Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Iron(III)-Catalyzed Direct C−H Amination of (Hetero)Arenes

Bin Lv[a], Pan Gao[a], Shuwei Zhang[a], Xiaodong Jia[a], Minyan Wang[b,*], Yu Yuan[a,*]

[a]College of Chemistry and Chemical Engineering, Yangzhou University, Yangzhou 225002, China

[b]State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, China

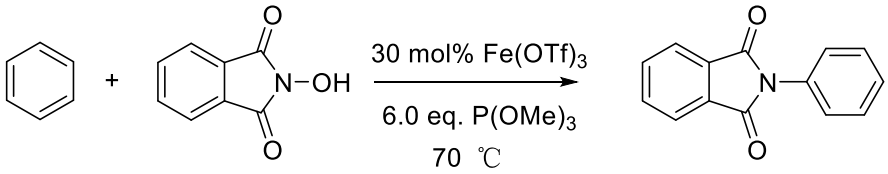
yyuan@yzu.edu.cn

Table of Contents

1. General Information.

All new compounds were fully characterized. ^{1}H NMR and ^{13}C NMR spectra were obtained with an Agilent Technologies 400 or 600 spectrometer in $CDCl_3$ with TMS as an internal standard. Mass spectra were obtained on a Bruker Dalton maXis instrument. IR spectra were recorded on a FT–IR spectrometer. All reactions were carried out under air atmosphere. Unless otherwise noted, materials obtained from commercial suppliers without further purification. All reactions under standard conditions were monitored by thin–layer chromatography (TLC) on gel F254 plates. All reactions were monitored by TLC. Flash column chromatograph was carried out using 300–400 mesh silica gel at medium pressure.

2. Optimization the Reaction Conditions



Entry[a]	Fe (cat.)	Additive	T (℃)	Solvent	Yiled (%)[b]
1[a]	$FeCl_3$ (30 mol%)	$P(OEt)_3$ (5.0 eq.)	100	Benzene	20
2	$Fe(acac)_3$ (30 mol%)	$P(OEt)_3$ (5.0 eq.)	100	Benzene	< 10
3	$Fe(OTs)_3$ (30 mol%)	$P(OEt)_3$ (5.0 eq.)	100	Benzene	12
4	$Fe(OTf)_3$ (30 mol%)	$P(OEt)_3$ (5.0 eq.)	100	Benzene	52
5	$FeCl_2$ (30 mol%)	$P(OEt)_3$ (5.0 eq.)	100	Benzene	< 10
6	$FeBr_2$ (30 mol%)	$P(OEt)_3$ (5.0 eq.)	100	Benzene	< 10
7	$Fe(OAc)_2$ (30 mol%)	$P(OEt)_3$ (5.0 eq.)	100	Benzene	< 10
8	$Fe(OTf)_2$ (30 mol%)	$P(OEt)_3$ (5.0 eq.)	100	Benzene	49
9	$FePO_4$ (30 mol%)	$P(OEt)_3$ (5.0 eq.)	100	Benzene	< 10
10	$Fe(OTf)_3$ (50 mol%)	$P(OEt)_3$ (5.0 eq.)	100	Benzene	47
11	$Fe(OTf)_3$ (15 mol%)	$P(OEt)_3$ (5.0 eq.)	100	Benzene	52

12	$Fe(OTf)_3$ (5 mol%)	$P(OEt)_3$ (5.0 eq.)	100	Benzene	28
13	--	$P(OEt)_3$ (5.0 eq.)	100	Benzene	< 10
14	$Fe(OTf)_3$ (30 mol%)	$P(OEt)_3$ (8.0 eq.)	100	Benzene	51
15	$Fe(OTf)_3$ (30 mol%)	$P(OEt)_3$ (6.0 eq.)	100	Benzene	62
16	$Fe(OTf)_3$(30 mol%)	$P(OEt)_3$ (3.0 eq.)	100	Benzene	21
17	$Fe(OTf)_3$(30 mol%)	$P(OEt)_3$ (1.5 eq.)	100	Benzene	< 10
18	$Fe(OTf)_3$ (30 mol%)	--	100	Benzene	NR
19	$Fe(OTf)_3$ (30 mol%)	$P(OMe)_3$ (6.0 eq.)	100	Benzene	76
20	$Fe(OTf)_3$ (30 mol%)	$P(OPh)_3$ (6.0 eq.)	100	Benzene	39
21	$Fe(OTf)_3$ (30 mol%)	$OP(OEt)_3$ (6.0 eq.)	100	Benzene	< 10
22	$Fe(OTf)_3$ (30 mol%)	P(t–Bu)$_3$ (6.0 eq.)	100	Benzene	< 10
23[c]	$Fe(OTf)_3$ (30 mol%)	$P(OMe)_3$ (6.0 eq.)	100	DCM	53
24[c]	$Fe(OTf)_3$ (30 mol%)	$P(OMe)_3$ (6.0 eq.)	100	DCE	50
25[c]	$Fe(OTf)_3$ (30 mol%)	$P(OMe)_3$ (6.0 eq.)	100	CH_3CN	43
26[c]	$Fe(OTf)_3$ (30 mol%)	$P(OMe)_3$ (6.0 eq.)	100	THF	< 10
27[c]	$Fe(OTf)_3$ (30 mol%)	$P(OMe)_3$ (6.0 eq.)	100	DMF	NR
28[c]	$Fe(OTf)_3$ (30 mol%)	$P(OMe)_3$ (6.0 eq.)	100	DMSO	NR
29[c]	$Fe(OTf)_3$ (30 mol%)	$P(OMe)_3$ (6.0 eq.)	100	1,4–dioxane	NR
30[c]	$Fe(OTf)_3$ (30 mol%)	$P(OMe)_3$ (6.0 eq.)	100	Ethanol	NR
31	$Fe(OTf)_3$ (30 mol%)	$P(OMe)_3$ (6.0 eq.)	r.t.	Benzene	NR
32	$Fe(OTf)_3$ (30 mol%)	$P(OMe)_3$ (6.0 eq.)	50	Benzene	43
33	$Fe(OTf)_3$ (30 mol%)	$P(OMe)_3$ (6.0 eq.)	70	Benzene	88
34[d]	$Fe(OTf)_3$ (30 mol%)	$P(OMe)_3$ (6.0 eq.)	70	Benzene	75

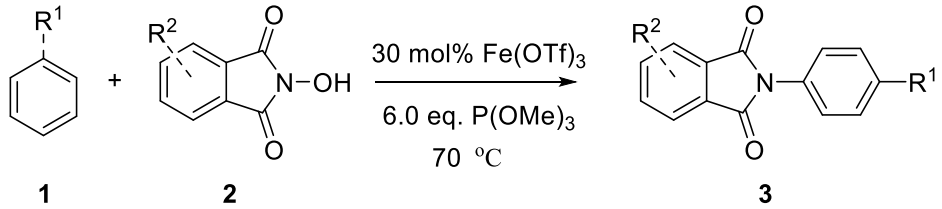
[a] *N*–hydroxyphthalimide (0.1 mmol), Fe (cat.) (30 mol%), additive, benzene (2.0 mL), 70 ℃, air.

[b] Yield after purification.

[c] *N*–hydroxyphthalimide (0.1 mmol), benzene (1.0 mmol), $Fe(OTf)_3$ (30 mol%), $P(OMe)_3$ (6.0 eq), solvent (2.0 mL),70 ℃, air.

[d] *N*–hydroxyphthalimide (0.1 mmol), benzene (1.0 mmol), $Fe(OTf)_3$ (30 mol%), $P(OMe)_3$ (6.0 eq), solvent (2.0 mL),70 ℃, N_2.

3. General Procedure for Arylamine

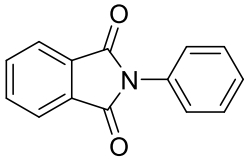


1 **2** **3**

To a 15 mL sealed tube was added *N*-hydroxyphthalimide **2** (0.1 mmol), $Fe(OTf)_3$ (0.03 mmol), trimethyl phosphite (0.6 mmol) and (hetero)arene **1** (2 mL). The formed mixture was stirred at 70 °C under air for 12 h monitored by TLC. The solution was then cooled to room temperature and the solvent was removed under vaccum directly. The crude products were purified by column chromatography on silica gel to afford the desired product **3**.

4. Characterization of Products

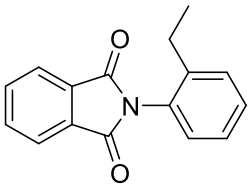
2-Phenylisoindoline-1,3-dione (3aa)[2]



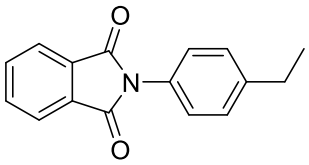
3aa

Following the general procedure, the reaction of *N*-hydroxyphthalimide **2a** (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in benzene (2 mL) at 70 °C under air for 12 h. The crude product was purified by column chromatography on silica gel to afford **3aa** (19.7 mg, 88%) as a white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.96 – 7.94 (m, 2H), 7.82 – 7.75 (m, 2H), 7.53-7.49 (m, 2H), 7.47 – 7.35 (m, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 167.26, 134.37, 131.73, 131.64, 129.09, 128.08, 126.55, 123.73. **IR (ν, cm^{-1})** 1730, 1700, 1382, 1100, 1068, 877, 704. **HRMS m/z (ESI)**: calcd for $C_{14}H_9NaO_2$ $(M + Na)^+$ 246.0531, found 246.0523.

2-(2-Ethylphenyl)isoindoline-1,3-dione (3baa) and 2-(4-ethylphenyl)isoindoline-1,3-dione (3bab)[2]



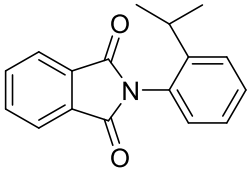
3baa



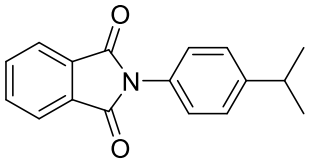
3bab

Following the general procedure, the reaction of *N*–hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in ethylbenzene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3ba** (24.6 mg, 98%, **3baa**:**3bab** = 1:7) as a white solid. The isomer ratio was determined by ^{1}H NMR spectroscopy. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.96 – 7.93 (m, 2H), 7.82 – 7.74 (m, 2H), 7.41 (t, *J* = 8.1 Hz, 1H [**3bab**]), 7.33 (s, 2H [**3bab**]), 7.27 – 7.20 (m, 3H), 7.17 (d, *J* = 7.6 Hz, 1H [**3baa**]), 2.76 – 2.65 (m, 2H [**3bab**]), 2.52 (d, *J* = 7.6 Hz, 2H [**3baa**]), 1.27 (t, *J* = 7.6 Hz, 3H [**3bab**]), 1.16 (t, *J* = 7.6 Hz, 3H [**3baa**]). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 167.45, 167.40, 145.36, 144.37, 134.32, 134.30, 131.81, 131.52, 129.27, 128.97, 128.60, 127.82, 126.47, 126.13, 123.93, 123.76, 123.68, 28.68, 28.58, 15.40, 15.25. **IR (ν, cm^{-1})** 1744, 1710, 1518, 1379, 1111, 1081, 883, 715. **HRMS m/z (ESI)**: calcd for $C_{16}H_{13}NNaO_2$ $(M + Na)^+$ 274.0844, found 274.0840.

2-(2-Isopropylphenyl)isoindoline-1,3-dione (3caa) and 2-(4-isopropylphenyl)isoindoline-1,3-dione (3cab)[3]



3caa

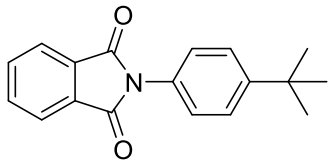


3cab

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in cumene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3ca** (16.2 mg, 61%, **3caa**:**3cab** = 1:8) as a white solid. The isomer ratio was determined by ^{1}H NMR spectroscopy. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.96 – 7.92 (m, 2H), 7.80–7.76 (m, 2H), 7.47 (d, *J* = 1.0 Hz, 1H [**3caa**]), 7.42 (t, *J* = 8.1 Hz, 1H [**3cab**]), 7.35 (d, *J* = 1.8 Hz, 1H), 7.27 (dd, *J* = 5.0, 2.9 Hz, 1H), 7.25 – 7.21 (m, 1H

[**3cab**]), 7.15 (d, *J* = 7.6 Hz, 1H [**3caa**]), 3.00 – 2.93 (m, 1H [**3cbb**]), 2.86 – 2.75 (m, 1H [**3caa**]), 1.28 (dd, *J* = 6.9, 1.7 Hz, 6H [**3cab**]), 1.19 (d, *J* = 6.9 Hz, 6H [**3caa**]). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 167.41, 167.37, 149.92, 148.83, 134.29, 134.27, 131.74, 131.48, 129.94, 129.47, 129.10, 128.92, 127.15, 126.72, 126.66, 126.38, 126.31, 124.81, 123.97, 123.72, 123.62, 120.29, 115.23, 33.95, 33.86, 23.86, 23.80. **IR (ν, cm^{-1})** 1744, 1707, 1375,1232, 1113, 1081, 832, 719. **HRMS m/z (ESI)**: calcd for $C_{17}H_{15}NNaO_2$ $(M + Na)^+$ 288.1000, found 288.0997.

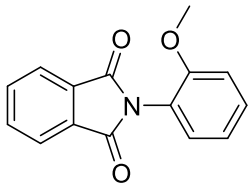
2-(4-(*Tert*-butyl)phenyl)isoindoline-1,3-dione (3da)[4]



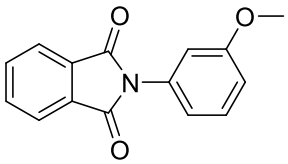
3da

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in *tert*-butylbenzene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3da** (21.0 mg, 75%) as a white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.98 – 7.89 (m, 2H), 7.81 – 7.74 (m, 2H), 7.55 – 7.49 (m, 1H), 7.44-7.42 (m, 2H), 7.39 – 7.32 (m, 1H), 1.36 (s, 9H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 167.42, 152.26, 151.06, 134.28, 131.75, 131.28, 128.65, 126.10, 126.00, 125.24, 123.84, 123.62, 34.80, 34.67, 31.25, 31.21. **IR (ν, cm^{-1})** 1754, 1720, 1428, 1115, 1078, 871, 724. **HRMS m/z (ESI)**: calcd for $C_{18}H_{17}NNaO_2$ $(M + Na)^+$ 302.1157, found 302.1153.

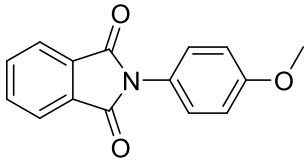
2-(2-Methoxyphenyl)isoindoline-1,3-dione (3eaa), 2-(3-methoxyphenyl)isoindoline-1,3-dione (3eab), and 2-(4-methoxyphenyl)isoindoline-1,3-dione(3eac)[2]



3eaa



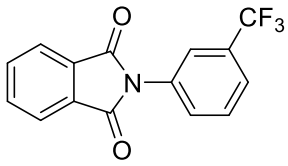
3eab



3eac

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (10.0 equiv., 1.0 mmol, 124.1 mg) in anisole (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3ea** (16.5 mg, 65%, **3eaa**:**3eab**:**3eac** = 13:1:12) as a white solid. The isomer ratio was determined by ^{1}H NMR spectroscopy. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.93 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.77 (dt, *J* = 5.6, 2.8 Hz, 2H), 7.43 (td, *J* = 7.9, 1.7 Hz, 1H [**3eaa**]), 7.36 – 7.29 (m, 1H), 7.25 (d, *J* = 3.1 Hz, 1H), 7.11 – 6.98 (m, 2H), 3.84 (s, 3H [**3eac**]), 3.83 (s, 3H [**3eab**]), 3.79 (s, 3H [**3eaa**]). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 167.56, 167.35, 159.28, 155.86, 134.28, 134.07, 132.31, 131.85, 130.65, 129.99, 127.93, 124.30, 123.65, 120.86, 120.33, 114.49, 112.17, 55.83, 55.50. **IR (ν, cm^{-1})** 1734, 1708, 1512, 1386, 1113, 1024, 883, 715. **HRMS m/z (ESI)**: calcd for $C_{15}H_{11}NNaO_3$ $(M + Na)^+$ 276.0637, found 276.0631.

2-(3-(Trifluoromethyl)phenyl)isoindoline-1,3-dione (3fa)[2]

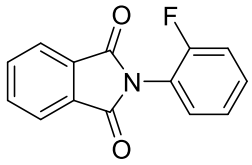


3fa

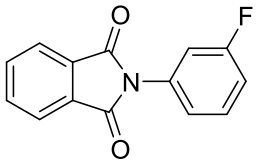
Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphate (6.0 equiv., 0.6 mmol, 74.4 mg) in trifluorotoluene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3fa** (17.8 mg, 60%) as a white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.01 – 7.94 (m, 2H), 7.84 – 7.79 (m, 2H), 7.79 – 7.60 (m, 4H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 165.34, 135.33, 132.28, 131.72, 131.40, 129.63, 126.40, 126.14, 124.93, 124.69, 123.95, 123.36, 122.21. **^{19}F NMR (376 MHz, $CDCl_3$)** δ -62.46. **IR (ν, cm^{-1})** 1735, 1712, 1512, 1388, 1323, 1012, 1069, 805,

714. **HRMS m/z (ESI)**: calcd for $C_{15}H_8F_3NNaO_2$ $(M + Na)^+$ 314.0405, found 314.0397.

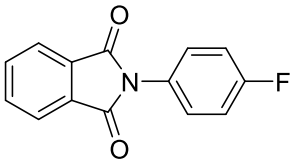
2-(2-Fluorophenyl)isoindoline-1,3-dione (3gaa), 2-(3-fluorophenyl)isoindoline-1,3-dione (3gab), and 2-(4-fluorophenyl)isoindoline-1,3-dione (3gac)[2]



3gaa



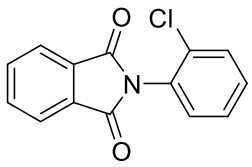
3gab



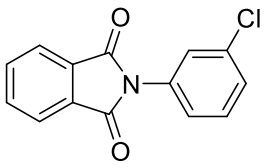
3gac

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (10.0 equiv., 1.0 mmol, 124.1 mg) in fluorobenzene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3ga** (14.7 mg, 61%, **3gaa**:**3gab**:**3gac** = 1:5:2) as a white solid. The isomer ratio was determined by ^{19}F NMR spectroscopy. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.98 – 7.90 (m, 2H), 7.83 – 7.74 (m, 2H), 7.53 – 7.32 (m, 2H [**3gaa**+**3gab**]), 7.31 – 7.15 (m, 2H), 7.14 – 7.06 (m, 1H [**3gac**]). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 167.80, 166.83, 166.50, 134.59, 134.49, 134.44, 131.94, 131.63, 131.54, 130.75, 130.67, 130.23, 130.13, 129.85, 128.40, 128.31, 124.64, 124.60, 123.92, 123.89, 123.80, 122.00, 121.97, 116.85, 116.65, 116.23, 116.00, 115.10, 114.89, 114.04, 113.79. **^{19}F NMR (376 MHz, $CDCl_3$)** δ -111.17 [**3gab**], -113.06 [**3gac**], -118.68 [**3gaa**]. **IR (ν, cm^{-1})** 1746, 1713, 1594, 1387, 1109, 1086, 857, 715. **HRMS m/z (ESI)**: calcd for $C_{14}H_8FNNaO_2$ $(M + Na)^+$ 264.0437, found 264.0429.

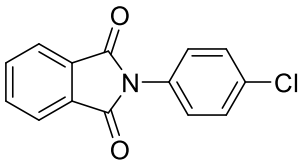
2-(2-Chlorophenyl)isoindoline-1,3-dione (3haa), 2-(3-chlorophenyl)isoindoline-1,3-dione (3hab), and 2-(4-chlorophenyl)isoindoline-1,3-dione (3hac) [2]



3haa



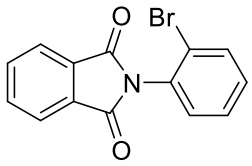
3hab



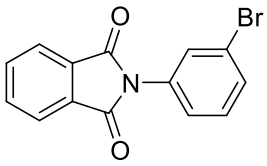
3hac

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in chlorobenzene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3ha** (12.9 mg, 50%, **3haa**:**3hab**:**3hac** = 1:4:2) as a white solid. The isomer ratio was determined by ^{1}H NMR spectroscopy. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.97 – 7.94 (m, 2H), 7.85 – 7.75 (m, 2H), 7.57 (dt, *J* = 6.0, 2.1 Hz, 2H [**3haa**]), 7.51 – 7.47 (m, 2H [**3hac**]), 7.47 – 7.31 (m, 2H [**3haa**] + 2H [**3hac**] + 4H [**3hac**]). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.97, 166.66, 166.46, 134.60, 134.55, 134.45, 133.83, 133.47, 130.64, 130.43, 130.18, 130.01, 129.30, 128.24, 127.71, 127.65, 126.67, 125.01, 123.95, 123.90, 123.85. **IR (ν, cm^{-1})** 1730, 1713, 1495, 1386, 1120, 1015, 885, 715. **HRMS m/z (ESI)**: calcd for $C_{14}H_8ClNNaO_2$ $(M + Na)^+$ 280.0141, found 280.0132.

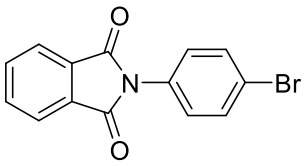
2-(2-Bromophenyl)isoindoline-1,3-dione (3iaa), 2-(3-bromophenyl)isoindoline-1,3-dione (3iab), and 2-(4-bromophenyl)isoindoline-1,3-dione (3iac) [2]



3iaa



3iab

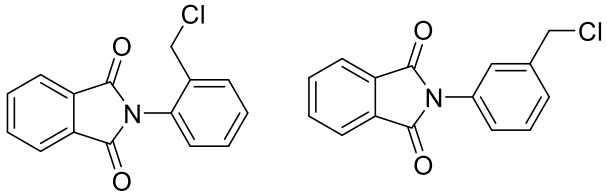


3iac

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (10.0 equiv., 1.0 mmol, 124.1 mg) in bromobenzene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford

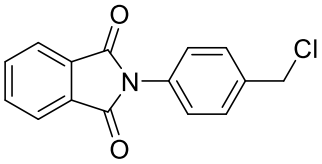
3ia (15.4 mg, 51%, **3iab**:**3iac** = 1:6) as a white solid. The isomer ratio was determined by ^{1}H NMR spectroscopy. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.99 – 7.92 (m, 2H), 7.83 – 7.76 (m, 2H), 7.64 – 7.61 (m, 2H [**3iab**]), 7.56 – 7.49 (m, 2H [**3iac**]), 7.44 – 7.34 (m, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.90, 134.61, 134.57, 132.27, 131.59, 131.12, 130.72, 130.28, 129.86, 127.31, 125.52, 123.90, 123.86, 122.21. **IR (ν, cm^{-1})** 1732, 1711, 1493, 1386, 1119, 1081, 850, 715. **HRMS m/z (ESI)**: calcd for $C_{14}H_8BrNNaO_2$ $(M + Na)^+$ 323.9636, found 323.9628.

2-(2-(Chloromethyl)phenyl)isoindoline-1,3-dione (3jaa), 2-(3-(chloromethyl)phenyl)isoindoline-1,3-dione (3jab), and 2-(4-(chloromethyl)phenyl)isoindoline-1,3-dione (3jac) [5]



3jaa

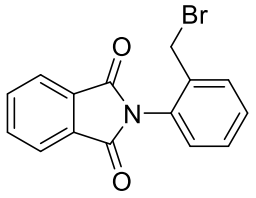
3jab



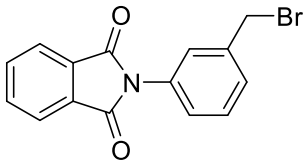
3jac

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (10.0 equiv., 1.0 mmol, 124.1 mg) in benzyl chloride (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3ja** (11.4 mg, 42%, **3jaa**:**3jab**:**3jac** = 1:2:3) as a white solid. The isomer ratio was determined by ^{1}H NMR spectroscopy. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.98 – 7.04 (m, 2H), 7.82 – 7.79 (m, 2H), 7.59 – 7.25 (m, 4H), 4.63 (s, 2H [**3jab**]), 4.62 (s, 2H [**3jaa**]), 4.53 (s, 2H [**3jac**]). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 167.22, 167.06, 138.54, 137.19, 135.62, 134.48, 132.04, 131.91, 131.68, 131.66, 130.69, 130.62, 129.73, 129.68, 129.65, 129.43, 129.28, 128.07, 126.65, 126.50, 126.36, 123.93, 123.79, 45.51, 42.84. **IR (ν, cm^{-1})** 1739, 1717, 1380, 1110, 1077, 875, 718. **HRMS m/z (ESI)**: calcd for $C_{15}H_{10}ClNNaO_2$ $(M + Na)^+$ 294.0298, found 294.0292.

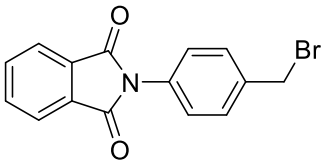
2-(2-(Bromomethyl)phenyl)isoindoline-1,3-dione (3kaa), 2-(3-(bromomethyl)phenyl)isoindoline-1,3-dione (3kab), and 2-(4-(bromomethyl)phenyl)isoindoline-1,3-dione (3kac) [6]



3kaa



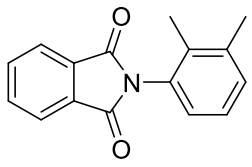
3kab



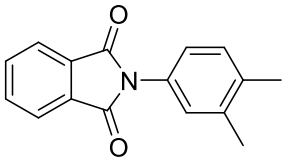
3kac

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (10.0 equiv., 1.0 mmol, 124.1 mg) in benzyl bromide (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3ka** (17.9 mg, 57%, **3kaa**:**3kab**:**3kac** = 1:3:5) as a white solid. The isomer ratio was determined by ^{1}H NMR spectroscopy. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.00 – 7.91 (m, 2H), 7.82 – 7.78 (m, 2H), 7.58 – 7.24 (m, 4H), 4.52 (s, 2H [**3kab**]), 4.51 (s, 2H [**3kaa**]), 4.42 (s, 2H [**3kac**]). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 167.22, 167.06, 138.54, 137.19, 135.62, 134.48, 132.04, 131.91, 131.68, 131.66, 130.69, 130.62, 129.73, 129.68, 129.65, 129.43, 129.28, 128.07, 126.65, 126.50, 126.36, 123.93, 123.79, 44.71, 42.32. **IR (ν, cm^{-1})** 1760, 1721, 1379, 1110, 1053, 876, 716. **HRMS m/z (ESI)**: calcd for $C_{15}H_{10}BrNNaO_2$ $(M + Na)^+$ 337.9793, found 337.9788.

2-(2,3-Dimethylphenyl)isoindoline-1,3-dione (3laa) and 2-(3,4-dimethylphenyl)isoindoline-1,3-dione (3lab) [2]



3laa

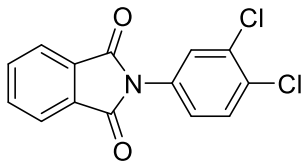


3lab

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in *o*-xylene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to

afford **3la** (21.3 mg, 85%, **3laa**:**3lab** = 1:1) as a white solid. The isomer ratio was determined by ^{1}H NMR spectroscopy. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.96 – 7.92 (m, 2H), 7.84 – 7.71 (m, 2H), 7.28 – 7.19 (m, 2H [**3laa**] + 1H [**3lab**]), 7.17 (d, *J* = 2.2 Hz, 1H [**3lab**]), 7.14 – 7.12 (m, 1H [**3lab**]), 7.06 (d, *J* = 1.6 Hz, 1H [**3laa**]), 2.35 (s, 3H [**3laa**]), 2.30 (d, *J* = 2.9 Hz, 6H [**3lab**]), 2.08 (s, 3H [**3laa**]). **^{13}C NMR (151 MHz, $CDCl_3$)** δ 167.51, 137.61, 137.01, 134.25, 131.90, 131.41, 130.25, 128.71, 127.74, 126.26, 124.13, 123.73, 20.39, 19.85, 19.49, 14.62. **IR (ν, cm^{-1})** 1771, 1716, 1377, 1107, 1084, 872, 715. **HRMS m/z (ESI)**: calcd for $C_{16}H_{13}NNaO_2$ $(M + Na)^+$ 274.0844, found 274.0832.

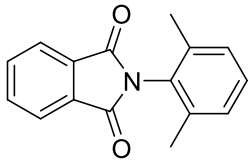
2-(3,4-Dichlorophenyl)isoindoline-1,3-dione (3ma)[7]



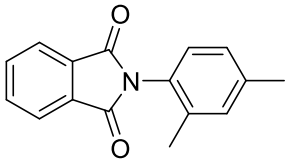
3ma

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in *o*-dichlorobenzene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3ma** (9.6 mg, 33%) as a white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.00 – 7.91 (m, 2H), 7.86 – 7.77 (m, 2H), 7.63 (dd, *J* = 2.4, 0.9 Hz, 1H), 7.57 (d, *J* = 8.6 Hz, 1H), 7.37 (ddd, *J* = 8.6, 2.4, 0.9 Hz, 1H).**^{13}C NMR (151 MHz, $CDCl_3$)** δ166.60, 134.73, 133.01, 132.10, 131.45, 131.09, 130.67, 128.14, 125.50, 123.98. **IR (ν, cm^{-1})** 1774, 1711, 1379, 1112, 1079, 869, 715. **HRMS m/z (ESI)**: calcd for $C_{14}H_9NaO_2$ $(M + Na)^+$ 313.9752, found 313.9791.

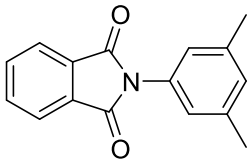
2-(2,6-Dimethylphenyl)isoindoline-1,3-dione (3naa), 2-(2,4-dimethylphenyl)isoindoline-1,3-dione (3nab), and 2-(3,5-dimethylphenyl)isoindoline-1,3-dione (3nac) [2]



3naa



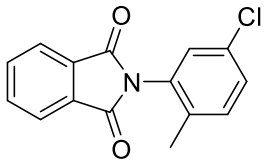
3nab



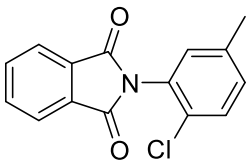
3nac

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in *m*-xylene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3na** (22.6 mg, 90%, **3naa**:**3nab**:**3nac** = 6:11:1) as a white solid. The isomer ratio was determined by ^{1}H NMR spectroscopy. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.97 – 7.94 (m, 2H), 7.81 – 7.78 (m, 2H), 7.29–7.26 (m, 1H [**3naa**]), 7.19–7.12 (m, 2H [**3naa**] + 1H [**3nab**]), 7.15 – 7.11 (m, 1H [**3nab**]), 7.08 (d, *J* = 7.8 Hz, 1H [**3nab**]), 7.05 (s, 1H [**3nac**]), 7.02 (s, 2H [**3nac**]), 2.38 (s, 3H [**3nab**], 6H [**3nac**]), 2.16 (d, *J* = 2.1 Hz, 6H [**3naa**], 3H [**3nab**]). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 167.51, 167.21, 139.95, 139.01, 137.36, 136.12, 134.31, 134.23, 132.04, 131.96, 131.86, 130.80, 130.09, 129.44, 129.05, 128.45, 128.42, 127.83, 127.60, 124.48, 123.75, 123.69, 21.27, 20.71, 18.04, 17.90. **IR (ν, cm^{-1})** 1780, 1723, 1377, 1108, 1084, 883, 723. **HRMS m/z (ESI)**: calcd for $C_{16}H_{13}NNaO_2$ $(M + Na)^+$ 274.0844, found 274.0840.

2-(5-Chloro-2-methylphenyl)isoindoline-1,3-dione (3oaa)[8] **and 2-(2-chloro-5-methylphenyl)isoindoline-1,3-dione (3oab)**



3oaa

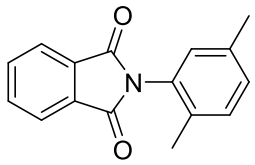


3oab

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in *p*-chlorotoluene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3oa** (17.1 mg, 63%, **3oaa**:**3oab** = 1:1) as a white solid. The isomer ratio

was determined by ^{1}H NMR spectroscopy. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.99 – 7.91 (m, 2H), 7.80 – 7.77 (m, 2H), 7.28 – 7.21 (m, 2H), 7.18 – 7.16 (m, 1H [**3oaa**]), 7.01 (s, 1H [**3oab**]), 2.35 (s, 3H [**3oab**]), 2.15 (s, 3H [**3oaa**]). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.91, 135.19, 134.51, 133.90, 132.07, 131.92, 131.80, 131.26, 129.54, 128.85, 123.90, 18.39, 17.62. **IR (ν, cm^{-1})** 1766, 1726, 1374, 1111, 1074, 889, 718. **HRMS m/z (ESI)**: calcd for $C_{15}H_{10}ClNNaO_2$ $(M + Na)^+$ 294.0298, found 294.0290.

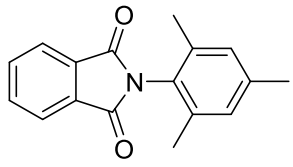
2-(2,5-Dimethylphenyl)isoindoline-1,3-dione (3pa)[2]



3pa

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in *p*-xylene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3pa** (23.6 mg, 94%) as a white solid. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.97 – 7.93 (m, 2H), 7.80–7.77 (m, 2H), 7.26 – 7.23 (m, 1H), 7.18 (d, *J* = 8.0 Hz, 1H), 7.02 (s, 1H), 2.36 (s, 3H), 2.16 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.79, 136.61, 134.22, 133.19, 131.95, 130.86, 130.24, 129.08, 123.64, 20.74, 17.47. **IR (ν, cm^{-1})** 1775, 1718, 1370, 1112, 1082, 873, 718. **HRMS m/z (ESI)**: calcd for $C_{16}H_{13}NNaO_2$ $(M + Na)^+$ 274.0844, found 274.0836.

2-Mesitylisoindoline-1,3-dione (3qa)[2]

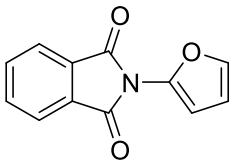


3qa

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in mesitylene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3qa** (17.8 mg, 67%) as a white solid. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.98 – 7.95(m, 2H), 7.83 – 7.77 (m, 2H), 7.01 (s, 2H), 2.34 (s, 3H), 2.12 (s, 6H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.75, 139.33, 136.41, 134.23, 132.42, 129.67, 127.00,

123.69, 21.09, 17.92. **IR (ν, cm^{-1})** 1779, 1723, 1375, 1113, 1083, 882, 718. **HRMS m/z (ESI)**: calcd for $C_{17}H_{15}NNaO_2$ $(M + Na)^+$ 288.1000, found 288.0995.

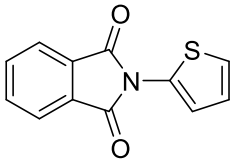
2-(Furan-2-yl)isoindoline-1,3-dione (3ra)[7]



3ra

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in furan (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3ra** (8.7 mg, 41%) as a light yellow solid. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.99-7.96 (m, 2H), 7.85 – 7.80 (m, 2H), 7.47 (dd, *J* = 2.1, 1.0 Hz, 1H), 6.55 (dd, *J* = 3.3, 2.1 Hz, 1H), 6.46 (dd, *J* = 3.4, 1.0 Hz, 1H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.75, 139.33, 136.41, 134.23, 132.42, 129.67, 127.00, 123.69, 21.09, 17.92. **IR (ν, cm^{-1})** 1782, 1728, 1388, 1100, 1082, 882, 716. **HRMS m/z (ESI)**: calcd for $C_{12}H_7NNaO_3$ $(M + Na)^+$ 236.0324, found 236.0316.

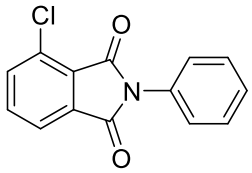
2-(Thiophen-2-yl)isoindoline-1,3-dione (3sa)[7]



3sa

Following the general procedure, the reaction of *N*-hydroxyphthalimide (1.0 equiv., 0.1 mmol, 16.3 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in thiophene (2 mL) at 70 °C under air for 24 h. The crude product was purified by column chromatography on silica gel to afford **3ra** (7.1 mg, 31%) as a yellow solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.94 - 9.91 (m, 2H), 7.81 – 7.74 (m, 2H), 7.52 (ddq, *J* = 5.3, 2.7, 1.2 Hz, 1H), 7.27 – 7.23 (m, 1H), 7.04 (ddt, *J* = 5.4, 3.8, 1.3 Hz, 1H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 165.96, 135.58, 133.99, 131.42, 128.39, 125.25, 123.89, 121.91, 120.40, 77.32, 77.00, 76.68. **IR (ν, cm^{-1})** 1780, 1723, 1377, 1110, 1064, 883, 711. **HRMS m/z (ESI)**: calcd for $C_{12}H_7NNaO_2S$ $(M + Na)^+$ 252.0095, found 252.0084.

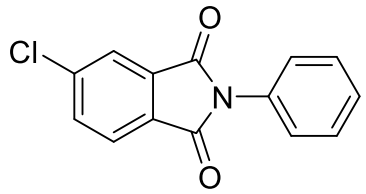
4-Chloro-2-phenylisoindoline-1,3-dione (3ab) [1], [9]



3ab

Following the general procedure, the reaction of 4-chloro-2-hydroxyisoindoline-1,3-dione (1.0 equiv., 0.1 mmol, 19.7 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in benzene (2 mL) at 70 °C under air for 12 h. The crude product was purified by column chromatography on silica gel to afford **3ab** (20.8 mg, 81%) as a white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.86 (dd, *J* = 4.7, 3.5 Hz, 1H), 7.75 – 7.66 (m, 2H), 7.54 – 7.46 (m, 2H), 7.42 (dt, *J* = 8.2, 2.0 Hz, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 165.82, 164.82, 136.12, 135.25, 133.84, 131.89, 131.32, 129.11, 128.29, 127.37, 126.55, 122.22. **IR (ν, cm^{-1})** 1762, 1713, 1378, 1112, 1070, 869, 737. **HRMS m/z (ESI)**: calcd for $C_{14}H_8ClNNaO_2$ $(M + Na)^+$ 280.0141, found 280.0132.

5-Chloro-2-phenylisoindoline-1,3-dione (3ac) [1], [10]

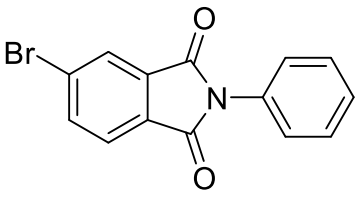


3ca

Following the general procedure, the reaction of 5-chloro-2-hydroxyisoindoline-1,3-dione (1.0 equiv., 0.1 mmol, 19.7 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in benzene (2 mL) at 70 °C under air for 12 h. The crude product was purified by column chromatography on silica gel to afford **3ac** (20.0 mg, 78%) as a white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.97 – 7.84 (m, 2H), 7.73 (dd, *J* = 7.9, 1.8 Hz, 1H), 7.54 – 7.45 (m, 2H), 7.45 – 7.36 (m, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.29, 165.97, 141.10, 134.46, 133.40, 131.39, 129.78, 129.15, 128.29, 126.45, 125.00, 124.14. **IR (ν, cm^{-1})** 1781, 1715, 1387, 1118, 1068, 846, 739. **HRMS m/z (ESI)**: calcd for $C_{14}H_8ClNNaO_2$ $(M + Na)^+$ 280.0141, found 280.0133.

5-Bromo-2-phenylisoindoline-1,3-dione (3ad) [1], [11]

Following the general procedure, the reaction of 5-bromo-2-hydroxyisoindoline-1,3-



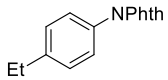
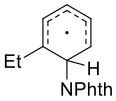
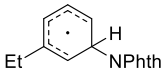
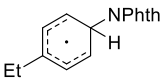
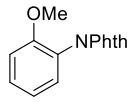
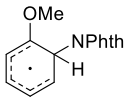
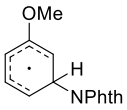
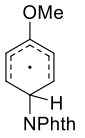
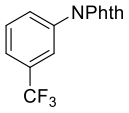
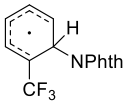
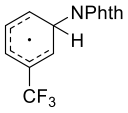
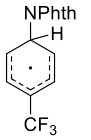
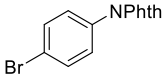
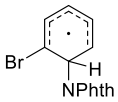
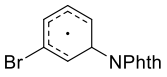
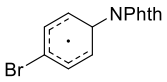
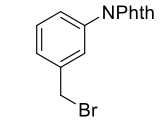
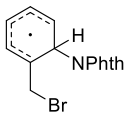
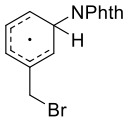
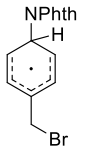
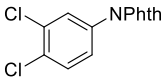
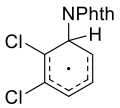
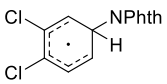
3ad

dione (1.0 equiv., 0.1 mmol, 19.7 mg), $Fe(OTf)_3$ (30 mol%, 0.03 mmol, 15.1 mg), trimethyl phosphite (6.0 equiv., 0.6 mmol, 74.4 mg) in benzene (2 mL) at 70 ^oC under air for 12 h. The crude product was purified by column chromatography on silica gel to afford **3ad** (25.6 mg, 85%) as a white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.05 (s, 1H), 7.90 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.79 (d, *J* = 7.9 Hz, 1H), 7.49 (dd, *J* = 8.6, 7.0 Hz, 2H), 7.40 (d, *J* = 7.8 Hz, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.43, 165.05, 138.01, 133.34, 131.36, 130.24, 129.30, 128.28, 127.06, 126.44, 124.93, 77.37, 77.05, 76.73. **IR (ν, cm^{-1})** 1777, 1719, 1384, 1247, 1067, 843, 735. **HRMS m/z (ESI)**: calcd for $C_{14}H_8BrNNaO_2$ $(M + Na)^+$ 323.9636, found 323.9629.

5. The Theoretical Regioselectivity Calculations

Density functional theory (DFT) calculations were carried out to elaborate the regioselectivity of the Fe-catalyzed direct C–H amination of arenes with *N*-hydroxyphthalimide using GAUSSIAN 09 software.[12] B3LYP-D3[13] functional combined with 6-31G*[14] basis set were implemented for optimization of all geometries (no imaginary frequency) and frequency computations (one imaginary frequency). All the stationary points and the thermal correction to free energies at 298.15 K and 1 atm were also identified at this level of theory. Furthermore, single-point solvation energy was calculated by B3LYP-D3 functional and 6-311+G (d,p)[15] basis set as well as continuum model SMD[16] (benzene as solvent).

Table S1. The calculated energies for the regioselectivity of the reaction

Product	TS-o	TS-m	TS-p
 **3ba** (*o/p* = 1/7)	 5.5 (2.4)	 6.4 (2.6)	 4.8 (1.4)
 **3ea** (*o/m/p* = 13/1/12)	 3.3 (0.9)	 3.8 (0.6)	 3.5 (1.0)
 **3fa** (*m*)	 8.5 (3.9)	 7.3 (3.8)	 7.6 (4.4)
 **3ia** (*o/m/p* = 0/1/6)	 6.2 (3.2)	 6.2 (3.4)	 6.0 (3.3)
 **3ka** (*o/m/p* = 1/3/5)	 8.5 (2.7)	 6.2 (2.4)	 5.9 (3.6)
 **3ma** (*m*)	 6.4 (4.0)	 5.9 (3.4)	

Note: For the ratio of the selectivity and the relative free energies, the best one is marked in blue, the second one in black, the last one in red. The energies listed inside the brackets was calculated by B3LYP-D3/6-31G* level and the energies listed outside the brackets was calculated by B3LYP-D3/6-311(d,p)/SMD level.

Table S2. The calculated energies of stationary points (in Hartree/Particle), and vibrational frequencies of transitions states (in cm^{-1})

	G_{gas}	E_{ele}	E_0	E	H	G
7	-1159.194999	-1159.683851	-1159.490461	-1159.473849	-1159.472905	-1159.536398
8	-512.330595	-512.560421	-512.458804	-512.450745	-512.449801	-512.493395
9	-646.855177	-647.110741	-647.022964	-647.015079	-647.014135	-647.055682
1a	-232.175592	-232.324415	-232.223619	-232.219230	-232.218286	-232.251084
TS10	-744.501303	-744.895621	-744.691870	-744.678474	-744.677530	-744.735035
10	-744.529764	-744.926535	-744.720407	-744.707325	-744.706381	-744.761944
11	-744.290781	-744.722361	-744.514884	-744.501761	-744.500817	-744.556964
TS12	-744.285811	-744.713429	-744.509345	-744.496904	-744.495960	-744.549014
12	744.328114	-744.759975	-744.550510	-744.537785	-744.536841	-744.590296
1b	-310.759485	-310.983350	-310.825706	-310.818442	-310.817498	-310.857732
TS3ba-o	-823.086200	-823.558911	-823.297328	-823.281416	-823.280472	-823.342305
10-3ba-o	-823.116523	-823.589038	-823.325523	-823.309710	-823.308766	-823.370195
TS3ba-m	-823.085993	-823.557384	-823.295948	-823.280094	-823.279150	-823.340943
10-3ba-m	-823.114253	-823.585830	-823.322847	-823.306831	-823.305887	-823.368409
TS3ba-p	-823.087802	-823.559428	-823.297978	-823.281987	-823.281043	-823.343511
10-3ba-p	-823.115702	-823.586629	-823.323591	-823.307495	-823.306551	-823.370559
1e	-346.671538	-346.885570	-346.751798	-346.744993	-346.744049	-346.782801
TS3ea-o	-859.000647	-859.464068	-859.226419	-859.210870	-859.209925	-859.270893
10-3ea-o	-859.030817	-859.493750	-859.254181	-859.238596	-859.237652	-859.299096
TS3ea-m	-859.001188	-859.461748	-859.224154	-859.208607	-859.207662	-859.270121
10-3ea-m	-859.026491	-859.488737	-859.249600	-859.234009	-859.233065	-859.294388
TS3ea-p	-859.000571	-859.463276	-859.226089	-859.210501	-859.209557	-859.270661
10-3ea-p	-859.026785	-859.489203	-859.249755	-859.234168	-859.233224	-859.294599
1f	-569.216959	-569.478131	-569.372369	-569.364503	-569.363559	-569.406550
TS3fa-o	-1081.541418	-1082.049016	-1081.839683	-1081.823051	-1081.822107	-1081.886388
10-3fa-o	-1081.573655	-1082.082284	-1081.870885	-1081.854339	-1081.853395	-1081.917502
TS3fa-m	-1081.541495	-1082.048373	-1081.839216	-1081.822410	-1081.821466	-1081.888363

10-3fa-m	-1081.570365	-1082.080150	-1081.869128	-1081.852437	-1081.851493	-1081.916721
TS3fa-p	-1081.540507	-1082.048313	-1081.839121	-1081.822332	-1081.821387	-1081.887768
10-3fa-p	-1081.572062	-1082.081619	-1081.870419	-1081.853738	-1081.852794	-1081.918741
1i	-2802.994999	-2805.871894	-2805.780952	-2805.775269	-2805.774325	-2805.811815
TS3ia-o	-3315.320499	-3318.444855	-3318.250498	-3318.235937	-3318.234993	-3318.295296
10-3ia-o	-3315.352243	-3318.477480	-3318.281031	-3318.266557	-3318.265613	-3318.325350
TS3ia-m	-3315.320144	-3318.443576	-3318.249285	-3318.234669	-3318.233725	-3318.295337
10-3ia-m	-3315.348831	-3318.473920	-3318.277826	-3318.263312	-3318.262367	-3318.322552
TS3ia-p	-3315.320278	-3318.445150	-3318.250646	-3318.236145	-3318.235200	-3318.295655
10-3ia-p	-3315.350298	-3318.475378	-3318.278930	-3318.264433	-3318.263489	-3318.323762
1k	-2842.288020	-2845.206413	-2845.086826	-2845.079755	-2845.078811	-2845.120541
TS3ka-o	-3354.614311	-3357.776442	-3357.553690	-3357.537780	-3357.536836	-3357.600445
10-3ka-o	-3354.647848	-3357.813804	-3357.588432	-3357.572744	-3357.571799	-3357.633943
TS3ka-m	-3354.614773	-3357.778879	-3357.555734	-3357.539800	-3357.538855	-3357.604012
10-3ka-m	-3354.642606	-3357.808462	-3357.583660	-3357.567746	-3357.566801	-3357.631294
TS3ka-p	-3354.613833	-3357.779225	-3357.556162	-3357.540207	-3357.539263	-3357.604560
10-3ka-p	-3354.646359	-3357.813072	-3357.587971	-3357.572040	-3357.571095	-3357.635975
1m	-1151.383285	-1151.570756	-1151.489078	-1151.482433	-1151.481489	-1151.520968
TS3ma-o	-1663.707491	-1664.143396	-1663.958326	-1663.942764	-1663.941819	-1664.004188
10-3ma-o	-1663.739955	-1664.176430	-1663.989178	-1663.973700	-1663.972756	-1664.034517
TS3ma-m	-1663.708432	-1664.143421	-1663.958284	-1663.942701	-1663.941757	-1664.004918
10-3ma-m	-1663.737973	-1664.173975	-1663.986834	-1663.971319	-1663.970375	-1664.032584

Notes: Ggas was the sum of electronic and thermal free energies in gas phase. E_{ele}, E_0, E, H, and G were the electronic energies, sum of electronic and zero-point energies, sum of electronic and thermal energies, sum of electronic and thermal ethalpies, and sum of electronic and thermal free energies in solvent, respectively.

Cartesian coordinates of the optimized structures

7

C	-2.253161	-0.778682	-0.007428
C	-2.229288	0.656974	-0.124533
C	-3.420286	1.391810	-0.006628
C	-4.611462	0.718432	0.219926
C	-4.635058	-0.704479	0.337595
C	-3.466913	-1.444461	0.227533
H	-3.391367	2.475712	-0.096875
H	-5.542049	1.276144	0.310683
H	-5.583133	-1.208842	0.516409
H	-3.474230	-2.528902	0.316041
C	-0.878599	1.105871	-0.361793
C	-0.916408	-1.298166	-0.168999
O	-0.395282	2.236566	-0.559478
O	-0.438948	-2.443325	-0.167730
N	-0.136731	-0.107642	-0.304415
O	1.178978	-0.169309	-0.768523
P	2.227873	-0.486948	0.506967
O	3.471042	-0.749889	-0.592381
O	2.605348	1.015744	1.064906
C	4.750152	-0.975906	-0.025062
H	5.406752	-1.326479	-0.828248
H	5.173872	-0.055554	0.402939
H	4.727282	-1.742776	0.765407
C	2.744135	2.131612	0.156988
H	1.761579	2.396269	-0.245130
H	3.160138	2.956621	0.743782
H	3.432403	1.879186	-0.658570

8

C	-0.143709	-0.698496	-0.000003
C	-0.143716	0.698501	-0.000075
C	-1.327912	1.428072	0.000048
C	-2.523656	0.703828	0.000243
C	-2.523650	-0.703839	0.000318
C	-1.327899	-1.428073	0.000196
H	-1.313890	2.513329	-0.000005
H	-3.472482	1.232722	0.000346
H	-3.472471	-1.232741	0.000474
H	-1.313868	-2.513330	0.000251
C	1.278829	1.146894	-0.000284
C	1.278844	-1.146873	-0.000177
O	1.701770	2.288456	-0.000193
O	1.701766	-2.288455	0.000042
N	2.134520	-0.000011	-0.000208

9

O	-1.318383	-0.159822	-0.699566
O	1.322547	-0.157695	-0.696593
C	-1.716033	-1.059135	0.308277
H	-2.806084	-1.222845	0.247257
H	-1.228164	-2.046424	0.197779
H	-1.471632	-0.669192	1.306754
C	1.712630	-1.062340	0.309469
H	1.221411	-2.047298	0.193366
H	2.802256	-1.229980	0.252131
H	1.465943	-0.675170	1.308483
P	0.000838	0.947983	-0.356790

O	-0.001150	1.117518	1.163609	N	-0.391271	1.358472	-1.356647
				C	1.472761	0.731644	-0.018380
1a				C	-0.043539	0.002987	-1.631032
C	-1.064838	-0.904542	0.000005	C	0.491318	1.812953	-0.327538
C	0.251079	-1.374313	0.000069	O	-0.628747	-0.697877	-2.436675
C	1.315819	-0.469879	-0.000056	O	0.419323	2.912866	0.188053
C	1.064761	0.904631	0.000008	C	1.139813	-0.373089	-0.803214
C	-0.250963	1.374331	0.000062	C	1.855345	-1.562933	-0.728427
C	-1.315859	0.469773	-0.000057	H	1.583979	-2.413582	-1.345674
H	-1.892888	-1.608249	-0.000066	C	2.921958	-1.612680	0.174097
H	0.446169	-2.443359	0.000079	H	3.504008	-2.525009	0.270476
H	2.339236	-0.835217	-0.000153	C	3.257551	-0.498782	0.965540
H	1.892980	1.608127	0.000008	H	4.092596	-0.572868	1.656675
H	-0.446295	2.443326	0.000018	C	2.535066	0.695465	0.877404
H	-2.339195	0.835364	-0.000063	H	2.782203	1.562087	1.482655

TS10				**10**			
C	-2.976705	-0.228963	-0.274735	C	2.434259	0.398027	1.257899
C	-1.654843	0.645039	1.566137	C	2.434181	0.398107	-1.257937
C	-1.285007	-0.651633	1.917868	C	3.573733	-0.353387	-1.226695
C	-1.758048	-1.737628	1.171650	C	4.169835	-0.742077	-0.000113
C	-2.606971	-1.525405	0.078780	C	3.573839	-0.353460	1.226511
H	-3.608212	-0.058722	-1.140843	H	1.972791	0.686673	2.198315
H	-1.271117	1.495520	2.121566	H	1.972563	0.686811	-2.198258
H	-0.620023	-0.819243	2.760520	H	4.032947	-0.665808	-2.161537
H	-1.460191	-2.748321	1.437718	H	5.070419	-1.347638	-0.000161
H	-2.961061	-2.369413	-0.505658	H	4.033126	-0.665925	2.161303
C	-2.492699	0.860966	0.460223	C	1.748863	0.862929	0.000029
H	-2.763901	1.872692	0.177829	H	1.695539	1.965174	0.000077

N	0.318173	0.481428	0.000086	N	0.294587	0.363937	-0.000595
C	-1.987251	0.618126	0.000006	C	-1.981054	0.648159	-0.000449
C	-0.154782	-0.845769	0.000109	C	-0.248445	-0.941064	0.000337
C	-0.728230	1.418661	0.000046	C	-0.692312	1.381110	-0.001409
O	0.532409	-1.844901	0.000135	O	0.440108	-1.940060	0.000554
O	-0.593744	2.627406	0.000106	O	-0.419993	2.562644	-0.002738
C	-1.645084	-0.734948	0.000039	C	-1.717366	-0.733742	0.000684
C	-2.612852	-1.728103	0.000003	C	-2.742707	-1.667359	0.001727
H	-2.332235	-2.776744	0.000046	H	-2.531591	-2.731694	0.002589
C	-3.954217	-1.320435	-0.000067	C	-4.057708	-1.177779	0.001594
H	-4.742169	-2.068301	-0.000102	H	-4.887257	-1.877958	0.002390
C	-4.297441	0.038698	-0.000097	C	-4.320437	0.198131	0.000423
H	-5.345884	0.323168	-0.000162	H	-5.349586	0.543424	0.000326
C	-3.310292	1.034024	-0.000061	C	-3.278412	1.137961	-0.000637
H	-3.560991	2.090187	-0.000076	H	-3.474062	2.205254	-0.001569

11				**TS12**			
C	2.397958	0.237340	1.254174	C	2.425775	0.035341	1.242253
C	2.397487	0.230416	-1.254829	C	2.425212	0.034510	-1.242117
C	3.679381	-0.255235	-1.239070	C	3.803573	-0.044013	-1.229767
C	4.313019	-0.487853	0.001270	C	4.484622	-0.084230	-0.000366
C	3.679767	-0.248473	1.240600	C	3.804125	-0.043192	1.229321
H	1.862738	0.409823	2.183710	H	1.864050	0.051000	2.171224
H	1.861904	0.397582	-2.185124	H	1.863069	0.049533	-2.170847
H	4.194570	-0.497287	-2.162593	H	4.357588	-0.102165	-2.160670
H	5.322780	-0.891701	0.002212	H	5.568539	-0.160778	-0.000585
H	4.195329	-0.485433	2.165238	H	4.358568	-0.100717	2.160008
C	1.708122	0.620447	-0.001302	C	1.701799	0.177680	0.000187
H	1.758397	1.747399	-0.004216	H	1.483663	1.454576	-0.000267

N	0.286191	-0.060028	0.000577	O	0.080400	-2.338514	0.377508
C	-1.882953	0.699743	0.000042	N	-0.321909	-0.042549	0.003793
C	-0.519621	-1.246940	0.000340	C	-1.755925	-0.036270	0.010608
C	-0.475161	1.095332	0.000090	C	-2.447873	-0.889980	-0.852371
O	-0.092380	-2.371018	0.000255	C	-2.427162	0.831106	0.883812
O	0.128253	2.180989	-0.000366	C	-3.841587	-0.861992	-0.843589
C	-1.913527	-0.710159	0.000184	H	-1.905681	-1.560896	-1.509428
C	-3.112909	-1.400825	0.000113	C	-3.822862	0.858305	0.865767
H	-3.133267	-2.485717	0.000207	H	-1.871722	1.434164	1.598156
C	-4.295349	-0.640970	-0.000094	C	-4.527101	0.014019	0.004216
H	-5.254073	-1.150197	-0.000152	H	-4.392550	-1.523444	-1.504403
C	-4.263475	0.758912	-0.000238	H	-4.354710	1.523143	1.538775
H	-5.196256	1.313668	-0.000402	H	-5.612363	0.030768	-0.000050
C	-3.046755	1.457092	-0.000179	O	0.042230	2.227405	-0.422344
H	-3.014334	2.541550	-0.000297	H	-0.940119	2.270539	-0.457736

12				**1b**			
C	1.864185	0.658596	-0.109402	C	2.321451	0.000093	0.240013
C	1.917826	-0.726391	0.129411	C	0.266341	1.203265	-0.189272
C	3.125495	-1.390529	0.246140	C	-0.436758	-0.000088	-0.336608
C	4.296621	-0.620406	0.117671	C	0.266472	-1.203355	-0.189167
C	4.241689	0.757787	-0.121311	C	1.632943	-1.206543	0.096167
C	3.013634	1.427406	-0.241298	H	3.385957	0.000161	0.458826
H	3.163829	-2.459266	0.429181	H	2.160665	-2.151043	0.202092
H	5.263302	-1.106187	0.205414	H	-0.263632	-2.146958	-0.302649
H	5.164973	1.320086	-0.215699	H	-0.263860	2.146805	-0.302859
H	2.966710	2.495087	-0.427515	C	-1.928219	-0.000159	-0.595029
C	0.534751	-1.247172	0.208352	H	-2.200480	0.879446	-1.192366
C	0.460084	1.019308	-0.185433	H	-2.200471	-0.880037	-1.191966

C	-2.744381	0.000119	0.710333	C	-4.161653	0.627987	-0.602020
H	-2.510753	0.884607	1.313931	H	-5.061043	1.189184	-0.840370
H	-3.821028	0.000074	0.503800	C	-3.200746	1.187815	0.248687
H	-2.510744	-0.884115	1.314303	H	-3.325384	2.173926	0.685341
C	1.632806	1.206642	0.096065	C	1.417927	1.957268	-0.933711
H	2.160419	2.151213	0.201878	H	0.869567	1.859896	-1.879150
				H	0.711557	2.329463	-0.184970
TS3ba-o				C	2.553689	2.985163	-1.105333
C	2.752028	-0.913605	1.244828	H	3.268512	2.656764	-1.868378
C	1.948634	0.606625	-0.515485	H	2.152252	3.959651	-1.404928
C	2.309715	-0.353871	-1.460421	H	3.102951	3.117587	-0.166340
C	2.885116	-1.566983	-1.068285	H	3.149706	-2.303208	-1.822237
C	3.119039	-1.843522	0.286423				
H	2.890192	-1.119962	2.301240	**10-3ba-o**			
H	2.145765	-0.151811	-2.516274	C	2.080210	-0.937608	1.538884
H	3.560583	-2.790824	0.579719	C	2.306183	0.415549	-0.597473
C	2.142232	0.300737	0.857351	C	3.416234	-0.337480	-0.877400
H	1.913266	1.054701	1.603639	C	3.885749	-1.359463	-0.017431
N	-0.081900	-0.439277	1.396823	C	3.190317	-1.646022	1.183718
C	-2.066324	0.430803	0.511206	H	1.535755	-1.156063	2.453525
C	-0.568893	-1.362937	0.449080	H	3.952310	-0.148709	-1.805614
C	-0.852107	0.733471	1.336700	H	3.545318	-2.446504	1.828269
O	-0.030134	-2.403903	0.121482	C	1.549104	0.192545	0.698823
O	-0.569067	1.801156	1.857613	H	1.579390	1.120670	1.293974
C	-1.887613	-0.837881	-0.041941	N	0.098288	0.027923	0.452846
C	-2.837748	-1.406405	-0.879465	C	-2.178021	0.412073	0.409751
H	-2.686736	-2.395511	-1.300846	C	-0.467055	-1.035633	-0.277683
C	-3.982811	-0.649617	-1.157743	C	-0.869043	0.947252	0.884714
H	-4.747189	-1.053225	-1.816189	O	0.145438	-1.950257	-0.786241

O	-0.646622	1.967801	1.510167	N	-0.076155	-1.117311	-1.335821
C	-1.938159	-0.773912	-0.286067	C	1.673665	-0.959299	0.210817
C	-2.971499	-1.503228	-0.854287	C	0.639169	0.064720	-1.613238
H	-2.770598	-2.423496	-1.393829	C	0.402029	-1.678390	-0.132317
C	-4.272364	-1.002938	-0.701965	O	0.348995	0.907654	-2.444384
H	-5.109331	-1.545677	-1.132201	O	-0.096330	-2.600294	0.485776
C	-4.512794	0.188356	-0.003397	C	1.824348	0.089065	-0.697351
H	-5.532085	0.550373	0.096914	C	2.910150	0.953021	-0.641228
C	-3.459791	0.918030	0.565885	H	3.012580	1.765013	-1.354353
H	-3.630278	1.842514	1.108624	C	3.848393	0.735647	0.374504
C	1.804741	1.492755	-1.522960	H	4.707631	1.394714	0.463030
H	2.409763	1.484334	-2.437463	C	3.697733	-0.321131	1.288485
H	0.775019	1.260837	-1.834150	H	4.442958	-0.458711	2.067152
C	1.822600	2.906423	-0.906653	C	2.604863	-1.193027	1.214290
H	2.834297	3.174829	-0.581409	H	2.476131	-2.014405	1.912246
H	1.494305	3.647453	-1.644172	H	-2.572631	0.444683	2.564501
H	1.154667	2.978476	-0.042261	H	-1.968033	1.444716	-1.566378
H	4.764467	-1.935048	-0.290295	C	-1.823106	2.525677	0.933984
				H	-2.330257	3.253546	0.287545
TS3ba-m				H	-2.144769	2.739541	1.960662
C	-2.842667	-1.549522	-0.173556	C	-0.299486	2.720705	0.814170
C	-2.237911	0.733280	-0.793012	H	0.033316	2.550701	-0.215495
C	-2.239712	1.123240	0.546663	H	-0.009648	3.736767	1.105384
C	-2.566863	0.159827	1.514635	H	0.236660	2.012996	1.456818
C	-2.877635	-1.160675	1.157705				
H	-3.043305	-2.577314	-0.455068	**10-3ba-m**			
H	-3.120905	-1.883736	1.930340	C	-1.566913	-1.673708	1.256874
C	-2.495068	-0.604690	-1.159337	C	-1.999457	-0.505305	-0.927374
H	-2.515384	-0.876906	-2.208060	C	-3.175053	-0.017445	-0.428640

C	-3.573523	-0.358713	0.895627	H	-4.098200	2.519659	0.276130
C	-2.758620	-1.182982	1.708417				
H	-0.934845	-2.297302	1.882917	**TS3ba-p**			
H	-3.091270	-1.426063	2.714886	C	-1.407907	1.401262	-1.225606
C	-1.060604	-1.364135	-0.125415	C	-2.446223	1.601681	0.978209
H	-0.864142	-2.306438	-0.663093	C	-3.175621	0.454500	0.727508
N	0.287421	-0.746383	-0.069930	C	-3.013789	-0.259385	-0.475836
C	2.564823	-0.428200	-0.287055	C	-2.138405	0.249280	-1.456546
C	0.556206	0.536068	0.445579	H	-0.716935	1.785587	-1.969428
C	1.448669	-1.388522	-0.530124	H	-2.551418	2.128280	1.921306
O	-0.261718	1.306122	0.904075	H	-3.860932	0.072481	1.479396
O	1.493547	-2.500150	-1.021435	H	-2.030826	-0.284106	-2.398081
C	2.031536	0.722571	0.295301	C	-1.502591	2.063073	0.026889
C	2.833083	1.801488	0.636223	H	-1.000268	3.013345	0.162973
H	2.404592	2.690393	1.088592	N	0.384751	1.188841	0.907885
C	4.205860	1.692500	0.373094	C	2.387681	0.471337	-0.053046
H	4.867550	2.516237	0.625775	C	0.427187	-0.208116	1.027629
C	4.741112	0.536485	-0.211785	C	1.444542	1.629049	0.100576
H	5.809071	0.482210	-0.403291	O	-0.441881	-0.924074	1.495514
C	3.920724	-0.548040	-0.552557	O	1.557043	2.739917	-0.390508
H	4.320923	-1.449257	-1.006446	C	1.762568	-0.648657	0.496883
H	-4.509655	0.030087	1.286737	C	2.370554	-1.896089	0.493639
H	-1.673922	-0.246353	-1.932377	H	1.872233	-2.758554	0.925673
C	-4.025330	0.942078	-1.233582	C	3.639472	-1.990423	-0.092913
H	-3.778408	0.852945	-2.298523	H	4.147623	-2.950453	-0.123558
H	-5.085963	0.674605	-1.132958	C	4.267808	-0.864024	-0.647051
C	-3.817269	2.396995	-0.775996	H	5.251262	-0.971854	-1.096418
H	-2.763049	2.679965	-0.867109	C	3.646636	0.391642	-0.632506
H	-4.420727	3.089401	-1.374384	H	4.120221	1.270765	-1.058597

C	-3.684708	-1.593830	-0.675278	C	-4.581977	-1.563352	0.000305
H	-4.027445	-1.692157	-1.713721	H	-5.303452	-2.375587	0.000319
H	-4.572967	-1.664333	-0.035930	C	-5.039741	-0.238412	0.000406
C	-2.717044	-2.750072	-0.342597	H	-6.108616	-0.044358	0.000475
H	-3.225494	-3.716837	-0.430416	C	-4.140751	0.837216	0.000397
H	-1.862489	-2.746249	-1.028395	H	-4.480215	1.868299	0.000436
H	-2.318056	-2.641917	0.670219	C	4.776909	-1.081051	0.000102
				H	4.847446	-1.734673	-0.879156
10-3ba-p				H	4.849074	-1.731897	0.881265
C	1.639195	0.685809	1.254300	C	5.968847	-0.101556	-0.002588
C	1.639129	0.685498	-1.254120	H	6.922618	-0.642255	-0.002677
C	2.818295	0.001520	-1.220076	H	5.939979	0.543419	-0.888228
C	3.449514	-0.369455	0.000193	H	5.941679	0.546185	0.881081
C	2.818384	0.001813	1.220369				
H	1.166398	0.946257	2.197378	**1e**			
H	1.166275	0.945710	-2.197235	C	1.851651	-1.001831	-0.000088
H	3.296328	-0.279589	-2.156912	C	1.337587	1.351717	0.000032
H	3.296454	-0.279055	2.157255	C	-0.032097	1.064860	0.000109
C	0.916727	1.098042	0.000059	C	-0.455212	-0.270056	0.000135
H	0.769953	2.191089	-0.000076	C	0.494262	-1.303423	0.000033
N	-0.478119	0.595431	0.000143	H	2.577466	-1.810896	-0.000123
C	-2.787165	0.535161	0.000276	H	0.139064	-2.329241	0.000037
C	-0.836390	-0.766806	0.000251	H	1.657955	2.390498	-0.000033
C	-1.600491	1.439860	0.000102	H	-0.748192	1.878655	0.000164
O	-0.068091	-1.705197	0.000041	O	-1.761341	-0.671881	0.000117
O	-1.570347	2.655767	0.000274	C	-2.769646	0.324565	-0.000163
C	-2.331023	-0.783696	0.000217	H	-2.712366	0.960264	-0.894831
C	-3.210764	-1.855540	0.000206	H	-3.721470	-0.210463	-0.000339
H	-2.841767	-2.876433	0.000165	H	-2.712752	0.960361	0.894460

C	2.284427	0.329683	-0.000090
H	3.345194	0.562780	-0.000076

TS3ea-o

C	-3.112321	0.008593	-1.204576
C	-1.767061	0.775100	0.694673
C	-2.319870	-0.230887	1.490156
C	-3.258911	-1.098952	0.931548
C	-3.664430	-0.978183	-0.409876
H	-3.398242	0.112986	-2.245981
H	-2.030115	-0.345475	2.527710
H	-4.401400	-1.664012	-0.815235
C	-2.120637	0.873084	-0.685388
H	-1.784739	1.743339	-1.237246
N	-0.223096	-0.036290	-1.462775
C	1.569320	-0.954326	-0.265544
C	0.747520	0.966901	-1.307351
C	0.163275	-1.182383	-0.747915
O	0.643065	2.125436	-1.673470
O	-0.513922	-2.177756	-0.559875
C	1.925317	0.349317	-0.611512
C	3.170701	0.873280	-0.291181
H	3.433936	1.889401	-0.568843
C	4.058045	0.041837	0.404336
H	5.040363	0.415370	0.680968
C	3.699779	-1.270156	0.753355
H	4.411197	-1.888966	1.293700
C	2.443129	-1.790153	0.416822
H	2.152422	-2.803388	0.677505
H	-3.682340	-1.884249	1.551128
O	-0.852177	1.678087	1.108337
C	-0.234609	1.496128	2.379847
H	0.235649	0.507322	2.447208
H	0.530381	2.270346	2.447513
H	-0.956658	1.620023	3.196707

10-3ea-o

C	2.042876	-1.494470	1.211414
C	2.248157	0.658209	-0.068378
C	3.376902	0.168579	-0.670407
C	3.852118	-1.130601	-0.362551
C	3.165131	-1.940388	0.573758
H	1.511318	-2.111946	1.929477
H	3.914597	0.767383	-1.397426
H	3.541387	-2.937396	0.789113
C	1.468387	-0.126737	0.960337
H	1.441805	0.454643	1.896572
N	0.039777	-0.193400	0.588000
C	-2.240245	0.167476	0.593382
C	-0.441201	-0.705385	-0.629916
C	-0.980745	0.376060	1.366490
O	0.232755	-1.207410	-1.505326
O	-0.831130	0.913215	2.446576
C	-1.918033	-0.480205	-0.599980
C	-2.889970	-0.808024	-1.533125
H	-2.624761	-1.311434	-2.457624
C	-4.214944	-0.463481	-1.231300
H	-5.005636	-0.703494	-1.936642

C	-4.538267	0.187512	-0.032635	H	4.158176	1.550900	-0.337109
H	-5.574300	0.442161	0.172342	C	4.384662	-0.582100	-0.722118
C	-3.546796	0.514329	0.902990	H	5.396416	-0.494620	-1.108693
H	-3.781719	1.019178	1.834813	C	3.781168	-1.848411	-0.660430
H	4.740354	-1.504729	-0.860783	H	4.336585	-2.718150	-1.000809
O	1.677883	1.869904	-0.282618	C	2.477992	-2.006270	-0.171106
C	2.247029	2.712476	-1.275747	H	1.999624	-2.979263	-0.115313
H	2.240661	2.221907	-2.257668	H	-2.651377	-0.099777	-2.628970
H	1.622618	3.606969	-1.306191	H	-2.977507	0.021308	1.656115
H	3.276766	2.992778	-1.017052	O	-3.572645	-1.331607	-0.645744
				C	-3.814387	-2.114936	0.524271
TS3ea-m				H	-4.548627	-1.631088	1.182005
C	-1.368249	2.188257	-0.455222	H	-4.223722	-3.061087	0.166259
C	-2.639851	0.451727	0.722964	H	-2.878642	-2.286895	1.066673
C	-2.894130	-0.170805	-0.494777				
C	-2.424362	0.410133	-1.698010	**10-3ea-m**			
C	-1.670528	1.579458	-1.672521	C	-1.607718	-1.610598	1.278230
H	-0.738692	3.068535	-0.404960	C	-2.062784	-0.185541	-0.755213
H	-1.306518	2.005737	-2.602628	C	-3.191167	0.273532	-0.138005
C	-1.837796	1.603134	0.748648	C	-3.564746	-0.185591	1.162643
H	-1.674920	2.118508	1.687043	C	-2.757548	-1.122052	1.837465
N	0.322407	0.665911	1.190594	H	-0.977130	-2.321241	1.804283
C	1.809685	-0.860448	0.237093	H	-3.057431	-1.456421	2.827426
C	1.409753	1.396753	0.684180	C	-1.149022	-1.176420	-0.086305
C	0.430494	-0.676135	0.804617	H	-1.041685	-2.065702	-0.729572
O	1.524532	2.610222	0.671908	N	0.241137	-0.661519	-0.033370
O	-0.413786	-1.548423	0.941107	C	2.506414	-0.420847	-0.413539
C	2.409921	0.397643	0.177333	C	0.640398	0.484045	0.681594
C	3.703552	0.565830	-0.296911	C	1.309828	-1.258007	-0.721486

O	-0.080228	1.189452	1.355347	N	-0.158241	-2.322385	0.510838
O	1.235625	-2.252738	-1.417685	C	1.592131	-0.901065	-0.248084
C	2.106391	0.621153	0.424261	C	0.036275	-1.276982	1.443245
C	3.007140	1.570574	0.882479	C	0.760877	-2.109497	-0.553036
H	2.681688	2.375545	1.534020	O	-0.596047	-1.146676	2.479408
C	4.341311	1.444206	0.470597	O	0.833479	-2.804764	-1.551232
H	5.077815	2.168071	0.807959	C	1.133616	-0.380546	0.960853
C	4.742765	0.397463	-0.370911	C	1.668417	0.781301	1.505128
H	5.783968	0.326278	-0.672586	H	1.295259	1.176802	2.444555
C	3.822908	-0.556687	-0.827925	C	2.689354	1.414424	0.787251
H	4.119292	-1.372513	-1.479810	H	3.133544	2.327681	1.174087
H	-4.469019	0.214211	1.607305	C	3.154199	0.888021	-0.431741
H	-1.764047	0.149262	-1.741158	H	3.950226	1.403387	-0.962549
O	-4.065600	1.179097	-0.668006	C	2.608553	-0.284422	-0.967772
C	-3.757473	1.730297	-1.937388	H	2.954989	-0.700606	-1.908877
H	-3.726494	0.955660	-2.716417	H	-1.254165	-1.118129	-2.475558
H	-4.558193	2.437369	-2.162646	H	-0.501451	1.201275	-2.135086
H	-2.795286	2.260472	-1.921449	O	-1.180470	2.688304	0.062223
				C	-0.233854	3.343964	-0.777012
TS3ea-p				H	-0.638272	3.506392	-1.784288
C	-2.863652	-0.485347	0.459476	H	-0.039987	4.308694	-0.305538
C	-1.600682	-0.564777	-1.608754	H	0.699026	2.770987	-0.840021
C	-1.168750	0.743730	-1.415230				
C	-1.574494	1.434386	-0.260501	**10-3ea-p**			
C	-2.442408	0.816434	0.666470	C	1.599459	1.095292	1.300464
H	-3.492873	-0.969814	1.198513	C	1.711365	0.864955	-1.193541
H	-2.733467	1.376724	1.548380	C	2.895042	0.189311	-1.057845
C	-2.424230	-1.201756	-0.665771	C	3.444153	-0.057849	0.222326
H	-2.732961	-2.228811	-0.819812	C	2.777101	0.424864	1.385659

H	1.098145	1.457775	2.193390	C	-2.137736	1.210318	0.001930
H	3.249938	0.240888	2.346275	C	-0.743251	1.212728	-0.023868
C	0.904366	1.334272	-0.013884	C	-0.049417	-0.000096	-0.036924
H	0.660550	2.402376	-0.122946	C	-0.743380	-1.212829	-0.023867
N	-0.445734	0.706537	-0.015380	H	-2.679028	-2.152113	0.007987
C	-2.740378	0.441092	-0.075368	H	-0.192739	-2.147607	-0.042406
C	-0.685169	-0.677845	0.083537	H	-2.678782	2.152229	0.008017
C	-1.636286	1.444725	-0.114466	H	-0.192500	2.147449	-0.042421
O	0.159017	-1.543849	0.178066	C	1.454420	-0.000043	-0.002321
O	-1.712645	2.654871	-0.211713	F	1.973362	1.090329	-0.611467
C	-2.172120	-0.827677	0.043703	F	1.922242	0.001650	1.268721
C	-2.955061	-1.970520	0.105362	F	1.973460	-1.091911	-0.608646
H	-2.499125	-2.951297	0.198403	C	-2.835523	0.000063	0.015903
C	-4.345542	-1.802922	0.043157	H	-3.921910	0.000129	0.034728
H	-4.993513	-2.673776	0.088560				
C	-4.916067	-0.528058	-0.076697	**TS3fa-o**			
H	-5.997114	-0.430651	-0.122277	C	2.596932	-1.219952	1.490842
C	-4.114262	0.620212	-0.137980	C	2.063883	0.428582	-0.225651
H	-4.541839	1.613706	-0.230555	C	2.731307	-0.339657	-1.168135
H	1.293544	1.052867	-2.178333	C	3.336466	-1.543504	-0.783629
H	3.412329	-0.148563	-1.949628	C	3.273230	-1.977716	0.545928
O	4.607794	-0.723356	0.459627	H	2.528187	-1.547844	2.522616
C	5.312373	-1.273160	-0.643440	H	3.750327	-2.909233	0.834919
H	5.650548	-0.490937	-1.336758	C	1.948048	-0.018386	1.113580
H	6.182311	-1.779905	-0.221553	H	1.561604	0.655399	1.870907
H	4.697182	-1.999733	-1.190681	N	-0.149178	-0.793376	1.148405
				C	-2.248416	0.070678	0.655078
1f				C	-0.582420	-1.423351	-0.032894
C	-2.137882	-1.210258	0.001917	C	-1.011971	0.268081	1.478753

O	0.055329	-2.210076	-0.705675	C	-2.341118	0.109948	0.609752
O	-0.787540	1.150931	2.285732	C	-0.630737	-1.034340	-0.513281
C	-1.986665	-0.947645	-0.264229	C	-1.068037	0.291201	1.363788
C	-2.939852	-1.357915	-1.185354	O	-0.002161	-1.691042	-1.315702
H	-2.723116	-2.150457	-1.894792	O	-0.862087	0.916026	2.384591
C	-4.177141	-0.701478	-1.163350	C	-2.080208	-0.681242	-0.510842
H	-4.947896	-0.984184	-1.875066	C	-3.080676	-1.017277	-1.410286
C	-4.439375	0.322437	-0.239441	H	-2.863622	-1.631351	-2.278627
H	-5.408012	0.814392	-0.252928	C	-4.369261	-0.529818	-1.151956
C	-3.473013	0.722532	0.692212	H	-5.179773	-0.769165	-1.834513
H	-3.661161	1.514488	1.410252	C	-4.630791	0.264706	-0.027046
H	2.791471	0.000024	-2.196348	H	-5.639686	0.628870	0.144755
H	3.855575	-2.141711	-1.526264	C	-3.611835	0.597428	0.876108
C	1.368254	1.695434	-0.641894	H	-3.798824	1.213506	1.749978
F	1.349265	2.608741	0.347455	H	3.780836	0.223509	-1.439885
F	0.074479	1.453576	-0.983552	H	4.507811	-2.065595	-0.792615
F	1.953961	2.260691	-1.719845	C	1.685820	1.636998	-0.503886
				F	1.398698	2.399949	0.579420
10-3fa-o				F	0.546271	1.594659	-1.248498
C	1.838300	-1.797488	1.296663	F	2.606142	2.296258	-1.238196
C	2.142942	0.272302	-0.096111				
C	3.229438	-0.318650	-0.678284	**TS3fa-m**			
C	3.646555	-1.618240	-0.307952	C	0.589085	2.118691	0.963078
C	2.929197	-2.337968	0.680886	C	1.930124	1.034773	-0.776027
H	1.277390	-2.350836	2.044216	C	2.574748	0.297177	0.201360
H	3.252094	-3.341269	0.946096	C	2.236720	0.455776	1.554412
C	1.334117	-0.415711	0.980955	C	1.246812	1.370560	1.930556
H	1.360054	0.200861	1.894776	H	-0.189924	2.824977	1.230213
N	-0.100646	-0.436756	0.647018	H	0.999696	1.495280	2.980521

C	0.893552	1.929128	-0.408773	C	2.050540	1.501181	1.945727
H	0.483072	2.615688	-1.139312	H	0.182825	2.544379	1.823791
N	-0.849319	0.675936	-0.985113	H	2.279865	1.876106	2.939668
C	-3.017675	0.308346	-0.234713	C	0.507629	1.385144	-0.036657
C	-0.895715	-0.647303	-0.511844	H	0.358376	2.246853	-0.709274
C	-2.028750	1.357700	-0.647220	N	-0.827825	0.753985	-0.026052
O	0.033481	-1.429149	-0.446847	C	-3.058506	0.334311	-0.444726
O	-2.194406	2.564501	-0.683437	C	-1.144474	-0.425015	0.678476
C	-2.329679	-0.904145	-0.143381	C	-1.932336	1.270432	-0.726666
C	-2.969610	-2.077646	0.229722	O	-0.374900	-1.068322	1.359858
H	-2.422875	-3.013187	0.294854	O	-1.923594	2.276395	-1.408960
C	-4.337198	-1.996507	0.522823	C	-2.588242	-0.678403	0.393918
H	-4.874559	-2.889922	0.828654	C	-3.414953	-1.703643	0.827934
C	-5.028348	-0.777982	0.432193	H	-3.035870	-2.485215	1.478842
H	-6.088444	-0.750147	0.668548	C	-4.746997	-1.684982	0.391310
C	-4.374060	0.398956	0.046139	H	-5.426286	-2.470969	0.708793
H	-4.896751	1.347441	-0.028747	C	-5.218876	-0.668227	-0.450392
H	2.752523	-0.134401	2.305293	H	-6.256349	-0.681973	-0.771974
H	2.182157	0.899931	-1.820778	C	-4.373980	0.363284	-0.883195
C	3.608193	-0.734604	-0.163876	H	-4.725566	1.156417	-1.535533
F	4.008891	-0.622279	-1.447524	H	3.875331	0.319307	1.818320
F	4.708711	-0.615861	0.619575	H	1.311040	0.055530	-1.623492
F	3.137793	-1.984921	0.011519	C	3.681600	-0.792277	-0.619521
				F	3.230618	-1.352478	-1.761492
10-3fa-m				F	4.819189	-0.121564	-0.921279
C	0.887996	1.878860	1.334284	F	4.033896	-1.794913	0.216579
C	1.527888	0.459552	-0.640936				
C	2.669498	0.120900	0.020543	**TS3fa-p**			
C	2.964218	0.625161	1.316865	C	-1.586005	1.914657	-1.210830

C	-0.841622	1.591264	1.099027
C	-1.765828	0.571304	1.249235
C	-2.597078	0.221616	0.173148
C	-2.513236	0.897777	-1.050561
H	-1.501070	2.436321	-2.158126
H	-3.170549	0.615227	-1.864559
C	-0.706429	2.248913	-0.151555
H	-0.080459	3.131310	-0.216078
N	1.144857	1.215327	-0.837315
C	3.012508	0.270784	0.176074
C	1.068154	-0.173806	-1.053425
C	2.169621	1.506767	0.078855
O	0.165248	-0.772659	-1.604506
O	2.321608	2.561151	0.670446
C	2.340124	-0.750050	-0.500367
C	2.860194	-2.034161	-0.582384
H	2.327016	-2.817756	-1.111583
C	4.087360	-2.269994	0.050647
H	4.525208	-3.263853	0.019562
C	4.763001	-1.244170	0.730734
H	5.711971	-1.462345	1.212660
C	4.232667	0.050270	0.800680
H	4.744481	0.852395	1.323201
H	-0.186791	1.878001	1.915256
H	-1.864617	0.047444	2.194438
C	-3.551456	-0.930693	0.345399
F	-4.160786	-0.885368	1.553464
F	-4.516367	-0.939504	-0.597968
F	-2.905723	-2.114554	0.276820

10-3fa-p

C	-1.038252	0.929655	-1.252658
C	-1.036838	0.932273	1.261382
C	-2.283924	0.382708	1.236724
C	-2.932706	0.099600	0.007225
C	-2.284023	0.379873	-1.224832
H	-0.534123	1.128351	-2.193965
H	-2.792208	0.134843	-2.152294
C	-0.287963	1.283493	0.003648
H	-0.070423	2.365804	0.002386
N	1.060981	0.685606	0.003319
C	3.357266	0.452981	-0.001909
C	1.315193	-0.700773	0.005240
C	2.244110	1.445483	-0.001212
O	0.472342	-1.572489	0.008980
O	2.299107	2.659785	-0.003971
C	2.802762	-0.828697	0.001815
C	3.599014	-1.964007	0.001785
H	3.154681	-2.954353	0.004608
C	4.988218	-1.775736	-0.002141
H	5.646279	-2.640013	-0.002390
C	5.544607	-0.489112	-0.005795
H	6.624985	-0.376383	-0.008765
C	4.729884	0.651689	-0.005715
H	5.146951	1.653808	-0.008543
H	-0.531675	1.132732	2.201735
H	-2.791220	0.141165	2.165186
C	-4.331507	-0.432535	-0.001342

F	-4.624056	-1.111933	1.130496	C	-2.196214	0.073898	0.698434
F	-5.246957	0.565527	-0.105591	C	-0.513643	1.518962	-0.047708
F	-4.547514	-1.263031	-1.047633	C	-0.978075	-0.066795	1.559723
				O	0.132334	2.268825	-0.754587
1i				O	-0.781651	-0.891031	2.434758
C	-2.181877	1.208219	-0.000073	C	-1.912773	1.028667	-0.280523
C	-2.181877	-1.208219	-0.000073	C	-2.845182	1.376712	-1.248085
C	-0.785435	-1.216374	-0.000052	H	-2.611616	2.120888	-2.003142
C	-0.785435	1.216374	-0.000052	C	-4.083149	0.723048	-1.210120
H	-2.719582	2.152384	-0.000127	H	-4.837781	0.957591	-1.955860
H	-0.233767	2.150158	-0.000111	C	-4.367702	-0.236943	-0.225248
H	-2.719582	-2.152384	-0.000127	H	-5.337018	-0.727823	-0.227182
H	-0.233767	-2.150158	-0.000111	C	-3.423277	-0.573410	0.752264
C	-2.882331	0.000000	0.000179	H	-3.628827	-1.314184	1.518608
H	-3.968525	0.000000	0.000226	H	3.855805	1.872159	-1.753741
C	-0.103065	0.000000	0.000031	H	2.555795	-0.175609	-2.276638
Br	1.811295	0.000000	0.000014	Br	0.944029	-2.040687	-0.631997

TS3ia-o				**10-3ia-o**			
C	2.752469	1.157190	1.376028	C	-1.746540	-1.869104	1.276381
C	1.954379	-0.477436	-0.236274	C	-2.131034	0.198056	-0.078386
C	2.613124	0.191650	-1.258398	C	-3.182467	-0.418438	-0.696173
C	3.345498	1.343805	-0.953771	C	-3.534451	-1.745131	-0.358347
C	3.421095	1.822543	0.362406	C	-2.800764	-2.446259	0.633540
H	2.785083	1.518138	2.398744	H	-1.177760	-2.404929	2.030860
H	3.995974	2.716957	0.581166	H	-3.085933	-3.465179	0.882044
C	1.976971	0.005639	1.091773	C	-1.283138	-0.464910	0.978914
H	1.566822	-0.594270	1.895989	H	-1.311876	0.140206	1.899452
N	-0.093120	0.957523	1.173944	N	0.144937	-0.442319	0.620909

C	2.385086	0.109110	0.603432	C	2.595504	0.056281	-0.599177
C	0.680140	-1.015342	-0.549303	C	1.145790	1.027465	0.964558
C	1.109287	0.267993	1.358585	C	1.611035	0.949910	-1.291913
O	0.058314	-1.655277	-1.370429	O	0.537704	1.238459	1.996420
O	0.901670	0.865739	2.395456	O	1.425387	1.064803	-2.491259
C	2.129508	-0.657855	-0.534916	C	2.307470	0.095186	0.767009
C	3.133644	-0.972559	-1.438054	C	3.040228	-0.642486	1.685968
H	2.920720	-1.568708	-2.319837	H	2.805384	-0.603126	2.745067
C	4.420741	-0.489543	-1.164147	C	4.079404	-1.438411	1.186646
H	5.234377	-0.713820	-1.848118	H	4.671705	-2.039530	1.871010
C	4.676993	0.280656	-0.021234	C	4.368115	-1.478202	-0.186550
H	5.684959	0.641474	0.162738	H	5.179121	-2.108605	-0.540548
C	3.654145	0.592439	0.885048	C	3.626480	-0.723763	-1.104651
H	3.837253	1.188690	1.773400	H	3.838290	-0.745866	-2.169100
H	-4.364458	-2.223749	-0.867296	H	-1.146002	-0.050329	-1.898956
H	-3.748231	0.116689	-1.451986	H	-3.352349	0.211142	1.788557
Br	-1.650011	1.985348	-0.519425	Br	-2.701973	-1.917269	-0.164995

TS3ia-m

C	-1.685622	2.668007	0.126428
C	-1.516829	0.526456	-1.059975
C	-2.281620	-0.056708	-0.064752
C	-2.760003	0.693554	1.019208
C	-2.463392	2.060618	1.098947
H	-1.434325	3.721001	0.193110
H	-2.837374	2.635814	1.940115
C	-1.166763	1.897232	-0.945854
H	-0.700193	2.380083	-1.796700
N	0.920185	1.638129	-0.282056

10-3ia-m

C	-0.814360	2.035521	1.171309
C	-1.481678	0.442312	-0.663174
C	-2.617092	0.185562	0.042672
C	-2.906812	0.804364	1.283824
C	-1.977591	1.730881	1.817831
H	-0.100755	2.737364	1.592841
H	-2.203352	2.202961	2.770484
C	-0.446840	1.409649	-0.146760
H	-0.291541	2.202256	-0.898232
N	0.882052	0.767667	-0.080793

C	3.090392	0.249695	-0.508106	C	-3.021000	0.201645	0.188386
C	1.201195	-0.316560	0.761634	C	-1.129718	-0.057388	-1.165647
C	1.970404	1.162350	-0.878436	C	-2.263427	1.492446	0.099308
O	0.444036	-0.849914	1.544032	O	-0.224653	-0.572648	-1.794412
O	1.956061	2.067386	-1.689998	O	-2.447491	2.505825	0.751274
C	2.631373	-0.633669	0.471018	C	-2.325495	-0.743170	-0.569545
C	3.455964	-1.607848	1.013221	C	-2.764669	-2.055659	-0.677376
H	3.085990	-2.288568	1.773485	H	-2.214280	-2.779451	-1.270386
C	4.773649	-1.672906	0.539009	C	-3.932710	-2.399478	0.014569
H	5.450656	-2.422679	0.938474	H	-4.305983	-3.418694	-0.034682
C	5.234101	-0.786032	-0.444078	C	-4.631433	-1.449717	0.777765
H	6.260538	-0.862279	-0.791335	H	-5.532853	-1.751267	1.304092
C	4.391587	0.195113	-0.985020	C	-4.183539	-0.126410	0.873427
H	4.734136	0.888070	-1.747075	H	-4.713345	0.617628	1.460118
H	-1.278854	-0.046172	-1.609443	H	1.490996	2.641094	-1.995481
H	-3.820353	0.561261	1.812108	H	3.117307	0.772637	-1.790666
Br	-3.892496	-1.065036	-0.655934	Br	3.705142	-1.185586	0.348425

TS3ia-p

C	0.715835	1.579384	1.164686
C	1.538288	2.055996	-1.083021
C	2.445608	1.014213	-0.975203
C	2.472637	0.254555	0.201541
C	1.616902	0.530642	1.276244
H	0.034599	1.808644	1.977779
H	1.667094	-0.070616	2.176980
C	0.641806	2.335624	-0.027913
H	-0.001033	3.206629	-0.064915
N	-1.274261	1.315341	-0.885135

10-3ia-p

C	0.976207	1.037931	1.256659
C	0.976200	1.038066	-1.256549
C	2.218385	0.477404	-1.234451
C	2.853474	0.189806	0.000002
C	2.218392	0.477268	1.234489
H	0.481595	1.253432	2.199428
H	2.732895	0.244173	2.161136
C	0.215776	1.370146	0.000075
H	-0.043775	2.441837	0.000132
N	-1.113929	0.721634	0.000049

C	-3.401686	0.409804	-0.000012	H	-0.969920	-0.891646	1.722525
C	-1.320852	-0.672667	-0.000017	H	-0.969874	0.893407	1.721632
C	-2.322468	1.439573	0.000094	Br	-2.146388	-0.000113	-0.313877
O	-0.451104	-1.517530	0.000099	C	3.229352	-0.000307	-0.486933
O	-2.421478	2.651354	-0.000009	H	4.236071	-0.000533	-0.895806
C	-2.803629	-0.851730	0.000010				
C	-3.560321	-2.013780	0.000011	**TS3ka-o**			
H	-3.081837	-2.988131	0.000024	C	1.568569	2.767980	0.015881
C	-4.955178	-1.873698	-0.000044	C	-0.647119	1.759100	-0.160719
H	-5.583122	-2.760143	-0.000061	C	-0.398220	1.496106	-1.509079
C	-5.555483	-0.606913	-0.000090	C	0.822522	1.859637	-2.088221
H	-6.639138	-0.531321	-0.000128	C	1.806218	2.500343	-1.331382
C	-4.780361	0.561145	-0.000077	H	2.336886	3.227743	0.628630
H	-5.231667	1.548360	-0.000090	H	2.759450	2.762626	-1.779465
H	0.481582	1.253658	-2.199286	C	0.355994	2.387593	0.602734
H	2.732880	0.244407	-2.161118	H	0.191738	2.570743	1.660258
Br	4.582229	-0.592069	-0.000049	N	1.907937	0.279134	1.730387
				C	0.628305	-1.471625	0.759911
1k				C	2.584022	-0.216647	0.573218
C	2.580600	-1.209208	-0.222456	C	0.669349	-0.427391	1.821517
C	2.580938	1.208879	-0.222960	O	3.647712	0.219503	0.173934
C	1.289211	1.208216	0.302050	O	-0.188094	-0.176934	2.651096
C	0.631905	0.000274	0.572219	C	1.786867	-1.334119	-0.008434
C	1.288877	-1.207968	0.302549	C	2.035382	-2.151976	-1.105066
H	3.080937	-2.152203	-0.425052	H	2.939206	-2.032533	-1.694030
H	0.780865	-2.148637	0.501169	C	1.072608	-3.117934	-1.412219
H	3.081534	2.151651	-0.425955	H	1.221371	-3.773517	-2.265732
H	0.781473	2.149114	0.500284	C	-0.094131	-3.255964	-0.637506
C	-0.750466	0.000582	1.136681	H	-0.823767	-4.013164	-0.910090

C	-0.332900	-2.432041	0.465964	H	-4.946855	-0.786114	-1.863620
H	-1.236007	-2.514098	1.060010	C	-4.417916	-0.314355	0.169656
H	1.003228	1.635266	-3.135901	H	-5.441104	-0.076073	0.446017
H	-1.151425	0.988585	-2.102686	C	-3.400022	-0.208672	1.127411
C	-1.957622	1.461304	0.523177	H	-3.601632	0.109101	2.145477
H	-1.808986	1.229005	1.577731	H	4.877059	-0.967300	-1.334943
H	-2.662219	2.289804	0.424769	H	3.841836	1.206373	-0.748728
Br	-2.948601	-0.103176	-0.206717	C	1.676544	1.666151	0.784438
				H	1.165950	1.642900	1.746848
10-3ka-o				H	2.388554	2.488300	0.737306
C	2.276736	-2.163461	0.497795	Br	0.192097	2.273805	-0.494916
C	2.261677	0.366748	0.399365				
C	3.391639	0.285562	-0.383264	**TS3ka-m**			
C	3.984028	-0.947120	-0.718802	C	0.211693	2.531771	0.453664
C	3.407126	-2.162646	-0.261835	C	1.404042	0.766845	-0.756745
H	1.815186	-3.090306	0.825871	C	1.892001	0.260397	0.446374
H	3.869889	-3.106462	-0.537685	C	1.563080	0.915448	1.641189
C	1.593737	-0.892336	0.920400	C	0.730995	2.048315	1.642626
H	1.581314	-0.841694	2.022994	H	-0.463421	3.379360	0.434612
N	0.156168	-0.928248	0.589734	H	0.492982	2.537412	2.582736
C	-2.111306	-0.521537	0.722699	C	0.518398	1.868653	-0.763437
C	-0.363229	-1.163983	-0.701611	H	0.224293	2.319824	-1.703119
C	-0.831891	-0.483843	1.482855	N	-1.321734	0.578778	-1.066533
O	0.281008	-1.497266	-1.672255	C	-3.439049	0.195636	-0.197247
O	-0.629954	-0.134928	2.631861	C	-1.339247	-0.750392	-0.632839
C	-1.831036	-0.923881	-0.584075	C	-2.482388	1.254049	-0.666944
C	-2.829136	-1.030111	-1.540096	O	-0.418764	-1.550522	-0.652844
H	-2.595811	-1.337597	-2.554563	O	-2.673919	2.456077	-0.706710
C	-4.136853	-0.718019	-1.142920	C	-2.746131	-1.016605	-0.173278

C	-3.358177	-2.197833	0.219887
H	-2.808298	-3.133727	0.230462
C	-4.703510	-2.124307	0.605829
H	-5.218403	-3.024088	0.931095
C	-5.399612	-0.906116	0.582884
H	-6.441473	-0.884109	0.890342
C	-4.773265	0.278913	0.173489
H	-5.300413	1.227539	0.148540
H	1.651201	0.273865	-1.690482
H	1.949687	0.531911	2.582165
C	2.694371	-1.000163	0.454254
H	2.785648	-1.432737	1.450059
H	2.283141	-1.735541	-0.236153
Br	4.577127	-0.688664	-0.155895

10-3ka-m

C	0.326779	1.313794	1.813438
C	1.046287	0.334039	-0.387013
C	2.122575	-0.229961	0.235929
C	2.335252	-0.033797	1.632743
C	1.424797	0.737029	2.388914
H	-0.377574	1.899270	2.397378
H	1.603457	0.870140	3.452929
C	0.027234	1.162663	0.346272
H	-0.034706	2.160385	-0.120067
N	-1.336024	0.627146	0.133561
C	-3.561505	0.466553	-0.461078
C	-1.750692	-0.665606	0.508235
C	-2.374410	1.370039	-0.454917
O	-1.055015	-1.508208	1.035263
O	-2.280218	2.511614	-0.862023
C	-3.189002	-0.749879	0.113923
C	-4.089231	-1.796435	0.244953
H	-3.786053	-2.737076	0.693944
C	-5.393695	-1.586134	-0.223650
H	-6.128612	-2.381654	-0.139101
C	-5.767438	-0.364609	-0.800865
H	-6.785984	-0.232381	-1.154534
C	-4.848635	0.686517	-0.928338
H	-5.123767	1.637534	-1.373455
H	0.876421	0.187631	-1.450700
H	3.207072	-0.475209	2.104873
C	3.073652	-1.088059	-0.537825
H	3.292864	-2.027317	-0.029099
H	2.731033	-1.287091	-1.552620
Br	4.864802	-0.210526	-0.745564

TS3ka-p

C	-0.564646	2.268802	-1.175432
C	-1.250760	2.520771	1.160991
C	-2.257801	1.593090	0.956783
C	-2.423803	0.983248	-0.298735
C	-1.571796	1.341269	-1.363961
H	0.110458	2.535558	-1.980830
H	-1.707470	0.870526	-2.334155
C	-0.352309	2.834331	0.110737
H	0.351348	3.650463	0.218666
N	1.384069	1.569845	0.763518

C	2.833091	0.060228	-0.258456	C	-0.103250	1.021752	-0.000255
C	1.086513	0.297407	1.284272	H	-0.209906	2.119803	0.000121
C	2.294810	1.459538	-0.298429	N	-1.507281	0.563361	-0.000174
O	0.217327	0.025817	2.091010	C	-3.815888	0.570990	0.000158
O	2.580056	2.337869	-1.094474	C	-1.904511	-0.788283	-0.000220
C	2.090233	-0.647709	0.688278	C	-2.605227	1.441818	0.000014
C	2.331653	-1.988896	0.949888	O	-1.159004	-1.745103	-0.000431
H	1.743739	-2.525600	1.687814	O	-2.535286	2.655371	0.000037
C	3.348468	-2.611738	0.214733	C	-3.397984	-0.761154	0.000052
H	3.562114	-3.664408	0.378531	C	-4.308583	-1.806975	0.000241
C	4.096137	-1.900272	-0.737136	H	-3.969949	-2.838290	0.000165
H	4.876488	-2.414467	-1.291471	C	-5.670705	-1.474912	0.000543
C	3.849293	-0.544040	-0.985854	H	-6.415369	-2.265808	0.000712
H	4.419539	0.017758	-1.719159	C	-6.089749	-0.137278	0.000642
H	-1.108379	2.970547	2.137487	H	-7.152441	0.087818	0.000877
H	-2.909817	1.310130	1.777992	C	-5.160153	0.912011	0.000447
C	-3.468359	-0.061846	-0.497636	H	-5.469935	1.952342	0.000523
H	-4.269866	-0.009332	0.238399	H	0.135779	0.864241	-2.197731
H	-3.881457	-0.065951	-1.506242	H	2.258875	-0.377392	-2.162161
Br	-2.671388	-1.891392	-0.269263	C	3.669217	-1.216795	-0.001404
				H	3.833254	-1.813957	0.894318
10-3ka-p				H	3.833987	-1.811880	-0.898374
C	0.607301	0.594005	1.255714	Br	5.263368	0.078537	0.000844
C	0.606973	0.594842	-1.256663				
C	1.776254	-0.098362	-1.228249	**1m**			
C	2.394383	-0.481688	-0.001075	C	2.391999	0.697828	0.000112
C	1.776493	-0.099181	1.226588	C	1.185088	-1.394766	-0.000041
H	0.136294	0.862831	2.197048	C	-0.028553	-0.701277	-0.000096
H	2.259404	-0.378906	2.160144	C	-0.028720	0.701443	-0.000106

C	1.185166	1.394538	0.000092	H	4.665511	-2.546860	0.739922
H	3.327806	1.248478	0.000318	C	4.494357	-0.733647	-0.411104
H	1.168482	2.479140	0.000344	H	5.458869	-0.876492	-0.890423
H	1.167997	-2.479307	0.000056	C	3.721729	0.389326	-0.732152
C	2.391832	-0.698020	-0.000185	H	4.057806	1.131569	-1.449336
H	3.327848	-1.248528	0.000013	Cl	-2.808305	-2.200795	-0.743179
Cl	-1.516955	-1.619716	0.000080	H	-3.834668	-1.020225	1.595228
Cl	-1.516752	1.619818	-0.000044	Cl	-0.942196	-0.003445	-2.214207

TS3ma-o

C	-2.245784	1.934855	1.071462
C	-1.761067	0.340301	-0.719205
C	-2.568275	-0.603743	-0.083495
C	-3.215655	-0.270889	1.114241
C	-3.061185	0.997865	1.682438
H	-2.095546	2.917521	1.504919
H	-3.576165	1.233911	2.608014
C	-1.550865	1.605952	-0.117439
H	-1.034975	2.373290	-0.684390
N	0.481248	1.294556	0.774151
C	2.491369	0.514195	-0.101166
C	0.690413	0.006865	1.305059
C	1.428055	1.562115	-0.232229
O	-0.075108	-0.606097	2.024241
O	1.380520	2.477397	-1.034020
C	2.041807	-0.431647	0.823422
C	2.803477	-1.543409	1.155293
H	2.441366	-2.271309	1.874582
C	4.042339	-1.685075	0.517581

10-3ma-o

C	1.373051	0.743922	2.137187
C	1.847545	-0.566983	0.040257
C	2.956158	0.216473	-0.157775
C	3.293780	1.251169	0.748030
C	2.489852	1.484203	1.889388
H	0.749156	0.925262	3.006992
H	2.778208	2.274365	2.577073
C	0.912405	-0.348301	1.210718
H	0.819302	-1.294753	1.766917
N	-0.462716	-0.102117	0.747310
C	-2.701820	-0.407412	0.284560
C	-0.839783	0.969608	-0.086606
C	-1.529614	-0.984094	1.002700
O	-0.104255	1.852008	-0.474671
O	-1.461343	-1.990262	1.679469
C	-2.290634	0.758596	-0.364908
C	-3.170602	1.515322	-1.123927
H	-2.837000	2.418494	-1.625094
C	-4.494462	1.063639	-1.215403

H	-5.214000	1.627817	-1.801886	H	-4.577190	-2.948022	-0.601150
C	-4.906909	-0.106805	-0.563455	C	-4.624064	-1.111113	0.523498
H	-5.939420	-0.431559	-0.655049	H	-5.562568	-1.362966	1.009474
C	-4.008855	-0.863864	0.201516	C	-3.992068	0.101979	0.824985
H	-4.313641	-1.773291	0.709651	H	-4.413652	0.807703	1.533919
Cl	4.016031	-0.027551	-1.531008	H	0.623417	1.173113	1.997053
H	4.171262	1.854946	0.550921	Cl	3.896073	-1.389772	-0.588674
Cl	1.393926	-1.862641	-1.022684	Cl	2.171388	-1.197027	2.135190

TS3ma-m

C	1.849763	2.006014	-1.090215
C	1.206480	1.099787	1.086047
C	2.057575	0.022553	0.891092
C	2.816684	-0.061936	-0.295650
C	2.711394	0.942472	-1.272364
H	1.753957	2.769079	-1.854782
H	3.307274	0.855107	-2.173792
C	1.047444	2.077881	0.075782
H	0.485103	2.974422	0.307953
N	-0.897847	1.376909	-0.720557
C	-2.790498	0.368246	0.182817
C	-0.944796	0.064282	-1.225871
C	-1.857010	1.535938	0.293259
O	-0.112210	-0.465070	-1.937181
O	-1.896246	2.447503	1.101822
C	-2.232154	-0.529512	-0.730402
C	-2.852887	-1.731386	-1.040772
H	-2.406936	-2.421137	-1.750525
C	-4.063145	-2.013463	-0.394228

10-3ma-m

C	1.101614	1.079632	-1.584938
C	1.351885	0.837626	0.901113
C	2.544875	0.209128	0.698411
C	3.049202	-0.002710	-0.618868
C	2.299940	0.454796	-1.736991
H	0.535717	1.415115	-2.448680
H	2.711992	0.289994	-2.727462
C	0.486255	1.313595	-0.233970
H	0.274814	2.387564	-0.103657
N	-0.858813	0.707915	-0.151620
C	-3.141158	0.460047	0.084741
C	-1.116990	-0.674267	-0.259541
C	-2.031379	1.455706	0.058877
O	-0.282910	-1.535417	-0.440062
O	-2.080251	2.663407	0.187331
C	-2.595528	-0.811441	-0.104649
C	-3.391270	-1.946923	-0.126716
H	-2.953530	-2.929193	-0.274182
C	-4.770771	-1.769636	0.049050

H	-5.428015	-2.634443	0.038549
C	-5.318277	-0.493235	0.238809
H	-6.391206	-0.388678	0.372306
C	-4.504226	0.647807	0.259448
H	-4.914808	1.641861	0.406076
H	0.979349	0.990036	1.908054
Cl	4.560202	-0.804459	-0.907748
Cl	3.458483	-0.331560	2.093838

6. Reference

[1] S. Zhao, Y. Zhu, Y. C. Wu, T. Lu and Q. F. Zhou, Phosphine-Catalyzed Domino Reactions of Allenoates with *N*-Hydroxyphthalimides: Direct Method to 3a-Hydroxyisoxazolo[3,2-*a*]isoindol-8(3 *aH*)-one Derivatives. *ChemistrySelect*, 2017, **2**, 1700.

[2] T. Kuribara, M.Nakajima and T. Nemoto, Visible-Light-Induced Metal-/Photocatalyst-Free C−H Bond Imidation of Arenes. *Org. Lett.*, 2020, **22**, 2235.

[3] R. Shrestha, P. Mukherjee, Y. Tan, Z. C. Litman and J. F. Hartwig, Sterically Controlled, Palladium-Catalyzed Intermolecular Amination of Arenes. *J. Am. Chem. Soc.*, 2013, **135**, 8480.

[4] Y. S. Shi, F. Liao, H. Niu and A. W. Lei, Selective Formation of Phthalimides from Amines, Aldehydes and CO by Pd-Catalyzed Oxidative C–H Aminocarbonylation. *Org. Chem. Front.*, 2018, **5**, 1957.

[5] L. Marchetti, A. Kantak,; R. Davis and B. DeBoef, Regioselective Gold-Catalyzed Oxidative C−N Bond Formation. *Org. Lett.*, 2015, **17**, 358.

[6] a) R. K. P. Subramanya, K. U. Sunil and S. J. Branko, Microwave-Assisted Benzyl Mono- and Dibromination in Diethyl Carbonate as Environmentally Friendly Alternative to Radical Bromination in Carbon Tetrachloride. *Green Chem.*, 2011, **13**, 928. b) X. F. Zhang, D. G. Huang, Y. S. Chen and R. H. Holm, Synthesis of Binucleating Macrocycles and Their Nickel(II) Hydroxo- and Cyano-Bridged Complexes with Divalent Ions: Anatomical Variation of Ligand Features. *Inorg. Chem*., 2012, **51**, 20, 11017. c) K. U. Sunil and S. J. Branko, Microwave-Assisted NBS Bromination of *p*-Iminotoluenes: Preparation of New Alcohol, Mercapto, and Amino Protection Groups. *Synth. Commun.*, 2011, **41**, 3177.

[7] L. J. Allen, P. J. Cabrera, M. Lee and M. S. Sanford, 3-Substituted Phthalic Acid Derivatives by Sonogashira Coupling Reaction. *J. Am. Chem. Soc*.,2014, **136**, 5607.

[8] G. Jean, L. Stéphane, P. Alain, R. Pierre, P. Bruno, B. A. Paola and M. Claude,

Synthesis and Biological Activity of 6*H*-Isoindolo[2,1-*a*] Indol-6-ones, Analogues of Batracylin, and Related Compounds. *Eur. Med. Chem.*, 2006, **41**, 379.

[9] Y. C. Yuan, K. Raghu, B. O. Christian, L. Thierry, R. Thierry and G. D. Rafael, Orcid Unmasking Amides: Ruthenium-Catalyzed Protodecarbonylation of *N*-Substituted Phthalimide Derivatives. *Org. Lett.*, 2017, **19**, 6404.

[10] D. S. Suman and A. Lutz, Ruthenium(II)-Catalyzed C–H Activation with Isocyanates: A Versatile Route to Phthalimides. *Chem. Eur. J.*, 2014, **20**, 13932.

[11] W. Oliver and R. W. Siegfried, 3-Substituted Phthalic Acid Derivatives by Sonogashira Coupling Reaction. *Synthesis*, 2007, **5**, 761.

[12] Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

[13] A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648. b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev.*, *B* 1988, **37**, 785.

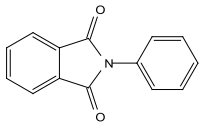
[14] a) R. Ditchfield, W. J. Hehre and J. A. Pople, *J. Chem. Phys.*, 1971, **54**, 724. b) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257. c) P. C. Hariharan and J. A. Pople, *Theor. Chem. Acc.*, 1973, **28**, 213.

[15] a) T. Clark, J. Chandrasekhar, G. W. Spitznagel and P. Von R. Schleyer, *J. Comput. Chem.*, 1983, **4**, 294. b) R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Chem.*

Phys., 1980, **72**, 650.

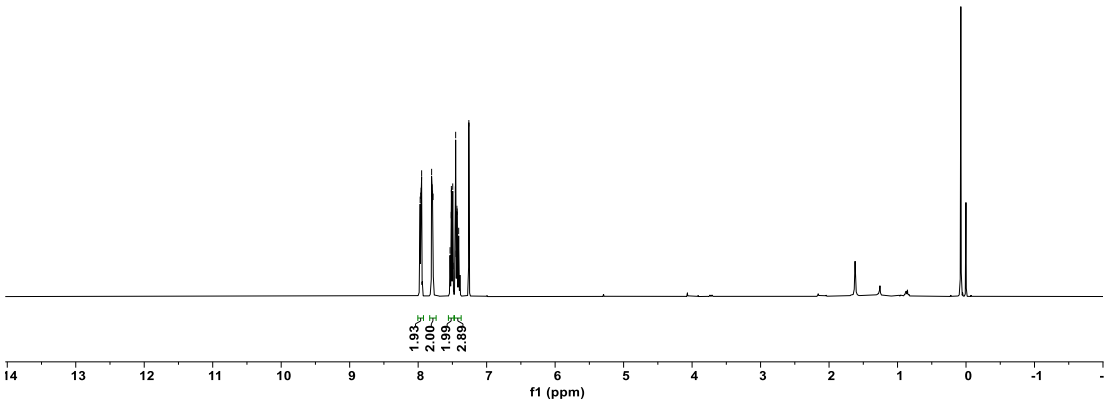
[16] A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B.*, 2009, **113**, 6378.

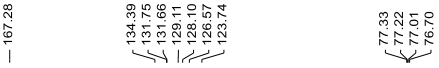
7. Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR Spectra.

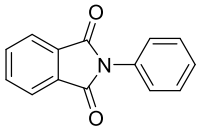


3aa

^{1}H NMR (400 MHz, $CDCl_3$)

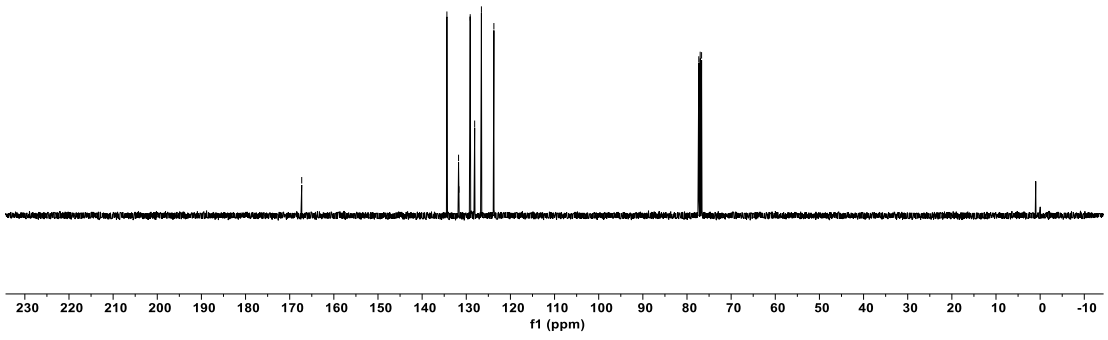


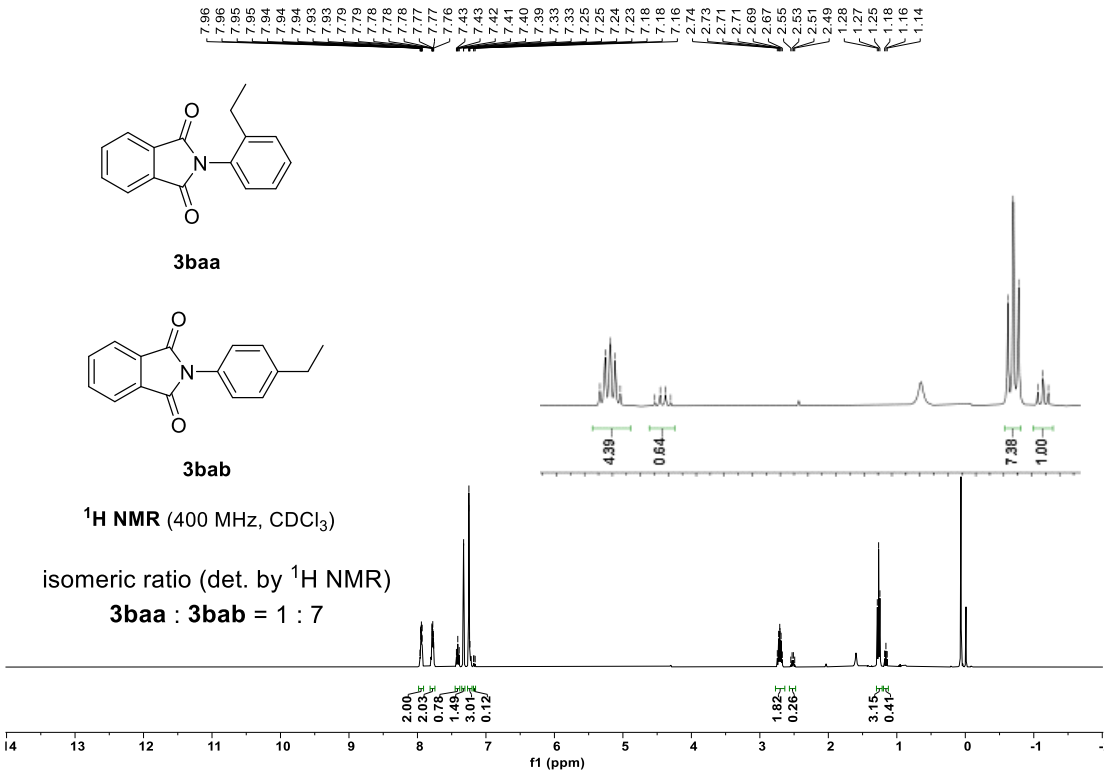


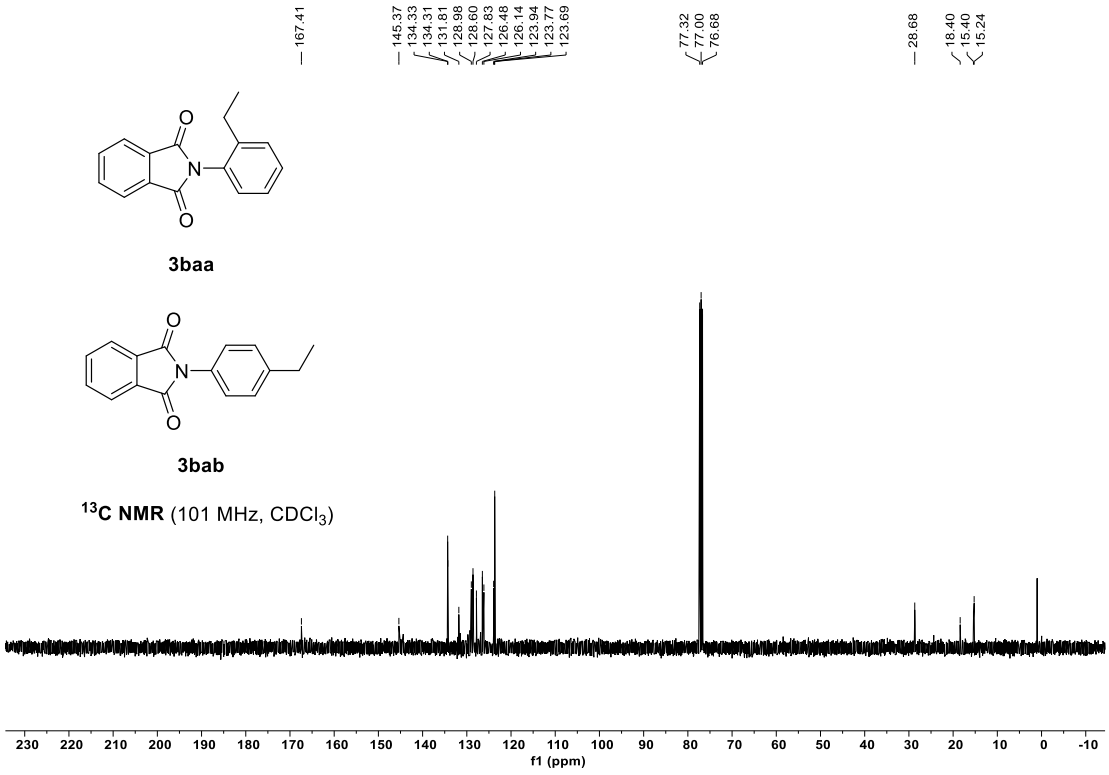


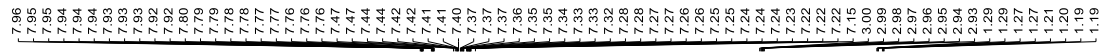
3aa

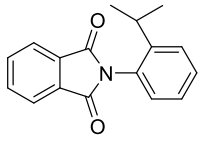
^{13}C NMR (101 MHz, $CDCl_3$)



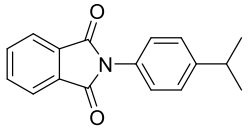

7.96 7.96 7.95 7.95 7.94 7.94 7.94 7.93 7.93 7.79 7.78 7.78 7.78 7.77 7.77 7.76 7.43 7.43 7.42 7.41 7.40 7.39 7.33 7.33 7.25 7.25 7.24 7.23 7.18 7.18 7.16 2.74 2.73 2.71 2.71 2.69 2.67 2.55 2.53 2.51 2.49 1.28 1.27 1.25 1.18 1.16 1.14
3baa
3bab
4.39 0.64 7.38 1.00
1H NMR (400 MHz, CDCl3)
isomeric ratio (det. by 1H NMR)
3baa : 3bab = 1 : 7
2.00 2.03 0.78 1.49 3.01 0.12 1.82 0.26 3.15 0.41
f1 (ppm)


167.41 145.37 134.33 134.31 131.81 128.98 128.60 127.83 126.48 126.14 123.94 123.77 123.69 77.32 77.00 76.68 28.68 18.40 15.40 15.24
3baa
3bab
13C NMR (101 MHz, CDCl3)
f1 (ppm)





3caa

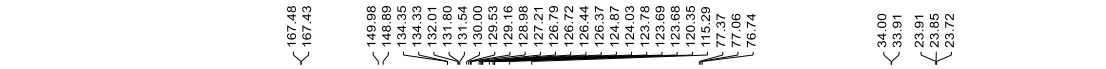


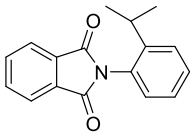
3cab

^{1}H NMR (400 MHz, $CDCl_3$)

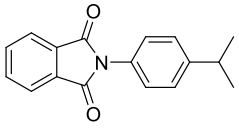
isomeric ratio (det. by ^{1}H NMR)

3caa : **3cab** = 1 : 8



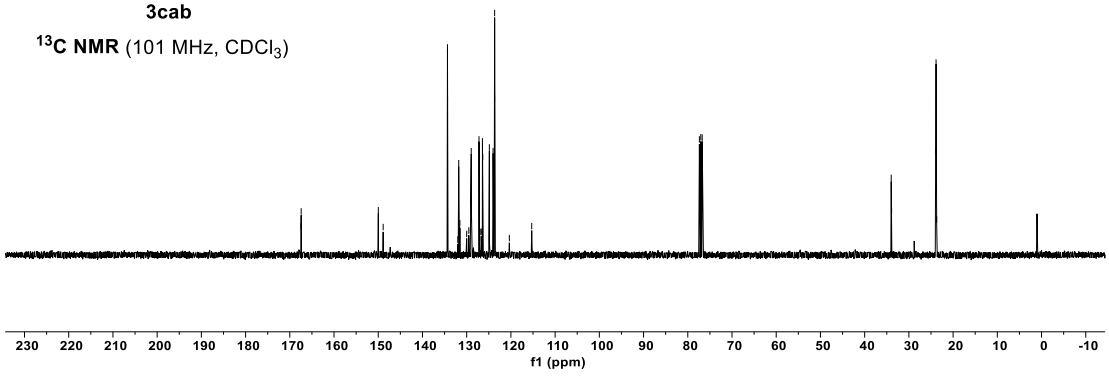


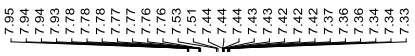
3caa

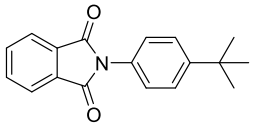


3cab

^{13}C NMR (101 MHz, $CDCl_3$)

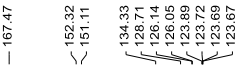


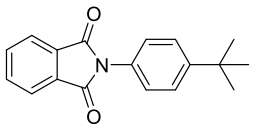




3da

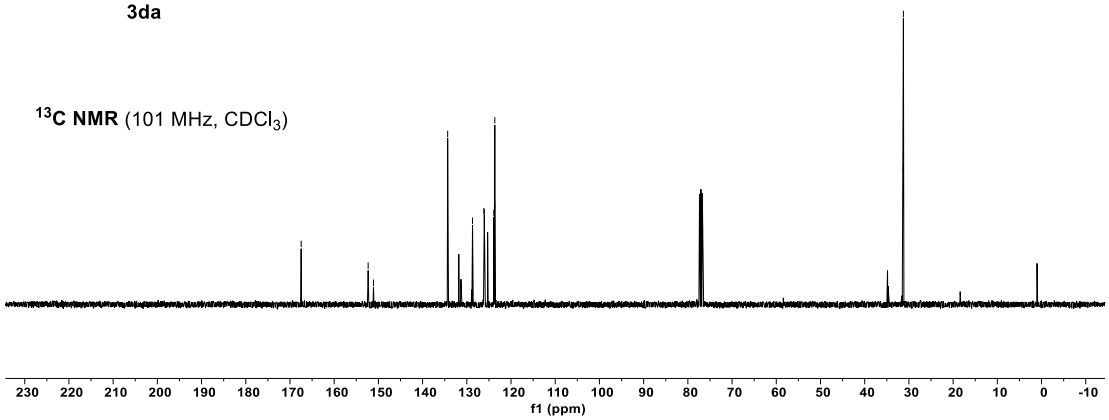
^{1}H NMR (400 MHz, $CDCl_3$)

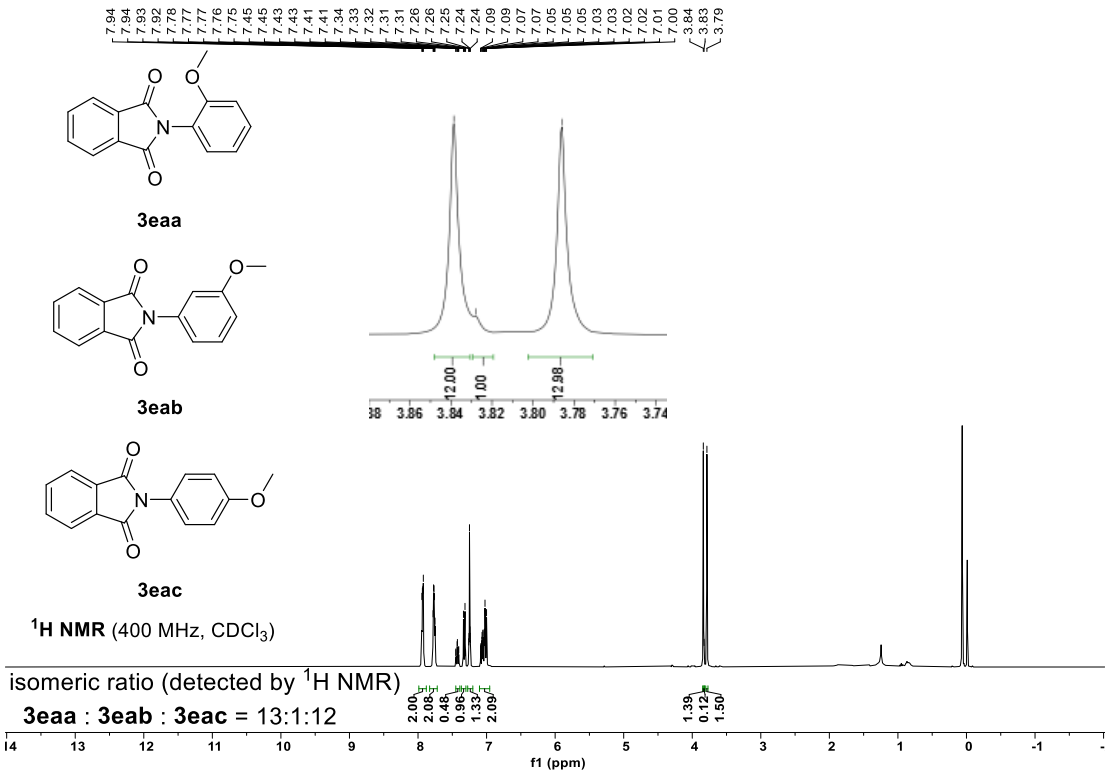


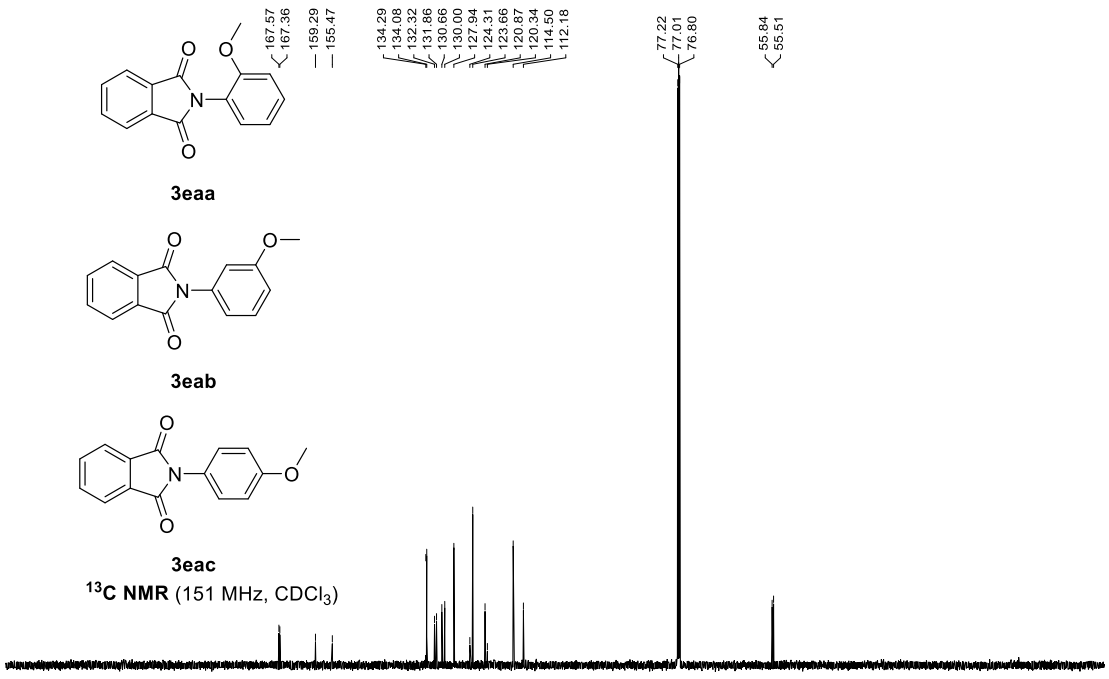


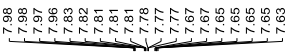
3da

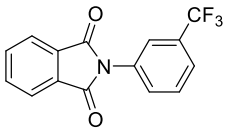
^{13}C NMR (101 MHz, $CDCl_3$)




3eaa
3eab
3eac
1H NMR (400 MHz, CDCl3)
isomeric ratio (detected by 1H NMR)
3eaa : 3eab : 3eac = 13:1:12
f1 (ppm)

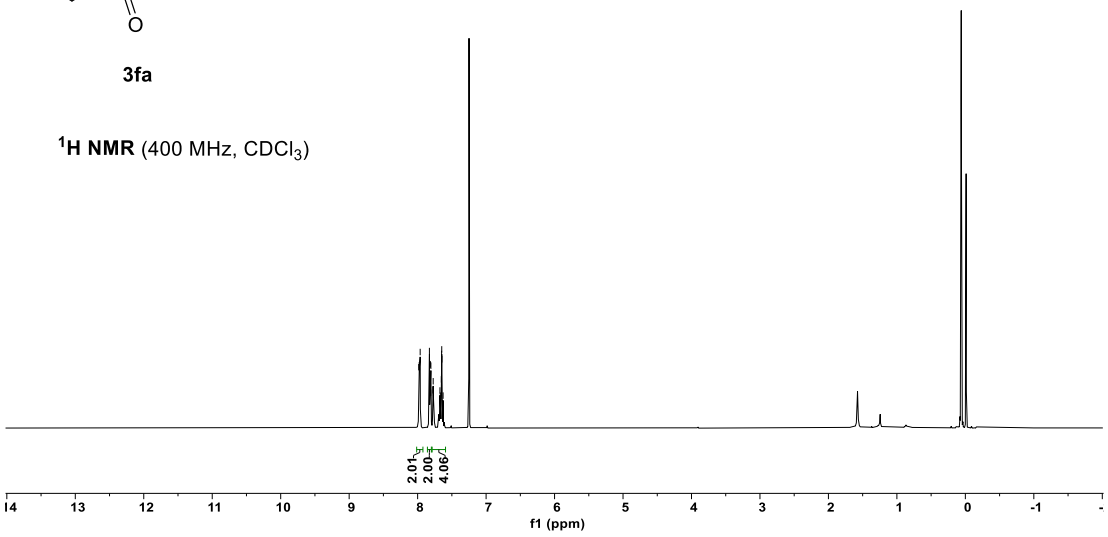

3eaa
3eab
3eac
13C NMR (151 MHz, CDCl3)

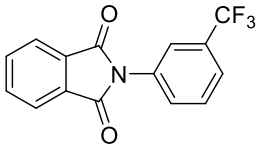




3fa

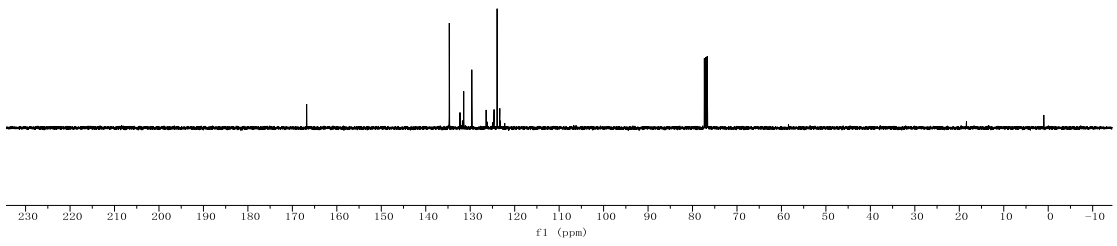
^{1}H NMR (400 MHz, $CDCl_3$)

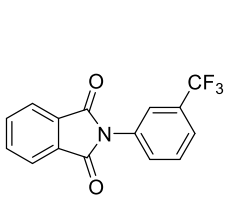




3fa

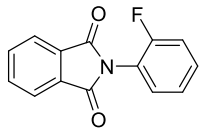
^{13}C NMR (101 MHz, $CDCl_3$)



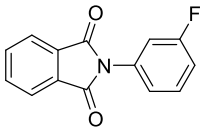


3fa

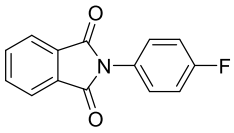
^{19}F NMR (376 MHz, $CDCl_3$)



3gaa

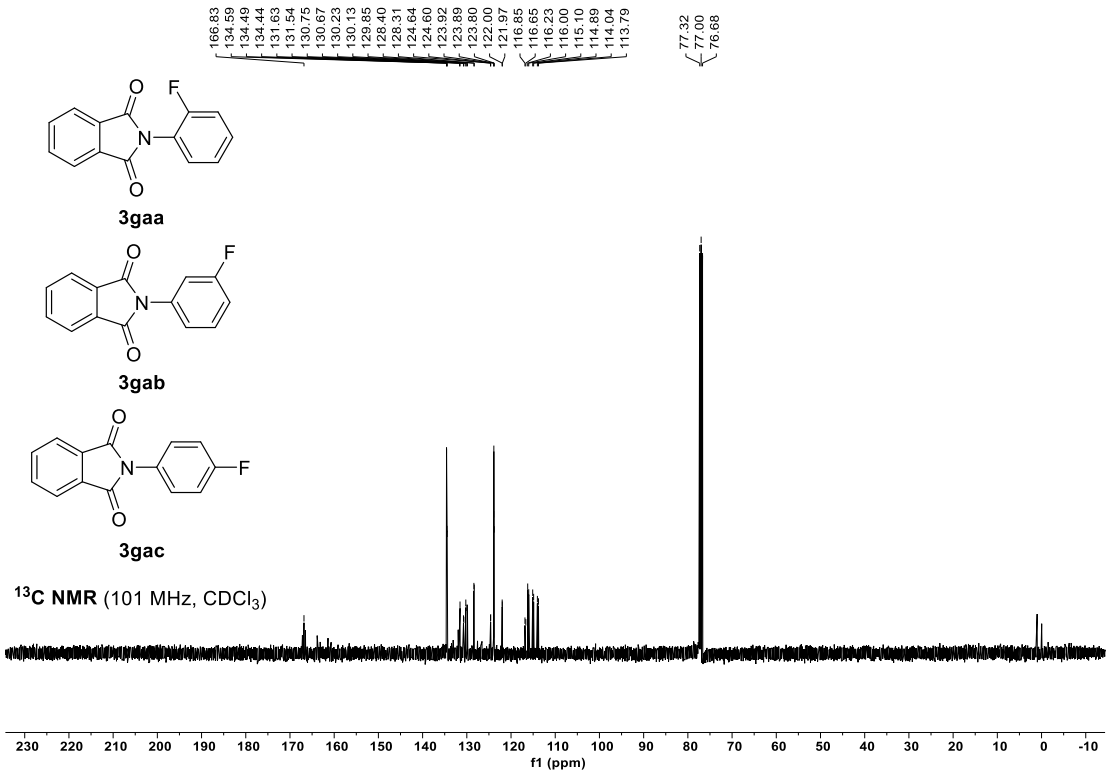


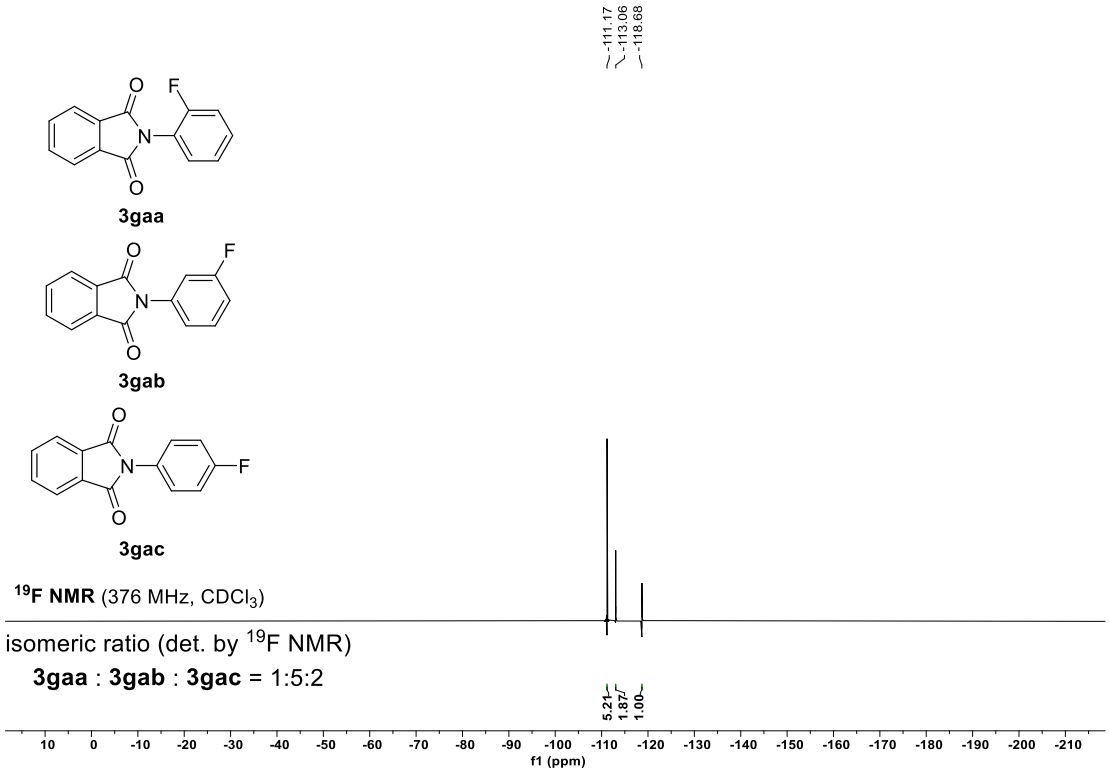
3gab

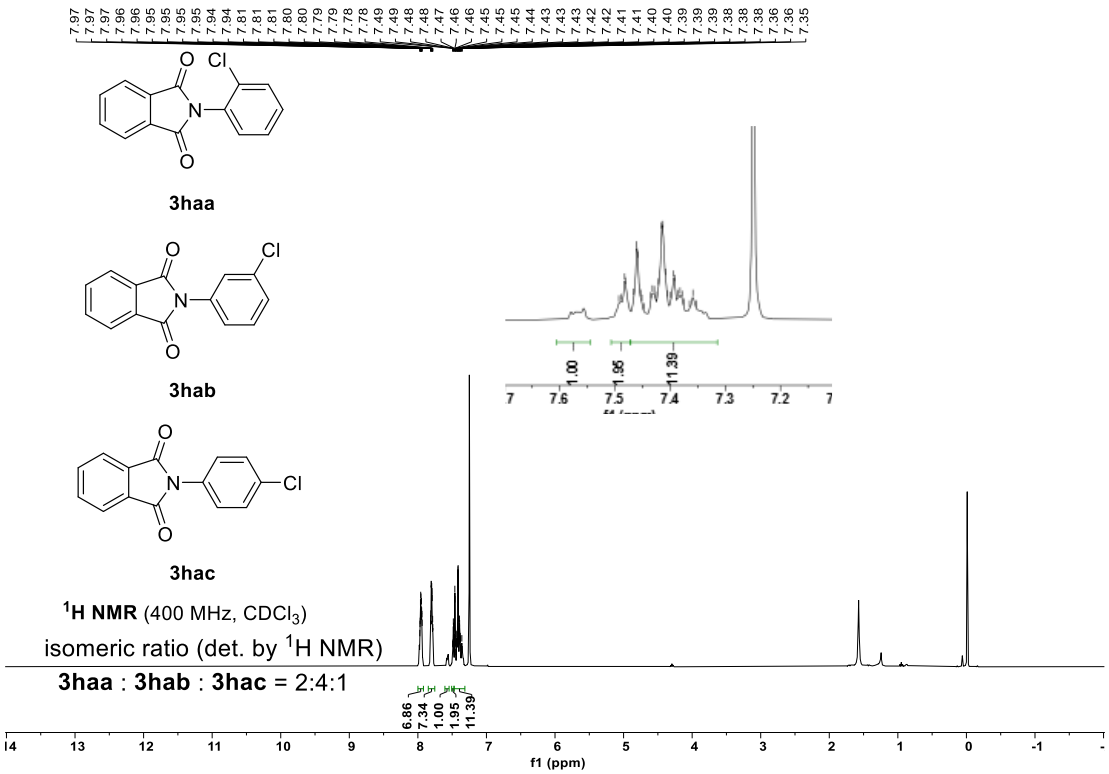


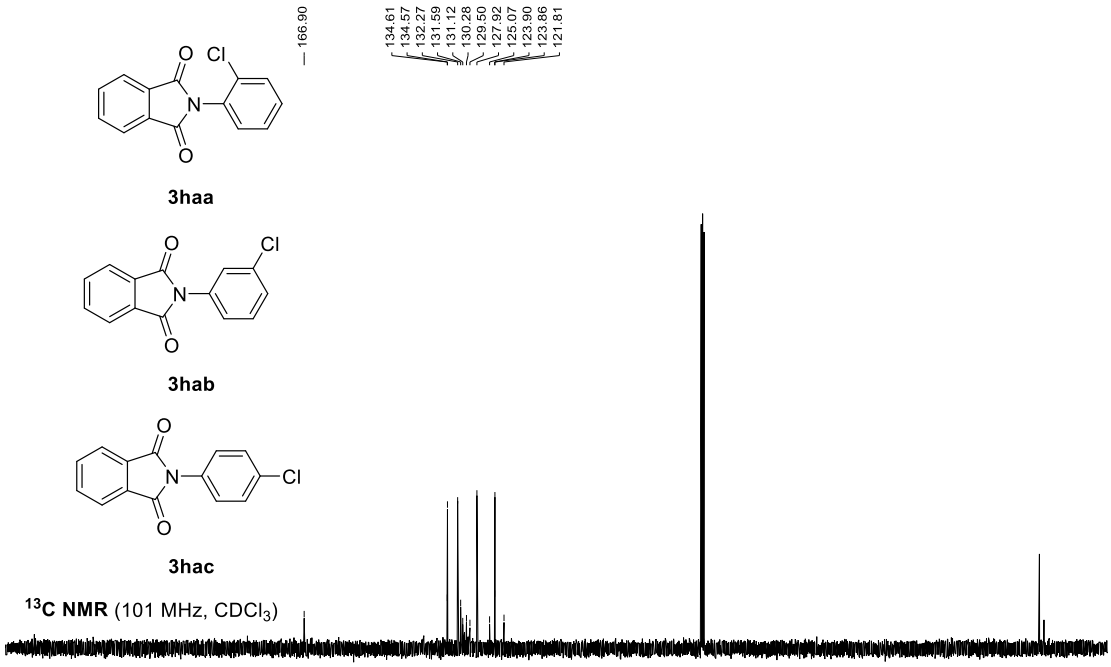
3gac

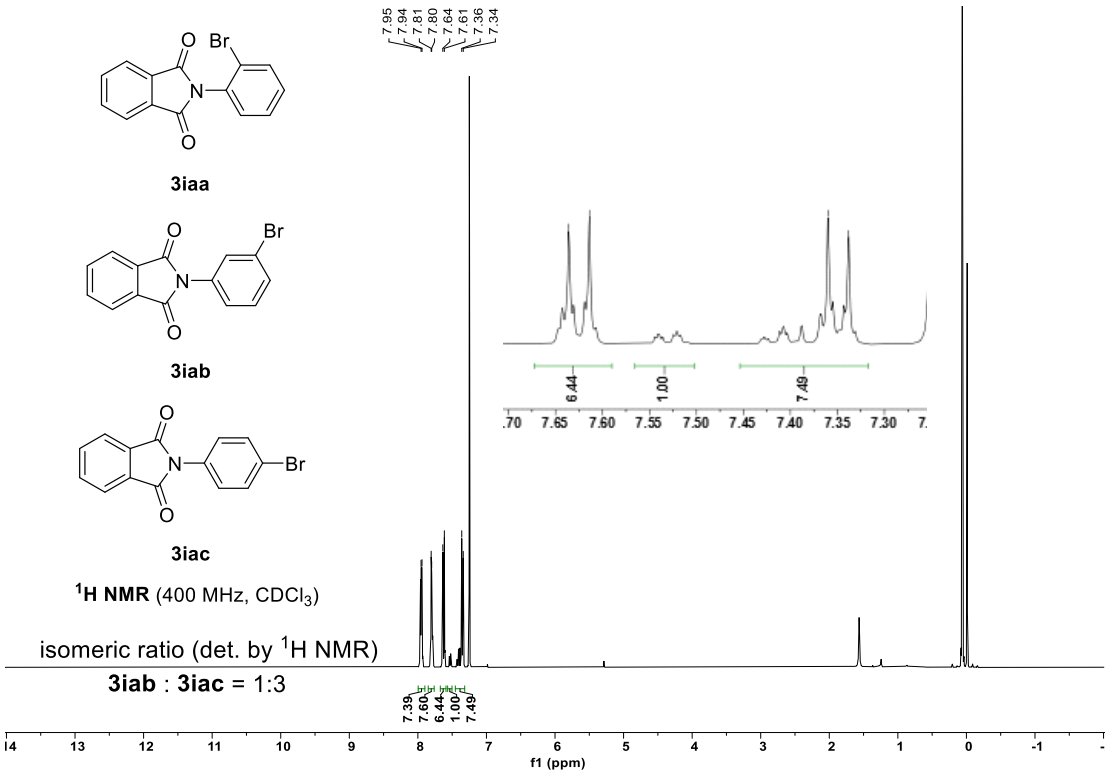
^{1}H NMR (400 MHz, $CDCl_3$)

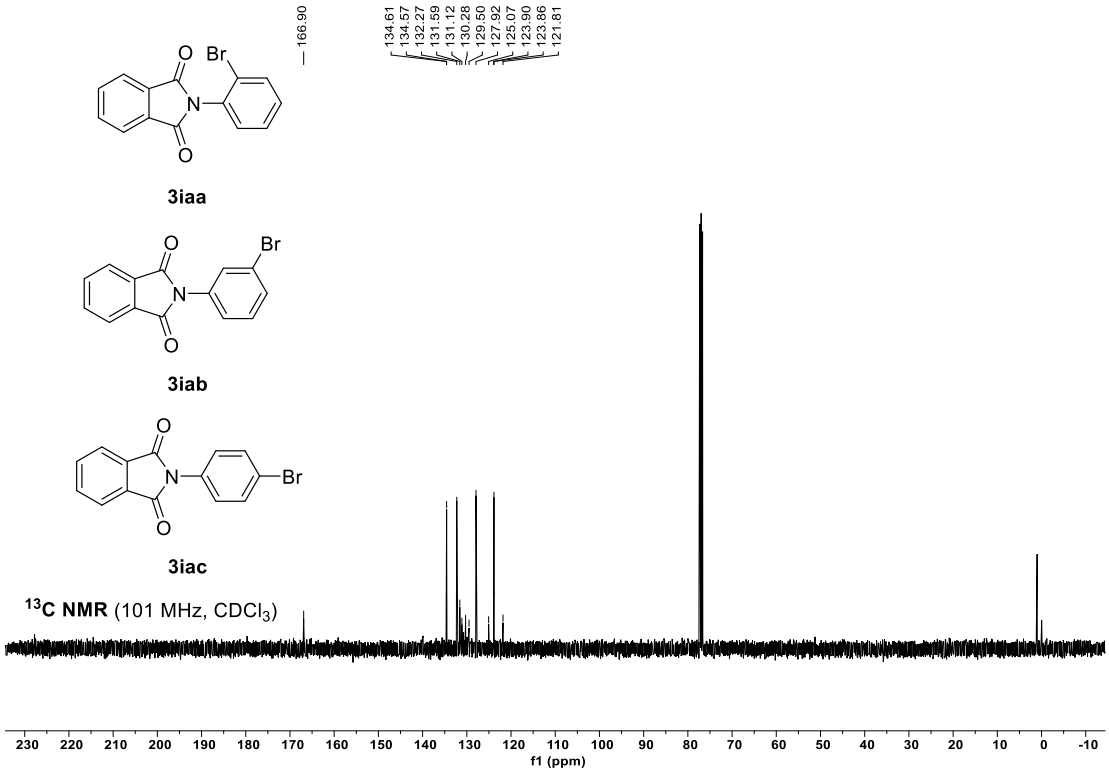

166.83
134.59
134.49
134.44
131.63
131.54
130.75
130.67
130.23
130.13
129.85
128.40
128.31
124.64
124.60
123.92
123.89
123.80
122.00
121.97
116.85
116.65
116.23
116.00
115.10
114.89
114.04
113.79
77.32
77.00
76.68
3gaa
3gab
3gac
13C NMR (101 MHz, CDCl3)
f1 (ppm)

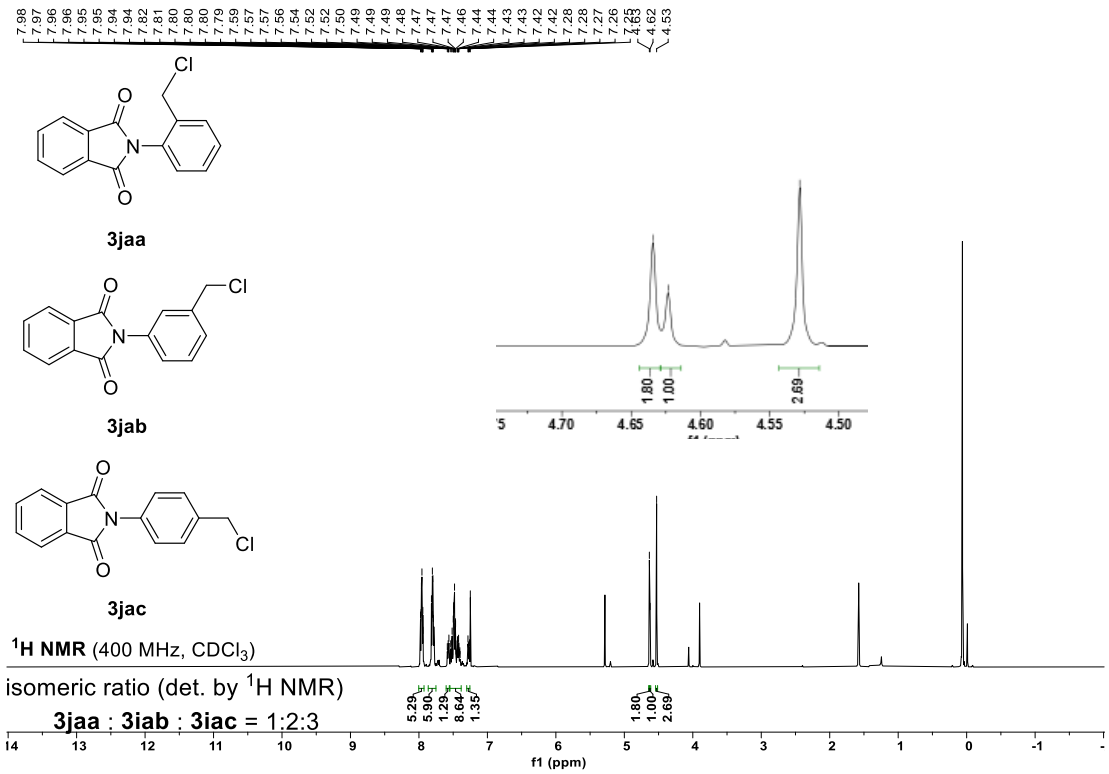

-111.17
-113.06
-118.68
3gaa
3gab
3gac
19F NMR (376 MHz, CDCl3)
isomeric ratio (det. by 19F NMR)
3gaa : 3gab : 3gac = 1:5:2
5.21
1.87
1.00
f1 (ppm)

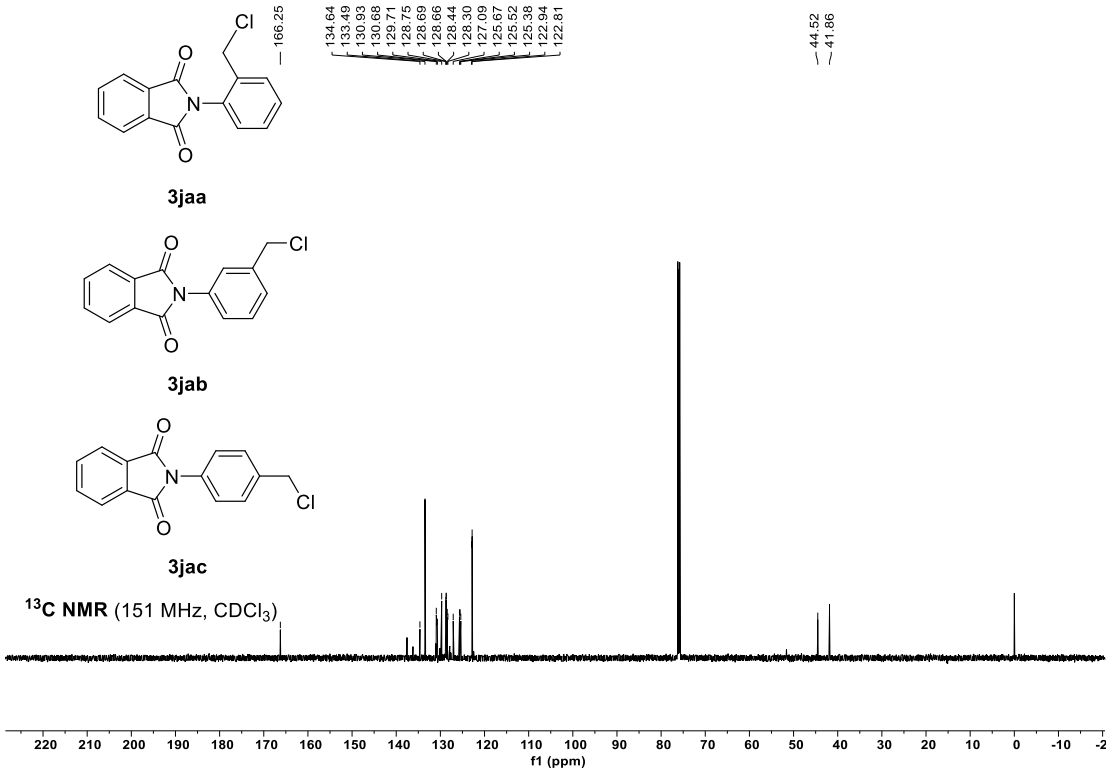

3haa
3hab
3hac
1H NMR (400 MHz, CDCl3)
isomeric ratio (det. by 1H NMR)
3haa : 3hab : 3hac = 2:4:1
f1 (ppm)

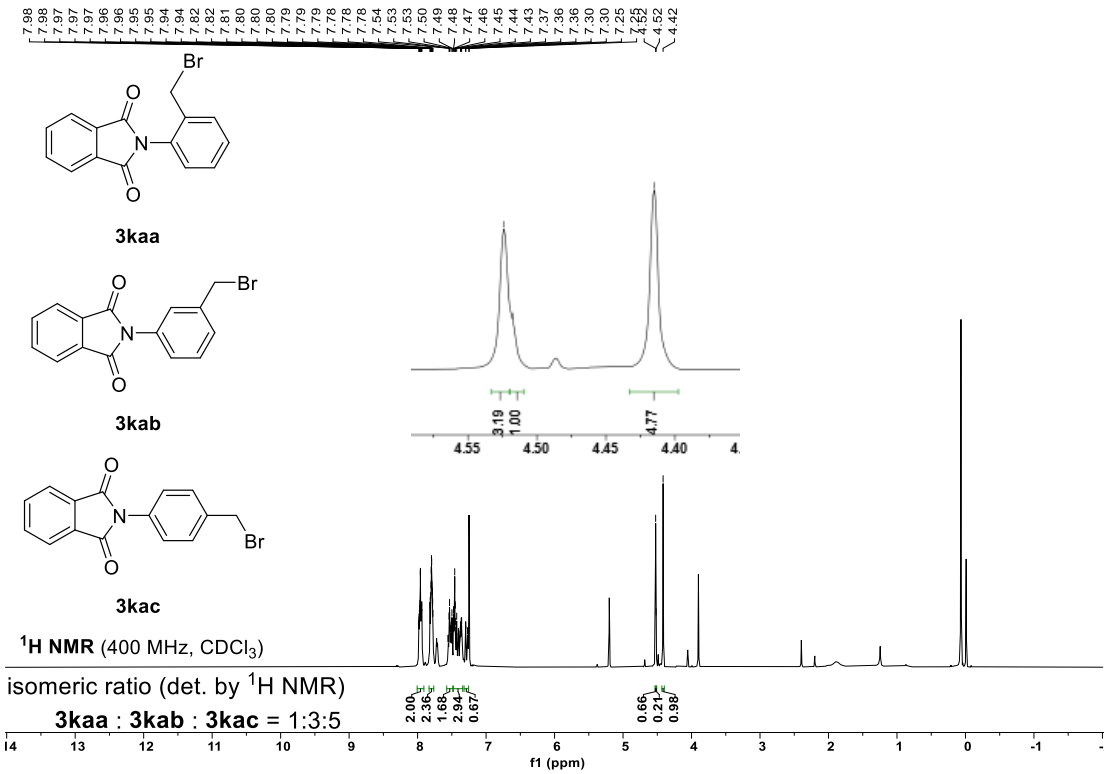

3haa
3hab
3hac
13C NMR (101 MHz, CDCl3)

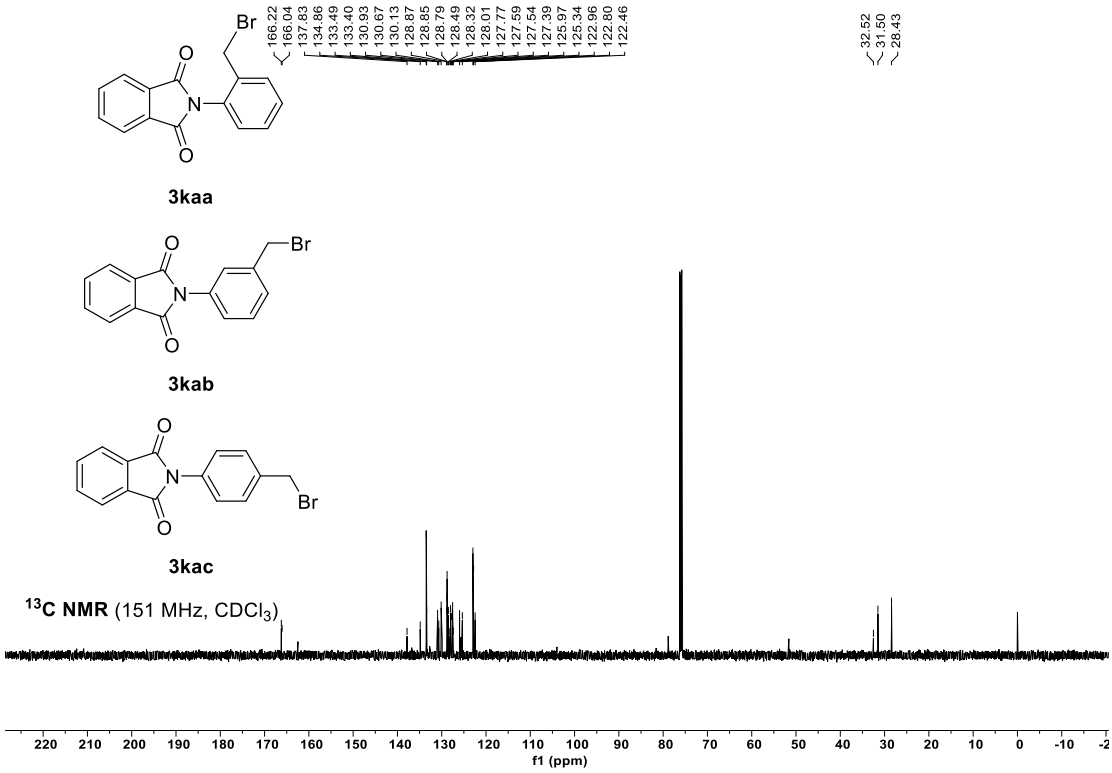

3iaa
3iab
3iac
1H NMR (400 MHz, CDCl3)
isomeric ratio (det. by 1H NMR)
3iab : 3iac = 1:3
f1 (ppm)

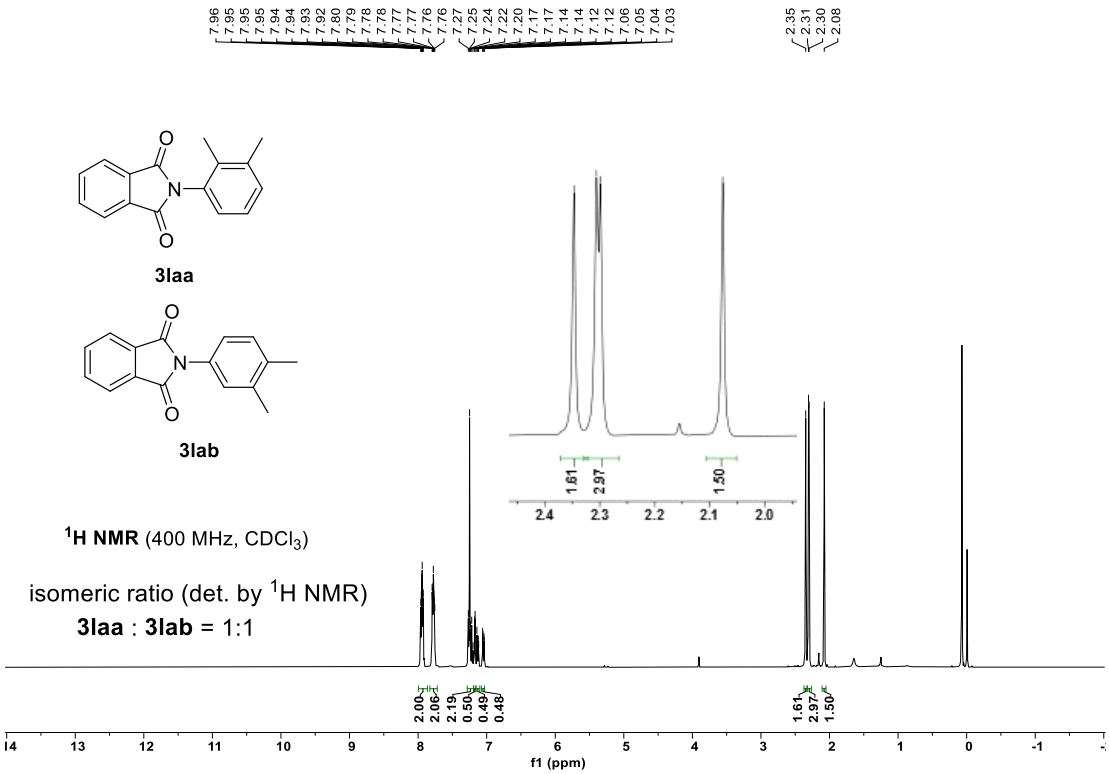

3iaa
3iab
3iac
13C NMR (101 MHz, CDCl3)
f1 (ppm)

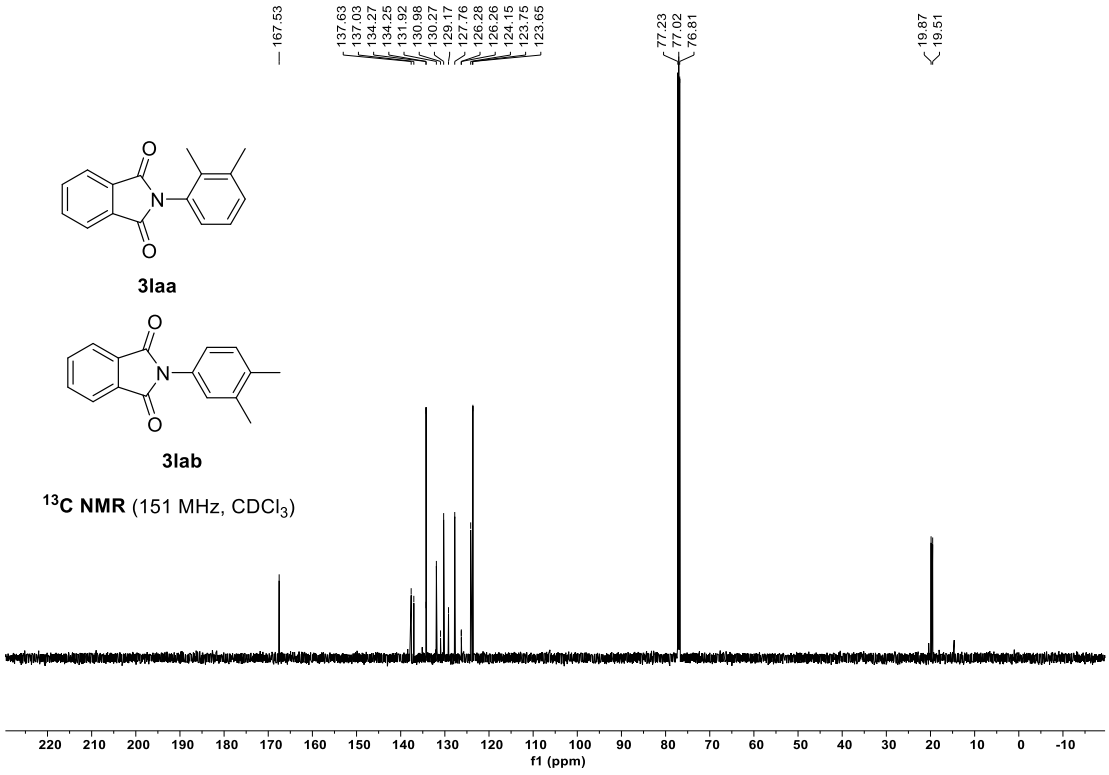

3jaa
3jab
3jac
1H NMR (400 MHz, CDCl3)
isomeric ratio (det. by 1H NMR)
3jaa ; 3jab ; 3iac = 1:2:3
f1 (ppm)

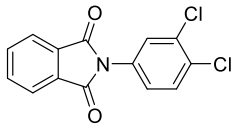

3jaa
3jab
3jac
13C NMR (151 MHz, CDCl3)
f1 (ppm)


3kaa
3kab
3kac
1H NMR (400 MHz, CDCl3)
isomeric ratio (det. by 1H NMR)
3kaa : 3kab : 3kac = 1:3:5
f1 (ppm)


3kaa
3kab
3kac
13C NMR (151 MHz, CDCl3)
f1 (ppm)

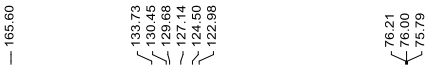

7.96
7.95
7.95
7.95
7.94
7.94
7.93
7.92
7.80
7.79
7.78
7.78
7.77
7.77
7.76
7.76
7.27
7.25
7.24
7.22
7.20
7.17
7.17
7.14
7.12
7.12
7.06
7.05
7.04
7.03
2.35
2.31
2.30
2.08
3laa
3lab
1.61
2.97
1.50
2.4
2.3
2.2
2.1
2.0
1H NMR (400 MHz, CDCl3)
isomeric ratio (det. by 1H NMR)
3laa : 3lab = 1:1
2.00
2.06
2.19
0.50
0.49
0.48
1.61
2.97
1.50
f1 (ppm)

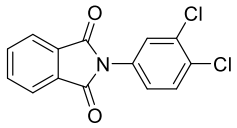

167.53
137.63
137.03
134.27
134.25
131.92
130.98
130.27
129.17
127.76
126.28
126.26
124.15
123.75
123.65
77.23
77.02
76.81
19.87
19.51
3laa
3lab
13C NMR (151 MHz, CDCl3)
f1 (ppm)



3ma

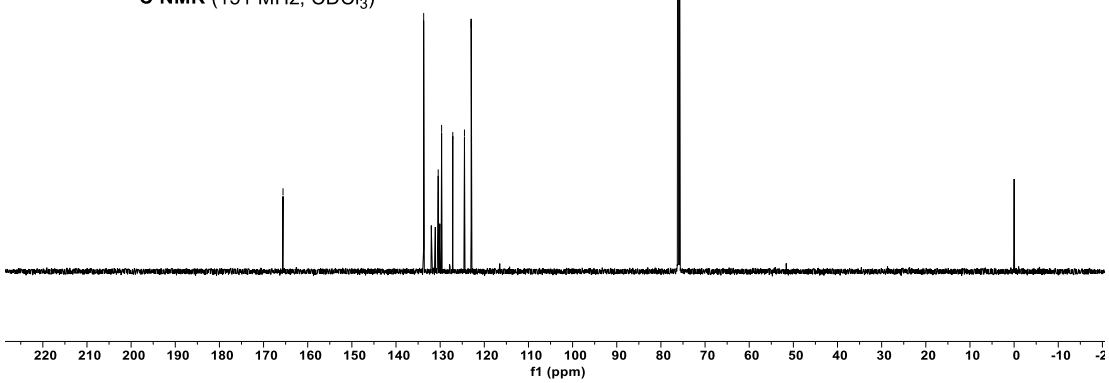
^{1}H NMR (400 MHz, $CDCl_3$)

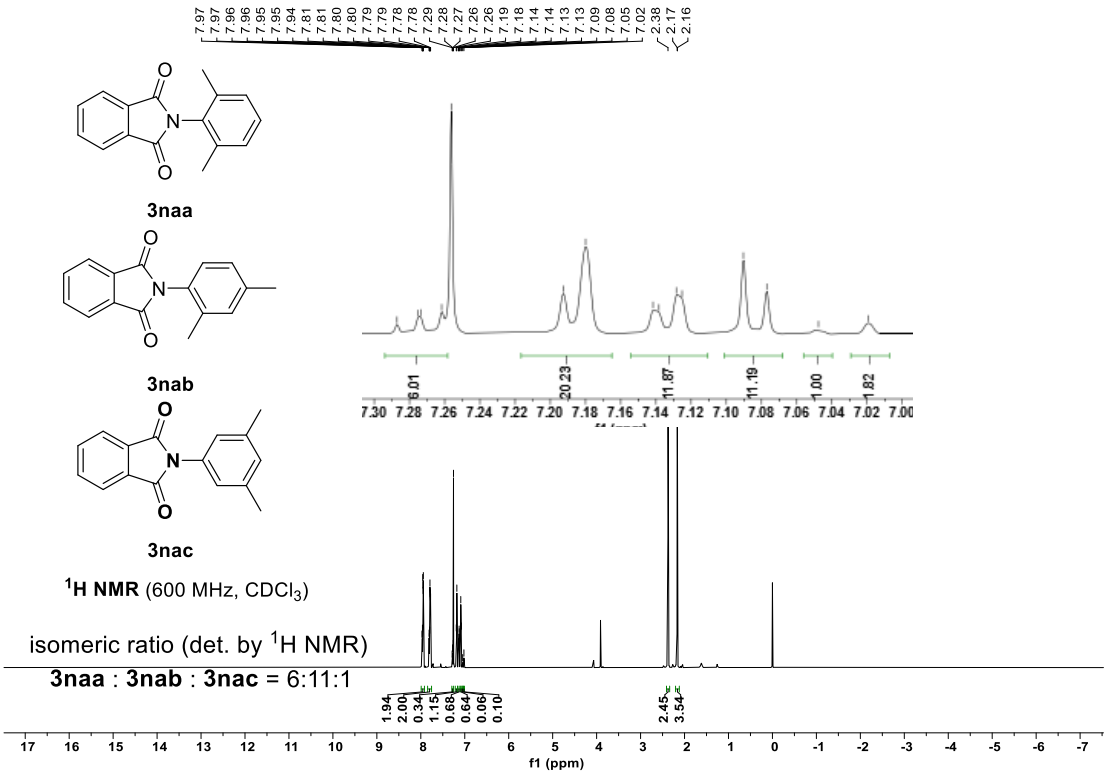


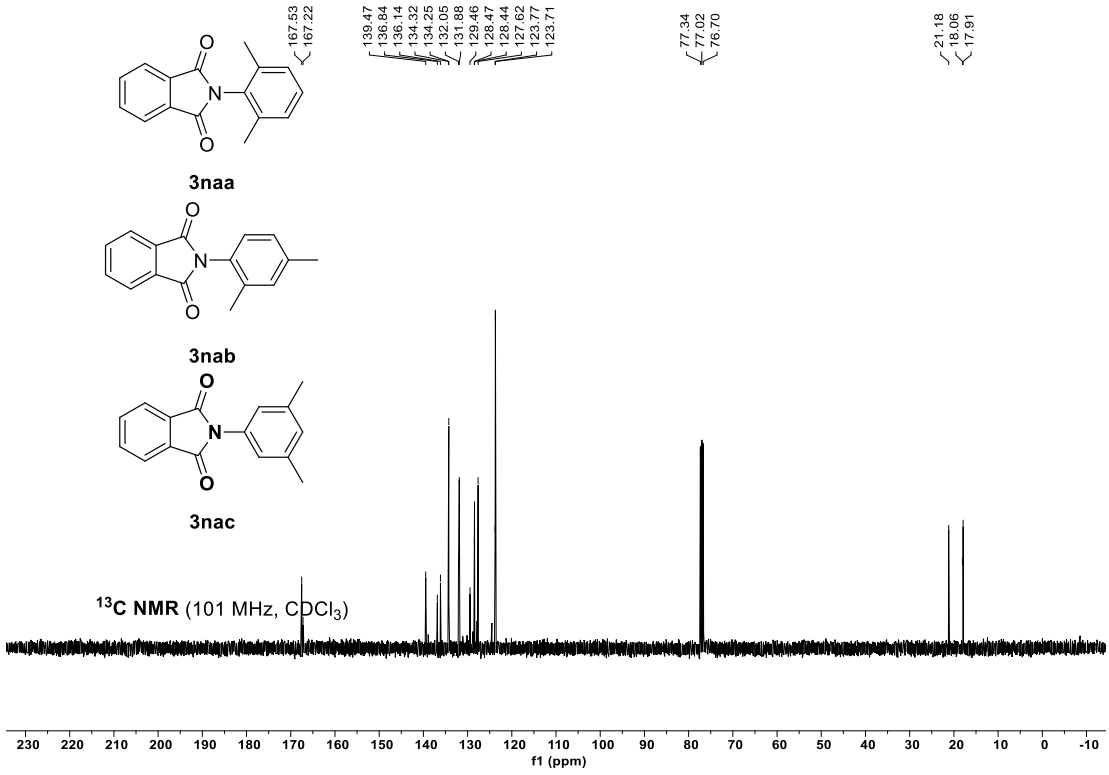


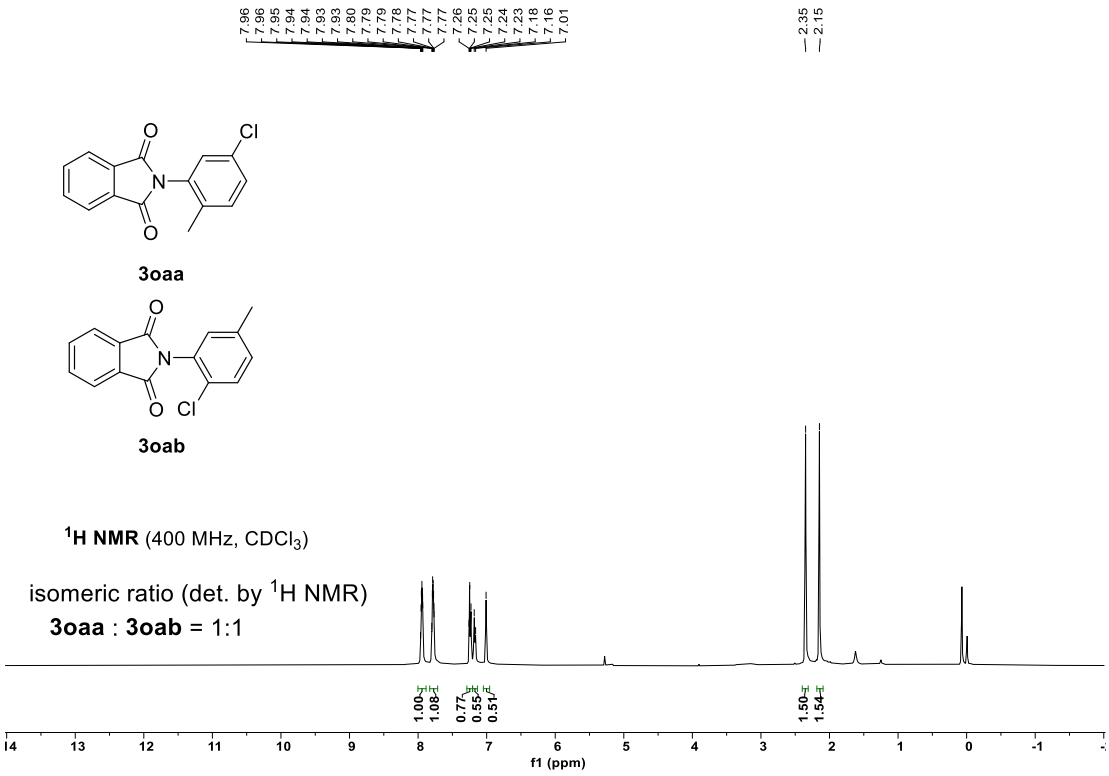
3ma

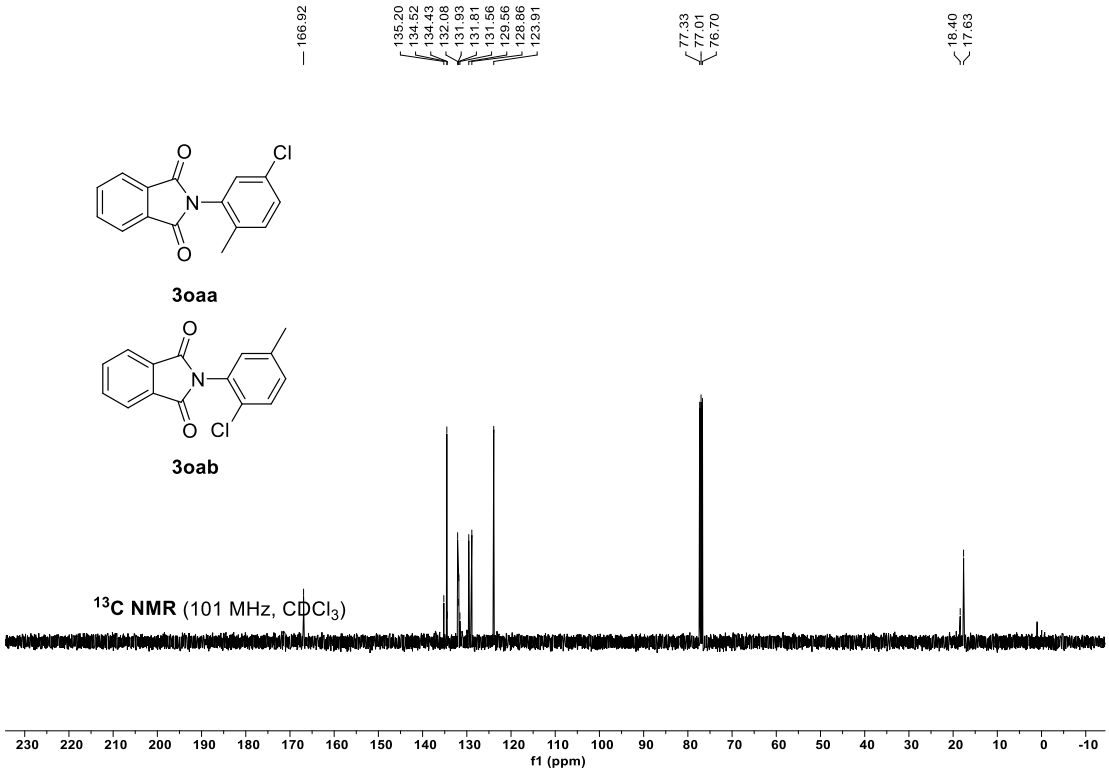
^{13}C NMR (151 MHz, $CDCl_3$)

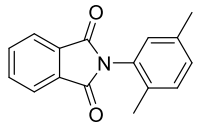



3naa
3nab
3nac
1H NMR (600 MHz, CDCl3)
isomeric ratio (det. by 1H NMR)
3naa : 3nab : 3nac = 6:11:1
f1 (ppm)


3naa
3nab
3nac
13C NMR (101 MHz, CDCl3)
f1 (ppm)

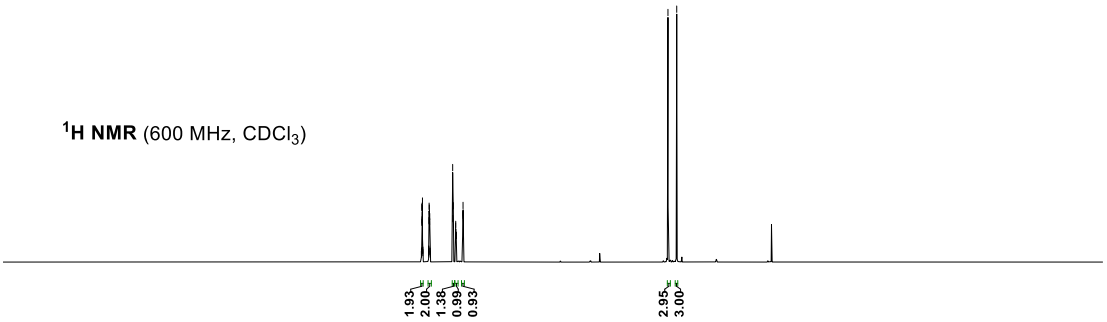

7.96
7.96
7.95
7.94
7.94
7.93
7.93
7.80
7.79
7.79
7.78
7.77
7.77
7.77
7.26
7.25
7.25
7.24
7.23
7.18
7.16
7.01
2.35
2.15
3oaa
3oab
1H NMR (400 MHz, CDCl3)
isomeric ratio (det. by 1H NMR)
3oaa : 3oab = 1:1
1.00
1.08
0.77
0.55
0.51
1.50
1.54
f1 (ppm)

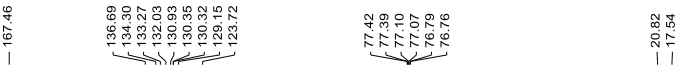

166.92
135.20
134.52
134.43
132.08
131.93
131.81
131.56
129.56
128.86
123.91
77.33
77.01
76.70
18.40
17.63
3oaa
3oab
13C NMR (101 MHz, CDCl3)
f1 (ppm)

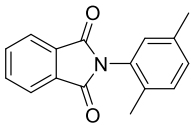


3pa

^{1}H NMR (600 MHz, $CDCl_3$)

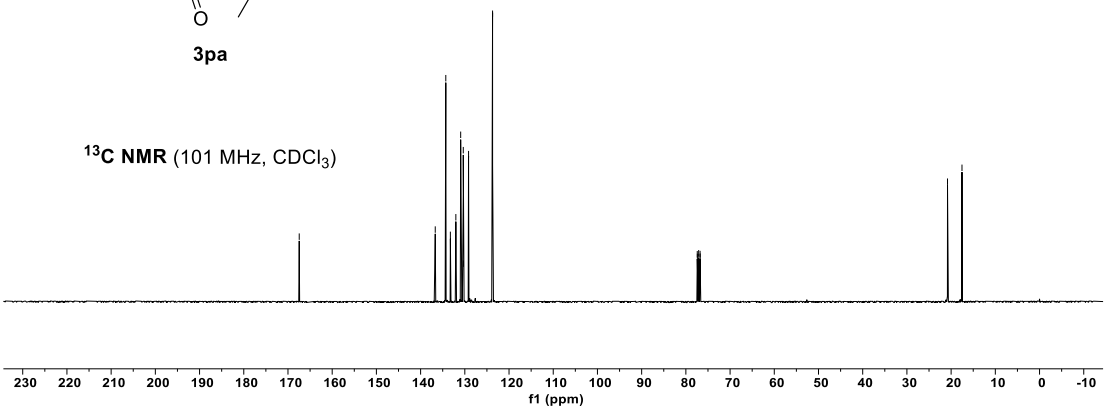


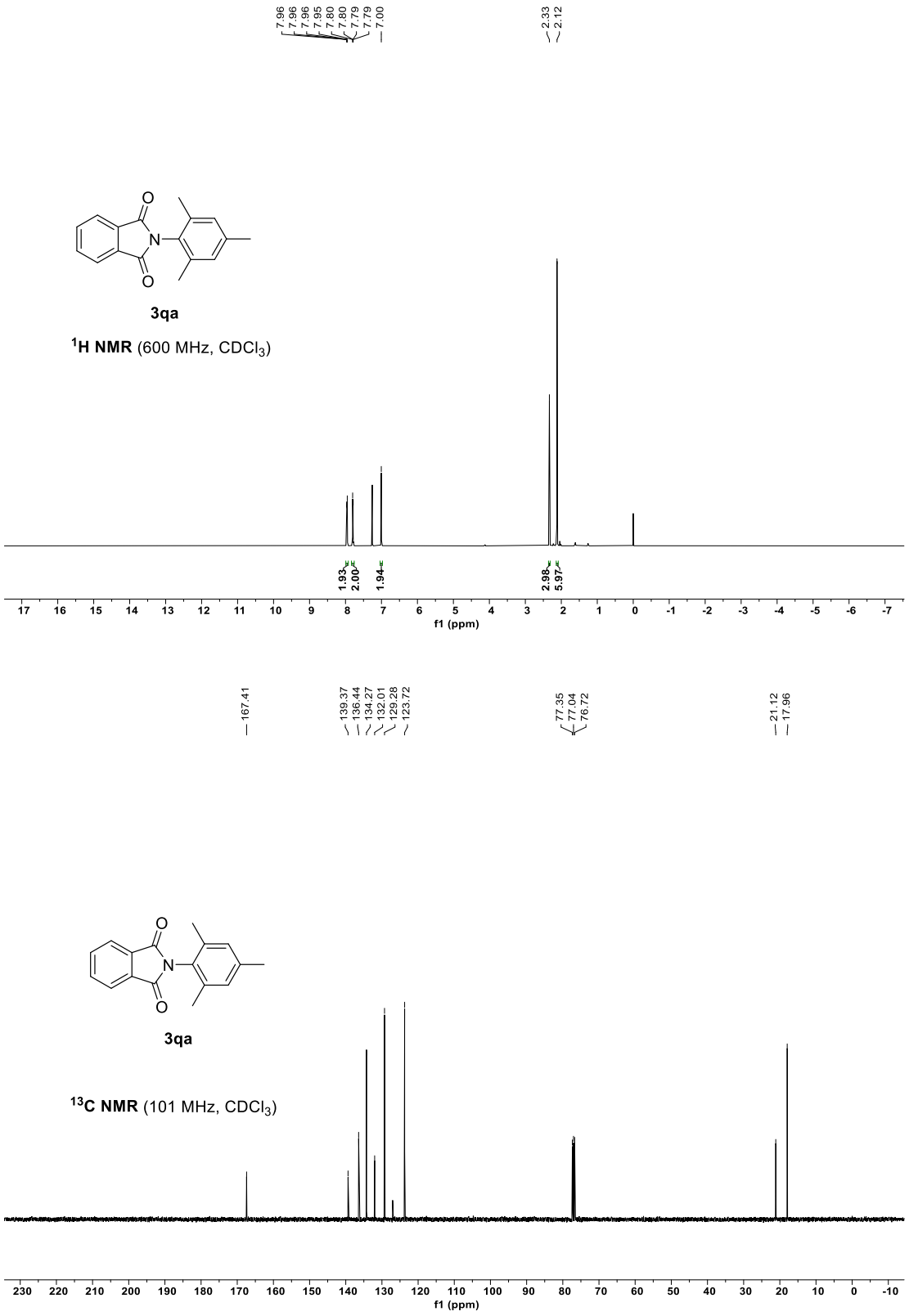


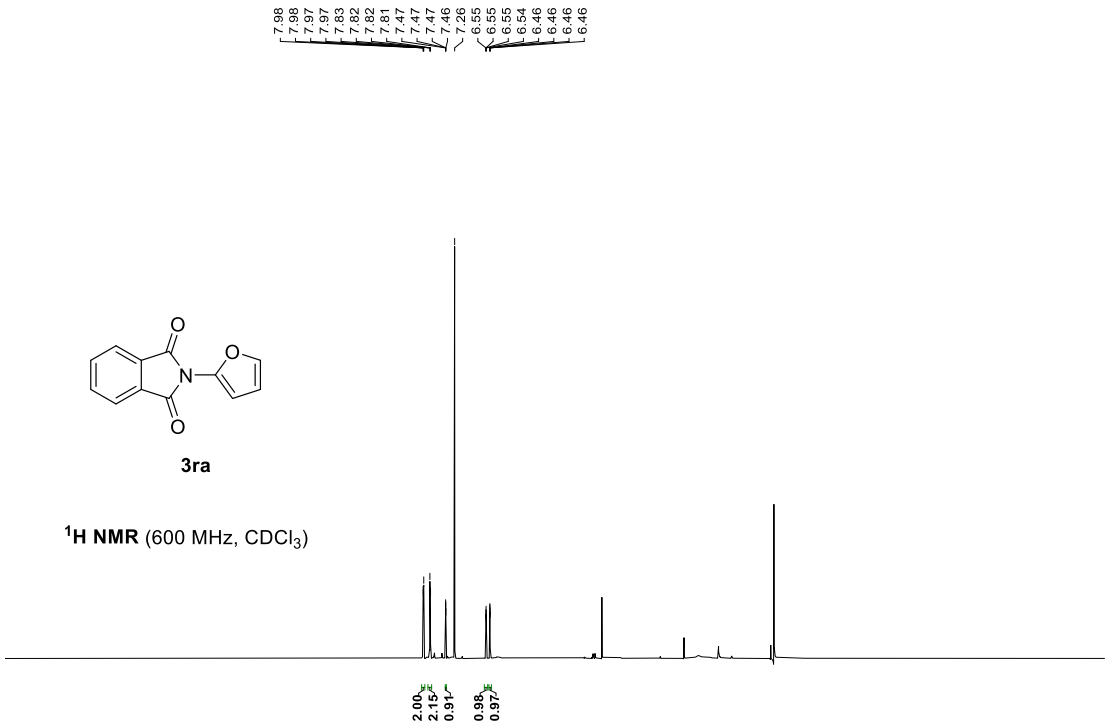


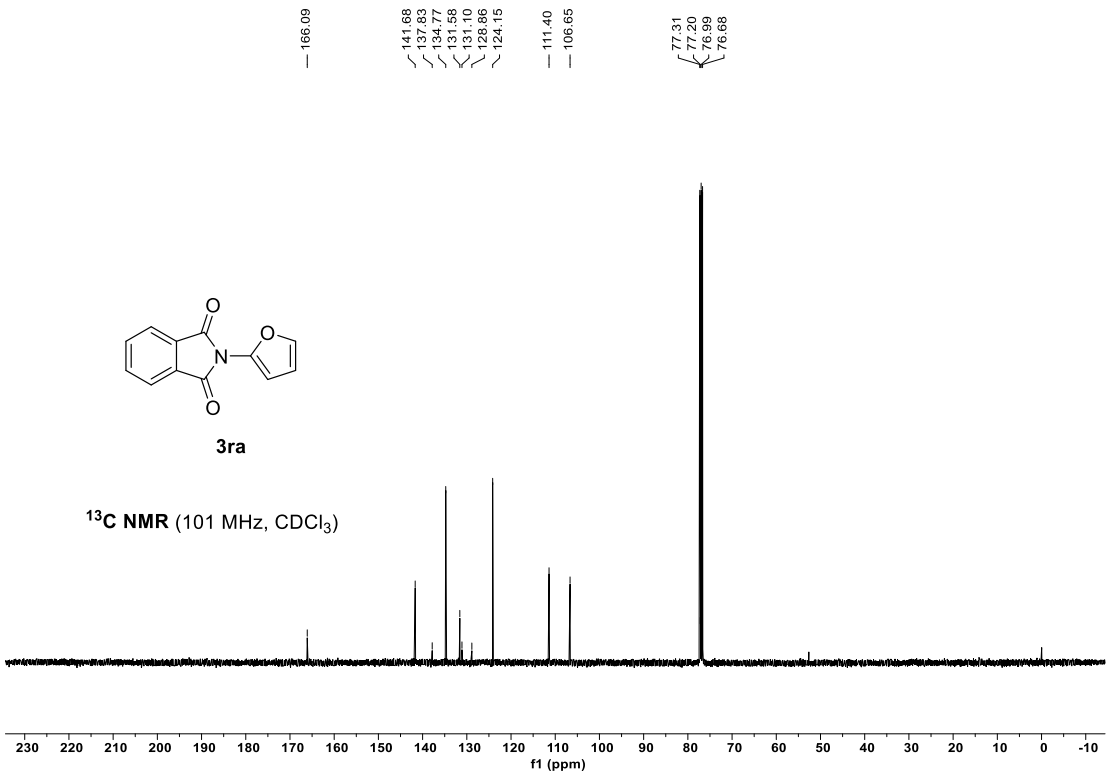
3pa

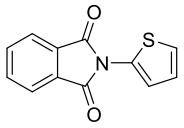
^{13}C NMR (101 MHz, $CDCl_3$)




7.96
7.96
7.96
7.95
7.80
7.80
7.79
7.79
7.00
2.33
2.12
3qa
1H NMR (600 MHz, CDCl3)
1.93
2.00
1.94
2.98
5.97
f1 (ppm)
167.41
139.37
136.44
134.27
132.01
129.28
123.72
77.35
77.04
76.72
21.12
17.96
3qa
13C NMR (101 MHz, CDCl3)
f1 (ppm)

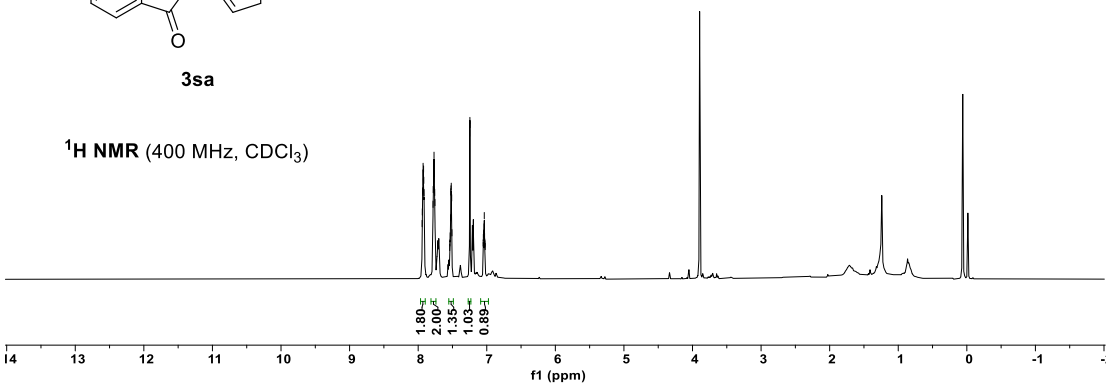

7.98
7.98
7.97
7.97
7.83
7.82
7.82
7.81
7.47
7.47
7.47
7.46
7.26
6.55
6.55
6.55
6.54
6.46
6.46
6.46
6.46
O
N
O
O
3ra
1H NMR (600 MHz, CDCl3)
2.00
2.15
0.91
0.98
0.97

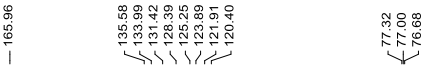

166.09
141.68
137.83
134.77
131.58
131.10
128.86
124.15
111.40
106.65
77.31
77.20
76.99
76.68
O
N
O
O
3ra
13C NMR (101 MHz, CDCl3)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

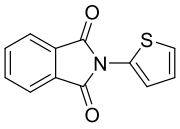


3sa

^{1}H NMR (400 MHz, $CDCl_3$)

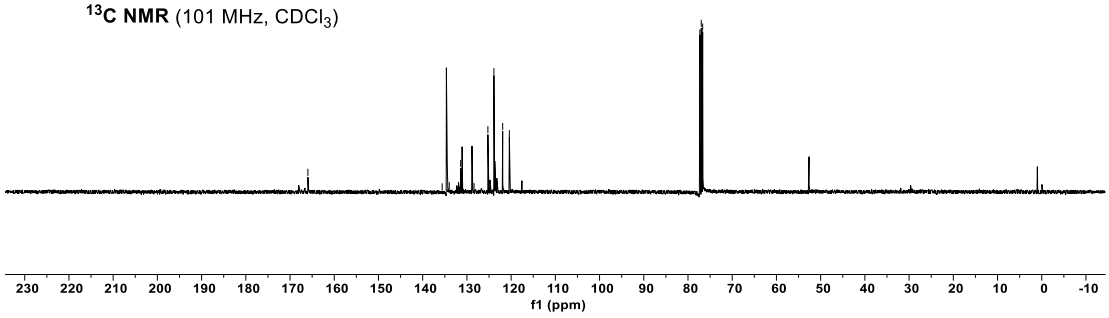




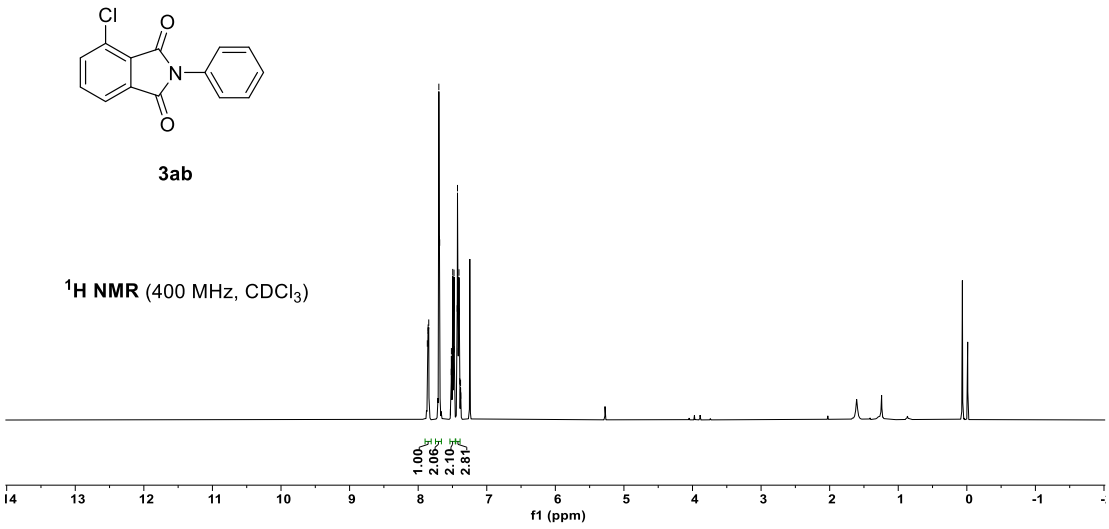


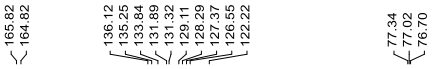
3sa

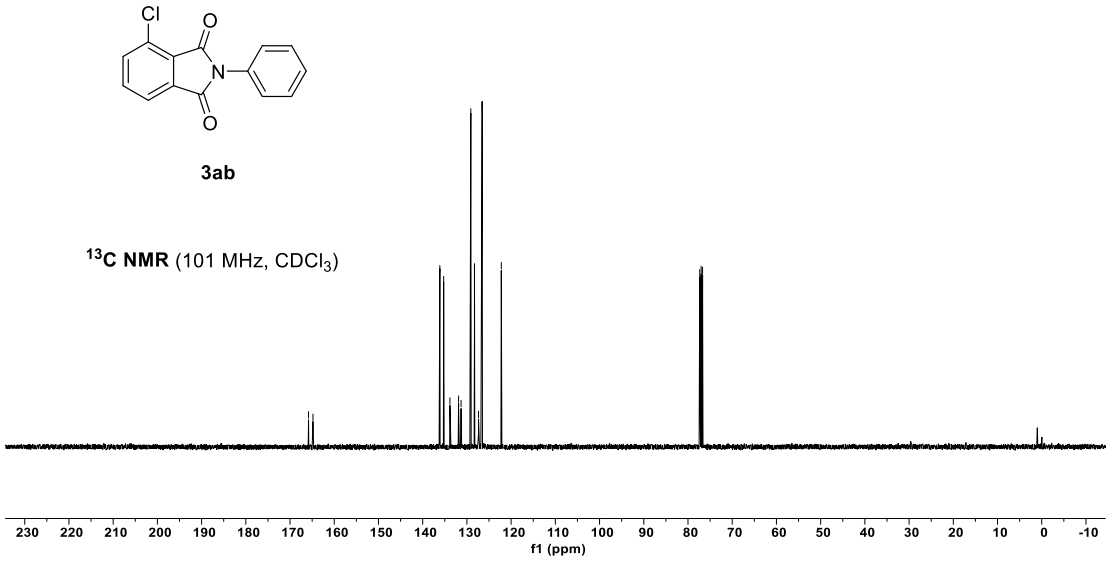
^{13}C NMR (101 MHz, $CDCl_3$)



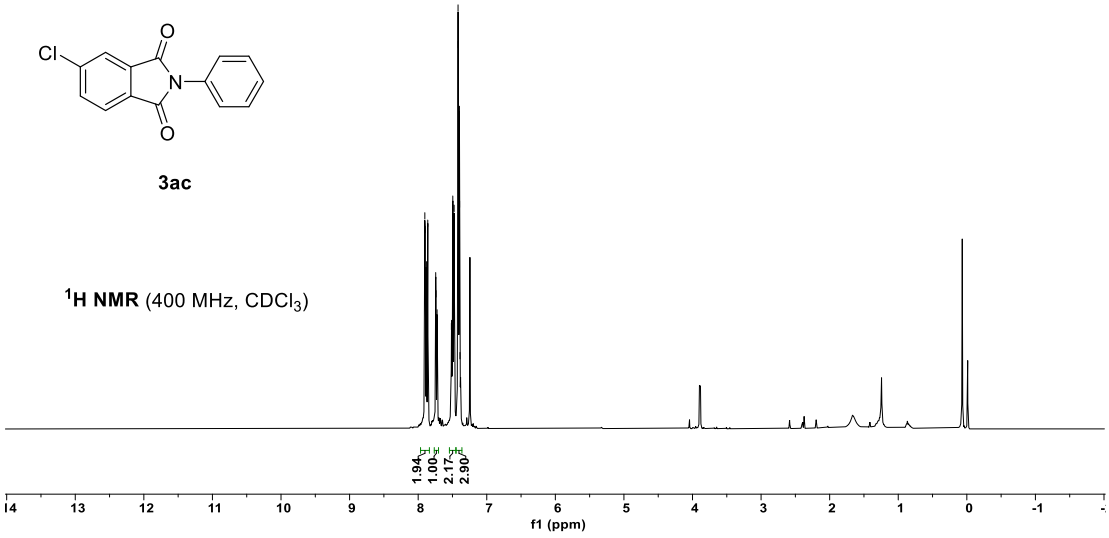

7.87
7.86
7.85
7.85
7.70
7.69
7.69
7.53
7.52
7.52
7.51
7.50
7.50
7.50
7.49
7.49
7.48
7.48
7.47
7.43
7.43
7.42
7.41
7.41
7.41
7.40
7.39
7.39
7.38
7.38

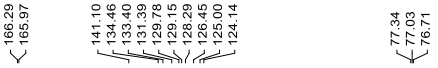

Cl
O
N
O
3ab
1H NMR (400 MHz, CDCl3)
1.00
2.06
2.10
2.81
f1 (ppm)

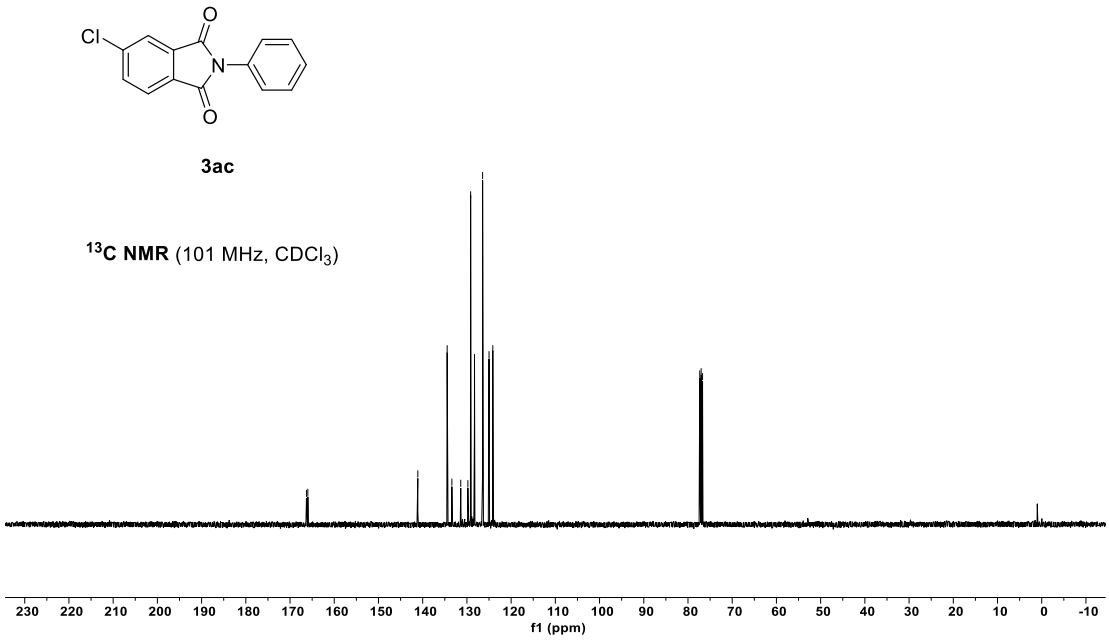

165.82
164.82
136.12
135.25
133.84
131.89
131.32
129.11
128.29
127.37
126.55
122.22
77.34
77.02
76.70

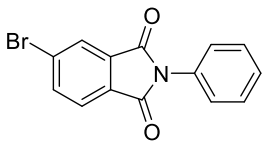

Cl
O
N
O
3ab
13C NMR (101 MHz, CDCl3)
f1 (ppm)


7.90
7.90
7.88
7.86
7.74
7.74
7.72
7.72
7.52
7.51
7.51
7.50
7.50
7.49
7.49
7.48
7.48
7.42
7.42
7.41
7.40
7.40
7.40
7.39


Cl
O
N
O
3ac
1H NMR (400 MHz, CDCl3)
1.94
1.00
2.17
2.90
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

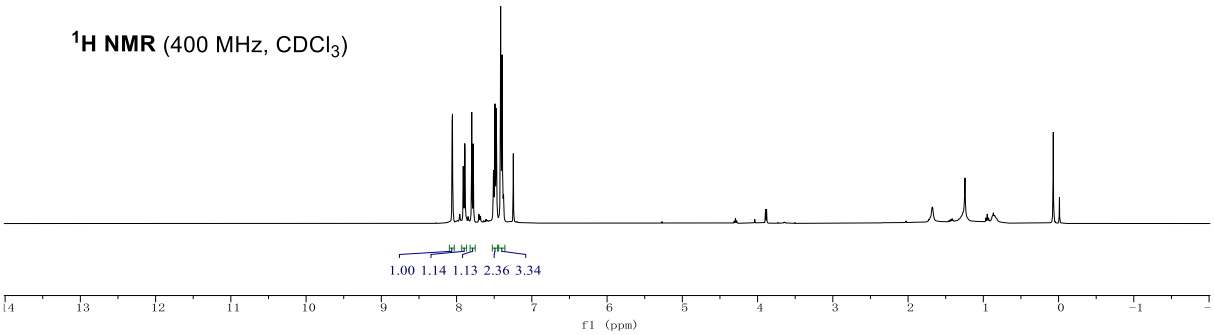

166.29
165.97
141.10
134.46
133.40
131.39
129.78
129.15
128.29
126.45
125.00
124.14
77.34
77.03
76.71


Cl
O
N
O
3ac
13C NMR (101 MHz, CDCl3)
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

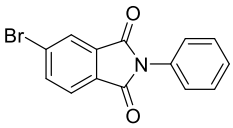


3ad

^{1}H NMR (400 MHz, $CDCl_3$)



166.43
165.05
138.01
133.34
131.36
130.24
129.30
128.28
127.06
126.44
124.93
77.37
77.05
76.73



3ad

^{13}C NMR (101 MHz, $CDCl_3$)