Supporting Information

Trifluoromethylselenolation and *N*-Acylation of Indoles with $[Me_4N][SeCF_3]$

Kai-Li Tan, Hao-Nan Wang, Tao Dong, Cheng-Pan Zhang*
School of Chemistry, Chemical Engineering and Life Science, Wuhan University of Technology, Wuhan 430070, China.
E-mail: cpzhang@whut.edu.cn, zhangchengpan1982@hotmail.com.

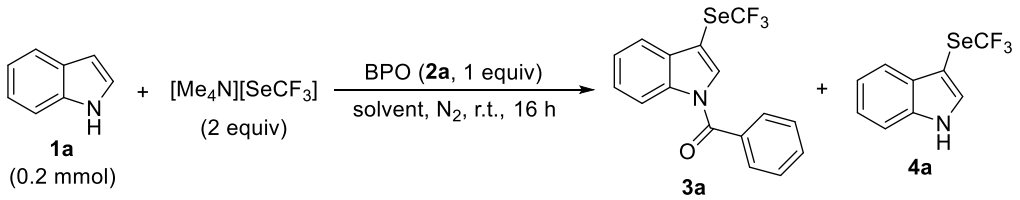
Table of contents

1. General information

All reactions were carried out under a nitrogen atmosphere. Unless otherwise specified, NMR spectra were recorded in $CDCl_3$ or acetone-d_6 on a 500 MHz (for ^1H), 471 MHz (for ^{19}F), and 126 MHz (for ^{13}C) spectrometer. All chemical shifts were reported in ppm relative to TMS (0 ppm) for ^1H NMR and $PhOCF_3$ (-58.0 ppm) for ^{19}F NMR as an internal or external standard. The HPLC experiments were carried out on a Wufeng LC-100 II instrument (column: Shodex, C18, 5 μm, 4.6 × 250 mm), and yields of the products were determined by using the corresponding pure compounds as the external standards, respectively. Melting points were measured and uncorrected. MS experiments were performed on a TOF-Q ESI or DART instrument. $[Me_4N][SeCF_3]$ was prepared according to the literature.[1] The starting materials (**2b-i**[2], **5a**[3] and **5j**[3]) were synthesized according to the literatures. Solvents were dried before use according to the literature.[4] Other reagents in the reactions were all purchased from the commercial sources and used without further purification.

2. Screening of the optimal reaction conditions for trifluoromethylselenolation / *N*-acylation of indole (1a) with $[Me_4N][SeCF_3]$

Table S1. Trifluoromethylselenolation/*N*-acylation of **1a** with $[Me_4N][SeCF_3]$ and BPO in different solvents.

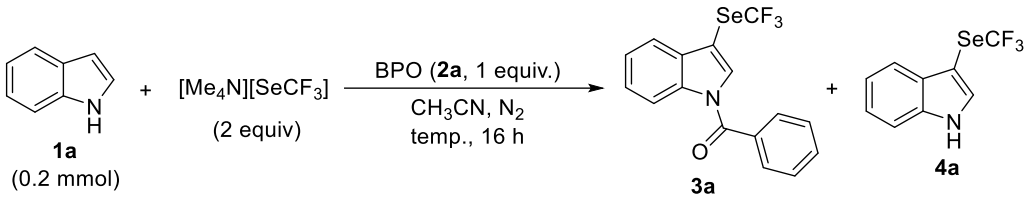


Entry [a]	Solvent	Yield (**3a**, %) [b]	Yield (**4a**, %) [b]
1	CH_3CN	94 (93)	5 (5)
2	DMF	62	10
3	DCM	27	22
4	THF	64	16
5	toluene	8	47
6	DMSO	28	63
7	1, 4-dioxane	39	18

[a] Reaction conditions: to a solution of **1a** (0.2 mmol) and $[Me_4N][SeCF_3]$ (0.4 mmol)

in solvent (1 mL) was added BPO (0.2 mmol) and solvent (1 mL). The mixture was reacted at room temperature under N_2 for 16 h. [b] Yields were determined by HPLC (λ = 249 nm, methanol/water = 90:10 (v/v)) using **3a** (t_R = 7.92 min) and **4a** (t_R = 4.58 min) as external standards, respectively. Isolated yields were depicted in the parentheses.

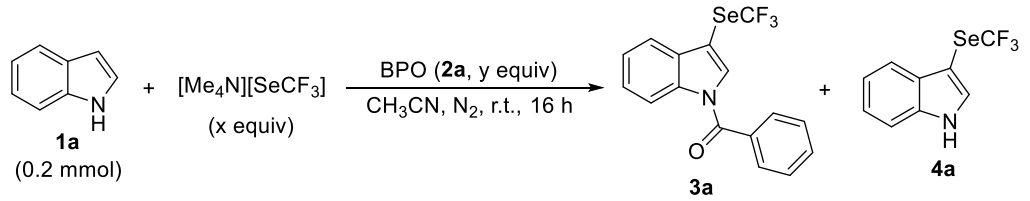
Table S2. Trifluoromethylselenolation/*N*-acylation of **1a** with $[Me_4N][SeCF_3]$ and BPO at different temperatures.



Entry [a]	Temperature	Yield (**3a**, %) [b]	Yield (**4a**, %) [b]
1	0 °C	36	53
2	r.t.	94 (93)	5 (5)
3	40 °C	84	9
4	60 °C	62	22
5	80 °C	52	48

[a] Reaction conditions: to a solution of **1a** (0.2 mmol) and $[Me_4N][SeCF_3]$ (0.4 mmol) in CH_3CN (1 mL) was added BPO (0.2 mmol) and CH_3CN (1 mL). The mixture was reacted under N_2 for 16 h. [b] Yields were determined by HPLC (λ = 249 nm, methanol/water = 90:10 (v/v)) using **3a** (t_R = 7.92 min) and **4a** (t_R = 4.58 min) as external standards, respectively. Isolated yields were depicted in the parentheses.

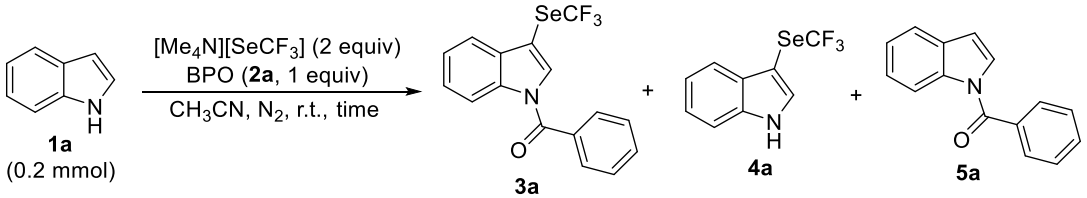
Table S3. Trifluoromethylselenolation/*N*-acylation of **1a** with different equivalents of $[Me_4N][SeCF_3]$ and BPO.



Entry [a]	1 : x : y	Yield (**3a**, %) [b]	Yield (**4a**, %) [b]
1	1 : 3 : 1.5	88	3
2	1 : 2.5 : 2	5	89
3	1 : 2.5 : 1	86	9
4	1 : 2.5 : 1.5	83	15
5	1 : 2 : 1	94 (93)	5 (5)
6	1 : 2 : 2	6	94
7	1 : 2 : 1.5	5	89
8	1 : 1.5 : 1	26	26
9	1 : 1 : 1	5	94
10	1 : 1 : 0.5	40	21

[a] Reaction conditions: to a solution of **1a** (0.2 mmol) and [Me_4N][$SeCF_3$] (0.6, 0.5, 0.4, 0.3 or 0.2 mmol) in CH_3CN (1 mL) was added BPO (0.3, 0.4, 0.2 or 0.1 mmol) and CH_3CN (1 mL). The mixture was reacted at room temperature under N_2 for 16 h. [b] Yields were determined by HPLC (λ = 249 nm, methanol/water = 90:10 (v/v)) using **3a** (t_R = 7.92 min) and **4a** (t_R = 4.58 min) as external standards, respectively. Isolated yields were depicted in the parentheses.

Table S4. Trifluoromethylselenolation/*N*-acylation of **1a** with [Me_4N][$SeCF_3$] and BPO at different times.

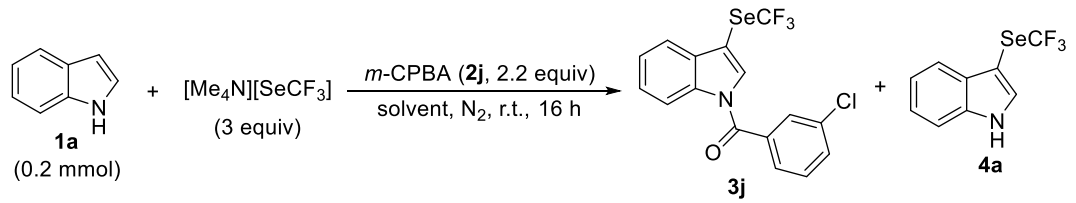


Entry [a]	Time	Yield (**1a**, %) [b]	Yield (**5a**, %) [b]	Yield (**3a**, %) [b]	Yield (**4a**, %) [b]
1	5 min	trace	0	< 1	> 99
2	15 min	0	0	5	91
3	30 min	0	0	19	80
4	45 min	0	0	37	63

5	1 h	0	0	46	53
6	2 h	0	0	62	37
7	3 h	0	0	66	30
8	4 h	0	0	78	18
9	8 h	0	0	85 (84)	13
10	12 h	0	0	90 (88)	5 (5)
11	16 h	0	0	94 (93)	5 (5)
12	20 h	0	0	93	6
13	24 h	0	0	88	11

[a] Reaction conditions: to a solution of **1a** (0.2 mmol) and $[Me_4N][SeCF_3]$ (0.4 mmol) in CH_3CN (1 mL) was added BPO (0.2 mmol) and CH_3CN (1 mL). The mixture was reacted at room temperature under N_2 atmosphere. [b] Yields were determined by HPLC (λ = 249 nm, methanol/water = 90:10 (v/v)) using **1a** (t_R = 3.61 min), **5a** (t_R = 5.37 min), **3a** (t_R = 7.92 min) and **4a** (t_R = 4.58 min) as external standards, respectively. Isolated yields were depicted in the parentheses.

Table S5. Trifluoromethylselenolation/*N*-acylation of **1a** with $[Me_4N][SeCF_3]$ and *m*-CPBA in different solvents.

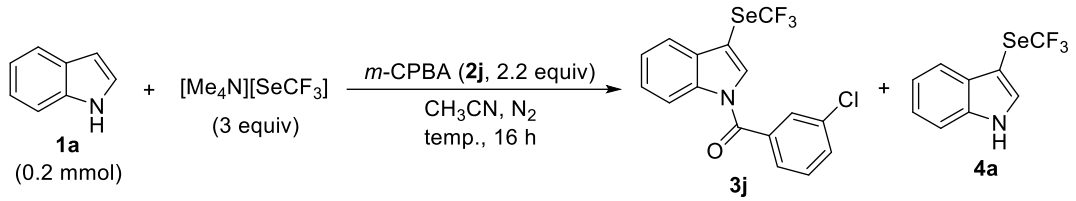


Entry [a]	Solvent	Yield (**3j**, %) [b]	Yield (**4a**, %) [b]
1	CH_3CN	83	5
2	DMF	61	18
3	DCM	37	29
4	THF	62	26
5	toluene	18	6
6	DMSO	23	42
7	1, 4-dioxane	58	12

[a] Reaction conditions: to a solution of **1a** (0.2 mmol) and $[Me_4N][SeCF_3]$ (0.6 mmol)

in solvent (1 mL) was added *m*-CPBA (0.44 mmol) and solvent (1 mL). The mixture was reacted at room temperature under N_2 for 16 h. [b] Yields were determined by HPLC (λ = 250 nm, methanol/water = 90:10 (v/v)) using **3j** (t_R = 9.85 min) and **4a** (t_R = 4.58 min) as external standards, respectively.

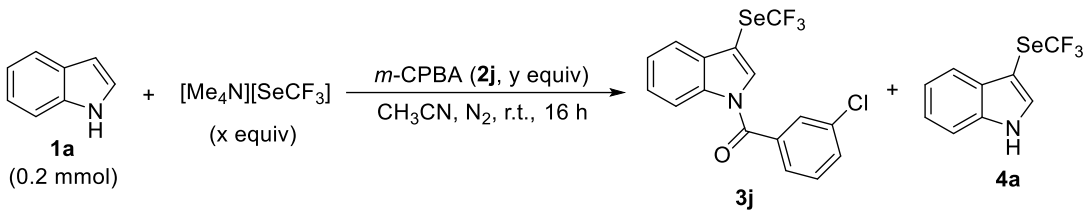
Table S6. Trifluoromethylselenolation/*N*-acylation of **1a** with $[Me_4N][SeCF_3]$ and *m*-CPBA at different temperatures.



Entry [a]	Temperature	Yield (**3j**, %) [b]	Yield (**4a**, %) [b]
1	0 °C	6	79
2	r.t.	83	5
3	40 °C	77	18
4	60 °C	71	20

[a] Reaction conditions: to a solution of **1a** (0.2 mmol) and $[Me_4N][SeCF_3]$ (0.6 mmol) in CH_3CN (1 mL) was added *m*-CPBA (0.44 mmol) and CH_3CN (1 mL). The mixture was reacted under N_2 for 16 h. [b] Yields were determined by HPLC (λ = 250 nm, methanol/water = 90:10 (v/v)) using **3j** (t_R = 9.85 min) and **4a** (t_R = 4.58 min) as external standards, respectively.

Table S7. Trifluoromethylselenolation/*N*-acylation of **1a** with different equivalents of $[Me_4N][SeCF_3]$ and *m*-CPBA.

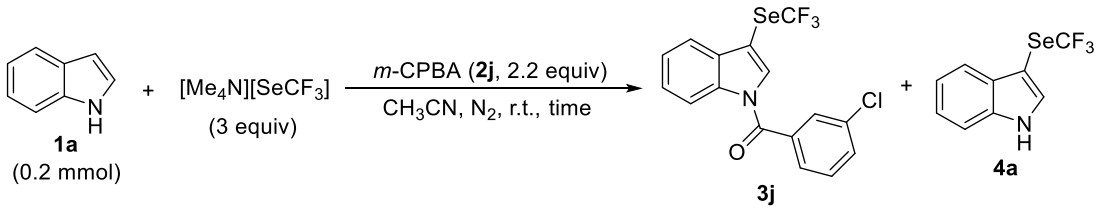


Entry [a]	1 : x : y	Yield (**3j**, %) [b]	Yield (**4a**, %) [b]

1	1 : 3 : 2.2	83	5
2	1 : 3 : 2	67	9
3	1 : 3 : 1.5	65	25
4	1 : 3 : 1	54	17

[a] Reaction conditions: to a solution of **1a** (0.2 mmol) and $[Me_4N][SeCF_3]$ (0.6 mmol) in CH_3CN (1 mL) was added *m*-CPBA (0.44, 0.4, 0.3 or 0.2 mmol) and CH_3CN (1 mL). The mixture was reacted at room temperature under N_2 for 16 h. [b] Yields were determined by HPLC (λ = 250 nm, methanol/water = 90:10 (v/v)) using **3j** (t_R = 9.85 min) and **4a** (t_R = 4.58 min) as external standards, respectively.

Table S8. Trifluoromethylselenolation/*N*-acylation of **1a** with $[Me_4N][SeCF_3]$ and *m*-CPBA at different times.



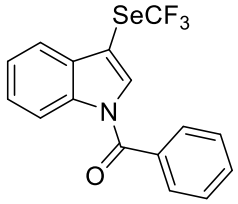
Entry [a]	Time (h)	Yield (**3j**, %) [b]	Yield (**4a**, %) [b]
1	4	36	60
2	8	93 (88)	trace (10)
3	12	87	3
4	16	83	5
5	20	86	2
6	24	88	8

[a] Reaction conditions: to a solution of **1a** (0.2 mmol) and $[Me_4N][SeCF_3]$ (0.6 mmol) in CH_3CN (1 mL) was added *m*-CPBA (0.44 mmol) and CH_3CN (1 mL). The mixture was reacted at room temperature under N_2 atmosphere. [b] Yields were determined by HPLC (λ = 250 nm, methanol/water = 90:10 (v/v)) using **3j** (t_R = 9.85 min) and **4a** (t_R = 4.58 min) as external standards, respectively. Isolated yields were depicted in the parentheses.

3. General procedure for trifluoromethylselenolation/*N*-acylation of indoles (1) with [Me_4N][$SeCF_3$] and an oxidant (2).

Under a nitrogen atmosphere, a Schlenk tube was charged with **1** (0.2 mmol), [Me_4N][$SeCF_3$] (0.4 or 0.6 mmol) and CH_3CN (1 mL), followed by addition of **2** (0.2 or 0.44 mmol) and CH_3CN (1 mL), with vigorous stirring. The mixture was reacted at room temperature under N_2 for 16 h or 8 h and concentrated to dryness under reduced pressure. The residue was purified by flash column chromatography on silica gel using a mixture of petroleum ether and ethyl acetate or dichloromethane as eluents to give the trifluoromethylselenolation/*N*-acylation products (**3**).

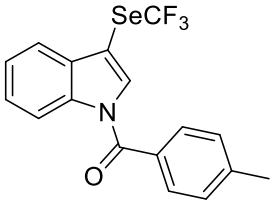
Phenyl(3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)methanone (**3a**)



White solid, 68.4 mg (93%, **1a** : [Me_4N][$SeCF_3$] : **2a** = 1 : 2 : 1) or 7.4 mg (10%, **1a** : [Me_4N][$SeCF_3$] : **2k** = 1 : 3 : 2.2), petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents for column chromatography. M.p.: 56-57 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, *J* = 7.9 Hz, 1H), 7.78-7.75 (m, 3H), 7.69-7.66 (m, 2H), 7.58 (t, *J* = 7.8 Hz, 2H), 7.50-7.44 (m, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -36.0 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.1, 136.2, 135.5, 133.6, 132.6, 131.9, 129.4, 128.9, 126.1, 124.9, 122.0 (q, *J* = 335.1 Hz), 120.4, 116.4, 100.4 (q, *J* = 1.7 Hz). IR (KBr): 3364, 3143, 3076, 3060, 3033, 1693, 1639, 1601, 1526, 1474, 1448, 1352, 1335, 1312, 1247, 1214, 1180, 1156, 1139, 1107, 1091, 1077, 1055, 1029, 1013, 1002, 964, 943, 927, 870, 848, 821, 796, 762, 737, 723, 708, 693, 658, 595 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{16}H_{11}F_3NOSe$ ($[M + H]^+$): 369.9952; found: 369.9967.

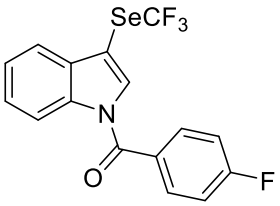
As an example, 37.9 mg (0.31 mmol) of benzoic acid was isolated from this reaction.[5] White solid. The compound was purified by prepared TLC plate (silica) using petroleum ether / ethyl acetate = 2 : 1 (v/v) as eluents. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.92 (s, br, 1H), 7.94 (d, *J* = 7.8 Hz, 2H), 7.62 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 167.8, 133.3, 131.2, 129.7, 129.0.

p-Tolyl(3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)methanone (**3b**)



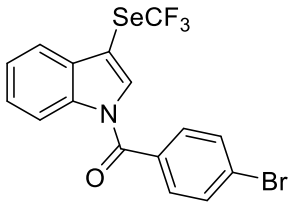
Light yellow solid, 71.1 mg (93%, **1a** : $[Me_4N][SeCF_3]$: **2b** = 1 : 2 : 1), petroleum ether / dichloromethane = 3 : 1 (v/v) as eluents for column chromatography. M.p.: 142-143 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (d, *J* = 7.9 Hz, 1H), 7.75 (d, *J* = 7.5 Hz, 1H), 7.70 (s, 1H), 7.68 (d, *J* = 7.5 Hz, 2H), 7.49-7.42 (m, 2H), 7.38 (d, *J* = 7.7 Hz, 2H), 2.49 (s, 3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -36.1 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.2, 143.6, 136.2, 135.7, 131.9, 130.6, 129.7, 129.6, 125.9, 124.7, 122.0 (q, *J* = 335.1 Hz), 120.4, 116.3, 100.0 (q, *J* = 1.5 Hz), 21.7. IR (KBr): 3366, 3150, 3054, 2923, 2853, 1685, 1608, 1527, 1509, 1468, 1444, 1410, 1350, 1329, 1312, 1293, 1247, 1210, 1182, 1154, 1139, 1100, 1086, 1055, 1016, 961, 863, 849, 828, 811, 789, 769, 751, 707, 635, 610 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{17}H_{13}F_3NOSe$ ($[M + H]^+$): 384.0109; found: 384.0115.

(4-Fluorophenyl)(3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)methanone (**3c**)



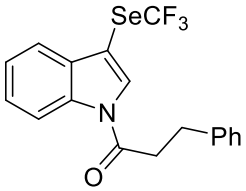
Light yellow solid, 55.3 mg (72%, **1a** : $[Me_4N][SeCF_3]$: **2c** = 1 : 2 : 1), petroleum ether / dichloromethane = 4 : 1 (v/v) as eluents for column chromatography. M.p.: 95-96 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (d, *J* = 7.9 Hz, 1H), 7.83 (m, 2H), 7.78 (d, *J* = 7.4 Hz, 1H), 7.67 (s, 1H), 7.52-7.46 (m, 2H), 7.29 (t, *J* = 8.4 Hz, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -36.0 (s, 3F), -104.8 (s, 1F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.0, 165.3 (d, *J* = 255.1 Hz), 136.2, 135.2, 132.1 (d, *J* = 9.1 Hz), 131.9, 129.7 (d, *J* = 3.3 Hz), 126.1, 124.9, 121.9 (q, *J* = 335.1 Hz), 120.5, 116.3 (d, *J* = 22.1 Hz), 116.2, 100.7. IR (KBr): 3141, 3077, 1696, 1603, 1524, 1509, 1471, 1448, 1433, 1410, 1352, 1334, 1313, 1250, 1239, 1230, 1214, 1160, 1141, 1128, 1102, 1090, 1056, 1014, 966, 878, 886, 851, 826, 810, 773, 756, 736, 709, 693, 631, 607 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{16}H_{10}F_4NOSe$ ($[M + H]^+$): 387.9858; found: 387.9856.

(4-Bromophenyl)(3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)methanone (**3d**)



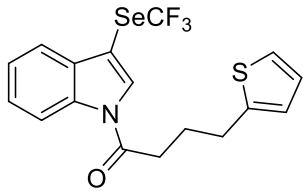
Light yellow solid, 82.2 mg (92%, **1a** : $[Me_4N][SeCF_3]$: **2d** = 1 : 2 : 1), petroleum ether / dichloromethane = 4 : 1 (v/v) as eluents for column chromatography. M.p.: 136-137 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, *J* = 7.9 Hz, 1H), 7.76 (d, *J* = 7.6 Hz, 1H), 7.73 (d, *J* = 8.3 Hz, 2H), 7.65-7.63 (m, 3H), 7.50-7.44 (m, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.9 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.1, 136.1, 135.0, 132.3, 132.3, 131.9, 130.9, 127.7, 126.2, 125.0, 121.9 (q, *J* = 335.1 Hz), 120.5, 116.3, 101.0 (q, *J* = 1.5 Hz). IR (KBr): 3154, 1681, 1647, 1589, 1531, 1483, 1471, 1446, 1357, 1332, 1313, 1292, 1280, 1244, 1209, 1151, 1137, 1101, 1089, 1072, 1014, 963, 872, 846, 832, 801, 769, 754, 737, 682, 627, 605 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{16}H_{10}BrF_3NOSe$ ($[M + H]^+$): 447.9058; found: 447.9056.

3-Phenyl-1-(3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)propan-1-one (**3e**)



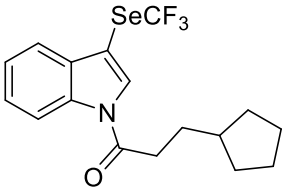
Light yellow solid, 66.5 mg (84%, **1a** : $[Me_4N][SeCF_3]$: **2e** = 1 : 2 : 1), petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents for column chromatography. M.p.: 107-108 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.1 Hz, 1H), 7.72 (s, 1H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.41 (t, *J* = 8.1 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 7.3 Hz, 2H), 7.26 (d, *J* = 7.6 Hz, 2H), 7.22 (t, *J* = 7.2 Hz, 1H), 3.24 (t, *J* = 7.4 Hz, 2H), 3.15 (t, *J* = 7.4 Hz, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.9 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.2, 140.0, 135.8, 132.6, 131.5, 128.8, 128.5, 126.7, 126.3, 124.6, 121.9 (q, *J* = 335.0 Hz), 120.4, 116.7, 101.1 (q, *J* = 1.5 Hz), 37.7, 30.3. IR (KBr): 3405, 3149, 3087, 3060, 3029, 2939, 2920, 1710, 1604, 1531, 1498, 1474, 1445, 1425, 1391, 1350, 1334, 1331, 1320, 1307, 1295, 1218, 1201, 1155, 1135, 1109, 1089, 1056, 1033, 1016, 979, 922, 906, 798, 789, 786, 761, 750, 736, 717, 696, 672 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{18}H_{15}F_3NOSe$ ($[M + H]^+$): 398.0265; found: 398.0279.

4-(Thiophen-2-yl)-1-(3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)butan-1-one (**3f**)



White solid, 71.9 mg (86%, **1a** : $[Me_4N][SeCF_3]$: **2f** = 1 : 2 : 1), petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents for column chromatography. M.p.: 104-105 ^oC. ^1H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.1 Hz, 1H), 7.74 (s, 1H), 7.70 (d, *J* = 7.7 Hz, 1H), 7.45 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.17 (d, *J* = 5.1 Hz, 1H), 6.96 (m, 1H), 6.86 (m, 1H), 3.04 (t, *J* = 7.3 Hz, 2H), 3.01 (t, *J* = 7.3 Hz, 2H), 2.26 (m, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.9 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.6, 143.6, 135.7, 132.7, 131.5, 127.0, 126.3, 124.9, 124.6, 123.6, 122.0 (q, *J* = 335.4 Hz), 120.4, 116.6, 101.0 (q, *J* = 1.5 Hz), 34.5, 28.9, 26.2. IR (KBr): 3410, 3153, 3141, 3111, 2960, 2943, 2930, 2916, 2849, 1713, 1532, 1473, 1443, 1415, 1407, 1387, 1368, 1307, 1230, 1218, 1199, 1155, 1143, 1111, 1092, 1077, 1054, 1016, 1003, 971, 954, 921, 903, 878, 845, 838, 765, 751, 736, 707, 671, 655, 600 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{17}H_{15}F_3NOSSe$ $([M + H]^+)$: 417.9986; found: 418.0000.

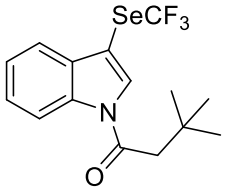
3-Cyclopentyl-1-(3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)propan-1-one (**3g**)



Light yellow solid, 58.7 mg (76%, **1a** : $[Me_4N][SeCF_3]$: **2g** = 1 : 2 : 1), petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents for column chromatography. M.p.: 71-72 ^oC. ^1H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.1 Hz, 1H), 7.83 (s, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.46-7.39 (m, 2H), 2.98 (t, *J* = 7.4 Hz, 2H), 1.95-1.86 (m, 5H), 1.67 (m, 2H), 1.58 (m, 2H), 1.19 (m, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -36.0 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.3, 135.8, 132.8, 131.5, 126.2, 124.5, 122.0 (q, *J* = 335.2 Hz), 120.3, 116.7, 100.8 (q, *J* = 1.6 Hz), 39.5, 35.2, 32.6, 30.7, 25.1. IR (KBr): 3419, 3160, 3138, 3123, 3106, 3075, 3051, 2946, 2863, 1716, 1632, 1604, 1526, 1474, 1445, 1417, 1382, 1362, 1331, 1315, 1299, 1223, 1198, 1183, 1157, 1113, 1099, 1056,

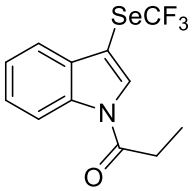
1017, 974, 948, 916, 814, 792, 762, 750, 737, 670, 601 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{17}H_{19}F_3NOSe$ ($[M + H]^+$): 390.0578; found: 390.0583.

3,3-Dimethyl-1-(3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)butan-1-one (**3h**)



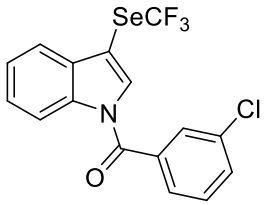
Light yellow liquid, 51.7 mg (71%, **1a** : $[Me_4N][SeCF_3]$: **2h** = 1 : 2 : 1), petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents for column chromatography. ^1H NMR (500 MHz, $CDCl_3$) δ 8.55 (d, *J* = 7.9 Hz, 1H), 7.83 (s, 1H), 7.71 (d, *J* = 7.7 Hz, 1H), 7.46-7.39 (m, 2H), 2.84 (s, 2H), 1.17 (s, 9H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -36.1 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.0, 135.9, 133.5, 131.6, 126.2, 124.5, 121.9 (q, *J* = 335.1 Hz), 120.3, 116.9, 100.4 (q, *J* = 1.6 Hz), 47.9, 31.8, 29.8. IR (KBr): 3412, 3140, 3066, 3031, 2986, 2961, 2934, 2913, 2870, 1712, 1655, 1601, 1526, 1473, 1465, 1449, 1406, 1394, 1372, 1361, 1345, 1297, 1253, 1218, 1160, 1130, 1109, 1089, 1055, 1017, 989, 946, 936, 895, 831, 799, 765, 747, 735, 676 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{15}H_{17}F_3NOSe$ ($[M + H]^+$): 364.0422; found: 364.0432.

1-(3-((Trifluoromethyl)selanyl)-1*H*-indol-1-yl)propan-1-one (**3i**)



Light yellow solid, 45.9 mg (72%, **1a** : $[Me_4N][SeCF_3]$: **2i** = 1 : 2 : 1), petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents for column chromatography. M.p.: 87-88 ^oC. ^1H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.1 Hz, 1H), 7.83 (s, 1H), 7.71 (d, *J* = 7.7 Hz, 1H), 7.46-7.39 (m, 2H), 3.01 (q, *J* = 7.3 Hz, 2H), 1.38 (t, *J* = 7.3 Hz, 3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -36.0 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.8, 135.8, 132.7, 131.5, 126.2, 124.5, 121.9 (q, *J* = 335.2 Hz), 120.3, 116.6, 100.9 (q, *J* = 1.5 Hz), 29.3, 8.6. IR (KBr): 3441, 3424, 3163, 3119, 2981, 2938, 2917, 1731, 1721, 1529, 1471, 1462, 1443, 1371, 1295, 1222, 1178, 1159, 1146, 1108, 1077, 1053, 1009, 966, 894, 808, 762, 756, 736, 655, 602 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{12}H_{11}F_3NOSe$ ($[M + H]^+$): 321.9952; found: 321.9957.

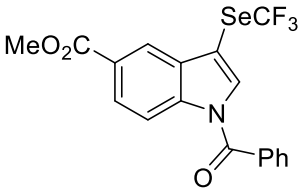
(3-Chlorophenyl)(3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)methanone (**3j**)



White solid, 70.8 mg (88%, **1a** : $[Me_4N][SeCF_3]$: **2j** = 1 : 3 : 2.2), petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents for column chromatography. M.p.: 95-96 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.1 Hz, 1H), 7.76-7.75 (m, 2H), 7.65-7.62 (m, 3H), 7.52 (t, *J* = 7.9 Hz, 1H), 7.50-7.45 (m, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.9 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.6, 136.1, 135.3, 135.2, 134.9, 132.7, 131.9, 130.2, 129.4, 127.3, 126.3, 125.1, 121.9 (q, *J* = 335.1 Hz), 120.6, 116.3, 101.2 (q, *J* = 1.8 Hz). IR (KBr): 3347, 3142, 3077, 2924, 2853, 1680, 1571, 1529, 1471, 1447, 1421, 1365, 1359, 1332, 1311, 1293, 1244, 1209, 1141, 1095, 1056, 1016, 1000, 970, 907, 895, 822, 816, 807, 767, 754, 736, 700, 684, 651, 593 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{16}H_{10}ClF_3NOSe$ ($[M + H]^+$): 403.9563; found: 403.9561.

As an example, 28.2 mg (0.18 mmol) of 3-chlorobenzoic acid was isolated from this reaction.[6] White solid. The compound was purified by prepared TLC plate (silica) using petroleum ether / ethyl acetate = 1 : 1 (v/v) as eluents. ^{1}H NMR (500 MHz, DMSO-d_6) δ 13.33 (s, br, 1H), 7.89 (m, 2H), 7.69 (d, *J* = 7.4 Hz, 1H), 7.54 (t, *J* = 8.0 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 166.5, 133.8, 133.4, 133.1, 131.1, 129.3, 128.4.

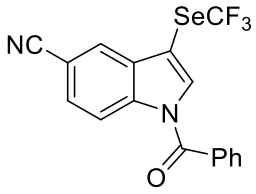
Methyl 1-benzoyl-3-((trifluoromethyl)selanyl)-1*H*-indole-5-carboxylate (**3k**)



Light yellow solid, 54.4 mg (64%, **1b** : $[Me_4N][SeCF_3]$: **2a** = 1 : 2 : 1), petroleum ether / dichloromethane = 1 : 1 (v/v) as eluents for column chromatography. M.p.: 126-127 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.41 (d, *J* = 8.7 Hz, 1H), 8.16 (d, *J* = 8.8 Hz, 1H), 7.78 (d, *J* = 7.8 Hz, 2H), 7.75 (s, 1H), 7.69 (t, *J* = 7.7 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 2H), 3.99 (s, 3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.9 (s, 3F). ^{13}C NMR (126 MHz, acetone-d_6) δ 168.0, 166.2, 138.8, 137.8, 133.2, 132.9,

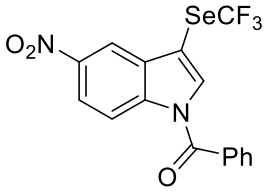
131.8, 129.6, 128.9, 126.7, 126.6, 122.3 (q, J = 334.1 Hz), 121.8, 116.2, 99.7 (q, J = 1.8 Hz), 51.6. IR (KBr): 3406, 3155, 3061, 3040, 2995, 2947, 2922, 2852, 1714, 1703, 1670, 1612, 1601, 1520, 1469, 1449, 1438, 1356, 1336, 1309, 1282, 1262, 1237, 1211, 1189, 1158, 1136, 1124, 1103, 1093, 1064, 987, 955, 945, 905, 889, 844, 830, 819, 797, 775, 768, 747, 725, 699, 667 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{18}H_{13}F_3NO_3Se$ ($[M + H]^+$): 428.0007; found: 428.0013.

1-Benzoyl-3-((trifluoromethyl)selanyl)-1*H*-indole-5-carbonitrile (**3l**)



Light yellow solid, 44.9 mg (53%, **1c** : $[Me_4N][SeCF_3]$: **2a** = 1 : 2 : 1), petroleum ether / dichloromethane = 1 : 1 (v/v) as eluents for column chromatography. M.p.: 158-160 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (d, J = 8.6 Hz, 1H), 8.09 (s, 1H), 7.81 (s, 1H), 7.78 (d, J = 7.8 Hz, 2H), 7.74-7.71 (m, 2H), 7.61 (t, J = 7.4 Hz, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.8 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.8, 138.1, 137.4, 133.4, 132.5, 132.2, 129.6, 129.2, 129.1, 125.4, 120.3 (q, J = 335.3 Hz), 119.1, 117.3, 108.5, 99.9. IR (KBr): 3447, 3146, 2958, 2923, 2852, 2228, 1698, 1656, 1610, 1601, 1581, 1524, 1460, 1447, 1435, 1349, 1334, 1327, 1309, 1276, 1253, 1212, 1179, 1146, 1131, 1113, 1103, 1089, 1055, 999, 977, 952, 937, 897, 837, 819, 794, 769, 736, 723, 701, 669, 635 cm^{-1}. HRMS-DART (m/z) calcd. for $C_{17}H_{13}F_3N_3OSe$ ($[M + NH_4]^+$): 412.0170; found: 412.0165.

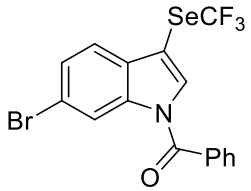
(5-Nitro-3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)(phenyl)methanone (**3m**)



Light yellow solid, 43.5 mg (53%, **1d** : $[Me_4N][SeCF_3]$: **2a** = 1 : 2 : 1), petroleum ether / dichloromethane = 1 : 1 (v/v) as eluents for column chromatography. M.p.: 124-125 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.66 (s, 1H), 8.52 (d, J = 9.1 Hz, 1H), 8.36 (d, J = 9.1 Hz, 1H), 7.86 (s, 1H), 7.80 (d, J = 7.8 Hz, 2H), 7.73 (t, J = 7.5 Hz, 1H), 7.62 (t, J = 7.5 Hz, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.8 (s, 3F). ^{13}C NMR

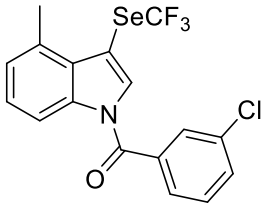
(126 MHz, $CDCl_3$) δ 167.8, 145.3, 139.2, 138.2, 133.5, 132.4, 132.3, 129.6, 129.2, 121.8 (q, *J* = 334.9 Hz), 121.2, 116.9, 116.9, 100.8 (q, *J* = 1.6 Hz). IR (KBr): 3393, 3144, 3098, 3072, 3034, 2923, 2852, 1706, 1610, 1600, 1582, 1522, 1440, 1366, 1350, 1332, 1306, 1264, 1247, 1206, 1180, 1143, 1136, 1120, 1102, 1089, 1075, 974, 938, 908, 899, 840, 825, 798, 777, 757, 735, 720, 696, 666, 641, 605 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{16}H_{10}F_3N_2O_3Se$ ($[M + H]^+$): 414.9803; found: 414.9804.

(6-Bromo-3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)(phenyl)methanone (**3n**)



Light yellow solid, 58.3 mg (65%, **1e** : $[Me_4N][SeCF_3]$: **2a** = 1 : 2 : 1), petroleum ether / dichloromethane = 3 : 1 (v/v) as eluents for column chromatography. M.p.: 120-121 °C. ^1H NMR (500 MHz, $CDCl_3$) δ 8.64 (s, 1H), 7.76 (d, *J* = 7.7 Hz, 2H), 7.69 (t, *J* = 7.7 Hz, 1H), 7.64 (s, 1H), 7.61-7.56 (m, 4H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.9 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.9, 136.8, 135.8, 133.0, 132.9, 130.8, 129.4, 129.0, 128.3, 121.9 (q, *J* = 334.8 Hz), 121.6, 120.0, 119.5, 100.2 (q, *J* = 1.6 Hz). IR (KBr): 3375, 3362, 3145, 3132, 3123, 3081, 3066, 3051, 2923, 2852, 1697, 1689, 1632, 1599, 1525, 1517, 1466, 1447, 1423, 1360, 1348, 1316, 1276, 1238, 1210, 1182, 1160, 1129, 1117, 1104, 1092, 1028, 999, 960, 931, 881, 870, 819, 810, 782, 746, 735, 718, 698, 664, 622, 614 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{16}H_{10}BrF_3NOSe$ ($[M + H]^+$): 447.9058; found: 447.9060.

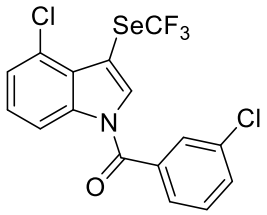
(3-Chlorophenyl)(4-methyl-3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)methanone (**3p**)



White solid, 75.6 mg (94%, **1g** : $[Me_4N][SeCF_3]$: **2j** = 1 : 3 : 2.2), petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents for column chromatography. M.p.: 118-119 °C. ^1H NMR (500 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.4 Hz, 1H), 7.75 (s, 1H), 7.65-7.60 (m, 3H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.36 (t, *J* = 7.7 Hz, 1H), 7.17 (d, *J* = 7.4 Hz, 1H). 2.84 (s,

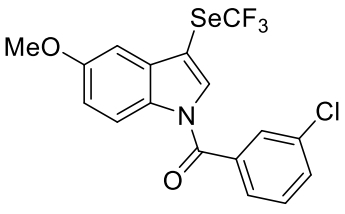
3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -37.6 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.6, 136.5, 135.3, 135.2, 132.7, 132.0, 130.2, 129.5, 128.5, 127.4, 127.2, 126.1, 121.7 (q, *J* = 334.0 Hz), 114.2, 99.5 (q, *J* = 1.5 Hz), 19.4. IR (KBr): 3371, 3154, 2965, 2928, 2853, 1689, 1655, 1633, 1595, 1581, 1571, 1528, 1483, 1466, 1454, 1421, 1411, 1387, 1355, 1327, 1300, 1274, 1249, 1227, 1187, 1168, 1109, 1019, 985, 970, 949, 916, 900, 866, 811, 783, 752, 736, 719, 688, 661, 621 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{17}H_{12}ClF_3NOSe$ ($[M + H]^+$): 417.9719; found: 417.9721.

(4-Chloro-3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)(3-chlorophenyl)methanone (**3q**)



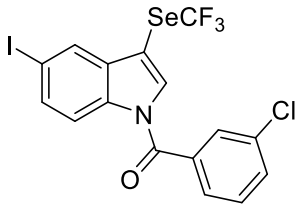
Light yellow solid, 66.9 mg (77%, **1h** : $[Me_4N][SeCF_3]$: **2j** = 1 : 3 : 2.2), petroleum ether / dichloromethane = 3 : 1 (v/v) as eluents for column chromatography. M.p.: 125-126 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (m, 1H), 7.76 (s, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.62-7.61 (m, 2H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.39-7.36 (m, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -37.2 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.4, 137.4, 136.2, 135.4, 134.7, 133.0, 130.3, 129.6, 127.4, 127.3, 127.0, 126.8, 126.4, 121.8 (q, *J* = 334.6 Hz), 115.1, 99.2 (q, *J* = 1.7 Hz). IR (KBr): 3377, 3146, 3107, 3091, 3068, 3033, 2924, 2852, 1692, 1659, 1650, 1569, 1524, 1474, 1461, 1415, 1352, 1329, 1299, 1265, 1242, 1185, 1169, 1148, 1129, 1094, 1058, 999, 966, 929, 916, 901, 845, 809, 783, 752, 743, 736, 710, 685, 658, 600 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{16}H_9Cl_2F_3NOSe$ ($[M + H]^+$): 437.9173; found: 437.9182.

(3-Chlorophenyl)(5-methoxy-3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)methanone (**3r**)



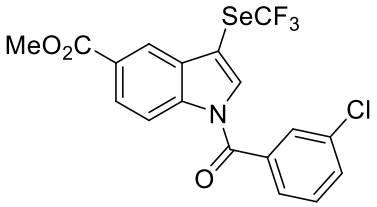
Light yellow solid, 84.2 mg (97%, **1i** : $[Me_4N][SeCF_3]$: **2j** = 1 : 3 : 2.2), petroleum ether / dichloromethane = 3 : 1 (v/v) as eluents for column chromatography. M.p.: 106-108 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (d, *J* = 9.0 Hz, 1H), 7.75 (s, 1H), 7.64-7.60 (m, 2H), 7.57 (s, 1H), 7.51 (t, *J* = 7.9 Hz, 1H), 7.17 (s, 1H), 7.08 (d, *J* = 9.0 Hz, 1H), 3.93 (s, 3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.9 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.3, 157.7, 135.5, 135.2, 133.1, 132.6, 130.6, 130.2, 129.4, 127.2, 121.9 (q, *J* = 335.2 Hz), 117.4, 115.2, 102.7, 101.0 (q, *J* = 1.5 Hz), 55.8. IR (KBr): 3391, 3144, 3056, 2998, 2958, 2919, 2882, 2853, 2834, 1702, 1611, 1587, 1568, 1526, 1474, 1444, 1414, 1365, 1334, 1277, 1254, 1211, 1178, 1156, 1134, 1095, 1033, 977, 946, 924, 908, 836, 819, 806, 775, 755, 741, 728, 683, 668, 654, 631 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{17}H_{12}ClF_3NO_2Se$ ($[M + H]^+$): 433.9668; found: 433.9675.

(3-Chlorophenyl)(5-iodo-3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)methanone (**3s**)



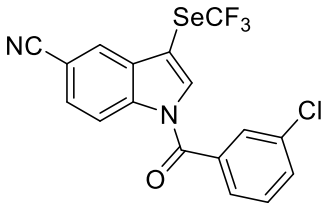
Light yellow solid, 92.1 mg (87%, **1j** : $[Me_4N][SeCF_3]$: **2j** = 1 : 3 : 2.2), petroleum ether / dichloromethane = 4 : 1 (v/v) as eluents for column chromatography. M.p.: 121-122 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.7 Hz, 1H), 8.08 (s, 1H), 7.77-7.75 (m, 2H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.61 (d, *J* = 7.5 Hz, 1H), 7.59 (s, 1H), 7.53 (t, *J* = 7.9 Hz, 1H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.8 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.4, 135.5, 135.4, 135.4, 134.9, 134.8, 134.0, 132.9, 130.3, 129.5, 129.4, 127.3, 121.8 (q, *J* = 335.2 Hz), 118.1, 99.9 (q, *J* = 1.6 Hz), 89.4. IR (KBr): 3368, 3151, 3120, 3061, 3033, 2992, 2962, 2924, 2852, 1697, 1600, 1564, 1557, 1531, 1450, 1437, 1423, 1381, 1350, 1312, 1295, 1263, 1239, 1220, 1208, 1167, 1146, 1137, 1117, 1094, 1070, 1057, 1030, 1022, 1000, 968, 927, 897, 886, 873, 804, 792, 782, 754, 748, 736, 729, 706, 683, 668, 653, 630, 603 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{16}H_9ClF_3INOSe$ ($[M + H]^+$): 529.8529; found: 529.8532.

Methyl 1-(3-chlorobenzoyl)-3-((trifluoromethyl)selanyl)-1*H*-indole-5-carboxylate (**3t**)



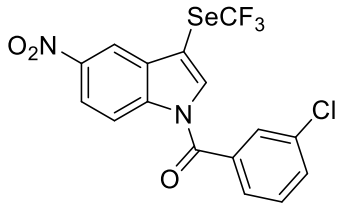
Light yellow solid, 78.8 mg (86%, **1b** : $[Me_4N][SeCF_3]$: **2j** = 1 : 3 : 2.2), petroleum ether / dichloromethane = 1 : 1 (v/v) as eluents for column chromatography. M.p.: 125-126 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.41 (d, *J* = 8.8 Hz, 1H), 8.17 (d, *J* = 8.8 Hz, 1H), 7.77 (s, 1H), 7.70 (s, 1H), 7.66 (d, *J* = 8.2 Hz, 1H), 7.64 (d, *J* = 7.7 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 3.99 (s, 3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.8 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.8, 166.5, 138.7, 136.1, 135.4, 134.7, 133.1, 131.9, 130.3, 129.5, 127.5, 127.4, 127.2, 122.7, 121.8 (q, *J* = 334.5 Hz), 116.2, 101.5 (q, *J* = 1.6 Hz), 52.4. IR (KBr): 3419, 3140, 3112, 3060, 2956, 2926, 2850, 1719, 1696, 1613, 1570, 1529, 1468, 1434, 1358, 1337, 1291, 1251, 1228, 1162, 1149, 1134, 1104, 1088, 986, 964, 902, 880, 827, 806, 777, 765, 750, 737, 714, 683, 654, 639, 607 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{18}H_{12}ClF_3NO_3Se$ ($[M + H]^+$): 461.9618; found: 461.9622.

1-(3-Chlorobenzoyl)-3-((trifluoromethyl)selanyl)-1*H*-indole-5-carbonitrile (**3u**)



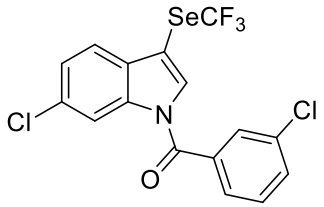
Light yellow solid, 59.2 mg (69%, **1c** : $[Me_4N][SeCF_3]$: **2j** = 1 : 3 : 2.2), petroleum ether / dichloromethane = 1 : 1 (v/v) as eluents for column chromatography. M.p.: 136-137 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (d, *J* = 8.6 Hz, 1H), 8.09 (s, 1H), 7.77 (s, 1H), 7.76 (s, 1H), 7.74 (d, *J* = 8.7 Hz, 1H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 1H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.6 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.4, 137.0, 135.9, 134.5, 133.2, 132.4, 131.2, 129.4, 128.5, 128.3, 126.4, 124.5, 120.7 (q, *J* = 335.1 Hz), 117.9, 116.3, 107.8, 99.6 (q, *J* = 1.7 Hz). IR (KBr): 3143, 3074, 2955, 2926, 2855, 2225, 1705, 1610, 1569, 1527, 1460, 1435, 1421, 1344, 1330, 1310, 1279, 1250, 1213, 1167, 1140, 1088, 1060, 981, 915, 891, 817, 803, 774, 757, 745, 738, 720, 655, 635 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{17}H_9ClF_3N_2OSe$ ($[M + H]^+$): 428.9515; found: 428.9515.

(3-Chlorophenyl)(5-nitro-3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)methanone (**3v**)



Light yellow solid, 41.2 mg (46%, **1d** : $[Me_4N][SeCF_3]$: **2j** = 1 : 3 : 2.2), petroleum ether / ethyl acetate = 4 : 1 (v/v) as eluents for column chromatography. M.p.: 113-114 ^oC. ^1H NMR (500 MHz, $CDCl_3$) δ 8.66 (s, 1H), 8.52 (d, *J* = 9.1 Hz, 1H), 8.38 (d, *J* = 9.1 Hz, 1H), 7.81 (s, 1H), 7.79 (s, 1H), 7.70 (d, *J* = 7.9 Hz, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.57 (t, *J* = 7.9 Hz, 1H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.6 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.4, 145.5, 139.1, 137.6, 135.6, 134.0, 133.5, 132.3, 130.5, 129.6, 127.5, 121.7 (q, *J* = 334.8 Hz), 121.4, 116.9, 101.5 (q, *J* = 1.7 Hz). IR (KBr): 3142, 3077, 2956, 2925, 2854, 1709, 1612, 1570, 1522, 1469, 1454, 1439, 1419, 1412, 1365, 1350, 1335, 1306, 1279, 1263, 1244, 1206, 1168, 1144, 1089, 999, 977, 956, 911, 901, 892, 852, 824, 800, 783, 763, 756, 736, 717, 683, 654, 642, 603 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{16}H_9ClF_3N_2O_3Se$ ($[M + H]^+$): 448.9414; found: 448.9424.

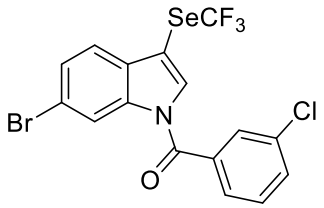
(6-Chloro-3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)(3-chlorophenyl)methanone (**3w**)



Light yellow liquid, 66.9 mg (77%, **1k** : $[Me_4N][SeCF_3]$: **2j** = 1 : 3 : 2.2), petroleum ether / dichloromethane = 3 : 1 (v/v) as eluents for column chromatography. ^1H NMR (500 MHz, $CDCl_3$) δ 8.47 (s, 1H), 7.76 (s, 1H), 7.66 (d, *J* = 8.2 Hz, 2H), 7.62 (d, *J* = 7.5 Hz, 1H), 7.60 (s, 1H), 7.53 (t, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 8.4 Hz, 1H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.8 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.4, 136.4, 135.4, 135.3, 134.7, 132.9, 132.5, 130.4, 130.3, 129.4, 127.3, 125.8, 121.8 (q, *J* = 334.9 Hz), 121.4, 116.7, 100.9. IR (KBr): 3434, 3145, 3109, 3058, 2924, 2854, 1747, 1705, 1651, 1632, 1603, 1573, 1526, 1475, 1455, 1427, 1415, 1345, 1316, 1275, 1237, 1211, 1167,

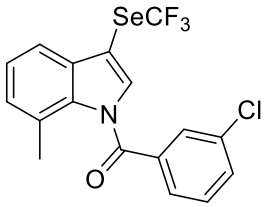
1151, 1121, 1097, 1065, 1060, 965, 901, 875, 816, 794, 774, 748, 737, 720, 632 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{16}H_9Cl_2F_3NOSe$ ($[M + H]^+$): 437.9173; found: 437.9179.

(6-Bromo-3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)(3-chlorophenyl)methanone (**3x**)



Light yellow solid, 81.5 mg (85%, **1e** : $[Me_4N][SeCF_3]$: **2j** = 1 : 3 : 2.2), petroleum ether / dichloromethane = 3 : 1 (v/v) as eluents for column chromatography. M.p.: 66-68 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.64 (s, 1H), 7.75 (s, 1H), 7.66 (d, *J* = 7.9 Hz, 1H), 7.62-7.57 (m, 4H), 7.54 (t, *J* = 7.9 Hz, 1H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.8 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.4, 136.7, 135.4, 135.2, 134.7, 132.9, 130.8, 130.3, 129.4, 128.5, 127.3, 121.8 (q, *J* = 334.4 Hz), 121.7, 120.3, 119.5, 100.9 (q, *J* = 1.6 Hz). IR (KBr): 3138, 3124, 3078, 3064, 2924, 2852, 1694, 1571, 1521, 1472, 1451, 1421, 1353, 1317, 1275, 1235, 1235, 1207, 1161, 1131, 1117, 1096, 964, 893, 871, 820, 791, 771, 758, 749, 735, 707, 683, 655, 626 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{16}H_9BrClF_3NOSe$ ($[M + H]^+$): 481.8668; found: 481.8673.

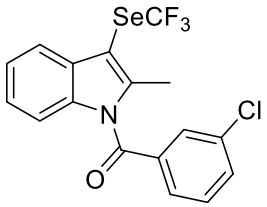
(3-Chlorophenyl)(7-methyl-3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)methanone (**3y**)



Light yellow solid, 22.5 mg (27%, **1l** : $[Me_4N][SeCF_3]$: **2j** = 1 : 3 : 2.2), petroleum ether / dichloromethane = 5 : 1 (v/v) as eluents for column chromatography. M.p.: 111-113 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 7.9 Hz, 1H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.54 (s, 1H), 7.53 (t, *J* = 7.9 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.29 (d, *J* = 7.3 Hz, 1H), 2.48 (s, 3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -36.0 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.6, 136.2, 135.9,

135.4, 134.7, 133.8, 133.1, 130.6, 130.3, 128.8, 128.6, 126.0, 125.1, 121.9 (q, J = 334.9 Hz), 118.4, 100.1 (q, J = 1.5 Hz), 21.4. IR (KBr): 3397, 3151, 2961, 2924, 2852, 1706, 1652, 1616, 1596, 1570, 1534. 1485, 1475, 1449, 1442, 1415, 1401, 1378, 1339, 1309, 1268, 1248, 1216, 1169, 1150, 1124, 1115, 1096, 1057, 1000, 979, 919, 909, 890, 861, 810, 802, 786, 770, 753, 740, 690, 676, 651 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{17}H_{12}ClF_3NOSe$ ($[M + H]^+$): 417.9719; found: 417.9725.

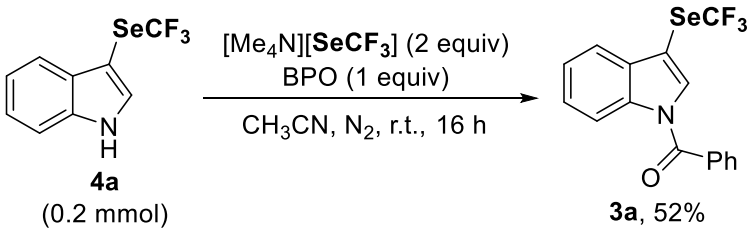
(3-Chlorophenyl)(2-methyl-3-((trifluoromethyl)selanyl)-1*H*-indol-1-yl)methanone (**3z**)



Light yellow solid, 28.8 mg (35%, **1m** : $[Me_4N][SeCF_3]$: **2j** = 1 : 3 : 2.2), petroleum ether / dichloromethane = 5 : 1 (v/v) as eluents for column chromatography. M.p.: 82-84 ^oC. ^1H NMR (500 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.70 (d, J = 7.9 Hz, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.60 (d, J = 7.7 Hz, 1H), 7.46 (t, J = 7.9 Hz, 1H), 7.30 (t, J = 7.6 Hz, 1H), 7.15 (t, J = 8.1 Hz, 1H), 7.00 (d, J = 8.3 Hz, 1H), 2.65 (s, 3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -35.9 (s, 3F). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.1, 144.9, 136.4, 136.2, 135.4, 133.7, 131.3, 130.3, 129.9, 128.1, 124.3, 123.7, 122.4 (q, J = 336.9 Hz), 120.2, 113.9, 101.3 (q, J = 1.5 Hz), 14.9. IR (KBr): 3440, 3361, 3060, 2924, 2851, 1689, 1595, 1570, 1561, 1474, 1450, 1435, 1381, 1353, 1310, 1293, 1274, 1250, 1217, 1165, 1145, 1115, 1089, 1055, 1031, 970, 938, 922, 903, 884, 852, 799, 789, 754, 745, 737, 681, 666, 650, 632, 612 cm^{-1}. HRMS- DART (m/z) calcd. for $C_{17}H_{12}ClF_3NOSe$ ($[M + H]^+$): 417.9719; found: 417.9711.

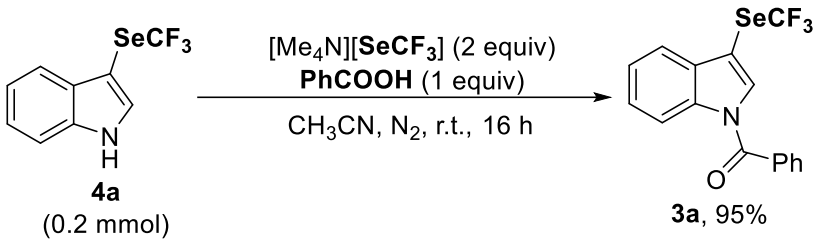
4. The control experiments for mechanistic insights

4.1. *N*-Acylation of 4a with $[Me_4N][SeCF_3]$ (2 equiv) and BPO (1 equiv) under the standard condition.



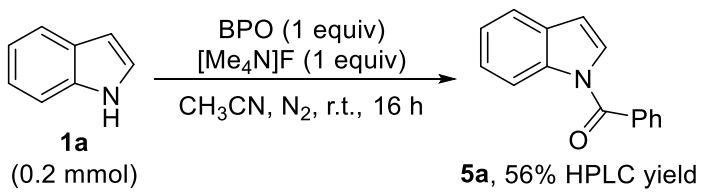
Procedure: Under a nitrogen atmosphere, a Schlenk tube was charged with **4a** (52.8 mg, 0.2 mmol), $[Me_4N][SeCF_3]$ (88.8 mg, 0.4 mmol) and CH_3CN (1 mL), followed by addition of BPO (64.6 mg, 75%, 0.2 mmol) and CH_3CN (1 mL), with vigorous stirring. The mixture was reacted at room temperature under N_2 for 16 h and concentrated to dryness under reduced pressure. The residue was purified by flash column chromatography on silica gel using a mixture of petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents to give **3a** as a white solid (38.2 mg, 52% yield).

4.2. *N*-Acylation of 4a with $[Me_4N][SeCF_3]$ (2 equiv) and $PhCO_2H$ (1 equiv) under the standard condition.



Procedure: Under a nitrogen atmosphere, a Schlenk tube was charged with **4a** (52.8 mg, 0.2 mmol), $[Me_4N][SeCF_3]$ (88.8 mg, 0.4 mmol) and CH_3CN (1 mL), followed by addition of benzoic acid (24.4 mg, 0.2 mmol) and CH_3CN (1 mL), with vigorous stirring. The mixture was reacted at room temperature under N_2 for 16 h and concentrated to dryness under reduced pressure. The residue was purified by flash column chromatography on silica gel using petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents to give **3a** as a white solid (69.9 mg, 95% yield).

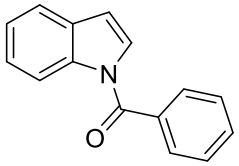
4.3. *N*-Acylation of 1a with $[Me_4N]F$ (1 equiv) and BPO (1 equiv) under the standard condition.



Procedure: Under a nitrogen atmosphere, a sealed tube was charged with **1a** (23.4 mg, 0.2 mmol), BPO (64.6 mg, 75%, 0.2 mmol), $[Me_4N]F$ (18.6 mg, 0.2 mmol) and CH_3CN (2 mL) with vigorous stirring. The mixture was reacted at room temperature under N_2 for 16 h and analyzed by HPLC (λ = 249 nm, methanol/water = 70:30 (v/v))

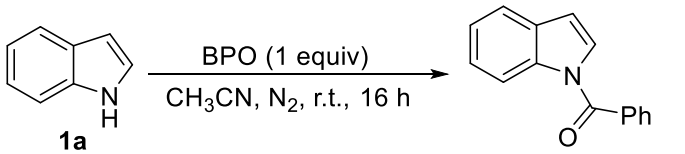
using **5a** (t_R = 9.23 min) as an external standard. The HPLC yield of **5a** in this reaction was determined to be 56%.

Compound **5a** (as reference for HPLC analysis of the reaction mixtures or as starting material in section 4.7) was synthesized according to the literature.[3]



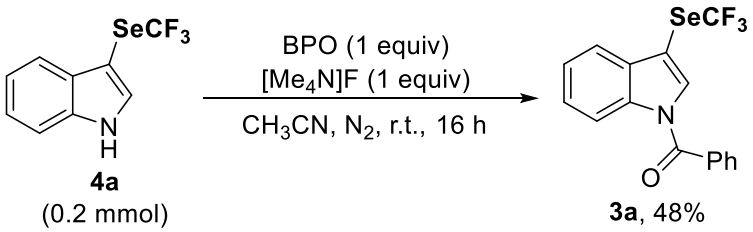
White solid. M.p.: 70-71 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.46 (d, *J* = 8.3 Hz, 1H), 7.76 (d, *J* = 7.6 Hz, 2H), 7.64-7.60 (m, 2H), 7.54 (t, *J* = 7.6 Hz, 2H), 7.42 (t, *J* = 7.7 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 3.7 Hz, 1H), 6.63 (d, *J* = 3.7 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.8, 136.1, 134.6, 131.9, 130.8, 129.2, 128.6, 127.6, 125.0, 124.0, 120.9, 116.4, 108.6.

4.4. *N*-Acylation of 1a with BPO (1 equiv) under the standard condition.



Procedure: Under a nitrogen atmosphere, a sealed tube was charged with **1a** (23.4 mg, 0.2 mmol), BPO (64.6 mg, 75%, 0.2 mmol) and CH_3CN (2 mL) with vigorous stirring. The mixture was reacted at room temperature under N_2 for 16 h and analyzed by HPLC (λ = 249 nm, methanol/water = 70:30 (v/v)) using **5a** (t_R = 9.23 min) as an external standard. The HPLC yield of **5a** in this reaction was determined to be 60%.

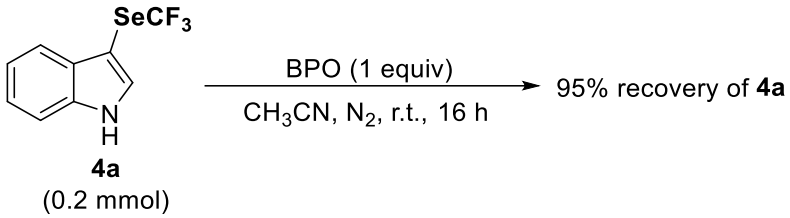
4.5. *N*-Acylation of 4a with [Me$_4$N]F (1 equiv) and BPO (1 equiv) under the standard condition.



Procedure: Under a nitrogen atmosphere, a sealed tube was charged with **4a** (52.8 mg, 0.2 mmol), BPO (64.6 mg, 75%, 0.2 mmol), [Me$_4$N]F (18.6 mg, 0.2 mmol) and CH_3CN (2 mL) with vigorous stirring. The mixture was reacted at room temperature

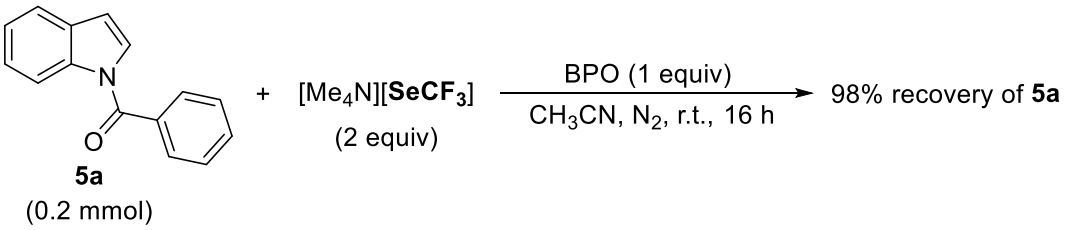
under N_2 for 16 h and concentrated to dryness under reduced pressure. The residue was purified by flash column chromatography on silica gel using a mixture of petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents to give **3a** as a white solid (35.3 mg, 48% yield).

4.6. *N*-Acylation of 4a with BPO (1 equiv) under the standard condition.



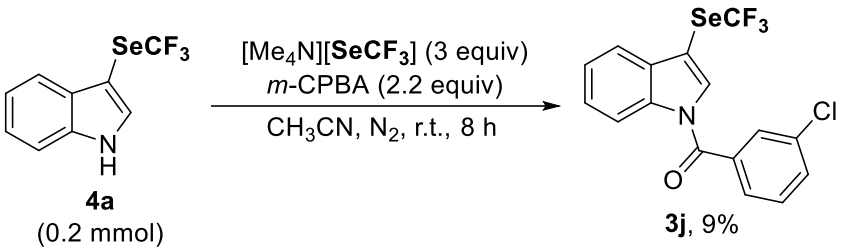
Procedure: Under a nitrogen atmosphere, a sealed tube was charged with **4a** (52.8 mg, 0.2 mmol), BPO (64.6 mg, 75%, 0.2 mmol) and CH_3CN (2 mL) with vigorous stirring. The mixture was reacted at room temperature under N_2 for 16 h and concentrated to dryness under reduced pressure. The residue was purified by flash column chromatography on silica gel using a mixture of petroleum ether / ethyl acetate = 10 : 1 (v/v) as eluents to recover 50.2 mg of **4a** (95% yield).

4.7. Trifluoromethylselenolation of 5a with [Me4N][SeCF3] (2 equiv) and BPO (1 equiv) under the standard condition.



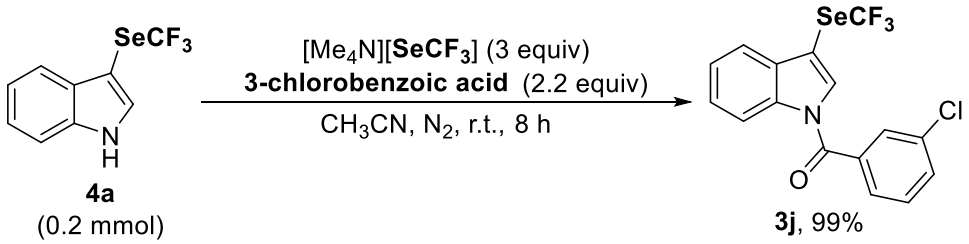
Procedure: Under a nitrogen atmosphere, a Schlenk tube was charged with **5a** (44.3 mg, 0.2 mmol), $[Me_4N][SeCF_3]$ (88.8 mg, 0.4 mmol) and CH_3CN (1 mL), followed by addition of BPO (64.6 mg, 75%, 0.2 mmol) and CH_3CN (1 mL), with vigorous stirring. The mixture was reacted at room temperature under N_2 for 16 h and concentrated to dryness under reduced pressure. The residue was purified by flash column chromatography on silica gel using petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents to recover 43.4 mg of **5a** (98% yield).

4.8. *N*-Acylation of 4a with [Me4N][SeCF3] (3 equiv) and *m*-CPBA (2.2 equiv) under the optimized condition.



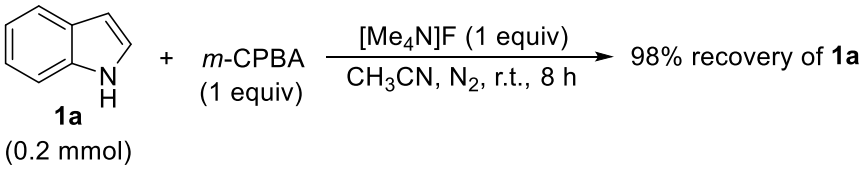
Procedure: Under a nitrogen atmosphere, a Schlenk tube was charged with **4a** (52.8 mg, 0.2 mmol), $[Me_4N][SeCF_3]$ (133.2 mg, 0.6 mmol) and CH_3CN (1 mL), followed by addition of *m*-CPBA (89.3 mg, 85%, 0.44 mmol) and CH_3CN (1 mL), with vigorous stirring. The mixture was reacted at room temperature under N_2 for 8 h and concentrated to dryness under reduced pressure. The residue was purified by flash column chromatography on silica gel using a mixture of petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents to give **3j** as a white solid (7.2 mg, 9% yield).

4.9. *N*-Acylation of 4a with $[Me_4N][SeCF_3]$ (3 equiv) and 3-chlorobenzoic acid (2.2 equiv) under the optimized condition.



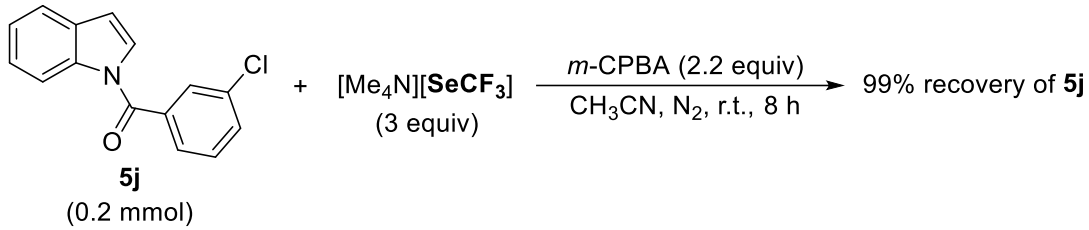
Procedure: Under a nitrogen atmosphere, a Schlenk tube was charged with **4a** (52.8 mg, 0.2 mmol), $[Me_4N][SeCF_3]$ (133.2 mg, 0.6 mmol) and CH_3CN (1 mL), followed by addition of 3-chlorobenzoic acid (68.9 mg, 0.44 mmol) and CH_3CN (1 mL), with vigorous stirring. The mixture was reacted at room temperature under N_2 for 8 h and concentrated to dryness under reduced pressure. The residue was purified by flash column chromatography on silica gel using a mixture of petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents to give **3j** as a white solid (79.7 mg, 99% yield).

4.10. *N*-Acylation of 1a with $[Me_4N]F$ (1 equiv) and *m*-CPBA (1 equiv) under the optimized condition.



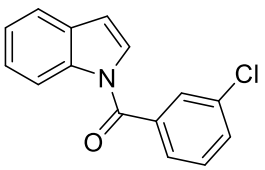
Procedure: Under a nitrogen atmosphere, a sealed tube was charged with **1a** (23.4 mg, 0.2 mmol), *m*-CPBA (40.6 mg, 85%, 0.2 mmol), $[Me_4N]F$ (18.6 mg, 0.2 mmol) and CH_3CN (2 mL) with vigorous stirring. The mixture was reacted at room temperature under N_2 for 16 h and concentrated to dryness under reduced pressure. The residue was purified by flash column chromatography on silica gel using a mixture of petroleum ether / ethyl acetate = 10 : 1 (v/v) as eluents to recover 22.9 mg of **1a** (98% yield).

4.11. Trifluoromethylselenolation of 5j with $[Me_4N][SeCF_3]$ (3 equiv) and *m*-CPBA (2.2 equiv) under the optimized condition.



Procedure: Under a nitrogen atmosphere, a Schlenk tube was charged with **5j** (51.1 mg, 0.2 mmol), $[Me_4N][SeCF_3]$ (133.2 mg, 0.6 mmol) and CH_3CN (1 mL), followed by addition of *m*-CPBA (89.3 mg, 85%, 0.44 mmol) and CH_3CN (1 mL), with vigorous stirring. The mixture was reacted at room temperature under N_2 for 8 h and concentrated to dryness under reduced pressure. The residue was purified by flash column chromatography on silica gel using a mixture of petroleum ether / ethyl acetate = 20 : 1 (v/v) as eluents to recover 50.6 mg of **5j** (99% yield).

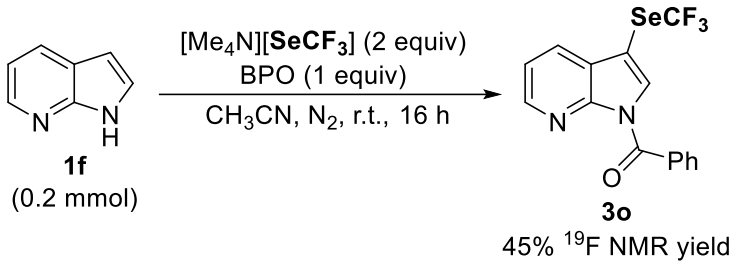
Compound **5j** was synthesized according to the literature.[3]



(3-Chlorophenyl)(1*H*-indol-1-yl)methanone (**5j**): White solid. M.p.: 81-82 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41 (d, *J* = 8.3 Hz, 1H), 7.74 (s, 1H), 7.63-7.58 (m, 3H), 7.48 (t, *J* = 7.8 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.25 (d, *J* = 3.7 Hz, 1H), 6.65 (d, *J* = 3.7 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.1, 136.3, 136.0, 134.9, 131.9, 130.8, 130.0, 129.2, 127.2, 125.2, 124.2, 121.0, 116.4, 109.2. IR (KBr): 3322, 3153, 3113, 3065, 3052, 3035, 1674, 1607, 1587, 1567, 1540, 1472, 1455, 1419, 1383, 1351, 1296, 1243, 1203, 1166, 1149, 1127, 1092, 1078, 1018, 929,

910, 889, 805, 771, 751, 731, 686, 665, 632 cm^{-1}. HRMS-ESI (m/z) calcd. for $C_{15}H_{11}ClNO$ ($[M + H]^+$): 256.0524; found: 256.0533.

5. ^{19}F NMR analysis of the reaction mixture of 7-azaindole (1f), $[Me_4N][SeCF_3]$ and BPO



Procedure: Under a nitrogen atmosphere, a Schlenk tube was charged with **1f** (23.6 mg, 0.2 mmol), $[Me_4N][SeCF_3]$ (88.8 mg, 0.4 mmol) and CH_3CN (1 mL), followed by addition of BPO (64.6 mg, 75%, 0.2 mmol) and CH_3CN (1 mL), with vigorous stirring. The mixture was reacted at room temperature under N_2 for 16 h and analyzed by ^{19}F NMR using $PhOCF_3$ (27.3 mg, 0.17 mmol) as an internal standard.

Figure S1. ^{19}F NMR spectrum of the above reaction mixture.

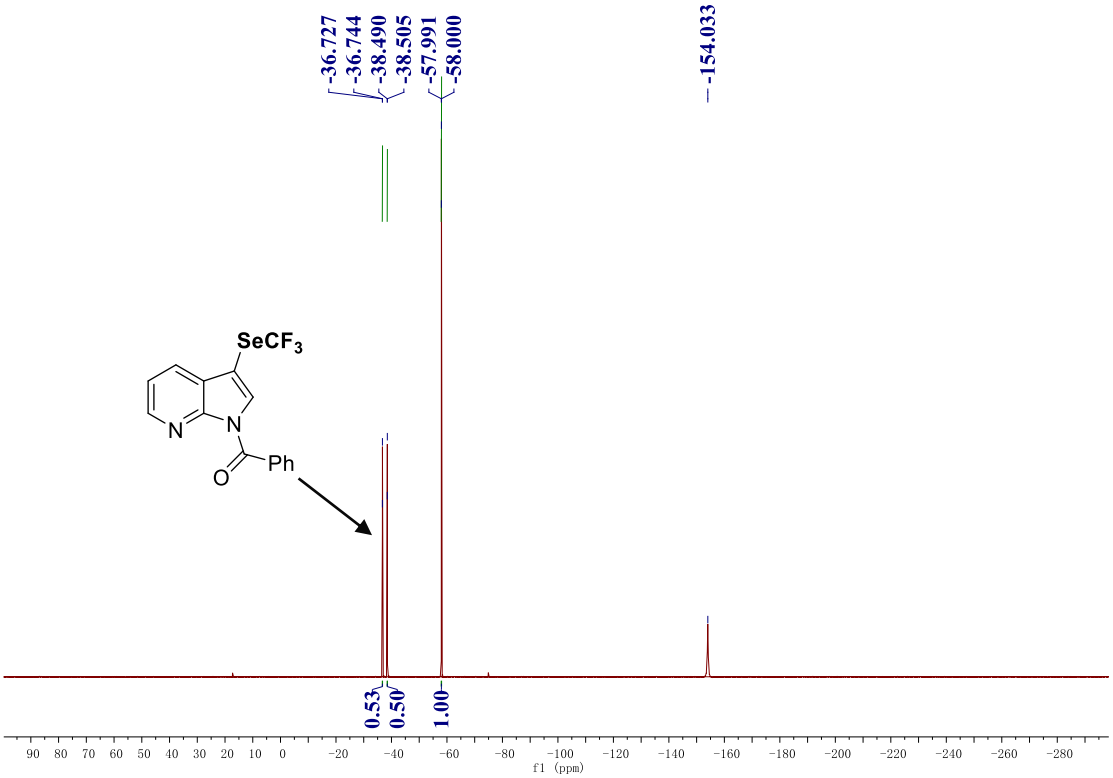
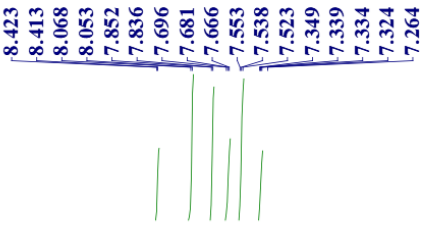
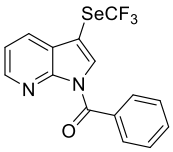


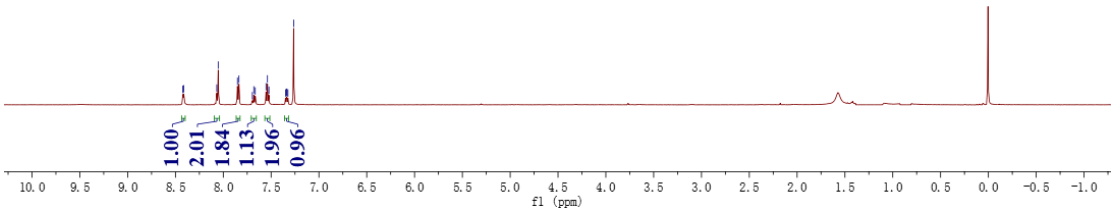
Figure S2. NMR spectra of the isolated product (with minor deacylated byproduct) from the above reaction.

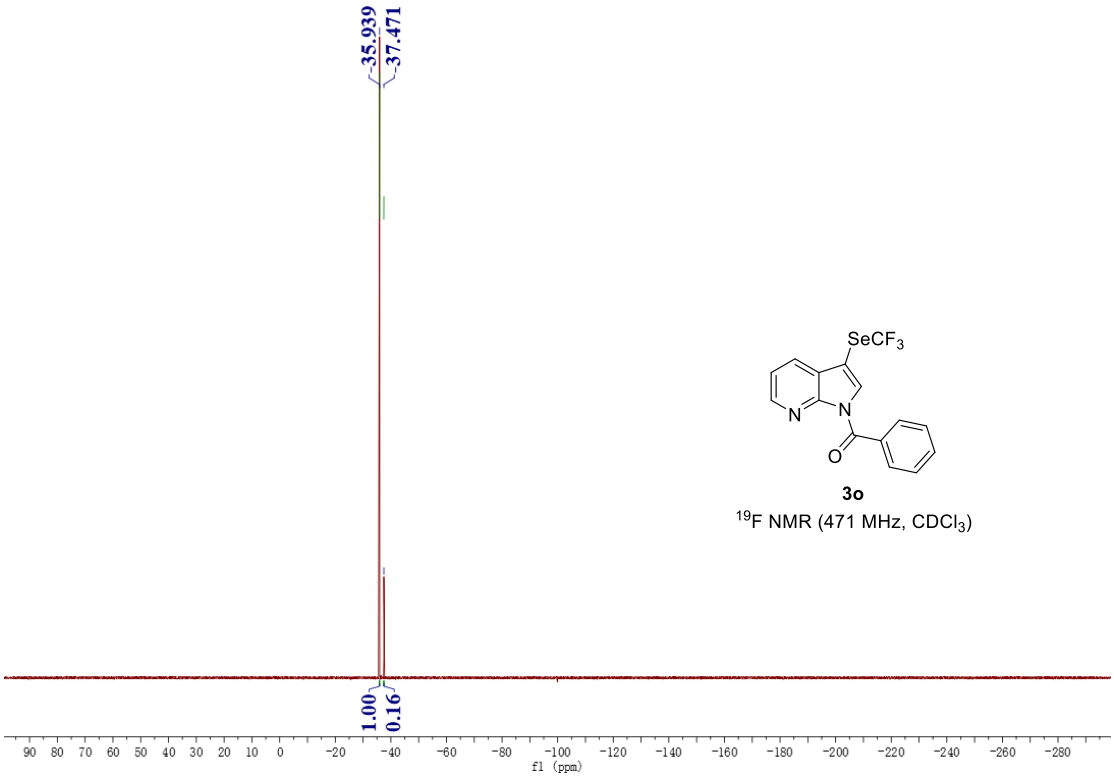




3o

^{1}H NMR (500 MHz, $CDCl_3$)





3o

^{19}F NMR (471 MHz, $CDCl_3$)

6. Trifluoromethylselenolation/*N*-acylation of pyrrole with BPO under the standard condition.

Procedure: Under a nitrogen atmosphere, a Schlenk tube was charged with pyrrole (13.4 mg, 0.2 mmol), $[Me_4N][SeCF_3]$ (88.8 mg, 0.4 mmol) and CH_3CN (1 mL), followed by addition of BPO (64.6 mg, 75%, 0.2 mmol) and CH_3CN (1 mL), with vigorous stirring. The mixture was reacted at room temperature under N_2 for 16 h and concentrated to dryness under reduced pressure. The residue was purified by prepared TLC plate (silica) using petroleum ether / dichloromethane = 4 : 1 (v/v) as eluents to give a mixture of impure (2,4-bis((trifluoromethyl)selanyl)-1*H*-pyrrol-1-yl)(phenyl) methanone (5.7 mg), phenyl(2-((trifluoromethyl)selanyl)-1*H*-pyrrol-1-yl)methanone (6.7 mg), and phenyl(3-((trifluoromethyl)selanyl)-1*H*-pyrrol-1-yl)methanone (5.0 mg).

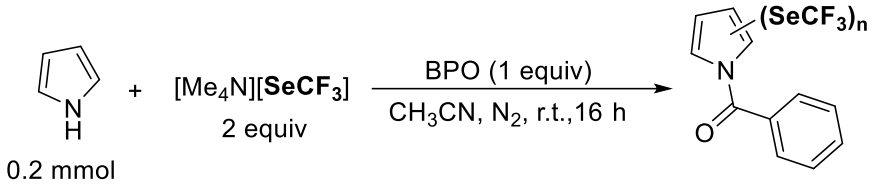
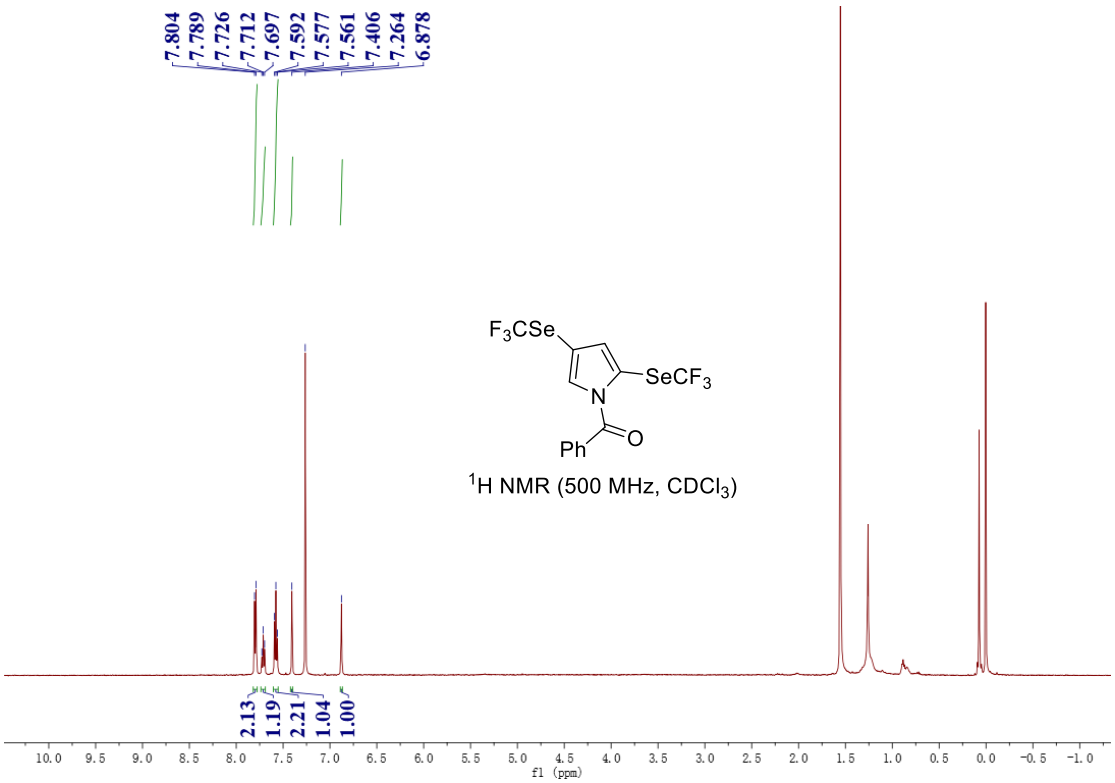
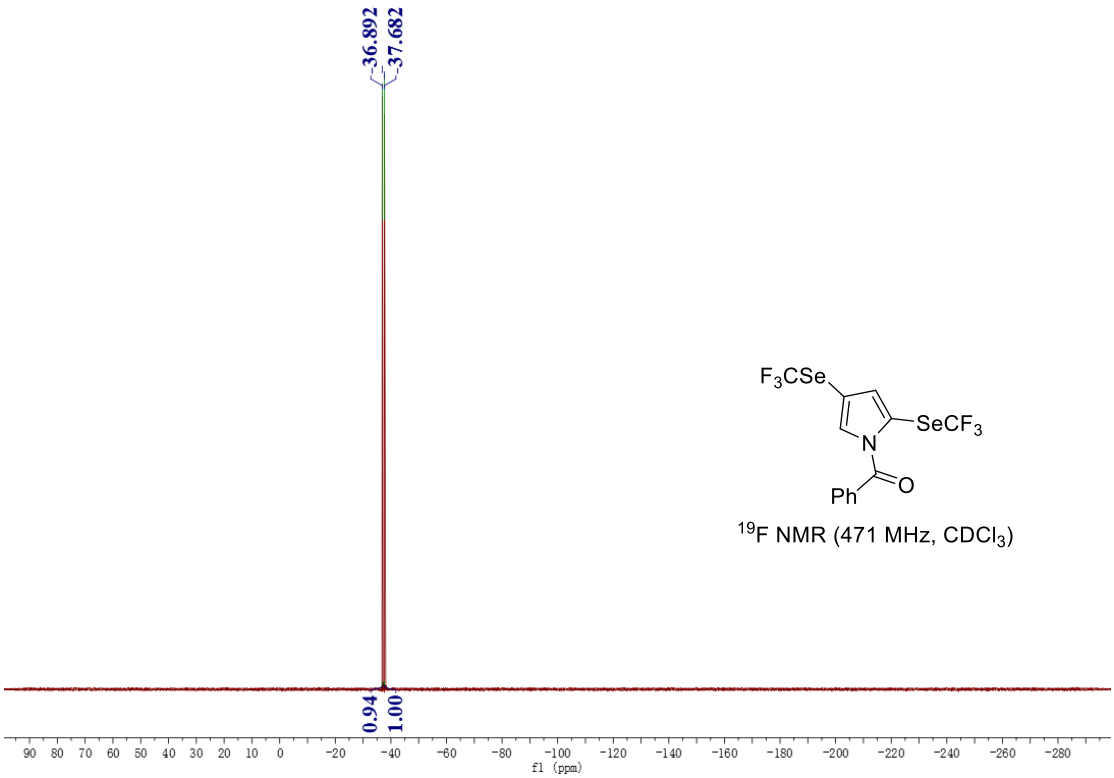
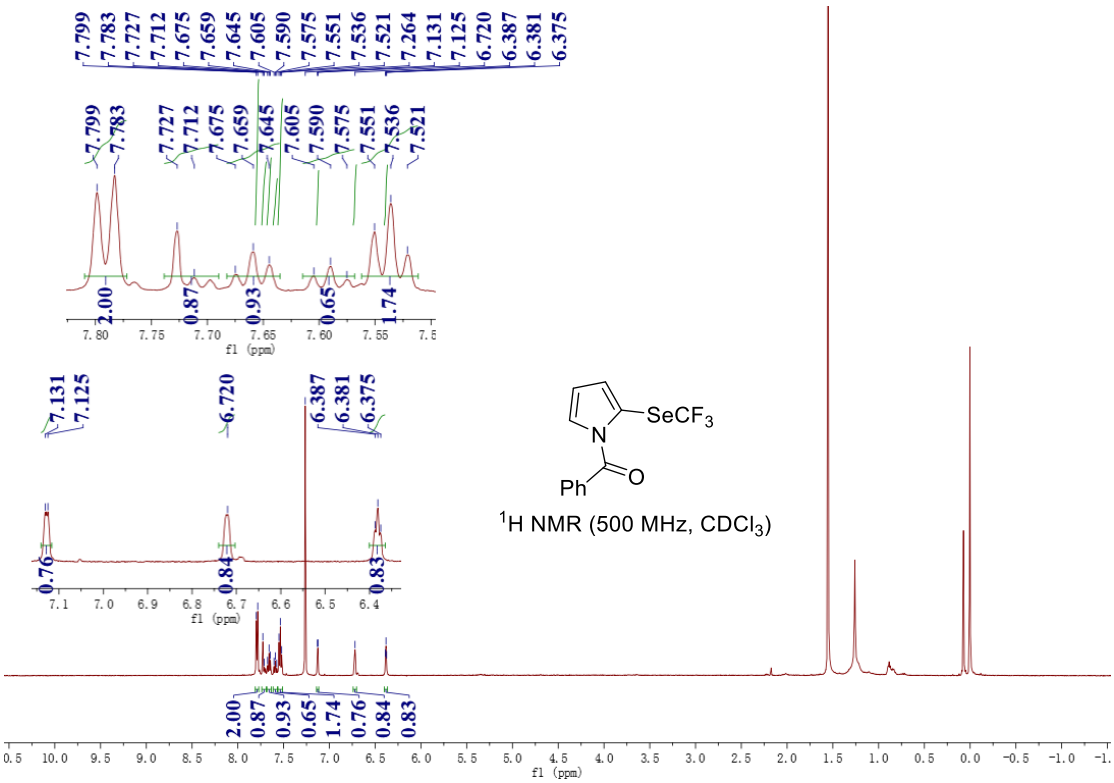


Figure S3. NMR spectra of the impure products.

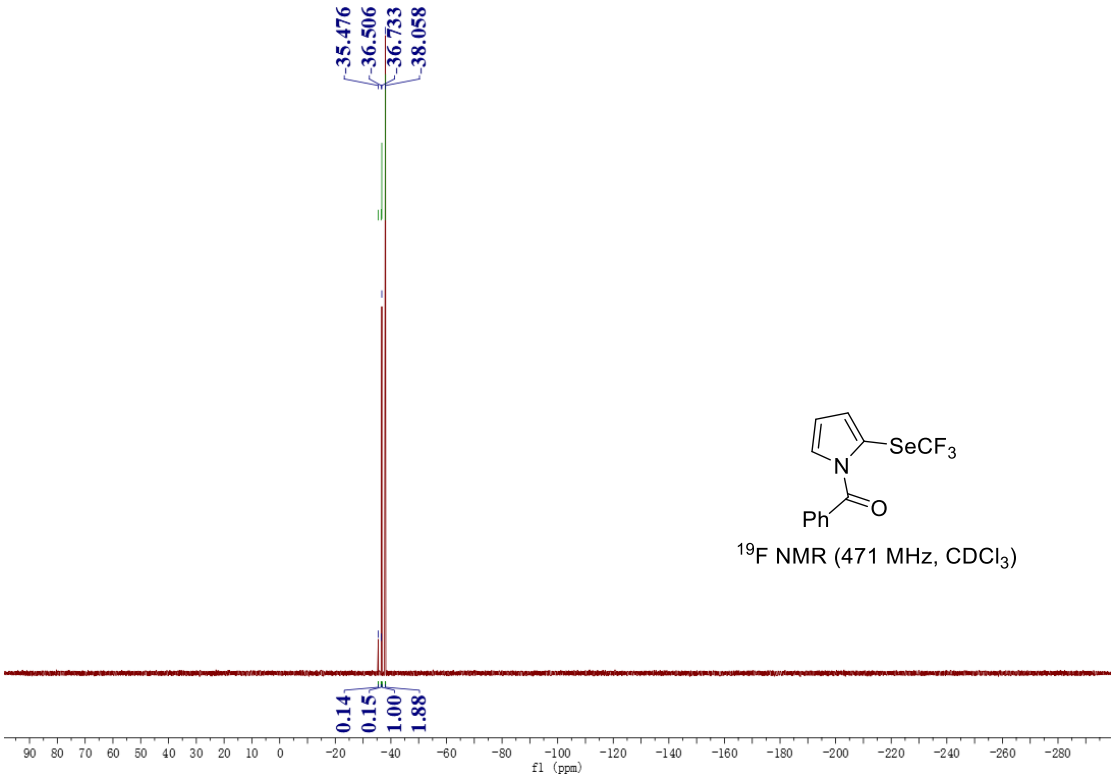




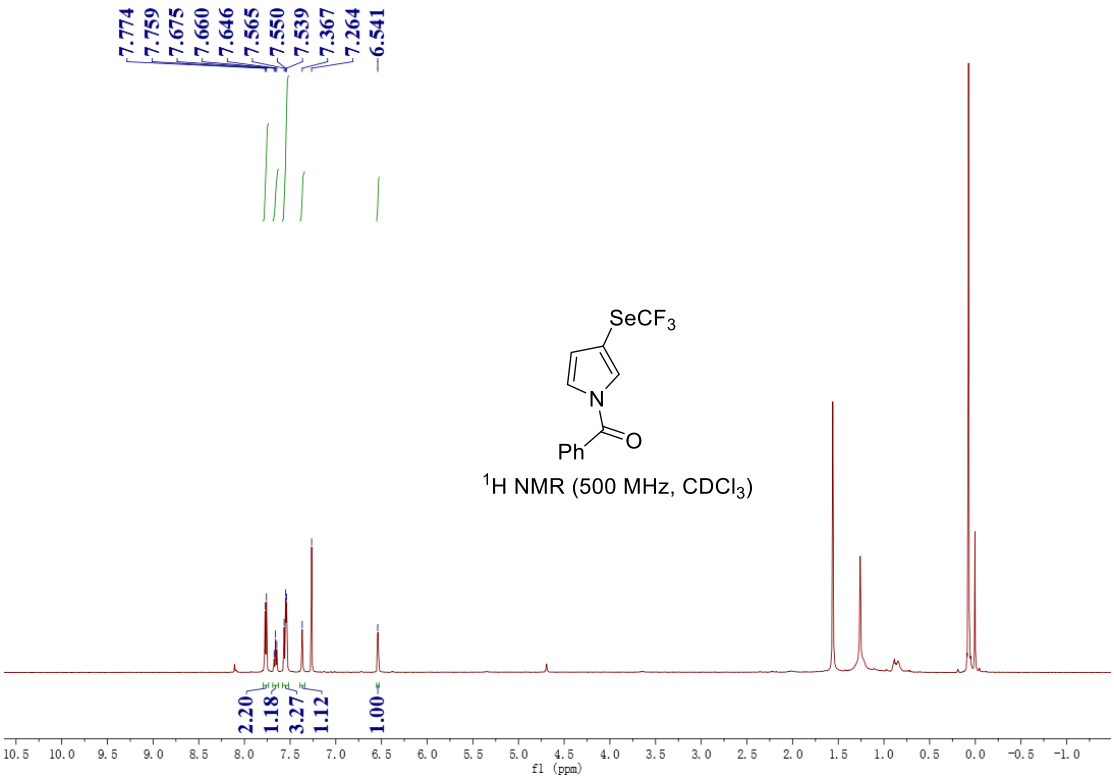
^{19}F NMR (471 MHz, $CDCl_3$)



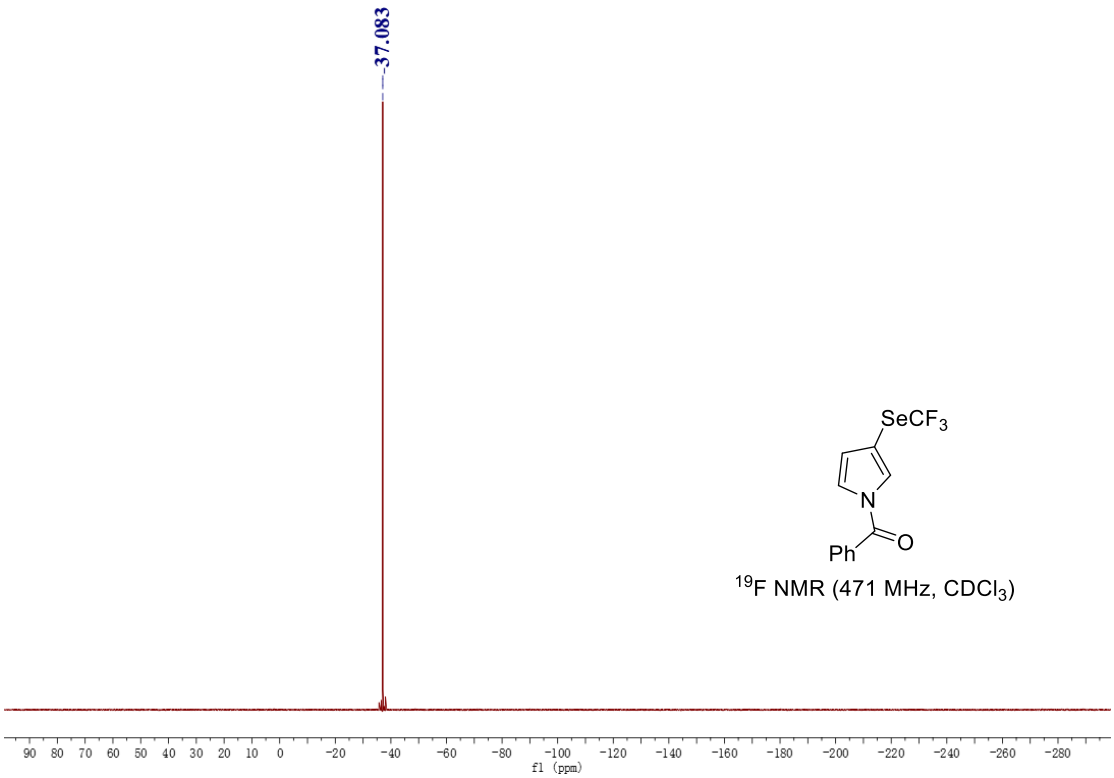
^{1}H NMR (500 MHz, $CDCl_3$)



^{19}F NMR (471 MHz, $CDCl_3$)



^{1}H NMR (500 MHz, $CDCl_3$)



^{19}F NMR (471 MHz, $CDCl_3$)

Reference:

[1] W. Tyrra, D. Naumann, Y. L. Yagupolskii, *J. Fluorine Chem.* **2003**, *123*, 183-187.

[2] H. Tian, W.-T. Xu, Y.-X. Liu, Q.-M. Wang, *Org. Lett.* **2020**, *22*, 5005-5008.

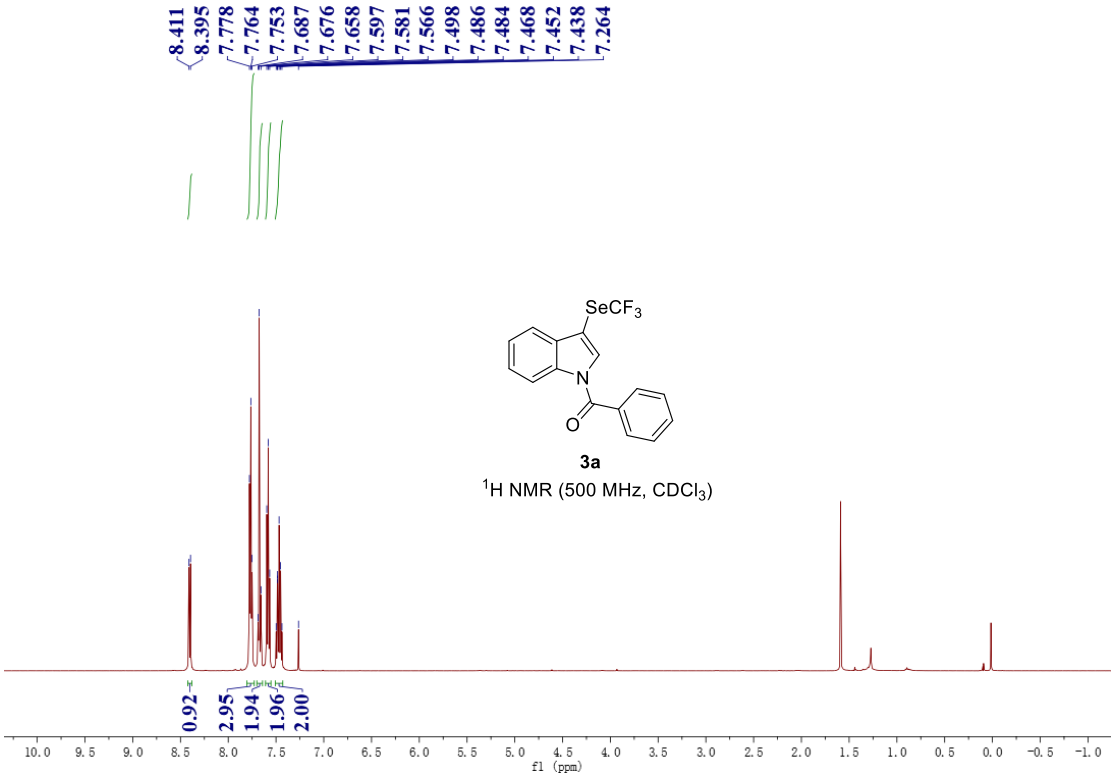
[3] S. A. Iqbal, J. Cid, R. J. Procter, M. Uzelac, K. Yuan, M. J. Ingleson, *Angew. Chem. Int. Ed.* **2019**, *58*, 15381-15385.

[4] W. L. F. Armarego, C. L. L. Chai, *Purification of Laboratory Chemicals*, 5th ed; Butterworth Heinemann: Oxford, **2003**.

[5] R. Ueno, T. Shimizu, E. Shirakawa, *Synlett* **2016**, *27*, 741-744.

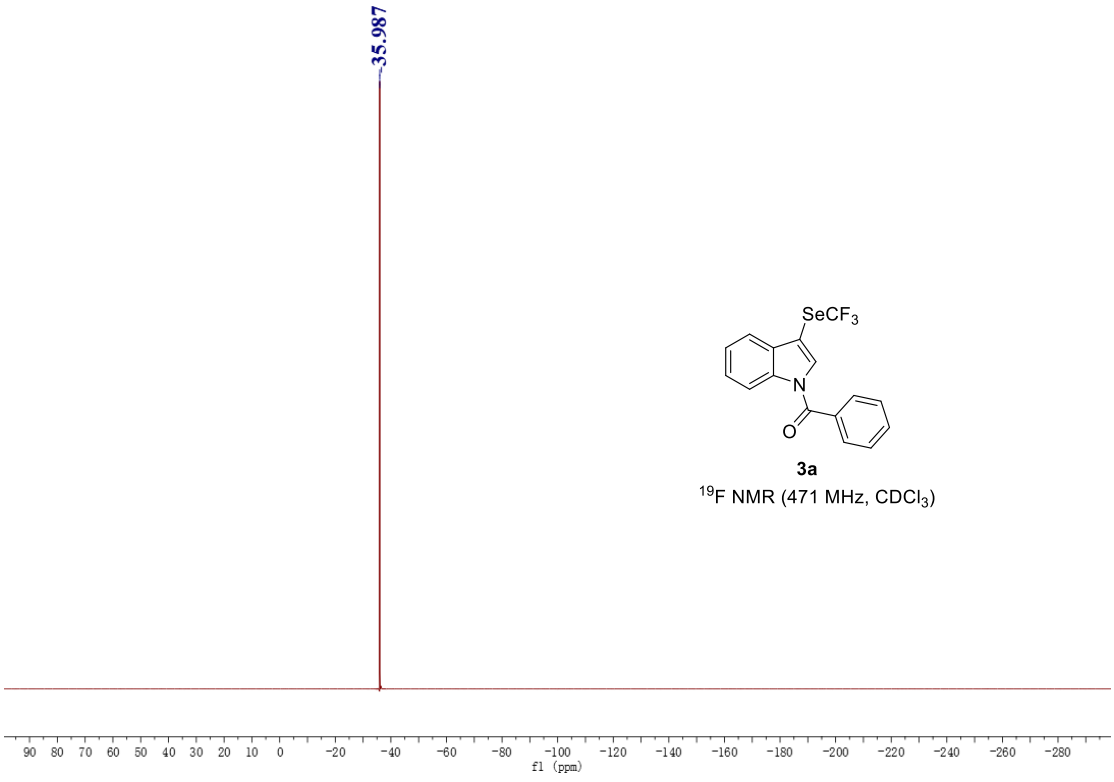
[6] D.-S. Yang, H.-J. Yang, H. Fu, *Chem. Commun.* **2011**, *47*, 2348-2350.

7. NMR spectra of the products



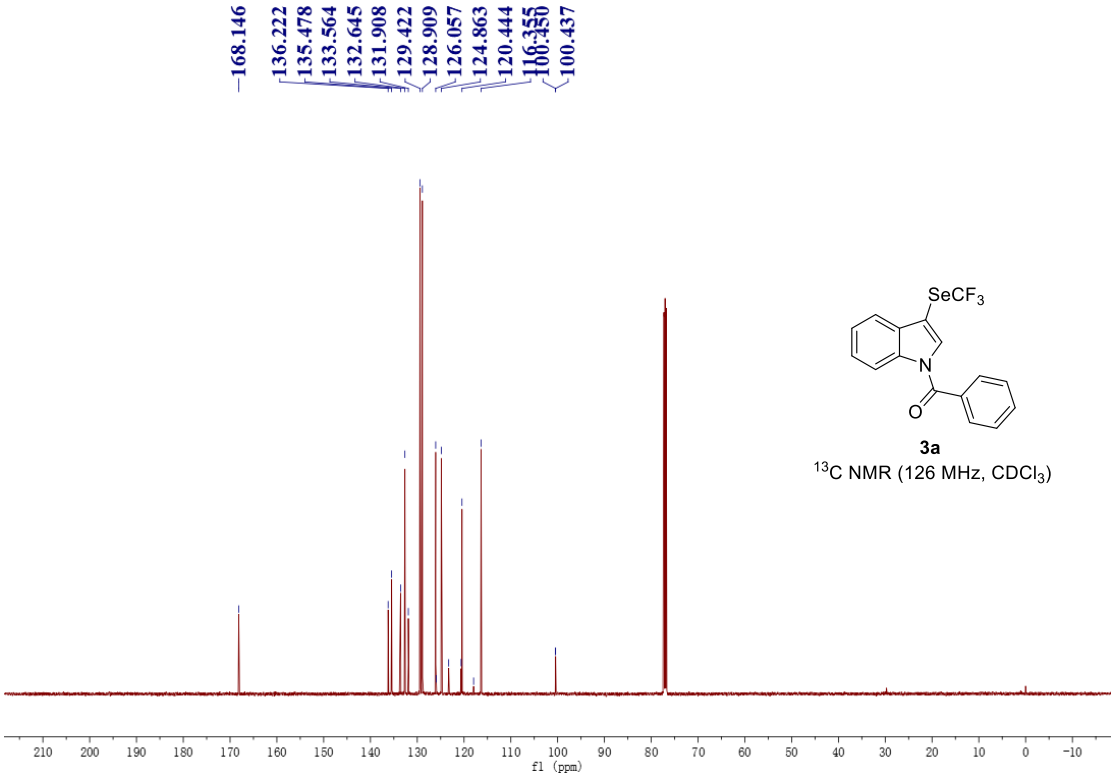
3a

^{1}H NMR (500 MHz, $CDCl_3$)



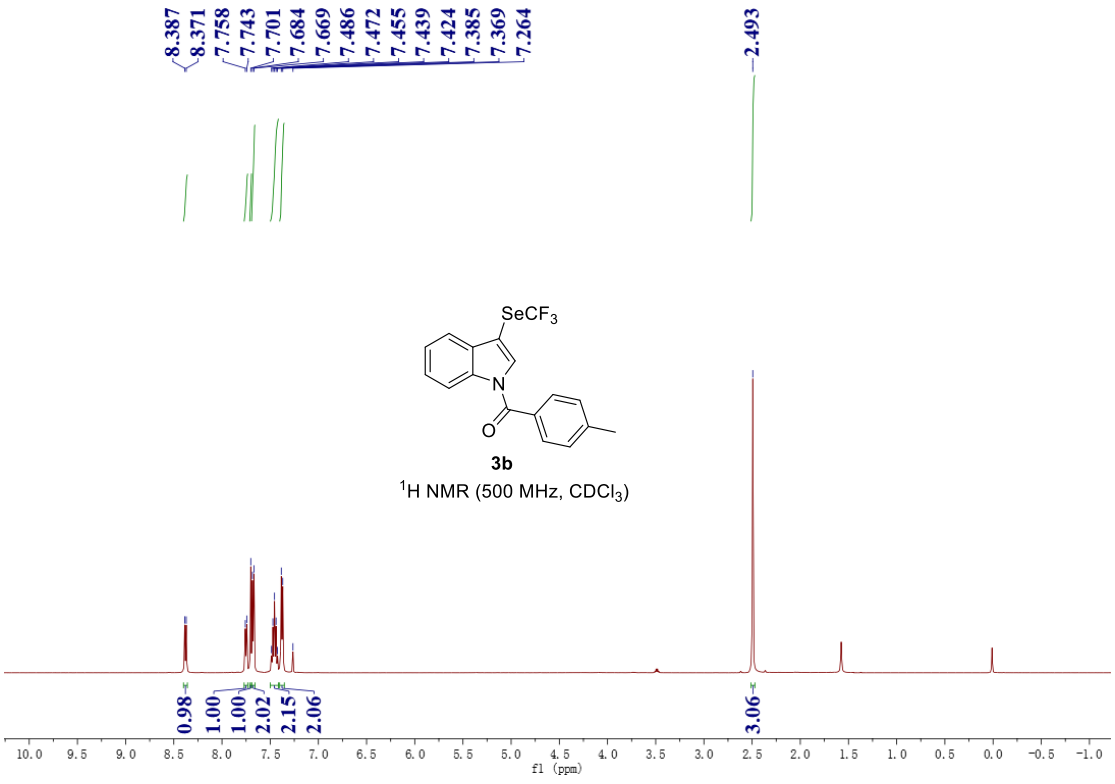
3a

^{19}F NMR (471 MHz, $CDCl_3$)



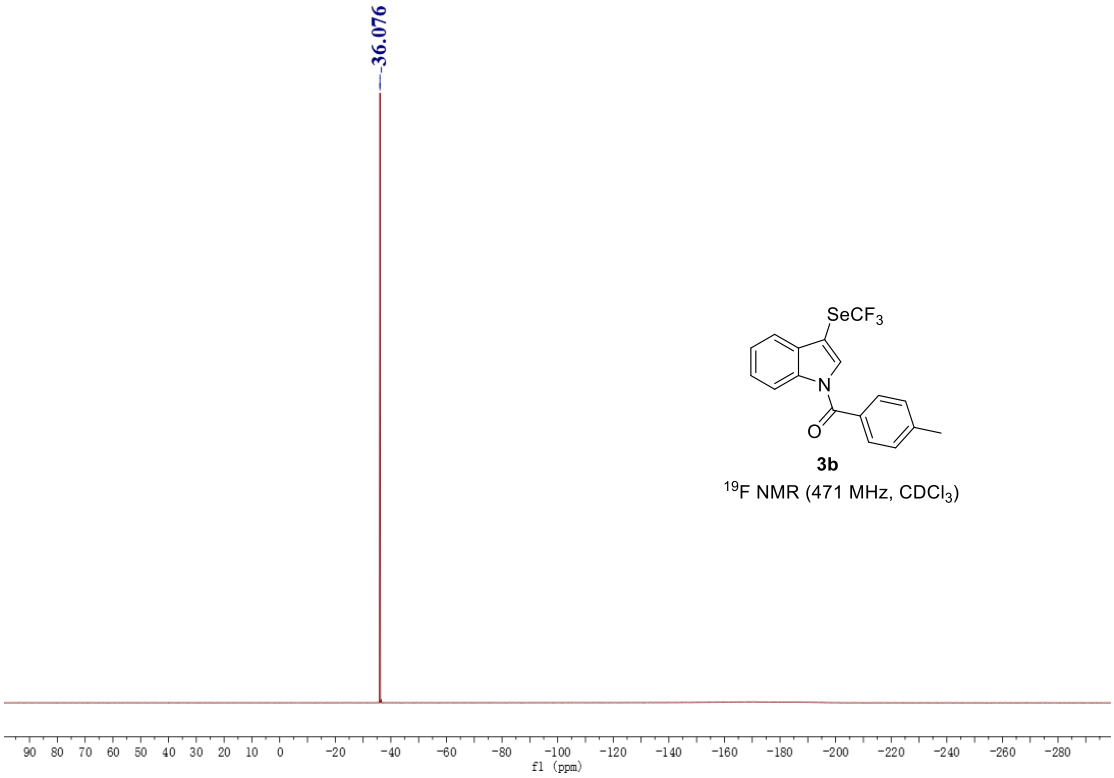
3a

^{13}C NMR (126 MHz, $CDCl_3$)



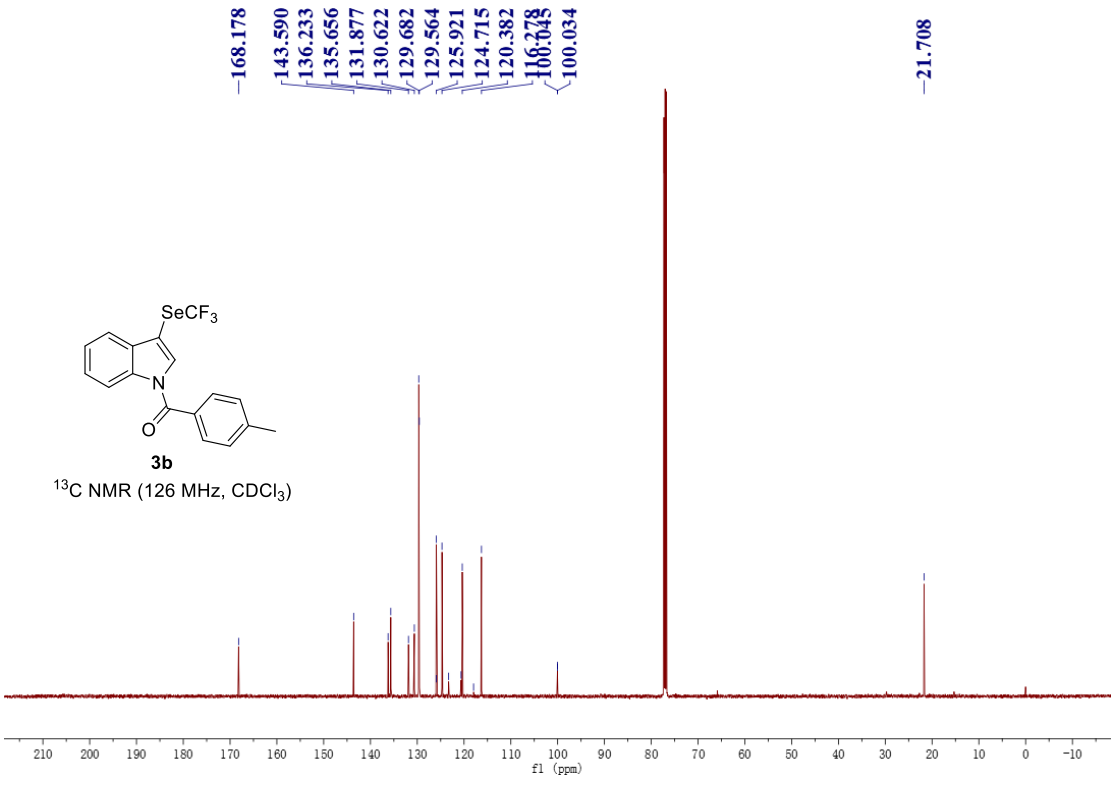
3b

^{1}H NMR (500 MHz, $CDCl_3$)



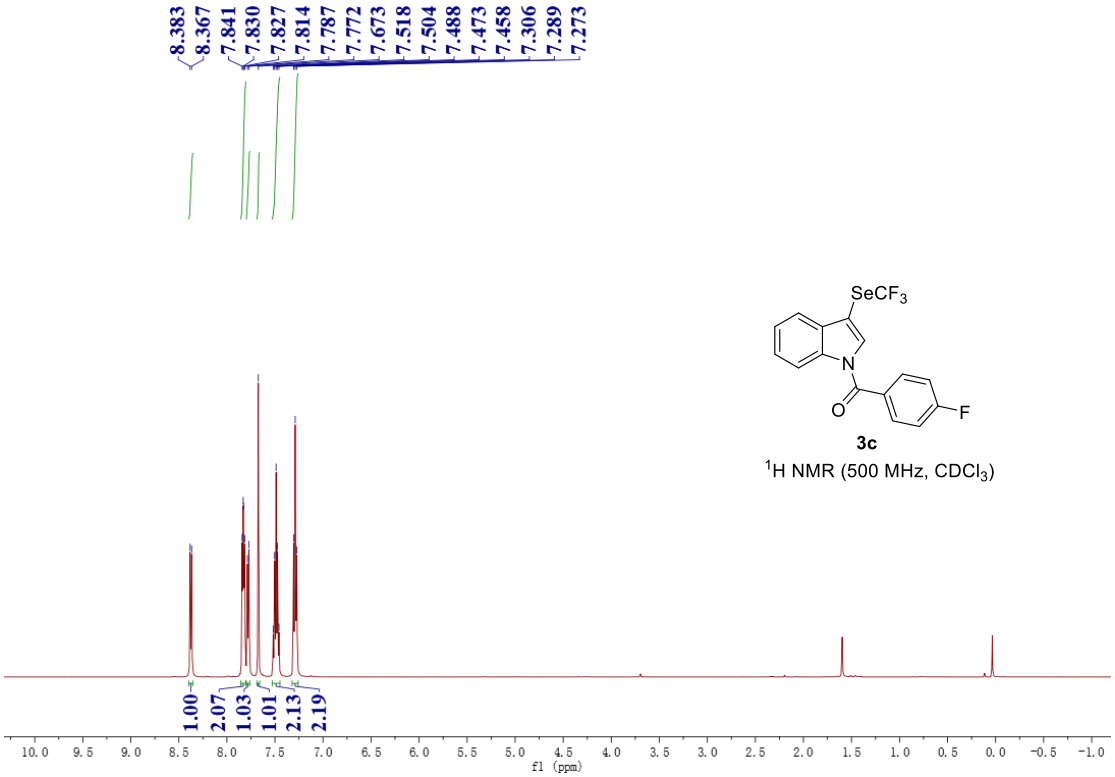
3b

^{19}F NMR (471 MHz, $CDCl_3$)



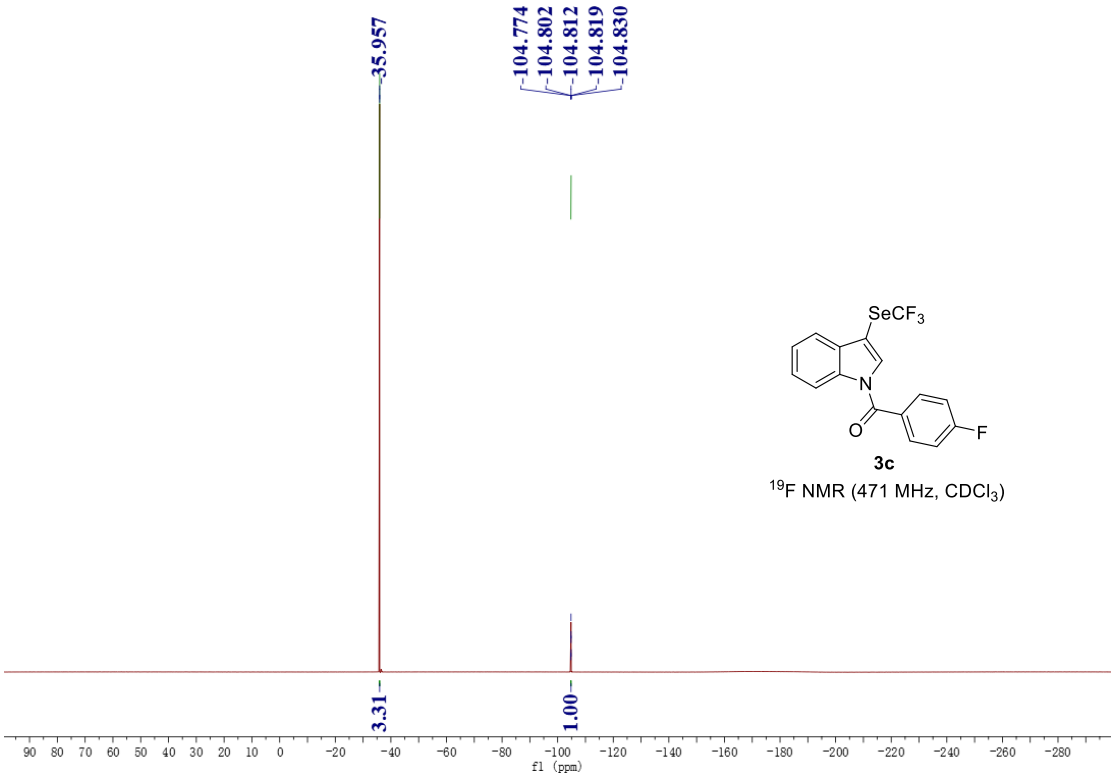
3b

^{13}C NMR (126 MHz, $CDCl_3$)



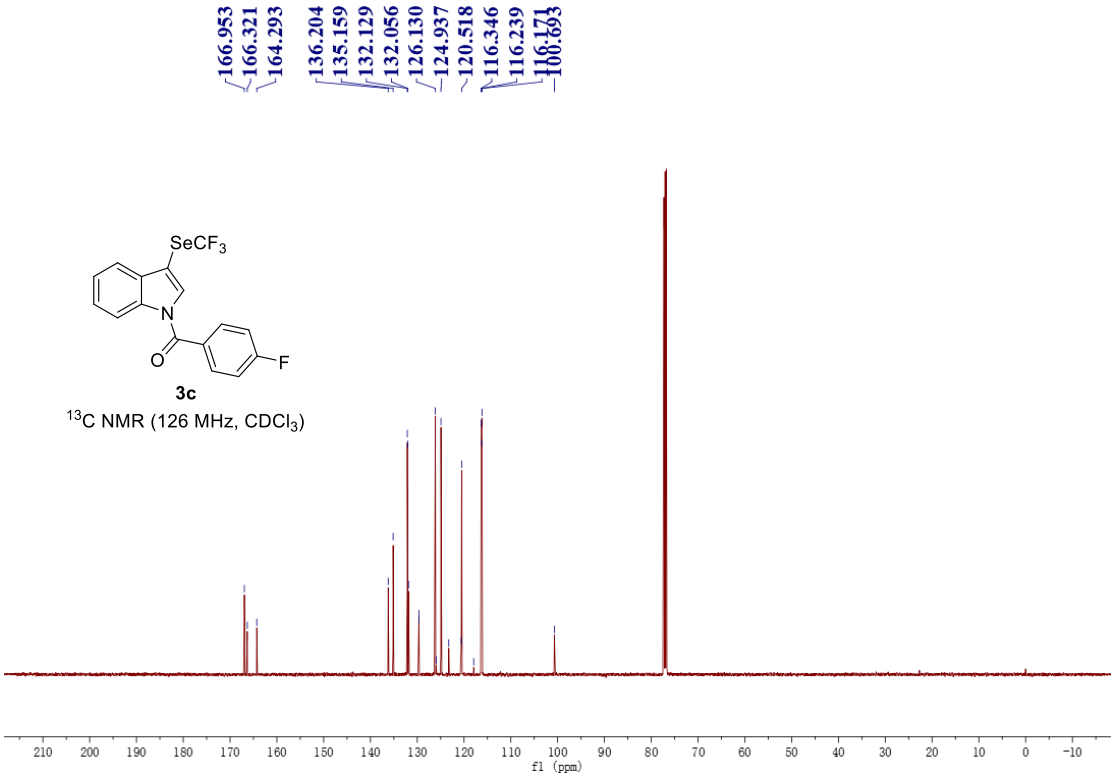
3c

^{1}H NMR (500 MHz, $CDCl_3$)



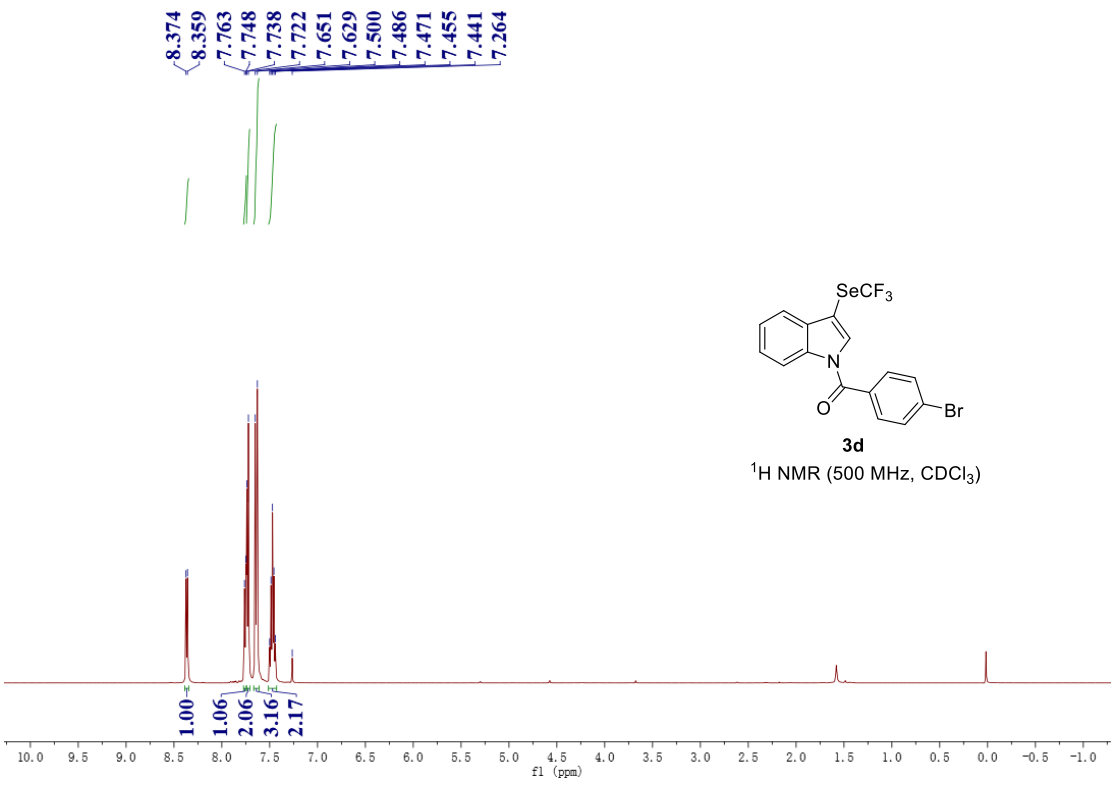
3c

^{19}F NMR (471 MHz, $CDCl_3$)



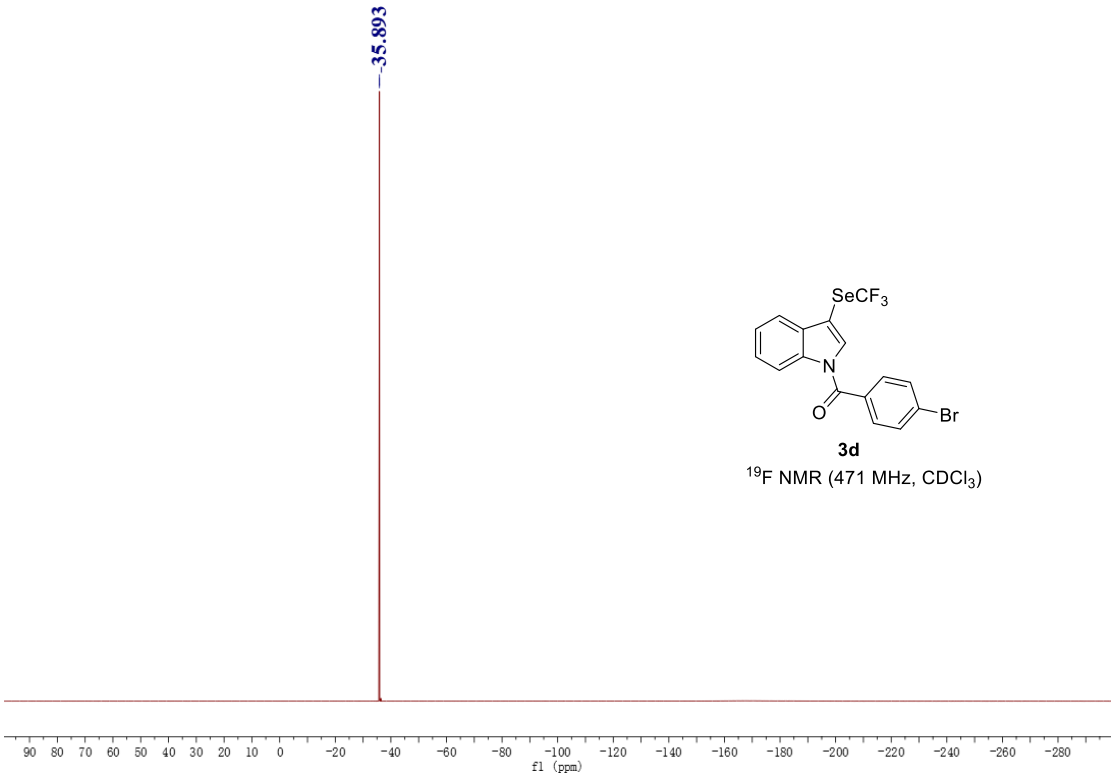
3c

^{13}C NMR (126 MHz, $CDCl_3$)



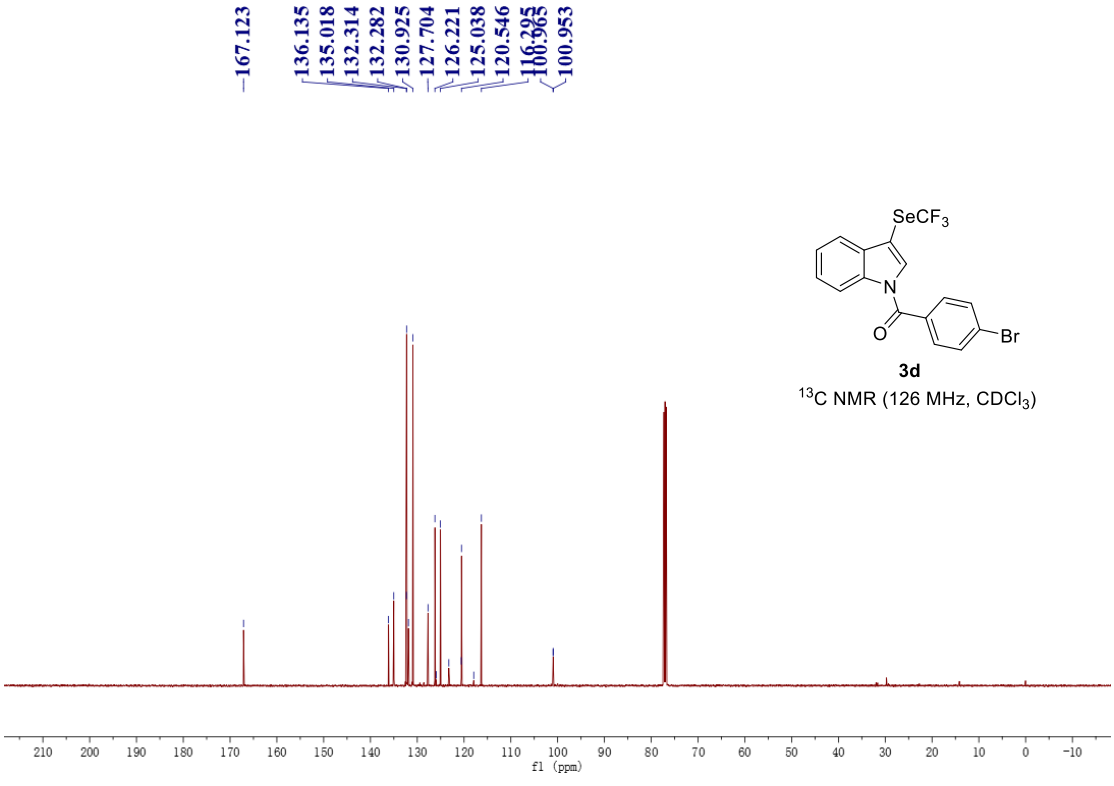
3d

^{1}H NMR (500 MHz, $CDCl_3$)



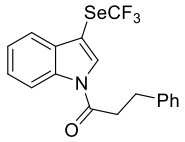
3d

^{19}F NMR (471 MHz, $CDCl_3$)



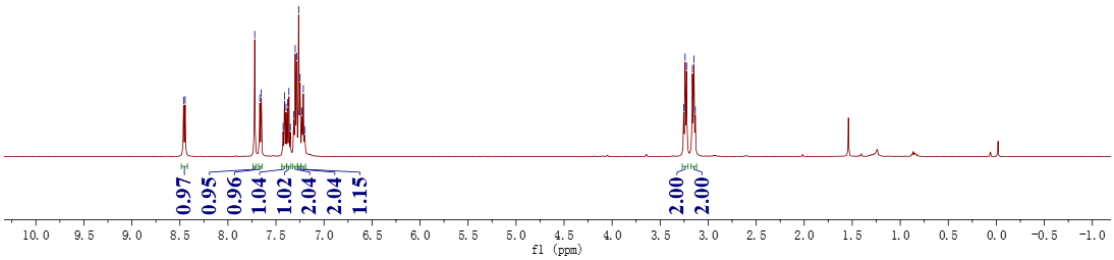
3d

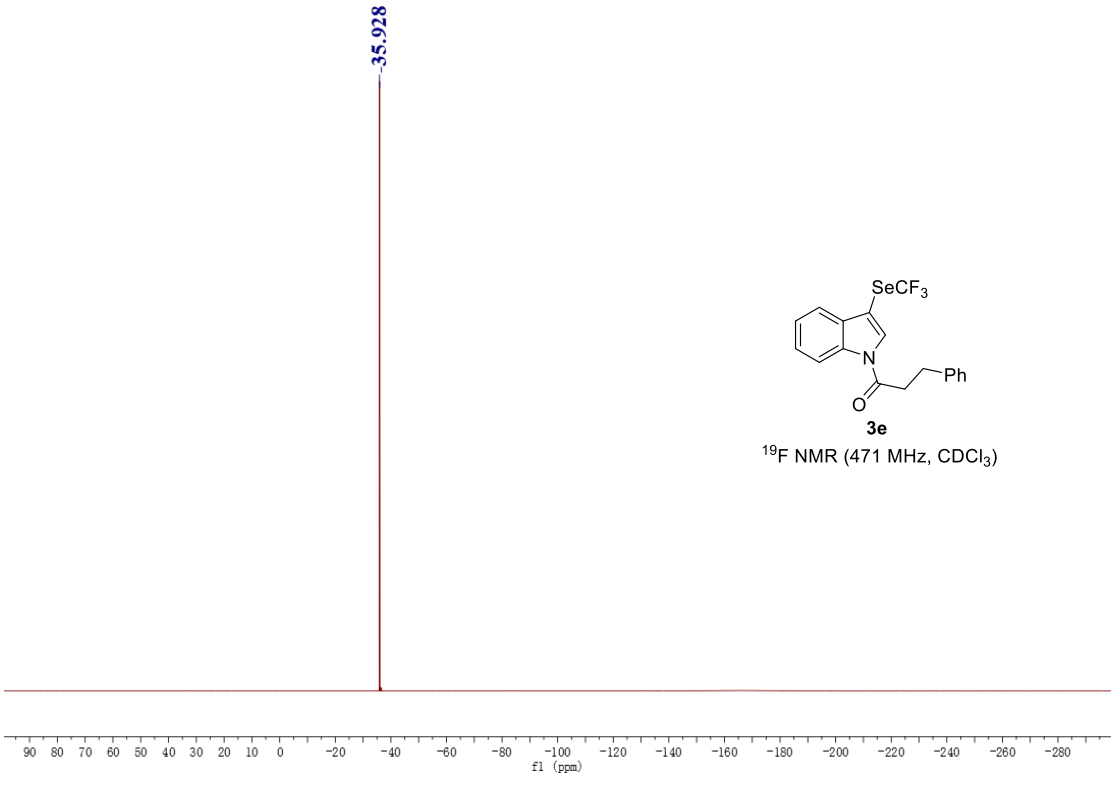
^{13}C NMR (126 MHz, $CDCl_3$)



3e

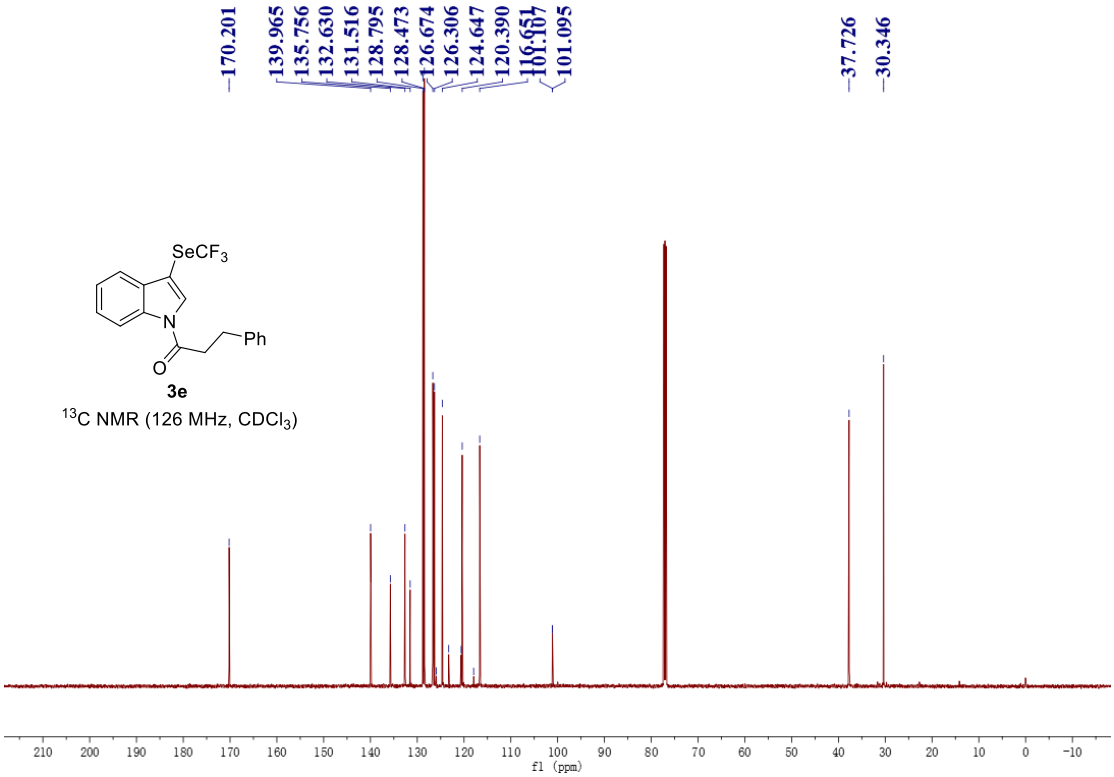
^{1}H NMR (500 MHz, $CDCl_3$)

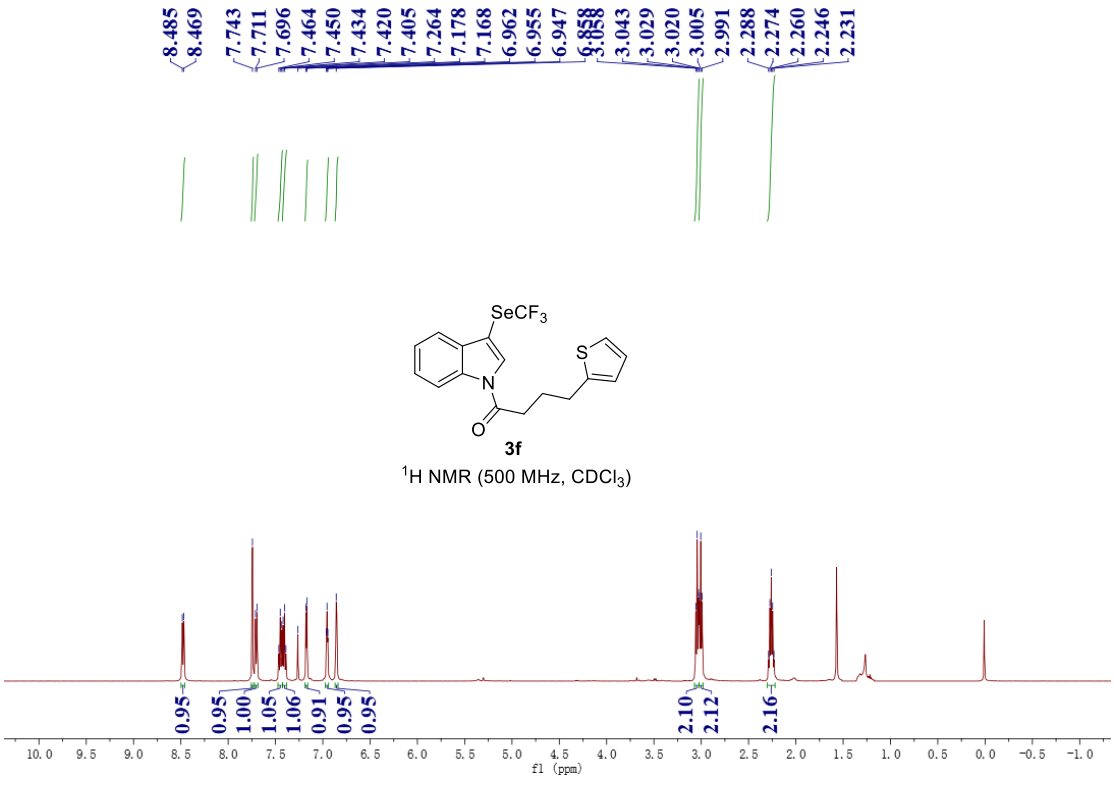


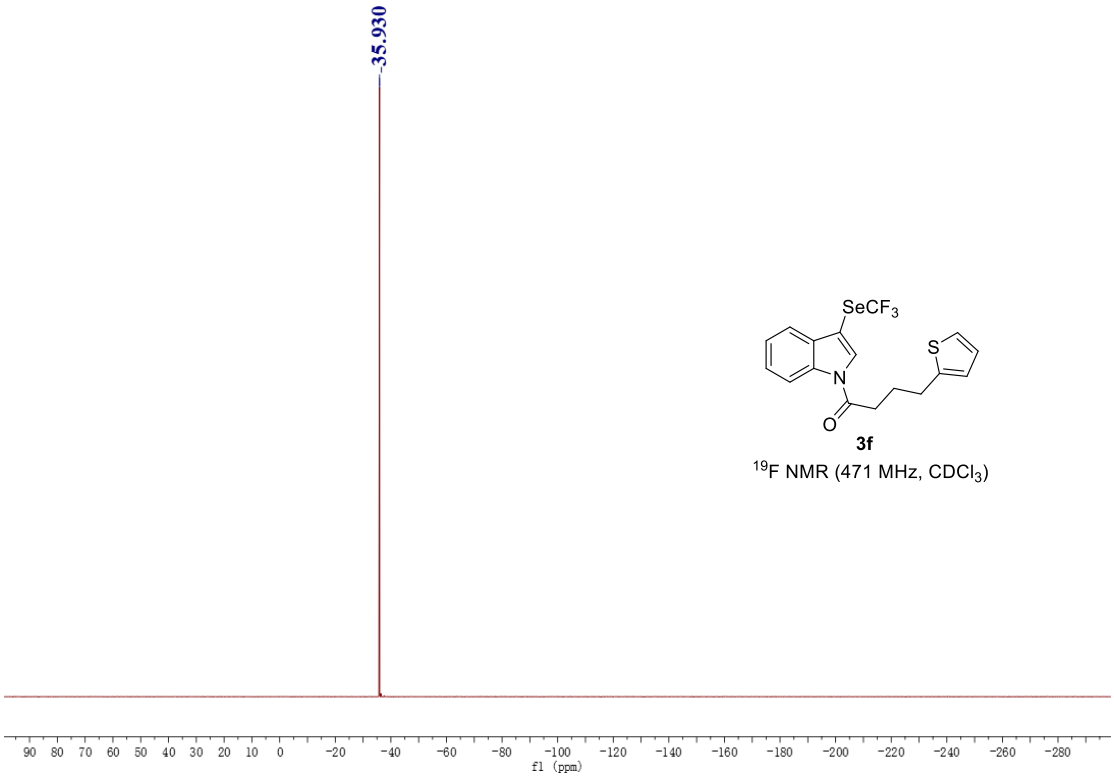


3e

^{19}F NMR (471 MHz, $CDCl_3$)

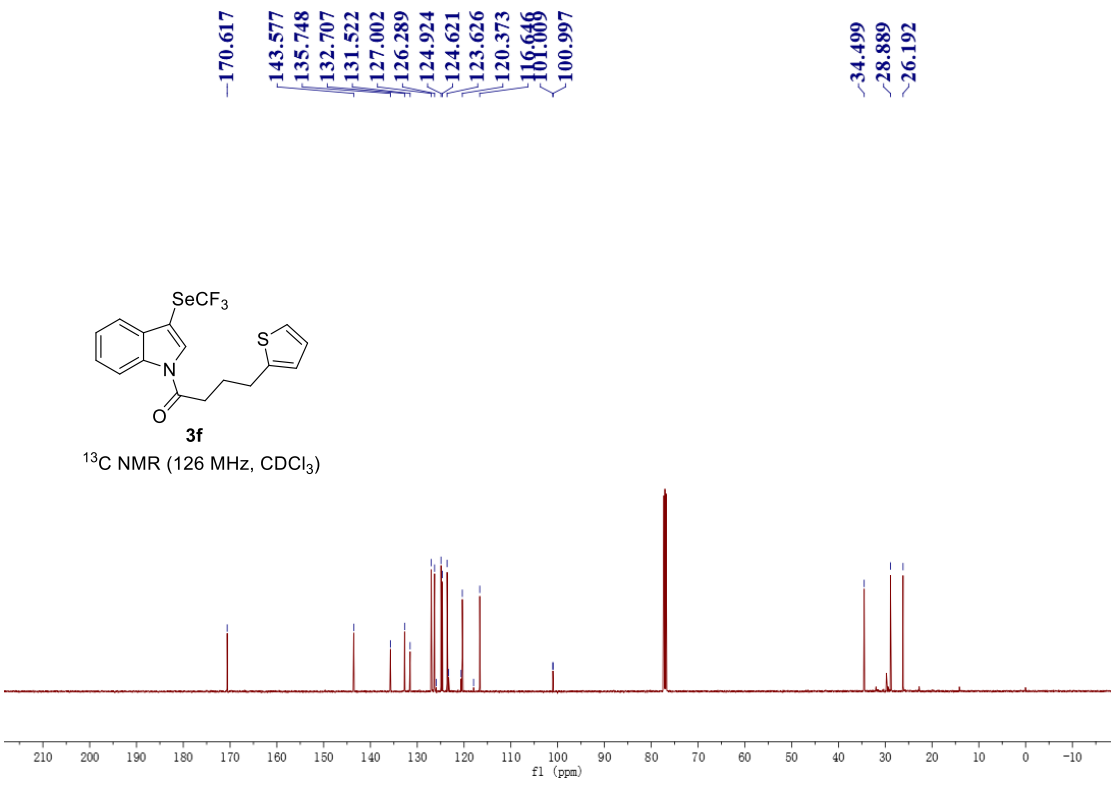

170.201
139.965
135.756
132.630
131.516
128.795
128.473
126.674
126.306
124.647
120.390
116.651
101.107
101.095
37.726
30.346
SeCF3
N
O
Ph
3e
13C NMR (126 MHz, CDCl3)
f1 (ppm)


8.485
8.469
7.743
7.711
7.696
7.464
7.450
7.434
7.420
7.405
7.264
7.178
7.168
6.962
6.955
6.947
3.043
3.029
3.020
3.005
2.991
2.288
2.274
2.260
2.246
2.231
SeCF3
N
S
O
3f
1H NMR (500 MHz, CDCl3)
0.95
0.95
1.00
1.05
1.06
0.91
0.95
0.95
2.10
2.12
2.16
f1 (ppm)



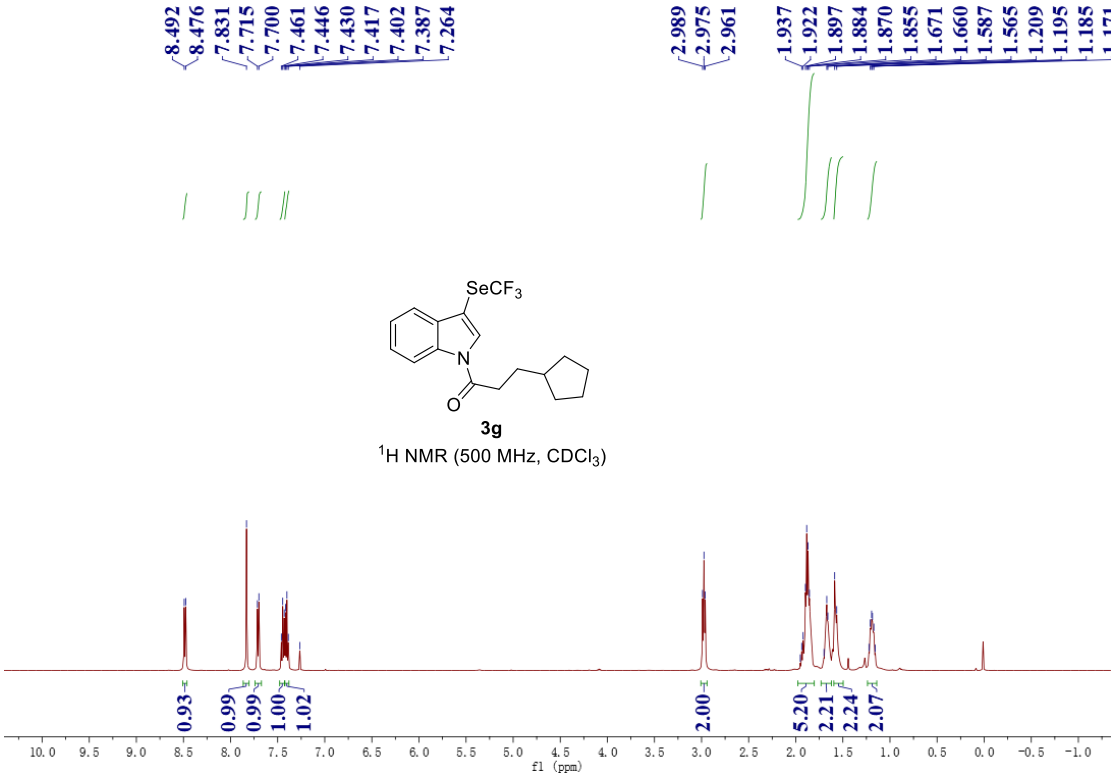
3f

^{19}F NMR (471 MHz, $CDCl_3$)



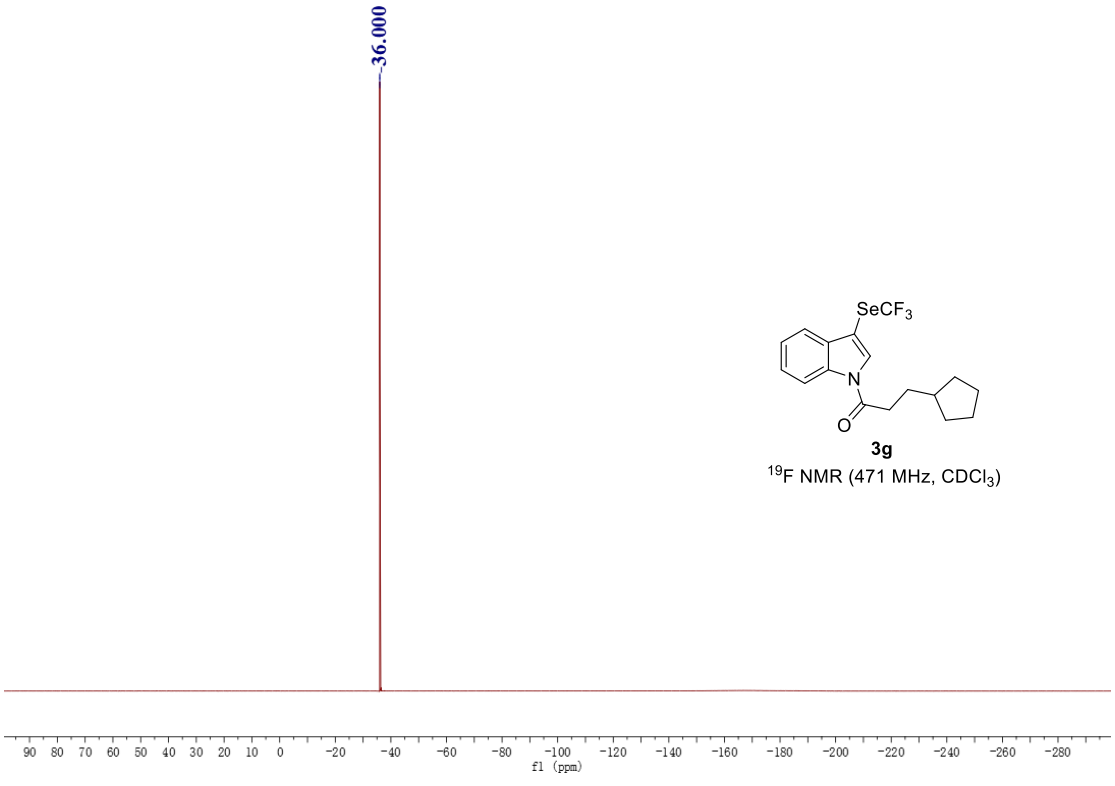
3f

^{13}C NMR (126 MHz, $CDCl_3$)



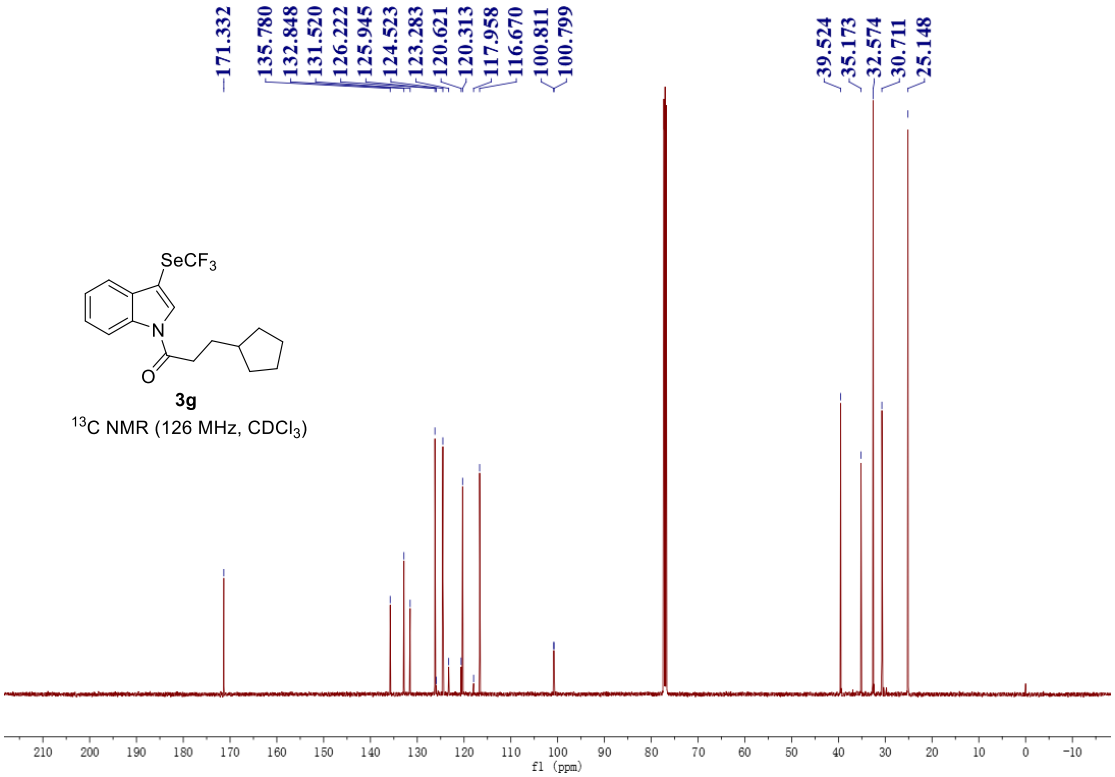
3g

^{1}H NMR (500 MHz, $CDCl_3$)



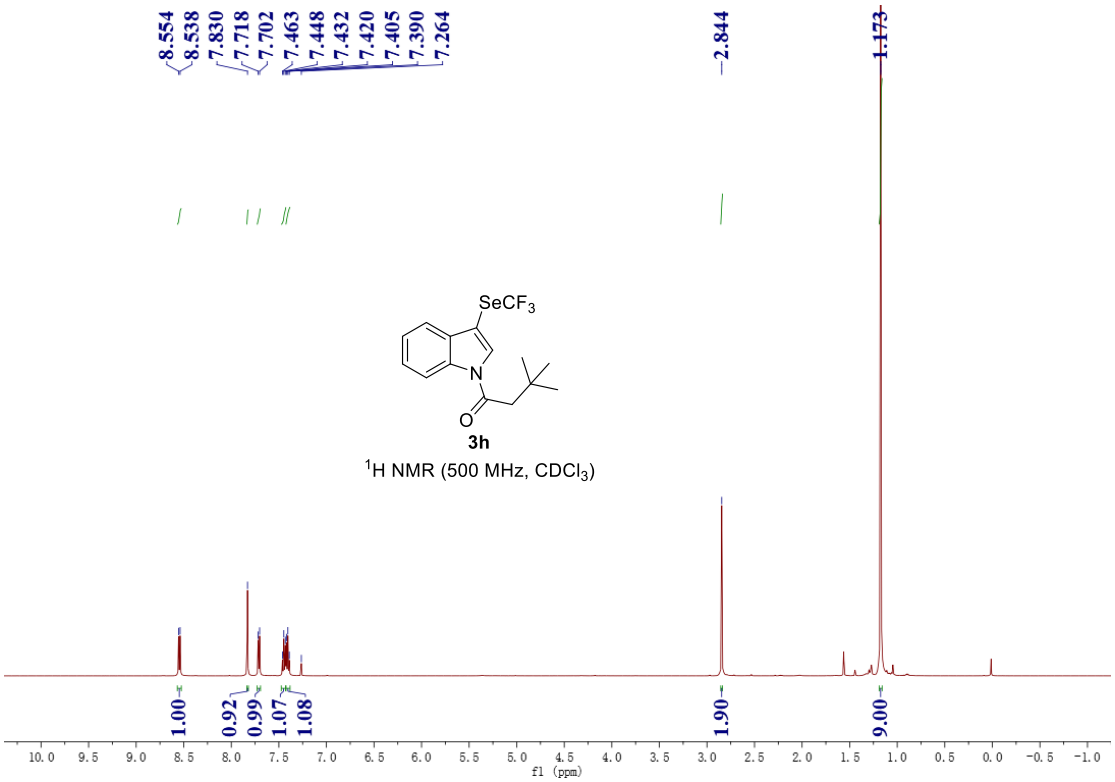
3g

^{19}F NMR (471 MHz, $CDCl_3$)



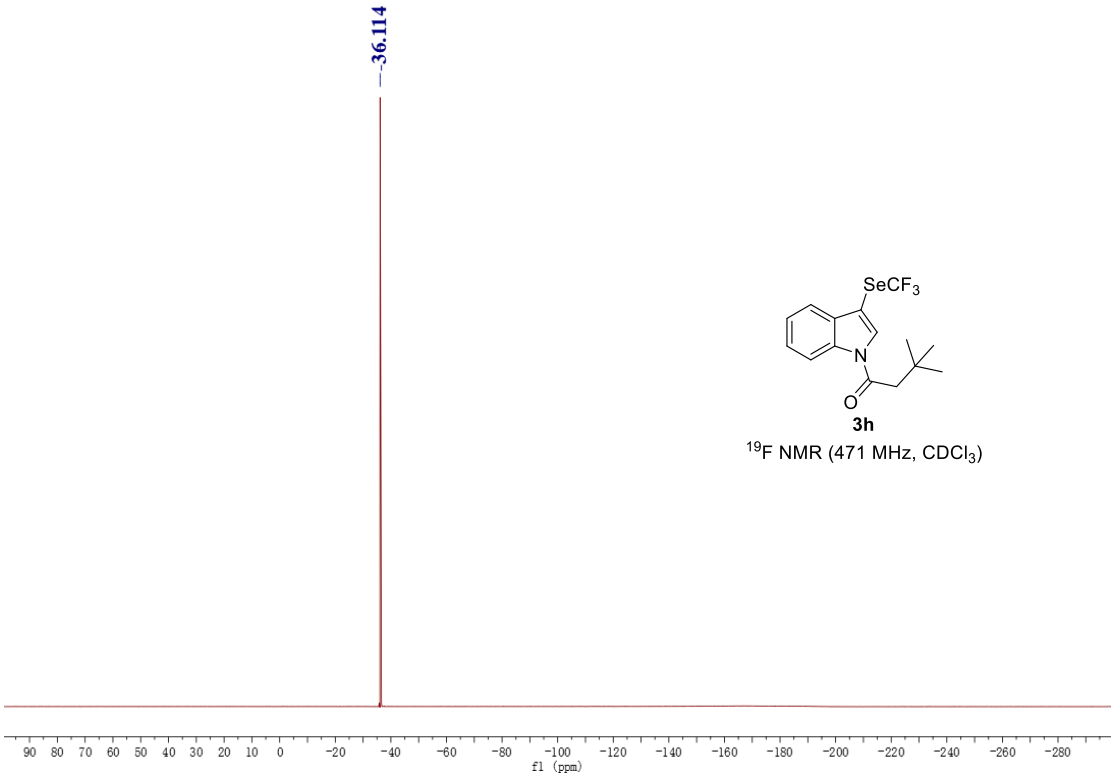
3g

^{13}C NMR (126 MHz, $CDCl_3$)



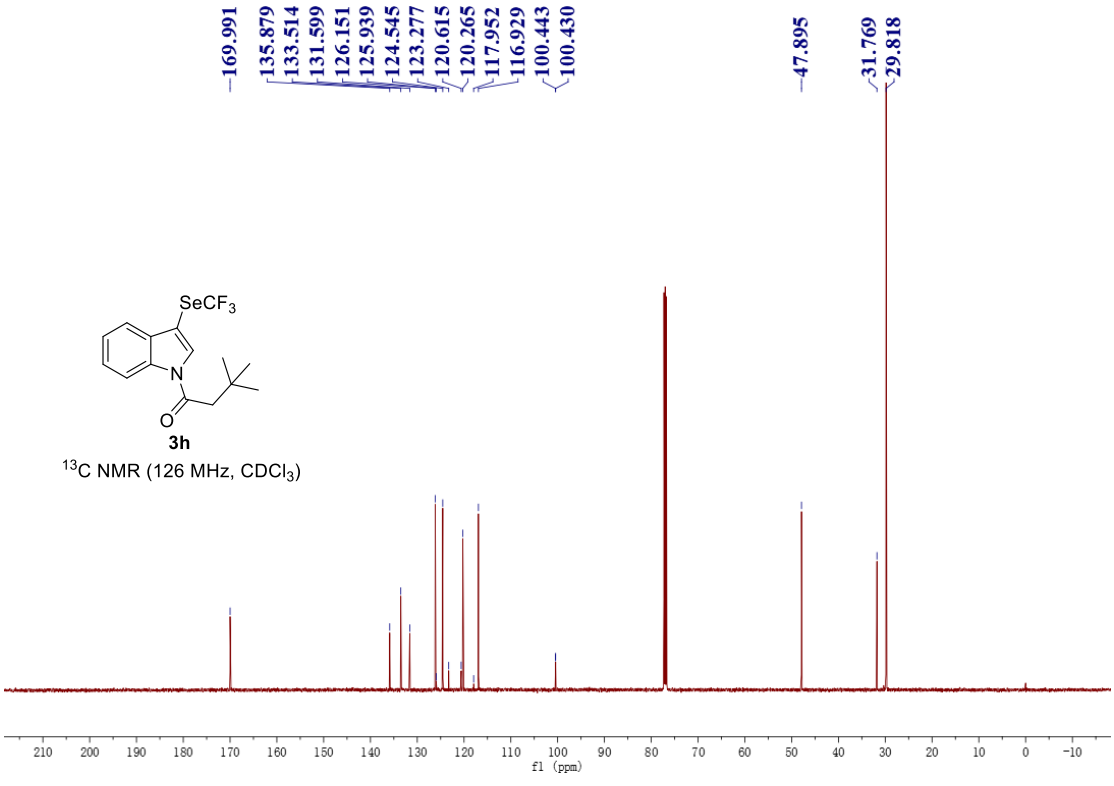
3h

^{1}H NMR (500 MHz, $CDCl_3$)



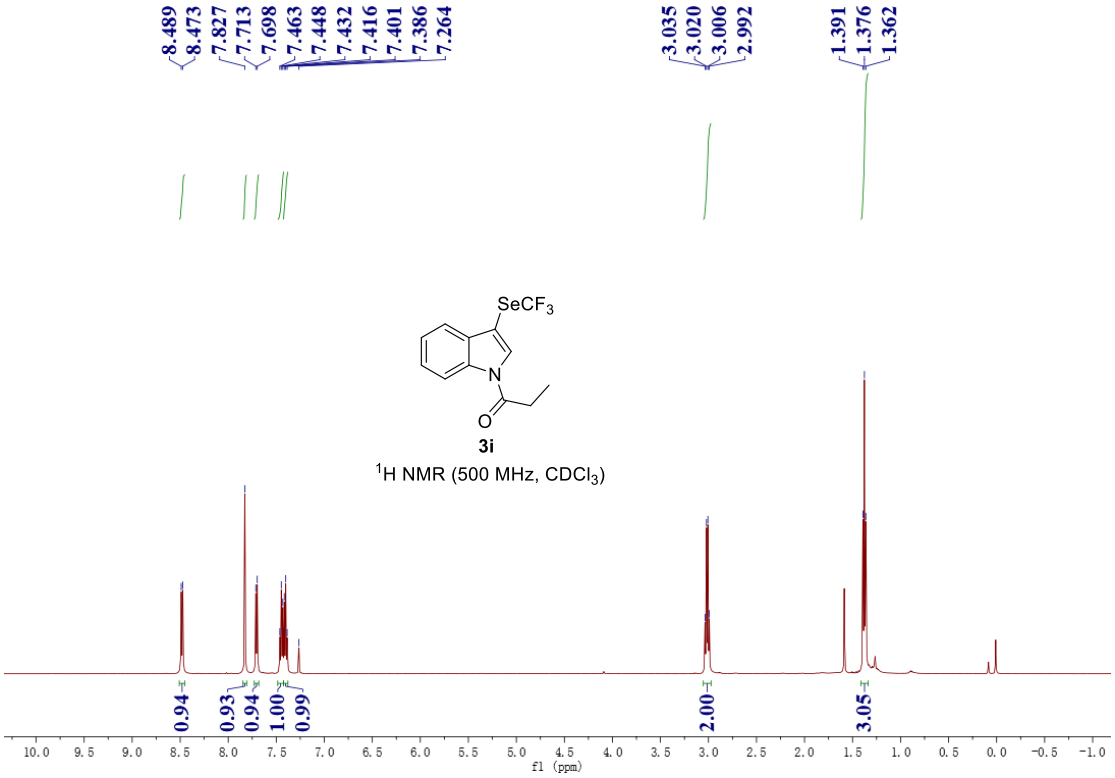
3h

^{19}F NMR (471 MHz, $CDCl_3$)



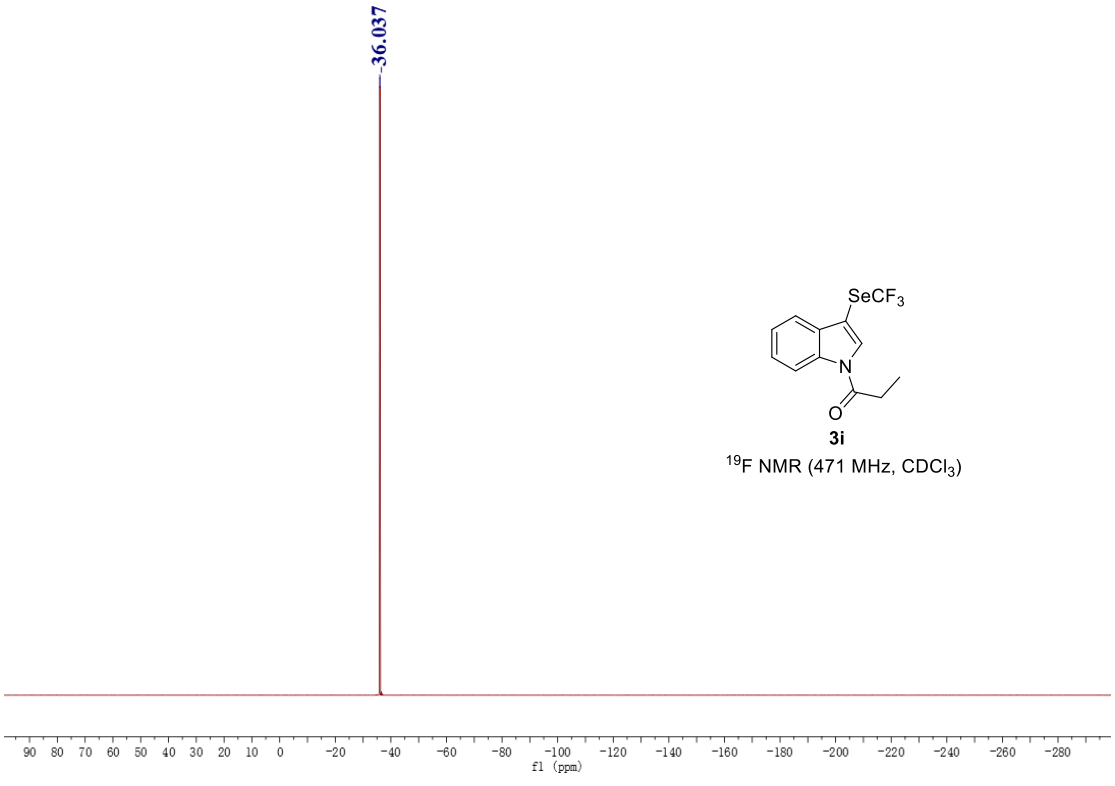
3h

^{13}C NMR (126 MHz, $CDCl_3$)



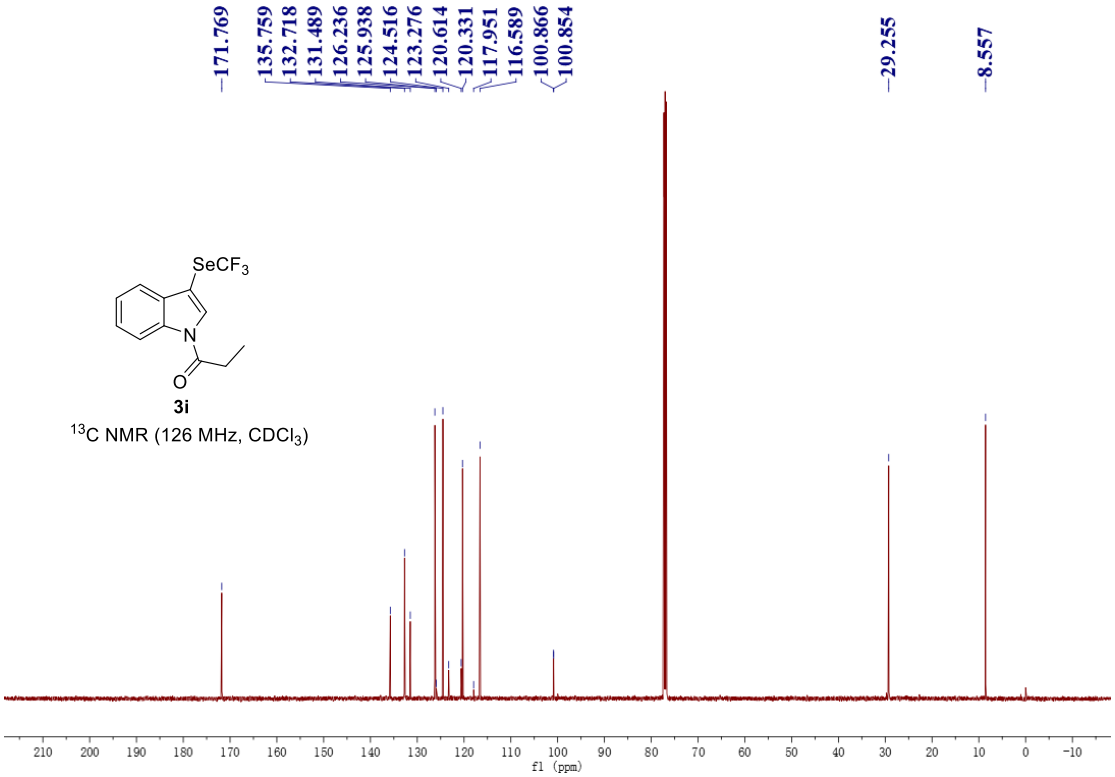
3i

^{1}H NMR (500 MHz, $CDCl_3$)



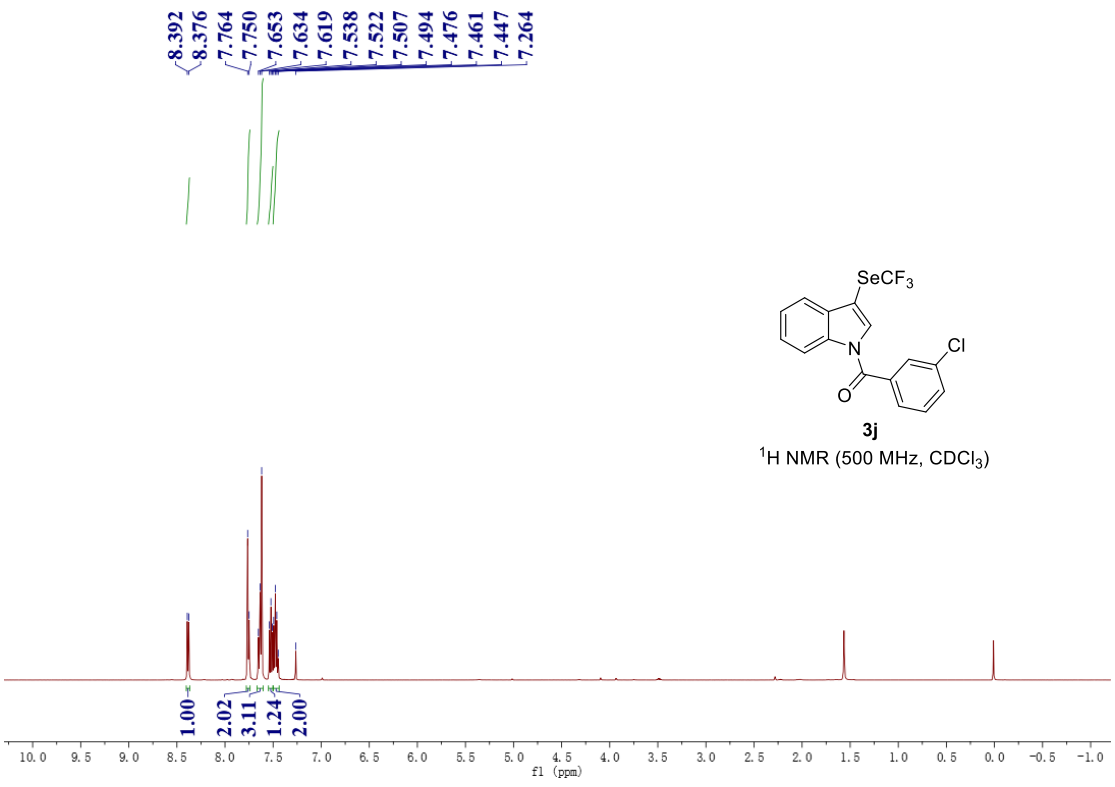
3i

^{19}F NMR (471 MHz, $CDCl_3$)



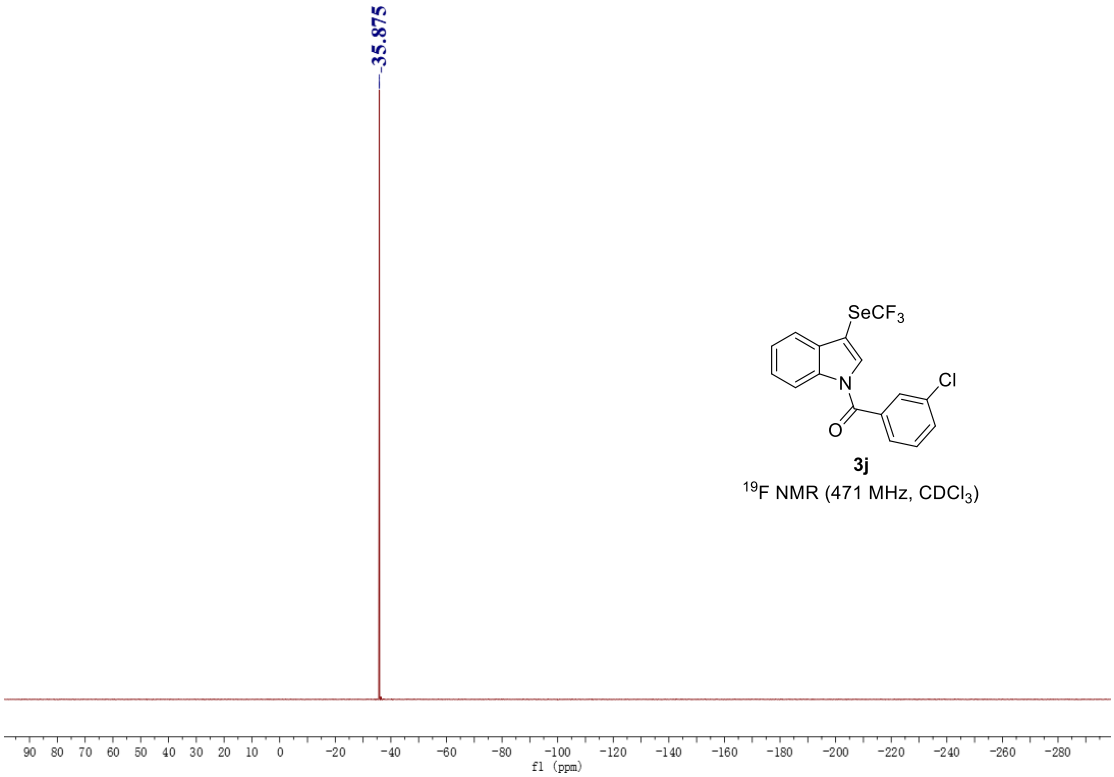
3i

^{13}C NMR (126 MHz, $CDCl_3$)



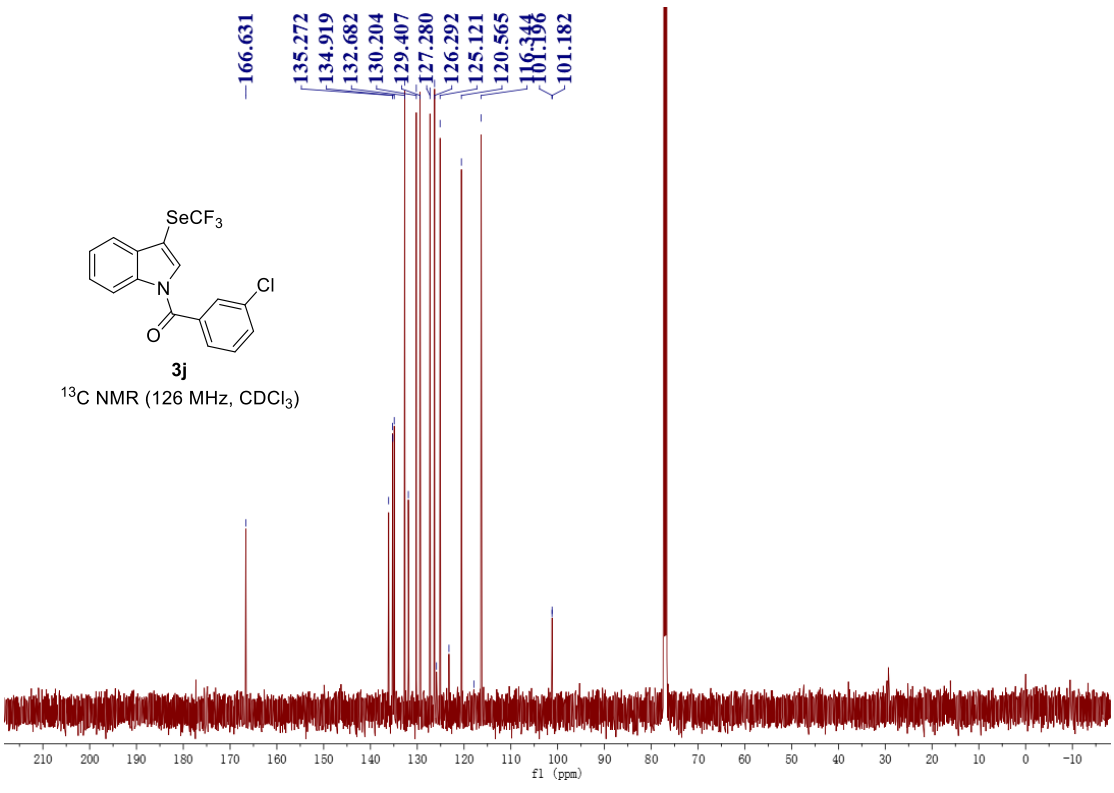
3j

^{1}H NMR (500 MHz, $CDCl_3$)



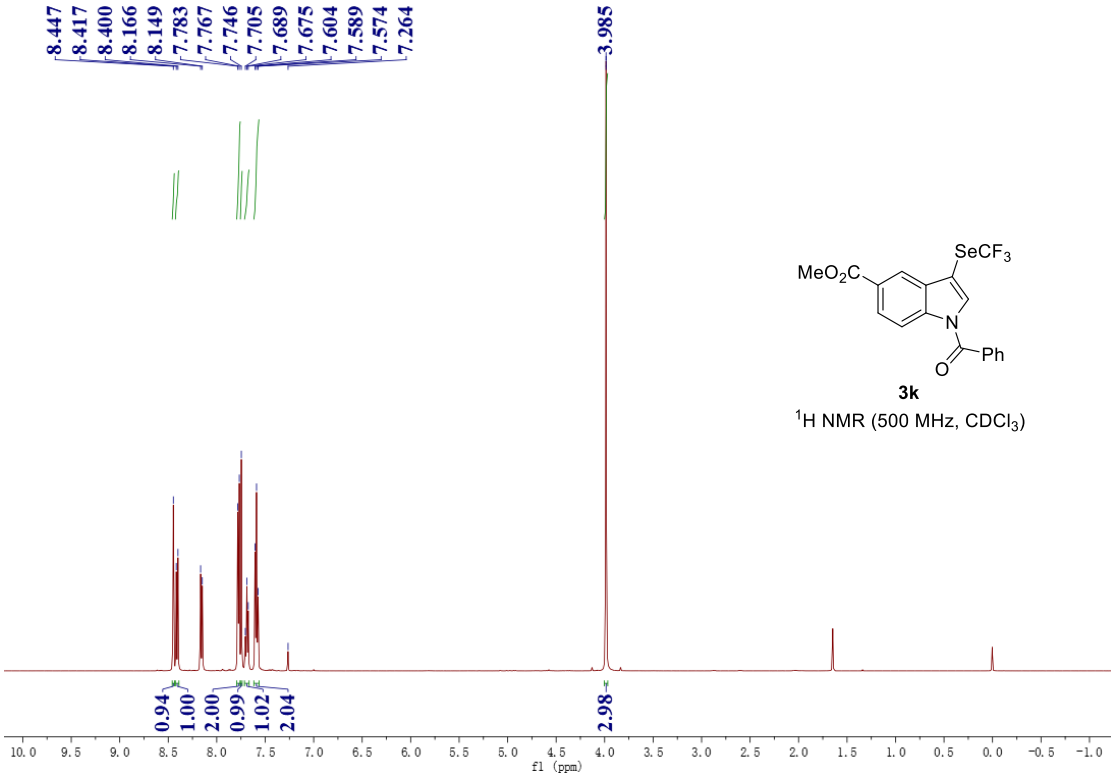
3j

^{19}F NMR (471 MHz, $CDCl_3$)



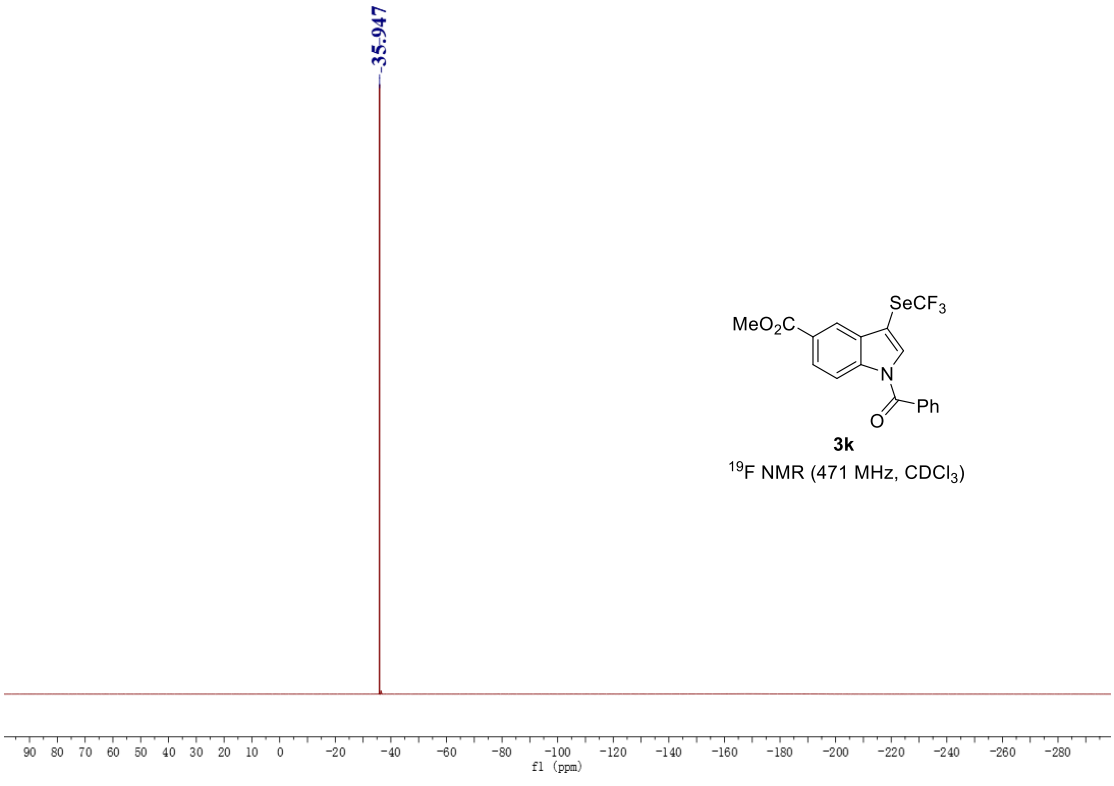
3j

^{13}C NMR (126 MHz, $CDCl_3$)



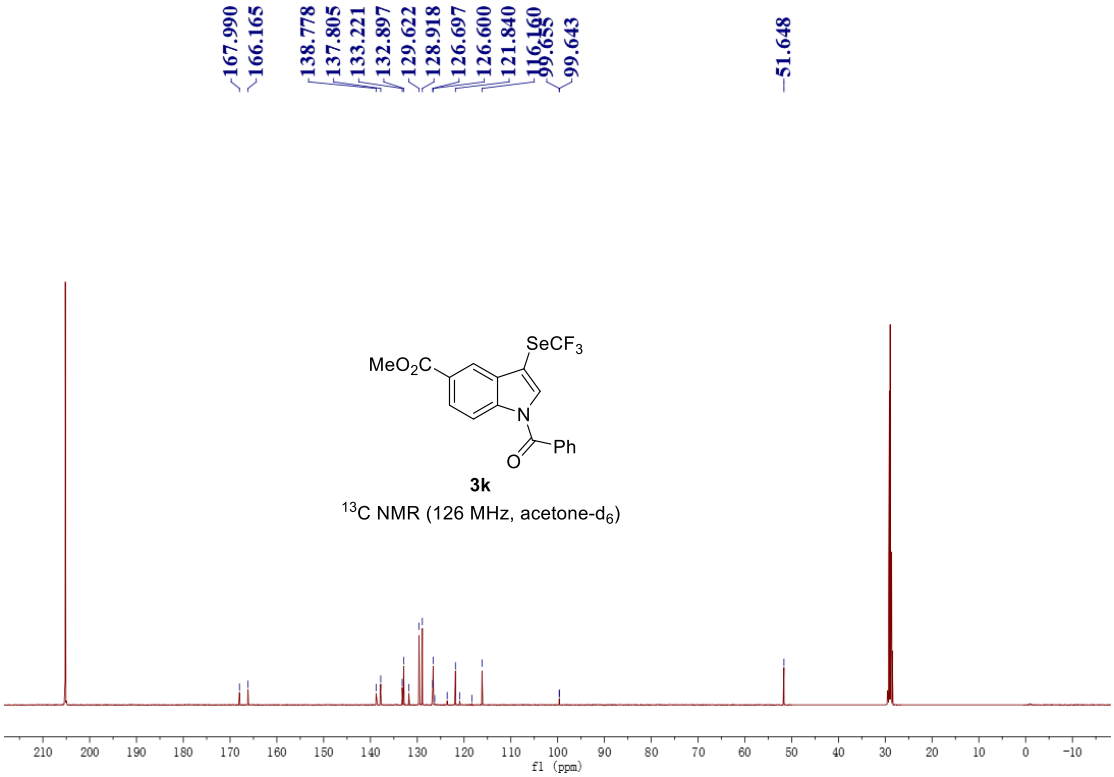
3k

^{1}H NMR (500 MHz, $CDCl_3$)



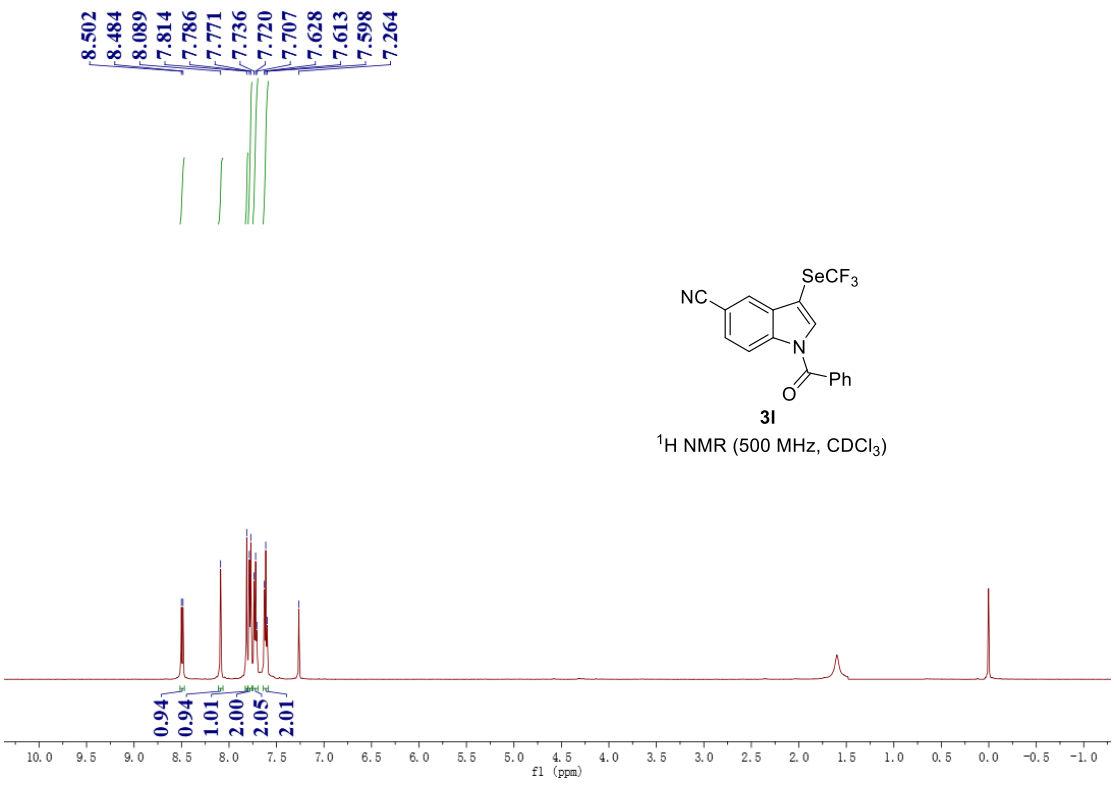
3k

^{19}F NMR (471 MHz, $CDCl_3$)



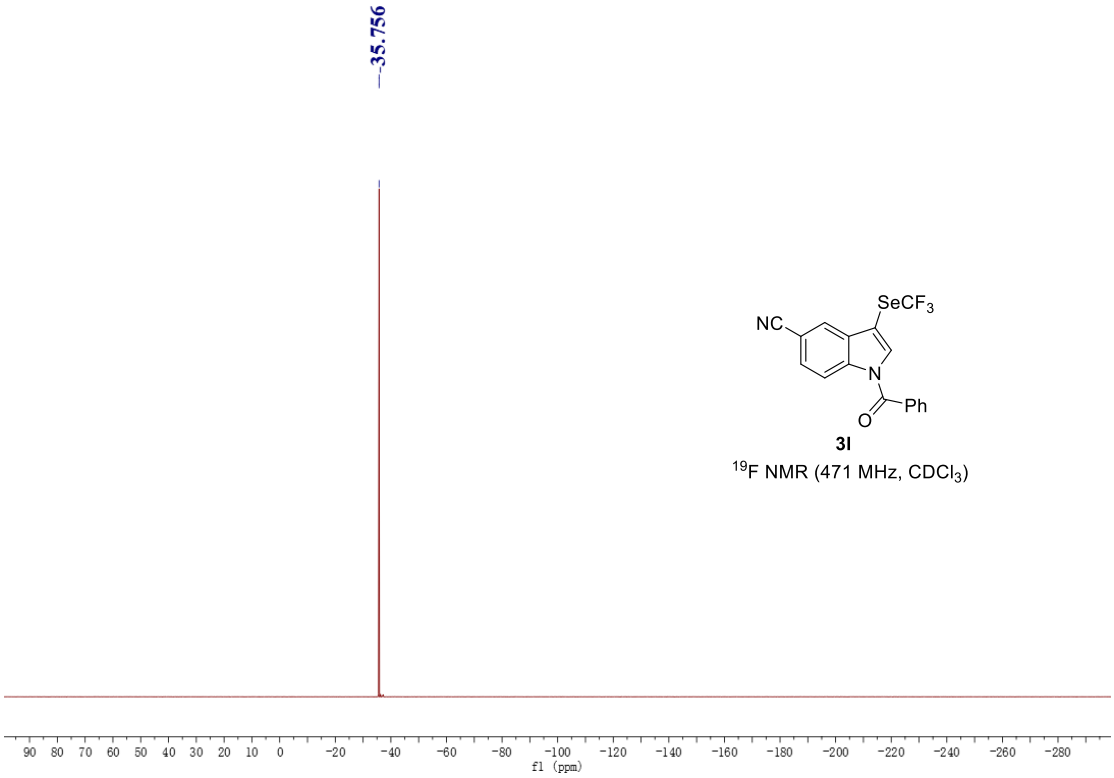
3k

^{13}C NMR (126 MHz, acetone-d_6)



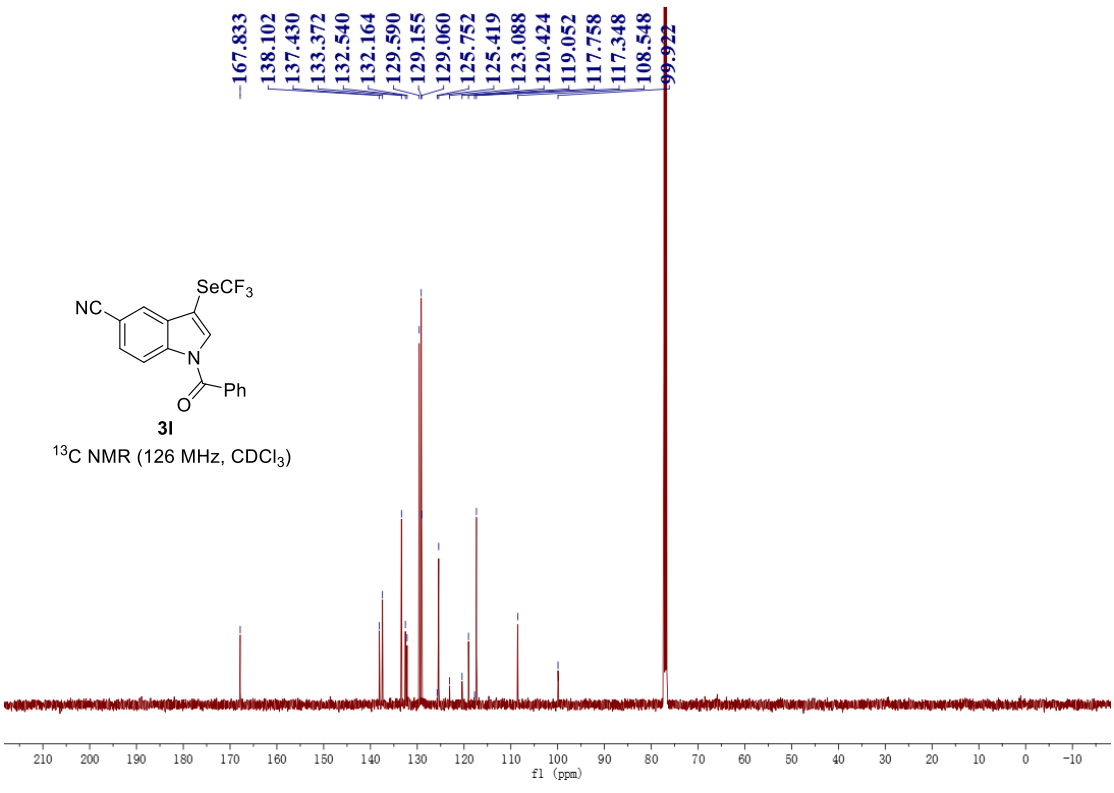
3l

^{1}H NMR (500 MHz, $CDCl_3$)



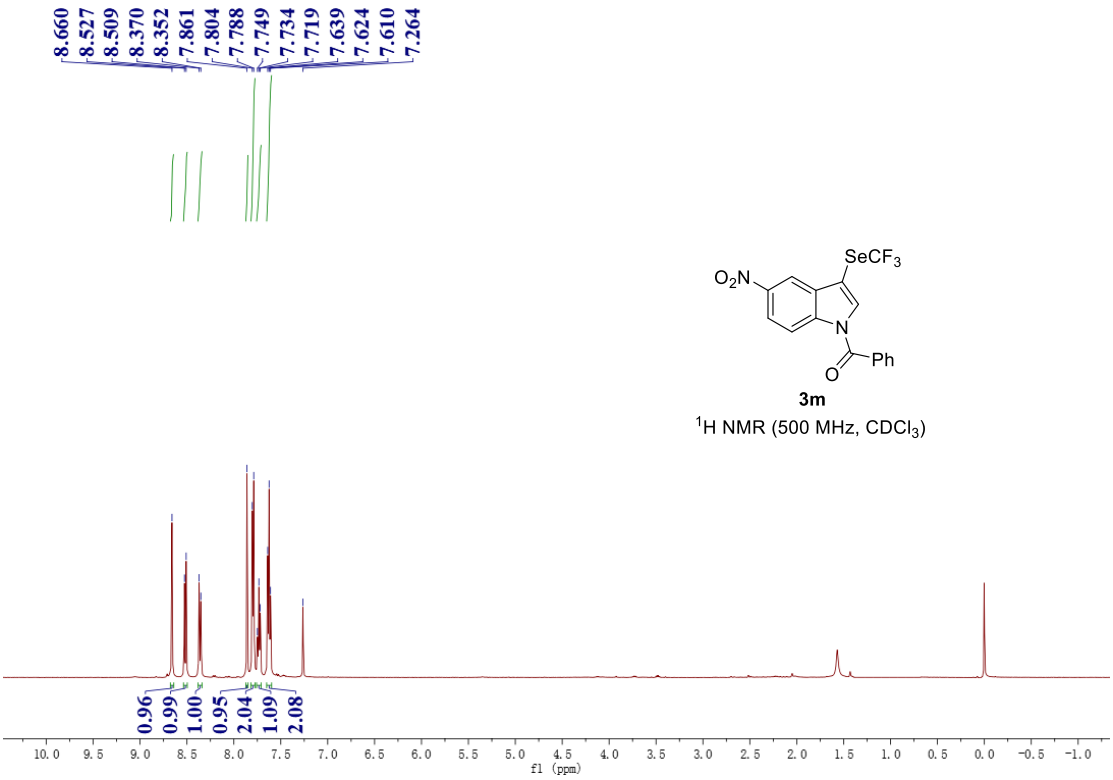
3l

^{19}F NMR (471 MHz, $CDCl_3$)



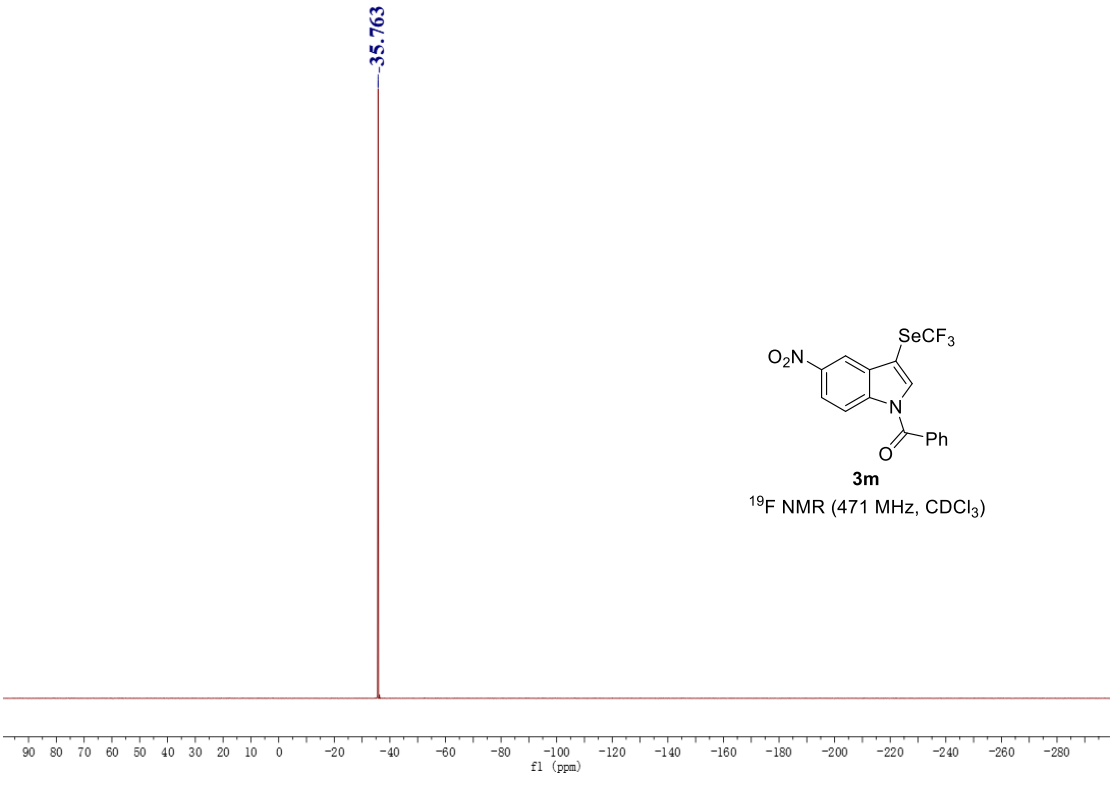
3l

^{13}C NMR (126 MHz, $CDCl_3$)



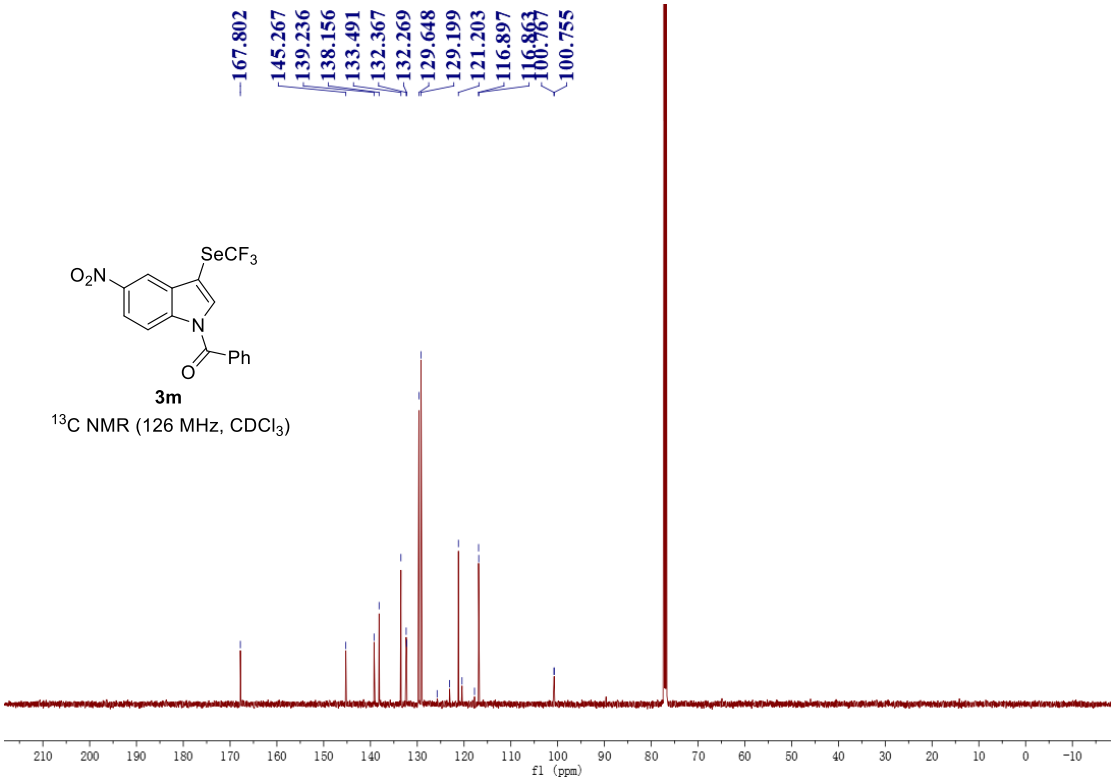
3m

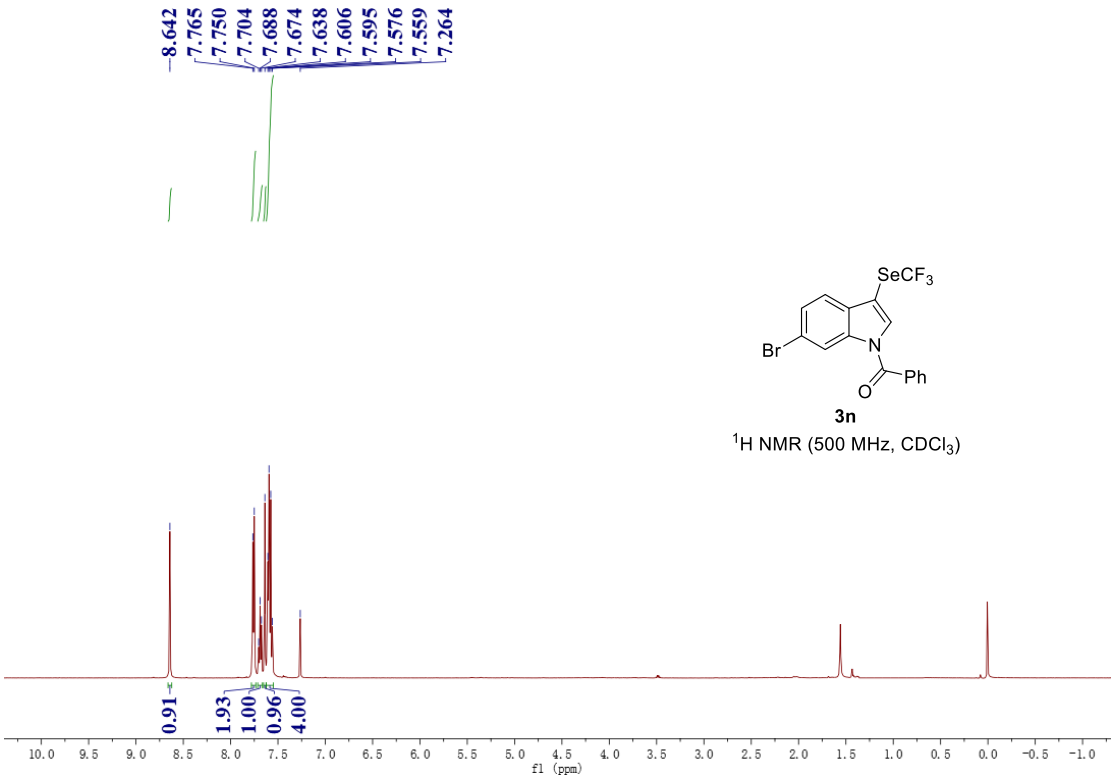
^{1}H NMR (500 MHz, $CDCl_3$)

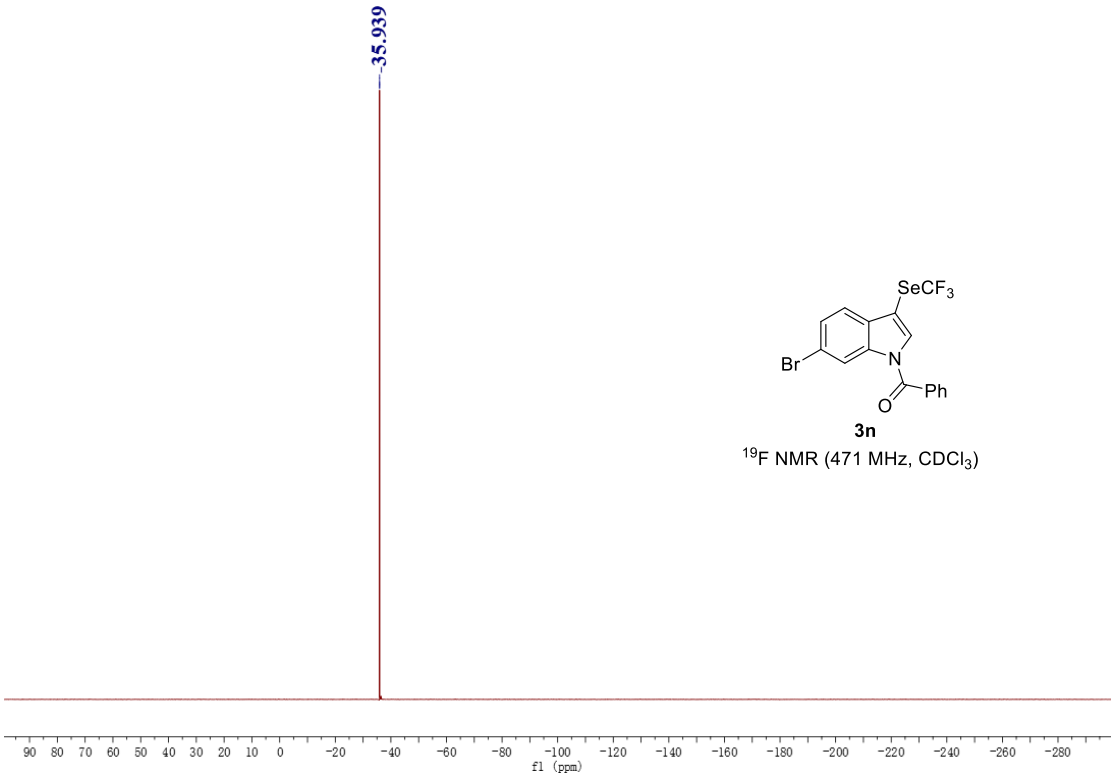


3m

^{19}F NMR (471 MHz, $CDCl_3$)

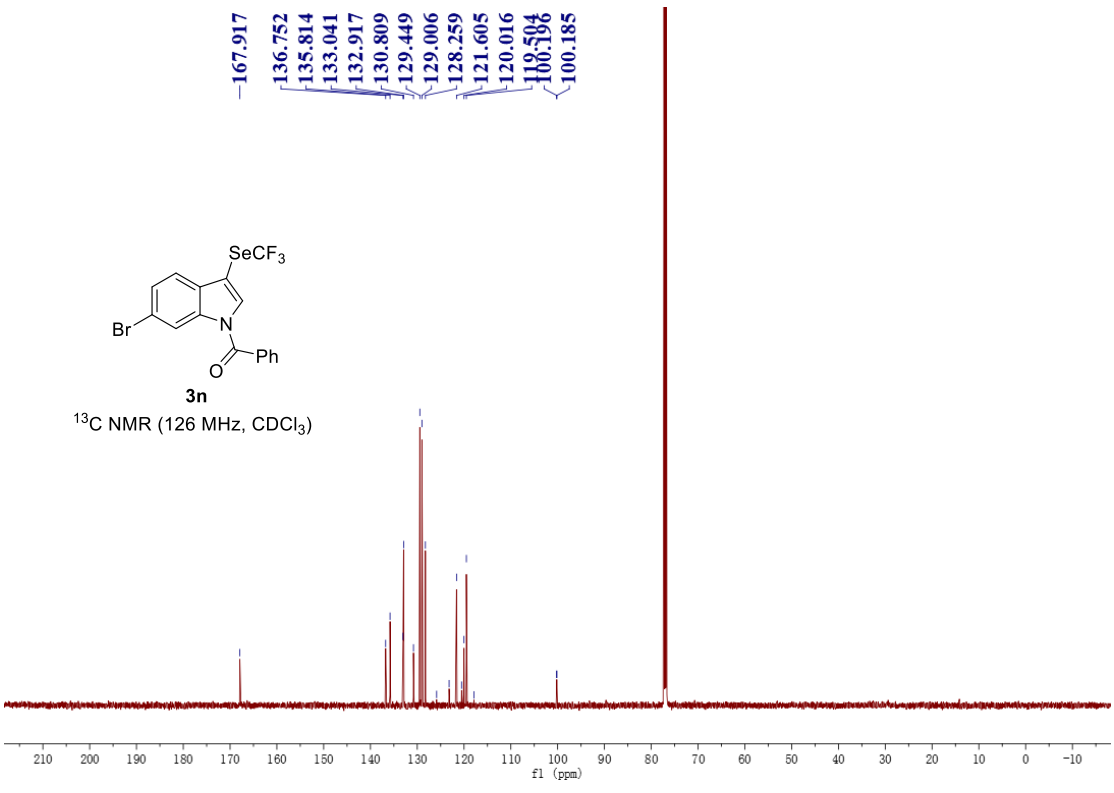

167.802
145.267
139.236
138.156
133.491
132.367
132.269
129.648
129.199
121.203
116.897
116.863
100.767
100.755
SeCF3
O2N
N
O
Ph
3m
13C NMR (126 MHz, CDCl3)
f1 (ppm)


8.642
7.765
7.750
7.704
7.688
7.674
7.638
7.606
7.595
7.576
7.559
7.264
SeCF3
Br
N
O
Ph
3n
1H NMR (500 MHz, CDCl3)
0.91
1.93
1.00
0.96
4.00
f1 (ppm)



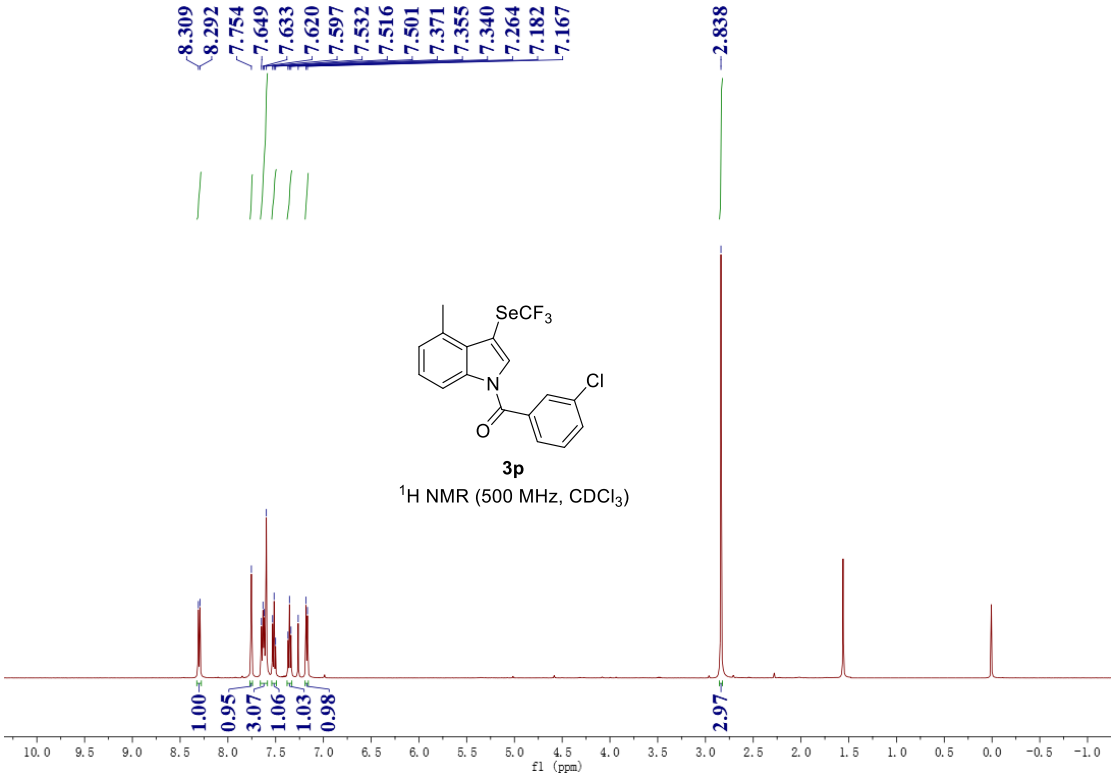
3n

^{19}F NMR (471 MHz, $CDCl_3$)



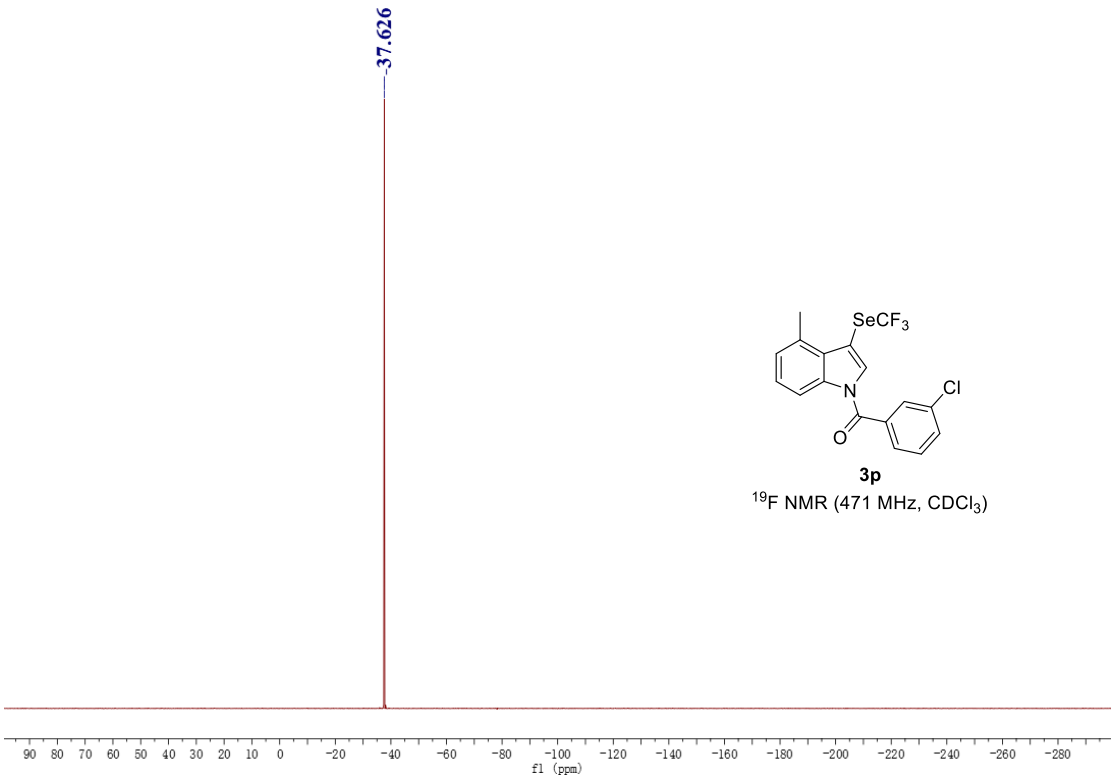
3n

^{13}C NMR (126 MHz, $CDCl_3$)



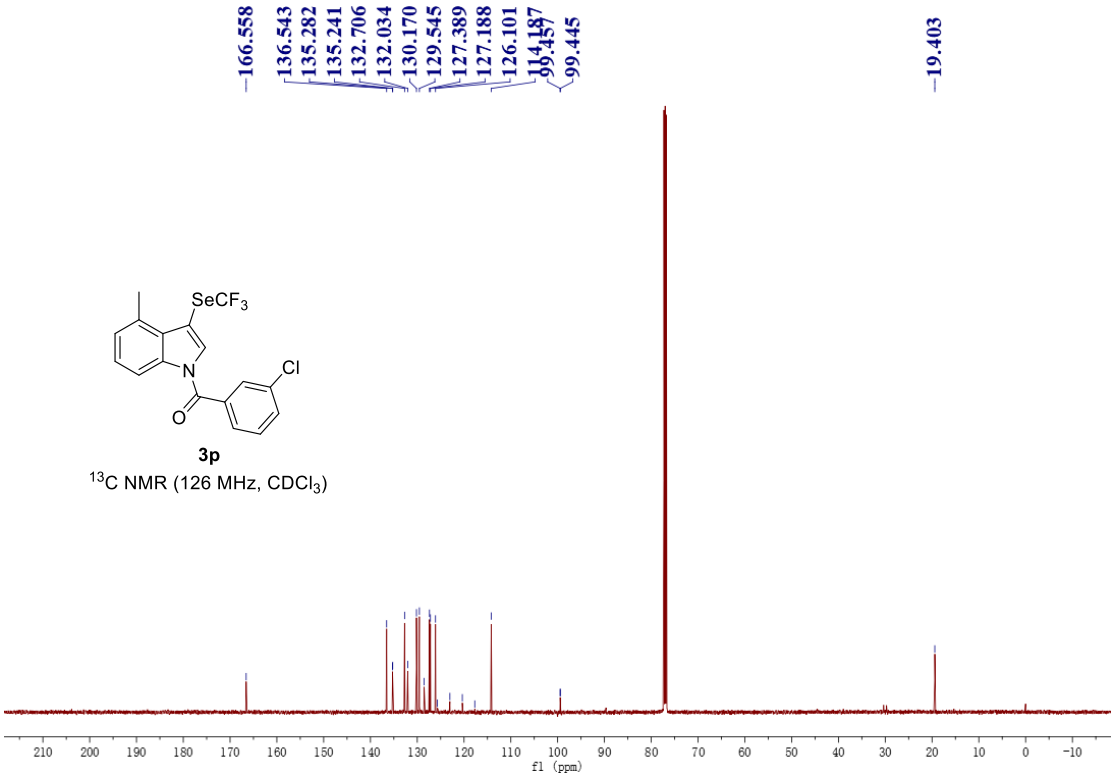
3p

^{1}H NMR (500 MHz, $CDCl_3$)



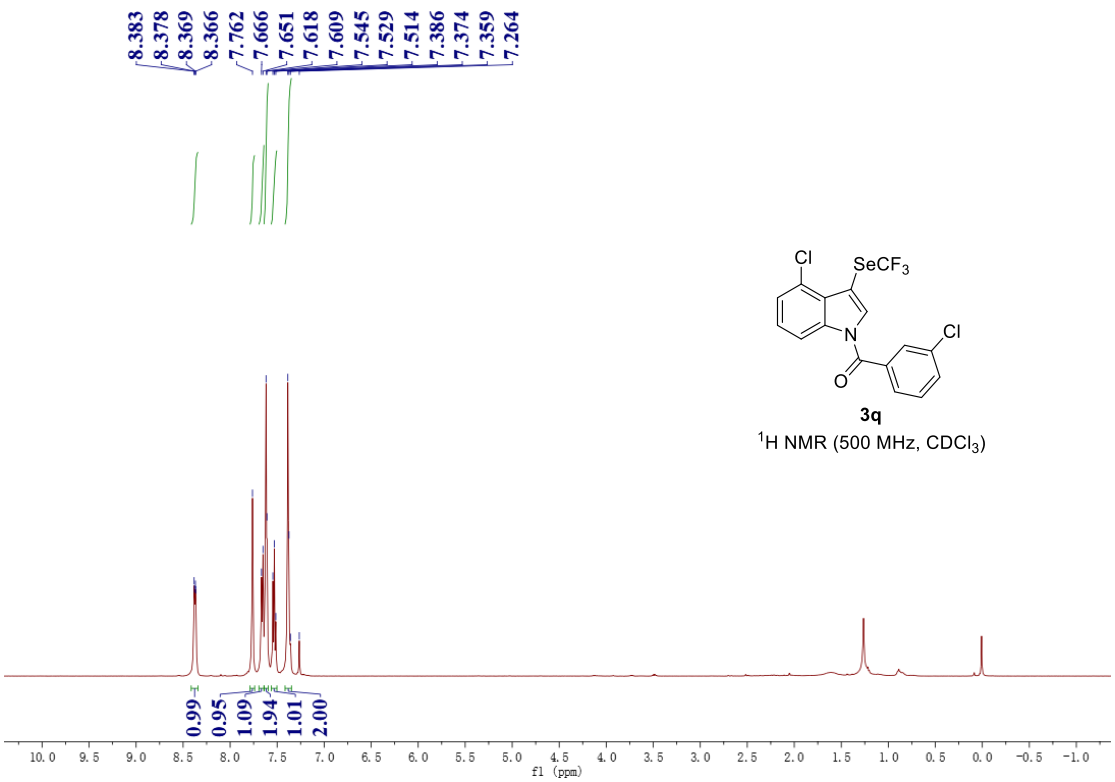
3p

^{19}F NMR (471 MHz, $CDCl_3$)



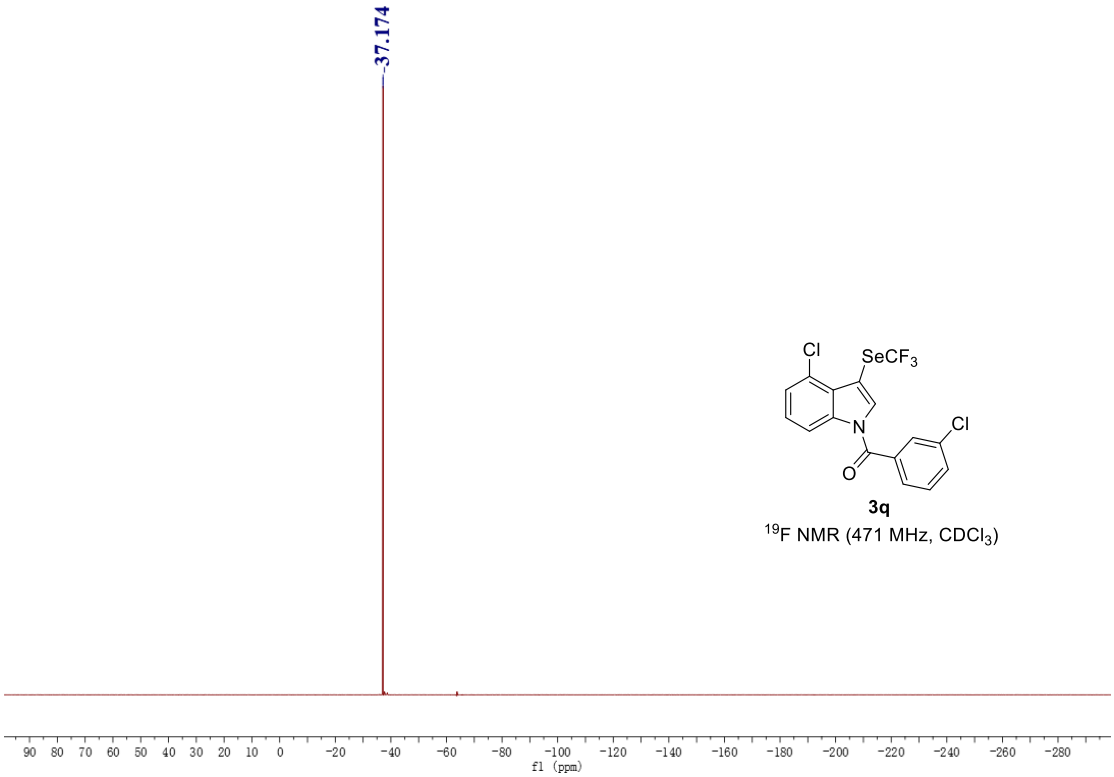
3p

^{13}C NMR (126 MHz, $CDCl_3$)



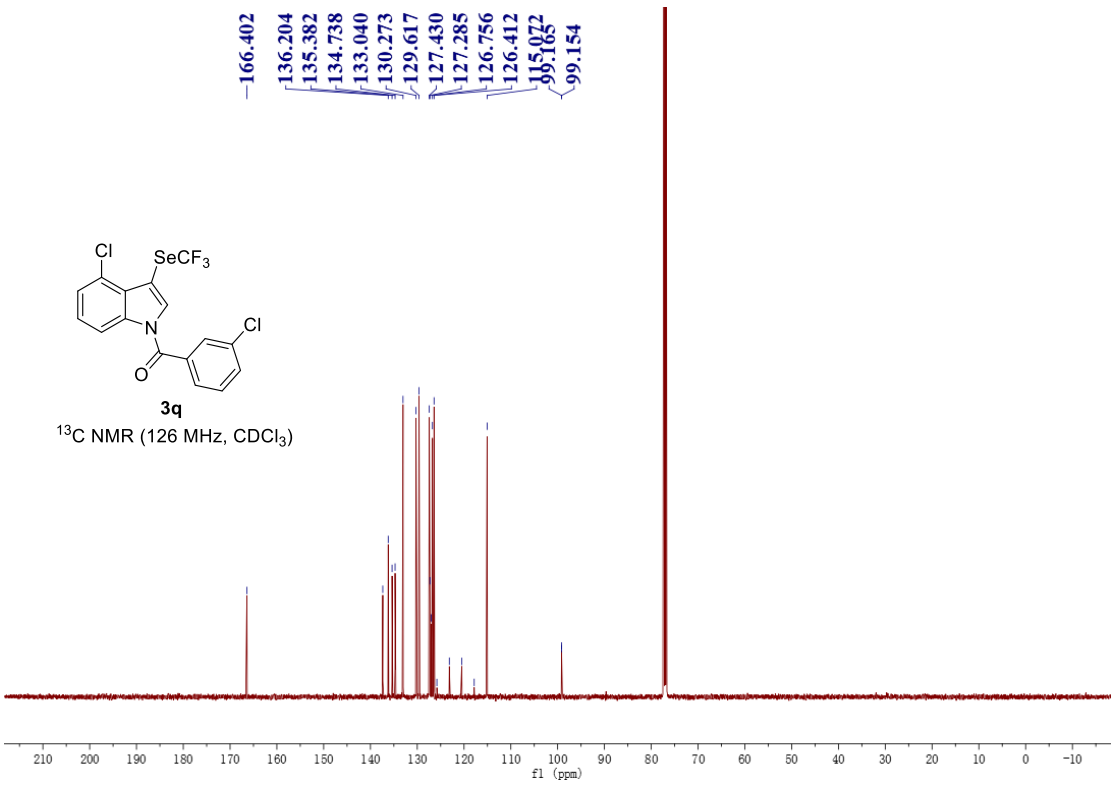
3q

^{1}H NMR (500 MHz, $CDCl_3$)



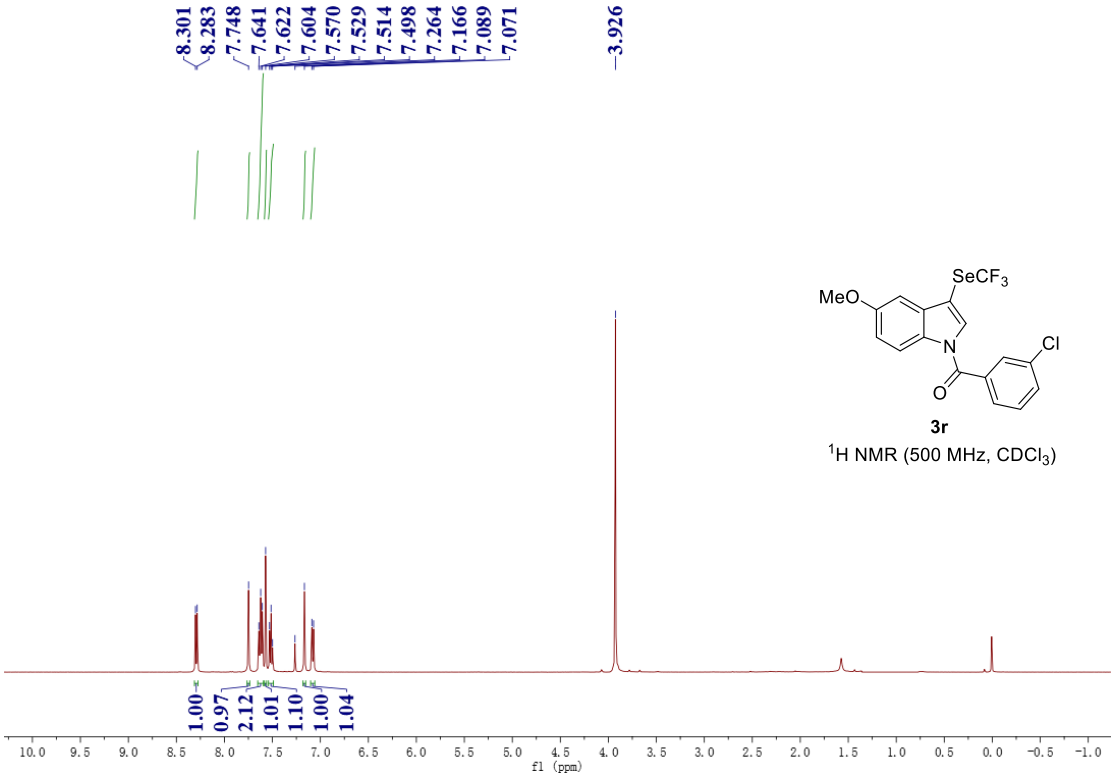
3q

^{19}F NMR (471 MHz, $CDCl_3$)



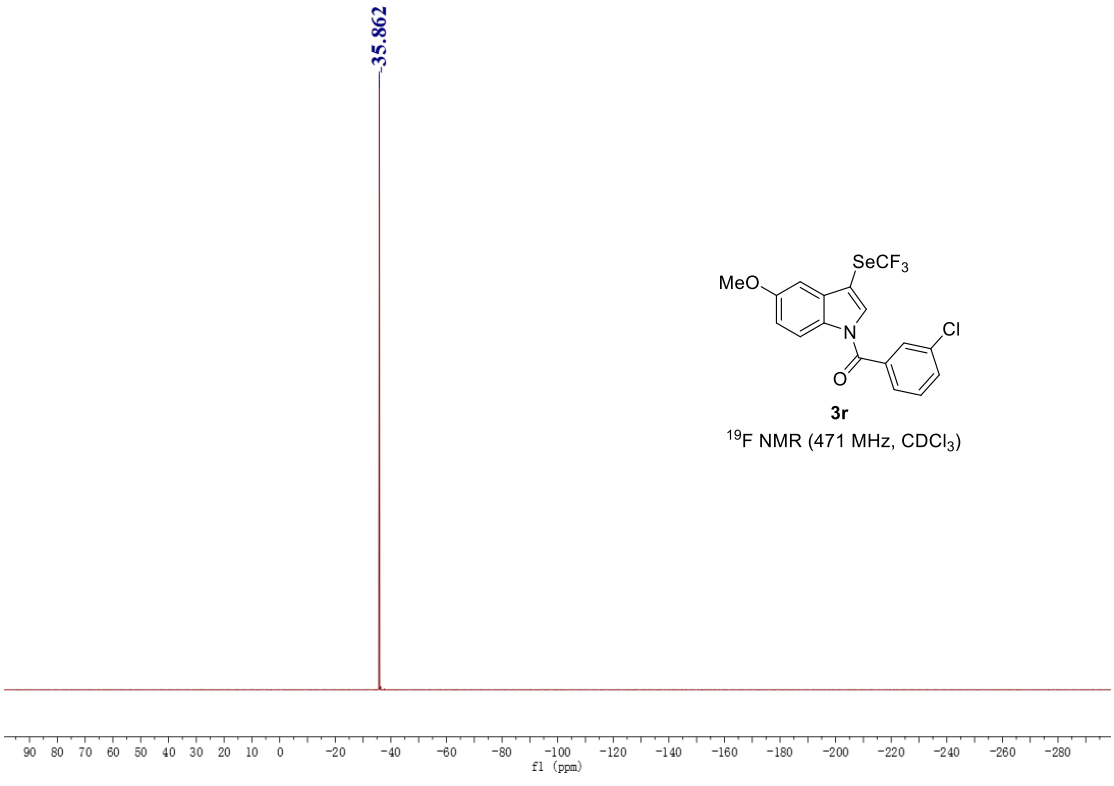
3q

^{13}C NMR (126 MHz, $CDCl_3$)



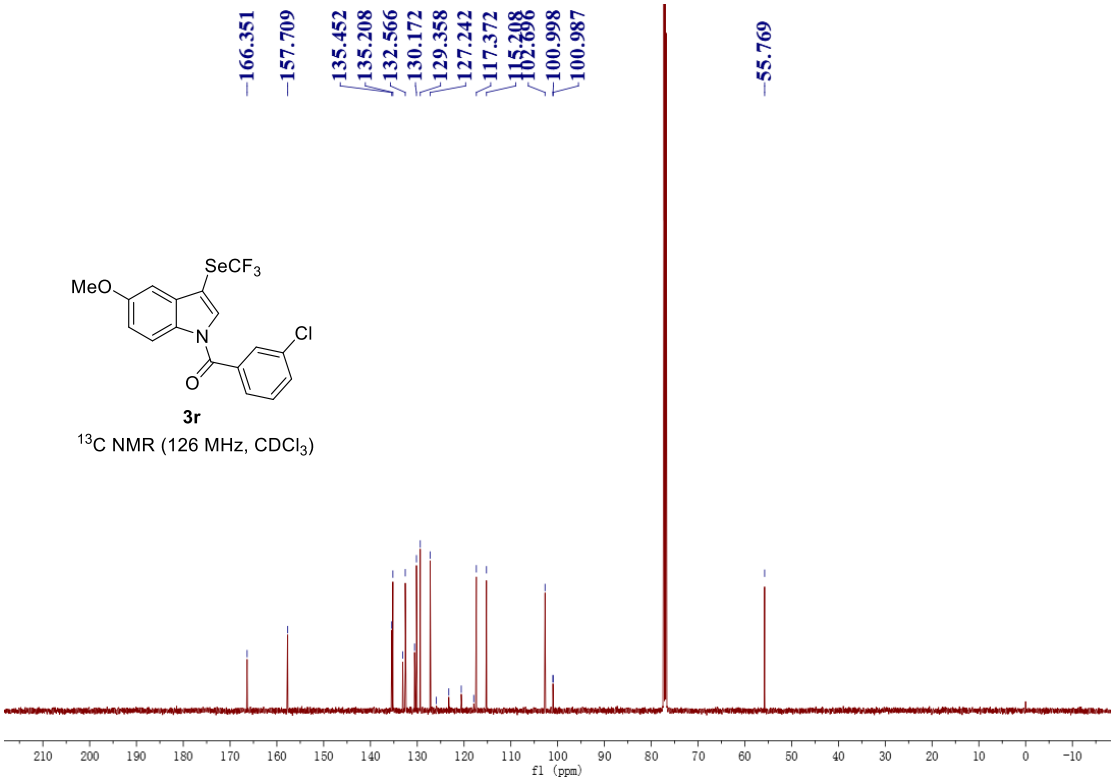
3r

^{1}H NMR (500 MHz, $CDCl_3$)



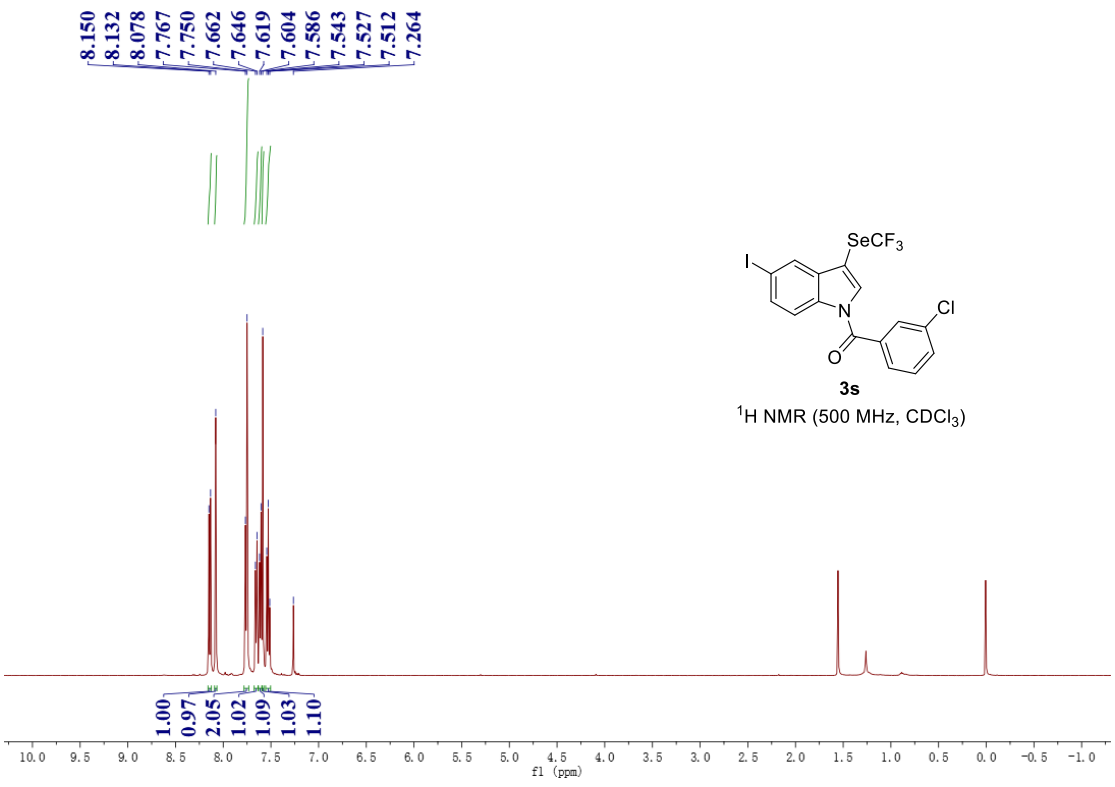
3r

^{19}F NMR (471 MHz, $CDCl_3$)



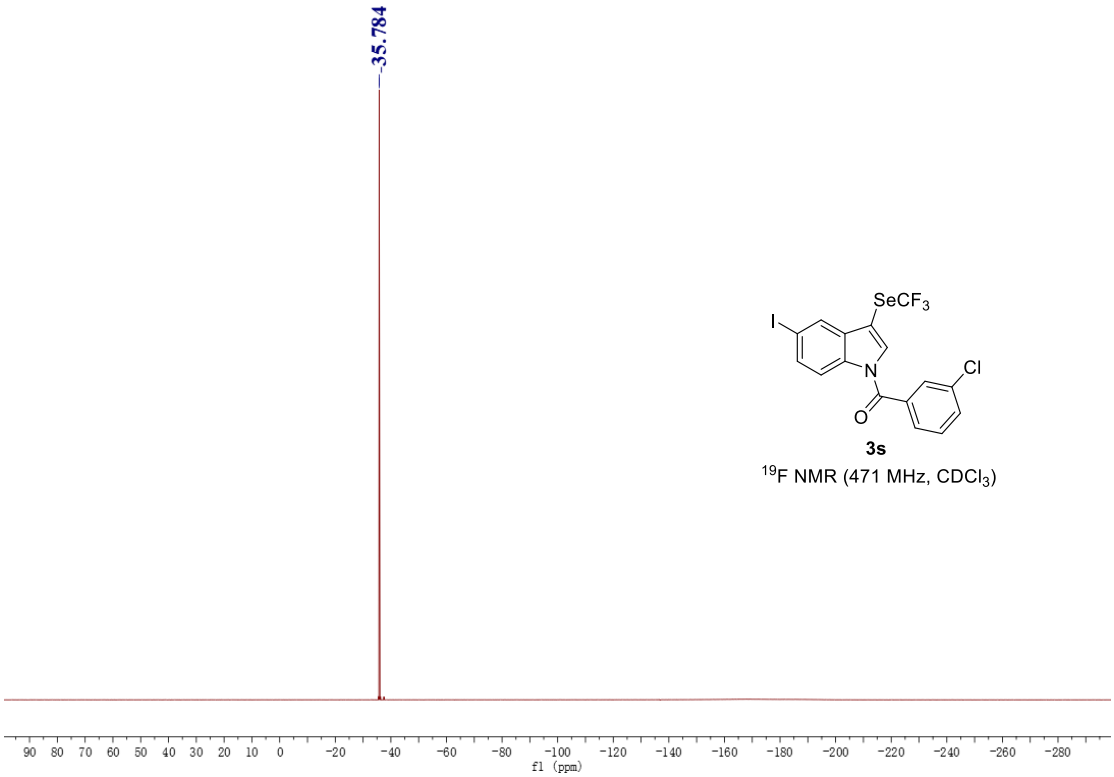
3r

^{13}C NMR (126 MHz, $CDCl_3$)



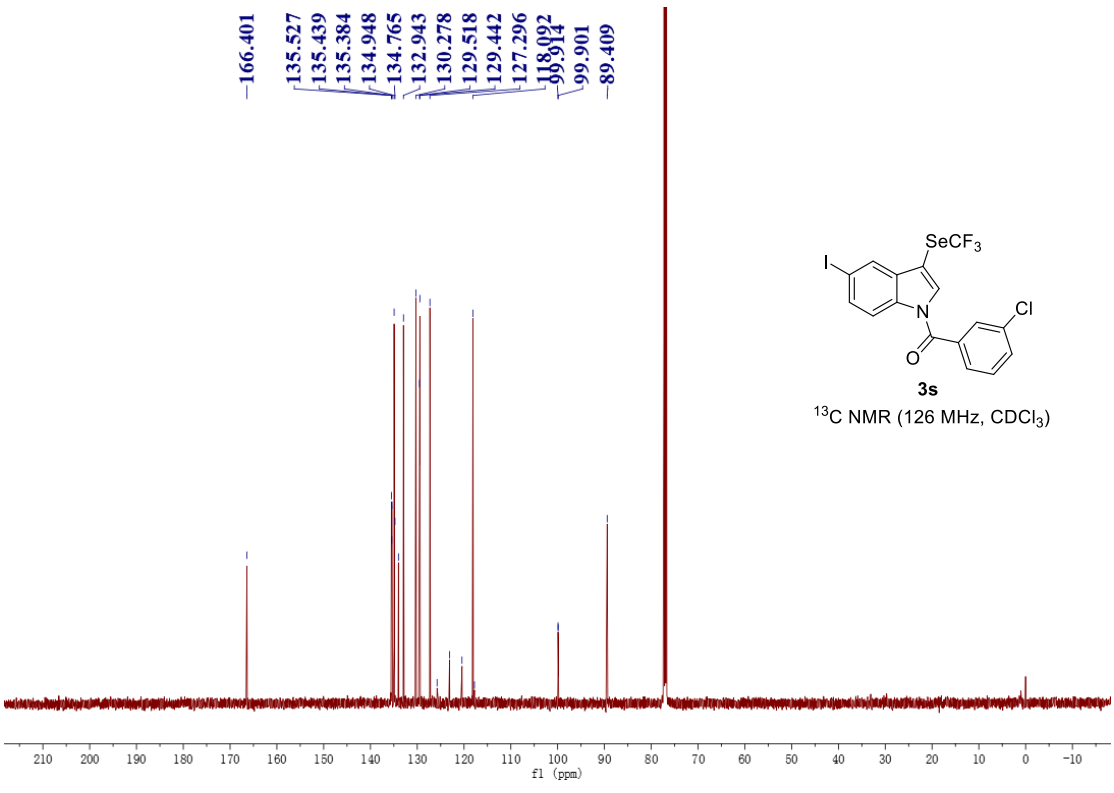
3s

^{1}H NMR (500 MHz, $CDCl_3$)



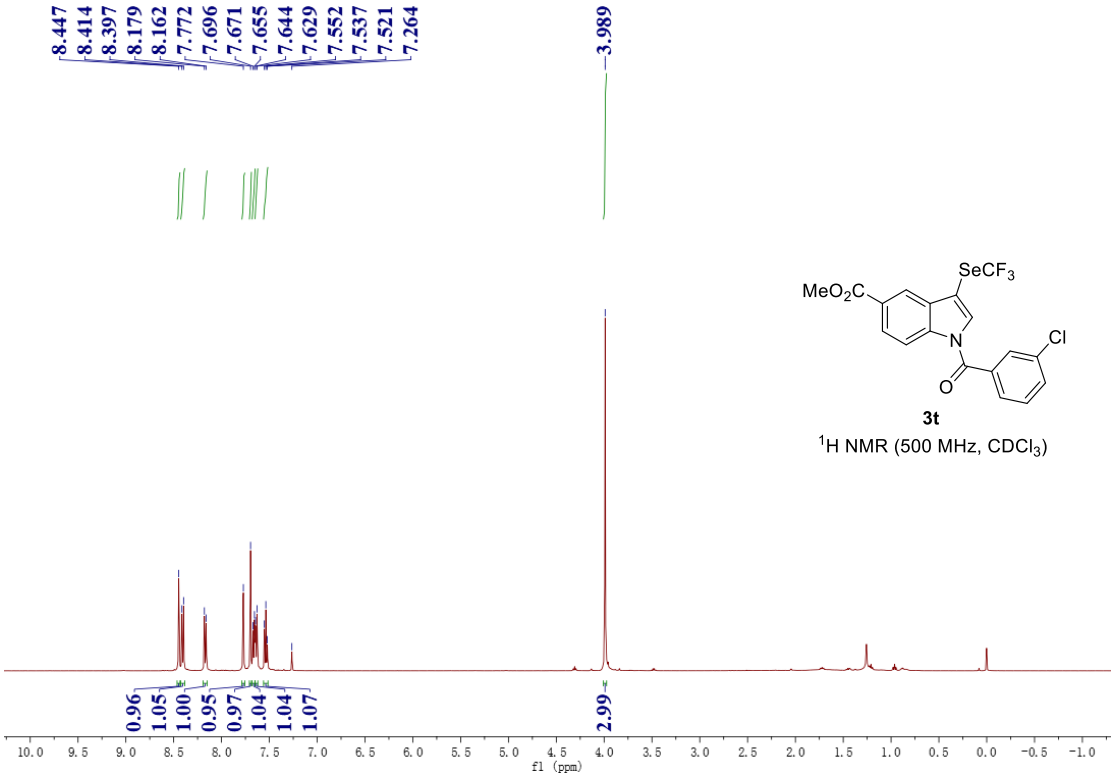
3s

^{19}F NMR (471 MHz, $CDCl_3$)



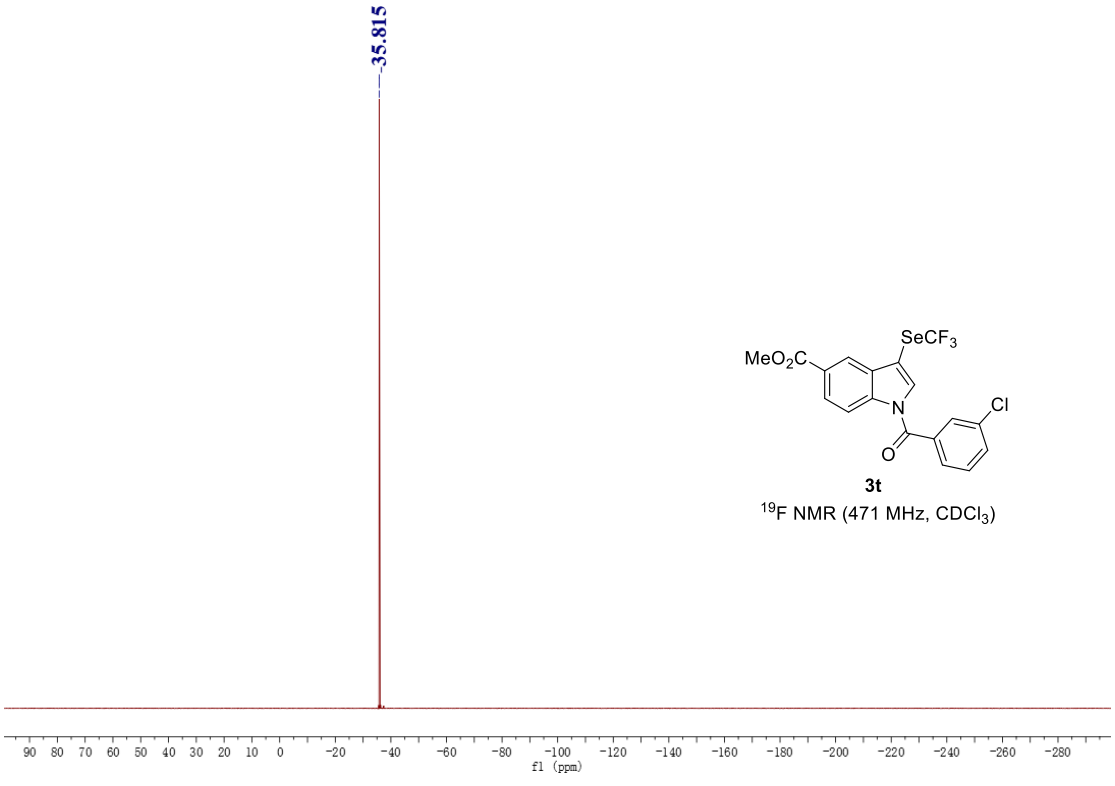
3s

^{13}C NMR (126 MHz, $CDCl_3$)



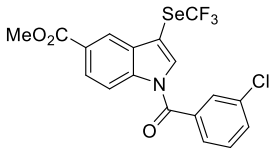
3t

^{1}H NMR (500 MHz, $CDCl_3$)



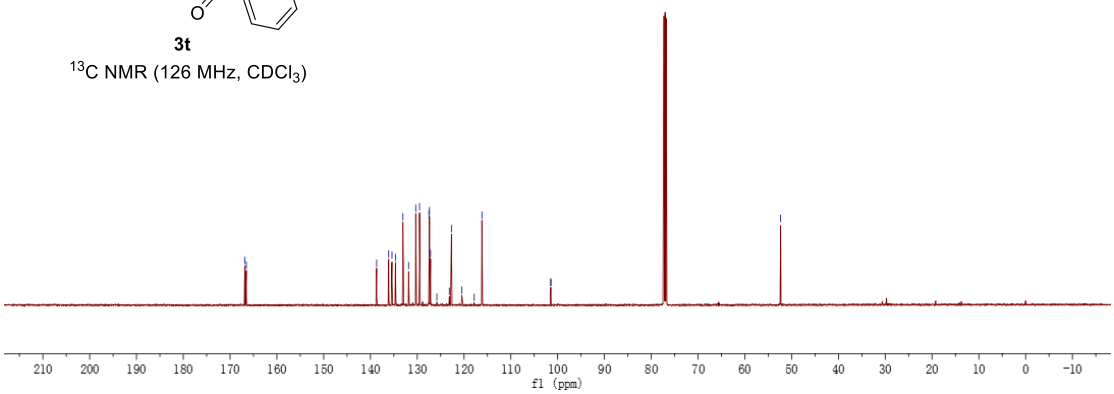
3t

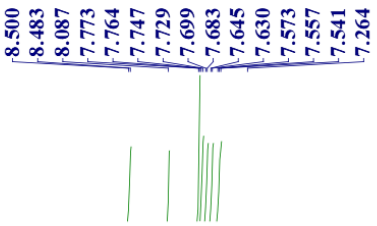
^{19}F NMR (471 MHz, $CDCl_3$)

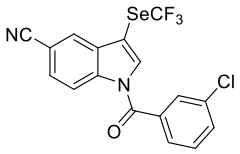


3t

^{13}C NMR (126 MHz, $CDCl_3$)

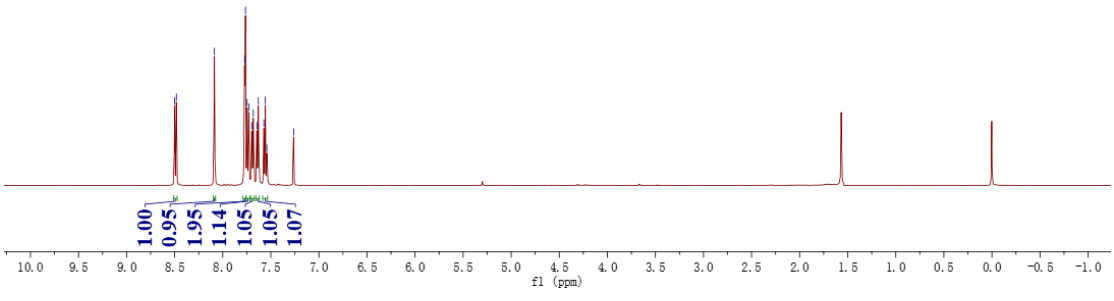


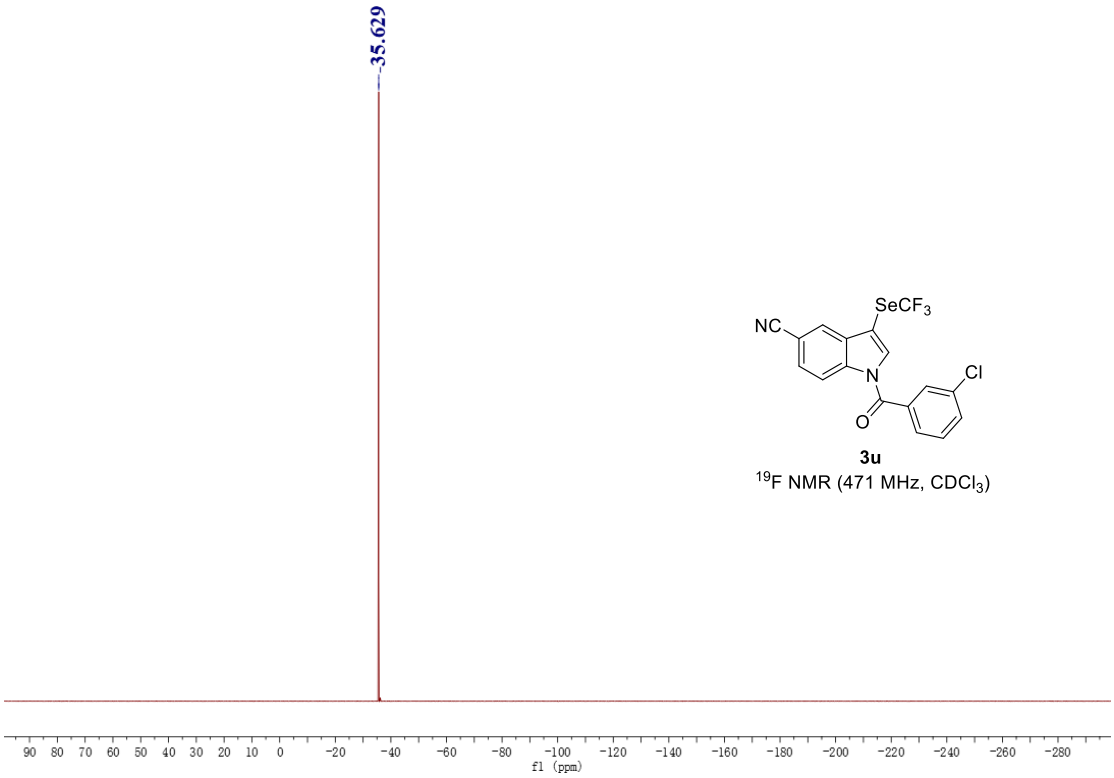




3u

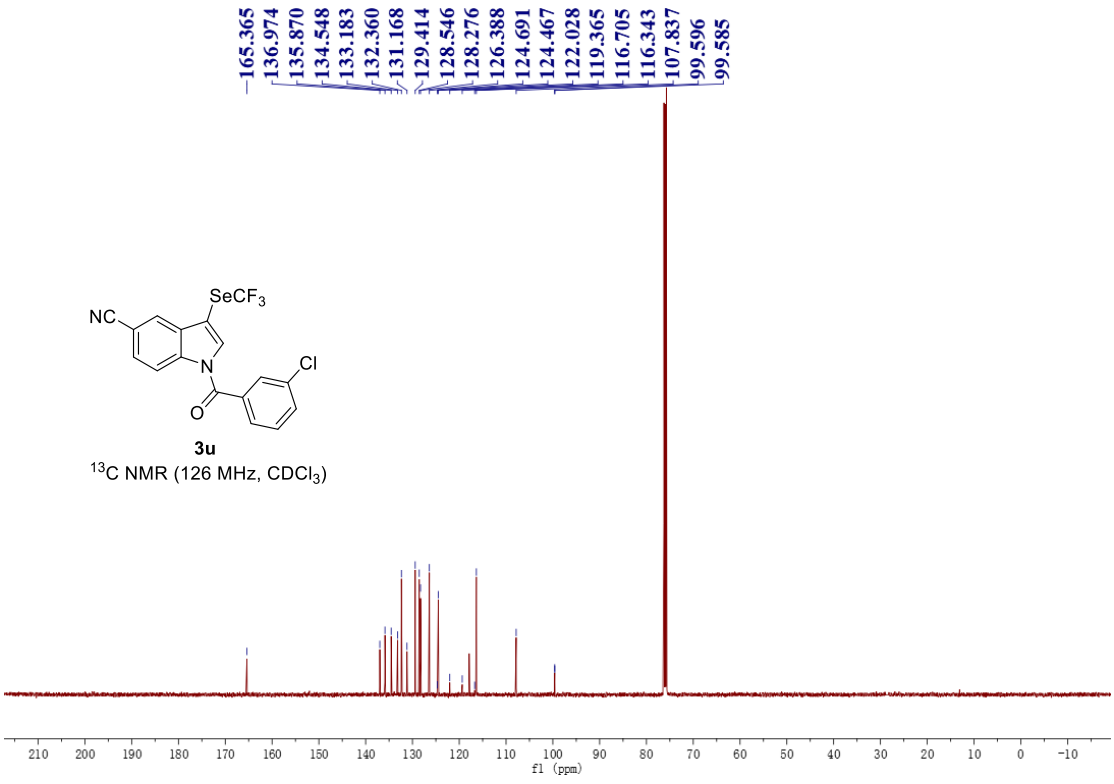
^{1}H NMR (500 MHz, $CDCl_3$)





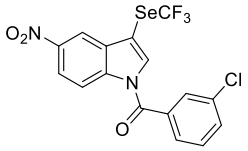
3u

^{19}F NMR (471 MHz, $CDCl_3$)



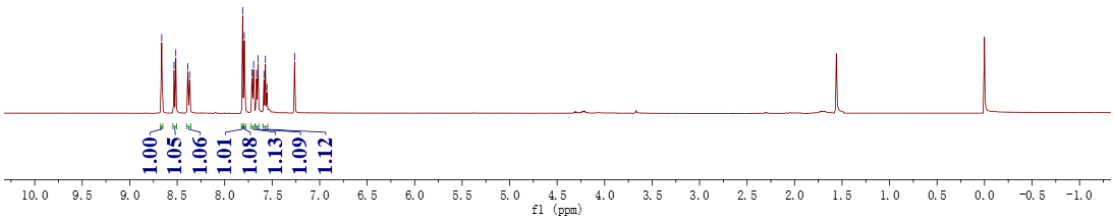
3u

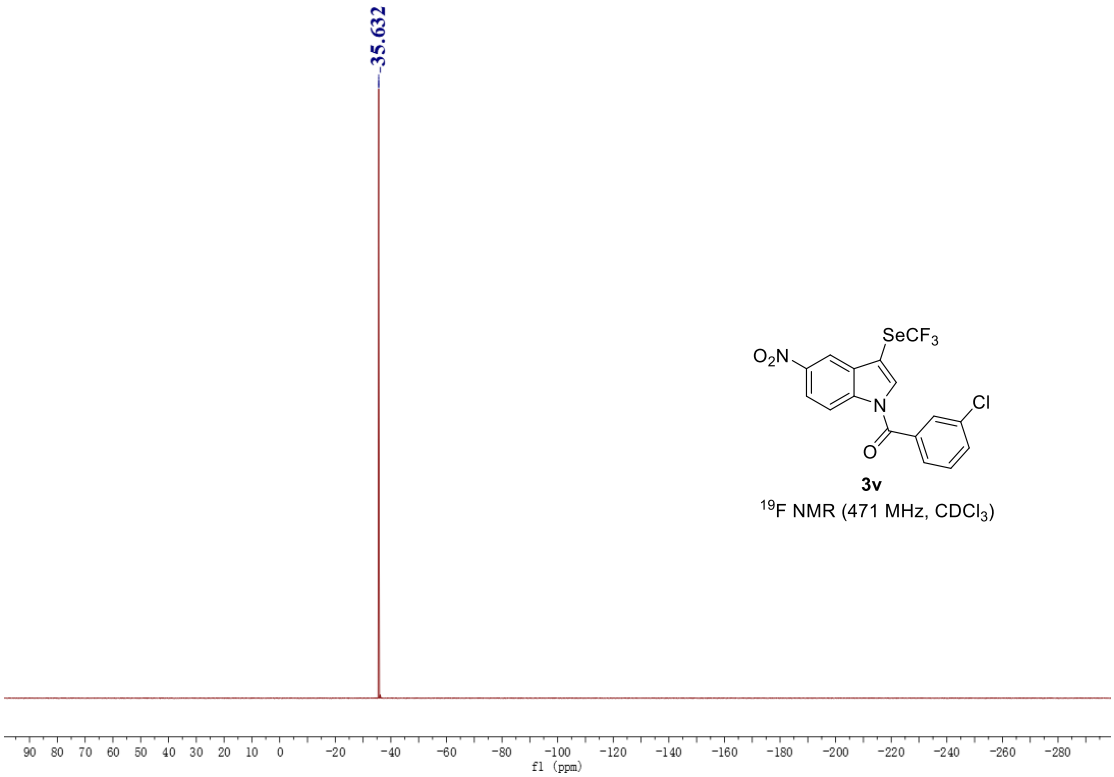
^{13}C NMR (126 MHz, $CDCl_3$)



3v

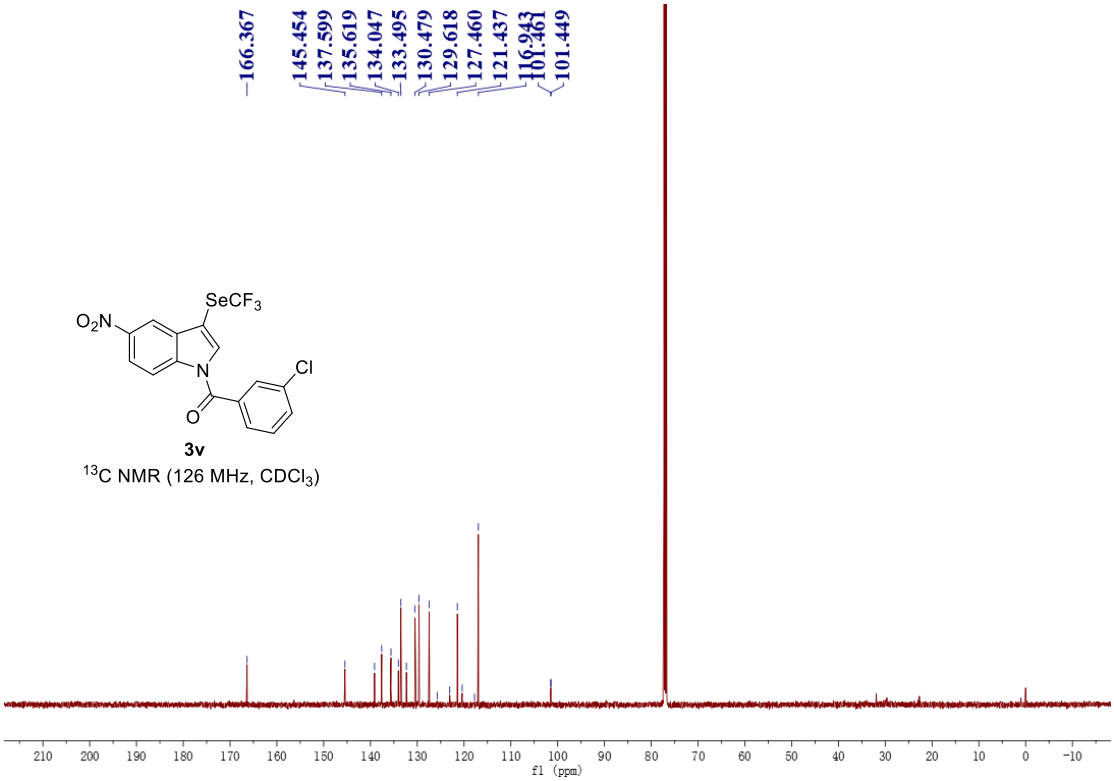
^{1}H NMR (500 MHz, $CDCl_3$)





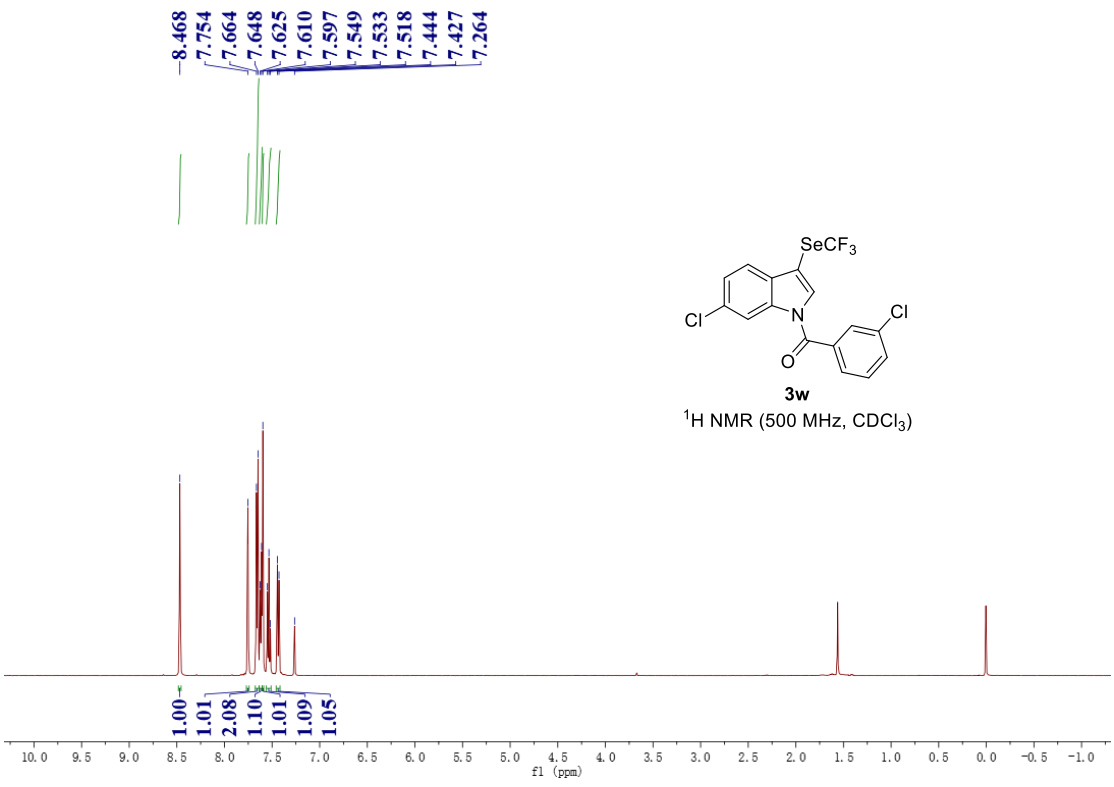
3v

^{19}F NMR (471 MHz, $CDCl_3$)



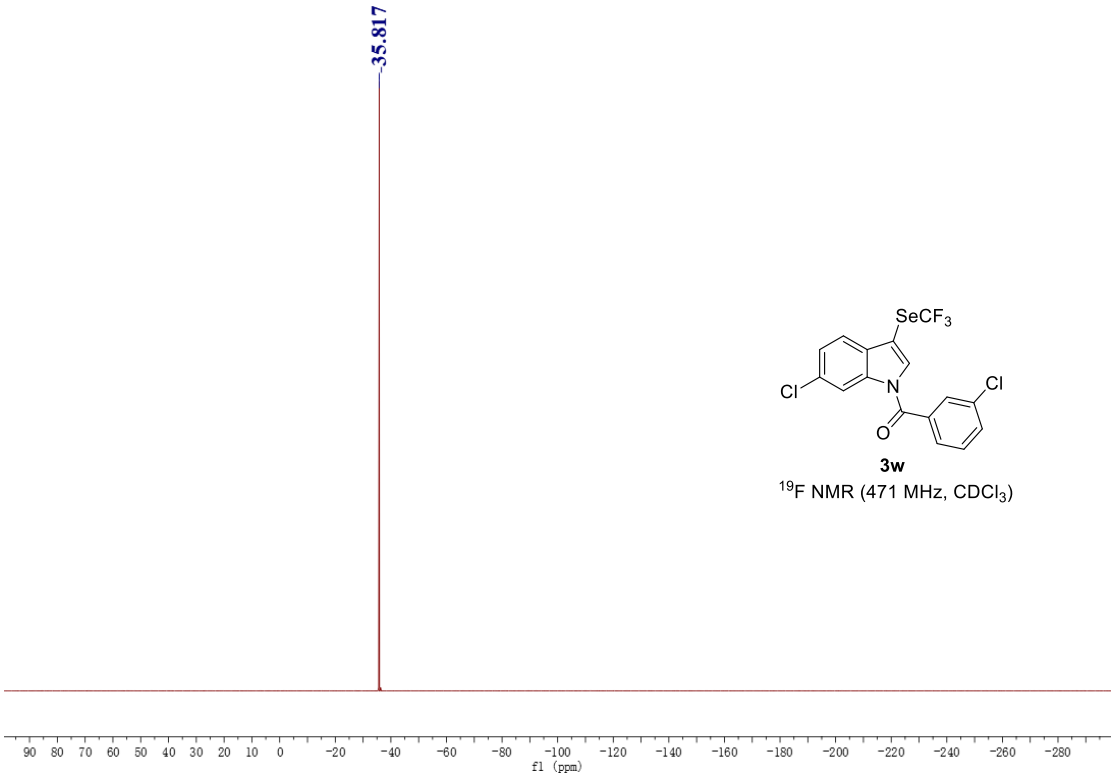
3v

^{13}C NMR (126 MHz, $CDCl_3$)



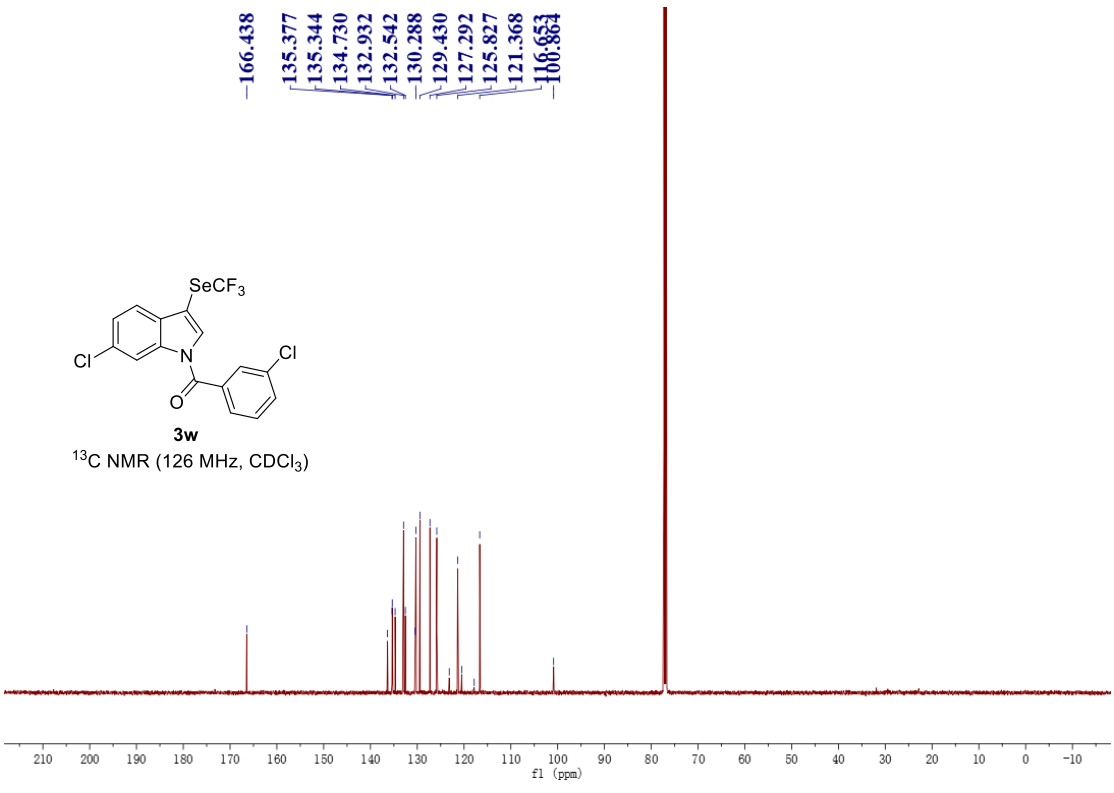
3w

^{1}H NMR (500 MHz, $CDCl_3$)



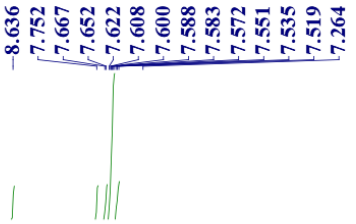
3w

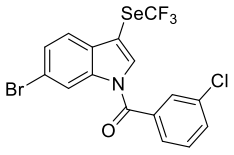
^{19}F NMR (471 MHz, $CDCl_3$)



3w

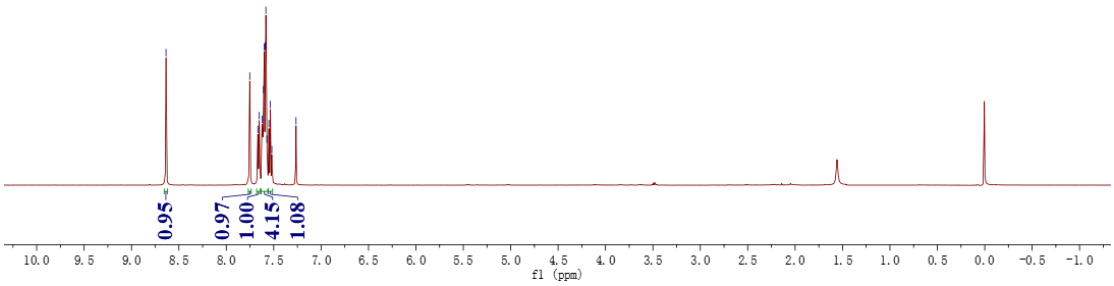
^{13}C NMR (126 MHz, $CDCl_3$)

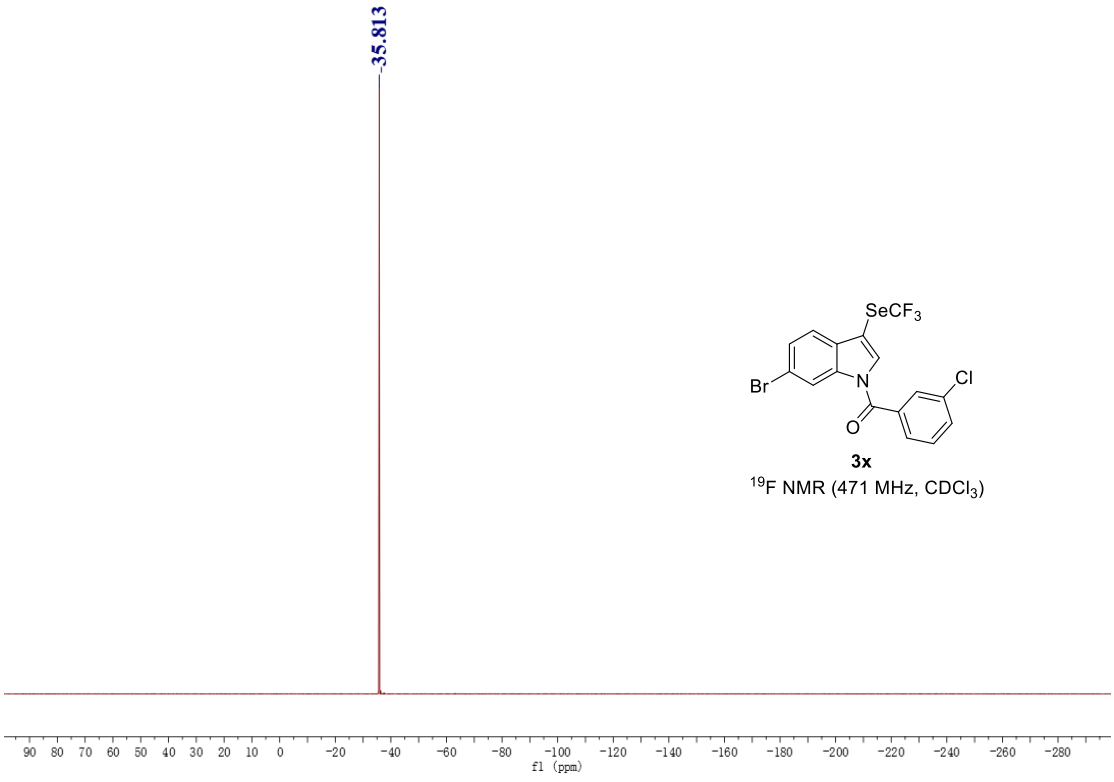




3x

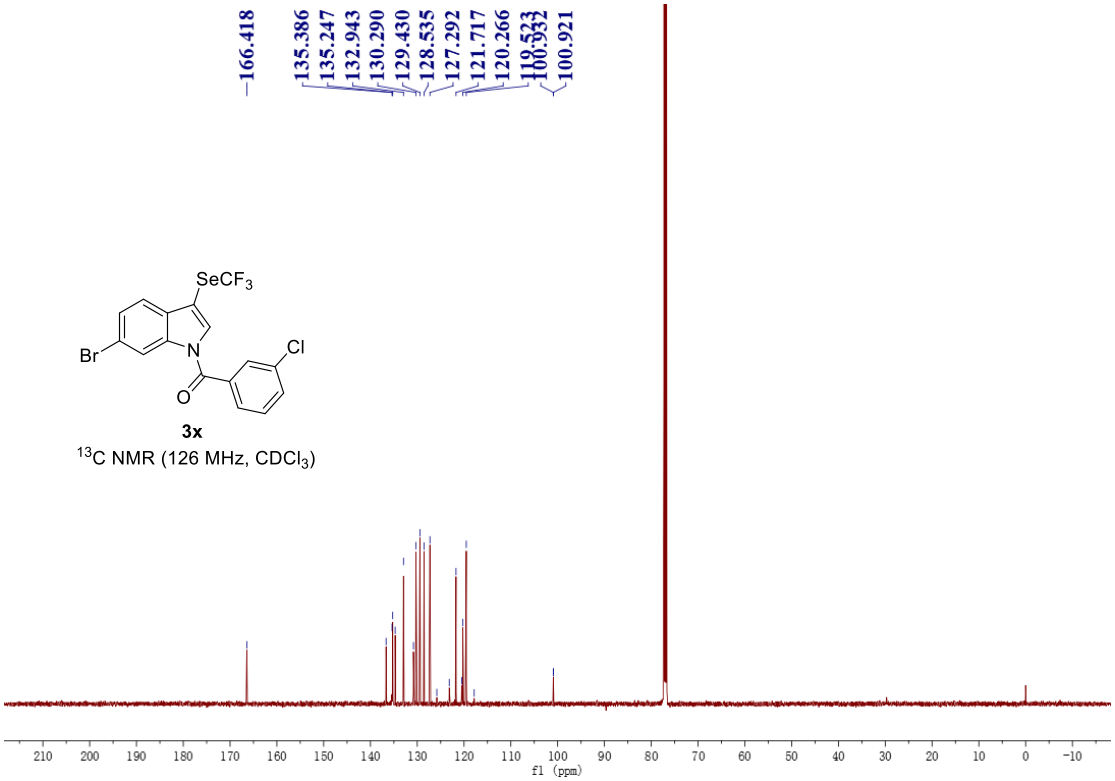
^{1}H NMR (500 MHz, $CDCl_3$)





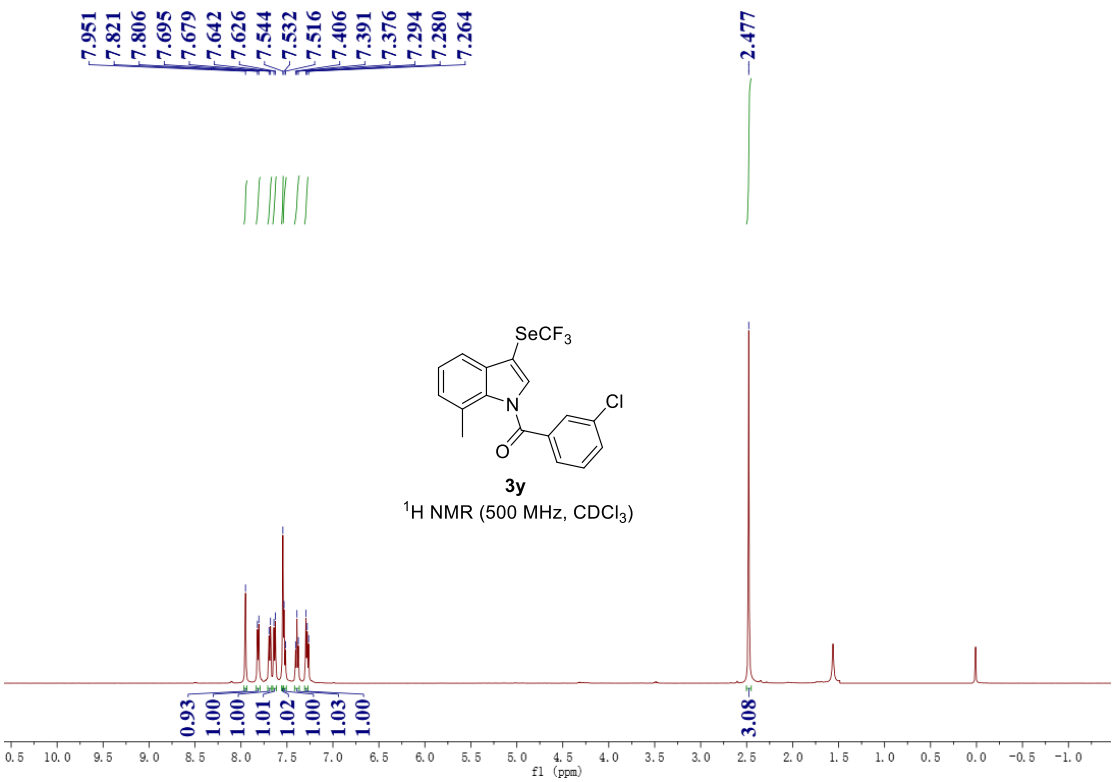
3x

^{19}F NMR (471 MHz, $CDCl_3$)



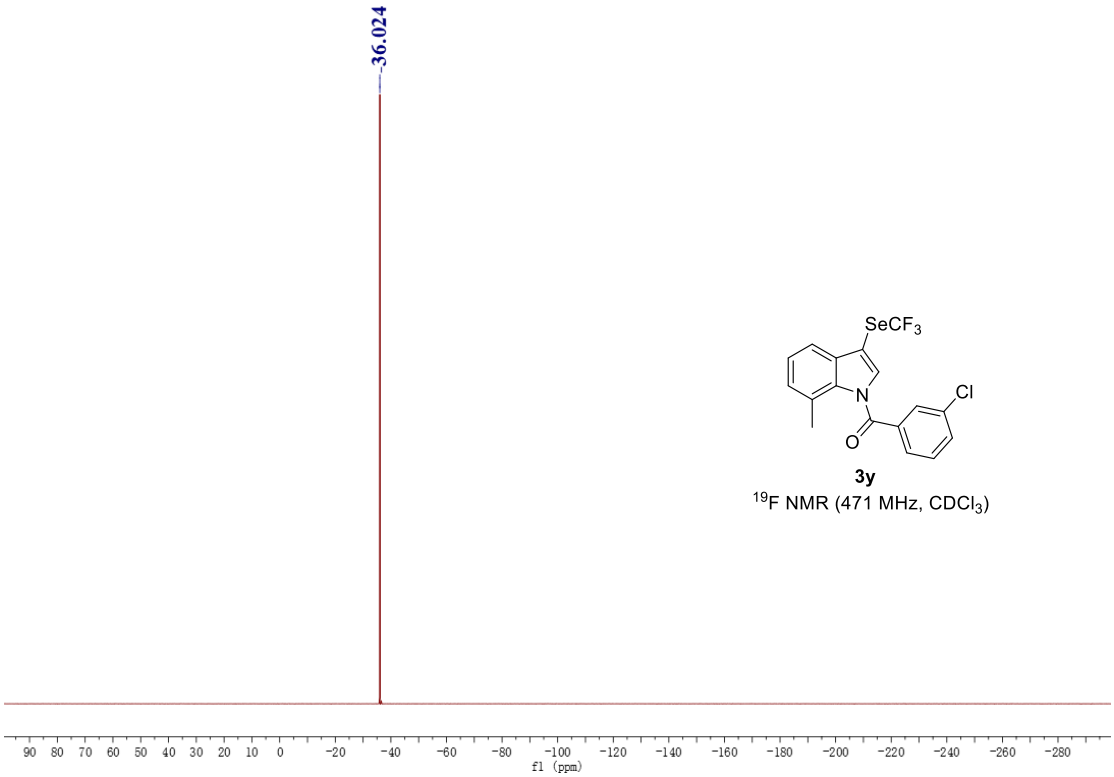
3x

^{13}C NMR (126 MHz, $CDCl_3$)



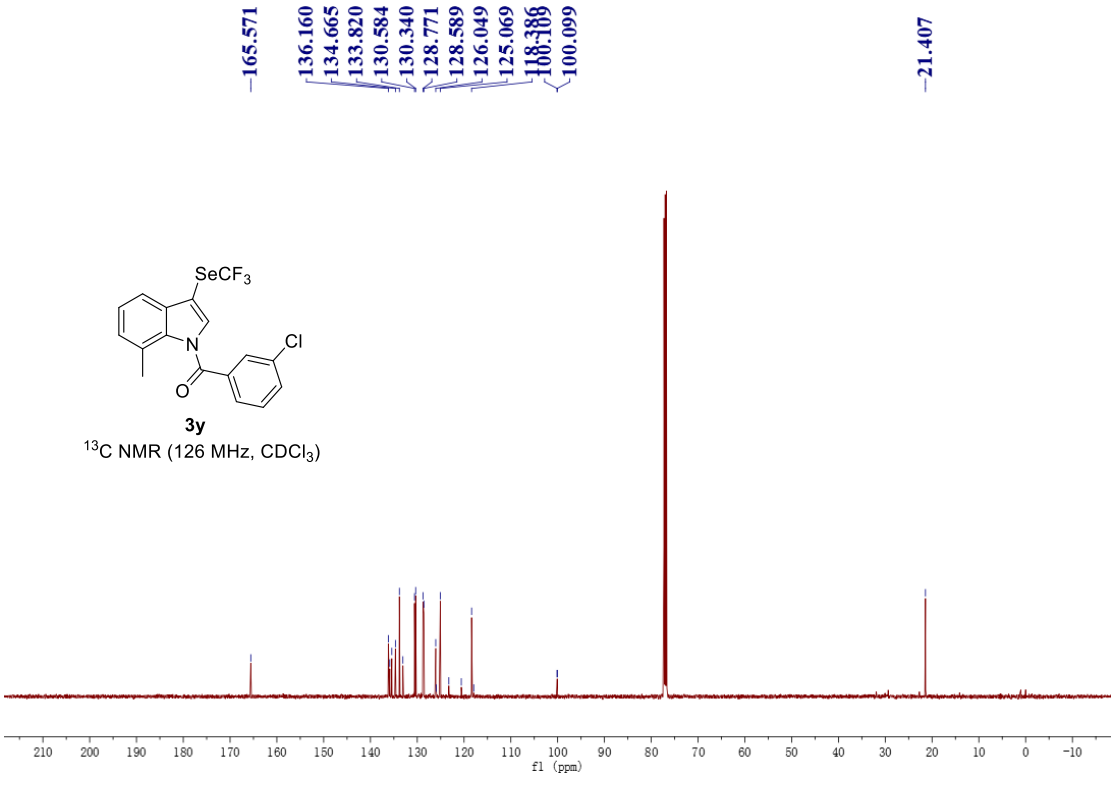
3y

^{1}H NMR (500 MHz, $CDCl_3$)



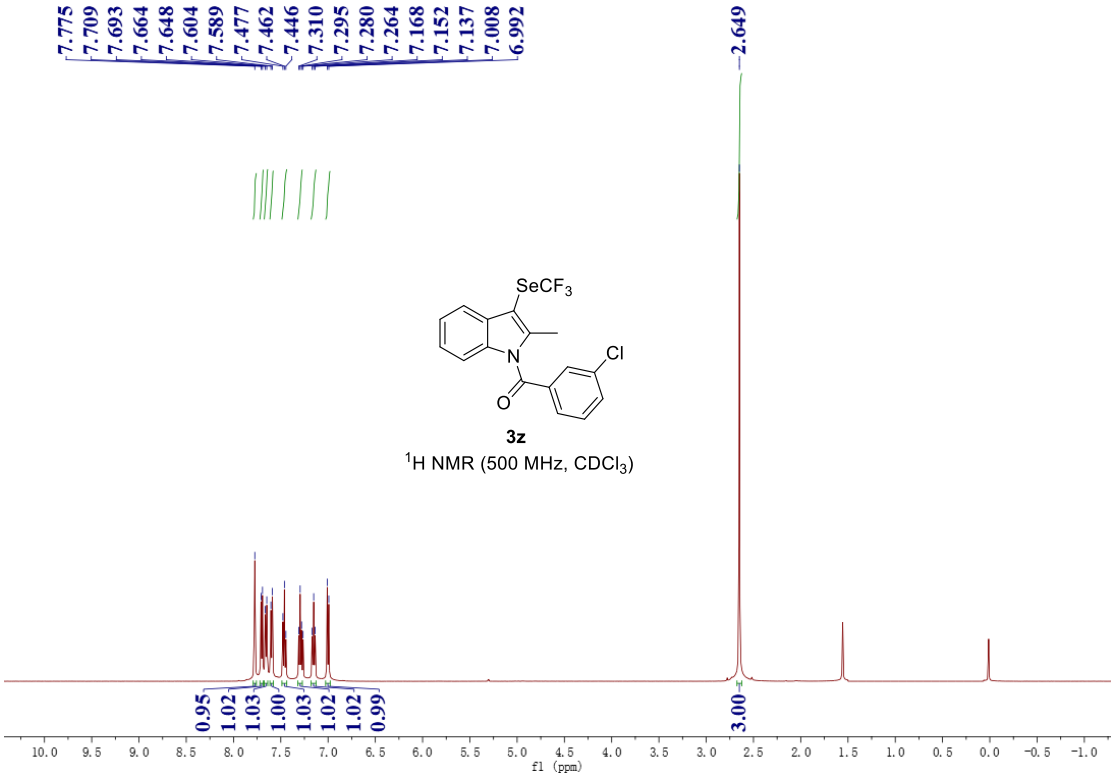
3y

^{19}F NMR (471 MHz, $CDCl_3$)



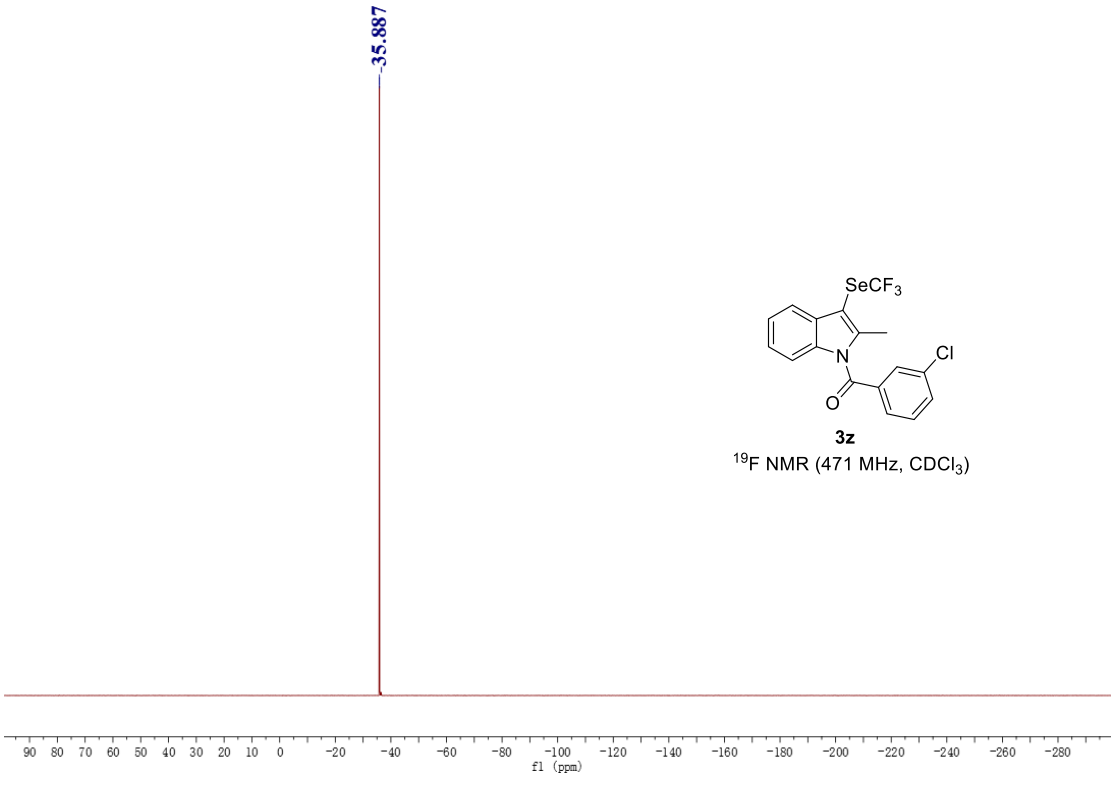
3y

^{13}C NMR (126 MHz, $CDCl_3$)



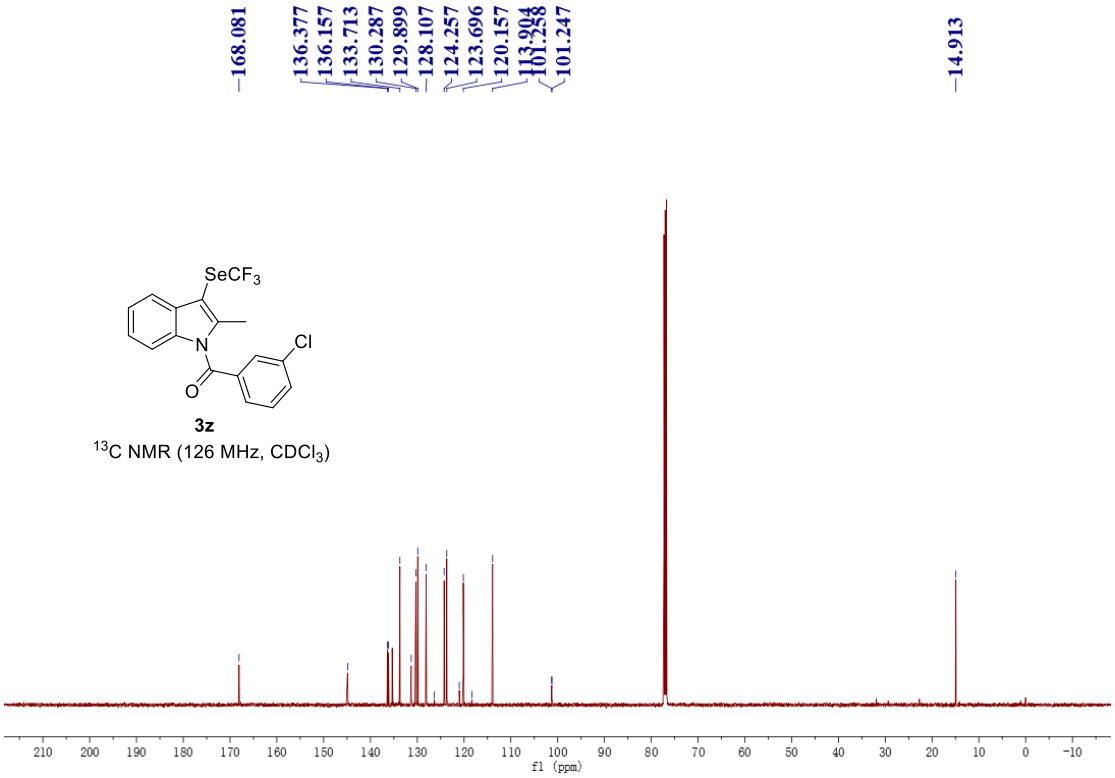
3z

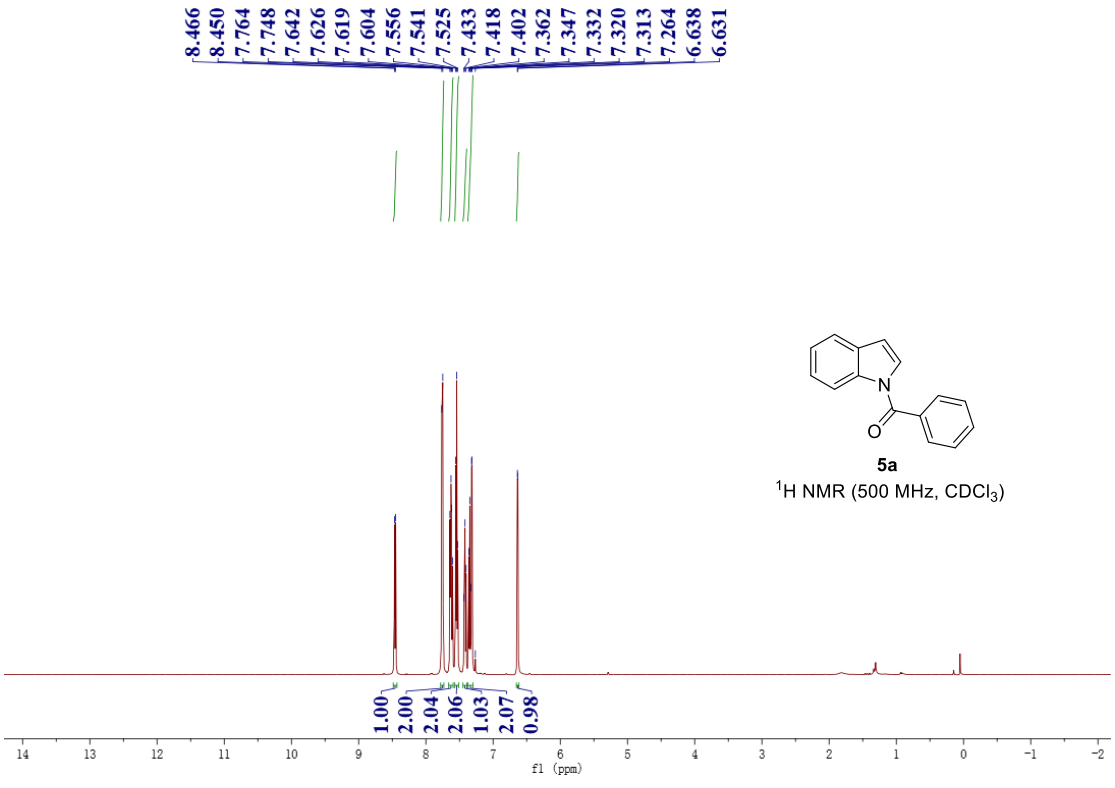
^{1}H NMR (500 MHz, $CDCl_3$)

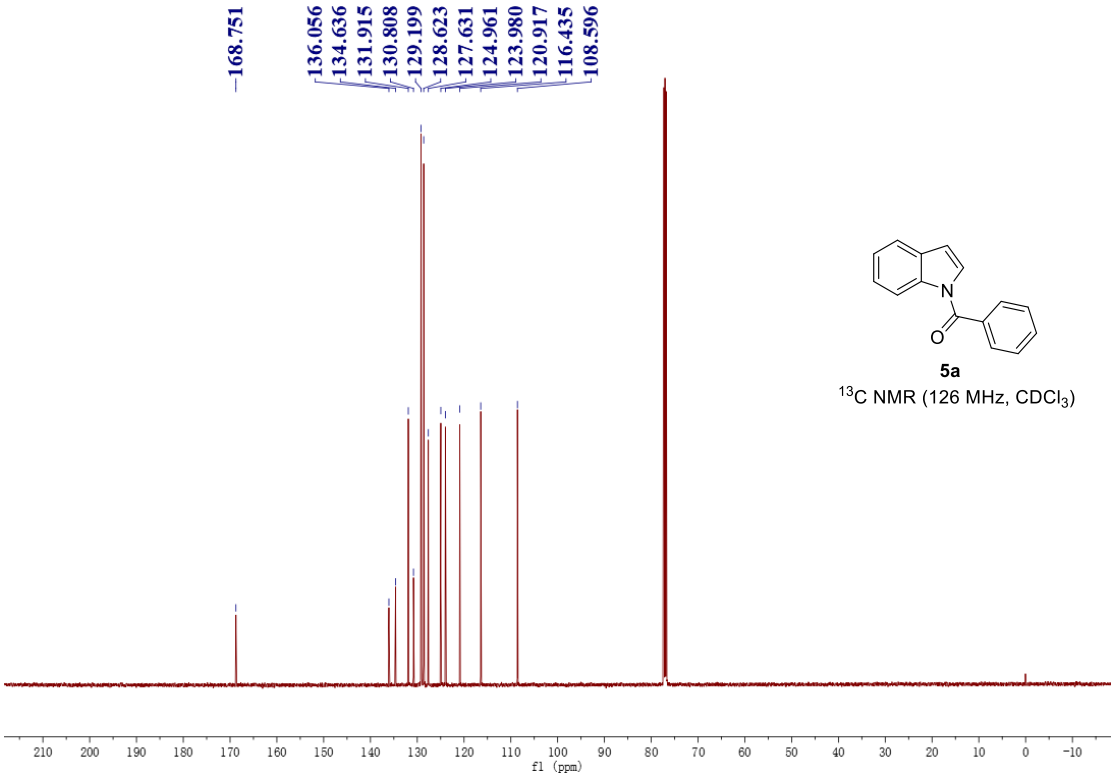


3z

^{19}F NMR (471 MHz, $CDCl_3$)

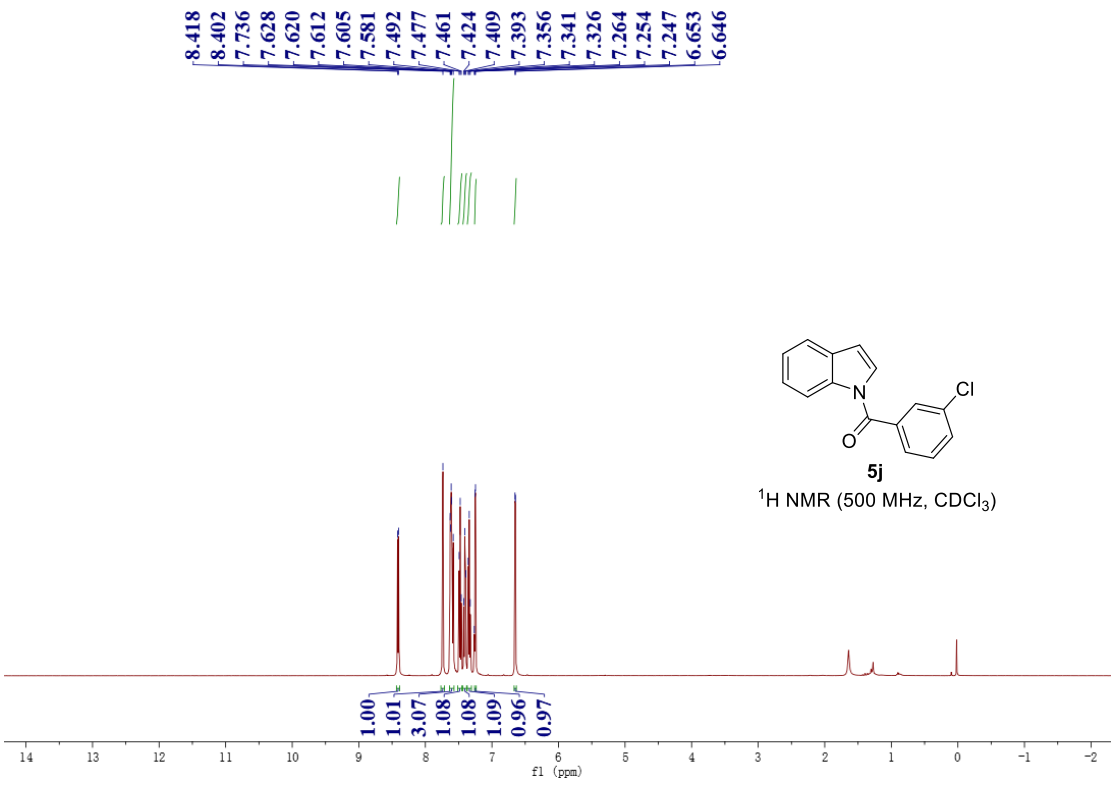

168.081
136.377
136.157
133.713
130.287
129.899
128.107
124.257
123.696
120.157
113.904
101.258
101.247
14.913
SeCF3
N
Cl
O
3z
13C NMR (126 MHz, CDCl3)
f1 (ppm)


8.466
8.450
7.764
7.748
7.642
7.626
7.619
7.604
7.556
7.541
7.525
7.433
7.418
7.402
7.362
7.347
7.332
7.320
7.313
7.264
6.638
6.631
1.00
2.00
2.04
2.06
1.03
2.07
0.98
N
O
5a
1H NMR (500 MHz, CDCl3)
f1 (ppm)



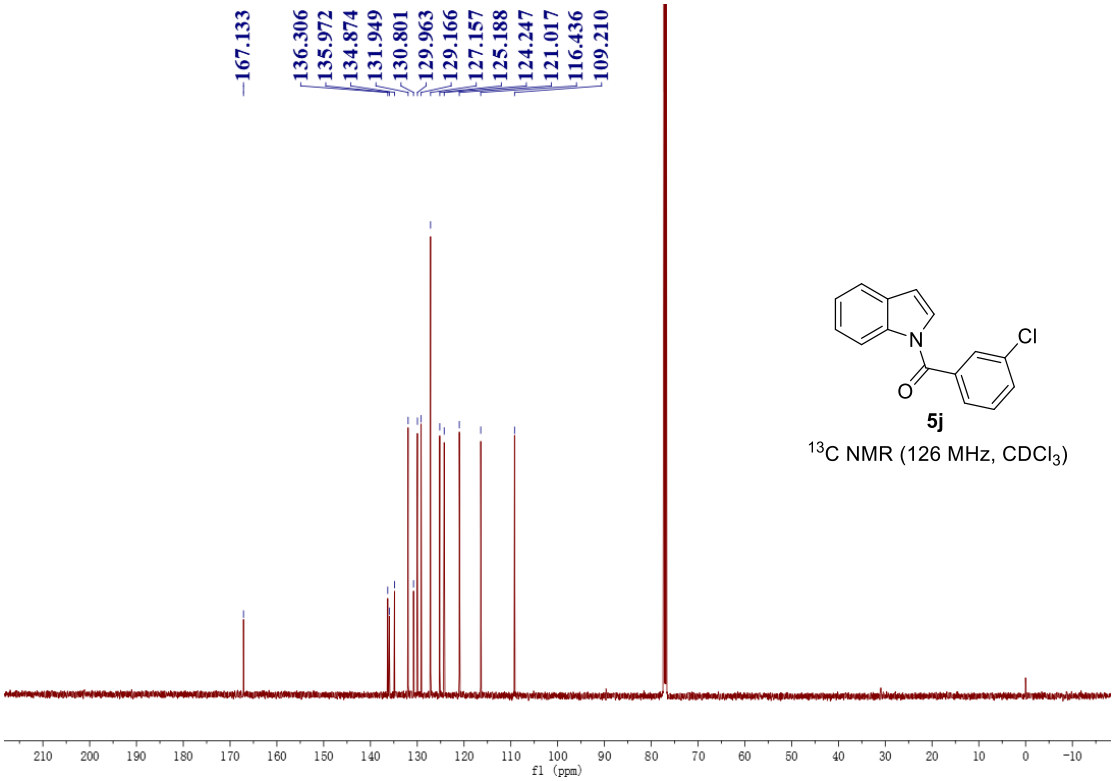
5a

^{13}C NMR (126 MHz, $CDCl_3$)



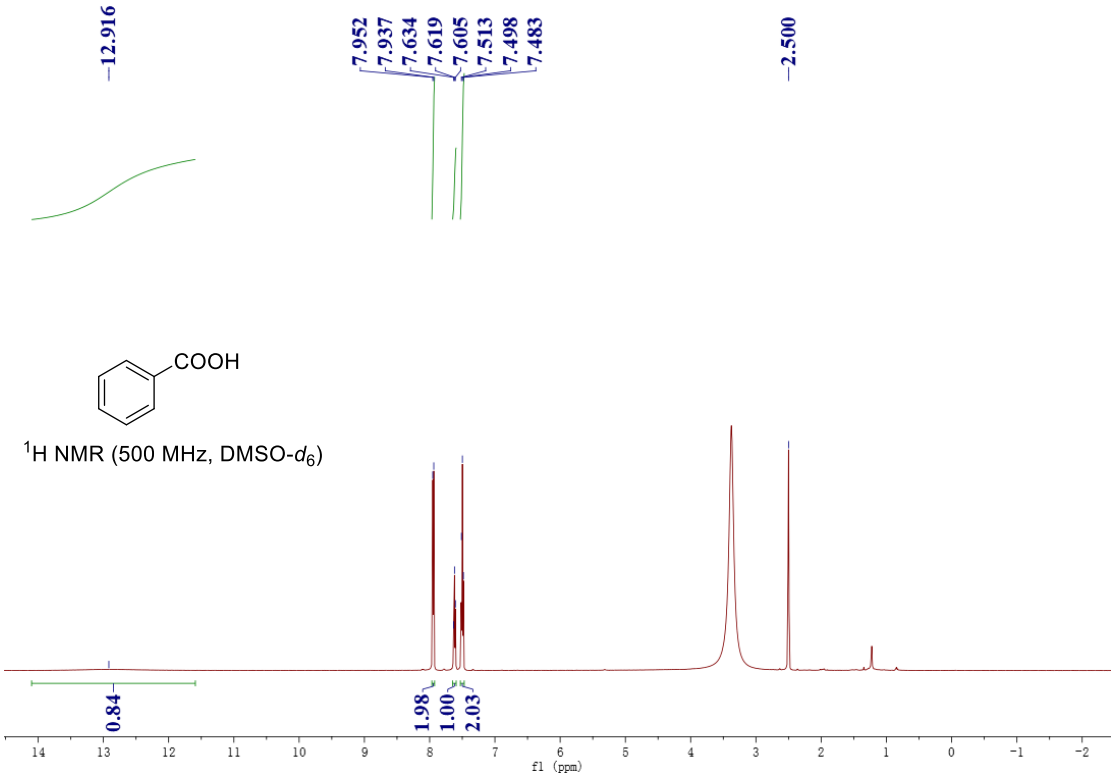
5j

^{1}H NMR (500 MHz, $CDCl_3$)

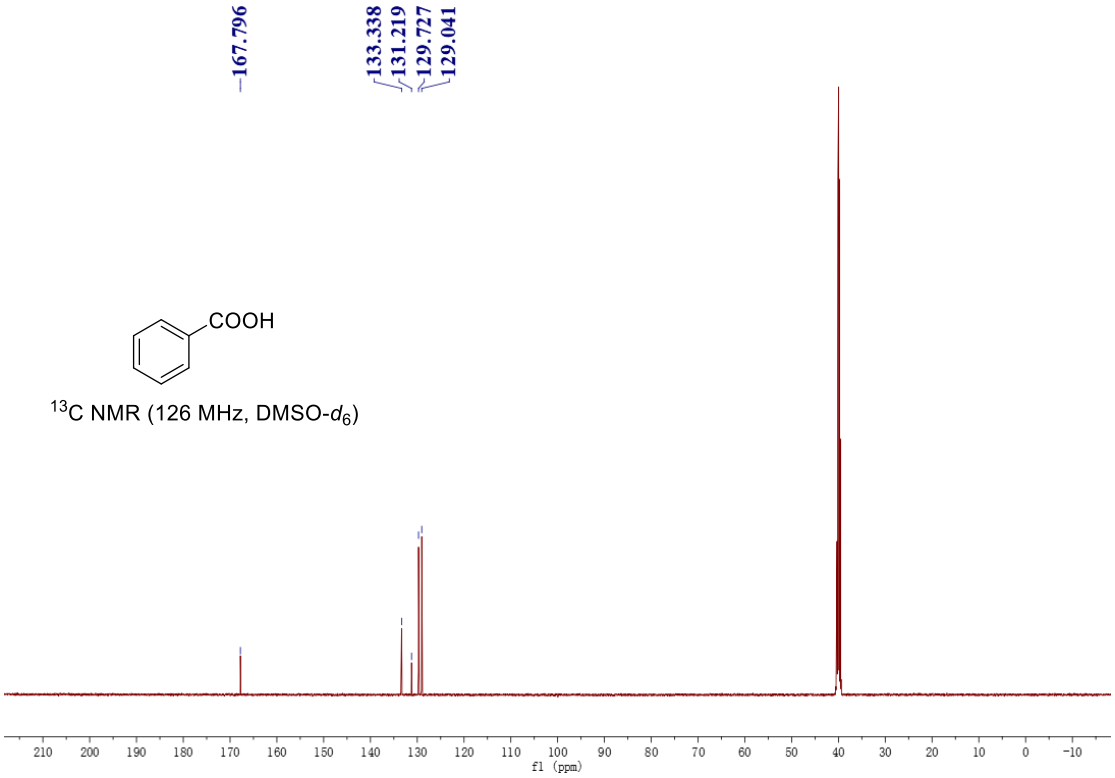


5j

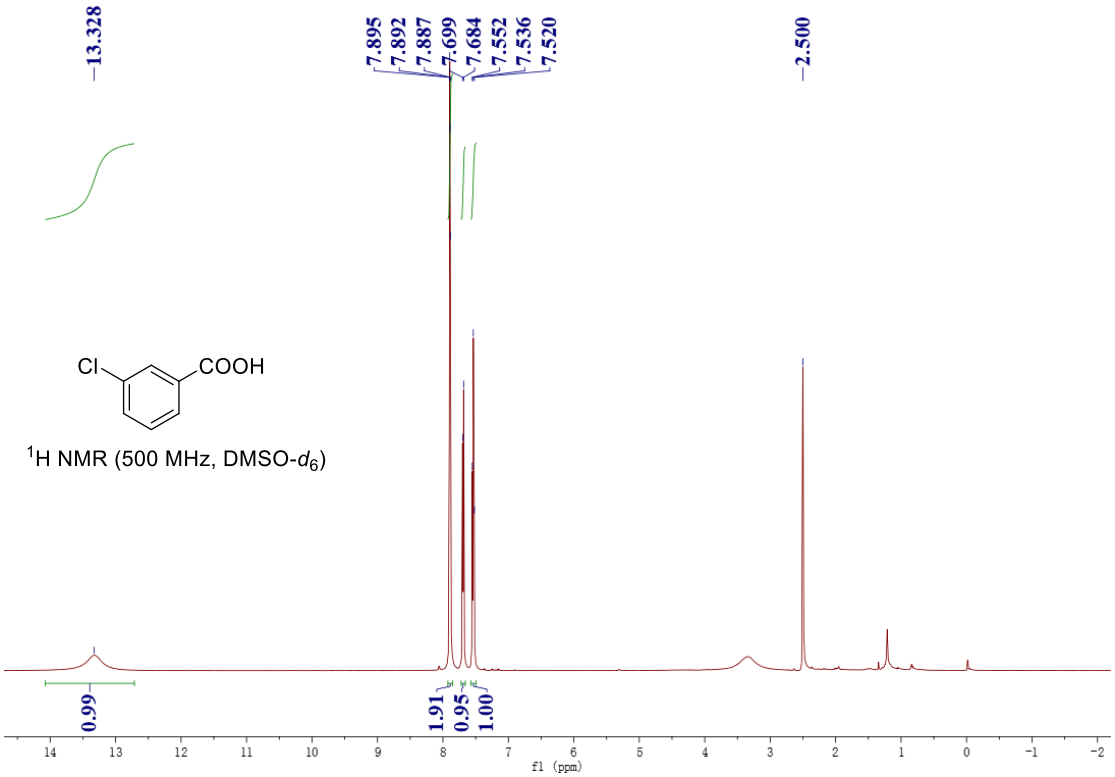
^{13}C NMR (126 MHz, $CDCl_3$)



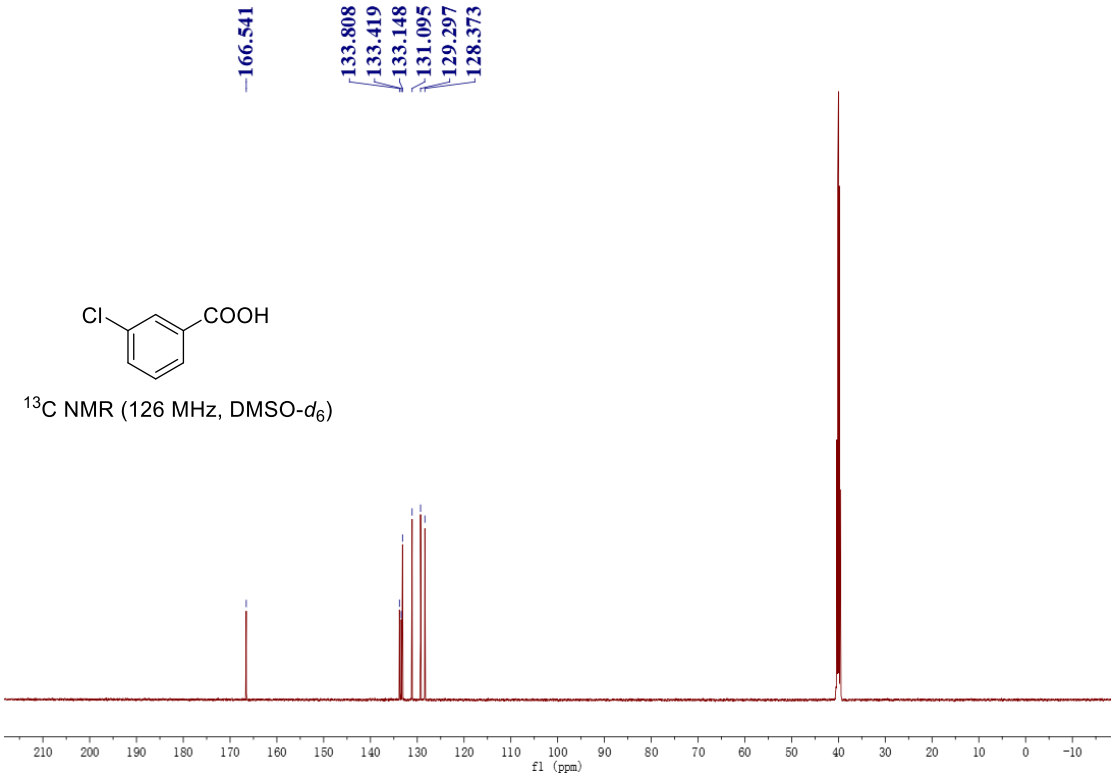
^{1}H NMR (500 MHz, DMSO-d_6)



^{13}C NMR (126 MHz, DMSO-d_6)



^{1}H NMR (500 MHz, DMSO-d_6)



^{13}C NMR (126 MHz, DMSO-d_6)