Supporting Information

Three-Component Friedel–Crafts-Type Difuncitonalization of Ynamides with (Hetero)arenes and Iodine(III) Electrophile

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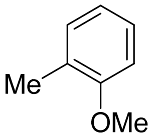
1. Materials and Methods

General. All reactions dealing with air- or moisture-sensitive compounds were performed by standard Schlenk technique in oven-dried reaction vessels under an argon atmosphere. Analytical thin-layer chromatography (TLC) was performed on Merck 60 F254 silica gel plates. Flash chromatography was performed using 40-50 μm silica gel (silica gel 60N, Kanto Chemical). ^{1}H, ^{13}C{^{1}H}, and ^{19}F{^{1}H} NMR spectra were recorded on JEOL JNM-ECA600 (600 MHz) spectrometers. ^{1}H and ^{13}C{^{1}H} NMR spectra are reported in parts per million (ppm) downfield from an internal standard, tetramethylsilane (0 ppm) and $CHCl_3$ (77.0 ppm), respectively. ^{19}F{^{1}H} NMR spectra are referenced to external standard (CF_3CO_2H, –76.6 ppm). Structural assignments were made with additional information from COSY, HMQC, HMBC, and NOESY experiments. Melting points were determined with a MPA100 OptiMelt apparatus. High-resolution mass spectra (HRMS) were recorded on a JEOL JMS-700 equipped with a double-focusing mass analyzer or a JMS-T100GC spectrometer equipped with a TOF mass analyzer.

Materials. Unless otherwise noted, commercial reagents were purchased from TCI, Kanto Chemical, Sigma-Aldrich, or other commercial suppliers and used as received. Anhydrous MeCN was purchased from FUJIFILM Wako Pure Chemical and was used as received. DMF and toluene were distilled over CaH_2 and stored under argon in the presence of molecular sieves 4Å. Ynamides **2a–2g**,[1] heteroarenes **1q**[2] and **1r**[3], and 3,3-bis(trifluoromethyl)-1λ^{3}-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl trifluoromethanesulfonate (benziodoxole triflate, BXT)[4] were prepared according to the literature procedures.



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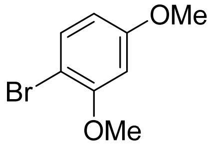

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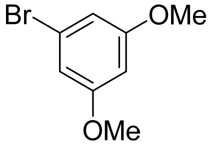

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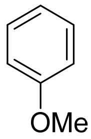

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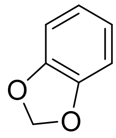

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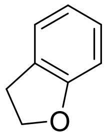

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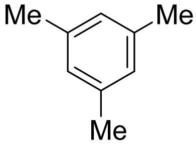

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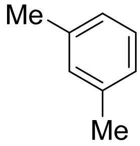

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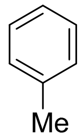

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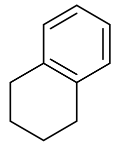

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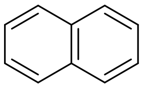

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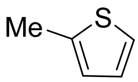

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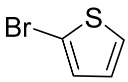

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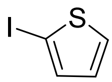

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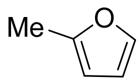

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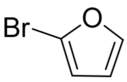

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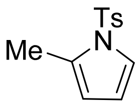

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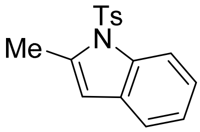

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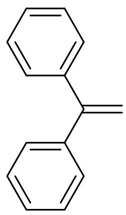

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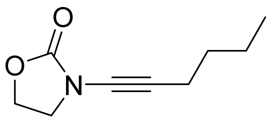

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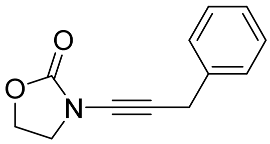

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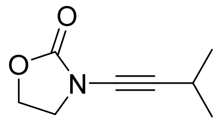

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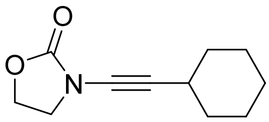

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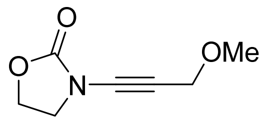

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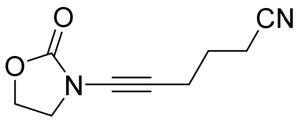

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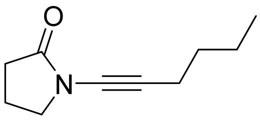

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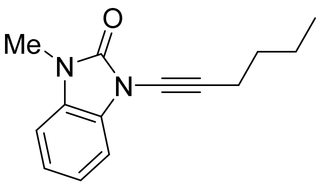

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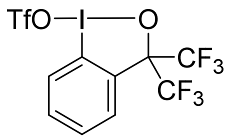
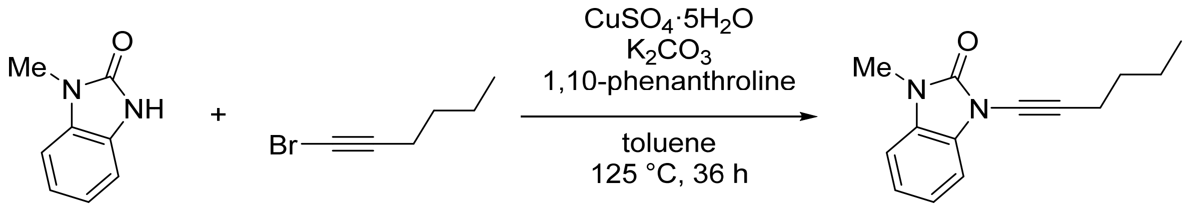


BXT

Figure S1. Starting materials used in this study.

2. Preparation of Ynamide



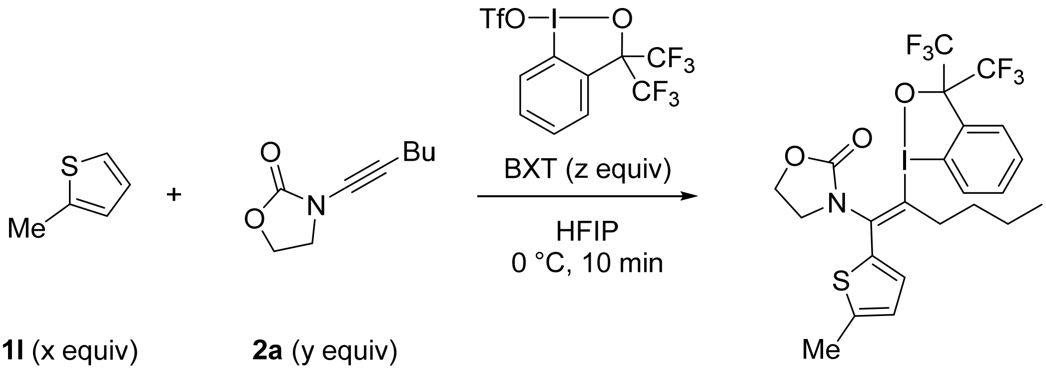
2h

1-(Hex-1-yn-1-yl)-3-methyl-1,3-dihydro-2*H*-benzo[*d*]imidazol-2-one (2h): Under an argon atmosphere, a 10 mL vial equipped with a magnetic stir bar was charged with 1-methyl-1,3-dihydro-2*H*-benzo[*d*]imidazol-2-one[5] (133.3 mg, 0.9 mmol, 1.0 equiv), K_2CO_3 (248.8 mg, 1.8 mmol, 2.0 equiv), $CuSO_4{\cdot}5H_2O$ (44.9 mg, 0.18 mmol, 20 mol%) and 1,10-phenanthroline (32.4 mg, 0.18 mmol, 20 mol%). To the resulting mixture was added toluene (1.5 mL) and 1-bromohex-1-yne[1a] (159.4 mg, 0.99 mmol, 1.1 equiv), and the mixture was stirred at 125 °C for 36 h. The reaction mixture was then cooled to room temperature, filtered through a plug of Celite, washed with EtOAc, and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to afford the corresponding product **2h** as a colorless oil (127.4 mg, 62%).

R_f 0.25 (hexane/EtOAc = 4/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.19-7.12 (m, 3H), 6.97-6.94 (m, 1H), 3.41 (s, 3H), 2.49 (t, *J* = 7.2 Hz, 2H), 1.66-1.60 (m, 2H), 1.54-1.47 (m, 2H), 0.96 (t, *J* = 7.5 Hz, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 153.6, 129.4, 128.5, 123.0, 121.9, 109.5, 107.7, 75.3, 66.5, 30.8, 27.4, 21.9, 18.3, 13.6; HRMS (EI) *m*/*z*: $[M]^+$ calcd for $C_{14}H_{16}N_2O$ 228.1257; found, 228.1257.

3. Iodo(III)arylation of Ynamides

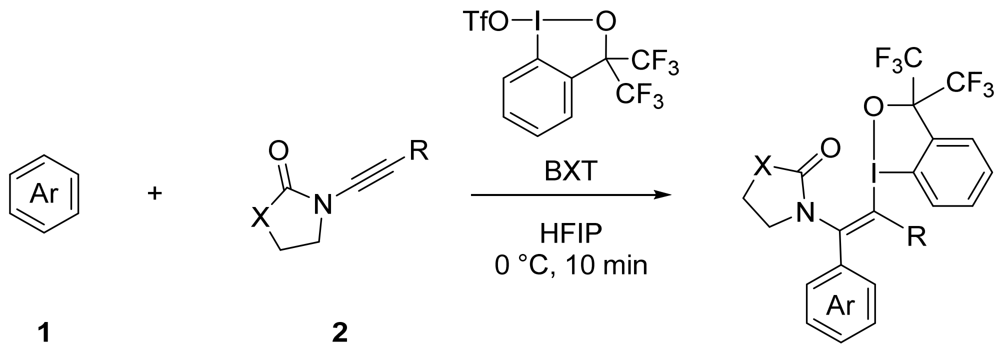
Table S1. Optimization of Reaction Conditions for Iodo(III)arylation of **1l**[a].



1l (x equiv) **2a** (y equiv) **3al**

Entry	x	y	z	Conc. [M]	Yield [%][b]
1	1.2	1.0	1.2	0.2	48
2	1.2	1.0	1.2	0.1	53
3	1.2	1.0	1.2	0.05	82[c]

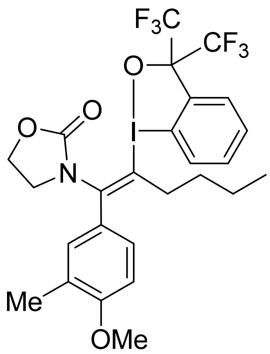
[a] The reaction was performed on a 0.1 mmol scale. [b] Determined by ^{1}H NMR using 1,1,2,2-tetrachloroethane as an internal standard. [c] Isolated yield.



1 **2** **3**

General Procedure A: Under an argon atmosphere, a 4 mL vial equipped with a magnetic stir bar was charged sequentially with arene **1** (0.1 mmol), ynamide **2** (0.2 mmol, 2.0 equiv), and HFIP (2.0 mL), followed by the addition of BXT (103.6 mg, 0.2 mmol, 2.0 equiv) at 0 °C. The resulting mixture was stirred at 0 °C for 10 min. Saturated Na_2CO_3 aq. (4 mL) was added, and then the mixture was extracted with EtOAc (5 mL × 3). The combined organic layer was washed with H_2O (5 mL) and brine (5 mL), dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel to afford the desired product.

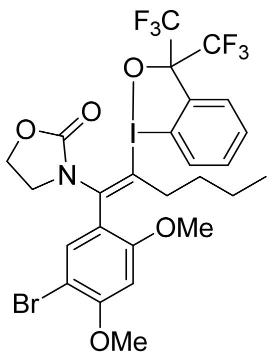
General Procedure B: Under an argon atmosphere, a 4 mL vial equipped with a magnetic stir bar was charged sequentially with heteroarene **1** (0.12 mmol, 1.2 equiv), ynamide **2** (0.1 mmol), and HFIP (2.0 mL), followed by the addition of BXT (62.2 mg, 0.12 mmol, 1.2 equiv) at 0 °C. The resulting mixture was stirred at 0 °C for 10 min. Saturated Na_2CO_3 aq. (4 mL) was added, and then the mixture was extracted with EtOAc (5 mL × 3). The combined organic layer was washed with H_2O (5 mL) and brine (5 mL), dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel to afford the desired product.



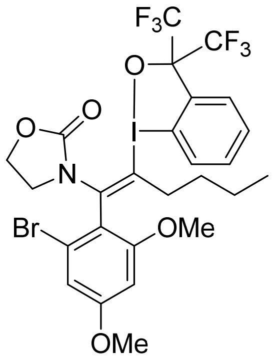
(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(4-methoxy-3-methylphenyl)hex-1-en-1-yl)oxazolidin-2-one (3aa): Synthesized by the general procedure A (60.5 mg, 92% yield); white solid; R_f 0.27 (hexane/EtOAc = 1/1); m.p. 164.2-165.1 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89-7.84 (m, 1H), 7.65-7.57 (m, 3H), 7.12 (dd, *J* = 8.4 Hz, 1.8 Hz, 1H), 7.04 (s, 1H), 6.91 (d, *J* = 8.4 Hz, 1H), 4.34 (t, *J* = 8.4 Hz, 2H), 3.90 (s, 3H), 3.44 (t, *J* = 7.8 Hz, 2H), 2.65-2.51 (m, 2H), 2.27 (s, 3H), 1.48-1.41 (m, 2H), 1.23-1.15 (m, 2H), 0.72 (t, *J* = 7.2 Hz, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 158.9, 157.3, 144.2, 133.5, 131.5, 130.6, 130.4, 130.1, 128.6, 128.0, 127.8, 126.8, 124.2 (q, J_{C-F} = 291.3 Hz), 123.5, 110.9, 110.2, 81.8-

81.4 (m), 62.4, 55.4, 45.0, 34.8, 32.5, 21.5, 16.3, 13.5; $^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$) δ -75.7; HRMS (FAB) *m*/*z*: $[M + H]^+$ calcd for $C_{26}H_{27}F_6INO_4$ 658.0883; found, 658.0893.

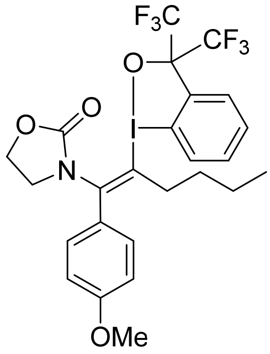
1 mmol-scale synthesis of 3aa: Under an argon atmosphere, a 20 mL two-necked flask equipped with a magnetic stir bar was charged sequentially with 1-methoxy-2-methylbenzene (**1a**, 122.2 mg, 1.0 mmol), 3-(hex-1-yn-1-yl)oxazolidin-2-one (**2a**, 334.4 mg, 2.0 mmol, 2.0 equiv), and HFIP (20 mL), followed by the addition of BXT (1.04 g, 2.0 mmol, 2.0 equiv) at 0 °C. The resulting mixture was stirred at 0 °C for 10 min. Saturated Na_2CO_3 aq. (5 mL) was added, and then the mixture was extracted with EtOAc (15 mL × 3). The combined organic layer was washed with H_2O (15 mL) and brine (15 mL), dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel to afford **3aa** (525.9 mg, 80% yield).



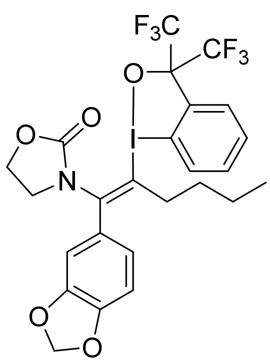
(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(5-bromo-2,4-dimethoxyphenyl)hex-1-en-1-yl)oxazolidin-2-one (3ab): Synthesized by the general procedure A (56.4 mg, 75% yield); white solid; R_f 0.23 (hexane/EtOAc = 1/1); m.p. 91.4-92.4 °C; ^1H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.2 Hz, 1H), 7.81-7.69 (m, 1H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.34 (s, 1H), 6.57 (s, 1H), 4.33 (t, *J* = 7.8 Hz, 2H), 3.99 (s, 3H), 3.95 (s, 3H), 3.40 (t, *J* = 7.8 Hz, 2H), 2.48-2.37 (m, 2H), 1.45-1.37 (m, 2H), 1.23-1.14 (m, 2H), 0.71 (t, *J* = 7.5 Hz, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 158.3, 157.6, 157.5, 139.1, 134.1, 133.9, 131.4, 130.5, 130.0, 129.1, 128.4, 124.3 (q, J_{C-F} = 291.7 Hz), 114.1, 111.5, 103.1, 96.5, 82.0-81.6 (m), 62.3, 56.5, 56.1, 44.7, 35.0, 32.2, 21.5, 13.5; $^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$) δ -75.7, -75.8; HRMS (FAB) *m/z*: $[M + H]^+$ calcd for $C_{26}H_{26}BrF_6INO_5$ 751.9938; found, 751.9940.



(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ³-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(2-bromo-4,6-dimethoxyphenyl)hex-1-en-1-yl)oxazolidin-2-one (3ac): Synthesized by the general procedure A (57.2 mg, 76% yield); white solid; R_f 0.22 (hexane/EtOAc = 1/1); m.p. 149.0-151.7 °C; ^1H NMR (600 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.4 Hz, 1H), 7.83 (d, *J* = 7.2 Hz, 1H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 1H), 6.84 (d, *J* = 1.2 Hz, 1H), 6.53 (s, 1H), 4.38-4.29 (m, 2H), 4.00-3.87 (m, 6H), 3.51-3.31 (m, 2H), 2.45-2.27 (m, 2H), 1.47-1.37 (m, 2H), 1.24-1.17 (m, 2H), 0.72 (t, *J* = 7.2 Hz, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 162.1, 159.1, 157.6, 134.3, 131.1, 130.7, 130.1, 129.7, 124.6, 124.3 (q, J_{C-F} = 290.2 Hz), 114.1, 112.2, 109.9, 108.1, 98.3, 82.0-81.5 (m), 62.3, 56.1, 55.8, 44.5, 35.0, 32.2, 21.6, 13.6, one carbon could not be found due to overlapping; $^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$, 45 °C) δ -75.7; HRMS (FAB) *m/z*: $[M + H]^+$ calcd for $C_{26}H_{26}BrF_6INO_5$ 751.9938; found, 751.9955.

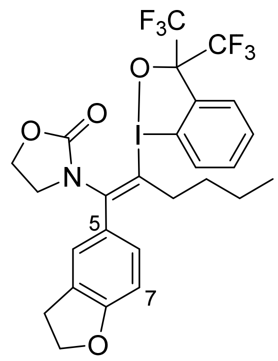


(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(4-methoxyphenyl)hex-1-en-1-yl)oxazolidin-2-one (3ad): Synthesized by the general procedure A (37.3 mg, 58% yield, regioisomer ratio = 3:1 as determined by ^{1}H NMR); the major isomer was isolated by recrystallization from hexane/CH_2Cl_2 (22.2 mg, 35%); white solid; R_f 0.23 (hexane/EtOAc = 1/1); m.p. 151.2-152.6 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (d, J = 7.8 Hz, 1H), 7.63-7.55 (m, 3H), 7.26-7.23 (m, 2H), 7.02-6.99 (m, 2H), 4.35 (t, J = 8.4 Hz, 2H), 3.88 (s, 3H), 3.44 (t, J = 8.0 Hz, 2H), 2.64-2.53 (m, 2H), 1.49-1.42 (m, 2H), 1.23-1.15 (m, 2H), 0.72 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 160.7, 157.3, 143.9, 133.5, 131.5, 130.5, 130.3, 130.1, 128.5, 127.4, 124.2 (q, $J_{C\text{-}F}$ = 291.3 Hz), 124.0, 114.7, 110.9, 81.8-81.4 (m), 62.4, 55.4, 45.0, 34.9, 32.5, 21.6, 13.5; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$) δ -75.7; HRMS (FAB) *m*/*z*: [M + H]$^+$ calcd for $C_{25}H_{25}F_6INO_4$ 644.0727; found, 644.0744.



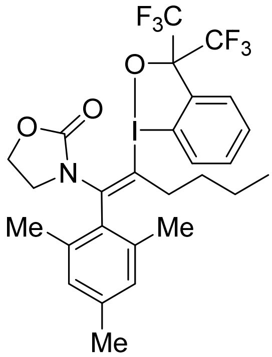
(*Z*)-3-(1-(Benzo[*d*][1,3]dioxol-5-yl)-2-(3,3-bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)hex-1-en-1-yl)oxazolidin-2-one (3ae): Synthesized by the general procedure A (43.3 mg, 66% yield); white solid; R_f 0.40 (hexane/EtOAc = 1/2); m.p. 88.2-92.0 °C; ^{1}H NMR (600

MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.2 Hz, 1H), 7.63-7.56 (m, 3H), 6.93 (d, *J* = 8.4 Hz, 1H), 6.81 (dd, *J* = 7.8 Hz, 1.8 Hz, 1H), 6.75 (d, *J* = 1.2 Hz, 1H), 6.08 (s, 2H), 4.36 (t, *J* = 7.8 Hz, 2H), 3.46 (t, *J* = 7.8 Hz, 2H), 2.66-2.54 (m, 2H), 1.49-1.43 (m, 2H), 1.25-1.17 (m, 2H), 0.74 (t, *J* = 7.2 Hz, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 157.2, 149.0, 148.5, 143.5, 133.4, 131.6, 130.5, 130.1, 128.5, 127.8, 125.5, 124.2 (q, $J_{C\text{-}F}$ = 291.6 Hz), 123.1, 110.9, 108.9, 108.7, 101.8, 82.0-81.2 (m), 62.4, 44.9, 34.8, 32.4, 21.5, 13.5; $^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$) δ -75.7; HRMS (FAB) *m/z*: $[M + H]^+$ calcd for $C_{25}H_{23}F_6INO_5$ 658.0520; found, 658.0534.

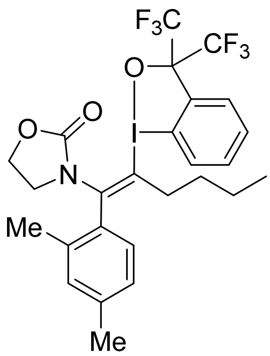


(C5:C7 = 23:1)

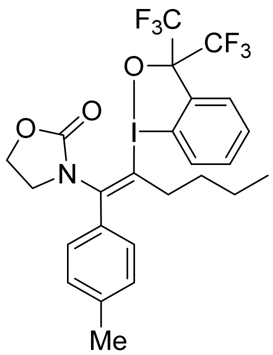
(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ³-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(2,3-dihydrobenzofuran-5-yl)hex-1-en-1-yl)oxazolidin-2-one (3af): Synthesized by the general procedure A (43.9 mg, 67% yield, regioisomer ratio =23:1 as determined by ^1H NMR); white solid; R_f 0.41 (hexane/EtOAc = 1/2); m.p. 87.4-89.3 °C; ^1H NMR (600 MHz, $CDCl_3$, major isomer) δ 7.88 (d, *J* = 7.2 Hz, 1H), 7.63-7.55 (m, 3H), 7.11 (d, *J* = 1.2 Hz, 1H), 7.07 (dd, *J* = 7.8 Hz, 2.1 Hz, 1H), 6.87 (d, *J* = 8.4 Hz, 1H), 4.67 (t, *J* = 8.4 Hz, 2H), 4.36 (t, *J* = 8.0 Hz, 2H), 3.45 (t, *J* = 7.8 Hz, 2H), 3.29 (t, *J* = 8.0 Hz, 2H), 2.68-2.54 (m, 2H), 1.50-1.42 (m, 2H), 1.24-1.16 (m, 2H), 0.73 (t, *J* = 7.2 Hz, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$, major isomer) δ 161.5, 157.3, 144.2, 133.6, 131.5, 130.5, 130.1, 129.4, 128.6, 128.5, 127.4, 125.3, 124.2 (q, $J_{C\text{-}F}$ = 291.3 Hz), 124.0, 110.9, 109.9, 81.9-81.5 (m), 71.8, 62.4, 45.0, 34.9, 32.5, 29.5, 21.6, 13.6; $^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$, major isomer) δ -75.7; HRMS (FAB) *m/z*: $[M + H]^+$ calcd for $C_{26}H_{25}F_6INO_4$ 656.0727; found, 656.0730.



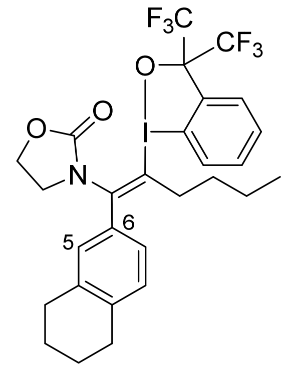
(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-mesitylhex-1-en-1-yl)oxazolidin-2-one (3ag): Synthesized by the general procedure A (63.6 mg, 97% yield); white solid; R_f 0.26 (hexane/EtOAc = 1/1); m.p. 177.7-179.2 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.2 Hz, 1H), 7.60-7.54 (m, 2H), 7.50-7.46 (m, 1H), 6.97 (s, 2H), 4.34 (t, *J* = 7.8 Hz, 2H), 3.39-3.33 (m, 2H), 2.33 (s, 3H), 2.28 (s, 6H), 1.72-1.65 (m, 2H), 1.42-1.34 (m, 2H), 1.21-1.13 (m, 2H), 0.71 (t, *J* = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 157.3, 141.4, 139.5, 136.2, 134.6, 131.1, 130.4, 129.9, 129.4, 128.3, 124.3, 124.2 (q, J_{C-F} = 291.7 Hz), 111.8, 82.0-81.2 (m), 62.7, 44.6, 34.3, 32.2, 21.8, 21.0, 20.5, 13.4, one carbon could not be found due to overlapping; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$) δ -75.7; HRMS (FAB) *m*/*z*: $[M + H]^+$ calcd for $C_{27}H_{29}F_6INO_3$ 656.1091; found, 656.1098.



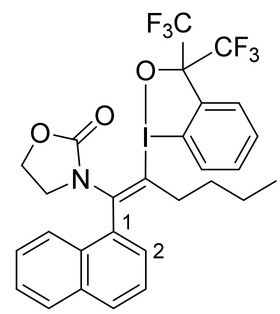
(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(2,4-dimethylphenyl)hex-1-en-1-yl)oxazolidin-2-one (3ah): Synthesized by the general procedure (39.1 mg, 61% yield); white solid; R_f 0.25 (hexane/EtOAc = 1/1); m.p. 91.6-94.3 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (d, J = 7.2 Hz, 1H), 7.62-7.55 (m, 3H), 7.15-7.11 (m, 2H), 7.09 (d, J = 7.8 Hz, 1H), 4.36-4.31 (m, 2H), 3.43-3.36 (m, 1H), 3.33-3.27 (m, 1H), 2.58-2.48 (m, 1H), 2.39 (s, 3H), 2.30-2.22 (m, 4H), 1.47-1.39 (m, 1H), 1.39-1.31 (m, 1H), 1.22-1.12 (m, 2H), 0.70 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 157.2, 143.6, 140.2, 136.1, 134.1, 132.0, 131.3, 130.5, 130.0, 129.9, 129.0, 128.9, 127.5, 124.3 (q, $J_{C\text{-}F}$ = 295.4 Hz), 124.2 (q, $J_{C\text{-}F}$ = 291.0 Hz), 111.4, 82.0-81.6 (m), 62.4, 44.8, 34.8, 32.4, 21.6, 21.2, 19.6, 13.5, one carbon could not be found due to overlapping; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$) δ -75.4, -75.9; HRMS (FAB) m/z: [M + H]$^+$ calcd for $C_{26}H_{27}F_6INO_3$ 642.0934; found, 642.0942.



(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(*p*-tolyl)hex-1-en-1-yl)oxazolidin-2-one (3ai): Synthesized by the general procedure A modified using 0.3 mmol of toluene (**1i**) and 0.1 mmol each of **2a** and BXT (23.8 mg, 38% yield); white solid; R_f 0.23 (hexane/EtOAc = 1/1); m.p. 138.2-140.1 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (d, J = 7.2 Hz, 1H), 7.64-7.56 (m, 3H), 7.30 (d, J = 7.8 Hz, 2H), 7.20 (d, J = 7.8 Hz, 2H), 4.35 (t, J = 8.0 Hz, 2H), 3.42 (t, J = 7.8 Hz, 2H), 2.62-2.50 (m, 1H), 2.43 (s, 3H), 1.48-1.41 (m, 1H), 1.23-1.13 (m, 2H), 0.71 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 157.3, 144.1, 140.3, 133.6, 131.5, 130.6, 130.1, 130.0, 129.2, 128.7, 128.5, 127.9, 124.2 (q, $J_{C\text{-}F}$ = 291.7 Hz), 111.0, 81.9-81.5 (m), 62.4, 45.0, 34.8, 32.5, 21.6, 21.4, 13.5; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$) δ -75.7; HRMS (FAB) m/z: [M + H]$^+$ calcd for $C_{25}H_{25}F_6INO_3$ 628.0778; found, 628.0774.

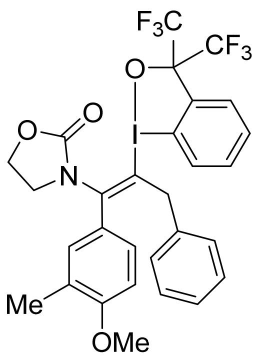


(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(5,6,7,8-tetrahydronaphthalen-2-yl)hex-1-en-1-yl)oxazolidin-2-one (3aj): Synthesized by the general procedure A (55.4 mg, 83% yield, regioisomer ratio = 11:1 as determined by ^{1}H NMR); white solid; R_f 0.38 (hexane/EtOAc = 1/1); m.p. 91.1-96.5 °C; ^{1}H NMR (600 MHz, $CDCl_3$, major isomer) δ 7.87 (d, *J* = 7.2 Hz, 1H), 7.64-7.56 (m, 3H), 7.16 (d, *J* = 7.8 Hz, 1H), 7.00 (d, *J* = 7.8 Hz, 1H), 6.96 (s, 1H), 4.34 (t, *J* = 8.4 Hz, 2H), 3.43 (t, *J* = 8.4 Hz, 2H), 2.85-2.77 (m, 4H), 2.62-2.51 (m, 2H), 1.88-1.81 (m, 4H), 1.49-1.42 (m, 2H), 1.24-1.17 (m, 2H), 0.73 (t, *J* = 7.8 Hz, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$, major isomer) δ 157.3, 144.4, 139.5, 138.4, 133.6, 131.5, 130.5, 130.1, 130.0, 129.2, 129.1, 128.6, 127.7, 125.8, 124.3 (q, $J_{C\text{-}F}$ = 292.5 Hz), 110.9, 81.9-81.5 (m), 62.4, 45.0, 34.8, 32.5, 29.4, 29.3, 22.9, 22.8, 21.6, 13.5; $^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$, major isomer) δ -75.7; HRMS (FAB) *m*/*z*: $[M + H]^+$ calcd for $C_{28}H_{29}F_6INO_3$ 668.1091; found, 668.1093.



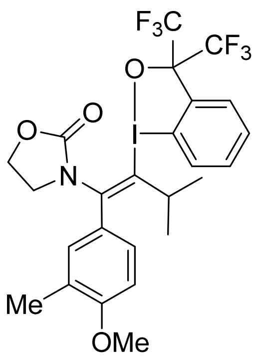
(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(naphthalen-1-

yl)hex-1-en-1-yl)oxazolidin-2-one (3ak): Synthesized by the general procedure A (58.4 mg, 88% yield, regioisomer ratio = 5:1 as determined by ^{1}H NMR); white solid; R_f 0.43 (hexane/EtOAc = 1/1); m.p. 113.4-115.6 °C; ^{1}H NMR (600 MHz, $CDCl_3$, major isomer) δ 8.01 (d, J = 8.4 Hz, 1H), 7.99-7.95 (m, 1H), 7.91-7.87 (m, 1H), 7.86-7.81 (m, 1H), 7.76-7.70 (m, 1H), 7.66-7.58 (m, 5H), 7.50 (d, J = 6.6 Hz, 1H), 4.32-4.27 (m, 1H), 4.23-4.16 (m, 1H), 3.50-3.41 (m, 1H), 3.18-3.09 (m, 1H), 2.59-2.50 (m, 1H), 2.30-2.24 (m, 1H), 1.50-1.39 (m, 1H), 1.36-1.27 (m, 1H), 1.13-1.07 (m, 1H), 1.07-1.00 (m, 1H), 0.56 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$, major isomer) δ 157.3, 142.8, 133.9, 133.8, 131.6, 131.0, 130.6, 130.5, 130.3, 130.1, 129.2, 128.9, 128.3, 128.0, 127.1, 125.3, 124.3 (q, $J_{C\text{-}F}$ = 291.6 Hz), 124.2, 124.1 (q, $J_{C\text{-}F}$ = 291.6 Hz), 111.4, 82.0-81.4 (m), 62.5, 45.1, 35.1, 32.7, 21.6, 13.4, one carbon could not be found due to overlapping; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$, major isomer) δ -75.3, -76.0; ^{1}H NMR (600 MHz, $CDCl_3$, minor isomer) δ 7.99-7.97 (m, 1H), 7.95-7.92 (m, 2H), 7.91-7.87 (m, 1H), 7.85-7.81 (m, 1H), 7.75-7.71 (m, 1H), 7.67-7.58 (m, 4H), 7.37 (dd, J = 8.4 Hz, 1.2 Hz, 1H), 4.36 (t, J = 7.8 Hz, 2H), 3.50-3.41 (m, 2H), 2.67-2.60 (m, 2H), 1.51-1.39 (m, 2H), 1.18-1.13 (m, 2H), 0.67 (t, J = 7.5 Hz, 3H); ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$, minor isomer) δ -75.6; HRMS (FAB) *m/z*: $[M + H]^+$ calcd for $C_{28}H_{25}F_6INO_3$ 664.0778; found, 664.0788.



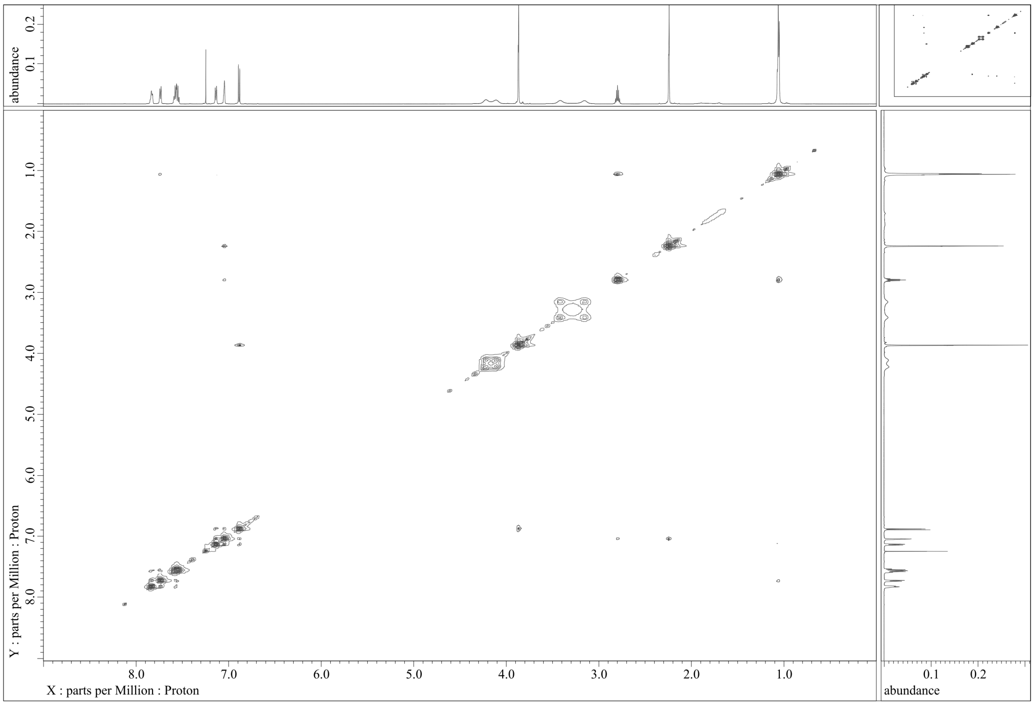
(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^{3}-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(4-methoxy-3-methylphenyl)-3-phenylprop-1-en-1-yl)oxazolidin-2-one (3ba): Synthesized by the general procedure A (53.9 mg, 78% yield); white solid; R_f 0.31 (hexane/EtOAc = 1/1); m.p. 82.9-

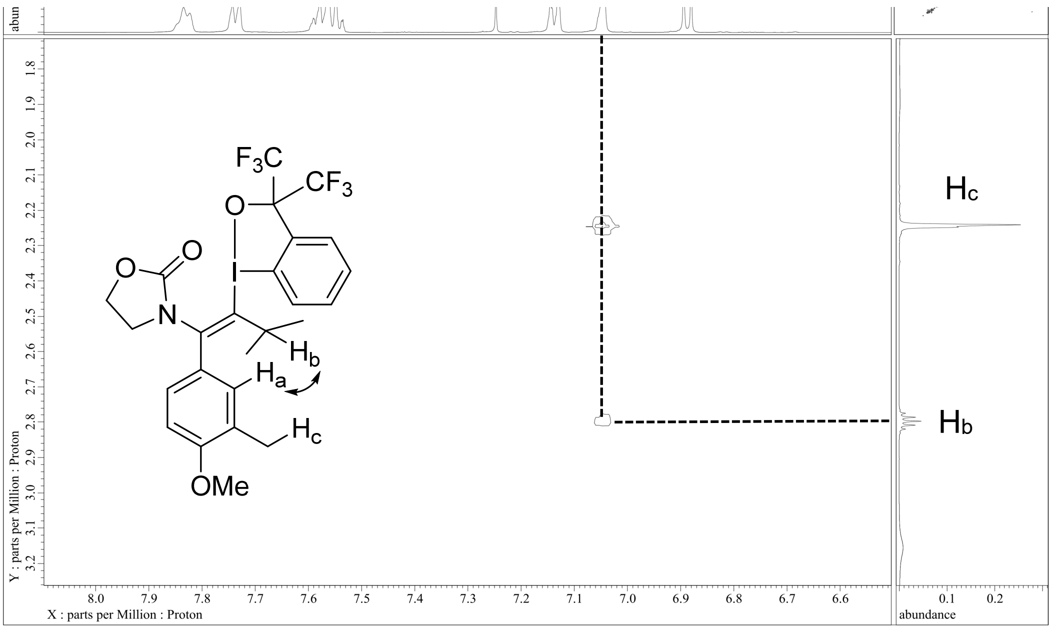
85.9 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86-7.82 (m, 1H), 7.72-7.69 (m, 1H), 7.62-7.58 (m, 2H), 7.24-7.16 (m, 4H), 7.13 (d, J = 1.8 Hz, 1H), 7.05 (d, J = 7.2 Hz, 2H), 6.92 (d, J = 8.4 Hz, 1H), 4.32 (t, J = 7.8 Hz, 2H), 4.04-3.96 (m, 2H), 3.88 (s, 3H), 3.45 (t, J = 7.8 Hz, 2H), 2.28 (s, 3H); $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) δ 159.2, 157.2, 145.1, 137.4, 133.4, 131.6, 130.8, 130.5, 130.1, 128.9, 128.6, 128.23, 128.21, 128.1, 127.2, 125.9, 124.1 (q, $J_{C\text{-}F}$ = 292.3 Hz), 123.3, 111.3, 110.4, 81.8-81.4 (m), 62.5, 55.5, 45.1, 41.0, 16.4; $^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) δ -75.7; HRMS (FAB) m/z: $[M + H]^+$ calcd for $C_{29}H_{25}F_6INO_4$ 692.0727; found, 692.0722.

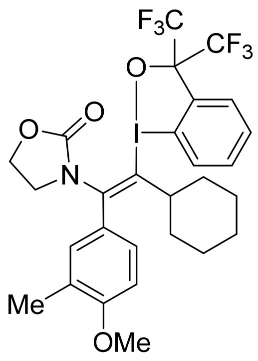


(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ³-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(4-methoxy-3-methylphenyl)-3-methylbut-1-en-1-yl)oxazolidin-2-one (3ca): Synthesized by the general procedure A (51.5 mg, 80% yield); white solid; R_f 0.23 (hexane/EtOAc = 1/1); m.p. 150.3-152.5 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90-7.85 (m, 1H), 7.77 (d, J = 7.2 Hz, 1H), 7.63-7.56 (m, 2H), 7.18-7.15 (m, 1H), 7.09-7.06 (m, 1H), 6.92 (d, J = 8.4 Hz, 1H), 4.30-4.20 (m, 1H), 4.19-4.07 (m, 1H), 3.90 (s, 3H), 3.52-3.36 (m, 1H), 3.26-3.12 (m, 1H), 2.83 (sept, J = 6.6 Hz, 1H), 2.27 (s, 3H), 1.11-1.06 (m, 6H); $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) δ 159.1, 156.8, 143.8, 138.5, 132.9, 131.4, 130.35, 130.30, 128.1, 128.0, 127.4, 124.3 (q, $J_{C\text{-}F}$ = 292.6 Hz), 124.0, 111.6, 110.2, 81.9-81.2 (m), 62.3, 55.4, 45.0, 33.9, 24.5, 21.6, 16.4, one carbon could not be found due to overlapping; $^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) δ -75.7; HRMS (FAB) m/z: $[M + H]^+$ calcd for $C_{25}H_{25}F_6INO_4$ 644.0727; found, 644.0734. The stereochemistry was determined to be *Z* based on NOESY analysis (see below). The stereochemistry of the rest of the iodo(III)arylation products was assigned by analogy.

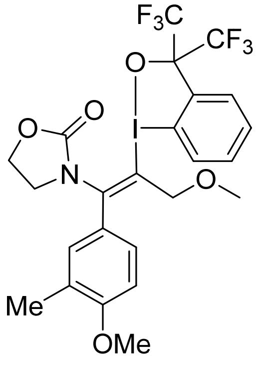
NOESY spectra of **3ca**



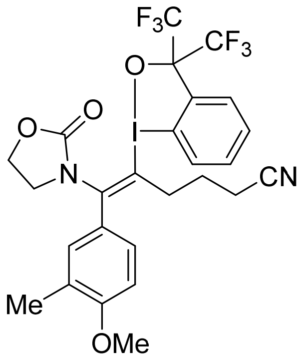




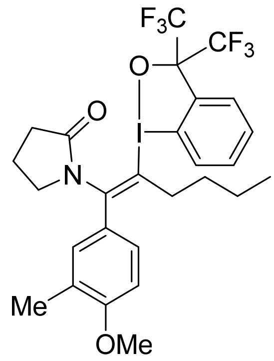
(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ³-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-2-cyclohexyl-1-(4-methoxy-3-methylphenyl)vinyl)oxazolidin-2-one (3da): Synthesized by the general procedure A (48.5 mg, 71% yield); white solid; R_f 0.23 (hexane/EtOAc = 1/1); m.p. 112.3-115.1 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.8 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.57-7.53 (m, 1H), 7.15 (d, *J* = 8.4 Hz, 1H), 7.07 (s, 1H), 6.91 (d, *J* = 8.4 Hz, 1H), 4.30-4.16 (m, 1H), 4.16-4.05 (m, 1H), 3.91-3.89 (m, 3H), 3.48-3.35 (m, 1H), 3.19-3.08 (m, 1H), 2.45 (tt, *J* = 12.0 Hz, 3.0 Hz, 1H), 2.27 (s, 3H), 1.85-1.73 (m, 2H), 1.73-1.65 (m, 3H), 1.47-1.34 (m, 2H), 1.28-1.06 (m, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 159.1, 156.7, 144.0, 137.5, 132.9, 131.3, 130.4, 130.32, 130.26, 128.1, 128.0, 127.4, 124.3 (q, $J_{C\text{-}F}$ = 292.0 Hz), 124.2, 111.8, 110.2, 81.8-81.4 (m), 62.2, 55.4, 45.0, 43.9, 34.4, 31.7, 25.5, 25.2, 16.3, one carbon could not be found due to overlapping; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$) δ -75.5, -75.8; HRMS (FAB) *m*/*z*: $[M + H]^+$ calcd for $C_{28}H_{29}F_6INO_4$ 684.1040; found, 684.1057.



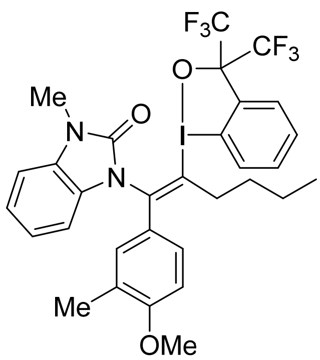
(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ³-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-3-methoxy-1-(4-methoxy-3-methylphenyl)prop-1-en-1-yl)oxazolidin-2-one (3ea): Synthesized by the general procedure A (36.8 mg, 57% yield); white solid; R_f 0.37 (hexane/EtOAc = 1/2); m.p. 196.3-199.5 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84 (d, J = 7.2 Hz, 1H), 7.70 (dd, J = 8.4 Hz, 1.2 Hz, 1H), 7.60-7.57 (m, 1H), 7.56-7.52 (m, 1H), 7.20 (dd, J = 8.4 Hz, 2.4 Hz, 1H), 7.10 (d, J = 1.2 Hz, 1H), 6.91 (d, J = 8.4 Hz, 1H), 4.33 (t, J = 7.8 Hz, 2H), 4.23 (s, 2H), 3.90 (s, 3H), 3.45 (t, J = 8.0 Hz, 2H), 3.25 (s, 3H), 2.27 (s, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 159.7, 156.5, 147.7, 132.8, 131.4, 130.7, 130.2, 130.1, 128.8, 128.11, 128.06, 124.2 (q, $J_{C\text{-}F}$ = 292.5 Hz), 123.1, 122.8, 111.7, 110.2, 81.8-81.4 (m), 72.7, 62.5, 58.3, 55.5, 45.4, 16.3; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$) δ -75.7; HRMS (FAB) m/z: $[M + H]^+$ calcd for $C_{24}H_{23}F_6INO_5$ 646.0520; found, 646.0530.



(*Z*)-5-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-6-(4-methoxy-3-methylphenyl)-6-(2-oxooxazolidin-3-yl)hex-5-enenitrile (3fa): Synthesized by the general procedure A (35.4 mg, 53% yield); white solid; R_f 0.4 (hexane/EtOAc = 1/2); m.p. 95.1-97.0 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91-7.85 (m, 1H), 7.66-7.59 (m, 3H), 7.13 (dd, J = 8.4 Hz, 1.8 Hz, 1H), 7.04-7.02 (m, 1H), 6.94 (d, J = 8.4 Hz, 1H), 4.43-4.38 (m, 2H), 3.90 (s, 3H), 3.49 (t, J = 8.1 Hz, 2H), 2.88-2.69 (m, 2H), 2.31-2.25 (m, 5H), 1.84-1.77 (m, 2H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 159.4, 157.7, 146.0, 133.6, 131.8, 130.7, 130.6, 130.3, 128.6, 128.4, 127.9, 124.1 (q, $J_{C\text{-}F}$ = 291.3 Hz), 122.7, 122.5, 118.5, 111.0, 110.6, 81.8-81.4 (m), 62.7, 55.5, 44.9, 33.5, 26.0, 16.4, 15.6; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$) δ -75.6; HRMS (FAB) m/z: $[M + H]^+$ calcd for $C_{26}H_{24}F_6IN_2O_4$ 669.0679; found, 669.0679.

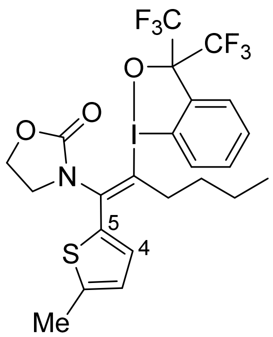


(*Z*)-1-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(4-methoxy-3-methylphenyl)hex-1-en-1-yl)pyrrolidin-2-one (3ga): Synthesized by the general procedure A (41.9 mg, 64% yield); white solid; R_f 0.22 (hexane/EtOAc = 1/1); m.p. 87.0-87.9 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, J = 7.2 Hz, 1H), 7.67-7.65 (m, 1H), 7.61-7.56 (m, 2H), 7.08 (dd, J = 8.4 Hz, 2.4 Hz, 1H), 6.99 (dd, J = 1.8 Hz, 1H), 6.88 (d, J = 8.4 Hz, 1H), 3.89 (s, 3H), 3.26 (t, J = 7.2 Hz, 2H), 2.70-2.50 (m, 4H), 2.26 (s, 3H), 2.03-1.96 (m, 2H), 1.48-1.41 (m, 2H), 1.23-1.14 (m, 2H), 0.71 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 175.6, 158.7, 144.4, 133.8, 131.4, 130.7, 130.4, 129.9, 129.1, 127.8, 127.7, 125.2, 124.5, 124.3 (q, J_{C-F} = 291.3 Hz), 111.4, 110.0, 81.9-81.5 (m), 55.4, 48.2, 34.8, 32.6, 31.2, 21.5, 18.1, 16.3, 13.5; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$) δ -75.7; HRMS (FAB) *m*/*z*: [M + H]$^+$ calcd for $C_{27}H_{29}F_6INO_3$ 656.1091; found, 656.1097.



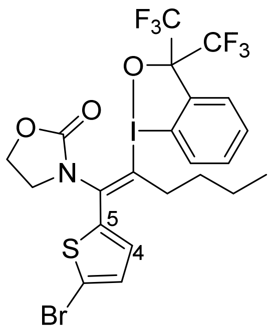
(*Z*)-1-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(4-methoxy-3-methylphenyl)hex-1-en-1-yl)-3-methyl-1,3-dihydro-2*H*-benzo[*d*]imidazol-2-one (3ha): Synthesized by the general procedure A (53.9 mg, 75% yield); white solid; R_f 0.42

(hexane/EtOAc = 1/1); m.p. 189.2-190.6 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.8 Hz, 1H), 7.74 (d, *J* = 7.2 Hz, 1H), 7.61-7.54 (m, 2H), 7.14 (d, *J* = 9.0 Hz, 1H), 7.08-7.04 (m, 2H), 6.98 (d, *J* = 7.8 Hz, 1H), 6.87 (t, *J* = 7.5 Hz, 1H), 6.81 (d, *J* = 7.8 Hz, 1H), 6.51 (d, *J* = 7.8 Hz, 1H), 3.84 (s, 3H), 3.48 (s, 3H), 3.16-3.02 (m, 1H), 2.65-2.52 (m, 1H), 2.20 (s, 3H), 1.58-1.51 (m, 2H), 1.40-1.31 (m, 1H), 1.22-1.14 (m, 1H), 0.75 (t, *J* = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 158.8, 153.8, 141.2, 133.8, 131.4, 131.1, 130.3, 129.92, 129.87, 128.9, 128.3 (2C), 127.5, 124.8, 124.4 (q, J_{C-F} = 292.8 Hz), 124.1 (q, J_{C-F} = 291.3 Hz), 122.7, 121.8, 111.4, 110.2, 109.9, 108.1, 82.1-81.3 (m), 55.4, 34.9, 32.7, 27.7, 21.5, 16.3, 13.5, one carbon could not be found due to overlapping; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$) δ -75.1, -76.3; HRMS (FAB) *m*/*z*: $[M + H]^+$ calcd for $C_{31}H_{30}F_6IN_2O_3$ 719.1200; found, 719.1198.



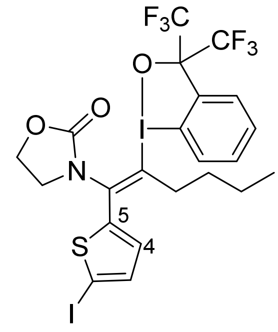
(C5:C4 = 16:1)

(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(5-methylthiophen-2-yl)hex-1-en-1-yl)oxazolidin-2-one (3al): Synthesized by the general procedure B (51.9 mg, 82% yield, regioisomer ratio = 16:1 as determined by ^{1}H NMR); white solid; R_f 0.24 (hexane/EtOAc = 1/1); m.p. 121.2-121.8 °C; ^{1}H NMR (600 MHz, $CDCl_3$, major isomer) δ 7.86 (d, *J* = 7.2 Hz, 1H), 7.61 (td, *J* = 7.8 Hz, 1.8 Hz, 1H), 7.58-7.52 (m, 2H), 6.99 (d, *J* = 3.6 Hz, 1H), 6.80-6.78 (m, 1H), 4.39 (t, *J* = 7.8 Hz, 2H), 3.61 (t, *J* = 7.5 Hz, 2H), 2.90-2.73 (m, 2H), 2.55 (s, 3H), 1.60-1.53 (m, 2H), 1.36-1.29 (m, 2H), 0.83 (t, *J* = 7.5 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$, major isomer) δ 156.8, 144.0, 137.6, 132.9, 131.8, 130.7, 130.5, 130.4, 130.3, 130.1, 128.5, 126.0, 124.2 (q, J_{C-F} = 295.4 Hz), 110.8, 81.6-81.2 (m), 62.5, 45.4, 35.8, 32.3, 21.9, 15.4, 13.6; $^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$, major isomer) δ -75.7; HRMS (FAB) *m*/*z*: $[M + H]^+$ calcd for $C_{23}H_{23}F_6INO_3S$ 634.0342; found, 634.0344.



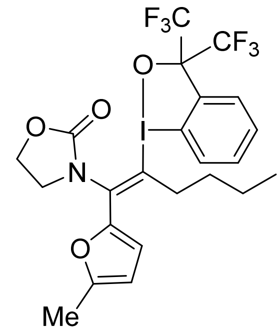
(C5:C4 = 17:1)

(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(5-bromothiophen-2-yl)hex-1-en-1-yl)oxazolidin-2-one (3am): Synthesized by the general procedure B (23.0 mg, 33% yield, regioisomer ratio = 17:1 as determined by ^1H NMR); white solid; R_f 0.25 (hexane/EtOAc = 1/1); m.p. 134.4-136.2 °C; ^1H NMR (600 MHz, $CDCl_3$, major isomer) δ 7.87 (d, *J* = 7.8 Hz, 1H), 7.64-7.60 (m, 1H), 7.58-7.54 (m, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.11 (d, *J* = 1.8 Hz, 1H), 6.96 (d, *J* = 1.8 Hz, 1H), 4.40 (t, *J* = 7.8 Hz, 2H), 3.61 (t, *J* = 7.5 Hz, 2H), 2.81-2.73 (m, 2H), 1.60-1.53 (m, 2H), 1.36-1.30 (m, 2H), 0.84 (t, *J* = 7.5 Hz, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$, major isomer) δ 156.7, 136.2, 134.5, 133.7, 133.0, 132.0, 130.7 (2C), 130.5, 130.2, 128.6, 124.2 (q, J_{C-F} = 285.5 Hz), 116.1, 110.8, 81.7-81.3 (m), 62.6, 45.4, 35.9, 32.4, 22.0, 13.7; $^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$, major isomer) δ -75.7; HRMS (FAB) *m*/*z*: $[M + H]^+$ calcd for $C_{22}H_{20}BrF_6INO_3S$ 697.9291; found, 697.9306.

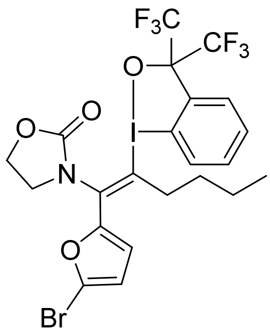


(C5:C4 = 16:1)

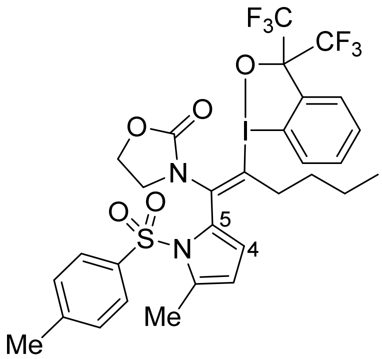
(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(5-iodothiophen-2-yl)hex-1-en-1-yl)oxazolidin-2-one (3an): Synthesized by the general procedure B (44.7 mg, 60% yield, regioisomer ratio = 16:1 as determined by ^{1}H NMR); white solid; R_f 0.25 (hexane/EtOAc = 1/1); m.p. 170.6-175.6 °C; ^{1}H NMR (600 MHz, $CDCl_3$, major isomer) δ 7.86 (d, *J* = 7.2 Hz, 1H), 7.64-7.60 (m, 1H), 7.58-7.54 (m, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 3.6 Hz, 1H), 6.86 (d, *J* = 3.0 Hz, 1H), 4.40 (t, *J* = 7.8 Hz, 2H), 3.60 (t, *J* = 7.2 Hz, 2H), 2.85-2.70 (m, 2H), 1.60-1.53 (m, 2H), 1.35-1.29 (m, 2H), 0.84 (t, *J* = 7.2 Hz, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$, major isomer) δ 156.7, 138.9, 137.6, 135.9, 133.5, 132.9, 131.9, 131.1, 130.6, 130.5, 128.5, 124.1 (q, J_{C-F} = 292.3 Hz), 110.7, 81.6-81.2 (m), 77.5, 62.5, 45.3, 35.8, 32.3, 21.9, 13.6; ^{19}F NMR (565 MHz, $CDCl_3$, major isomer) δ -75.7; HRMS (FAB) *m*/*z*: $[M + H]^+$ calcd for $C_{22}H_{20}F_6I_2NO_3S$ 745.9152; found, 745.9156.



(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(5-methylfuran-2-yl)hex-1-en-1-yl)oxazolidin-2-one (3ao): Synthesized by the general procedure B (22.2 mg, 36% yield); white solid; R_f 0.29 (hexane/EtOAc = 1/2); m.p. 93.8-95.1 °C; ^{1}H NMR (600 MHz, CDCl3) δ 7.85 (d, *J* = 7.2 Hz, 1H), 7.62-7.58 (m, 1H), 7.57-7.51 (m, 2H), 6.48 (d, *J* = 3.6 Hz, 1H), 6.16 (d, *J* = 3.0 Hz, 1H), 4.43 (t, *J* = 7.8 Hz, 2H), 3.73-3.67 (m, 2H), 3.13-2.93 (m, 2H), 2.40 (s, 3H), 1.67-1.60 (m, 2H), 1.44-1.36 (m, 2H), 0.90 (t, *J* = 7.2 Hz, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, CDCl3) δ 157.0, 155.1, 143.7, 134.2, 132.3, 132.0, 130.50, 130.47, 128.5, 124.1 (q, J_{C-F} = 292.8Hz), 115.2, 110.4, 108.4, 81.3-81.1 (m), 62.5, 46.5, 35.8, 31.8, 22.2, 13.9, 13.7, one carbon could not be found due to overlapping; $^{19}F\{^1H\}$ NMR (565 MHz, CDCl3) δ -75.7; HRMS (FAB) *m*/*z*: $[M + H]^+$ calcd for $C_{23}H_{23}F_6INO_4$ 618.0570; found, 618.0573.

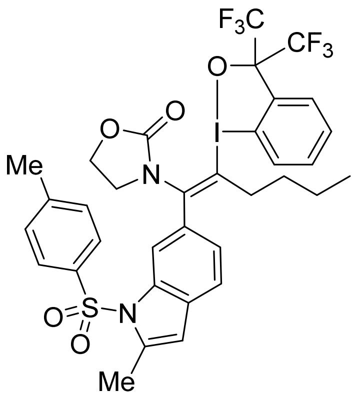


(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ³-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(5-bromofuran-2-yl)hex-1-en-1-yl)oxazolidin-2-one (3ap): Synthesized by the general procedure B (15.0 mg, 22% yield); white solid; R_f 0.36 (hexane/EtOAc = 1/2); m.p. 137.3-139.0 °C; ^1H NMR (600 MHz, CDCl3) δ 7.85 (d, *J* = 7.2 Hz, 1H), 7.65-7.60 (m, 1H), 8.58-8.54 (m, 1H), 7.52 (d, *J* = 7.8 Hz, 1H), 6.57-6.54 (m, 1H), 6.50 (d, *J* = 3.6 Hz, 1H), 4.46-4.41 (m, 2H), 3.71 (t, *J* = 7.8 Hz, 2H), 3.10-2.90 (m, 2H), 1.67-1.59 (m, 2H), 1.45-1.37 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, CDCl3) δ 156.8, 147.0, 133.6, 132.7, 132.2, 132.1, 130.6, 130.5, 128.5, 124.9, 124.1 (q, J_{C-F} = 292.0 Hz), 115.9, 113.9, 110.3, 81.4-81.0 (m), 62.6, 46.3, 35.8, 31.8, 22.2, 13.6; $^{19}F\{^1H\}$ NMR (565 MHz, CDCl3) δ -76.0; HRMS (FAB) *m*/*z*: $[M + H]^+$ calcd for $C_{22}H_{20}BrF_6INO_4$ 681.9519; found, 681.9529.



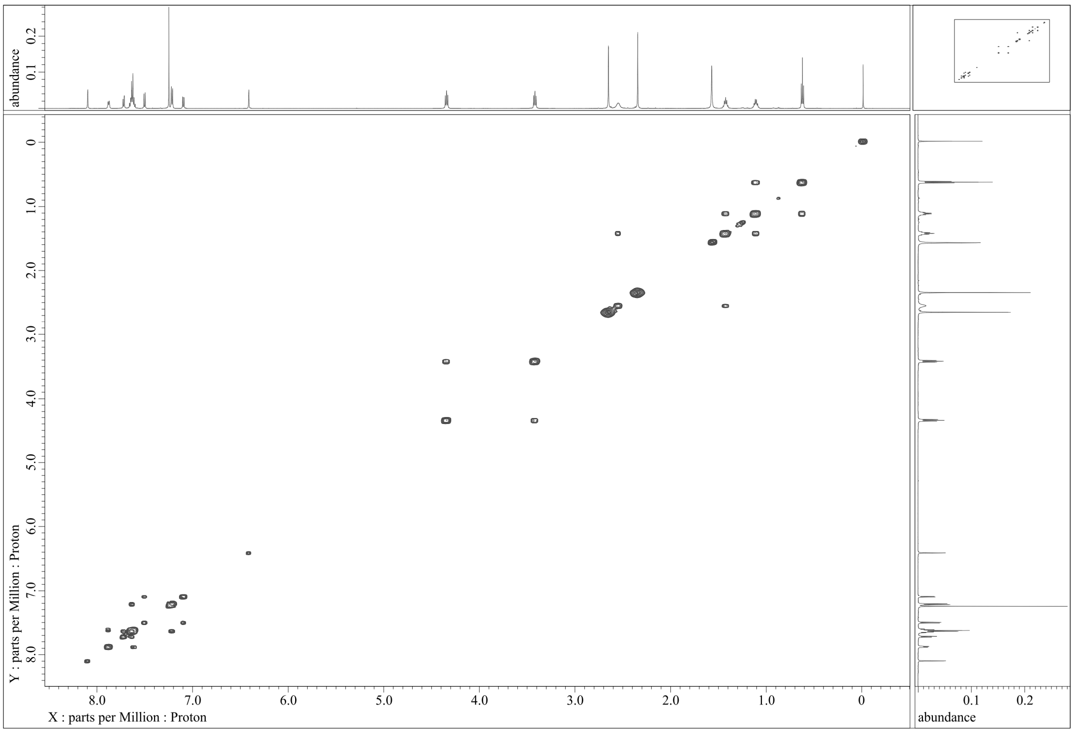
(C5:C4 = 14:1)

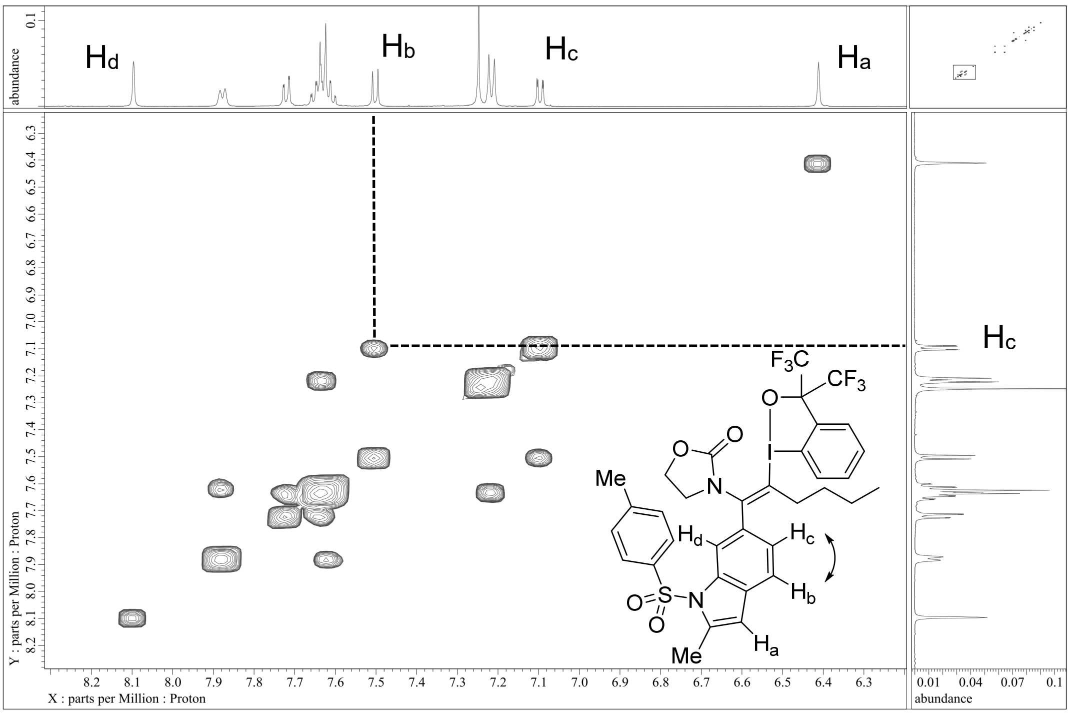
(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(2-methyl-1-tosyl-1*H*-pyrrol-3-yl)hex-1-en-1-yl)oxazolidin-2-one (3aq): Synthesized by the general procedure B (42.2 mg, 55% yield, regioisomer ratio = 14:1 as determined by ^{1}H NMR); yellow solid; R_f 0.22 (hexane/EtOAc = 1/1); m.p. 91.9-95.7 °C; ^{1}H NMR (600 MHz, $CDCl_3$, major isomer) δ 7.83 (d, *J* = 7.8 Hz, 1H), 7.68-7.63 (m, 1H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.56-7.52 (m, 1H), 7.46-7.42 (m, 1H), 7.33 (d, *J* = 8.4 Hz, 2H), 6.33 (d, *J* = 3.6 Hz, 1H), 6.13-6.11 (m, 1H), 4.38-4.25 (m, 2H), 3.69 (dd, *J* = 15.0 Hz, 8.4 Hz, 1H), 3.57-3.50 (m, 1H), 2.44-2.41 (m, 6H), 2.35-2.25 (m, 1H), 2.19-2.11 (m, 1H), 1.38-1.21 (m, 2H), 1.11-0.99 (m, 2H), 0.70 (t, *J* = 7.5 Hz, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$, 45 °C, major isomer) δ 157.5, 145.7, 136.7, 136.0, 135.5, 134.0, 131.3, 130.4, 130.2, 130.0, 129.7, 127.1, 126.6, 126.0, 124.3 (q, J_{C-F} = 291.4 Hz), 118.9, 113.1, 112.0, 82.1-81.7 (m), 62.5, 45.4, 35.8, 33.0, 22.2, 21.6, 15.3, 13.5; $^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$, major isomer) δ -75.7; HRMS (FAB) *m*/*z*: $[M + H]^+$ calcd for $C_{30}H_{30}F_6IN_2O_5S$ 771.0819; found, 771.0812.



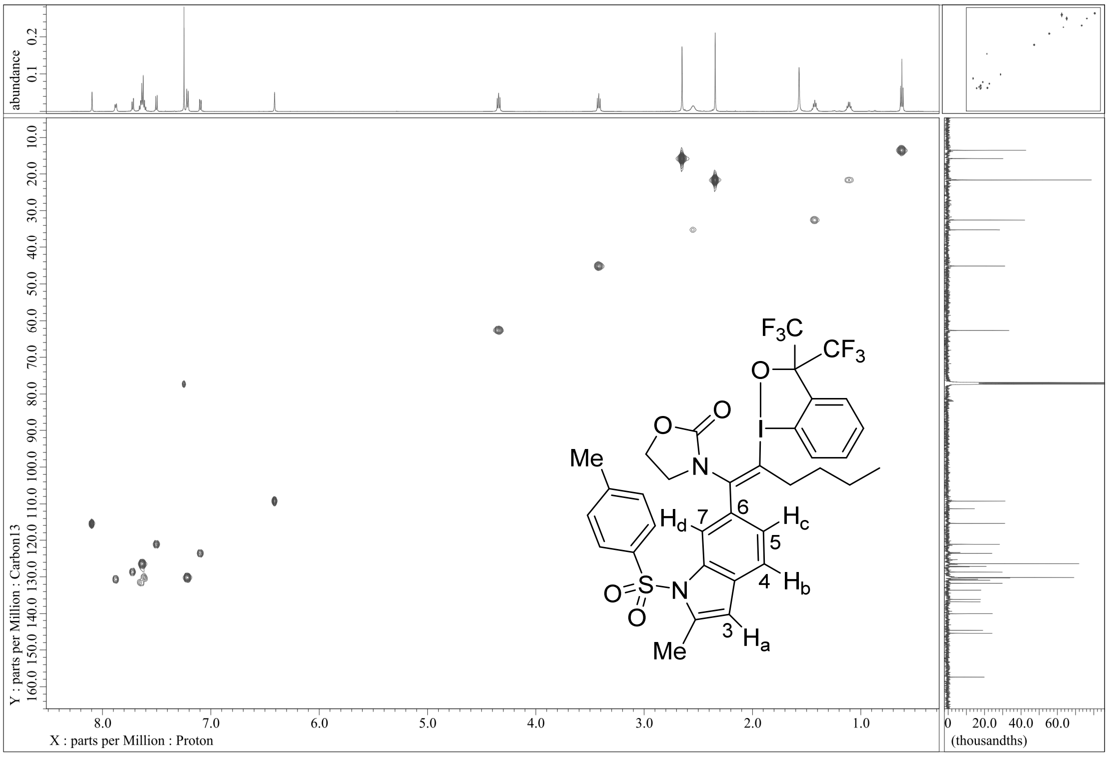
(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(2-methyl-1-tosyl-1*H*-indol-6-yl)hex-1-en-1-yl)oxazolidin-2-one (3ar): Synthesized by the general procedure B (46.0 mg, 56% yield); white solid; R_f 0.46 (hexane/EtOAc = 1/2); m.p. 117.4-121.2 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.89 (d, *J* = 7.2 Hz, 1H), 7.74 (dd, *J* = 8.4 Hz, 1.2 Hz, 1H), 7.68-7.61 (m, 4H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.23 (d, *J* = 8.4 Hz, 2H), 7.11 (dd, *J* = 8.4 Hz, 1.5 Hz, 1H), 6.43 (s, 1H), 4.36 (m, 2H), 3.43 (m, 2H), 2.67 (s, 3H), 2.61-2.51 (m, 2H), 2.36 (s, 3H), 1.47-1.40 (m, 2H), 1.16-1.08 (m, 2H), 0.64 (t, *J* = 7.5 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 157.3, 145.4, 144.6, 139.9, 136.7, 136.0, 133.5, 131.6, 130.8, 130.6, 130.2, 130.1, 128.6, 127.2, 127.0, 126.3, 124.2 (q, $J_{C\text{-}F}$ = 292.8 Hz), 123.5, 121.0, 115.4, 111.2, 109.2, 81.9-81.5 (m), 62.5, 45.1, 35.1, 32.5, 21.6, 15.7, 13.5, one carbon could not be found due to overlapping; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$) δ -75.7; HRMS (FAB) *m*/*z*: [M + H]$^+$ calcd for $C_{34}H_{32}F_6IN_2O_5S$ 821.0975; found, 821.0981. The regioselectivity was determined by ^{1}H–^{1}H COSY, ^{1}H–^{13}C HMQC, and ^{1}H–^{13}C HMBC analyses (see below).

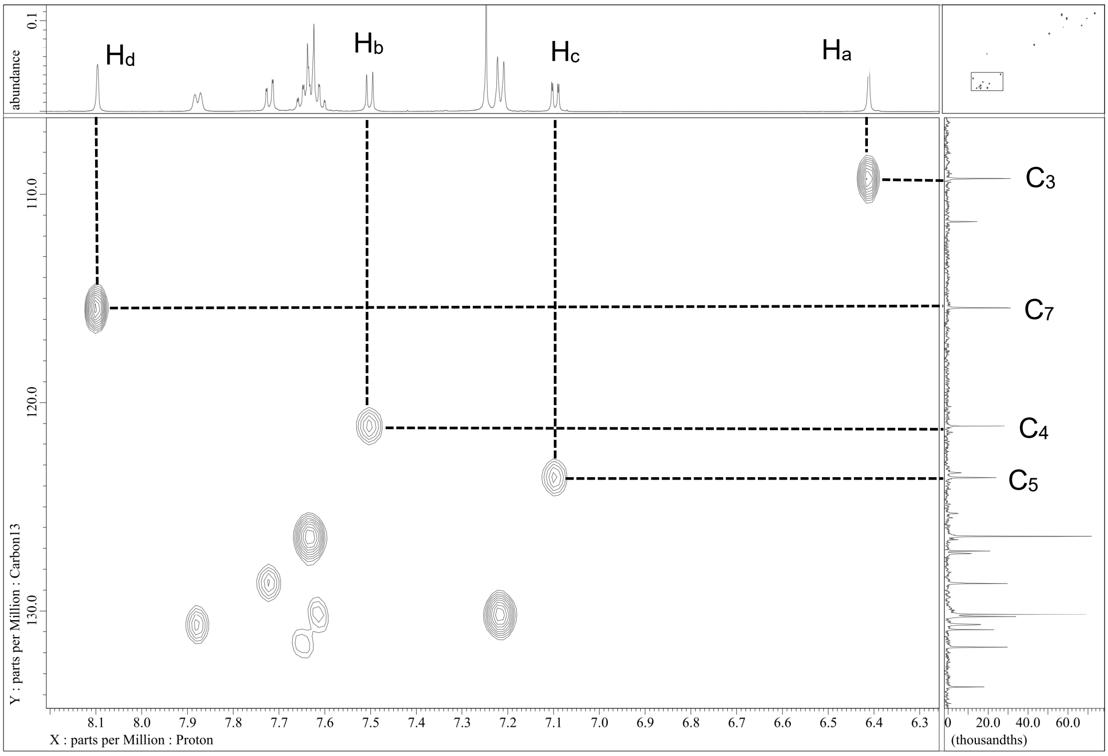
COSY spectra of **3ar**



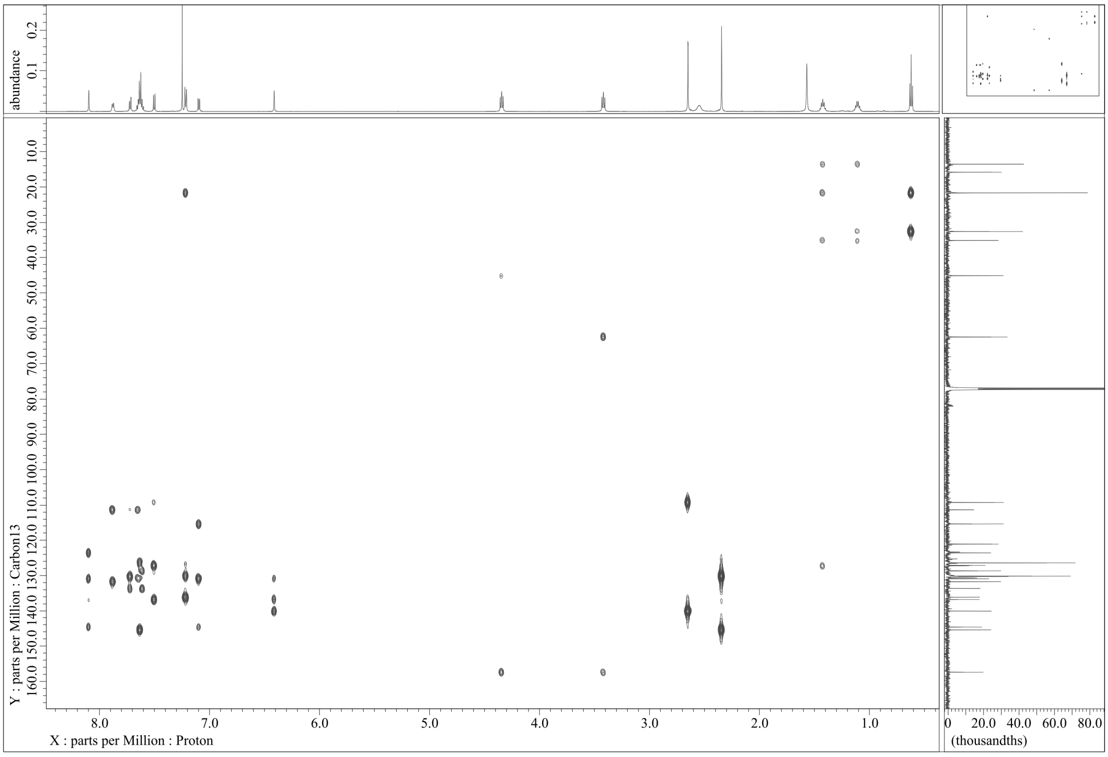


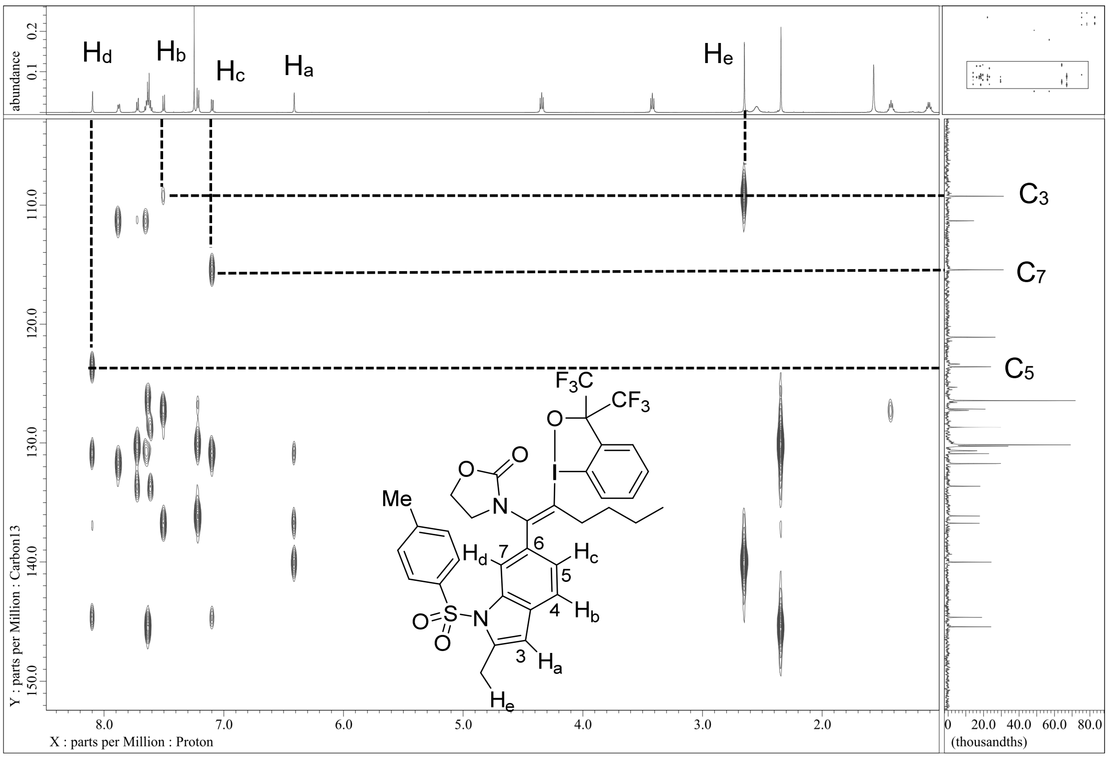
HMQC spectra of **3ar**

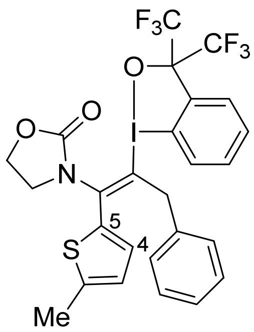




HMBC spectra of **3ar**

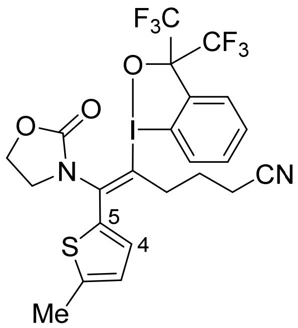






(C5:C4 = 14:1)

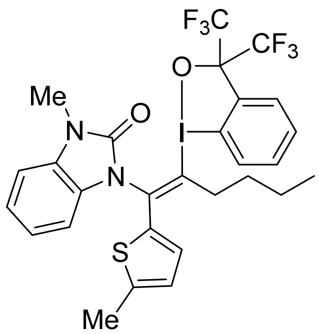
(*Z*)-3-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(5-methylthiophen-2-yl)-3-phenylprop-1-en-1-yl)oxazolidin-2-one (3bl): Synthesized by the general procedure B (47.4 mg, 71% yield, regioisomer ratio = 14:1 as determined by ^{1}H NMR); white solid; R_f 0.26 (hexane/EtOAc = 1/1); m.p. 148.7-149.4 °C; ^{1}H NMR (600 MHz, $CDCl_3$, major isomer) δ 7.83 (d, J = 7.2 Hz, 1H), 7.62-7.53 (m, 3H), 7.28-7.25 (m, 2H), 7.24-7.20 (m, 1H), 7.12 (d, J = 7.8 Hz, 2H), 7.09 (d, J = 3.6 Hz, 1H), 6.81-6.78 (m, 1H), 4.38 (t, J = 7.8 Hz, 2H), 4.27-4.18 (m, 2H), 3.63 (t, J = 7.8 Hz, 2H), 2.54 (s, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$, major isomer) δ 156.7, 144.4, 138.5, 136.9, 132.9, 131.8, 130.6, 130.5, 130.3, 130.2, 129.5, 129.1, 128.7, 128.3, 127.5, 126.1, 124.1 (q, $J_{C\text{-}F}$ = 292.6 Hz), 111.2, 81.7-81.2 (m), 62.5, 45.4, 41.6, 15.4; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$, major isomer) δ -75.7; HRMS (FAB) *m*/*z*: [M + H]$^+$ calcd for $C_{26}H_{21}F_6INO_3S$ 668.0186; found, 668.0181.



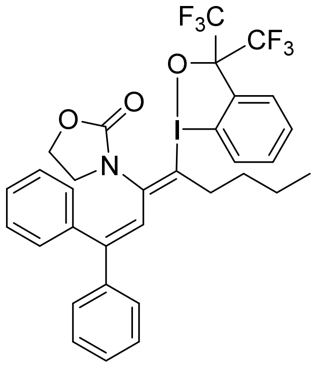
(C5:C4 = 21:1)

(*Z*)-5-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-6-(5-methylthiophen-2-yl)-6-(2-oxooxazolidin-3-yl)hex-5-enenitrile (3fl): Synthesized by the general procedure B (29.6 mg, 46% yield, regioisomer ratio = 21:1 as determined by ^{1}H NMR);

white solid; R_f 0.40 (hexane/EtOAc = 1/1); m.p. 95.7-96.2 °C; ^{1}H NMR (600 MHz, $CDCl_3$, major isomer) δ 7.88 (d, J = 7.8 Hz, 1H), 7.65-7.62 (m, 1H), 7.61-7.57 (m, 1H), 7.49 (d, J = 7.8 Hz, 1H), 7.04 (d, J = 3.0 Hz, 1H), 6.84-6.82 (m, 1H), 4.43 (t, J = 7.8 Hz, 2H), 3.69-3.62 (m, 2H), 3.16-2.82 (m, 2H), 2.56 (s, 3H), 2.37 (t, J = 6.9 Hz, 2H), 1.93-1.86 (m, 2H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$, major isomer) δ 157.1, 144.9, 139.1, 133.3, 132.0, 130.7, 130.5, 129.4, 128.3, 126.3, 126.2, 124.1 (q, $J_{C\text{-}F}$ = 291.7 Hz), 118.5, 110.9, 81.7-81.3 (m), 62.7, 45.0, 34.2, 25.8, 15.9, 15.5; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$, major isomer) δ -75.7; HRMS (FAB) m/z[M + H]$^+$ calcd for $C_{23}H_{20}F_6IN_2O_3S$ 645.0138; found, 645.0153.

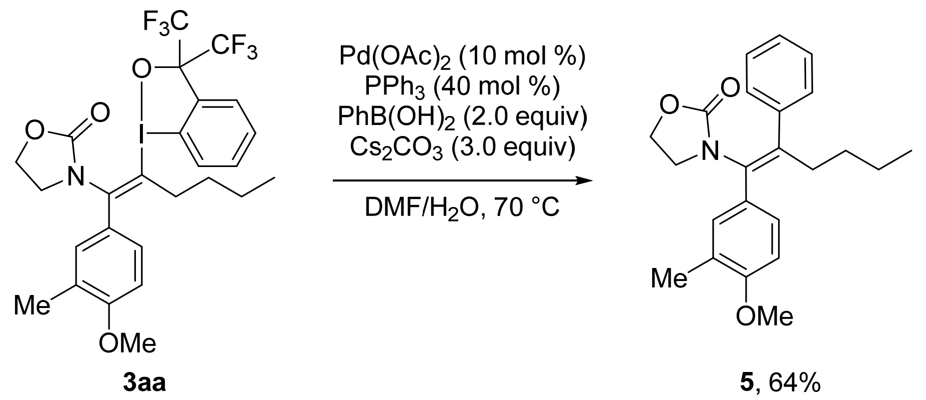


(*Z*)-1-(2-(3,3-Bis(trifluoromethyl)-1λ^3-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1-(5-methylthiophen-2-yl)hex-1-en-1-yl)-3-methyl-1,3-dihydro-2*H*-benzo[*d*]imidazol-2-one (3hl): Synthesized by the general procedure B (61.2 mg, 84% yield); white solid; R_f 0.50 (hexane/EtOAc = 1/1); m.p. 178.3-180.5 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.80-7.75 (m, 1H), 7.67-7.60 (m, 1H), 7.58-7.53 (m, 2H), 7.10 (t, J = 7.2 Hz, 1H), 7.01 (d, J = 7.5 Hz, 1H), 6.94 (t, J = 7.8 Hz, 1H), 6.88 (d, J = 4.2 Hz, 1H), 6.70-6.67 (m, 1H), 6.62 (d, J = 7.2 Hz, 1H), 3.44 (s, 3H), 3.30-3.07 (m, 1H), 3.07-2.77 (m, 1H), 2.49 (s, 3H), 1.73-1.66 (m, 2H), 1.51-1.34 (m, 2H), 0.88 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 153.2, 144.2, 134.9, 133.1, 132.0, 131.7, 130.7, 130.3, 130.2, 129.8, 129.0, 128.7, 125.8, 124.2 (q, $J_{C\text{-}F}$ = 291.7 Hz), 124.0 (q, $J_{C\text{-}F}$ = 291.0 Hz), 122.8, 121.9, 111.0, 109.3, 108.2, 81.6-81.2 (m), 35.9, 32.2, 27.6, 22.0, 15.4, 13.7, one carbon could not be found due to overlapping; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$) δ -75.5, -76.0; HRMS (FAB) m/z: [M + H]$^+$ calcd for $C_{28}H_{26}F_6IN_2O_2S$ 695.0658; found, 695.0656.



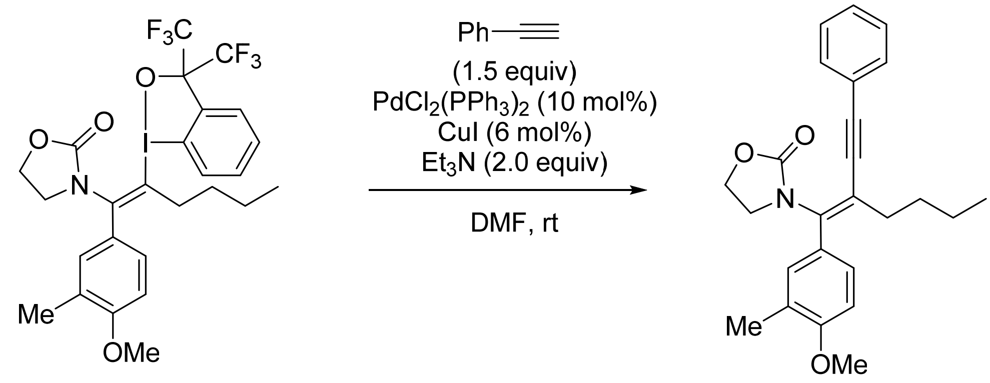
(*Z*)-3-(4-(3,3-Bis(trifluoromethyl)-1λ[3]-benzo[*d*][1,2]iodaoxol-1(3*H*)-yl)-1,1-diphenylocta-1,3-dien-3-yl)oxazolidin-2-one (3as): Synthesized by the general procedure A (25.8 mg, 36% yield); white solid; R_f 0.44 (hexane/EtOAc = 1/1); m.p. 131.1-132.2 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.4 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 1H), 7.49-7.41 (m, 4H), 7.41-7.35 (m, 3H), 7.31-7.27 (m, 2H), 7.23-7.20 (m, 2H), 7.08 (d, *J* = 8.4 Hz, 1H), 6.55 (s, 1H), 3.90-3.55 (m, 2H), 3.50 (t, *J* = 8.4 Hz, 2H), 3.00-2.30 (m, 2H), 1.65-1.59 (m, 2H), 1.44-1.36 (m, 2H), 0.89 (t, *J* = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 156.8, 150.0, 141.5, 140.2, 138.3, 133.9, 131.5, 130.4, 130.0, 129.5, 129.20, 129.16, 129.0, 128.7, 128.5, 124.2 (q, $J_{C\text{-}F}$ = 291.3 Hz), 116.8, 111.8, 81.8-81.4 (m), 61.8, 44.8, 35.8, 32.6, 22.0, 13.7, two carbons could not be found due to overlapping; ^{19}F{^{1}H} NMR (565 MHz, $CDCl_3$) δ -75.7; HRMS (FAB) *m*/*z*: [M + H]$^+$ calcd for $C_{32}H_{29}F_6INO_3$ 716.1091; found, 716.1086.

4. Product Transformations



(*Z*)-3-(1-(4-Methoxy-3-methylphenyl)-2-phenylhex-1-en-1-yl)oxazolidin-2-one (5): Under an argon atmosphere, a 4 mL vial equipped with a stir bar was charged with **3aa** (65.7 mg, 0.10 mmol), $Pd(OAc)_2$ (2.2 mg, 0.010 mmol, 10 mol%), PPh_3 (10.5 mg, 0.040 mmol, 40 mol%), and Cs_2CO_3 (97.7 mg, 0.30 mmol, 3.0 equiv), followed by the addition of DMF (0.80 mL) and H_2O (0.20 mL). Then phenylboronic acid (24.4 mg, 0.20 mmol, 2.0 equiv) was added. The resulting mixture was then placed on an aluminum block preheated at 70 °C and stirred for 24 h. The mixture was cooled to room temperature, diluted with Et_2O (10 mL), and washed with H_2O (5 mL) and brine (5 mL). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to afford the title compound **5** as a colorless oil (23.4 mg, 64% yield).

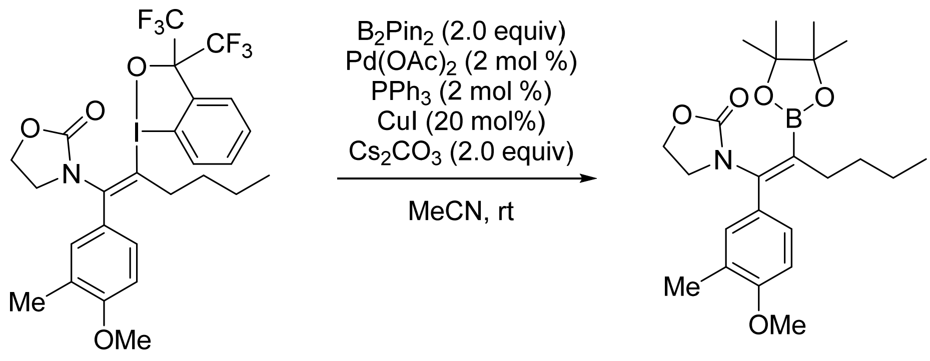
R_f 0.36 (hexane/EtOAc = 2/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37-7.33 (m, 2H), 7.32-7.29 (m, 2H), 7.29-7.25 (m, 1H), 7.22 (dd, *J* = 8.4 Hz, 2.4 Hz, 1H), 7.17 (d, *J* = 1.8 Hz, 1H), 6.83 (d, *J* = 8.4 Hz, 1H), 4.02 (t, *J* = 8.0 Hz, 2H), 3.85 (s, 3H), 3.35-3.31 (m, 2H), 2.44-2.40 (m, 2H), 2.23 (s, 3H), 1.33-1.27 (m, 2H), 1.27-1.20 (m, 2H), 0.78 (t, *J* = 7.5 Hz, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 157.5, 156.3, 142.0, 140.4, 130.9, 130.4, 128.4, 128.2, 127.5, 127.4, 127.1, 126.5, 109.5, 61.8, 55.2, 46.0, 33.9, 30.6, 22.5, 16.2, 13.7; HRMS (EI) *m/z*: $[M]^+$ calcd for $C_{23}H_{27}NO_3$ 365.1985; found, 365.1983.



3aa → **6**, 76% (*Z*/*E* = 11:1)

(*Z*)-3-(1-(4-Methoxy-3-methylphenyl)-2-(phenylethynyl)hex-1-en-1-yl)oxazolidin-2-one (6): Under an argon atmosphere, a 4 mL vial equipped with a stir bar was charged with **3aa** (65.7 mg, 0.10 mmol), $PdCl_2(PPh_3)_2$ (7.0 mg, 0.01 mol, 10 mol%), CuI (1.1 mg, 0.006 mmol, 6 mol%), and DMF (0.5 mL). To the mixture was added ethynylbenzene (15.3 mg, 0.15 mmol, 1.5 equiv) and Et_3N (20.2 mg, 0.2 mmol, 2.0 equiv), and the resulting mixture was stirred at room temperature for 24 h. The mixture was diluted with Et_2O (5 mL) and washed with H_2O (5 mL) and brine (5 mL). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to afford the title compound **6** as a yellow oil (29.6 mg, 76% yield, *Z*/*E* = 11:1).

R_f 0.46 (hexane/EtOAc = 1/1); ^{1}H NMR (600 MHz, $CDCl_3$, major isomer) δ 7.49-7.45 (m, 2H), 7.35-7.30 (m, 3H), 7.16 (dd, *J* = 8.4 Hz, 2.4 Hz, 1H), 7.12 (d, *J* = 1.2 Hz, 1H), 6.82 (d, *J* = 8.4 Hz, 1H), 4.43-4.38 (m, 2H), 3.86 (s, 3H), 3.80-3.76 (m, 2H), 2.35 (t, *J* = 7.2 Hz, 2H), 2.23 (s, 3H), 1.71-1.64 (m, 2H), 1.39-1.32 (m, 2H), 0.88 (t, *J* = 7.8 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$, major isomer) δ 158.1, 155.9, 138.9, 131.5, 130.9, 128.33, 128.27, 127.7, 126.9, 126.7, 123.4, 121.7, 109.5, 96.3, 87.9, 62.3, 55.3, 46.0, 31.9, 31.1, 22.2, 16.3, 13.9; HRMS (EI) *m*/*z*: $[M]^+$ calcd for $C_{25}H_{27}NO_3$ 389.1985; found, 389.2002.

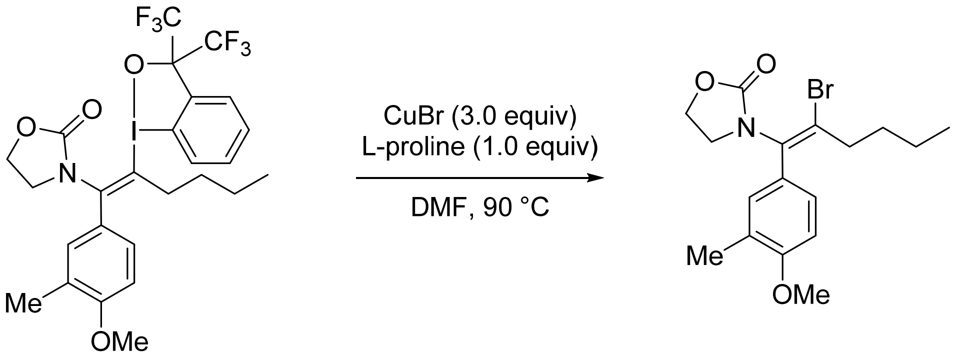


3aa

7, 26%

(*E*)-3-(1-(4-Methoxy-3-methylphenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)oxazolidin-2-one (7): Under an argon atmosphere, a 4 mL vial equipped with a stir bar was charged with **3aa** (65.7 mg, 0.10 mmol), bis(pinacolato)diboron (50.8 mg, 0.20 mmol), $Pd(OAc)_2$ (0.4 mg, 0.002 mmol), PPh_3 (0.5 mg, 0.002 mmol), CuI (3.8 mg, 0.02 mmol), Cs_2CO_3 (65.2 mg, 0.20 mmol), and MeCN (1.0 mL). The resulting mixture was stirred at room temperature for 24 h. The mixture was diluted with CH_2Cl_2 (10 mL) and washed with H_2O (5 mL) and brine (5 mL).The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to afford the title compound **7** as a colorless oil (10.8 mg, 26% yield).

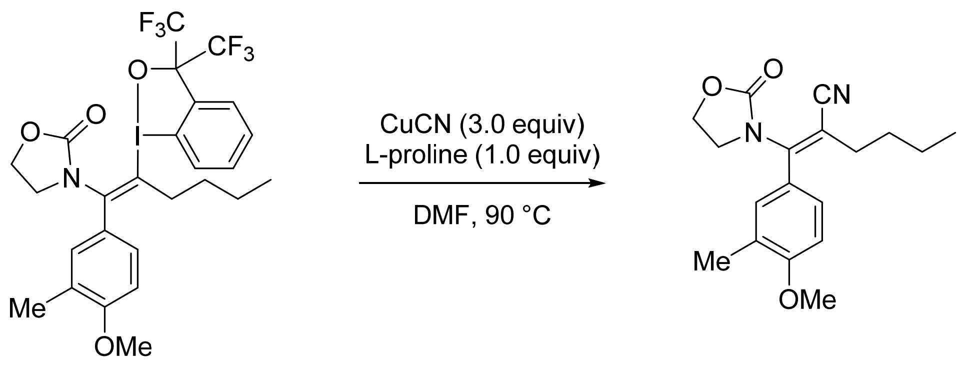
R_f 0.32 (hexane/EtOAc = 2/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.09 (dd, *J* = 8.4 Hz, 2.4 Hz, 1H), 7.06 (d, *J* = 1.2 Hz, 1H), 6.79 (d, *J* = 8.4 Hz, 1H), 4.31-4.26 (m, 2H), 3.84 (s, 3H), 3.52-3.48 (m, 2H), 2.22-2.17 (m, 5H), 1.47-1.39 (m, 2H), 1.34-1.28 (m, 14H), 0.87 (t, *J* = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 157.7, 157.5, 142.6, 131.0, 127.9, 127.5, 126.4, 109.4, 83.2, 61.7, 55.3, 46.0, 32.8, 31.3, 25.1, 22.8, 16.2, 14.0, one carbon could not be found due to overlapping; HRMS (EI) *m*/*z*: $[M]^+$ calcd for $C_{23}H_{34}BNO_5$ 415.2525; found, 415.2531.



3aa **8**, 87%

(*Z*)-3-(2-Bromo-1-(4-methoxy-3-methylphenyl)hex-1-en-1-yl)oxazolidin-2-one (8): Under an argon atmosphere, a 4 mL vial equipped with a stir bar was charged with **3aa** (65.7 mg, 0.1 mmol), CuBr (43.0 mg, 0.3 mmol), L-proline (11.5 mg, 0.1 mmol), and DMF (1.0 mL). The resulting mixture was then placed on an aluminum block preheated at 90 °C and stirred for 24 h. The mixture was cooled to room temperature, diluted with EtOAc (10 mL), and washed with H_2O (5 mL) and brine (5 mL). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to afford the title compound **8** as a colorless oil (32.1 mg, 87% yield).

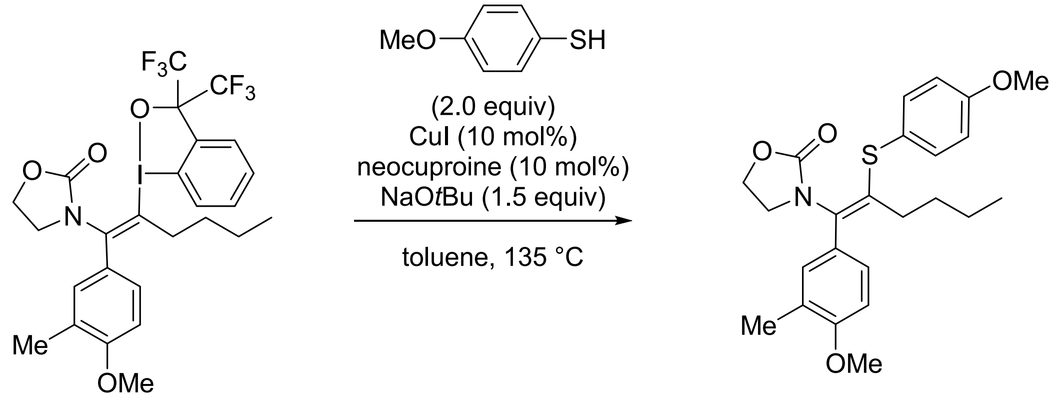
R_f 0.55 (hexane/EtOAc = 1/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.11 (dd, *J* = 8.4 Hz, 2.4 Hz, 1H), 7.08-7.06 (m, 1H), 6.80 (d, *J* = 8.4 Hz, 1H), 4.38 (t, *J* = 8.0 Hz, 2H), 3.85 (s, 3H), 3.63-3.59 (m, 2H), 2.53-2.49 (m, 2H), 2.21 (s, 3H), 1.65-1.58 (m, 2H), 1.33-1.25 (m, 2H), 0.84 (t, *J* = 7.5 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 158.0, 155.4, 133.0, 130.8, 130.2, 127.5, 127.0, 126.5, 109.7, 62.3, 55.3, 44.6, 36.6, 31.0, 21.6, 16.2, 13.8; HRMS (EI) *m/z*: $[M]^+$ calcd for $C_{17}H_{22}BrNO_3$ 367.0778; found, 367.0783.



3aa **9**, 91%

(*Z*)-2-((4-Methoxy-3-methylphenyl)(2-oxooxazolidin-3-yl)methylene)hexanenitrile (9): Under an argon atmosphere, a 4 mL vial equipped with a stir bar was charged with **3aa** (65.7 mg, 0.1 mmol), CuCN (26.9 mg, 0.3 mmol), L-proline (11.5 mg, 0.1 mmol), and DMF (1.0 mL). The resulting mixture was then placed on an aluminum block preheated at 90 °C and stirred for 16 h. The mixture was cooled to room temperature, diluted with EtOAc (10 mL), and washed with H_2O (5 mL) and brine (5 mL). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to afford the title compound **9** as a colorless oil (28.6 mg, 91% yield).

R_f 0.35 (hexane/Et_2O = 1/8); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.10 (dd, J = 8.4 Hz, 2.4 Hz, 1H), 7.04-7.02 (m, 1H), 6.86 (d, J = 8.4 Hz, 1H), 4.46-4.42 (m, 2H), 3.87 (s, 3H), 3.70-3.66 (m, 2H), 2.34-2.30 (m, 2H), 2.22 (s, 3H), 1.64-1.58 (m, 2H), 1.36-1.29 (m, 2H), 0.86 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 159.3, 155.1, 147.0, 130.6, 127.8, 127.5, 123.6, 117.8, 110.2, 109.9, 62.4, 55.4, 45.7, 30.6, 29.8, 21.8, 16.2, 13.6; HRMS (EI) *m*/*z*: $[M]^+$ calcd for $C_{18}H_{22}N_2O_3$ 314.1625; found, 314.1630.



(*Z*)-3-(1-(4-Methoxy-3-methylphenyl)-2-((4-methoxyphenyl)thio)hex-1-en-1-yl)oxazolidin-2-one (10): Under an argon atmosphere, a 4 mL vial equipped with a stir bar was charged with **3aa** (65.8 mg, 0.10 mmol), CuI (1.9 mg, 0.01 mmol), neocuproine (2.1 mg, 0.01 mmol), and NaO*t*Bu (14.4 mg, 0.15 mmol), followed by the addition of toluene (1.0 mL) and 4-methoxybenzenethiol (28.0 mg, 0.20 mmol). The resulting mixture was then placed on an aluminum block preheated at 135 °C and stirred for 18 h. The mixture was diluted with EtOAc (10 mL) and washed with water (5 mL x 3). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to afford the title compound **10** as a colorless oil (12.0 mg, 28% yield).

R_f 0.35 (hexane/EtOAc = 2/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.48-7.45 (m, 2H), 7.11 (dd, J = 8.4 Hz, 2.0 Hz, 1H), 7.09-7.07 (m, 1H), 6.88-6.85 (m, 2H), 6.79 (d, J = 8.4 Hz, 1H), 4.33-4.29 (m, 2H), 3.84 (s, 3H), 3.81 (s, 3H), 3.57-3.53 (m, 2H), 2.21 (s, 3H), 2.13-2.10 (m, 2H), 1.50-1.43 (m, 2H), 1.14-1.07 (m, 2H), 0.69 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 159.5, 157.7, 156.1, 138.5, 134.8, 131.9, 131.1, 127.74, 127.67, 126.7, 123.9, 114.5, 109.5, 62.1, 55.33, 55.30, 45.2, 31.0, 30.9, 21.9, 16.2, 13.7; HRMS (EI) *m/z*: $[M]^+$ calcd for $C_{24}H_{29}NO_4S$ 427.1817; found, 427.1814.

5. DFT Calculation

All the density functional theory (DFT) calculations were performed with the Gaussian 16 program.[6] Geometry optimizations were performed with the M06-2X functional[7] and a combined basis set B1 (i.e. the SDD effective core potential[8] for iodine, the 6-31+G(d,p) basis set for all other atoms). Harmonic frequency calculations were performed for each stationary point to ensure that it is either an energy minimum (no imaginary frequency) or a transition state (only one imaginary frequency). For each transition state, intrinsic reaction coordinate (IRC)[9] analysis was performed to ensure that it connects the correct reactant and product. The single-point energy calculations were further performed with the M06-2X functional and a combined basis set B2 (i.e., the SDD effective core potential for iodine, the 6-311+G(2df,2p) basis set for all other atoms). The CPCM model[10] with 1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) as the solvent was used for all the calculations. Because HIFP solvent is not available in the list of default/pre-defined solvents in *Gaussian 16* software, it is herein parametrised using a set of seven parameters.[11] These include the static dielectric constant of the solvent at 25 °C (*Eps* = 16.7);[12,13,14] dynamic (optical) dielectric constant – the square of the refractive index value of 1.275 at 20 °C was used[15] (*EpsInf = 1.625625*); hydrogen bond acidity (*HBondAcidity = 1.96*) and basicity (*HBondBasicity = 0.00*),[12] which are Abraham's *A* and *B* values respectively; the surface tension of the solvent at interface (*SurfaceTensionAtInterface = 23.23*);[13] carbon aromaticity–the fraction of aromatic carbons (*CarbonAromaticity = 0.00*) and electronegative halogenicity–the fraction of halogens (*Electronegative Halogenicity = 0.60*). These parameters were specified using the keyword "SCRF = (CPCM, Solvent= Generic, Read)" in *Gaussian 16*. The single-point energies corrected by the thermal correction to Gibbs free energies (TCG, obtained from frequency calculations) were used as the Gibbs free energies reported in this work, corresponding to the reference state of 1 mol/L, 298.15 K.

The Single point energy calculations were conducted using the M06-2X functional and the def2-TZVP basis set[16] for quantum theory of atoms in molecules (QTAIM) analysis. The QTAIM analysis was carried out with the Multiwfn program[17], utilizing the corresponding formatted Gaussian checkpoint (fchk) files.

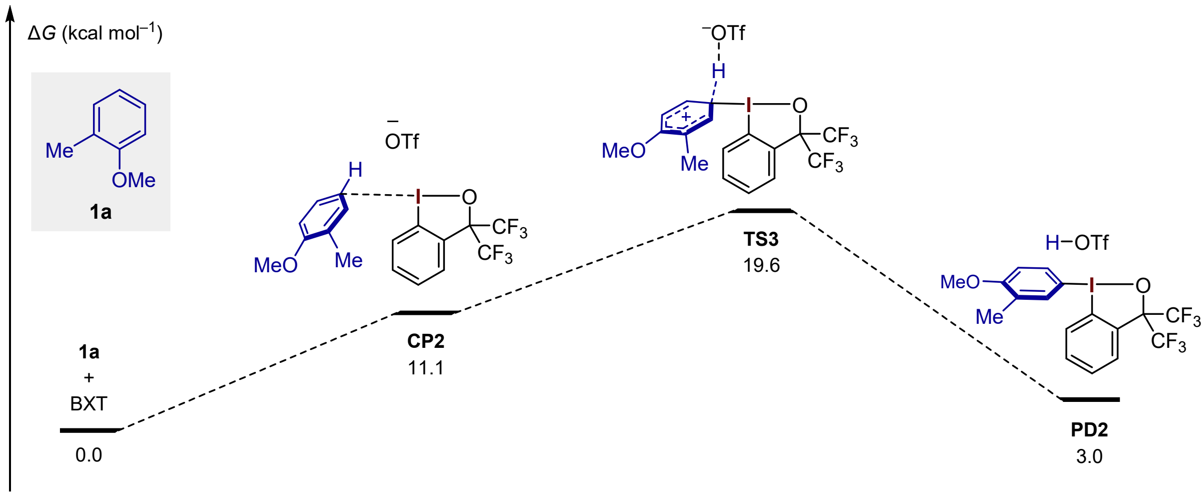


Figure S2. The energy profile of C–H λ^3-iodanation of 1-methoxy-2-methylbenzene (**1a**) with BXT (M06-2X(CPCM, HFIP)/6-311+G(2df,2p)-SDD(for I)//M06-2X/6-31+G(d,p)-SDD(for I)). The figure shows that the activation energy of 19.6 kcal mol^{-1} is higher than that in the three-component coupling between **1a**, ynamide **2a'**, and BXT.

Table S2. The nature of bond critical points (BCPs) between the ynamide β-carbon and iodine in **CP0** and **PD** (M06-2X(CPCM, HFIP)/def2-TZVP//M06-2X/6-31+G(d,p)-SDD(for I)).[a]

Structure	ρ**(r) (a.u.)**	$\nabla^2\rho$**(r) (a.u.)**	G**(r) (a.u.)**	V**(r) (a.u.)**	H**(r) (a.u.)**
CP0	0.0752	0.0283	0.0309	-0.0548	-0.0239
PD	0.1148	-0.0404	0.0445	-0.0992	-0.0546

[a] ρ(r): Electron density at BCPs; $\nabla^2\rho$(r): Laplacian of electron density at BCPs; G(r): kinetic energy at BCPs; V(r): potential energy density at BCPs; H(r): energy density at BCPs.

Table S3. Energy data (hartrees).

Structure	**E(M06-2X/6-31+G(d,p))**	**TCG**	**E(M06-2X(CPCM)/ 6-311+G(2df,2p))**	**TCG+ E(M06-2X(CPCM)/ 6-311+G(2df,2p))**	**Imaginary Frequency (cm^{-1})**
1a	-385.935287	0.12955	-386.049808	-385.920258	
2a’	-437.831585	0.091028	-1992.45537	-1992.35825	
BXT	-1991.823477	0.097118	-437.981852	-437.890824	
CP0	-2429.671908	0.210084	-2430.457234	-2430.24715	
CP1t	-2815.625396	0.362459	-2816.522384	-2816.15993	
CP1c	-2815.626316	0.363851	-2816.524907	-2816.16106	
TS1t	-2815.618302	0.366206	-2816.515503	-2816.1493	-165.63
TS1c	-2815.609668	0.366597	-2816.507531	-2816.14093	-218.13
INT1t	-2815.633423	0.367498	-2816.537645	-2816.17015	
INT1c	-2815.629895	0.363982	-2816.536673	-2816.17269	
TS2	-2815.630513	0.366442	-2816.530806	-2816.16436	-138.17
PD	-2815.670740	0.366864	-2816.561581	-2816.19472	
[**2a’**–I]$^{+}$	-448.932186	0.089050	-449.153735	-449.064685	
[**2a’**–H]$^{+}$	-438.173463	0.103557	-438.389935	-438.286378	
CP2	-2377.753276	0.245434	-2378.506197	-2378.26076	
TS3	-2377.731492	0.242929	-2378.490182	-2378.24725	-600.34
PD2	-2377.764570	0.243534	-2378.51732	-2378.27379	

Cartesian coordinate

1a

C	-2.28418000	-0.66984000	-0.00003300
C	-1.84096600	0.65594000	0.00002500
C	-0.48711600	0.97312200	0.00001400
C	0.44141500	-0.08469300	-0.00000500
C	0.01668600	-1.41255400	-0.00001200
C	-1.35168600	-1.69800800	0.00000000
H	-3.34644300	-0.88991700	0.00007300
H	-2.56455400	1.46721100	0.00003500
H	0.73175200	-2.22647800	0.00004300
H	-1.67694700	-2.73363400	-0.00003000
C	0.00931500	2.39262300	-0.00000800
H	0.63288000	2.58881400	0.87751700
H	0.63059700	2.58957600	-0.87900900
H	-0.82880800	3.09286100	0.00133100
O	1.75062800	0.29679500	0.00003500
C	2.73253800	-0.71731700	-0.00000700
H	2.65278300	-1.34605400	-0.89481400
H	3.69479100	-0.20630900	-0.00007000
H	2.65288800	-1.34606700	0.89480400

2a’

O	2.26547400	0.47869300	0.10254700
C	2.35157900	-0.93069600	-0.12473500
C	0.93657500	-1.45465600	0.14275800
H	2.65252700	-1.09659600	-1.16327300
H	3.10233700	-1.34026900	0.55003300
H	0.64406600	-2.25379400	-0.54023600
H	0.79658000	-1.78749200	1.17766800
C	0.97607400	0.89390600	0.00125800
O	0.62737700	2.03802300	0.01480600
N	0.17270300	-0.23984300	-0.11356300
C	-1.17774100	-0.18508500	-0.05908400
C	-2.38426300	-0.16787800	-0.02452900
C	-3.84503300	-0.10936000	0.01983300
H	-4.16938200	0.93349600	0.06435300
H	-4.28790600	-0.56564400	-0.86910600
H	-4.23309000	-0.62192200	0.90367900

BXT

C	0.02512500	3.39749700	0.14420400
C	-1.29401200	3.42922900	0.58967900
C	-2.08389900	2.28186500	0.56316400
C	-1.55094400	1.08637800	0.07789500
C	-0.23251200	1.10246900	-0.34717000
C	0.58674400	2.21272200	-0.33666100
H	0.63603500	4.29324400	0.16972100
H	-1.71553800	4.35489800	0.96588800
H	-3.10655700	2.31120800	0.92095400
H	1.61762800	2.17447800	-0.66982100
I	0.39181500	-0.82553800	-1.00415500
O	-1.60740300	-1.18384800	-0.74676300
C	-2.29779400	-0.24138100	0.00891400
C	-3.66087300	-0.07721300	-0.70285100
C	-2.46577900	-0.81425800	1.43662800
F	-3.13964600	-1.96112800	1.43275100
F	-1.24595900	-1.04920000	1.94461100
F	-3.09337300	0.03888600	2.25362800
F	-4.23088100	-1.25410900	-0.93823900
F	-4.51272100	0.65526800	0.03157800
F	-3.48417700	0.54356400	-1.87203900
C	3.21942600	-0.48550800	1.17970600
F	2.95411100	-1.78327600	1.01934800
F	4.20613800	-0.34438100	2.04761900
F	2.12178700	0.10874900	1.66179700
O	4.80014400	-0.48964800	-0.93184900
O	3.80882600	1.69461500	-0.16612800
S	3.67926700	0.27608300	-0.44168200
O	2.40887500	0.01165600	-1.28152800

CP0

C	-2.65263700	3.21198300	-1.44740900
C	-3.94114700	2.74370500	-1.20479200
C	-4.14076400	1.49503900	-0.62158200
C	-3.04416900	0.70074300	-0.28107000
C	-1.77542800	1.18057500	-0.56931700
C	-1.54499700	2.42456600	-1.13166800
H	-2.49632900	4.19609200	-1.87593400
H	-4.79871600	3.35733700	-1.45834300
H	-5.14543500	1.13866500	-0.42569700
H	-0.54194600	2.80169600	-1.29488000
I	-0.22315500	-0.19112400	-0.02457100
O	-1.91204800	-1.07317700	0.88522500
C	-3.13574300	-0.66594200	0.39906800
C	-3.63532400	-1.71352700	-0.62513000
C	-4.06998200	-0.60419700	1.63171800
F	-4.00592000	-1.72265100	2.34597700
F	-3.71256900	0.41537500	2.41894100
F	-5.35510700	-0.41787200	1.27975500
F	-3.77645700	-2.91777500	-0.07852800
F	-4.80632900	-1.36846200	-1.18035000
F	-2.73224600	-1.80858200	-1.61501700
C	4.14458800	-2.75715600	0.22475500
F	3.28186400	-3.63524300	0.73278200
F	4.80471100	-3.33677000	-0.77513100
F	5.02104900	-2.42548900	1.17568100
O	2.31273800	-1.75281400	-1.37828600
O	4.32696900	-0.37783500	-0.87291300
O	3.04761800	4.16288200	1.45467500
C	4.21251500	3.31049100	1.53943900
C	3.74783200	1.94130700	1.03962400
H	4.98748700	3.74810400	0.90644200
H	4.53474100	3.30136800	2.57860500
H	4.46980300	1.39951600	0.42858600
H	3.38308500	1.28223100	1.82904300
C	2.15789700	3.68315100	0.59548800
O	1.16499700	4.20975100	0.19854900
N	2.59500800	2.36082400	0.21345800
C	1.95455300	1.69443200	-0.68510900
C	1.21939700	1.03878700	-1.46409000
C	1.06246600	0.68648400	-2.89989900
H	0.01053100	0.75145600	-3.19160400
H	1.66008600	1.34903800	-3.52725100
H	1.40635200	-0.34619800	-3.01592900
S	3.25984500	-1.25411800	-0.37202300
O	2.58593700	-0.74068500	0.84652900

CP1t

C	2.29011700	3.32562900	1.81025500
C	3.57838400	3.48416100	1.30859200
C	4.19683100	2.44781000	0.61334900
C	3.52704000	1.23818800	0.42098700
C	2.24068200	1.11287700	0.92621500
C	1.60367500	2.12604800	1.62093200
H	1.80132000	4.13378100	2.34354700
H	4.10694700	4.42017700	1.45307700
H	5.19633500	2.57874800	0.21532400
H	0.59114200	2.01909800	1.98940500
I	1.35252000	-0.79565300	0.51471900
O	3.34683700	-1.09318700	-0.14716500
C	4.10296600	0.04005400	-0.33451100
C	5.52096500	-0.30661300	0.17858200
C	4.12321500	0.36388500	-1.84858100
F	4.64632500	-0.62731400	-2.56502100
F	2.85630000	0.55003500	-2.26261800
F	4.80427600	1.48413700	-2.13065900
F	5.95634900	-1.45365500	-0.33196900
F	6.41879100	0.64564400	-0.13647600
F	5.50301100	-0.42224800	1.51050000
C	-2.28639900	-4.49844600	-0.41587800
F	-1.45389800	-4.81601200	-1.40724700
F	-2.14145000	-5.39017200	0.56253000
F	-3.53756600	-4.57271400	-0.87510200
O	-0.53296400	-2.87484500	0.65760800
O	-2.91091500	-2.59231800	1.27982400
O	-1.94183800	3.12645400	-1.56527300
C	-2.50145400	2.08752300	-2.39811500
C	-2.09118200	0.75482500	-1.75391200
H	-3.58161100	2.23782700	-2.40632600
H	-2.08809300	2.21686100	-3.39739300
H	-2.90552000	0.04394800	-1.63462300
H	-1.26137300	0.26060500	-2.26343500
C	-1.49975900	2.66044900	-0.40577300
O	-1.06050500	3.29344700	0.50493700
N	-1.62012100	1.22280000	-0.43538100
C	-1.27090000	0.52403500	0.59233200
C	-0.66749200	-0.07512200	1.52528700
C	-0.89713800	-0.60034200	2.89707200
H	0.02194900	-0.54088600	3.48475400
H	-1.68339800	-0.02541500	3.38949900
H	-1.20627800	-1.64731900	2.81653900
C	-4.00064300	0.28938500	1.75517900

C	-4.62566300	-0.04822000	0.54962600
C	-5.05528700	0.92723800	-0.34341200
C	-4.80770000	2.27934600	-0.02323400
C	-4.18310300	2.63229900	1.17403000
C	-3.79151200	1.62854700	2.06624400
H	-3.69389100	-0.51228000	2.41811200
H	-4.76425300	-1.09916900	0.31126400
H	-3.99306700	3.67013400	1.42035500
H	-3.31541000	1.91426100	3.00046100
C	-5.78256100	0.57068600	-1.61209800
H	-6.77739000	1.02588500	-1.62832100
H	-5.26490000	0.93498200	-2.50657100
H	-5.88867200	-0.51253700	-1.69556800
O	-5.21603600	3.18117200	-0.96208300
C	-5.00381200	4.55660500	-0.69493200
H	-3.93506700	4.77651000	-0.58801500
H	-5.40301800	5.09369500	-1.55449300
H	-5.53861000	4.86630100	0.20973700
S	-1.93914000	-2.79489000	0.20103000
O	-2.12439000	-1.94464500	-0.98673400

CP1c

C	2.37476400	-2.31692700	-2.53554600
C	3.66158900	-2.33434800	-2.00637300
C	4.03701500	-1.40342000	-1.04064500
C	3.12162600	-0.44684000	-0.59613800
C	1.84820600	-0.44966600	-1.14862300
C	1.44953500	-1.36415300	-2.10874600
H	2.07067100	-3.05239500	-3.27301000
H	4.37814500	-3.07706900	-2.34000700
H	5.04140700	-1.41601000	-0.63311200
H	0.44205400	-1.38049800	-2.50290700
I	0.59451900	1.11966900	-0.39545700
O	2.28981400	1.24307400	0.89468100
C	3.43337900	0.62799500	0.44756700
C	4.35425300	1.69745200	-0.19072100
C	4.09983800	0.00494800	1.69804900
F	4.18347000	0.88049900	2.69339600
F	3.37783200	-1.04028300	2.12305500
F	5.34355800	-0.43998800	1.44101500
F	4.70621600	2.63713700	0.68358800
F	5.47518400	1.17360900	-0.70939700
F	3.68772900	2.29238400	-1.19430800
O	-1.56881600	3.07967900	-0.60400100
O	-2.53120300	1.38204900	0.89893900
O	-3.43217000	-3.17594600	-1.03395600
C	-4.45627000	-2.29066100	-0.53113300
C	-3.78920800	-0.92175100	-0.34935200
H	-5.26231800	-2.27650300	-1.26712700
H	-4.81054000	-2.70756900	0.41117600
H	-4.35696000	-0.07812800	-0.74321500
H	-3.48712300	-0.70993400	0.67565400
C	-2.36351000	-2.52082100	-1.46014900
O	-1.41060900	-2.95991500	-2.02353000
N	-2.56514700	-1.11500600	-1.15577100
C	-1.78500100	-0.21839400	-1.63373500
C	-0.95993900	0.63999600	-2.05782000
C	-0.86051200	1.51018800	-3.26710900
H	-1.03618100	2.53811300	-2.93454600
H	0.14231600	1.43879500	-3.69670200
H	-1.60627500	1.23530800	-4.01370200
C	-1.00722300	-1.13131200	2.34607800
C	0.00046400	-1.78141600	1.62559800
C	-0.17788700	-3.05545900	1.09546400
C	-1.41283200	-3.69774900	1.31820200
C	-2.41532800	-3.07969700	2.06807300
C	-2.20586700	-1.79188500	2.57679300
H	-0.85326500	-0.12569300	2.72223200
H	0.96635500	-1.29891000	1.49519400
H	-2.98960800	-1.31005300	3.15439300
O	-1.52721800	-4.93572900	0.76608300
C	-2.71065900	-5.66540900	1.01064700
H	-3.58460700	-5.15012800	0.59454200
H	-2.58466500	-6.62213900	0.50506700
H	-2.85627500	-5.83395500	2.08428200
S	-2.79922400	2.44657600	-0.08605400
C	-3.60704000	3.78231300	0.89584100
F	-4.74724500	3.33434900	1.42653100
F	-3.88367600	4.82991100	0.12218200
F	-2.80911100	4.18117800	1.88486000
O	-3.79249700	2.09401000	-1.11058800
H	-3.34717800	-3.59411600	2.27671300
C	0.90519700	-3.76824500	0.33571800
H	1.14524800	-4.72466600	0.81022500
H	0.58093000	-3.98708500	-0.68706600
H	1.81042400	-3.15533200	0.29743800

TS1t

C	2.58647500	2.63778600	2.48812700
C	3.82900600	2.78111100	1.87810000
C	4.26065300	1.85502300	0.93184700
C	3.45183000	0.76759800	0.59683100
C	2.21148400	0.66119600	1.20734800
C	1.75888900	1.56843800	2.14966300
H	2.24595600	3.36182200	3.22045000
H	4.46762000	3.61913200	2.13599100
H	5.22527400	1.97609200	0.45270100
H	0.77592800	1.47864000	2.59669600
I	1.06909900	-1.04798200	0.59150500
O	3.03131100	-1.42269100	-0.28641000
C	3.82659200	-0.32151000	-0.41656600
C	5.28264900	-0.80030000	-0.19969600
C	3.65569800	0.26131700	-1.84351200
F	4.01147000	-0.60585800	-2.78884500
F	2.35322900	0.56251000	-2.03558400
F	4.35092100	1.39220300	-2.03809700
F	5.55285100	-1.87705400	-0.93156100
F	6.18903600	0.14410200	-0.52567700
F	5.47441500	-1.11252300	1.08663500
C	-3.09755400	-4.25845000	-0.44040400
F	-2.33842600	-4.72898700	-1.42904200
F	-3.08949800	-5.13947900	0.55857500
F	-4.34922900	-4.13858900	-0.88926100
O	-1.09581900	-2.91449700	0.58566300
O	-3.39440500	-2.24162300	1.21249200
O	-0.76120600	3.09110100	-1.54420200
C	-1.48225400	2.20471800	-2.42286300
C	-1.51852200	0.85457500	-1.70213600
H	-2.47917400	2.62995600	-2.56398500
H	-0.94640600	2.16857400	-3.36996400
H	-2.46696700	0.32651000	-1.77462200
H	-0.71781900	0.17833800	-2.01555100
C	-0.70935700	2.60380500	-0.30182100
O	-0.27777100	3.17371400	0.65756100
N	-1.25726000	1.29085300	-0.32036100
C	-1.39232500	0.59370300	0.79472300
C	-0.77115200	-0.19126800	1.62205600
C	-1.11513600	-0.74954000	2.95830900
H	-0.20732800	-0.91101900	3.54492300
H	-1.77365100	-0.07567700	3.51281800
H	-1.61625900	-1.71401500	2.82101000
C	-3.46819400	0.75901400	1.49481400
C	-4.18385200	0.63955400	0.27792800
C	-4.40490000	1.73331400	-0.52936800
C	-3.90094200	2.99463800	-0.10043400
C	-3.29195200	3.15555300	1.14832900
C	-3.09115700	2.03802300	1.95098500
H	-3.42564600	-0.11928800	2.12790300
H	-4.51817100	-0.34945700	-0.02138900
H	-2.93573000	4.12324400	1.47673700
H	-2.61218600	2.15559300	2.91875900
C	-5.15445200	1.62962400	-1.82822800
H	-6.04713700	2.26181700	-1.81094900
H	-4.55023000	1.97079900	-2.67491600
H	-5.45413300	0.59594800	-2.00832500
O	-4.06923100	3.99746300	-0.98264600
C	-3.54092500	5.27990700	-0.66216200
H	-2.45989700	5.22177400	-0.49639400
H	-3.74918100	5.90817400	-1.52627100
H	-4.03791200	5.69354500	0.22089200
S	-2.47071900	-2.62124700	0.13364400
O	-2.54330500	-1.77189100	-1.06590500

TS1c

C	2.28191100	-2.67181000	-2.21190700
C	3.60950300	-2.76620500	-1.80316500
C	4.17095400	-1.77164200	-1.00723000
C	3.41317500	-0.65947300	-0.62888200
C	2.09613800	-0.59059200	-1.05343000
C	1.50551800	-1.57830900	-1.82966200
H	1.83188800	-3.45016800	-2.81961000
H	4.21030200	-3.62069200	-2.09576800
H	5.19795200	-1.85947300	-0.67244600
H	0.46168600	-1.54337400	-2.12001700
I	1.02995000	1.14750600	-0.36043100
O	3.09406300	1.54689200	0.26311700
C	3.92785600	0.47304300	0.27468900
C	5.31257800	0.96996200	-0.20572400
C	4.01480900	-0.07518700	1.72287900
F	4.48538400	0.83156900	2.57516200
F	2.77339800	-0.41512100	2.12607600

F	4.77668400	-1.17633900	1.83107500
F	5.68953700	2.06399100	0.44895800
F	6.28194900	0.04697300	-0.03584800
F	5.26360100	1.26126400	-1.51107600
O	-1.30018700	2.82564100	0.00944300
O	-3.19152200	1.72054200	1.17024200
O	-4.04899100	-2.86663900	-1.50789400
C	-4.93268700	-1.97342700	-0.80002800
C	-4.16627800	-0.65566000	-0.66071900
H	-5.84328800	-1.87769400	-1.38932000
H	-5.15803000	-2.42631500	0.16824600
H	-4.42175300	0.09293100	-1.41449400
H	-4.23073700	-0.18314500	0.32090600
C	-2.79499900	-2.41130100	-1.52580700
O	-1.84339100	-2.95352100	-2.00397300
N	-2.79435600	-1.11942200	-0.91519800
C	-1.69383900	-0.44783700	-0.71894500
C	-0.79403400	0.30876200	-1.27275900
C	-1.04561400	0.81529200	-2.67459200
H	-1.18468200	1.89902700	-2.61819000
H	-0.17807400	0.59004700	-3.30390700
H	-1.94504100	0.37666300	-3.11213900
C	-1.31621000	-0.69426200	1.56019200
C	-0.47852100	-1.73390100	1.09282500
C	-0.91604100	-3.04932800	0.99523500
C	-2.22688000	-3.32996900	1.41838000
C	-3.04122400	-2.32809800	1.99179400
C	-2.58030600	-1.02644300	2.07733800
H	-0.94821800	0.31677400	1.70030500
H	0.54855700	-1.52133800	0.81336100
H	-3.19147100	-0.24360800	2.51254000
O	-2.61649100	-4.60998700	1.26311800
C	-3.89674400	-5.00445000	1.72605500
H	-4.68992800	-4.47056300	1.19108300
H	-3.97403500	-6.06891000	1.51205000
H	-3.99450400	-4.83699000	2.80364900
S	-2.75295300	2.56236100	0.04477800
C	-3.47909000	4.21781400	0.41296500
F	-4.80939300	4.13126100	0.48003900
F	-3.16049500	5.09023300	-0.54220100
F	-3.02679800	4.67814100	1.57815200
O	-3.33824900	2.19265700	-1.25364300
H	-4.01899600	-2.57876700	2.38862300
C	-0.04744700	-4.14328600	0.44566200
H	-0.02083100	-5.00017400	1.12387500
H	-0.44224400	-4.49154200	-0.51468000
H	0.97001200	-3.77694100	0.29144100

INT1t

C	1.88641100	3.48506900	1.12202000
C	3.15132600	3.64152900	0.56073100
C	3.88179000	2.52823200	0.15557600
C	3.35591400	1.24035700	0.30434400
C	2.08717100	1.12036200	0.84621500
C	1.34418300	2.21033700	1.27054400
H	1.30575400	4.34719900	1.43268100
H	3.57264800	4.63327800	0.43494100
H	4.86459500	2.65596500	-0.28311900
H	0.35090000	2.08759700	1.68681400
I	1.29810800	-0.88100900	0.92154500
O	3.48829200	-1.15317100	0.38993600
C	4.09215000	-0.05271200	-0.10410200
C	5.54483200	-0.02872700	0.43624800
C	4.10380000	-0.12786300	-1.65437500
F	4.79146600	-1.17438700	-2.10566700
F	2.83101200	-0.25675700	-2.09070700
F	4.60148900	0.97307700	-2.24788000
F	6.14488000	-1.20443700	0.27036900
F	6.31788900	0.89992500	-0.16997500
F	5.54287700	0.25322300	1.74567200
C	-2.89059100	-4.39900700	-0.34003500
F	-2.10389000	-5.00764700	-1.22555100
F	-2.97142300	-5.15921900	0.75119000
F	-4.11266300	-4.28773700	-0.86789600
O	-0.89506300	-3.00993000	0.64194400
O	-3.21078000	-2.19904600	1.04188700
O	-0.52631500	2.67459700	-2.04214300
C	0.08364900	1.49365800	-2.60641200
C	-0.61004000	0.33975400	-1.88559100
H	-0.08340500	1.50833500	-3.68199000
H	1.15408700	1.52387100	-2.38317300
H	-1.53866700	0.02658300	-2.37344100
H	0.02193000	-0.53874200	-1.75824800
C	-0.98720600	2.36969000	-0.81743800
O	-1.43113800	3.18410700	-0.03161800
N	-0.88717300	1.01573600	-0.61072900
C	-1.44734300	0.46734800	0.57343500
C	-0.71474100	-0.20678400	1.46221300
C	-1.16432100	-0.75030700	2.78145000
H	-0.56119400	-0.30079800	3.57916800
H	-2.21997800	-0.56042300	2.98954300
H	-1.02062100	-1.83461300	2.80871000
C	-2.94826100	0.74221500	0.78010600
C	-3.74969500	0.58721400	-0.44995300
C	-4.75214900	1.43527200	-0.79649100
C	-5.01059900	2.54580400	0.07851300
C	-4.27218200	2.78009600	1.26907200
C	-3.24126800	1.94511200	1.56855400
H	-3.29603800	-0.14017800	1.37267200
H	-3.52876500	-0.29939100	-1.04589000
H	-4.47566100	3.64636100	1.88413400
H	-2.61800400	2.13849300	2.43783200
C	-5.59830400	1.25950300	-2.02581200
H	-6.65429700	1.15610700	-1.76162500
H	-5.50949600	2.12597500	-2.68687200
H	-5.28395800	0.36674600	-2.56751700
O	-5.98799000	3.32690300	-0.31240100
C	-6.35293800	4.48440100	0.45002600
H	-5.51144200	5.17862000	0.50336400
H	-7.17814900	4.93582700	-0.09512000
H	-6.67940900	4.18915200	1.44982700
S	-2.22483600	-2.73031300	0.07960500
O	-2.21541000	-2.01912500	-1.21162500

INT1c

C	2.11096900	-3.22814600	-1.76280600
C	3.46301000	-3.33518300	-1.44958200
C	4.10452300	-2.31028000	-0.76040800
C	3.40224500	-1.16312200	-0.37512600
C	2.06446800	-1.07488300	-0.72195900
C	1.39645900	-2.08603300	-1.40172800
H	1.59653700	-4.02395700	-2.29182800
H	4.02240400	-4.21880300	-1.73833300
H	5.15624600	-2.39889900	-0.51553000
H	0.34228300	-2.02584300	-1.65171900
I	1.06625900	0.74275200	-0.11673300
O	3.10906400	0.90228800	0.82187200
C	4.02915700	-0.00341400	0.42778500
C	5.07672700	0.70489300	-0.46931200
C	4.70032200	-0.56796600	1.70653000
F	5.11696900	0.40606700	2.51147300
F	3.81509200	-1.31319000	2.38818900
F	5.76622200	-1.35620700	1.45155200
F	5.69041600	1.69868700	0.17285200
F	6.03222300	-0.12389500	-0.93480400
F	4.45345700	1.22513900	-1.53846400
O	-1.37144400	2.16440400	1.07604600
O	-3.48086900	2.34439400	-0.18809400
O	-3.78267500	-2.18625400	-3.01357600
C	-4.65186600	-1.05094200	-2.86458000
C	-3.82945400	-0.01153400	-2.09253800
H	-4.95203100	-0.72101100	-3.85828100
H	-5.53226100	-1.37232200	-2.30015700
H	-3.33263400	0.71999300	-2.74070800
H	-4.40527100	0.54161800	-1.35030000
C	-2.76485000	-2.09816600	-2.13035700
O	-1.92855800	-2.95837100	-1.96976100
N	-2.84961800	-0.89722800	-1.46428500
C	-1.73955100	-0.44315200	-0.69363100
C	-0.66873400	0.09580700	-1.27730100
C	-0.53822000	0.34144100	-2.74800900
H	-0.67525200	1.41432400	-2.92551700
H	0.45878900	0.06043700	-3.10159400
H	-1.27439200	-0.22007500	-3.33064600
C	-1.87331600	-0.76219900	0.80730800
C	-1.56847000	-2.19989100	0.98311700
C	-2.44488500	-3.09796600	1.49845300
C	-3.70891100	-2.58360300	1.94952100
C	-4.05597600	-1.20028100	1.88854500
C	-3.17983600	-0.32413400	1.33414100
H	-1.12434400	-0.14020800	1.32783500
H	-0.60058600	-2.54147000	0.62021400
H	-3.41461100	0.73508800	1.24133700
O	-4.51822900	-3.49001000	2.43300500
C	-5.81792200	-3.13652800	2.92909400
H	-6.41580900	-2.69075700	2.13149400
H	-6.26208300	-4.07444300	3.25267300
H	-5.72347200	-2.45199500	3.77457500
S	-2.10356100	2.84366600	-0.01607000
C	-2.33980200	4.55687300	0.62543500
F	-3.00529600	5.29814300	-0.26011800
F	-1.16421200	5.13350600	0.86495200

F	-3.03919600	4.53187700	1.76305200
O	-1.33000800	3.01303900	-1.24903400
H	-5.00762400	-0.85617400	2.27305000
C	-2.17018700	-4.57076300	1.59471600
H	-2.25483200	-4.92351400	2.62594400
H	-2.88668300	-5.13370900	0.99003400
H	-1.16653500	-4.78419800	1.22576500

TS2

C	1.91341800	-3.52073400	-0.38729400
C	3.21566800	-3.60838600	0.09753300
C	3.99856600	-2.46405100	0.21862000
C	3.48761500	-1.21107600	-0.13736200
C	2.18186400	-1.15756100	-0.59367000
C	1.38428700	-2.28127200	-0.74265100
H	1.29439000	-4.40653800	-0.48382800
H	3.62719200	-4.57086000	0.38239900
H	5.01233700	-2.53882300	0.59397000
H	0.36980000	-2.21213000	-1.11684200
I	1.42998800	0.82115900	-1.01214500
O	3.64922600	1.12844700	-0.65756100
C	4.28869300	0.10630800	-0.05338800
C	5.66016500	-0.07077900	-0.75464500
C	4.49260700	0.45066200	1.44558200
F	5.22419100	1.55035300	1.61333100
F	3.28545300	0.67198000	2.00630100
F	5.07292400	-0.53514000	2.15481300
F	6.30724400	1.08755600	-0.85642400
F	6.48033900	-0.92782900	-0.10828200
F	5.48020700	-0.55356500	-1.99162200
C	-3.39180300	4.10546100	0.31834100
F	-2.74253200	4.84258300	1.21635700
F	-3.53640300	4.81661000	-0.79713700
F	-4.60193300	3.81692300	0.79963600
O	-1.16573000	2.99944300	-0.54972700
O	-3.33518000	1.86885000	-1.01626100
O	-0.75749000	-2.20710800	2.66690400
C	-0.46857600	-0.87634800	3.13787400
C	-0.07876200	-0.10443000	1.87697600
H	-1.37523500	-0.47178200	3.59887600
H	0.33292100	-0.94363700	3.87140600
H	-0.41260900	0.93395400	1.88110700
H	1.00024700	-0.16948200	1.70623800
C	-1.09732600	-2.14500900	1.36468100
O	-1.57977200	-3.06310200	0.73860300
N	-0.82140400	-0.88460300	0.88252700
C	-1.32253900	-0.49118600	-0.37409900
C	-0.61264000	0.13235800	-1.32219000
C	-1.12275800	0.61898200	-2.64870300
H	-0.59753900	0.09995100	-3.45914100
H	-2.19828400	0.48856500	-2.77574600
H	-0.93241200	1.69273300	-2.75137900
C	-2.80402900	-0.82331600	-0.57787700
C	-3.65385700	-0.86778200	0.60555300
C	-4.78277500	-1.63146200	0.68539900
C	-5.06534500	-2.49879600	-0.40925700
C	-4.23264400	-2.57074400	-1.55616900
C	-3.11598000	-1.78976300	-1.61042900
H	-3.20414300	0.22840900	-0.95113400
H	-3.40491200	-0.16851600	1.40213900
H	-4.45365400	-3.26488100	-2.35634500
H	-2.43965400	-1.87219400	-2.45713300
C	-5.70570000	-1.61396800	1.87042200
H	-6.72078200	-1.34076200	1.56937300
H	-5.75633600	-2.60205600	2.33613100
H	-5.35407000	-0.89231600	2.60863300
O	-6.15500600	-3.22837600	-0.27005600
C	-6.54221900	-4.15215300	-1.28986900
H	-5.77291800	-4.91724400	-1.42044600
H	-7.46234700	-4.60735300	-0.93110600
H	-6.72745200	-3.62565100	-2.22964200
S	-2.45491900	2.55285000	-0.02240800
O	-2.41434300	1.85820000	1.27484200

PD

C	2.19514500	-3.55166000	-0.07762800
C	3.50925700	-3.49414300	0.37860800
C	4.20950800	-2.29102000	0.35986300
C	3.60100800	-1.12054400	-0.10596800
C	2.28422000	-1.21130000	-0.52263900
C	1.56766200	-2.39642900	-0.54188400
H	1.63902800	-4.48309200	-0.06576600
H	3.99570100	-4.38999900	0.74958200
H	5.23422300	-2.25509400	0.71079600
H	0.54366100	-2.44089400	-0.89344000
I	1.37157500	0.65756000	-1.09980600
O	3.58521000	1.15026500	-0.89001800
C	4.30575100	0.25163200	-0.18899700
C	5.67679400	0.09237900	-0.89590800
C	4.50771300	0.77775000	1.25664900
F	5.16855200	1.93389100	1.28369000
F	3.29567500	0.98775700	1.81391600
F	5.15837600	-0.08089400	2.06220300
F	6.23270900	1.27527600	-1.14820100
F	6.56861800	-0.61781700	-0.17127800
F	5.51764800	-0.54606600	-2.06275200
C	-3.52497700	3.96892000	0.34557000
F	-2.84032600	4.82170900	1.09190100
F	-3.81596800	4.52405300	-0.81948100
F	-4.64310600	3.62666500	0.96985500
O	-1.35406500	2.86857000	-0.71110300
O	-3.51308600	1.65184900	-0.81899900
O	-0.33557000	-2.22197100	2.92449200
C	-0.16249500	-0.83805400	3.26162400
C	0.09513300	-0.16409200	1.91559500
H	-1.08333400	-0.47510800	3.73049600
H	0.67356300	-0.75729600	3.95451400
H	-0.28273000	0.85628200	1.86092700
H	1.16440900	-0.18737700	1.68152500
C	-0.75352500	-2.31830400	1.64159700
O	-1.11384700	-3.34335300	1.12323800
N	-0.66870900	-1.06378000	1.05122700
C	-1.24948800	-0.82720300	-0.21423900
C	-0.64072500	-0.16624500	-1.21815300
C	-1.26175700	0.22020800	-2.53304500
H	-0.83651500	-0.37992100	-3.34597100
H	-2.34494000	0.09089600	-2.53542800
H	-1.05740000	1.27245000	-2.76080900
C	-2.64214600	-1.35187300	-0.33406100
C	-3.56813600	-1.09718600	0.69475700
C	-4.89057700	-1.52180000	0.62057400
C	-5.29086300	-2.25270600	-0.51661800
C	-4.37935200	-2.54123600	-1.53309500
C	-3.06356500	-2.08954500	-1.43569900
H	-3.73897400	0.78894100	-0.39911400
H	-3.23943600	-0.55423100	1.57919800
H	-4.67527300	-3.12494900	-2.39620300
H	-2.35399000	-2.33950800	-2.21854700
C	-5.88315500	-1.25120400	1.71609500
H	-6.75717300	-0.71851000	1.33024000
H	-6.24809200	-2.19016200	2.14287500
H	-5.42796200	-0.65761100	2.51130000
O	-6.58775500	-2.64562400	-0.52199500
C	-7.04600700	-3.41465900	-1.61805400
H	-6.49173600	-4.35668400	-1.69547100
H	-8.09577200	-3.62461900	-1.41883700
H	-6.95587000	-2.85537400	-2.55629000
S	-2.48692400	2.46219600	0.08051900
O	-2.33529300	1.81417000	1.36550200

[2a'–I]$^+$

I	-2.11590400	-0.49384200	-0.08045500
O	3.64866100	-0.56077500	0.52222100
C	3.92389400	-0.15810000	-0.83531700
C	2.54508900	-0.00735800	-1.49438600
H	4.47626600	0.78246300	-0.79955400
H	4.53060000	-0.93858800	-1.28915400
H	2.47958900	0.82749900	-2.19069700
H	2.20512500	-0.93097200	-1.96844000
C	2.44191700	-0.23272500	0.92783800
O	1.93723800	-0.27762400	1.99152500
N	1.70313300	0.23599000	-0.30336800
C	0.52633300	0.68090600	-0.22816800
C	-0.68626400	1.07595900	-0.01868600
C	-1.14284300	2.48010600	0.24548900
H	-1.64453800	2.50496800	1.21613900
H	-0.30171300	3.17484400	0.25237000
H	-1.86032600	2.77595600	-0.52358500

[2a'–H]$^+$

O	-2.17840900	0.55565500	0.18440100
C	-2.29623300	-0.86663300	0.39752800
C	-1.05028800	-1.47321400	-0.26367000
H	-2.32731800	-1.04169800	1.47424500
H	-3.22522900	-1.18837600	-0.06786100
H	-0.63101300	-2.31850600	0.28003200
H	-1.21863600	-1.73274700	-1.31085000
C	-0.94412000	0.95248600	-0.02734600
O	-0.46817800	2.02676700	-0.09427800
N	-0.13063900	-0.31393400	-0.21946000

C	1.11799200	-0.27544300	-0.35763400
C	2.39672800	-0.13245600	-0.49461500
C	3.40188400	-0.15819500	0.62813200
H	3.93965000	0.79299500	0.62731900
H	2.93073000	-0.30750000	1.59823300
H	4.12181200	-0.95804600	0.44069000
H	2.74139300	0.01277000	-1.52093100

CP2

C	1.97414500	3.47993300	0.38776200
C	0.89314800	4.34956900	0.52158700
C	-0.41358100	3.88674700	0.38075500
C	-0.63362900	2.53788200	0.10221900
C	0.45641200	1.68867600	-0.01143200
C	1.76316600	2.12746500	0.11931900
H	2.98916000	3.84984100	0.49028400
H	1.06537800	5.39907600	0.73392700
H	-1.25103800	4.56688000	0.48609600
H	2.59859900	1.44523900	0.01353300
I	-0.12226000	-0.32174500	-0.38812700
O	-1.90507200	0.59511300	-0.61056500
C	-1.99801300	1.88838300	-0.07871900
C	-2.85202400	2.65836000	-1.11391000
C	-2.71728200	1.77461700	1.28619600
F	-3.93135100	1.25043200	1.16719400
F	-1.99084100	0.97700600	2.08331700
F	-2.82871800	2.96518900	1.88819700
F	-3.95898400	1.99740300	-1.42559700
F	-3.20531200	3.86387800	-0.64064300
F	-2.14295300	2.84365400	-2.22981600
O	-1.76940100	-2.08220700	-0.92190500
O	0.39470200	-3.18478600	-0.76825700
C	2.59075400	-1.52643600	0.66408100
C	3.32183900	-0.77351300	1.59666900
C	4.38586600	0.02904500	1.20940500
C	4.71638300	0.08335600	-0.16519800
C	3.99038200	-0.64213000	-1.10933300
C	2.93102500	-1.45629400	-0.68940600
H	1.82534000	-2.22543800	0.98856700
H	3.06647500	-0.83126100	2.65135700
H	4.24683000	-0.60433900	-2.16108500
H	2.39999500	-2.07808400	-1.40500100
C	5.18551700	0.83753500	2.19173600
H	6.24467600	0.56851200	2.14637100
H	5.12275700	1.90631700	1.96205700
H	4.82236300	0.67601800	3.20828000
O	5.75983100	0.89466600	-0.46927400
C	6.17892600	0.96251900	-1.82041200
H	5.38336700	1.36156600	-2.45998900
H	7.03249200	1.63849600	-1.83575500
H	6.48451400	-0.02396700	-2.18577000
S	-1.06161700	-3.40759300	-0.85620700
C	-1.49815800	-3.98292100	0.84203500
O	-1.55367500	-4.42254000	-1.75928600
F	-1.08005200	-3.07221800	1.73444800
F	-2.81009300	-4.13247700	0.97586000
F	-0.89898400	-5.13882400	1.11274000

TS3

C	-1.79468800	3.40262700	-0.86145800
C	-3.17695600	3.23756500	-0.84763800
C	-3.73361300	1.99001700	-0.58120500
C	-2.90798400	0.89159200	-0.32772200
C	-1.53728100	1.09436100	-0.32981000
C	-0.95454400	2.32163500	-0.59526000
H	-1.35970400	4.37239000	-1.07933300
H	-3.82776400	4.08172100	-1.04823400
H	-4.81002000	1.86464100	-0.56931700
H	0.11978300	2.44985300	-0.60847000
I	-0.40282800	-0.66921500	0.12915500
O	-2.40057000	-1.44148800	-0.06682300
C	-3.41521000	-0.52450800	-0.03706300
C	-4.43316900	-0.96699200	-1.11658900
C	-4.05839700	-0.54391700	1.37186400
F	-4.55770900	-1.73887400	1.67587500
F	-3.11288600	-0.24513300	2.27912900
F	-5.04144300	0.36115900	1.50749200
F	-4.74893200	-2.25112800	-0.98861500
F	-5.57855100	-0.25984100	-1.05896000
F	-3.90833500	-0.78456600	-2.33333700
O	2.38299600	-1.84027400	1.06495200
O	2.40459400	-2.09069400	-1.36834200
C	1.57392900	0.55253400	0.29544500
C	1.60640500	1.49485600	1.36571800
C	2.21666200	2.72368600	1.25182800
C	2.81382000	3.04559600	0.00137900
C	2.77454400	2.15953700	-1.09024400
C	2.15271500	0.93298600	-0.94290200
H	2.00949400	-0.55843100	0.66654400
H	1.16055000	1.21851100	2.31981600
H	3.23815500	2.41882300	-2.03376900
H	2.14811600	0.21885100	-1.76249700
C	2.28886200	3.71339400	2.37961100
H	3.32879700	3.93659400	2.63397900
H	1.81689700	4.65951500	2.09925900
H	1.78728200	3.31904800	3.26469700
O	3.40176000	4.24322800	-0.04374600
C	4.06565700	4.64938700	-1.23619400
H	3.35883100	4.71840600	-2.06856900
H	4.47840400	5.63275000	-1.02072700
H	4.87271100	3.95354200	-1.48323200
S	2.95898100	-2.60270400	-0.11387600
C	4.69673900	-1.98047200	-0.11060900
O	3.04737300	-4.02932800	0.09829700
F	4.68691500	-0.64064900	-0.20062700
F	5.32745900	-2.31842900	1.00847600
F	5.37020300	-2.46358300	-1.14975900

PD2

C	-2.07267400	3.68534200	-0.64009000
C	-3.43029600	3.40915600	-0.77642500
C	-3.90971900	2.12117100	-0.55812200
C	-3.03681500	1.08956900	-0.19548600
C	-1.69183500	1.39494000	-0.08762500
C	-1.18386800	2.66788200	-0.29608200
H	-1.69596100	4.69016200	-0.80065200
H	-4.12191300	4.19839200	-1.05141300
H	-4.96690200	1.91126200	-0.66833700
H	-0.12590200	2.87848100	-0.19404600
I	-0.40271900	-0.25500200	0.43108600
O	-2.48461900	-1.11440900	0.58900100
C	-3.48477400	-0.36064800	0.08596500
C	-3.96125400	-0.98740800	-1.25007500
C	-4.63472200	-0.35617900	1.12556200
F	-4.95322000	-1.59164100	1.50484100
F	-4.25415300	0.32507700	2.21555300
F	-5.76583100	0.22314200	0.66952300
F	-4.39230700	-2.23803300	-1.08826300
F	-4.94919000	-0.29397700	-1.84755300
F	-2.92768200	-1.01634200	-2.10976700
O	4.15509700	-0.80971200	0.42552800
O	2.11552400	-1.86006900	1.36899100
C	1.35369200	0.97146400	0.12975600
C	2.00542800	1.54949200	1.22678100
C	3.16316700	2.30988500	1.07159100
C	3.66829600	2.49435400	-0.23479000
C	3.02779700	1.92124800	-1.33688500
C	1.86919400	1.16156700	-1.14709600
H	3.52628000	-0.05749200	0.43805700
H	1.61436300	1.39829400	2.23066200
H	3.41865900	2.05110300	-2.33871400
H	1.37962000	0.72065100	-2.01123500
C	3.88238100	2.92725000	2.23727700
H	4.91132600	2.56050400	2.29624400
H	3.93853600	4.01368500	2.12393900
H	3.37071400	2.69505700	3.17281600
O	4.79153500	3.24152500	-0.31402000
C	5.37476200	3.44293700	-1.58975100
H	4.68567900	3.97222400	-2.25700600
H	6.25940700	4.05419600	-1.41973200
H	5.66874000	2.48864200	-2.04036500
S	3.40558600	-2.16331600	0.78802300
C	3.07377700	-2.78970300	-0.91994500
O	4.35286900	-3.05616100	1.39025500
F	2.30557100	-1.91354100	-1.56269700
F	4.21163800	-2.94149100	-1.57795200
F	2.44446400	-3.94989300	-0.83496800

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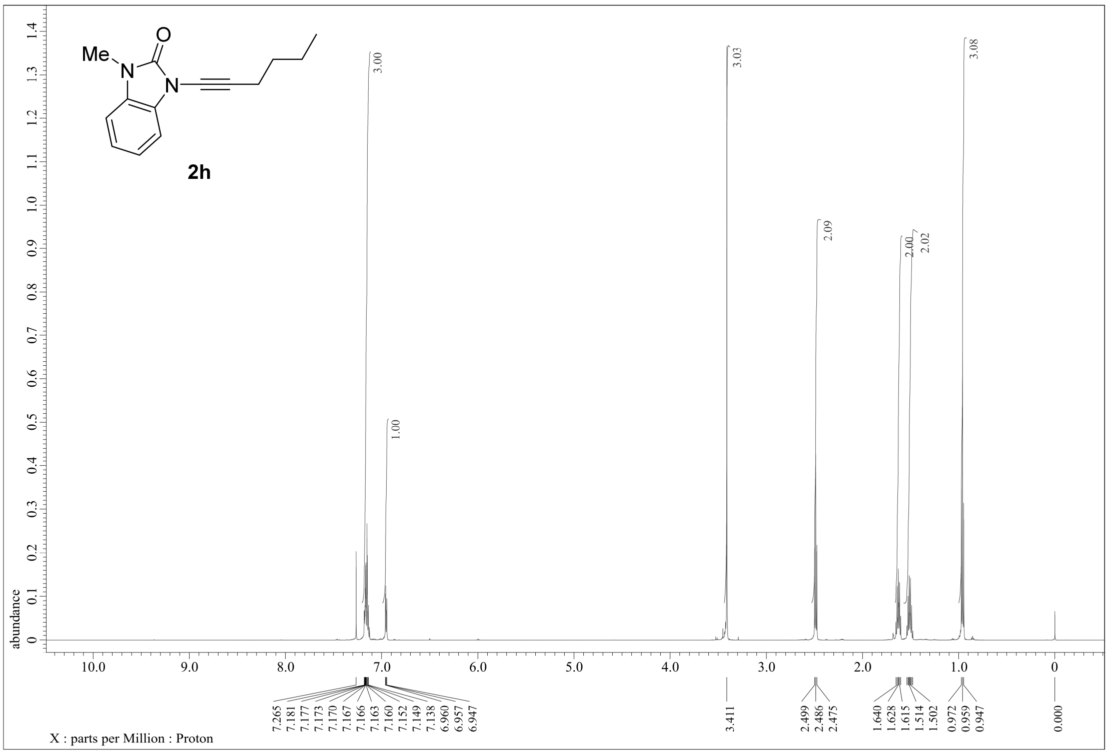
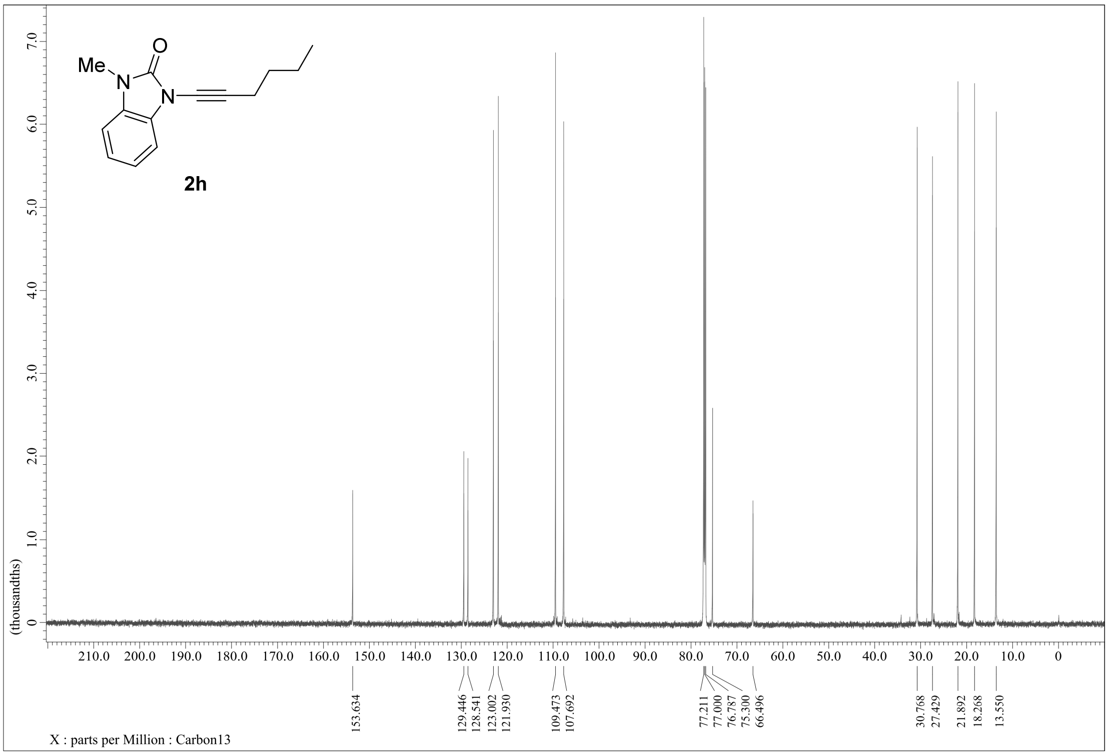
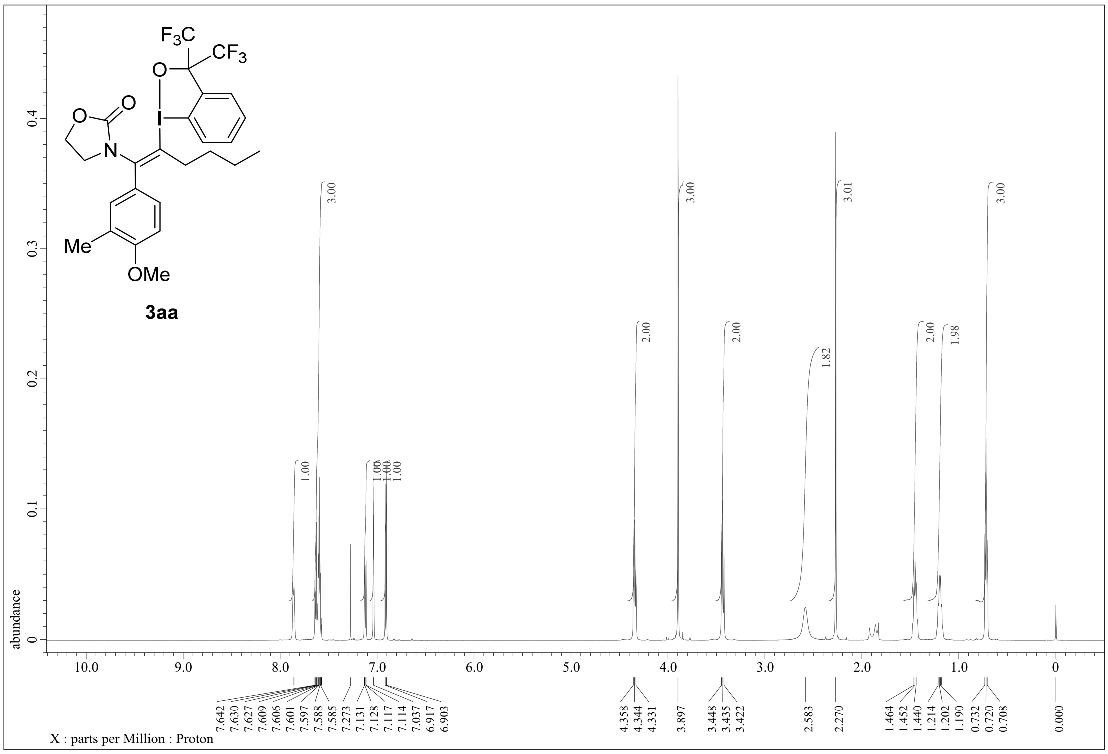
7. NMR Spectra

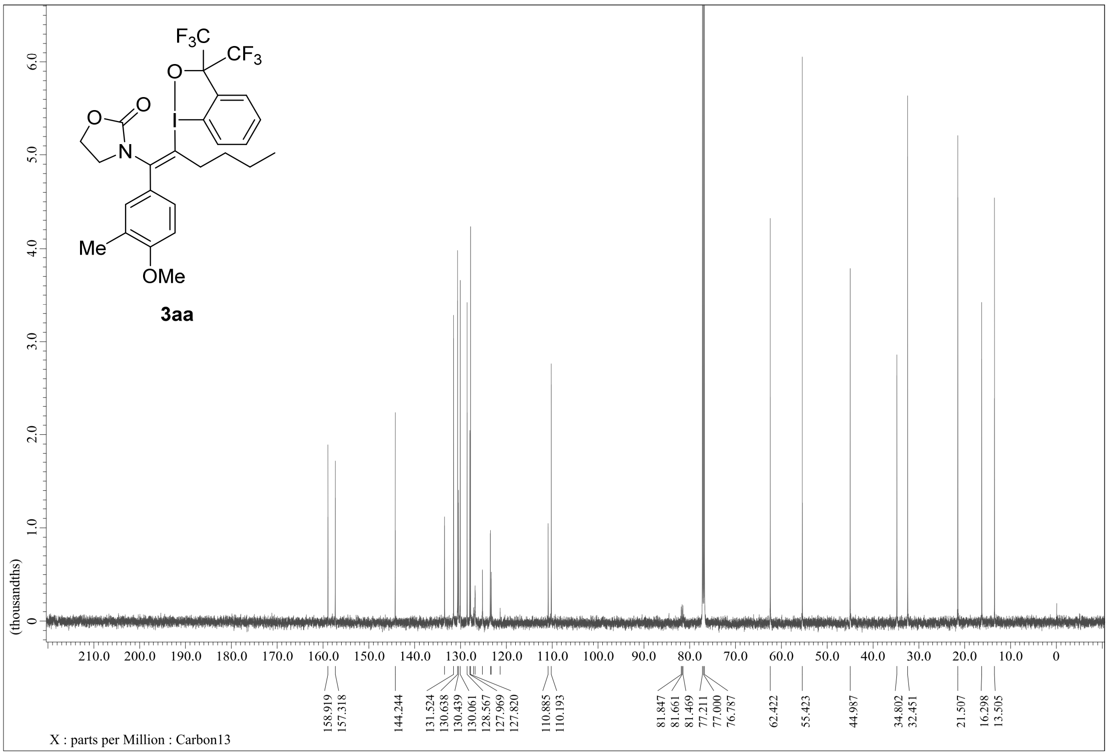
^{1}H NMR (600 MHz, CDCl$_3$) and ^{13}C{^{1}H} NMR (151 MHz, CDCl$_3$) spectra of **2h**



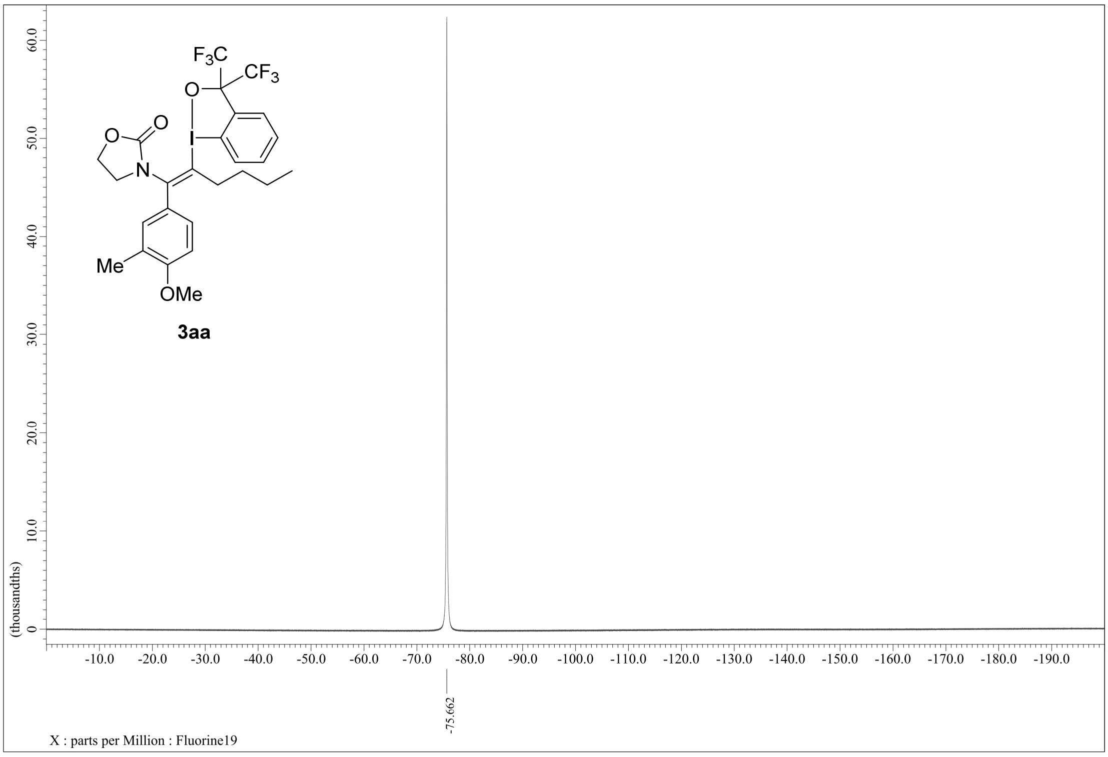


[1]H NMR (600 MHz, $CDCl_3$) and [13]C{[1]H} NMR (151 MHz, $CDCl_3$) spectra of **3aa**

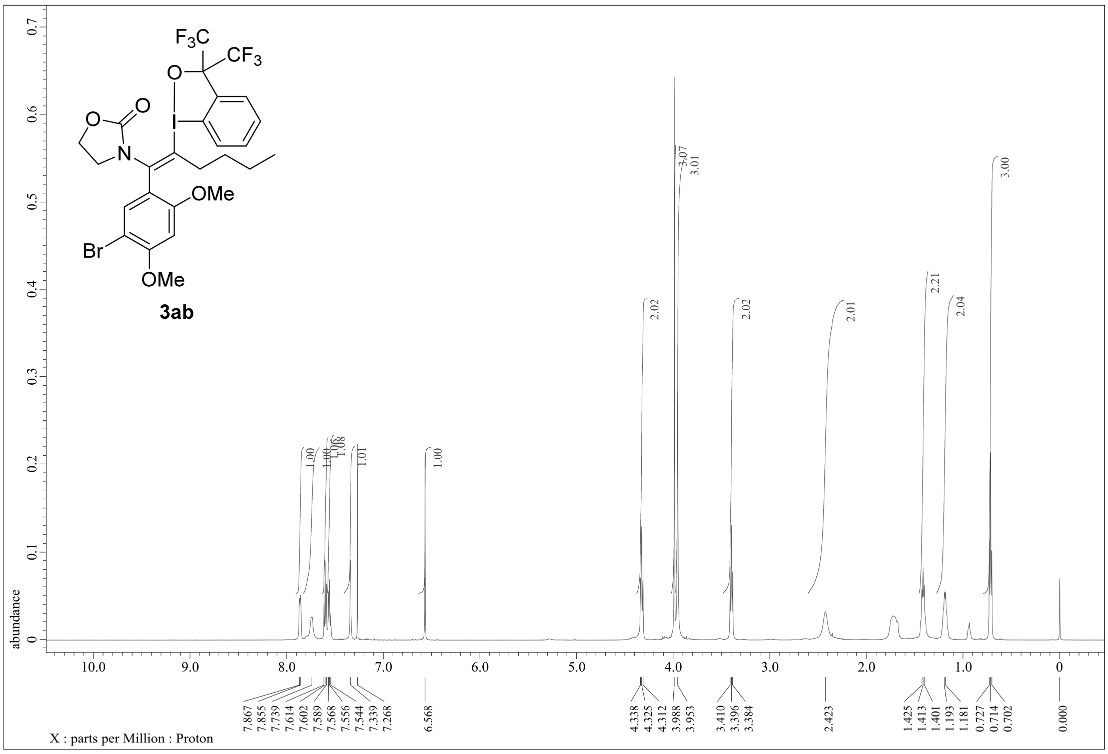


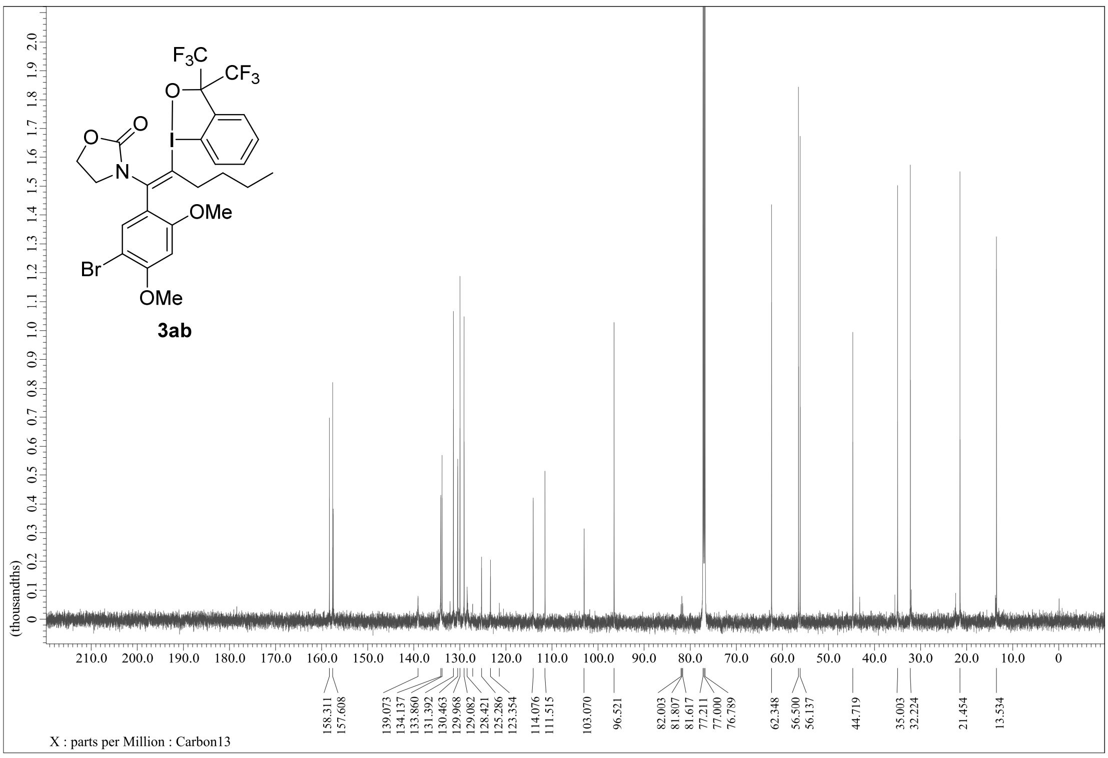


[19]F{[1]H} NMR (565 MHz, $CDCl_3$) spectrum of **3aa**

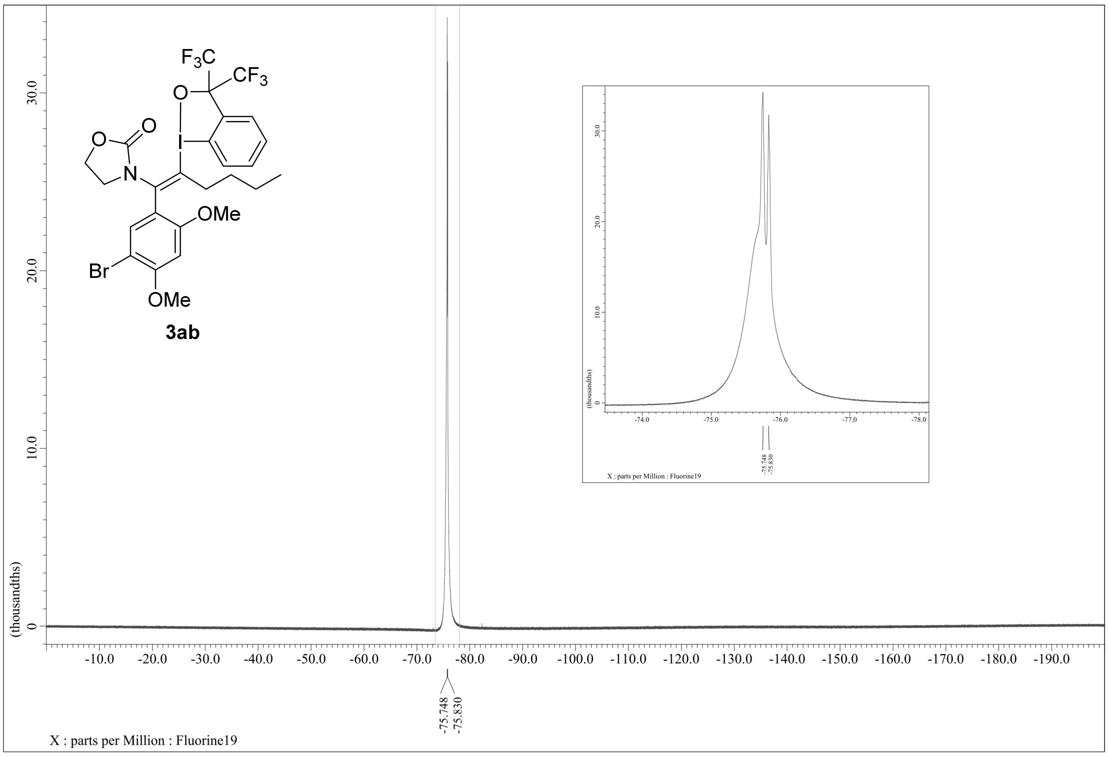


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3ab**

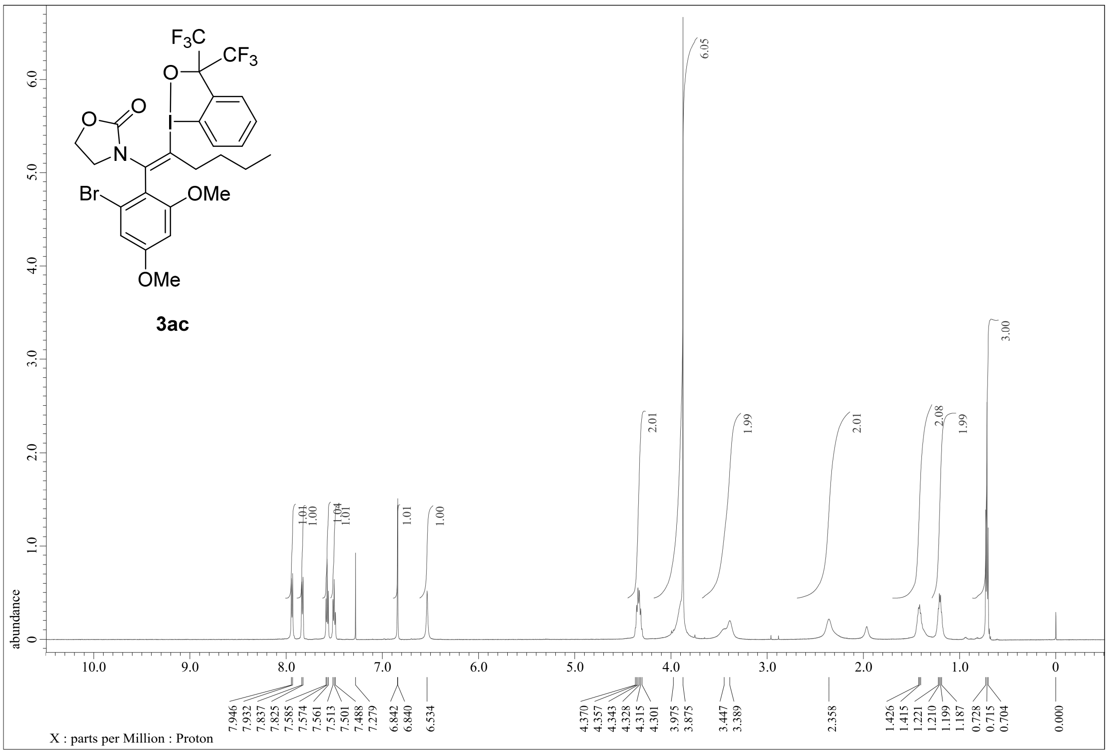


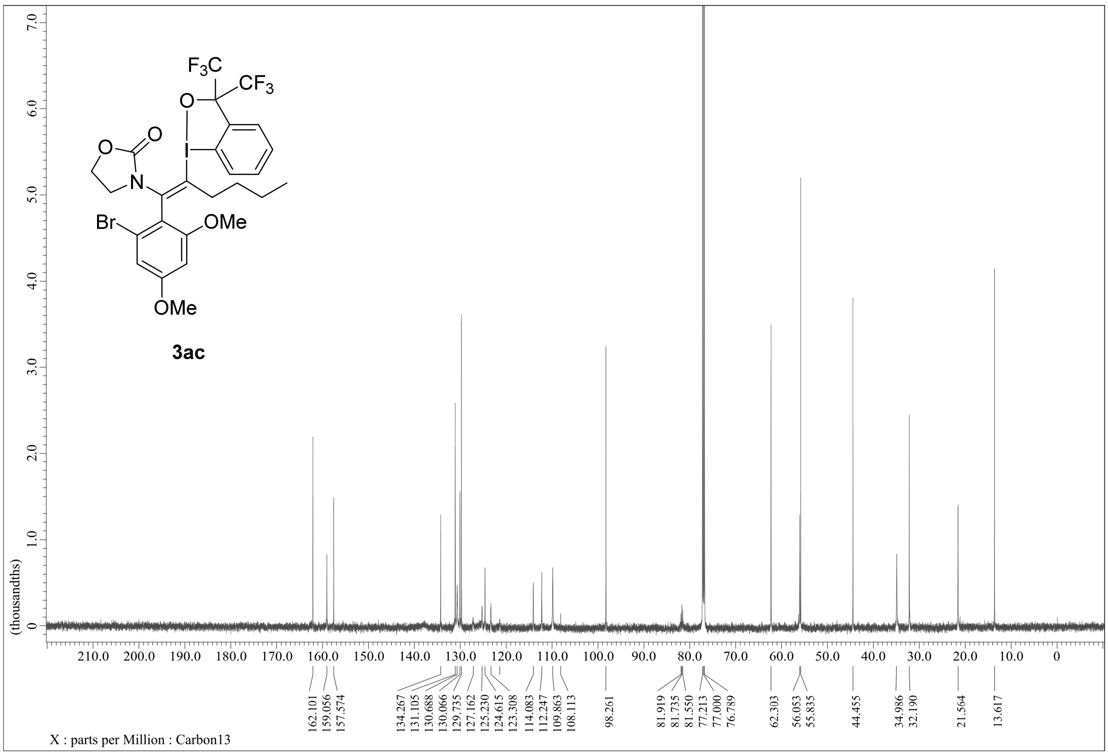


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ab**

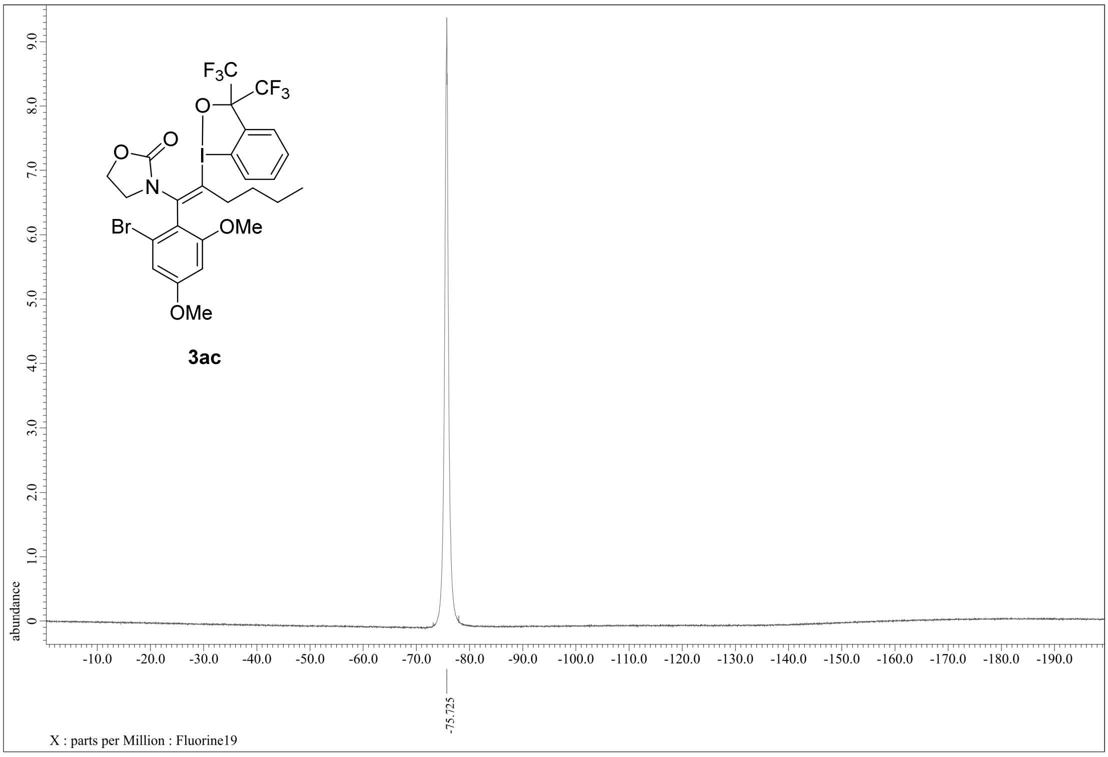


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3ac**

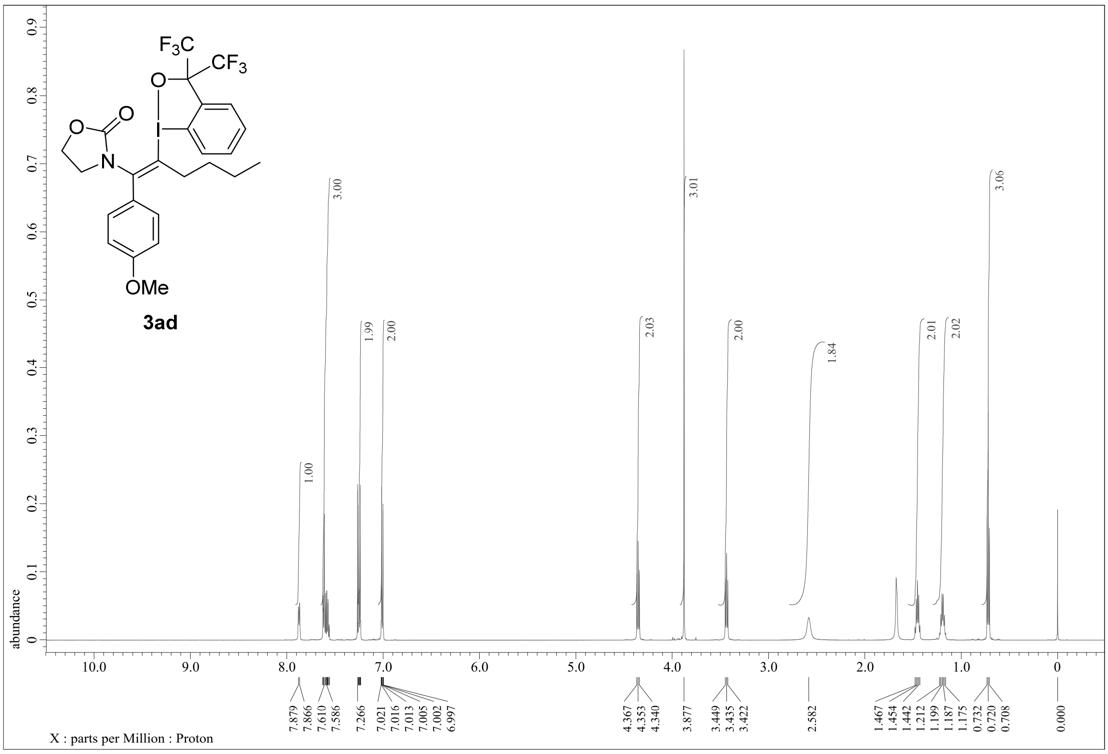


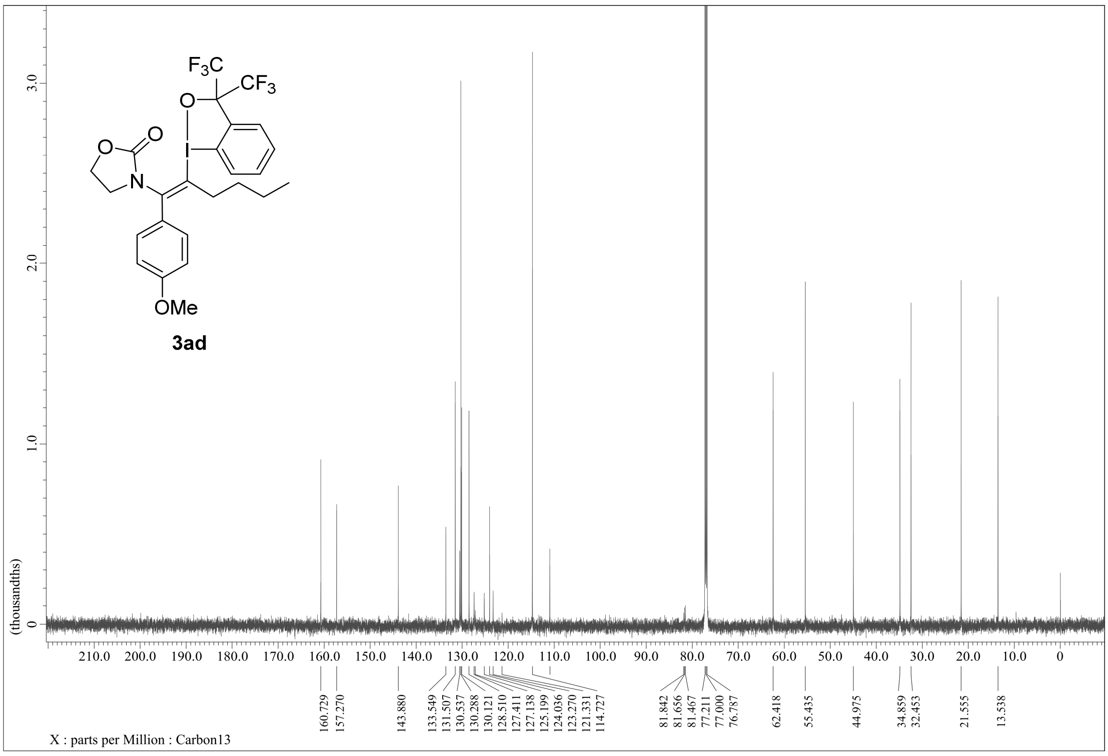


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ac**

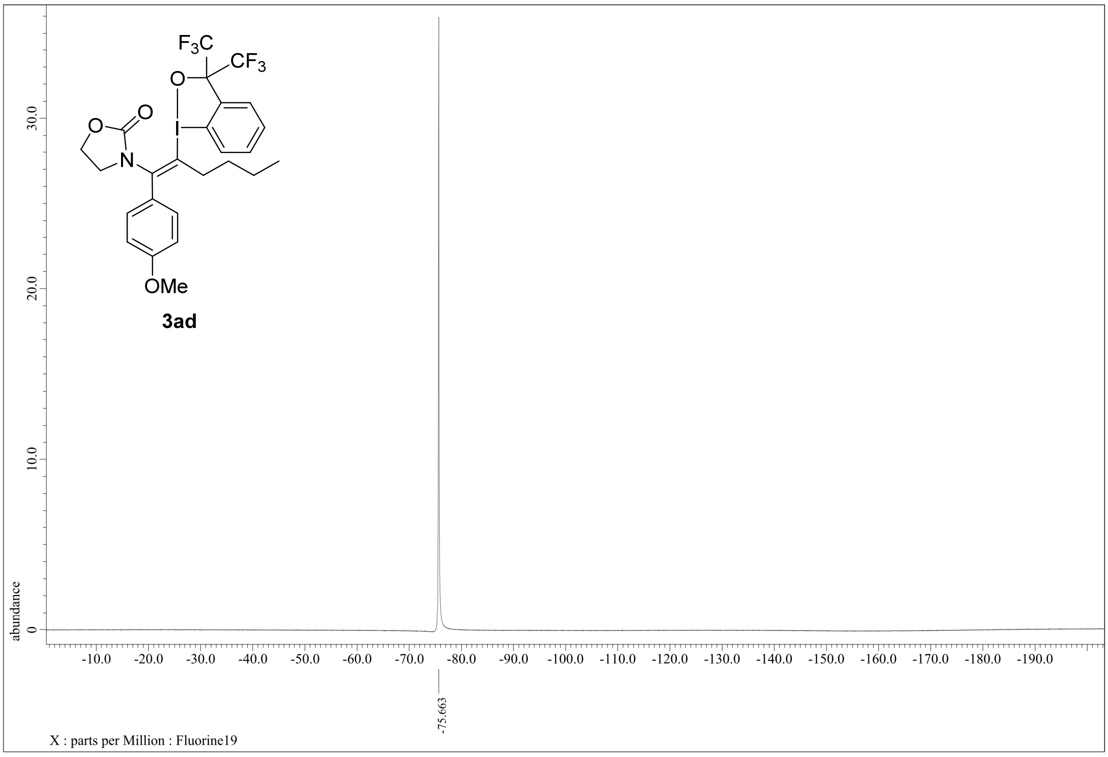


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3ad**

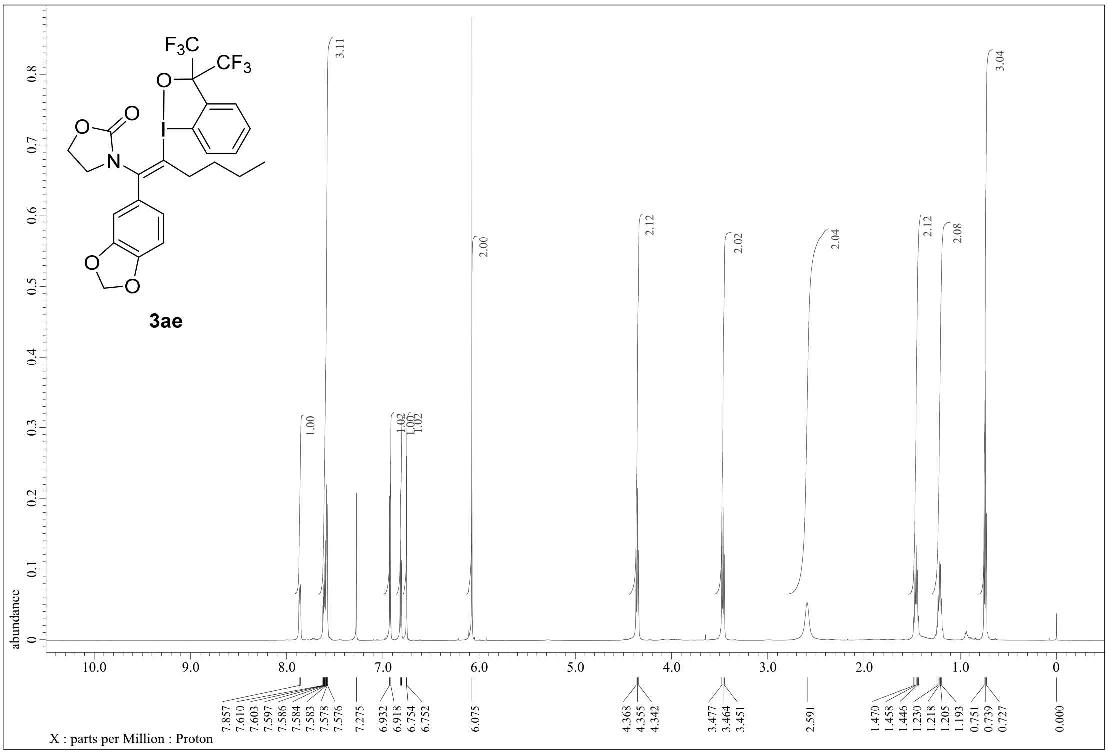


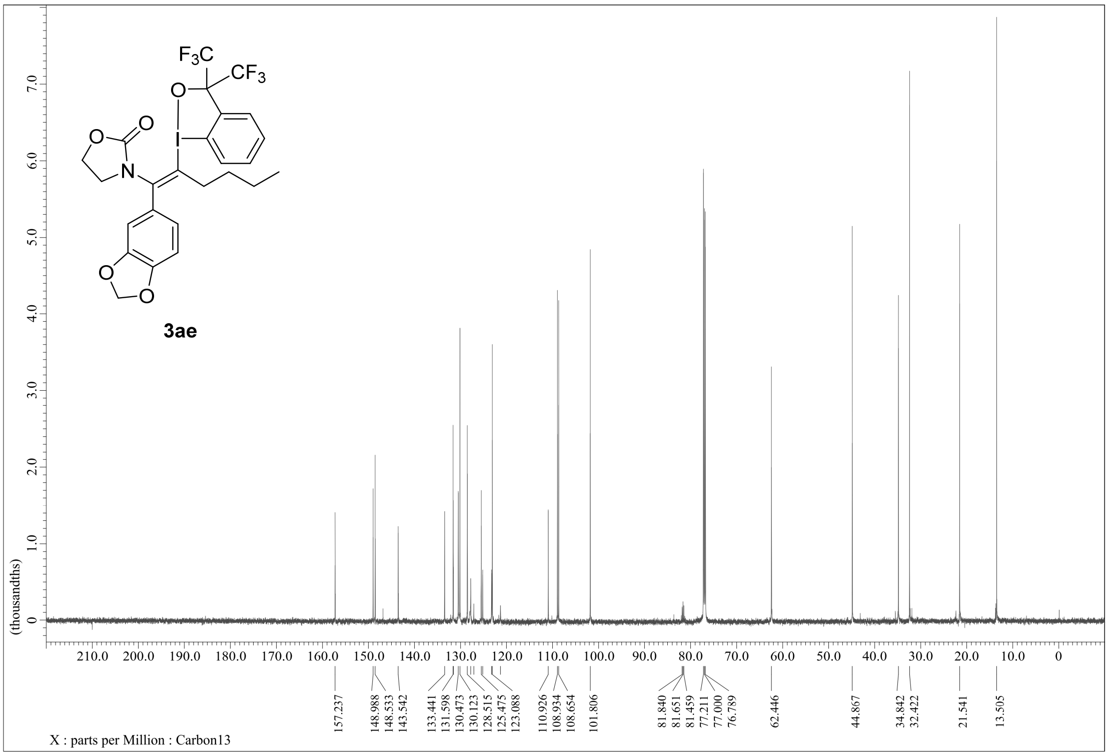


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ad**

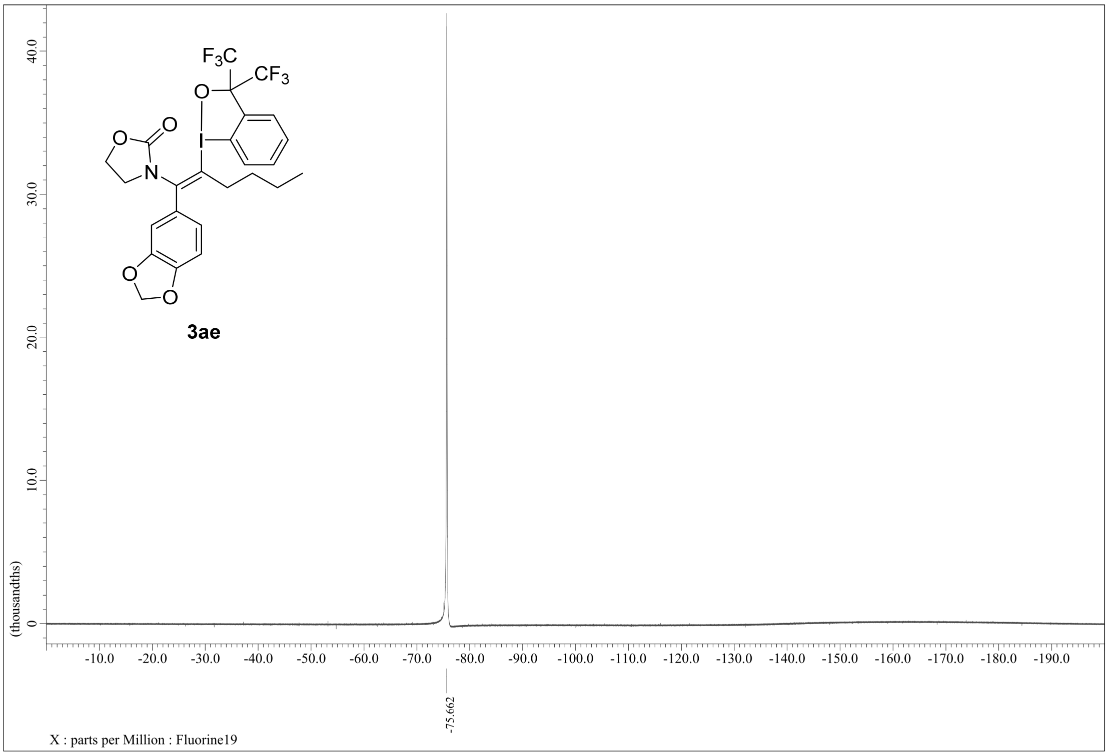


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3ae**

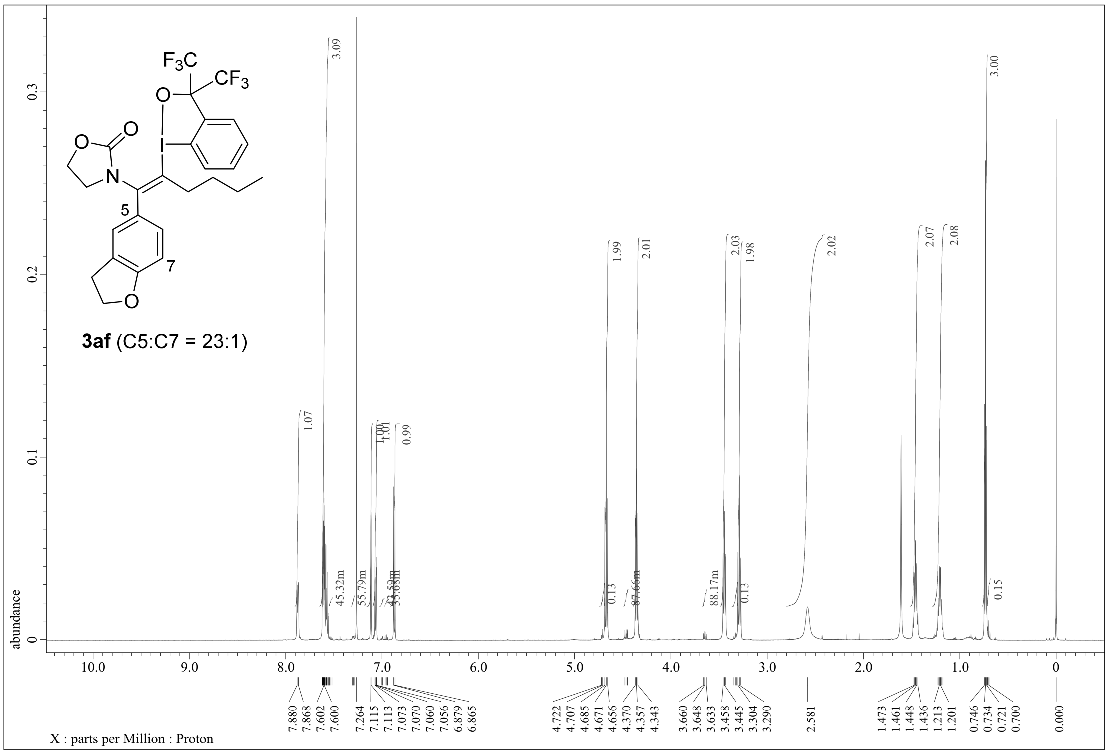


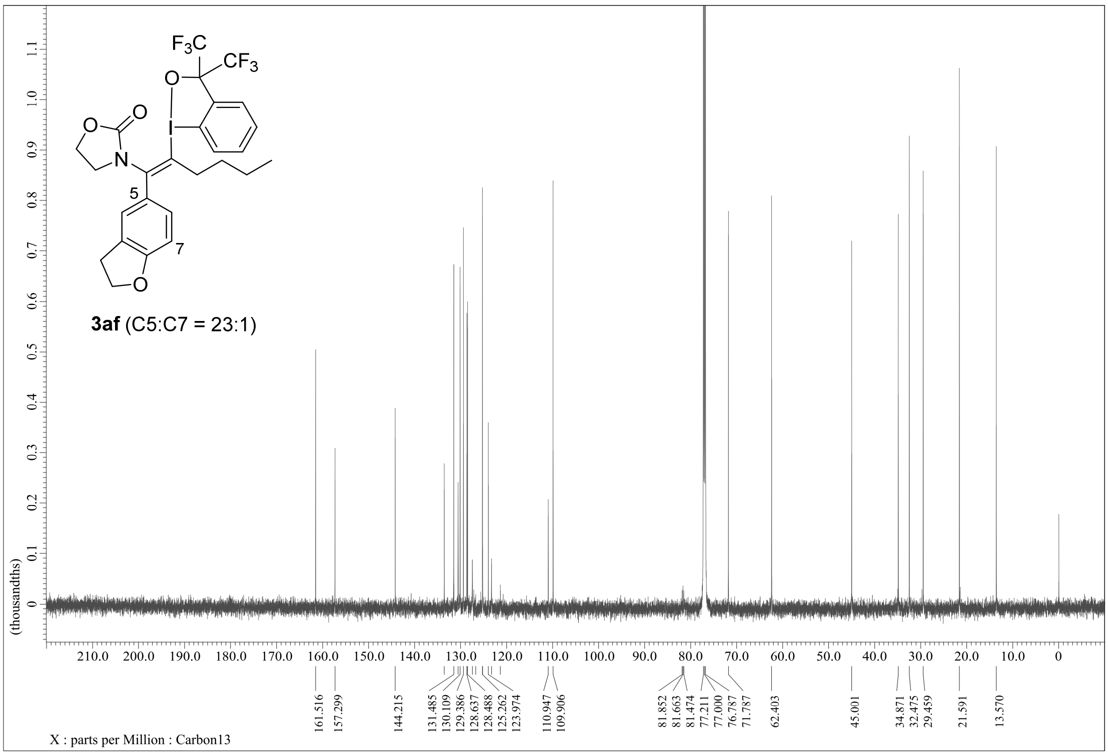


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ae**

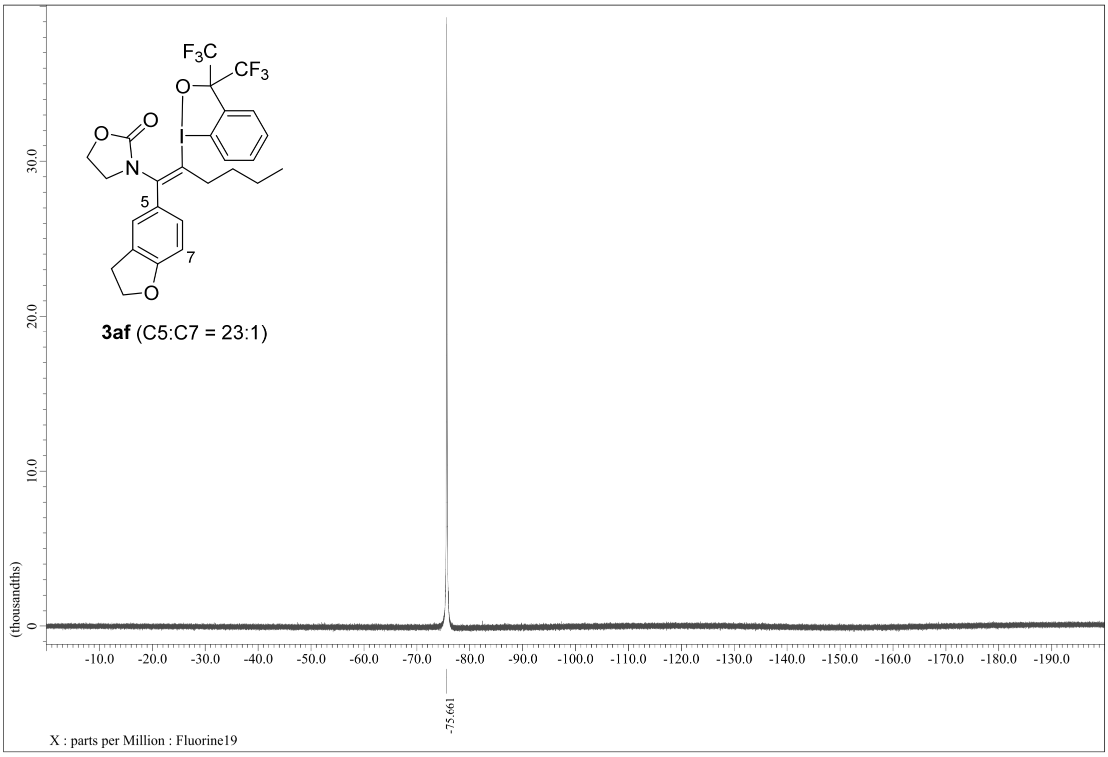


[1]H NMR (600 MHz, $CDCl_3$) and [13]C{[1]H} NMR (151 MHz, $CDCl_3$) spectra of **3af**

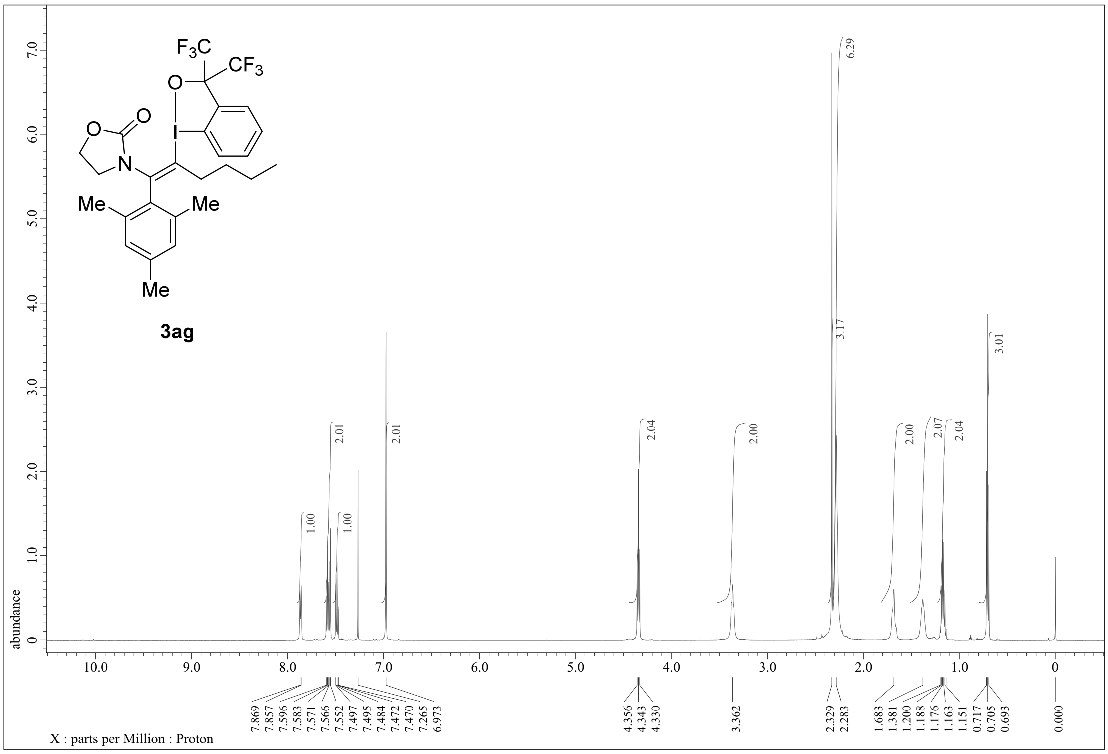


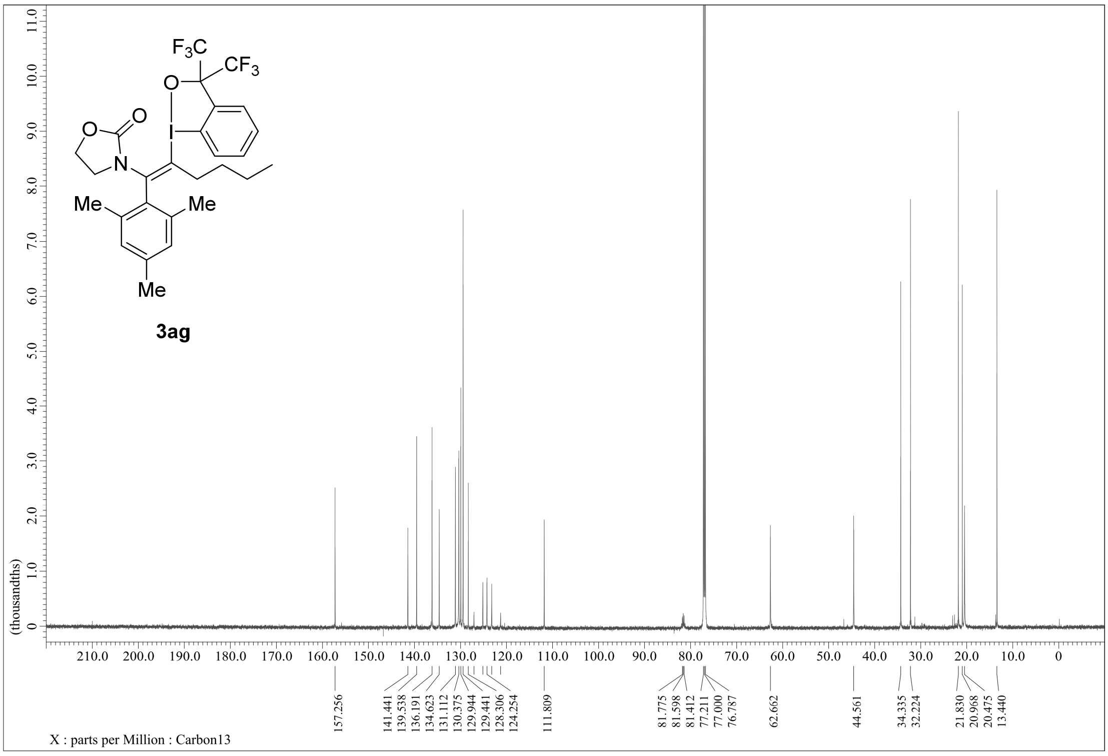


$^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3af**

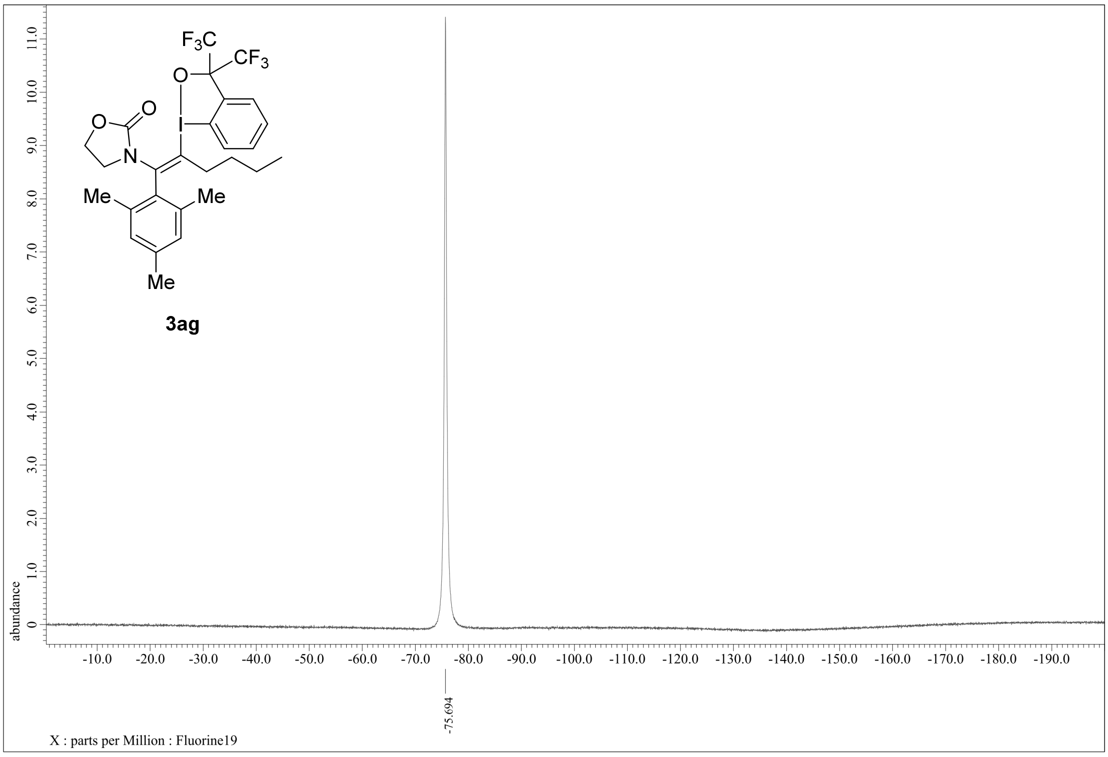


[1]H NMR (600 MHz, $CDCl_3$) and [13]C{[1]H} NMR (151 MHz, $CDCl_3$) spectra of **3ag**

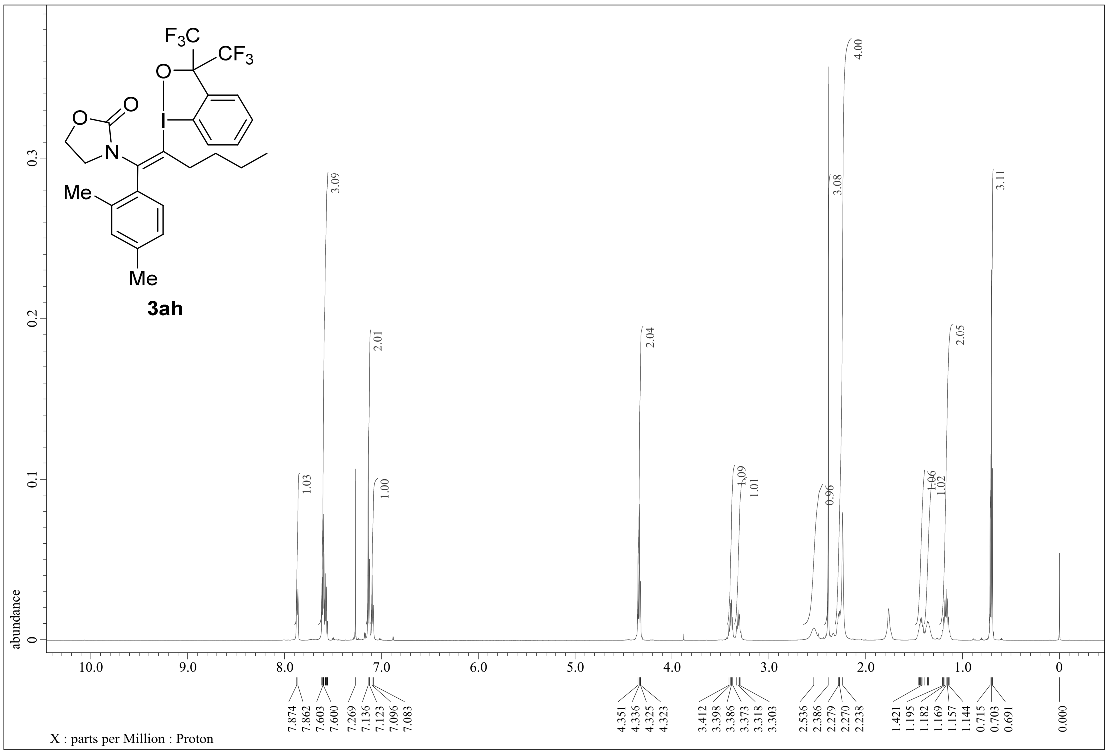


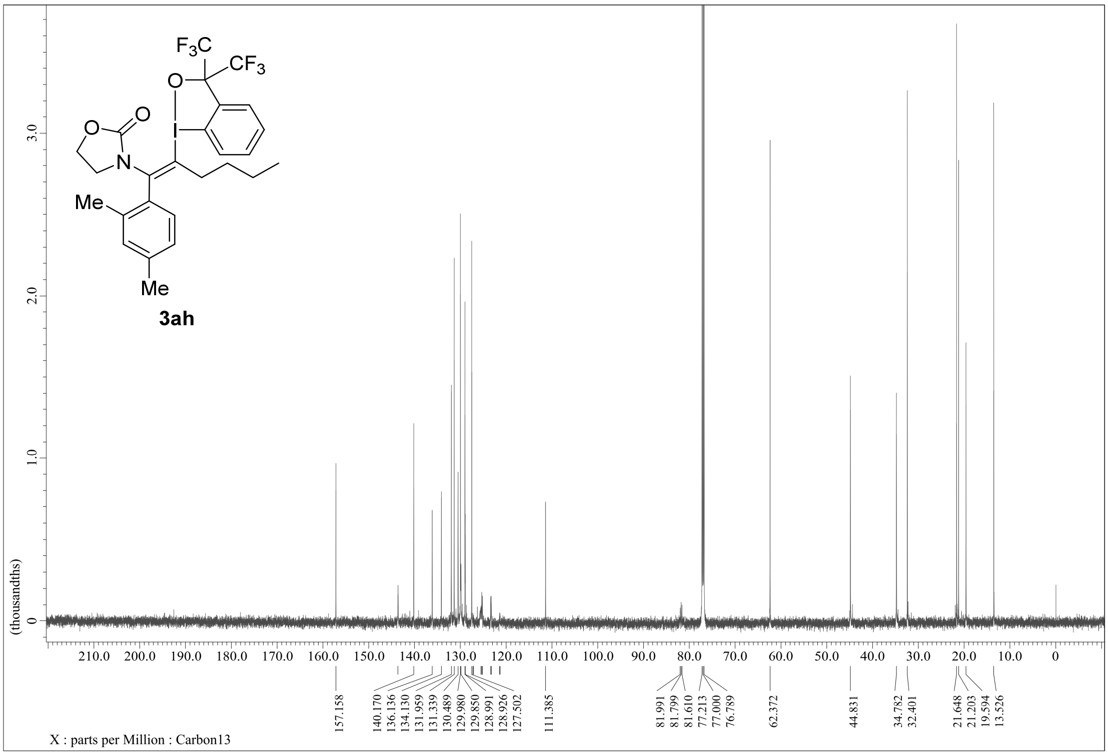


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ag**

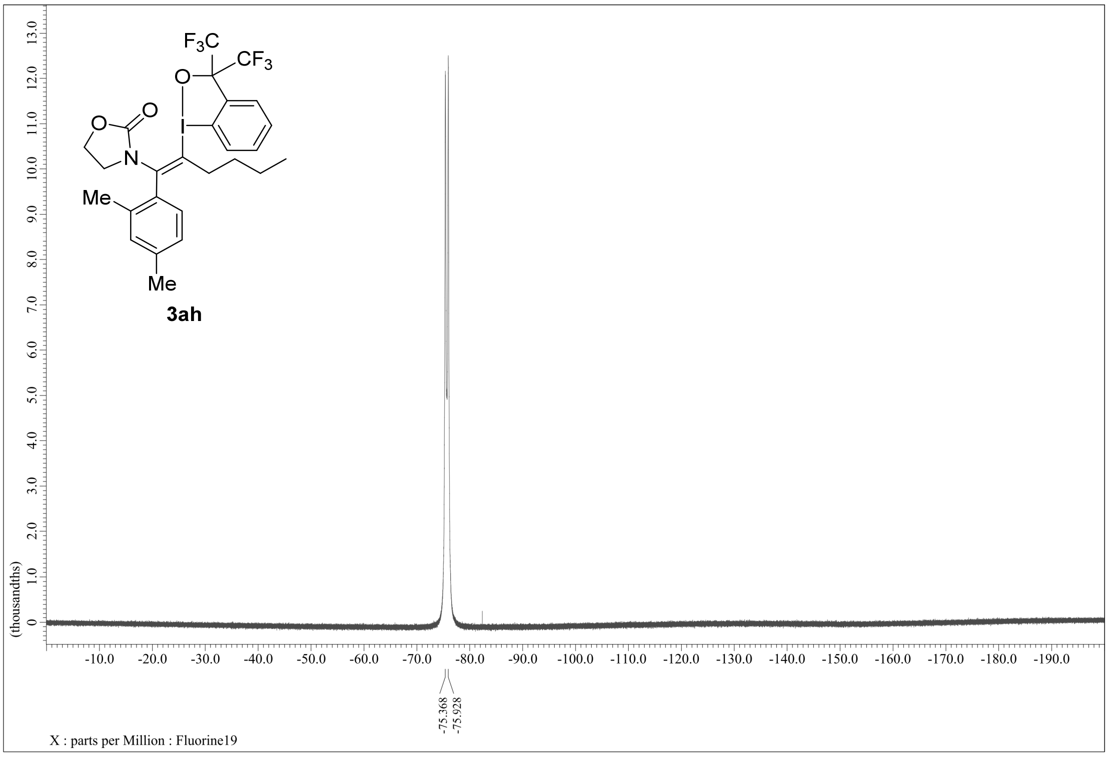


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3ah**

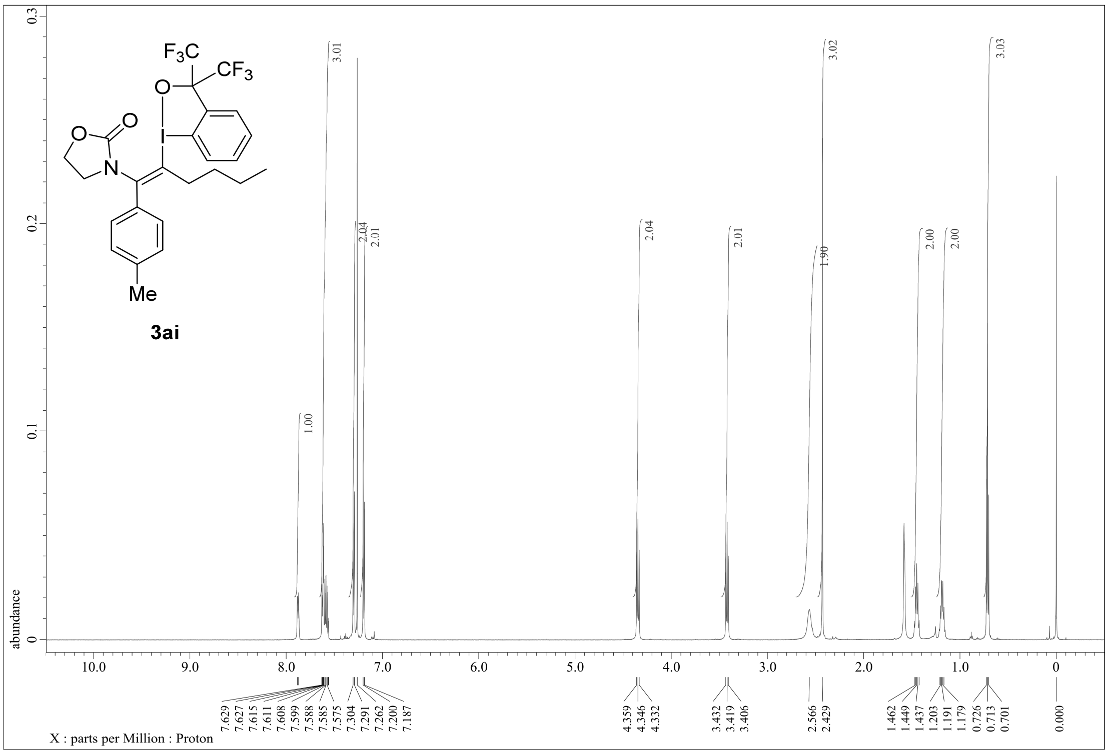


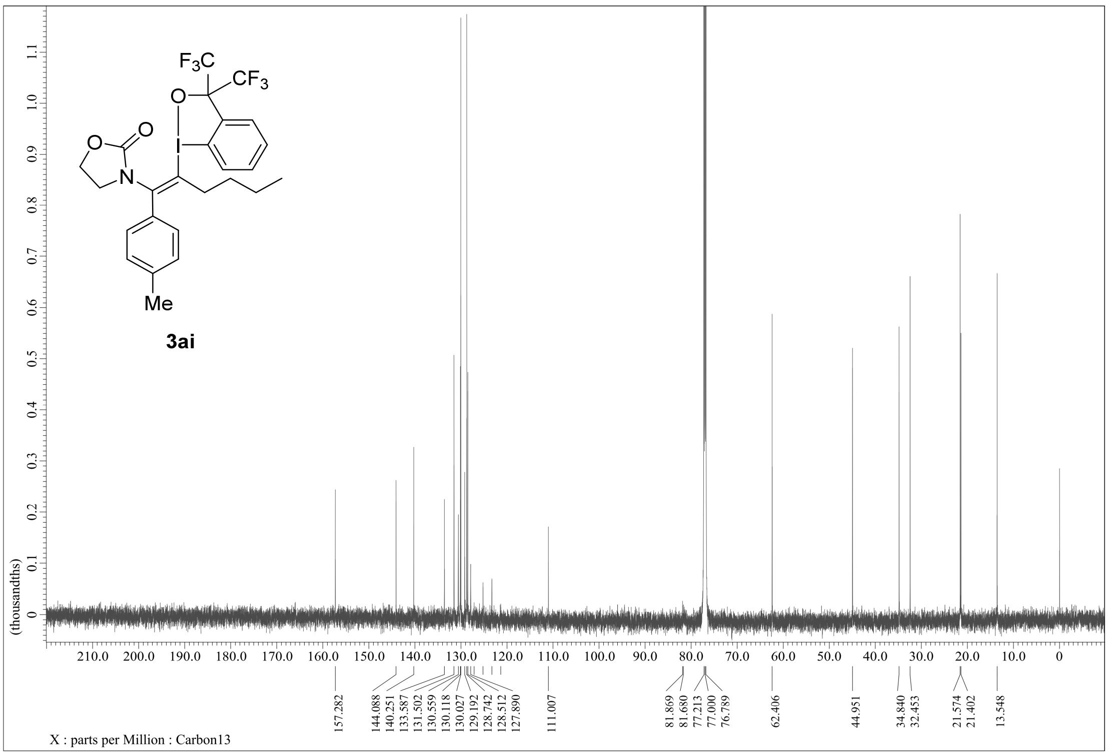


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ah**

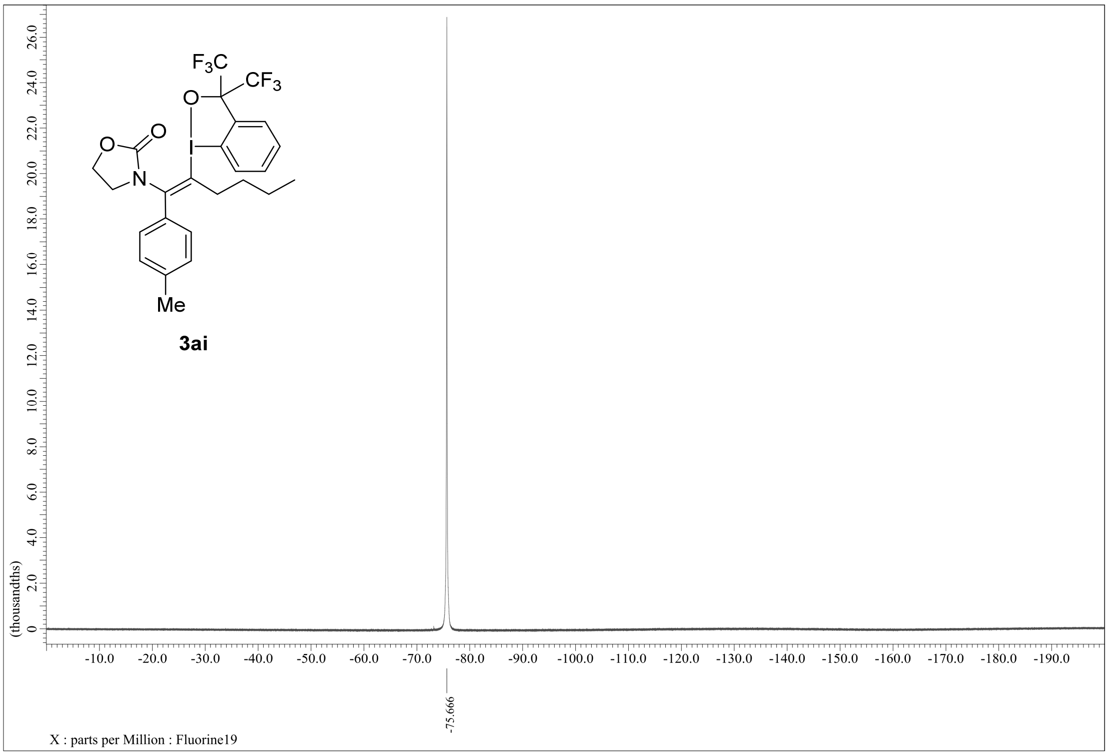


[1]H NMR (600 MHz, $CDCl_3$) and [13]C{[1]H} NMR (151 MHz, $CDCl_3$) spectra of **3ai**

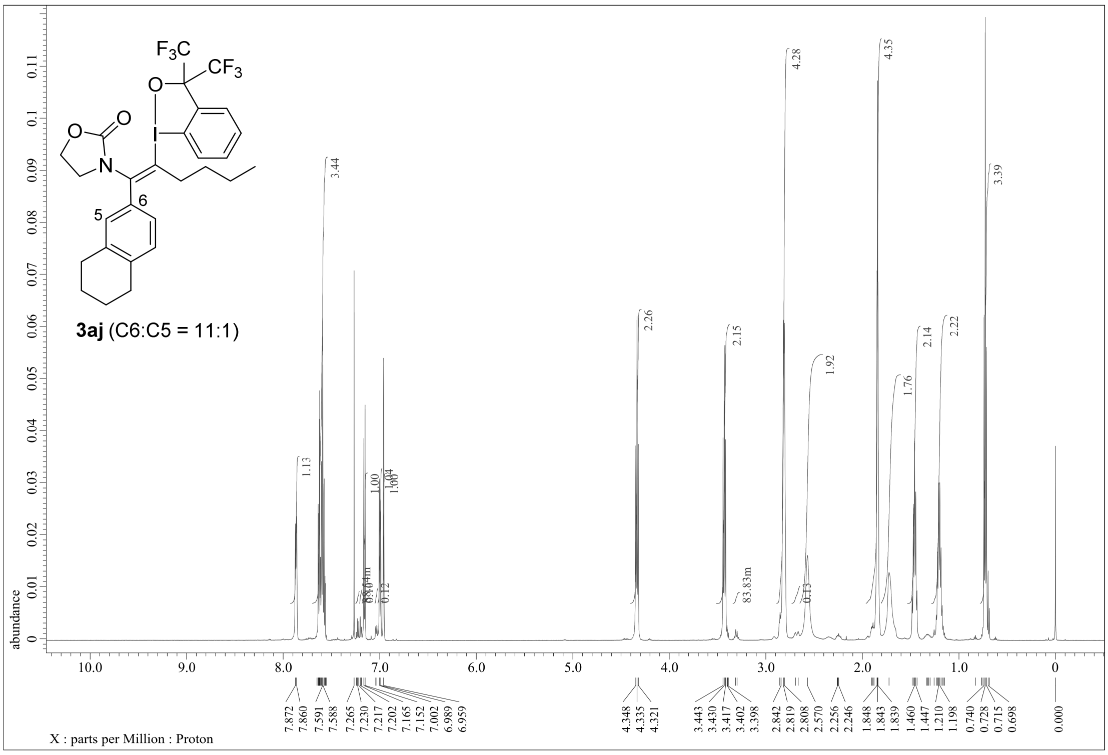


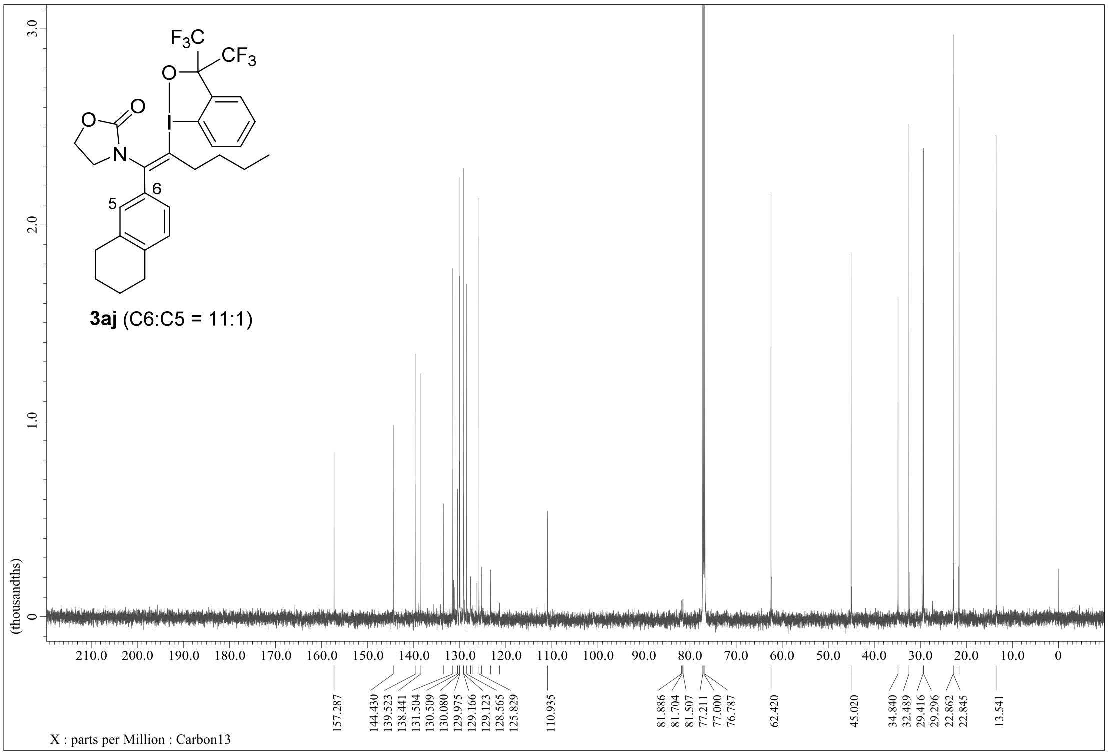


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ai**

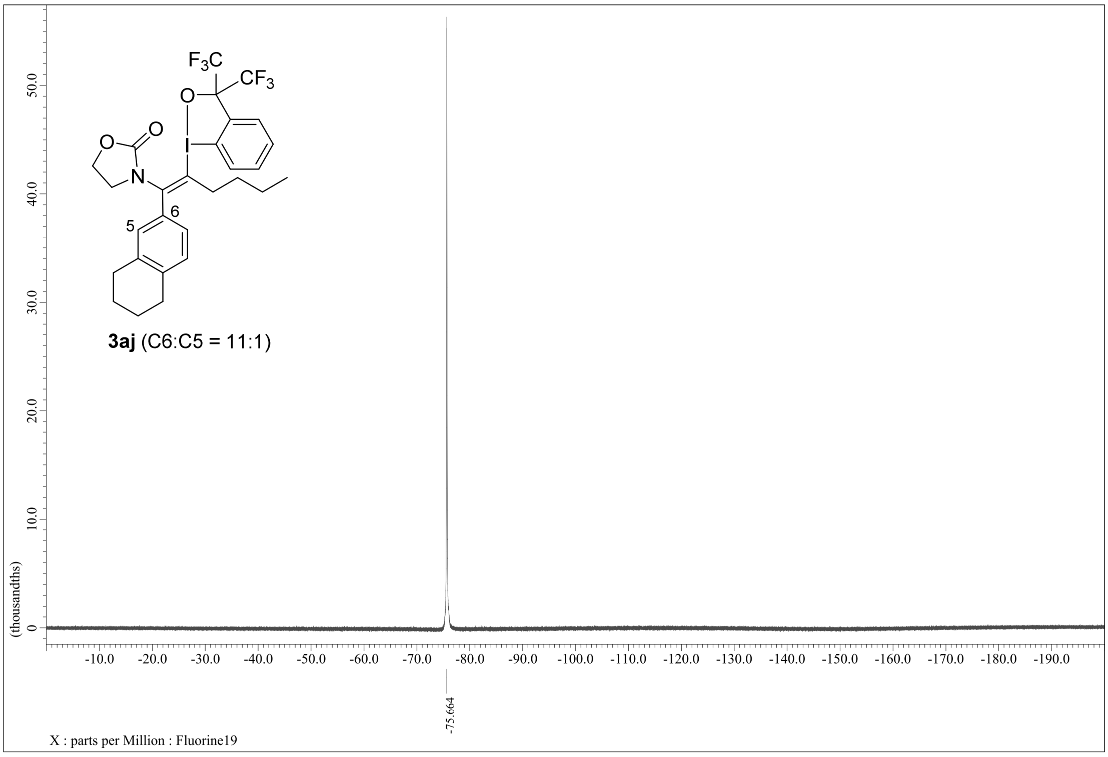


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3aj**

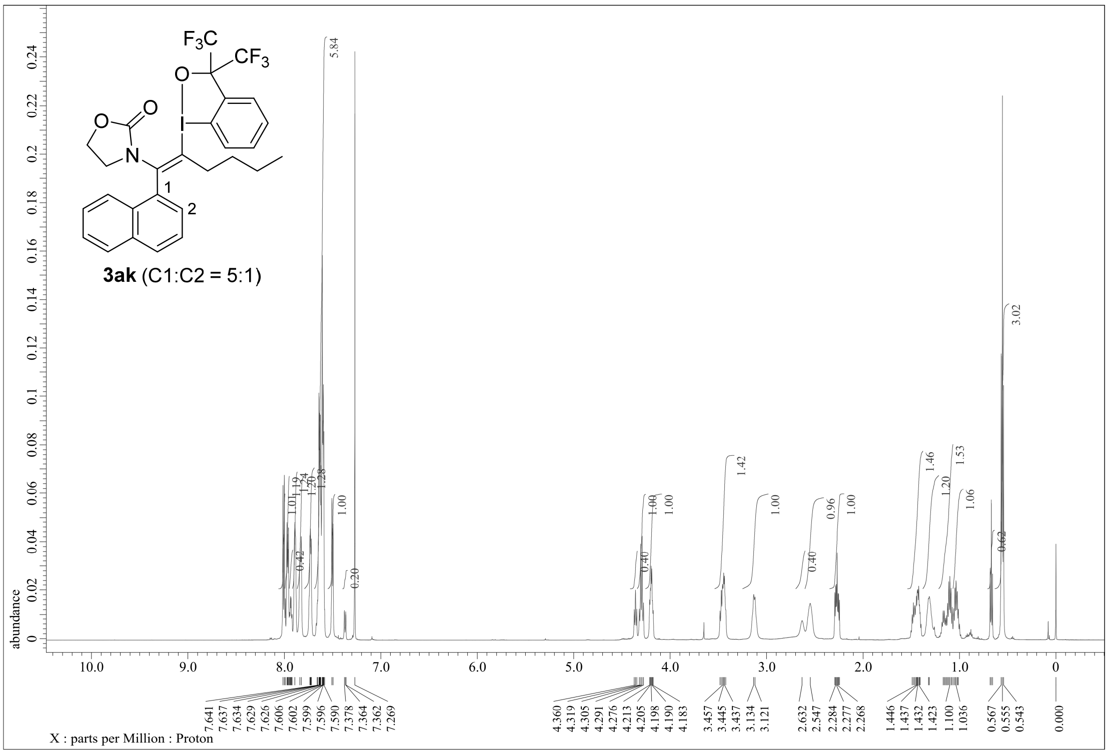


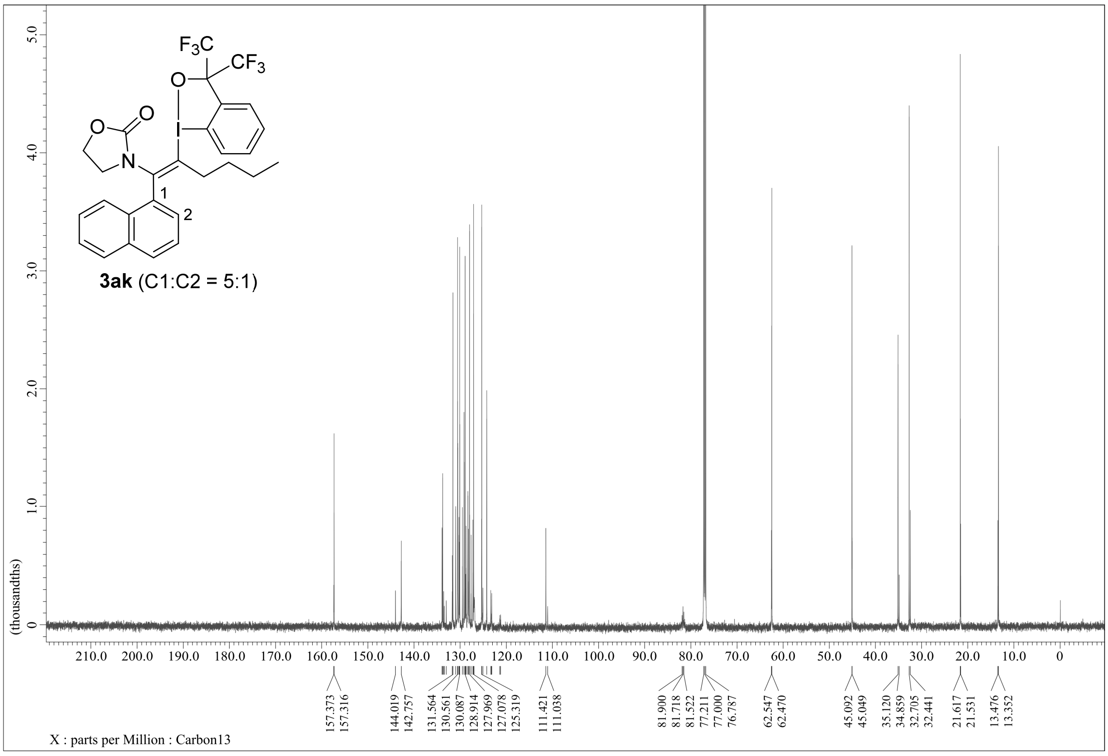


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3aj**

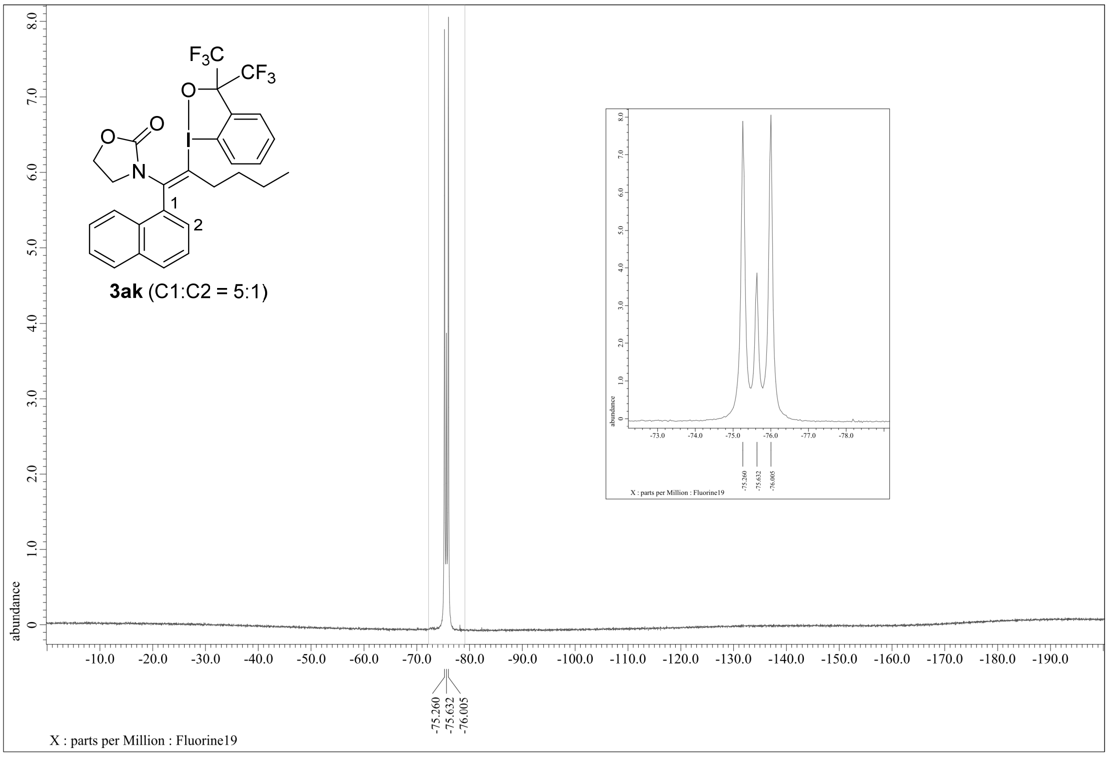


[1]H NMR (600 MHz, $CDCl_3$) and [13]C{[1]H} NMR (151 MHz, $CDCl_3$) spectra of **3ak**

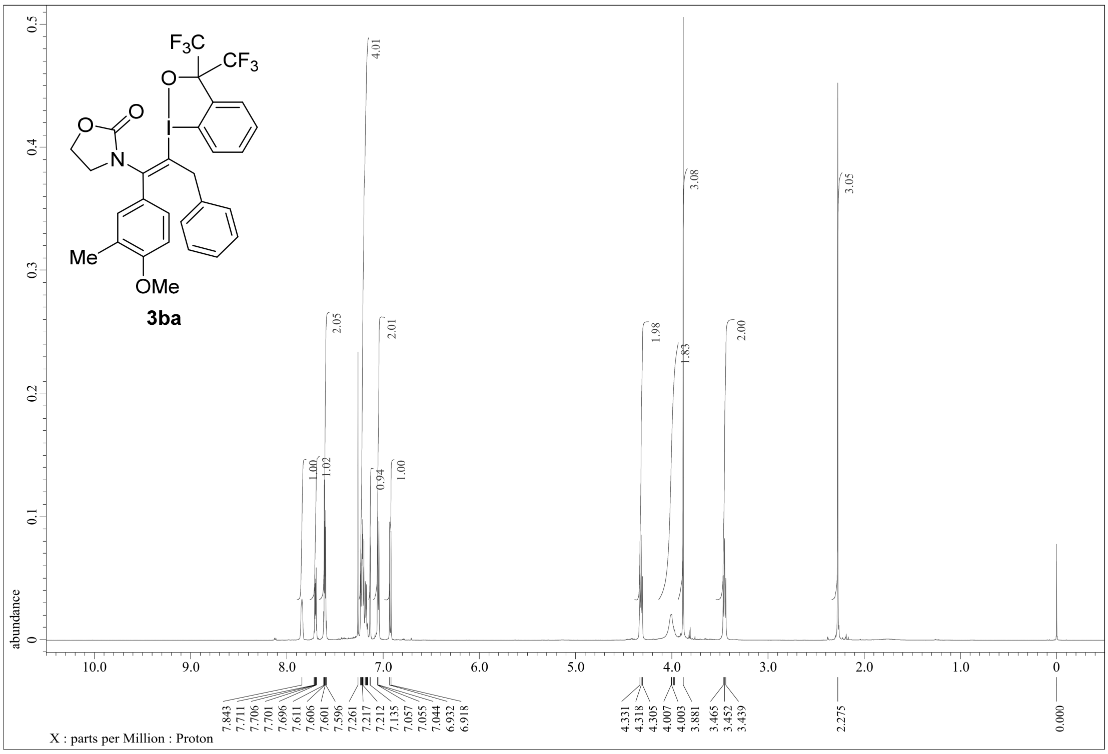


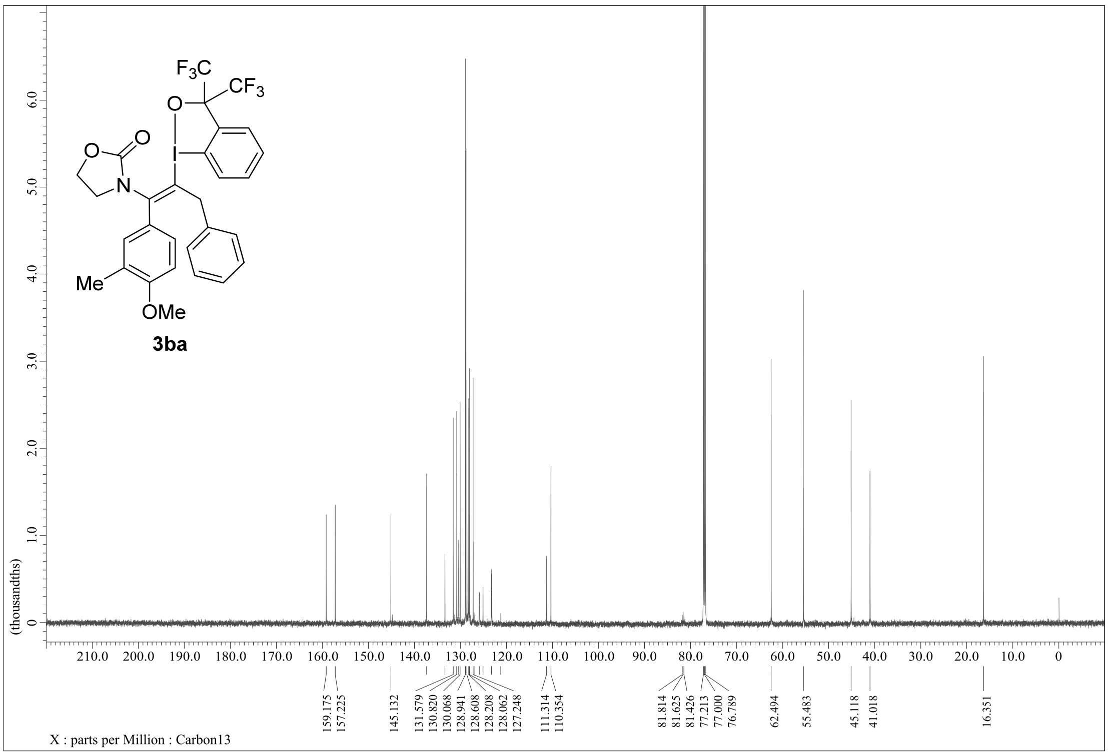


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ak**

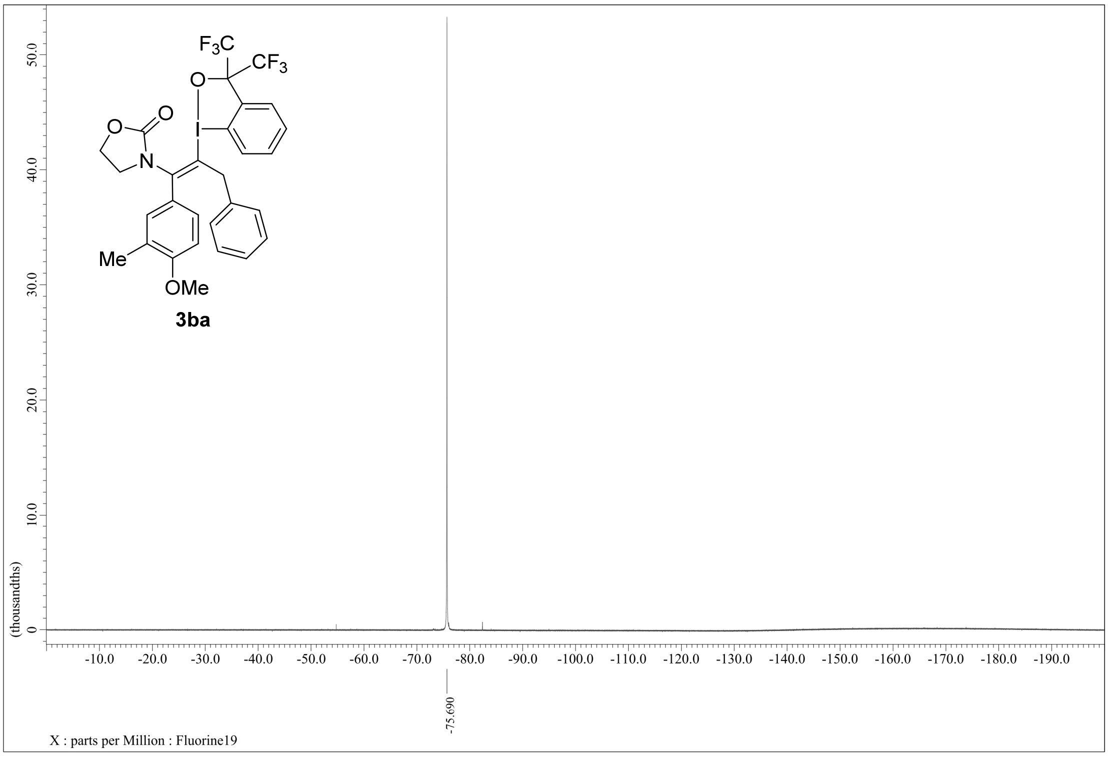


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3ba**

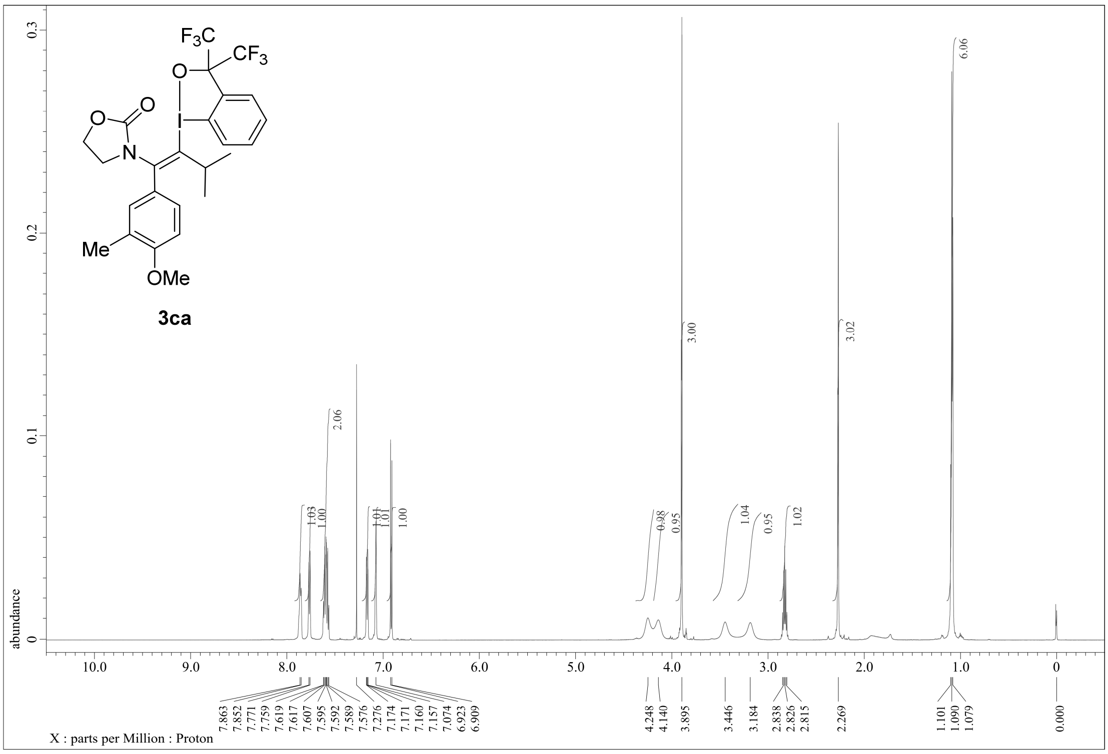


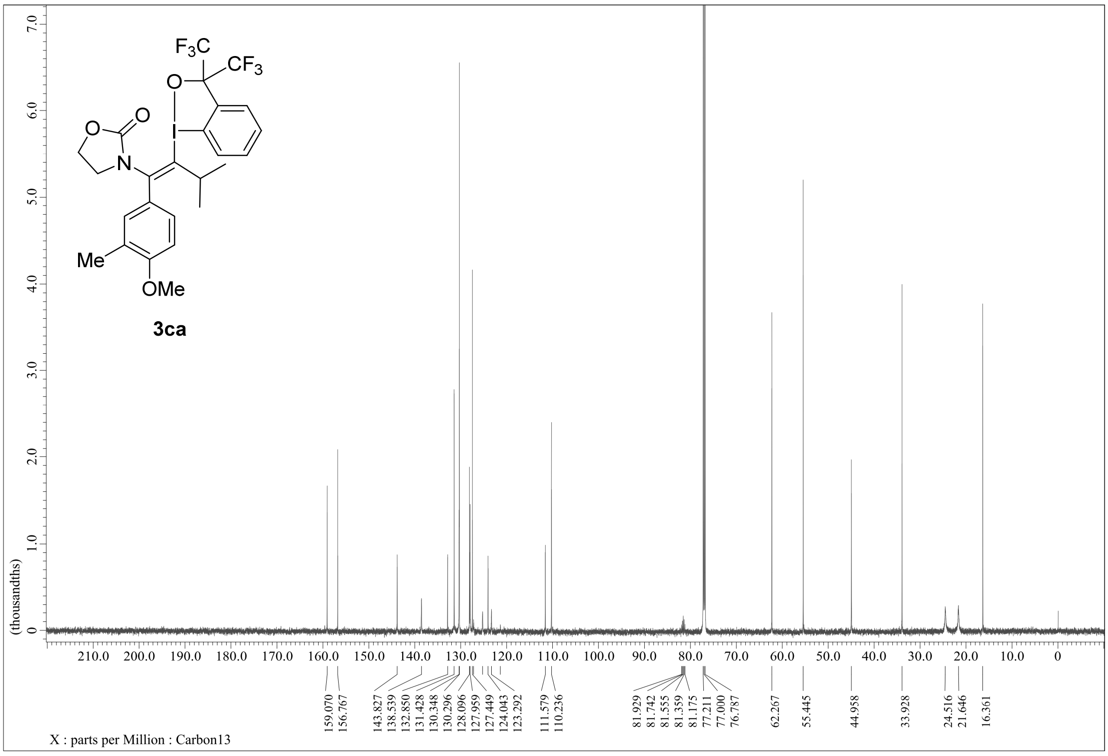


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ba**

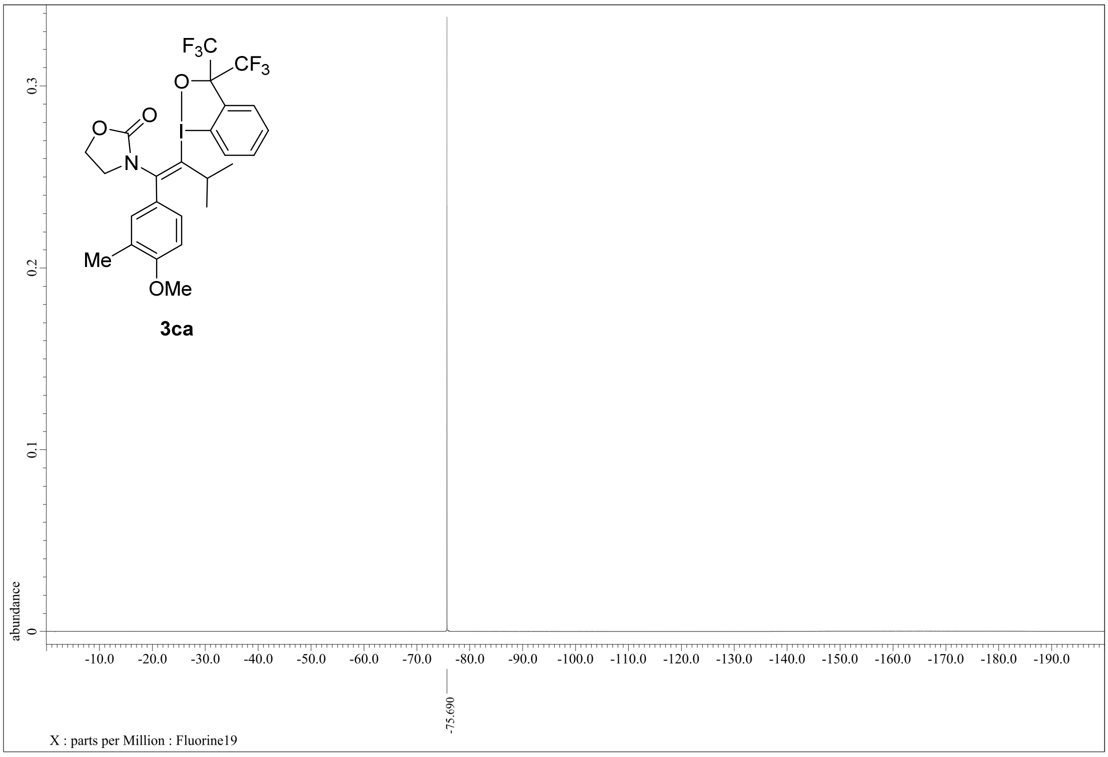


[1]H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3ca**

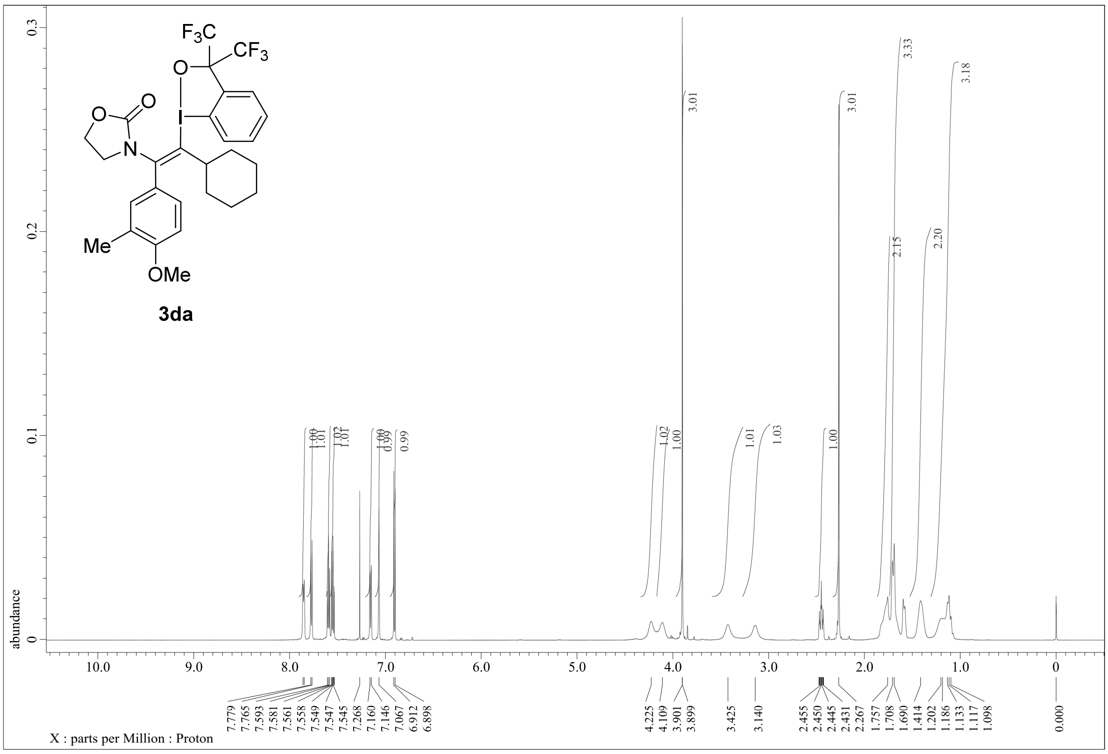


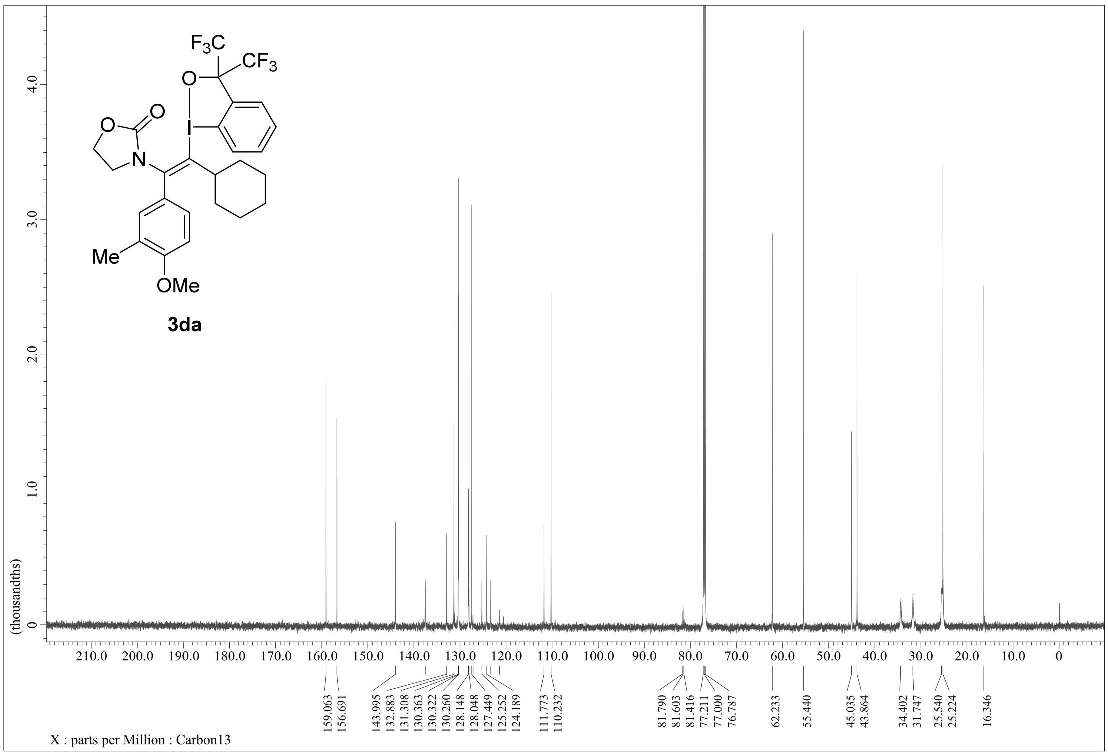


$^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ca**

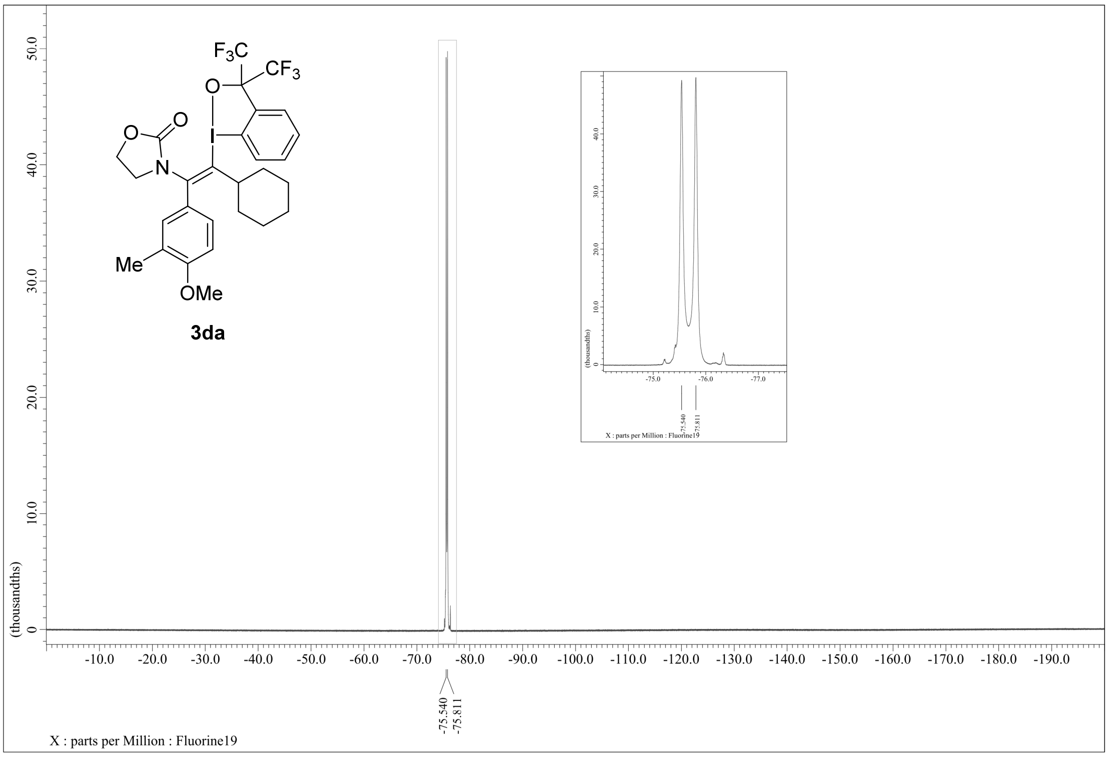


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3da**

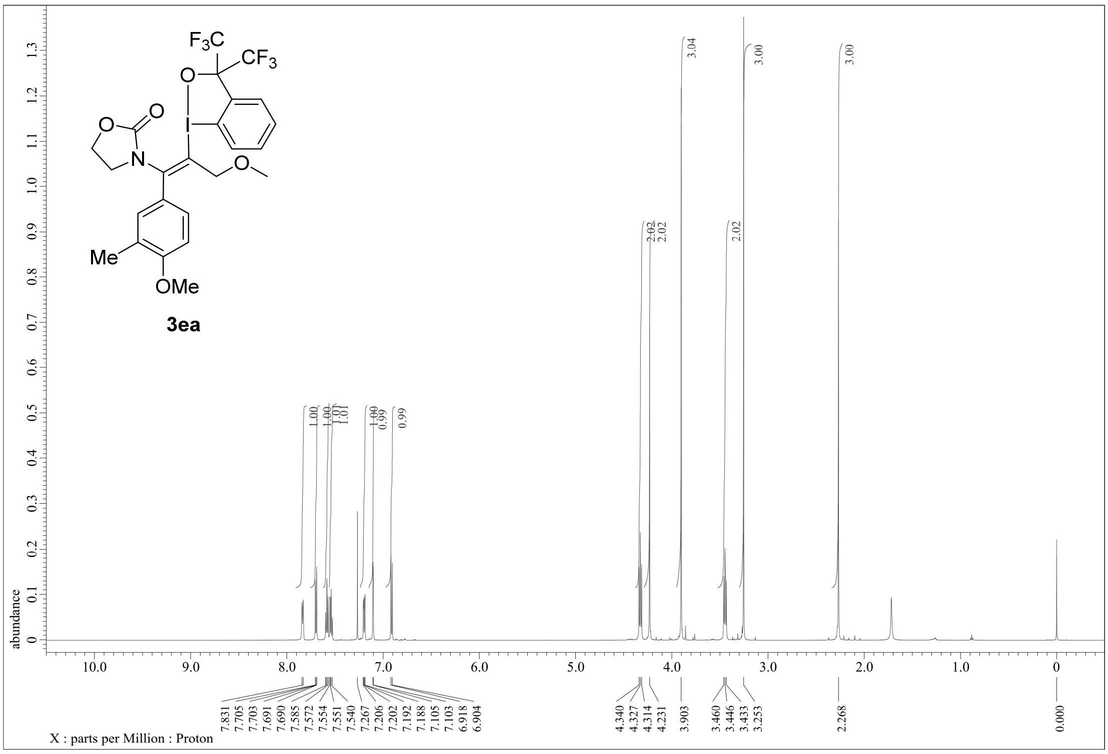


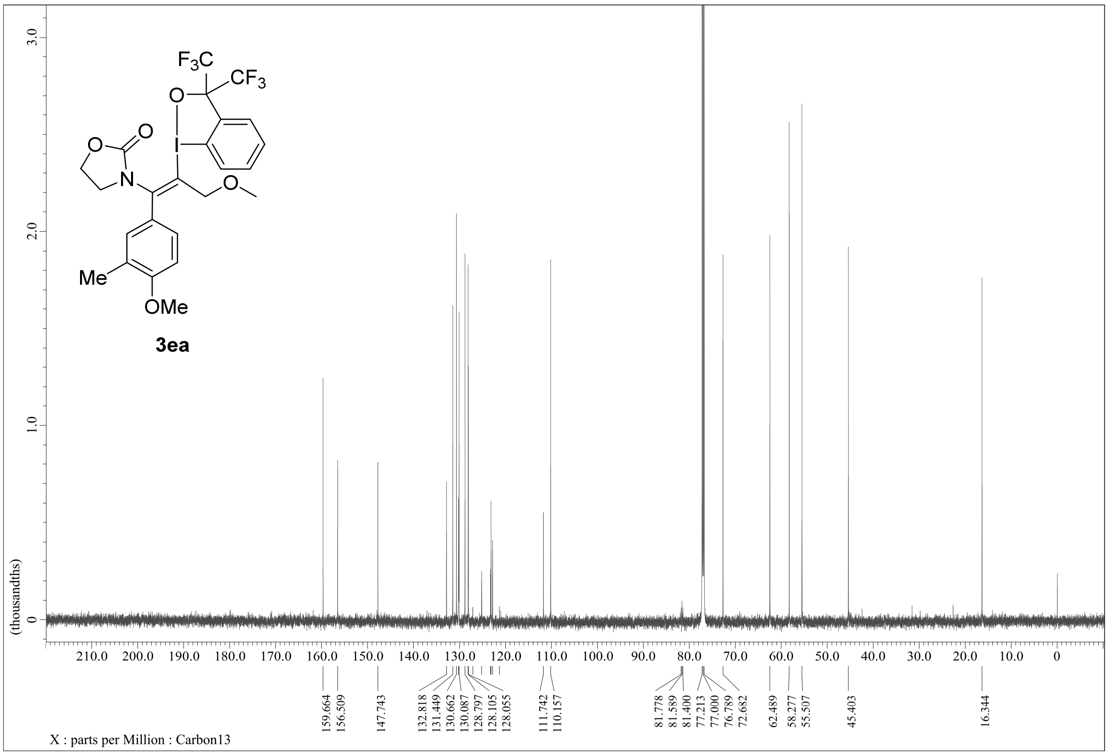


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3da**

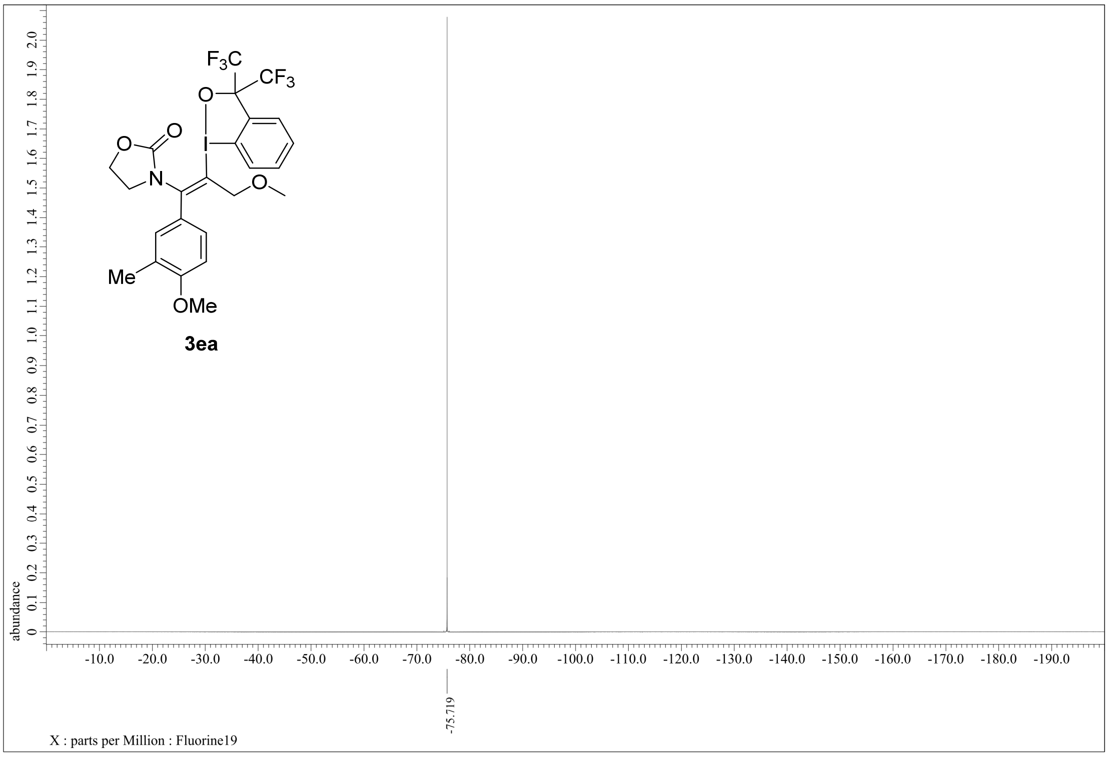


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3ea**

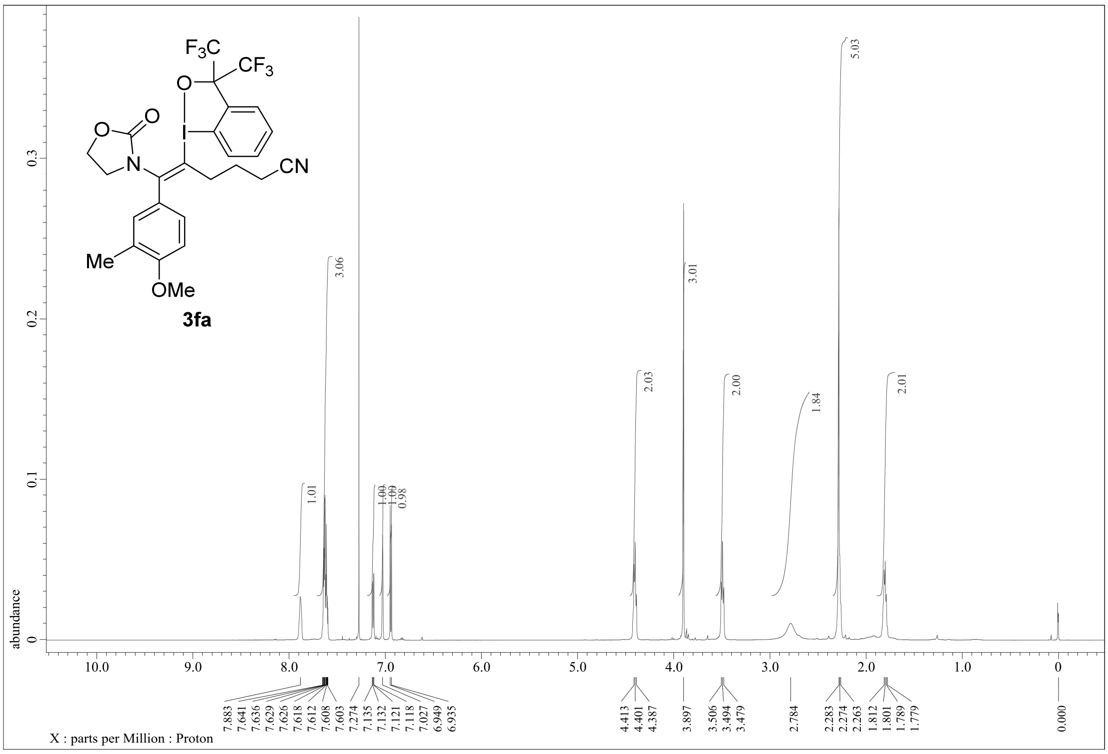


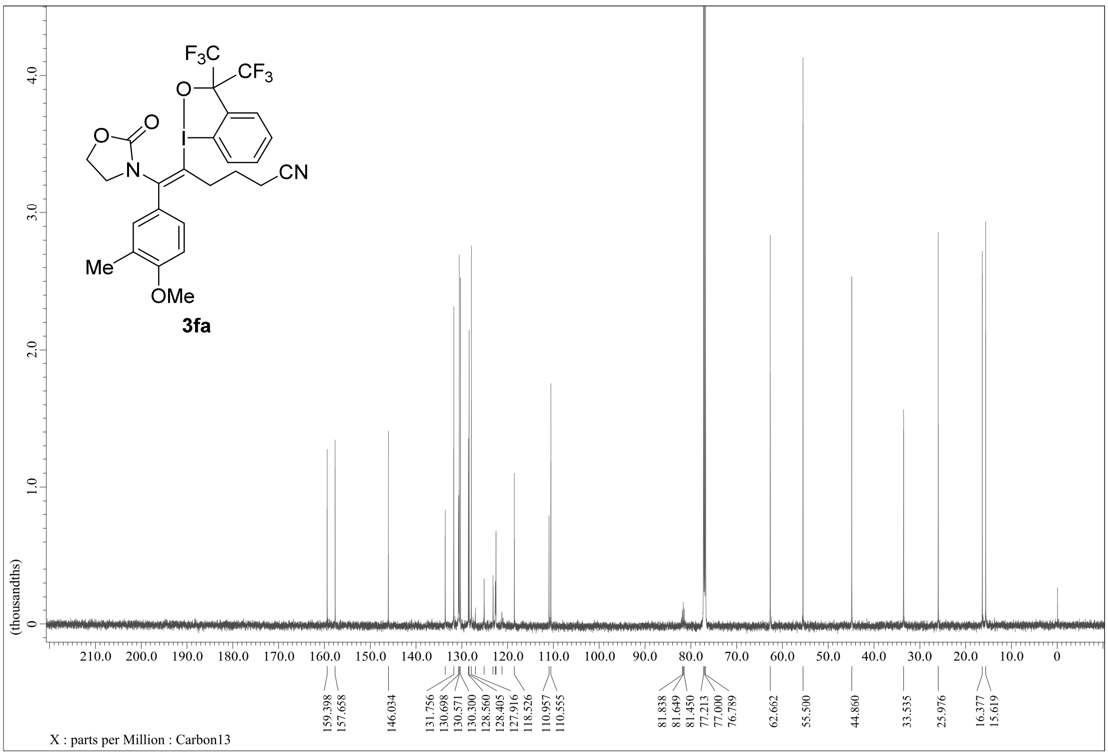


[19]F{[1]H} NMR (565 MHz, $CDCl_3$) spectrum of **3ea**

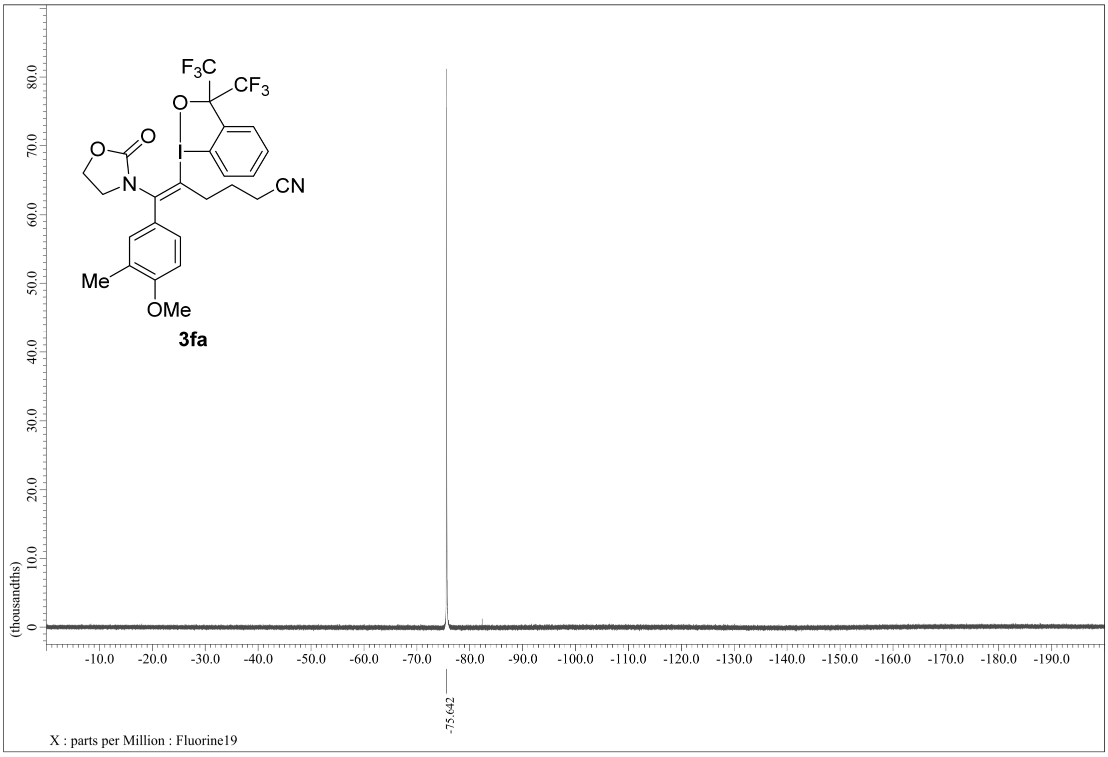


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3fa**

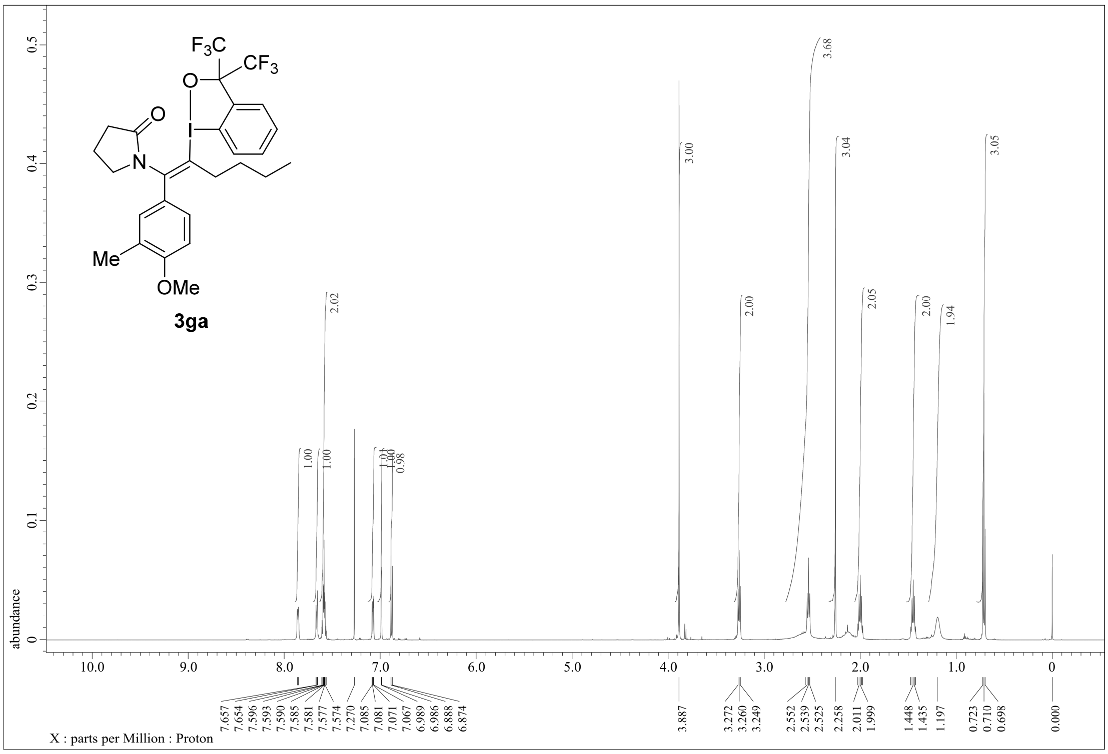


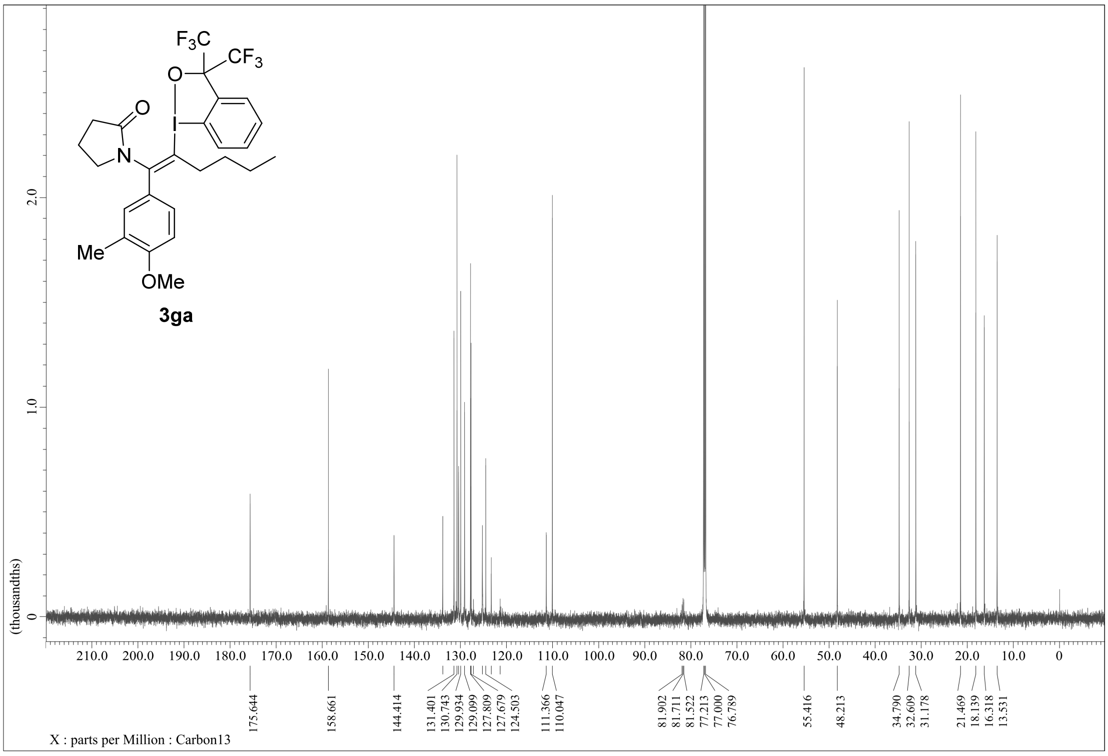


$^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3fa**

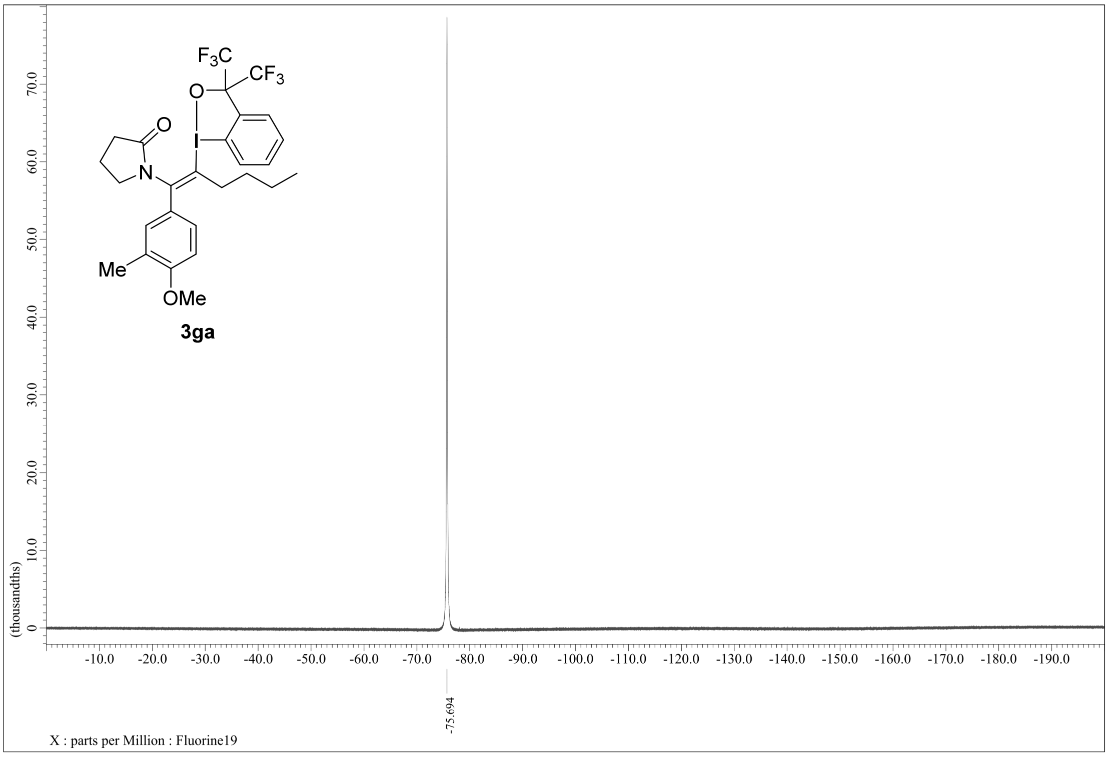


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3ga**

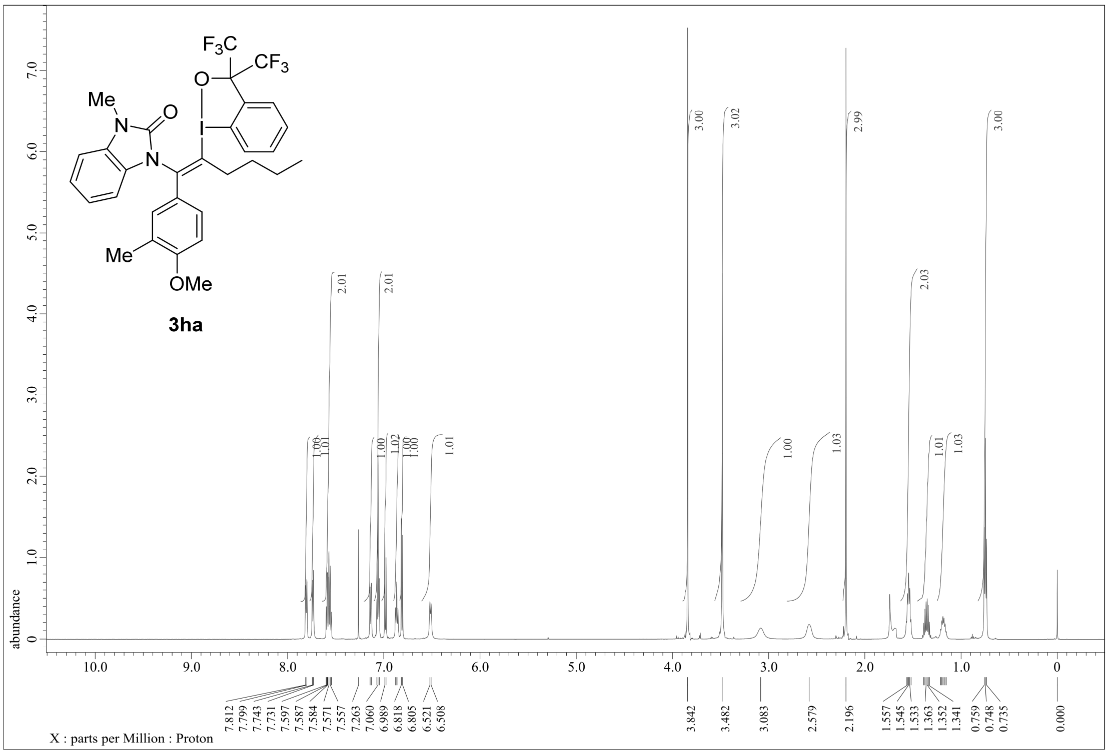


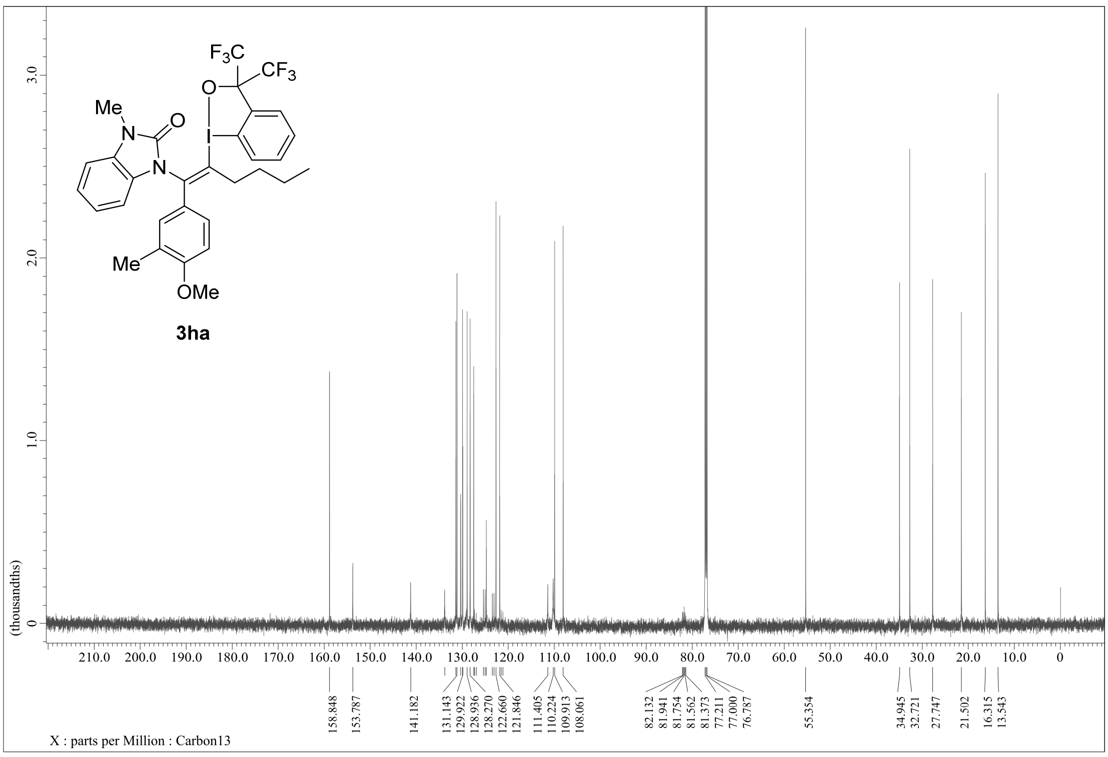


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ga**

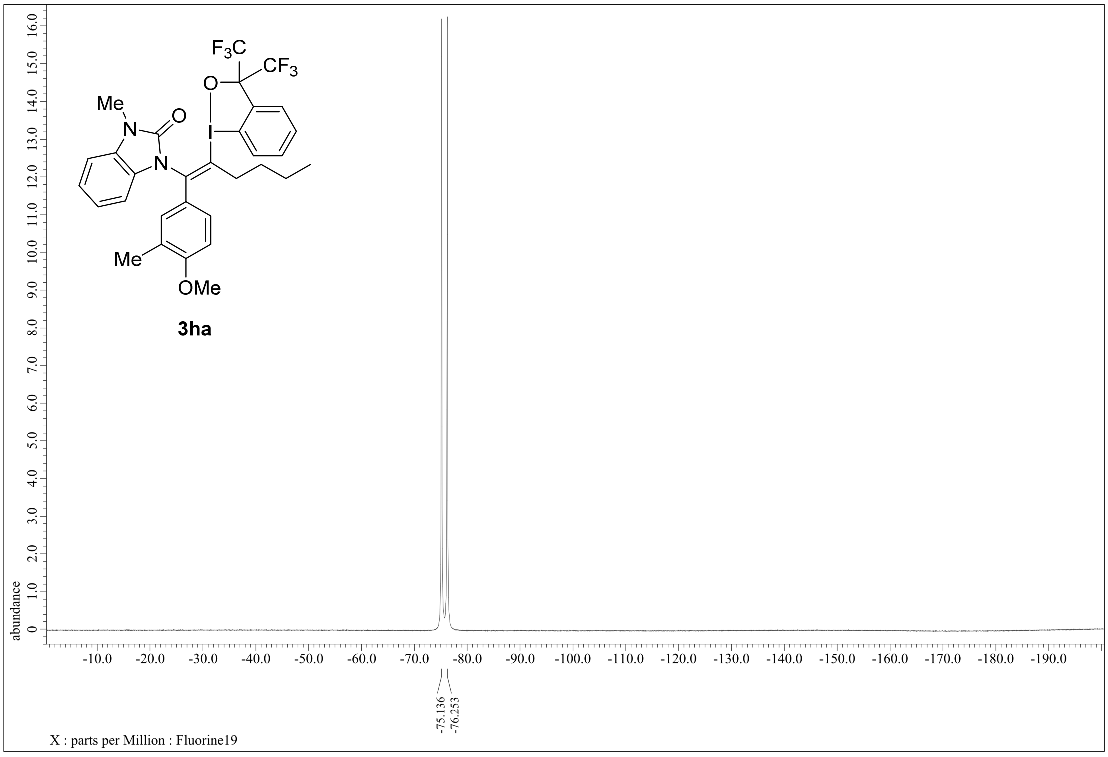


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3ha**

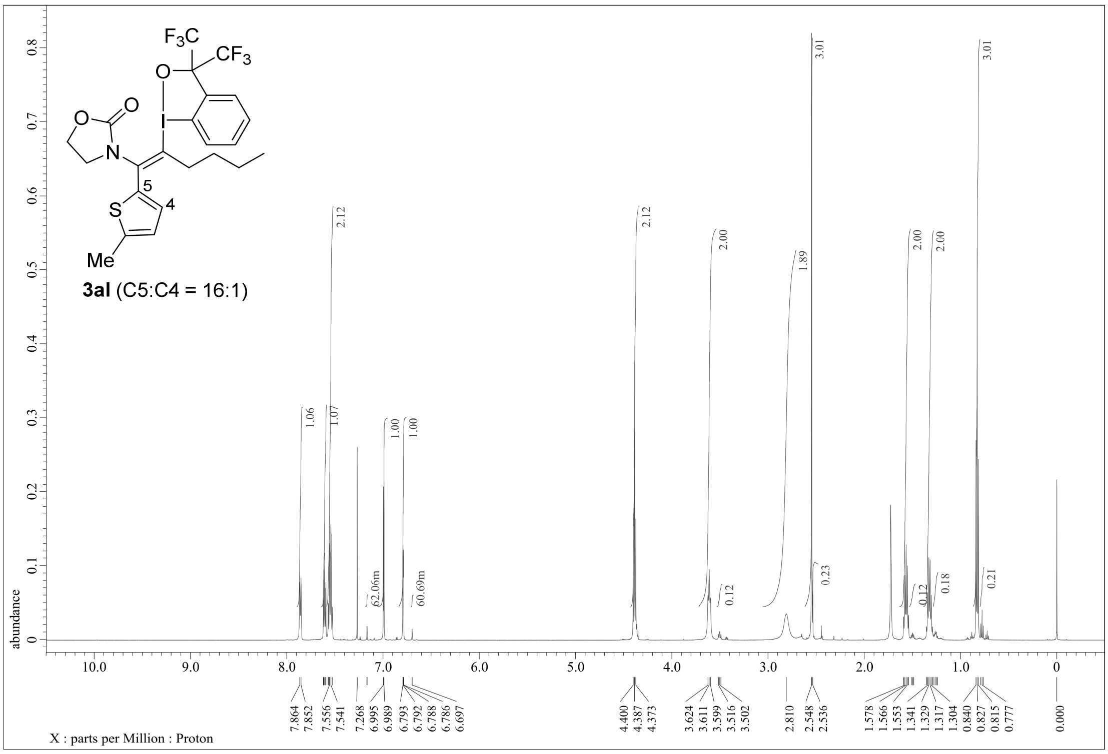


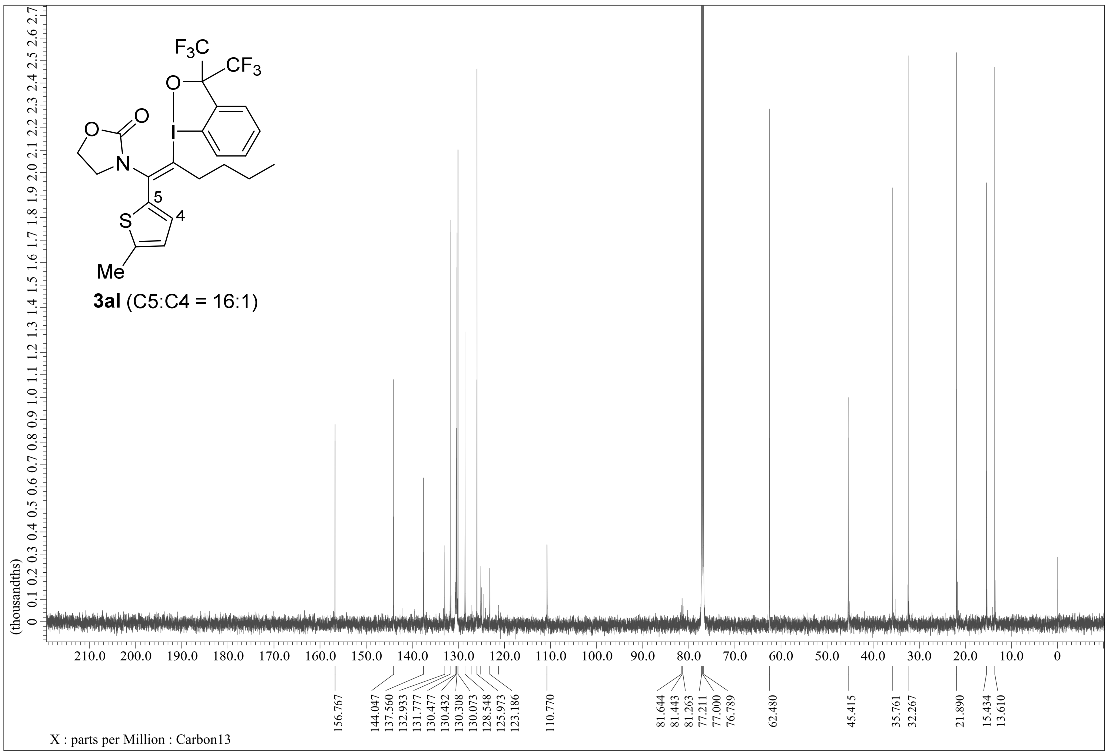


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ha**

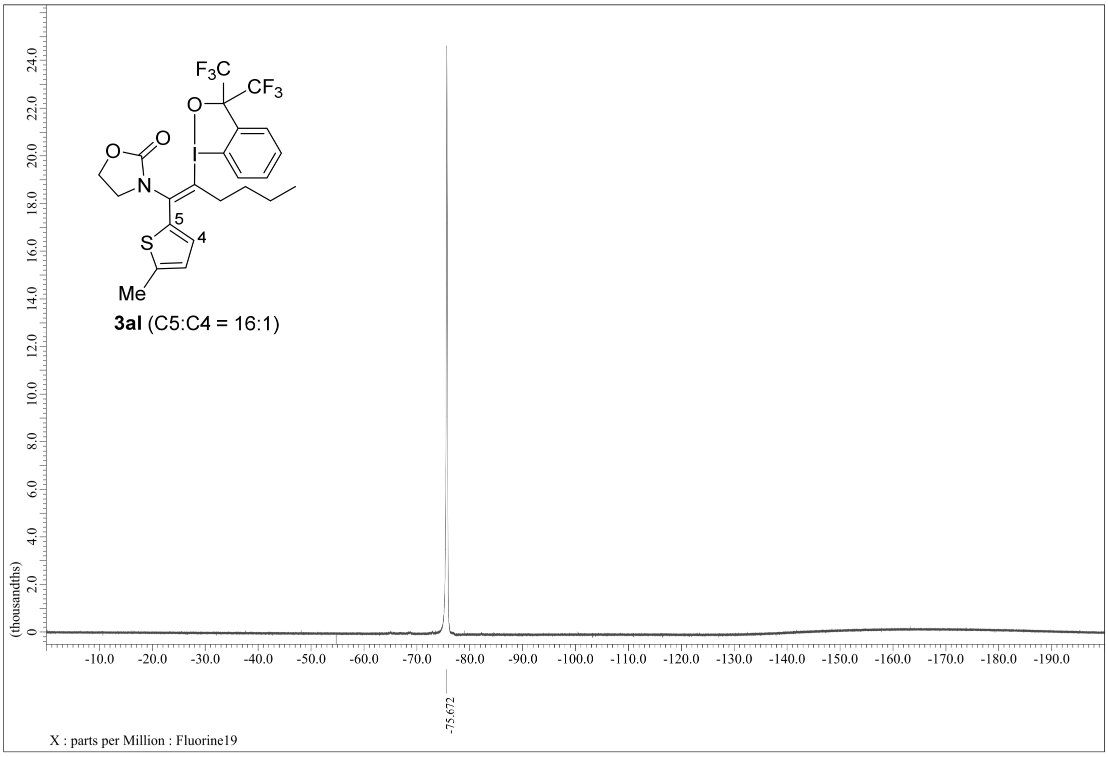


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3al**

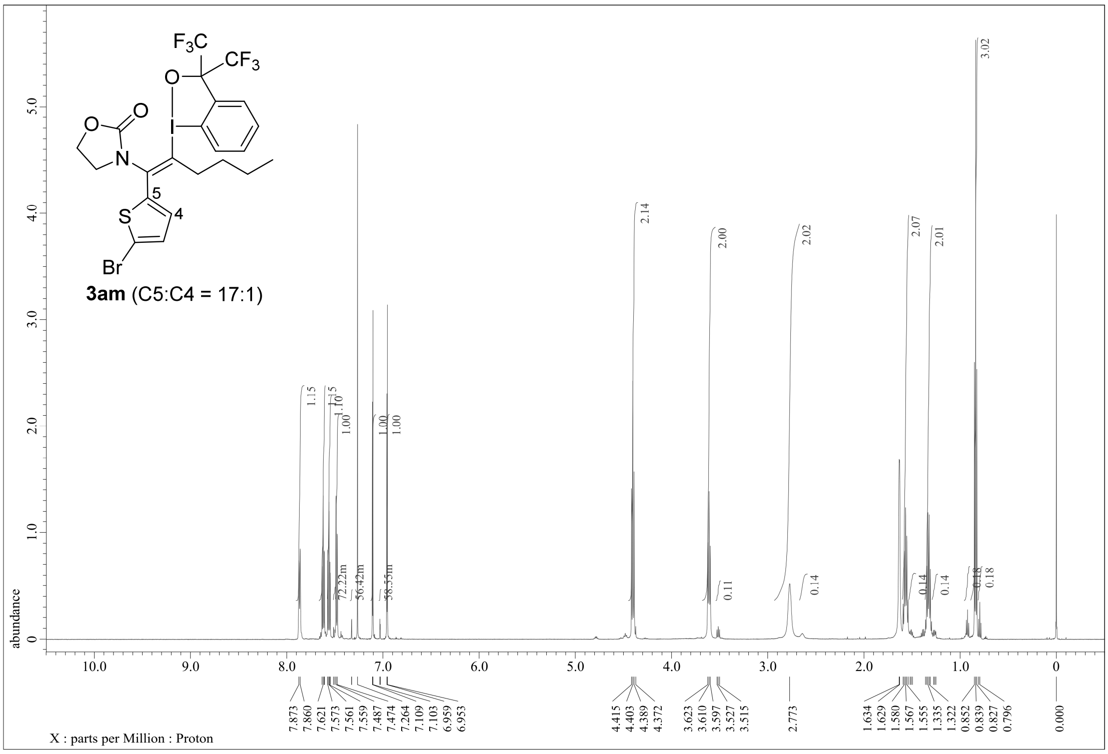


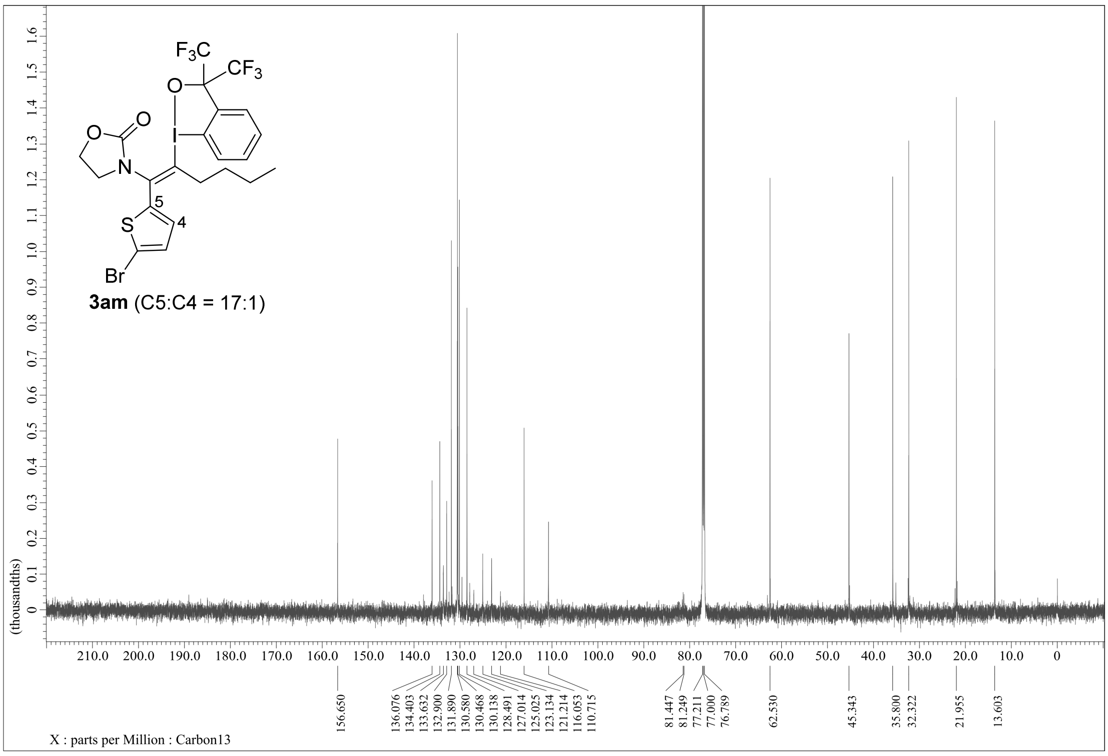


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3al**

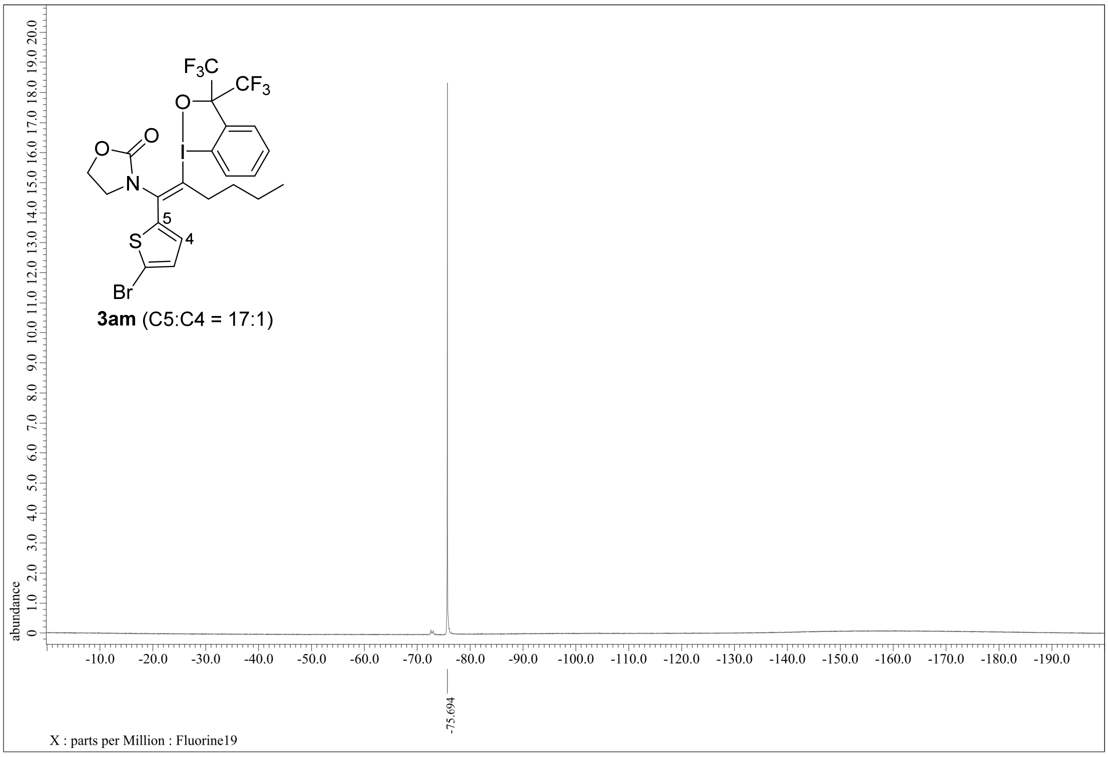


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3am**

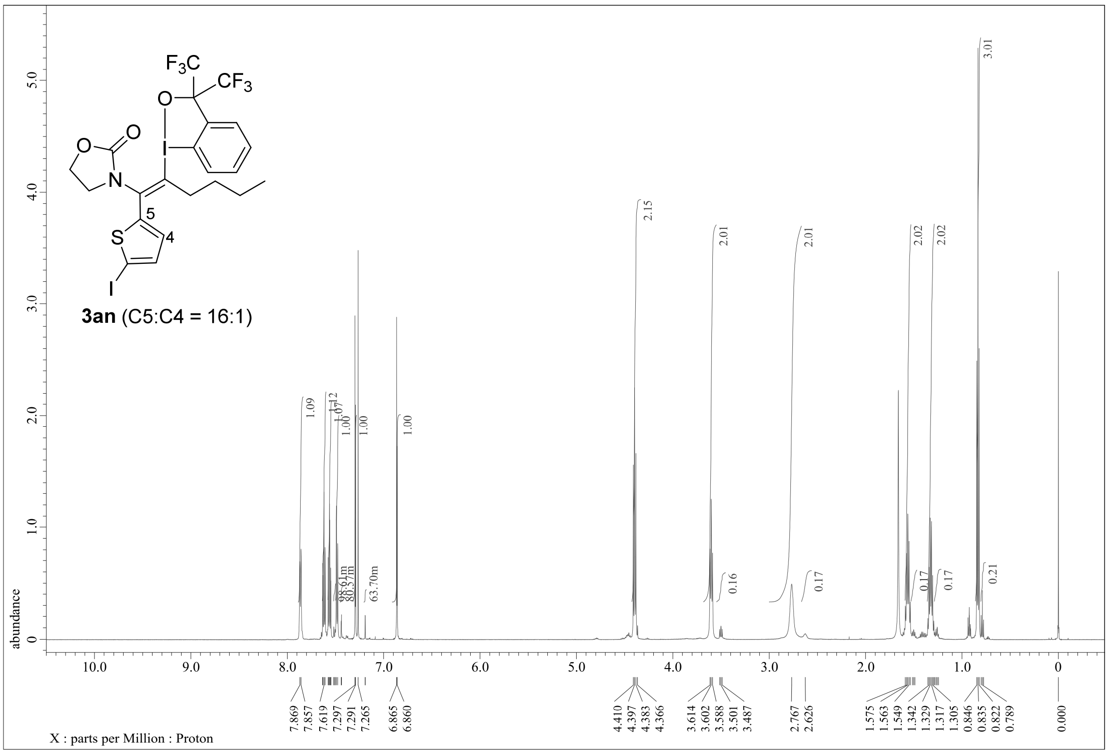


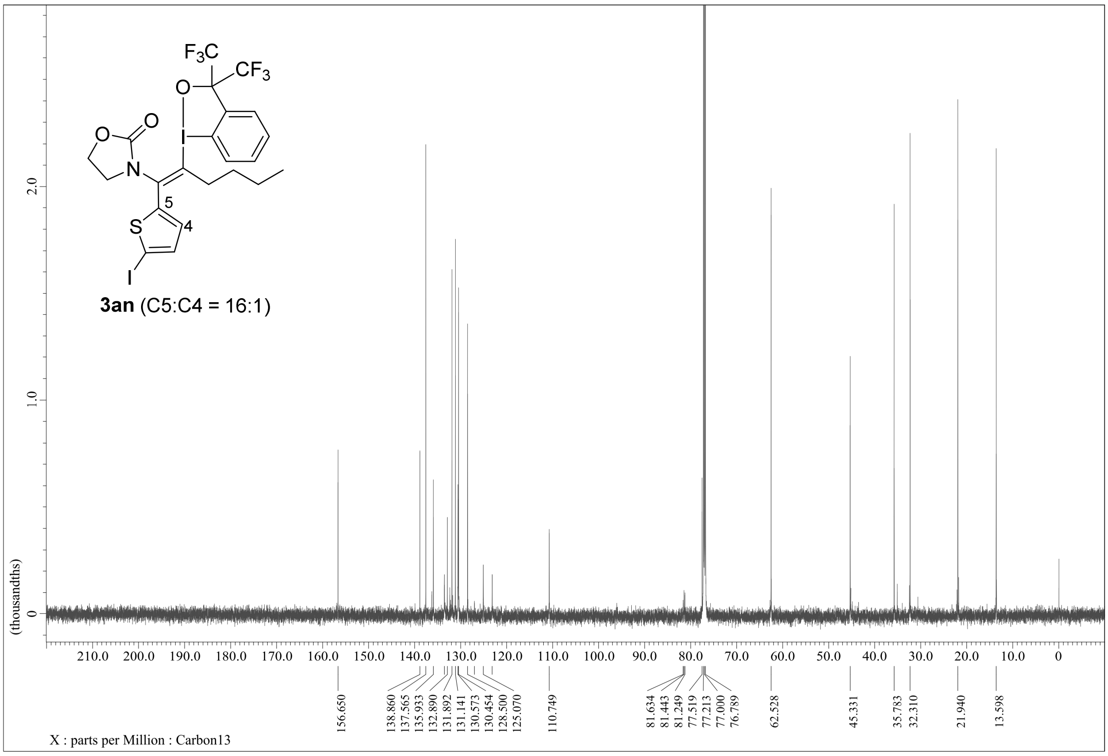


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3am**

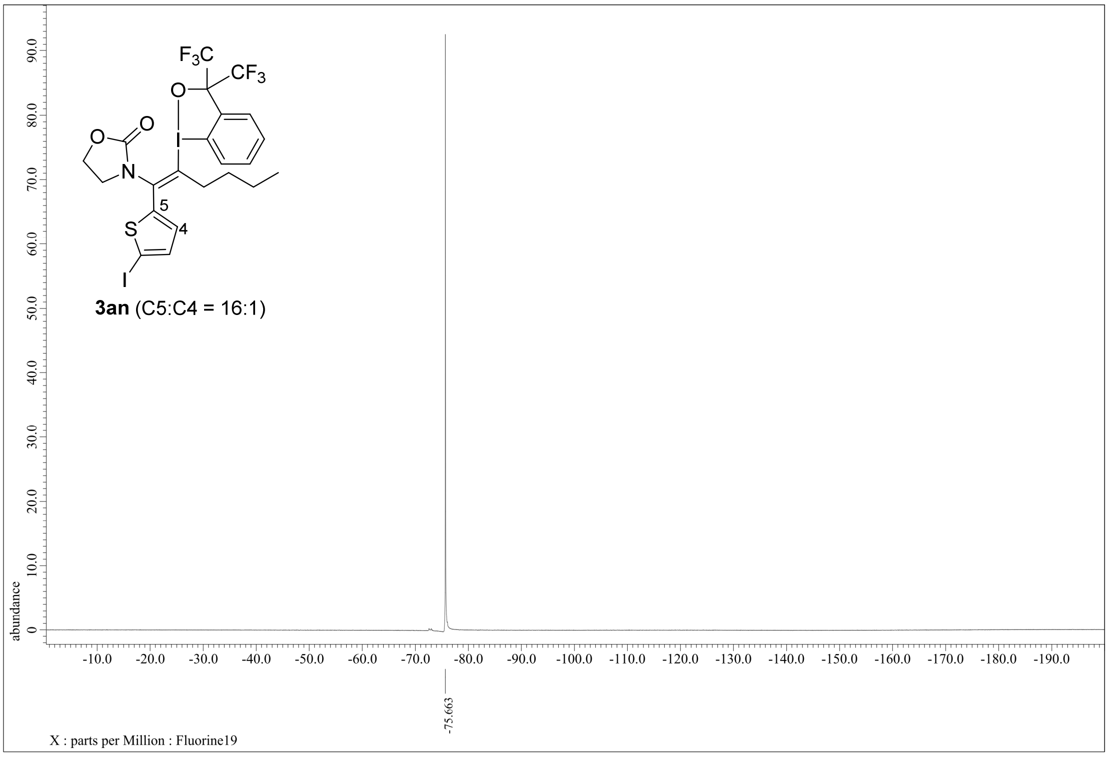


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3an**

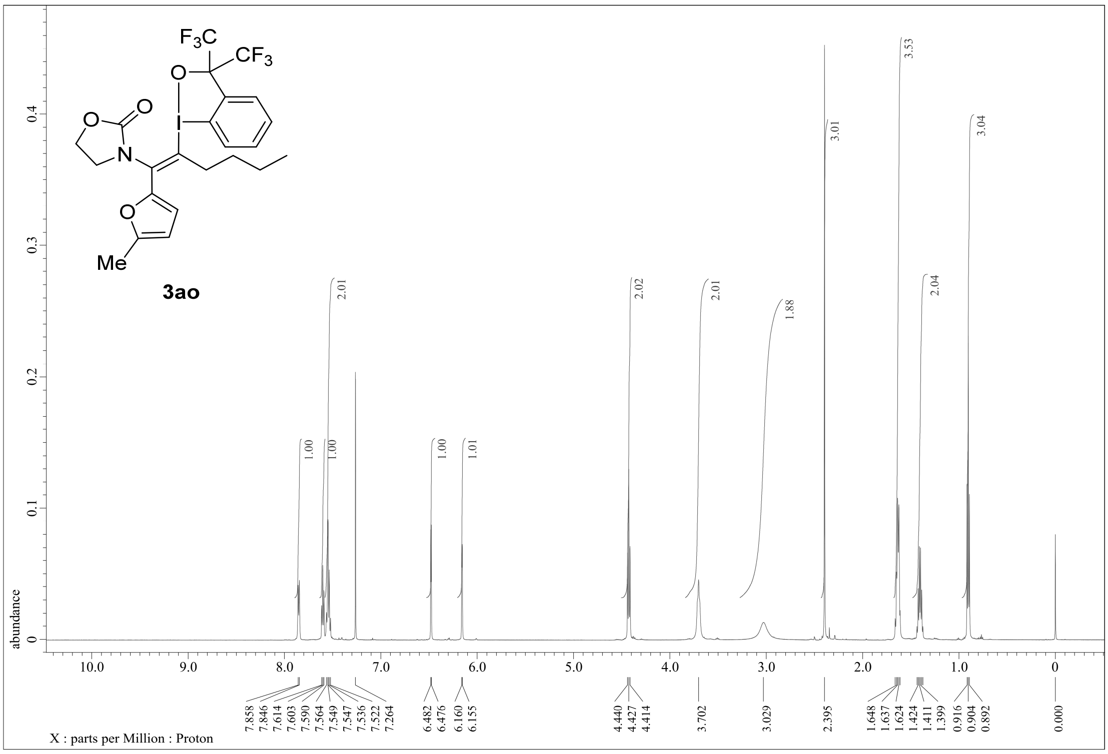


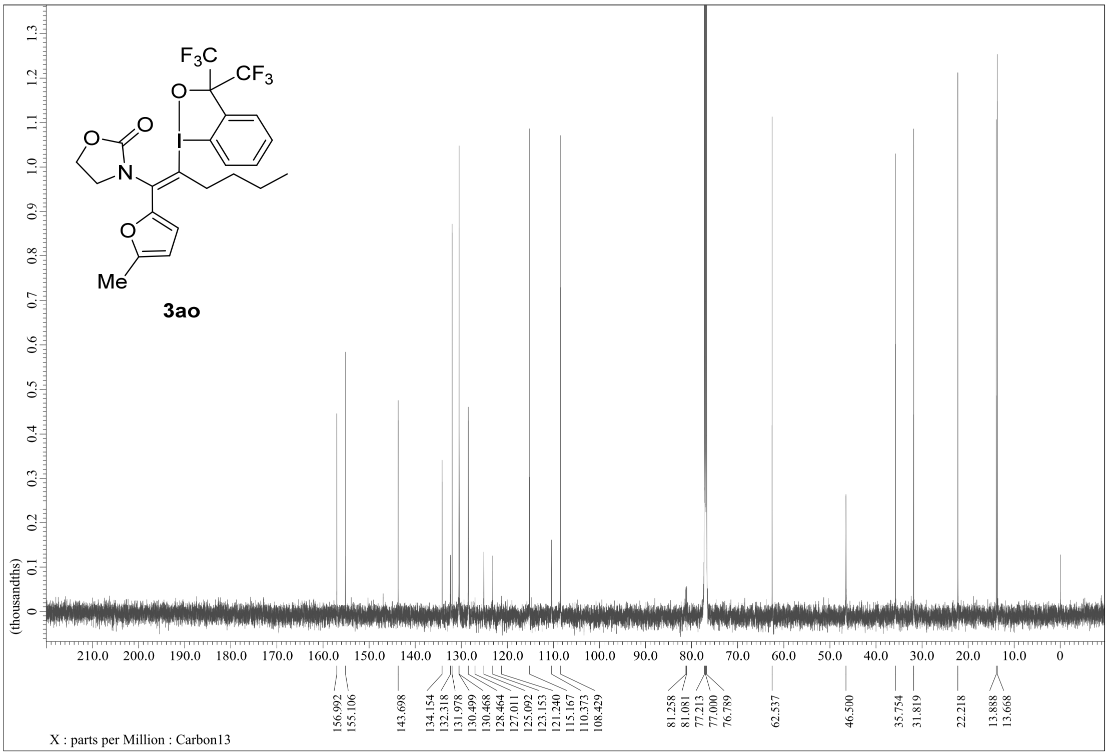


$^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3an**

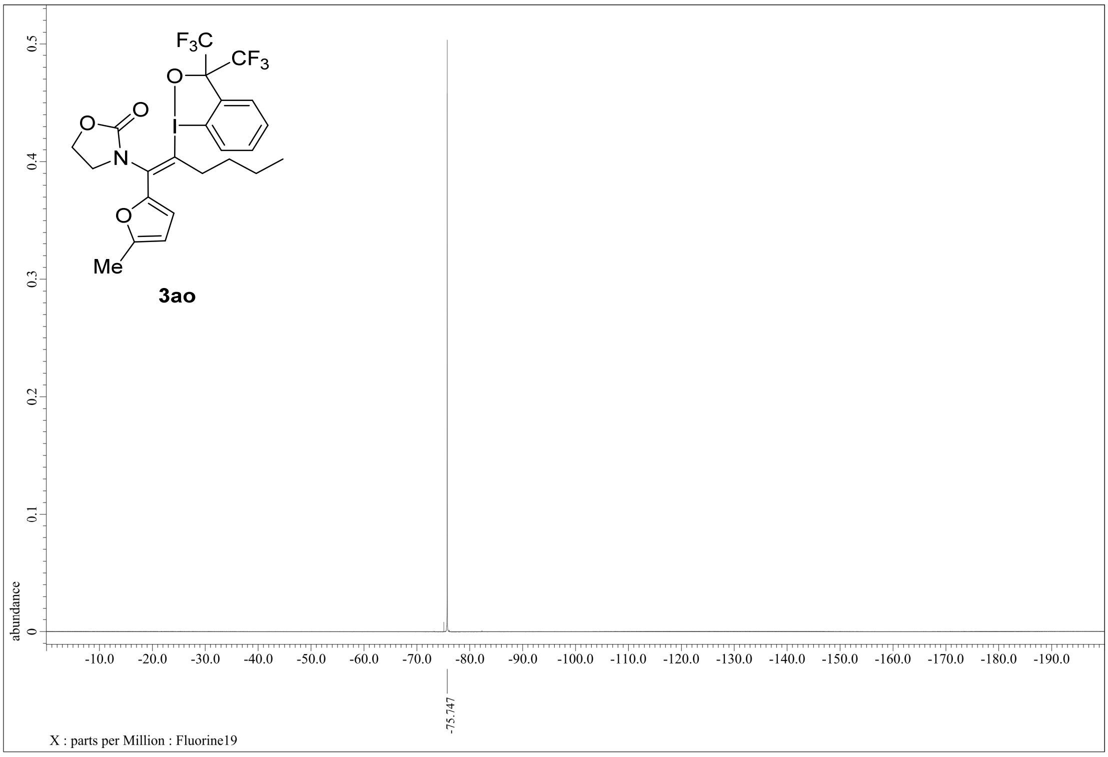


[1]H NMR (600 MHz, $CDCl_3$) and [13]C{[1]H} NMR (151 MHz, $CDCl_3$) spectra of **3ao**

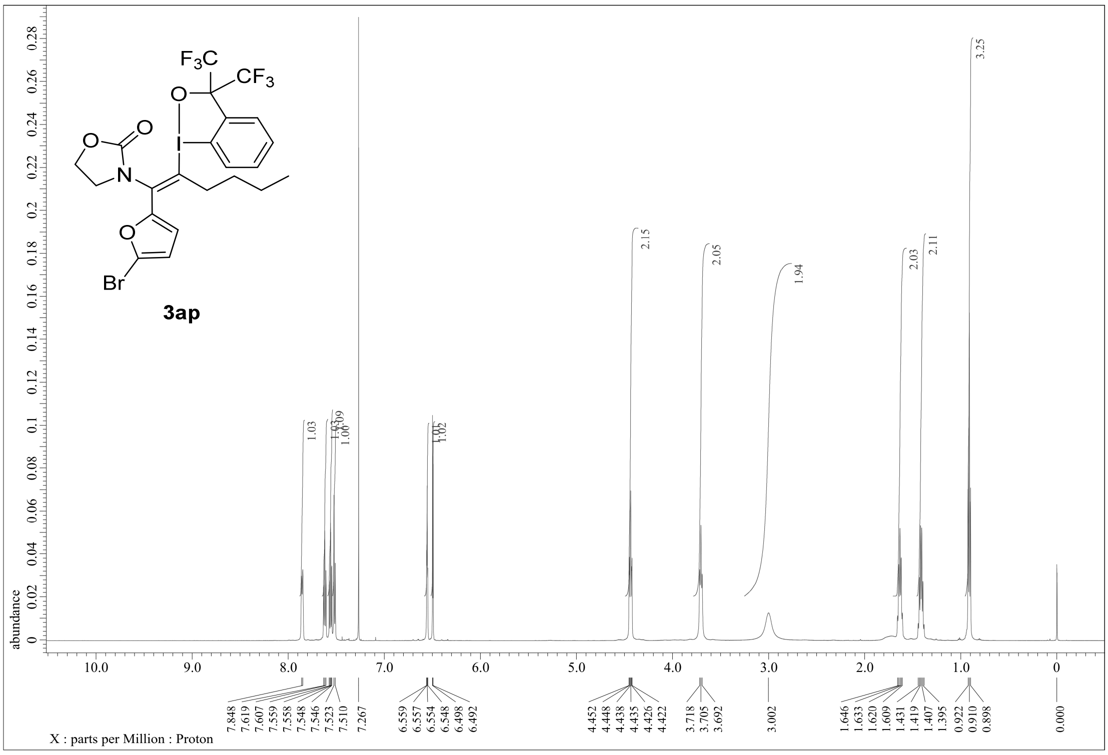


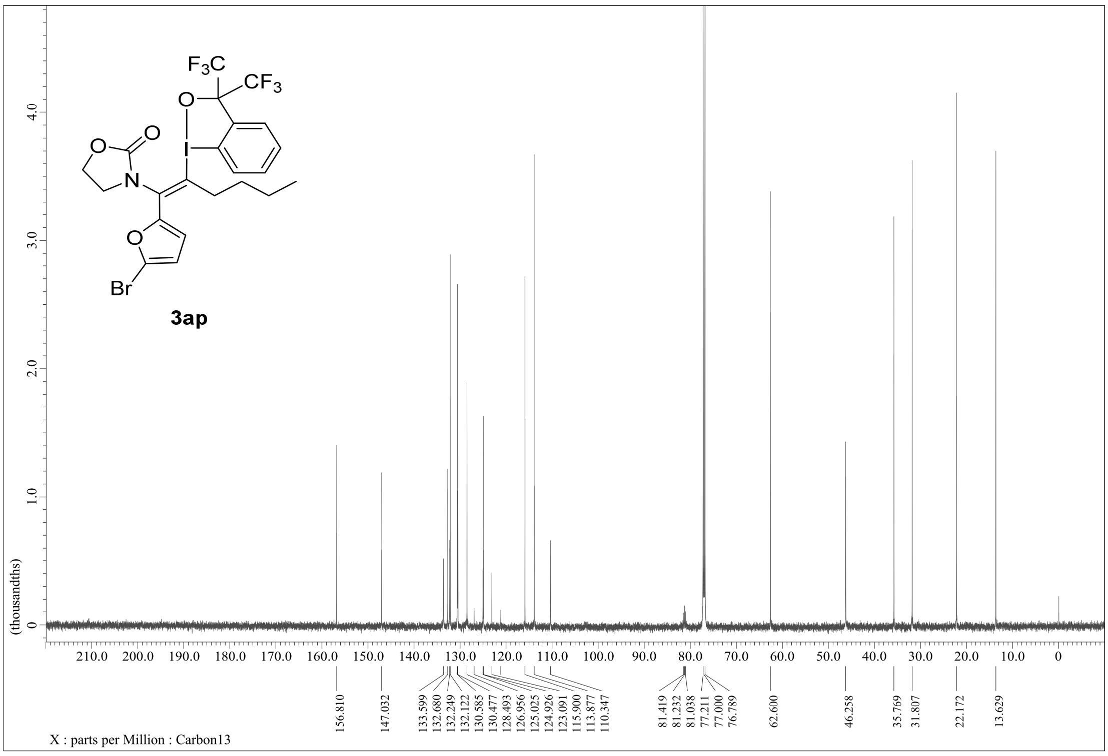


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ao**

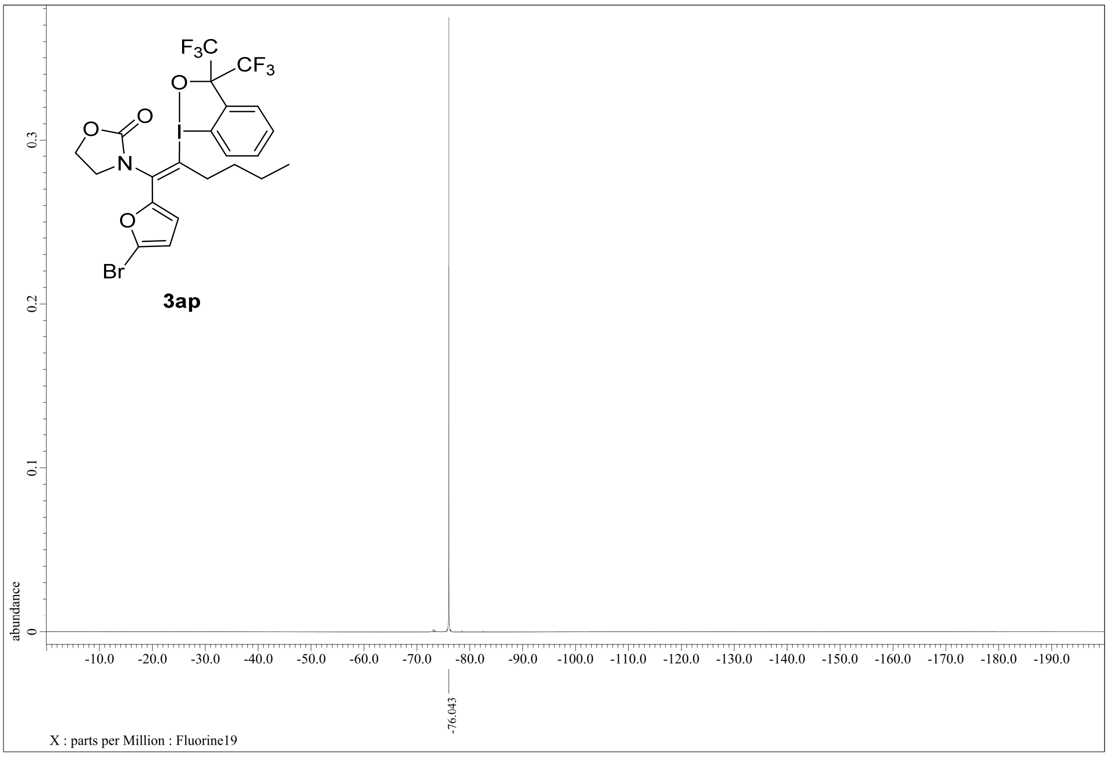


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3ap**

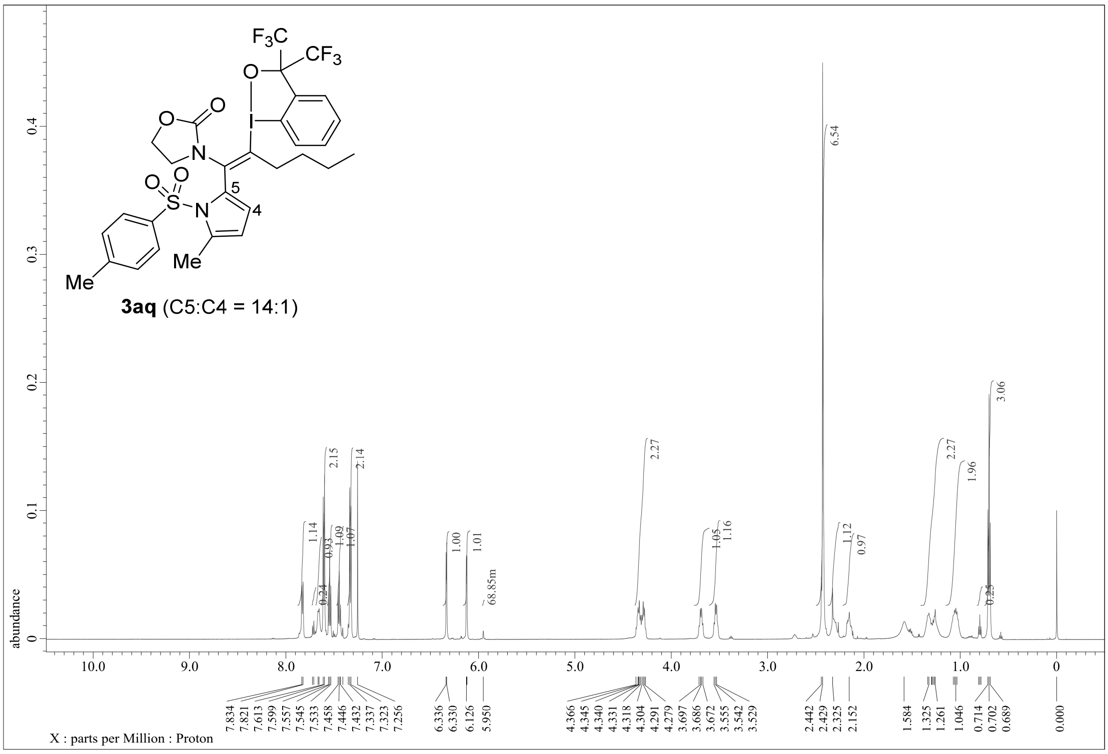


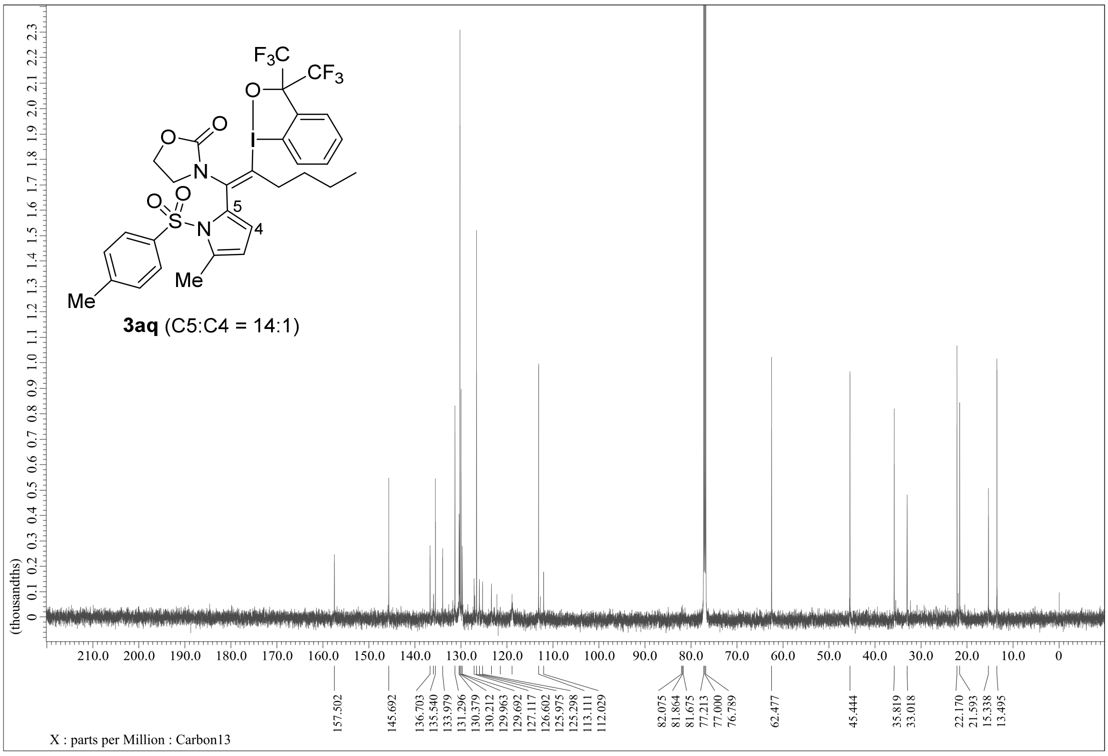


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ap**

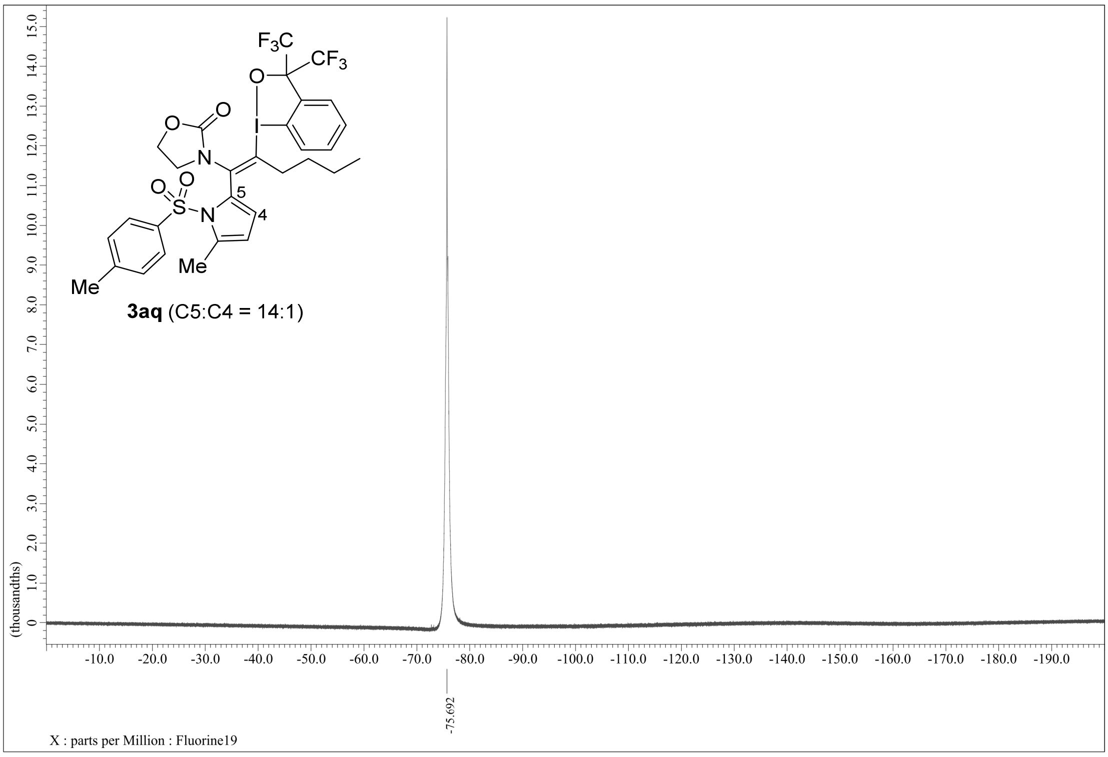


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3aq**

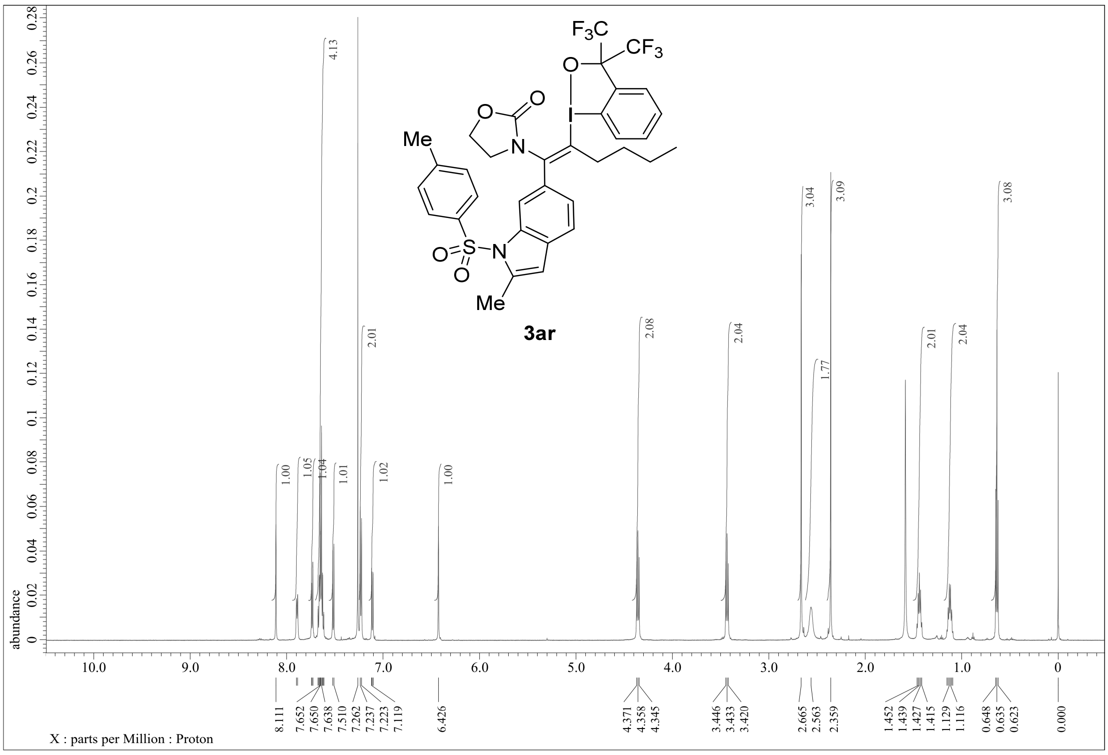


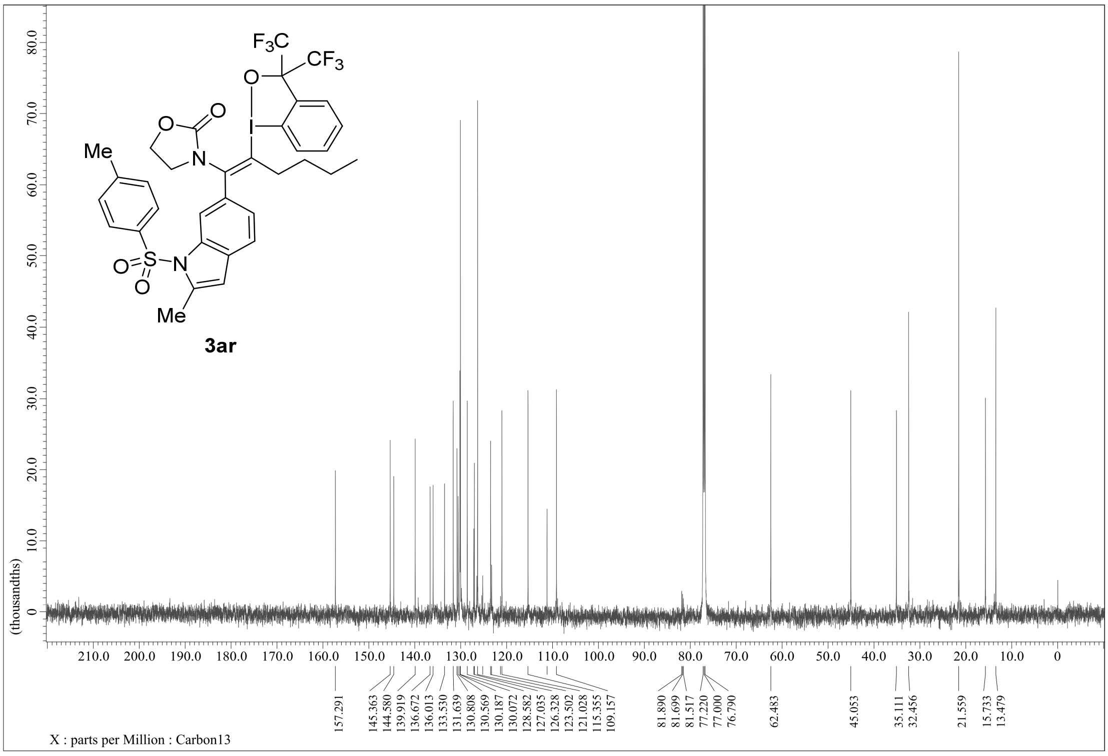


$^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3aq**

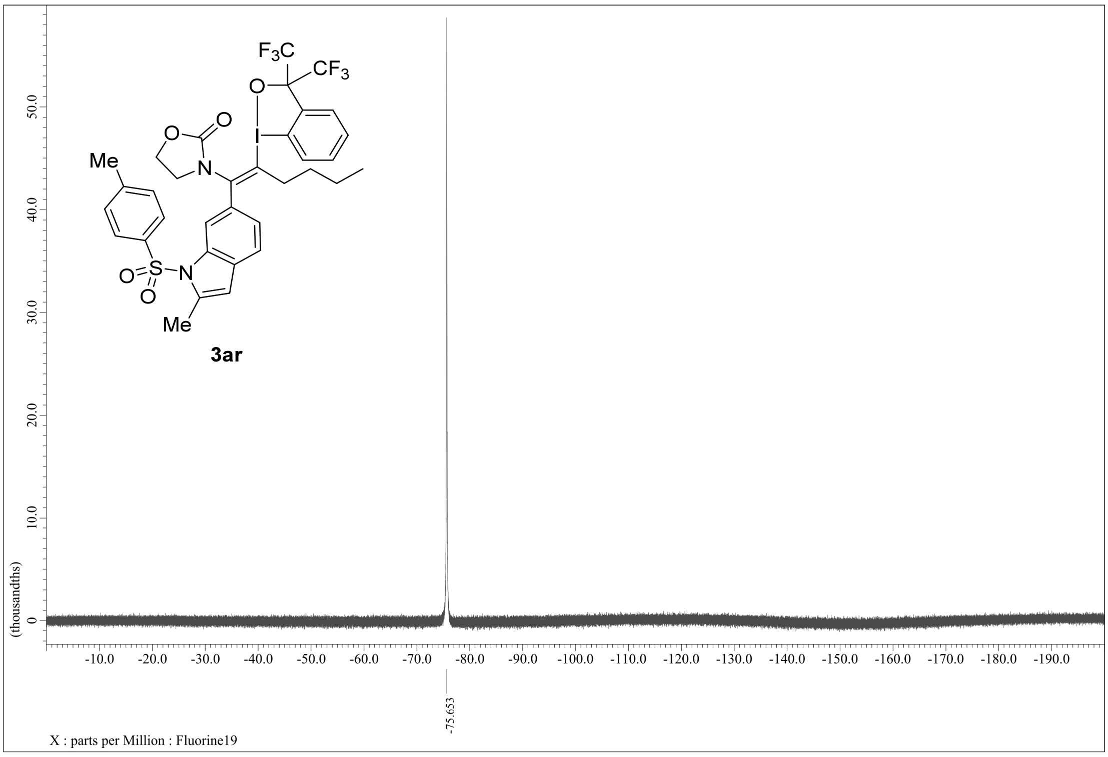


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3ar**

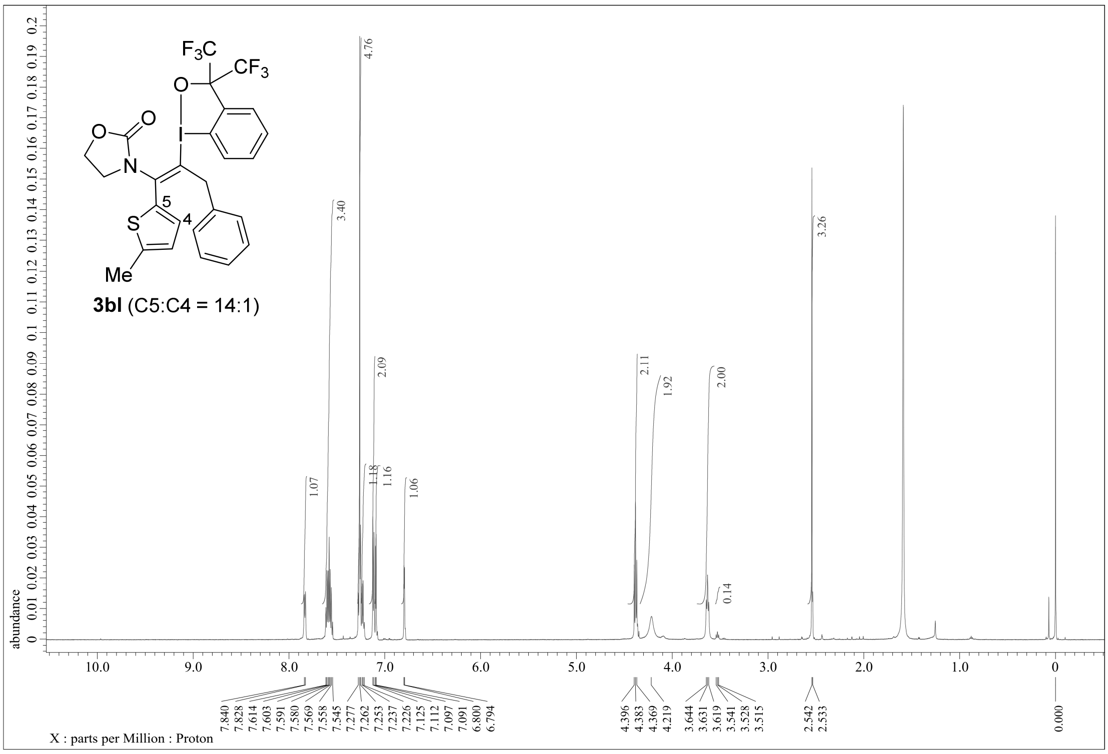


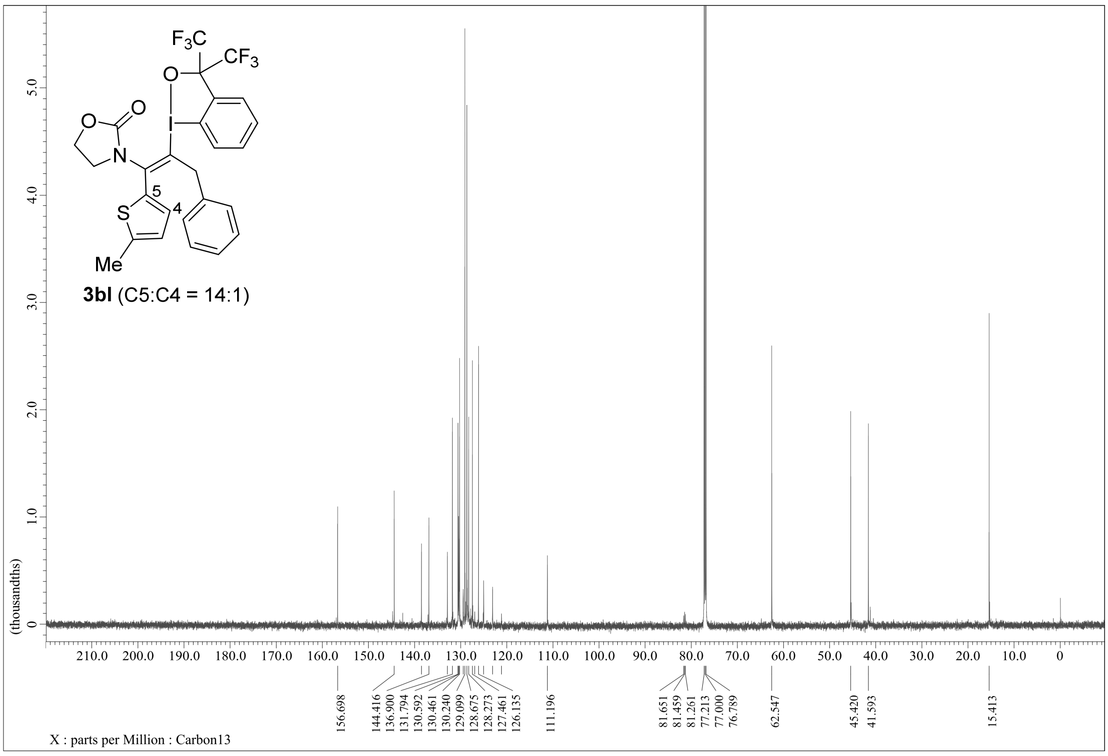


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3ar**

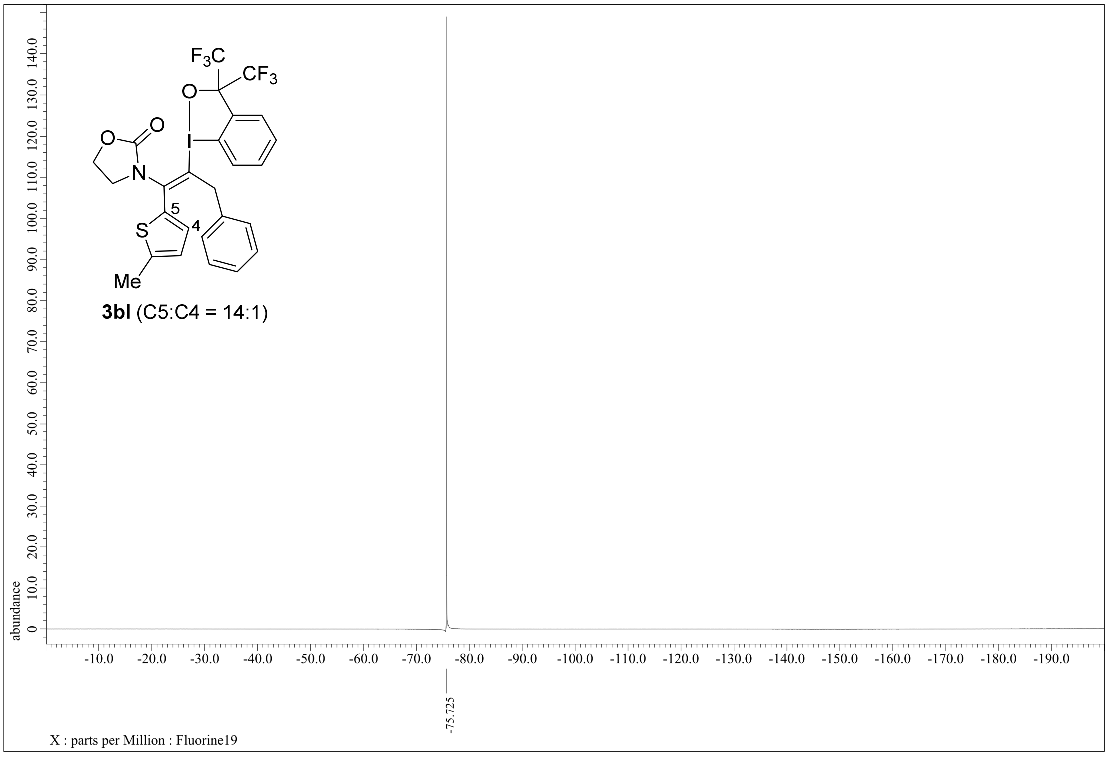


[1]H NMR (600 MHz, $CDCl_3$) and [13]C{[1]H} NMR (151 MHz, $CDCl_3$) spectra of **3bl**

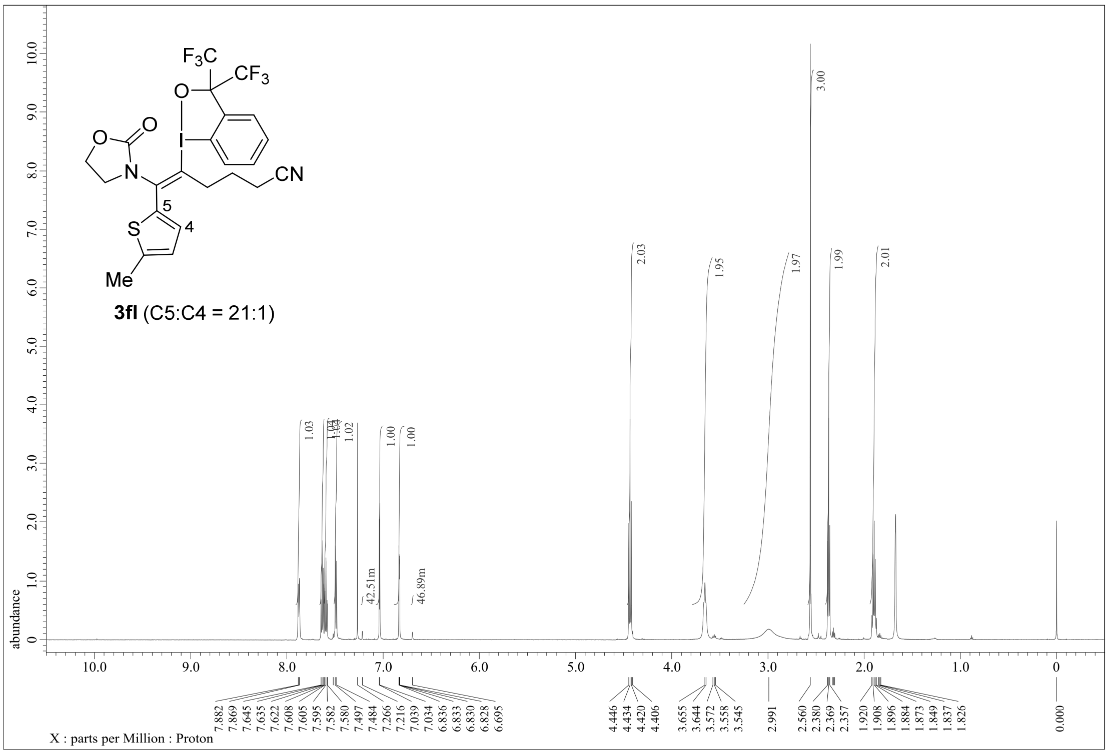


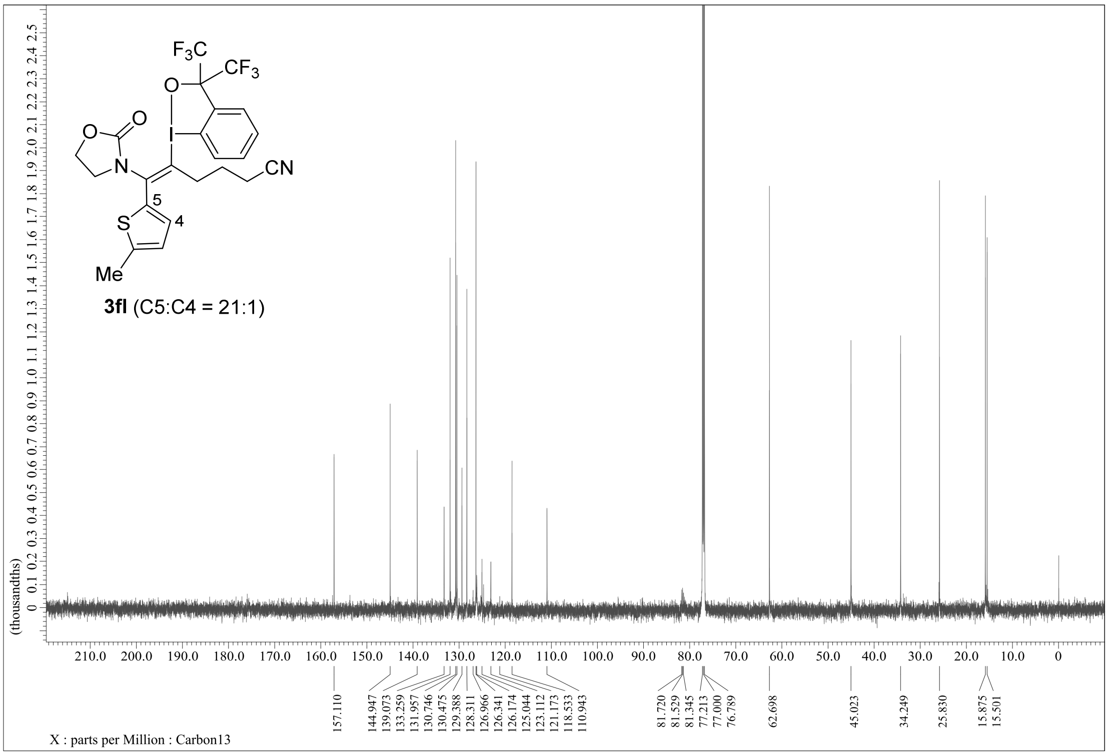


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3bl**

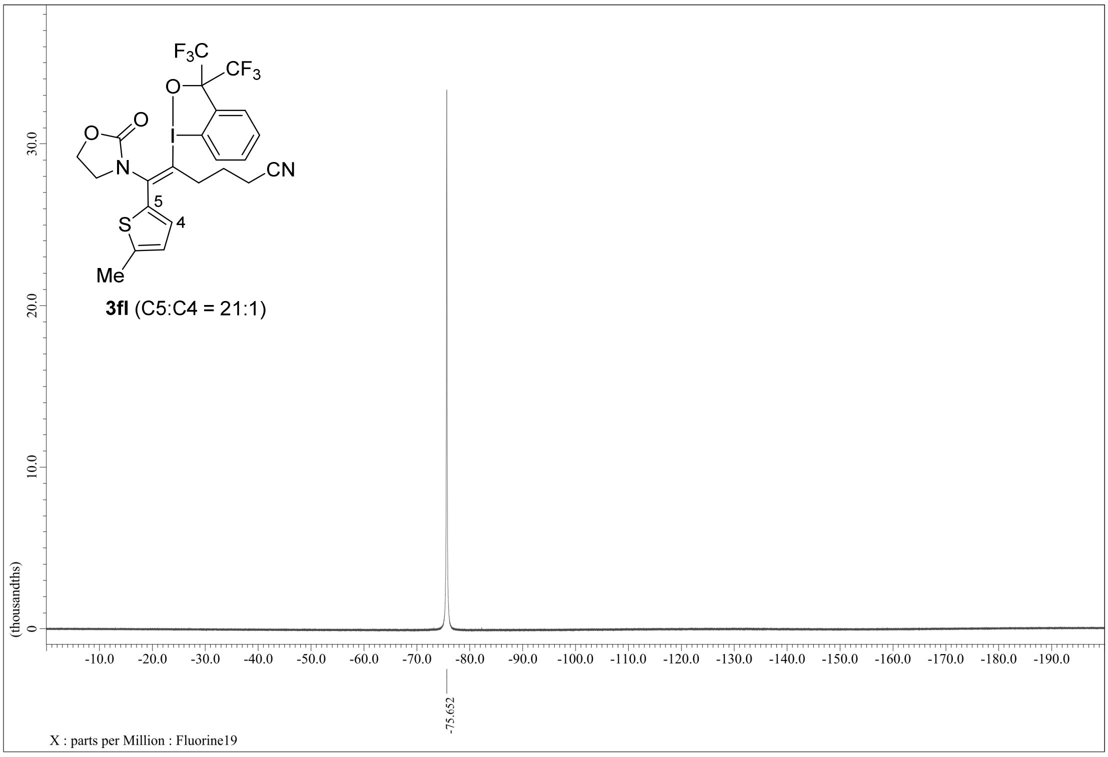


[1]H NMR (600 MHz, $CDCl_3$) and [13]C{[1]H} NMR (151 MHz, $CDCl_3$) spectra of **3fl**

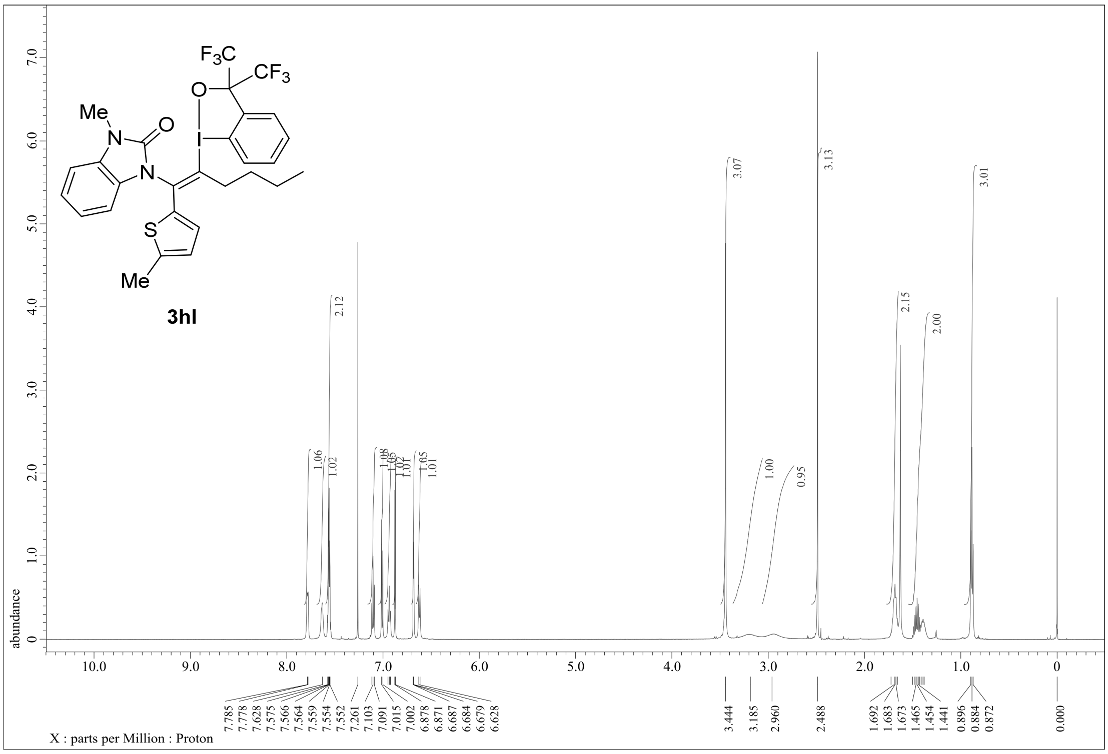


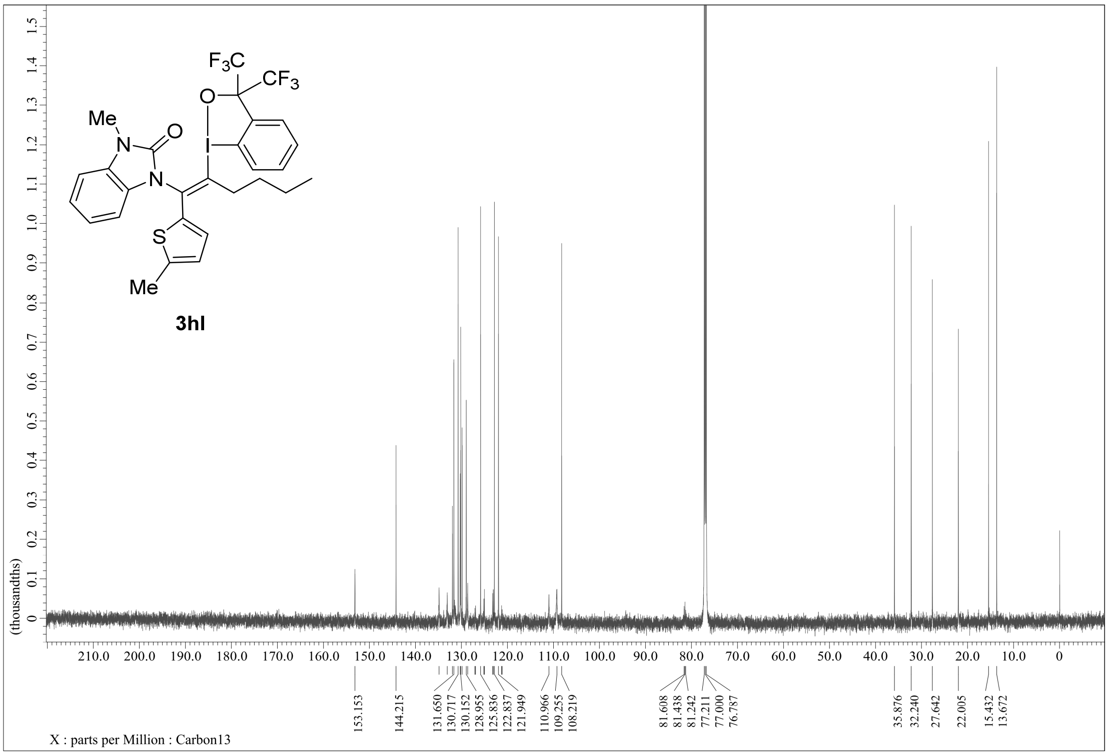


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3fl**

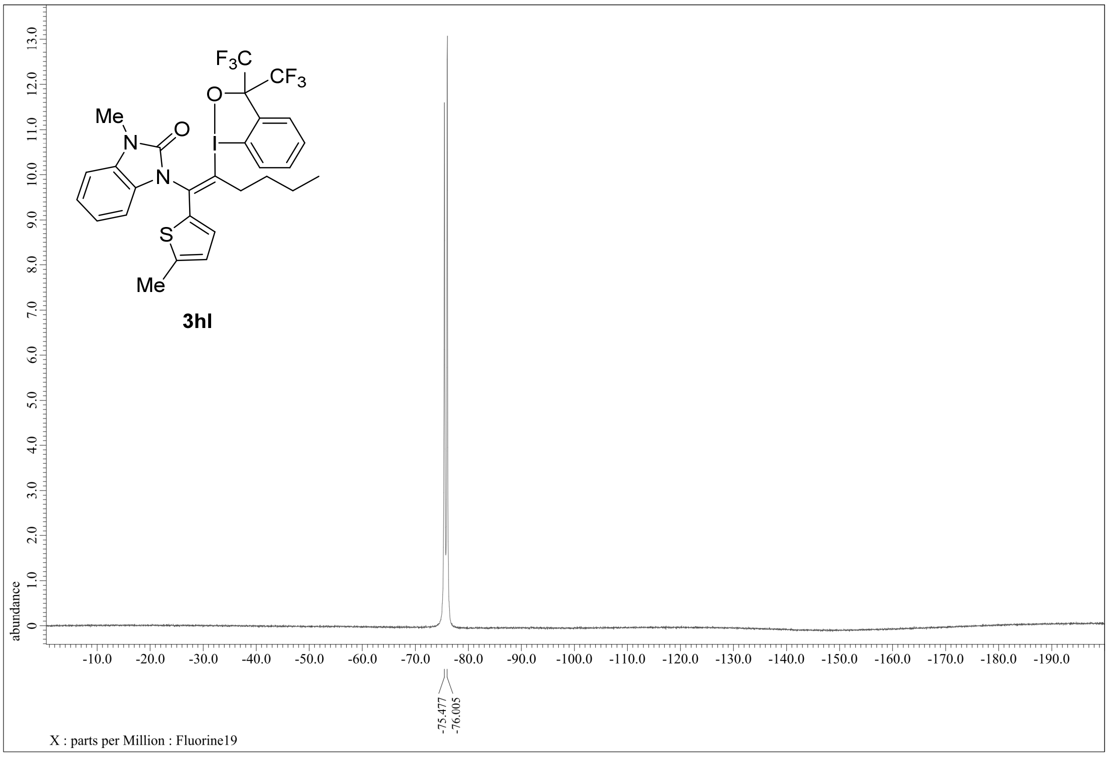


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3hl**

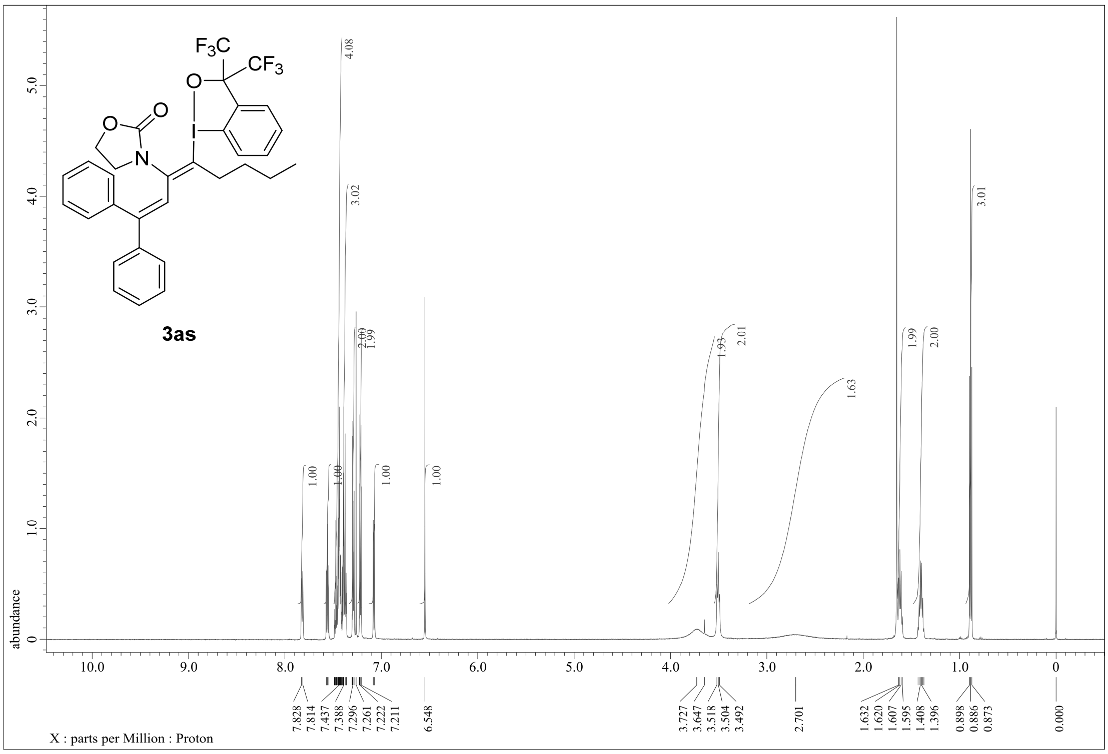


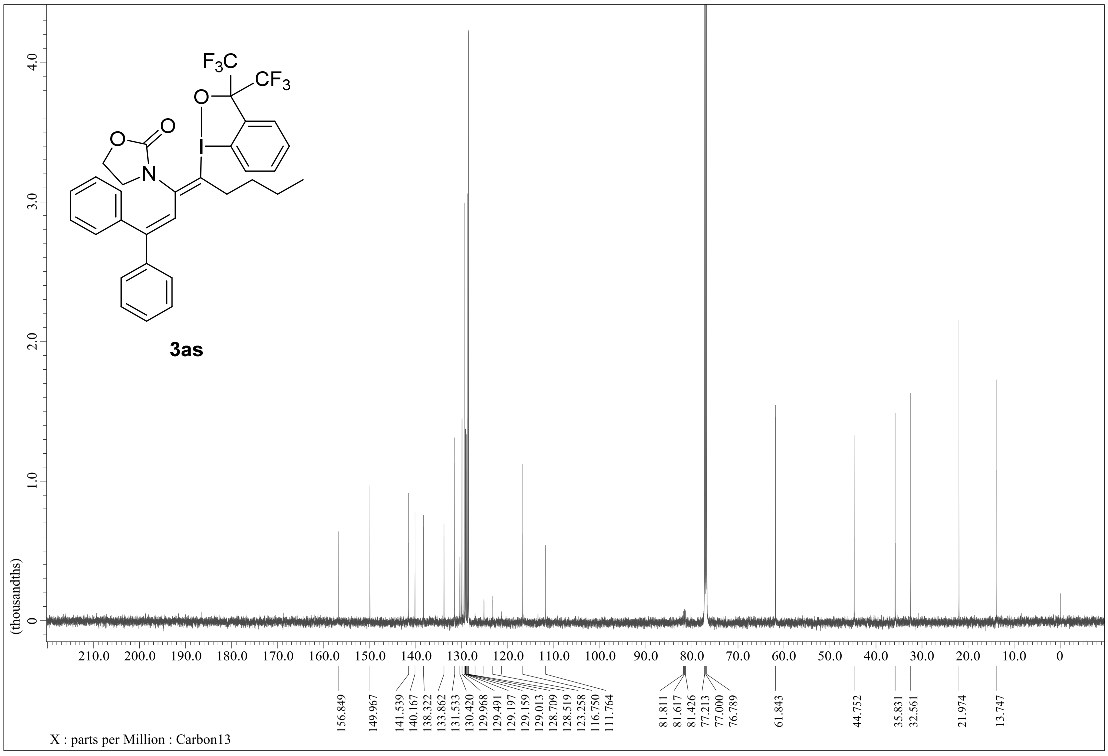


$^{19}F\{^1H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3hl**

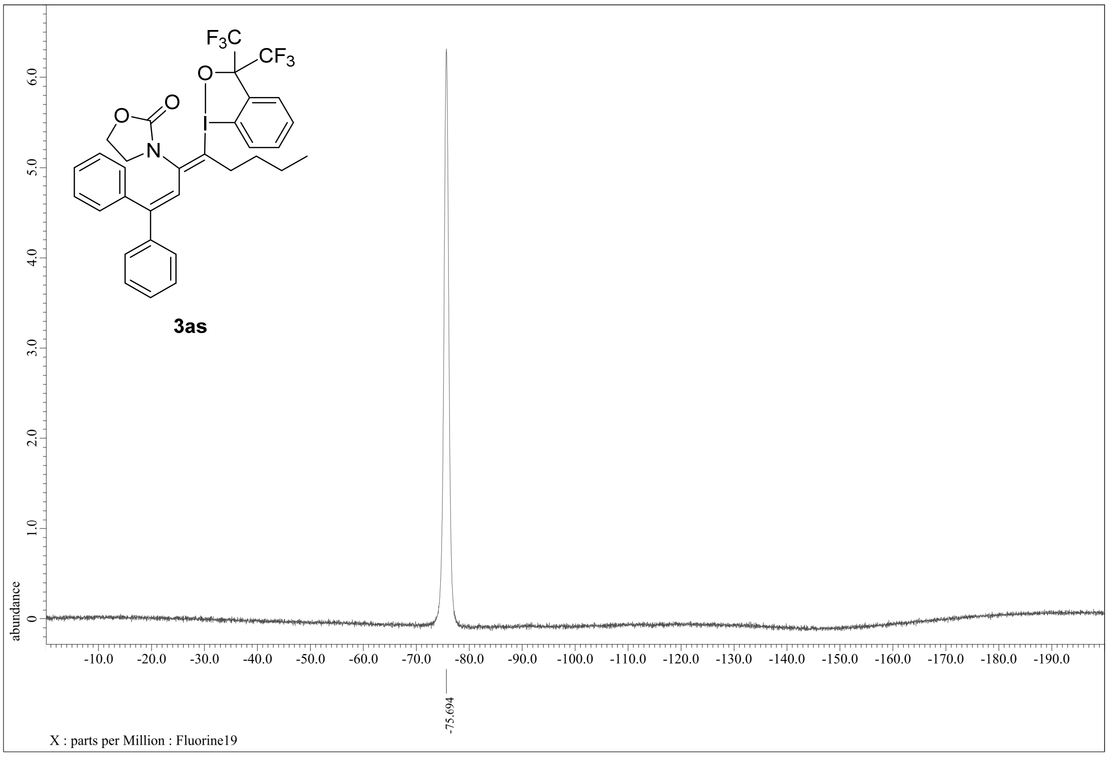


^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **3as**

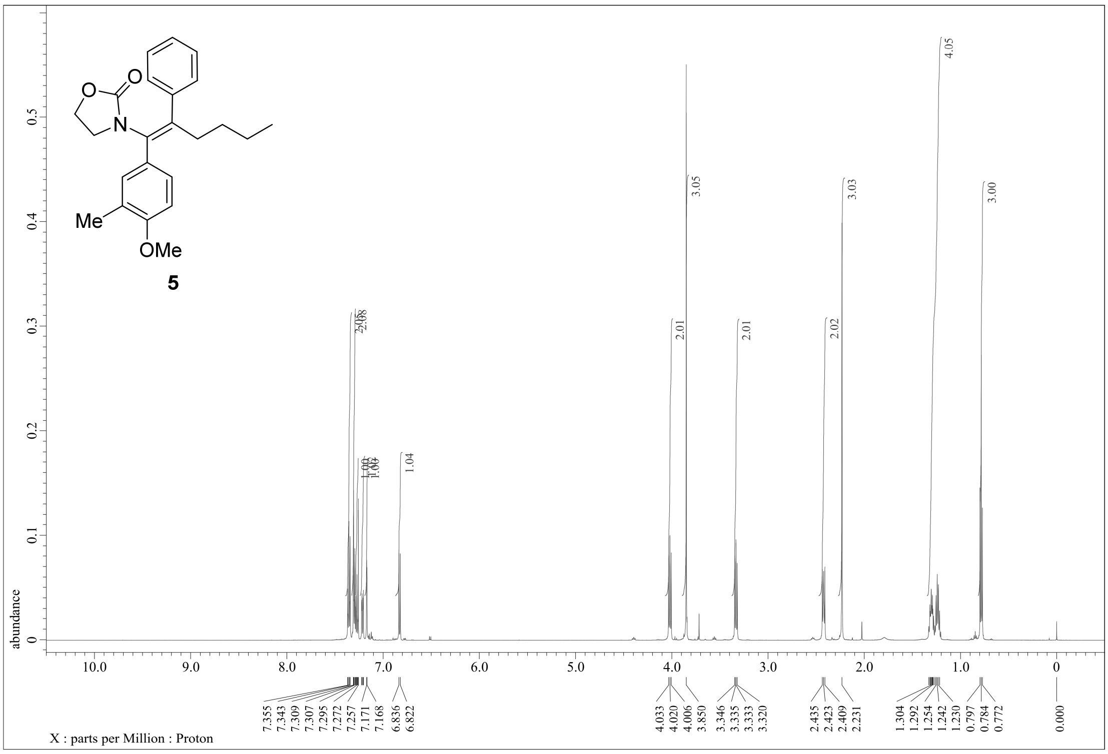


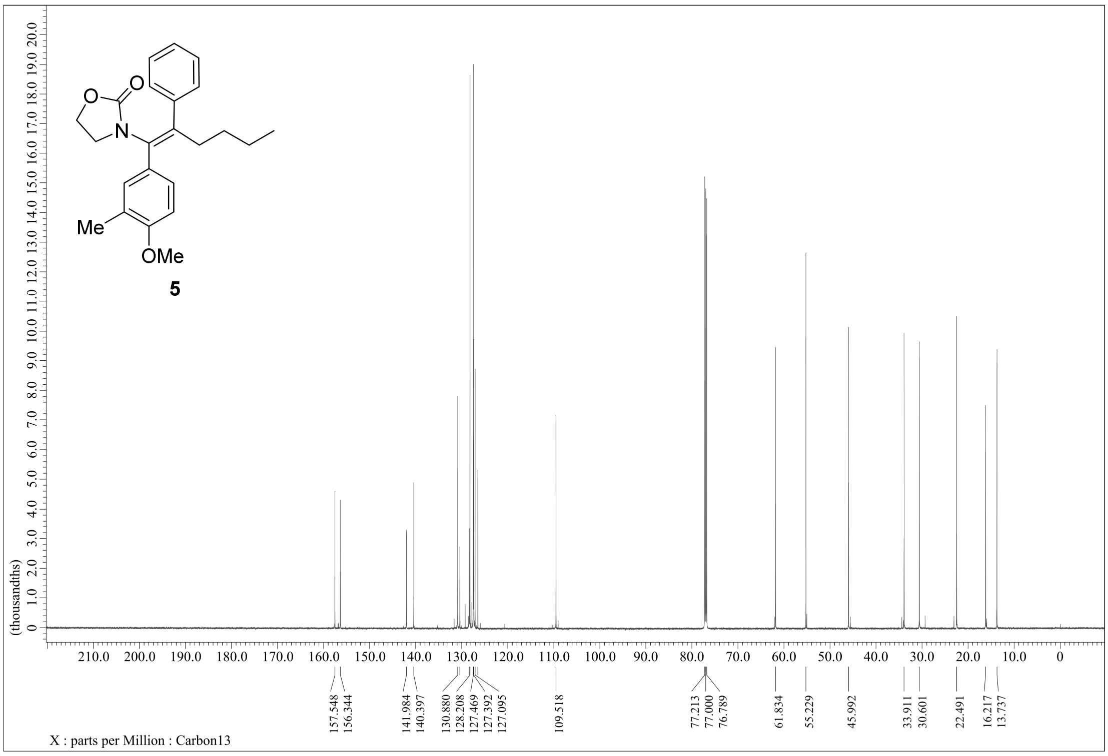


$^{19}F\{^{1}H\}$ NMR (565 MHz, $CDCl_3$) spectrum of **3as**

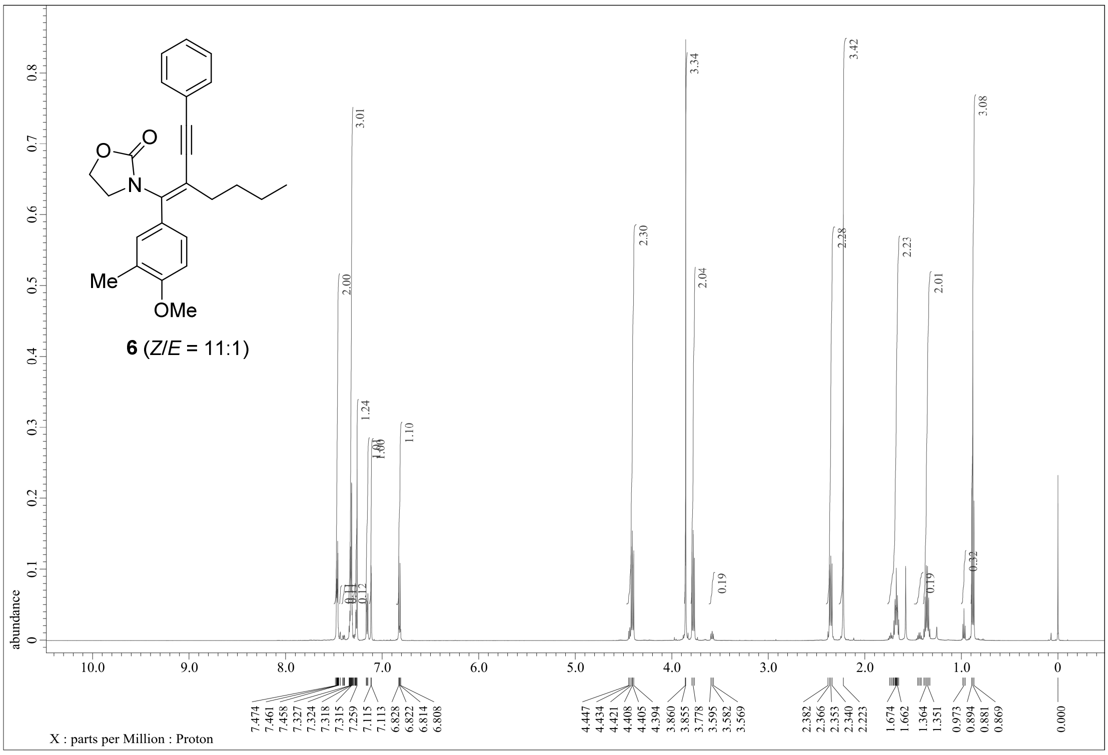


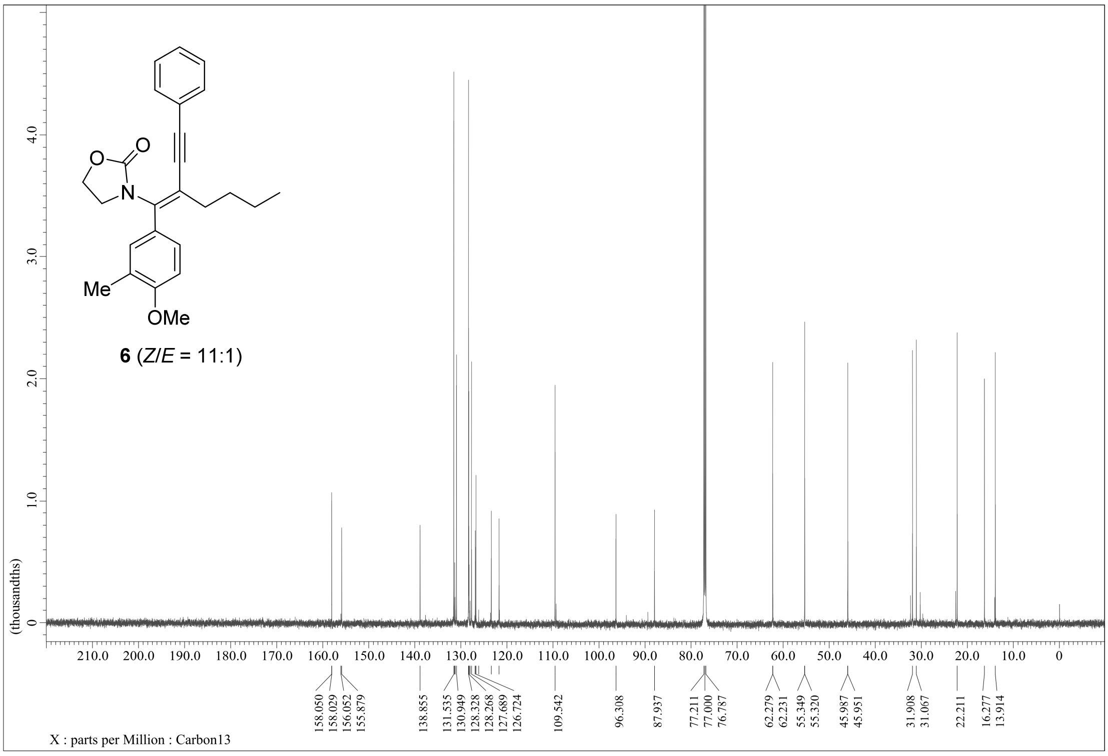
^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **5**



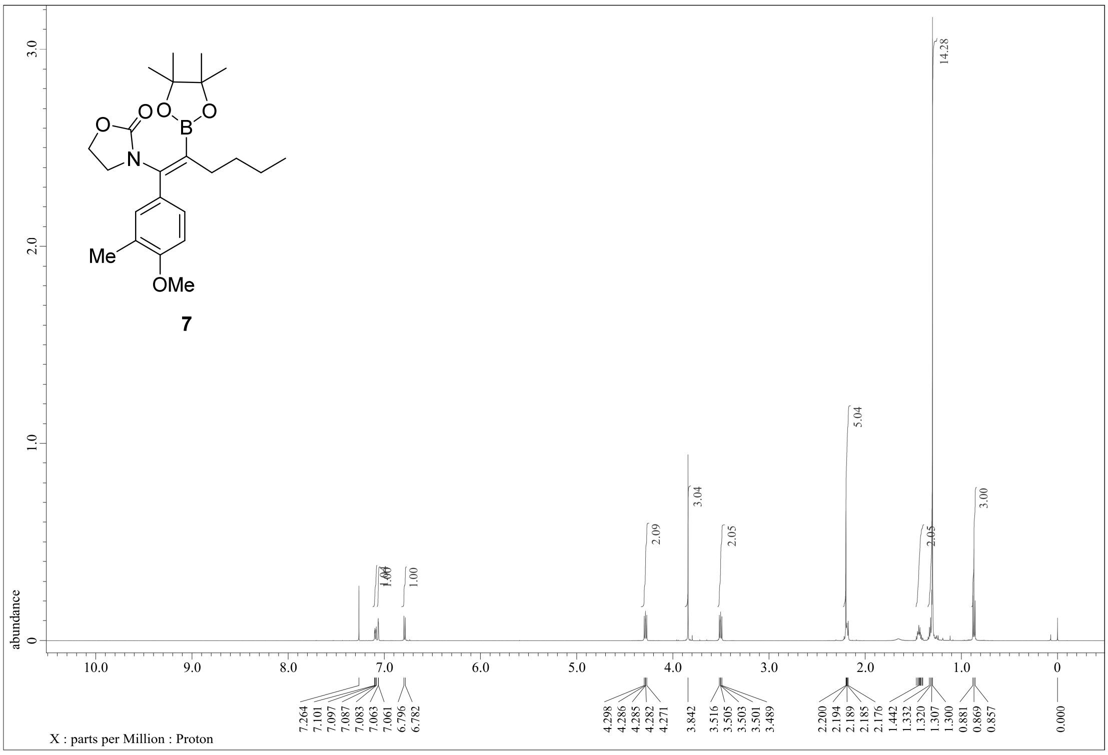


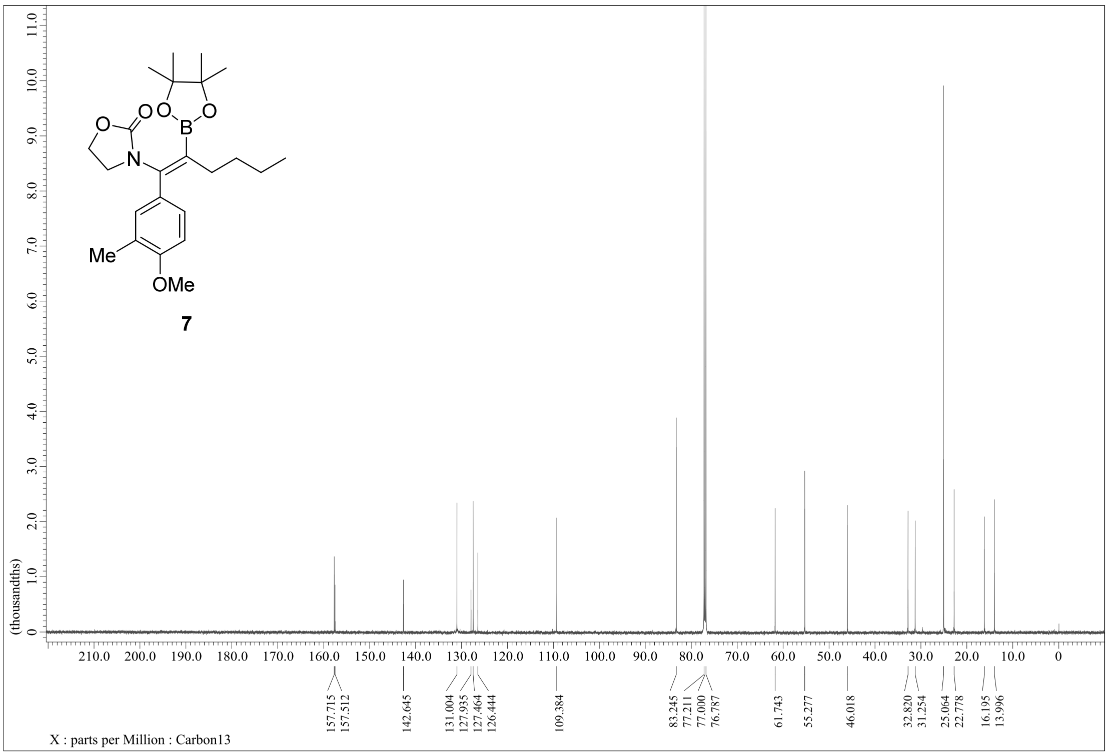
^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **6**



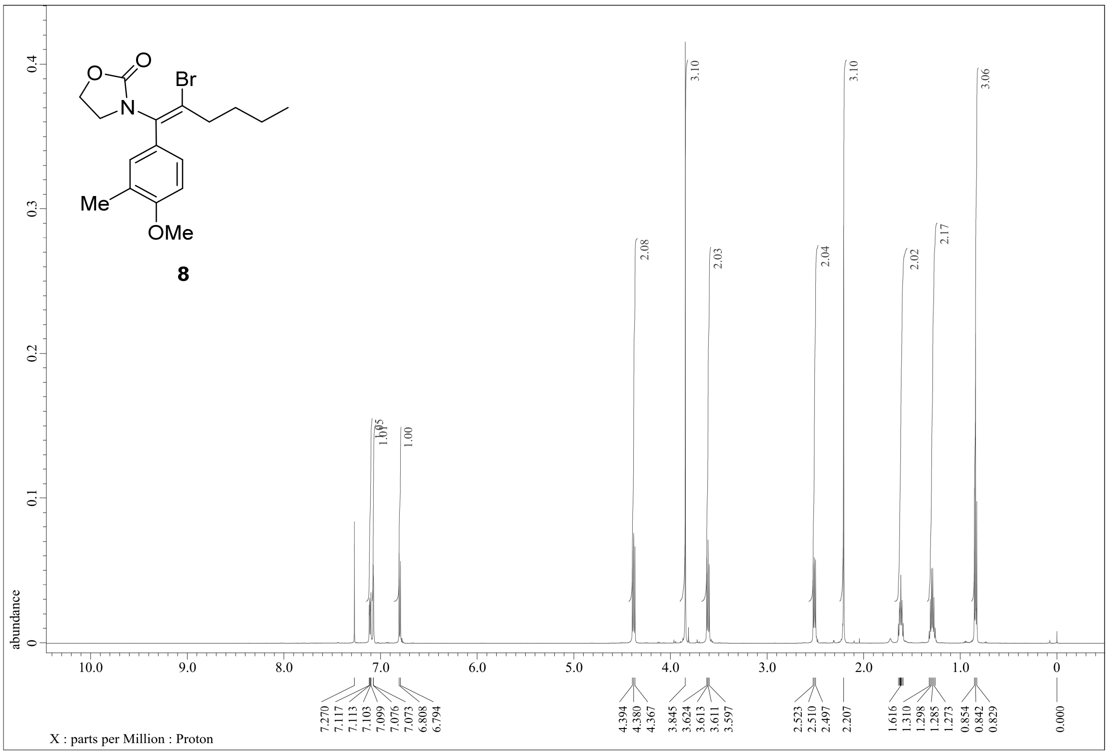


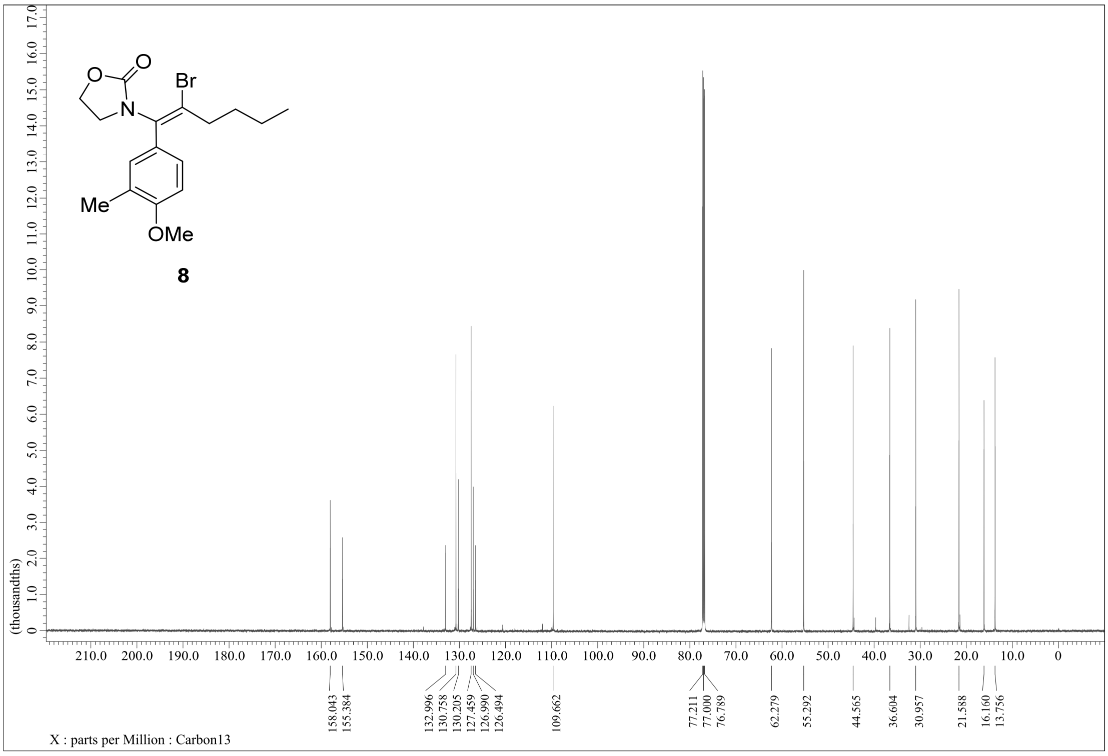
^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **7**



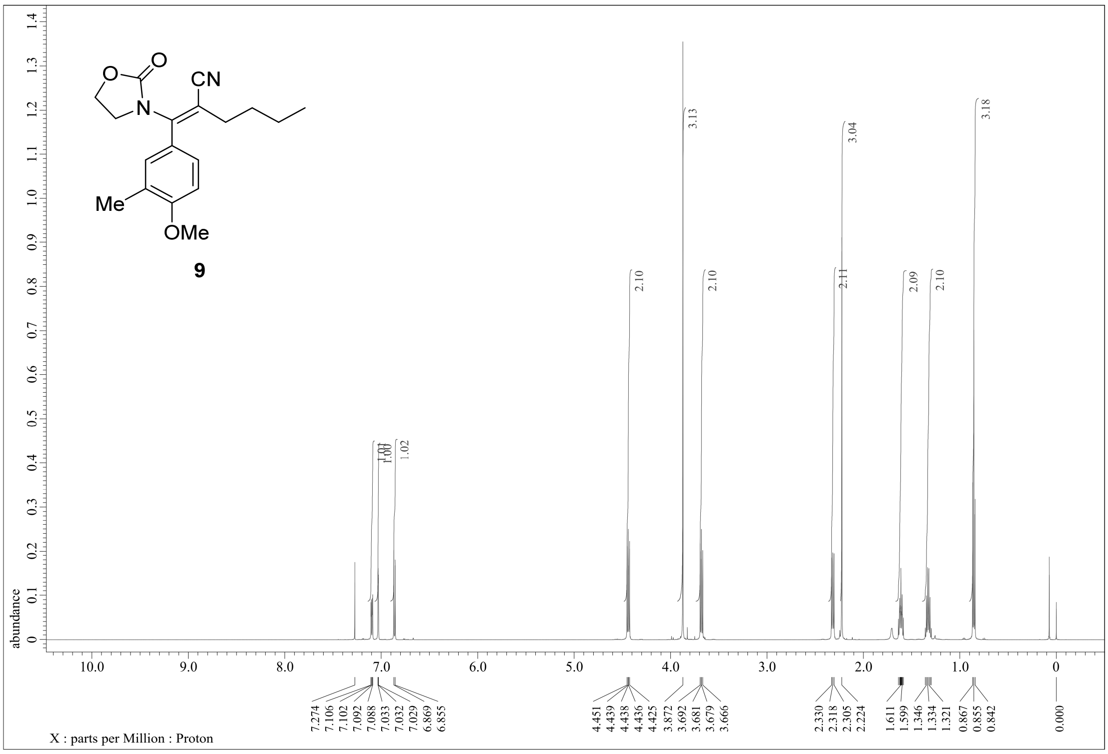


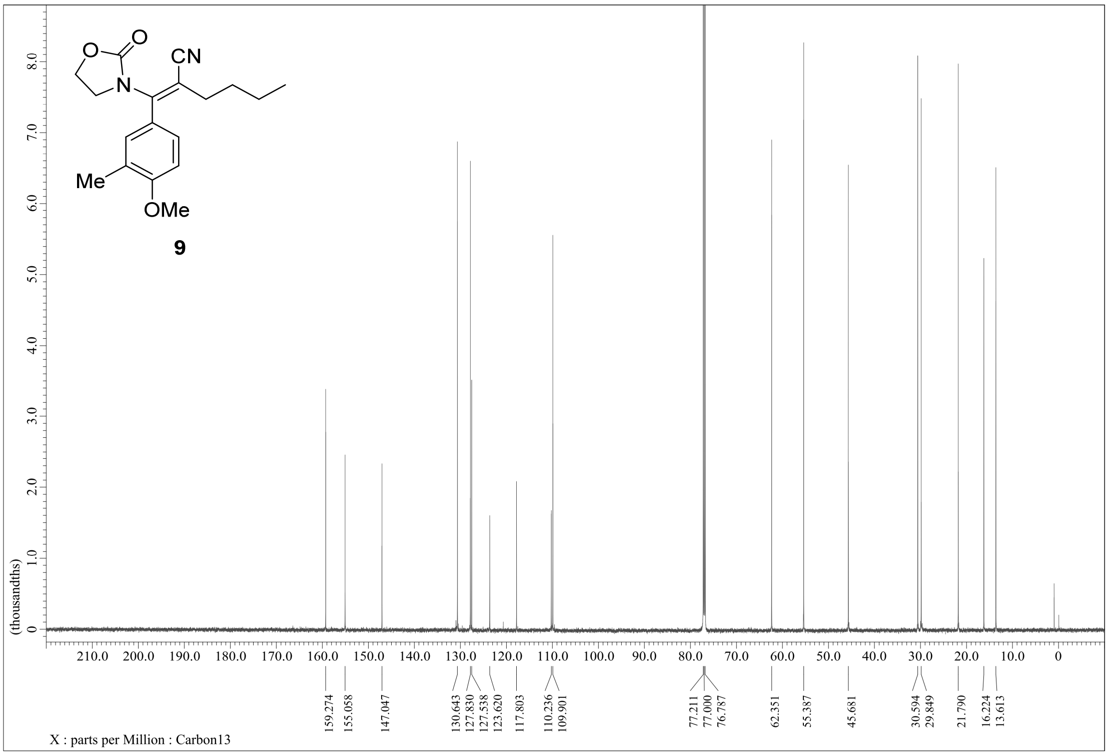
^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **8**





[1]H NMR (600 MHz, $CDCl_3$) and [13]C{[1]H} NMR (151 MHz, $CDCl_3$) spectra of **9**





^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) spectra of **10**