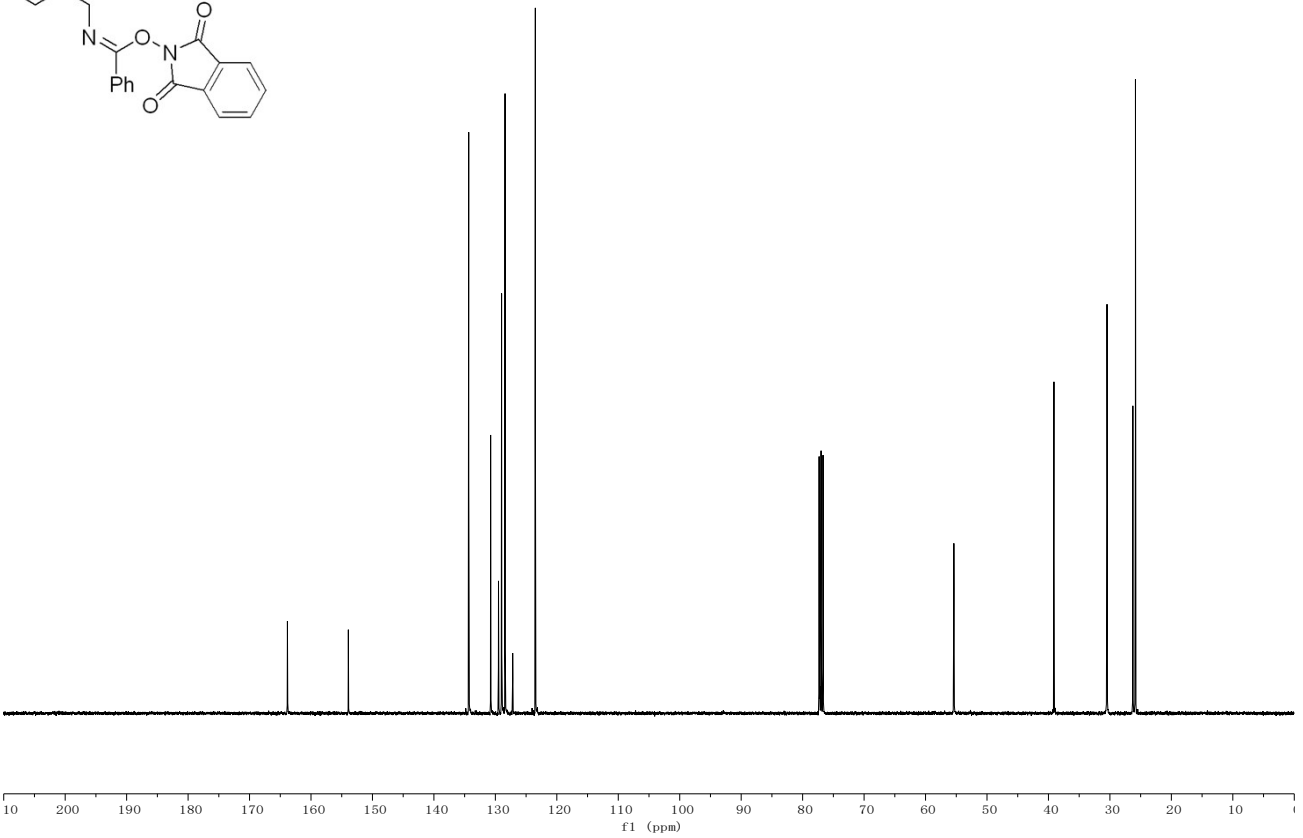


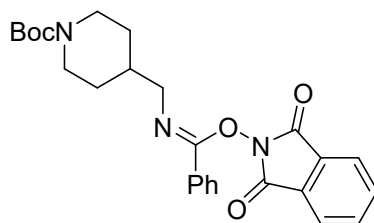
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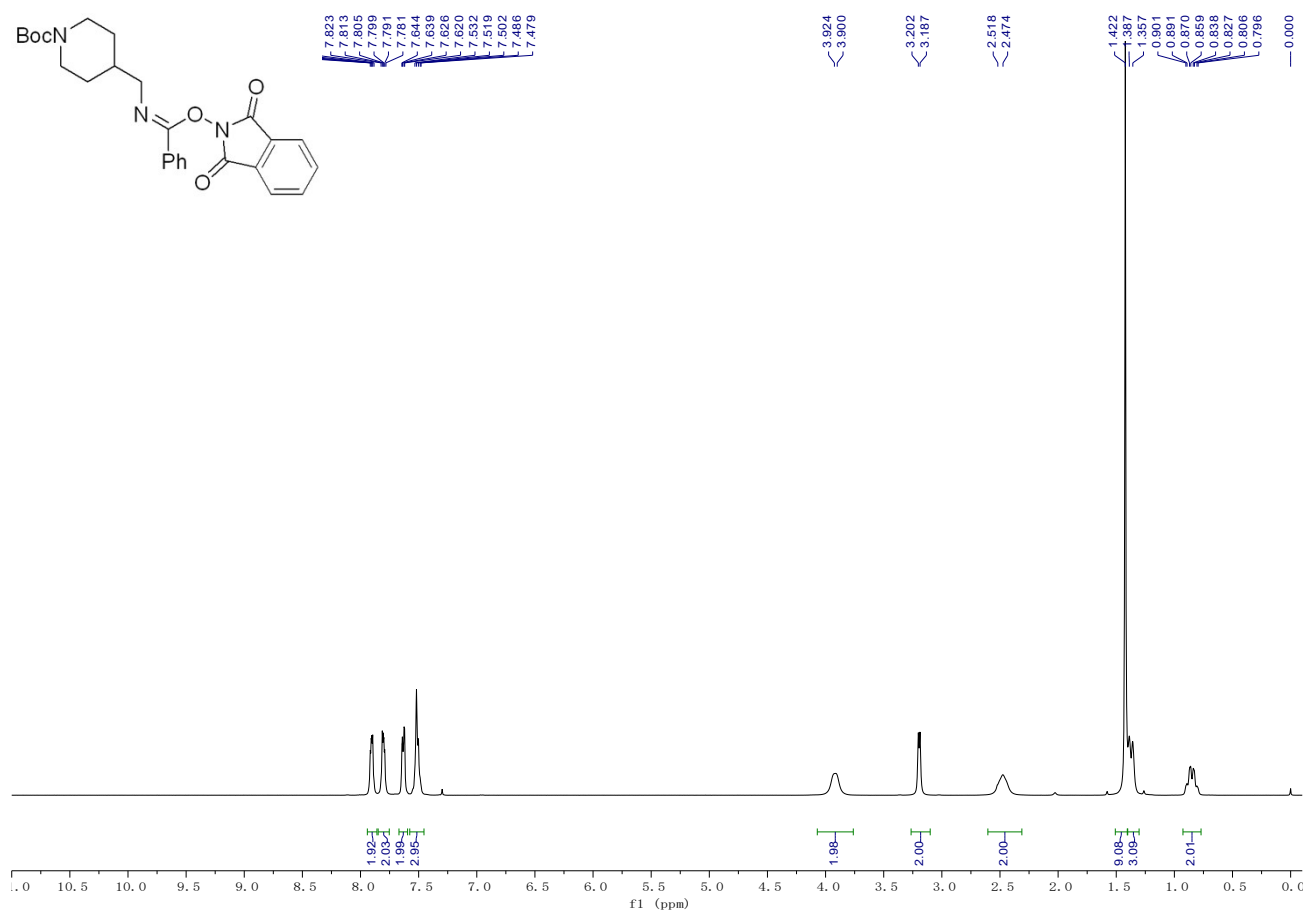
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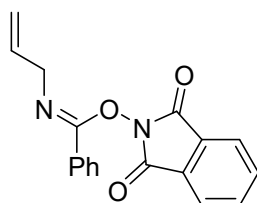
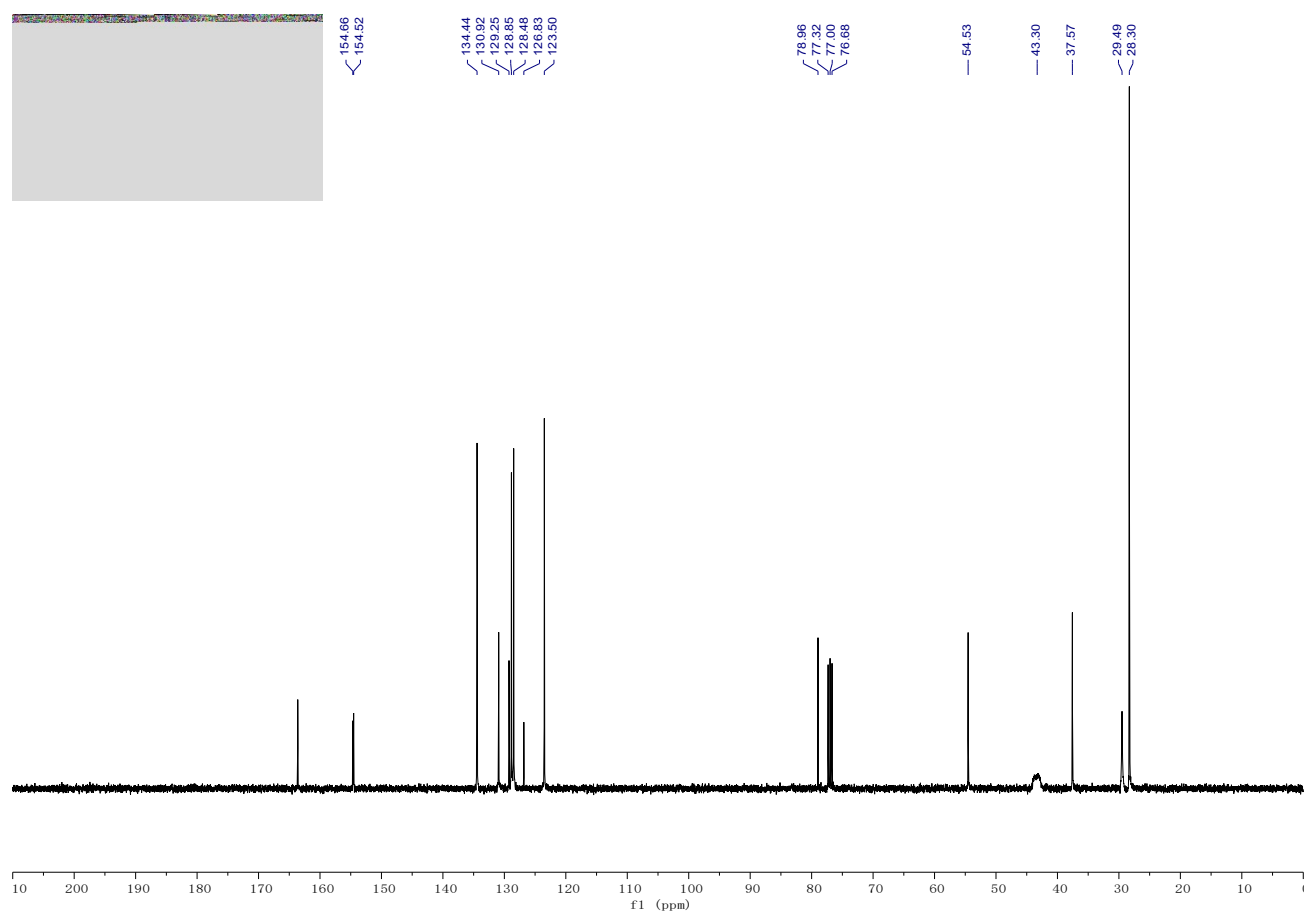
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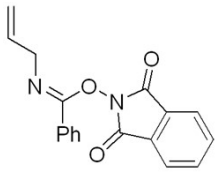


tert-butyl (Z)-4-((((1,3-dioxoisindolin-2-yl)oxy)(phenyl)methylene)amino)methyl)piperidine-1-carboxylate (1m). A white solid, 1.97 g, 85% yield; M.p.: 117-118 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.94-7.86 (m, 2H), 7.80 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.67-7.60 (m, 2H), 7.58-7.45 (m, 3H), 4.07-3.76 (m, 2H), 3.19 (d, $J = 5.9$ Hz, 2H), 2.60-2.31 (m, 2H), 1.42 (s, 9H), 1.40-1.30 (m, 3H), 0.93-0.77 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 163.6, 154.7, 154.5, 134.4, 130.9, 129.2, 128.9, 128.5, 126.8, 123.5, 79.0, 54.5, 43.3, 37.6, 29.5, 28.3; IR (neat) ν 2975, 2917, 2843, 1733, 1678, 1479, 1365, 1289, 1238, 1220, 1186, 1076, 1016 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{26}\text{H}_{29}\text{N}_3\text{O}_5\text{Na}^+$ Requires: 486.1999, Found: 486.2006.



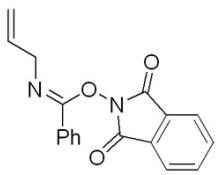
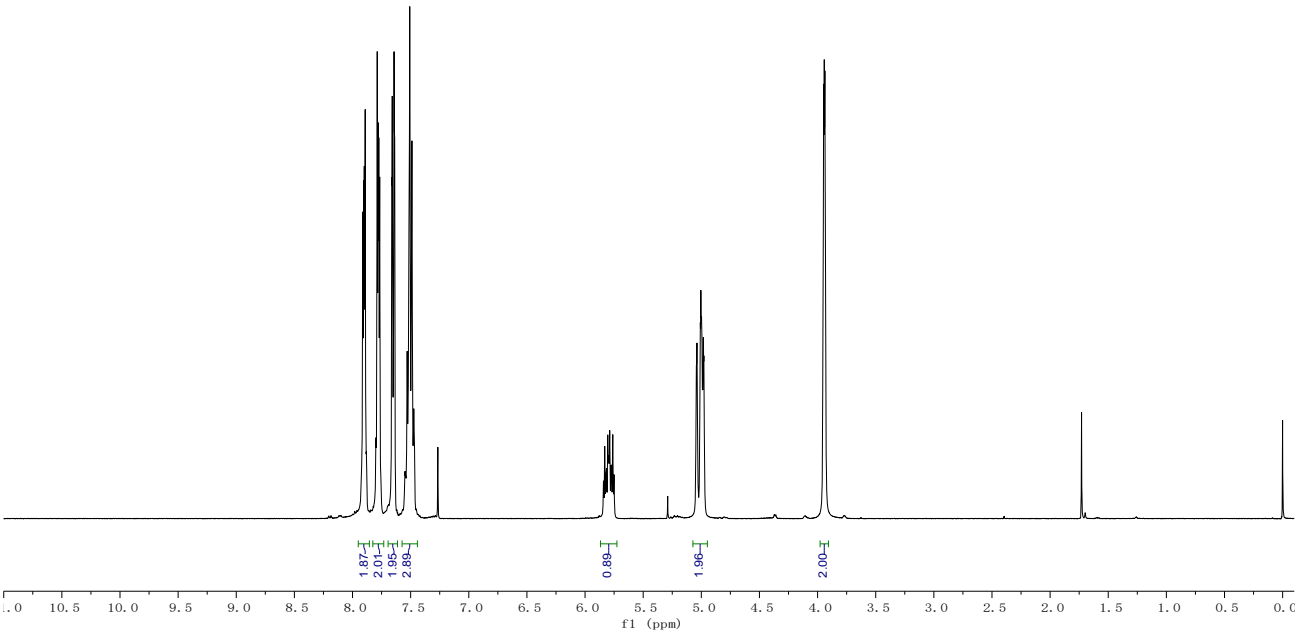


1,3-dioxoisindolin-2-yl (Z)-N-allylbenzimidate (1n). A white solid, 1.24 g, 81% yield; M.p.: 142-144 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.90 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.78 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.69-7.61 (m, 2H), 7.57-7.44 (m, 3H), 5.87-5.73 (m, 1H), 5.07-4.95 (m, 2H), 3.98-3.91 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 163.2, 156.2, 135.1, 134.4, 131.1, 129.3, 128.7, 128.5, 126.8, 123.7, 114.7, 51.3; IR (neat) ν 1790, 1739, 1716, 1641, 1600, 1467, 1446, 1354, 1250, 1186, 1142, 1052, 979, 913 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{18}\text{H}_{15}\text{N}_2\text{O}_3^+$ Requires: 307.1077, Found: 307.1068.

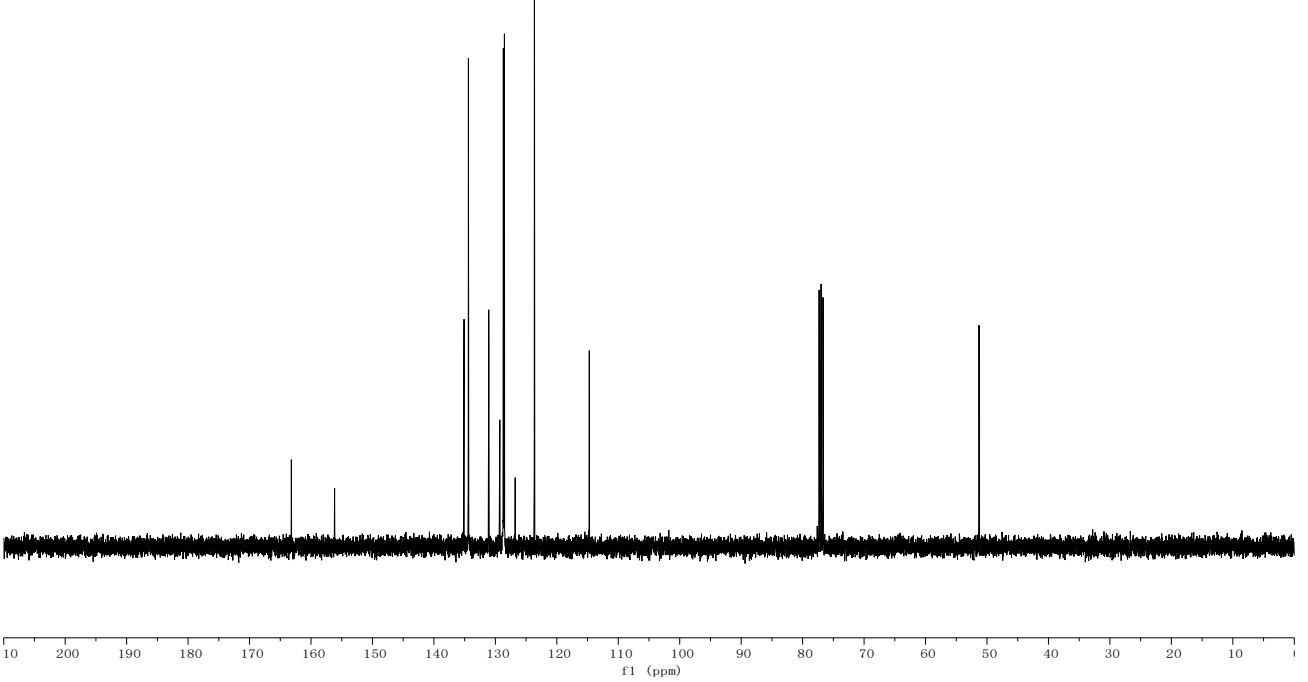


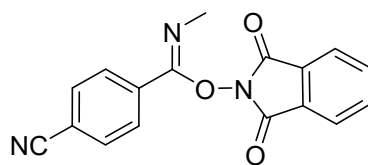
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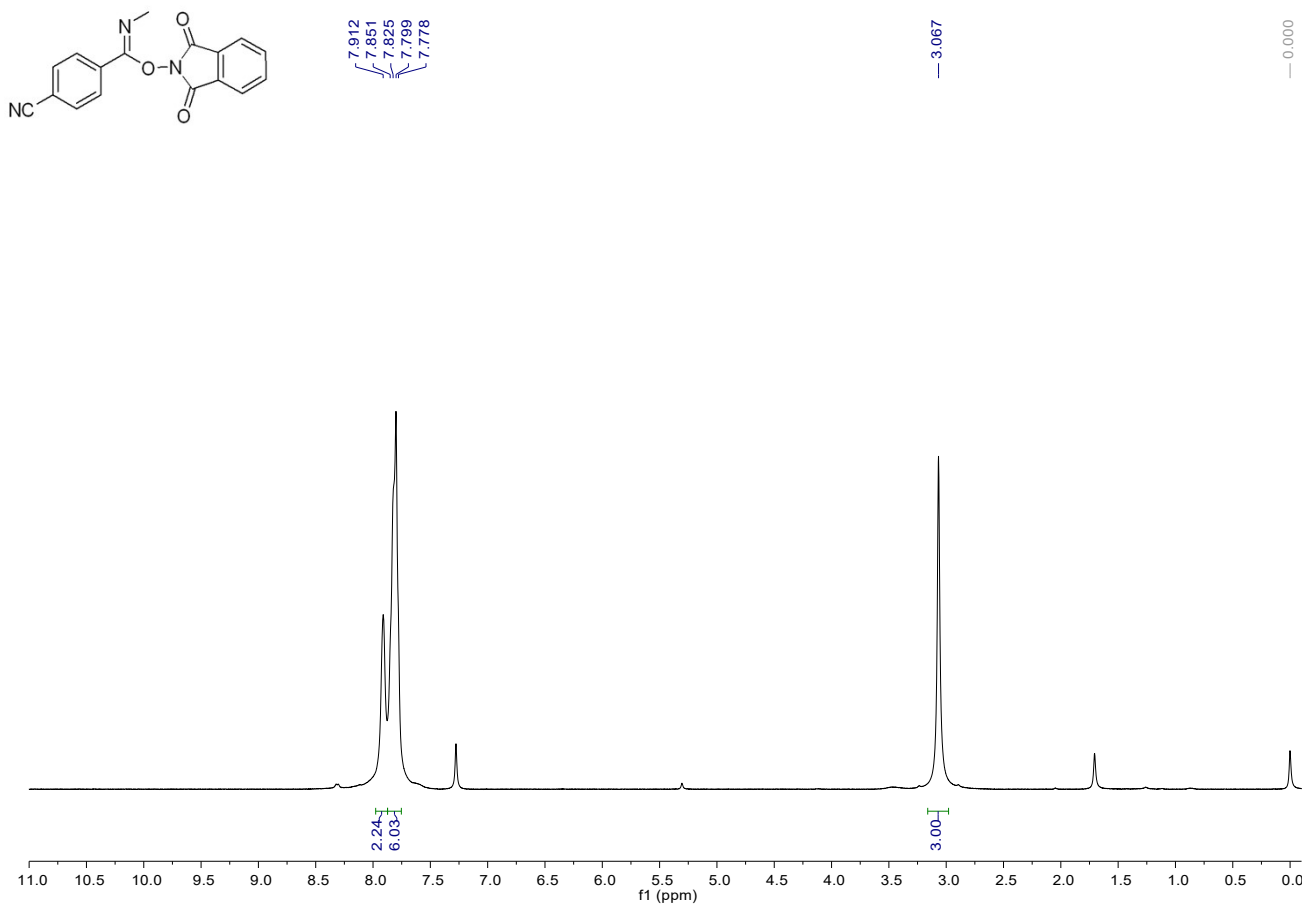


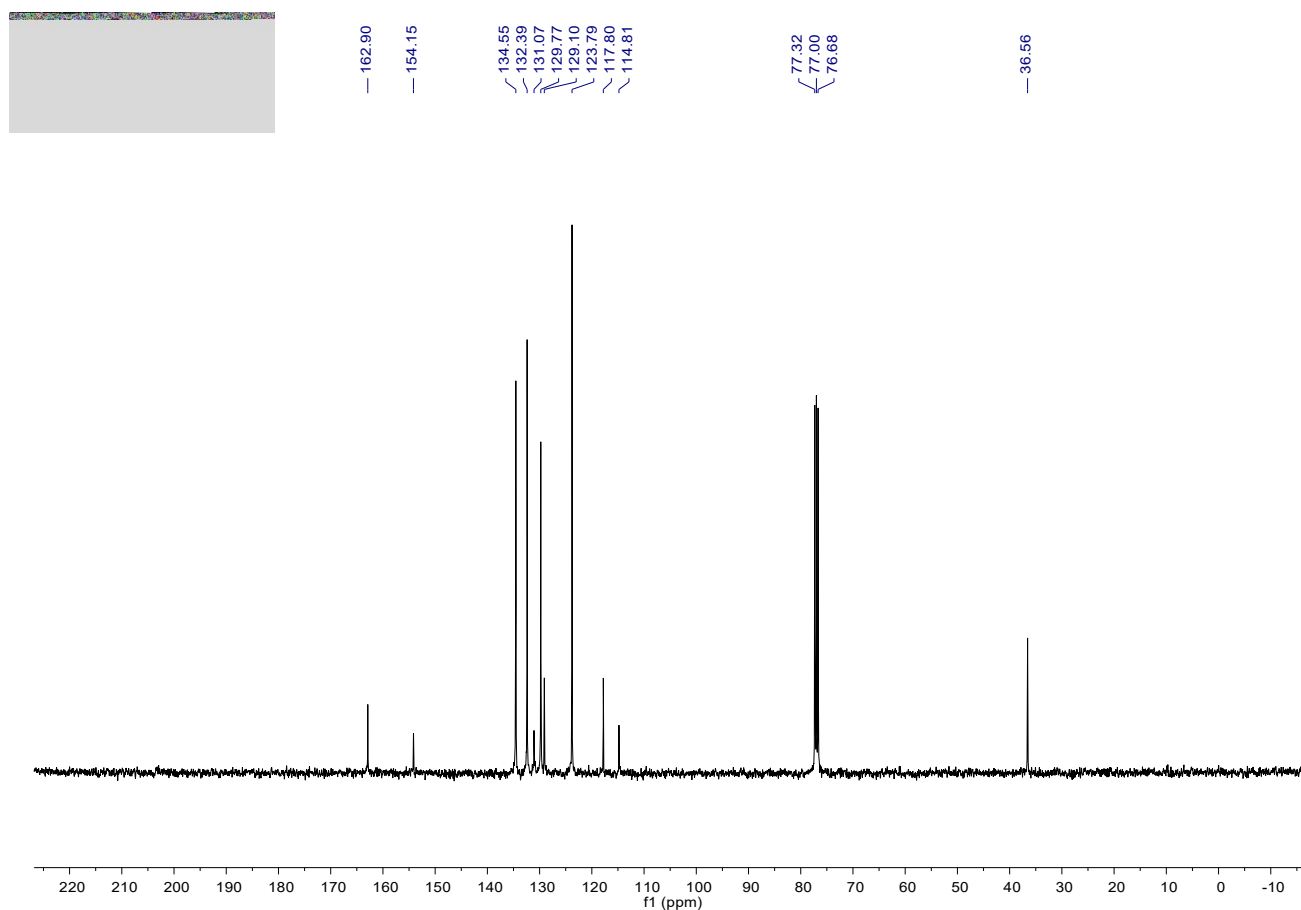
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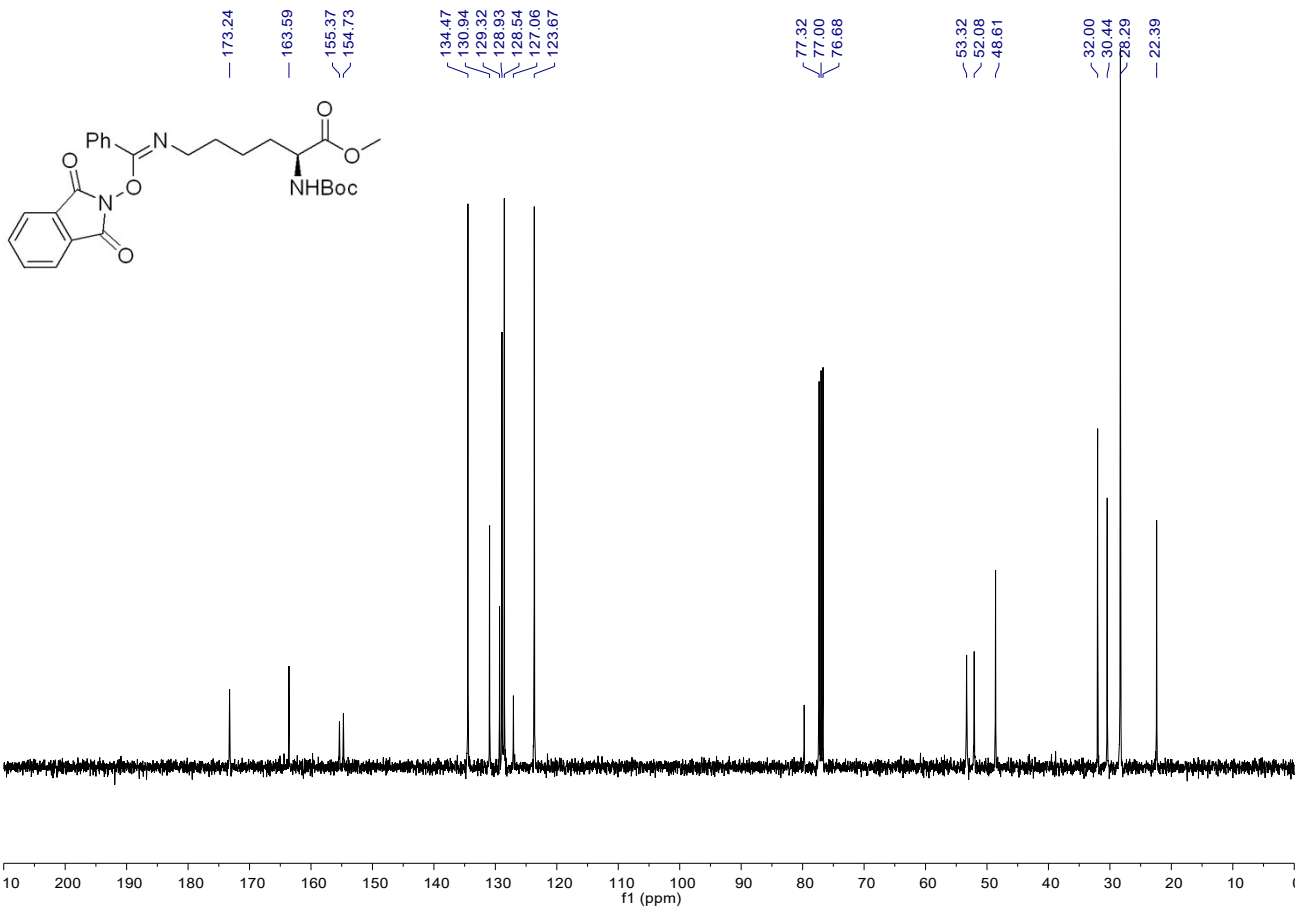
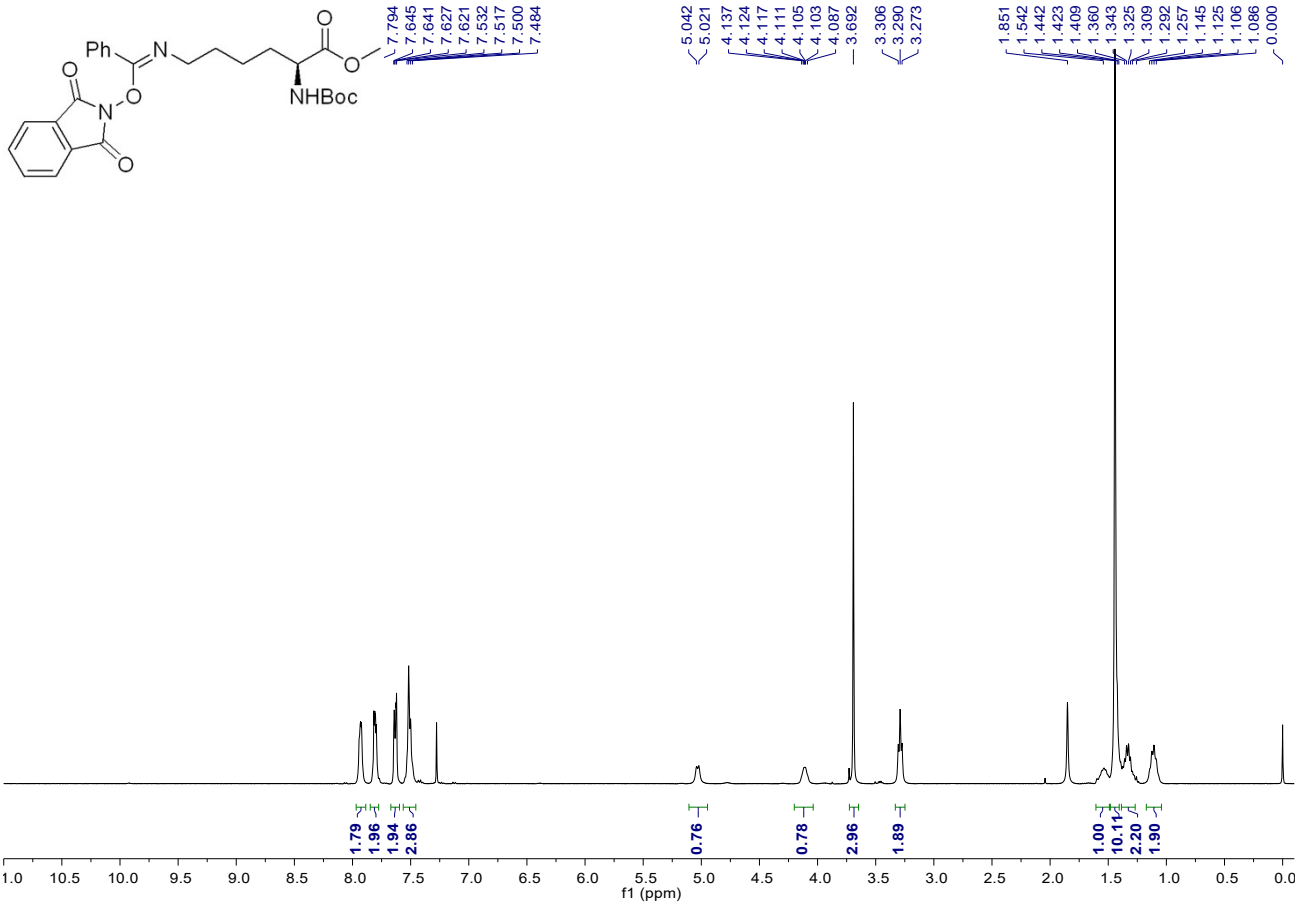


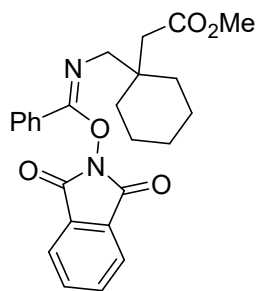
1,3-dioxoisindolin-2-yl (Z)-4-cyano-N-methylbenzimidate (1r). A white solid, 1.2 g, 77% yield; M.p.: 198-200 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.98-7.87 (m, 2H), 7.87-7.75 (m, 6H), 3.07 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 162.9, 154.2, 134.5, 132.4, 131.1, 129.8, 129.1, 123.8, 117.8, 114.8, 36.6; IR (neat) ν 2228, 1730, 1707, 1378, 1239, 1145, 1008, 880, 782, 691 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{19}\text{H}_{12}\text{N}_3\text{O}_3^+$ Requires: 306.0873, Found: 306.0867.



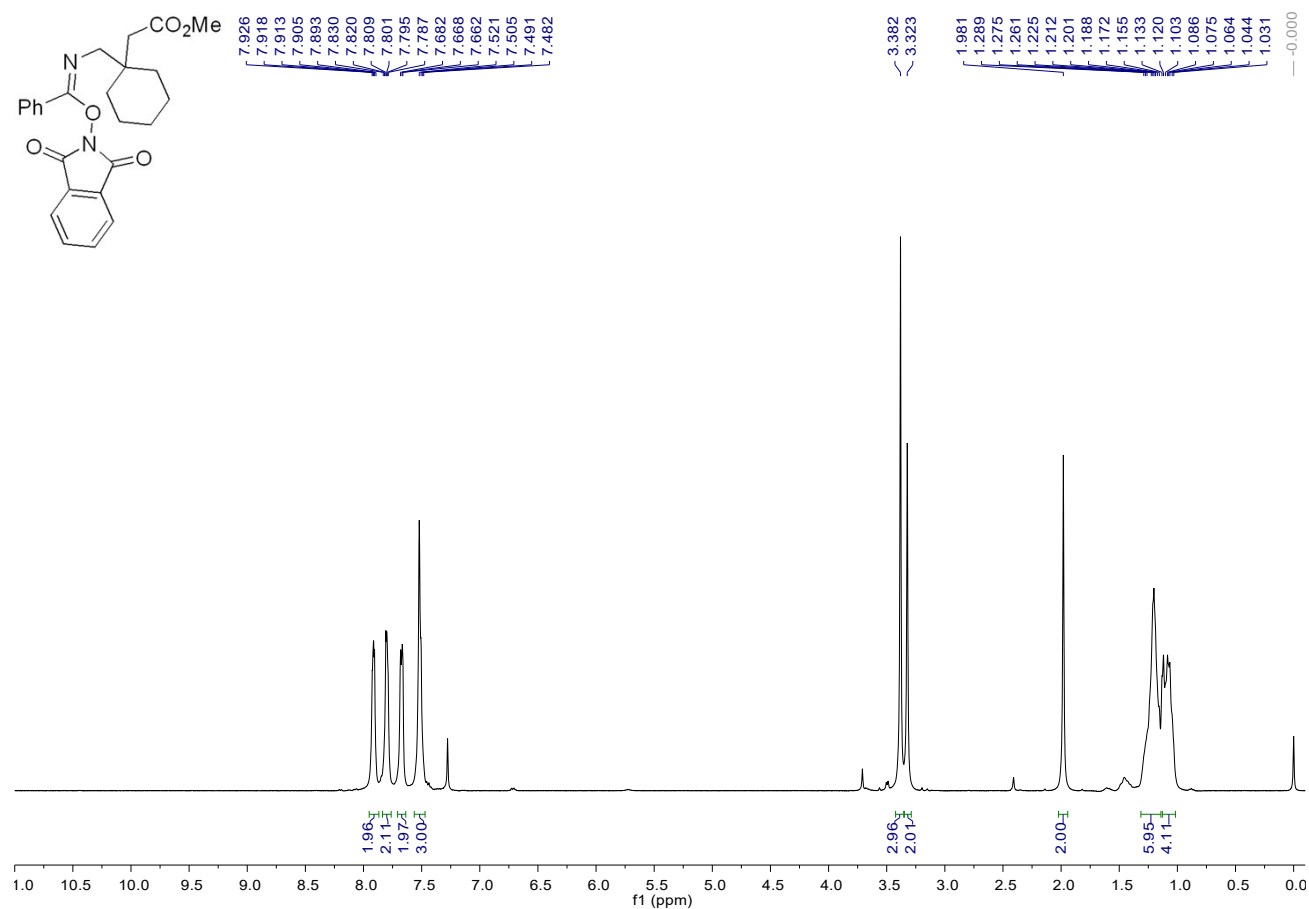


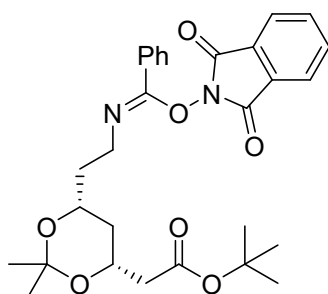
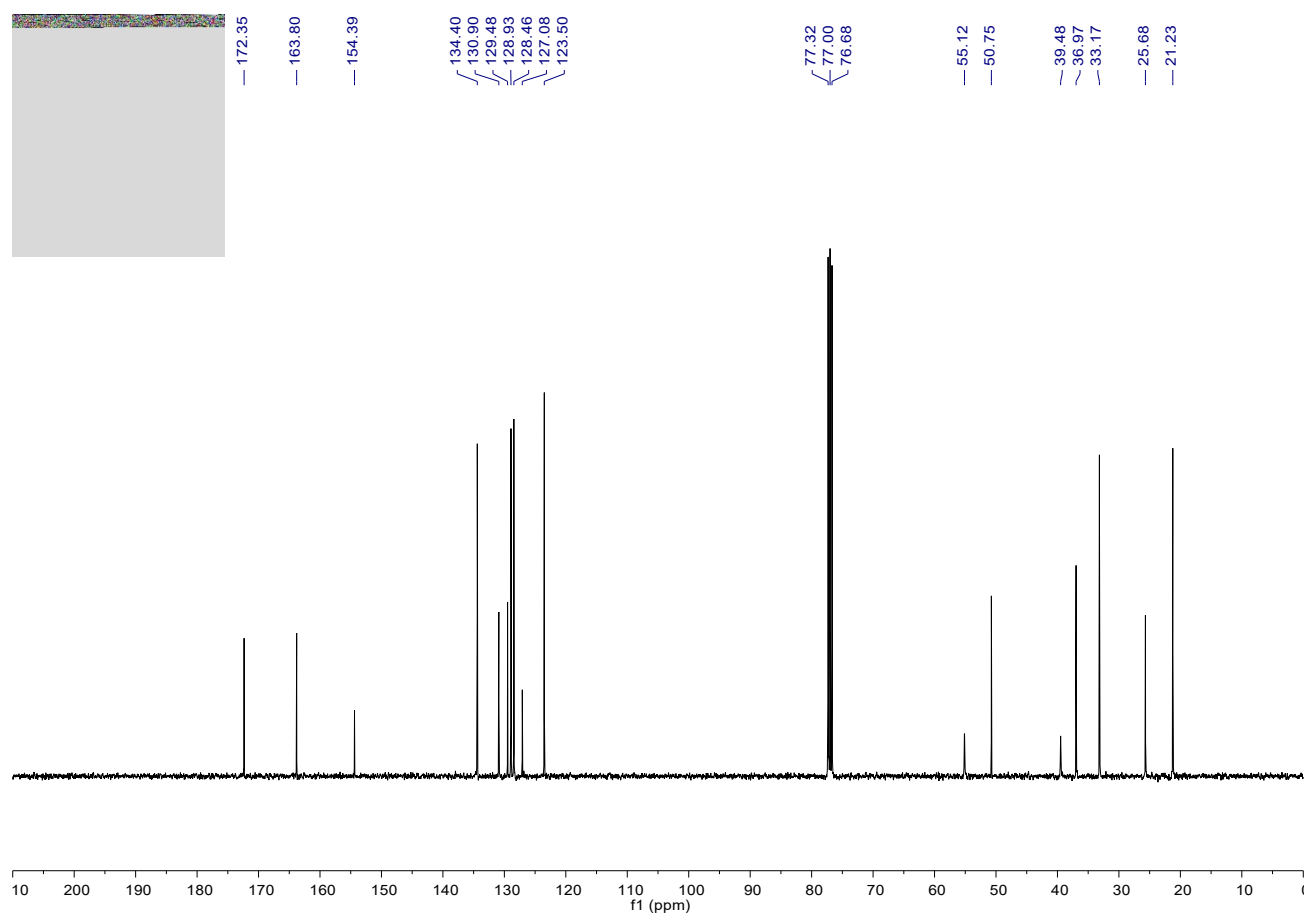
methyl (Z)-N²-(tert-butoxycarbonyl)-N⁶-(((1,3-dioxoisindolin-2-yl)oxy)(phenyl)methylene)-L-lysinate (1ac). A pale yellow oil, 2.14 g, 84% yield; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.93 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.81 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.67-7.60 (m, 2H), 7.56-7.46 (m, 3H), 5.03 (d, *J* = 8.5 Hz, 1H), 4.20-4.04 (m, 1H), 3.69 (s, 3H), 3.29 (t, *J* = 6.6 Hz, 2H), 1.61-1.49 (m, 1H), 1.48-1.41 (m, 10H), 1.39-1.27 (m, 2H), 1.17-1.04 (m, 2H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 173.2, 163.6, 155.4, 154.7, 134.5, 130.9, 129.3, 128.9, 128.5, 127.1, 123.7, 79.7, 53.3, 52.1, 48.6, 32.0, 30.4, 28.3, 22.4; IR (neat) ν 2935, 2867, 1796, 1737, 1708, 1579, 1516, 1491, 1364, 1239, 1160, 1017, 697 cm⁻¹; HRMS (ESI) Calcd. for C₂₇H₃₂N₃O₇⁺ Requires: 510.2235, Found: 510.2234.





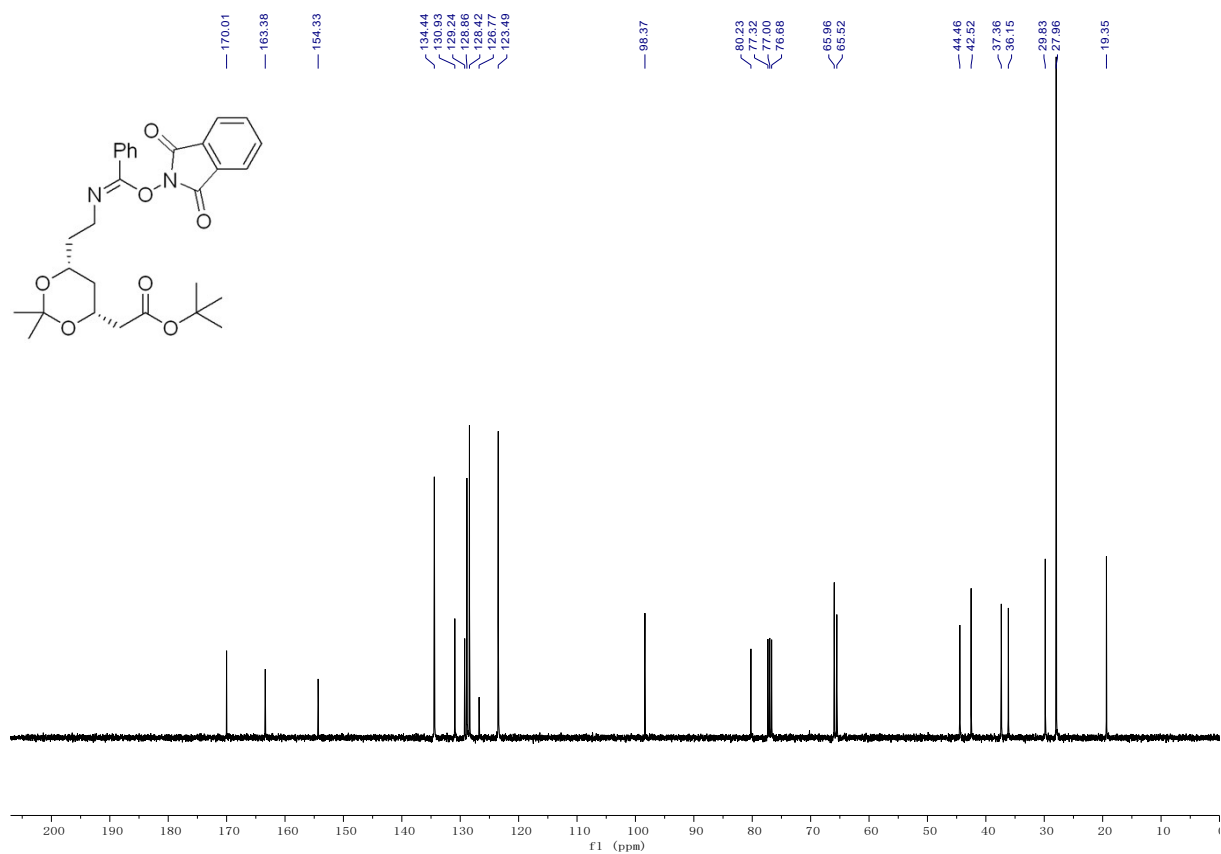
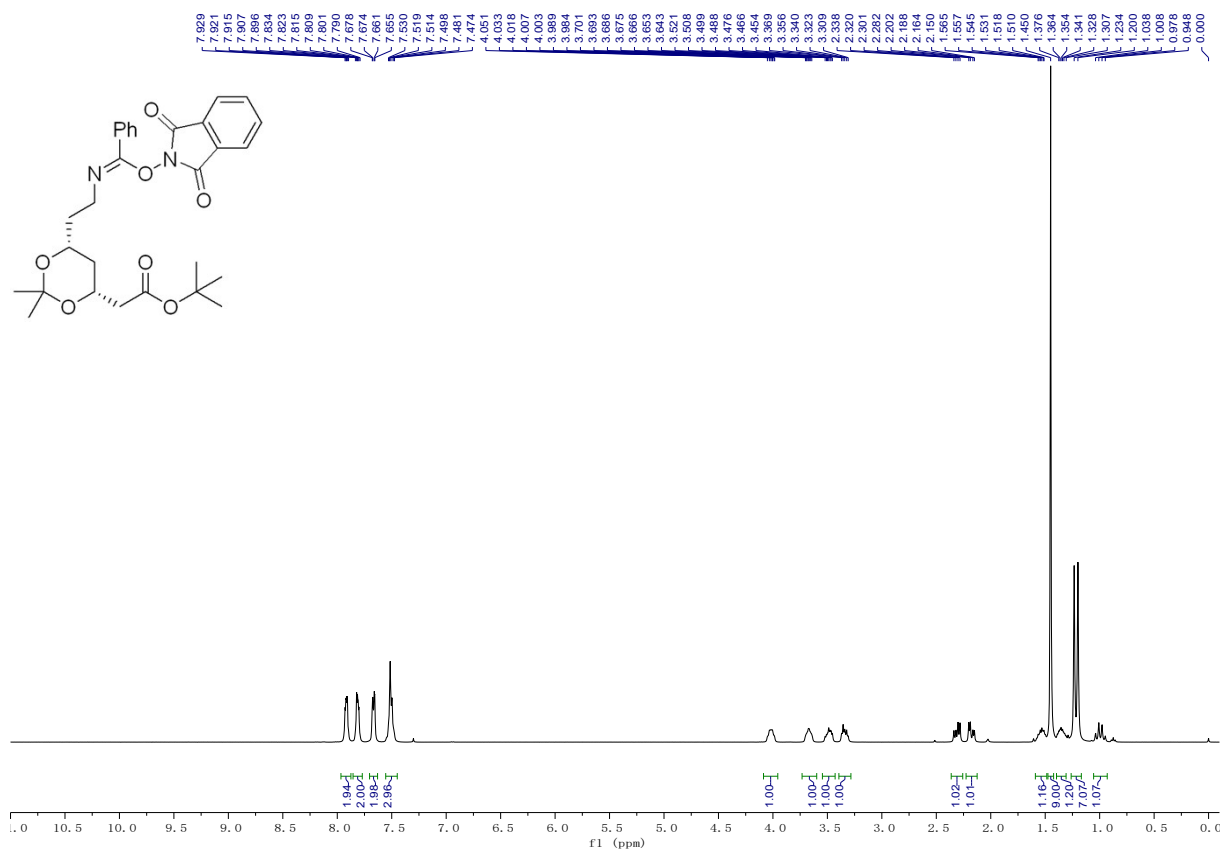
methyl (Z)-2-(1-((((1,3-dioxisoindolin-2-yl)oxy)(phenyl)methylene)amino)methyl)cyclohexyl)acetate (1ad). A white solid, 977 mg, 45% yield; M.p.: 69-70 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.92 (dd, *J* = 5.5, 3.2 Hz, 2H), 7.84-7.76 (m, 2H), 7.71-7.64 (m, 2H), 7.56-7.47 (m, 3H), 3.38 (s, 3H), 3.32 (s, 2H), 1.98 (s, 2H), 1.31-1.14 (m, 6H), 1.13-1.02 (m, 4H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 172.3, 163.8, 154.4, 134.4, 130.9, 129.5, 128.9, 128.5, 127.1, 123.5, 55.1, 50.8, 39.5, 37.0, 33.2, 25.7, 21.2; IR (neat) ν 2935, 2861, 1792, 1739, 1580, 1532, 1467, 1354, 1239, 1130, 1032, 907, 879 cm⁻¹; HRMS (ESI) Calcd. for C₂₅H₂₇N₂O₅⁺ Requires: 435.1915, Found: 435.1918.

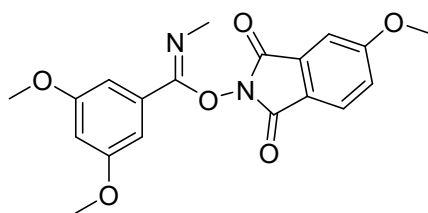




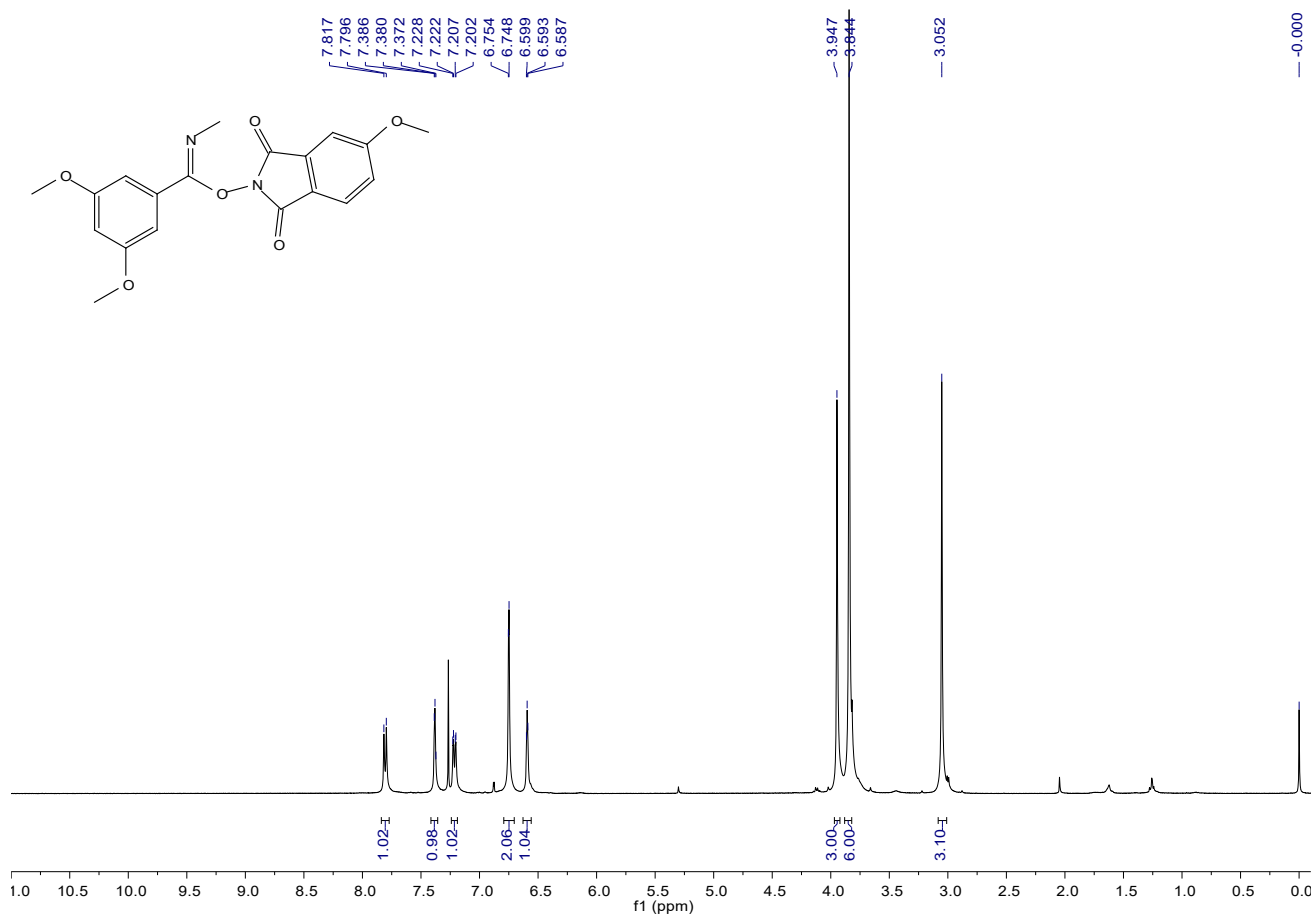
tert-butyl 2-(((4R,6R)-6-(2-(((Z)-((1,3-dioxisoindolin-2-yl)oxy)(phenyl)methylene)amino)ethyl)-2,2-dimethyl-1,3-dioxan-4-yl)acetate (1ae). A white solid, 1.86 g, 78% yield; M.p.: 125-126 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.92 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.81 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.70-7.63 (m, 2H), 7.51 (s, 3H), 4.08-3.92 (m, 1H), 3.73-3.58 (m, 1H), 3.56-3.41 (m, 1H), 3.39-3.26 (m, 1H), 2.31 (dd, $J = 15.0, 7.3$ Hz, 1H), 2.17 (dd, $J = 15.0, 5.7$ Hz, 1H), 1.59-1.48 (m, 1H), 1.45 (s, 9H), 1.39-1.31 (m, 1H), 1.26-1.15 (m, 7H), 1.06-0.92 (m, 1H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 170.2, 163.5, 154.4, 134.5, 131.0, 129.4, 129.0, 128.5, 126.9, 123.6, 98.5, 80.4, 66.1, 65.7, 44.6, 42.6, 37.5, 36.3, 29.9, 28.1, 19.5; IR (neat) ν 2978, 2929, 1799, 1740, 1722, 1467, 1429, 1377, 1286, 1262,

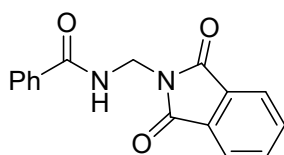
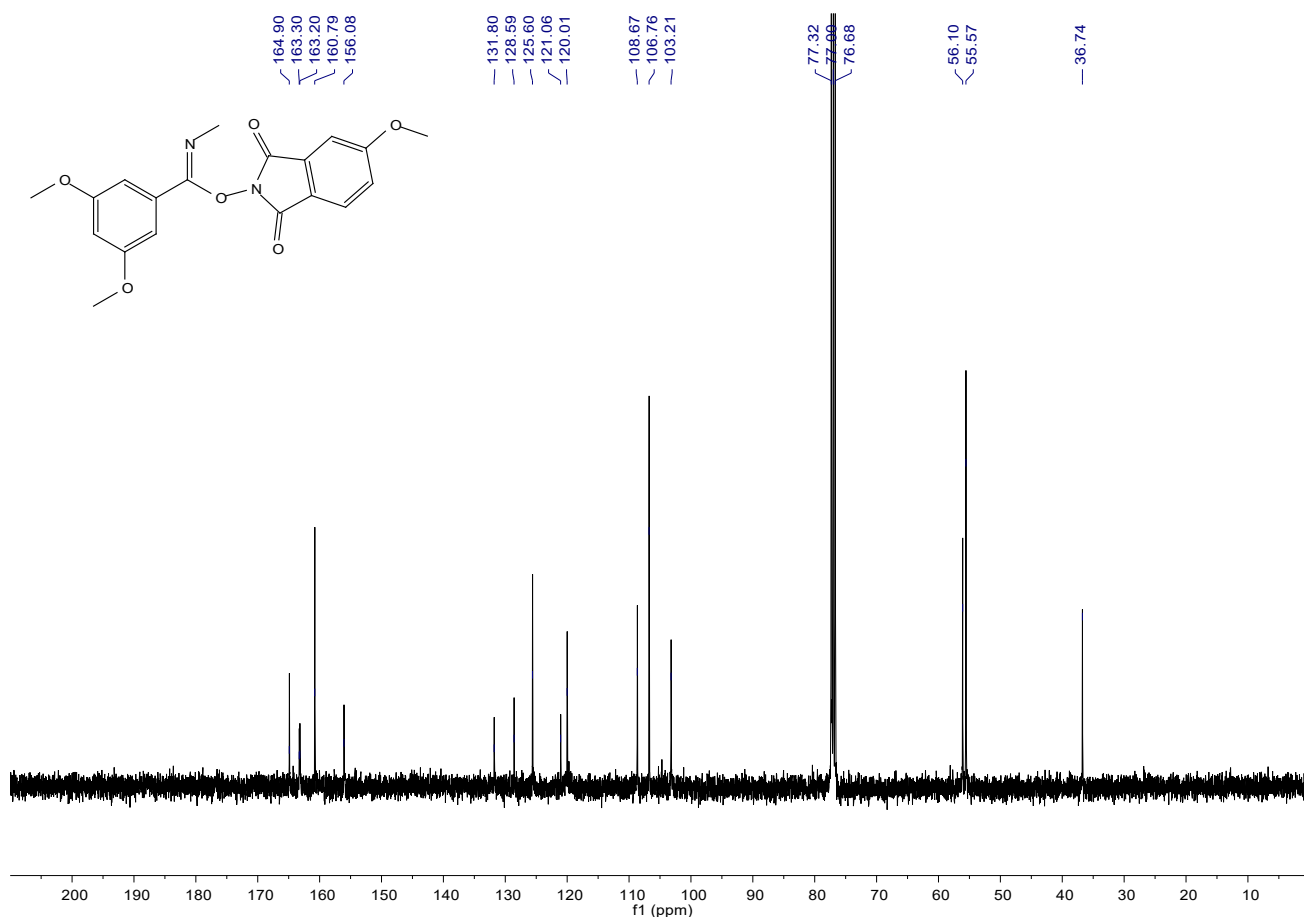
1184, 1131, 1107, 1005, 980 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{29}\text{H}_{35}\text{N}_2\text{O}_7^+$ Requires: 523.2439, Found: 523.2433.





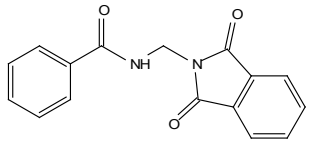
5-methoxy-1,3-dioxoisindolin-2-yl (Z)-3,5-dimethoxy-N-methylbenzimidate (1ah). A white solid, 218.3 mg, 59% yield; M.p.: 175-177 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.81 (d, $J = 8.4$ Hz, 1H), 7.41 – 7.36 (m, 1H), 7.21 (dd, $J = 8.3, 2.3$ Hz, 1H), 6.75 (d, $J = 2.3$ Hz, 2H), 6.59 (t, $J = 2.4$ Hz, 1H), 3.95 (s, 3H), 3.84 (s, 6H), 3.05 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 164.9, 163.3, 163.2, 160.8, 156.1, 131.8, 128.6, 125.6, 121.1, 120.0, 108.7, 106.8, 103.2, 56.1, 55.6, 36.7; IR (neat) ν 2836, 1792, 1734, 1593, 1488, 1450, 1358, 1288, 1205, 1158, 1023, 981, 842, 715 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{19}\text{H}_{18}\text{N}_2\text{O}_6\text{Na}^+$ Requires: 393.1057, Found: 393.1066.



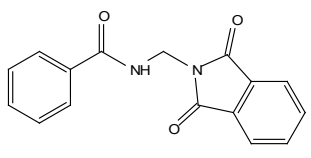
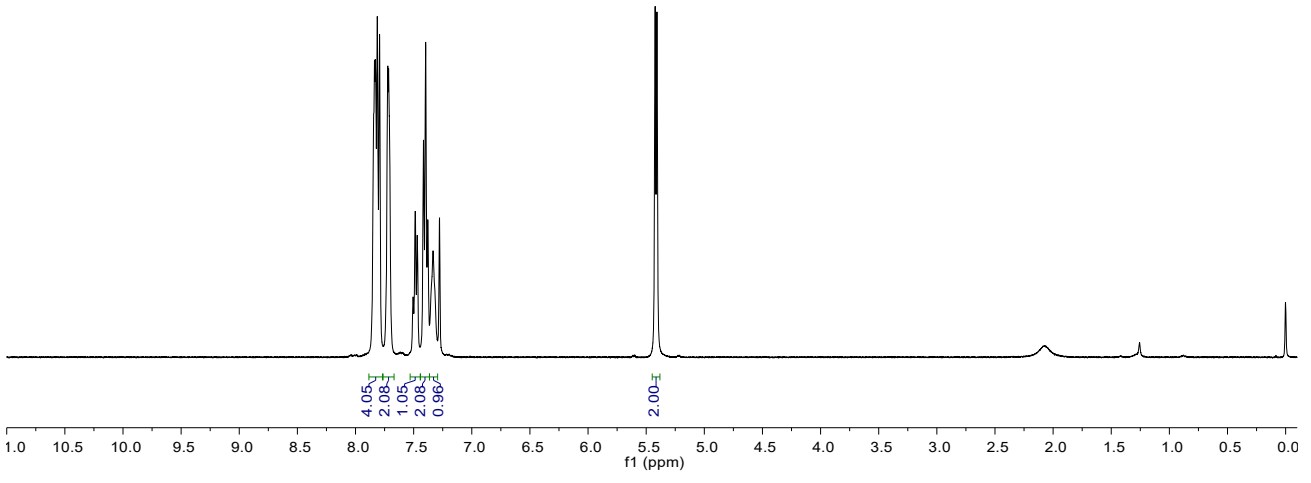


***N*-((1,3-dioxisoindolin-2-yl)methyl)benzamide (2a)**. A white solid, 54 mg, 97% yield; M.p.: 194-196 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.88-7.77 (m, 4H), 7.76-7.67 (m, 2H), 7.53-7.44 (m, 1H), 7.40 (t, $J = 7.3$ Hz, 2H), 7.36-7.29 (m, 1H), 5.41 (d, $J = 6.5$ Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.5, 166.8, 134.2, 133.2, 131.9, 131.7, 128.5, 127.2, 123.5, 42.9; IR (neat) ν 3337, 3055, 2958, 1774, 1708, 1652, 1524, 1472, 1411, 1328, 1305, 1175, 1049, 905, 805, 728 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{16}\text{H}_{13}\text{N}_2\text{O}_3^+$ Requires: 281.0921, Found: 281.0920.

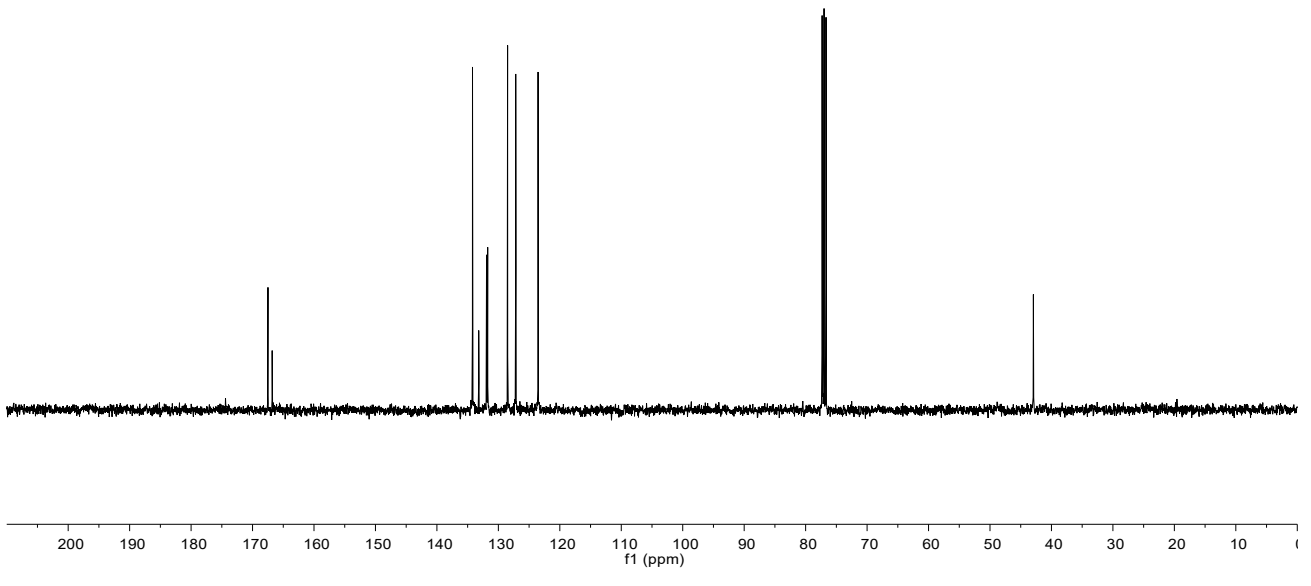
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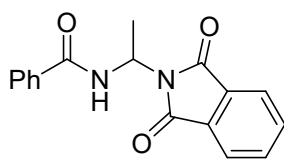


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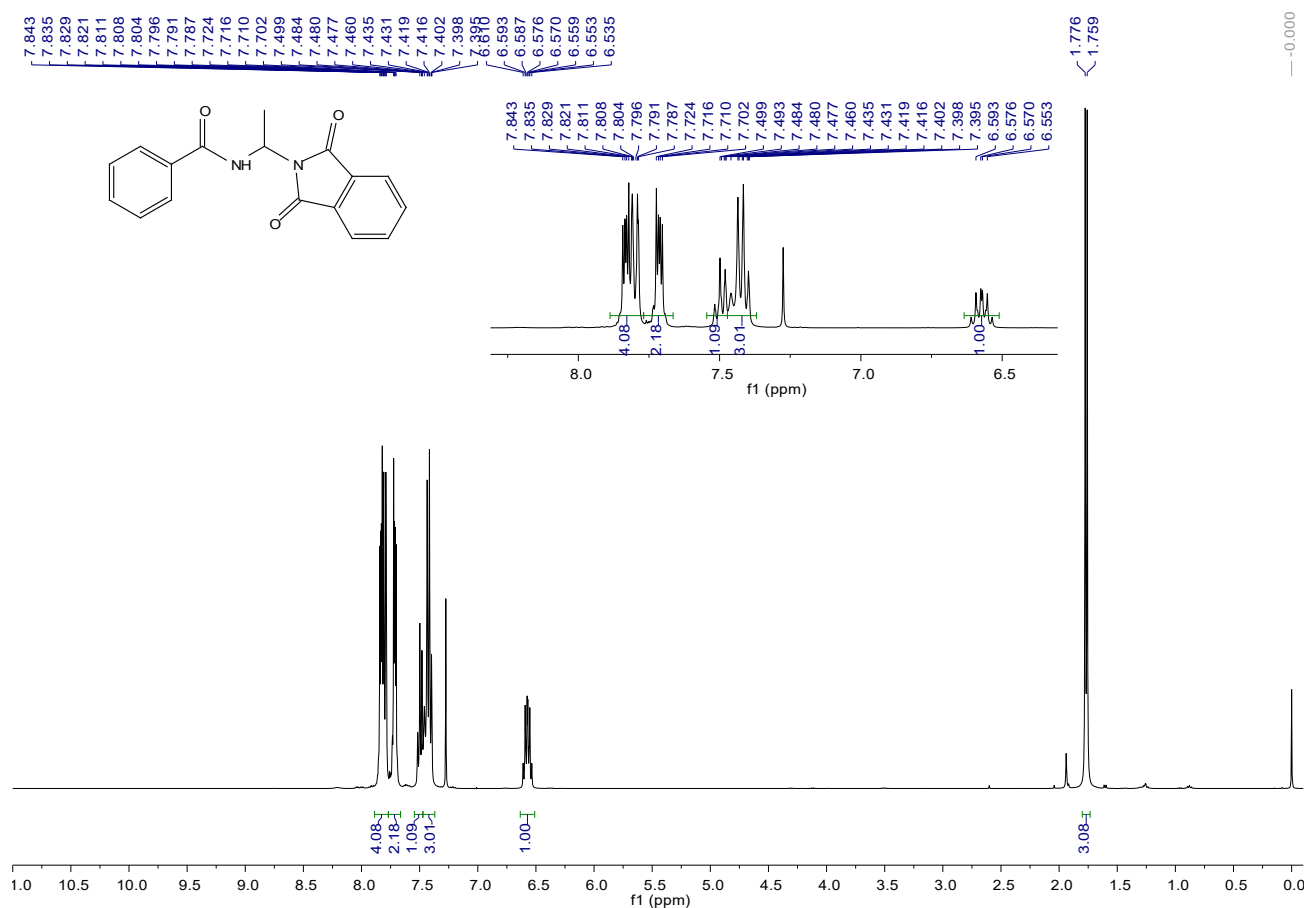


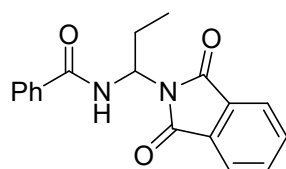
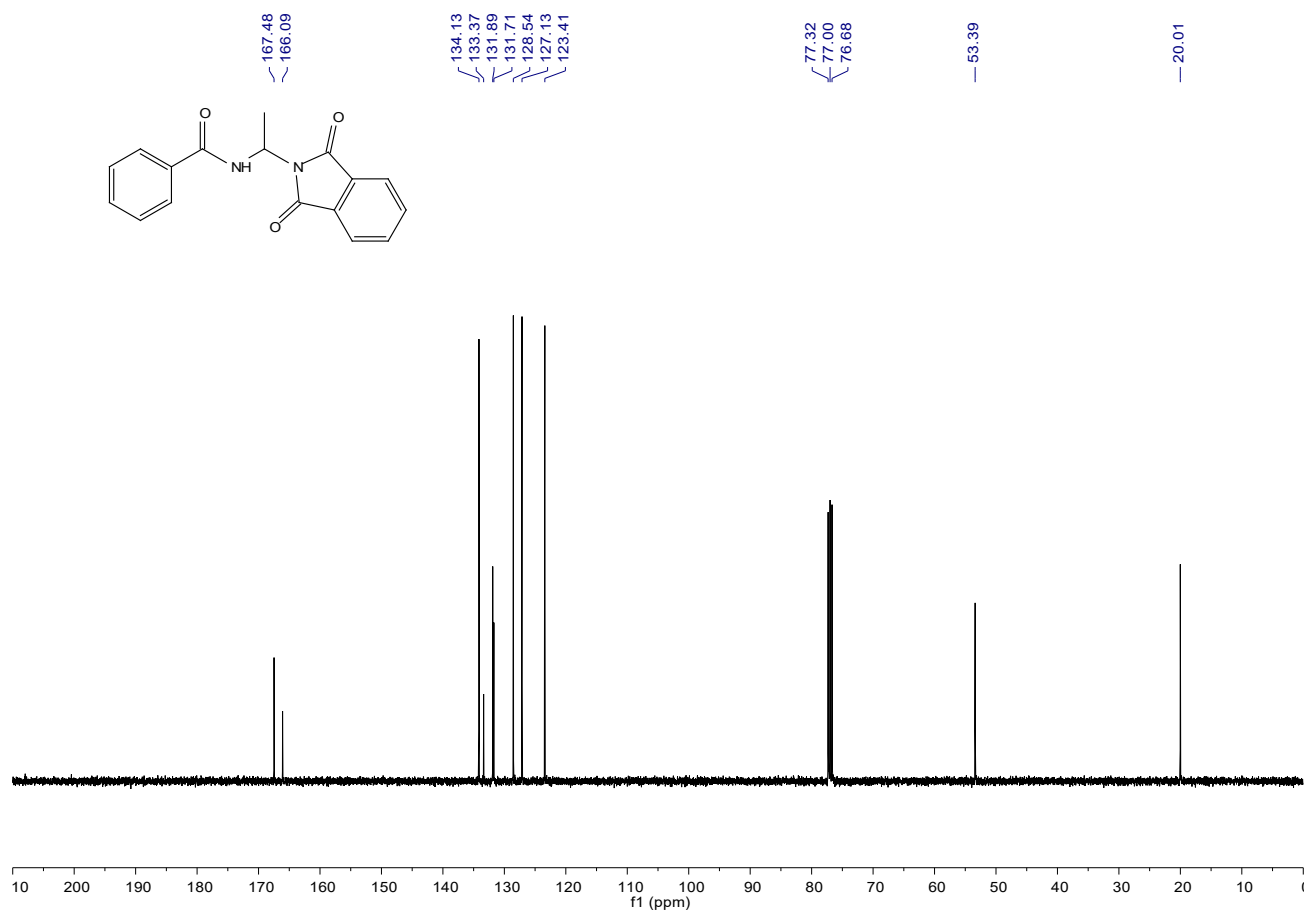
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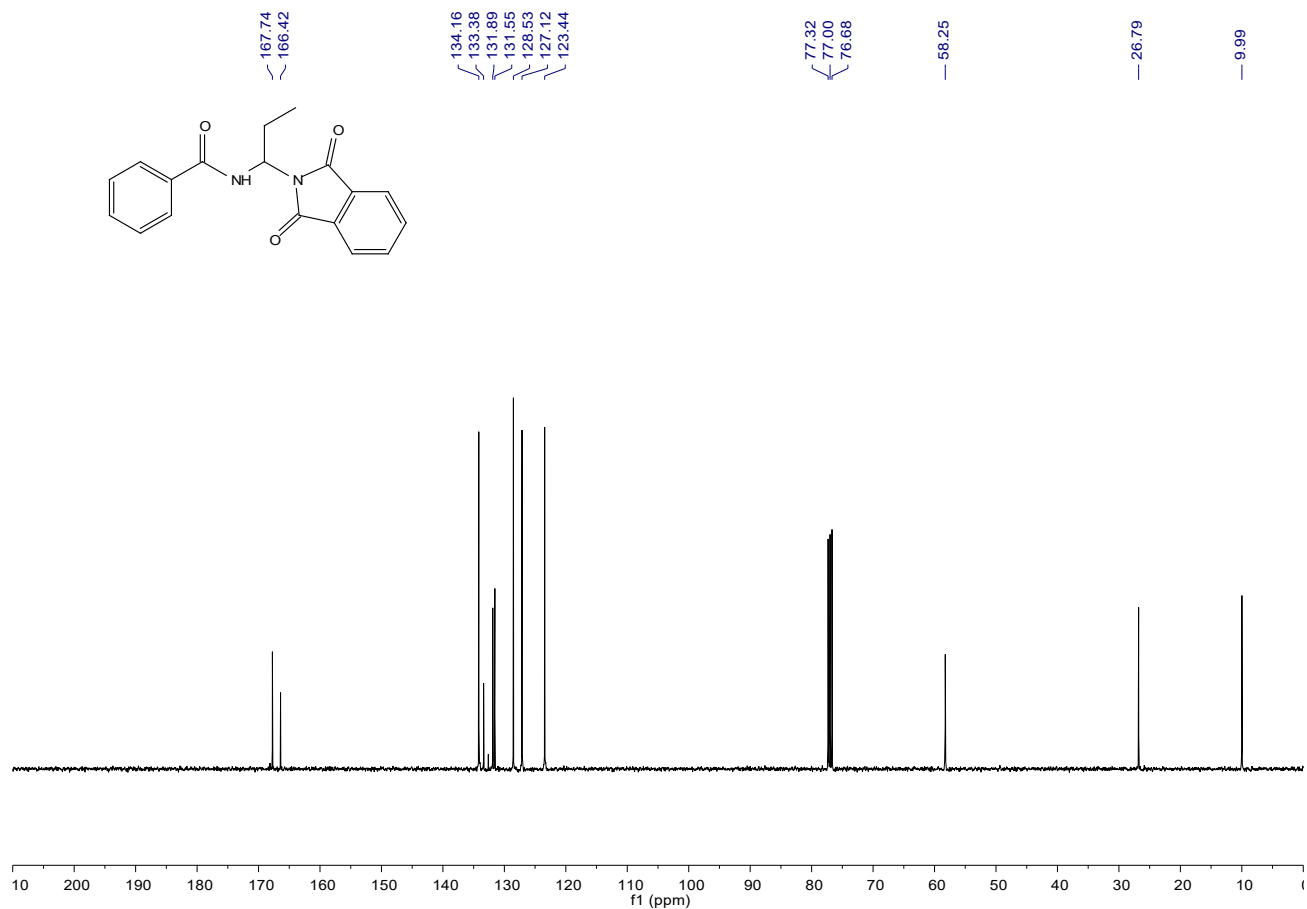
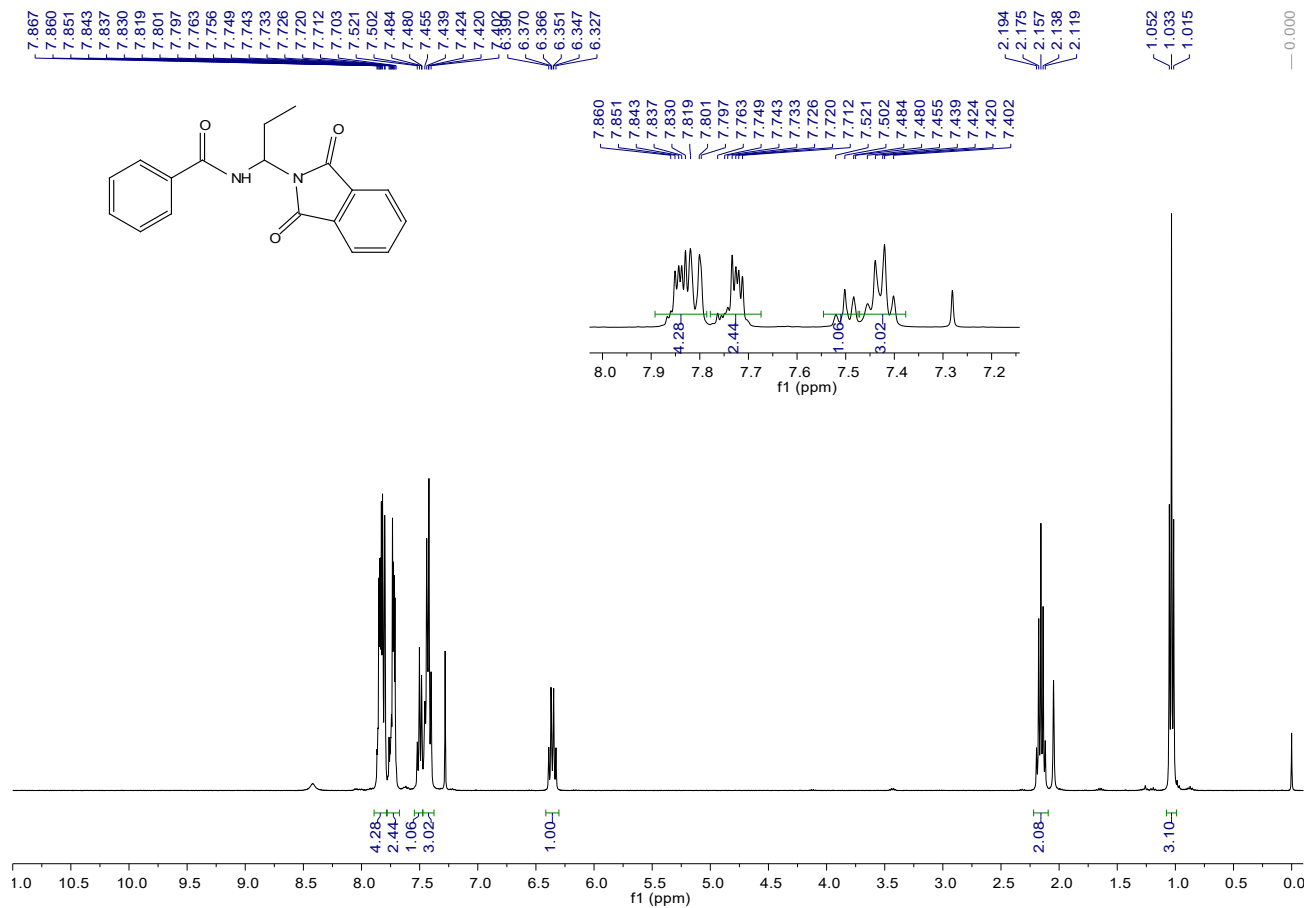


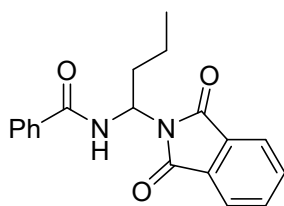
***N*-(1-(1,3-dioxisoindolin-2-yl)ethyl)benzamide (2b)**. A white solid, 57 mg, 97% yield; M.p.: 212-214 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.89-7.77 (m, 4H), 7.77-7.66 (m, 2H), 7.55-7.47 (m, 1H), 7.47-7.37 (m, 3H), 6.57 (dq, $J = 9.3, 6.8$ Hz, 1H), 1.77 (d, $J = 6.8$ Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.5, 166.1, 134.1, 133.4, 131.9, 131.7, 128.5, 127.1, 123.4, 53.4, 20.0; IR (neat) ν 3332, 3058, 2993, 1737, 1701, 1650, 1602, 1527, 1384, 1322, 1284, 1122, 1055, 893, 861 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{17}\text{H}_{15}\text{N}_2\text{O}_3^+$ Requires: 295.1077, Found: 295.1077.



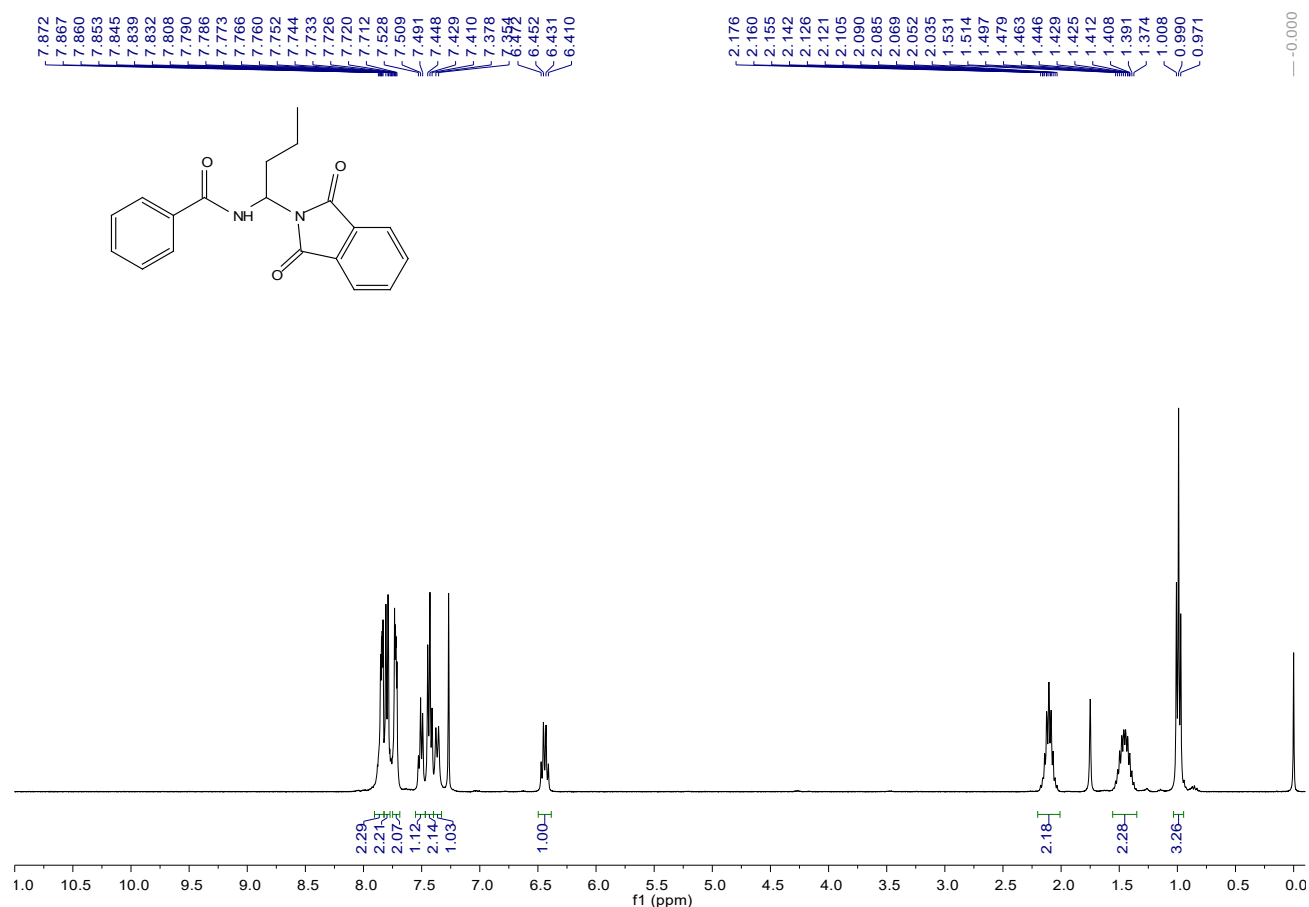


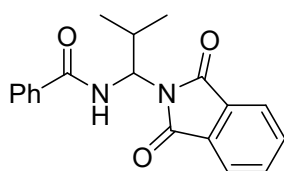
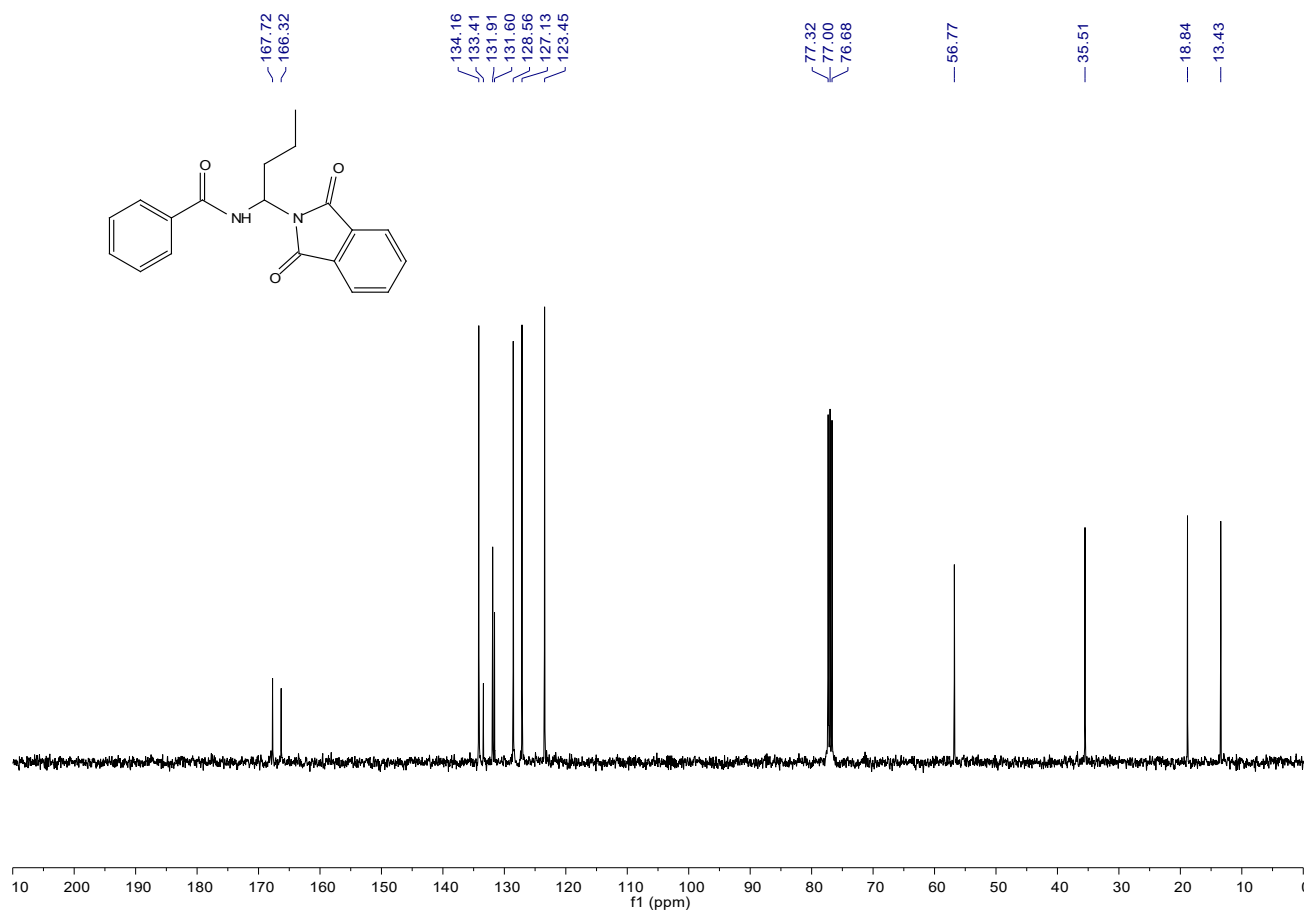
***N*-(1-(1,3-dioxisoindolin-2-yl)propyl)benzamide (2c)**. A white solid, 56 mg, 90% yield; M.p.: 164-166 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.89-7.79 (m, 4H), 7.78-7.67 (m, 2H), 7.55-7.47 (m, 1H), 7.47-7.38 (m, 3H), 6.36 (dt, *J* = 9.6, 7.8 Hz, 1H), 2.22-2.09 (m, 2H), 1.03 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 167.7, 166.4, 134.2, 133.4, 131.9, 131.5, 128.5, 127.1, 123.4, 58.3, 26.8, 10.0; IR (neat) ν 3334, 2982, 2930, 1772, 1702, 1647, 1579, 1529, 1490, 1318, 1152, 1113, 1089, 1011, 969 cm⁻¹; HRMS (ESI) Calcd. for C₁₈H₁₇N₂O₃⁺ Requires: 309.1234, Found: 309.1234.



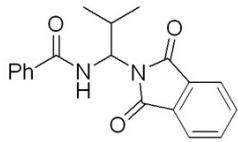


***N*-(1-(1,3-dioxisoindolin-2-yl)butyl)benzamide (2d)**. A white solid, 52 mg, 80% yield; M.p.: 188-192 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.91-7.82 (m, 2H), 7.82-7.77 (m, 2H), 7.72 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.37 (d, *J* = 9.4 Hz, 1H), 6.44 (t, *J* = 9.3, 7.8 Hz, 1H), 2.20-2.01 (m, 2H), 1.56-1.35 (m, 2H), 0.99 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 167.7, 166.3, 134.2, 133.4, 131.9, 131.6, 128.6, 127.1, 123.5, 56.8, 35.5, 18.8, 13.4; IR (neat) ν 3381, 3065, 2929, 2872, 1772, 1703, 1580, 1532, 1490, 1398, 1325, 1150, 1088, 1026 cm⁻¹; HRMS (ESI) Calcd. for C₁₉H₁₉N₂O₃⁺ Requires: 323.1390, Found: 323.1390.





***N*-(1-(1,3-dioxisoindolin-2-yl)-2-methylpropyl)benzamide (2e)**. A white solid, 52 mg, 81% yield; M.p.: 185-187 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.87-7.78 (m, 4H), 7.72 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.54-7.38 (m, 4H), 6.11 (dd, $J = 9.3$ Hz, 1H), 2.63-2.48 (m, 1H), 1.15 (d, $J = 6.7$ Hz, 3H), 0.99 (d, $J = 6.7$ Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.8, 166.5, 134.2, 133.5, 131.9, 131.4, 128.5, 127.1, 123.4, 62.3, 31.8, 19.1, 18.7; IR (neat) ν 3379, 2959, 1776, 1702, 1665, 1602, 1522, 1489, 1403, 1334, 1294, 1253, 1172, 1087, 1024, 986, 879 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{19}\text{H}_{19}\text{N}_2\text{O}_3^+$ Requires: 323.1390, Found: 323.1391.

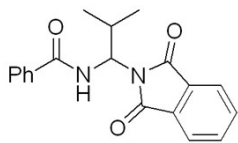
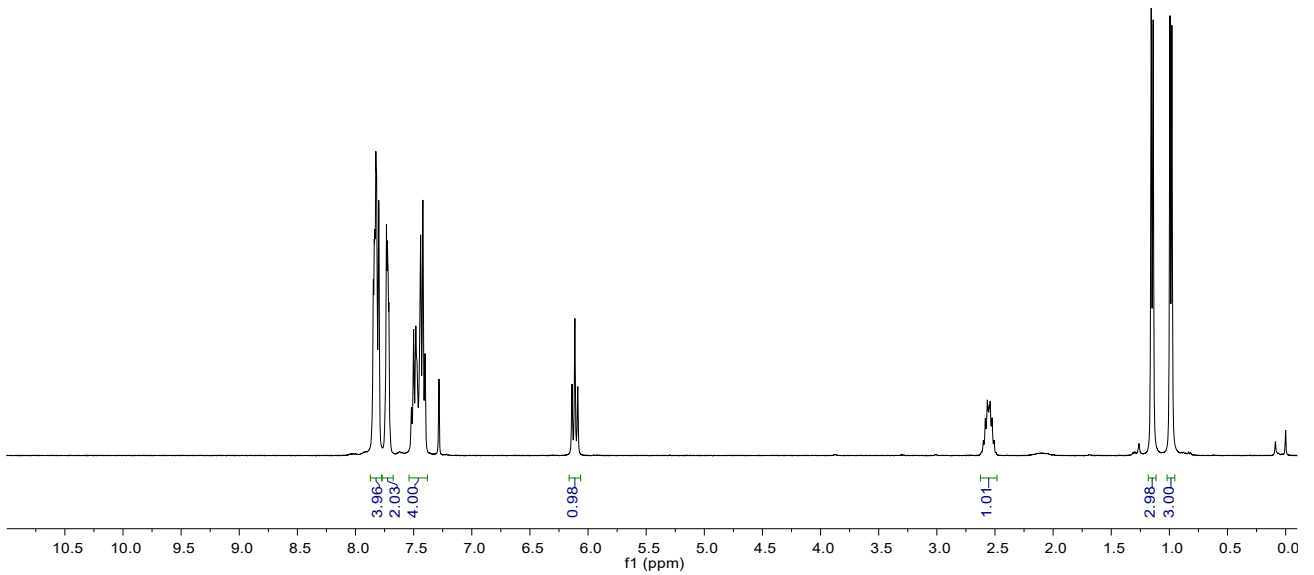


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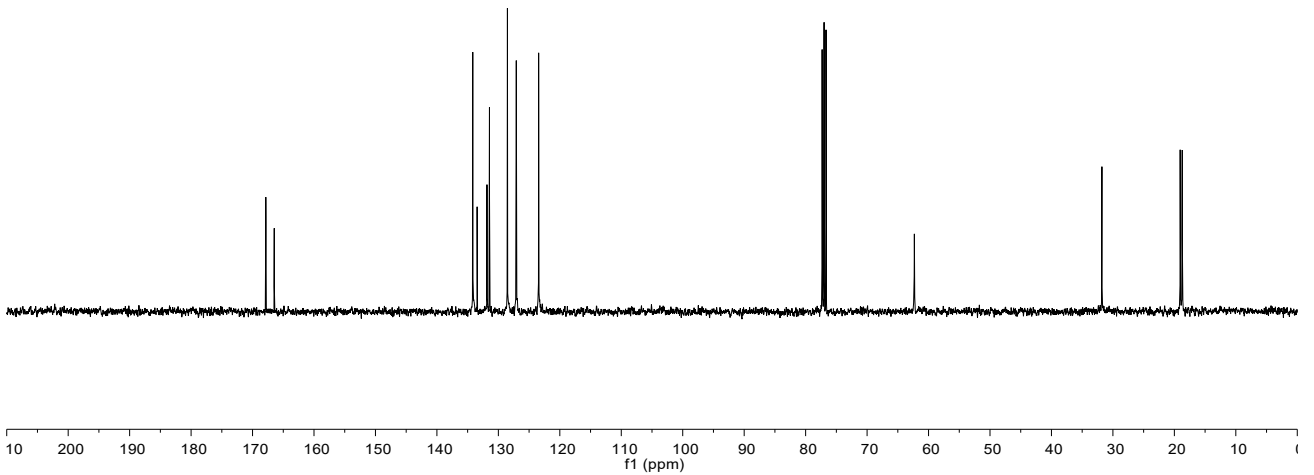
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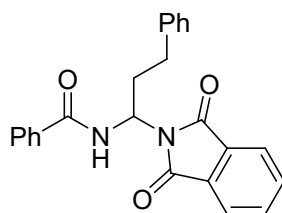
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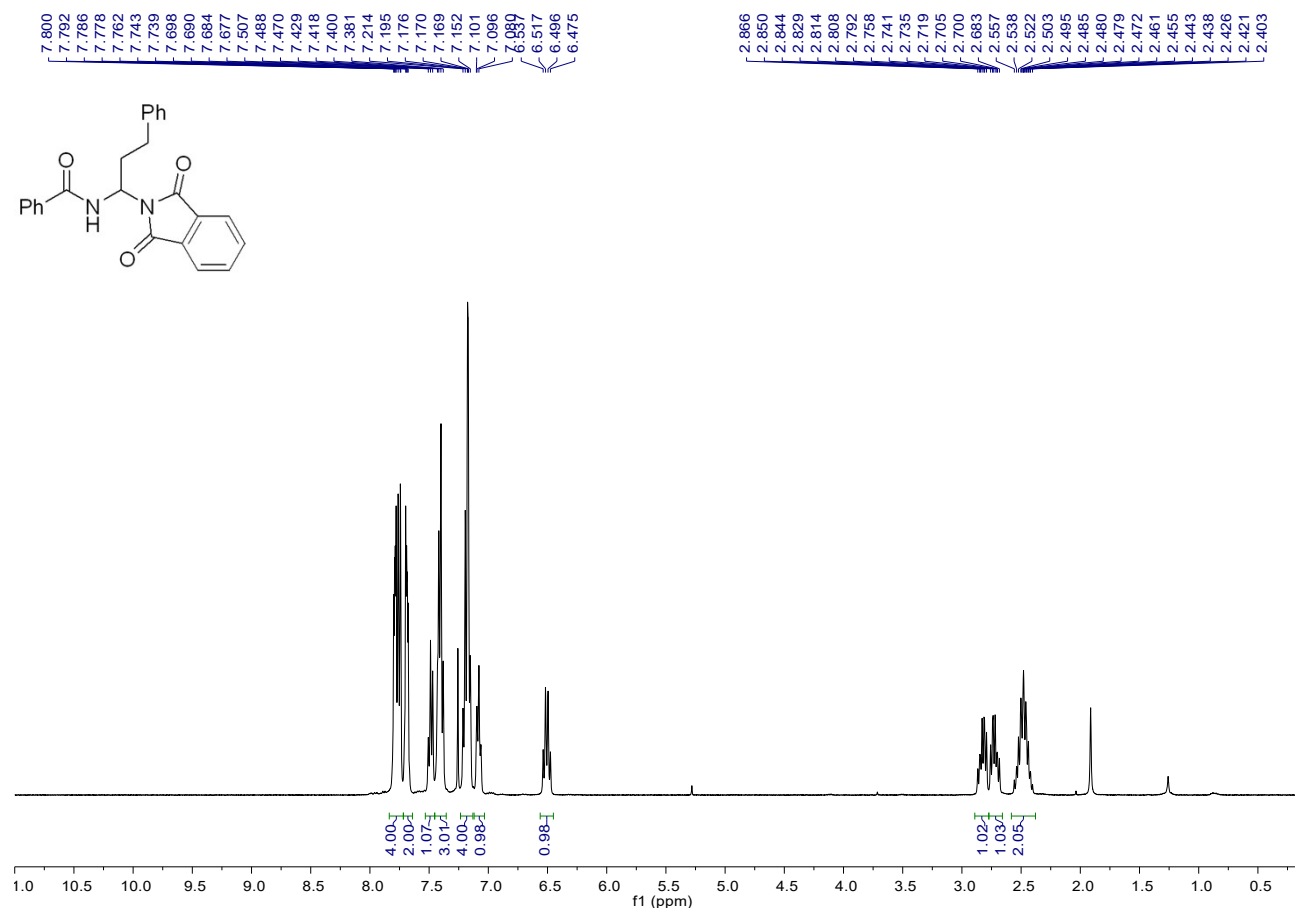
31.79

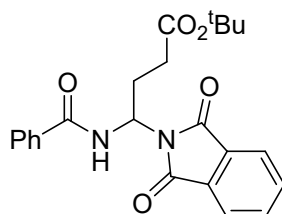
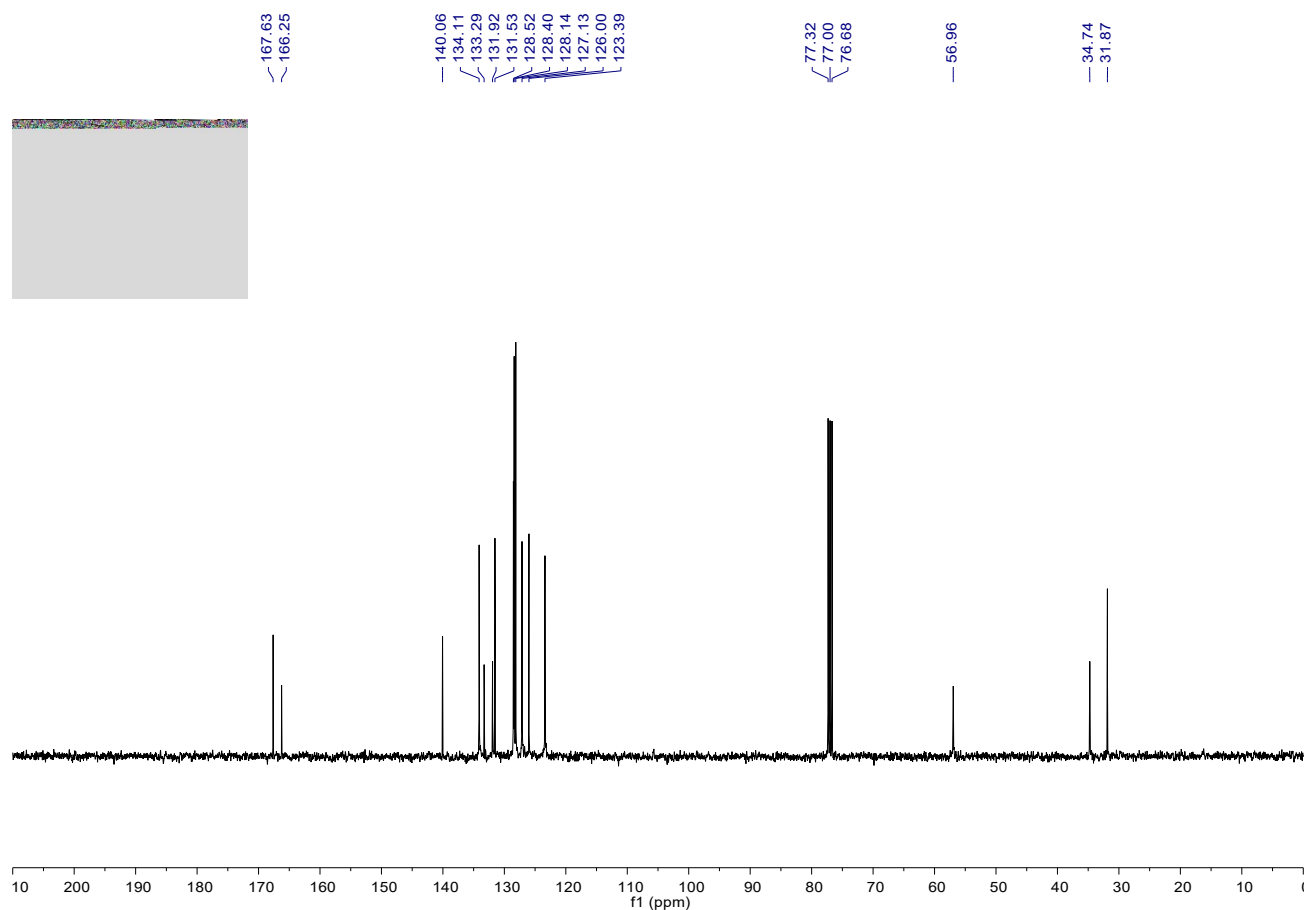
19.05
18.72



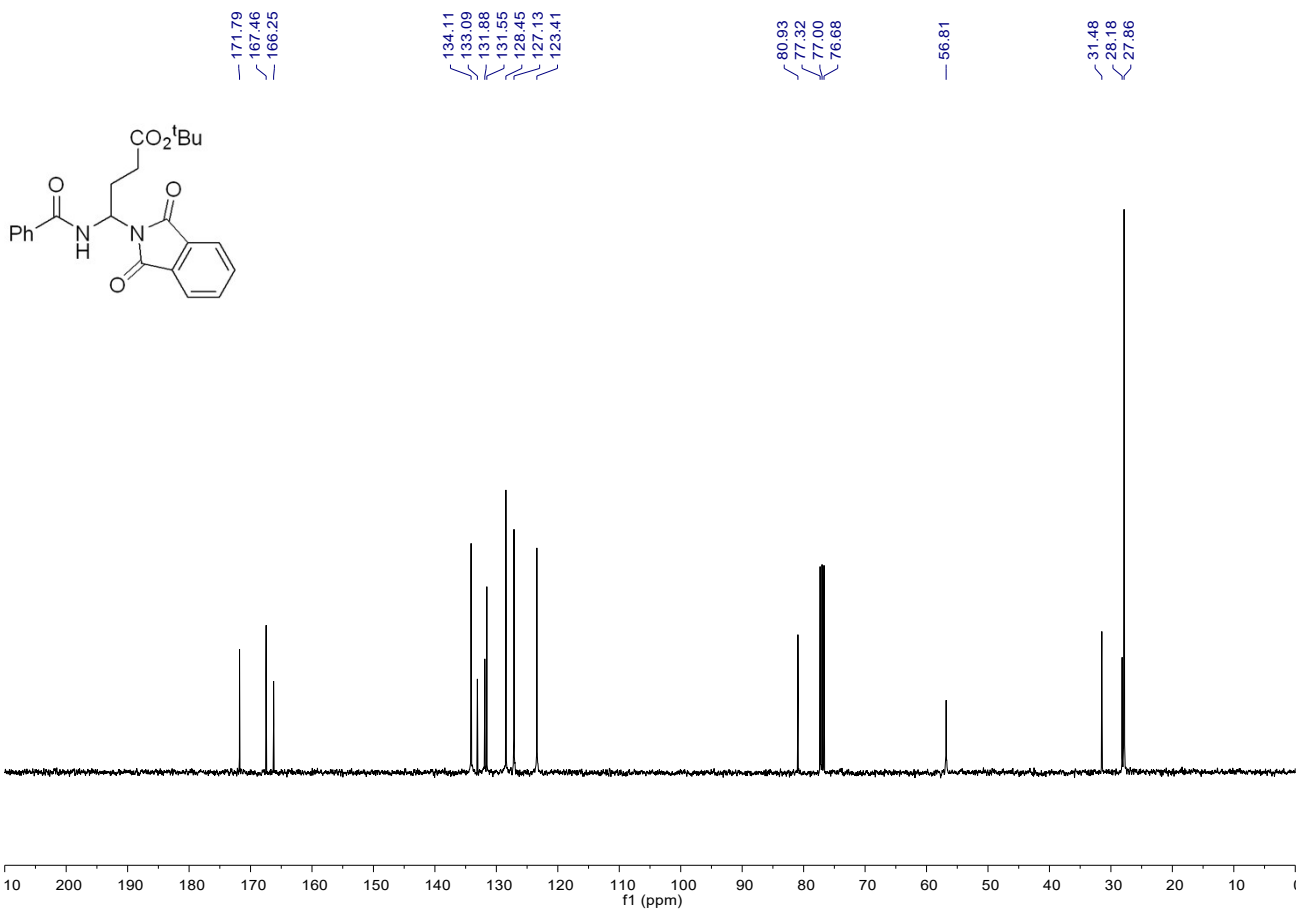
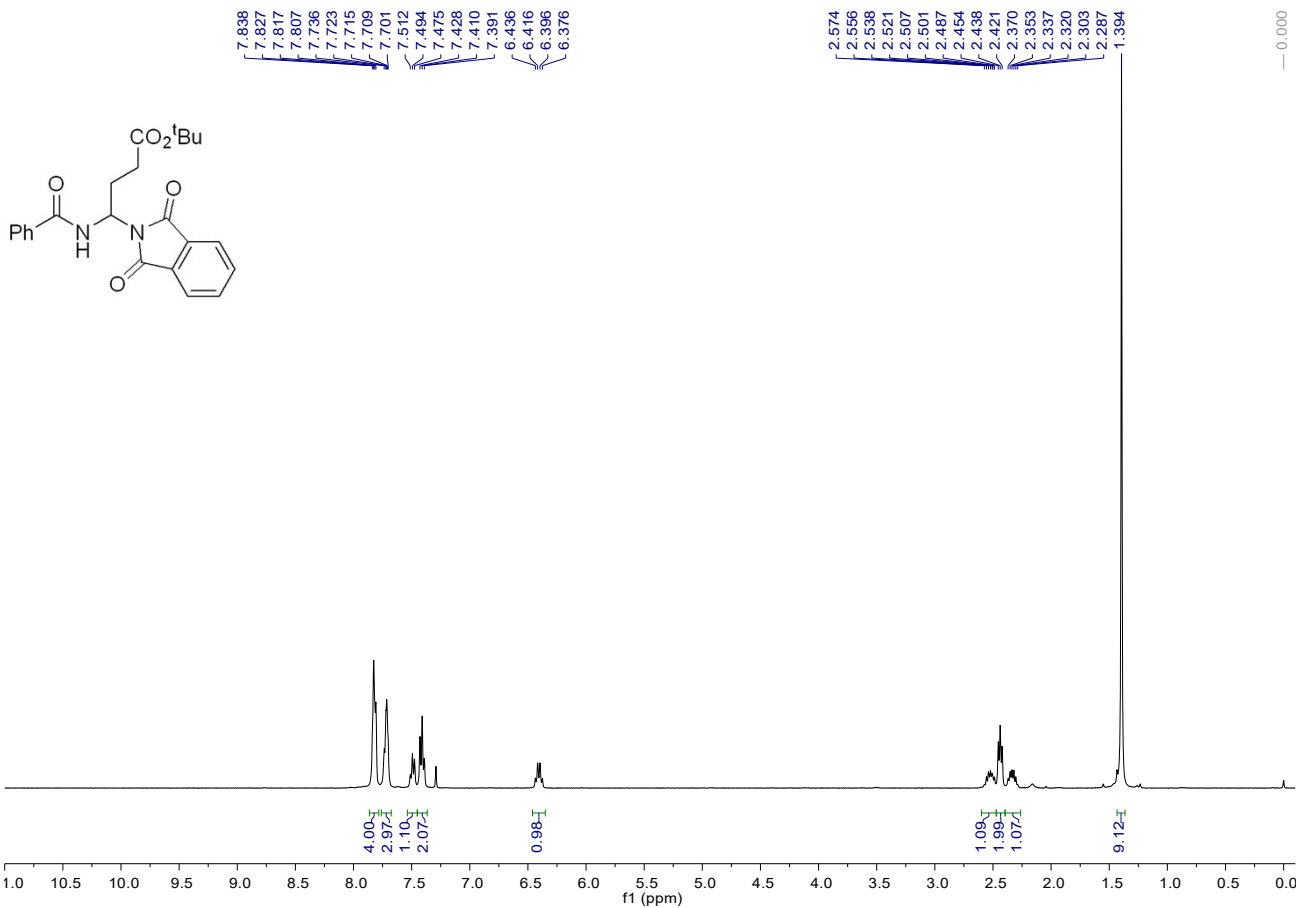


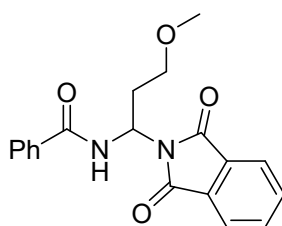
***N*-(1-(1,3-dioxisoindolin-2-yl)-3-phenylpropyl)benzamide (2f)**. A white solid, 54 mg, 70% yield; M.p.: 214-218 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.84-7.72 (m, 4H), 7.69 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.49 (t, $J = 7.4$ Hz, 1H), 7.45-7.36 (m, 3H), 7.24-7.13 (m, 4H), 7.12-7.03 (m, 1H), 6.51 (q, $J = 8.1$ Hz, 1H), 2.89-2.77 (m, 1H), 2.77-2.66 (m, 1H), 2.58-2.38 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.6, 166.2, 140.1, 134.1, 133.3, 131.9, 131.5, 128.5, 128.4, 128.1, 127.1, 126.0, 123.4, 57.0, 34.7, 31.9; IR (neat) ν 3380, 2930, 1774, 1704, 1580, 1525, 1490, 1404, 1374, 1325, 1184, 1119, 1084, 1003 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{24}\text{H}_{21}\text{N}_2\text{O}_3^+$ Requires: 385.1547, Found: 385.1548.



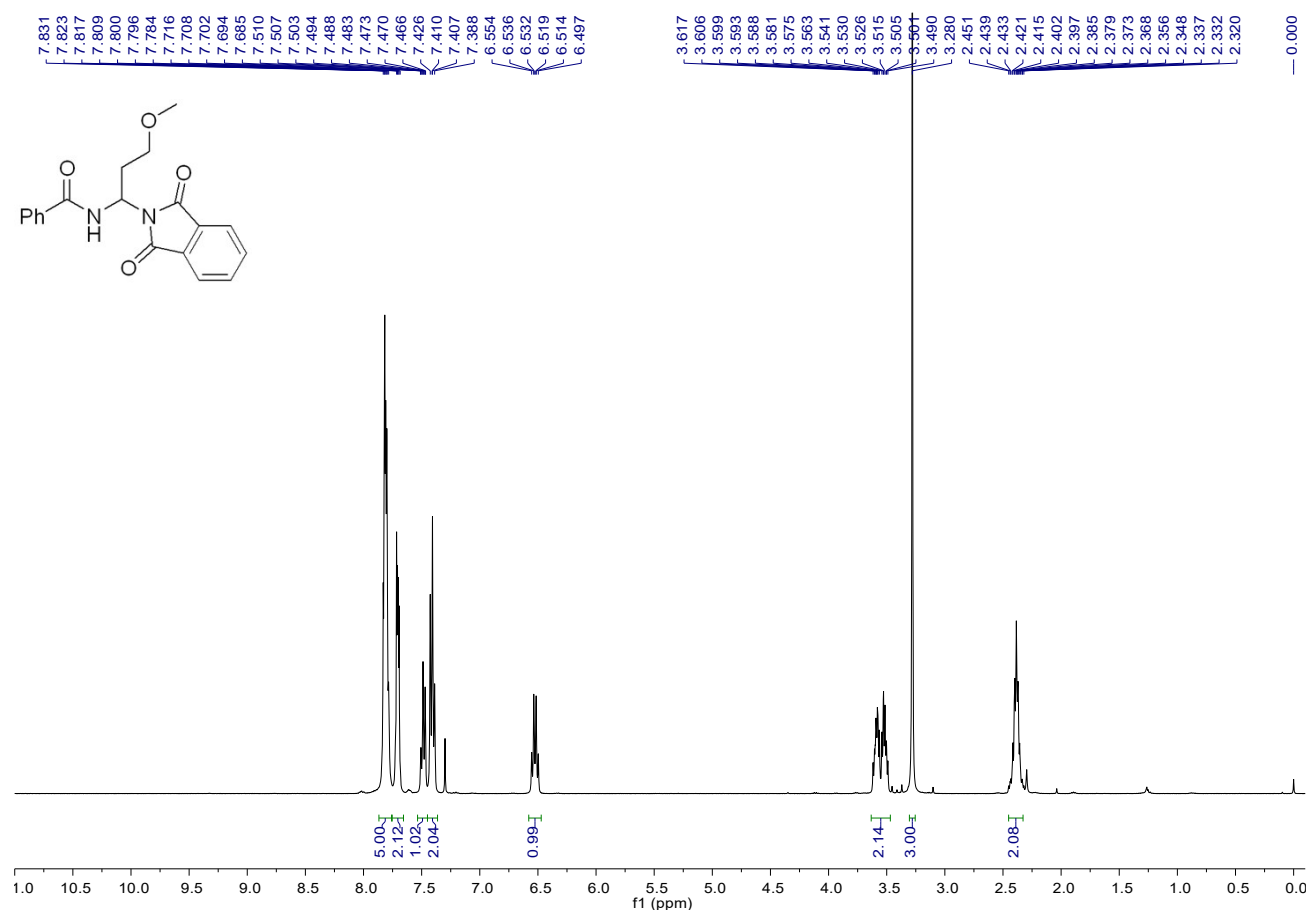


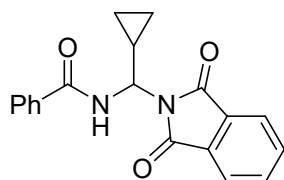
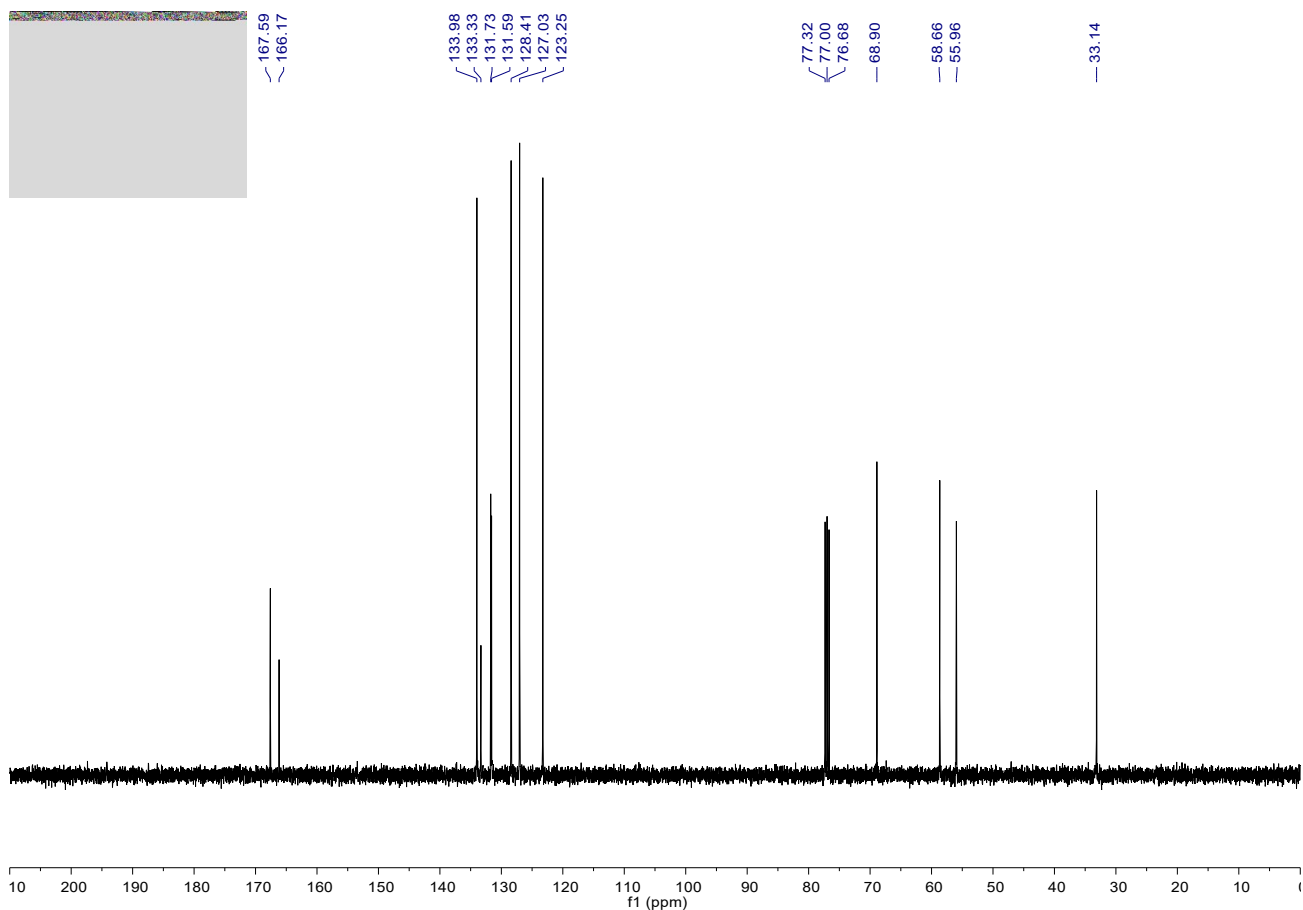
tert-butyl 4-benzamido-4-(1,3-dioxisoindolin-2-yl)butanoate (2g). A white solid, 70 mg, 86% yield; M.p.: 164-166 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.86-7.78 (m, 4H), 7.76-7.68 (m, 3H), 7.49 (t, $J = 7.4$ Hz, 1H), 7.41 (t, $J = 7.5$ Hz, 2H), 6.41 (q, $J = 7.9$ Hz, 1H), 2.60-2.47 (m, 1H), 2.44 (t, $J = 6.7$ Hz, 2H), 2.40-2.26 (m, 1H), 1.39 (s, 9H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 171.8, 167.5, 166.2, 134.1, 133.1, 131.9, 131.5, 128.5, 127.1, 123.4, 80.9, 56.8, 31.5, 28.2, 27.9; IR (neat) ν 3370, 2981, 1777, 1706, 1656, 1579, 1523, 1490, 1324, 1271, 1168, 1079, 970 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{23}\text{H}_{24}\text{N}_2\text{O}_5\text{Na}^+$ Requires: 431.1577, Found: 431.1579.



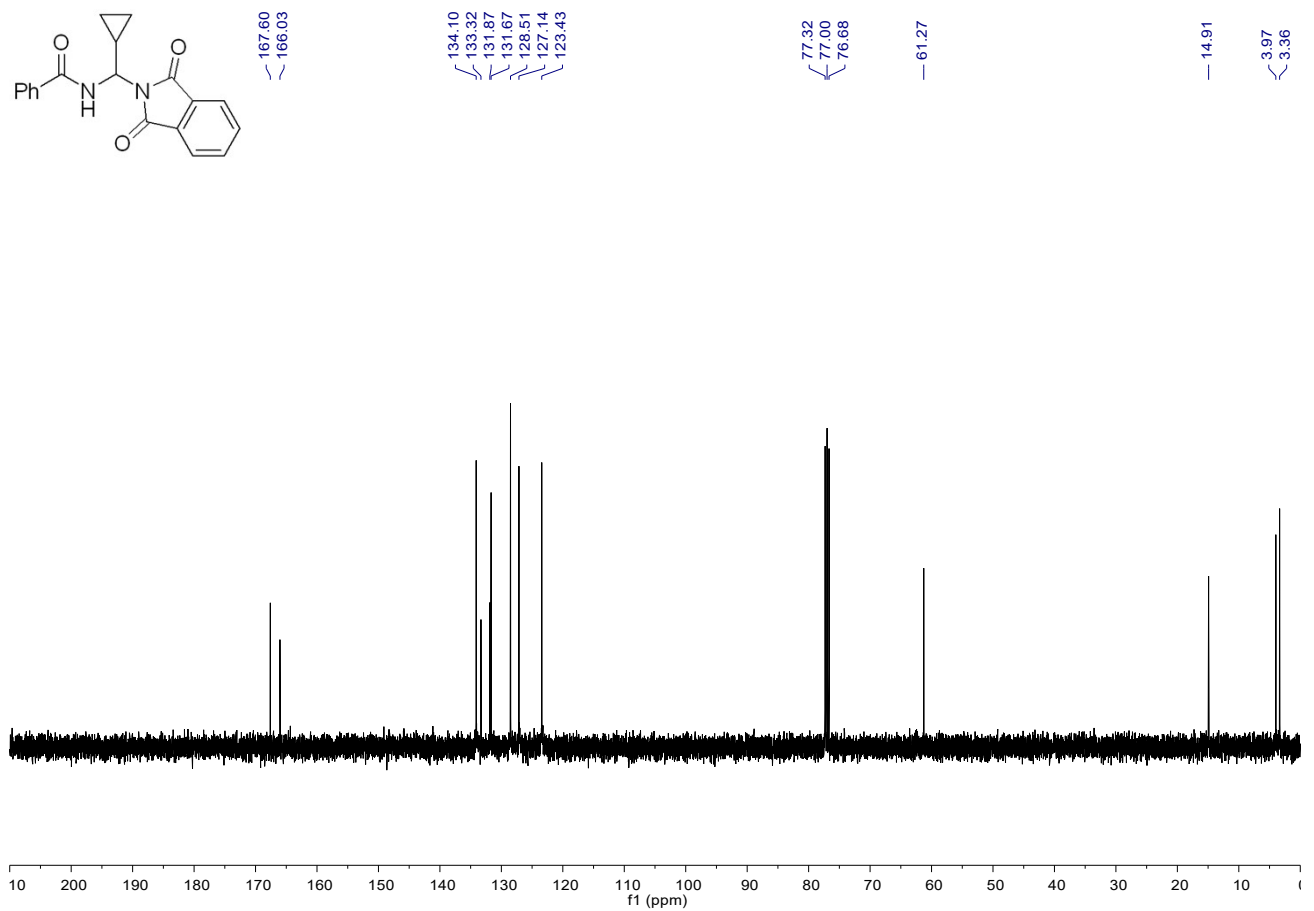
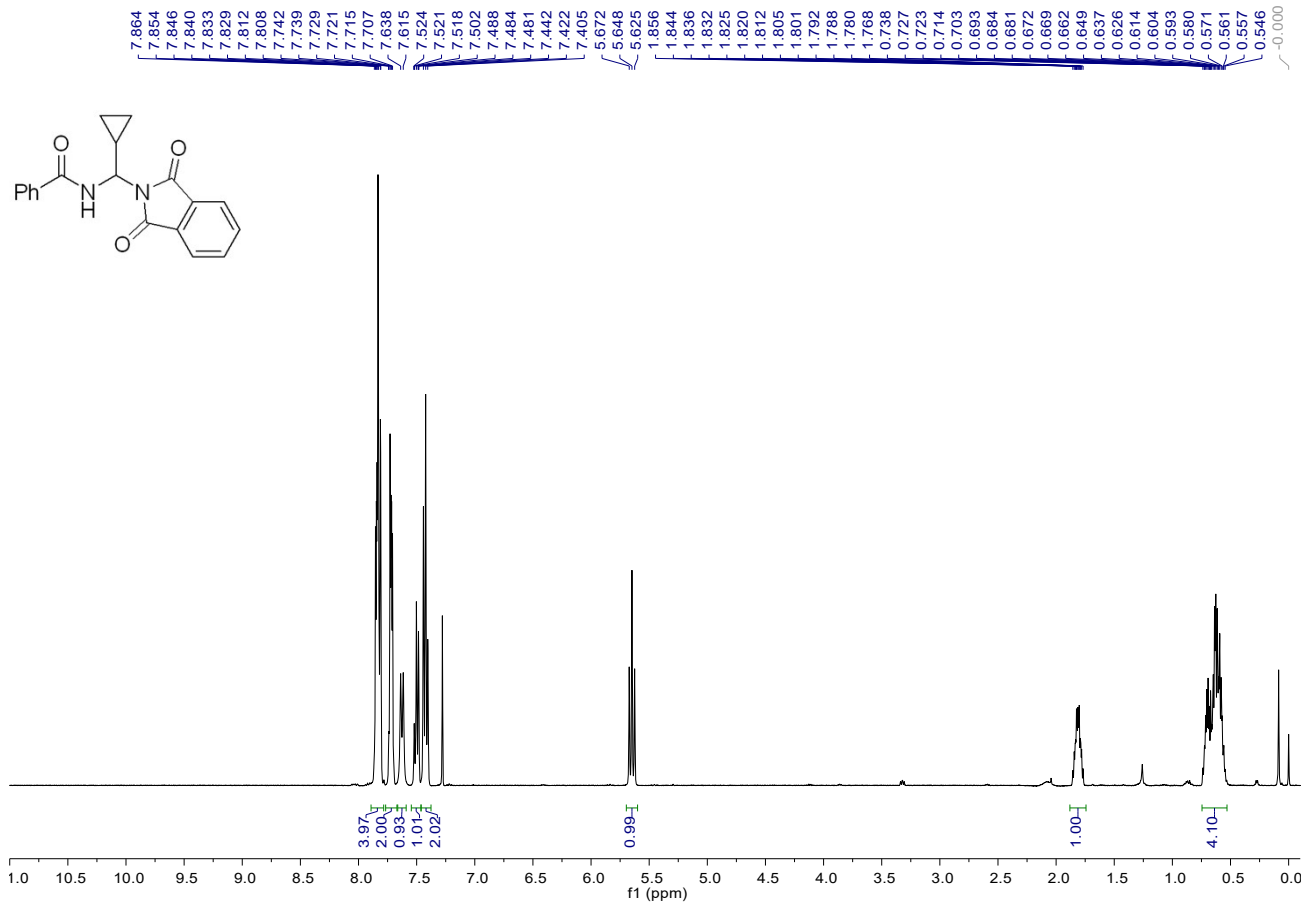


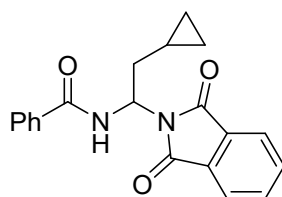
***N*-(1-(1,3-dioxisoindolin-2-yl)-3-methoxypropyl)benzamide (2h)**. A white solid, 45 mg, 66% yield; M.p.: 158-162 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.87-7.76 (m, 5H), 7.70 (dd, $J = 5.5$, 3.0 Hz, 2H), 7.54-7.45 (m, 1H), 7.45-7.36 (m, 2H), 6.53 (dt, $J = 8.7$, 7.1 Hz, 1H), 3.63-3.47 (m, 2H), 3.28 (s, 3H), 2.45-2.33 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.6, 166.2, 134.0, 133.3, 131.7, 131.6, 128.4, 127.0, 123.3, 68.9, 58.7, 56.0, 33.1; IR (neat) ν 3374, 2862, 2832, 1773, 1705, 1665, 1602, 1530, 1491, 1402, 1335, 1198, 1145, 1088, 959 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{19}\text{H}_{19}\text{N}_2\text{O}_4^+$ Requires: 339.1339, Found: 339.1340.



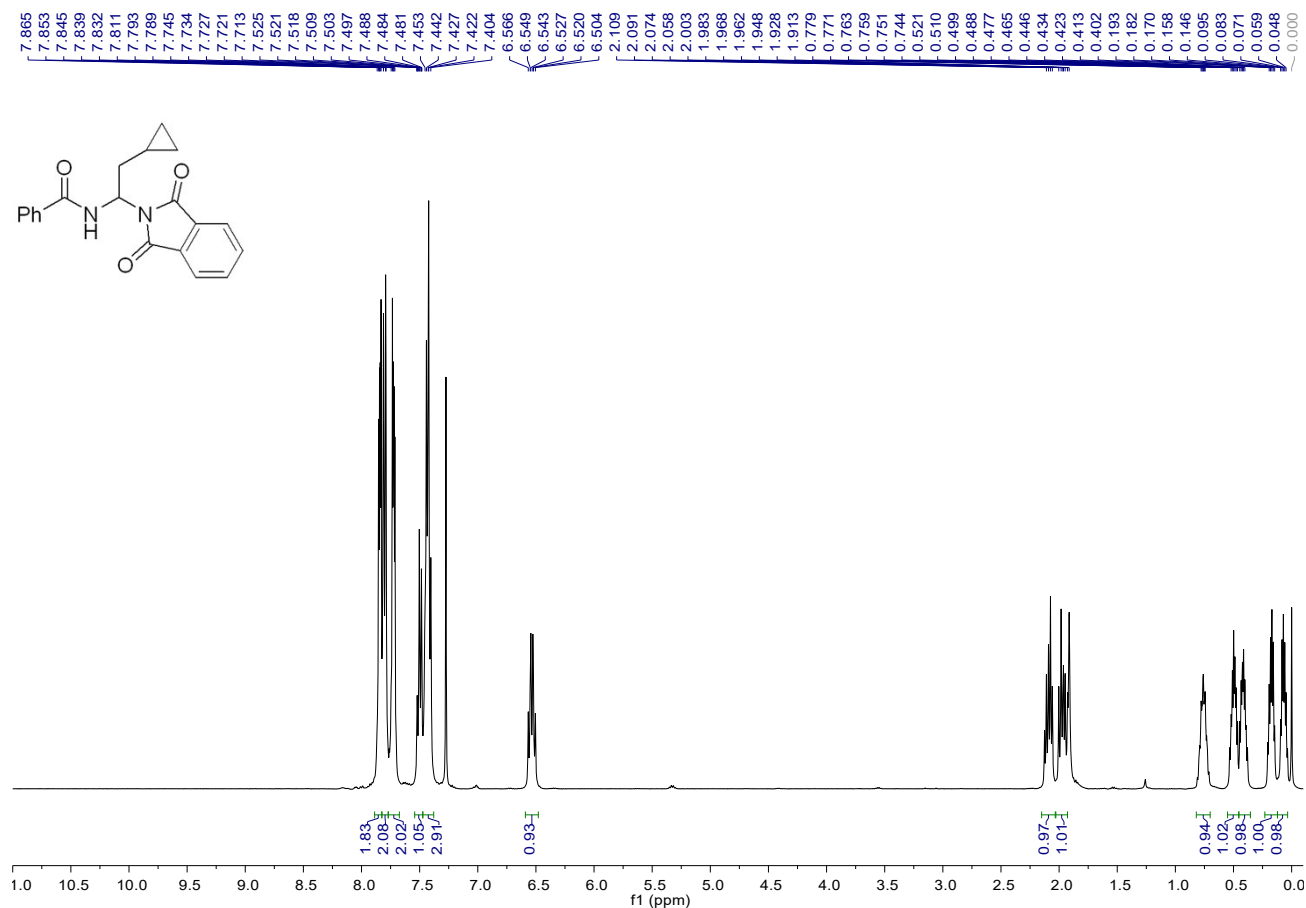


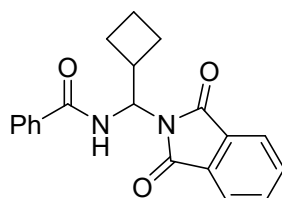
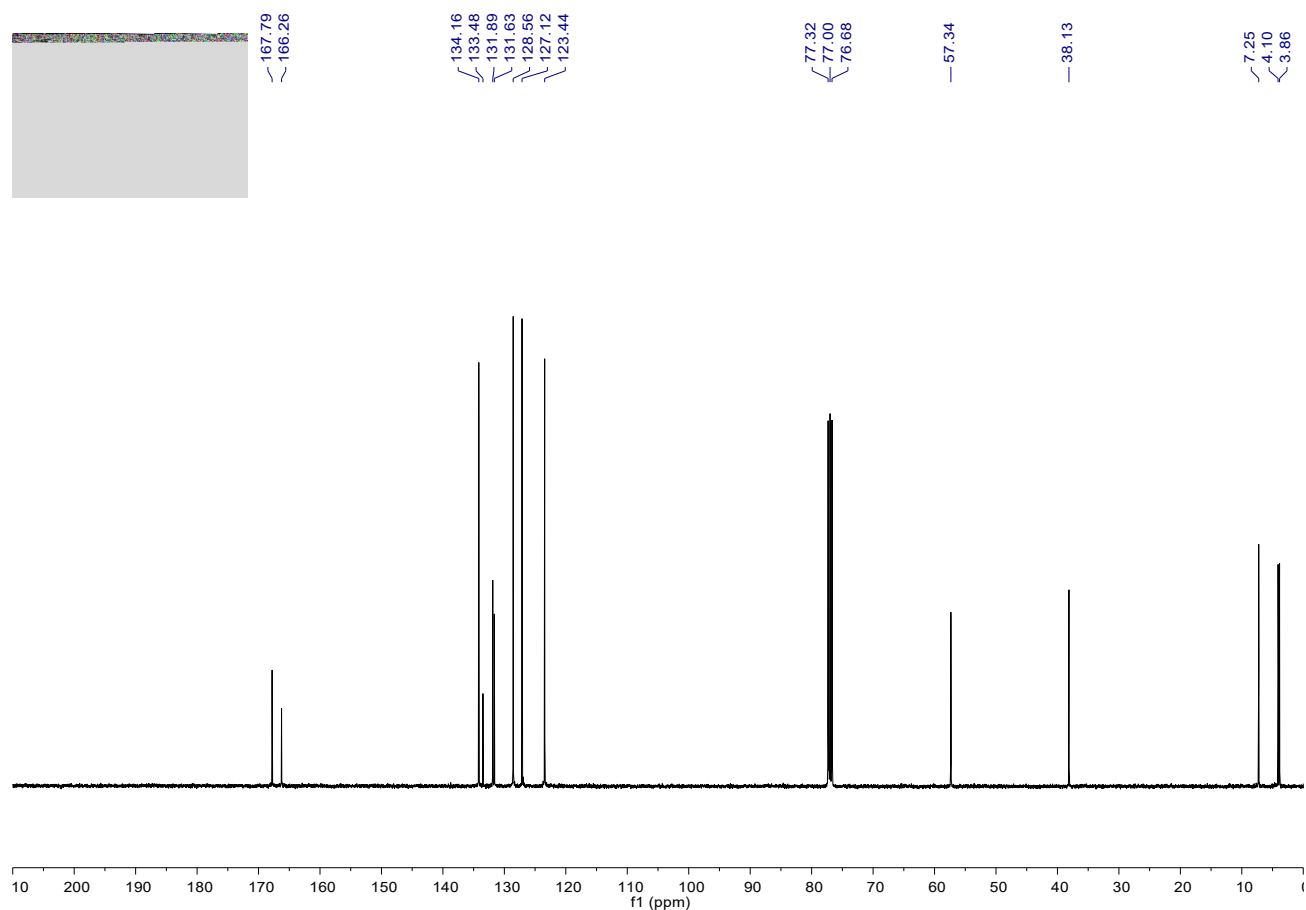
***N*-(cyclopropyl(1,3-dioxoisoindolin-2-yl)methyl)benzamide (2i)**. A white solid, 44 mg, 68% yield; M.p.: 189-191 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.89-7.78 (m, 4H), 7.72 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.63 (d, $J = 9.0$ Hz, 1H), 7.55-7.46 (m, 1H), 7.42 (t, $J = 7.4$ Hz, 2H), 5.65 (t, $J = 9.3$ Hz, 1H), 1.88-1.74 (m, 1H), 0.75-0.53 (m, 4H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.6, 166.0, 134.1, 133.3, 131.9, 131.7, 128.5, 127.1, 123.4, 61.3, 14.9, 4.0, 3.4; IR (neat) ν 3334, 1774, 1704, 1650, 1525, 1381, 1308, 1169, 1078, 1025, 897, 834, 803, 716 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{19}\text{H}_{17}\text{N}_2\text{O}_3^+$ Requires: 321.1234, Found: 321.1234.



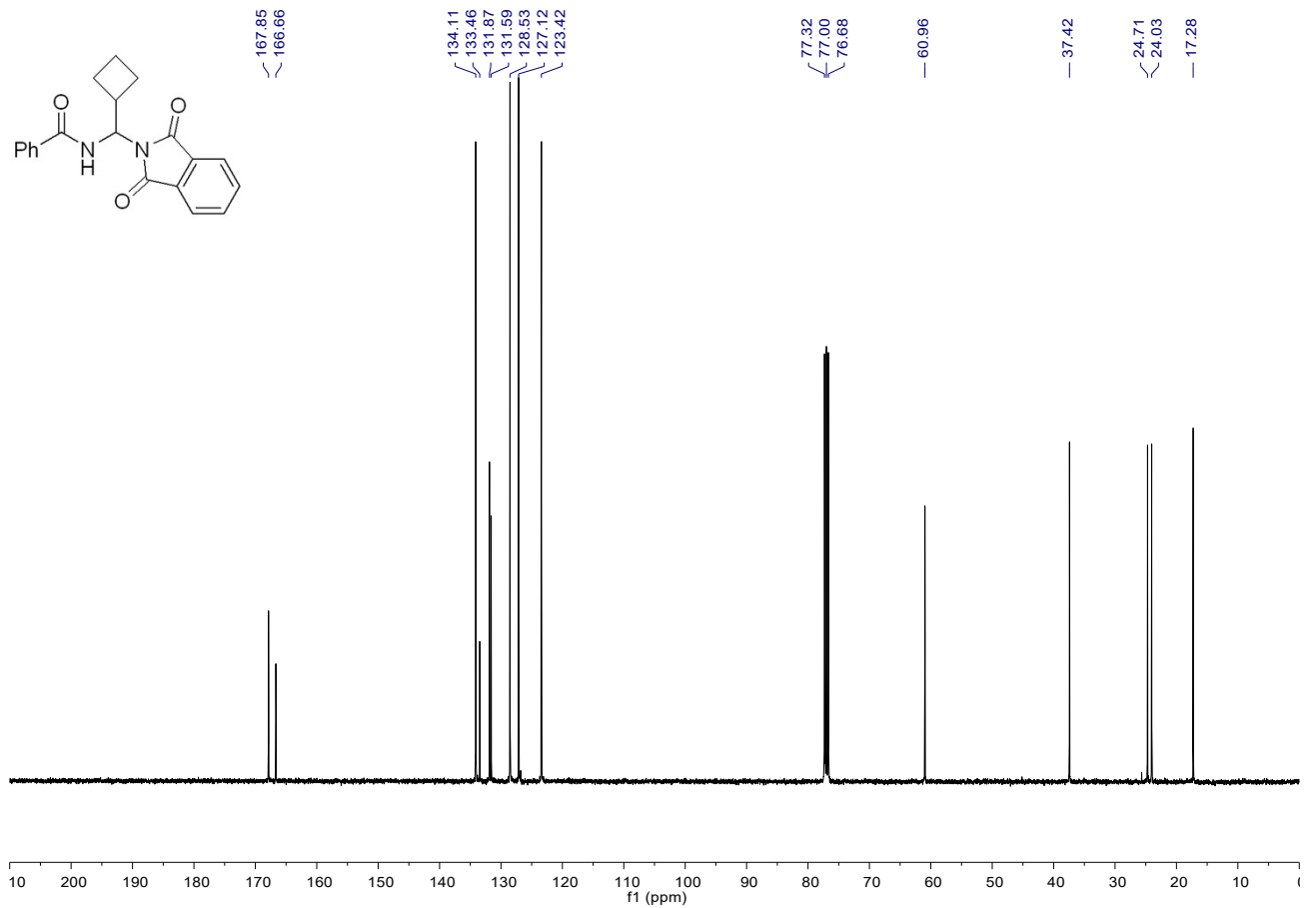
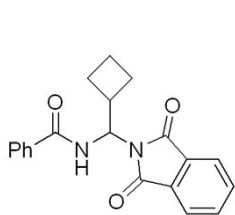
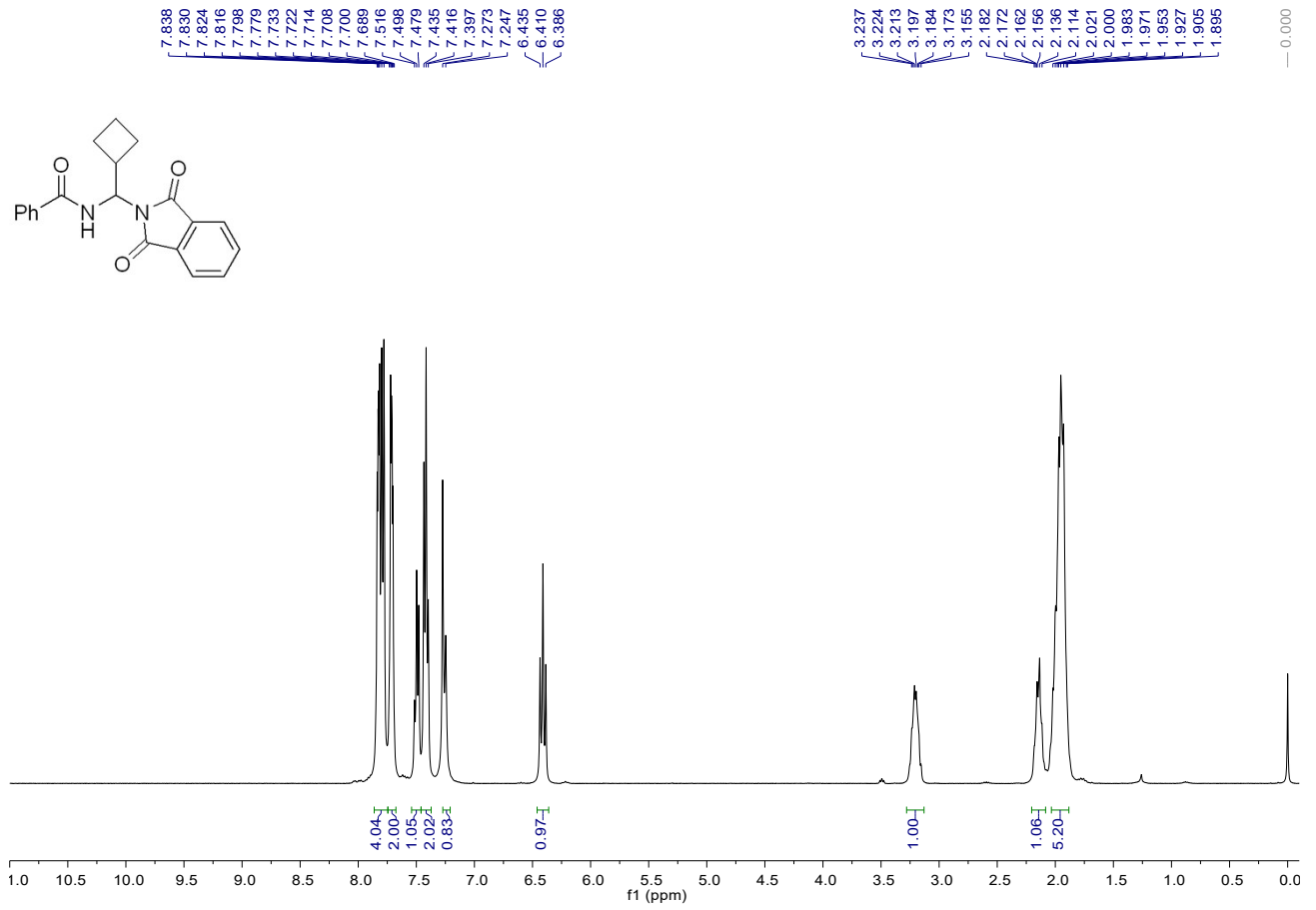
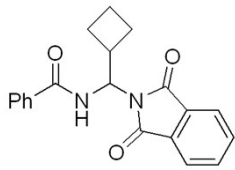


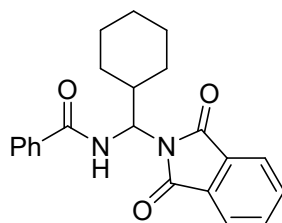
***N*-(2-cyclopropyl-1-(1,3-dioxoisindolin-2-yl)ethyl)benzamide (2j)**. A white solid, 55 mg, 82% yield; M.p.: 199-201 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.84 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.83-7.77 (m, 2H), 7.77-7.67 (m, 2H), 7.54-7.47 (m, 1H), 7.47-7.38 (m, 3H), 6.53 (td, *J* = 9.0, 6.6 Hz, 1H), 2.09 (dt, *J* = 13.3, 6.5 Hz, 1H), 2.03-1.92 (m, 1H), 0.82-0.70 (m, 1H), 0.55-0.45 (m, 1H), 0.45-0.35 (m, 1H), 0.23-0.12 (m, 1H), 0.12-0.03 (m, 1H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 167.8, 166.3, 134.2, 133.5, 131.9, 131.6, 128.6, 127.1, 123.4, 57.3, 38.1, 7.2, 4.1, 3.9; IR (neat) ν 3375, 3003, 2919, 1773, 1699, 1660, 1526, 1490, 1442, 1374, 1288, 1178, 1108 cm⁻¹; HRMS (ESI) Calcd. for C₂₀H₁₈N₂O₃Na⁺ Requires: 357.1210, Found: 357.1209.



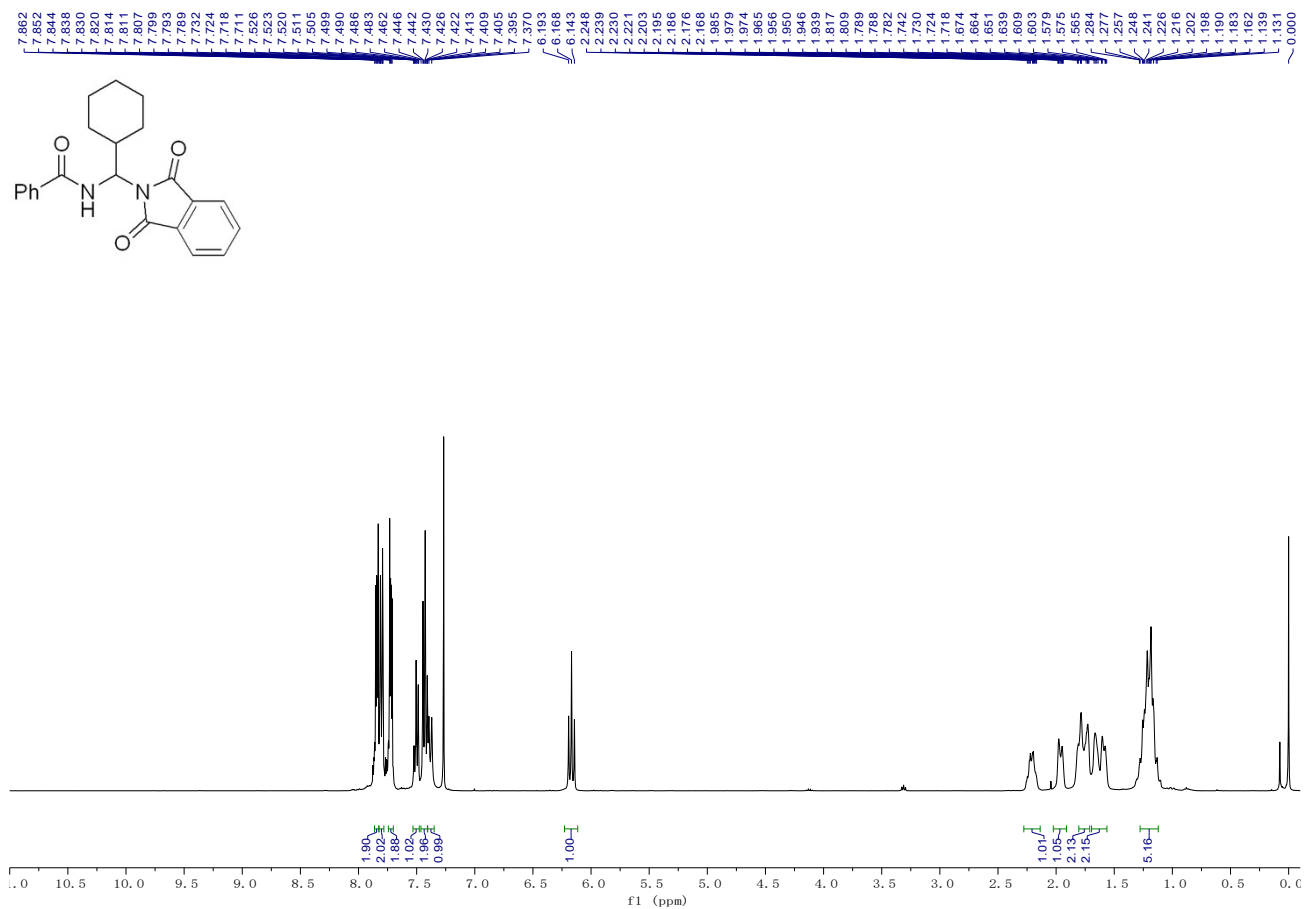


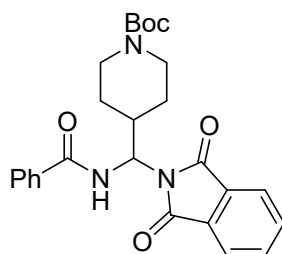
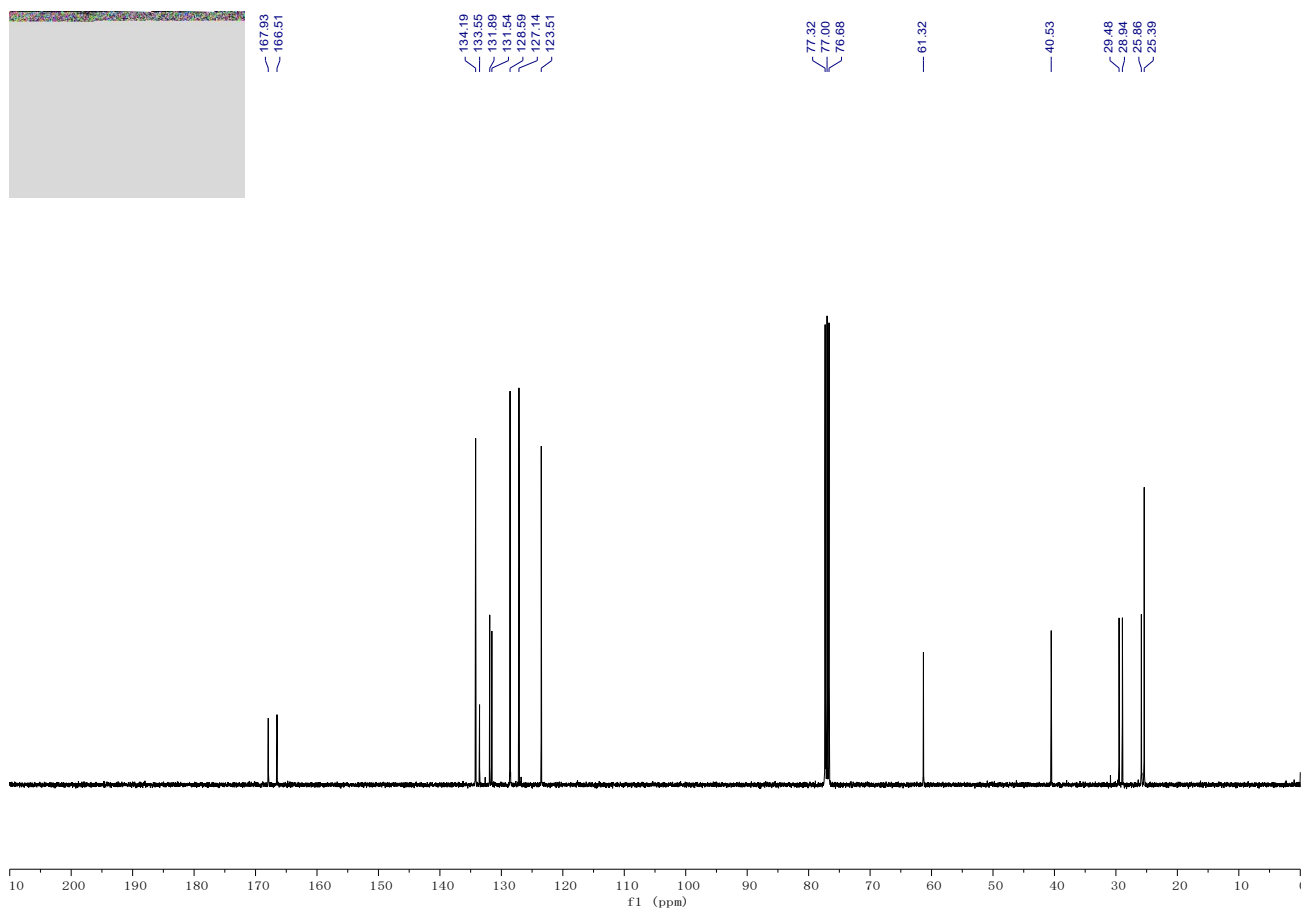
***N*-(cyclobutyl(1,3-dioxoisindolin-2-yl)methyl)benzamide (2k)**. A white solid, 54 mg, 80% yield; M.p.: 202-204 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.86-7.74 (m, 4H), 7.71 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.50 (t, $J = 7.3$ Hz, 1H), 7.42 (t, $J = 7.5$ Hz, 2H), 7.25 (s, 1H), 6.41 (t, $J = 9.9$ Hz, 1H), 3.28-3.13 (m, 1H), 2.20-2.08 (m, 1H), 2.03-1.88 (m, 5H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.9, 166.7, 134.1, 133.5, 131.9, 131.6, 128.5, 127.1, 123.4, 61.0, 37.4, 24.7, 24.0, 17.3; IR (neat) ν 3368, 2934, 1775, 1701, 1602, 1523, 1403, 1334, 1265, 1119, 1021, 944 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{20}\text{H}_{18}\text{N}_2\text{O}_3\text{Na}^+$ Requires: 357.1210, Found: 357.1207.



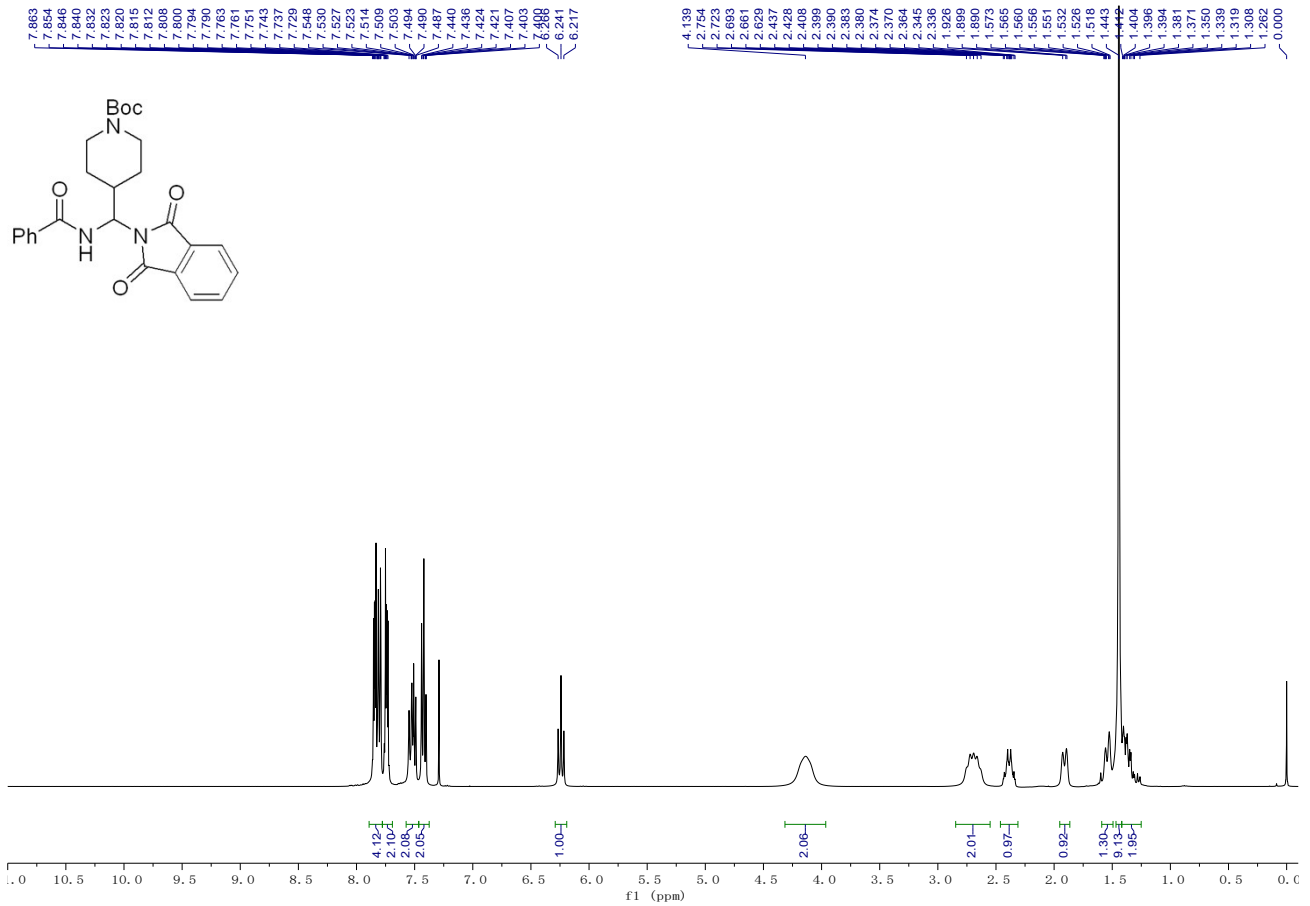


***N*-(cyclohexyl(1,3-dioxisoindolin-2-yl)methyl)benzamide (21)**. A white solid, 53 mg, 73% yield; M.p.: 236-238 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.84 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.82-7.78 (m, 2H), 7.72 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.53-7.48 (m, 1H), 7.46-7.41 (m, 2H), 7.38 (d, *J* = 9.7 Hz, 1H), 6.17 (t, *J* = 10.0 Hz, 1H), 2.28-2.14 (m, 1H), 2.02-1.91 (m, 1H), 1.80-1.71 (m, 2H), 1.70-1.56 (m, 2H), 1.28-1.12 (m, 5H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 167.9, 166.5, 134.2, 133.5, 131.9, 131.5, 128.6, 127.1, 123.5, 61.3, 40.5, 29.5, 28.9, 25.9, 25.4; IR (neat) ν 3385, 2924, 2851, 1774, 1702, 1667, 1602, 1519, 1488, 1406, 1375, 1303, 1162 cm⁻¹; HRMS (ESI) Calcd. for C₂₂H₂₂N₂O₃Na⁺ Requires: 385.1523, Found: 385.1517.

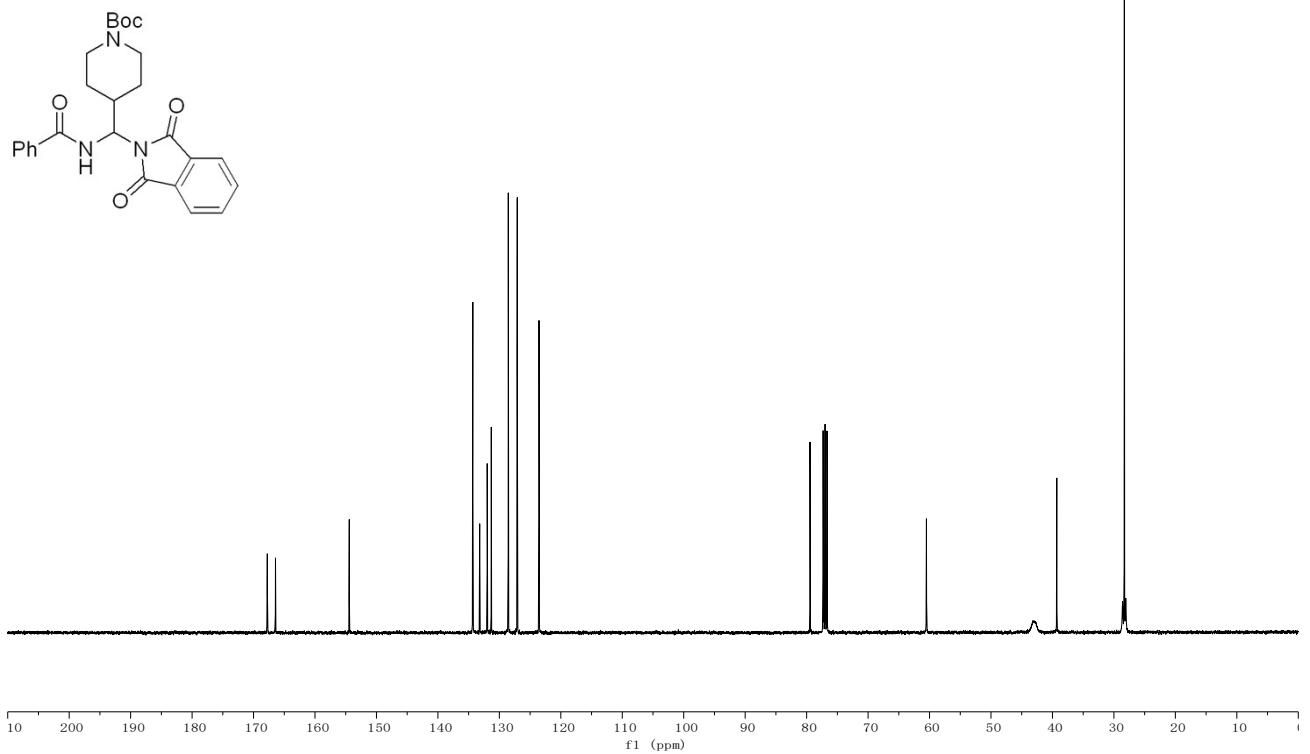


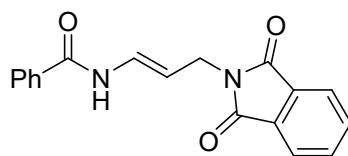


tert-butyl-4-(benzamido(1,3-dioxoisindolin-2-yl)methyl)piperidine-1-carboxylate (2m). A white solid, 67 mg, 72% yield; M.p.: 205-206 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.89-7.78 (m, 4H), 7.78-7.69 (m, 2H), 7.57-7.46 (m, 2H), 7.46-7.38 (m, 2H), 6.24 (t, $J = 9.8$ Hz, 1H), 4.32-3.96 (m, 2H), 2.85-2.55 (m, 2H), 2.46-2.31 (m, 1H), 1.95-1.86 (m, 1H), 1.59-1.49 (m, 1H), 1.44 (s, 9H), 1.42-1.25 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.8, 166.4, 154.4, 134.3, 133.2, 132.0, 131.3, 128.5, 127.1, 123.5, 79.5, 60.5, 43.0, 39.3, 28.6, 28.3, 28.1; IR (neat) ν 3385, 2979, 2851, 1779, 1704, 1651, 1578, 1414, 1357, 1295, 1150, 1116, 1065, 1029 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{26}\text{H}_{29}\text{N}_3\text{O}_5\text{Na}^+$ Requires: 486.1999, Found: 486.1994.

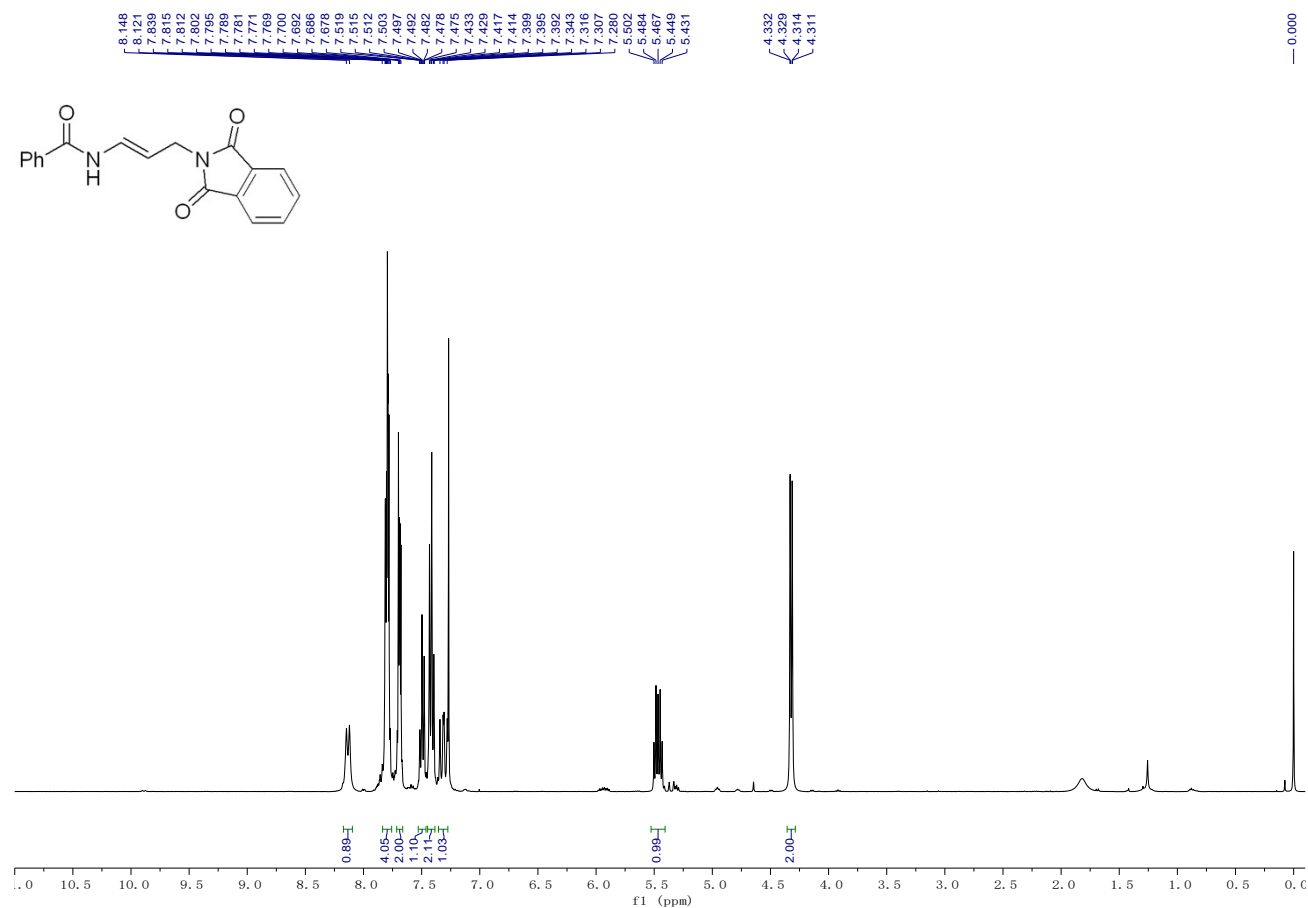


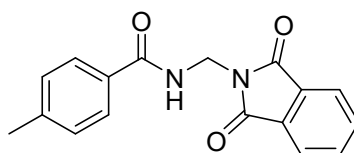
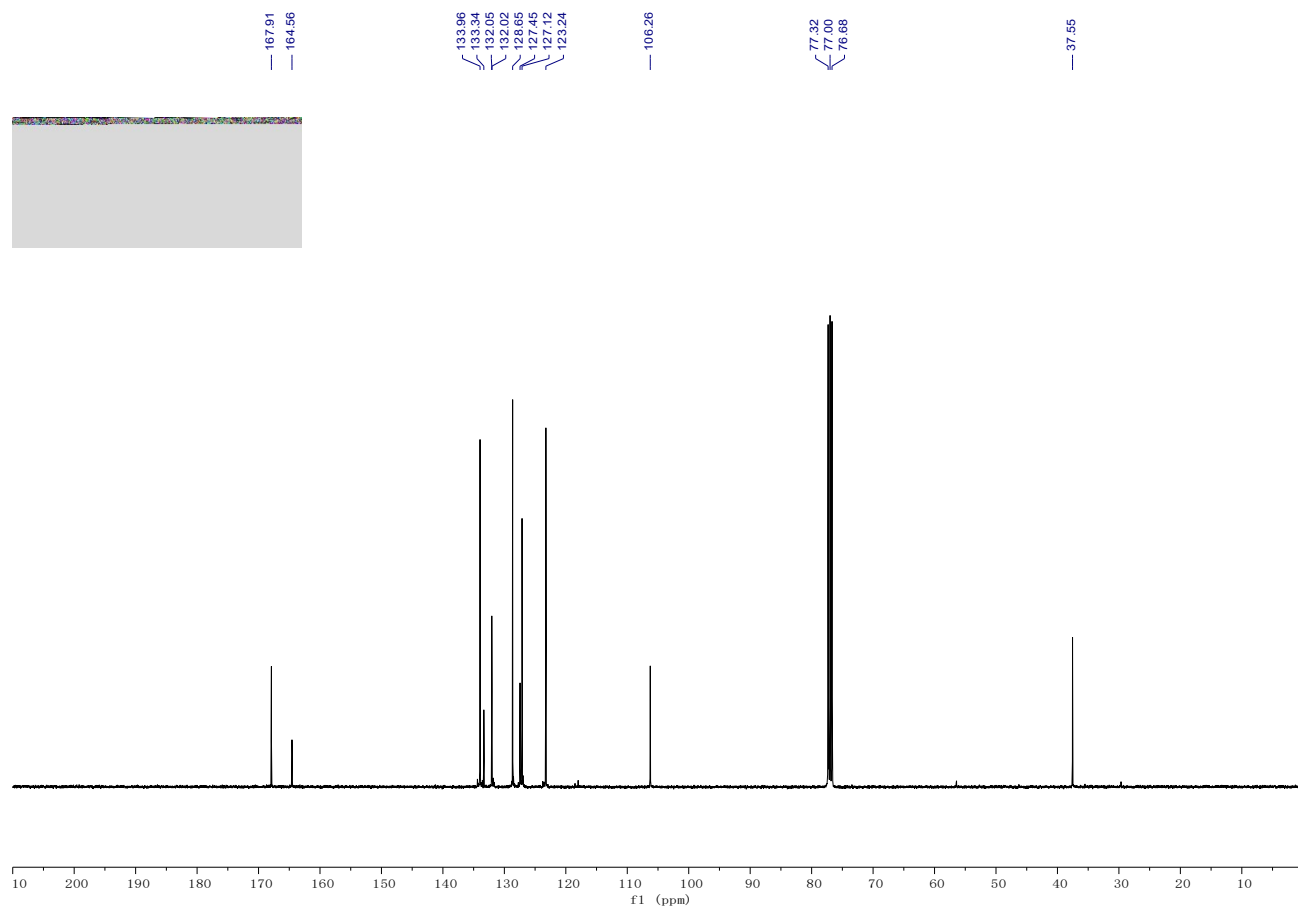
167.76, 166.43, 154.42, 134.32, 133.20, 131.98, 131.31, 128.55, 127.09, 123.55, 79.45, 77.32, 77.00, 76.68, 60.50, 43.14, 39.29, 28.59, 28.30, 28.07



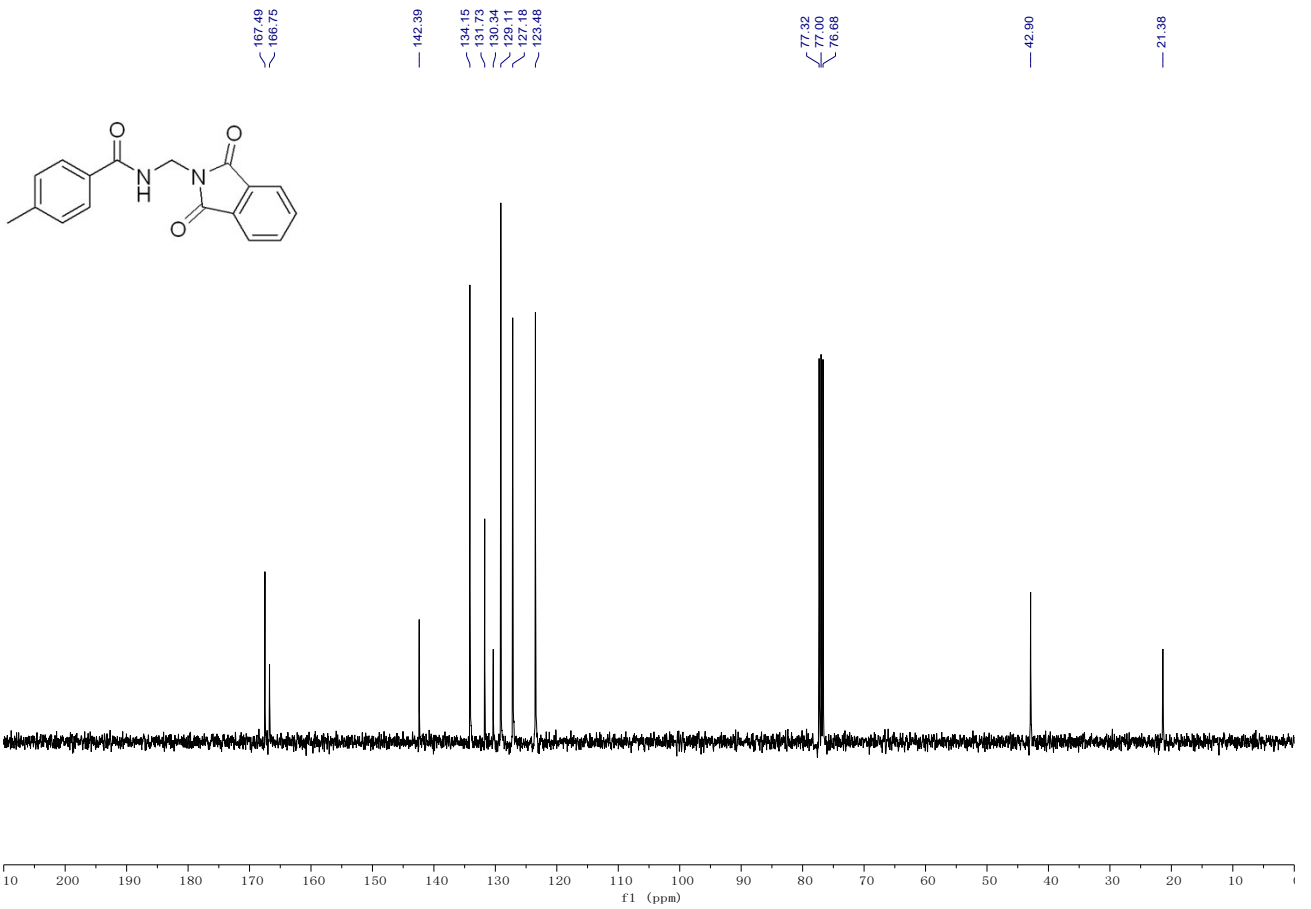
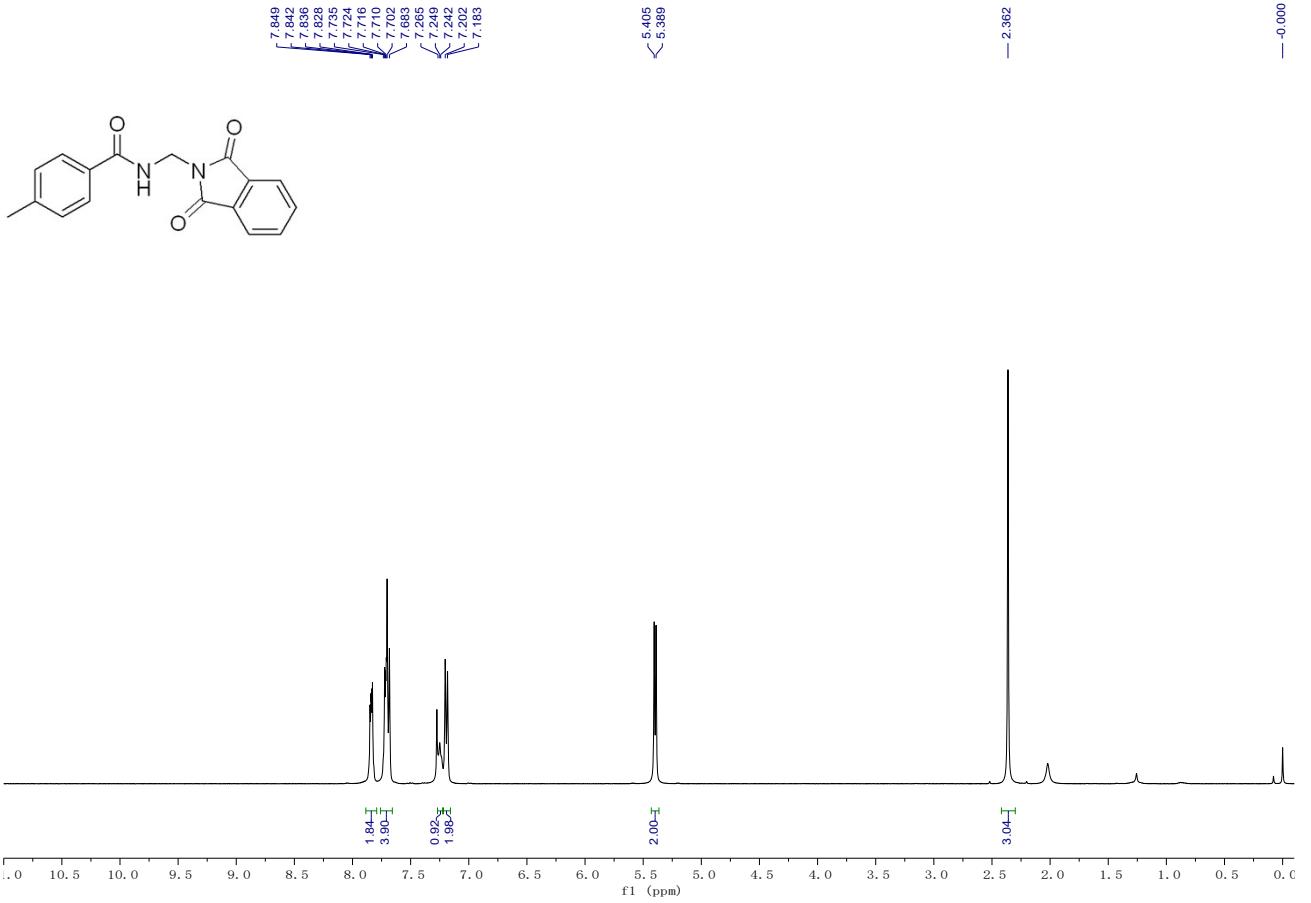


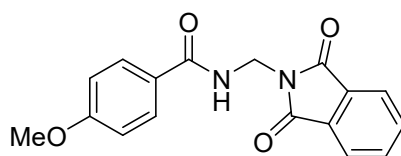
(E)-N-(3-(1,3-dioxisoindolin-2-yl)prop-1-en-1-yl)benzamide (2n). A white solid, 19 mg, 31% yield; M.p.: 201-203 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 8.13 (d, $J = 10.7$ Hz, 1H), 7.84-7.76 (m, 4H), 7.69 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.53-7.46 (m, 1H), 7.45-7.39 (m, 2H), 7.31 (dd, $J = 14.2, 10.6$ Hz, 1H), 5.47 (dt, $J = 14.1, 7.0$ Hz, 1H), 4.32 (dd, $J = 7.0, 1.2$ Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.9, 164.6, 134.0, 133.3, 132.0, 132.0, 128.7, 127.4, 127.1, 123.2, 106.3, 37.5; IR (neat) ν 3399, 3296, 1763, 1706, 1661, 1580, 1488, 1392, 1292, 1244, 1143, 1051, 925 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{18}\text{H}_{14}\text{N}_2\text{O}_3\text{Na}^+$ Requires: 329.0897, Found: 329.0893.



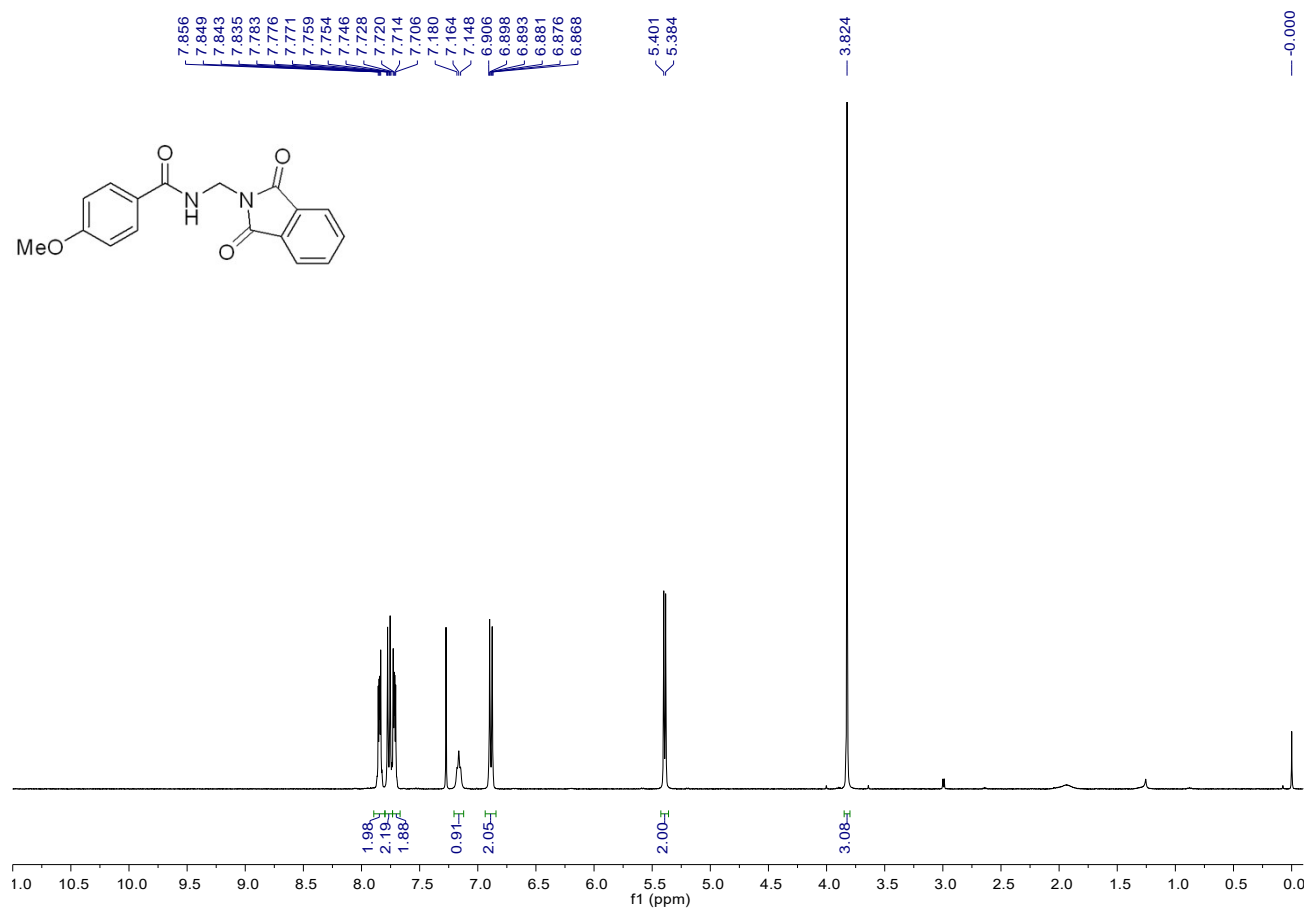


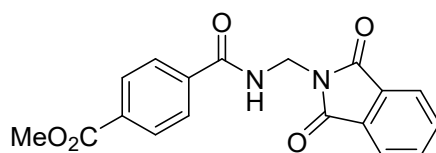
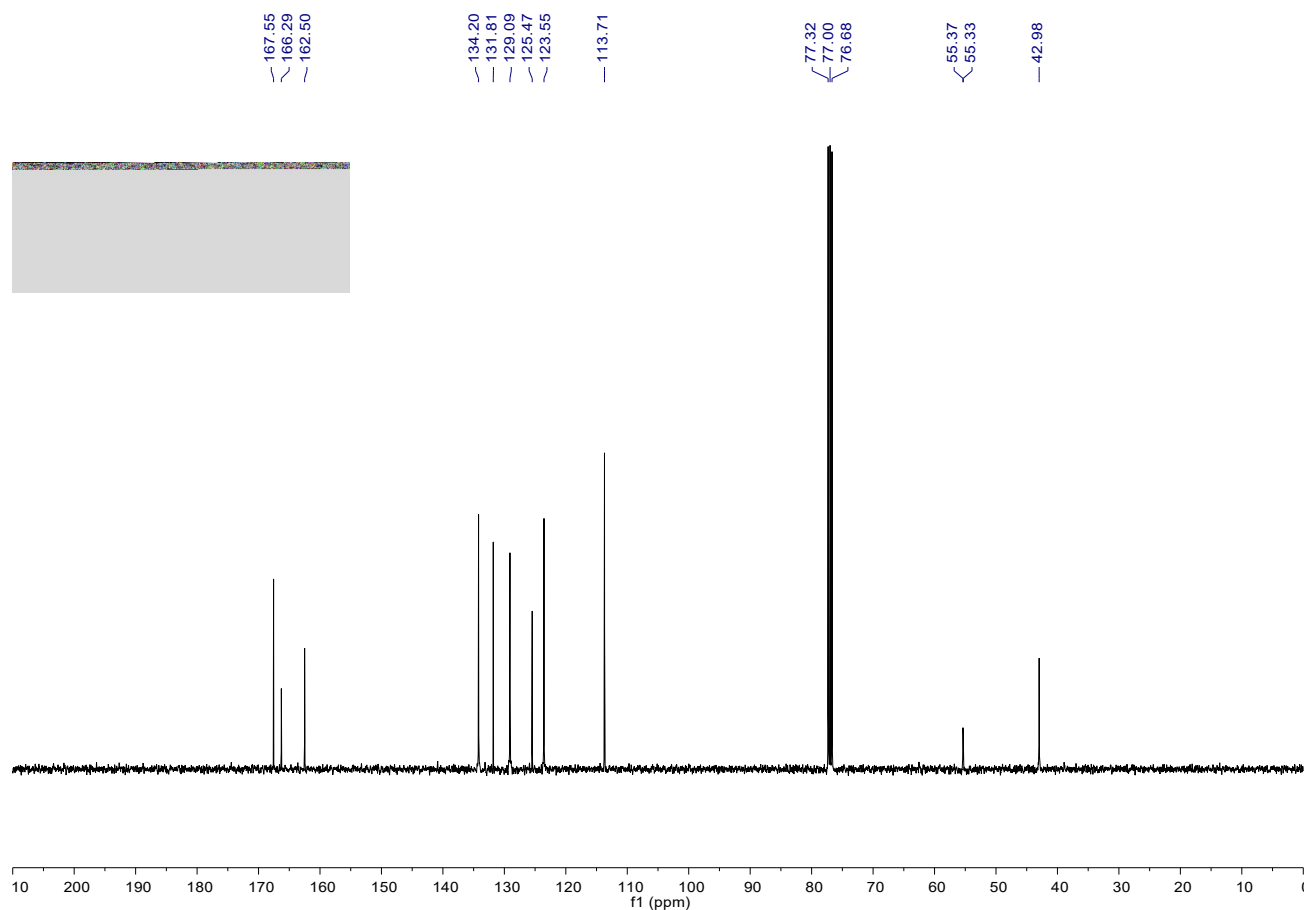
***N*-((1,3-dioxisoindolin-2-yl)methyl)-4-methylbenzamide (2o)**. A white solid, 58 mg, 99% yield; M.p.: 210-214 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.84 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.76-7.66 (m, 4H), 7.27-7.22 (m, 1H), 7.19 (d, *J* = 7.9 Hz, 2H), 5.40 (d, *J* = 6.4 Hz, 2H), 2.36 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 167.5, 166.7, 142.4, 134.1, 131.7, 130.3, 129.1, 127.2, 123.5, 42.9, 21.4; IR (neat) ν 3313, 2957, 1774, 1713, 1643, 1573, 1528, 1444, 1397, 1369, 1276, 1215, 1165, 1120, 994 cm⁻¹; HRMS (ESI) Calcd. for C₁₇H₁₅N₂O₃⁺ Requires: 295.1077, Found: 295.1078.



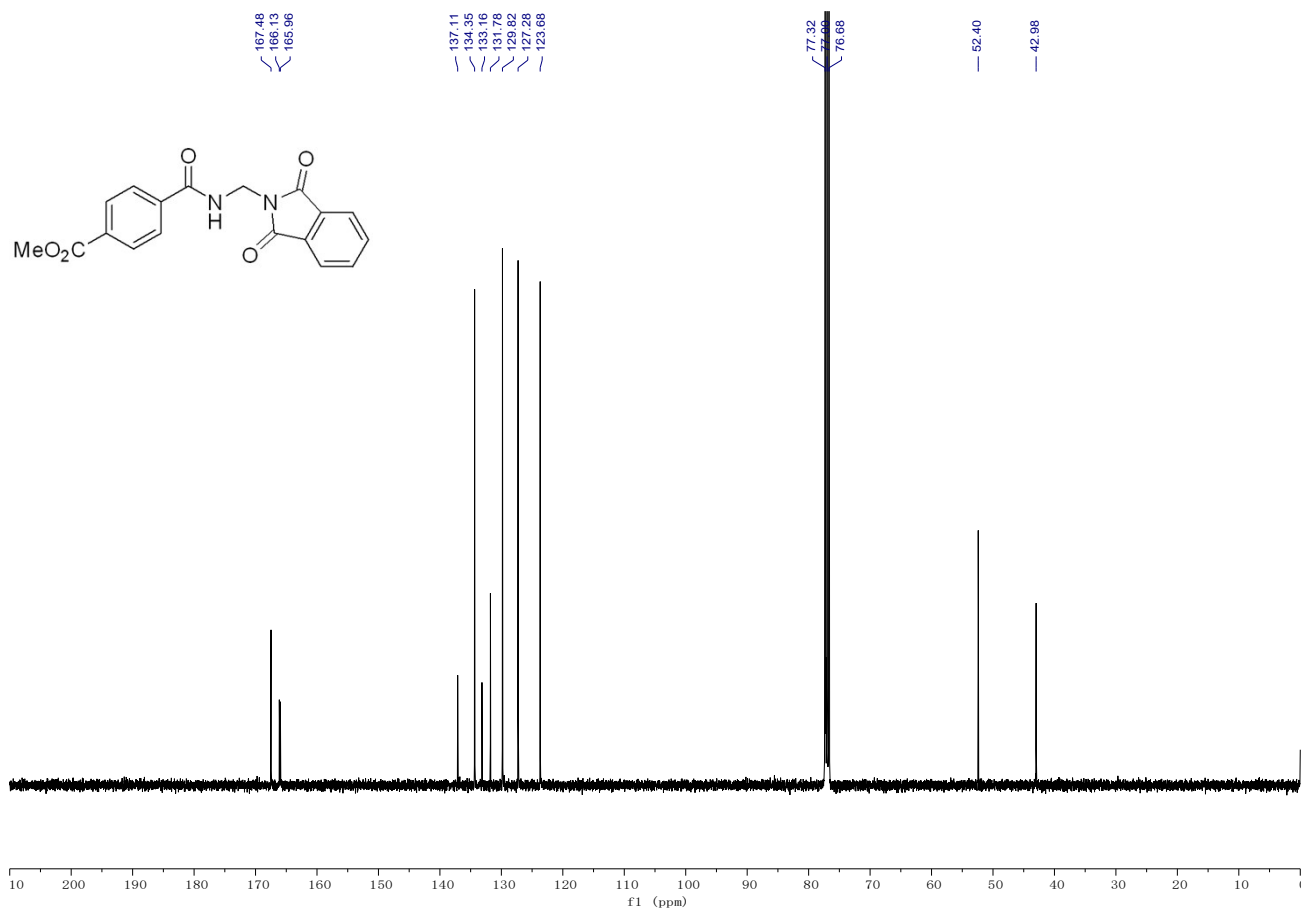
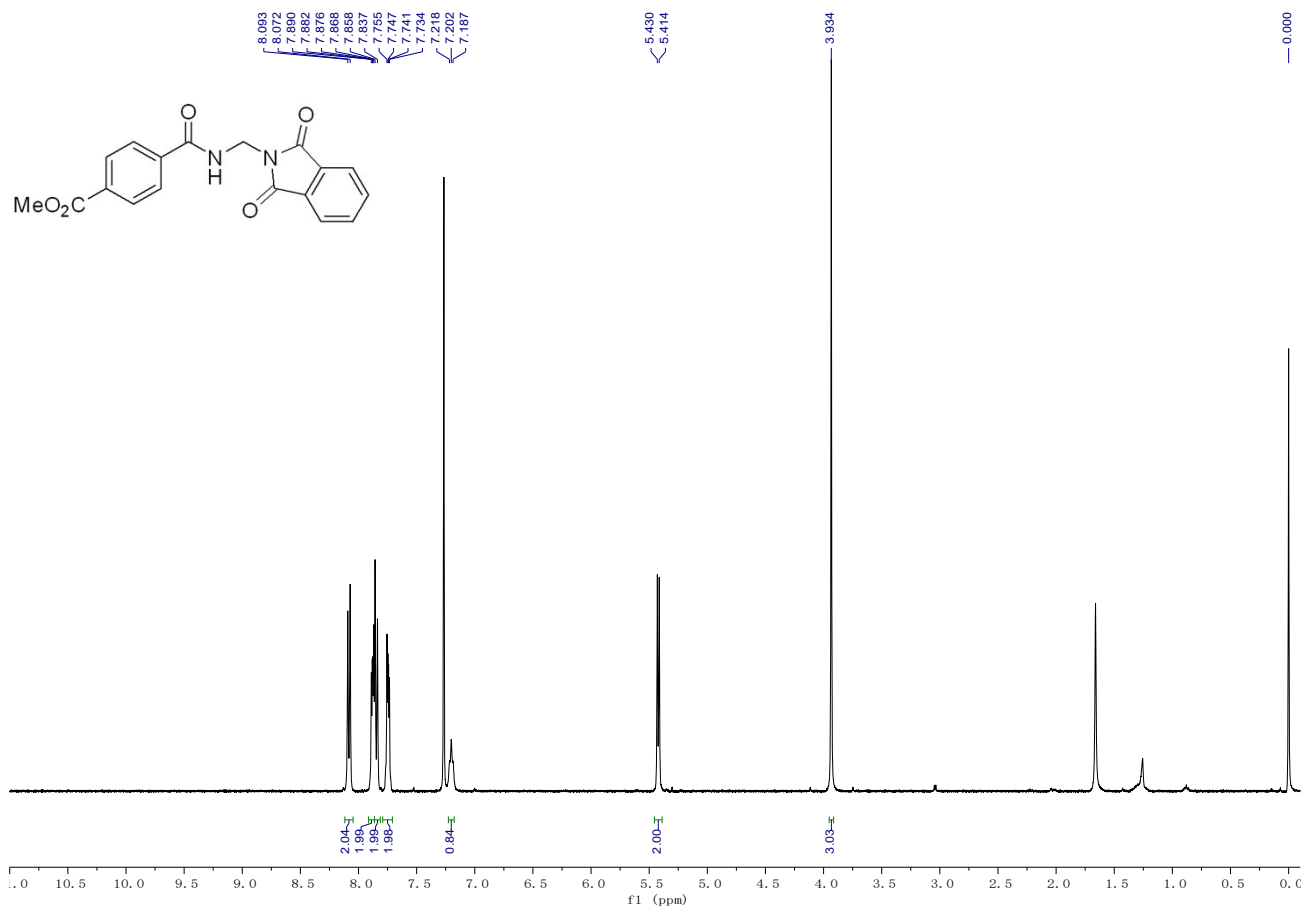


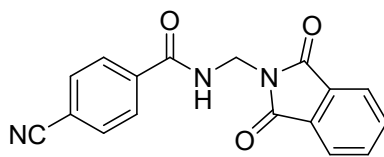
***N*-((1,3-dioxisoindolin-2-yl)methyl)-4-methoxybenzamide (2p)**. A white solid, 55 mg, 88% yield; M.p.: 206-210 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.85 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.80-7.73 (m, 2H), 7.72 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.16 (t, *J* = 6.4 Hz, 1H), 6.94-6.84 (m, 2H), 5.39 (d, *J* = 6.4 Hz, 2H), 3.82 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 167.6, 166.3, 162.5, 134.2, 131.8, 129.1, 125.5, 123.6, 113.7, 55.4, 55.3, 43.0; IR (neat) ν 3343, 2961, 1775, 1711, 1640, 1607, 1505, 1470, 1411, 1293, 1256, 1178, 1025, 878 cm⁻¹; HRMS (ESI) Calcd. for C₁₇H₁₅N₂O₄⁺ Requires: 311.1026, Found: 311.1026.



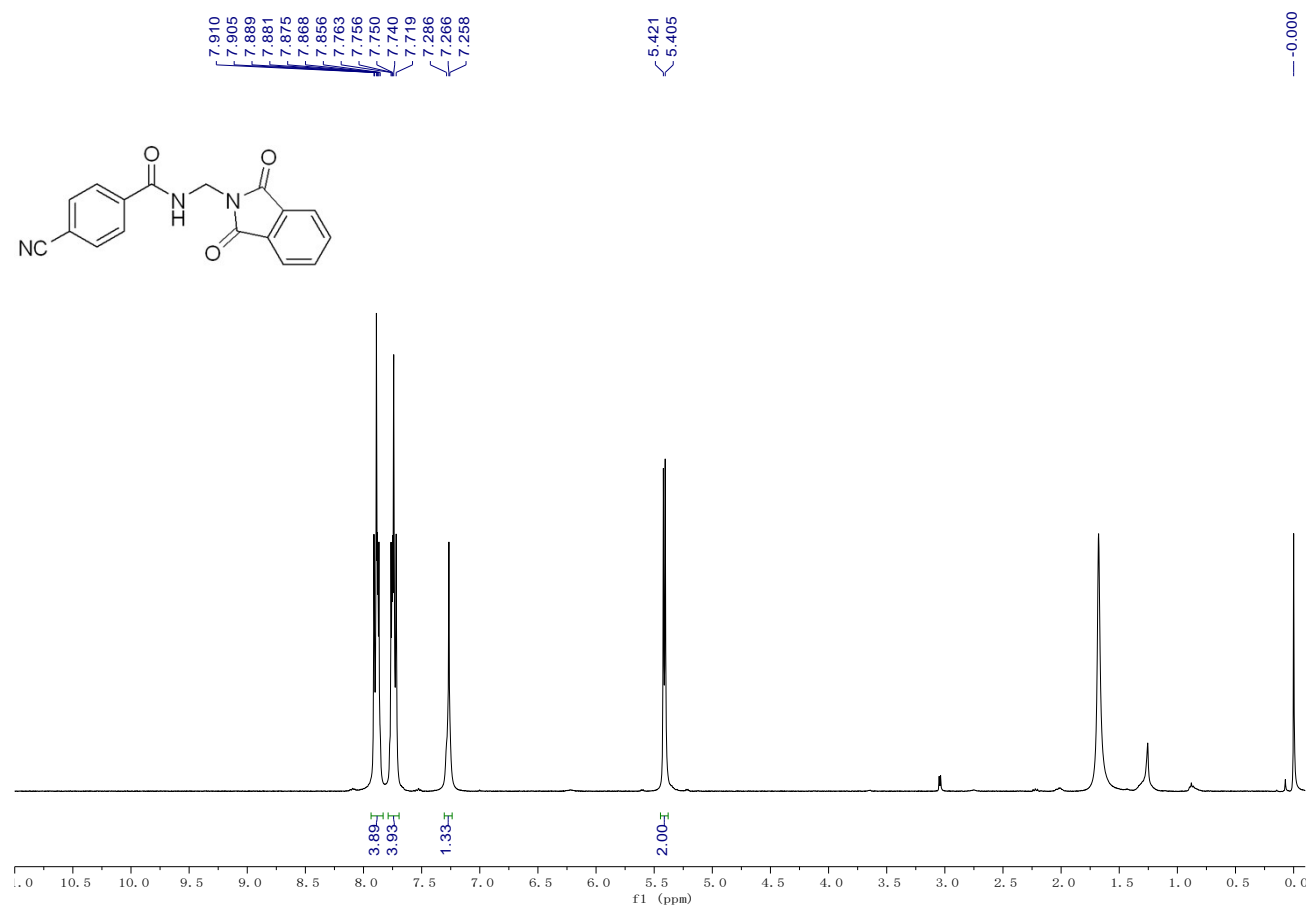


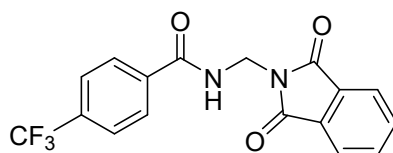
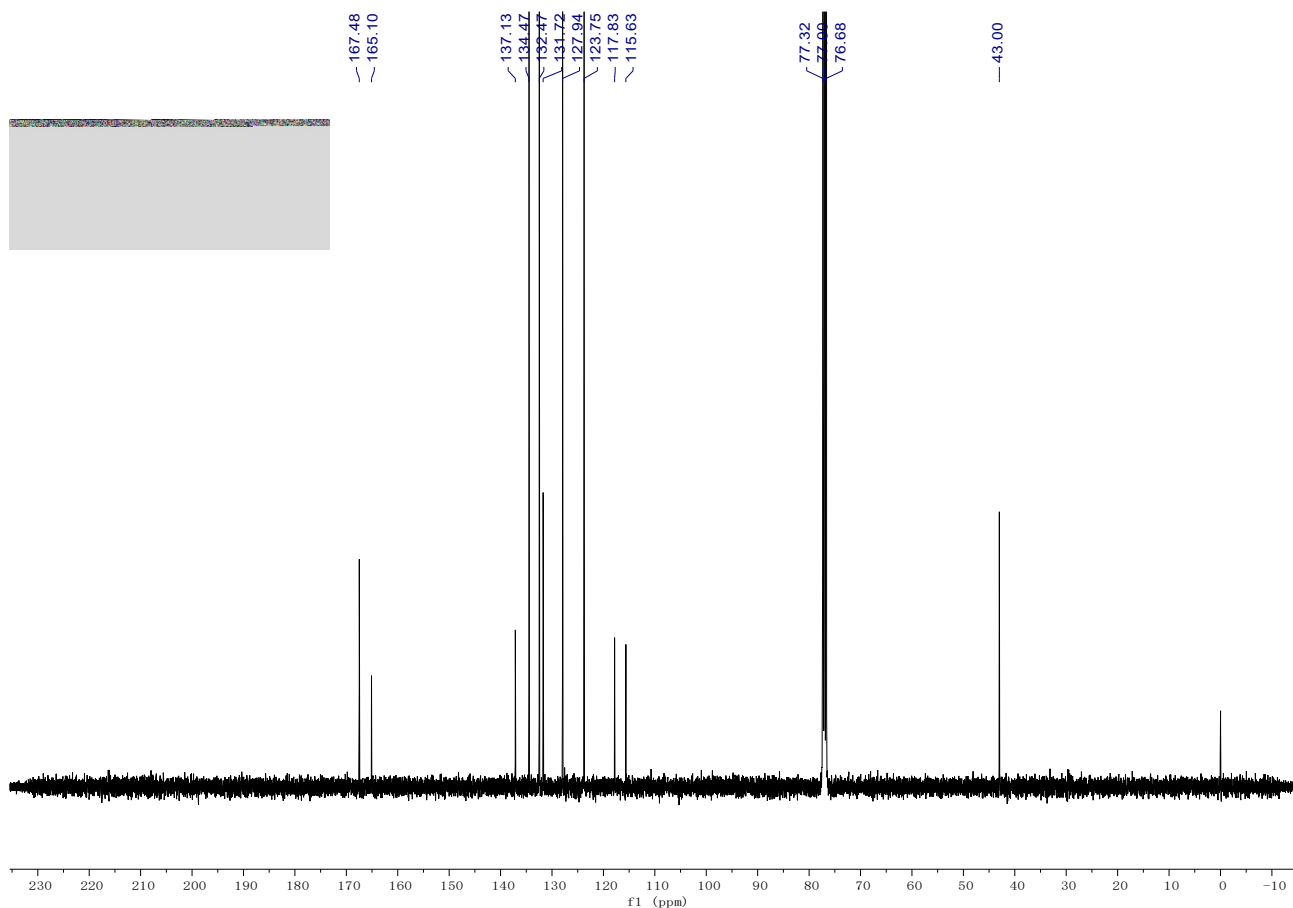
methyl 4-(((1,3-dioxoisindolin-2-yl)methyl)carbamoyl)benzoate (2q). A white solid, 67 mg, 99% yield; M.p.: 230-234 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 8.08 (d, $J = 8.4$ Hz, 2H), 7.88 (dd, $J = 5.4, 3.1$ Hz, 2H), 7.85 (d, $J = 8.1$ Hz, 2H), 7.74 (dd, $J = 5.6, 3.1$ Hz, 2H), 7.20 (t, $J = 6.2$ Hz, 1H), 5.42 (d, $J = 6.4$ Hz, 2H), 3.93 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.5, 166.1, 166.0, 137.1, 134.4, 133.2, 131.8, 129.8, 127.3, 123.7, 52.4, 43.0; IR (neat) ν 3296, 2952, 1773, 1702, 1648, 1572, 1471, 1447, 1404, 1330, 1275, 1191, 1108, 1016, 958 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{18}\text{H}_{15}\text{N}_2\text{O}_5^+$ Requires: 339.0975, Found: 339.0975.



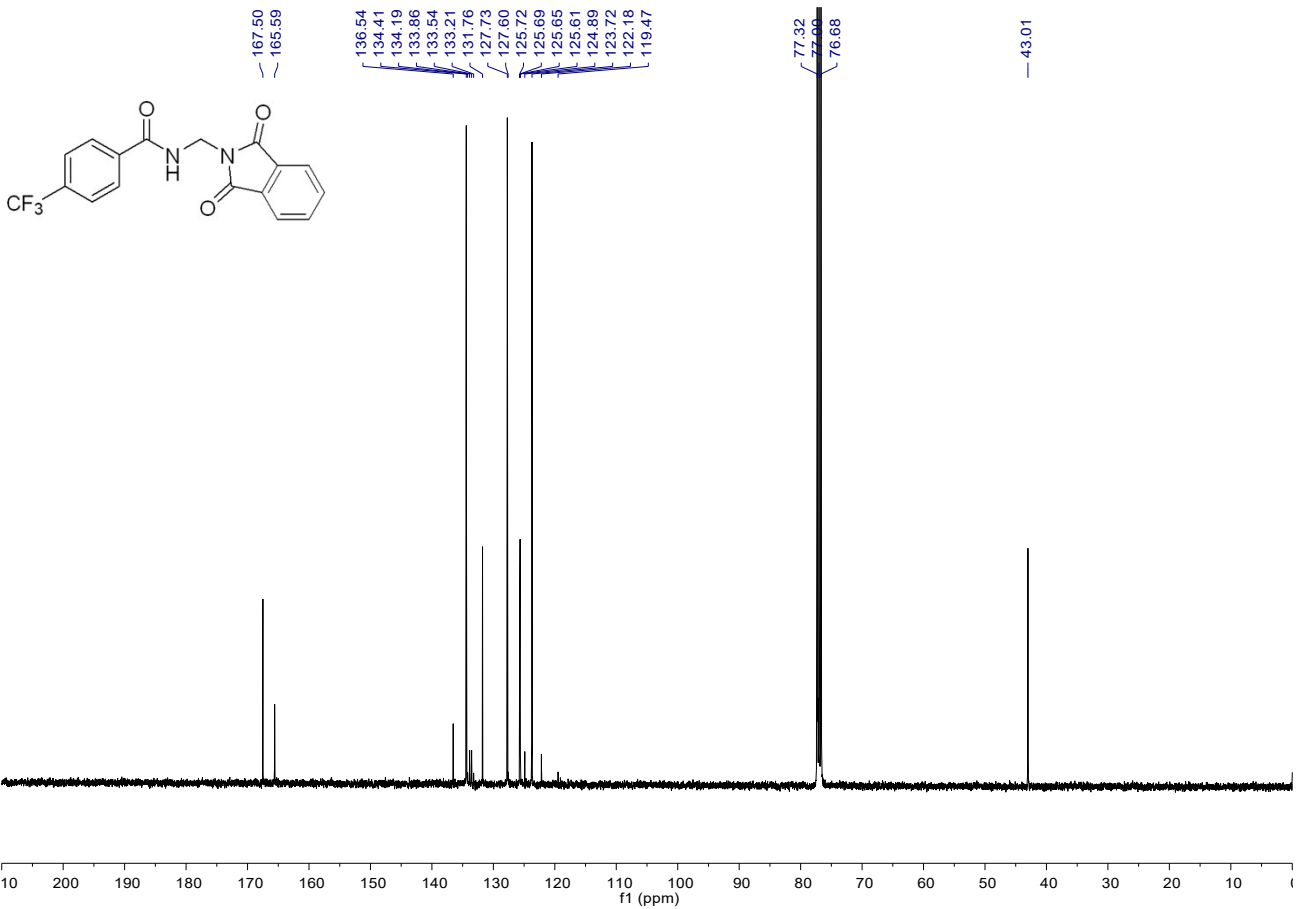
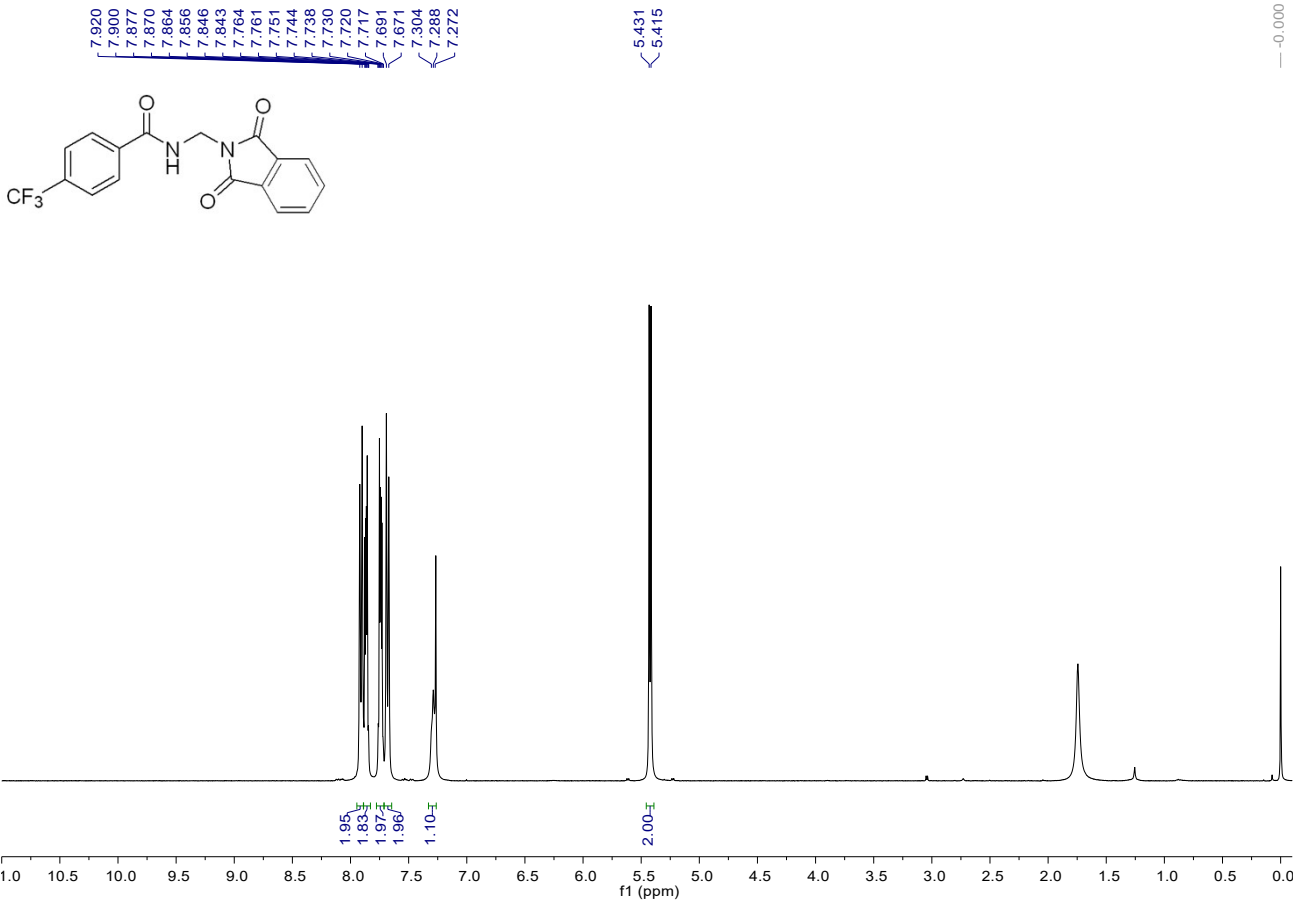


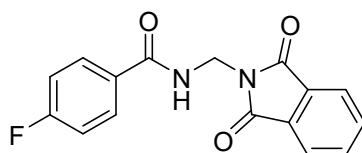
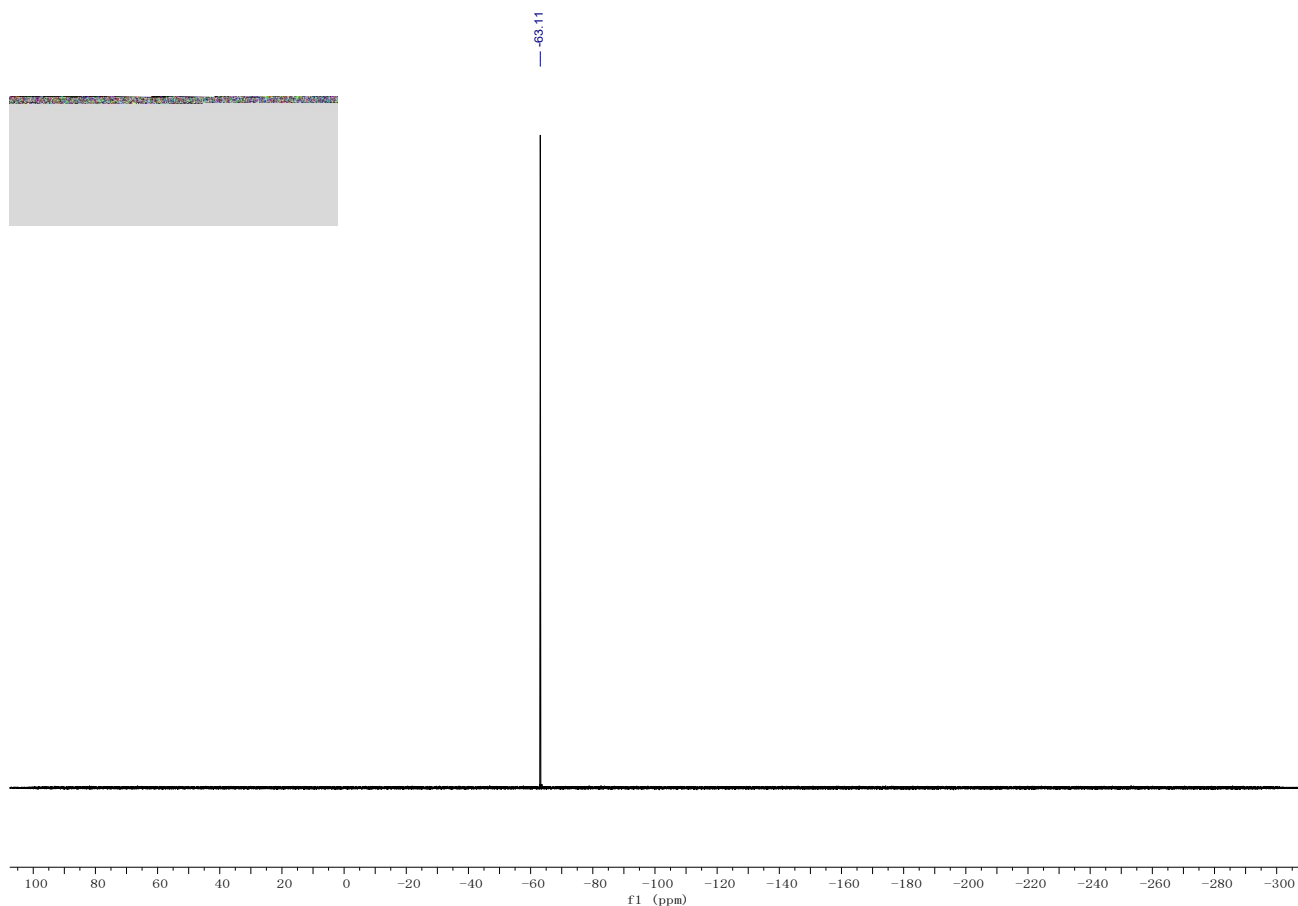
4-cyano-*N*-((1,3-dioxisoindolin-2-yl)methyl)benzamide (2r). A white solid, 61 mg, quant. yield; M.p.: 240-244 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.94-7.83 (m, 4H), 7.79-7.69 (m, 4H), 7.31-7.24 (m, 1H), 5.41 (d, *J* = 6.4 Hz, 2H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 167.5, 165.1, 137.1, 134.5, 132.5, 131.7, 127.9, 123.8, 117.8, 115.6, 43.0; IR (neat) ν 3285, 2230, 1779, 1712, 1648, 1544, 1497, 1428, 1309, 1281, 1164, 1090, 1014, 956 cm⁻¹; HRMS (ESI) Calcd. for C₁₇H₁₂N₃O₃⁺ Requires: 306.0873, Found: 306.0873.



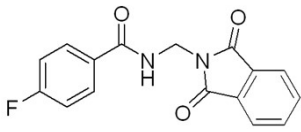


***N*-((1,3-dioxoisindolin-2-yl)methyl)-4-(trifluoromethyl)benzamide (2s)**. A white solid, 70 mg, quant. yield; M.p.: 224-228 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.91 (d, $J = 8.2$ Hz, 2H), 7.89-7.83 (m, 2H), 7.78-7.71 (m, 2H), 7.68 (d, $J = 8.2$ Hz, 2H), 7.33-7.26 (m, 1H), 5.42 (d, $J = 6.4$ Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.5, 165.6, 136.5, 134.4, 133.7 (q, $J = 32.9$ Hz), 131.8, 127.7, 125.6 (q, $J = 3.7$ Hz), 124.5 (q, $J = 272.8$ Hz), 123.7, 43.0; ^{19}F NMR (CDCl_3 , 376 MHz, CFCl_3) δ -63.1; IR (neat) ν 3298, 1773, 1703, 1651, 1546, 1406, 1327, 1145, 1105, 1051, 1014, 993, 958 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{17}\text{H}_{12}\text{N}_2\text{O}_3\text{F}_3^+$ Requires: 349.0795, Found: 349.0795.



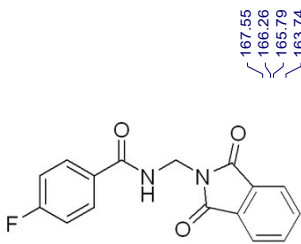
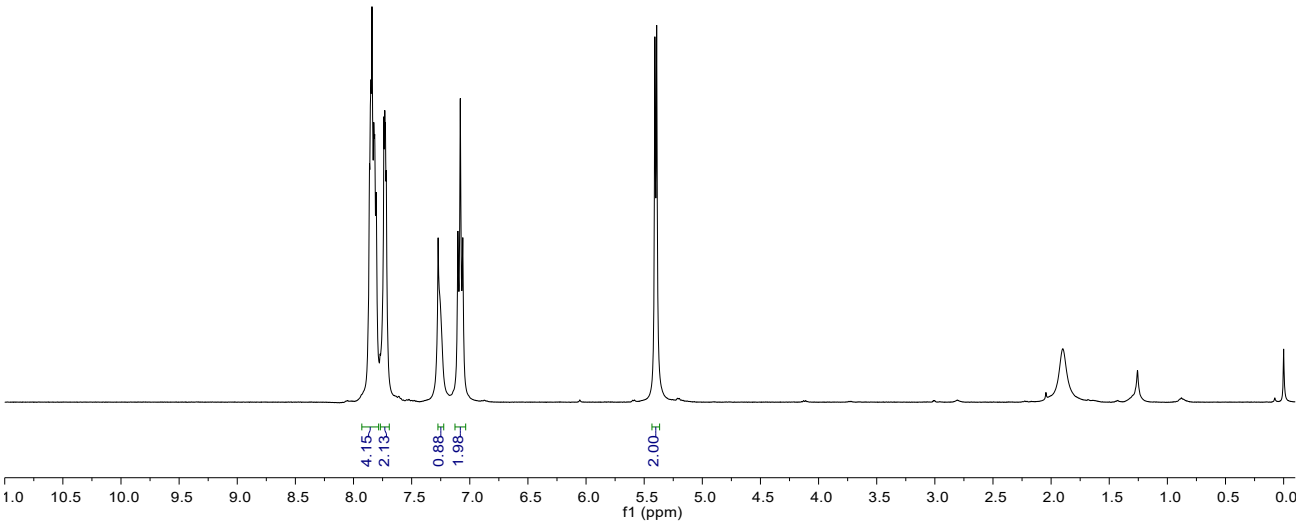


***N*-((1,3-dioxoisindolin-2-yl)methyl)-4-fluorobenzamide (2t).** A white solid, 59 mg, 99% yield; M.p.: 208-212 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.93-7.78 (m, 4H), 7.77-7.69 (m, 2H), 7.27-7.22 (m, 1H), 7.08 (dd, $J = 8.4, 8.4$ Hz, 2H), 5.40 (d, $J = 6.3$ Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.5, 165.8, 165.0 (d, $J = 252.8$ Hz), 134.3, 131.8, 129.7 (d, $J = 9.0$ Hz), 129.4 (d, $J = 3.1$ Hz), 123.6, 115.7 (d, $J = 22.0$ Hz), 43.0; ^{19}F NMR (CDCl_3 , 376 MHz, CFCl_3) δ -107.2 (tt, $J = 8.5, 5.2$ Hz); IR (neat) ν 3385, 1774, 1709, 1666, 1600, 1523, 1496, 1430, 1367, 1303, 1222, 1160, 1098, 1012, 954, 872 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{16}\text{H}_{12}\text{N}_2\text{O}_3\text{F}^+$ Requires: 299.0826, Found: 299.0828.

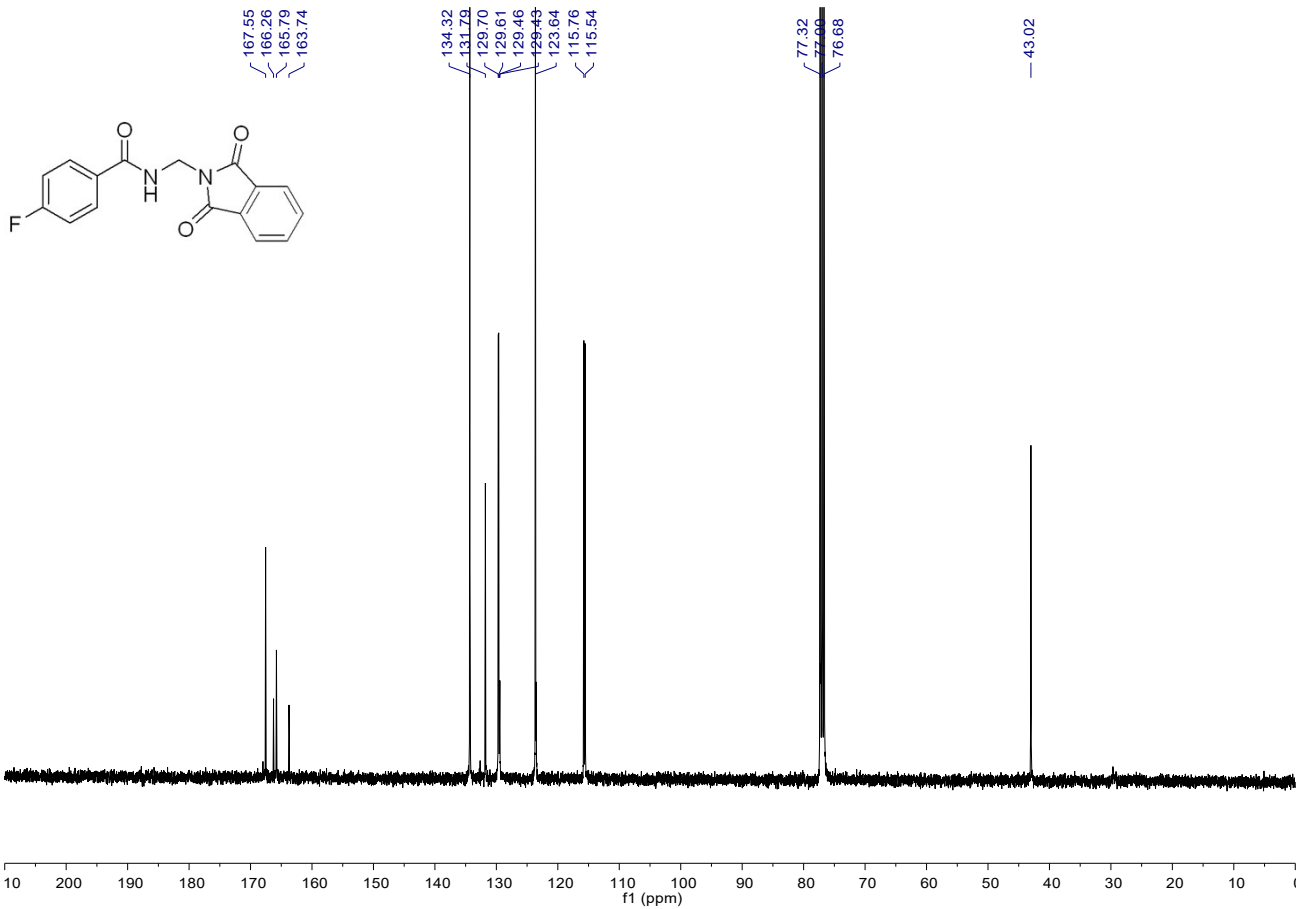


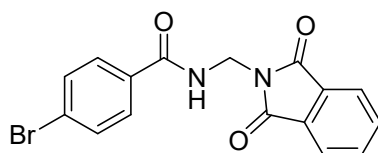
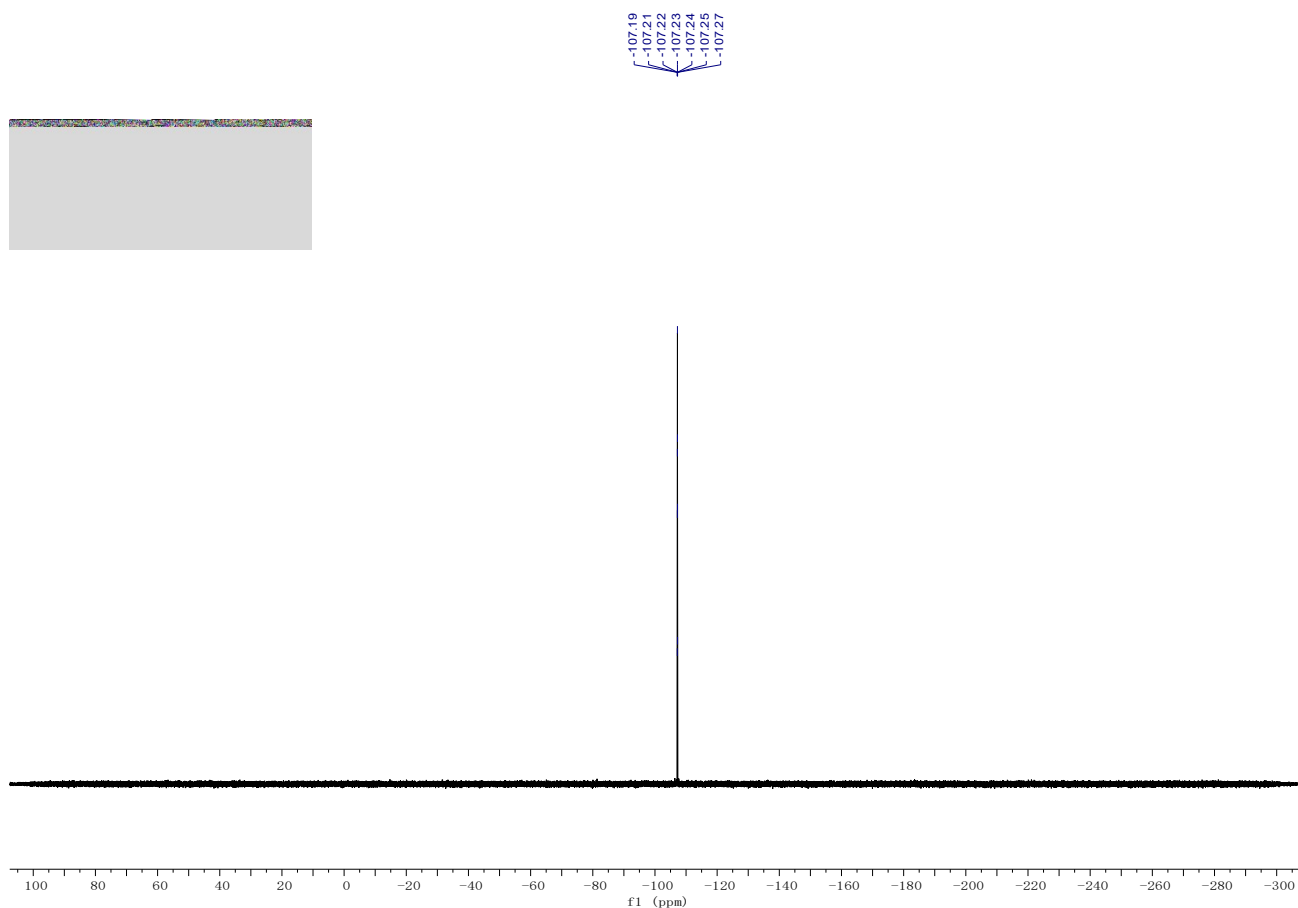
7.874
7.863
7.856
7.850
7.841
7.826
7.817
7.804
7.750
7.739
7.731
7.725
7.717
7.249
7.102
7.081
7.060
5.408
5.392

-0.000

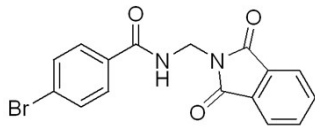


167.55
166.26
165.79
163.74
134.32
131.79
129.70
129.61
129.46
129.45
123.64
115.76
115.54
77.32
77.00
76.68
43.02

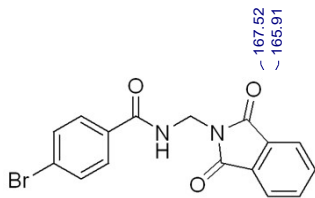
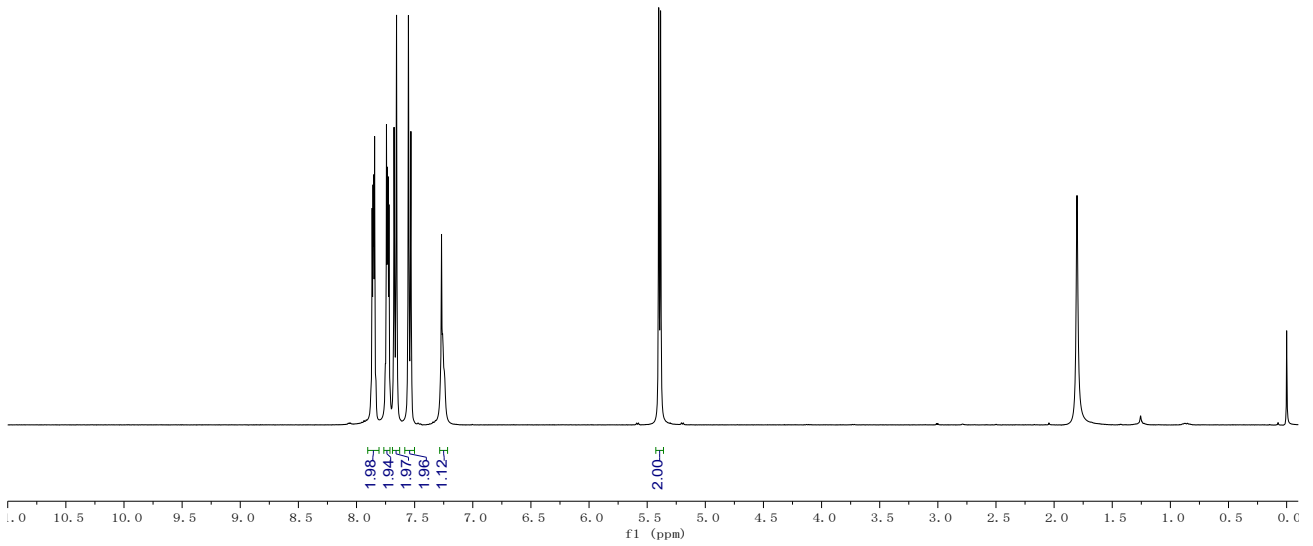




4-bromo-*N*-((1,3-dioxisoindolin-2-yl)methyl)benzamide (2u). A white solid, 71 mg, 99% yield; M.p.: 216-220 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.85 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.73 (dd, $J = 5.5, 3.0$ Hz, 2H), 7.69-7.63 (m, 2H), 7.58-7.50 (m, 2H), 7.28-7.22 (m, 1H), 5.39 (d, $J = 6.4$ Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.5, 165.9, 134.3, 132.1, 131.8, 131.83, 128.76, 126.8, 123.7, 43.0; IR (neat) ν 3322, 1779, 1700, 1655, 1589, 1540, 1443, 1370, 1327, 1302, 1179, 1073, 1045, 877 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{16}\text{H}_{12}\text{N}_2\text{O}_3\text{Br}^+$ Requires: 359.0026, Found: 359.0026.



7.879
7.875
7.866
7.858
7.852
7.844
7.834
7.831
7.755
7.752
7.742
7.735
7.729
7.721
7.712
7.684
7.677
7.673
7.661
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7.537
7.532
7.526
7.260
7.242
5.401
5.385

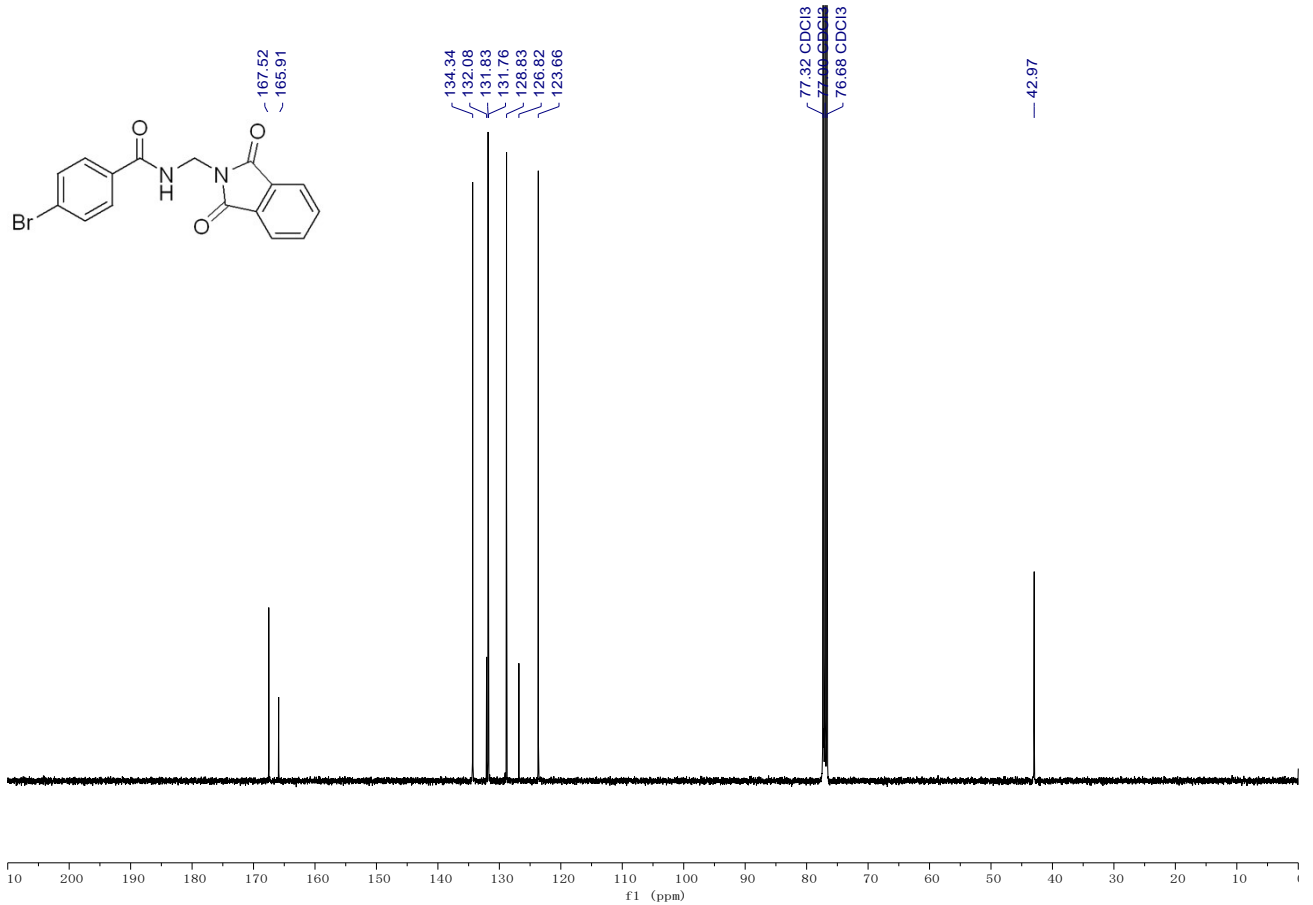


167.52
165.91

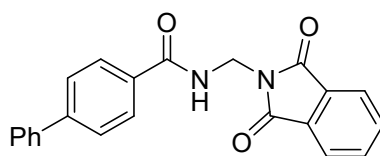
134.34
132.08
131.83
131.76
128.83
126.82
123.66

77.32 CDCl3
77.06 CDCl3
76.68 CDCl3

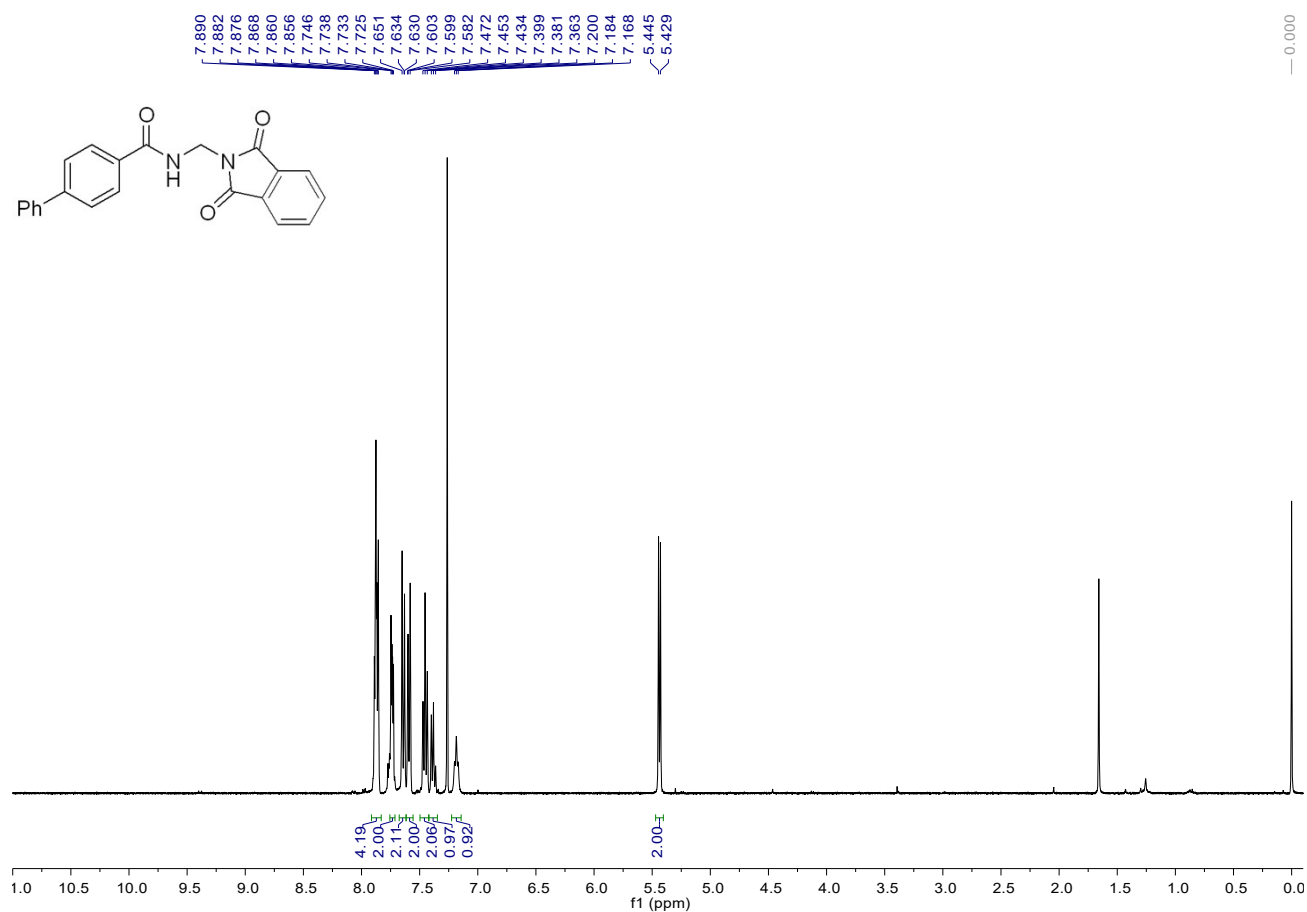
42.97

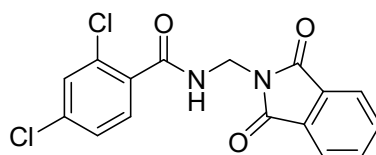
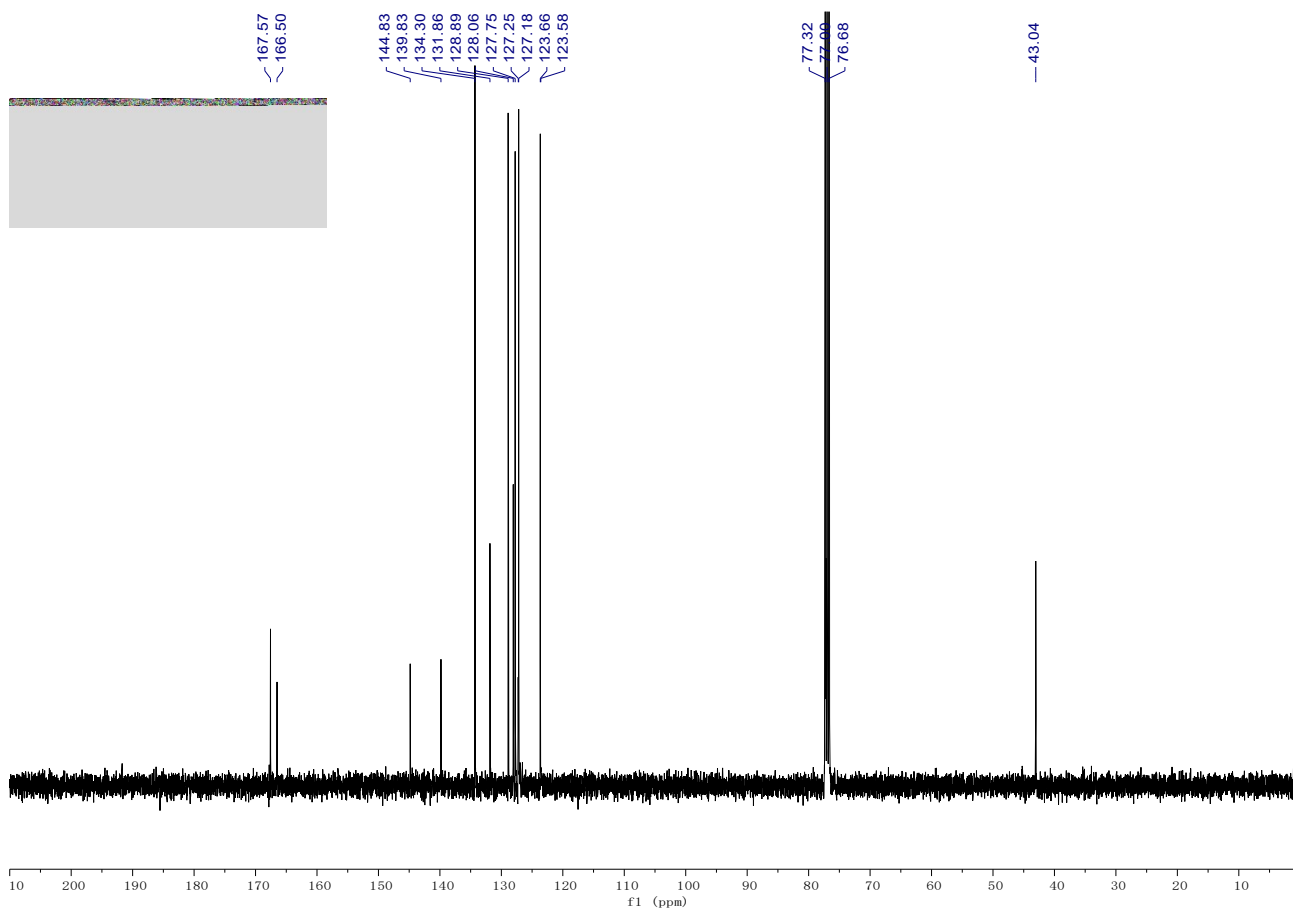


-0.000

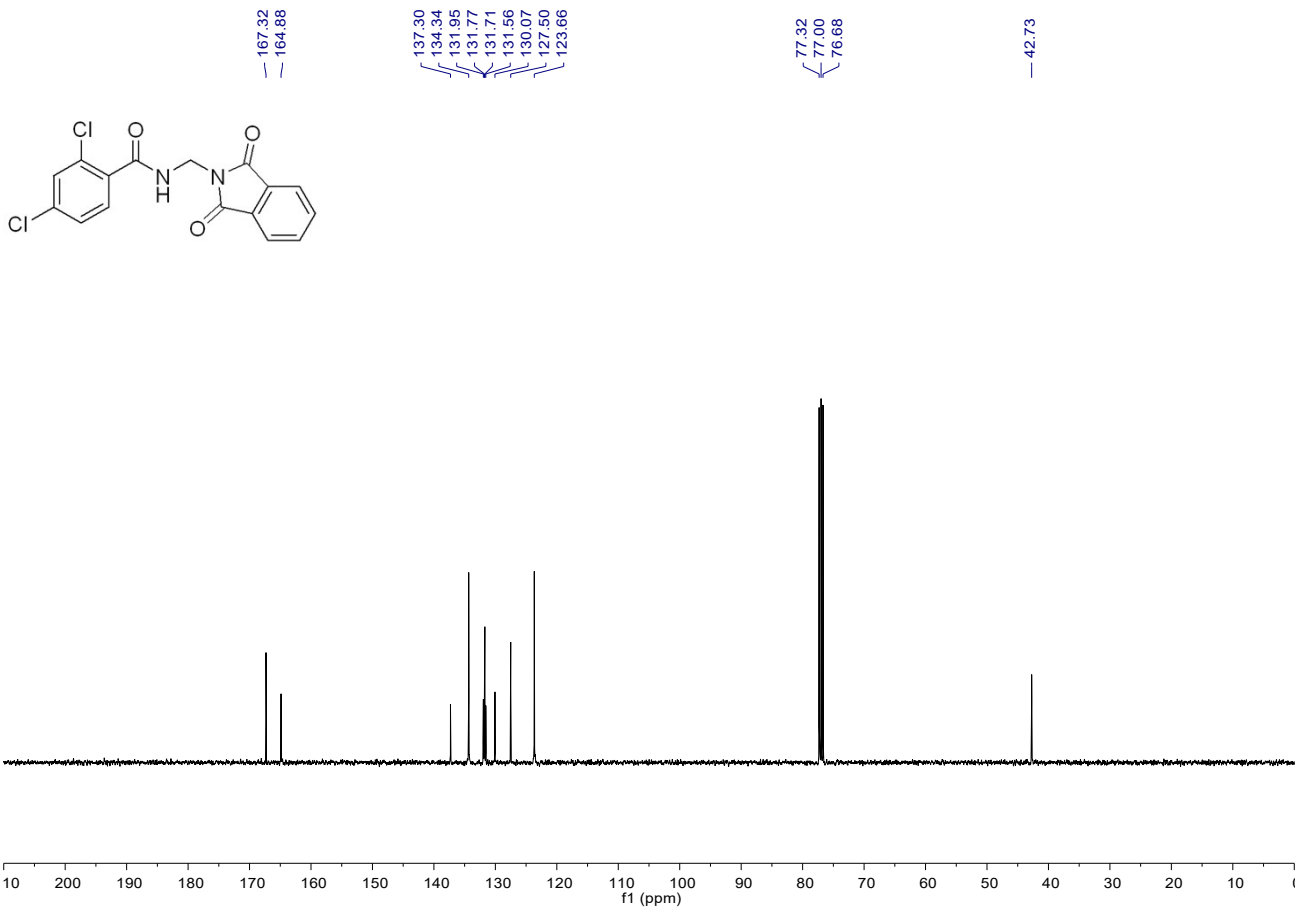
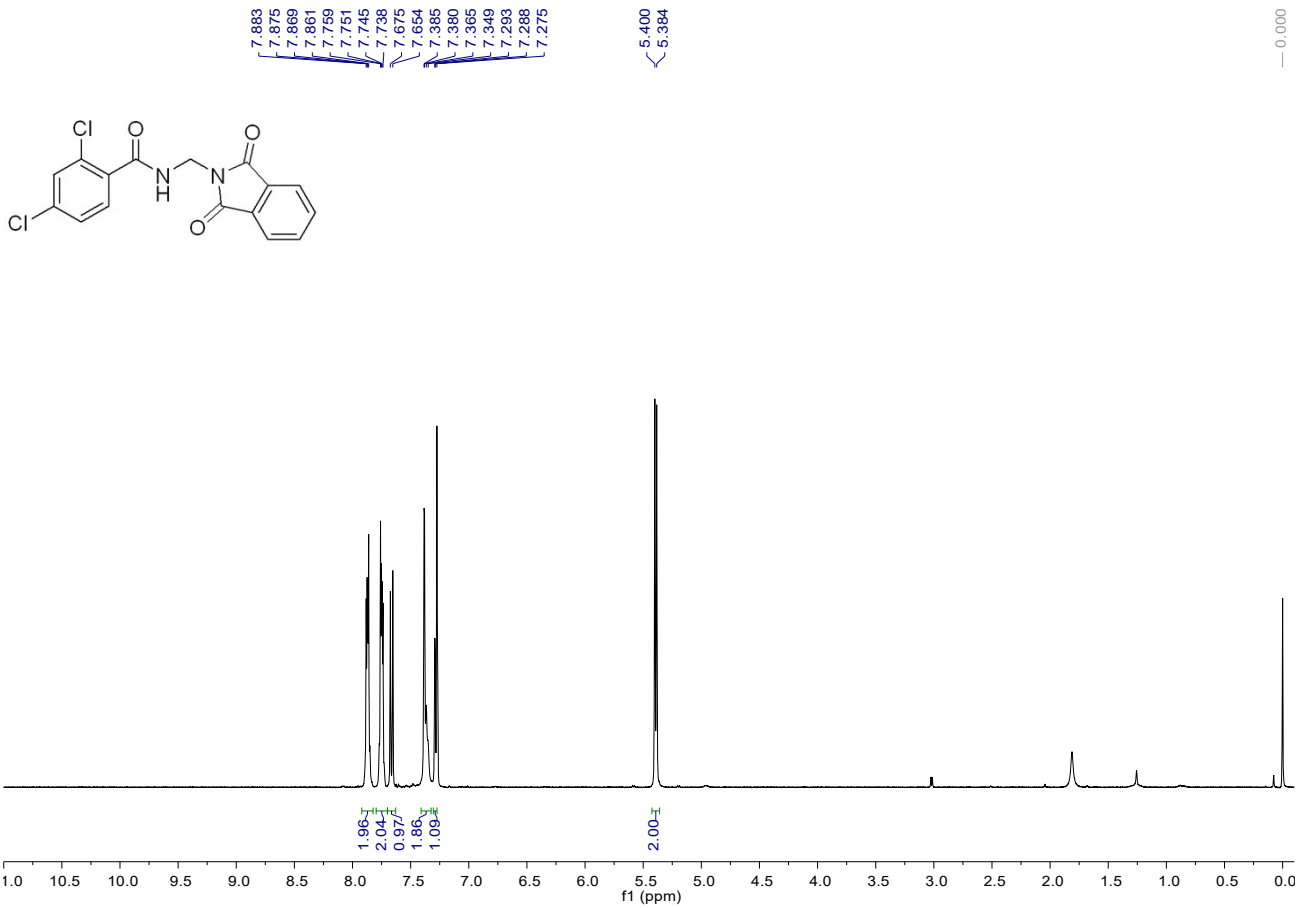


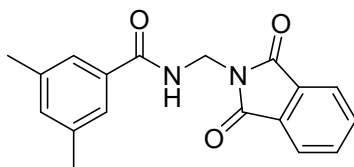
***N*-((1,3-dioxoisindolin-2-yl)methyl)-[1,1'-biphenyl]-4-carboxamide (2v)**. A white solid, 66 mg, 92% yield; M.p.: 246-250 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.91-7.83 (m, 4H), 7.74 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.64 (d, $J = 8.3$ Hz, 2H), 7.62-7.56 (m, 2H), 7.45 (t, $J = 7.5$ Hz, 2H), 7.38 (t, $J = 7.3$ Hz, 1H), 7.18 (t, $J = 6.4$ Hz, 1H), 5.44 (d, $J = 6.4$ Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.6, 166.5, 144.8, 139.8, 134.3, 131.9, 128.9, 128.1, 127.8, 127.2, 127.2, 123.7, 123.6, 43.0; IR (neat) ν 3316, 1774, 1712, 1648, 1582, 1485, 1468, 1400, 1325, 1274, 1171, 1146, 1065, 996 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{22}\text{H}_{17}\text{N}_2\text{O}_3^+$ Requires: 357.1234, Found: 357.1235.



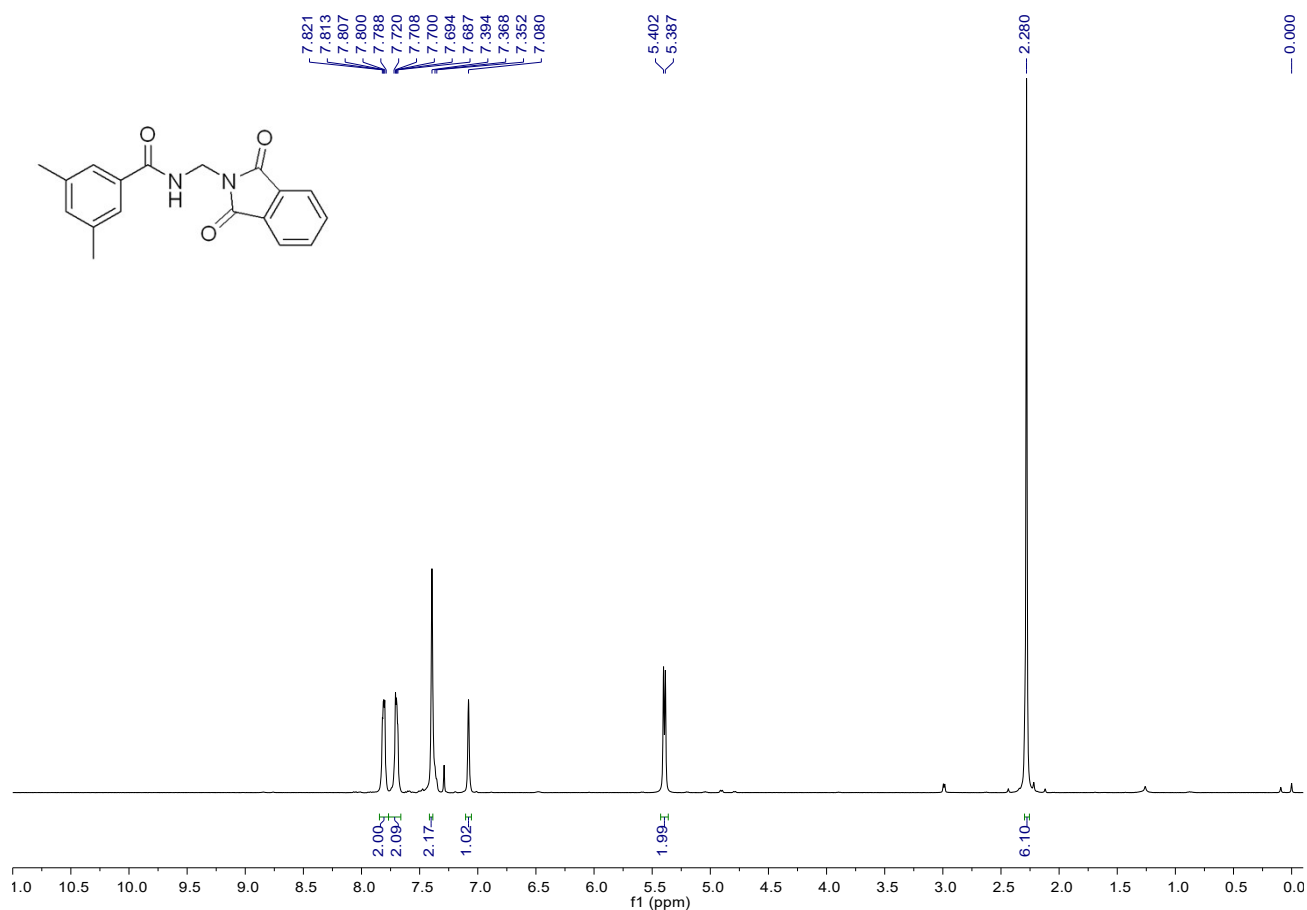


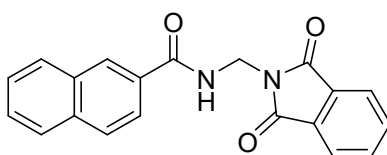
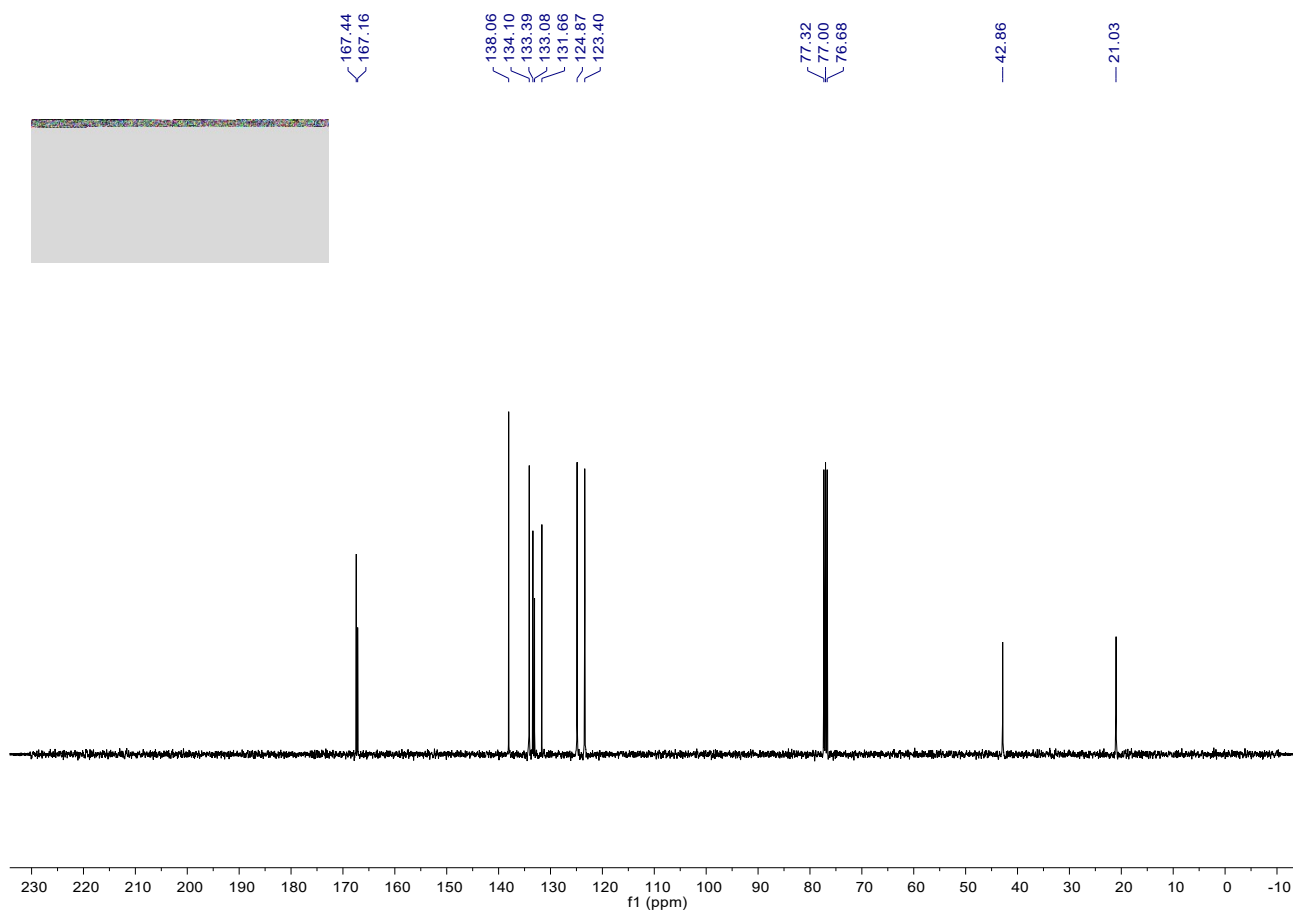
2,4-dichloro-*N*-((1,3-dioxoisindolin-2-yl)methyl)benzamide (2w). A white solid, 68 mg, 98% yield; M.p.: 197-200 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.87 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.75 (dd, *J* = 5.6, 3.1 Hz, 2H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.41-7.32 (m, 2H), 7.31-7.27 (m, 1H), 5.39 (d, *J* = 6.4 Hz, 2H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 167.3, 164.9, 137.3, 134.3, 131.9, 131.8, 131.7, 131.6, 130.1, 127.5, 123.7, 42.7; IR (neat) ν 3285, 3065, , 1770, 1700, 1655, 1559, 1439, 1365, 1290, 1248, 1104, 989 cm⁻¹; HRMS (ESI) Calcd. for C₁₆H₁₁N₂O₃Cl₂⁺ Requires: 349.0141, Found: 349.0143.



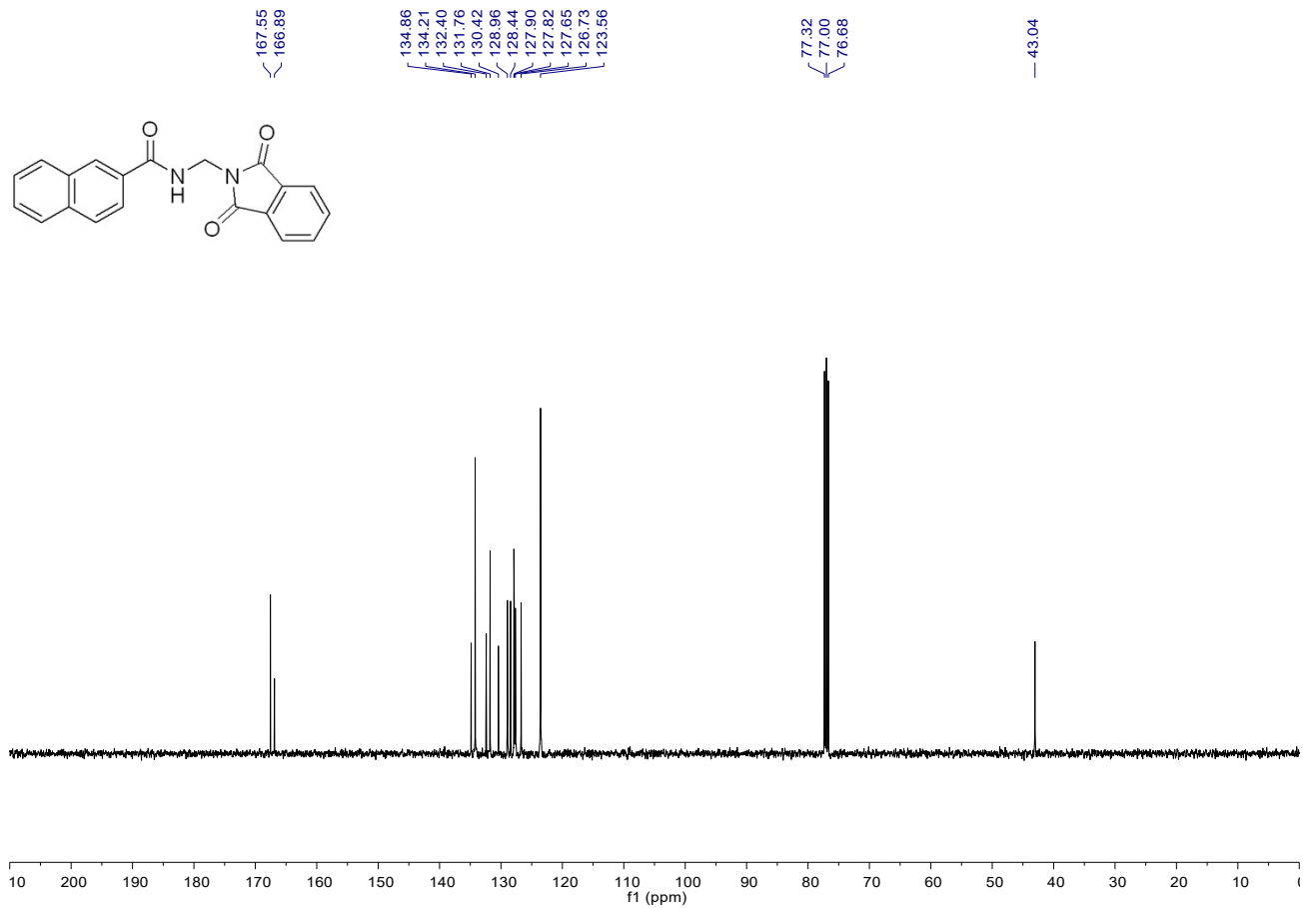
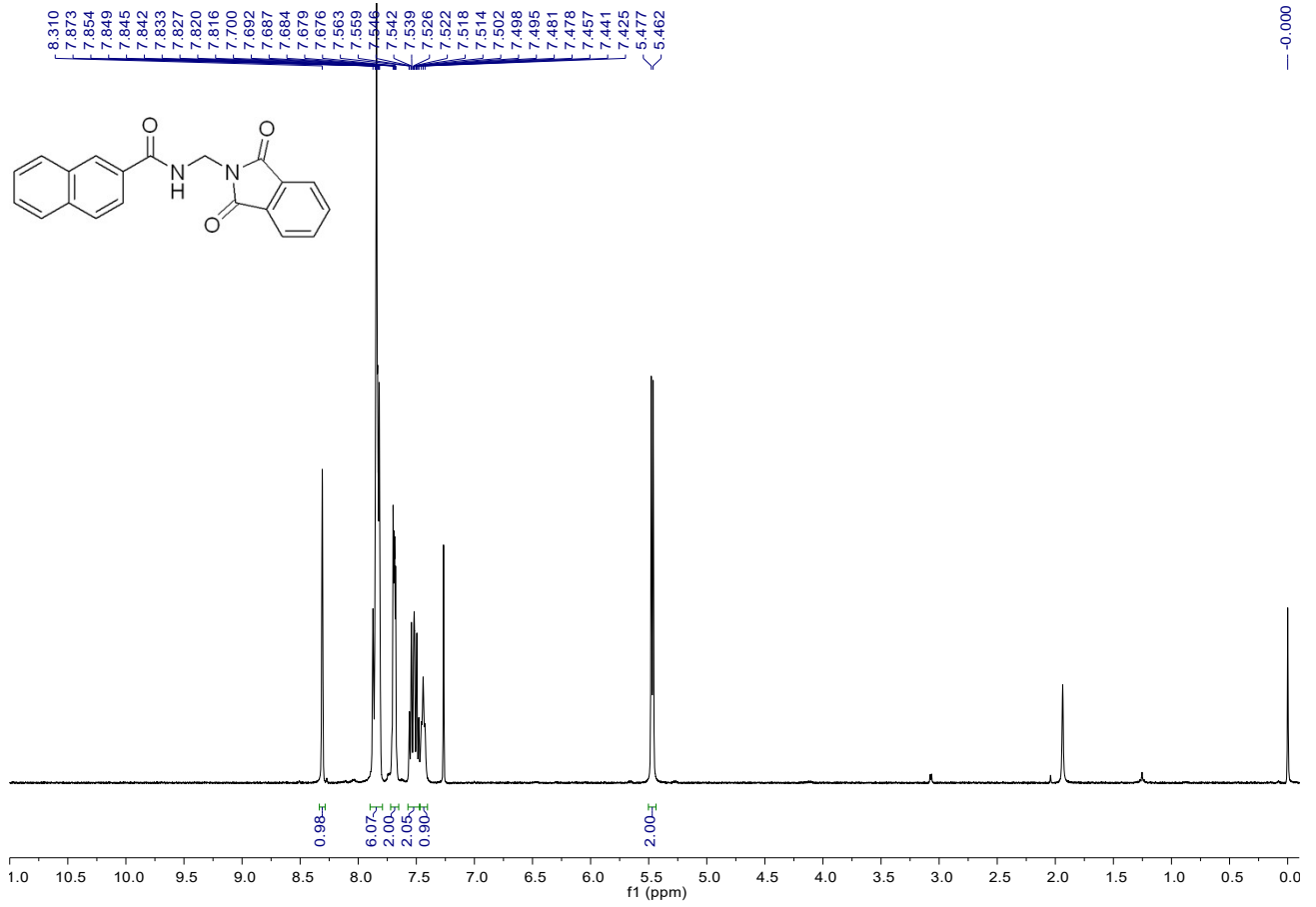


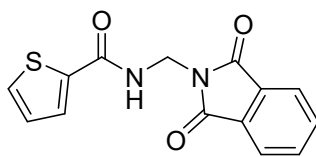
***N*-((1,3-dioxisoindolin-2-yl)methyl)-3,5-dimethylbenzamide (2x)**. A white solid, 58 mg, 94% yield; M.p.: 198-202 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.81 (dd, $J = 5.4, 3.1$ Hz, 2H), 7.70 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.39 (s, 2H), 7.08 (s, 1H), 5.39 (d, $J = 6.3$ Hz, 2H), 2.28 (s, 6H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.4, 167.2, 138.1, 134.1, 133.4, 133.1, 131.7, 124.9, 123.4, 42.9, 21.0; IR (neat) ν 3321, 1777, 1699, 1652, 1536, 1463, 1361, 1311, 1250, 1176, 1032, 868, 720 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_3^+$ Requires: 309.1234, Found: 309.1234.



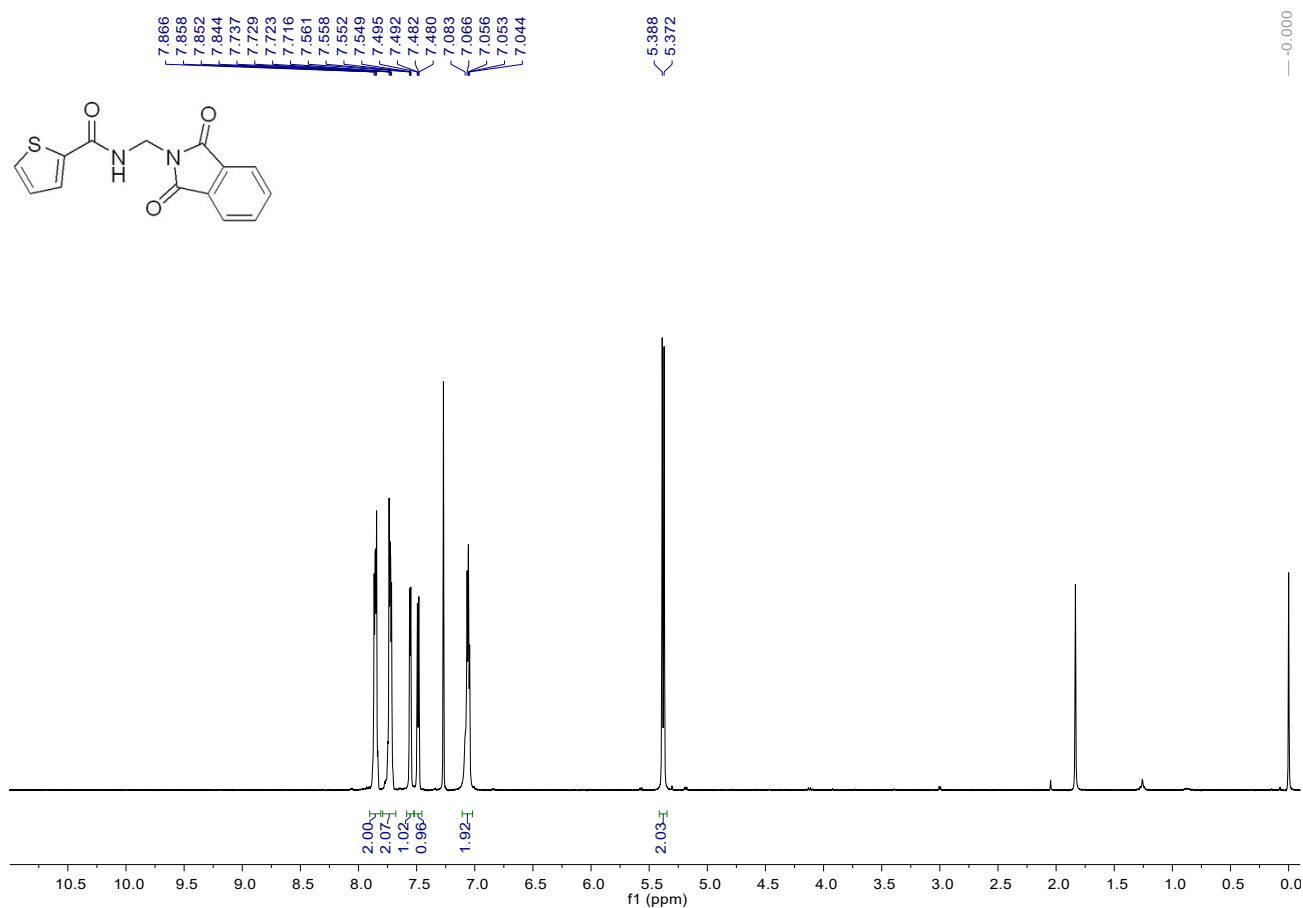


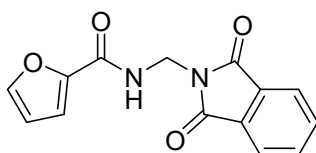
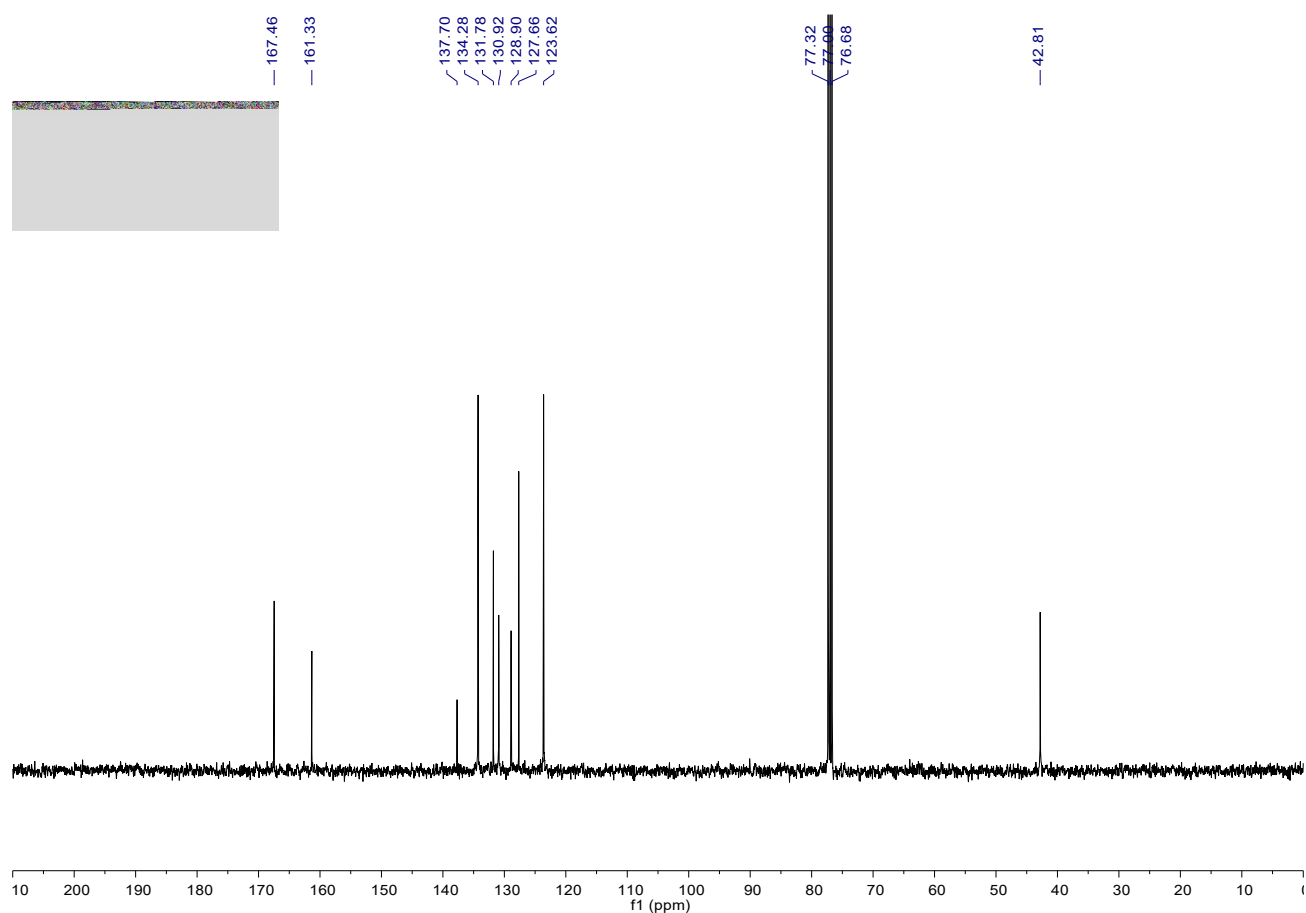
***N*-((1,3-dioxoisindolin-2-yl)methyl)-2-naphthamide (2y)**. A white solid, 65 mg, 99% yield; M.p.: 208-210 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 8.31 (s, 1H), 7.90-7.79 (m, 6H), 7.73-7.64 (m, 2H), 7.57-7.47 (m, 2H), 7.44 (t, $J = 6.4$ Hz, 1H), 5.47 (d, $J = 6.4$ Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.5, 166.9, 134.9, 134.2, 132.4, 131.8, 130.4, 129.0, 128.4, 127.9, 127.8, 127.7, 126.7, 123.6, 43.0; IR (neat) ν 3341, 3065, 2954, 1779, 1708, 1648, 1529, 1466, 1410, 1365, 1301, 1176, 1122, 1044, 1007 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{20}\text{H}_{15}\text{N}_2\text{O}_3^+$ Requires: 331.1077, Found: 331.1078.



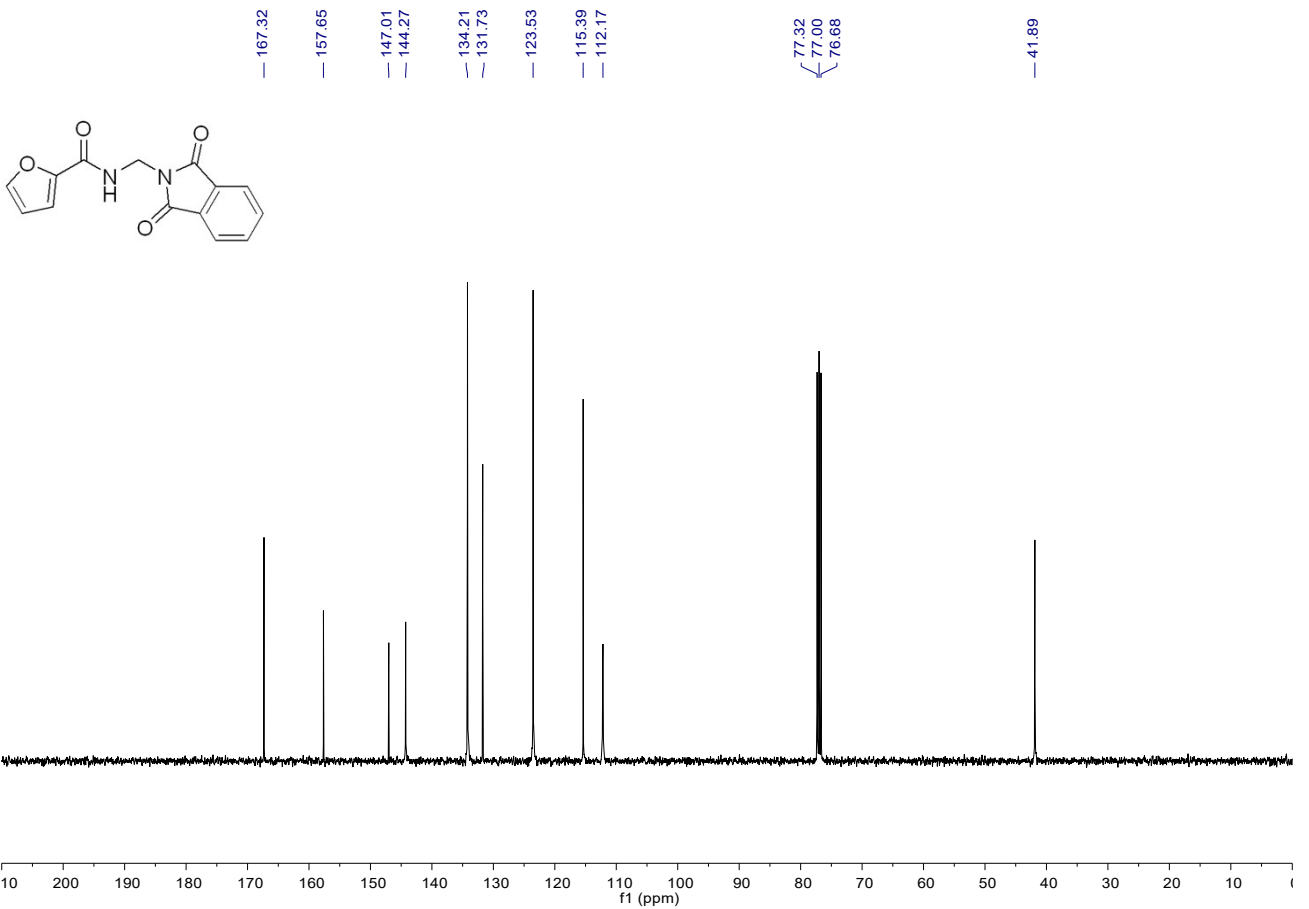
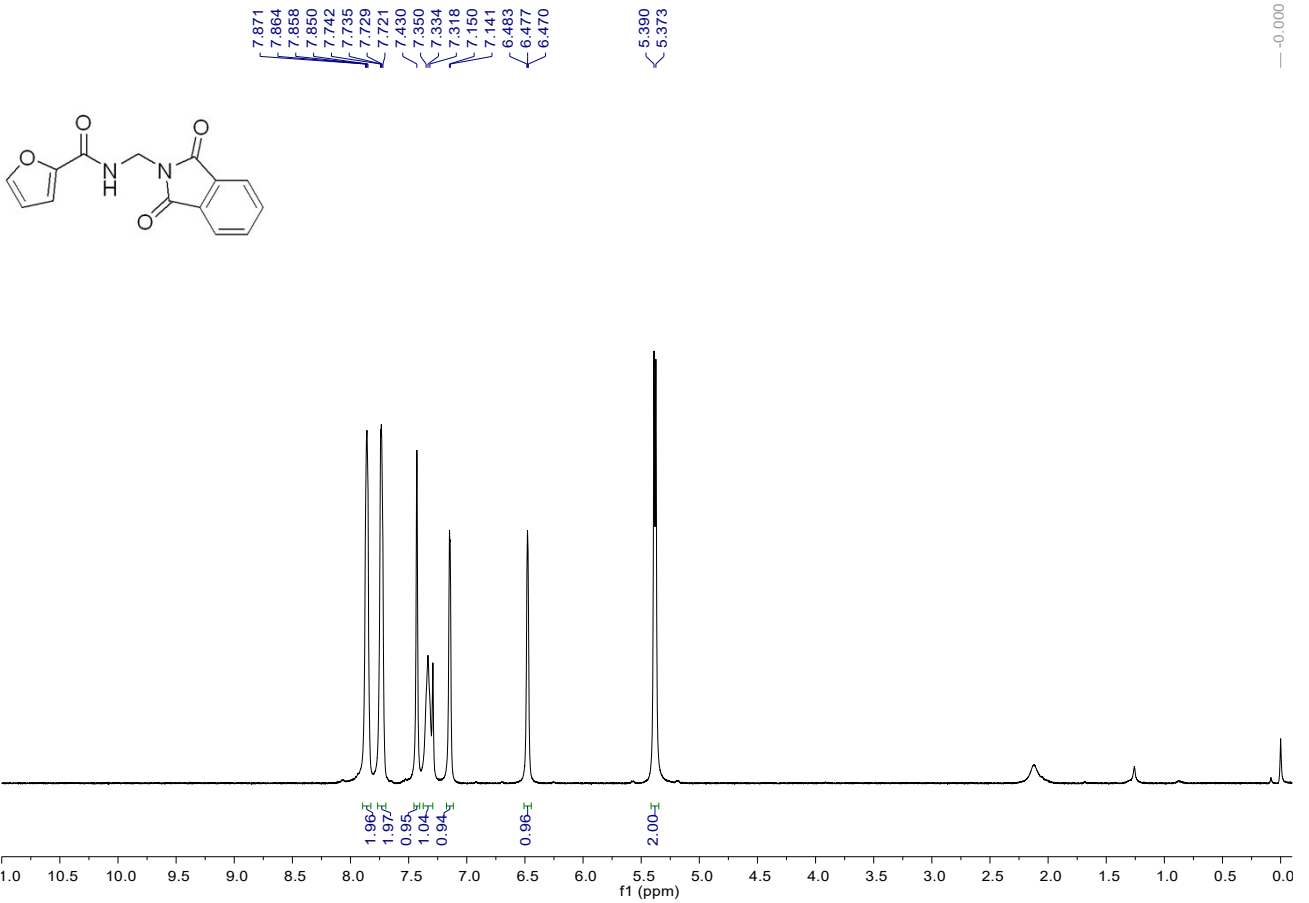


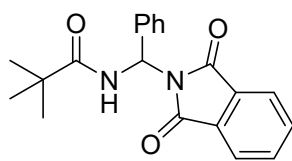
***N*-((1,3-dioxoisindolin-2-yl)methyl)thiophene-2-carboxamide (2z)**. A white solid, 57 mg, quant. yield; M.p.: 226-230 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.86 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.73 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.56 (dd, *J* = 3.7, 1.1 Hz, 1H), 7.49 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.11-7.02 (m, 2H), 5.38 (d, *J* = 6.5 Hz, 2H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 167.5, 161.3, 137.7, 134.3, 131.8, 130.9, 128.9, 127.7, 123.6, 42.8; IR (neat) ν 3384, 3364, 1773, 1703, 1652, 1537, 1463, 1418, 1364, 1350, 1264, 1132, 1032, 944 cm⁻¹; HRMS (ESI) Calcd. for C₁₄H₁₁N₂O₃S⁺ Requires: 287.0485, Found: 287.0485.



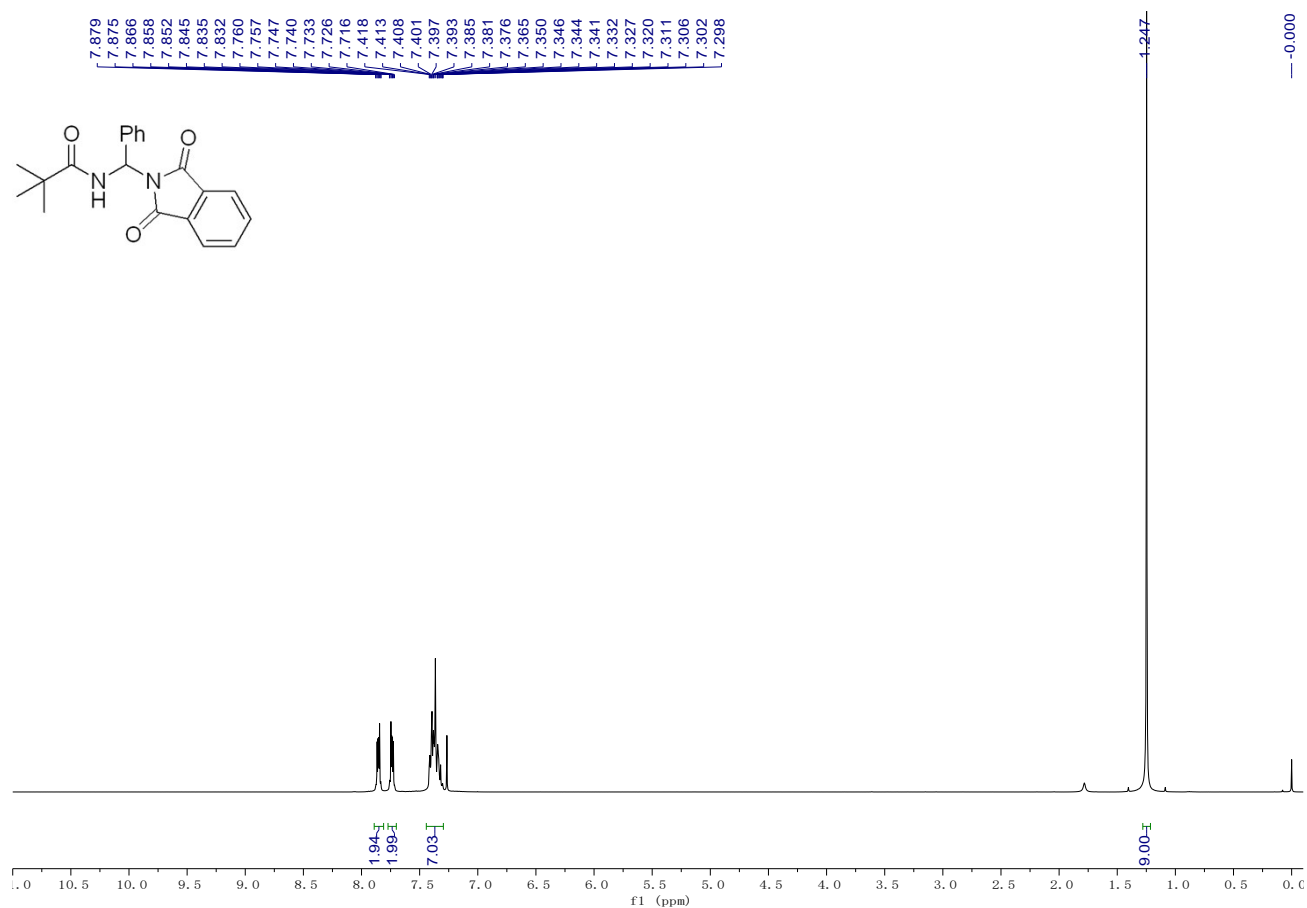


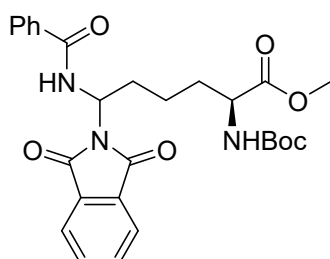
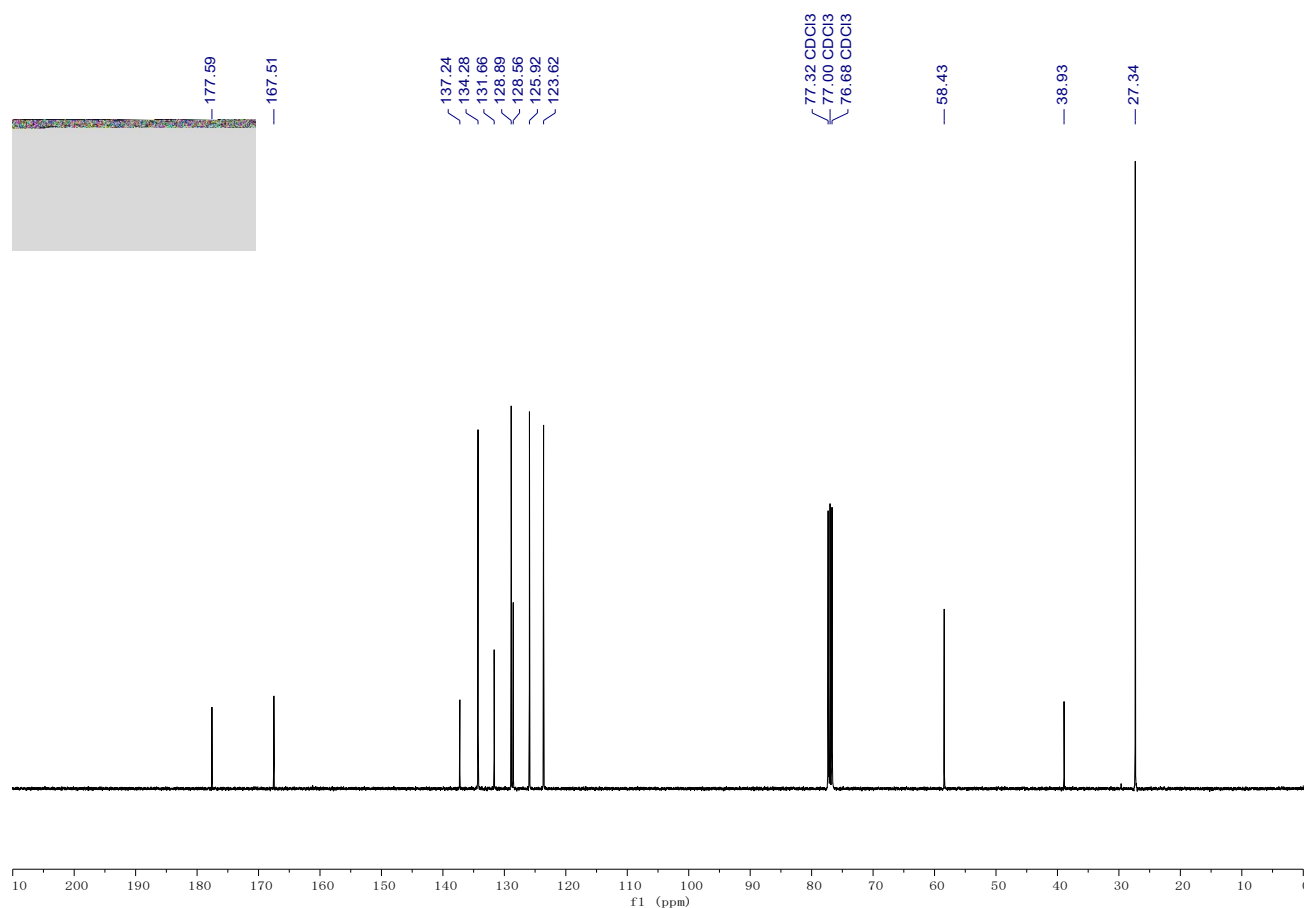
***N*-((1,3-dioxoisindolin-2-yl)methyl)furan-2-carboxamide (2aa).** A white solid, 48 mg, 89% yield; M.p.: 200-204 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.86 (dd, $J = 5.4, 3.0$ Hz, 2H), 7.77-7.70 (m, 2H), 7.43 (s, 1H), 7.33 (t, $J = 6.5$ Hz, 1H), 7.15 (d, $J = 3.5$ Hz, 1H), 6.48 (t, $J = 2.6$ Hz, 1H), 5.38 (d, $J = 6.5$ Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.3, 157.6, 147.0, 144.3, 134.2, 131.7, 123.5, 115.4, 112.2, 41.9; IR (neat) ν 3367, 3119, 1769, 1702, 1593, 1532, 1473, 1424, 1292, 1192, 1022, 1012, 957, 883, 759 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{14}\text{H}_{11}\text{N}_2\text{O}_4^+$ Requires: 271.0713, Found: 271.0715.



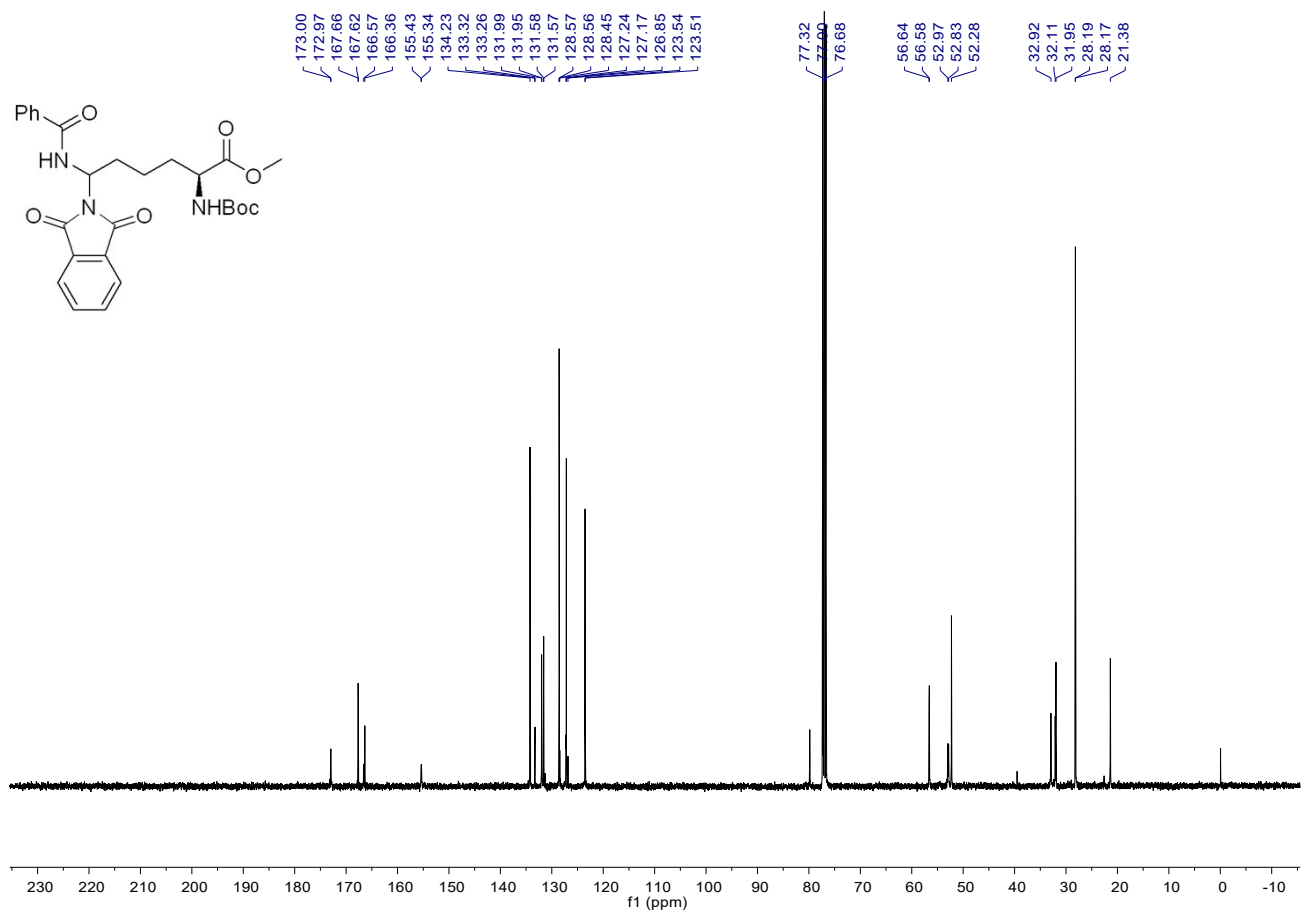
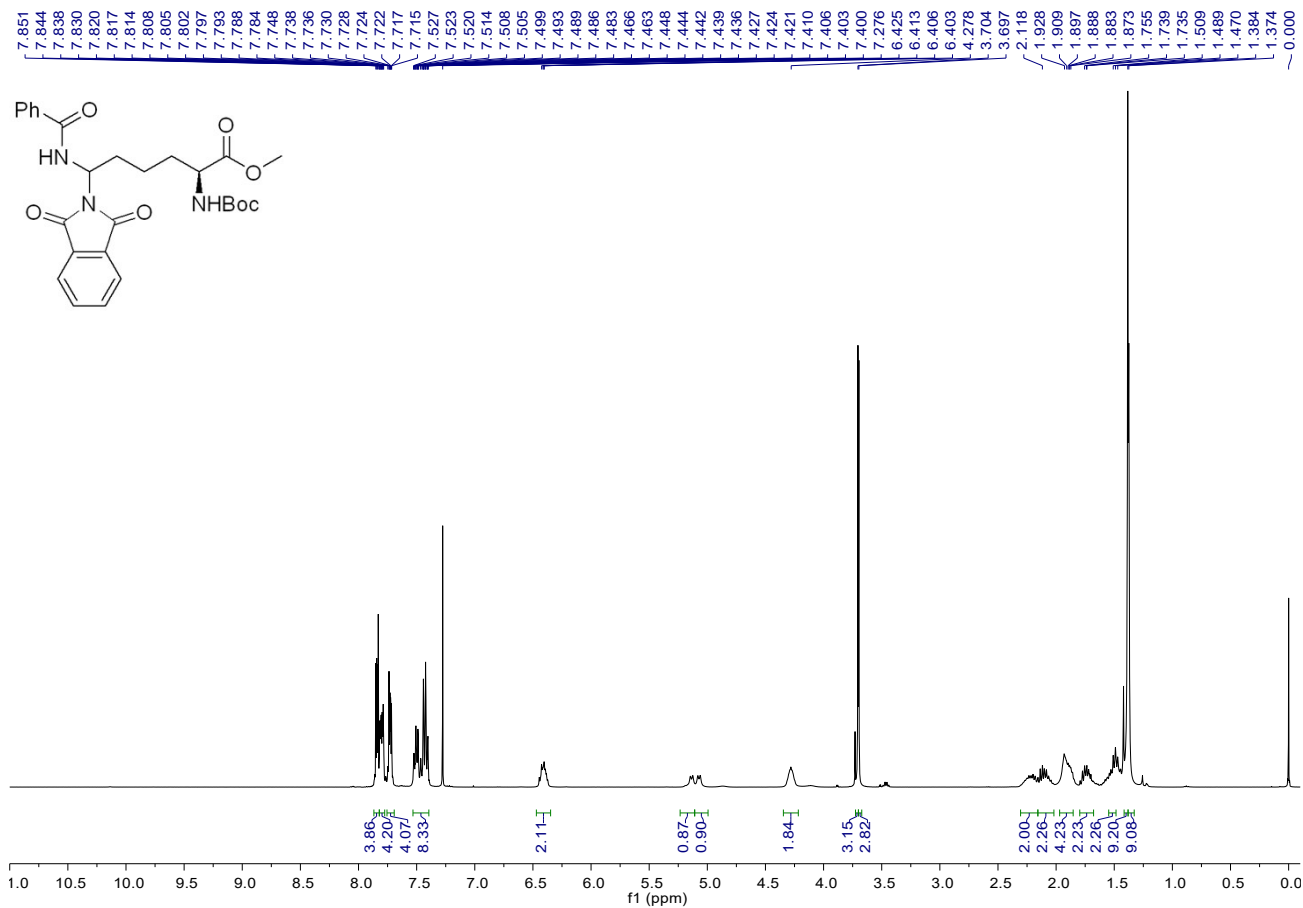


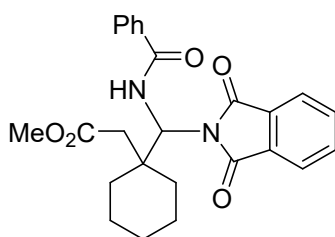
***N*-((1,3-dioxoisindolin-2-yl)(phenyl)methyl)pivalamide (2ab).** A white solid, 38 mg, 56% yield; M.p.: 144-146 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.86 (dd, *J* = 5.4, 3.0 Hz, 2H), 7.74 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.44-7.30 (m, 7H), 1.25 (s, 9H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 177.6, 167.5, 137.2, 134.3, 131.7, 128.9, 128.6, 125.9, 123.6, 58.4, 38.9, 27.3; IR (neat) ν 3452, 3394, 2958, 1759, 1707, 1679, 1609, 1508, 1488, 1392, 1355, 1174, 1108, 797 cm⁻¹; HRMS (ESI) Calcd. for C₂₀H₂₁N₂O₃⁺ Requires: 337.1547, Found: 337.1547.



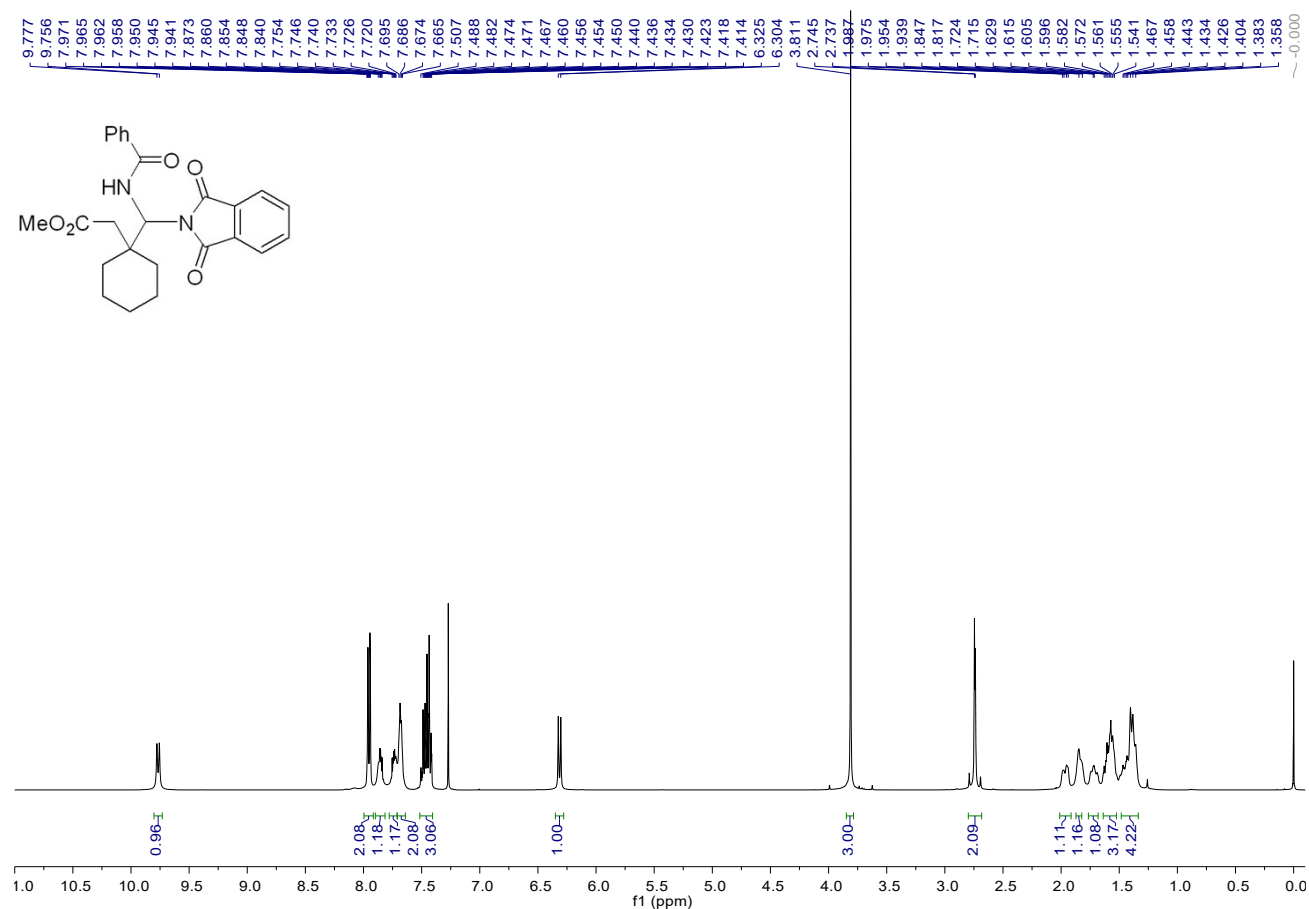


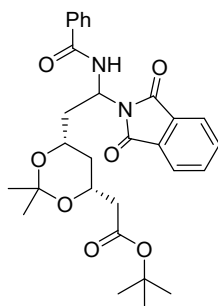
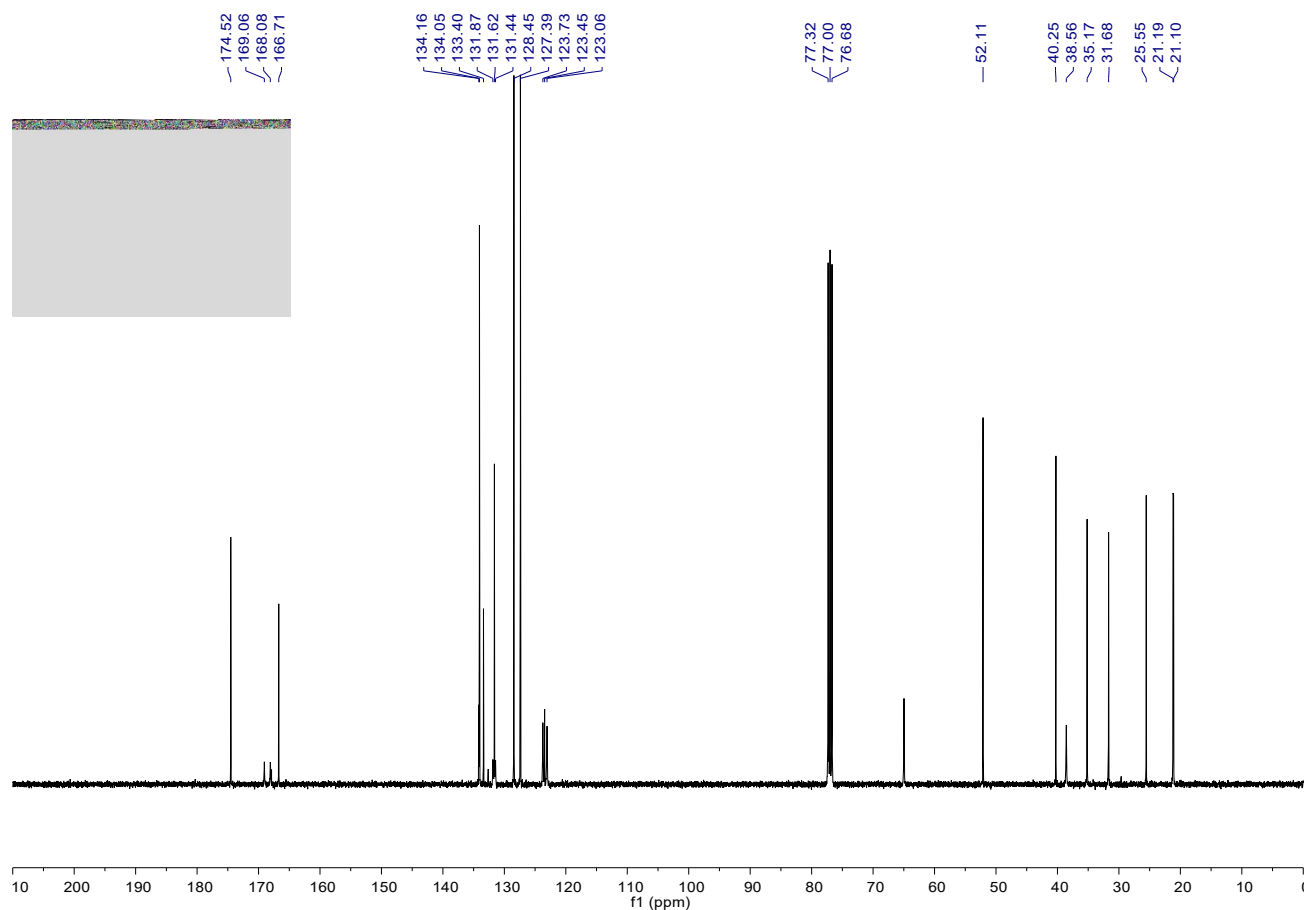
methyl(2S)-6-benzamido-2-((tert-butoxycarbonyl)amino)-6-(1,3-dioxisoindolin-2-yl)hexanoate (2ac). A white solid, 71 mg, 70% yield; M.p.: 155-157 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.84 (dd, *J* = 5.5, 3.0 Hz, 4H), 7.82-7.77 (m, 4H), 7.76-7.69 (m, 4H), 7.53-7.40 (m, 8H), 6.47-6.35 (m, 2H), 5.14 (d, *J* = 8.4 Hz, 1H), 5.07 (d, *J* = 8.5 Hz, 1H), 4.35-4.22 (m, 2H), 3.70 (s, 3H), 3.70 (s, 3H), 2.31-2.16 (m, 2H), 2.16-2.02 (m, 2H), 1.97-1.85 (m, 4H), 1.80-1.68 (m, 2H), 1.55-1.48 (m, 2H), 1.38 (s, 9H), 1.37 (s, 9H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 173.00, 173.97, 167.7, 167.6, 166.6, 166.4, 155.4, 155.3, 134.2, 133.32, 133.26, 131.99, 131.95, 131.58, 131.57, 128.57, 128.56, 128.4, 127.24, 127.17, 126.9, 123.54, 123.51, 79.8, 56.64, 56.58, 53.0, 52.8, 52.3, 32.9, 32.1, 31.9, 28.19, 28.17, 21.4; IR (neat) ν 3353, 2952, 2929, 1776, 1705, 1661, 1603, 1517, 1455, 1392, 1364, 1288, 1159, 1052 cm⁻¹; HRMS (ESI) Calcd. for C₂₇H₃₁N₃O₇Na⁺ Requires: 532.2054, Found: 532.2050.



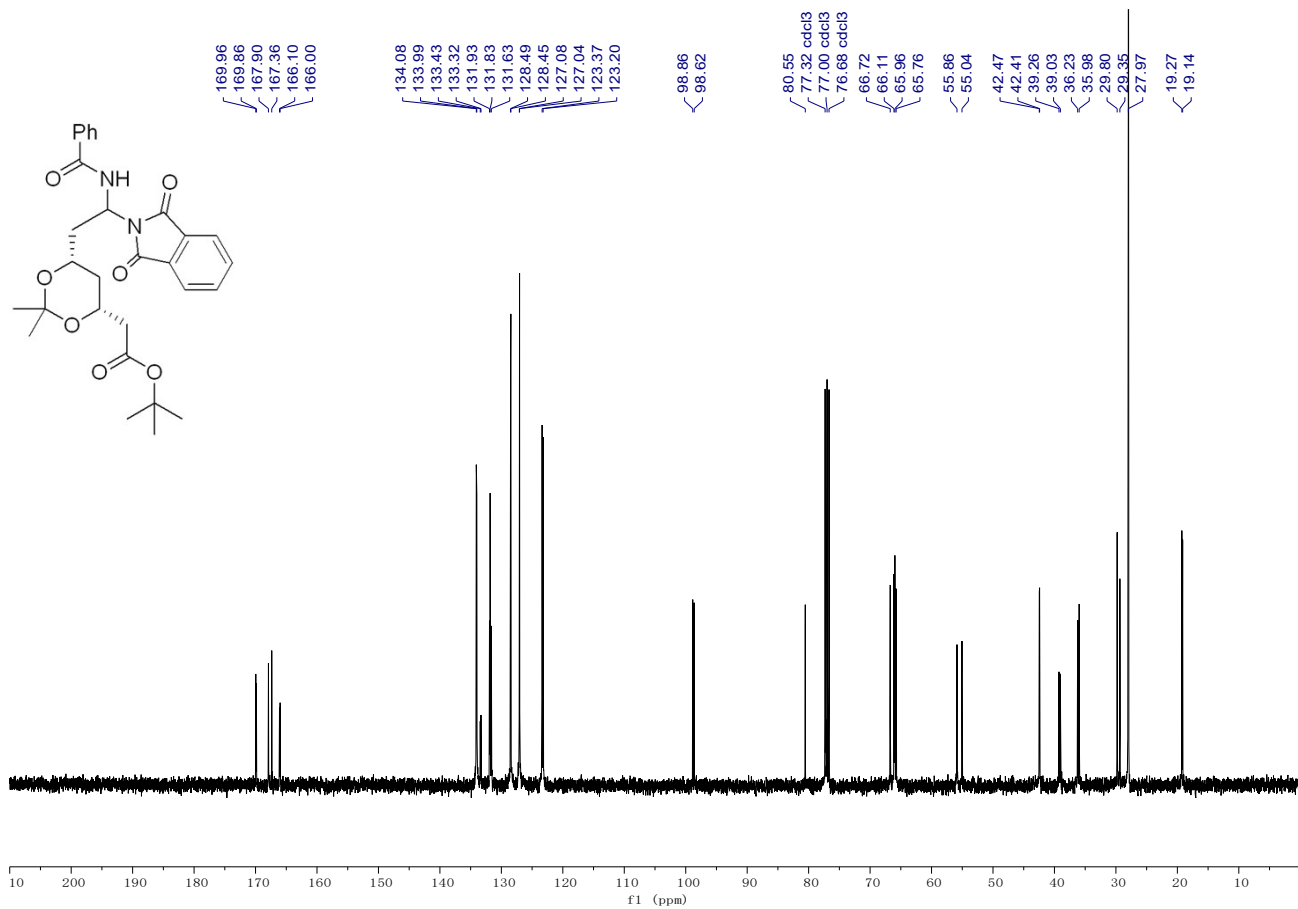
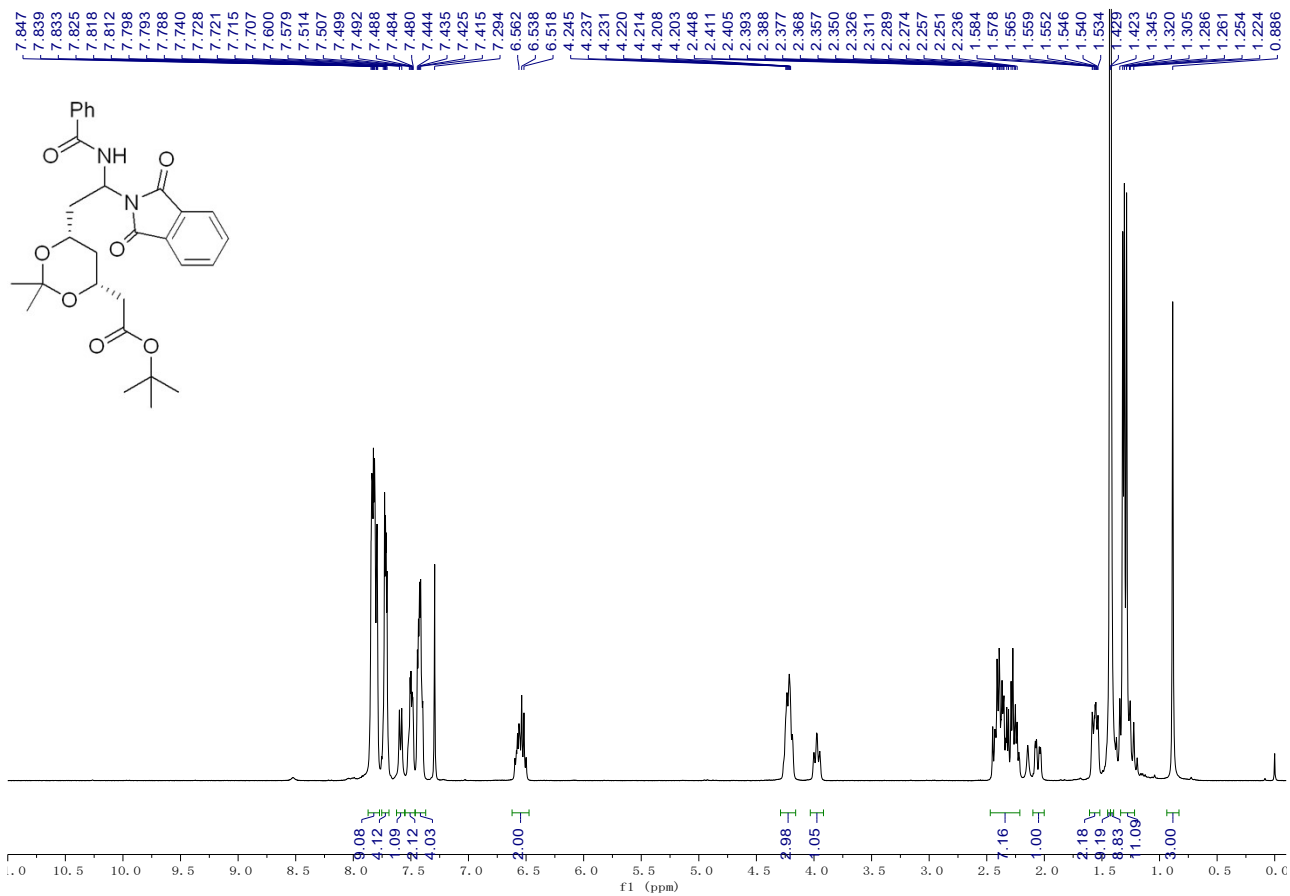


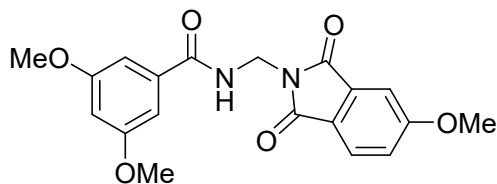
methyl 2-(1-(benzamido(1,3-dioxisoindolin-2-yl)methyl)cyclohexyl)acetate (2ad). A white solid, 80 mg, 92% yield; M.p.: 156-158 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 9.77 (d, $J = 8.5$ Hz, 1H), 8.00-7.92 (m, 2H), 7.90-7.82 (m, 1H), 7.78-7.71 (m, 1H), 7.71-7.64 (m, 2H), 7.52-7.41 (m, 3H), 6.31 (d, $J = 8.4$ Hz, 1H), 3.81 (s, 3H), 2.74 (d, $J = 3.2$ Hz, 2H), 1.96 (dd, $J = 13.7, 5.5$ Hz, 1H), 1.87-1.82 (m, 1H), 1.77-1.68 (m, 1H), 1.64-1.52 (m, 3H), 1.48-1.34 (m, 4H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 174.5, 169.1, 168.1, 166.7, 134.2, 134.1, 133.4, 131.9, 131.6, 131.4, 128.4, 127.4, 123.7, 123.4, 123.1, 65.0, 52.1, 40.3, 38.6, 35.2, 31.7, 25.6, 21.2, 21.1; IR (neat) ν 3319, 2924, 2853, 1775, 1712, 1659, 1605, 1520, 1464, 1373, 1344, 1213 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{25}\text{H}_{26}\text{N}_2\text{O}_5\text{Na}^+$ Requires: 457.1734, Found: 457.1729.



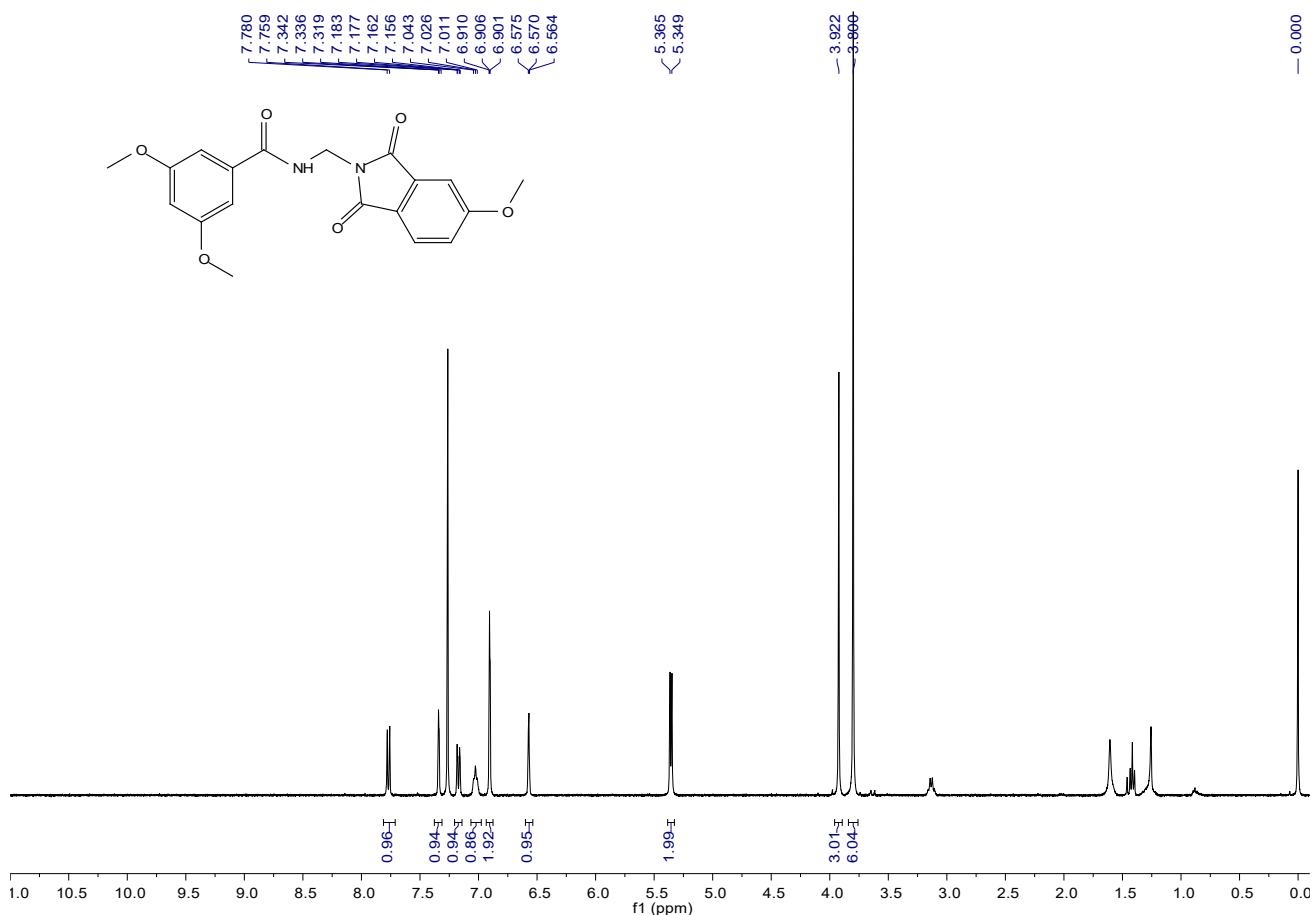


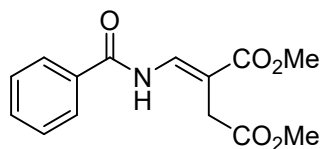
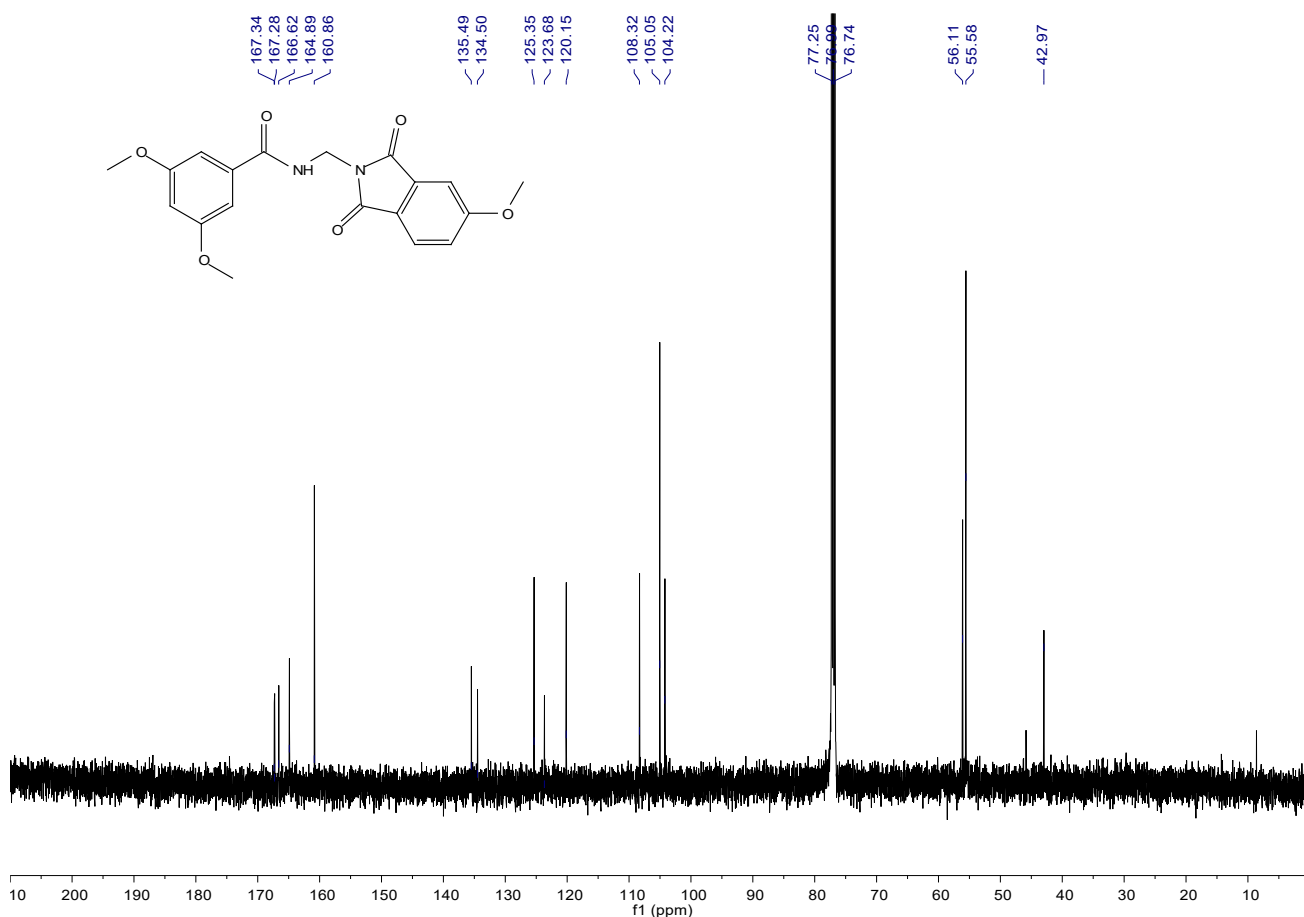
tert-butyl-2-((4R,6R)-6-(2-benzamido-2-(1,3-dioxoisindolin-2-yl)ethyl)-2,2-dimethyl-1,3-dioxan-4-yl)acetate (2ae). A white solid, 80 mg, 76% yield; M.p.: 150-152 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 7.87-7.77 (m, 9H), 7.75-7.69 (m, 4H), 7.59 (d, *J* = 8.2 Hz, 1H), 7.55-7.46 (m, 2H), 7.46-7.37 (m, 4H), 6.62-6.47 (m, 2H), 4.29-4.16 (m, 3H), 4.03-3.92 (m, 1H), 2.47-2.21 (m, 7H), 2.10-2.00 (m, 1H), 1.61-1.52 (m, 2H), 1.43 (s, 9H), 1.42 (s, 9H), 1.34-1.22 (m, 11H), 0.89 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 170.0, 169.9, 167.9, 167.4, 166.1, 166.0, 134.1, 134.0, 133.4, 133.3, 131.9, 131.8, 131.6, 128.49, 128.45, 127.1, 127.0, 123.4, 123.2, 98.9, 98.6, 80.5, 66.7, 66.1, 66.0, 65.8, 55.9, 55.0, 42.5, 42.4, 39.3, 39.0, 36.2, 36.0, 29.8, 29.4, 28.0, 19.3, 19.1; IR (neat) ν 3394, 2943, 1779, 1703, 1662, 1488, 1440, 1367, 1279, 1144, 1060, 1026, 972, 879, 819 cm⁻¹; HRMS (ESI) Calcd. for C₂₉H₃₄N₂O₇Na⁺ Requires: 545.2258, Found: 545.2254.



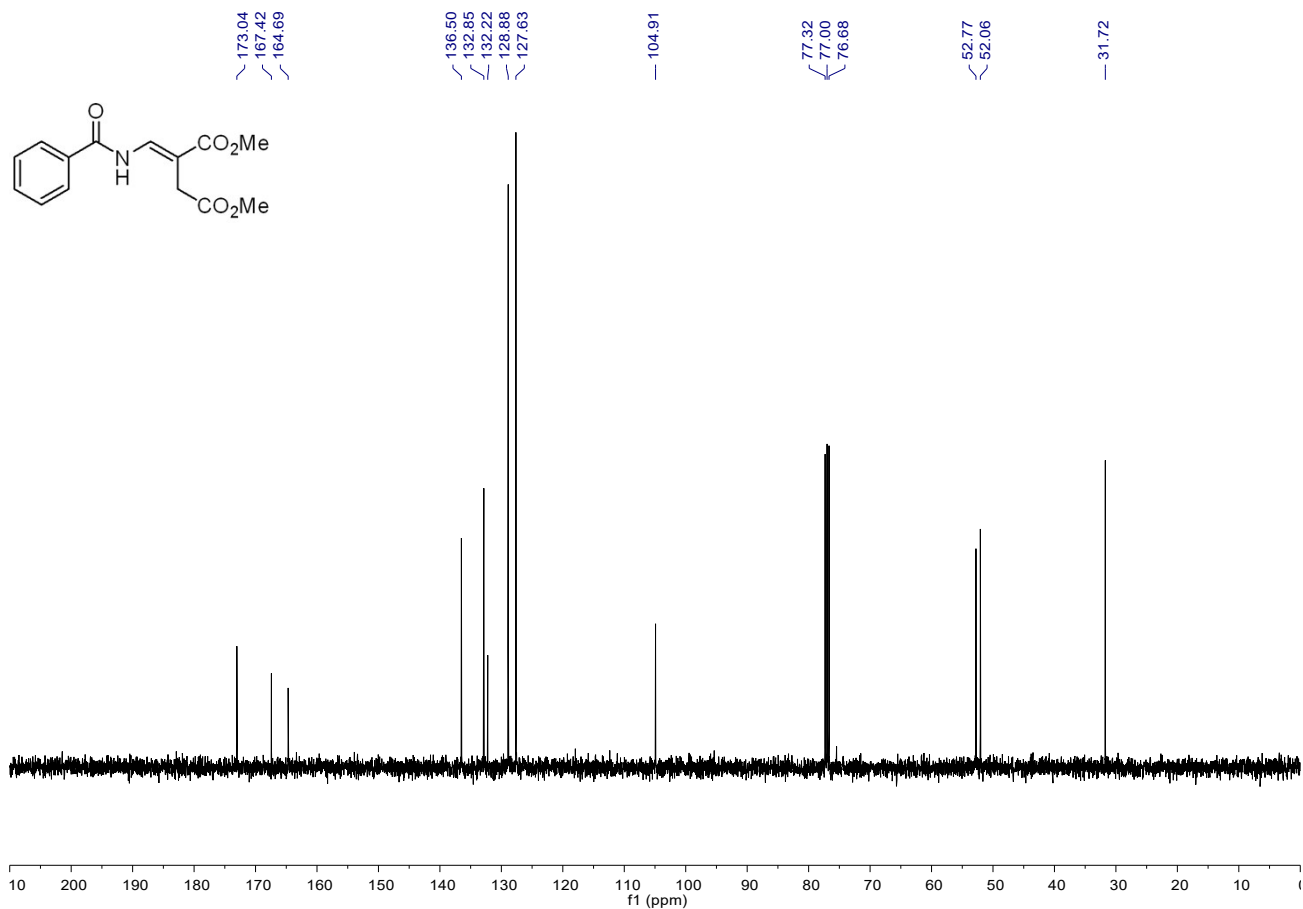
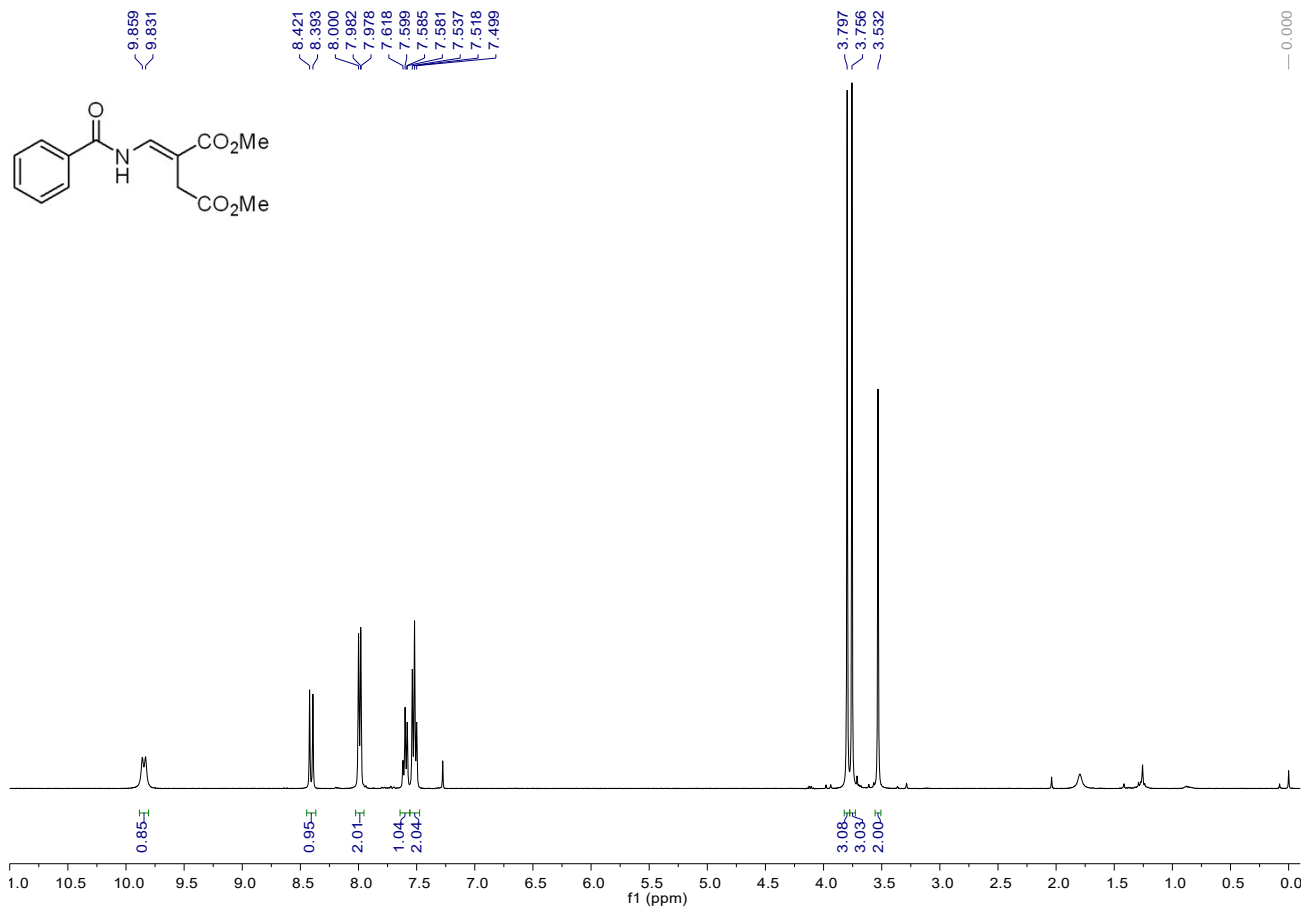


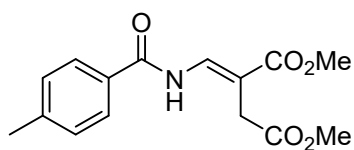
3,5-dimethoxy-N-((5-methoxy-1,3-dioxisoindolin-2-yl)methyl)benzamide (2ah). A white solid, 59.9 mg, 81% yield; M.p.: 215-217 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.77 (d, $J = 8.3$ Hz, 1H), 7.34 (d, $J = 2.2$ Hz, 1H), 7.17 (dd, $J = 8.4, 2.2$ Hz, 1H), 7.03 (t, $J = 6.5$ Hz, 1H), 6.91 (t, $J = 1.9$ Hz, 2H), 6.60 – 6.54 (m, 1H), 5.36 (d, $J = 6.4$ Hz, 2H), 3.92 (s, 3H), 3.80 (s, 6H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.3, 167.3, 166.6, 164.9, 160.9, 135.5, 134.5, 125.4, 123.7, 120.2, 108.3, 105.0, 104.2, 56.1, 55.6, 43.0; IR (neat) ν 2919, 2844, 1771, 1716, 1594, 1537, 1396, 1291, 1205, 1157, 1064, 845, 743 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{19}\text{H}_{18}\text{N}_2\text{O}_6\text{Na}^+$ Requires: 393.1057, Found: 393.1058.



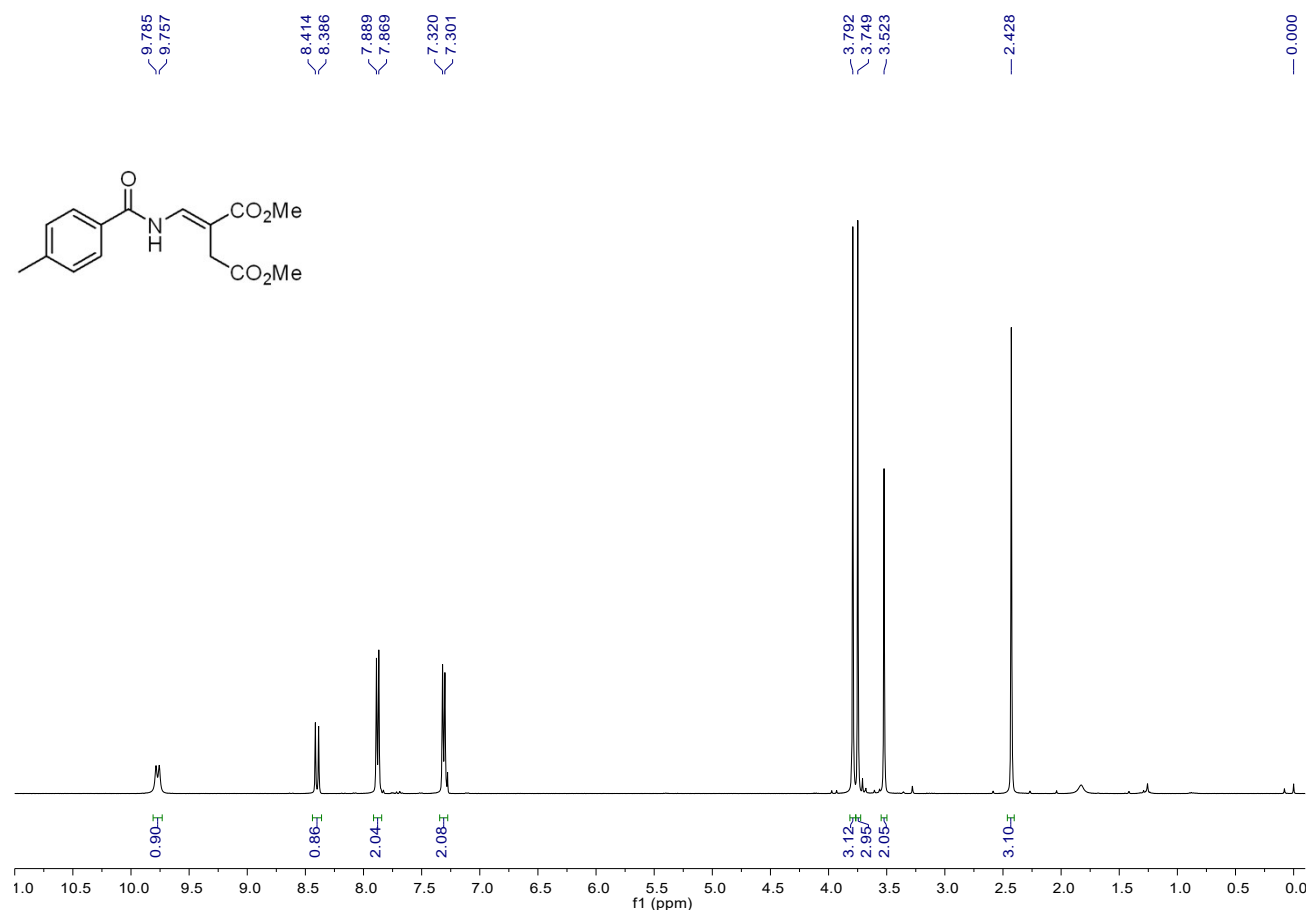


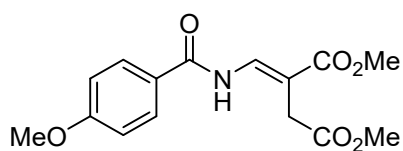
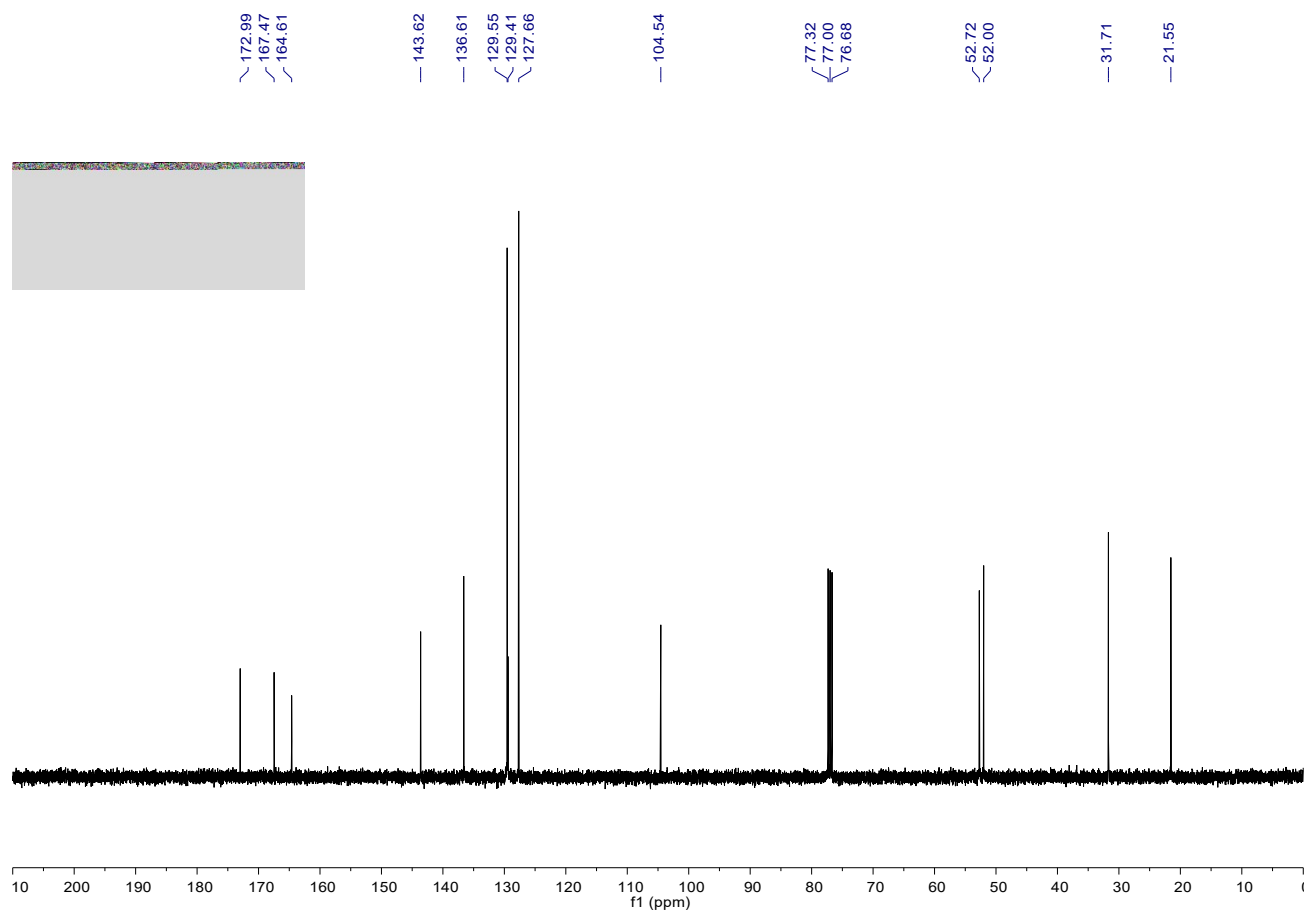
dimethyl (E)-2-(benzamidomethylene) succinate (4aa). A white solid, 39 mg, 70% yield; M.p.: 102-104 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 9.85 (d, $J = 11.2$ Hz, 1H), 8.41 (d, $J = 11.3$ Hz, 1H), 8.02-7.95 (m, 2H), 7.60 (t, $J = 7.5$ Hz, 1H), 7.52 (t, $J = 7.5$ Hz, 2H), 3.80 (s, 3H), 3.76 (s, 3H), 3.53 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 173.0, 167.4, 164.7, 136.5, 132.9, 132.2, 128.9, 127.6, 104.9, 52.8, 52.1, 31.7; IR (neat) ν 3364, 2957, 1716, 1687, 1651, 1479, 1195, 1113, 1025, 800, 700, 682 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{14}\text{H}_{15}\text{NO}_5\text{Na}^+$ Requires: 300.0842, Found: 300.0841.



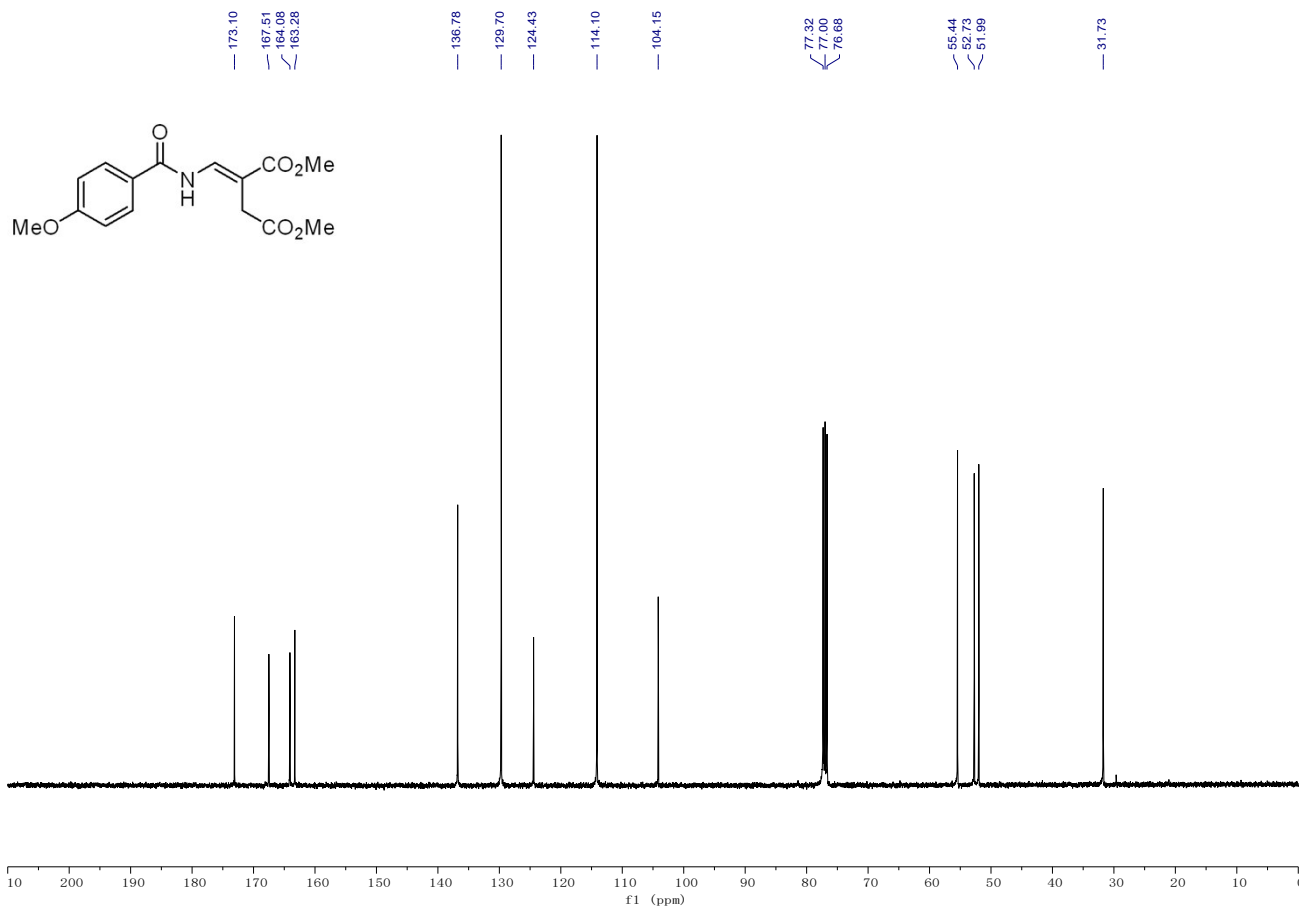
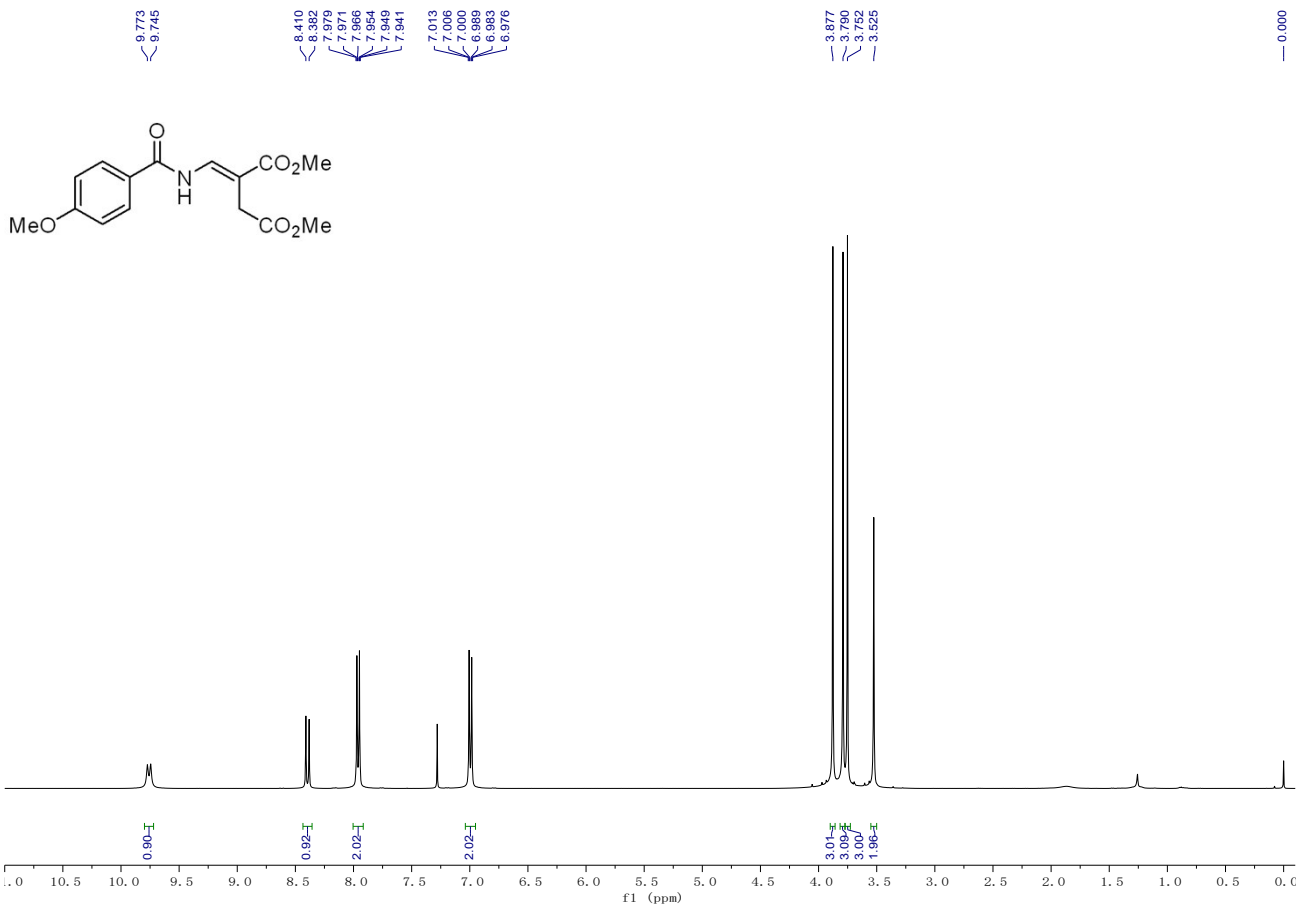


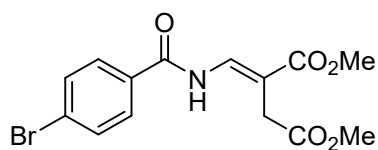
dimethyl (E)-2-((4-methylbenzamido)methylene) succinate (4ba). A white solid, 41 mg, 70% yield; M.p.: 170-172 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 9.77 (d, $J = 11.3$ Hz, 1H), 8.40 (d, $J = 11.3$ Hz, 1H), 7.88 (d, $J = 8.0$ Hz, 2H), 7.31 (d, $J = 7.8$ Hz, 2H), 3.79 (s, 3H), 3.75 (s, 3H), 3.52 (s, 2H), 2.43 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 173.0, 167.5, 164.6, 143.6, 136.6, 129.5, 129.4, 127.7, 104.5, 52.7, 52.0, 31.7, 21.5; IR (neat) ν 3369, 2956, 1712, 1689, 1655, 1483, 1374, 1339, 1185, 1127, 1021, 849, 740 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{15}\text{H}_{17}\text{NO}_5\text{Na}^+$ Requires: 314.0999, Found: 314.0994.



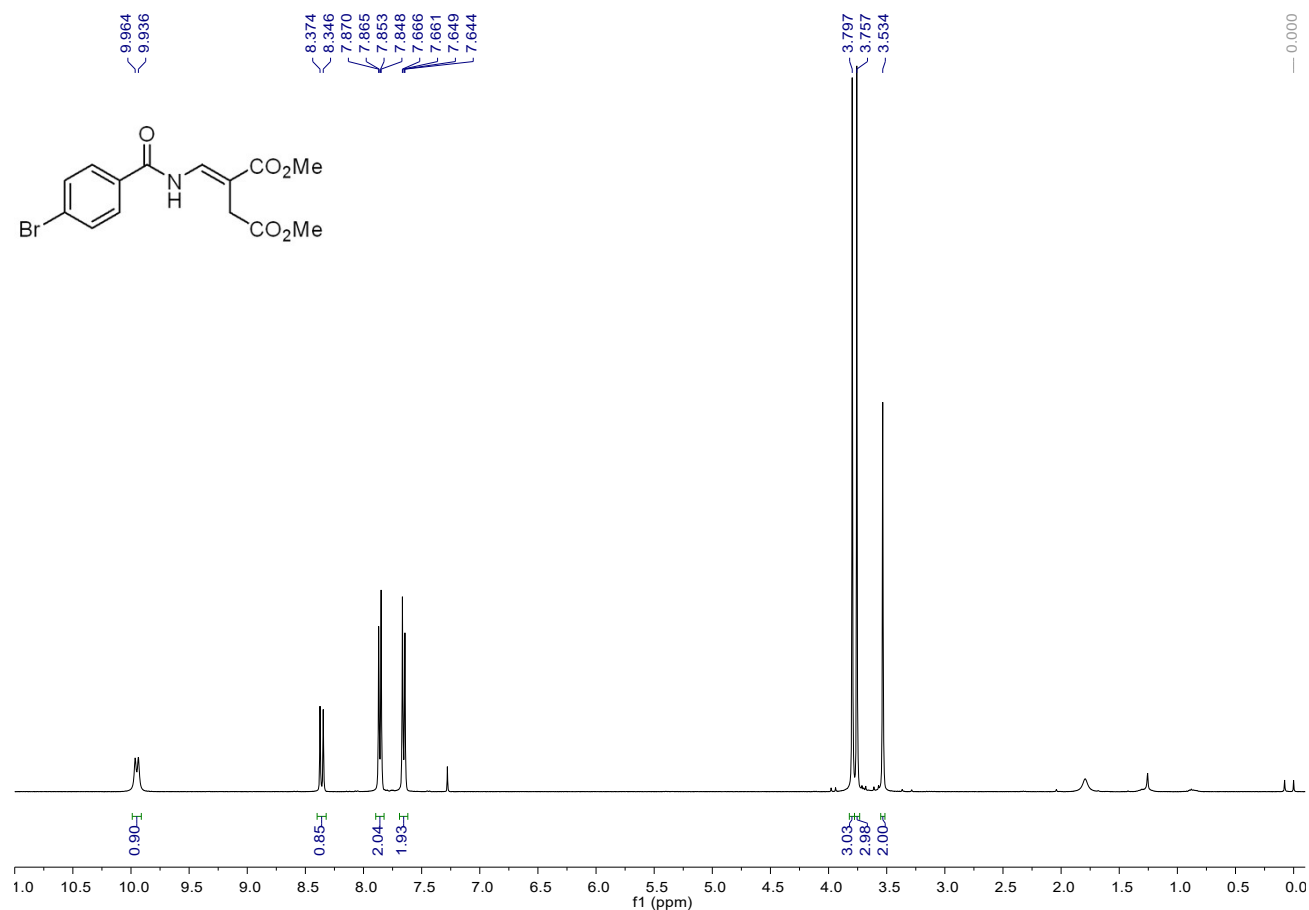


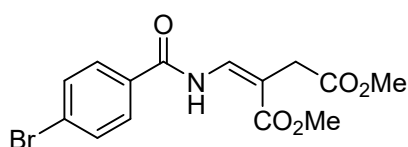
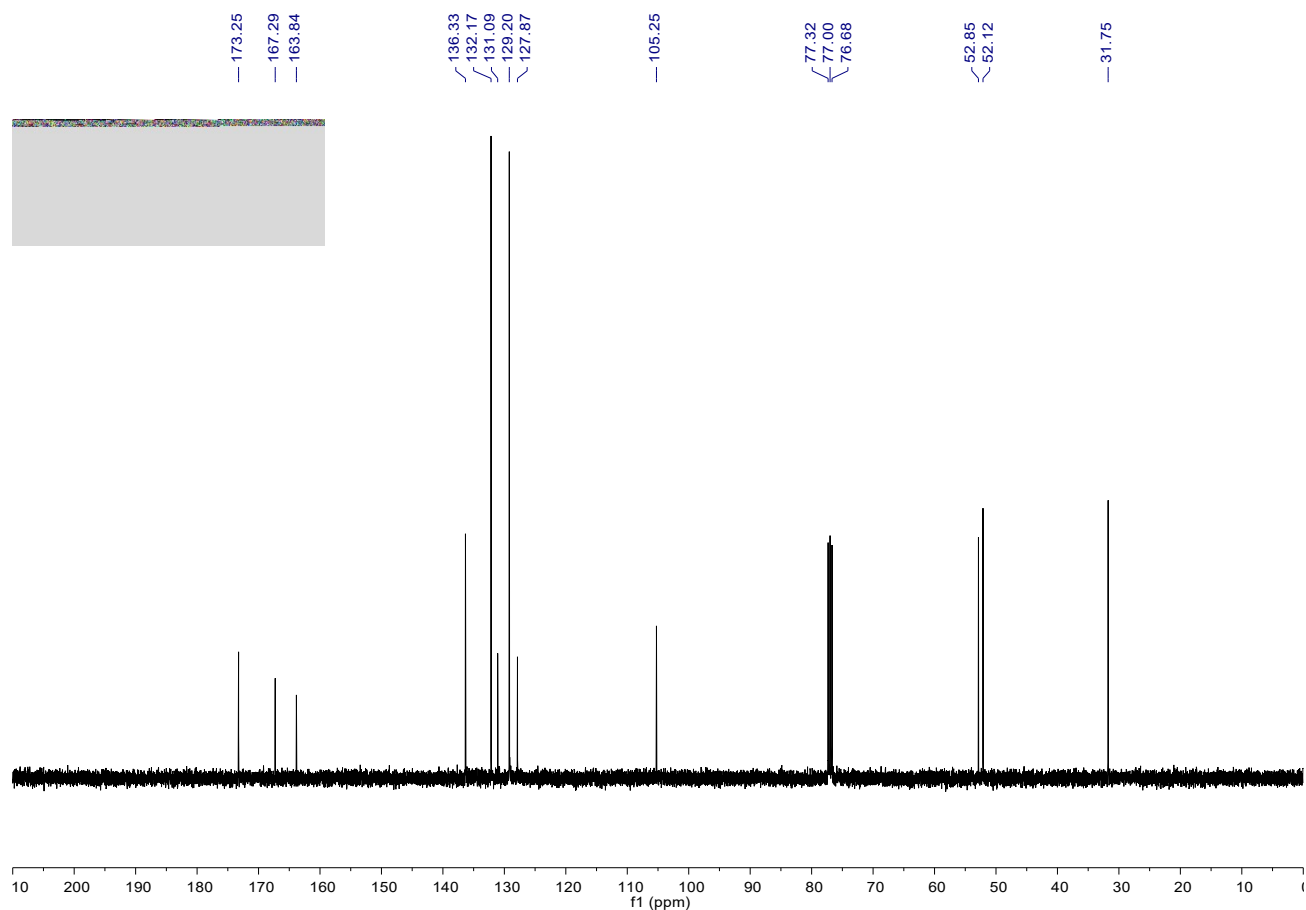
dimethyl (E)-2-((4-methoxybenzamido)methylene) succinate (4ca). A white solid, 36 mg, 59% yield; M.p.: 128-130 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 9.76 (d, $J = 11.3$ Hz, 1H), 8.40 (d, $J = 11.3$ Hz, 1H), 8.00-7.92 (m, 2H), 7.04-6.95 (m, 2H), 3.88 (s, 3H), 3.79 (s, 3H), 3.75 (s, 3H), 3.53 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 173.1, 167.5, 164.1, 163.3, 136.8, 129.7, 124.4, 114.1, 104.1, 55.4, 52.7, 52.0, 31.7; IR (neat) ν 3372, 2954, 1687, 1608, 1483, 1339, 1251, 1172, 1129, 1032, 1005, 7993, 758, 693 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{15}\text{H}_{17}\text{NO}_6\text{Na}^+$ Requires: 330.0948, Found: 330.0942.



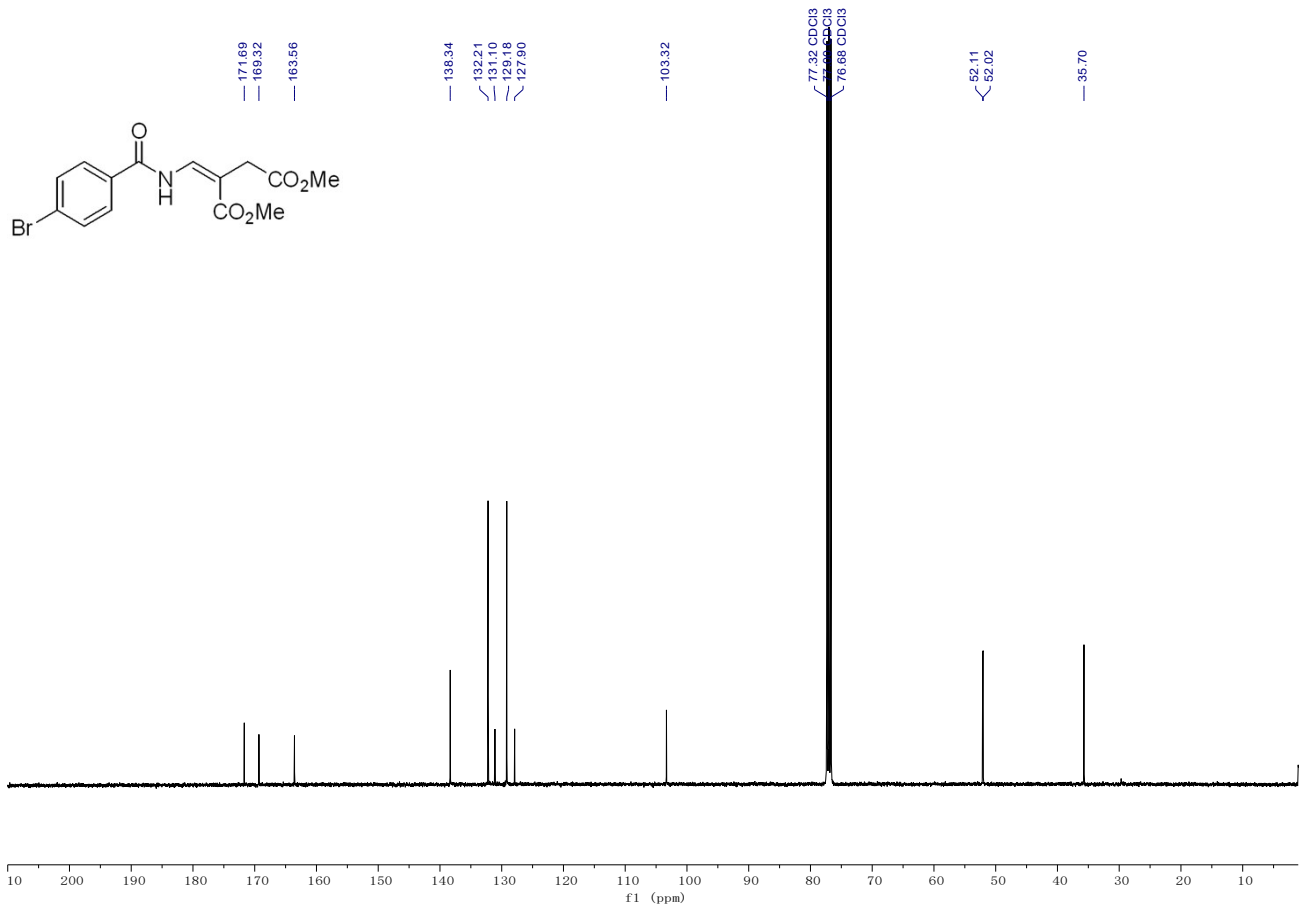
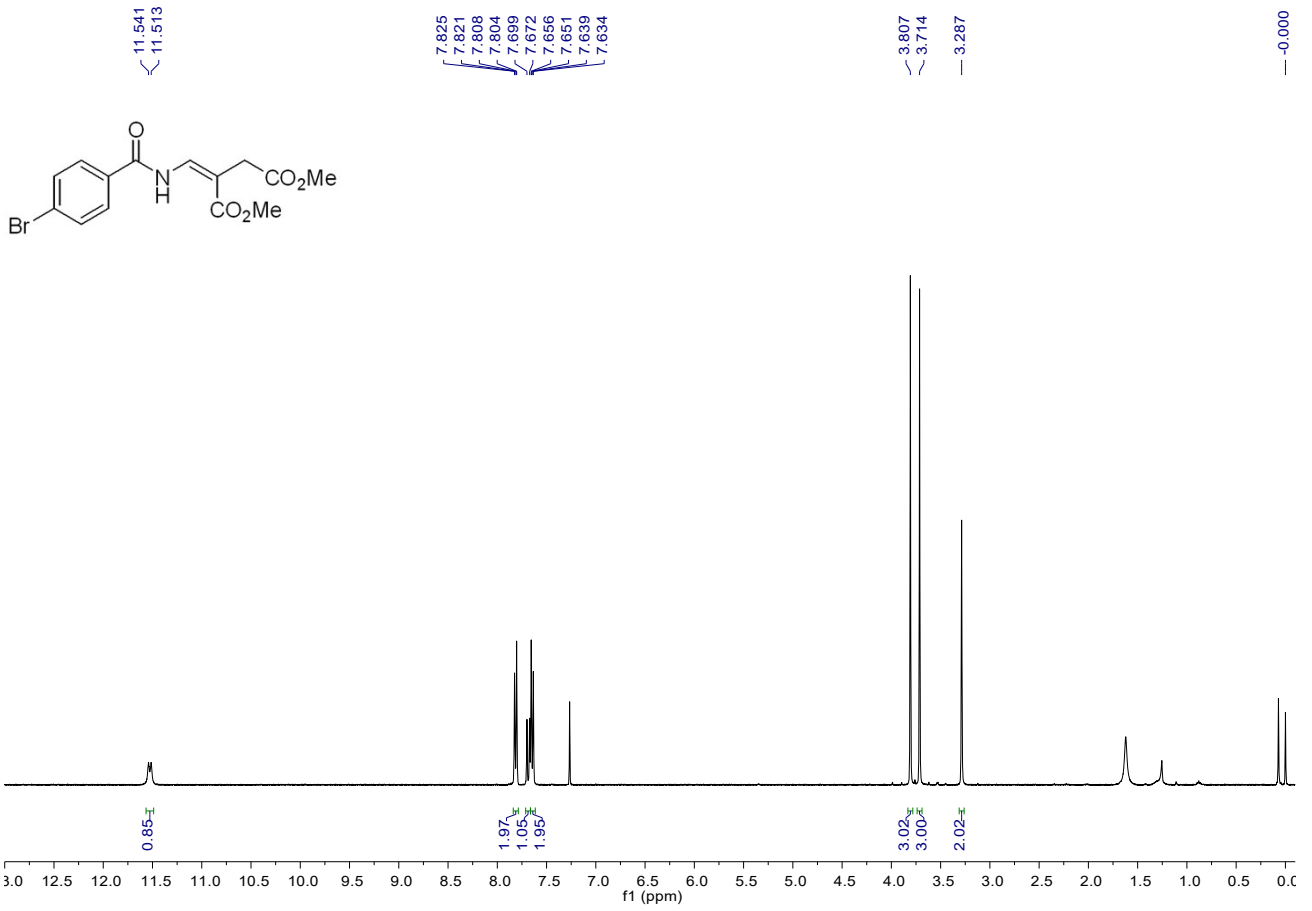


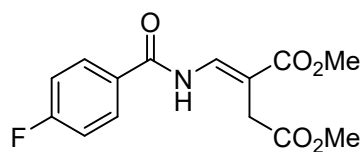
dimethyl (E)-2-((4-bromobenzamido)methylene) succinate (4da). A white solid, 43 mg, 61% yield; M.p.: 163-165 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 9.95 (d, $J = 11.2$ Hz, 1H), 8.36 (d, $J = 11.1$ Hz, 1H), 7.89-7.82 (m, 2H), 7.69-7.62 (m, 2H), 3.80 (s, 3H), 3.76 (s, 3H), 3.53 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 173.2, 167.3, 163.8, 136.3, 132.2, 131.1, 129.2, 127.9, 105.2, 52.9, 52.1, 31.8; IR (neat) ν 3365, 2954, 1712, 1690, 1478, 1435, 1257, 1184, 1119, 1106, 1009, 906, 744 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{14}\text{H}_{14}\text{NO}_5\text{NaBr}^+$ Requires: 377.9948, Found: 377.9955.



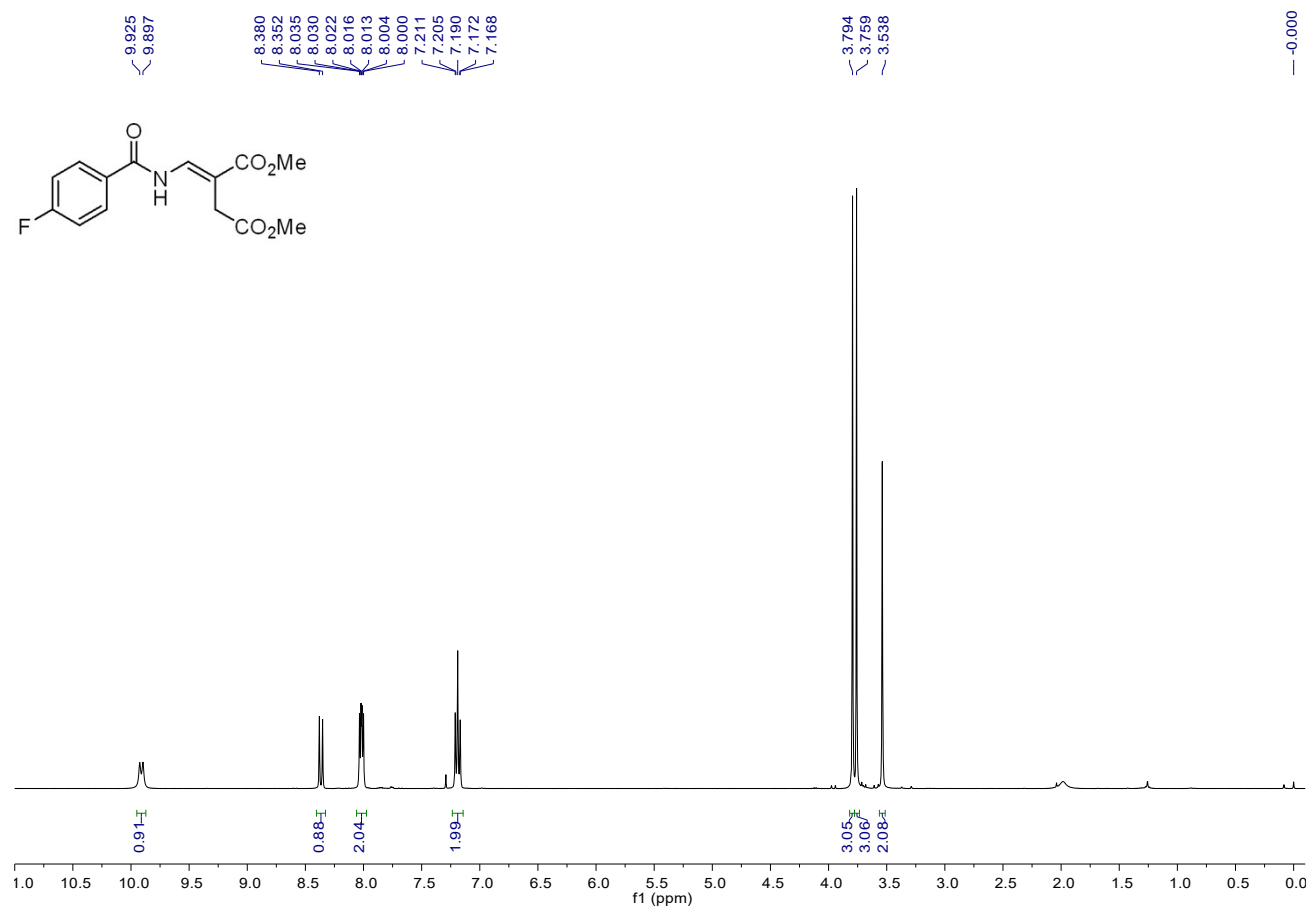


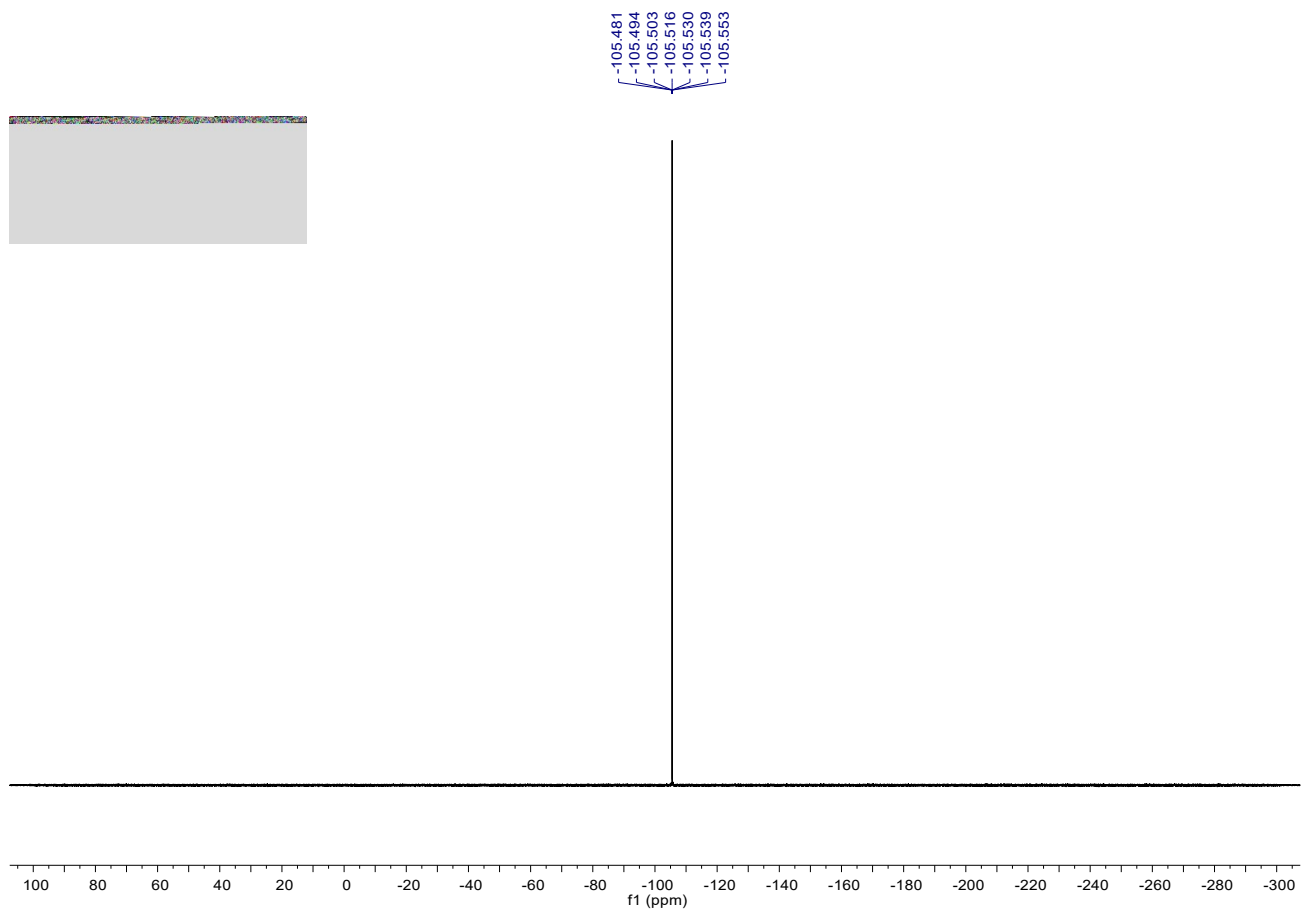
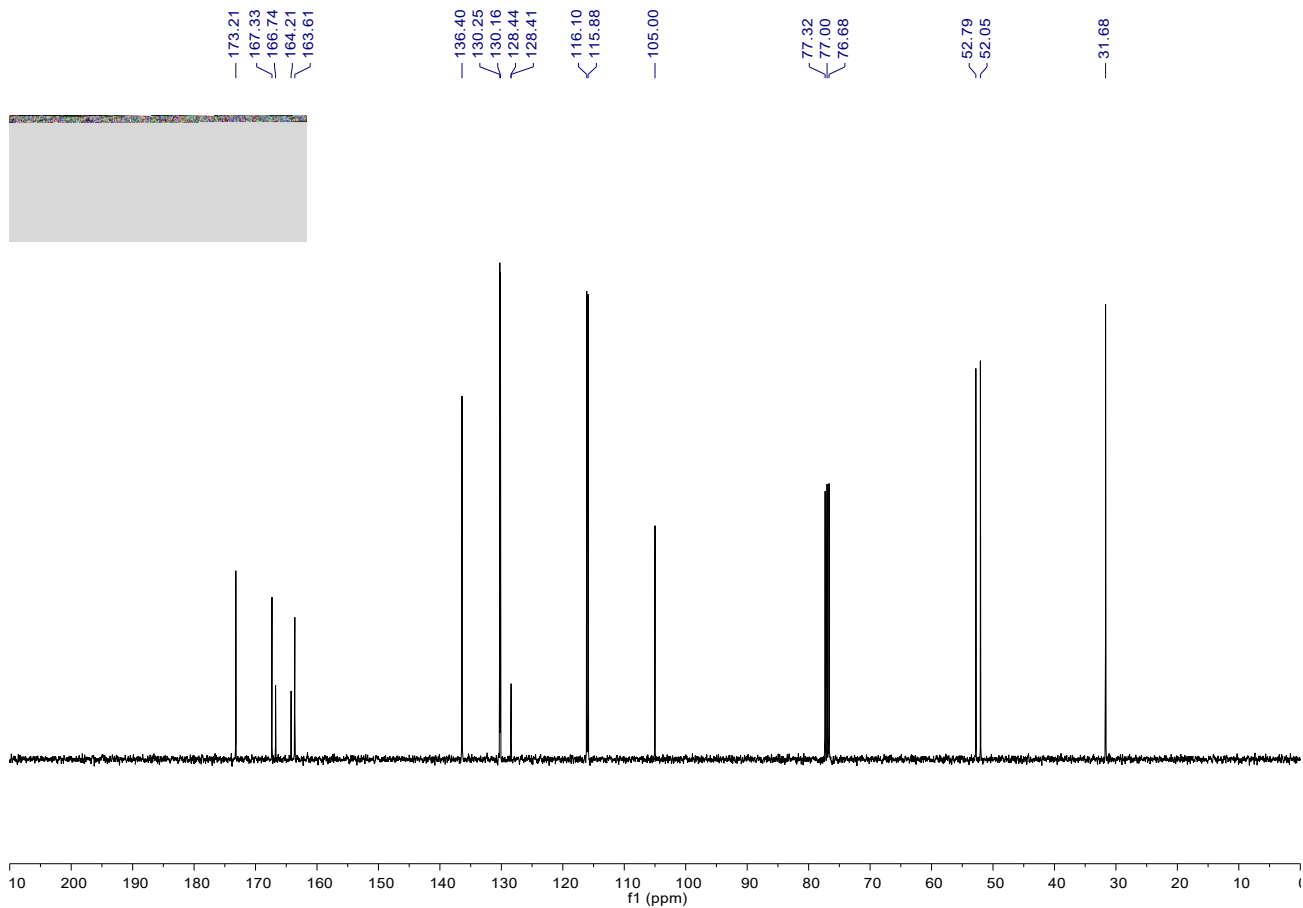
dimethyl (Z)-2-((4-bromobenzamido)methylene) succinate (4da'). A white solid, 7 mg, 10% yield; M.p.: 121 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 11.53 (d, $J = 10.9$ Hz, 1H), 7.84-7.79 (m, 2H), 7.69 (d, $J = 10.9$ Hz, 1H), 7.66-7.61 (m, 2H), 3.81 (s, 3H), 3.71 (s, 3H), 3.29 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 171.7, 169.3, 163.6, 138.3, 132.2, 131.1, 129.2, 127.9, 103.3, 52.1, 52.0, 35.7; IR (neat) ν 3283, 2921, 1737, 1691, 1630, 1499, 1437, 1351, 1240, 1208, 1173, 1114, 1010, 838 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{14}\text{H}_{14}\text{NO}_5\text{NaBr}^+$ Requires: 377.9948, Found: 377.9946.

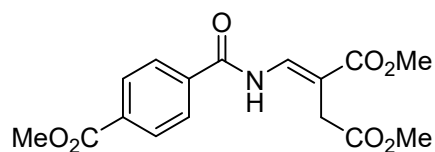




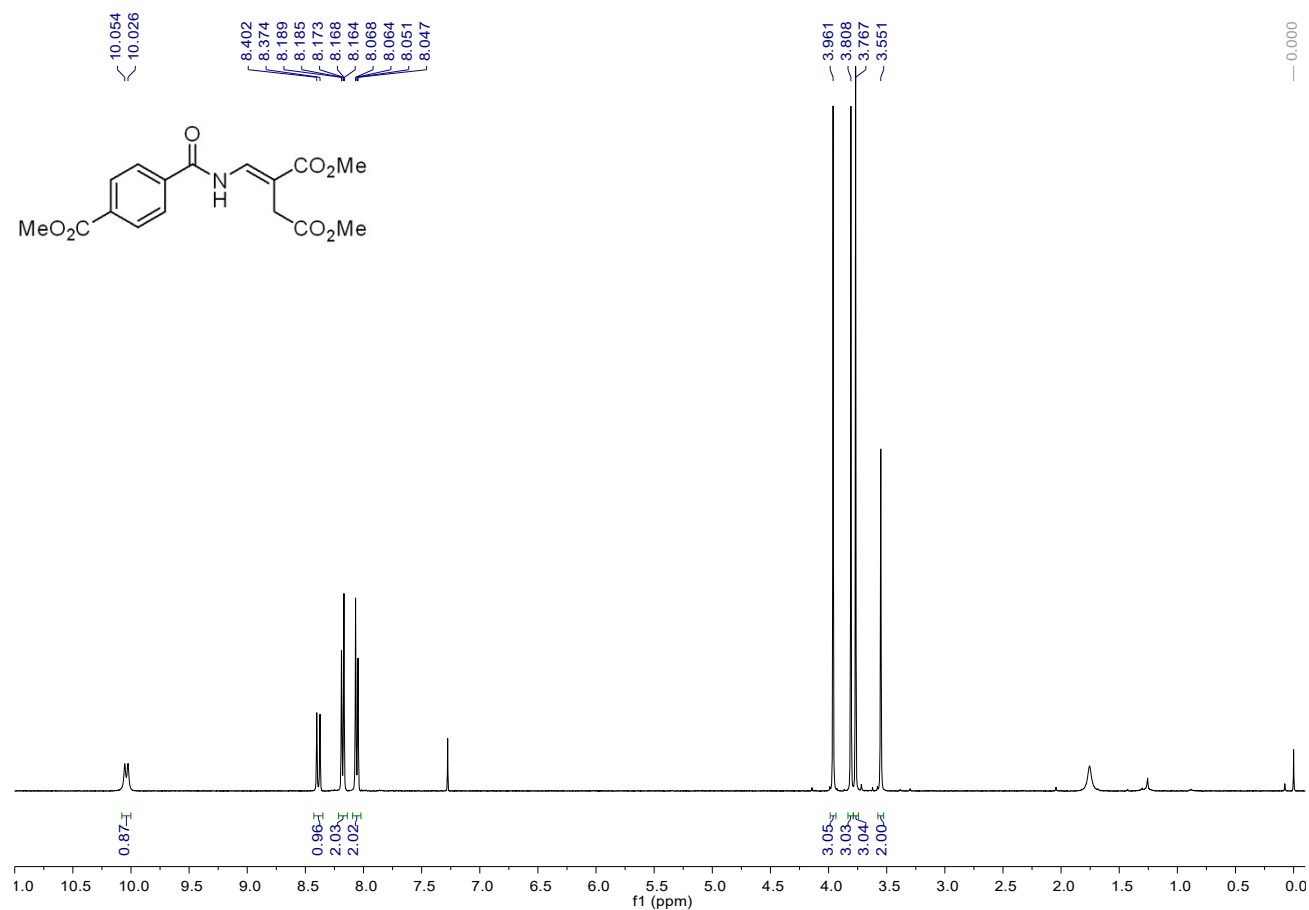
dimethyl (E)-2-((4-fluorobenzamido)methylene)succinate (4ea). A white solid, 39 mg, 66% yield; M.p.: 127-129 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 9.91 (d, $J = 11.1$ Hz, 1H), 8.37 (d, $J = 11.1$ Hz, 1H), 8.06-7.97 (m, 2H), 7.19 (t, $J = 8.6$ Hz, 2H), 3.79 (s, 3H), 3.76 (s, 3H), 3.54 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 173.2, 167.3, 165.5 (d, $J = 254.3$ Hz), 163.6, 136.4, 130.2 (d, $J = 9.3$ Hz), 128.4 (d, $J = 3.2$ Hz), 116.0 (d, $J = 22.1$ Hz), 105.0, 52.8, 52.1, 31.7; ^{19}F NMR (CDCl_3 , 376 MHz, CFC_3) δ -105.5 (ddd, $J = 13.6, 8.5, 5.2$ Hz); IR (neat) ν 3360, 2958, 1711, 1691, 1657, 1604, 1486, 1435, 1253, 1160, 1115, 981, 856, 755 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{14}\text{H}_{14}\text{NO}_5\text{FNa}^+$ Requires: 318.0748, Found: 318.0751.

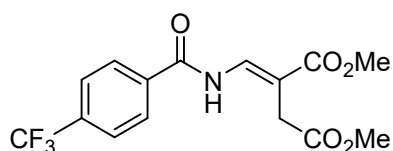
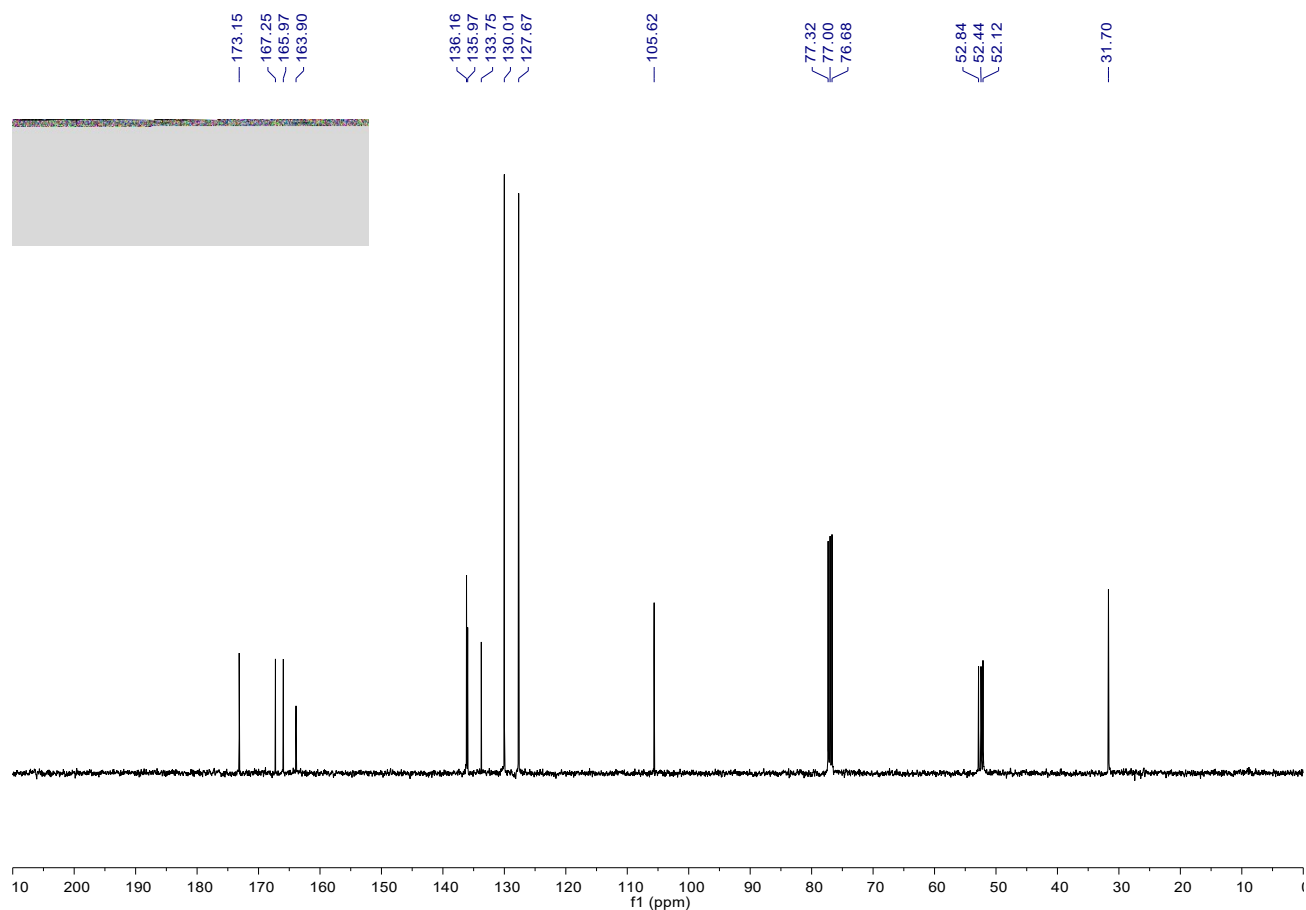




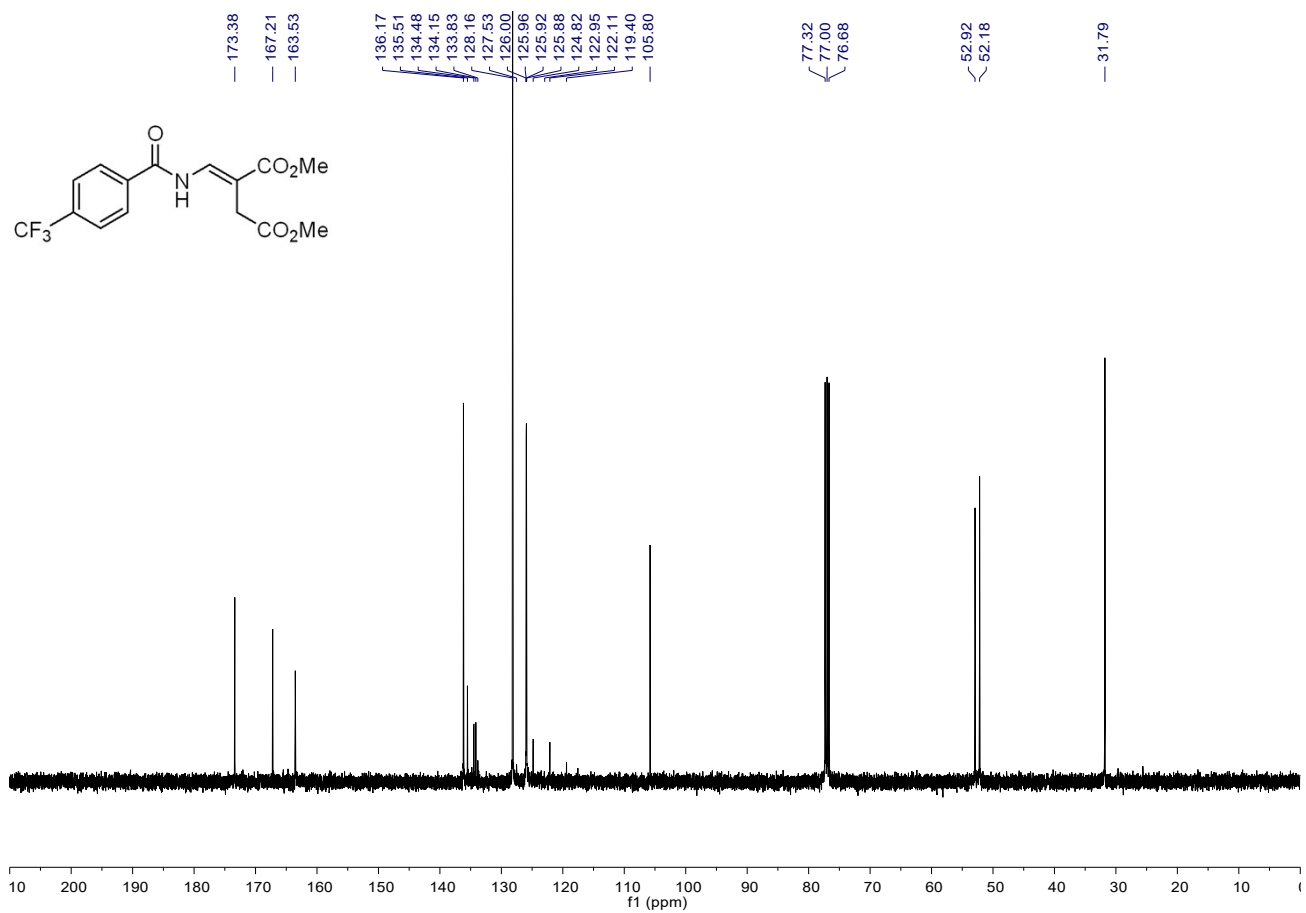
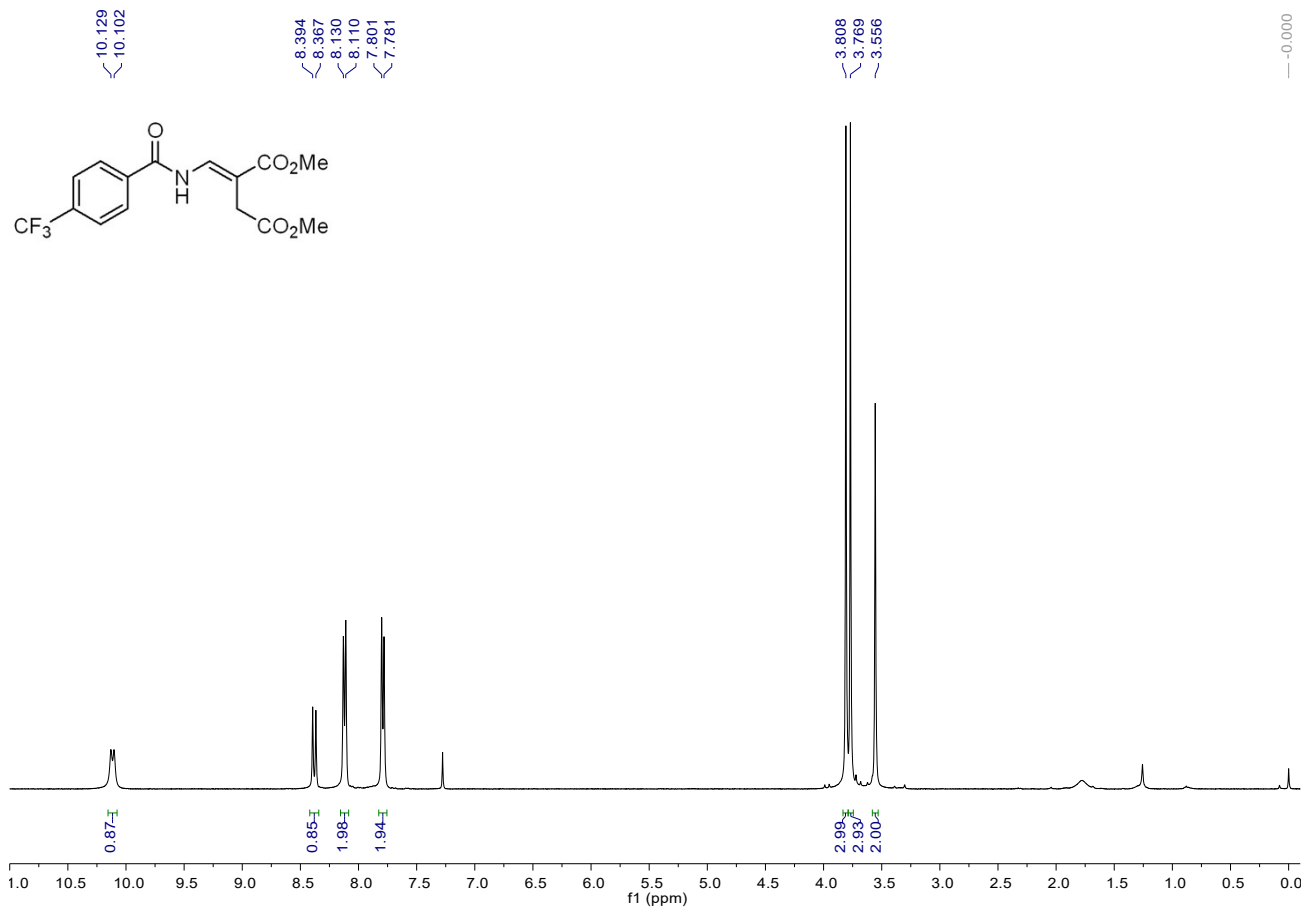


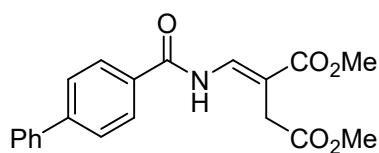
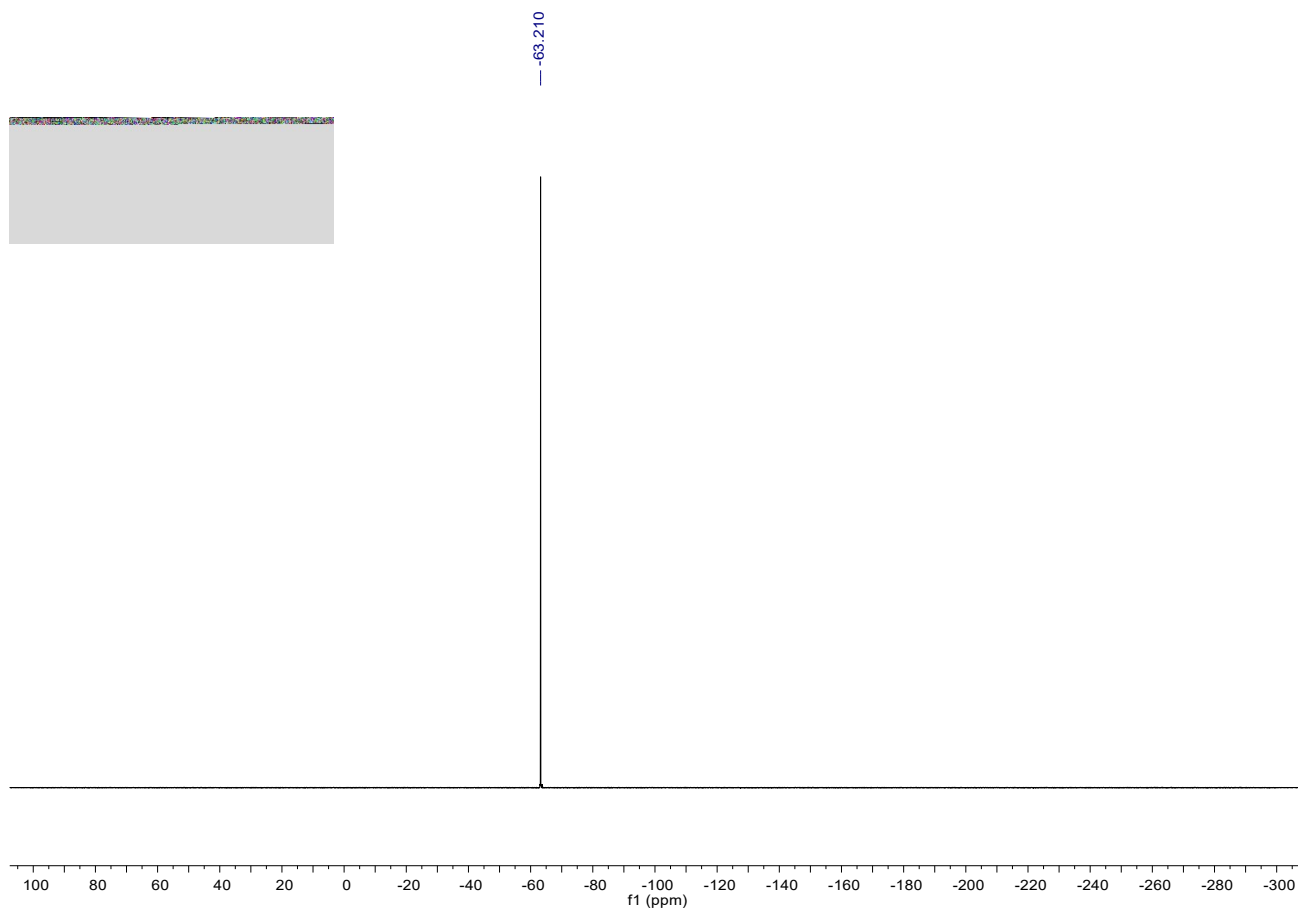
dimethyl (E)-2-((4-(methoxycarbonyl)benzamido)methylene) succinate (4fa). A white solid, 38 mg, 56% yield; M.p.: 128-130 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 10.04 (d, $J = 11.1$ Hz, 1H), 8.39 (d, $J = 11.1$ Hz, 1H), 8.21-8.14 (m, 2H), 8.09-8.02 (m, 2H), 3.96 (s, 3H), 3.81 (s, 3H), 3.77 (s, 3H), 3.55 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 173.1, 167.2, 166.0, 163.9, 136.2, 136.0, 133.8, 130.0, 127.7, 105.6, 52.8, 52.4, 52.1, 31.7; IR (neat) ν 3415, 2960, 1738, 1715, 1681, 1519, 1437, 1330, 1281, 1175, 1175, 1020, 922 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{16}\text{H}_{17}\text{NO}_7\text{Na}^+$ Requires: 358.0897, Found: 358.0904.



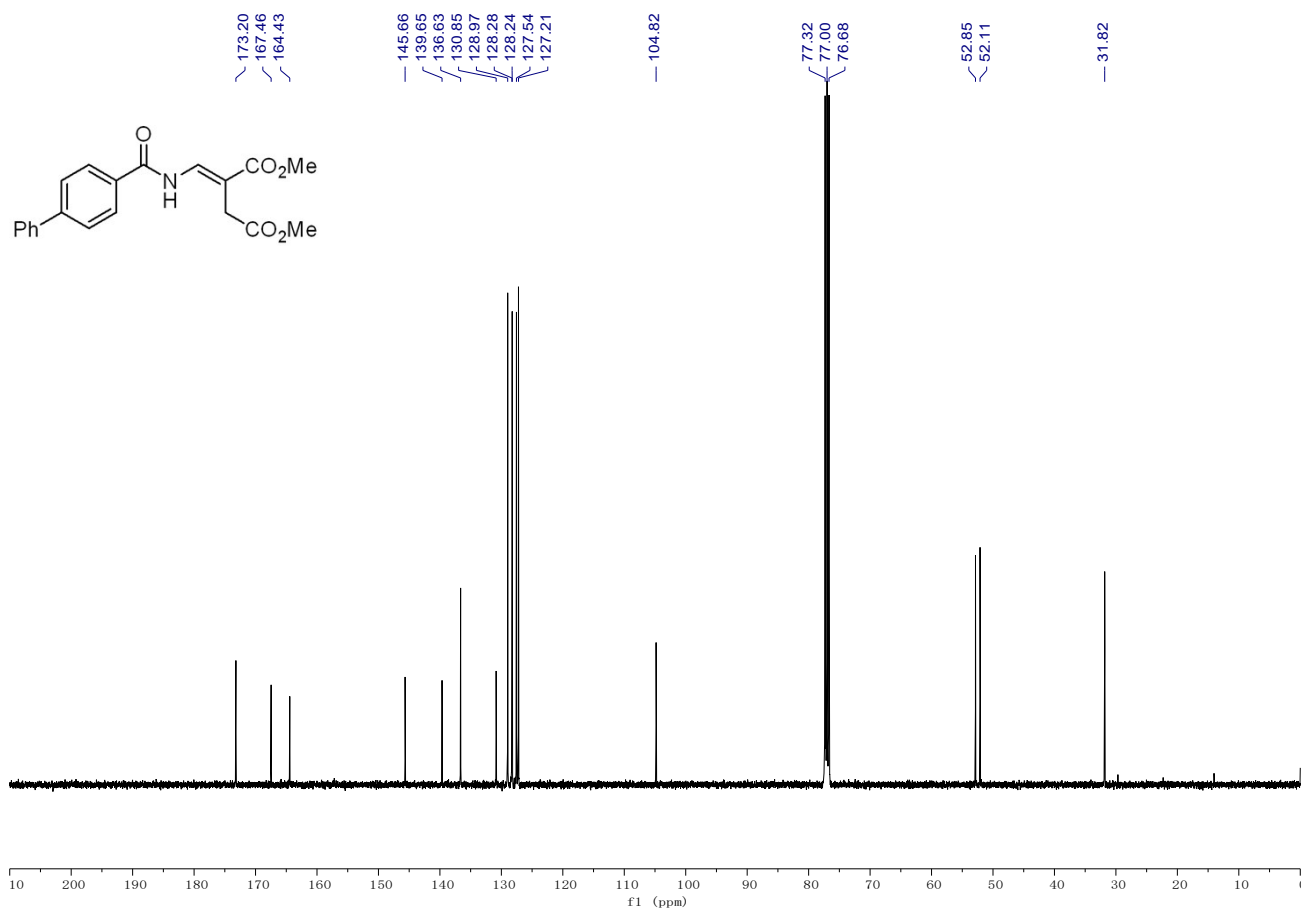
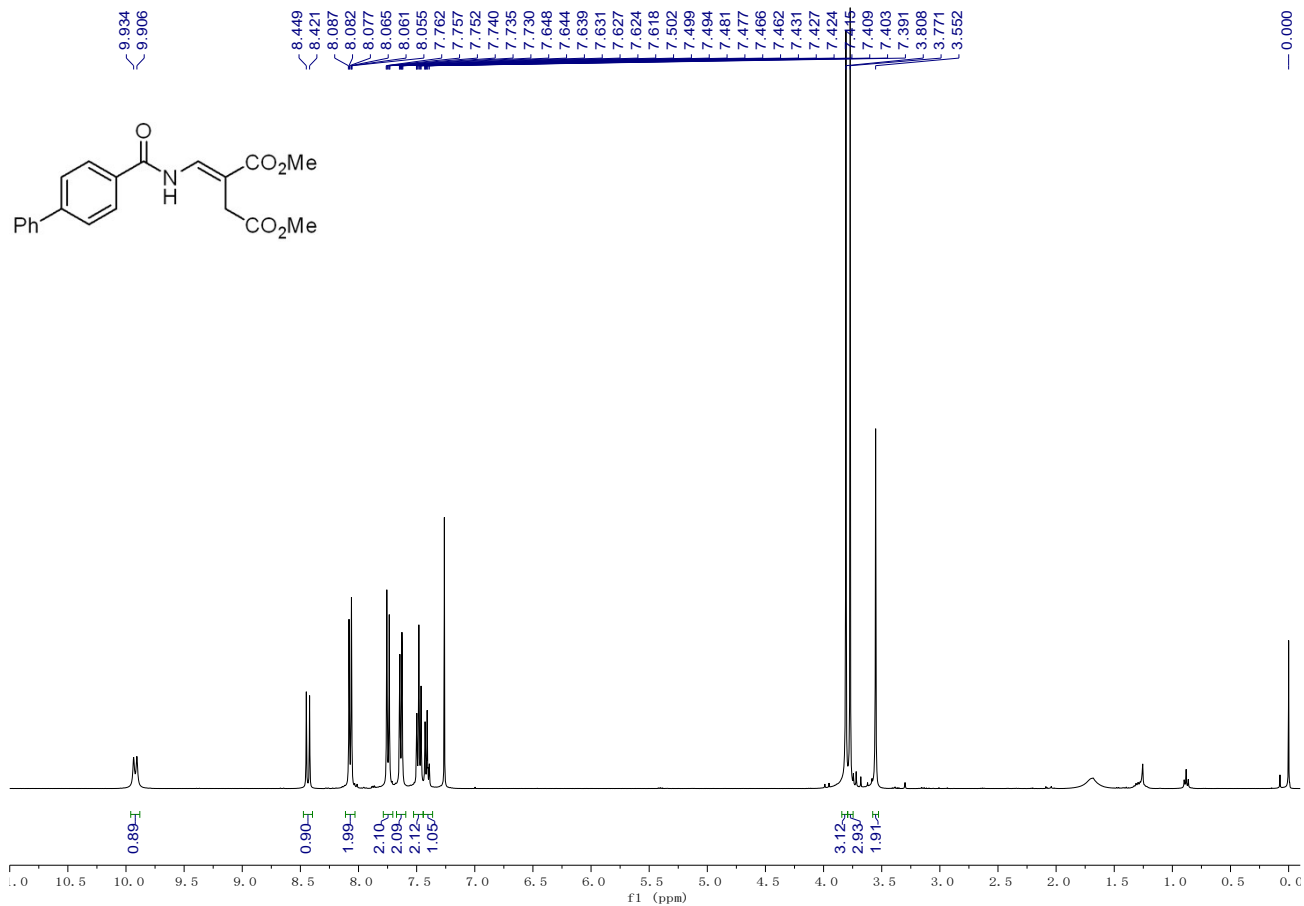


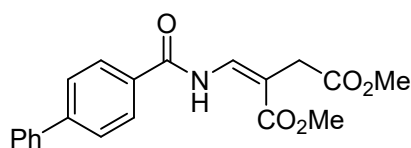
dimethyl (E)-2-((4-(trifluoromethyl)benzamido)methylene) succinate (4ga). A white solid, 30 mg, 44% yield; M.p.: 117-119 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 10.12 (d, $J = 11.1$ Hz, 1H), 8.38 (d, $J = 11.1$ Hz, 1H), 8.12 (d, $J = 8.1$ Hz, 2H), 7.79 (d, $J = 8.1$ Hz, 2H), 3.81 (s, 3H), 3.77 (s, 3H), 3.56 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 173.4, 167.2, 163.5, 136.2, 135.5, 134.3 (q, $J = 32.8$ Hz), 128.2, 125.9 (q, $J = 3.7$ Hz), 123.4 (q, $J = 272.9$ Hz), 105.8, 52.9, 52.2, 31.8; ^{19}F NMR (CDCl_3 , 376 MHz, CFCl_3) δ -63.2; IR (neat) ν 3361, 2959, 2853, 1716, 1705, 1662, 1488, 1332, 1284, 1207, 1106, 1060, 1017, 861, 778 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{15}\text{H}_{14}\text{NO}_5\text{F}_3\text{Na}^+$ Requires:368.0716, Found: 368.0720.



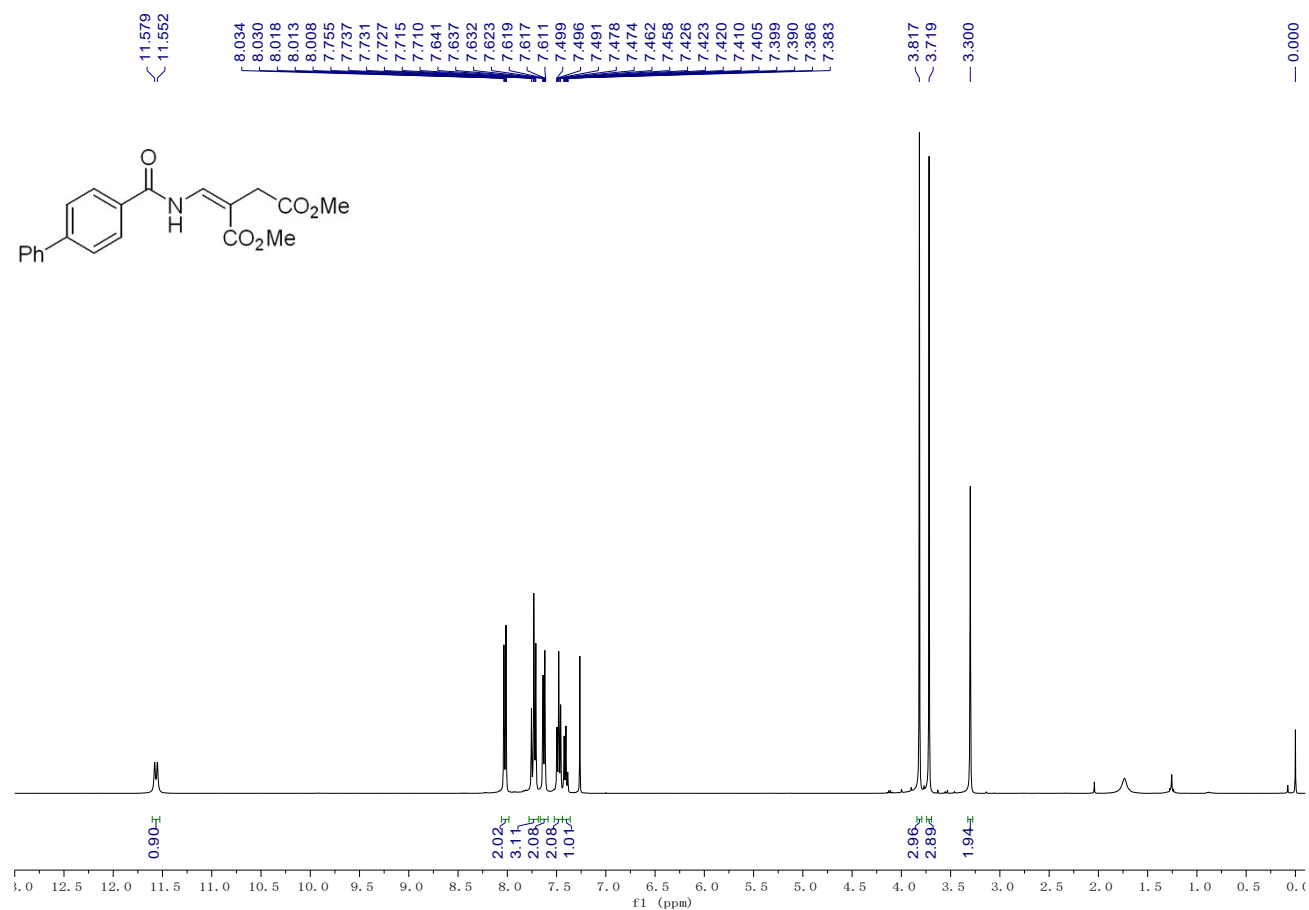


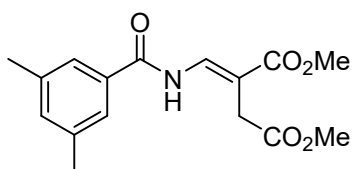
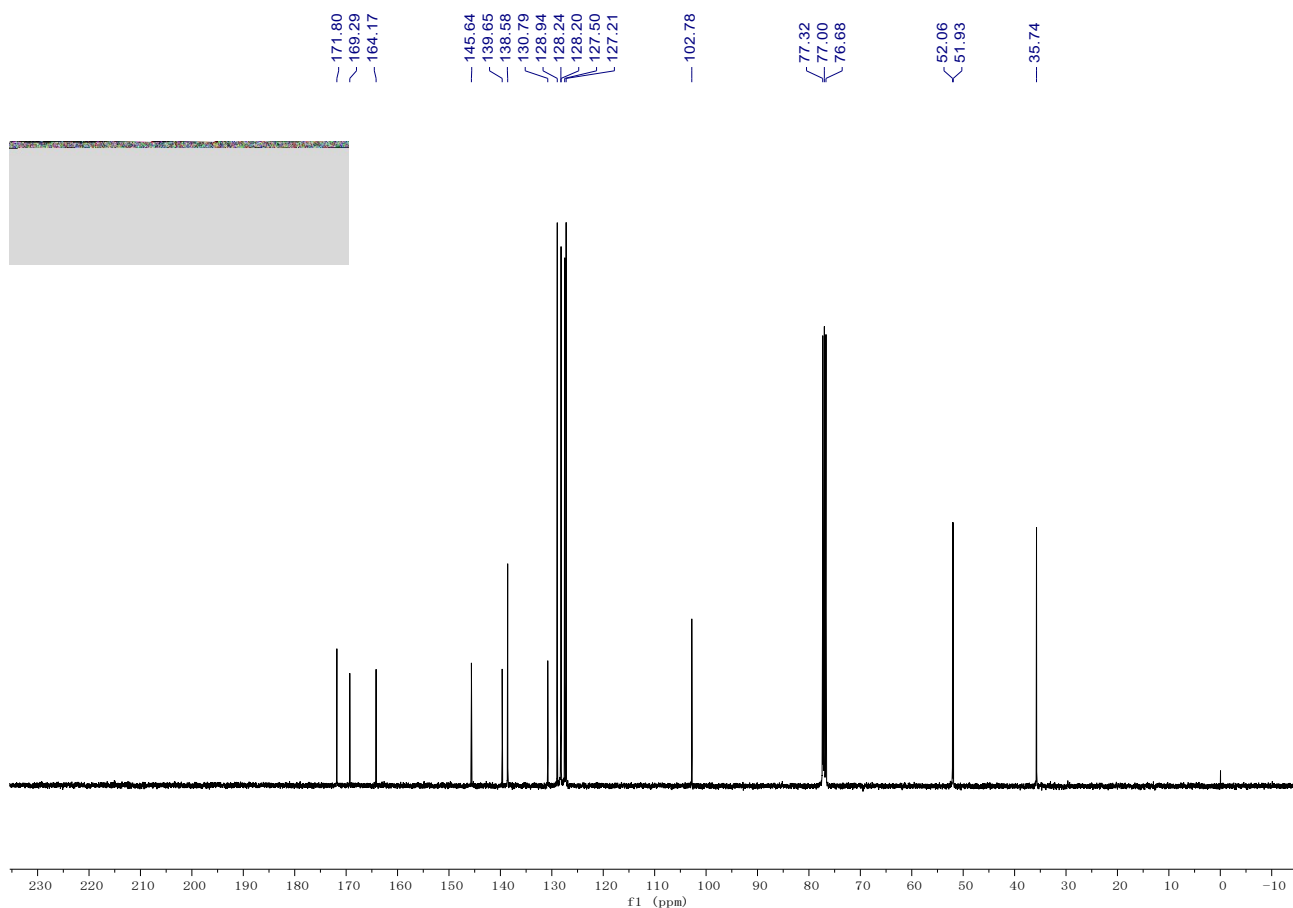
dimethyl (E)-2-([1,1'-biphenyl]-4-carboxamidomethylene) succinate (4ha). A white solid, 33 mg, 46% yield; M.p.: 108-110 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 9.92 (d, $J = 11.3$ Hz, 1H), 8.43 (d, $J = 11.3$ Hz, 1H), 8.11-8.03 (m, 2H), 7.79-7.70 (m, 2H), 7.67-7.59 (m, 2H), 7.53-7.44 (m, 2H), 7.44-7.36 (m, 1H), 3.81 (s, 3H), 3.77 (s, 3H), 3.55 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 173.2, 167.5, 164.4, 145.7, 139.7, 136.6, 130.8, 129.0, 128.3, 128.2, 127.5, 127.2, 104.8, 52.8, 52.1, 31.8; IR (neat) ν 3346, 2956, 1687, 1656, 1607, 1497, 1337, 1193, 1111, 1005, 958, 737, 694 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{20}\text{H}_{19}\text{NO}_5\text{Na}^+$ Requires: 376.1155, Found: 376.1153.



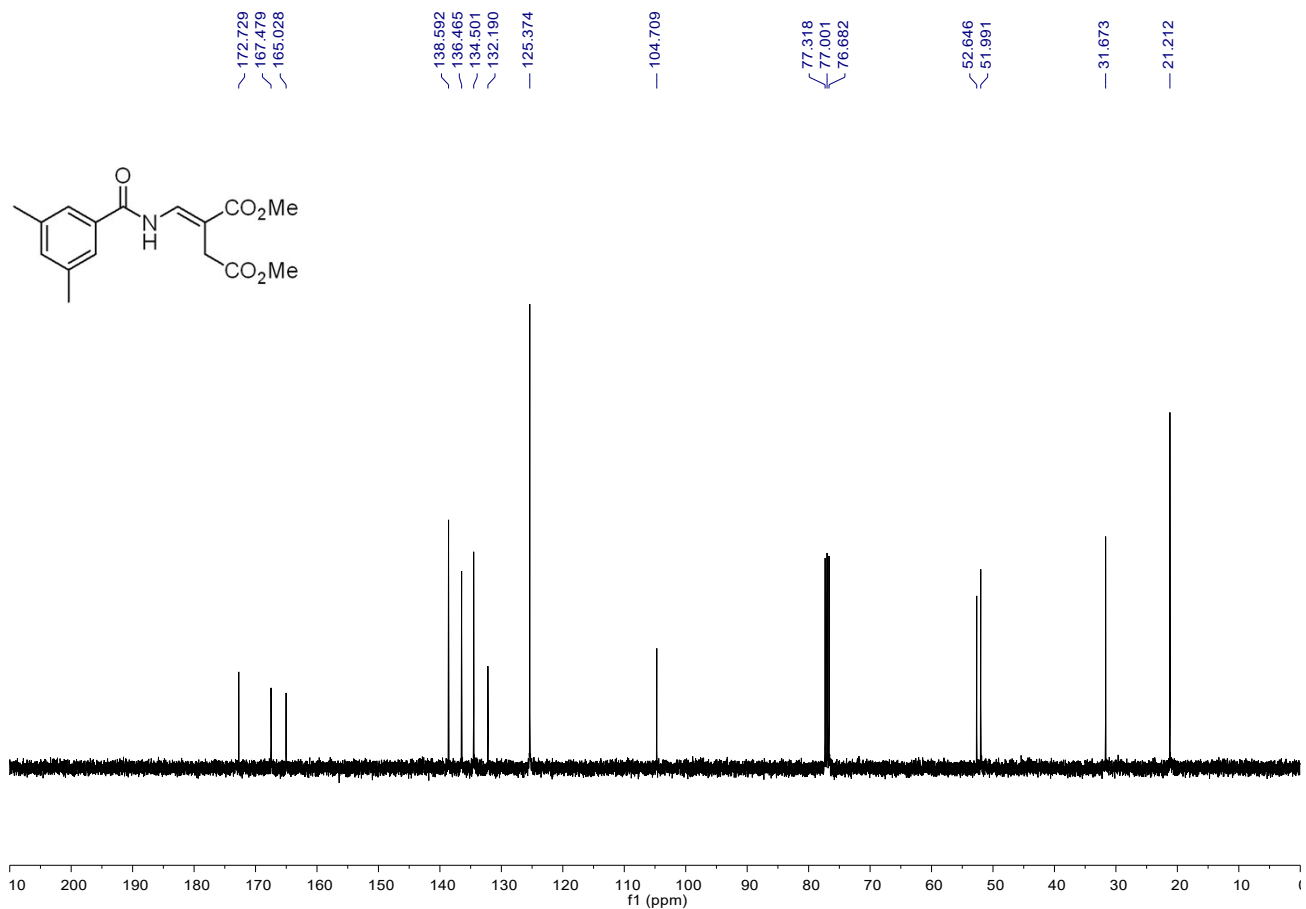
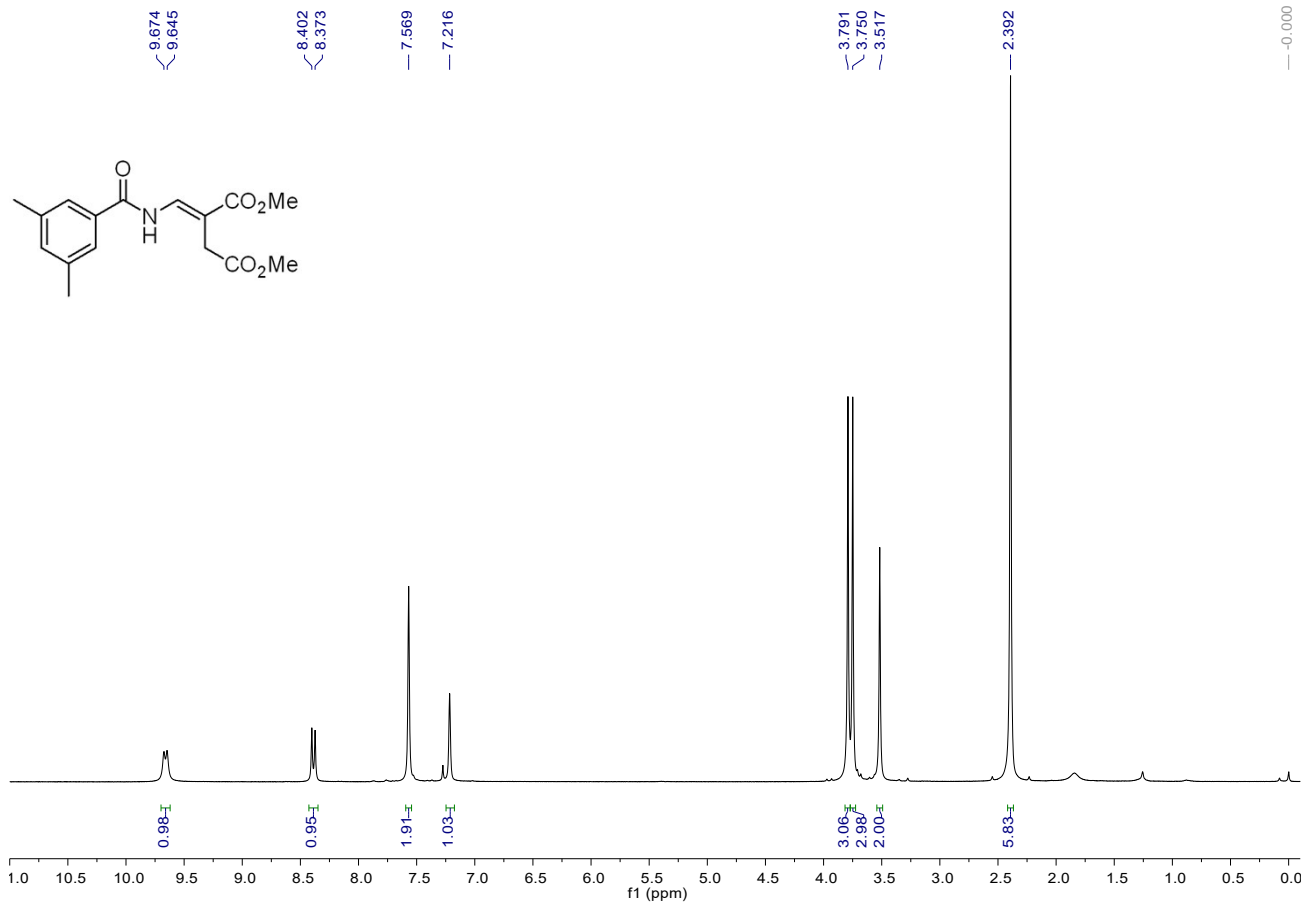


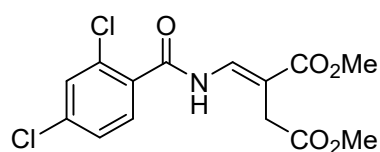
dimethyl (Z)-2-([1,1'-biphenyl]-4-carboxamidomethylene) succinate (4ha'). A white solid, 17 mg, 24% yield; M.p.: 165-167 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 11.57 (d, $J = 11.0$ Hz, 1H), 8.06-7.98 (m, 2H), 7.78-7.69 (m, 3H), 7.67-7.59 (m, 2H), 7.52-7.44 (m, 2H), 7.44-7.36 (m, 1H), 3.82 (s, 3H), 3.72 (s, 3H), 3.30 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 171.8, 169.3, 164.2, 145.6, 139.7, 138.6, 130.8, 128.9, 128.2, 128.2, 127.5, 127.2, 102.8, 52.1, 51.9, 35.7; IR (neat) ν 3284, 2954, 1744, 1680, 1609, 1581, 1439, 1362, 1192, 1150, 1015, 859, 784 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{20}\text{H}_{19}\text{NO}_5\text{Na}^+$ Requires: 376.1155, Found: 376.1154.



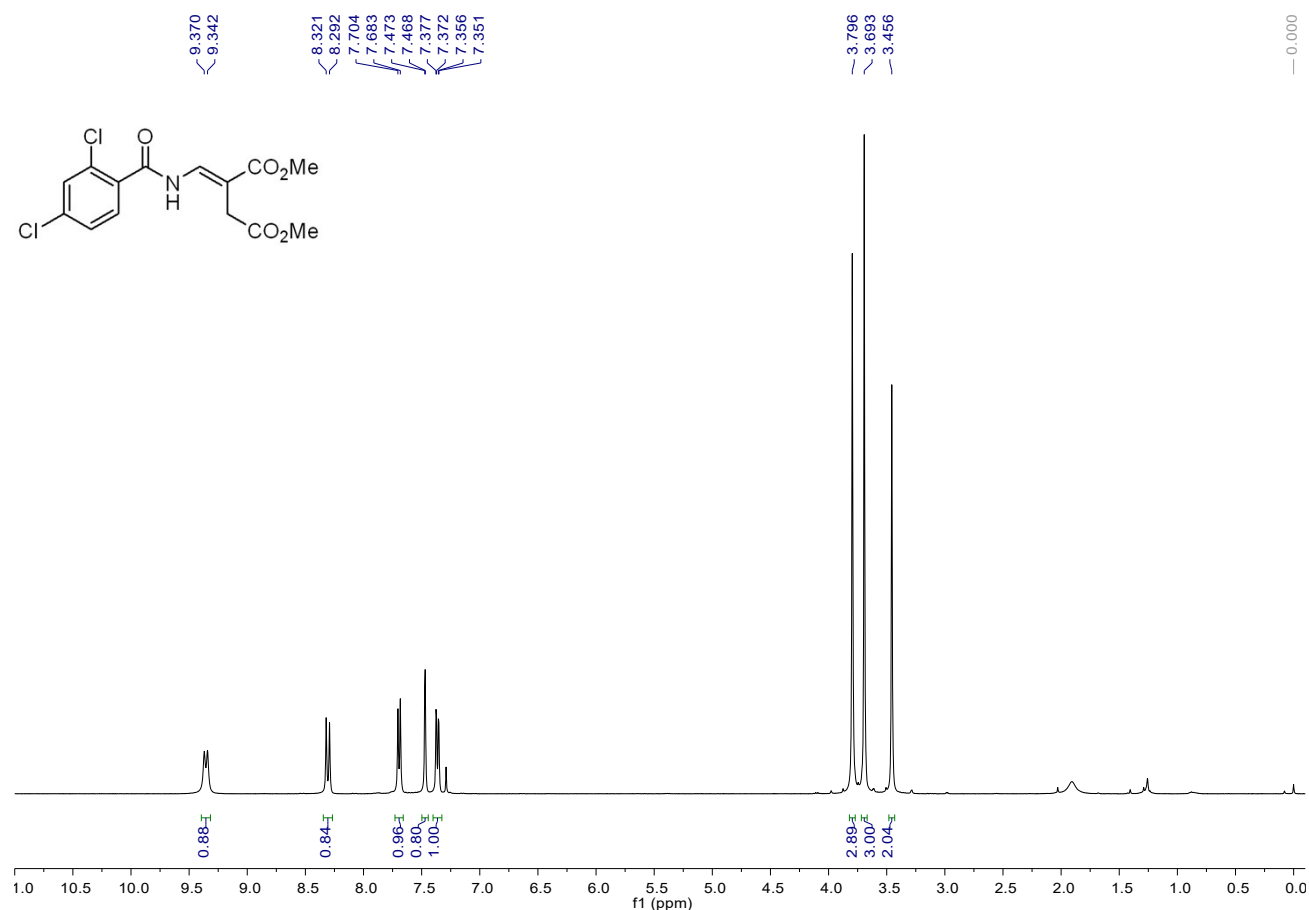


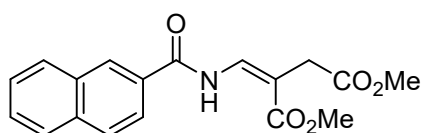
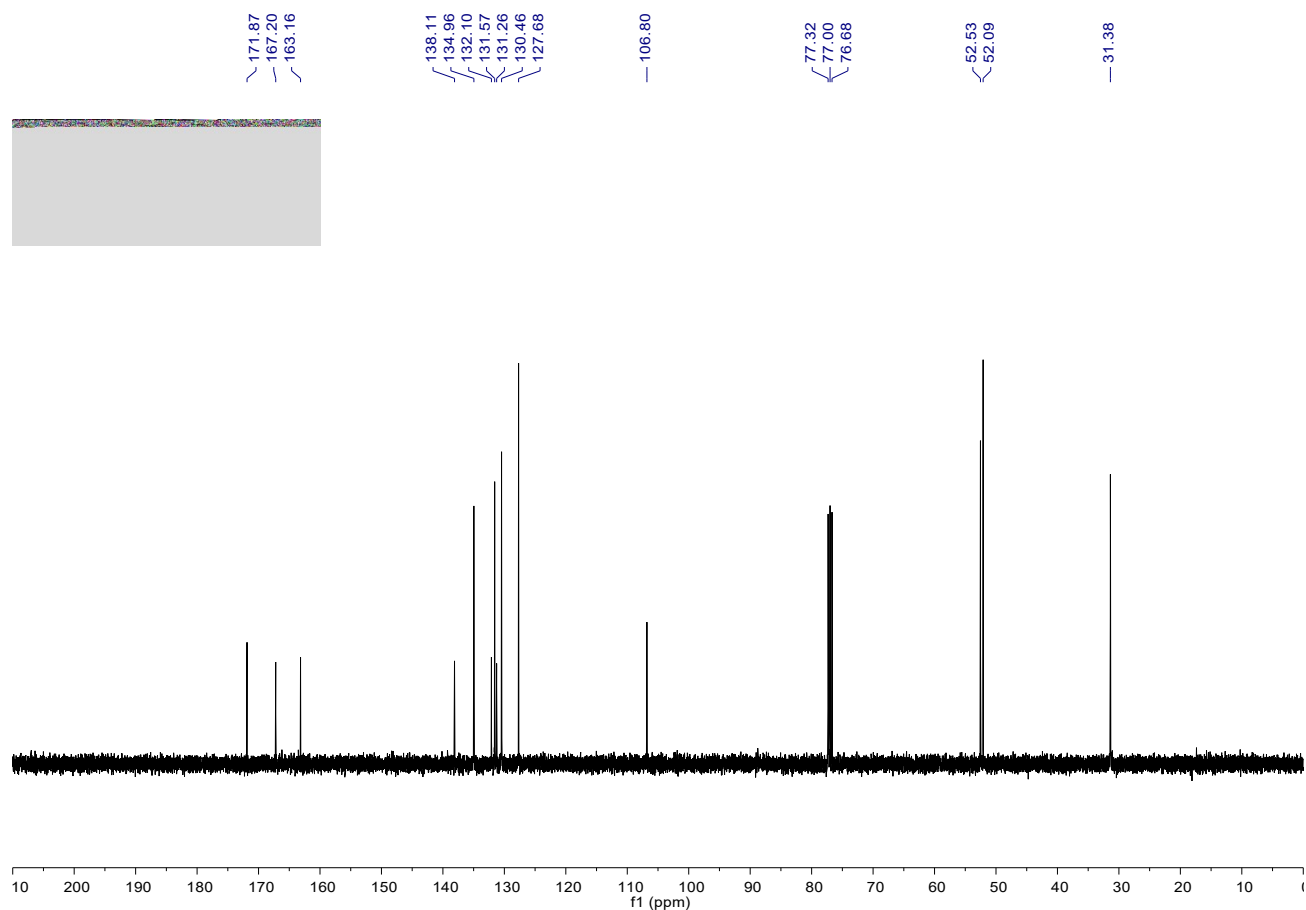
dimethyl (E)-2-((3,5-dimethylbenzamido)methylene) succinate (4ia). A white solid, 40 mg, 65% yield; M.p.: 186-188 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 9.66 (d, *J* = 11.4 Hz, 1H), 8.39 (d, *J* = 11.3 Hz, 1H), 7.57 (s, 2H), 7.22 (s, 1H), 3.79 (s, 3H), 3.75 (s, 3H), 3.52 (s, 2H), 2.39 (s, 6H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 172.7, 167.5, 165.0, 138.6, 136.5, 134.5, 132.2, 125.4, 104.7, 52.6, 52.0, 31.7, 21.2; IR (neat) ν 3359, 2953, 1739, 1694, 1671, 1651, 1491, 1300, 1217, 1191, 1166, 1114, 1006, 868, 772 cm⁻¹; HRMS (ESI) Calcd. for C₁₆H₁₉NO₅Na⁺ Requires: 328.1155, Found: 328.1149.



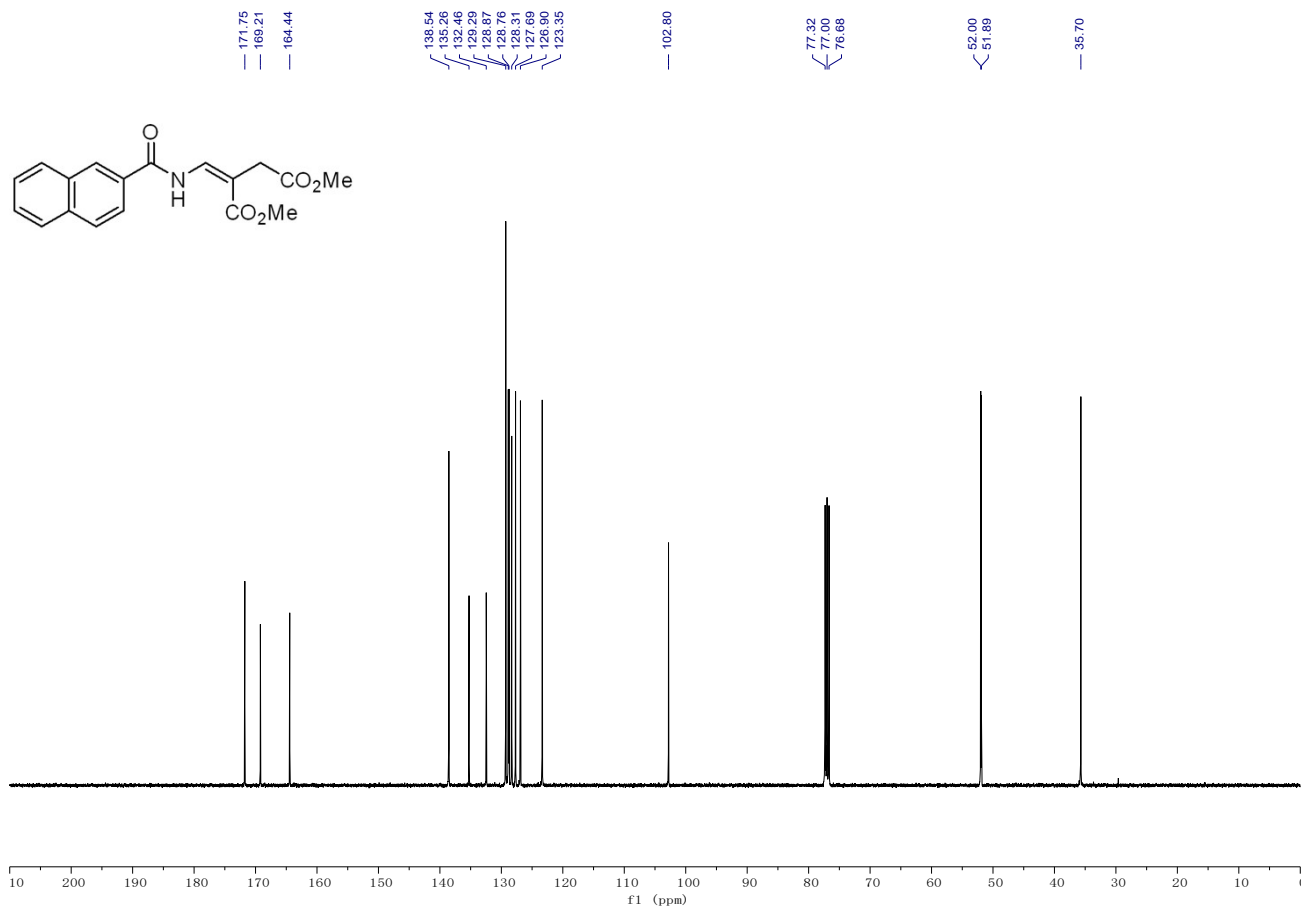
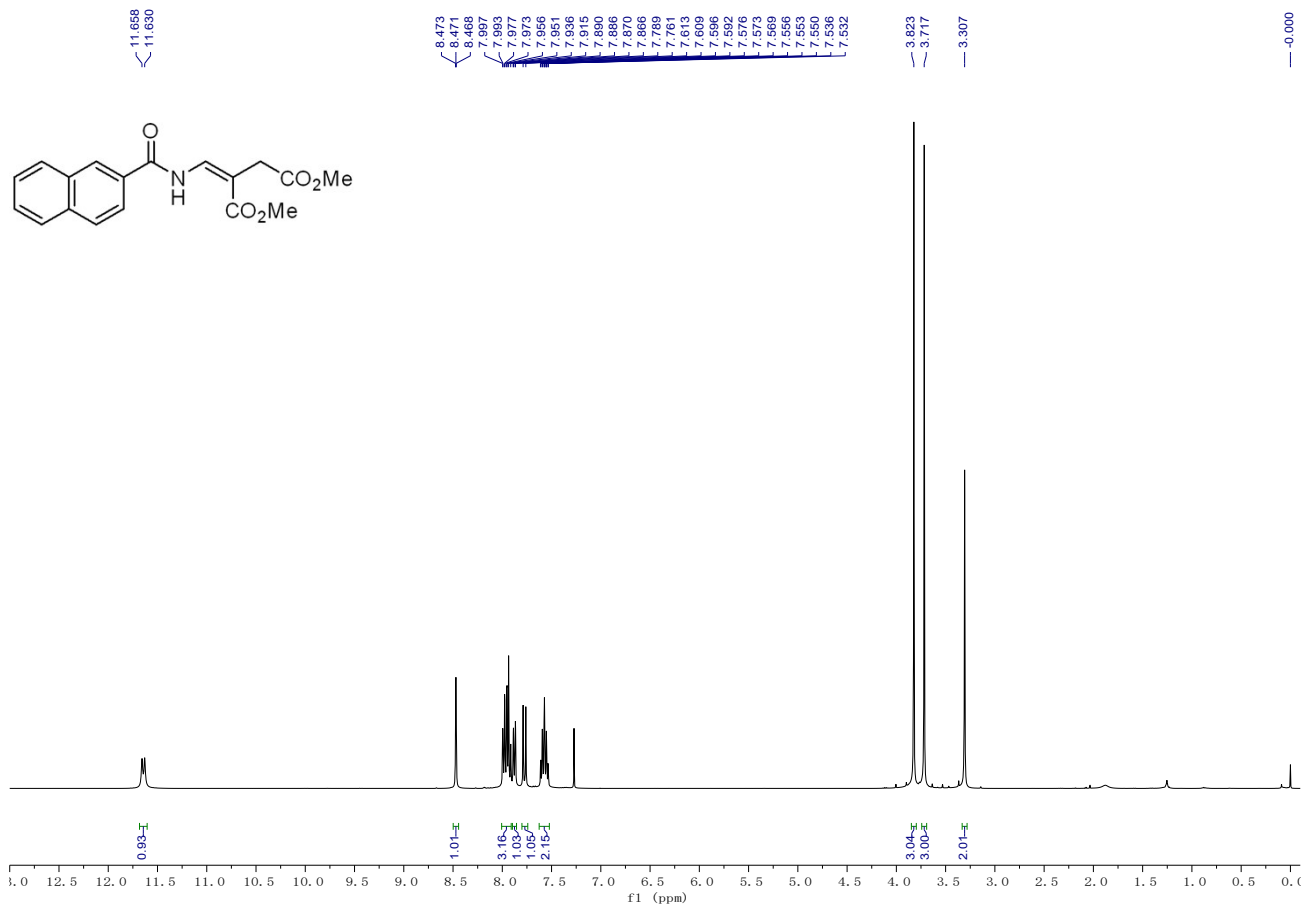


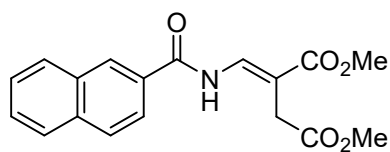
dimethyl (E)-2-((2,4-dichlorobenzamido)methylene)succinate (4ja). A white solid, 48 mg, 69% yield; M.p.: 105-107 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 9.36 (d, $J = 11.4$ Hz, 1H), 8.31 (d, $J = 11.4$ Hz, 1H), 7.69 (d, $J = 8.4$ Hz, 1H), 7.47 (d, $J = 2.0$ Hz, 1H), 7.36 (dd, $J = 8.4, 2.0$ Hz, 1H), 3.80 (s, 3H), 3.69 (s, 3H), 3.46 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 171.9, 167.2, 163.2, 138.1, 135.0, 132.1, 131.6, 131.3, 130.5, 127.7, 106.8, 52.5, 52.1, 31.4; IR (neat) ν 3341, 3083, 2955, 1727, 1677, 1631, 1506, 1362, 1271, 1168, 1124, 1078, 888, 693 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{14}\text{H}_{13}\text{NO}_5\text{NaCl}_2^+$ Requires: 368.0063, Found: 368.0061.



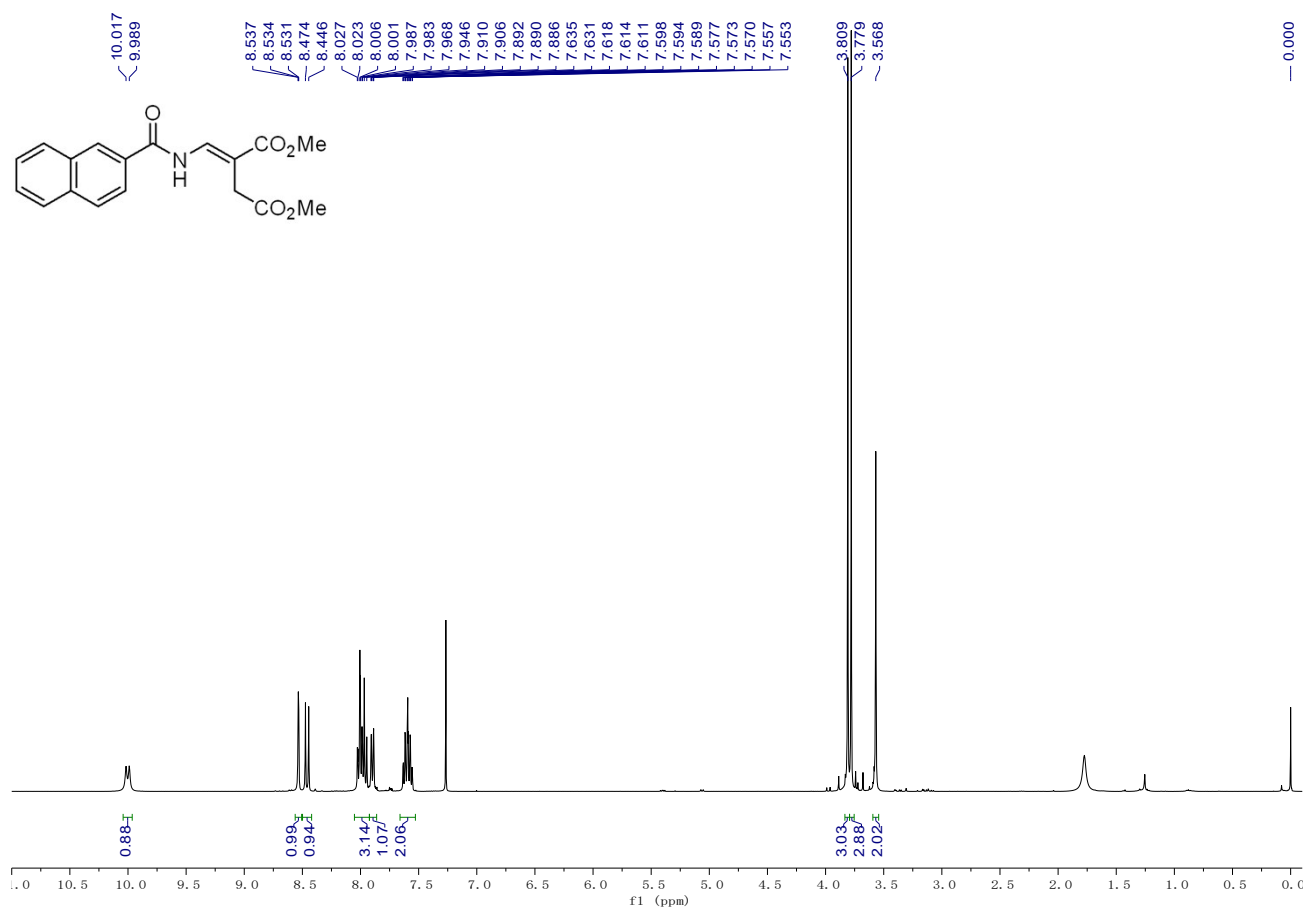


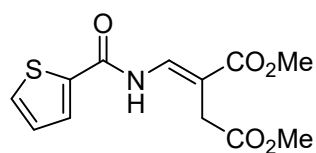
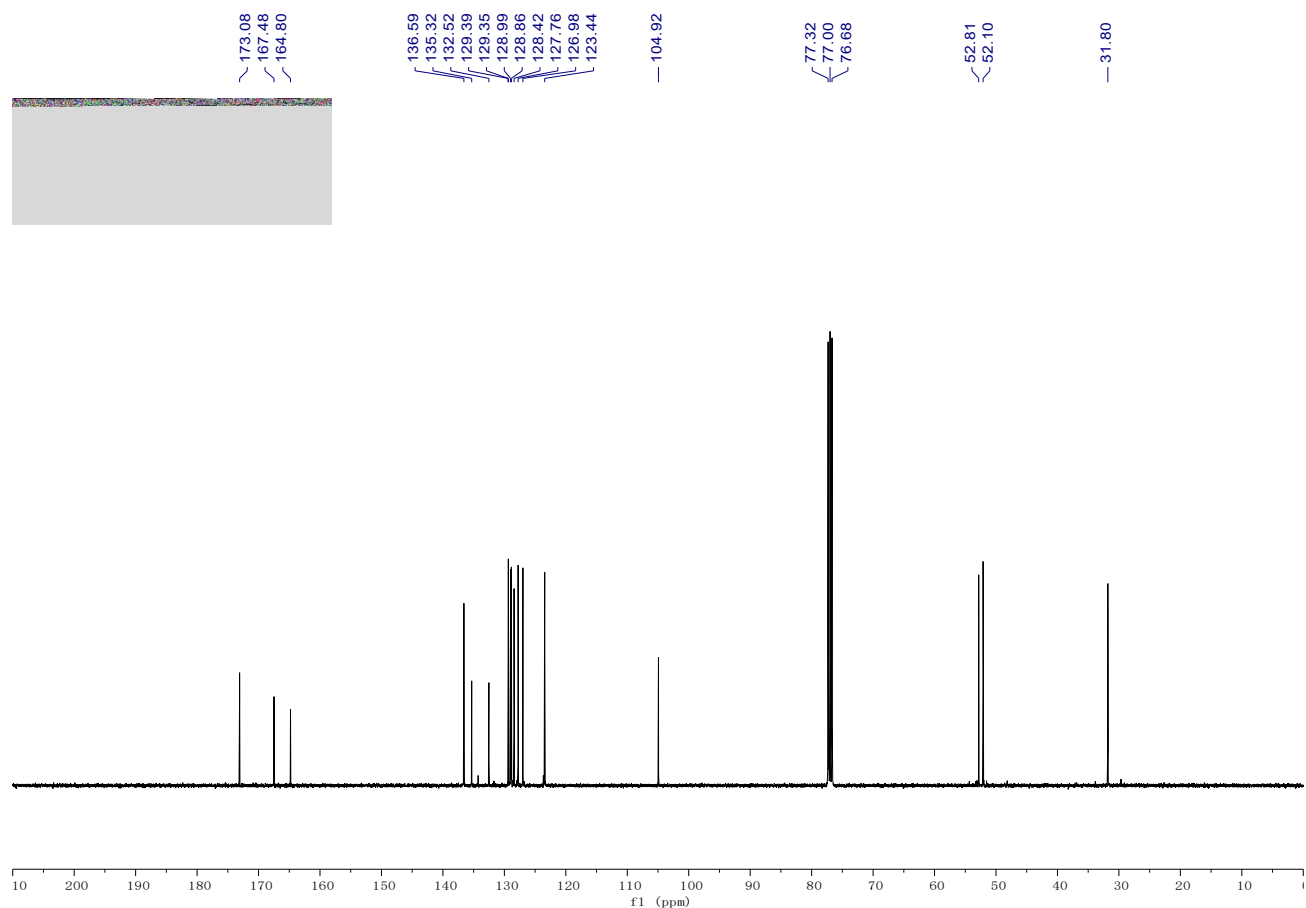
dimethyl (Z)-2-((2-naphthamido)methylene) succinate (4ka). A white solid, 28 mg, 42% yield; M.p.: 156-158 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 11.64 (d, $J = 11.0$ Hz, 1H), 8.50-8.44 (m, 1H), 8.01-7.91 (m, 3H), 7.90-7.86 (m, 1H), 7.77 (d, $J = 11.0$ Hz, 1H), 7.63-7.52 (m, 2H), 3.82 (s, 3H), 3.72 (s, 3H), 3.31 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 171.7, 169.2, 164.4, 138.5, 135.3, 132.5, 129.3, 128.9, 128.8, 128.3, 127.7, 126.9, 123.3, 102.8, 52.0, 51.9, 35.7; IR (neat) ν 3310, 2954, 1743, 1681, 1617, 1513, 1433, 1347, 1288, 1191, 1144, 1124, 994, 941, 808 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{18}\text{H}_{17}\text{NO}_5\text{Na}^+$ Requires: 350.0999, Found: 350.0992.



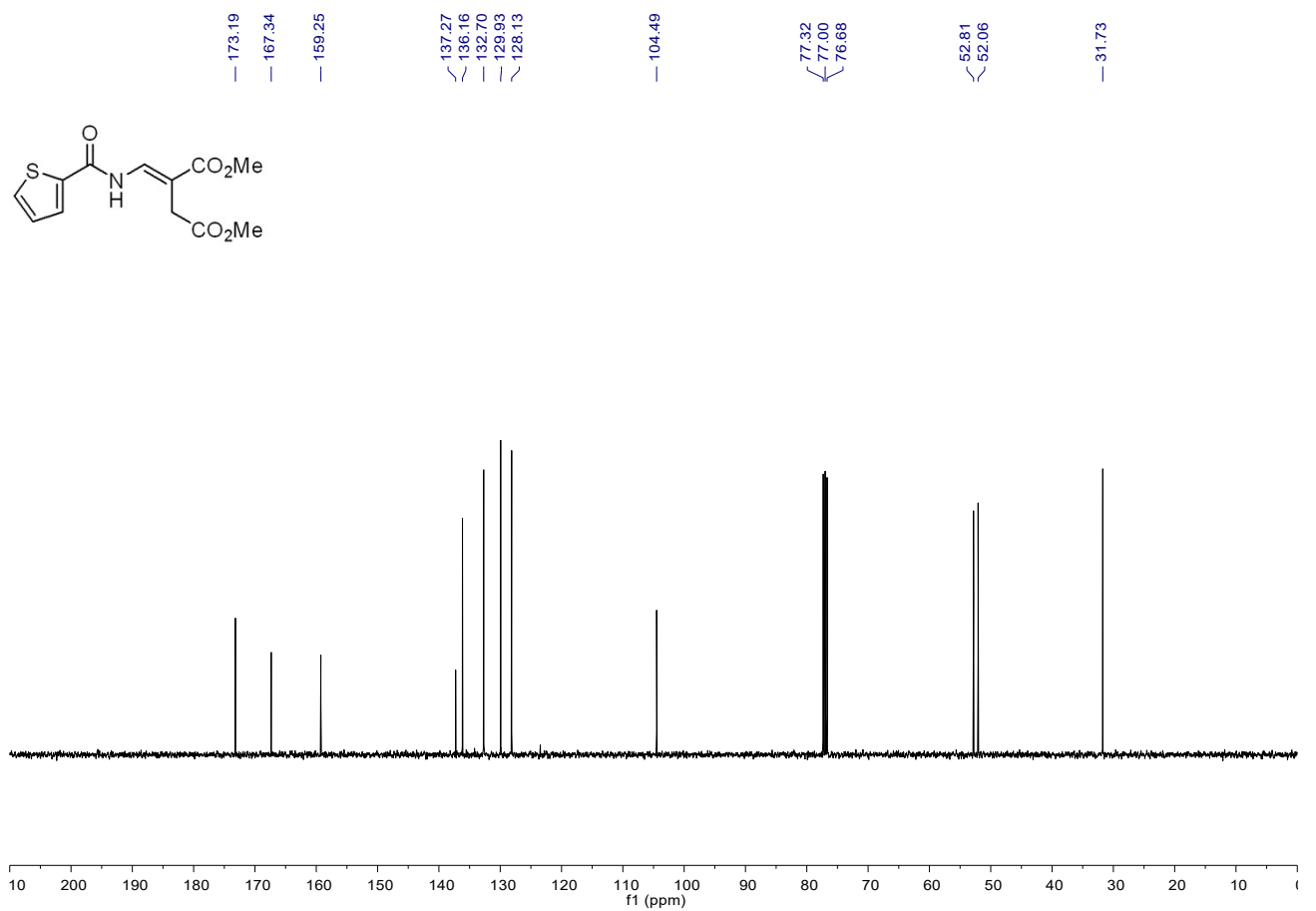
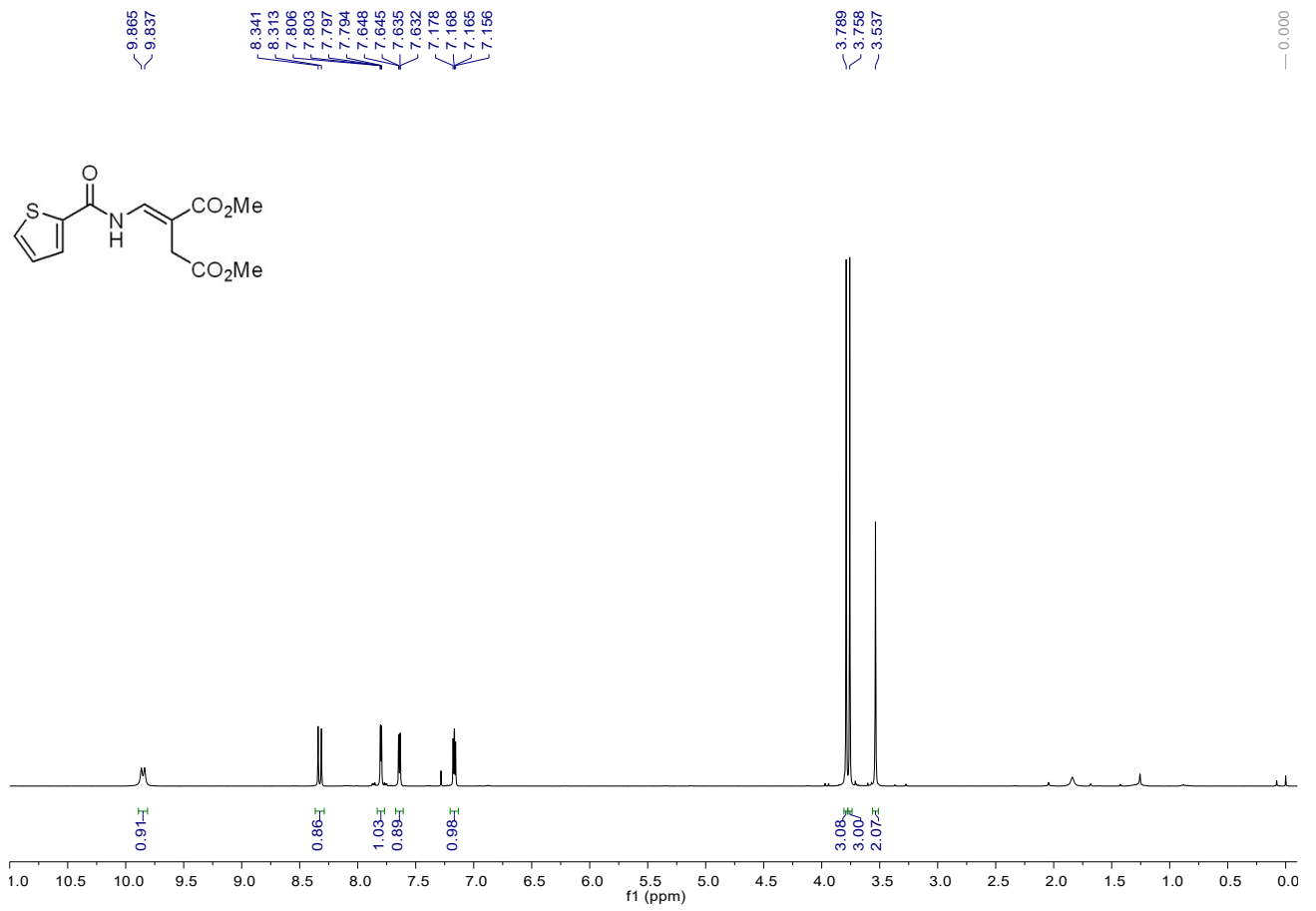


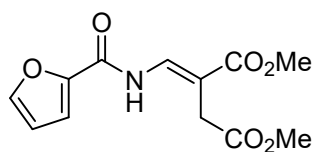
dimethyl (E)-2-((2-naphthamido)methylene) succinate (4ka'). A white solid, 21 mg, 32% yield; M.p.: 136-138 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 10.00 (d, $J = 11.3$ Hz, 1H), 8.56-8.51 (m, 1H), 8.46 (d, $J = 11.3$ Hz, 1H), 8.05-7.92 (m, 3H), 7.92-7.86 (m, 1H), 7.66-7.53 (m, 2H), 3.81 (s, 3H), 3.78 (s, 3H), 3.57 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 173.1, 167.5, 164.8, 136.6, 135.3, 132.5, 129.39, 129.35, 129.0, 128.9, 128.4, 127.8, 127.0, 123.4, 104.9, 52.8, 52.1, 31.8; IR (neat) ν 3332, 2958, 1715, 1690, 1641, 1513, 1434, 1285, 1213, 1189, 1127, 1099, 959 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{18}\text{H}_{17}\text{NO}_5\text{Na}^+$ Requires: 350.0999, Found: 350.0993.



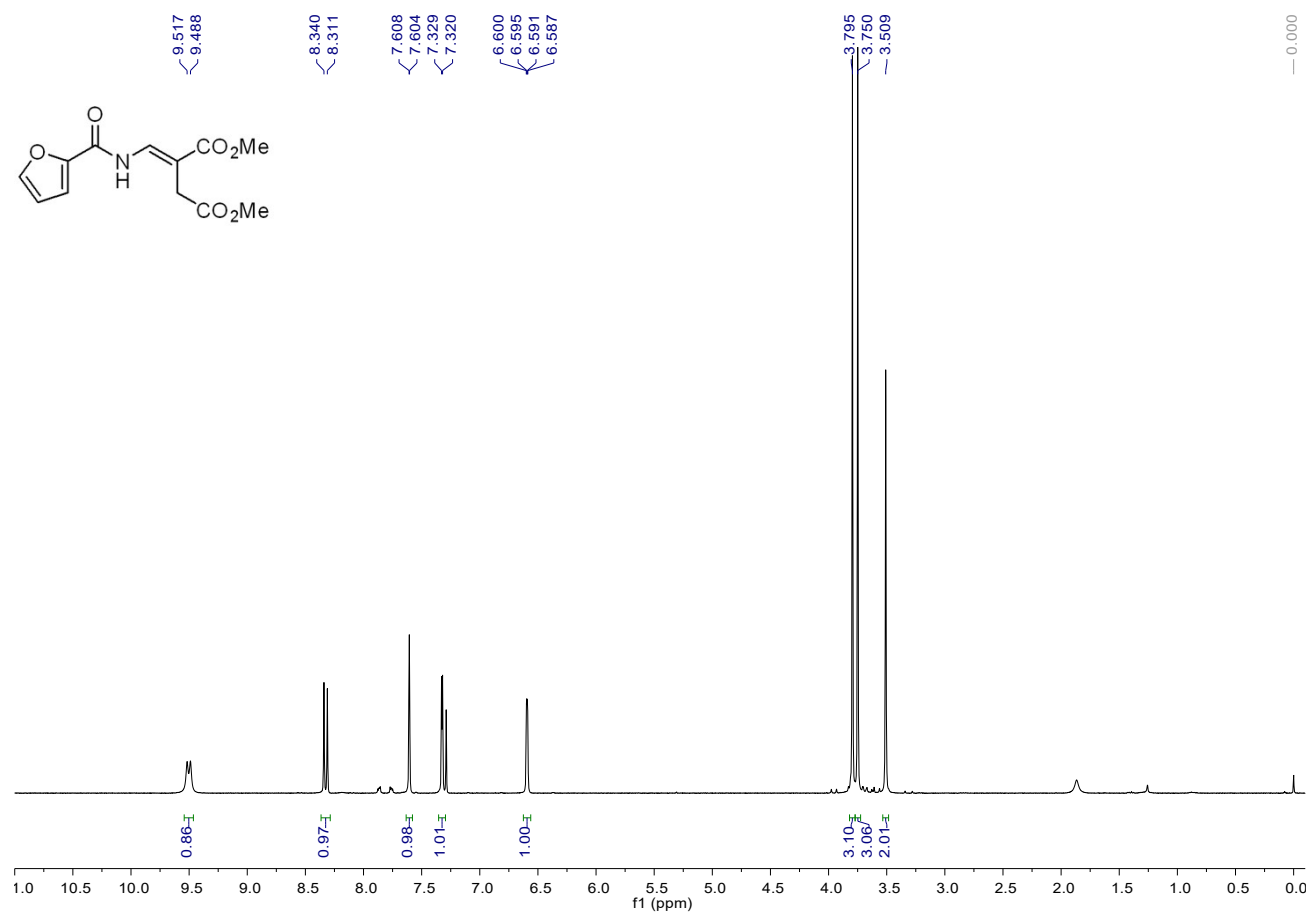


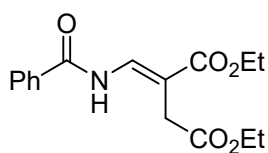
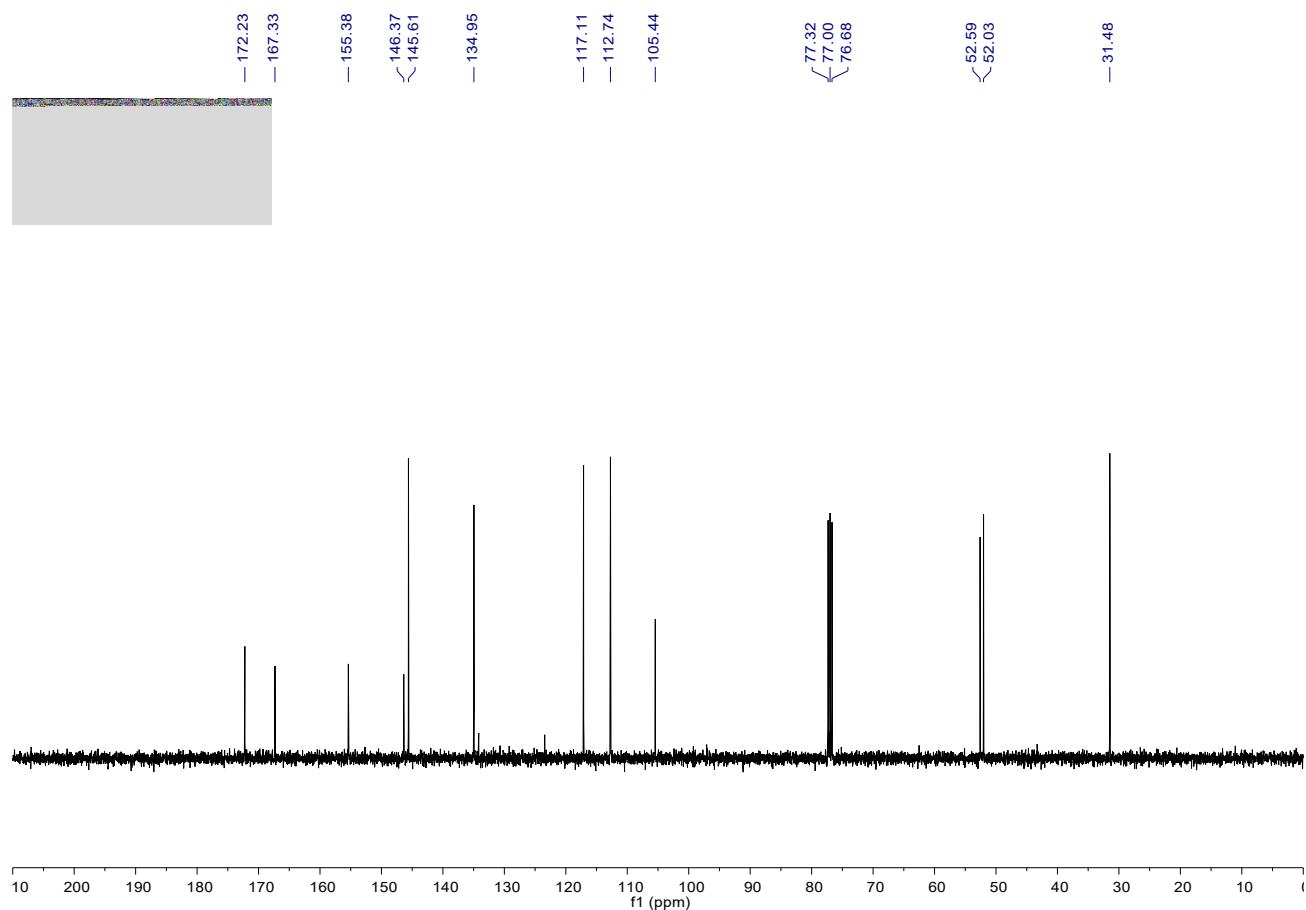
dimethyl (E)-2-((thiophene-2-carboxamido)methylene) succinate (41a). A white solid, 35 mg, 62% yield; M.p.: 114-116 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 9.85 (d, J = 11.3 Hz, 1H), 8.33 (d, J = 11.3 Hz, 1H), 7.80 (dd, J = 3.8, 1.2 Hz, 1H), 7.64 (dd, J = 5.0, 1.2 Hz, 1H), 7.17 (dd, J = 5.0, 3.8 Hz, 1H), 3.79 (s, 3H), 3.76 (s, 3H), 3.54 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 173.2, 167.3, 159.3, 137.3, 136.2, 132.7, 129.9, 128.1, 104.5, 52.8, 52.1, 31.7; IR (neat) ν 3350, 3094, 2960, 1709, 1678, 1489, 1441, 1355, 1261, 1202, 1178, 1109, 1025, 853 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{12}\text{H}_{13}\text{NO}_5\text{NaS}^+$ Requires: 306.0407, Found: 306.0398.



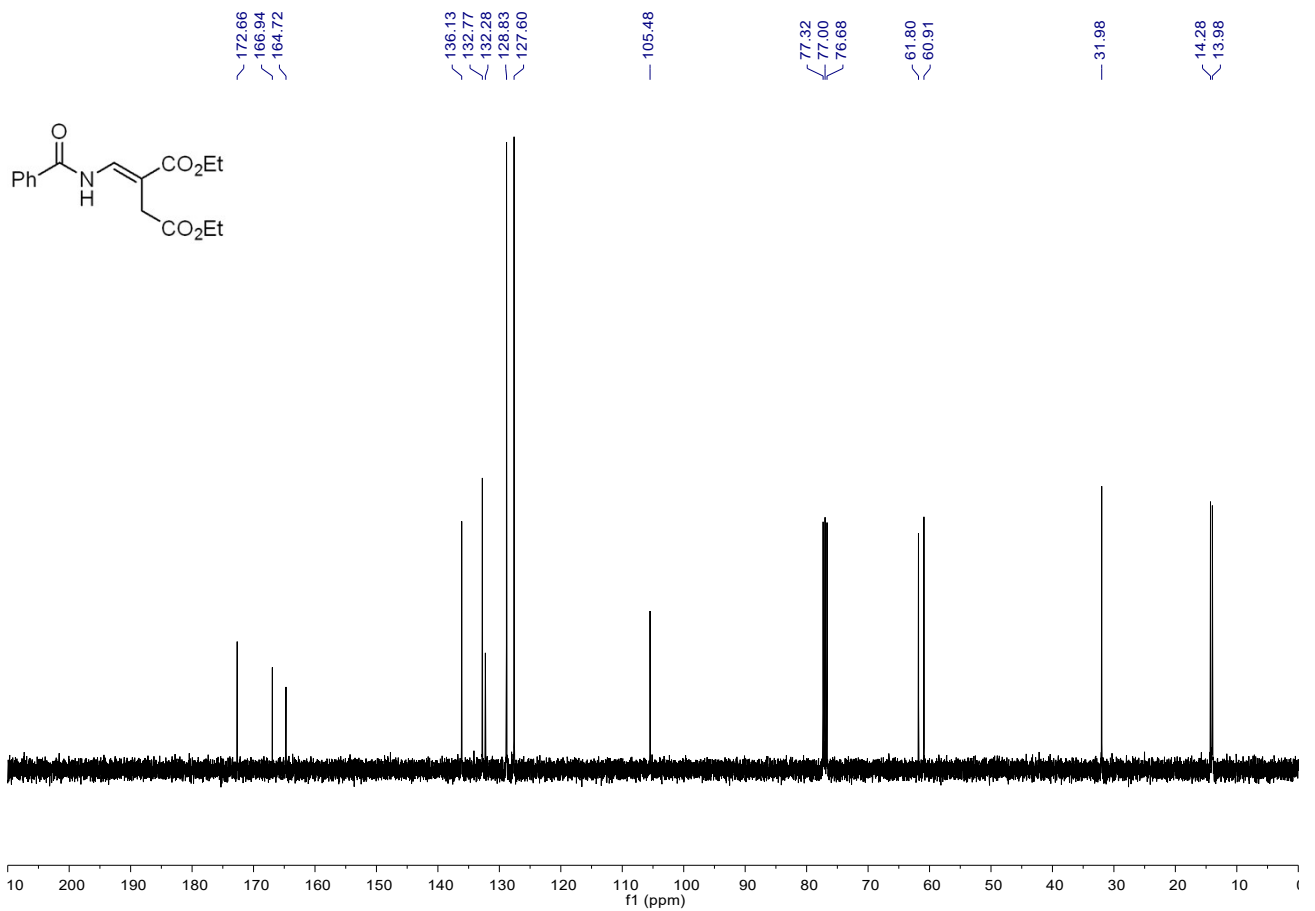
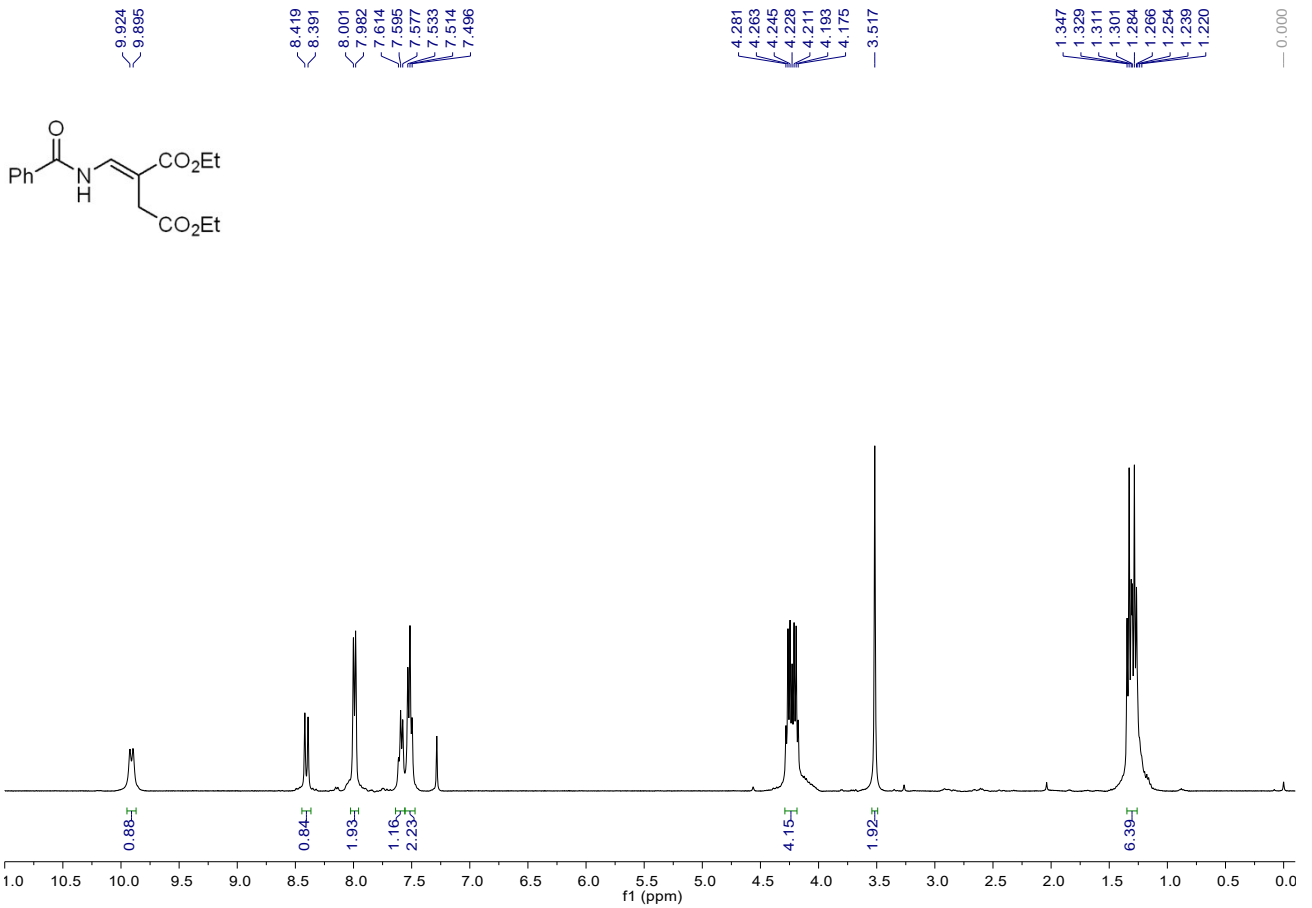


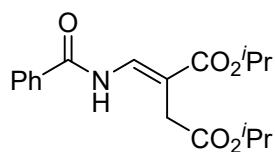
dimethyl (E)-2-((furan-2-carboxamido)methylene) succinate (4ma). A white solid, 33 mg, 61% yield; M.p.: 94-96 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 9.50 (d, $J = 11.6$ Hz, 1H), 8.33 (d, $J = 11.6$ Hz, 1H), 7.61 (d, $J = 1.6$ Hz, 1H), 7.32 (d, $J = 3.6$ Hz, 1H), 6.59 (dd, $J = 3.6, 1.7$ Hz, 1H), 3.79 (s, 3H), 3.75 (s, 3H), 3.51 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 172.2, 167.3, 155.4, 146.4, 145.6, 135.0, 117.1, 112.7, 105.4, 52.6, 52.0, 31.5; IR (neat) ν 3373, 3147, 3116, 2956, 1694, 1645, 1499, 1308, 1263, 1195, 1106, 1017, 948, 875, 775 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{12}\text{H}_{13}\text{NO}_6\text{Na}^+$ Requires: 290.0635, Found: 290.0630.



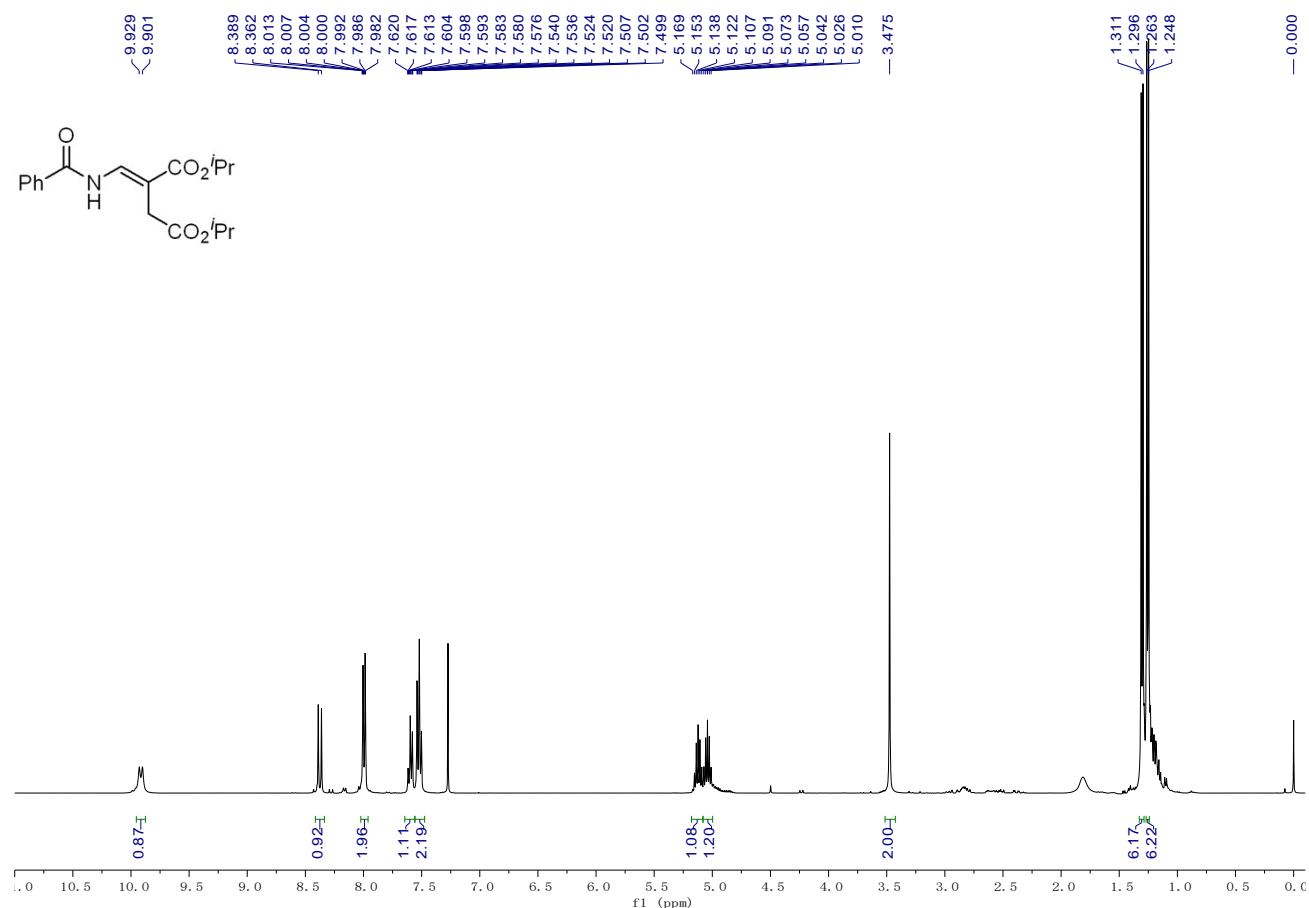


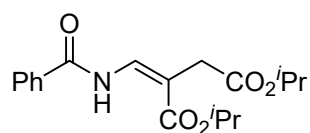
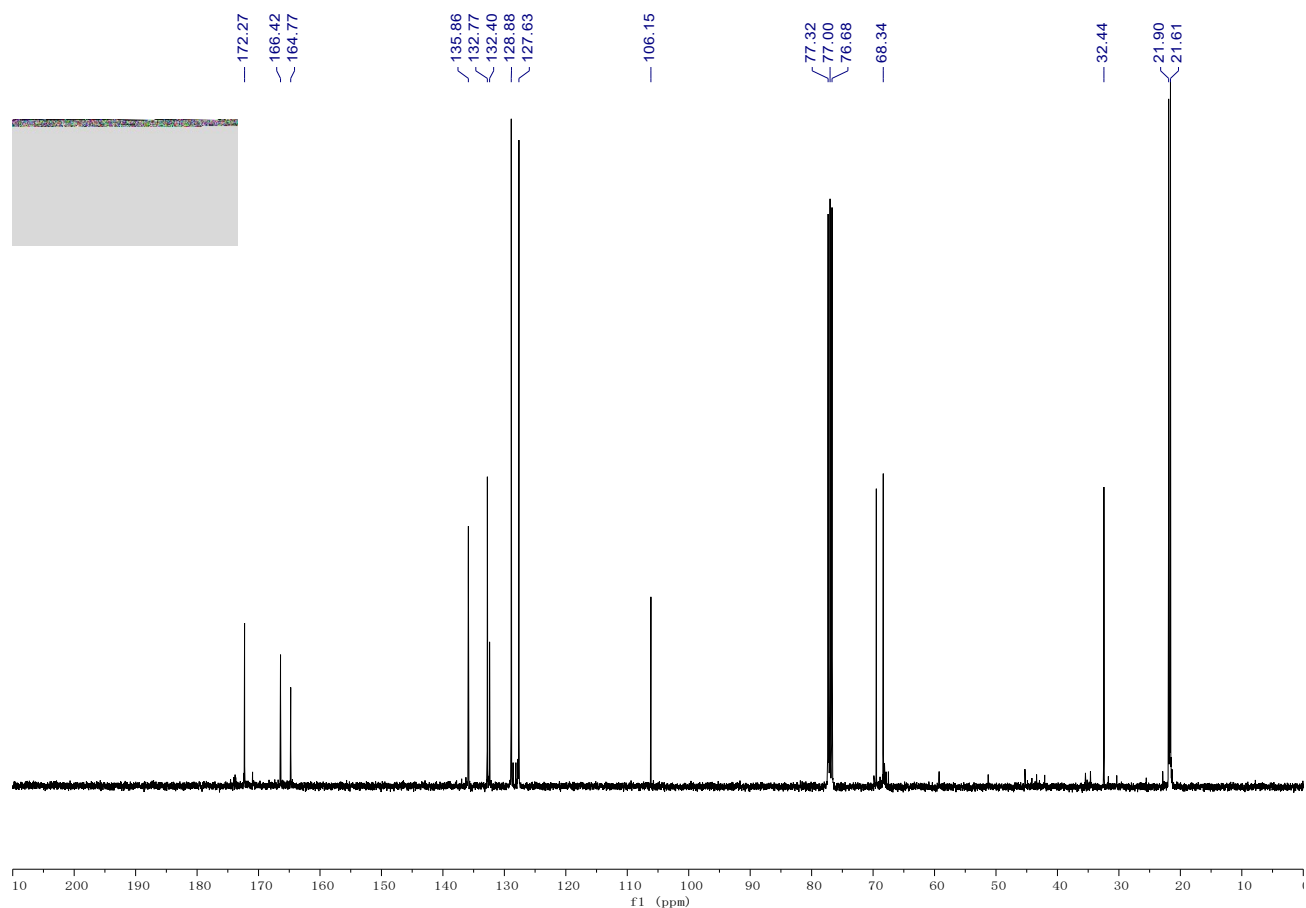
diethyl (E)-2-(benzamidomethylene) succinate (4ab). A white solid, 32 mg, 52% yield; M.p.: 79-81 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 9.91 (d, $J = 11.4$ Hz, 1H), 8.41 (d, $J = 11.1$ Hz, 1H), 7.99 (d, $J = 7.6$ Hz, 2H), 7.60 (t, $J = 7.4$ Hz, 1H), 7.51 (t, $J = 7.5$ Hz, 2H), 4.29-4.19 (m, 4H), 3.52 (s, 2H), 1.35-1.26 (m, 6H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 172.7, 166.9, 164.7, 136.1, 132.8, 132.3, 128.8, 127.6, 105.5, 61.8, 60.9, 32.0, 14.3, 14.0; IR (neat) ν 3354, 2982, 2932, 1734, 1670, 1602, 1478, 1399, 1288, 1258, 1178, 1112, 951 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{16}\text{H}_{19}\text{NO}_5\text{Na}^+$ Requires: 328.1155, Found: 328.1146.



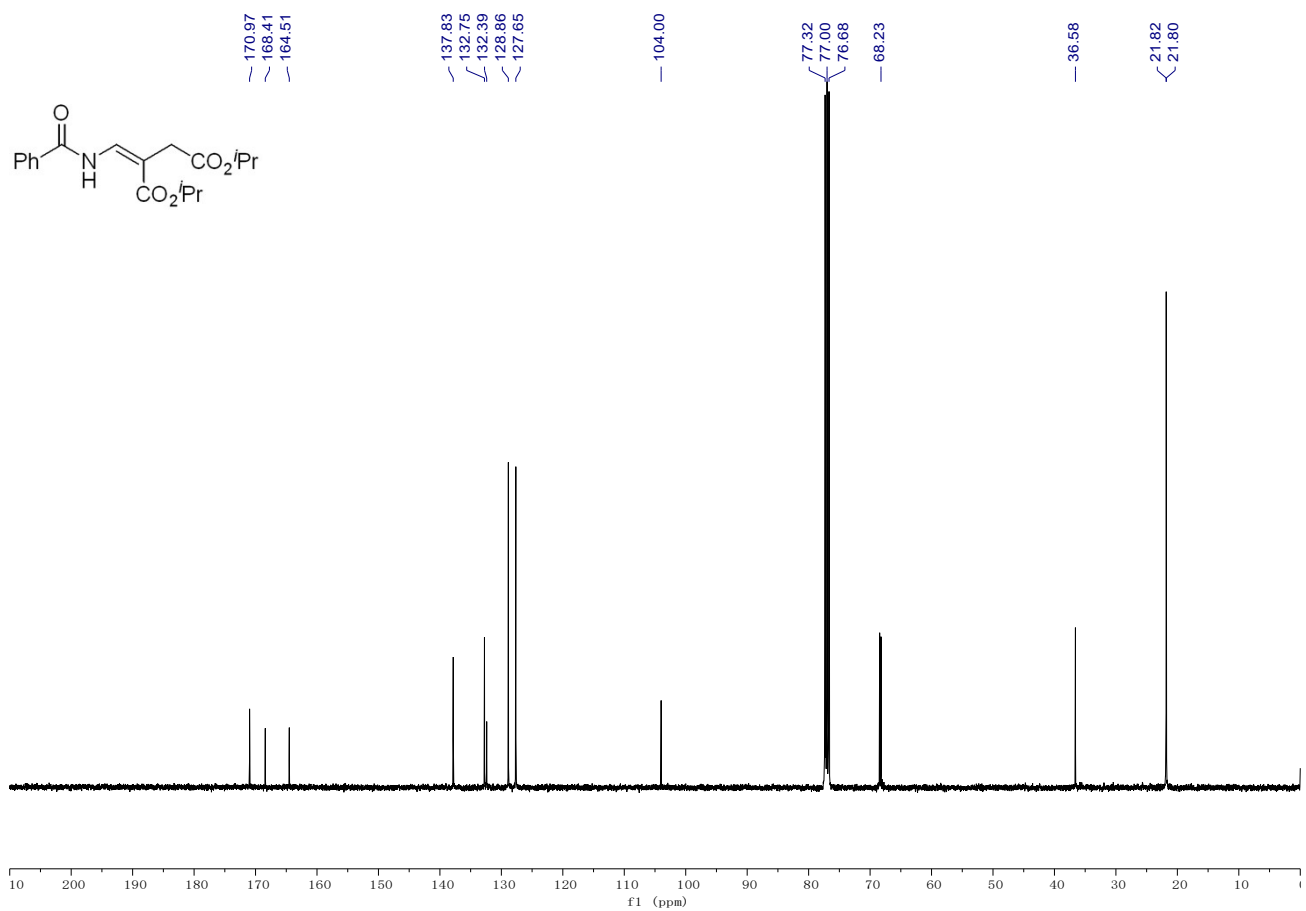
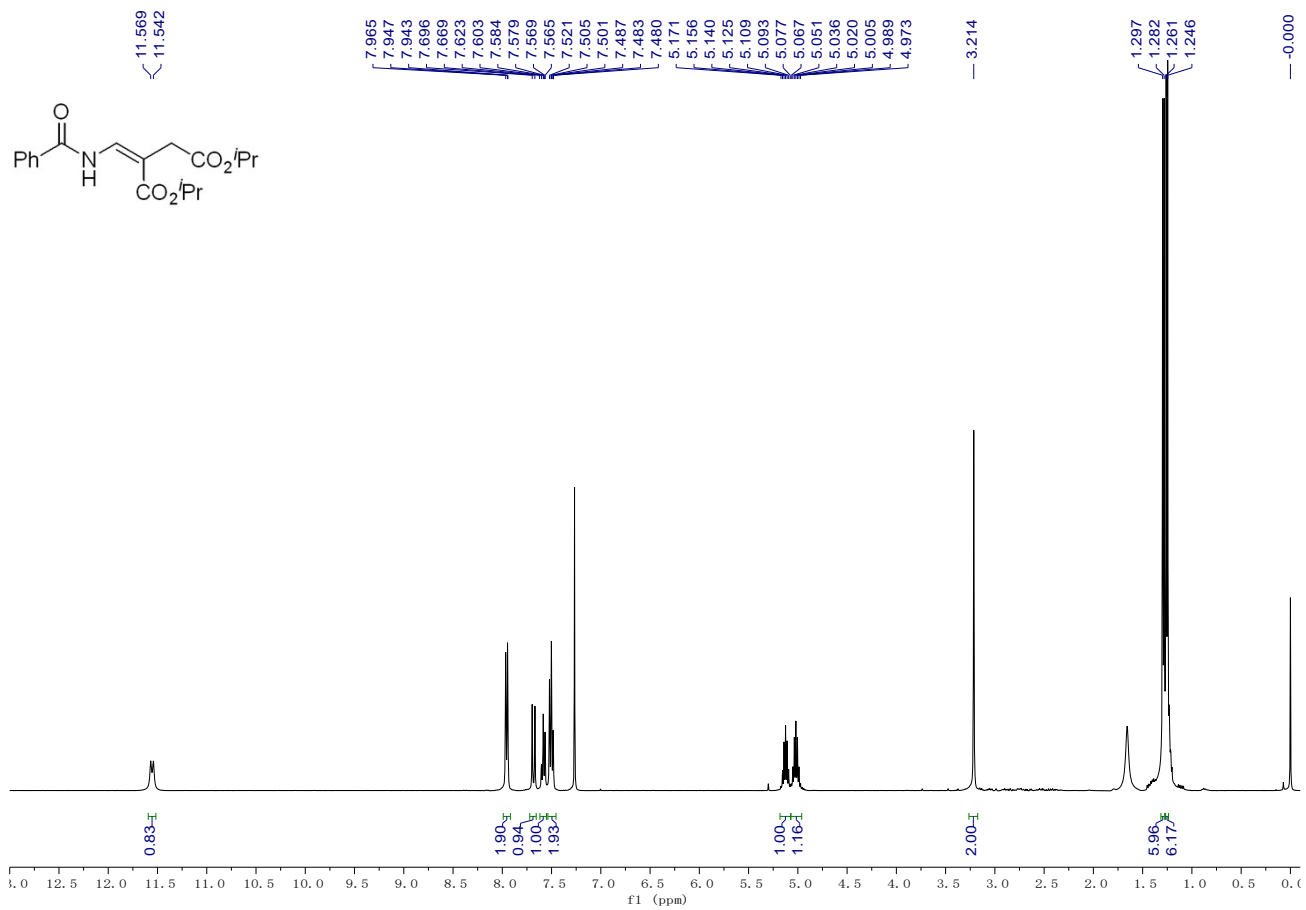


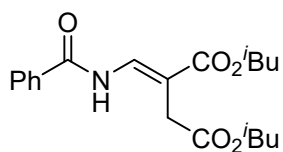
diisopropyl (E)-2-(benzamidomethylene) succinate (4ac). A white solid, 20 mg, 29% yield; M.p.: 97-99 °C; ¹H NMR (CDCl₃, 400 MHz, TMS) δ 9.92 (d, *J* = 11.2 Hz, 1H), 8.38 (d, *J* = 11.1 Hz, 1H), 8.02-7.96 (m, 2H), 7.65-7.56 (m, 1H), 7.52 (dd, *J* = 8.3, 6.8 Hz, 2H), 5.18-5.08 (m, 1H), 5.08-5.00 (m, 1H), 3.48 (s, 2H), 1.30 (d, *J* = 6.2 Hz, 6H), 1.26 (d, *J* = 6.3 Hz, 6H); ¹³C NMR (CDCl₃, 100 MHz, TMS) δ 172.3, 166.4, 164.8, 135.9, 132.8, 132.4, 128.9, 127.6, 106.2, 69.5, 68.3, 32.4, 21.9, 21.6; IR (neat) ν 3360, 2977, 1686, 1650, 1509, 1421, 1254, 1195, 1096, 1025, 815, 699 cm⁻¹; HRMS (ESI) Calcd. for C₁₈H₂₃NO₅Na⁺ Requires: 356.1468, Found: 356.1470.



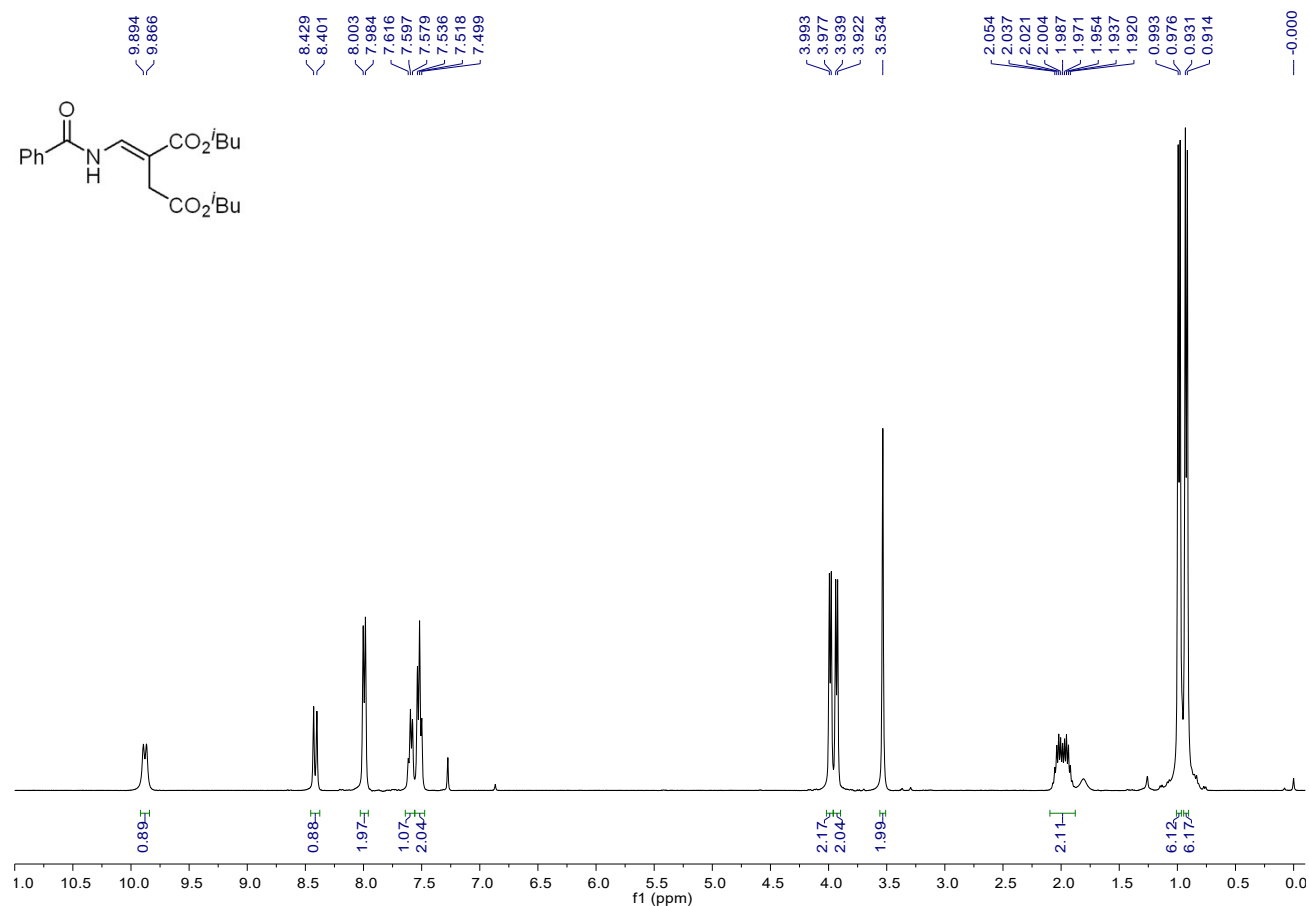


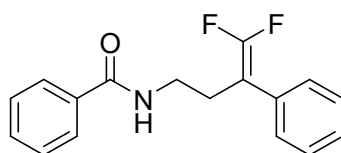
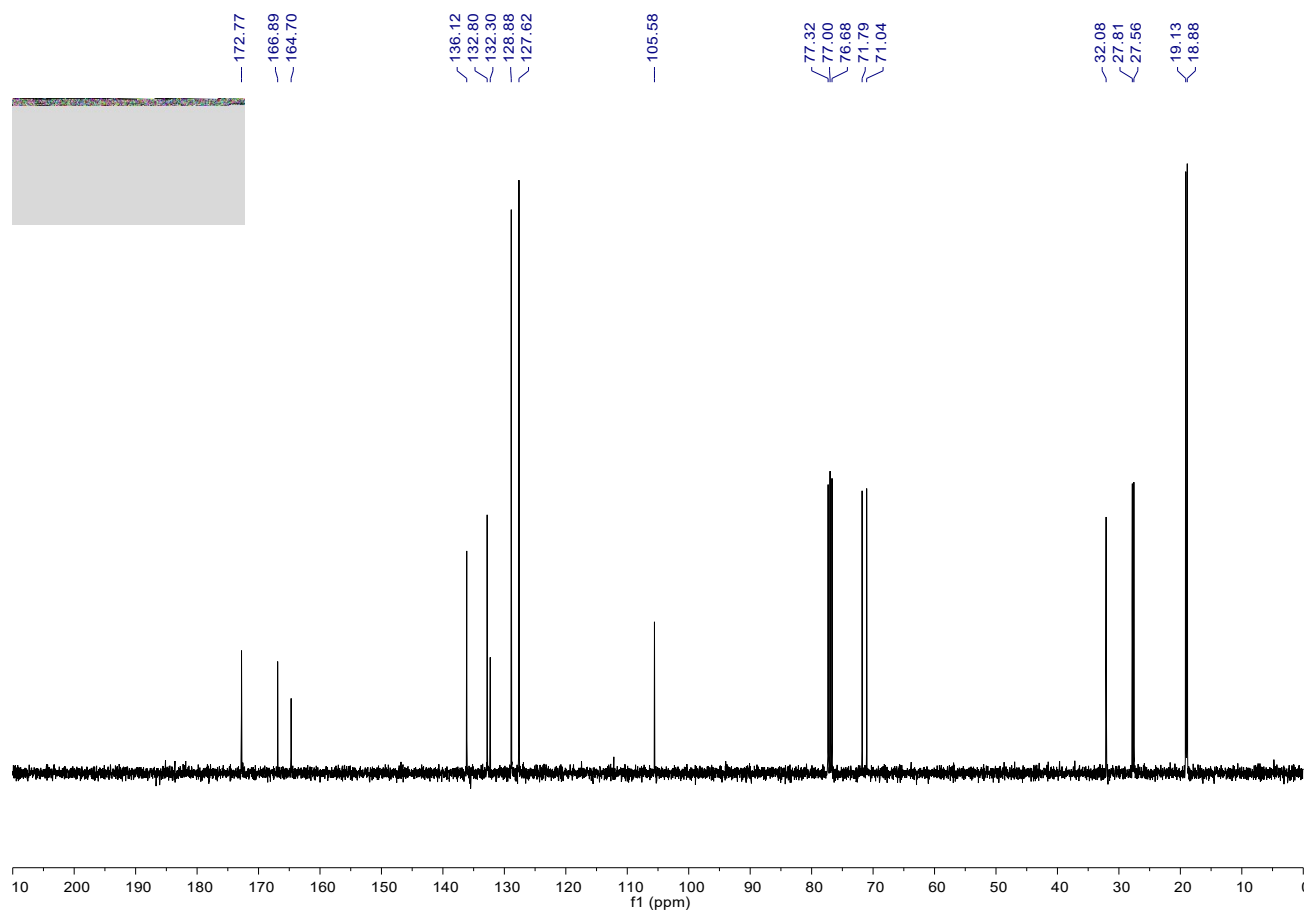
diisopropyl (Z)-2-(benzamidomethylene) succinate (4ac'). A white solid, 9 mg, 13% yield; M.p.: 77-79 °C; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 11.56 (d, $J = 10.9$ Hz, 1H), 7.99-7.92 (m, 2H), 7.68 (d, $J = 10.9$ Hz, 1H), 7.62-7.55 (m, 1H), 7.54-7.45 (m, 2H), 5.12 (hept, $J = 6.3$ Hz, 1H), 5.02 (hept, $J = 6.3$ Hz, 1H), 3.21 (s, 2H), 1.29 (d, $J = 6.3$ Hz, 6H), 1.25 (d, $J = 6.3$ Hz, 6H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 171.0, 168.4, 164.5, 137.8, 132.7, 132.4, 128.9, 127.6, 104.0, 68.4, 68.2, 36.6, 21.82, 21.80; IR (neat) ν 3318, 2974, 2937, 1728, 1693, 1623, 1473, 1371, 1337, 1191, 1106 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{18}\text{H}_{23}\text{NO}_5\text{Na}^+$ Requires: 356.1468, Found: 356.1470.



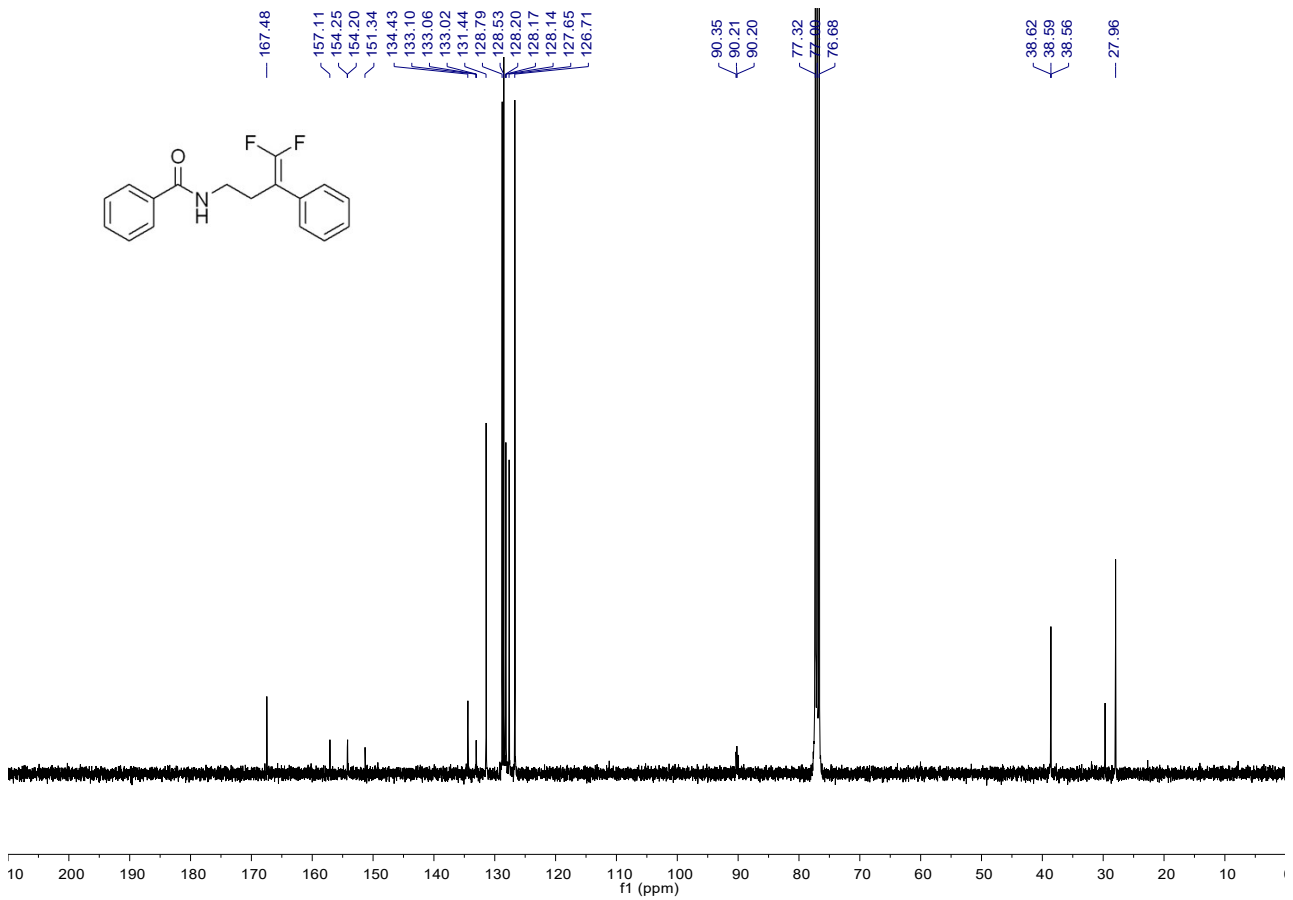
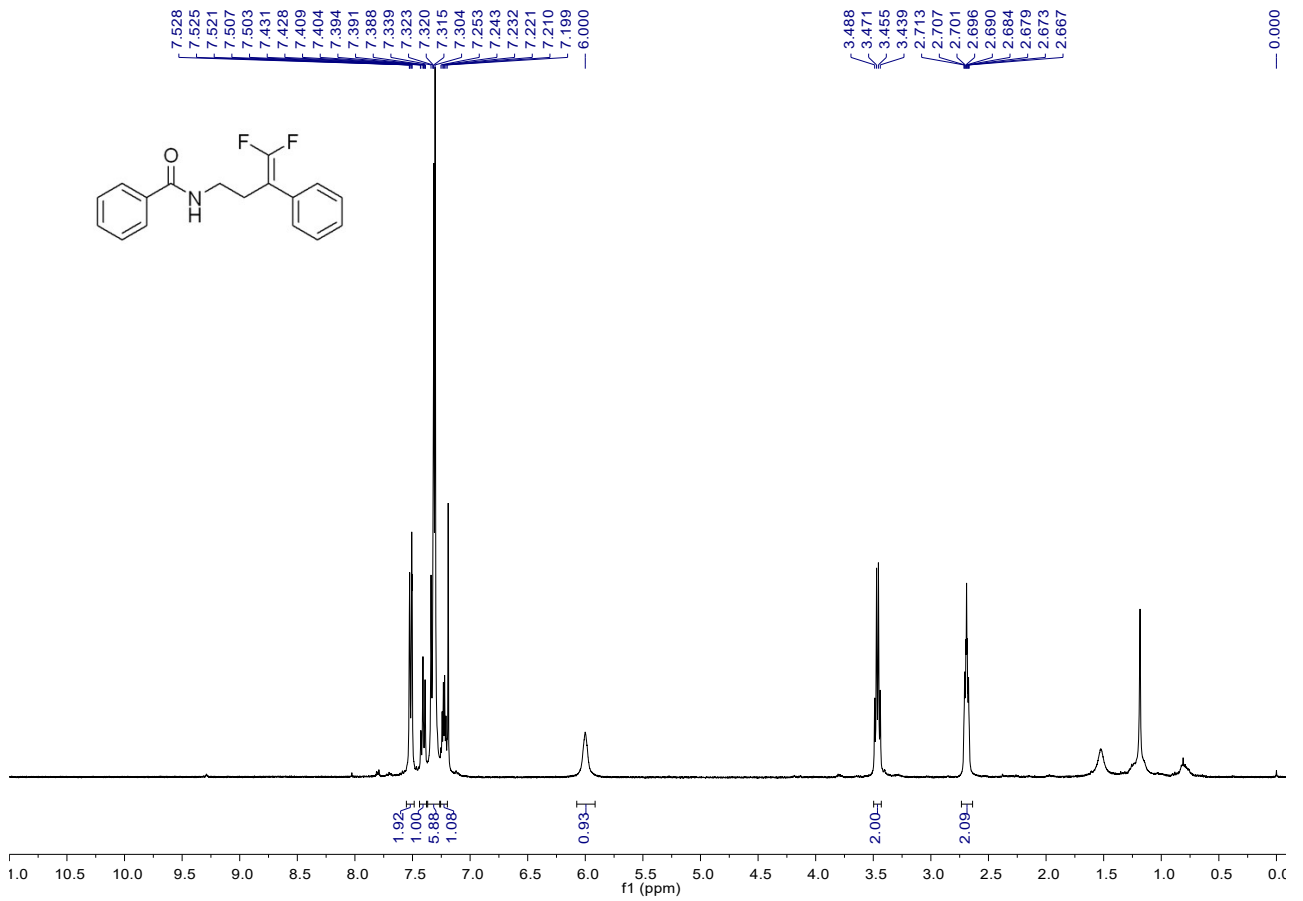


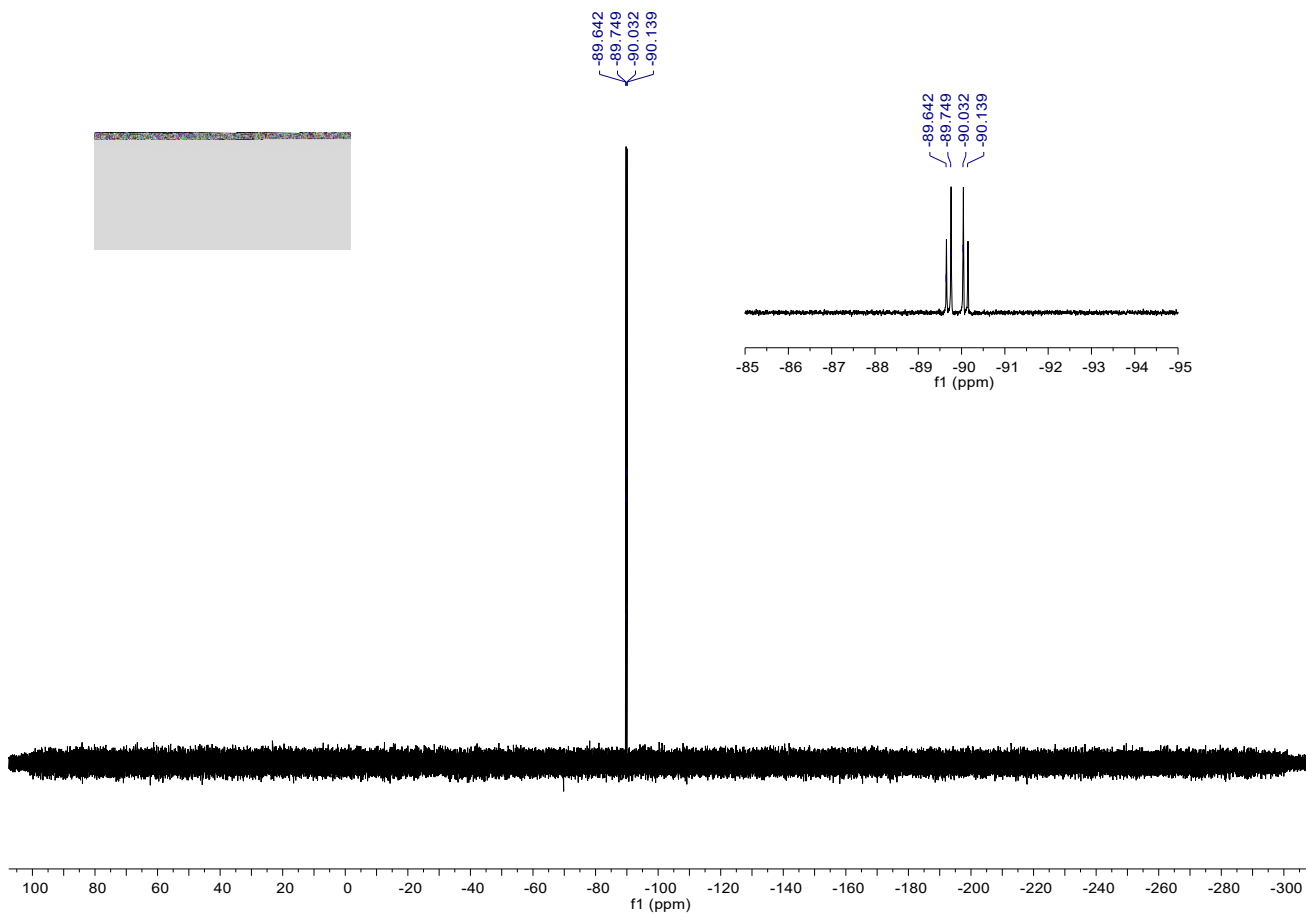
diisobutyl (E)-2-(benzamidomethylene) succinate (4ad). A pale yellow oil, 44 mg, 61% yield; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 9.88 (d, $J = 11.2$ Hz, 1H), 8.42 (d, $J = 11.2$ Hz, 1H), 7.99 (d, $J = 7.6$ Hz, 2H), 7.60 (t, $J = 7.4$ Hz, 1H), 7.52 (t, $J = 7.5$ Hz, 2H), 3.99 (d, $J = 6.6$ Hz, 2H), 3.93 (d, $J = 6.7$ Hz, 2H), 3.53 (s, 2H), 2.10-1.88 (m, 2H), 0.98 (d, $J = 6.7$ Hz, 6H), 0.92 (d, $J = 6.7$ Hz, 6H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 172.8, 166.9, 164.7, 136.1, 132.8, 132.3, 128.9, 127.6, 105.6, 71.8, 71.0, 32.1, 27.8, 27.6, 19.1, 18.9; IR (neat) ν 3324, 2961, 2875, 1697, 1641, 1582, 1508, 1395, 1257, 1172, 1109, 1002, 821 cm^{-1} ; HRMS (ESI) Calcd. for $\text{C}_{20}\text{H}_{27}\text{NO}_5\text{Na}^+$ Requires: 384.1781, Found: 384.1780.





N-(4,4-difluoro-3-phenylbut-3-en-1-yl)benzamide (S2a). A yellow oil, 12 mg, 21% yield; ^1H NMR (CDCl_3 , 400 MHz, TMS) δ 7.55 – 7.49 (m, 2H), 7.44 – 7.38 (m, 1H), 7.37 – 7.26 (m, 6H), 7.26 – 7.20 (m, 1H), 6.00 (s, 1H), 3.46 (dt, $J = 6.5, 6.5$ Hz, 2H), 2.73 – 2.64 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz, TMS) δ 167.47, 154.21 (dd, $J = 292.3, 287.9$ Hz), 134.42, 133.19 – 132.92 (m), 131.43, 128.79, 128.52, 128.16 (t, $J = 3.2$ Hz), 127.64, 126.71, 90.16 (dd, $J = 21.2, 14.5$ Hz), 38.71 – 38.45 (m), 27.95; ^{19}F NMR (376 MHz, CDCl_3) δ -89.7 (d, $J = 40.2$ Hz, 1F), -90.1 (d, $J = 40.0$ Hz, 1F); IR (neat): ν 3308, 3066, 2927, 1727, 1636, 1537, 1488, 1306, 1233, 1123, 930, 761, 692 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{17}\text{H}_{15}\text{NOF}_2\text{Na}^+$ Requires: 310.1014, Found: 310.1012.





(J) Reaction Quantum Yield Measurement²

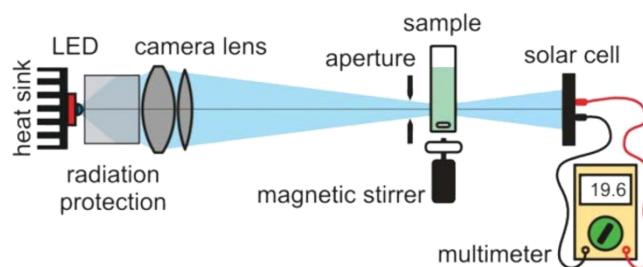


Fig. S2 Schematic of the setup²

In order to further study whether light irradiation involves a chain process, we measured the quantum yield of the reaction. The reaction setup is shown in Fig. S1.

The quantum yield Φ of the overall photoreaction is generally defined as the number N_{prod} of formed product molecules divided by the number of absorbed photons $N_{\text{ph,abs}}$:

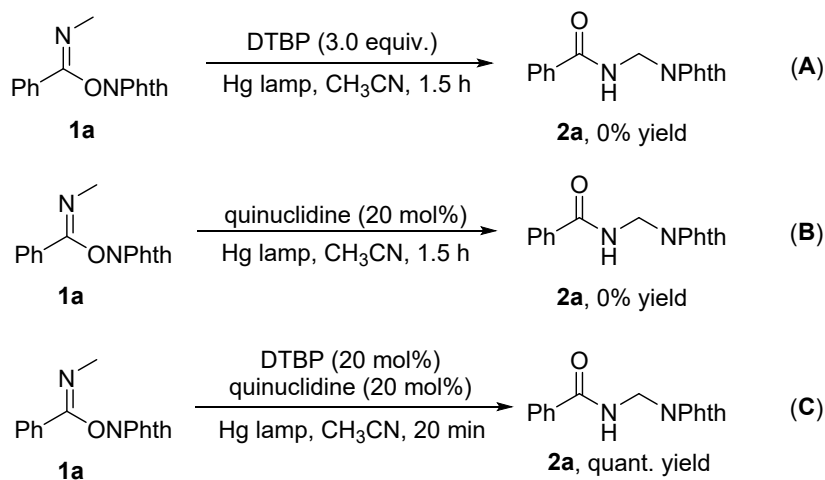
$$\Phi = \frac{N_{\text{prod}}}{N_{\text{ph,abs}}} = N_A h c \frac{c_{\text{prod}} V}{P_{\text{abs}} \Delta t \lambda_{\text{LED}}}$$

Here, N_A is the Avogadro constant, h is Planck's constant, c is the speed of light, c_{prod} is the product concentration, V is the sample volume, P_{abs} is the absorbed radiant power, Δt is the illumination time and λ_{LED} is the central wavelength of the LED. The reaction was measured with ILT1400 portable radiometer/photometer and c_{prod} is measured with ¹H NMR.

2 mL of DMSO-*d*₆ reaction solution ($c = 0.025$ M) that has been treated according to (D) *General Procedure*, with additional 2/3 equiv of methyl benzoate that will not affect the reaction as an internal standard, added to a 4 mL cuvette containing a stir bar. After irradiating the mixture with blue light of 6.0 mW/cm² at room temperature and stirring the mixture for 2 mins, the reaction yield at this time was measured to be 46%. The quantum yield of the reaction is calculated to be $\Phi = 20$:

$$\Phi = (6.022 \times 10^{23} \text{ mol}^{-1})(6.626 \times 10^{-34} \text{ J}\cdot\text{s})(3.0 \times 10^8 \text{ m/s}) \frac{(0.025 \times 0.46 \text{ mol/L})(2.0 \times 10^{-3} \text{ L})}{[(6.0 - 3.5) \times 10^{-3} \times 2 \text{ W}](120 \text{ s})(450 \text{ nm})} = 20$$

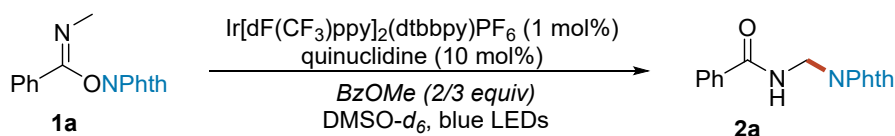
(K) High-Pressure Mercury Lamp Irradiation Experiments



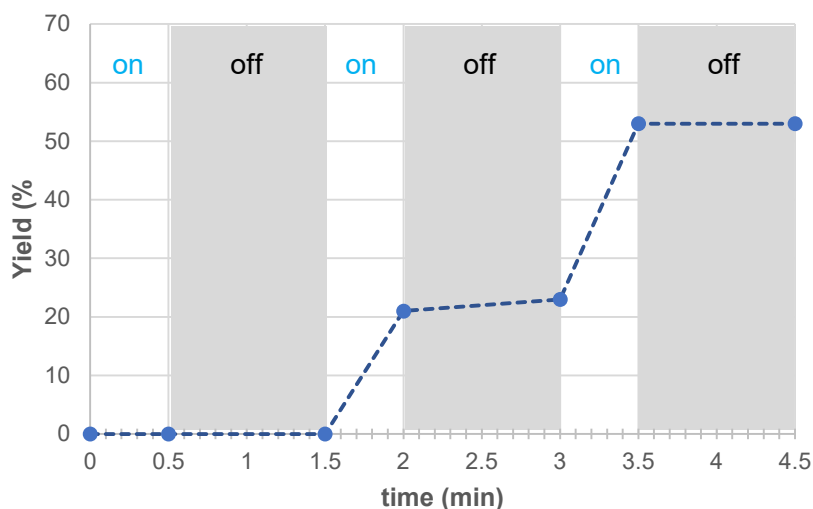
A dry 12 mL sealed bottle equipped with a Teflon cap and a magnetic stirrer was charged with NHPI imidate ester **1a** (0.2 mmol, 1.0 equiv) and a certain amount of quinuclidine, then injected 2.0 mL of dry acetonitrile through a syringe and the reaction system was degassed with argon bubbling for 10 minutes. Then a certain amount of DTBP was injected under argon, and the reaction flask was sealed with a Teflon cap. After that, the reaction mixture was put into a high-pressure mercury lamp reactor for reaction, and the progress of the reaction was detected by TLC and ^1H NMR spectroscopic analysis.

Note: The high-pressure mercury lamp emits ultraviolet rays, so be careful to avoid light; at the same time, the high-pressure mercury lamp emits a lot of heat, so it is necessary to adapt the condensing circulating water and the fan! !

(L) Light On/Off Reaction



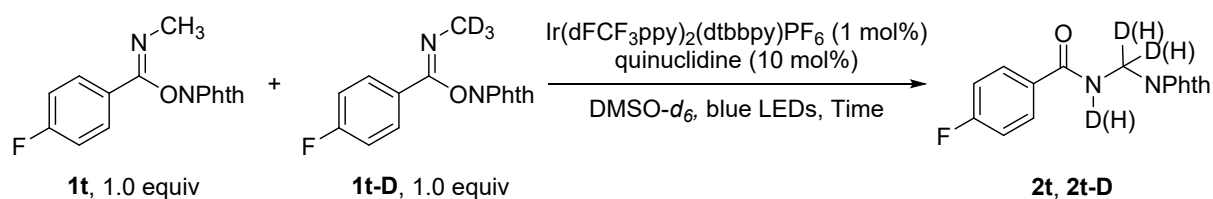
A dry 25 mL Schlenk tube equipped with rubber plug and a magnetic stirrer was charged with the photocatalyst Ir[dF(CF₃)ppy]₂(dtbbpy)PF₆ (0.004 mmol, 0.01 equiv), NHPI imidate ester **1a** (0.4 mmol, 1.0 equiv) and quinuclidine (0.04 mmol, 0.1 equiv), then injected 4.0 mL of dry DMSO-*d*₆ through a syringe. After the above mixture was degassed by bubbling argon for 10 minutes, 2/3 equiv of methyl benzoate was injected into the reaction tube, sealed with a rubber plug under argon and equipped with an argon balloon, then placed in the blue light of an 8 W blue LED strip with a timer at room temperature (using a fan to maintain the temperature). After stirring for a certain period of time, 0.4 mL of the reaction solution was taken out, and the yield was measured by ¹H NMR spectroscopy. The result is shown as below:



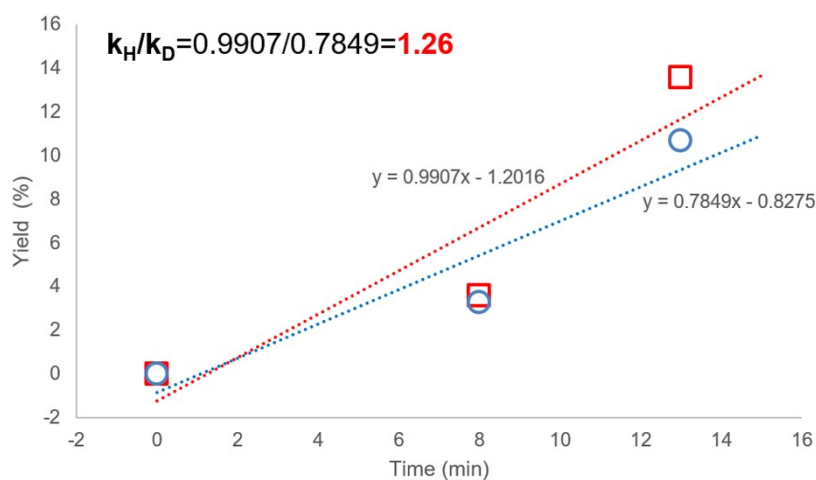
Chain reactions are generally terminated milliseconds after illumination is turned off. This experiment only offers qualitative evidence that light is necessary to trigger the reaction³. The light on/off experiment indicated that constant irradiation of visible light is needed, suggesting that photoredox catalysis and radical chain process coexist in the reaction.

It is possible that there are trace impurities or oxygen remaining in the reaction solution, which could quench the initially excited catalyst; thus, no product was produced in the first 0.5 min of the reaction.

(M) Kinetic Isotope Effect (KIE) Study of the Amination of **1t**



A dry 10 mL sealed tube equipped with a rubber plug and a magnetic stirrer was charged with the photocatalyst Ir[dF(CF₃)ppy]₂(dtbbpy)PF₆ (0.002 mmol, 0.01 equiv), NHPI imidate ester **1t** (0.2 mmol, 1.0 equiv), **1t-D** (0.2 mmol, 1.0 equiv) and quinuclidine (0.02 mmol, 0.1 equiv), and injected 4.0 mL of dry DMSO-*d*₆ through a syringe. After the above mixture was degassed by bubbling argon for 10 minutes, 2/3 equiv of methyl 4-fluorobenzoate was injected into the reaction tube, sealed with a rubber plug under argon and equipped with an argon balloon, then placed in the blue light of an 0.27 W blue LED strip at room temperature. After stirring for a certain period of time, 0.4 mL of the reaction solution was taken out, and the yield was measured by combining ¹H NMR and ¹⁹F NMR spectroscopy. The result is shown as below:



(N) Computational Details

Computational methods

All DFT calculations were performed with Gaussian 16 program.⁴ The geometries of all minima and transition states have been optimized at B3LYP/6-31G(d) level of theory. The subsequent frequency calculations on the stationary points were carried out at the same level of theory to ascertain the nature of the stationary points as minima or first-order saddle points on the respective potential energy surfaces. All transition states were characterized by one and only one imaginary frequency pertaining to the desired reaction coordinate. Thermochemical corrections to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at this same level. The solvent effect was estimated by the IEFPCM method with radii and nonelectrostatic terms for SMD solvation model in DMSO ($\epsilon = 46.826$) or in acetonitrile ($\epsilon = 35.688$). Solution-phase single point energy calculations were performed at B3LYP/6-311+G(d,p) level based on the gas phase optimized structures. The possible conformers for each species were searched manually, and the best conformer was used to calculate the reaction energy profile.

Table S1.^a

	$E_{\text{tot}} (E_{\text{h}})$	$H_{298, \text{DMSO}}$	$G_{298, \text{DMSO}}$
1a	-952.3318301	-952.06355	-952.128783
quinuclidinium radical cation	-329.2150822	-329.0122501	-329.0514021
TS1	-1281.530572	-1281.061425	-1281.145065
A	-951.6851626	-951.4309612	-951.4952752
quinuclidinium	-329.8820471	-329.6634625	-329.7020875
TS2	-951.6724798	-951.4201324	-951.4846644
B	-439.1522766	-439.0111622	-439.0544372
·NPhth	-512.556442	-512.4459902	-512.4895192
TS3	-1464.883305	-1464.505127	-1464.593462
HNPhth	-513.2559847	-513.1309835	-513.1726245
	$E_{\text{tot}} (E_{\text{h}})$	$H_{298, \text{acetonitrile}}$	$G_{298, \text{acetonitrile}}$
A	-951.6893751	-951.4348503	-951.4991463
TS2	-951.672680	-951.420003	-951.484601
B	-439.1551382	-439.0137946	-439.0570506
·NPhth	-512.5571978	-512.4466203	-512.4901733
3a	-534.5199463	-534.3685272	-534.4187022
TS4	-1486.191032	-1485.784497	-1485.878489
C	-1486.223250	-1485.813797	-1485.909294
D	-534.628448	-534.4801749	-534.5306749
TS5	-1486.330305	-1485.924932	-1486.018461
E	-1486.362634	-1485.954845	-1486.050423

a. Calculated at SMD/B3LYP/6-311+G(d,p)//B3LYP/6-31G(d)

Archive Entries

1a

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quinuclidinium radical cation

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TS1

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13N1)]\@

quinuclidinium

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(C7H14N1)]\ \@

TS2

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2.579692,-0.814513,0.242989\C,0,-3.937673,0.798455,-0.966117\C,0,-3.62
9542,-1.717638,0.337118\C,0,-5.004565,-0.103116,-0.870664\H,0,-4.04311
9,1.758709,-1.459902\C,0,-4.853056,-1.340467,-0.229403\H,0,-3.500306,-
2.672591,0.83548\H,0,-5.967667,0.159006,-1.297974\H,0,-5.701411,-2.015
562,-0.171086\N,0,-0.503893,0.198124,0.17838\O,0,-1.187219,2.290616,-0
.642973\O,0,-0.684081,-1.780439,1.43374\H,0,0.431143,3.263384,0.800812
\Version=ES64L-G09RevD.01\State=2-A\HF=-951.6726800\S2=0.773258\S2-1=
0.\S2A=0.750436\RMSD=2.932e-09\Dipole=-1.716267,-0.4295949,-0.9365976\
Quadrupole=17.9469141,-3.9919536,-13.9549605,0.8705766,-1.2896888,3.81
15991\PG=C01 [X(C16H11N2O3)]\ \@

B

1\1\GINC-B2128\SP\RB3LYP\6-311+G(d,p)\C8H7N1O1\ROOT\23-Jul-2021\0\#p
b3lyp/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=acetonitrile)\
Title Card Required\0,1\C,0,-0.0009467325,-0.0021508709,-0.0001349244
\C,0,-0.0025021187,-0.0047257522,1.4035687349\C,0,1.215329749,-0.00316
83484,2.100114892\C,0,2.4194511216,0.0066814476,1.3973606824\C,0,2.414
7504191,0.0123508096,0.000840401\C,0,1.2027403295,0.0069625877,-0.6974
867002\H,0,-0.9536287496,-0.0069730757,-0.5197463511\H,0,1.2063414502,
-0.0205285987,3.1842888115\H,0,3.3614328891,0.0049092075,1.938809333\H
,0,3.3547591917,0.0181875908,-0.5447673436\H,0,1.2005305502,0.00953759
82,-1.7839957699\C,0,-1.313427703,0.0038772744,2.1070578662\N,0,-1.224
8492519,0.1069310976,3.5305133179\C,0,-2.0957402594,0.8321273512,4.105
8054124\H,0,-2.0997209215,0.8977606465,5.1951123361\H,0,-2.858153279,1
.3982464986,3.5574571571\O,0,-2.3834153617,-0.1085009535,1.531040413\
Version=ES64L-G16RevA.03\State=1-A\HF=-439.1551382\RMSD=3.822e-09\Dipo
le=0.9162398,0.782288,0.3683926\Quadrupole=-0.6725226,-4.8337032,5.506
2258,-3.6186421,-6.3117593,3.1942776\PG=C01 [X(C8H7N1O1)]\ \@

•NPhth

```
1\1\GINC-B2175\SP\UB3LYP\6-311+G(d,p)\C8H4N1O2(2)\ROOT\04-Aug-2021\0\
#p b3lyp/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=acetonitrile
)\Title Card Required\0,2\C,0,0.,0.,0.\C,0,0.,0.,2.29323701\C,0,1.42
26784569,0.,0.4477965458\C,0,1.4226536687,-0.0001703937,1.8453795352\C
,0,2.6080457458,-0.0006145452,-0.2802657355\C,0,2.6079600167,-0.000992
2056,2.5735562384\C,0,3.8030003686,-0.0015453406,0.4434536382\H,0,2.59
64634488,-0.0004211623,-1.3651155414\C,0,3.802966943,-0.0017574724,1.8
499306247\H,0,2.5962673376,-0.0011124949,3.6584034107\H,0,4.7513555342
,-0.0022120851,-0.0851223977\H,0,4.7512953715,-0.0025902599,2.37855157
93\N,0,-0.8559453417,0.002002152,1.14642068\O,0,-0.4255658403,-0.00109
10301,-1.1404851752\O,0,-0.4256730653,-0.0013949571,3.4335538143\Vers
ion=ES64L-G16RevA.03\State=2-A\HF=-512.5571978\S2=0.762354\S2-1=0.\S2A
=0.750112\RMSD=9.206e-09\Dipole=3.7108881,-0.0008602,0.0006717\Quadrup
ole=1.2581443,2.6046612,-3.8628054,0.0008797,-0.0016749,0.0000998\PG=C
01 [X(C8H4N1O2)]\@
```

TS3

```
1\1\GINC-B2146\SP\UB3LYP\6-311+G(d,p)\C24H16N3O5(2)\ROOT\24-Aug-2021\0
\#p b3lyp/6-311+g(d,p) scrf=(iefpcm,smd,solvent=dms)\Title Card Req
uired\0,2\C,0,-3.672323,-1.556438,-0.203266\C,0,-2.358318,-2.047881,-
0.157446\C,0,-1.870333,-2.842942,-1.208397\C,0,-2.690595,-3.135572,-2.
293863\C,0,-3.999902,-2.647864,-2.337274\C,0,-4.487968,-1.861919,-1.29
1205\H,0,-4.054944,-0.954133,0.613578\H,0,-0.848427,-3.203877,-1.15935
3\H,0,-2.308271,-3.742928,-3.108753\H,0,-4.638492,-2.880742,-3.184653\
H,0,-5.507738,-1.489755,-1.318674\C,0,-1.473981,-1.798462,0.996129\N,0
,-0.623406,-2.643088,1.4016\C,0,0.340233,-2.349748,2.41427\H,0,0.42225
4,-3.189292,3.111242\H,0,0.218215,-1.400848,2.943594\O,0,-1.662436,-0.
585596,1.721525\C,0,-0.462517,1.121507,0.481648\C,0,-2.738543,1.476308
,1.007339\C,0,-0.847396,2.490017,0.037057\C,0,-2.19349,2.702441,0.3541
93\C,0,-0.08571,3.467433,-0.58541\C,0,-2.825922,3.900489,0.058788\C,0,
-0.715796,4.682931,-0.882897\H,0,0.957546,3.290953,-0.825118\C,0,-2.06
2886,4.895675,-0.56637\H,0,-3.870134,4.054894,0.309207\H,0,-0.151197,5
.474875,-1.365143\H,0,-2.522087,5.849099,-0.80843\N,0,-1.674541,0.5489
29,0.928892\O,0,0.615202,0.569222,0.472208\O,0,-3.82856,1.27396,1.4915
21\H,0,1.35584,-2.31724,1.900862\C,0,3.408726,-0.759917,1.454785\C,0,2
.535533,-1.815737,-0.402395\C,0,3.918574,-0.043407,0.242118\C,0,3.3890
43,-0.681535,-0.882058\C,0,4.767083,1.05053,0.125662\C,0,3.686106,-0.2
52348,-2.169517\C,0,5.061423,1.497884,-1.166086\H,0,5.175602,1.535529,
1.006116\C,0,4.529054,0.856056,-2.296714\H,0,3.272242,-0.758686,-3.035
344\H,0,5.712915,2.356113,-1.302025\H,0,4.779139,1.230402,-3.28503\N,0
,2.798443,-1.950729,0.982933\O,0,1.801239,-2.524461,-1.061124\O,0,3.52
4991,-0.436267,2.618296\Version=ES64L-G16RevA.03\State=2-A\HF=-1464.8
833047\S2=0.75785\S2-1=0.\S2A=0.750042\RMSD=3.289e-09\Dipole=0.3094774
,4.1531382,-3.1225641\Quadrupole=4.7103419,4.8200888,-9.5304306,8.7837
```

114,-5.8021886,-3.4860028\PG=C01 [X(C24H16N3O5)]\@

HNPhth

1\1\GINC-B2152\SP\RB3LYP\6-311+G(d,p)\C8H5N1O2\ROOT\24-Aug-2021\0\#p
b3lyp/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=dmsolvent)\Title Card
Required\0,1\C,0,-0.0065130847,0.0006472986,-0.0273818204\C,0,-0.0
065981678,0.000556485,2.3204595512\C,0,1.4115902456,-0.0002186662,0.44
78423644\C,0,1.4115377167,-0.0003606076,1.8453421476\C,0,2.5945464233,
-0.000870412,-0.277050531\C,0,2.5944389705,-0.0012021107,2.5703256882\
C,0,3.7942345614,-0.0016903606,0.4461230664\H,0,2.5827257101,-0.000755
624,-1.3626277612\C,0,3.7941819512,-0.001857082,1.8472432586\H,0,2.582
5355505,-0.0013009104,3.655901986\H,0,4.7412922862,-0.0022178867,-0.08
60321129\H,0,4.7411996672,-0.0024981177,2.3794693919\N,0,-0.7750643828
,0.0009335282,1.1465061095\O,0,-0.4369384125,0.001112578,-1.1610404082
\O,0,-0.4371204736,0.000588392,3.4540794099\H,0,-1.7864885192,0.001574
9587,1.1464718622\Version=ES64L-G16RevA.03\State=1-A\HF=-513.2559847\
RMSD=3.574e-09\Dipole=1.529699,-0.0008927,0.0000851\Quadrupole=9.16365
14,-0.4610484,-8.702603,-0.006023,0.0006245,0.0012686\PG=C01 [X(C8H5N1
O2)]\@

3a

1\1\GINC-B2071\SP\RB3LYP\6-311+G(d,p)\C6H8O4\ROOT\01-Jun-2021\0\#p b3
lyp/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=acetonitrile)\Ti
tle Card Required\0,1\C,0,-0.0074915471,0.0000259784,-0.006746797\C,0
,0.0074868037,0.000242726,1.3326368962\H,0,0.9120214961,-0.0004138858,
-0.5819200094\H,0,-0.9120275732,0.0006815478,1.9078082102\C,0,1.241316
1023,-0.0000821944,2.1587071205\O,0,1.2262224599,0.0005170098,3.373450
191\O,0,2.3725769539,-0.0001244862,1.4205328368\C,0,-1.2413188624,0.00
03559116,-0.8328073844\O,0,-1.2262336868,-0.0002778419,-2.0475474774\
O,0,-2.3725625746,0.000227187,-0.0946154342\C,0,-3.5957290975,-0.000101
8208,-0.8480718661\H,0,-3.6560449706,-0.8899357476,-1.4803038625\H,0,-
4.3947808871,-0.000250703,-0.106501633\H,0,-3.656460546,0.8896436152,-
1.4803900976\C,0,3.595733437,0.0000250523,2.1740054231\H,0,4.394794769
8,-0.000822174,1.4324459148\H,0,3.6565667397,0.8903030055,2.8055709024
\H,0,3.6559309528,-0.8892759399,2.8069910566\Version=ES64L-G16RevA.03
\State=1-A\HF=-534.5199463\RMSD=8.748e-09\Dipole=-0.0000126,-0.0000957
, -0.0000001\Quadrupole=15.7308071,-0.639984,-15.0908231,-0.0015664,1.9
707905,-0.0038013\PG=C01 [X(C6H8O4)]\@

TS4

1\1\GINC-B2071\SP\RB3LYP\6-311+G(d,p)\C6H8O4\ROOT\01-Jun-2021\0\#p b3
lyp/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=acetonitrile)\Ti
tle Card Required\0,1\C,0,-0.0074915471,0.0000259784,-0.006746797\C,0
,0.0074868037,0.000242726,1.3326368962\H,0,0.9120214961,-0.0004138858,

-0.5819200094\H,0,-0.9120275732,0.0006815478,1.9078082102\C,0,1.241316
1023,-0.0000821944,2.1587071205\O,0,1.2262224599,0.0005170098,3.373450
191\O,0,2.3725769539,-0.0001244862,1.4205328368\C,0,-1.2413188624,0.00
03559116,-0.8328073844\O,0,-1.2262336868,-0.0002778419,-2.0475474774\O
,0,-2.3725625746,0.000227187,-0.0946154342\C,0,-3.5957290975,-0.000101
8208,-0.8480718661\H,0,-3.6560449706,-0.8899357476,-1.4803038625\H,0,-
4.3947808871,-0.000250703,-0.106501633\H,0,-3.656460546,0.8896436152,-
1.4803900976\C,0,3.595733437,0.0000250523,2.1740054231\H,0,4.394794769
8,-0.000822174,1.4324459148\H,0,3.6565667397,0.8903030055,2.8055709024
\H,0,3.6559309528,-0.8892759399,2.8069910566\\Version=ES64L-G16RevA.03
\State=1-A\HF=-534.5199463\RMSD=8.748e-09\Dipole=-0.0000126,-0.0000957
, -0.0000001\Quadrupole=15.7308071,-0.639984,-15.0908231,-0.0015664,1.9
707905,-0.0038013\PG=C01 [X(C6H8O4)]\@

c

1\1\GINC-A761\SP\UB3LYP\6-311+G(d,p)\C22H19N2O7(2)\SIOC001\08-Apr-2021
\O\#\#p b3lyp/6-311+g(d,p) scrf=(iefpcm,smd,solvent=acetonitrile)\Titl
e Card Required\O,2\C,0,2.276372,2.701817,0.985663\C,0,1.027046,2.356
542,0.450008\C,0,0.475776,3.131326,-0.581903\C,0,1.171469,4.229178,-1.
079837\C,0,2.41838,4.568509,-0.548139\C,0,2.964949,3.806437,0.485556\H
,0,2.698785,2.119243,1.797009\H,0,-0.496803,2.859502,-0.977121\H,0,0.7
41801,4.820609,-1.882771\H,0,2.959869,5.426169,-0.93667\H,0,3.928174,4
.073922,0.909595\C,0,0.234696,1.228812,0.989706\N,0,-1.025347,1.242351
,1.048695\C,0,-1.79036,0.098748,1.51887\H,0,-1.221571,-0.837117,1.4724
16\O,0,0.950769,0.128256,1.544078\C,0,1.638614,-1.252362,-0.332214\C,0
,3.272666,-0.517987,1.208752\C,0,2.946281,-1.866583,-0.693935\C,0,3.91
196,-1.437718,0.223432\C,0,3.263638,-2.732144,-1.730013\C,0,5.230129,-
1.859305,0.136428\C,0,4.592445,-3.166528,-1.822276\H,0,2.506147,-3.058
68,-2.434621\C,0,5.559028,-2.737393,-0.904735\H,0,5.970914,-1.521001,0
.853145\H,0,4.878497,-3.848759,-2.616706\H,0,6.579969,-3.093298,-1.002
067\N,0,1.953096,-0.36514,0.724145\O,0,0.536167,-1.424029,-0.802129\O,
0,3.736447,0.007393,2.195076\H,0,-2.070222,0.270837,2.563415\C,0,-3.08
1274,-0.01873,0.677918\H,0,-3.646029,0.916304,0.773953\C,0,-2.795803,-
0.262987,-0.767154\H,0,-1.884389,-0.763029,-1.07597\C,0,-3.984098,-1.1
21696,1.245163\O,0,-4.299259,-2.142972,0.677876\O,0,-4.386497,-0.80427
3,2.496331\C,0,-5.24503,-1.769649,3.128187\H,0,-4.740268,-2.734739,3.2
16601\H,0,-5.469988,-1.362433,4.113589\H,0,-6.161563,-1.902553,2.54872
1\C,0,-3.775736,0.124036,-1.76161\O,0,-4.838279,0.682062,-1.516232\O,0
, -3.379215,-0.199697,-3.022306\C,0,-4.31297,0.140626,-4.053699\H,0,-4.
500912,1.217882,-4.069632\H,0,-3.851804,-0.179765,-4.988172\H,0,-5.264
974,-0.375192,-3.901148\\Version=ES64L-G09RevD.01\State=2-A\HF=-1486.2
232503\S2=0.755538\S2-1=0.\S2A=0.750022\RMSD=4.360e-09\Dipole=3.004968
1,-0.8593276,-0.9854568\Quadrupole=2.7677333,-2.4975366,-0.2701967,-7.
9871744,-16.1902297,-3.7321979\PG=C01 [X(C22H19N2O7)]\@

D

```
1\1\GINC-B2156\SP\UB3LYP\6-311+G(d,p)\C6H8O4(1-,2)\ROOT\19-Jul-2021\0\
\#p b3lyp/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=acetonitril
e)\Title Card Required\ -1,2\C,0,-0.0290760346,-0.0002226874,-0.03824
2874\C,0,0.0290594275,0.0000253859,1.3641330694\H,0,0.8927802884,-0.00
03074419,-0.6103071877\H,0,-0.8928030279,0.0001250056,1.9361896842\C,0
,1.2061103599,0.0001769898,2.1580978842\O,0,1.2837559126,0.0002967471,
3.398105945\O,0,2.3936565664,0.0000736274,1.3962782439\C,0,-1.20611441
89,-0.0003617305,-0.8321908065\O,0,-1.2837752959,-0.0005211322,-2.0721
95634\O,0,-2.3936440602,0.0000752938,-0.0703497924\C,0,-3.5743160397,0
.0001215509,-0.8424700343\H,0,-3.6456660715,-0.8843936829,-1.489812482
4\H,0,-4.4062763319,0.0004262673,-0.1286736204\H,0,-3.6453519323,0.884
3856075,-1.4901926596\C,0,3.5743288417,0.0001840844,2.1684014582\H,0,4
.4062896747,-0.0003802234,1.4546057404\H,0,3.6457520334,0.8849062731,2
.8154652014\H,0,3.645290087,-0.8838726897,2.816401865\Version=ES64L-G
16RevA.03\State=2-A\HF=-534.628448\S2=0.754042\S2-1=0.\S2A=0.750012\RM
SD=4.518e-09\Dipole=0.0000376,0.0002285,0.0000191\Quadrupole=11.027995
4,6.4865956,-17.514591,-0.0013177,-5.6800205,-0.0041162\PG=C01 [X(C6H8
O4)]\@
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TS5

```
1\1\GINC-B2178\SP\RB3LYP\6-311+G(d,p)\C22H19N2O7(1-)\ROOT\23-Jul-2021\
0\#p b3lyp/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=acetonitr
ile)\Title Card Required\ -1,1\C,0,0.0142656343,-0.0408052462,0.00175
38856\C,0,-0.0545633169,-0.0500401741,1.4139180958\C,0,1.1631650315,-0
.1415902727,2.1307572945\C,0,2.3809644244,-0.2087667023,1.4680082104\C
,0,2.4377803471,-0.1829933176,0.0676238635\C,0,1.2435538572,-0.1038137
981,-0.6522642103\H,0,-0.9004882855,-0.0293837268,-0.5805251014\H,0,1.
1140332544,-0.1560427412,3.2142334961\H,0,3.3005766617,-0.2745564673,2
.0470629974\H,0,3.3941139092,-0.2283001098,-0.4484145839\H,0,1.2642942
638,-0.1025635979,-1.7407390393\C,0,-1.3073212297,-0.0033448557,2.1439
556904\N,0,-1.452688608,-0.4442857812,3.3516103135\C,0,-2.5875375377,-
0.4121449384,4.0816924061\H,0,-3.5438397101,-0.1833236278,3.6124856791
\O,0,-2.4927024951,0.4031946632,1.4222859823\C,0,-2.264045106,2.866941
9037,1.4851401625\C,0,-2.8134409099,1.7767484141,-0.5306317867\C,0,-2.
5086968977,3.8984215015,0.4297620475\C,0,-2.8317444846,3.25171294,-0.7
646586062\C,0,-2.4435157232,5.2804133657,0.5119602588\C,0,-3.10652836,
3.9660150435,-1.9215219423\C,0,-2.7245694194,6.0120453914,-0.650152136
6\H,0,-2.1913101168,5.7669364398,1.4492188782\C,0,-3.050094497,5.36421
89454,-1.8486458618\H,0,-3.3562813758,3.4510098553,-2.8443354566\H,0,-
2.6931506128,7.0981542286,-0.6217925385\H,0,-3.2628827364,5.9569744234
,-2.7347131602\N,0,-2.4137147882,1.6382317896,0.8048342313\O,0,-1.9661
884081,3.0336375356,2.644994091\O,0,-3.0740621253,0.8813653214,-1.3113
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412607\H,0,-2.6143395216,-1.1023270467,4.9197595668\C,0,-2.7794673053,
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E

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8,-0.9830329,10.4883403,-9.352543\PG=C01 [X(C22H19N2O7)]\@

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