Supporting information for

Transition Metal Free Intramolecular Selective Oxidative C(sp^3)-N Coupling: Synthesis of *N*-Aryl-isoindolinones from 2-Alkylbenzamides

Ajay Verma, Saket Patel, Meenakshi, Amit Kumar, Abhimanyu Yadav, Shailesh Kumar, Sadhan Jana, Shubham Sharma, Ch. Durga Prasad, and Sangit Kumar*

Department of Chemistry, Indian Institute of Science Education and Research (IISER) Bhopal, Indore By-pass Road, Bhauri, Bhopal, Madhya Pradesh, India, Pin: 462 066.

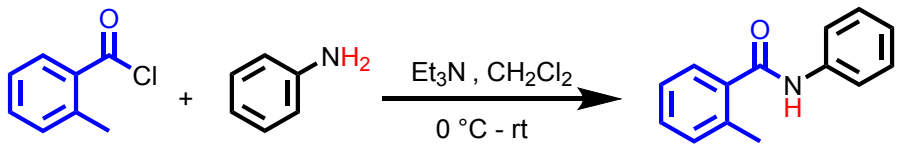
E-mail: *sangitkumar@iiserb.ac.in*

Table of contents **Page**

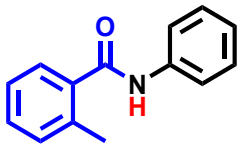
General Experimental Details

All NMR experiments were carried out on Bruker 400/500 MHz spectrometer in $CDCl_3$ and NMR chemical shifts are reported in ppm referenced to the solvent peaks of $CDCl_3$ (7.26 ppm for ^1H and 77 (± 0.07) ppm for ^{13}C) respectively. The following abbreviations were used to indicate multiplicity: s (singlet), brs (broad singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublets) td (triplet of doublet) and m (multiplet),. High resolution mass analysis is performed on quadrupole-time of flight Bruker MicroTOF-Q II mass spectrometer equipped with an ESI and APCI source; HR-GC mass analysis is performed on Agilent 7200 Accurate mass Q-TOF MS equipped with 7890A GC and LR-GC mass analysis is performed on Agilent Technologies MS-S975C inert XLEI/CIMSD with triple axis detector. Single crystal X-ray data for compounds **8**, **11** and **25** were collected on a Bruker D8 VENTURE diffractometer equipped with CMOS Photon 100 detector and Mo-Kα (λ = 0.71073 Å) radiation was used. 2-Toluenic acid, thionyl chloride and dry acetonitrile was purchased from Spectrochem Pvt. Ltd. . Di-*tert*-butyl peroxide and substituted anilines were purchased from Sigma Aldrich co. India and Spectrochem Pvt. Ltd. India respectivly. Dichloromethane used from MBRAUN solvent drying system. Silica gel (100-200 mesh size) was used for column chromatography purchased from RANKEM Pvt. Ltd. India. TLC analysis of reaction mixtures was performed using Merck silica gel (60 F_{254}) plates.

General Procedure for Amides

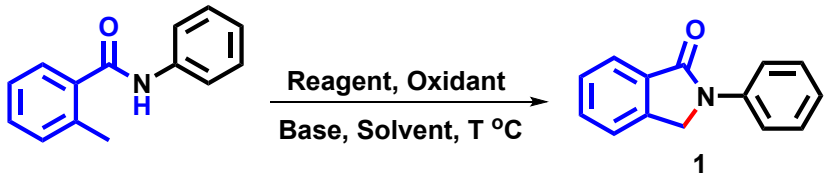


To a stirred solution of 2-methylbenzoyl chloride (309 mg, 2.0 mmol) in CH_2Cl_2 (25 mL), aniline (196 mg, 2.1 mmol) and triethylamine (406 mg, 4.0 mmol) in CH_2Cl_2 (15 mL) were added dropwise using a dropping funnel at 0 °C. After complete addition, the reaction mixture was stirred for 4-5 hours 0 °C to room temperature. After completion of the reaction, 10% HCl aqueous solution (30 mL) was added to the reaction mixture. The resulting solution was extracted with CH_2Cl_2 (30 mL × 3), organic layer layer was washed with brine (40 mL), dried over Na_2SO_4, and concentrated on a rotary evaporator under vacuum. A white solid was obtained, compound was pure enough and proceeded for next step.



2-Methyl-*N*-phenylbenzamide (substrate for 1).[1] White solid, yield 0.405 g (96%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.65 – 7.54 (m, 3H), 7.44 (d, *J* = 7.4 Hz, 1H), 7.34 (t, *J* = 7.8 Hz, 3H), 7.27 – 7.18 (m, 2H), 7.14 (t, *J* = 7.4 Hz, 1H), 2.48 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.1, 138.0, 136.5, 136.4, 131.3, 130.3, 129.1, 126.6, 125.9, 124.6, 119.9, 19.8; **GC-LRMS** *m/z* calcd for $C_{14}H_{13}NO$ $[M]^+$ 211.3, found 211.0.

Table S1. Optimization of reaction conditions



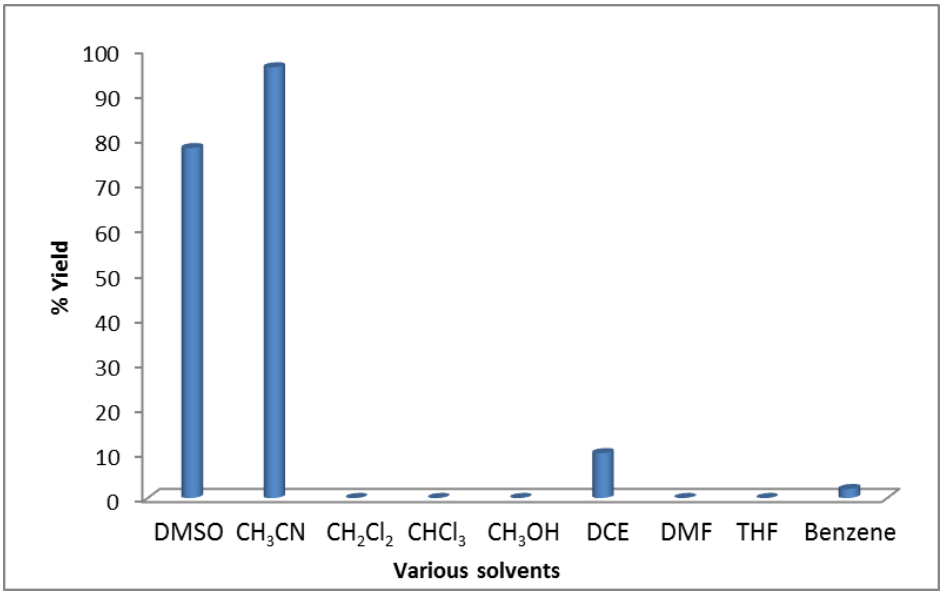
Entry	Reagent	Oxidant	Base	Solvent	T (°C)	Sub conv (%)	Yield of 1 (%)
1[a]	**$Pd(OAc)_2$**	DTBP	K_2CO_3	CH_3CN	140	<10	Trace
2[a]	**$Pd(PPh_3)_4$**	DTBP	$NaHCO_3$	CH_3CN	140	50	20
3[a,b]	**$Cu(OAc)_2$**	DTBP	K_2CO_3	CH_3CN	140	<10	Trace
4	**I_2**	**DTBP**	**K_2CO_3**	**CH_3CN**	**140**	**100**	**86**
5	I_2	DTBP	K_2CO_3	CH_3CN	**80**	35	20
6	I_2	DTBP	K_2CO_3	CH_3CN	**100**	65	58
7	**—**	**—**	K_2CO_3	CH_3CN	140	ND	—
8	I_2	DTBP	**—**	CH_3CN	140	ND	—
9	**—**	DTBP	K_2CO_3	CH_3CN	140	ND	—
10	**I_2 (1 equiv)**	DTBP	K_2CO_3	CH_3CN	140	40	52
11	**I_2 (3 equiv)**	DTBP	K_2CO_3	CH_3CN	140	40	67
12	I_2	DTBP	K_2CO_3	**DMSO**	140	90	78

Entry	Reagent	Oxidant	Base	Solvent	T (°C)	Sub conv (%)	Yield of 1 (%)
13	I_2	DTBP	K_2CO_3	**CH_3OH**	140	ND	—
14	I_2	DTBP	K_2CO_3	**Benzene**	140	10	Trace
15	I_2	DTBP	K_2CO_3	**$CHCl_3$**	140	ND	—
16	I_2	DTBP	K_2CO_3	**CH_2Cl_2**	140	ND	—
17	I_2	DTBP	K_2CO_3	**DCE**	140	18	10
18	I_2	DTBP	K_2CO_3	**DMF**	140	ND	—
20	I_2	**TBHP**	K_2CO_3	CH_3CN	140	ND	—
21	I_2	**H_2O_2**	K_2CO_3	CH_3CN	140	ND	—
22	I_2	**$K_2S_2O_8$**	K_2CO_3	CH_3CN	140	45	38
23	I_2	**$(NH_4)_2S_2O_8$**	K_2CO_3	CH_3CN	140	50	42
24	I_2	DTBP	**KO^tBu**	CH_3CN	140	ND	—
25	I_2	DTBP	**KOH**	CH_3CN	140	ND	—
26	I_2	DTBP	**K_3PO_4**	CH_3CN	140	90	80
27	I_2	DTBP	**Cs_2CO_3**	CH_3CN	140	70	64
28	I_2	DTBP	**$NaHCO_3$**	CH_3CN	140	82	73
29[c]	**NBS**	DTBP	K_2CO_3	CH_3CN	140	ND	—
30[c]	**$[(^nBu)_4N]^+I^-$**	DTBP	K_2CO_3	CH_3CN	140	ND	—
31[c]	**NCS**	DTBP	K_2CO_3	CH_3CN	140	ND	—

All reactions were carried out at 0.14 mmol of 2-methyl-*N*-phenyl benzamide using 2 equiv of reagent and base, excess of oxidant (8 equiv) in 2 mL of solvent at 140 °C in a sealed tube and the progress of reaction was monitored by TLC. [a] 10 mol % of transition metal salt was used; [b] two equiv of iodine was used, unless otherwise stated; [c] two equivalent of reagent was used; DTBP = di-*tert*-butyl peroxide, TBHP- *tert*-butyl hydroperoxide NBS = *N*-Bromosuccinimide, NCS = *N*-Chlorosuccinimide; ND = Not detected.

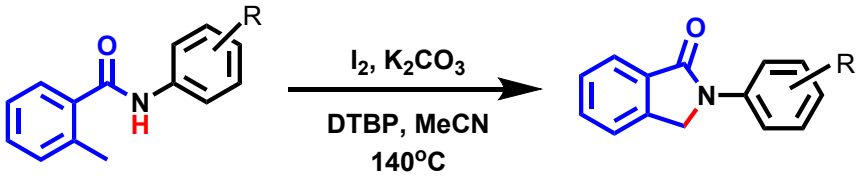
Optimization of reaction conditions. Synthesis of isoindolinone **1** from 2-methyl-*N*-phenyl benzamide was optimized by screening various reagents, oxidants, bases in various solvents in a sealed tube at 80-140 ^{o}C(Table S1, variation is shown by red color in Table for clarity). We began screening various transition metal catalysts for the oxidative coupling of C(sp^3)-H and N-H bonds in 2-methyl-*N*-phenylbenzamide. Transition metals noticed to inefficient promotor for the coupling as $Pd(PPh_3)_4$ yielded 20% of isoindolinone **1**. Again Pd(II) and Cu(II) catalysts were ineffective for the promotion of C-N coupling reaction as only traces of product **1** was observed. Next iodine in combination of DTBP offered quantitative yield (86%) of **1**. Worthnoting here is that although excess of DTBP was used, however, over oxidized product *N*-phenyl phthalimide **2** was not observed. We also studied the effect of the temperature on the rate of the reaction. Formation of isoindolinone **1** has not been observed at room temperature for 24 h. The yields 20% and 58% were obatained at 80 and 100 ^{o}C, respectively, when reaction was heated for 14h. Reaction completed in 30 h when reaction was heated at 100 ^{o}C. Reaction took 7 h for completion at 140 ^{o}C. As mentioned in entries 7-9, presence of I_2 and base K_2CO_3 is necessary to accomplish the transformation as absence of either one failed to provide any isoindolinone **1**. Also iodine and K_2CO_3 are not effective for the complete conversion of the substrate and addition of oxidant is required for the complete transformation of the substrate into product. Two equiv of iodine noticed to be optimum for the preparation of **1** as one or three equiv of iodine lower the yield of **1** considerably.

Yield of 1 in different solvents

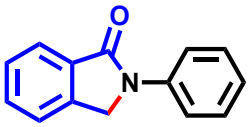


Next, various solvents were screened, nonetheless, acetonitrile found to be superior. Among various oxidants, protonated TBHP and H_2O_2 did not promot any C-N coupling as no product formation was observed. DTBP, potassium and ammonium persulfates noticed to be good for C-N coupling. Surprisingly, strong bases such as KO^{t}Bu, and KOH, noticed to be ineffective as no product formation was observed in these cases. K_3PO_4, Cs_2CO_3 and $NaHCO_3$ yielded 80, 64, 73% yield of **1**, respectively. We chose K_2CO_3 due to its ready availability. In the end, various other halogen reagents such as NBS, NCS and $[(^nBu)_4N]^+I^-$ were screened, however, none of them promoted C-N coupling.

Typical procedure for benzylic C-N coupling of 2-methylbenzamide.

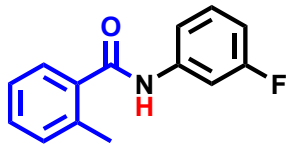


In a sealed tube, 2-methyl-*N*-phenylbenzamide (1 equiv. 0.5 mmol), iodine (2 equiv., 1 mmol), potassium carbonate (2 equiv. 1 mmol) were added followed by the addition of 2 mL dry acetonitrile. Reaction mixture was stirred at room temperature for 10 minutes. After that, di-*tert*-butyl peroxide, DTBP (8 equiv, 4 mmol) was added to the reaction mixture and reaction was heated to 140 °C. Progress of the reaction was monitored by thin layer chromatography. Reaction mixture was heated for 2-4 h (**27-31**) 4-10 h (**1, 5, 11, 19, 16-19, 21** and **24**) and 11-16 h (**3, 4, 6-10, 12-15, 20, 22, 23, 25,** and **26**). After completion, reaction mixture was poured into aqueous sodium sulfite solution (15 mL) followed by the extraction with dichloromethane (30 mL x 3). Combined organic layer was washed with brine solution (40 mL), dried over sodium sulfate. Organic layer was evaporated under reduced pressure at 40 °C. The obtained crude product was purified by column chromatography using ethyl acetate: hexane (1:9) over silica gel.

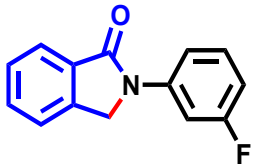


2-Phenylisoindolin-1-one (1).[2] Pale yellow solid, yield 0.090 g (86%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.91 (d, *J* = 7.4 Hz, 1 H), 7.85 (d, *J* = 7.9 Hz, 2H), 7.60 – 7.55 (m, 1H), 7.52 – 7.46 (m, 2H), 7.41 (t, *J* = 8.0 Hz, 2H), 7.16 (t, *J* = 7.4 Hz, 1H), 4.84 (s, 2H); **^{13}C NMR (100 MHz,**

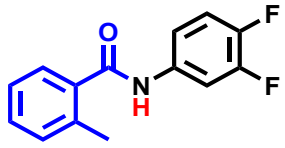
$CDCl_3$) δ 167.5, 140.1, 139.5, 133.3, 132.1, 129.2, 128.4, 124.5, 124.2, 122.6, 119.5, 50.8; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{11}NO$ $[M+H]^+$ 210.0913, found 210.0921.



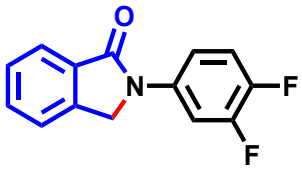
***N*-(3-Fluorophenyl)-2-methylbenzamide (substrate for 3)**.White solid, yield 421 mg (92%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.75 (s, 1H), 7.57 (d, *J* = 10.6 Hz, 1H), 7.40 (d, *J* = 7.5 Hz, 1H), 7.33 (t, *J* = 7.5 Hz, 1H), 7.30 – 7.15 (m, 4H), 6.82 (td, *J* = 8.2, 1.5 Hz, 1H), 2.44 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.2, 164.3, 161.8, 139.6, 139.5, 136.5, 136.0, 131.3, 130.5, 130.2, 130.1, 126.6, 125.9, 115.2, 111.3, 111.1, 107.6, 107.3, 19.8; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{12}FNO$ $[M+H]^+$ 230.0976, found 230.0996.



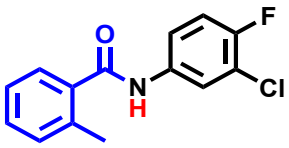
2-(3-Fluorophenyl)isoindolin-1-one (3). Pale yellow solid, yield 0.079 g (70%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.90 (d, *J* = 7.5 Hz, 1H), 7.82 – 7.76 (m, 1H), 7.62 – 7.53 (m, 2H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.34 (dd, *J* = 15.0, 8.2 Hz, 1H), 6.85 (td, *J* = 8.2, 2.0 Hz, 1H), 4.81 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.6, 164.4, 161.9, 141.1, 140.9, 139.9, 134.6, 132.9, 132.4, 130.3, 130.2, 128.5, 124.2, 123.9, 122.7, 114.2, 114.2, 111.1, 110.9, 106.8, 106.5, 50.7; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{10}FNO$ $[M+H]^+$ 228.0819, found 228.0843.



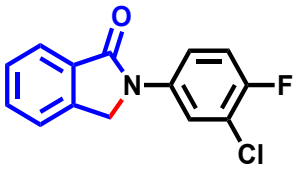
***N*-(3,4-Difluorophenyl)-2-methylbenzamide (substrate for 4)**. White solid, yield 0.464 g (94%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.78 (brs, 1H), 7.71 – 7.62 (m, 1H), 7.34 (dd, *J* = 18.7, 7.5 Hz, 2H), 7.26 – 7.16 (m, 2H), 7.10-7.03 (m, 2H), 2.42 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.9, 146.1, 146.0, 143.7, 143.5, 143.1, 143.0, 140.6, 140.5, 131.2, 130.4, 129.2, 129.2, 129.1, 129.1, 126.0, 125.3, 121.3, 120.6, 112.0, 111.8, 110.3, 104.6, 104.4, 14.4; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{11}F_2NO$ $[M+H]^+$ 248.0881, found 248.0911 .



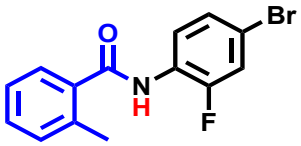
2-(3,4-Difluorophenyl)isoindolin-1-one (4). Yellow solid, yield 0.159 g (92%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.01 – 7.84 (m, 2H), 7.59 (t, *J* = 7.3 Hz, 1H), 7.53 – 7.40 (m, 3H), 7.17 (q, *J* = 9.2 Hz, 1H), 4.79 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.5, 151.6, 151.4, 149.1, 148.9, 148.3, 148.2, 145.9, 145.7, 139.7, 136.2, 136.1, 136.1, 136.0, 132.7, 132.5, 128.6, 124.3, 122.7, 117.4, 117.3, 114.6, 114.5, 114.5, 114.5, 109.1, 108.9, 50.7; **HRMS (ESI)** *m/z* calcd for $C_{14}H_9F_2NO$ $[M-H]^+$ 244.0568, found 244.0574 .



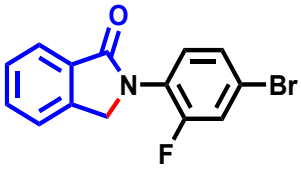
***N*-(3-Chloro-4-fluorophenyl)-2-methylbenzamide (substrate for 5)**. White solid, yield 0.515 g (98%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.77 (brs, 2H), 7.42 – 7.29 (m, 3H), 7.27 – 7.16 (m, 2H), 7.06 (t, *J* = 8.7 Hz, 1H), 2.42 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.2, 156.1, 153.7, 136.5, 135.7, 134.6, 134.6, 131.5, 130.6, 126.6, 125.9, 122.3, 121.3, 121.1, 119.7, 116.7, 116.5, 19.8; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{11}ClFNO$ $[M+H]^+$ 264.0586, found 264.0615.



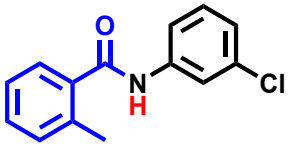
2-(3-Chloro-4-fluorophenyl)isoindolin-1-one (5). White solid, yield 0.091 g (70%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.96 (dd, *J* = 6.5, 2.7 Hz, 1H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.75 – 7.71 (m, 1H), 7.59 (t, *J* = 7.1 Hz, 1H), 7.54 – 7.46 (m, 2H), 7.15 (t, *J* = 8.8 Hz, 1H), 4.79 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.5, 156.1, 153.6, 139.8, 136.3, 136.2, 132.6, 132.5, 128.6, 124.3, 122.7, 121.5, 121.4, 121.3, 118.8, 118.8, 116.9, 116.7, 50.8; **HRMS (ESI)** *m/z* calcd for $C_{14}H_9ClFNO$ $[M+H]^+$ 262.0429, found 262.0414 .



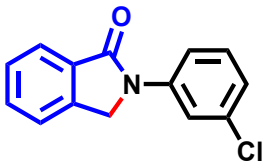
***N*-(4-Bromo-2-fluorophenyl)-2-methylbenzamide (substrate for 6)**. White solid, yield 0.554 g (90%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.43 (t, *J* = 8.3 Hz, 1H), 7.68 (brs, 1H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.46 – 7.39 (m, 1H), 7.39 – 7.27 (m, 4H), 2.55 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.8, 153.5, 151.1, 136.8, 135.5, 131.5, 130.8, 127.9, 127.8, 126.8, 126.0, 125.9, 125.8, 122.7, 118.6, 118.4, 116.1, 115.9, 19.9; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{11}BrFNO$ $[M+H]^+$ 308.0081, found 308.0088 .



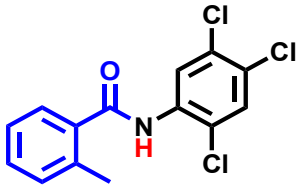
2-(4-bromo-2-fluorophenyl)isoindolin-1-one (6). Pale yellow solid, yield 0.137 g (90%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.94 (d, *J*=7.3 Hz, 1H), 7.63-7.49 (m, 4H), 7.38-7.35 (m, 2H), 4.85 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.9, 158.0, 155.5, 141.4, 132.3, 131.6, 129.0, 128.9, 128.4, 127.9, 127.9, 125.3, 124.5, 122.8, 120.5, 120.5, 120.2, 120.1, 52.0; **HRMS (ESI)** *m/z* calcd for $C_{14}H_9BrFNO$ $[M+H]^+$ 305.9924, found 305.9951.



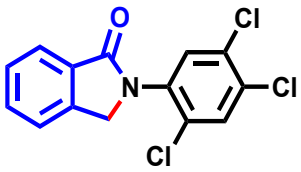
***N*-(3-Chlorophenyl)-2-methylbenzamide (substrate for 7)**. White solid, yield 0.447 g (91%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.78 (s, 1H), 7.69 (s, 1H), 7.45 (d, *J* = 7.6 Hz, 2H), 7.38 (dt, *J* = 7.5, 1.3 Hz, 1H), 7.32 – 7.25 (m, 3H), 7.15 (ddd, *J* = 8.0, 2.0, 0.9 Hz, 1H), 2.50 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.2, 139.1, 136.5, 135.9, 134.8, 131.4, 130.5, 130.1, 126.6, 125.9, 124.6, 120.0, 117.9, 19.83; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{12}ClNO$ $[M+H]^+$ 246.0680, found 246.0666.



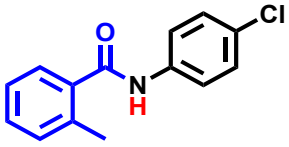
2-(3-Chlorophenyl)isoindolin-1-one (7).[3] White solid, yield 0.091 g (75%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.99 – 7.90 (m, 2H), 7.82 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.67 – 7.61 (m, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 8.2 Hz, 1H), 7.16 (dd, *J* = 8.0, 1.1 Hz, 1H), 4.85 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 167.6, 140.7, 139.9, 134.9, 132.8, 132.5, 130.2, 128.6, 124.34, 124.29, 122.7, 119.2, 117.1, 50.6; **HRMS (APCI)** *m/z* calcd for $C_{14}H_{10}ClNO$ $[M+H]^+$ 244.0524, found 244.0549



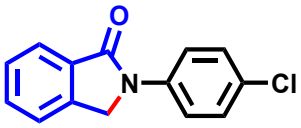
2-Methyl-*N*-(2,4,5-trichlorophenyl)benzamide (substrate for 8). White solid, yield 0.597 g (95%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.83 (s, 1H), 7.99 (s, 1H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.53 (s, 1H), 7.44 (td, *J*=7.6, 1.2 Hz, 1H), 7.33 (t, *J* = 7.4 Hz, 2H), 2.57 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 167.6, 137.1, 135.2, 134.2, 132.1, 131.7, 131.1, 129.8, 127.5, 126.8, 126.2, 122.3, 121.3, 20.1; **GC-HRMS** *m/z* calcd for $C_{14}H_{10}Cl_3NO$ $[M]^+$ 312.9828, found 312.9809.



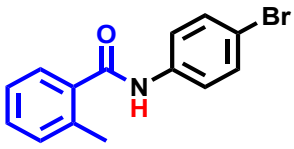
2-(2,4,5-Trichlorophenyl)isoindolin-1-one (8). Light brown solid, yield 0.103 g (66%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.97 (d, *J* = 7.5 Hz, 1H), 7.69 – 7.63 (m, 2H), 7.61 – 7.52 (m, 3H), 4.82 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.1, 141.5, 135.4, 132.9, 132.4, 131.8, 131.6, 131.5, 131.4, 131.3, 128.5, 124.6, 122.9, 52.0; **HRMS (ESI)** *m/z* calcd for $C_{14}H_8Cl_3NO$ $[M+H]^+$ 311.9744, found 311.9769 .



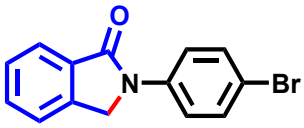
***N*-(4-Chlorophenyl)-2-methylbenzamide (substrate for 9)**. White solid, yield 0.417 g (85%);**^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.91 (s, 1H), 7.50 (d, *J* = 8.1 Hz, 2H), 7.38 – 7.28 (m, 2H), 7.25 (d, *J* = 8.6 Hz, 2H), 7.22 – 7.11 (m, 2H), 2.40 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.2, 136.6, 136.5, 136.0, 131.3, 130.5, 129.5, 129.1, 126.6, 125.9, 121.2, 19.8**. HRMS (ESI)** *m/z* calcd for $C_{14}H_{12}ClNO$ $[M+H]^+$ 246.0680, found 246.0692.



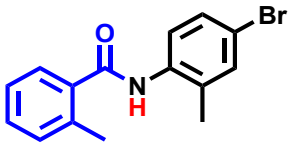
2-(4-Chlorophenyl)isoindolin-1-one (9).[2] White solid, yield 0.086 g (71%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 7.7 Hz, 1H), 7.74 (d, *J* = 8.9 Hz, 2H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 6.7 Hz, 2H), 7.28 (d, *J* = 8.9 Hz 2H), 4.72 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.5, 139.9, 138.1, 132.9, 132.2, 129.5, 129.1, 128.5, 124.2, 122.6, 120.3, 50.6; **GC-LRMS** *m/z* calcd for $C_{15}H_{13}NO$ $[M]^+$ 223.0997, found 223.1.



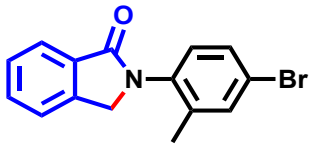
***N*-(4-Bromophenyl)-2-methylbenzamide (substrate for 10)**. White solid, yield 0.522 g (90%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.73 (brs, 1H), 7.52 – 7.29 (m, 6H), 7.20 (dd, *J* = 15.4, 7.6 Hz, 2H), 2.43 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.2, 137.1, 136.5, 136.0, 132.0, 131.3, 130.5, 126.6, 125.9, 121.5, 117.1, 19.8; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{12}BrNO$ $[M+H]^+$ 290.0175, found 290.0194



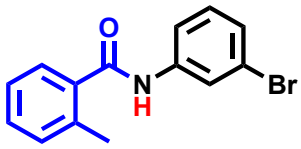
2-(4-Bromophenyl)isoindolin-1-one (10). Yellow solid, yield 0.187g (65%);**^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.89 (d, *J* = 8.1 Hz, 1H), 7.79 – 7.71 (m, 2H), 7.59 (td, *J* = 7.4, 3.6 Hz, 1H), 7.53 – 7.44 (m, 4H), 4.80 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.5, 139.9, 138.6, 132.9, 132.4, 132.1, 128.5, 124.2, 122.7, 120.7, 117.2, 50.6; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{10}BrNO$ $[M+H]^+$ 288.0019, found 288.0014.



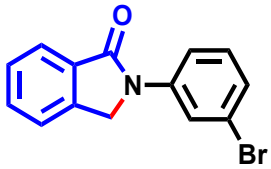
***N*-(4-Bromo-2-methylphenyl)-2-methylbenzamide (substrate for 11)**. White solid, yield 0.523 g (86%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.92 (d, *J* = 7.0 Hz, 1H), 7.52 (d, *J* = 7.2 Hz, 1H), 7.44 – 7.37 (m, 3H), 7.34 – 7.27 (m, 3H), 2.55 (s, 3H), 2.30 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.2, 136.6, 136.1, 134.9, 133.3, 131.5, 131.1, 130.5, 129.9, 126.7, 126.0, 124.4, 118.2,19.9, 17.8; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{14}BrNO$ $[M+H]^+$ 304.0332, found 304.0328 .



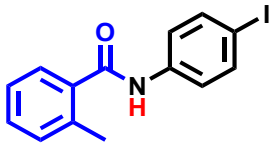
2-(4-Bromo-2-methylphenyl)isoindolin-1-one (11). Yellow solid, yield 0.119 g (79%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.96 (d, *J* = 7.6 Hz, 1H), 7.64 (td, *J* = 7.5, 1.1 Hz, 1H), 7.58 – 7.52 (m, 2H), 7.50 (d, *J* = 1.9 Hz, 1H), 7.42 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.14 (d, *J* = 8.4 Hz, 1H), 4.73 (s, 2H), 2.26 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 167.7, 141.5, 138.7, 136.2, 134.1, 132.1, 131.9, 129.9, 129.0, 128.4, 124.3, 122.9, 121.8, 52.9, 18.2; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{12}BrNO$ $[M+H]^+$ 302.0175, found 302.0204 .



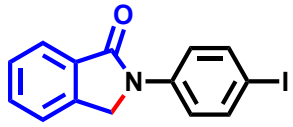
***N*-(3-Bromophenyl)-2-methylbenzamide (substrate for 12)**. White solid, yield 0.539 g (93%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.91 (s, 1H), 7.73 (s, 1H), 7.49 (d, *J* = 7.5 Hz, 1H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.38 (td, *J* = 7.6, 1.3 Hz, 1H), 7.32 – 7.20 (m, 4H), 2.49 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.2, 139.3, 136.5, 135.9, 131.4, 130.5, 130.4, 127.5, 126.6, 125.9, 122.8, 122.7, 118.4, 19.8; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{12}BrNO$ $[M+H]^+$ 290.0175, found 290.0183.



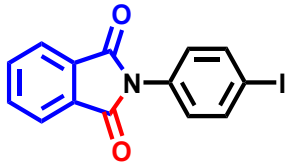
2-(3-Bromophenyl)isoindolin-1-one (12). White solid, yield 0.099 g (69%);**^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.12 – 8.03 (m, 1H), 7.96 – 7.83 (m, 2H), 7.65 – 7.60 (m, 1H), 7.55 – 7.50 (m, 2H), 7.37 – 7.20 (m, 2H), 4.83 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.6, 140.8, 139.9, 132.8, 132.4, 130.4, 128.5, 127.3, 124.3, 122.9, 122.7, 121.9, 117.6, 50.6; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{10}BrNO$ $[M+Na]^+$ 309.9838, found 309.9826.



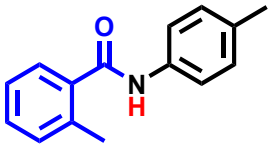
***N*-(4-Iodophenyl)-2-methylbenzamide (substrate for 13)**. White solid, yield 0.633 g (94%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.67 (d, *J* = 8.6 Hz, 2H), 7.60 (s, 1H), 7.49 – 7.36 (m, 4H), 7.33 – 7.23 (m, 2H), 2.50 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.1, 138.0, 137.8, 136.5, 136.0, 131.4, 130.5, 126.6, 125.9, 121.7, 87.7, 19.8; **GC-HRMS** *m/z* calcd for $C_{14}H_{12}INO$ $[M]^+$ 336.9964, found 336.9955 .



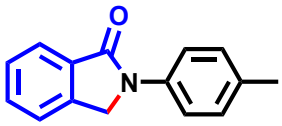
2-(4-Iodophenyl)isoindolin-1-one (13).[4] White solid, yield 0.105 g (63%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.91 (d, *J* = 7.7 Hz, 1H), 7.72 (d, *J* = 9.0 Hz, 2H), 7.66 (d, *J* = 9.0 Hz, 2H), 7.62 (t, *J* = 7.3 Hz, 1H), 7.56 – 7.49 (m, 2H), 4.81 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.6, 139.8, 139.3, 138.1, 132.9, 132.4, 128.5, 124.2, 122.7, 120.9, 87.9, 50.4; **GC-LRMS** *m/z* calcd for $C_{14}H_{10}INO$ $[M]^+$ 334.9, found 335.0.



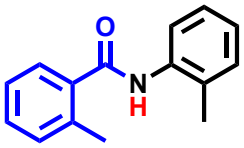
2-(4-Iodophenyl)isoindoline-1,3-dione. This iodo-phthalidamide was also formed along with the **13** in the reaction mixture. First fraction, yield 0.018g (10%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.95 – 7.93 (m, 2H), 7.83 – 7.78 (m, 4H), 7.21 (d, *J* = 8.6 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 166.9, 138.3, 134.6, 131.6, 131.5, 128.1, 123.9, 93.2; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{18}INO_2$ $[M+Na]^+$ 371.9492, found 371.9482.



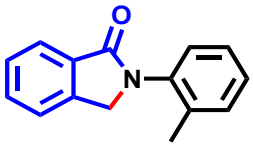
2-Methyl-*N*-(p-tolyl)benzamide (substrate for 14). White solid, yield 0.439g (91%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.49-7.43 (m, 4H), 7.24-7.22 (t, *J* = 7.2 Hz 1H), 7.24-7.22 (m, 2H), 7.16-7.14 (d, *J* = 7.9 Hz, 2H), 2.48 (s, 3H), 2.33 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.1, 136.6, 136.4, 135.5, 134.2, 131.2, 130.2, 129.6, 126.7, 125.9, 120.0, 20.9, 19.8.; **GC-LRMS** *m/z* calcd for $C_{15}H_{15}NO$ $[M]^+$ 225.1, found 225.1.



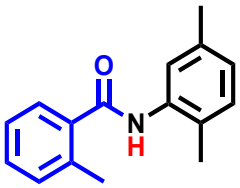
2-(*p*-Tolyl)isoindolin-1-one (14).[2] White solid, yield 0.080 g (67%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.90 (d, *J* = 7.8 Hz, 1H), 7.72(d *J* = 8.4 Hz, 2H), 7.56 (t, *J* = 7.0 Hz, 1H), 7.48 (t, *J* = 6.6 Hz, 2H), 7.21 (d, *J* = 8.4 Hz 2H), 4.79 (s, 2H), 2.33 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.3, 140.1, 134.0,134.1, 133.3, 131.9, 129.6, 128.3, 124.0, 122.5, 119.6, 50.8, 20.8; **GC-LRMS** *m/z* calcd for $C_{14}H_{10}ClNO$ $[M]^+$ 243.0450, found 243.1.



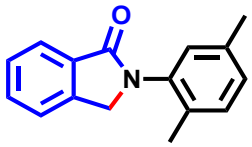
2-Methyl-*N*-(*o*-tolyl)benzamide (substrate for 15). White solid, yield 0.392g (87%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.95 (d, *J* = 6.0 Hz, 1H), 7.50 (d, *J* = 6.6 Hz, 1H), 7.35 (dd, *J* = 14.9, 7.4 Hz, 2H), 7.24 (dd, *J* = 19.0, 8.6 Hz, 4H), 7.11 (t, *J* = 7.4 Hz, 1H), 2.52 (s, 3H), 2.29 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.2, 136.5, 135.8, 131.3, 130.6, 130.3, 131.4, 129.2, 126.9, 126.7, 125.9, 125.4, 123.1, 19.9, 17.9; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{15}NO$ $[M+H]^+$ 226.1226, found 226.1246.



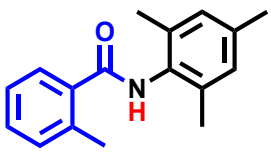
2-(o-Tolyl)isoindolin-1-one (15).[2] Brown semi solid, yield 0.089 g (80%);**^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.94 (d, *J* = 7.5 Hz, 1H), 7.63 – 7.56 (m, 1H), 7.51 (t, *J* = 7.9 Hz, 2H), 7.38 – 7.13 (m, 4H), 4.71 (s, 2H), 2.25 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.7, 141.6, 137.0, 136.4, 132.4, 131.7, 131.2, 128.3, 128.2, 127.5, 126.9, 124.3, 122.8, 53.1, 18.2; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{13}NO$ $[M+H]^+$ 224.1070, found 224.1065 .



***N*-(2,5-Dimethylphenyl)-2-methylbenzamide (substrate for 16)**. White solid, yield 0.425 g (89%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (brs, 1H), 7.50 (d, *J* = 7.1 Hz, 1H), 7.36 (t, *J* = 7.3 Hz, 1H), 7.30 – 7.21 (m, 3H), 7.09 (d, *J* = 7.7 Hz, 1H), 6.92 (d, *J* = 7.5 Hz, 1H), 2.53 (s, 3H), 2.35 (s, 3H), 2.24 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.1, 136.7, 136.6, 136.5, 135.6, 131.3, 130.4, 130.3, 126.7, 126.2, 126.0, 125.9, 123.5, 21.2, 19.9, 17.5; **HRMS (ESI)** *m/z* calcd for $C_{16}H_{17}NO$ $[M+H]^+$ 240.1383, found 240.1395 .

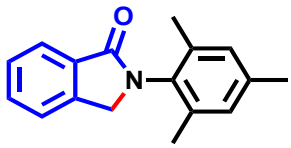


2-(2,5-Dimethylphenyl)isoindolin-1-one (16).[5] Brown semi solid, yield 0.059 g (50%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.94 (d, *J* = 7.4 Hz, 1H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 7.7 Hz, 1H), 7.12 – 7.04 (m, 2H), 4.69 (s, 2H), 2.32 (s, 3H), 2.19 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.7, 141.6, 136.8, 136.6, 133.1, 132.5, 131.7, 131.1, 129.0, 128.3, 128.0, 124.2, 122.8, 53.1, 20.8, 17.7; **HRMS (ESI)** *m/z* calcd for $C_{16}H_{15}NO$ $[M+H]^+$ 238.1226, found 238.1240.

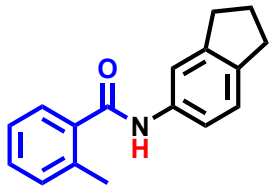


***N*-Mesityl-2-methylbenzamide (substrate for 17)**. White solid, yield 0.415 g (82%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.58 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.39 (dt, *J* = 7.5, 1.4 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.02 (brs, 1H), 6.97 (s, 2H), 2.56 (s, 3H), 2.32 (s, 9H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ

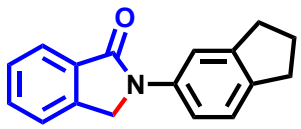
168.7, 137.3, 136.6, 136.5, 135.3, 131.2, 131.0, 130.1, 129.1, 126.7, 125.8, 21.0, 19.9, 18.6; **HRMS (ESI)** *m/z* calcd for $C_{17}H_{19}NO$ $[M+H]^+$ 254.1539, found 254.1551.



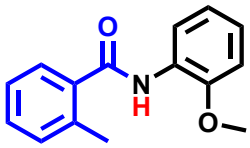
2-mesitylisoindolin-1-one (17). Yellow solid, yield 0.119 g (95%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.00 (dd, *J* = 7.1, 1.4 Hz, 1H), 7.67 – 7.60 (m, 1H), 7.55 (t, *J* = 7.2 Hz, 2H), 7.01 (s, 2H), 4.61 (s, 2H), 2.35 (s, 3H), 2.18 (s, 6H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.96, 141.72, 138.27, 136.46, 132.88, 132.47, 131.62, 129.33, 128.20, 124.35, 122.92, 51.34, 21.07, 17.91; **HRMS (ESI)** *m/z* calcd for $C_{17}H_{17}NO$ $[M+H]^+$ 252.1383, found 252.1364 .



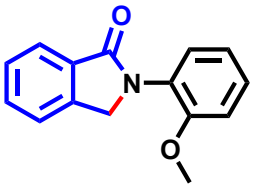
***N*-(2,3-Dihydro-1H-inden-5-yl)-2-methylbenzamide (substrate for 18)**. White solid, yield 0.360 g (80%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.63 (s, 1H), 7.56 (brs, 1H), 7.48 (d, *J* = 7.5 Hz, 1H), 7.37 (t, *J* = 7.2 Hz, 1H), 7.31 – 7.20 (m, 4H), 3.00 – 2.86 (m, 4H), 2.52 (s, 3H), 2.20 – 2.06 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.1, 145.3, 140.6, 136.7, 136.4, 136.1, 131.2, 130.2, 126.6, 125.9, 124.6, 118.1, 116.5, 33.1, 32.4, 25.7, 19.8; **HRMS (ESI)** *m/z* calcd for $C_{17}H_{17}NO$ $[M+H]^+$ 252.1383, found 252.1409 .



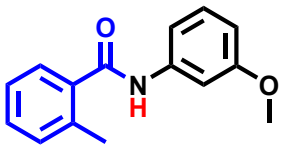
2-(2,3-Dihydro-1H-inden-5-yl)isoindolin-1-one (18).[6] White solid, yield 0.077 g (62%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.95 – 7.91 (m, 1H), 7.76 (s, 1H), 7.62 – 7.49 (m, 4H), 7.27 (d, *J* = 8.1 Hz, 1H), 4.81 (s, 2H), 2.94 (dt, *J* = 27.1, 7.4 Hz, 4H), 2.16 – 2.07 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 167.4, 145.3, 140.7, 140.3, 137.6, 133.4, 131.8, 128.3, 124.7, 124.0, 122.6, 117.9, 116.4, 51.3, 33.1, 32.4, 25.6; **HRMS (ESI)** *m/z* calcd for $C_{17}H_{15}NO$ $[M+H]^+$ 250.1226, found 250.1244 .



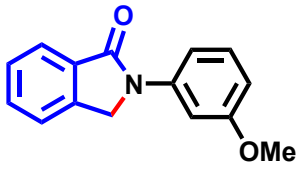
***N*-(2-Methoxyphenyl)-2-methylbenzamide (substrate for 19)**. White solid, yield 0.429g (89%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.59 (d, *J* = 7.7 Hz, 1H), 8.17 (brs, 1H), 7.59 – 7.53 (m, 1H), 7.44 – 7.38 (m, 1H), 7.30 (m, 2H), 7.13 (td, *J* = 7.8, 1.7 Hz, 1H), 7.06 (td, *J* = 7.6, 1.0 Hz, 1H), 6.94 (dd, *J* = 8.0, 1.4 Hz, 1H), 3.90 (s, 3H), 2.57 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.8, 148.1, 136.8, 136.5, 131.3, 130.2, 127.9, 126.9, 125.9, 123.9, 121.2, 119.8, 110.0, 55.7, 20.0; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{15}NO_2$ $[M+H]^+$ 242.1176, found 242.1191.



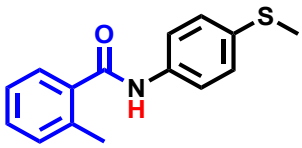
2-(2-Methoxyphenyl)isoindolin-1-one (19). White solid, yield 0.095 g (79%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.98 (dd, *J* = 7.3, 1.3 Hz, 1H), 7.63 – 7.59 (m, 1H), 7.54-7.51 (m, 2H), 7.46 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.36 (ddd, *J* = 7.6, 1.7, 0.7 Hz, 1H), 7.10 – 7.03 (m, 2H), 4.84 (s, 2H), 3.85 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.3, 155.1, 142.0, 132.6, 131.6, 129.1, 128.8, 127.9, 126.7, 124.2, 122.7, 120.9, 112.1, 55.7, 52.2; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{13}NO_2$ $[M+H]^+$ 240.1019, found 240.1023 .



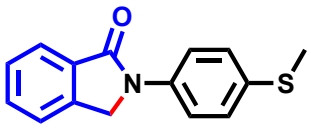
***N*-(3-Methoxyphenyl)-2-methylbenzamide (substrate for 20)**. White solid, yield 0.434 g (90%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.65 (brs, 1H), 7.48 – 7.41 (m, 2H), 7.37 (td, *J* = 7.6, 1.3 Hz, 1H), 7.29 – 7.23 (m, 3H), 7.10 (d, *J* = 7.6 Hz, 1H), 6.73 (dd, *J* = 8.3, 2.0 Hz, 1H), 3.84 (s, 3H), 2.50 (s, 3H); **^{13}C NMR (100MHz, $CDCl_3$)** δ 168.2, 160.2, 139.3, 136.4, 136.4, 131.2, 130.3, 129.8, 126.6, 125.9, 112.0, 110.4, 105.6, 55.4, 19.8; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{15}NO_2$ $[M+H]^+$ 242.1176, found 242.1200 .



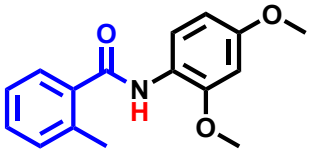
2-(3-Methoxyphenyl)isoindolin-1-one (20).[3] Pale yellow solid, yield 0.084 g (70%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.93 (d, *J* = 7.5 Hz, 1H), 7.70 (s, 1H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.54-7.51 (m, 2H), 7.38 – 7.31 (m, 2H), 6.75 (d, *J* = 6.4 Hz, 1H), 4.85 (s, 2H), 3.88 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 167.6, 160.2, 140.7, 140.1, 133.2, 132.2, 129.8, 128.4, 124.1, 122.6, 111.3, 110.3, 105.3, 55.4, 50.9; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{13}NO_2$ $[M+H]^+$ 240.1019, found 240.1014 .



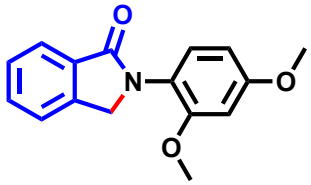
2-Methyl-*N*-(4-(methylthio)phenyl)benzamide (substrate for 21). White solid, yield 0.494 g (96%); **^{1}H NMR (400 MHz, $CDCl_3$) δ** 7.69 (s, 1H), 7.50 (d, *J* = 10.6 Hz, 2H), 7.39 (d, *J* = 7.4 Hz, 1H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.26 – 7.14 (m, 4H), 2.46 (s, 3H), 2.44 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ** 168.1, 136.4, 136.3, 135.7, 133.9, 131.2, 130.3, 128.0, 126.7, 125.9, 120.6, 19.8, 16.7; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{15}NOS$ $[M+H]^+$ 258.0947, found 258.0968.



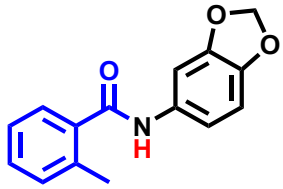
2-(4-(Methylthio)phenyl)isoindolin-1-one (21). Pale yellow solid, yield 0.064 g (50%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.90 (d, *J* = 7.2 Hz, 1H), 7.79 (d, *J* = 8.8 Hz, 2H), 7.58 (t, *J* = 7.0 Hz, 1H), 7.52 – 7.47 (m, 2H), 7.32 (d, *J* = 8.8 Hz, 2H), 4.82 (s, 2H), 2.48 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.4, 140.0, 137.1, 133.9, 133.2, 132.1, 128.4, 128.0, 124.2, 122.6, 119.9, 50.7, 16.6; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{13}NOS$ $[M+H]^+$ 256.0791, found 256.0806



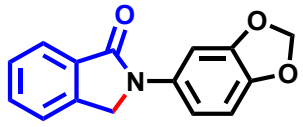
N-(2,4-Dimethoxyphenyl)-2-methylbenzamide(Substrate for 22) White solid, yield 0.499 g (92%);**^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.40 (d, *J* = 8.7 Hz, 1H), 8.04 – 7.85 (m, 1H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.39 – 7.29 (m, 1H), 7.25 (d, *J* = 7.2 Hz, 2H), 6.59 – 6.42 (m, 2H), 3.82 (s, 3H), 3.80 (s, 3H), 2.51 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.6, 156.6, 149.5, 136.9, 136.4, 131.2, 130.1, 126.9, 125.9, 121.4, 120.7, 103.8, 98.7, 55.7, 55.6, 20.0; **HRMS (ESI)** *m/z* calcd for $C_{16}H_{17}NO_3$ $[M+H]^+$ 272.1281, found 272.1299.



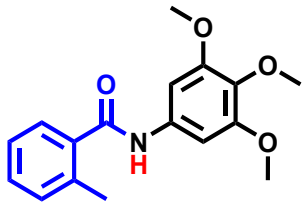
2-(2,4-Dimethoxyphenyl)isoindolin-1-one (22) Light brown solid, yield 0.096 g 72 %); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.92 (d, *J* = 7.4 Hz, 1H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.30 – 7.24 (m, 1H), 6.55 (s, 1H), 6.53 (d, *J* = 1.7 Hz, 1H), 4.73 (s, 2H), 3.82 (s, 3H), 3.77 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.5, 160.3, 156.2, 142.0, 132.7, 131.5, 129.6, 127.9, 124.2, 122.6, 119.8, 104.7, 99.9, 55.65, 55.59, 52.5; **HRMS (ESI)** *m/z* calcd for $C_{16}H_{15}NO_3$ $[M+H]^+$ 270.1125, found 270.1126.



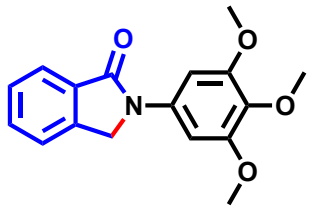
***N*-(Benzo[d][1,3]dioxol-5-yl)-2-methylbenzamide (substrate for 23)**.[7] White solid, yield 0.428 g (84%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.51 (brs, 1H), 7.46 (d, *J* = 7.5 Hz, 1H), 7.37 (t, *J* = 7.0 Hz, 2H), 7.30 – 7.21 (m, 2H), 6.90 (dd, *J* = 8.3, 1.6 Hz, 1H), 6.79 (d, *J* = 8.3 Hz, 1H), 5.98 (s, 2H), 2.50 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.0, 147.9, 144.5, 136.4, 132.2, 131.2, 130.2, 126.6, 125.9, 113.2, 108.1, 102.9, 101.3, 19.8; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{13}NO_3$ $[M+H]^+$ 255.08, found 255.1.



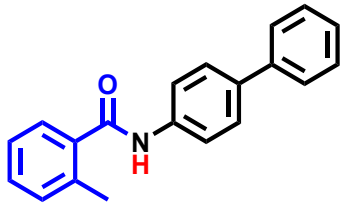
2-(Benzo[d][1,3]dioxol-5-yl)isoindolin-1-one (23).[6] White solid, yield 0.061 g (48%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.93 (d, *J* = 8.0 Hz, 1H), 7.60 (dd, *J* = 10.5, 4.3 Hz, 2H), 7.52 (t, *J* = 6.1 Hz, 2H), 7.11 (dd, *J* = 8.4, 2.1 Hz, 1H), 6.86 (d, *J* = 8.4 Hz, 1H), 6.00 (s, 2H), 4.81 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.3, 148.1, 144.6, 140.0, 133.8, 133.2, 131.9, 128.4, 124.1, 122.5, 112.9, 108.2, 102.6, 101.4, 51.5; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{11}NO_3$ $[M+H]^+$ 254.0812, found 254.0821.



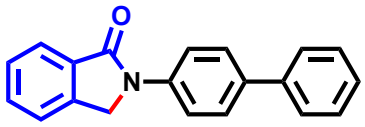
2-Methyl-*N*-(3,4,5-trimethoxyphenyl)benzamide (substrate for 24). White solid, yield 0.530 g (88%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.63 (s, 1H), 7.46 (d, *J* = 7.5 Hz, 1H), 7.36 (dt, *J* = 7.6, 1.1 Hz, 1H), 7.25 (dd, *J* = 16.7, 8.2 Hz, 2H), 6.95 (s, 2H), 3.86 (s, 6H), 3.82 (s, 3H), 2.51 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.2, 153.4, 136.4, 136.4, 134.8, 134.3, 131.3, 130.3, 126.6, 125.9, 97.5, 61.0, 56.1, 19.8; **HRMS (ESI)** *m/z* calcd for $C_{17}H_{19}NO$ $[M+H]^+$ 302.1387, found 302.1406 .



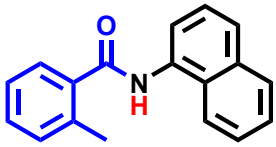
2-(3,4,5-Trimethoxyphenyl)isoindolin-1-one (24). Yellow solid, yield 0.118 g (79%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.92 – 7.89 (m, 1H), 7.64 – 7.58 (m, 1H), 7.56 – 7.49 (m, 2H), 7.17 (s, 2H), 4.85 (s, 2H), 3.92 (s, 6H), 3.87 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.9, 153.4, 139.9, 135.6, 135.2, 133.2, 132.2, 128.5, 124.0, 122.6, 97.6, 61.0, 56.3, 51.2; **HRMS (ESI)** *m/z* calcd for $C_{17}H_{17}NO_4$ $[M+H]^+$ 300.1230, found 300.1235 .



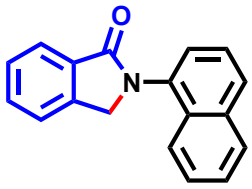
***N*-([1,1'-Biphenyl]-4-yl)-2-methylbenzamide (substrate for 25).** White solid, yield 0.534 g (93%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.73 (bd, *J* = 8.4 Hz, 3H), 7.66 – 7.60 (m, 4H), 7.51 (d, *J* = 7.5 Hz, 1H), 7.50 – 7.45 (m, 2H), 7.42 – 7.35 (m, 2H), 7.29 (dd, *J* = 8.8, 4.5 Hz, 2H), 2.54 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.2, 140.5, 137.5, 137.3, 136.5, 136.4, 131.3, 130.4, 128.9, 127.7, 127.2, 126.9, 126.7, 125.9, 120.3, 19.9; **HRMS (ESI)** *m/z* calcd for $C_{20}H_{17}NO$ $[M+H]^+$ 288.1383, found 288.1379.



2-([1,1'-Biphenyl]-4-yl)isoindolin-1-one (25).[8] White solid, yield 0.131 g (92%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.98 (dq, *J* = 7.2, 2.5 Hz, 3H), 7.71 – 7.67 (m, 2H), 7.66 – 7.61 (m, 3H), 7.57 – 7.52 (m, 2H), 7.50 – 7.45 (m, 2H), 7.40 – 7.35 (m, 1H), 4.92 (s, 2H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 167.6, 140.4, 140.1, 138.8, 137.2, 133.2, 132.2, 128.8, 128.5, 127.8, 127.2, 126.9, 124.2, 122.7, 119.7, 50.8; **HRMS (ESI)** *m/z* calcd for $C_{20}H_{15}NO$ $[M+Na]^+$ 308.1046, found 308.1068 .

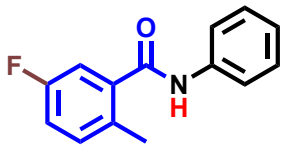


2-Methyl-*N*-(naphthalen-1-yl)benzamide (Substrate for 26) White solid, yield 0.470 g (90%);**^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.11 (s, 1H), 7.97 – 7.85 (m, 3H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.65 (s, 1H), 7.59 – 7.52 (m, 3H), 7.42 (d, *J* = 6.6 Hz, 1H), 7.34 (d, *J* = 6.8 Hz, 2H), 2.60 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.7, 136.7, 136.4, 136.4, 134.2, 132.3, 131.4, 130.4, 128.9, 127.1, 126.8, 126.5, 126.1, 126.0, 125.8, 120.6, 120.6, 20.0. **HRMS (ESI)** *m/z* calcd for $C_{18}H_{15}NO$ $[M+H]^+$ 262.1226, found 262.1246.

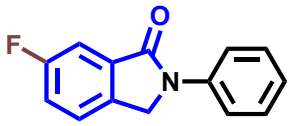


2-(Naphthalen-1-yl)isoindolin-1-one (26) White solid, yield 0.078 g (60%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.06 (d, *J* = 7.6 Hz, 1H), 7.98 – 7.93 (m, 2H), 7.75 (d, *J* = 8.2 Hz, 1H), 7.68 (td,

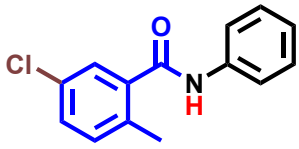
J = 7.5, 1.1 Hz, 1H), 7.63 – 7.50 (m, 6H), 4.92 (s, 2H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.9, 141.7, 135.0, 134.6, 132.4, 131.9, 130.4, 128.8, 128.6, 128.5, 126.9, 126.5, 125.65, 125.65, 124.5, 123.0, 122.89, 54.2; **HRMS (ESI)** *m/z* calcd for $C_{18}H_{13}NO$ $[M+Na]^+$ 282.0889, found 282.0877.



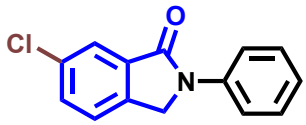
5-Fluoro-2-methyl-*N*-phenylbenzamide (substrate for 27). White solid, yield 0.426 g (93%)**; ^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.83 (s, 1H), 7.61 (d, *J* = 7.9 Hz, 2H), 7.37 (t, *J* = 7.9 Hz, 2H), 7.19 (dt, *J* = 8.7, 6.6 Hz, 2H), 7.13 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.05 (td, *J* = 8.4, 2.7 Hz, 1H), 2.43 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 166.9, 161.6, 159.7, 137.7, 137.6, 137.6, 132.7, 132.7, 131.8, 131.8, 129.1, 124.8, 120.1, 117.1, 116.9, 113.8, 113.6, 19.0; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{12}FNO$ $[M+H]^+$ 230.0976, found 230.1001.



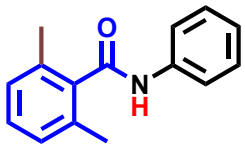
6-Fluoro-2-phenylisoindolin-1-one (27). Pale yellow solid, yield 0.102 g (90%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 7.9 Hz, 2H), 7.57 (dd, *J* = 7.6, 2.2 Hz, 1H), 7.50 – 7.38 (m, 3H), 7.28 (td, *J* = 8.7, 2.3 Hz, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 4.82 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 166.4, 164.3, 161.8, 139.3, 135.5, 135.5, 135.3, 135.3, 129.2, 124.8, 124.3, 124.2, 119.8, 119.6, 119.5, 110.9, 110.7, 50.4; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{10}FNO$ $[M+H]^+$ 228.0819, found 228.0841.



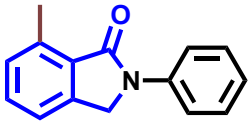
5-Chloro-2-methyl-*N*-phenylbenzamide (substrate for 28). White solid, yield 0.470 g (96%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.77 (s, 1H), 7.57 (d, *J* = 7.6 Hz, 2H), 7.39 – 7.30 (m, 3H), 7.27 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.14 (t, *J* = 7.6 Hz, 2H), 2.39 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 166.8, 137.8, 137.7, 134.8, 132.5, 131.5, 130.1, 129.1, 126.7, 124.8, 120.1, 19.2; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{12}ClNO$ $[M+H]^+$ 246.0680, found 246.0697.



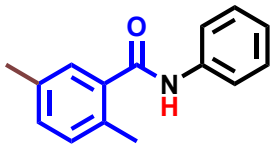
6-Chloro-2-phenylisoindolin-1-one (28). ^{1}H NMR (500 MHz, $CDCl_3$). White solid, yield 0.085 g (70%); δ 7.92 (d, *J* = 1.9 Hz, 1H), 7.88 – 7.85 (m, 2H), 7.61 – 7.56 (m, 1H), 7.50 – 7.43 (m, 3H), 7.25 – 7.20 (m, 1H), 4.86 (s, 2H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 166.1, 139.2, 138.2, 135.0, 134.8, 132.3, 129.3, 124.8, 124.3, 124.0, 119.5, 50.4; **HRMS (ESI)** *m/z* calcd for $C_{14}H_{10}ClNO$ $[M+H]^+$ 244.0524, found 245.0520.



2,6-Dimethyl-*N*-phenylbenzamide (substrate for 29). White solid, yield 0.382 g (85%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.59 (d, *J* = 7.9 Hz, 2H), 7.50 (brs, 1H), 7.35 (t, *J* = 7.9 Hz, 2H), 7.22 – 7.12 (m, 2H), 7.04 (d, *J* = 7.6 Hz, 2H), 2.36 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.7, 137.8, 137.6, 134.3, 129.2, 129.1, 127.7, 124.7, 120.0, 19.2; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{15}NO$ $[M+H]^+$ 226.1226, found 226.1255.

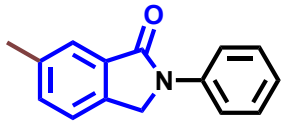


7-Methyl-2-phenylisoindolin-1-one (29). Pale yellow solid, yield 0.099 g (89%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.90 – 7.87 (m, 2H), 7.49 – 7.41 (m, 3H), 7.34 (d, *J* = 7.5 Hz, 1H), 7.25 (d, *J* = 7.5 Hz, 1H), 7.22 – 7.17 (m, 1H), 4.81 (s, 2H), 2.80 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.4, 140.7, 139.6, 138.4, 131.6, 130.4, 130.2, 129.1, 124.3, 120.1, 119.4, 50.1, 17.5; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{13}NO$ $[M+H]^+$ 224.1070, found 224.1091.

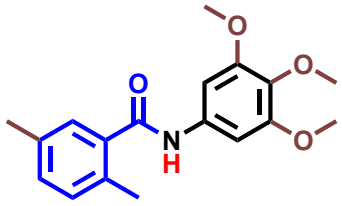


2,5-Dimethyl-*N*-phenylbenzamide (substrate for 30). White solid, yield 0.414 g (92%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.60 (d, *J* = 7.6 Hz, 3H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.25 (d, *J* = 3.2 Hz, 1H), 7.17 – 7.09 (m, 3H), 2.42 (s, 3H), 2.32 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.3,

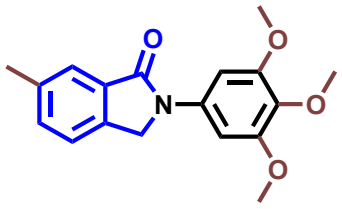
138.1, 136.3, 135.5, 133.2, 131.2, 131.0, 129.1, 127.3, 124.5, 119.9, 20.9, 19.3; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{15}NO$ $[M+H]^+$ 226.1226, found 226.1255.



6-Methyl-2-phenylisoindolin-1-one (30).[9] Pale yellow solid, yield 0.107 g (96%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.91 – 7.86 (m, 2H), 7.74 (s, 1H), 7.47 – 7.40 (m, 4H), 7.22 – 7.17 (m, 1H), 4.81 (s, 2H), 2.48 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 167.7, 139.6, 138.4, 137.4, 133.4, 133.1, 129.1, 124.4, 124.3, 122.4, 119.4, 50.5, 21.4; **GC-LRMS** *m/z* calcd for $C_{15}H_{13}NO$ $[M+H]^+$ 223.1, found 223.1.

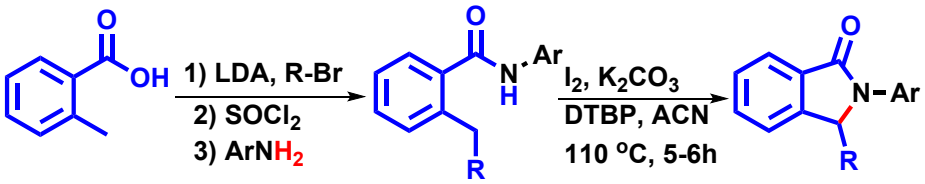


2,5-Dimethyl-*N*-(3,4,5-trimethoxyphenyl)benzamide (substrate for 31). White solid, yield 0.567 g (90%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.57 (s, 1H), 7.29 (s, 1H), 7.20 – 7.13 (m, 2H), 6.95 (s, 2H), 3.86 (s, 6H), 3.83 (s, 3H), 2.46 (s, 3H), 2.35 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.3, 153.4, 136.2, 135.5, 134.7, 134.3, 133.2, 131.2, 131.0, 127.2, 97.5, 61.0, 56.2, 20.9, 19.4; **HRMS (ESI)** *m/z* calcd for $C_{18}H_{21}NO_4$ $[M+H]^+$ 316.1543, found 316.1570.



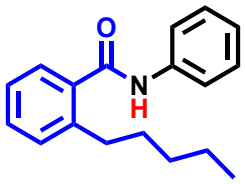
6-Methyl-2-(3,4,5-trimethoxyphenyl)isoindolin-1-one (31). White solid, yield 0.109 g (70%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.43 – 7.38 (m, 2H), 7.17 (s, 2H), 4.80 (s, 2H), 3.93 (s, 6H), 3.87 (s, 3H), 2.48 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 167.7, 153.4, 138.5, 137.2, 135.7, 135.0, 133.3, 133.2, 124.2, 124.1, 122.3, 97.5, 61.0, 56.2, 51.0, 21.4; **HRMS (APCI)** *m/z* calcd for $C_{18}H_{19}NO_4$ $[M+H]^+$ 314.1387, found 314.1396.

Preparation of 2-alkyl benzoic acids and respective isoindolinones[10]



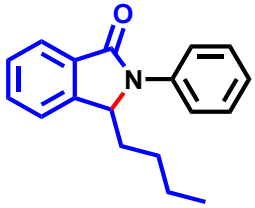
A solution of diisopropylamine (10.12 ml, 100 mmol) in anhydrous THF (30 mL) was cooled to -78 °C and 1.6 M n-BuLi (62 mL,100 mmol) was added dropwise by syringe. The solution was stirred under N_2 at 0 °C for 1.5 h. In a separate round bottom flask the solution of 2-methyl benzoic acid (2.7 g, 20 mmol) in THF (30 mL) was cooled to -78 °C under N_2. The LDA solution was transferred dropwise using syringe to the reaction mixture. After stirring the solution for 1.5 h at -78 °C, n-butyl bromide (6.85 g, 5.44 mL, 50 mmol) was added dropwise. The solution was stirred at -78 °C for 0.5 h and was warmed to rt. The reaction was quenched with 10% HCl (30 mL) and the reaction mixture was extracted with diethyl ether (3 x 60 mL). The combined organic extracts were concentrated under vacuum. The crude product was re-dissolved in diethyl ether (20 mL) and extracted with aqueous 20% KOH (3 x 30 mL) solution. The combined aqueous phase was washed with ether (30 mL x 3) and acidified with 2M HCl to pH 1. The aqueous phase was then extracted with ether (60 mL x 3). The combined organic extracts were washed with water (60 mL), brine (100 mL), dried over Na_2SO_4, filtered and concentrated under vacuum. This provided the mixture of mono alkylated (major) and dialkylated (minor) benzoic acids. Which was used for amide preparation without further purification.

2-Pentyl-*N*-phenylbenzamide (Substrate for 32). The crude 2-n-pentylbenzoic (400 mg, 1.41 mmol) acid was refluxed in excess of thionyl chloride (2 mL) for 2 h. After this, thionyl chloride was removed under vacuo which resulted in a dark brown liquid. To this liquid, 20 ml dry CH_2Cl_2 was added and reaction mixture was cooled to 0 °C. Aniline (232 mg, 2.5 mmol) and triethyl amine (840 mg, 8.32 mmol) in 15 ml of CH_2Cl_2 were added to the cold stirring mixture of aroyl chloride dropwise via dropping funnel. After complete addition, the resulted reaction mixture was stirred at 0 °C for 1 h and then at room temperature for 12 h. Standard work up, separation by column chromatography 0.331 g, 62% of product **27**.

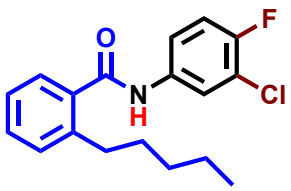


2-pentyl-*N*-phenylbenzamide (Substrate for 32).[11] White solid, yield 0.331 g (62%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.59 (d, *J* = 7.1 Hz, 3H), 7.41 (d, *J* = 7.5 Hz, 1H), 7.39 – 7.32 (m, 2H), 7.27 (d, *J* = 7.5 Hz, 1H), 7.21 (t, *J* = 7.4 Hz, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 2.80 (t, *J* = 7.7 Hz, 2H), 1.70 – 1.54 (m, 2H), 1.35 – 1.24 (m, 4H), 0.85 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.3, 141.3, 138.1, 136.5, 130.3, 130.2, 129.1, 126.7, 125.7, 124.5, 119.9, 33.2, 31.8, 31.4, 22.5, 14.0; **GC-LRMS** *m/z* calcd for $C_{18}H_{21}NO$ $[M]^+$ 267.1, found 267.1.

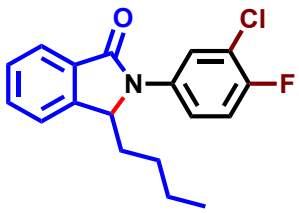
Procedure for the synthesis for the 3-substituted isoindolinones. In a sealed tube, 2-alkyl-*N*-arylbenzamide (1 equiv. 0.5 mmol), iodine (2 equiv., 1 mmol), potassium carbonate (2.5 equiv. 1.5 mmol) were added followed by the addition of 2 mL dry acetonitrile. Reaction mixture was stirred at room temperature for 10 minutes. After that, Di-*tert*-butyl peroxide (DTBP) (6 equiv, 3 mmol) was added and reaction was heated to 110 °C. Progress of the reaction was monitored by thin layer chromatography. After completion, reaction mixture was poured into aqueous sodium sulfite solution (15 mL) and extracted with dichloromethane (30 mL x 3). Combined organic layer was washed with brine solution (40 mL), dried over sodium sulfate. Organic layer was evaporated under reduced pressure at 40 °C. The obtained crude product was purified by column chromatography using ethyl acetate: hexane (1:9) over silica gel (230-400 mesh size).



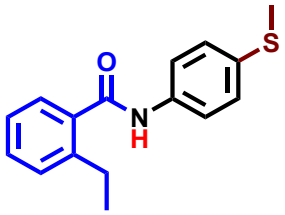
3-Butyl-2-phenylisoindolin-1-one (32) White solid, yield 0.086 g (65%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.96 (d, *J* = 7.5 Hz, 1H), 7.65 – 7.59 (m, 3H), 7.53 (t, *J* = 7.9 Hz, 2H), 7.50 – 7.46 (m, 2H), 7.27 (ddd, *J* = 8.5, 3.1, 2.0 Hz, 1H), 5.30 (dd, *J* = 5.4, 3.4 Hz, 1H), 2.00 – 1.86 (m, 2H), 1.18 – 1.01 (m, 2H), 0.93 – 0.77 (m, 2H), 0.72 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 167.4, 144.8, 137.1, 132.6, 132.0, 129.1, 128.3, 125.4, 124.1, 123.5, 122.1, 60.7, 30.5, 24.4, 22.4, 13.8; **HRMS (ESI)** *m/z* calcd for $C_{18}H_{19}NO$ $[M+H]^+$ 266.1539, found 266.1569.



***N*-(3-Chloro-4-fluorophenyl)-2-pentylbenzamide (Substrate for 33)** White solid, yield 0.357 g (56%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.82 (dd, *J* = 6.3, 2.1 Hz, 1H), 7.67 (s, 1H), 7.41 (t, *J* = 6.9 Hz, 3H), 7.31 (d, *J* = 7.5 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.13 (t, *J* = 8.7 Hz, 1H), 2.80 (t, *J* = 7.7 Hz, 2H), 1.75 – 1.57 (m, 2H), 1.43 – 1.26 (m, 4H), 0.88 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.3, 155.9, 153.9, 141.4, 135.7, 134.6, 134.6, 130.5, 130.4, 126.6, 125.9, 122.2, 121.3, 121.2, 119.7, 119.6, 116.8, 116.6, 33.2, 31.85, 31.4, 22.5, 14.0; **HRMS (ESI)** *m/z* calcd for $C_{18}H_{19}FClNO$ $[M+H]^+$ 320.1212, found 320.1236.

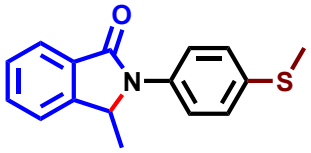


3-Butyl-2-(3-chloro-4-fluorophenyl)isoindolin-1-one (33) White solid, yield 0.155 g (98%);**^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.90 (dd, *J* = 7.3, 2.4 Hz, 1H), 7.68 (dd, *J* = 6.5, 2.6 Hz, 1H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.54 – 7.40 (m, 3H), 7.20 (td, *J* = 8.8, 3.1 Hz, 1H), 5.19 (brs, 1H), 2.01 – 1.79 (m, 2H), 1.11 (dd, *J* = 15.0, 7.5 Hz, 2H), 1.02 – 0.89 (m, 1H), 0.80 – 0.73 (m, 1H), 0.69 (td, *J* = 7.2, 1.8 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.4, 156.8, 154.3, 144.5, 133.9, 133.8, 132.4, 132.0, 128.5, 125.4, 124.2, 123.0, 122.9, 122.2, 121.5, 121.3, 116.9, 116.7, 60.8, 30.5, 24.3, 22.3, 13.7; **HRMS (ESI)** *m/z* calcd for $C_{18}H_{17}NOFCl$ $[M+H]^+$ 318.1055, found 318.1084.

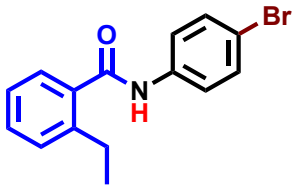


2-Ethyl-*N*-(4-(methylthio)phenyl)benzamide (Substrate for 34) White solid, yield 0.325 g (60%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.65 (s, 1H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.42 (m, 2H), 7.28 (m, 4H), 2.86 (q, *J* = 7.5 Hz, 2H), 2.50 (s, 3H), 1.27 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (125 MHz,**

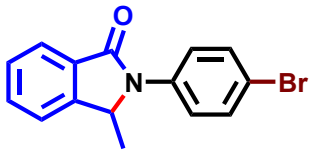
$CDCl_3$) δ 168.2, 142.6, 136.1, 135.7, 133.9, 130.4, 129.7, 128.1, 126.6, 125.9, 120.6, 26.4, 16.7, 15.9; **HRMS (ESI)** *m/z* calcd for $C_{16}H_{17}NOS$ $[M+H]^+$ 272.1104, found 272.1118.



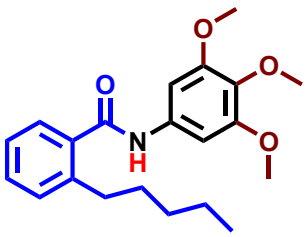
3-Methyl-2-(4-(methylthio)phenyl)isoindolin-1-one (34) White semi-solid, yield 0.114 g (85%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.94 (d, *J* = 7.6 Hz, 1H), 7.62 (td, *J* = 7.5, 1.1 Hz, 1H), 7.56 – 7.47 (m, 4H), 7.39 – 7.33 (m, 2H), 5.18 (q, *J* = 6.7 Hz, 1H), 2.52 (s, 3H), 1.46 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 166.92, 146.23, 135.21, 134.44, 132.14, 131.68, 128.45, 127.62, 124.12, 123.83, 122.02, 56.93, 18.76, 16.30; **HRMS (ESI)** *m/z* calcd for $C_{16}H_{16}NOS$ $[M+H]^+$ 270.0947 found.270.0971.



***N*-(4-Bromophenyl)-2-ethylbenzamide (Substrate for 35)** White solid, yield 0.350 g (58%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.64 (s, 1H), 7.53 (d, *J* = 8.7 Hz, 2H), 7.48 (d, *J* = 8.8 Hz, 2H), 7.46 – 7.38 (m, 2H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.26 (td, *J* = 7.5, 0.9 Hz, 1H), 2.85 (q, *J* = 7.5 Hz, 2H), 1.27 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.3, 142.7, 137.1, 135.8, 132.1, 130.6, 129.8, 126.6, 126.0, 121.4, 117.1, 26.4, 15.9; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{14}BrNO$ $[M+H]^+$ 304.0332 found.304.0331.

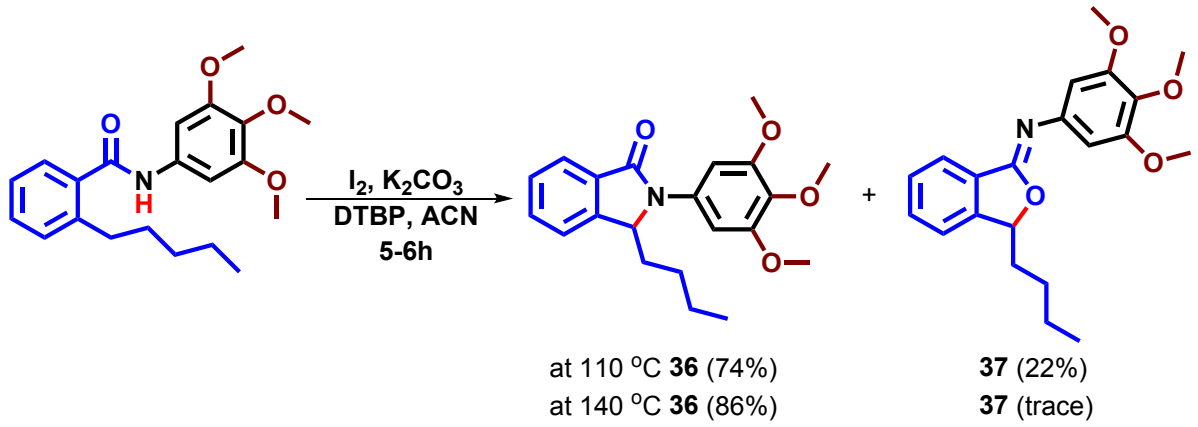


2-(4-Bromophenyl)-3-methylisoindolin-1-one (35) White solid, yield 136 g (90%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.94 (d, *J* = 7.6 Hz, 1H), 7.64 (td, *J* = 7.5, 1.1 Hz, 1H), 7.60 – 7.56 (m, 2H), 7.55 – 7.49 (m, 4H), 5.19 (q, *J* = 6.6 Hz, 1H), 1.48 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 166.9, 146.1, 136.3, 132.4, 132.2, 131.5, 128.6, 124.6, 124.2, 122.1, 118.3, 56.7, 18.7; **HRMS (ESI)** *m/z* calcd for $C_{15}H_{12}BrNO$ $[M+H]^+$ 302.0175 found.302.0205.



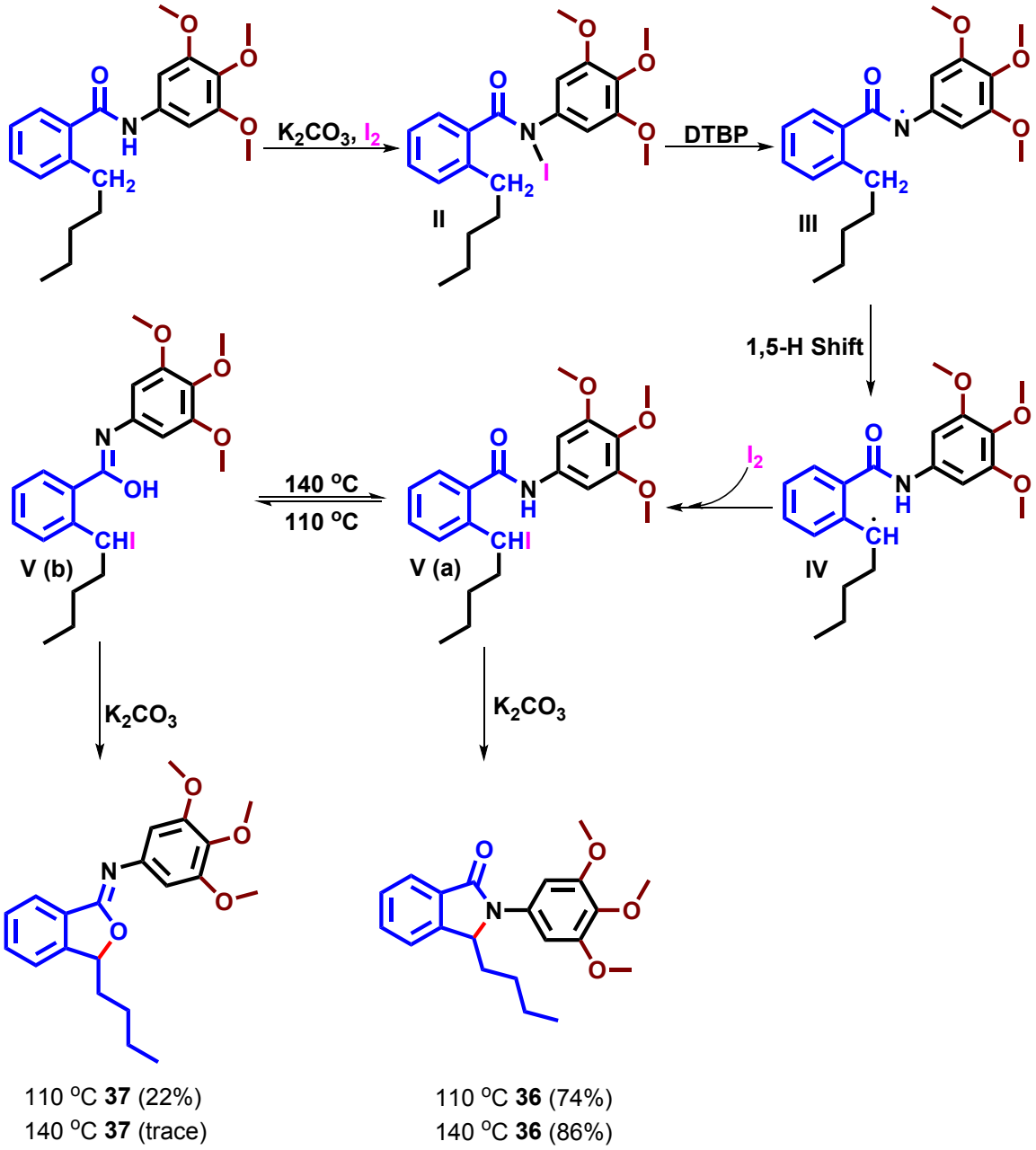
2-Pentyl-*N*-(3,4,5-trimethoxyphenyl)benzamide (Substrate for 36 and 37) White solid, yield 0.378 g (53%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.65 (s, 1H), 7.42 (d, *J* = 7.4 Hz, 1H), 7.40 – 7.35 (m, 1H), 7.32 – 7.26 (m, 1H), 7.22 (t, *J* = 7.4 Hz, 1H), 6.94 (s, 2H), 3.85 (s, 6H), 3.81 (s, 3H), 2.82 (t, *J* = 7.7 Hz, 2H), 1.69 – 1.57 (m, 2H), 1.39 – 1.29 (m, 4H), 0.92 – 0.86 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.4, 153.4, 141.2, 136.4, 134.7, 134.3, 130.3, 130.2, 126.7, 125.8, 97.6, 61.0, 56.1, 33.1, 31.8, 31.3, 22.5, 14.0; **HRMS (ESI)** *m/z* calcd for $C_{21}H_{27}NO_4$ $[M+H]^+$ 358.2013, found 358.2042.

Formation of 3-butyl-2-(3,4,5-trimethoxyphenyl)isoindolin-1-one (36) and 3-butyl-*N*-(2,4,6-trimethoxyphenyl)isobenzofuran-1(3H)-imine (37)



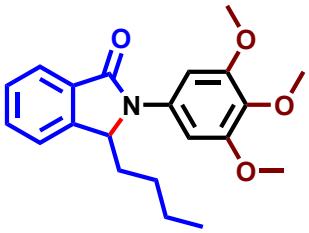
3-Butyl-2-(3,4,5-trimethoxyphenyl)isoindolin-1-one (**36**), second fraction and 3-butyl-*N*-(2,4,6-trimethoxyphenyl)isobenzofuran-1(3H)-imine (**37**), first fraction were obtained in 74 and 22% yields, respectively when reaction was perforemed at 110 °C by the following the procedure as described on S26. Similarly, formation of **38**, **39** and **40**, **41** was observed from respective benzamide substrate. The reaction provided 3-butyl-2-(3,4,5-trimethoxyphenyl)isoindolin-1-one (**36**) in quantitative yields when reaction was carried out at 140 °C.

Possible mechanism

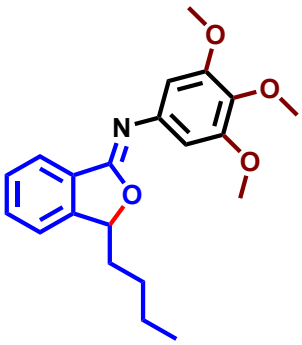


110 °C **37** (22%)
140 °C **37** (trace)

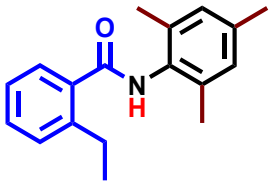
110 °C **36** (74%)
140 °C **36** (86%)



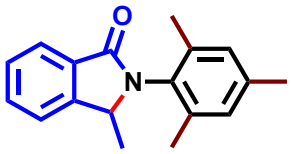
3-Butyl-2-(3,4,5-trimethoxyphenyl)isoindolin-1-one (36). Light brown semi-solid, yield 0.127g (74%) at 110 °C and 86% at 140 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.90 (d, *J* = 7.5 Hz, 1H), 7.59 (td, *J* = 7.4, 0.7 Hz, 1H), 7.49 (m, 2H), 6.79 (s, 2H), 5.22 – 5.10 (m, 1H), 3.87 (s, 6H), 3.84 (d, *J* = 9.0 Hz, 3H), 1.93 –1.87 (m, 1H), 1.68 – 1.60 (m, 1H), 1.15 – 1.09 (m, 2H), 0.94 – 0.83 (m, 3H), 0.72 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.5, 153.5, 144.7, 136.0, 132.9, 132.5, 132.0, 128.4, 124.1, 122.1, 101.8, 61.3, 61.0, 56.3, 36.7, 30.8, 22.4, 13.8; **HRMS (ESI)** *m/z* calcd for $C_{21}H_{25}NO_4$ $[M+H]^+$ 356.1856 found.356.1886.



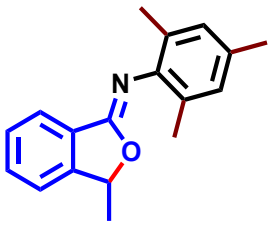
3-Butyl-*N*-(2,4,6-trimethoxyphenyl)isobenzofuran-1(3H)-imine (37). Light brown semi-solid, yield 0.039 g (22%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.93 (d, *J* = 7.6 Hz, 1H), 7.53 (dt, *J* = 7.4, 3.7 Hz, 1H), 7.47 (t, *J* = 6.8 Hz, 1H), 7.34 (d, *J* = 7.4 Hz, 1H), 6.69 (s, 2H), 5.57 (dd, *J* = 7.8, 4.0 Hz, 1H), 3.85 (s, 6H), 3.84 (s, 3H), 2.09 – 1.99 (m, 1H), 1.87 – 1.70 (m, 2H), 1.48 – 1.33 (m, 3H), 0.89 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 158.7, 153.0, 146.6, 142.4, 134.8, 131.9, 131.0, 128.8, 123.9, 121.2, 101.4, 84.7, 60.8, 55.9, 35.1, 27.2, 22.5, 14.0; **HRMS (ESI)** *m/z* calcd for $C_{21}H_{25}NO_4$ $[M+H]^+$ 356.1856 found.356.1891.



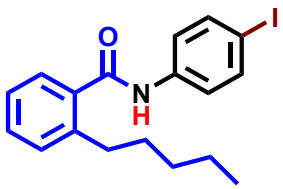
2-Ethyl-*N*-mesitylbenzamide (Substrate for 38 and 39) White solid, yield 0.267 g (60%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.53 (d, *J* = 7.5 Hz, 1H), 7.42 – 7.37 (m, 1H), 7.31 (d, *J* = 7.4 Hz, 1H), 7.25 (dd, *J* = 8.7, 6.1 Hz, 1H), 6.99 (s, 1H), 6.93 (s, 2H), 2.90 (q, *J* = 7.5 Hz, 2H), 2.29 (s, 6H), 2.28 (s, 3H), 1.28 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.8, 142.9, 137.3, 136.2, 135.3, 131.0, 130.3, 129.7, 129.1, 126.8, 125.8, 26.4, 20.9, 18.5, 16.2; **HRMS (ESI)** *m/z* calcd for $C_{18}H_{21}NO$ $[M+H]^+$ 268.1696, found 268.1717.



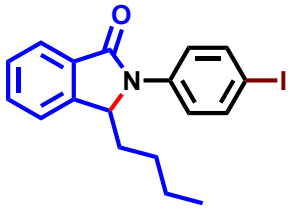
2-Mesityl-3-methylisoindolin-1-one (38). Light brown semi-solid, yield 0.086 g (65%) at 110 °C and 89% at 140 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.94 (d, *J* = 7.5 Hz, 1H), 7.59 (td, *J* = 7.4, 1.0 Hz, 1H), 7.53 – 7.45 (m, 2H), 6.96 (d, *J* = 15.4 Hz, 2H), 4.87 (q, *J* = 6.8 Hz, 1H), 2.30 (s, 3H), 2.19 (s, 3H), 2.10 (s, 3H), 1.38 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 167.4, 147.4, 138.0, 137.7, 136.1, 131.7, 131.6, 131.5, 129.6, 129.5, 128.2, 124.3, 122.1, 58.2, 21.0, 18.7, 18.2, 18.1; **HRMS (ESI)** *m/z* calcd for $C_{18}H_{19}NO$ $[M+H]^+$ 266.1539, found 266.1561.



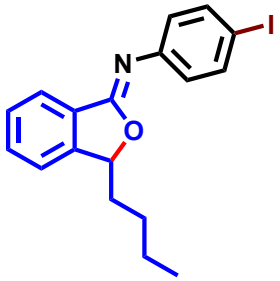
3-Butyl-*N*-mesitylisobenzofuran-1(3H)-imine (39) Semi-solid, yield 0.027 g (18%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.06 (d, *J* = 7.4 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.39 (d, *J* = 7.5 Hz, 1H), 6.92 (s, 2H), 5.59 (q, *J* = 6.5 Hz, 1H), 2.31 (s, 3H), 2.18 (d, *J* = 2.1 Hz, 6H), 1.59 (dd, *J* = 6.6, 0.8 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 157.4, 148.4, 142.6, 132.2, 131.9, 129.7, 128.8, 128.4, 128.1, 124.1, 121.2, 80.3, 21.6, 20.9, 18.3; **HRMS (ESI)** *m/z* calcd for $C_{18}H_{19}NO$ $[M+H]^+$ 266.1539, found 266.1549.



***N*-(4-Iodophenyl)-2-pentylbenzamide (Substrate for 40 and 41)** White solid, yield 0.526 g (67%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.63 (d, *J* = 8.6 Hz, 2H), 7.54 (s, 1H), 7.38 (dd, *J* = 11.7, 7.8 Hz, 4H), 7.27 (d, *J* = 7.5 Hz, 1H), 7.22 (dd, *J* = 13.4, 5.9 Hz, 1H), 2.77 (t, *J* = 7.7 Hz, 2H), 1.60 (m, 2H), 1.34 – 1.16 (m, 4H), 0.84 (t, *J* = 6.9 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.3, 141.4, 138.0, 137.8, 136.1, 130.4, 126.6, 125.9, 121.7, 87.7, 33.2, 31.8, 31.4, 22.5, 14.0; **HRMS (ESI)** *m/z* calcd for $C_{18}H_{20}INO$ $[M+H]^+$ 394.0662, found 394.0691.

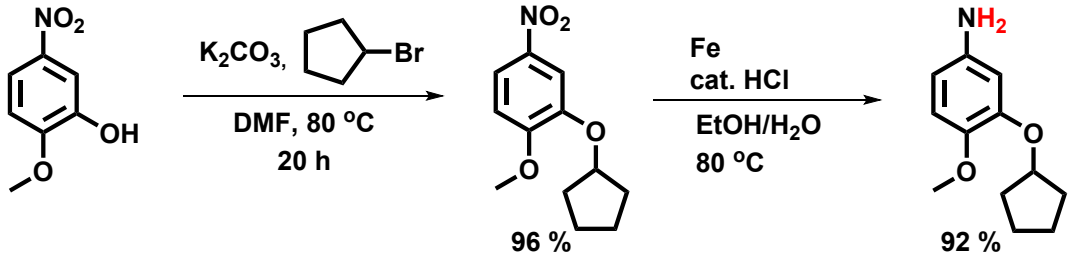


3-Butyl-2-(4-iodophenyl)isoindolin-1-one (40) White solid, yield 0.153 g (78%) at 110 °C and 90% at 140 °C; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.94 (d, *J* = 7.6 Hz, 1H), 7.80 – 7.76 (m, 2H), 7.64 (td, *J* = 7.5, 1.1 Hz, 1H), 7.55 – 7.50 (m, 2H), 7.44 – 7.39 (m, 2H), 5.26 (dd, *J* = 5.4, 3.3 Hz, 1H), 2.01 – 1.86 (m, 2H), 1.18 – 1.08 (m, 2H), 1.05 – 0.97 (m, 1H), 0.82 – 0.77 (m, 1H), 0.72 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 167.3, 144.5, 138.1, 137.0, 132.3, 132.3, 128.5, 124.9, 124.2, 122.2, 89.3, 60.4, 30.5, 24.3, 22.4, 13.8; **HRMS (ESI)** *m/z* calcd for $C_{18}H_{18}INO$ $[M+H]^+$ 392.0506, found 392.0515.

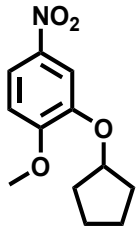


3-Butyl-*N*-(4-iodophenyl)isobenzofuran-1(3H)-imine (41) White solid, yield 0.015g (8%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.93 (d, *J* = 7.6 Hz, 1H), 7.62 (d, *J* = 8.6 Hz, 2H), 7.54 (dt, *J* = 7.5, 3.7 Hz, 1H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.34 (d, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 8.6 Hz, 2H), 5.55 (dd, *J* = 7.1, 4.4 Hz, 1H), 2.09 – 1.94 (m, 1H), 1.81 – 1.74 (m, 2H), 1.33 (m, 3H), 0.90 – 0.85 (m, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.3, 146.8, 146.5, 137.6, 132.0, 130.8, 128.8, 125.9, 124.0, 121.2, 87.7, 84.8, 34.8, 26.7, 22.5, 13.9; **HRMS (ESI)** *m/z* calcd for $C_{18}H_{18}INO$ $[M+H]^+$ 392.0506, found 392.0538.

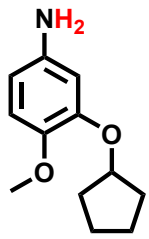
Preparation of 3-(cyclopentyloxy)-4-methoxyaniline



Compund 2-(cyclopentyloxy)-1-methoxy-4-nitrobenzene has been synthesized using standered procedure.[12] To a solution of 2-methoxy-5-nitrophenol (1.5 g, 8.87 mmol) in DMF (25 ml), potassium carbonate (2.7 g, 19.5 mmol), and cyclopentyl bromide (2.0 g, 13.3 mmol) were added and reaction mixture was stirred at 80 °C. After 20 h reaction mixture was cooled to room temperature, treated with 50 ml water, and extracted with diethyl ether (60mL x 3). The ether layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure and gives 2-(cyclopentyloxy)-1-methoxy-4-nitrobenzene in 96% yield. Crude reaction mixture was then subjected for the reduction of nitro group to amine group.



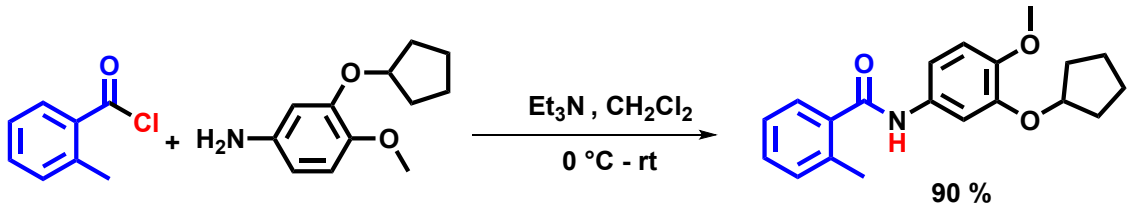
2-(Cyclopentyloxy)-1-methoxy-4-nitrobenzene: [12] White solid, yield 2.018 g (96%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.89 (dd, *J* = 8.9, 2.6 Hz, 1H), 7.74 (d, *J* = 2.6 Hz, 1H), 6.91 (d, *J* = 8.6 Hz, 1H), 4.86 (m, 1H), 3.96 (s, 3H), 2.09 – 1.99 (m, 2H), 1.96 – 1.81 (m, 4H), 1.71 – 1.63 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 155.4, 147.5, 141.3, 117.4, 110.1, 109.1, 81.0, 56.4, 32.7, 24.1; **GC-LRMS** *m/z* calcd for $C_{12}H_{15}NO_4$ $[M]^+$ 237.1, found 237.1.



3-(Cyclopentyloxy)-4-methoxyaniline. [12] In a 100 mL round-bottom flask 2-(cyclopentyloxy)-1-methoxy-4-nitrobenzene (1 g, 4.2 mmol, 1 equiv) was added to the stirring suspension of Fe

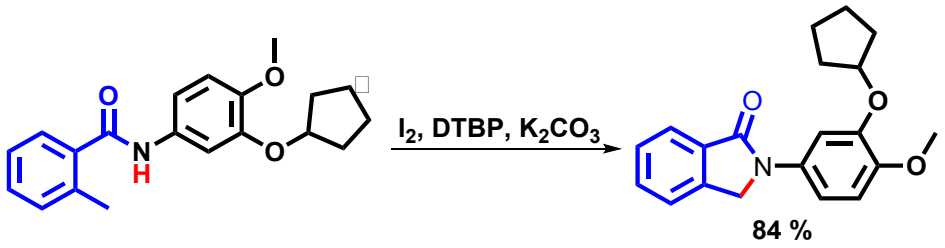
(2.4 g, 42.1 mmol) in ethanol/water (4:1), then HCl (0.1 ml) was added. The reaction mixture was heated under reflux for 4 hours and then cooled to room temperature. Reaction mixture was poured into aqueous saturated $NaHCO_3$ (80 ml), extracted with ethyl acetate (60 mL x 3), washed with brine, dried over Na_2SO_4, and the solvent was removed *in vacuo*. The resulted compound was purified by column chromatography gives 3-(cyclopentyloxy)-4-methoxyaniline in 92% yield. White solid, yield 0.803 g (92%), **^{1}H NMR (400 MHz, $CDCl_3$)** δ 6.69 (dd, *J* = 10.1, 5.5 Hz, 1H), 6.29 (d, *J* = 2.6 Hz, 1H), 6.19 (dd, *J* = 8.4, 2.6 Hz, 1H), 4.69 (m, 1H), 3.74 (s, 3H), 3.35 (s, 2H), 1.92 – 1.85 (m, 4H), 1.84 – 1.73 (m, 2H), 1.65 – 1.50 (m, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 148.8, 143.2, 140.7, 114.5, 106.7, 104.1, 80.3, 57.4, 32.9, 24.1; **GC-LRMS** *m/z* calcd for $C_{12}H_{17}NO_2$ $[M]^+$ 207.1, found 207.1.

Preparation of *N*-(3-(cyclopentyloxy)-4-methoxyphenyl)-2-methylbenzamide



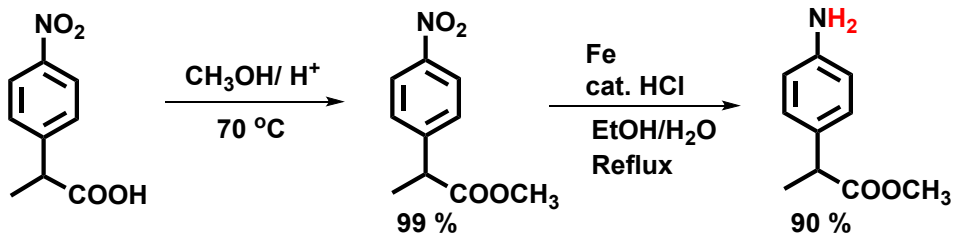
To a stirring solution of 2-methylbenzoyl chloride (226 mg, 2.0 mmol) in CH_2Cl_2 (25 mL), 3-(cyclopentyloxy)-4-methoxyaniline (300 mg, 1.45 mmol) and triethylamine (406 mg, 4.0 mmol) in CH_2Cl_2 (15 mL) were added using a dropping funnel at 0 °C. After complete addition, the reaction mixture was stirred for 4-5 hours at room temperature. After completion of reaction, 10% aqueous HCl solution (10 mL) was added to the reaction mixture. The resulting solution was extracted with CH_2Cl_2 (40 mL × 3), CH_2Cl_2 layer was washed with brine (40 mL) and dried over Na_2SO_4. The organic layer was concentrated on a rotary evaporator under vacuum. Purification of crude reaction mixture using column chromatography gives *N*-(3-(cyclopentyloxy)-4-methoxyphenyl)-2-methylbenzamide in 585 mg, 90 % yield. White solid, yield 0.585 g (90%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.48 – 7.42 (m, 2H), 7.39 (d, *J* = 2.0 Hz, 1H), 7.33 (t, *J* = 7.3 Hz, 1H), 7.22 (dd, *J* = 13.7, 7.2 Hz, 2H), 6.97 (dd, *J* = 8.6, 2.1 Hz, 1H), 6.81 (d, *J* = 8.6 Hz, 1H), 4.87 – 4.71 (m, 1H), 3.82 (s, 3H), 2.48 (s, 3H), 2.02 – 1.87 (m, 3H), 1.87 – 1.73 (m, 2H), 1.68 – 1.52 (m, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.9, 147.9, 146.7, 136.6, 136.4, 131.6, 131.2, 130.2, 126.7, 125.9, 112.3, 111.8, 108.0, 80.6, 56.4, 32.8, 24.1, 19.8; **HRMS (ESI)** *m/z* calcd for $C_{20}H_{23}NO_3$ $[M+H]^+$ 326.1751, found 326.1749.

Preparation of 2-(3-(cyclopentyloxy)-4-methoxyphenyl)isoindolin-1-one (DWP205190)



In a sealed tube, *N*-(3-(cyclopentyloxy)-4-methoxyphenyl)-2-methylbenzamide (1 equiv. 0.5 mmol), iodine (1.5 equiv., 1 mmol), potassium carbonate (2.5 equiv. 1.3 mmol) were added followed by the addition of 2 mL dry acetonitrile. Reaction mixture was stirred at room temperature for 10 minutes. After that, di-*tert*-butyl peroxide (DTBP) (8 equiv, 4 mmol) was added to the reaction mixture and reaction was heated to 125 °C. Progress of the reaction was monitored by thin layer chromatography. After 5 h, reaction mixture was poured into aqueous sodium sulfite solution (15 mL) followed by the extraction with dichloromethane (30 mL x 3). Combined organic layer was washed with brine solution (40 mL), dried over Na_2SO_4. Organic layer was evaporated under reduced pressure at 40 °C. The obtained crude product was purified by column chromatography using ethyl acetate: hexane (1:9) over silica gel gives 2-[3-(Cydopenty~xy)-4-melhoxyphenyl]-l-isoindolinone, **DWP205190** in 84 % yield. White solid, yield 0.109 g (84%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.94 – 7.89 (m, 2H), 7.60 (td, *J* = 7.5, 1.2 Hz, 1H), 7.54 – 7.49 (m, 2H), 7.03 (dd, *J* = 8.7, 2.6 Hz, 1H), 6.90 (d, *J* = 8.7 Hz, 1H), 4.91 – 4.86 (m, 1H), 4.83 (s, 2H), 3.88 (s, 3H), 2.11 – 2.02 (m, 2H), 2.00 – 1.92 (m, 2H), 1.90 – 1.82 (m, 2H), 1.69 – 1.59 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 167.4, 148.0, 147.0, 140.1, 133.4, 133.1, 131.9, 128.4, 123.9, 122.6, 112.0, 110.9, 107.9, 80.6, 56.3, 51.1, 32.9, 24.2.**HRMS (ESI)** *m/z* calcd for $C_{20}H_{11}NO_3$ $[M+H]^+$ 324.1594, found 324.1629.

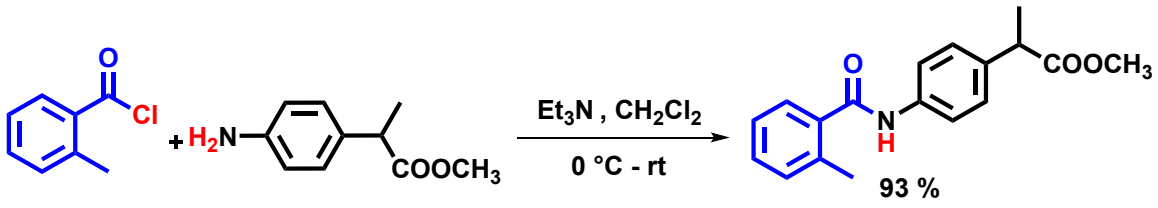
Preparation of methyl-2-(4-aminophenyl)propanoate



Methyl-2-(4-nitrophenyl)propanoate: In a 100 mL round bottom flask 2-(4-nitrophenyl)propanoic acid (1 g , 5.1 mmol), 80 mL methanol and 3-drops of conc. H_2SO_4 were added, resulted solution was refluxed at 70 ^oC for 5 h, reaction was quenched in saturated solution of sodium bicarbonate and extracted by ethyl acetate (60 mL x 3)), washed with brine, dried over Na_2SO_4 and the solvent was removed *in vacuo*. The resulted compound methyl-2-(4-nitrophenyl)propanoate was obtained in 1.034g, 99% yield. White solid, **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.23 – 8.15 (m, 2H), 7.51 – 7.45 (m, 2H), 3.86 (q, *J* = 7.3 Hz, 1H), 3.70 (s, 3H), 1.56 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 173.7, 147.7, 147.1, 128.6, 123.9, 52.4, 45.3, 18.4; **GC-LRMS** *m/z* calcd for $C_{10}H_{11}NO_4$ $[M]^+$ 209.0, found 209.0.

Methyl-2-(4-aminophenyl)propanoate: In a 100 mL round-bottom flask, methyl-2-(4-nitrophenyl)propanoate (1 g, 4.8 mmol, 1 equiv) was added to the stirring suspension of Fe (2.68 g, 47.8 mmol, 10 equiv) in ethanol/water (4:1), then HCl (0.1 ml) was added. The reaction mixture was heated under reflux for 4 h and then cooled to room temperature. Reaction mixture was poured into aqueous saturated sodium bicarbonate (80 mL), extracted with ethyl acetate (60 mL x 3), washed with brine, dried over Na_2SO_4 and the solvent was removed *in vacuo*. The crude reaction mixture was purified using column chromatography resulting in methyl-2-(4-aminophenyl)propanoate in 0.773 g, 90% yield. White solid, **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.07 (d, *J* = 8.4 Hz, 2H), 6.62 (d, *J* = 8.4 Hz, 2H), 3.63 (s, 3H), 3.62 – 3.57 (m, 1H), 1.44 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 175.5, 145.5, 130.5, 128.3, 115.3, 51.9, 44.6, 18.6; **GC-LRMS** *m/z* calcd for $C_{10}H_{13}NO_2$ $[M]^+$ 179.0, found 179.1.

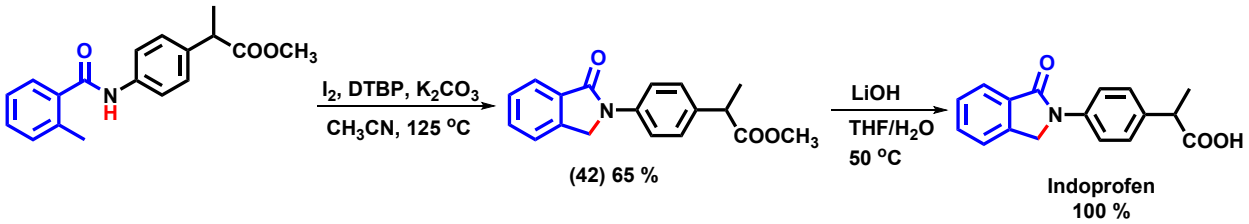
Preparation of methyl-(4-(2-methylbenzamido)phenyl)propanoate



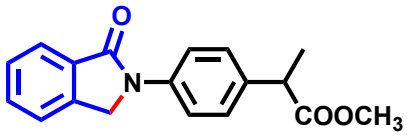
To a stirring solution of 2-methylbenzoyl chloride (459 mg, 2.94 mmol) in CH_2Cl_2 (25 mL), methyl-2-(4-aminophenyl)propanoate (631 mg, 3.53 mmol) and triethylamine (1.19 g, 4.0 mmol) in CH_2Cl_2 (15 mL) were added using a dropping funnel at 0 °C. After complete addition, the reaction mixture was stirred for 4-5 hours at room temperature. After completion of reaction 10% aqueous HCl solution (10 mL) was added to the reaction mixture. The resulting solution was extracted with CH_2Cl_2 (40 mL × 3), the combined organic layer was

washed with brine (40 mL) and dried over Na_2SO_4. The organic layer was concentrated on a rotary evaporator under vacuum. Crude reaction mixture was purified using column chromatography which provided methyl-(4-(2-methylbenzamido)phenyl)propanoate in 0.812 g, 93% yield. White solid, **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.63 (s, 1H), 7.55 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 7.5 Hz, 1H), 7.36 – 7.29 (m, 1H), 7.29 – 7.17 (m, 4H), 3.74 – 3.66 (m, 1H), 3.63 (s, 3H), 2.46 (s, 3H), 1.47 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 175.0, 168.1, 137.0, 136.7, 136.4, 136.3, 131.3, 130.3, 128.2, 126.6, 125.9, 120.2, 52.1, 44.9, 19.8, 18.5; **HRMS (ESI)** *m/z* calcd for $C_{18}H_{19}NO_3$ $[M+H]^+$ 298.1438, found 298.1464.

Preparation of Indoprofen

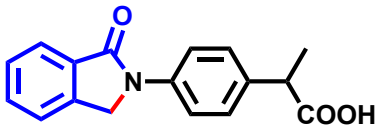


Methyl-2-(4-(1-oxoisoindolin-2-yl)phenyl)propanoate (42) In a sealed tube, methyl-(4-(2-methyl-benzamido)phenyl)propanoate (1 equiv. 0.5 mmol), iodine (1.5 equiv., 1 mmol), potassium carbonate (2.5 equiv. 1.3 mmol) were added followed by the addition of 2 mL dry acetonitrile. Reaction mixture was stirred at room temperature for 10 minutes. After that, DTBP (8 equiv, 4 mmol) was added to the reaction mixture and reaction was heated to 125 °C. Progress of the reaction was monitored by thin layer chromatography. After completion, reaction mixture was poured into aqueous sodium sulfite solution (15 mL) followed by the extraction with dichloromethane (30 mL x 3). Combined organic layer was washed with brine solution (40 mL), dried over sodium sulfate. Organic layer was evaporated under reduced pressure at 40 °C. The obtained crude product was purified by column chromatography using ethyl acetate: hexane (1:9) over silica gel gives compound **42** in 65 % yield.

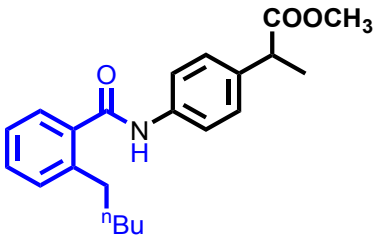


White solid, yield 0.095 g (65%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.94 (d, *J* = 7.5 Hz, 1H), 7.87 – 7.82 (m, 2H), 7.64 – 7.60 (m, 1H), 7.53 (m, 2H), 7.38 (dd, *J* = 9.0, 2.2 Hz, 2H), 4.86 (s, 2H), 3.80 – 3.74 (m, 1H), 3.69 (s, 3H), 1.54 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ

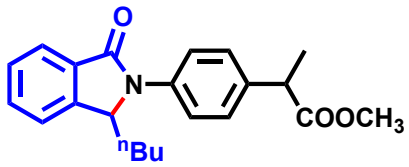
175.0, 167.5, 140.1, 138.5, 136.6, 133.2, 132.1, 128.4, 128.3, 124.2, 122.7, 119.7, 52.1, 50.7, 44.92, 18.5; **HRMS (ESI)** *m/z* calcd for $C_{18}H_{17}NO_3$ $[M+H]^+$ 296.1281, found 296.1290.



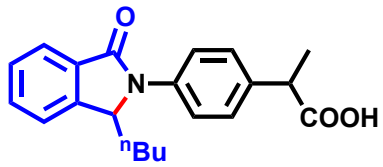
2-(4-(1-Oxoisoindolin-2-yl)phenyl)propanoic acid (Indoprofen): In a 25 mL RB flask, compound **42** (50 mg, 0.16 mmol), was dissolved in a 1:1 mixture of THF and water (6 + 6 mL) followed by addition of the LiOH (31 mg, 1.28 mmol). The resulted mixture was heated upto 50 ^oC for 10 h. Reaction mixture was then cooled to room temperature, quenched with 15 mL of 10% aqueous HCl, extracted with ethyl acetate (10 mL x 3), washed with brine, dried over sodium sulfate. The organic layer was concentrated on a rotary evaporator under vacuum. The resulted compound was pure in 100% yield. White solid, yield 0.045 g (100%); **^{1}H NMR (500 MHz, DMSO)** δ 12.36 (s, 1H), 7.89 – 7.84 (m, 2H), 7.79 (d, *J* = 7.6 Hz, 1H), 7.71 – 7.66 (m, 2H), 7.56 (m, 1H), 7.37 (d, *J* = 8.7 Hz, 2H), 5.02 (s, 2H), 3.70 (q, *J* = 7.1 Hz, 1H), 1.39 (d, *J* = 7.1 Hz, 3H); **^{13}C NMR (125 MHz, DMSO)** δ 175.9, 167.0, 141.5, 138.6, 137.5, 132.9, 132.7, 128.7, 128.4, 123.8, 123.7, 119.9, 50.9, 44.6, 19.0; **HRMS (ESI)** *m/z* calcd for $C_{17}H_{15}NO_3$ $[M+H]^+$ 282.1125, found 282.1149.



Methyl-2-(4-(2-pentylbenzamido)phenyl)propanoate (substrate for 43): White solid, yield 0.263 g (52%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.70 (s, 1H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.40 (m, 2H), 7.33 – 7.29 (m, 3H), 7.24 (t, *J* = 7.5 Hz, 1H), 3.74 (q, *J* = 7.2 Hz, 1H), 3.67 (s, 3H), 2.91 – 2.74 (t , *J* = 7.7 Hz, 2H), 1.73 – 1.57 (m, 2H), 1.52 (d, *J* = 7.2 Hz, 3H), 1.39 – 1.25 (m, 4H), 0.91 – 0.86 (m, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 175.0, 168.3, 141.3, 137.1, 136.7, 136.4, 130.3, 130.2, 128.2, 126.7, 125.9, 120.3, 52.1, 44.9, 33.2, 31.8, 31.4, 22.5, 18.6, 14.0; **HRMS (ESI)** *m/z* calcd for $C_{22}H_{27}NO_3$ $[M+Na]^+$ 376.1883, found 376.1896.



Methyl-2-(4-(1-butyl-3-oxoisoindolin-2-yl)phenyl)propanoate (43). Beige semi-solid, yield 0.131 g (75%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.92 (dd, *J* = 14.3, 5.2 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.54 – 7.44 (m, 4H), 7.36 (dd, *J* = 8.4, 1.3 Hz, 2H), 5.23 (dd, *J* = 5.1, 3.5 Hz, 1H), 3.73 (qd, *J* = 7.1, 1.5 Hz, 1H), 3.66 (d, *J* = 2.5 Hz, 3H), 1.97 – 1.80 (m, 2H), 1.53 – 1.47 (m, 3H), 1.15 – 1.04 (m, 2H), 0.92 – 0.71 (m, 2H), 0.67 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 174.9, 167.4, 144.7, 137.4, 136.2, 132.6, 131.9, 128.3, 128.2, 124.0, 123.5, 122.1, 60.7, 52.1, 44.9, 30.6, 24.4, 22.3, 18.7, 13.7; **HRMS (ESI)** *m/z* calcd for $C_{22}H_{25}NO_3$ $[M+Na]^+$ 374.1727, found 374.1755.



2-(4-(1-Butyl-3-oxoisoindolin-2-yl)phenyl)propanoic acid (44) White solid, yield 0.054 g (100%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.91 (d, *J* = 7.5 Hz, 1H), 7.58 (t, *J* = 7.3 Hz, 1H), 7.55 – 7.44 (m, 4H), 7.39 (d, *J* = 8.4 Hz, 2H), 5.27 – 5.20 (m, 1H), 3.82 – 3.71 (m, 1H), 1.96 – 1.83 (m, 2H), 1.52 (dd, *J* = 7.0, 4.2 Hz, 3H), 1.15 – 1.00 (m, 3H), 0.86 (m, 1H), 0.68 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 179.6, 167.6, 144.8, 137.1, 137.1, 136.1, 132.4, 132.1, 128.4, 124.2, 123.7, 122.1, 60.9, 44.9, 30.5, 24.4, 22.4, 18.2, 13.8; **HRMS (ESI)** *m/z* calcd for $C_{22}H_{25}NO_3$ $[M+Na]^+$ 374.1727, found 374.1755.

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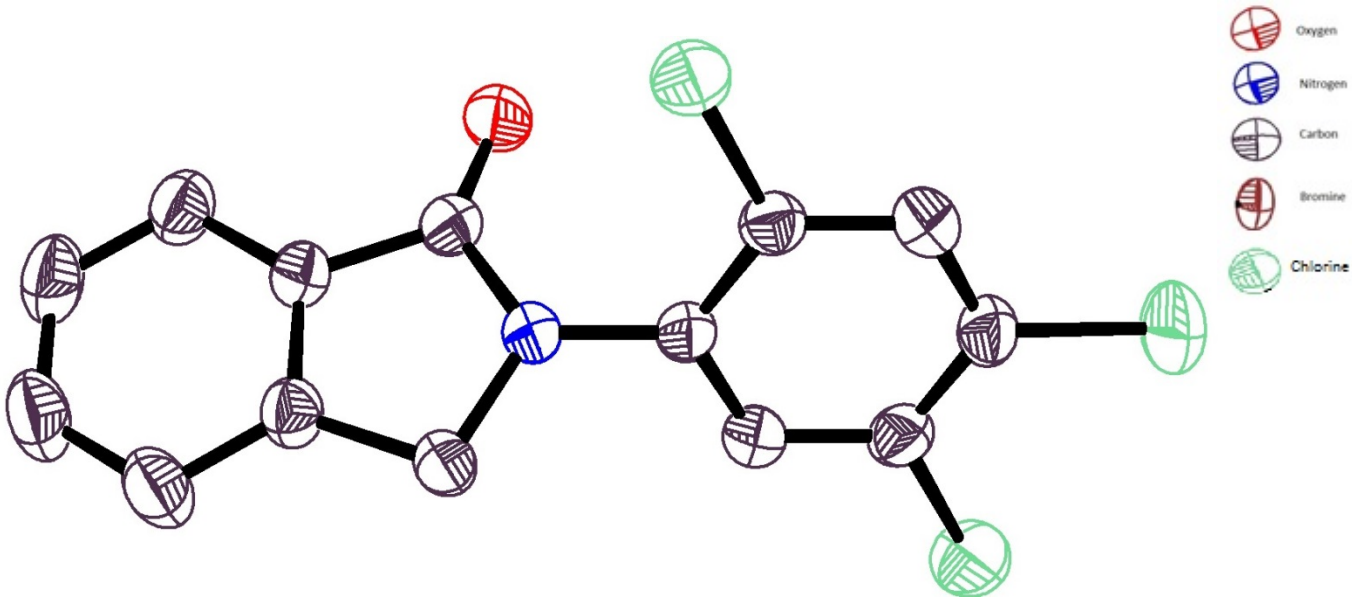
Crystal Structure of 2-(2,4,5-trichlorophenyl)isoindolin-1-one (8) (CCDC No.- 1021394)



Packing diagram of 2-(2,4,5-trichlorophenyl)isoindolin-1-one (8)

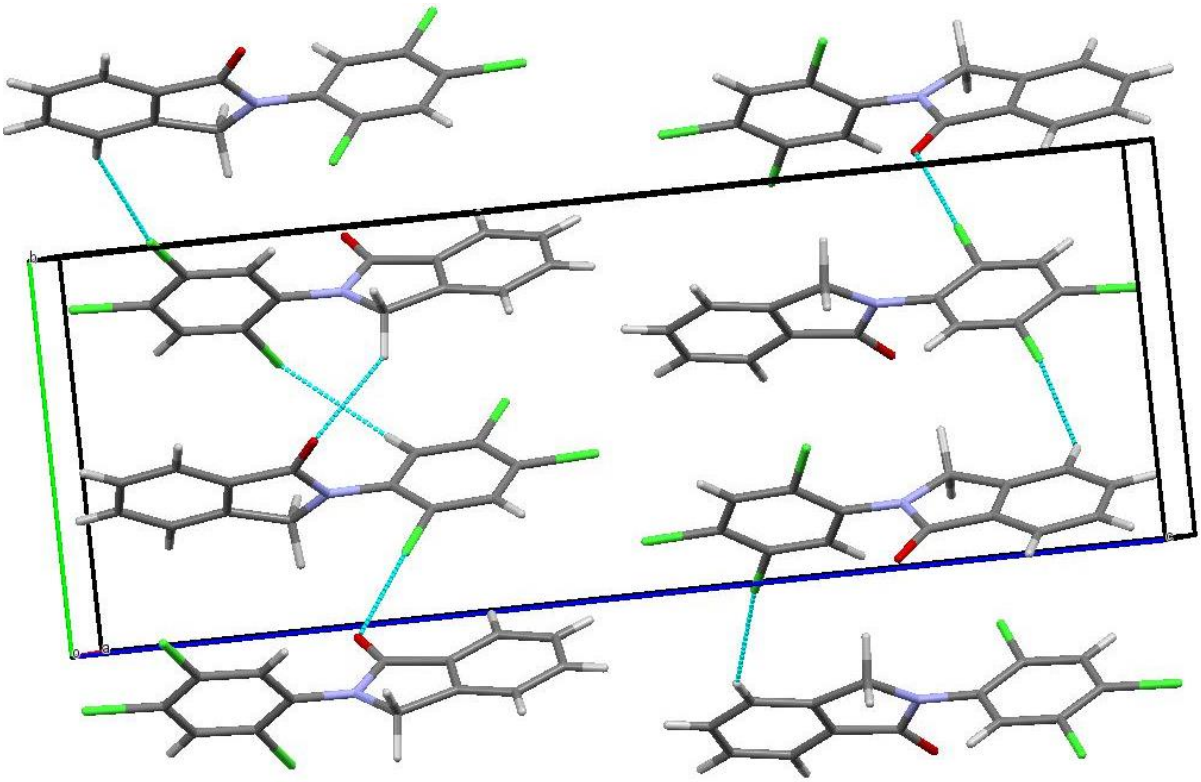


Table 1. Crystal data and structure refinement for 8

Identification code	2-(2,4,5-trichlorophenyl)isoindolin-1-one	
Empirical formula	C_{14} H_8 Cl_3 N O	
Formula weight	312.56	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 2_1 2_1 2_1	
Unit cell dimensions	a = 6.2868(5) Å	α= 90°.
	b = 8.7137(5) Å	β= 90°.
	c = 24.2013(17) Å	γ = 90°.
Volume	1325.78(15) $Å^3$	
Z	4	
Density (calculated)	1.566 Mg/m^3	
Absorption coefficient	0.679 mm^{-1}	
F(000)	632	
Theta range for data collection	2.484 to 29.992°.	
Index ranges	-8<=h<=8, -12<=k<=12, -34<=l<=7	
Reflections collected	7221	
Independent reflections	3773 [R(int) = 0.0238]	
Completeness to theta = 25.242°	99.5 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3773 / 0 / 172	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0355, wR2 = 0.0731	
R indices (all data)	R1 = 0.0658, wR2 = 0.0808	
Absolute structure parameter	0.45(2)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.293 and -0.177 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 8. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	1789(1)	1727(1)	3071(1)	48(1)
Cl(2)	6639(1)	3655(1)	4745(1)	72(1)
Cl(3)	9847(1)	5158(1)	3893(1)	68(1)
O(1)	1824(3)	4725(2)	2343(1)	49(1)
N(1)	4982(3)	3373(2)	2334(1)	37(1)
C(9)	5383(3)	3405(3)	2911(1)	35(1)
C(1)	3256(4)	4082(2)	2096(1)	36(1)
C(2)	3566(4)	3921(2)	1492(1)	37(1)
C(10)	7194(4)	4142(3)	3107(1)	40(1)
C(14)	4008(4)	2726(3)	3290(1)	36(1)
C(13)	4397(4)	2813(3)	3851(1)	44(1)
C(7)	5479(4)	3195(3)	1392(1)	39(1)
C(12)	6184(4)	3562(3)	4042(1)	43(1)
C(8)	6540(4)	2794(3)	1934(1)	40(1)
C(11)	7587(4)	4222(3)	3670(1)	42(1)
C(3)	2282(4)	4445(3)	1065(1)	48(1)
C(6)	6173(5)	2975(3)	855(1)	55(1)
C(4)	2984(5)	4211(3)	529(1)	57(1)
C(5)	4885(5)	3493(3)	429(1)	60(1)

Table 3. Bond lengths [Å] for 8

Cl1—C14	1.728 (2)	C2—C3	1.388 (3)
Cl2—C12	1.728 (2)	C10—C11	1.388 (3)
Cl3—C11	1.725 (2)	C14—C13	1.382 (3)
O1—C1	1.218 (3)	C13—C12	1.379 (4)
N1—C1	1.375 (3)	C7—C6	1.386 (3)
N1—C9	1.419 (3)	C7—C8	1.512 (3)
N1—C8	1.467 (3)	C12—C11	1.385 (3)
C9—C10	1.391 (3)	C3—C4	1.385 (4)
C9—C14	1.392 (3)	C6—C5	1.386 (4)
C1—C2	1.480 (3)	C4—C5	1.371 (4)
C2—C7	1.380 (3)		

Table 4. Bond angles [°] for 8

C1—N1—C9	122.99 (18)	C12—C13—C14	119.9 (2)
C1—N1—C8	113.87 (17)	C2—C7—C6	120.2 (2)
C9—N1—C8	122.48 (18)	C2—C7—C8	109.75 (19)
C10—C9—C14	118.67 (19)	C6—C7—C8	130.1 (2)
C10—C9—N1	119.35 (19)	C13—C12—C11	119.9 (2)
C14—C9—N1	121.98 (19)	C13—C12—Cl2	119.13 (19)
O1—C1—N1	125.7 (2)	C11—C12—Cl2	120.97 (19)
O1—C1—C2	128.8 (2)	N1—C8—C7	101.43 (18)
N1—C1—C2	105.52 (19)	C12—C11—C10	120.3 (2)
C7—C2—C3	121.8 (2)	C12—C11—Cl3	121.21 (18)
C7—C2—C1	109.3 (2)	C10—C11—Cl3	118.54 (18)

C3—C2—C1	128.8 (2)	C4—C3—C2	117.6 (2)
C11—C10—C9	120.3 (2)	C7—C6—C5	118.0 (3)
C13—C14—C9	121.0 (2)	C5—C4—C3	120.8 (2)
C13—C14—Cl1	118.15 (19)	C4—C5—C6	121.7 (2)
C9—C14—Cl1	120.86 (17)		

Table 5. Anisotropic displacement parameters ($Å^2$x 10^3) for 8. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	43(1)	52(1)	49(1)	-2(1)	-1(1)	-12(1)
Cl(2)	75(1)	111(1)	32(1)	-4(1)	-7(1)	-5(1)
Cl(3)	49(1)	96(1)	59(1)	-20(1)	-8(1)	-19(1)
O(1)	42(1)	62(1)	43(1)	-5(1)	2(1)	15(1)
N(1)	34(1)	49(1)	30(1)	0(1)	1(1)	5(1)
C(9)	32(1)	41(1)	32(1)	-2(1)	-1(1)	5(1)
C(1)	34(1)	39(1)	37(1)	0(1)	-2(1)	2(1)
C(2)	39(1)	37(1)	34(1)	-2(1)	-4(1)	-1(1)
C(10)	35(1)	49(1)	37(1)	1(1)	1(1)	-2(1)
C(14)	33(1)	38(1)	38(1)	-1(1)	-1(1)	2(1)
C(13)	42(1)	53(1)	36(1)	3(1)	5(1)	-2(1)
C(7)	44(1)	40(1)	33(1)	2(1)	-2(1)	3(1)
C(12)	45(1)	53(2)	30(1)	-4(1)	-3(1)	6(1)
C(8)	39(1)	48(1)	32(1)	2(1)	2(1)	9(1)
C(11)	34(1)	50(1)	41(1)	-7(1)	-5(1)	1(1)

C(3)	49(1)	54(1)	42(1)	-2(1)	-10(1)	7(1)
C(6)	64(2)	66(2)	37(1)	3(1)	9(1)	18(1)
C(4)	70(2)	64(2)	37(1)	3(1)	-15(1)	7(2)
C(5)	79(2)	71(2)	30(1)	0(1)	2(1)	10(2)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 8.

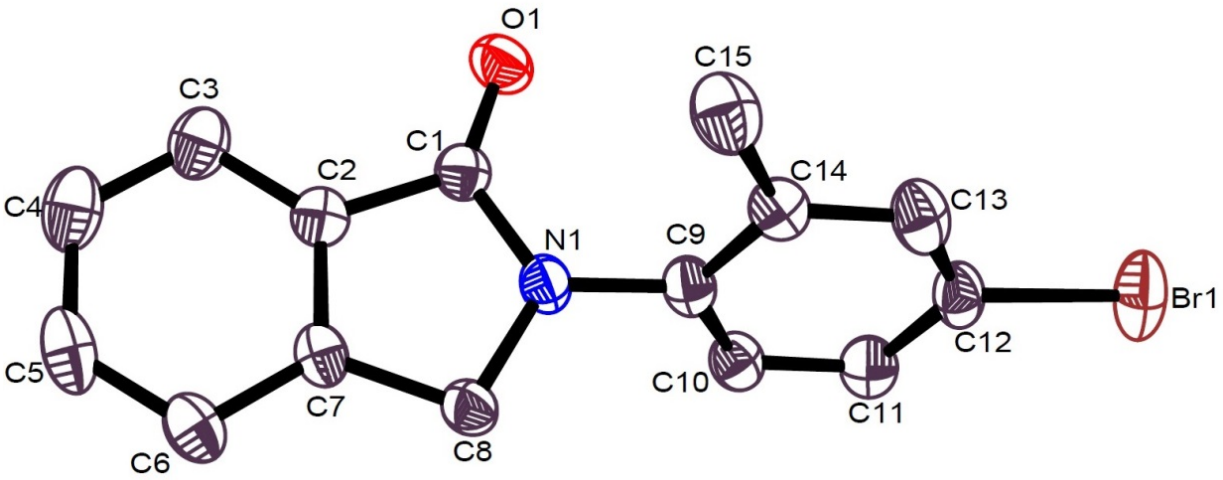
	x	y	z	U(eq)
H(10)	8166	4593	2854	48
H(13)	3434	2357	4105	53
H(8A)	6746	1672	1972	48
H(8B)	7929	3317	1974	48
H(3)	969	4945	1138	58
H(6)	7492	2485	780	67
H(4)	2139	4553	228	68
H(5)	5331	3345	57	72

Table 7. Torsion angles [°] for 8

C1—N1—C9—C10	−115.5 (2)	C3—C2—C7—C8	178.6 (2)
C8—N1—C9—C10	54.6 (3)	C1—C2—C7—C8	1.4 (3)
C1—N1—C9—C14	64.1 (3)	C14—C13—C12—C11	−0.2 (4)
C8—N1—C9—C14	−125.8 (2)	C14—C13—C12—Cl2	−179.9 (2)
C9—N1—C1—O1	−4.8 (4)	C1—N1—C8—C7	−2.2 (2)
C8—N1—C1—O1	−175.7 (2)	C9—N1—C8—C7	−173.07 (19)

C9—N1—C1—C2	173.86 (19)	C2—C7—C8—N1	0.4 (2)
C8—N1—C1—C2	3.0 (2)	C6—C7—C8—N1	178.5 (3)
O1—C1—C2—C7	176.0 (2)	C13—C12—C11—C10	0.5 (4)
N1—C1—C2—C7	−2.6 (2)	Cl2—C12—C11—C10	−179.77 (19)
O1—C1—C2—C3	−1.0 (4)	C13—C12—C11—Cl3	−179.58 (19)
N1—C1—C2—C3	−179.6 (2)	Cl2—C12—C11—Cl3	0.2 (3)
C14—C9—C10—C11	−1.3 (3)	C9—C10—C11—C12	0.3 (4)
N1—C9—C10—C11	178.2 (2)	C9—C10—C11—Cl3	−179.67 (17)
C10—C9—C14—C13	1.6 (3)	C7—C2—C3—C4	0.2 (4)
N1—C9—C14—C13	−177.9 (2)	C1—C2—C3—C4	176.8 (2)
C10—C9—C14—Cl1	−177.39 (17)	C2—C7—C6—C5	−0.5 (4)
N1—C9—C14—Cl1	3.1 (3)	C8—C7—C6—C5	−178.5 (3)
C9—C14—C13—C12	−0.9 (4)	C2—C3—C4—C5	−0.2 (4)
Cl1—C14—C13—C12	178.15 (19)	C3—C4—C5—C6	−0.1 (5)
C3—C2—C7—C6	0.2 (4)	C7—C6—C5—C4	0.4 (5)
C1—C2—C7—C6	−177.0 (2)		

Crystal Structure of 2-(4-bromo-2-methylphenyl)isoindolin-1-one (11) (CCDC- 1019580)



Packing diagram of 2-(4-bromo-2-methylphenyl)isoindolin-1-one 11

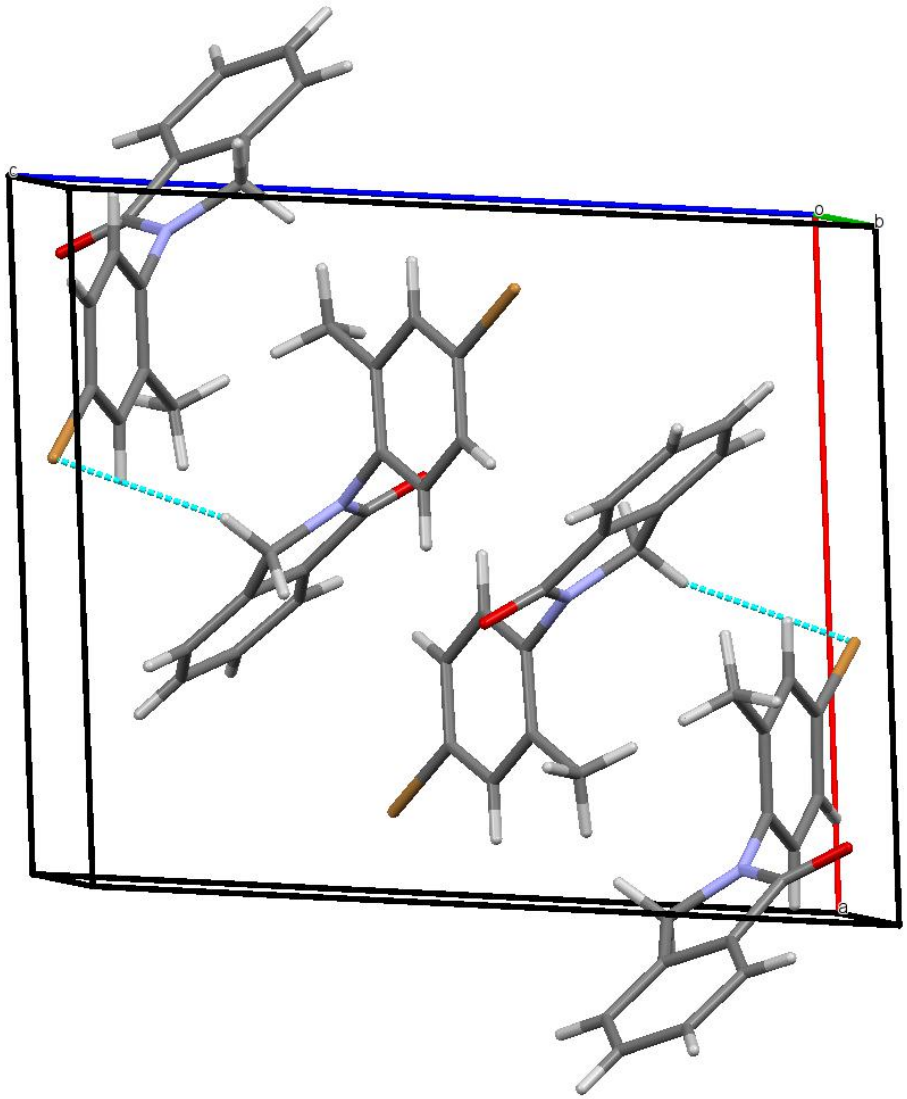


Table 8. Crystal data and structure refinement for 11

Identification code	2-(4-bromo-2-methylphenyl)isoindolin-1-one	
Empirical formula	C_{15} H_{12} Br N O	
Formula weight	302.17	
Temperature	160(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	a = 11.335(3) Å	α= 90°.
	b = 8.635(2) Å	β= 94.87(2)°.
	c = 13.184(4) Å	γ = 90°.
Volume	1285.8(6) $Å^3$	
Z	4	
Density (calculated)	1.561 Mg/m^3	
Absorption coefficient	3.183 mm^{-1}	
F(000)	608	
Theta range for data collection	2.476 to 28.051°.	
Index ranges	-14<=h<=14, 0<=k<=11, 0<=l<=17	
Reflections collected	3273	
Independent reflections	3070 [R(int) = 0.691]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3070 / 0 / 164	
Goodness-of-fit on F^2	1.093	
Final R indices [I>2sigma(I)]	R1 = 0.0570, wR2 = 0.1624	
R indices (all data)	R1 = 0.0884, wR2 = 0.1825	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.992 and -1.324 $e.Å^{-3}$	

Table 9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 11. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	3904(1)	8724(1)	10214(1)	54(1)
O(1)	1048(2)	1794(4)	9517(2)	40(1)
N(1)	640(3)	3771(4)	8351(2)	31(1)
C(4)	-1615(4)	-444(5)	7287(4)	44(1)
C(3)	-791(4)	19(5)	8058(3)	40(1)
C(2)	-357(3)	1509(4)	8017(3)	29(1)
C(1)	526(3)	2295(5)	8734(3)	29(1)
C(9)	1422(3)	4930(5)	8779(3)	31(1)
C(14)	2644(3)	4726(5)	8755(3)	32(1)
C(13)	3365(4)	5898(5)	9173(3)	39(1)
C(12)	2888(4)	7188(5)	9597(3)	36(1)
C(15)	3163(4)	3303(6)	8300(4)	45(1)
C(8)	-114(3)	4053(5)	7417(3)	31(1)
C(7)	-729(3)	2528(4)	7246(3)	29(1)
C(5)	-2001(4)	580(6)	6515(3)	42(1)
C(6)	-1572(3)	2083(5)	6476(3)	37(1)
C(10)	958(4)	6234(5)	9186(3)	33(1)
C(11)	1686(4)	7399(5)	9599(3)	37(1)

Table 10. Bond lengths [Å] for 11

Br1—C12	1.894 (4)	C13—C12	1.377 (6)
O1—C1	1.225 (5)	C13—H13	0.93
N1—C1	1.381 (5)	C12—C11	1.375 (6)
N1—C9	1.422 (5)	C15—H15A	0.96
N1—C8	1.458 (5)	C15—H15C	0.96
C4—C3	1.380 (6)	C15—H15B	0.96

C4—C5	1.390 (7)	C8—C7	1.498 (5)
C4—H4	0.93	C8—H8A	0.97
C3—C2	1.380 (5)	C8—H8B	0.97
C3—H3	0.93	C7—C6	1.388 (5)
C2—C7	1.384 (6)	C5—C6	1.389 (7)
C2—C1	1.481 (6)	C5—H5	0.93
C9—C10	1.371 (5)	C6—H6	0.93
C9—C14	1.399 (5)	C10—C11	1.383 (6)
C14—C13	1.386 (6)	C10—H10	0.93
C14—C15	1.509 (6)	C11—H11	0.93

Table 11. Bond angles [°] for 11

C1—N1—C9	125.4 (3)	C14—C15—H15A	109.5
C1—N1—C8	113.4 (3)	C14—C15—H15C	109.5
C9—N1—C8	121.2 (3)	H15A—C15—H15C	109.5
C3—C4—C5	120.4 (4)	C14—C15—H15B	109.5
C3—C4—H4	119.8	H15A—C15—H15B	109.5
C5—C4—H4	119.8	H15C—C15—H15B	109.5
C2—C3—C4	117.6 (4)	N1—C8—C7	102.2 (3)
C2—C3—H3	121.2	N1—C8—H8A	111.3
C4—C3—H3	121.2	C7—C8—H8A	111.3
C3—C2—C7	122.3 (4)	N1—C8—H8B	111.3
C3—C2—C1	128.8 (4)	C7—C8—H8B	111.3
C7—C2—C1	108.9 (3)	H8A—C8—H8B	109.2
O1—C1—N1	125.5 (4)	C2—C7—C6	120.6 (4)
O1—C1—C2	128.9 (4)	C2—C7—C8	109.9 (3)
N1—C1—C2	105.6 (3)	C6—C7—C8	129.5 (4)
C10—C9—C14	121.7 (4)	C6—C5—C4	122.2 (4)
C10—C9—N1	119.1 (3)	C6—C5—H5	118.9
C14—C9—N1	119.2 (4)	C4—C5—H5	118.9
C13—C14—C9	116.8 (4)	C7—C6—C5	117.0 (4)

C13—C14—C15	121.1 (4)	C7—C6—H6	121.5
C9—C14—C15	122.1 (4)	C5—C6—H6	121.5
C12—C13—C14	120.9 (4)	C9—C10—C11	121.1 (4)
C12—C13—H13	119.6	C9—C10—H10	119.5
C14—C13—H13	119.6	C11—C10—H10	119.5
C11—C12—C13	122.1 (4)	C12—C11—C10	117.4 (4)
C11—C12—Br1	118.2 (3)	C12—C11—H11	121.3
C13—C12—Br1	119.7 (3)	C10—C11—H11	121.3

Table 12. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 11. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	56(1)	61(1)	45(1)	-11(1)	7(1)	-32(1)
O(1)	37(2)	47(2)	35(2)	8(1)	-5(1)	-2(1)
N(1)	30(2)	35(2)	26(2)	2(1)	-1(1)	-7(1)
C(4)	41(2)	44(3)	50(3)	-12(2)	17(2)	-13(2)
C(3)	39(2)	38(3)	44(2)	-3(2)	11(2)	-7(2)
C(2)	26(2)	33(2)	30(2)	-2(2)	9(2)	1(2)
C(1)	26(2)	32(2)	31(2)	1(2)	5(2)	-1(2)
C(9)	31(2)	38(2)	24(2)	1(2)	2(2)	-7(2)
C(14)	31(2)	40(2)	26(2)	2(2)	6(2)	-2(2)
C(13)	30(2)	55(3)	32(2)	0(2)	9(2)	-10(2)
C(12)	35(2)	46(3)	29(2)	4(2)	2(2)	-15(2)
C(15)	32(2)	55(3)	49(3)	-9(2)	10(2)	0(2)
C(8)	32(2)	35(2)	26(2)	3(2)	-2(2)	-3(2)
C(7)	25(2)	35(2)	27(2)	-7(2)	4(2)	-2(2)
C(5)	31(2)	58(3)	37(2)	-20(2)	6(2)	-11(2)
C(6)	31(2)	48(3)	30(2)	-6(2)	2(2)	-1(2)
C(10)	28(2)	39(3)	32(2)	0(2)	5(2)	-2(2)
C(11)	39(2)	41(3)	31(2)	-1(2)	5(2)	-5(2)

Table 13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 11

	x	y	z	U(eq)
H(4)	-1914	-1447	7284	53
H(3)	-538	-648	8586	48
H(13)	4182	5813	9167	47
H(15A)	3987	3475	8220	67
H(15C)	2752	3093	7648	67
H(15B)	3081	2434	8743	67
H(8A)	352	4310	6856	37
H(8B)	-675	4880	7506	37
H(5)	-2564	247	6008	50
H(6)	-1837	2761	5958	44
H(10)	141	6337	9183	39
H(11)	1374	8290	9869	44

Table 14. Torsion angles [°] for 11

C5—C4—C3—C2	−1.3 (6)	C15—C14—C13—C12	−179.3 (4)
C4—C3—C2—C7	0.7 (6)	C14—C13—C12—C11	−2.0 (6)
C4—C3—C2—C1	−179.8 (4)	C14—C13—C12—Br1	177.3 (3)
C9—N1—C1—O1	3.0 (6)	C1—N1—C8—C7	−0.5 (4)
C8—N1—C1—O1	−178.6 (4)	C9—N1—C8—C7	178.1 (3)
C9—N1—C1—C2	−178.2 (3)	C3—C2—C7—C6	0.3 (6)
C8—N1—C1—C2	0.3 (4)	C1—C2—C7—C6	−179.3 (3)
C3—C2—C1—O1	−0.7 (6)	C3—C2—C7—C8	179.3 (3)
C7—C2—C1—O1	178.8 (4)	C1—C2—C7—C8	−0.3 (4)
C3—C2—C1—N1	−179.5 (4)	N1—C8—C7—C2	0.5 (4)
C7—C2—C1—N1	0.1 (4)	N1—C8—C7—C6	179.3 (3)
C1—N1—C9—C10	−113.3 (4)	C3—C4—C5—C6	0.9 (6)
C8—N1—C9—C10	68.3 (5)	C2—C7—C6—C5	−0.8 (5)

C1—N1—C9—C14	68.0 (5)	C8—C7—C6—C5	−179.5 (4)
C8—N1—C9—C14	−110.3 (4)	C4—C5—C6—C7	0.2 (6)
C10—C9—C14—C13	0.7 (6)	C14—C9—C10—C11	−0.6 (6)
N1—C9—C14—C13	179.3 (3)	N1—C9—C10—C11	−179.2 (4)
C10—C9—C14—C15	−179.4 (4)	C13—C12—C11—C10	2.1 (6)
N1—C9—C14—C15	−0.8 (6)	Br1—C12—C11—C10	−177.2 (3)
C9—C14—C13—C12	0.6 (6)	C9—C10—C11—C12	−0.8 (6)

Table 15. Hydrogen bonds for 11 [Å and °]

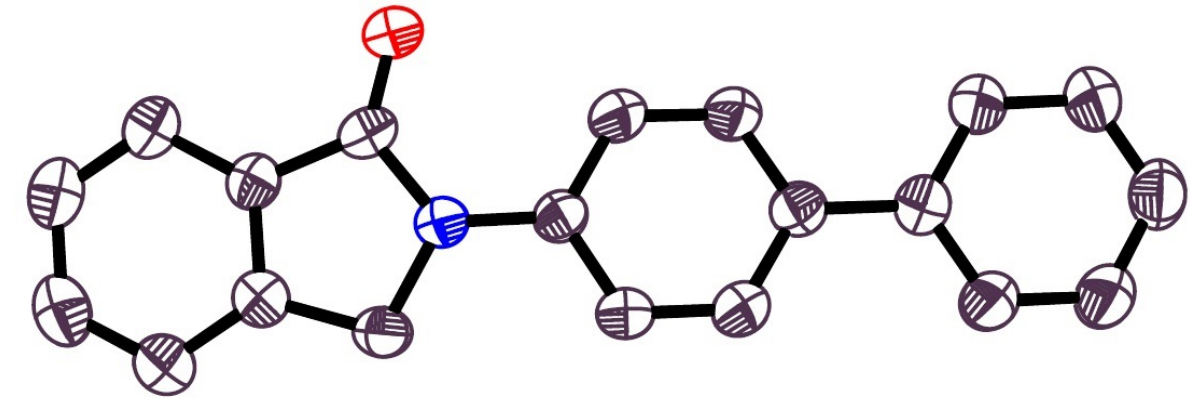
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8)-H(8A)...Br(1)#1	0.97	3.11	3.579(4)	111.5
C(8)-H(8A)...Br(1)#2	0.97	2.97	3.846(4)	151.3
C(8)-H(8A)...Br(1)#1	0.97	3.11	3.579(4)	111.5
C(8)-H(8A)...Br(1)#2	0.97	2.97	3.846(4)	151.3
C(8)-H(8A)...Br(1)#1	0.97	3.11	3.579(4)	111.5
C(8)-H(8A)...Br(1)#2	0.97	2.97	3.846(4)	151.3
C(8)-H(8A)...Br(1)#1	0.97	3.11	3.579(4)	111.5
C(8)-H(8A)...Br(1)#2	0.97	2.97	3.846(4)	151.3
C(8)-H(8A)...Br(1)#1	0.97	3.11	3.579(4)	111.5
C(8)-H(8A)...Br(1)#2	0.97	2.97	3.846(4)	151.3
C(8)-H(8A)...Br(1)#1	0.97	3.11	3.579(4)	111.5
C(8)-H(8A)...Br(1)#2	0.97	2.97	3.846(4)	151.3
C(8)-H(8A)...Br(1)#2	0.97	2.97	3.846(4)	151.3
C(8)-H(8A)...Br(1)#1	0.97	3.11	3.579(4)	111.5
C(8)-H(8A)...Br(1)#2	0.97	2.97	3.846(4)	151.3
C(8)-H(8A)...Br(1)#1	0.97	3.11	3.579(4)	111.5
C(8)-H(8A)...Br(1)#2	0.97	2.97	3.846(4)	151.3
C(8)-H(8A)...Br(1)#1	0.97	3.11	3.579(4)	111.5
C(8)-H(8A)...Br(1)#2	0.97	2.97	3.846(4)	151.3
C(8)-H(8A)...Br(1)#1	0.97	3.11	3.579(4)	111.5

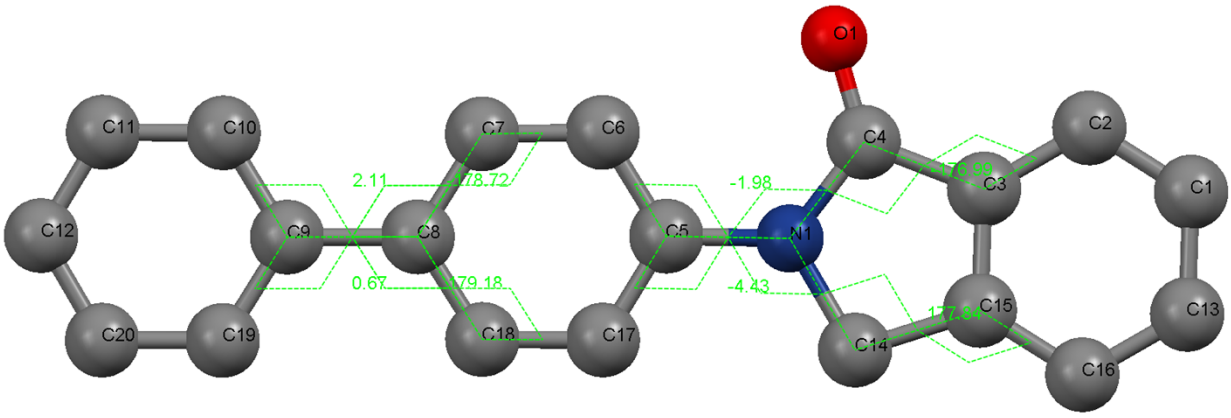
C(8)-H(8A)...Br(1)#2	0.97	2.97	3.846(4)	151.3
C(8)-H(8A)...Br(1)#1	0.97	3.11	3.579(4)	111.5

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,-y+3/2,z-1/2 #2 -x+1/2,y-1/2,-z+3/2

Crystal Structure of 2-([1,1'-biphenyl]-4-yl)isoindolin-1-one (25) (CCDC No.-1020238)





Packing diagram of 2-([1,1'-biphenyl]-4-yl)isoindolin-1-one 25

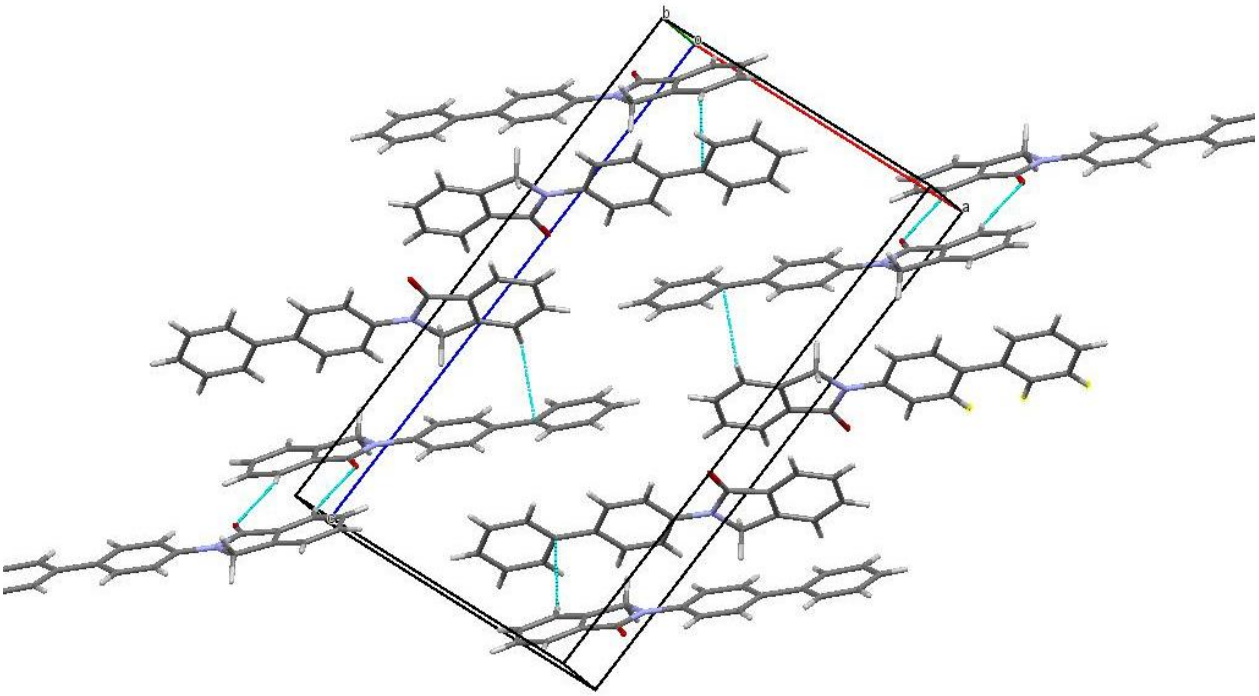


Table 16. Crystal data and structure refinement for 25

Identification code	2-([1,1'-biphenyl]-4-yl)isoindolin-1-one	
Empirical formula	C_{20} H_{15} N O	
Formula weight	285.33	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/c	
Unit cell dimensions	a = 11.4297(13) Å	α= 90°.
	b = 5.9995(6) Å	β= 96.386(8)°.
	c = 21.003(2) Å	γ = 90°.
Volume	1431.3(3) $Å^3$	
Z	4	
Density (calculated)	1.324 Mg/m^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	600	
Theta range for data collection	1.793 to 28.360°.	
Index ranges	-15<=h<=15, -7<=k<=7, -27<=l<=26	
Reflections collected	16331	

Independent reflections	3428 [R(int) = 0.0924]
Completeness to theta = 25.242°	99.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3428 / 0 / 200
Goodness-of-fit on F^2	0.938
Final R indices [I>2sigma(I)]	R1 = 0.0650, wR2 = 0.1426
R indices (all data)	R1 = 0.1331, wR2 = 0.1824
Extinction coefficient	0.015(3)
Largest diff. peak and hole	0.251 and -0.210 e.$Å^{-3}$

Table 17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 25. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	9198(1)	1134(2)	963(1)	53(1)
N(1)	9580(2)	4546(3)	1470(1)	41(1)
C(1)	12078(2)	3676(4)	-90(1)	56(1)
C(2)	11198(2)	2588(4)	180(1)	49(1)
C(3)	10725(2)	3622(3)	684(1)	40(1)
C(4)	9752(2)	2880(3)	1036(1)	42(1)
C(5)	8704(2)	4611(3)	1892(1)	40(1)
C(6)	7856(2)	2968(4)	1906(1)	57(1)
C(7)	7014(2)	3094(4)	2324(1)	58(1)
C(8)	6964(2)	4820(3)	2756(1)	43(1)
C(9)	6062(2)	4910(3)	3215(1)	44(1)
C(10)	5245(2)	3212(4)	3245(1)	60(1)
C(11)	4431(2)	3245(4)	3681(1)	66(1)
C(12)	4404(2)	4971(4)	4106(1)	63(1)
C(13)	12485(2)	5731(4)	146(1)	59(1)
C(14)	10410(2)	6403(3)	1434(1)	46(1)
C(15)	11116(2)	5682(3)	913(1)	43(1)

C(16)	12010(2)	6759(4)	645(1)	52(1)
C(17)	8653(2)	6366(4)	2315(1)	59(1)
C(18)	7808(2)	6451(4)	2733(1)	60(1)
C(19)	6006(2)	6650(4)	3643(1)	58(1)
C(20)	5197(2)	6686(4)	4082(1)	66(1)

Table 18. Bond lengths [Å] for 25

O1—C4	1.224 (2)	C9—C10	1.388 (3)
N1—C4	1.382 (2)	C10—C11	1.377 (3)
N1—C5	1.410 (3)	C10—H10	0.93
N1—C14	1.470 (2)	C11—C12	1.370 (3)
C1—C2	1.374 (3)	C11—H11	0.93
C1—C13	1.390 (3)	C12—C20	1.376 (3)
C1—H1	0.93	C12—H2	0.93
C2—C3	1.387 (3)	C13—C16	1.378 (3)
C2—H15	0.93	C13—H3	0.93
C3—C15	1.382 (3)	C14—C15	1.495 (3)
C3—C4	1.472 (3)	C14—H6	0.97
C5—C17	1.384 (3)	C14—H5	0.97
C5—C6	1.385 (3)	C15—C16	1.381 (3)
C6—C7	1.376 (3)	C16—H4	0.93
C6—H7	0.93	C17—C18	1.375 (3)
C7—C8	1.381 (3)	C17—H14	0.93
C7—H8	0.93	C18—H13	0.93
C8—C18	1.379 (3)	C19—C20	1.376 (3)
C8—C9	1.488 (3)	C19—H9	0.93
C9—C19	1.384 (3)	C20—H12	0.93

Table 19. Bond angles [°] for 25

C4—N1—C5	126.69 (17)	C12—C11—C10	120.7 (2)

C4—N1—C14	111.99 (17)	C12—C11—H11	119.7
C5—N1—C14	121.27 (16)	C10—C11—H11	119.7
C2—C1—C13	120.3 (2)	C11—C12—C20	118.6 (2)
C2—C1—H1	119.8	C11—C12—H2	120.7
C13—C1—H1	119.8	C20—C12—H2	120.7
C1—C2—C3	117.9 (2)	C16—C13—C1	121.7 (2)
C1—C2—H15	121.1	C16—C13—H3	119.2
C3—C2—H15	121.1	C1—C13—H3	119.2
C15—C3—C2	121.8 (2)	N1—C14—C15	102.83 (16)
C15—C3—C4	109.20 (18)	N1—C14—H6	111.2
C2—C3—C4	128.9 (2)	C15—C14—H6	111.2
O1—C4—N1	126.3 (2)	N1—C14—H5	111.2
O1—C4—C3	127.23 (19)	C15—C14—H5	111.2
N1—C4—C3	106.45 (18)	H6—C14—H5	109.1
C17—C5—C6	116.6 (2)	C16—C15—C3	120.2 (2)
C17—C5—N1	120.57 (19)	C16—C15—C14	130.3 (2)
C6—C5—N1	122.82 (19)	C3—C15—C14	109.52 (19)
C7—C6—C5	121.1 (2)	C13—C16—C15	118.1 (2)
C7—C6—H7	119.5	C13—C16—H4	120.9
C5—C6—H7	119.5	C15—C16—H4	120.9
C6—C7—C8	122.9 (2)	C18—C17—C5	121.4 (2)
C6—C7—H8	118.6	C18—C17—H14	119.3
C8—C7—H8	118.6	C5—C17—H14	119.3
C18—C8—C7	115.4 (2)	C17—C18—C8	122.7 (2)
C18—C8—C9	122.3 (2)	C17—C18—H13	118.7
C7—C8—C9	122.3 (2)	C8—C18—H13	118.7
C19—C9—C10	116.4 (2)	C20—C19—C9	122.0 (2)
C19—C9—C8	122.2 (2)	C20—C19—H9	119

C10—C9—C8	121.4 (2)	C9—C19—H9	119
C11—C10—C9	121.9 (2)	C12—C20—C19	120.5 (2)
C11—C10—H10	119.1	C12—C20—H12	119.7
C9—C10—H10	119.1	C19—C20—H12	119.7

Table 20. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 25. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	62(1)	41(1)	59(1)	-10(1)	15(1)	-5(1)
N(1)	44(1)	38(1)	41(1)	-3(1)	5(1)	-2(1)
C(1)	53(2)	64(2)	50(1)	3(1)	13(1)	13(1)
C(2)	49(1)	51(1)	46(1)	-3(1)	6(1)	8(1)
C(3)	41(1)	40(1)	39(1)	3(1)	3(1)	7(1)
C(4)	48(1)	36(1)	41(1)	-4(1)	-1(1)	5(1)
C(5)	42(1)	39(1)	37(1)	-2(1)	2(1)	1(1)
C(6)	57(2)	51(1)	65(2)	-21(1)	17(1)	-11(1)
C(7)	51(2)	55(2)	71(2)	-22(1)	19(1)	-15(1)
C(8)	41(1)	45(1)	41(1)	-2(1)	-1(1)	-1(1)
C(9)	39(1)	51(1)	40(1)	0(1)	0(1)	4(1)
C(10)	63(2)	61(2)	58(2)	-13(1)	19(1)	-15(1)
C(11)	69(2)	70(2)	64(2)	-8(1)	26(1)	-18(1)
C(12)	60(2)	77(2)	55(2)	-5(1)	18(1)	-4(1)
C(13)	50(2)	68(2)	60(2)	13(1)	14(1)	1(1)
C(14)	50(1)	39(1)	49(1)	-3(1)	5(1)	-7(1)
C(15)	41(1)	44(1)	42(1)	4(1)	1(1)	2(1)
C(16)	51(1)	53(1)	52(2)	3(1)	5(1)	-4(1)
C(17)	63(2)	52(1)	66(2)	-20(1)	22(1)	-19(1)
C(18)	64(2)	57(2)	61(2)	-21(1)	20(1)	-13(1)
C(19)	55(2)	58(2)	63(2)	-15(1)	15(1)	-6(1)
C(20)	64(2)	70(2)	68(2)	-20(1)	23(1)	-7(1)

Table 21. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 25

	x	y	z	U(eq)
H(1)	12404	3034	-433	67
H(15)	10927	1203	29	58
H(7)	7857	1759	1629	68
H(8)	6453	1968	2316	70
H(10)	5248	2019	2962	71
H(11)	3893	2083	3687	79
H(2)	3862	4983	4405	76
H(3)	13092	6430	-37	71
H(6)	10906	6592	1836	55
H(5)	9997	7787	1325	55
H(4)	12285	8140	798	62
H(14)	9201	7511	2318	71
H(13)	7806	7658	3010	72
H(9)	6532	7830	3635	70
H(12)	5186	7879	4364	79

Table 22. Torsion angles [°] for 25

C13—C1—C2—C3	0.9 (3)	C8—C9—C10—C11	177.9 (2)
C1—C2—C3—C15	0.1 (3)	C9—C10—C11—C12	−0.3 (4)
C1—C2—C3—C4	177.0 (2)	C10—C11—C12—C20	1.0 (4)
C5—N1—C4—O1	−3.2 (3)	C2—C1—C13—C16	−1.3 (4)
C14—N1—C4—O1	179.4 (2)	C4—N1—C14—C15	0.6 (2)
C5—N1—C4—C3	176.94 (17)	C5—N1—C14—C15	−177.04 (17)
C14—N1—C4—C3	−0.6 (2)	C2—C3—C15—C16	−0.9 (3)
C15—C3—C4—O1	−179.6 (2)	C4—C3—C15—C16	−178.36 (18)
C2—C3—C4—O1	3.1 (4)	C2—C3—C15—C14	177.60 (18)

C15—C3—C4—N1	0.3 (2)	C4—C3—C15—C14	0.1 (2)
C2—C3—C4—N1	−176.98 (19)	N1—C14—C15—C16	177.8 (2)
C4—N1—C5—C17	178.3 (2)	N1—C14—C15—C3	−0.4 (2)
C14—N1—C5—C17	−4.4 (3)	C1—C13—C16—C15	0.5 (3)
C4—N1—C5—C6	−2.0 (3)	C3—C15—C16—C13	0.6 (3)
C14—N1—C5—C6	175.30 (19)	C14—C15—C16—C13	−177.6 (2)
C17—C5—C6—C7	−0.1 (3)	C6—C5—C17—C18	0.6 (4)
N1—C5—C6—C7	−179.9 (2)	N1—C5—C17—C18	−179.7 (2)
C5—C6—C7—C8	−0.8 (4)	C5—C17—C18—C8	−0.2 (4)
C6—C7—C8—C18	1.2 (4)	C7—C8—C18—C17	−0.7 (4)
C6—C7—C8—C9	−178.7 (2)	C9—C8—C18—C17	179.2 (2)
C18—C8—C9—C19	0.6 (3)	C10—C9—C19—C20	0.8 (4)
C7—C8—C9—C19	−179.5 (2)	C8—C9—C19—C20	−177.7 (2)
C18—C8—C9—C10	−177.8 (2)	C11—C12—C20—C19	−0.7 (4)
C7—C8—C9—C10	2.1 (3)	C9—C19—C20—C12	−0.2 (4)
C19—C9—C10—C11	−0.6 (4)		

Table 23 Hydrogen bonds for 25 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1

C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1

C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1
C(6)-H(7)...O(1)	0.93	2.22	2.858(3)	125.1
C(14)-H(5)...O(1)#1	0.97	2.30	3.264(3)	172.1