**Supporting Information**

Synthesis, Bioactivity and Preliminary Mechanism of Action of Novel Trifluoromethyl Pyrimidine Derivatives

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Abbreviation

|  |  |  |
| --- | --- | --- |
|  | abbreviation | full name |
| 1 | 1H NMR | 1H nuclear magnetic resonance |
| 2 | 13C NMR | 13C nuclear magnetic resonance |
| 3 | 19F NMR | 19F nuclear magnetic resonance |
| 4 | HRMS | High-resolution mass spectroscopy |
| 5 | TMV | tobacco mosaic virus |
| 6 | MST | Microscale thermophoresis |
| 7 | *AB* | *Alternaria brassicae* |
| 8 | *FF* | *Fusarium fujikuroi* |
| 9 | *FO* | *Fusarium oxysporum f.sp.cucumerinum* |
| 10 | *CT* | *Colletotrichum truncatum* |
| 11 | *PC* | *Phytophthora capsici* |
| 12 | *CG* | *Colletotrichum gloeosporioides* |
| 13 | *RS* | *Rhizoctonia solani* |
| 14 | *FG* | *Fusarium graminearum* |
| 15 | *PS* | *Phytophthora soja* |
| 16 | *PP* | *Phytophthora* *palmivora* |
| 17 | *BC* | *Botrytis cinerea* |
| 18 | *PL* | *Phytophthora litchii* |
| 19 | DMSO | Dimethylsulfoxide |
| 20 | DMF | *N*,*N*-dimethylformamide |
| 21 | TLC | Thin Layer Chromatography |
| 22 | m.p. | Melting point |
| 23 | EC50 | 50% effective concentration |
| 24 | NB | Nutrient broth |
| 25 | OD | Optical density |
| 26 | PDA | Potato dextrose agar |
| 27 | TC | Thiodiazole-copper |
| 28 | BT | Bismerthiazol |
| 29 | SEM | Scanning electron microscope |

**Chemical synthesis**

***General Procedures for Preparing Target Compounds 5a–5v***

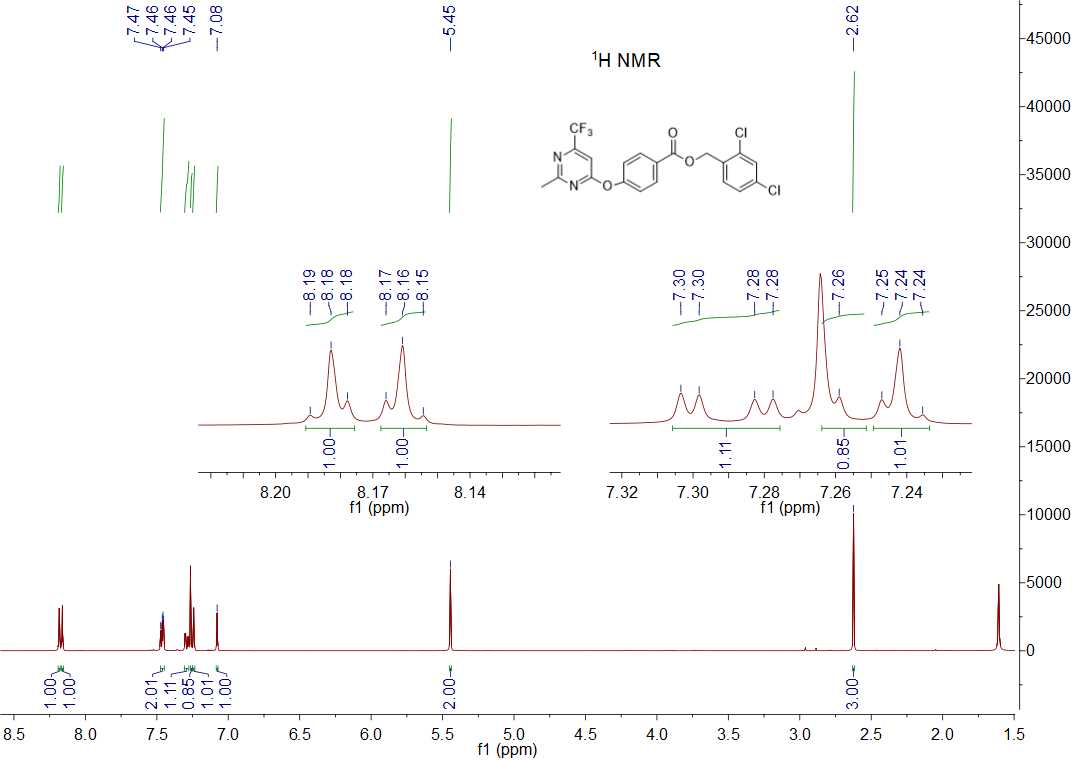
Intermediates **4** (1.69mmol), K2CO3 (2.30mmol) and DMF (20mL) were added to a 50mL round-bottom flask and stirred in ice bath for 30min, then DMF-dissolved chloride (1.53mmol) was added drop by drop for 6-8h reaction at room temperature, The reaction was monitored using TLC. Once the reaction was complete, the reaction solution was dumped into 30mL water and extracted with ethyl acetate for 3 times. The organic layer was combined and the solvent was removed by decompression to obtain the crude product. The crude product was purified using column chromatography (*V/V*, ethyl acetate: petroleum ether = 15:1 to 8:1) to obtain compounds **5a-5v** with a yield of 42% ~ 85%.

Crystal data of partly of the target compound **5d** and **5f**

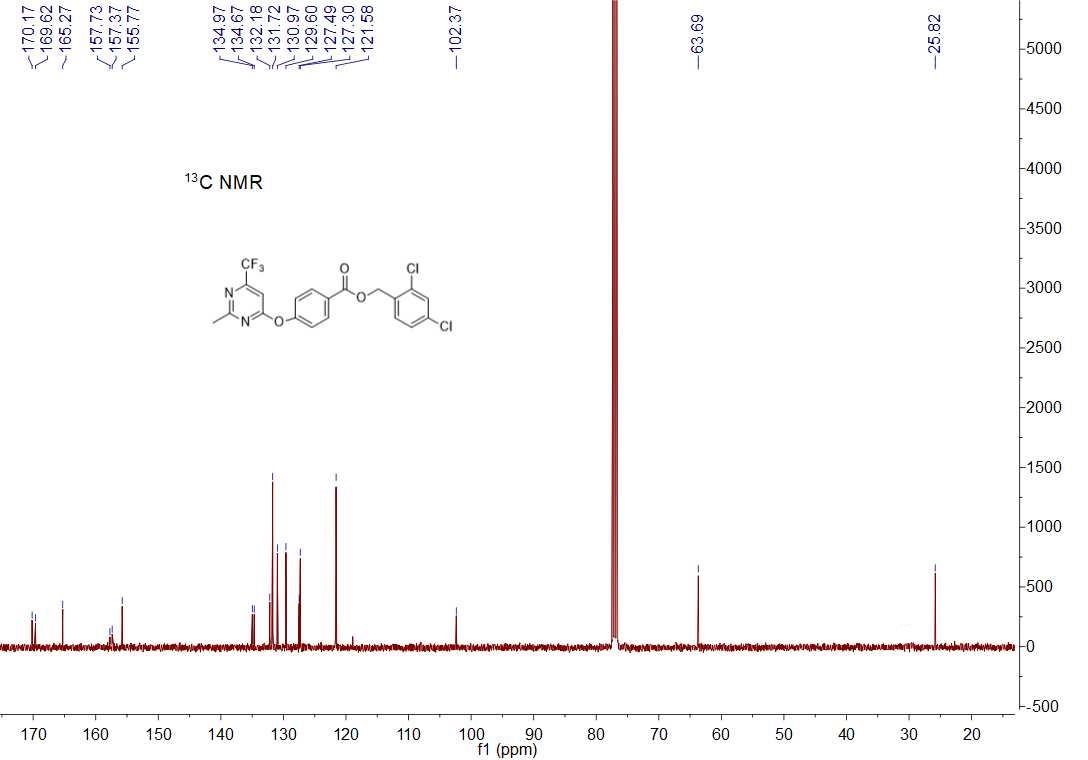
|  |  |  |
| --- | --- | --- |
| compound | **5d** | **5f** |
| Empirical formula | C20H14N2O3F3Cl | C20H13N2O3F4Cl |
| Formula weight | 422.78 | 440.77 |
| Temperature/K | 293(2) | 298.15 |
| Crystal system | monoclinic | monoclinic |
| Space group | C2/c | C2/c |
| a/Å | 33.696(3) | 29.278(3) |
| b/Å | 8.3255(8) | 9.6715(8) |
| c/Å | 16.0615(15) | 15.1518(14) |
| α/° | 90 | 90 |
| β/° | 112.950(5) | 111.425(5) |
| γ/° | 90 | 90 |
| Volume/Å3 | 4149.1(7) | 3993.9(6) |
| Z | 8 | 8 |
| ρcalcg/cm3 | 1.354 | 1.466 |
| μ/mm‑1 | 0.233 | 0.252 |
| F(000) | 1728.0 | 1792.0 |
| Crystal size/mm3 | 0.42 × 0.17 × 0.08 | 0.4 × 0.18 × 0.07 |
| Radiation | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 5.066 to 50.048 | 5.016 to 50.04 |
| Index ranges | -19 ≤ h ≤ 40, -9 ≤ k ≤ 9, -18 ≤ l ≤ 19 | -30 ≤ h ≤ 34, -11 ≤ k ≤ 11, -17 ≤ l ≤ 18 |
| Reflections collected | 9887 | 9466 |
| Independent reflections | 3643 [Rint = 0.1318, Rsigma = 0.1115] | 3478 [Rint = 0.0818, Rsigma = 0.0815] |
| Data/restraints/parameters | 3643/0/263 | 3478/354/301 |
| Goodness-of-fit on F2 | 0.897 | 0.886 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0764, wR2 = 0.1597 | R1 = 0.0726, wR2 = 0.1869 |
| Final R indexes [all data] | R1 = 0.2100, wR2 = 0.2142 | R1 = 0.1608, wR2 = 0.2322 |
| Largest diff. peak/hole / e Å-3 | 0.29/-0.27 | 0.35/-0.31 |

**1H NMR, 13C NMR, 19F NMR and HRMS spectrum of the title compounds**

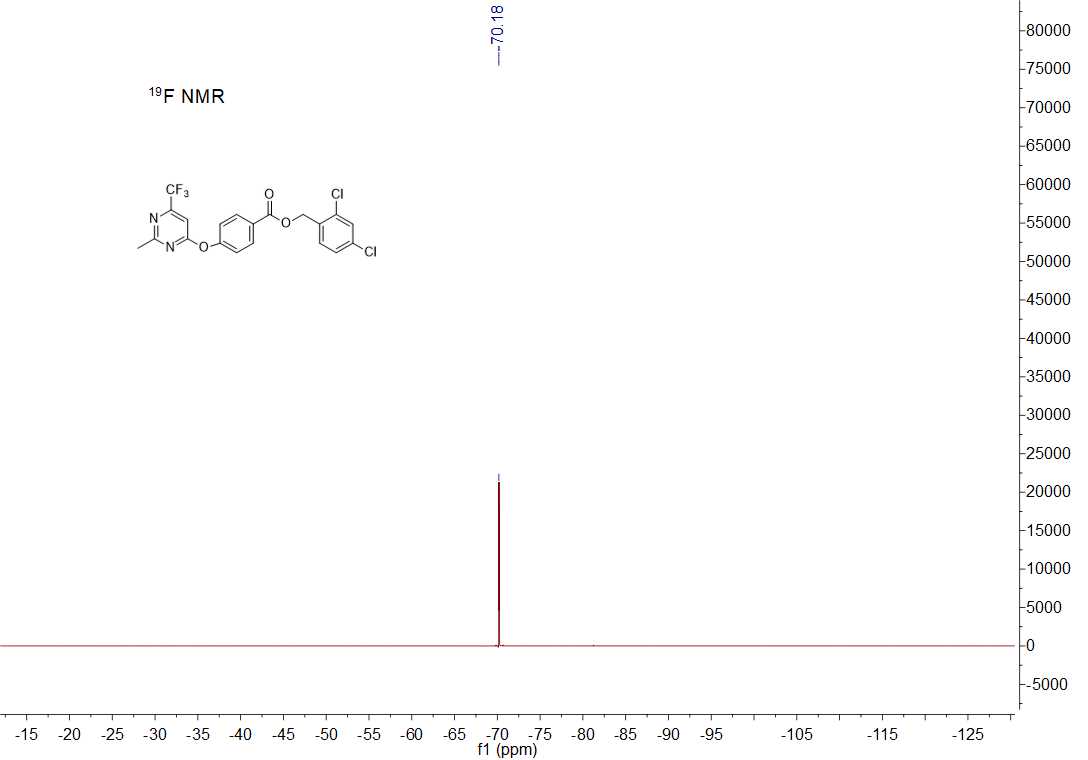
|  |  |
| --- | --- |
|  | **Physical and chemical data** |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.19 – 8.18 (m, 1H, Ph-H), 8.17 – 8.15 (m, 1H, Ph-H), 7.46 (dd, *J* = 5.2, 3.0 Hz, 2H, Ph-H), 7.29 (dd, *J* = 8.3, 2.1 Hz, 1H, Ph-H), 7.26 (s, 1H, Ph-H), 7.25 – 7.23 (m, 1H, Ph-H), 7.08 (s, 1H, Pyr-H), 5.45 (s, 2H, O-CH2-Ph), 2.62 (s, 3H, Pyr-CH3) ;  **13C NMR (101 MHz, CDCl3)** δ 170.17, 169.62, 165.27, 155.77, 134.97, 134.67, 132.18, 131.72, 130.97, 129.60, 127.49, 127.30, 121.58, 102.37, 63.69, 25.82;  **19F NMR (376 MHz, CDCl3)** δ-70.18;  **HRMS** (ESI) [M+H]+ calcd for C20H14O3N2Cl2F3: 457.0328, found: 457.0315; White solid; m.p.: 82.1-83.3. oC; yield, 50%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.19 – 8.14 (m, 2H, Ph-H), 7.49 (td, *J* = 7.5, 1.7 Hz, 1H, Ph-H), 7.36 (tdd, *J* = 7.3, 5.3, 1.8 Hz, 1H, Ph-H), 7.24 (d, *J* = 2.0 Hz, 1H, Ph-H), 7.22 (d, *J* = 2.0 Hz, 1H, Ph-H), 7.18 (td, *J* = 7.5, 1.1 Hz, 1H, Ph-H), 7.12 (ddd, *J* = 9.5, 8.3, 1.0 Hz, 1H, Ph-H), 7.07 (s, 1H, Pyr-H), 5.45 (s, 2H, O-CH2-Ph), 2.62 (s, 3H, Pyr-CH3);  **13C NMR (101 MHz, CDCl3)** δ170.18 , 169.68, 165.46 , 162.41 , 159.93 , 157.71 , 155.66 , 131.72 , 130.76, 130.40 , 127.76 , 124.23 , 122.96 , 121.51 , 115.52, 102.34 , 60.99, 25.82;  **19F NMR (376 MHz, CDCl3)** δ-70.18, -117.79;  **HRMS** (ESI) [M+H]+ calcd for C20H15O3N2F4: 407.1013, found: 407.1003; Yellow oil; yield, 65%. |
|  | **1H NMR (400 MHz, CDCl3)** δ8.18 – 8.16 (m, 1H, Ph-H), 8.16 – 8.14 (m, 1H, Ph-H), 7.35 (d, *J* = 8.0 Hz, 2H, Ph-H), 7.24 – 7.23 (m, 1H, Ph-H), 7.22 – 7.21 (m, 2H, Ph-H), 7.20 (d, *J* = 2.0 Hz, 1H, Ph-H), 7.06 (s, 1H, Pyr-H), 5.34 (s, 2H, O-CH2-Ph), 2.62 (s, 3H, Ph-CH3), 2.37 (s, 3H, Pyr-CH3);  **13C NMR (101 MHz, CDCl3)** δ170.18 , 169.71 , 165.61 , 157.35 , 155.56 , 138.30, 132.85, 131.67, 129.34, 128.50 , 128.04, 121.45, 102.35, 102.32, 66.95, 25.82, 21.26;  **19F NMR (376 MHz, CDCl3)** δ-70.18;  **HRMS** (ESI) [M+H]+ calcd for C21H18O3N2F3: 403.1264, found: 403.1257; White solid; m.p.: 47.3-48.9 oC; yield, 54%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.21 – 8.19 (m, 1H, Ph-H), 8.19 – 8.17 (m, 1H, Ph-H), 7.54 – 7.50 (m, 1H, Ph-H), 7.46 – 7.41 (m, 1H, Ph-H), 7.34 – 7.29 (m, 2H, Ph-H), 7.26 (d, *J* = 2.0 Hz, 1H, Ph-H), 7.24 (d, *J* = 2.0 Hz, 1H, Ph-H), 7.08 (s, 1H, Pyr-H), 5.49 (s, 2H, O-CH2-Ph), 2.62 (s, 3H, Pyr-CH3);  **13C NMR (101 MHz, CDCl3)** δ170.19, 169.67, 165.39, 157.35, 155.68, 133.96, 133.54, 131.75, 130.10, 129.73 , 127.73, 126.99, 121.56, 102.40, 64.3, 25.85;  **19F NMR (376 MHz, CDCl3)** δ -70.17;  **HRMS** (ESI) [M+H]+ calcd for C20H15O3N2ClF3: 423.0717, found: 423.0701; Brown solid; m.p.: 77.8-79.7 oC; yield, 67%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.29 – 8.27 (m, 1H, Ph-H), 8.26 – 8.25 (m, 1H, Ph-H), 8.20 (d, *J* = 2.0 Hz, 1H, Ph-H), 8.19 – 8.17 (m, 1H, Ph-H), 7.64 (s, 1H, Ph-H), 7.62 (s, 1H, Ph-H), 7.29 (d, *J* = 2.0 Hz, 1H, Ph-H), 7.27 (d, *J* = 2.1 Hz, 1H, Ph-H), 7.09 (s, 1H, Pyr-H), 5.48 (s, 2H, O-CH2-Ph), 2.63 (s, 3H, Pyr-CH3);  **13C NMR (101 MHz, CDCl3)** δ170.17, 169.60, 165.24, 157.78, 155.95, 147.82, 143.13, 131.73 , 128.48, 127.21, 123.94, 121.69, 102.43, 65.42, 25.83;  **19F NMR (376 MHz, CDCl3)** δ -70.18;  **HRMS** (ESI) [M+H]+ calcd for C20H15O5N3F3: 434.0958, found: 434.0941; Yellow solid; m.p.: 116.4-117.9 oC; yield, 42%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.16 – 8.14 (m, 1H, Ph-H), 8.13 – 8.12 (m, 1H, Ph-H), 7.37 – 7.27 (m, 2H, Ph-H), 7.24 – 7.22 (m, 1H, Ph-H), 7.22 – 7.20 (m, 1H, Ph-H), 7.10 – 7.07 (m, 1H, Ph-H), 7.06 – 7.05 (m, 1H, Pyr-H), 5.54 (s, 2H, O-CH2-Ph), 2.62 (s, 3H, Pyr-CH3);  **13C NMR (101 MHz, CDCl3)** δ170.18, 169.67, 165.39, 163.34, 157.68, 155.63, 136.58, 131.77, 130.95, 127.63, 125.61, 121.50, 118.94, 114.52, 102.37, 57.95, 25.84;  **19F NMR (376 MHz, CDCl3)** δ -70.18, -112.68;  **HRMS** (ESI) [M+H]+ calcd for C20H14O3N2ClF4: 441.0623, found: 441.0608; White solid; m.p.: 73.8-75.0 oC; yield, 45%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.20 – 8.18 (m, 1H, Ph-H), 8.18 – 8.16 (m, 1H, Ph-H), 7.32 (t, *J* = 7.9 Hz, 1H, Ph-H), 7.26 – 7.24 (m, 1H, Ph-H), 7.24 – 7.22 (m, 1H, Ph-H), 7.07 (s, 1H, , Pyr-H), 7.04 (d, *J* = 7.6 Hz, 1H, Ph-H), 7.01 – 6.99 (m, 1H, Ph-H), 6.92 – 6.88 (m, 1H, Ph-H), 5.36 (s, 2H, Ph-O-CH2), 3.84 (s, 3H, Ph-O-CH3), 2.62 (s, 3H, Pry-CH3);  **13C NMR (101 MHz, CDCl3)** δ170.19, 169.69, 165.54, 159.78, 157.69, 155.62, 137.38, 131.71, 129.76, 127.89, 121.51, 120.45, 118.94, 113.88, 113.65, 102.38, 66.81, 55.31, 25.85;  **19F NMR (376 MHz, CDCl3)** δ -70.17;  **HRMS** (ESI) [M+H]+ calcd for C21H18O4N2F3: 419.1213, found: 419.1199; Yellow oil; yield, 50%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.16 – 8.15 (m, 1H, Ph-H), 8.14 – 8.13 (m, 1H, Ph-H), 7.26 – 7.25 (m, 1H, Ph-H), 7.24 – 7.22 (m, 1H, Ph-H), 7.07 (s, 1H, Pyr-H), 3.95 (s, 3H, O-CH3), 2.63 (s, 3H, Pry-CH3);  **13C NMR (101 MHz, CDCl3)** δ170.19 , 169.71, 166.24, 157.69, 155.51, 131.56, 127.95, 121.47, 118.94, 102.33, 52.34, 25.84;  **19F NMR (376 MHz, CDCl3)** δ -70.18;  **HRMS** (ESI) [M+H]+ calcd for C14H12O3N2F3: 313.0794, found: 313.0785; White solid; m.p.: 111.1–112.4 oC; yield, 57%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.52 (d, *J* = 2.2 Hz, 1H, Ph-H), 8.17 – 8.15 (m, 1H, Ph-H), 8.14 – 8.13 (m, 1H, Ph-H), 7.78 (dd, *J* = 8.2, 2.5 Hz, 1H, Ph-H), 7.38 (d, *J* = 8.2 Hz, 1H, Ph-H), 7.26 (d, *J* = 2.0 Hz, 1H, Ph-H), 7.25 – 7.24 (m, 1H, Ph-H), 7.08 (s, 1H, Pyr-H), 5.38 (s, 2H, Ph-O-CH2), 2.62 (s, 3H, Pry-CH3);  **13C NMR (101 MHz, CDCl3)** δ170.17, 169.60, 165.31, 157.74, 155.88, 151.65, 149.74, 139.04, 131.71, 127.22, 124.38, 121.66, 118.92, 102.42, 63.50, 25.84;  **19F NMR (376 MHz, CDCl3)** δ -70.18;  **HRMS** (ESI) [M+H]+ calcd for C19H14O3N3ClF3: 424.0670, found: 424.0653; White solid; m.p.: 98.6–99.4 oC; yield, 49%; |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.19 – 8.17 (m, 1H, Ph-H), 8.17 – 8.15 (m, 1H, Ph-H), 7.26 (d, *J* = 2.0 Hz, 1H, Ph-H), 7.25 – 7.23 (m, 1H, Ph-H), 7.08 (s, 1H, Pyr-H), 6.06 (ddt, *J* = 17.1, 10.5, 5.7 Hz, 1H, Ph-H), 5.44 (dq, *J* = 17.2, 1.5 Hz, 1H, Ph-H), 5.32 (ddd, *J* = 10.5, 2.5, 1.2 Hz, 1H, Ph-H), 4.86 (t, *J* = 1.4 Hz, 1H, O-CH2), 4.85 (t, *J* = 1.4 Hz, 1H, O-CH2), 2.63 (s, 3H, Pyr-CH3);  **13C NMR (101 MHz, CDCl3)** δ170.19, 169.70, 165.40, 157.69, 155.57, 132.07, 131.63, 127.95, 121.49, 118.94, 118.54, 102.37, 65.81, 25.85;  **19F NMR (376 MHz, CDCl3)** δ -70.18;  **HRMS** (ESI) [M+H]+ calcd for C16H14O3N2F3: 339.0951, found: 339.0943; Yellow oil; yield, 41%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.16 – 8.14 (m, 1H, Ph-H), 8.13 (d, *J* = 2.1 Hz, 1H, Ph-H), 7.63 (s, 1H, Thia-H), 7.27 (d, *J* = 2.5 Hz, 1H, Ph-H), 7.25 – 7.24 (m, 1H, Ph-H), 7.08 (s, 1H, Pyr-H), 5.46 (s, 2H, O-CH2), 2.62 (s, 3H, Pyr-CH3);  **13C NMR (101 MHz, CDCl3)** δ170.17, 169.59, 165.36, 157.39, 155.99, 153.86, 141.90, 134.69, 131.78, 126.94, 121.68, 102.42, 58.57, 25.84;  **19F NMR (376 MHz, CDCl3)** δ -70.18;  **HRMS** (ESI) [M+H]+ calcd for C17H11O7NF3S: 430.0202, found: 430.0212; Brown solid; m.p.: 70.2–72.1 oC; yield, 62%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.88 (s, 1H, Pyr-H), 8.22 – 8.20 (m, 1H, Ph-H), 8.20 – 8.18 (m, 1H, Ph-H), 7.47 – 7.43 (m, 2H, Ph-H), 7.33 (d, *J* = 0.9 Hz, 1H, Ph-H), 7.30 (d, *J* = 2.1 Hz, 1H, Ph-H), 7.28 (t, *J* = 2.2 Hz, 1H, Ph-H), 7.26 – 7.25 (m, 1H, Pyr-H), 5.44 (s, 2H, Ph-O-CH2);  **13C NMR (101 MHz, CDCl3)** δ169.81, 165.12, 159.31, 157.34, 155.47, 134.95, 134.63, 132.13, 131.86, 130.91, 129.59, 127.87, 127.29, 121.66, 118.81, 105.82, 63.72;  **19F NMR (376 MHz, CDCl3)** δ -70.14;  **HRMS** (ESI) [M+H]+ calcd for C19H12O3N2Cl2F3: 443.0171, found: 443.0164; Brown solid; m.p.: 81.0–82.4 oC; yield, 71%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.88 (s, 1H, Pyr-H), 8.22 – 8.19 (m, 1H, Ph-H), 8.19 – 8.17 (m, 1H, Ph-H), 7.48 (td, *J* = 7.5, 1.6 Hz, 1H, Ph-H), 7.39 – 7.32 (m, 2H, Ph-H), 7.26 (d, *J* = 2.0 Hz, 1H, Ph-H), 7.25 – 7.23 (m, 1H, Ph-H), 7.17 (td, *J* = 7.5, 1.0 Hz, 1H, Ph-H), 7.14 – 7.09 (m, 1H, Pyr-H), 5.45 (s, 2H, Ph-O-CH2);  **13C NMR (101 MHz, CDCl3)** δ169.87, 165.32, 162.38, 159.91, 159.35, 157.33, 155.38, 131.87, 130.73, 130.42, 128.16, 124.34, 124.25, 122.93, 121.60, 115.52, 105.81, 60.98;  **19F NMR (376 MHz, CDCl3)** δ -70.16, -117.67;  **HRMS** (ESI) [M+H]+ calcd for C19H13O3N2F4: 393.0856, found: 393.0847; Brown solid; m.p.: 108.4–110.5 oC; yield, 66%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.87 (s, 1H, Pyr-H), 8.20 – 8.19 (m, 1H, Ph-H), 8.18 – 8.16 (m, 1H, Ph-H), 7.34 (d, *J* = 8.0 Hz, 2H, Ph-H), 7.31 (d, *J* = 0.9 Hz, 1H, Ph-H), 7.24 (d, *J* = 2.0 Hz, 1H, Ph-H), 7.23 (d, *J* = 2.0 Hz, 1H, Ph-H), 7.20 (d, *J* = 7.8 Hz, 2H, Ph-H, Pyr-H), 5.34 (s, 2H, Ph-O-CH2), 2.37 (s, 3H, Ph-CH3);  **13C NMR (101 MHz, CDCl3)** δ169.90, 165.46, 159.34, 157.71, 155.31, 138.28, 132.83, 131.80, 129.33, 128.44, 121.51, 118.85, 105.80, 66.96, 21.24;  **19F NMR (376 MHz, CDCl3)** δ -70.16;  **HRMS** (ESI) [M+H]+ calcd for C20H16O3N2F3: 389.1107, found: 389.1101; Yellow oil; yield, 57%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.88 (s, 1H, Pyr-H), 8.23 – 8.21 (m, 1H, Ph-H), 8.21 – 8.19 (m, 1H, Ph-H), 7.52 – 7.49 (m, 1H, Ph-H), 7.45 – 7.41 (m, 1H, Ph-H), 7.31 (ddd, *J* = 7.1, 3.9, 1.6 Hz, 3H, Ph-H), 7.28 – 7.27 (m, 1H, Ph-H), 7.26 – 7.24 (m, 1H, Pyr-H), 5.49 (s, 2H, Ph-O-CH2);  **13C NMR (101 MHz, CDCl3)** δ169.87, 165.24, 159.34, 157.37, 155.43, 133.94, 133.53, 131.87, 130.05, 129.72, 128.14, 126.97, 121.61, 118.85, 105.80, 64.39;  **19F NMR (376 MHz, CDCl3)** δ -70.16;  **HRMS** (ESI) [M+H]+ calcd for C19H13O3N2ClF3: 409.0561, found: 409.0546; White solid; m.p.: 99.6–100.6 oC; yield, 63%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.89 (s, 1H, Pyr-H), 8.29 – 8.27 (m, 1H, Ph-H), 8.26 – 8.25 (m, 1H, Ph-H), 8.24 – 8.22 (m, 1H, Ph-H), 8.21 – 8.20 (m, 1H, Ph-H), 7.63 (s, 1H, Ph-H), 7.61 (s, 1H, Ph-H), 7.35 (d, *J* = 0.9 Hz, 1H, Ph-H), 7.31 – 7.30 (m, 1H, Ph-H), 7.29 – 7.27 (m, 1H, Pyr-H), 5.49 (s, 2H, Ph-O-CH2);  **13C NMR (101 MHz, CDCl3)** δ169.77, 165.09, 159.30, 157.74, 155.63, 147.77, 143.07, 131.86, 128.42, 127.58, 123.93, 121.77, 105.86, 65.42;  **19F NMR (376 MHz, CDCl3)** δ -70.14;  **HRMS** (ESI) [M+H]+ calcd for C19H13O5N3F3: 420.0801, found: 420.0792; White solid; m.p.: 93.5–95.4 oC; yield, 68%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.87 (s, 1H, Pyr-H), 8.18 – 8.16 (m, 1H, Ph-H), 8.15 (d, *J* = 2.5 Hz, 1H, Ph-H), 7.39 – 7.32 (m, 1H, Ph-H), 7.32 (s, 1H, Ph-H), 7.24 (d, *J* = 2.6 Hz, 1H, Ph-H), 7.23 – 7.21 (m, 1H, Ph-H), 7.15 – 6.99 (m, 1H, Ph-H), 6.99 – 6.94 (m, 1H, Pyr-H), 5.54 (d, *J* = 1.7 Hz, 1H, O-CH2-Ph), 5.48 (s, 1H, O-CH2-Ph);  **13C NMR (101 MHz, CDCl3)** δ 169.87, 165.24, 163.33, 159.34, 157.32, 155.37, 136.62, 131.90, 131.04, 128.03, 125.60, 121.56, 118.84, 114.51, 114.28, 111.63, 105.79, 57.98, 54.85;  **19F NMR (376 MHz, CDCl3)** δ -70.16, -114.15;  **HRMS** (ESI) [M+H]+ calcd for C19H12O3N2ClF4: 427.0449, found: 427.0467; Yellow oil; yield, 73%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.88 (s, 1H, Pyr-H), 8.22 – 8.21 (m, 1H, Ph-H), 8.20 – 8.19 (m, 1H, Ph-H), 7.34 – 7.30 (m, 2H, Ph-H), 7.27 (d, *J* = 2.6 Hz, 1H, Ph-H), 7.25 – 7.23 (m, 1H, Ph-H), 7.03 (d, *J* = 7.6 Hz, 1H, Ph-H), 6.99 (d, *J* = 2.2 Hz, 1H, Ph-H), 6.90 (dd, *J* = 8.2, 2.1 Hz, 1H, Pyr-H), 5.36 (s, 2H, Ph-O-CH2), 3.83 (s, 3H, Ph-O-CH3);  **13C NMR (101 MHz, CDCl3)** δ169.85, 165.37, 159.75, 159.33, 157.66, 155.32, 137.32, 131.82, 129.73, 128.26, 121.56, 120.38, 118.82, 113.78, 113.67, 105.79, 66.81, 55.28;  **19F NMR (376 MHz, CDCl3)** δ -70.14;  **HRMS** (ESI) [M+H]+ calcd for C20H16O4N2F3: 405.1056, found: 405.1045; White solid; m.p.: 56.8–58.3 oC; yield, 55%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.89 (s, 1H, Pyr-H), 8.19 – 8.17 (m, 1H, Ph-H), 8.16 – 8.15 (m, 1H, Ph-H), 7.33 (d, *J* = 0.9 Hz, 1H, Ph-H), 7.27 (d, *J* = 2.7 Hz, 1H, Ph-H), 7.25 – 7.24 (m, 1H, Pyr-H), 3.95 (s, 3H, O-CH3);  **13C NMR (101 MHz, CDCl3)** δ169.88, 166.12, 159.36, 157.33, 155.25, 131.71, 128.33, 121.53, 118.85, 105.85, 52.39.;  **19F NMR (376 MHz, CDCl3)** δ -70.15;  **HRMS** (ESI) [M+H]+ calcd for C13H10O3N2F3: 299.0638, found: 299.0635; Yellow oil; yield, 82%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.88 (s, 1H, Pyr-H), 8.51 (d, *J* = 2.3 Hz, 1H, Ph-H), 8.19 – 8.18 (m, 1H, Ph-H), 8.17 – 8.15 (m, 1H, Ph-H), 7.77 (dd, *J* = 8.2, 2.5 Hz, 1H, Ph-H), 7.38 (d, *J* = 8.2 Hz, 1H, Ph-H), 7.34 (d, *J* = 0.8 Hz, 1H, Ph-H), 7.28 (d, *J* = 2.6 Hz, 1H, Ph-H), 7.27 (d, *J* = 1.3 Hz, 1H, Pyr-H), 5.38 (s, 2H, Ph-O-CH2);  **13C NMR (101 MHz, CDCl3)** δ169.80, 165.19, 159.33, 157.39, 155.61, 151.67, 149.72, 139.01, 131.85, 130.46, 127.62, 124.39, 121.75, 105.87, 63.54;  **19F NMR (376 MHz, CDCl3)** δ -70.14;  **HRMS** (ESI) [M+H]+ calcd for C18H12O3N2ClF3: 410.0513, found: 410.0502; Brown solid; m.p.: 85.3–86.9 oC; yield, 47%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.89 (s, 1H, Pyr-H), 8.22 – 8.19 (m, 1H, Ph-H), 8.19 – 8.17 (m, 1H, Ph-H), 7.33 (d, *J* = 0.9 Hz, 1H, Pyr-H), 7.27 (d, *J* = 2.6 Hz, 1H, Ph-H), 7.26 – 7.23 (m, 1H, Ph-H), 6.05 (ddt, *J* = 17.1, 10.5, 5.7 Hz, 1H, CH2=CH=CH2), 5.43 (dq, *J* = 17.2, 1.5 Hz, 1H, CH2=CH=CH2), 5.31 (ddd, *J* = 10.4, 2.5, 1.2 Hz, 1H, CH2=CH=CH2), 4.85 (dt, *J* = 5.7, 1.4 Hz, 2H, CH2=CH=CH2);  **13C NMR (101 MHz, CDCl3)** δ 169.89, 165.25, 159.36, 157.34, 155.31, 132.04, 131.76, 128.36, 121.55, 118.85, 118.51, 105.80, 65.81;  **19F NMR (376 MHz, CDCl3)** δ -70.15;  **HRMS** (ESI) [M+H]+ calcd for C15H12O3N2F3: 325.0794, found: 325.0786; Yellow oil; yield, 43%. |
|  | **1H NMR (400 MHz, CDCl3)** δ 8.88 (s, 1H, Pyr-H), 8.17 (s, 1H, Ph-H), 8.15 (s, 1H, Ph-H), 7.63 (s, 1H, Thia-H), 7.33 (s, 1H, Ph-H), 7.28 (s, 1H, Ph-H), 7.26 (s, 1H, Pyr-H), 5.46 (s, 2H, O-CH2).  **13C NMR (101 MHz, CDCl3)** δ169.79 165.23, 159.32, 155.72, 153.86, 141.90, 134.65, 131.91, 127.36, 121.76, 105.88, 58.61.  **19F NMR (376 MHz, CDCl3)** δ -70.15;  **HRMS** (ESI) [M+H]+ calcd for C16H10O3N3ClF3S: 416.0078, found: 416.0066; Yellow oil; yield, 57%. |



1H NMR spectrum of compound **5a**



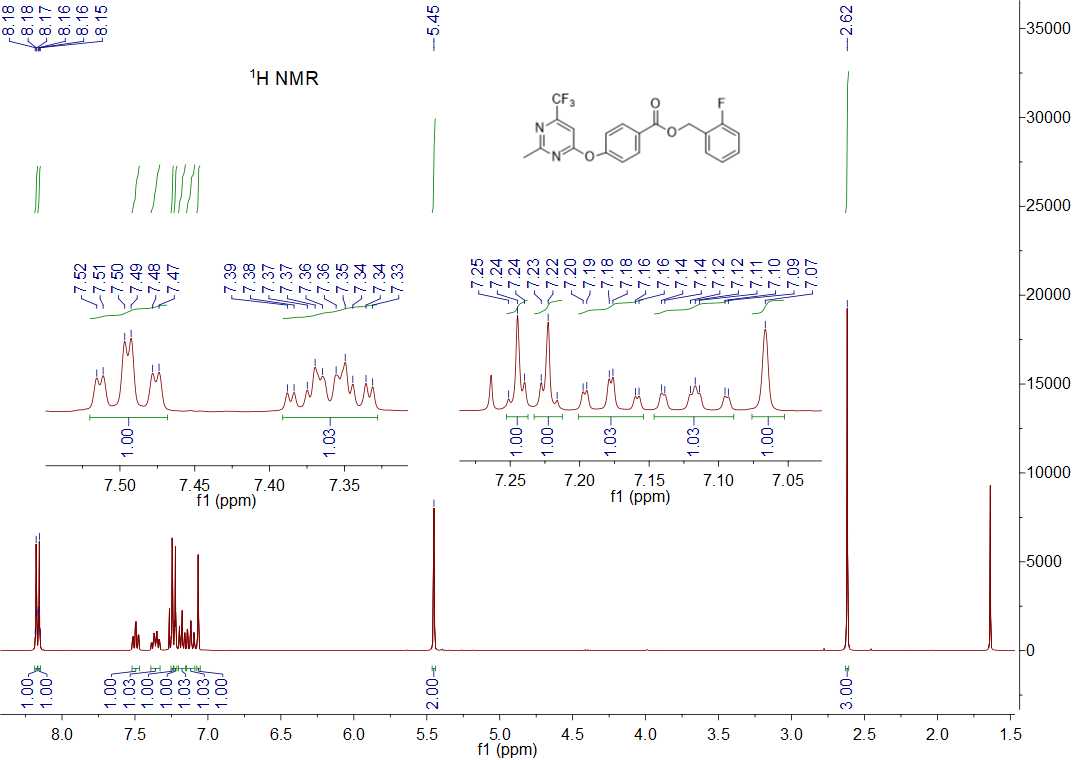
13C NMR spectrum of compound **5a**



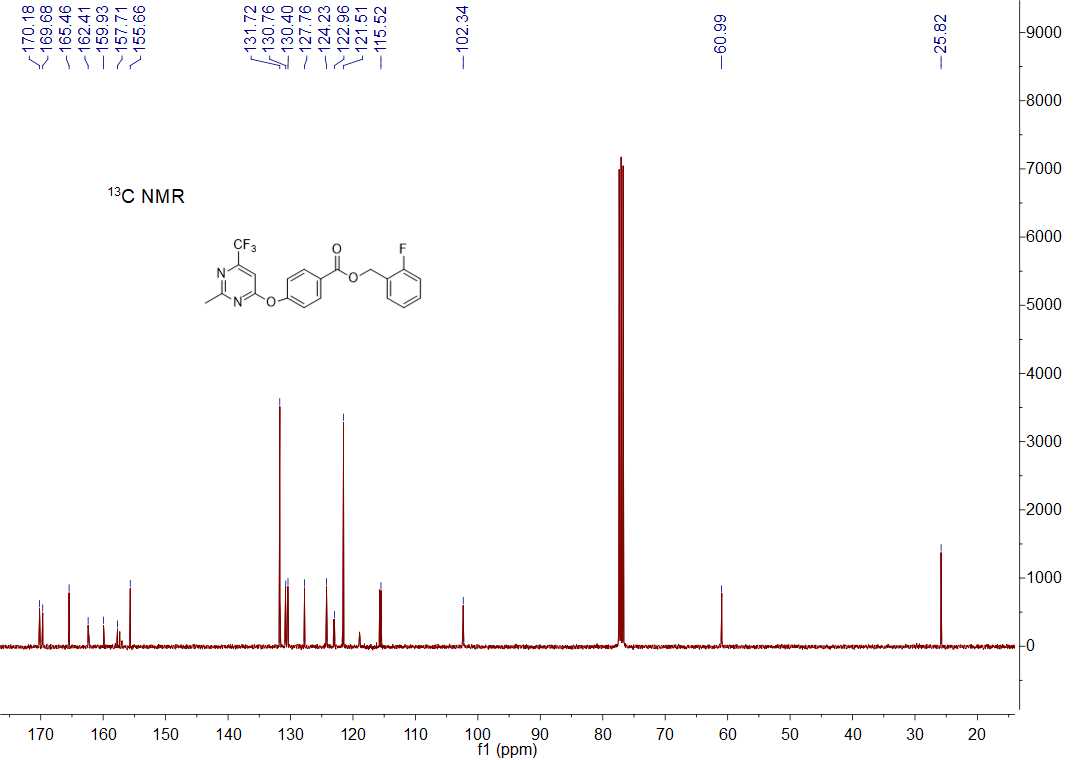
19F NMR spectrum of compound **5a**



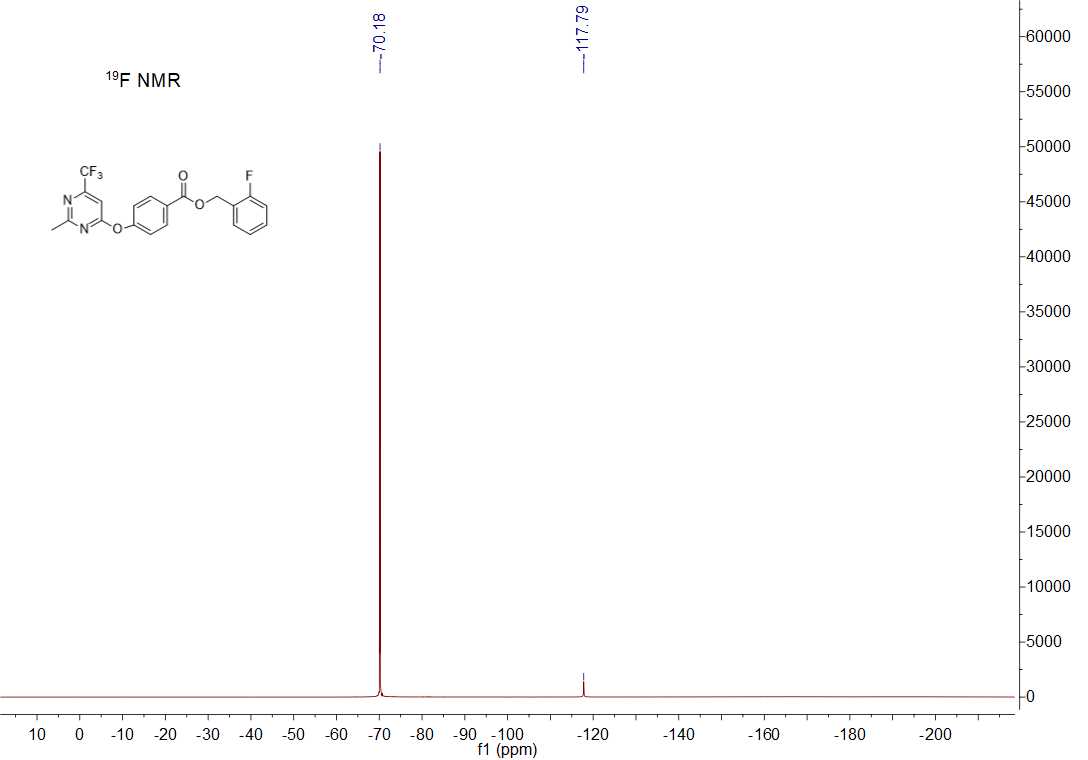
HRMS (ESI) spectrum of compound **5a**



1H NMR spectrum of compound **5b**



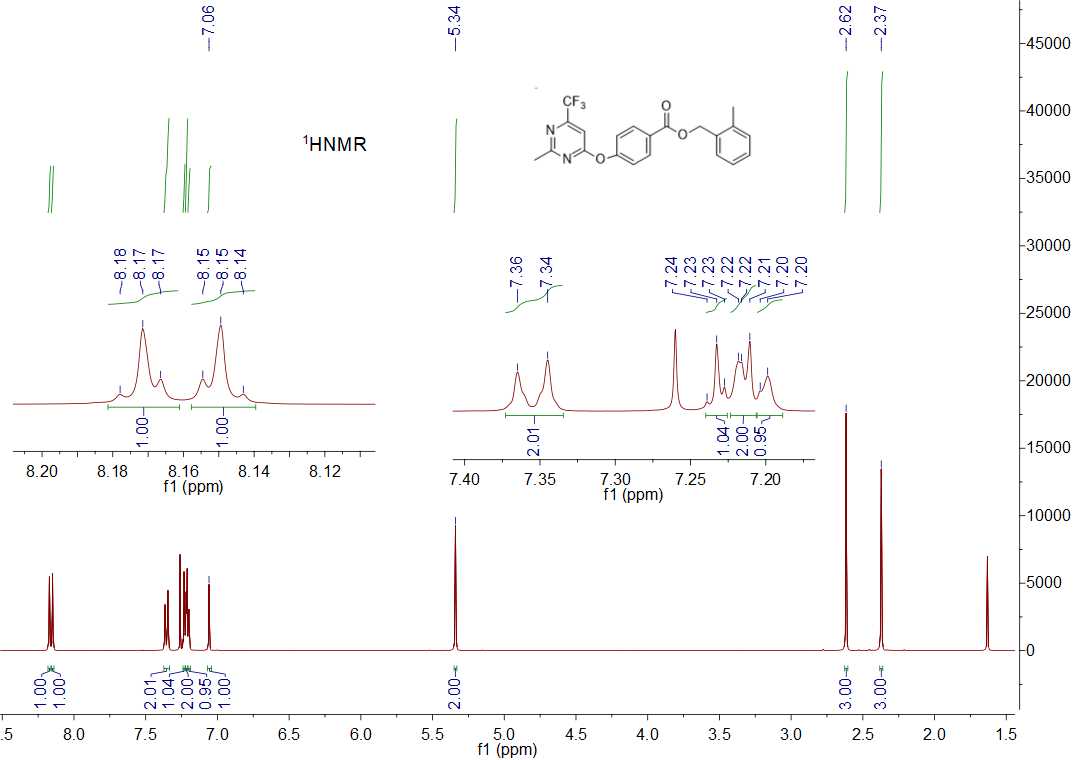
13C NMR spectrum of compound **5b**



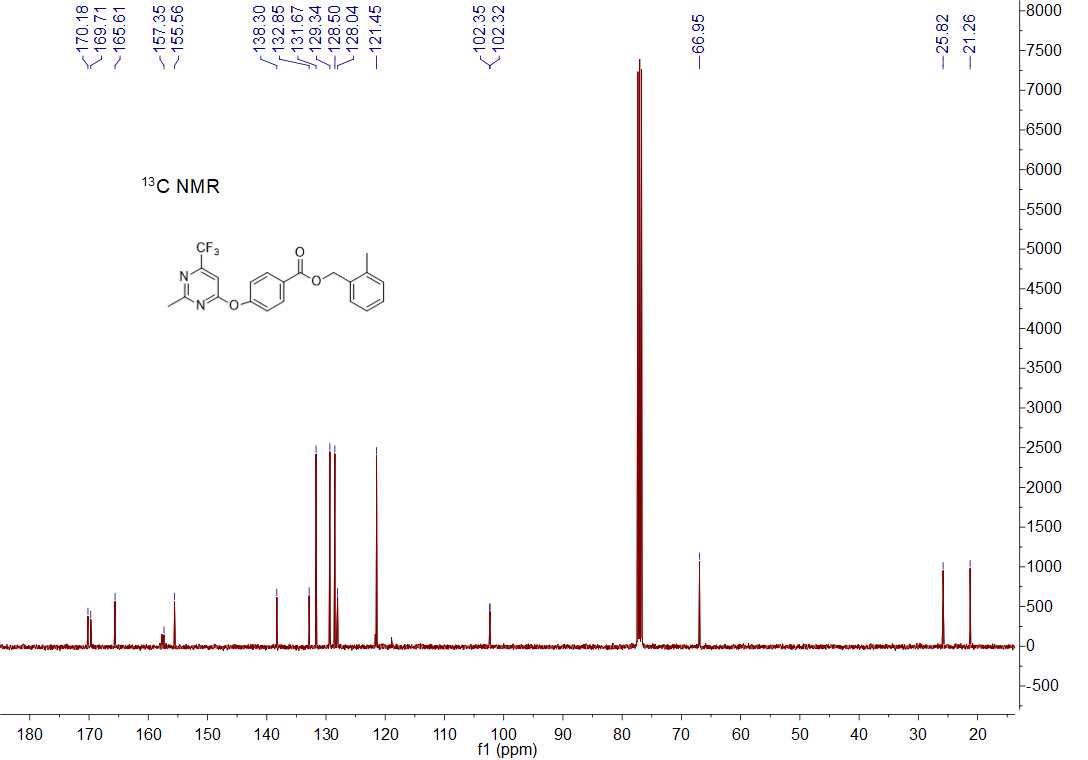
19F NMR spectrum of compound **5b**



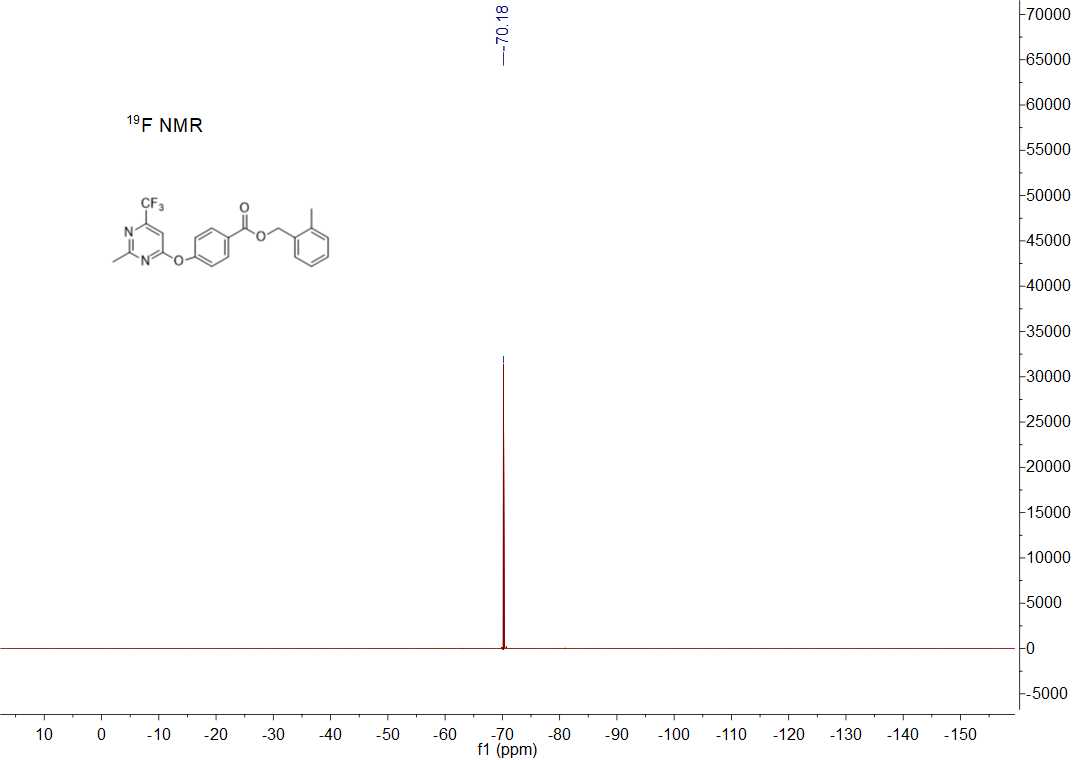
HRMS (ESI) spectrum of compound **5b**



1H NMR spectrum of compound **5c**



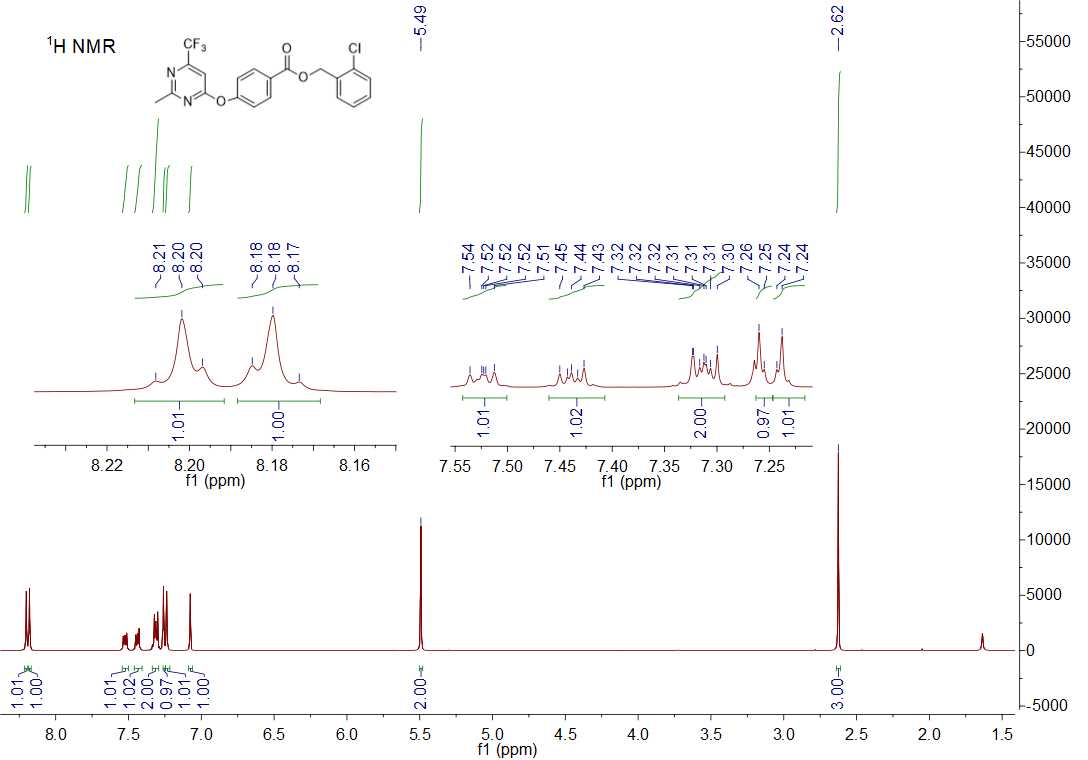
13C NMR spectrum of compound **5c**



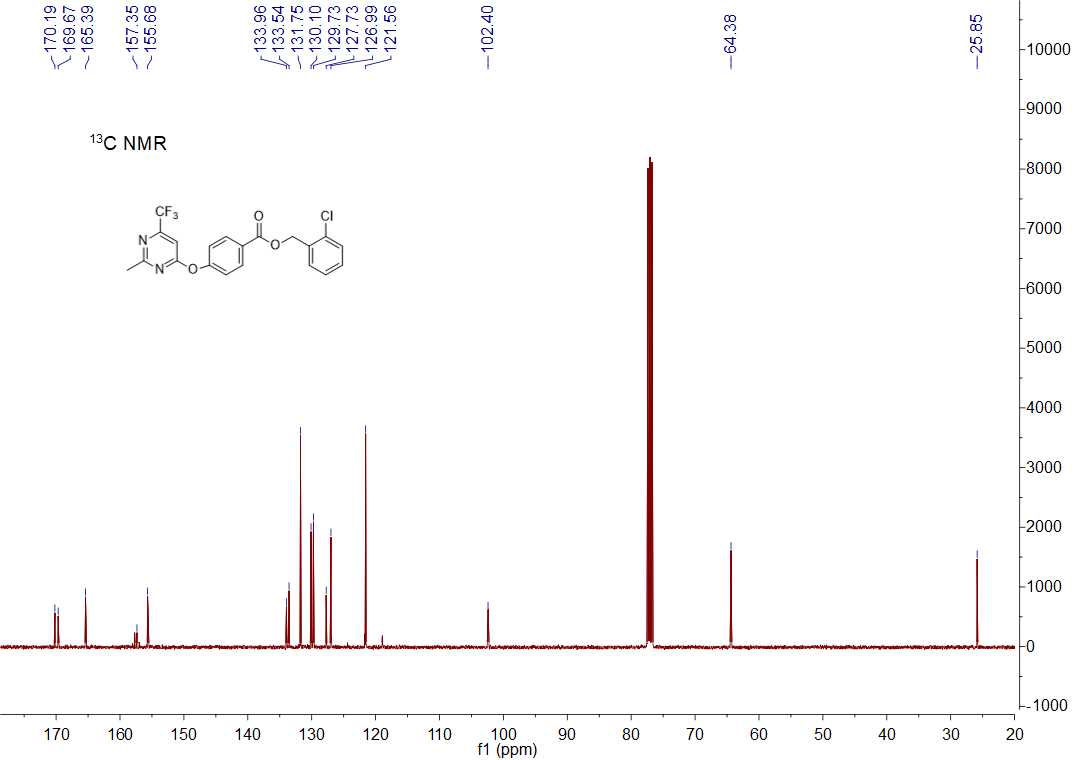
19F NMR spectrum of compound **5c**



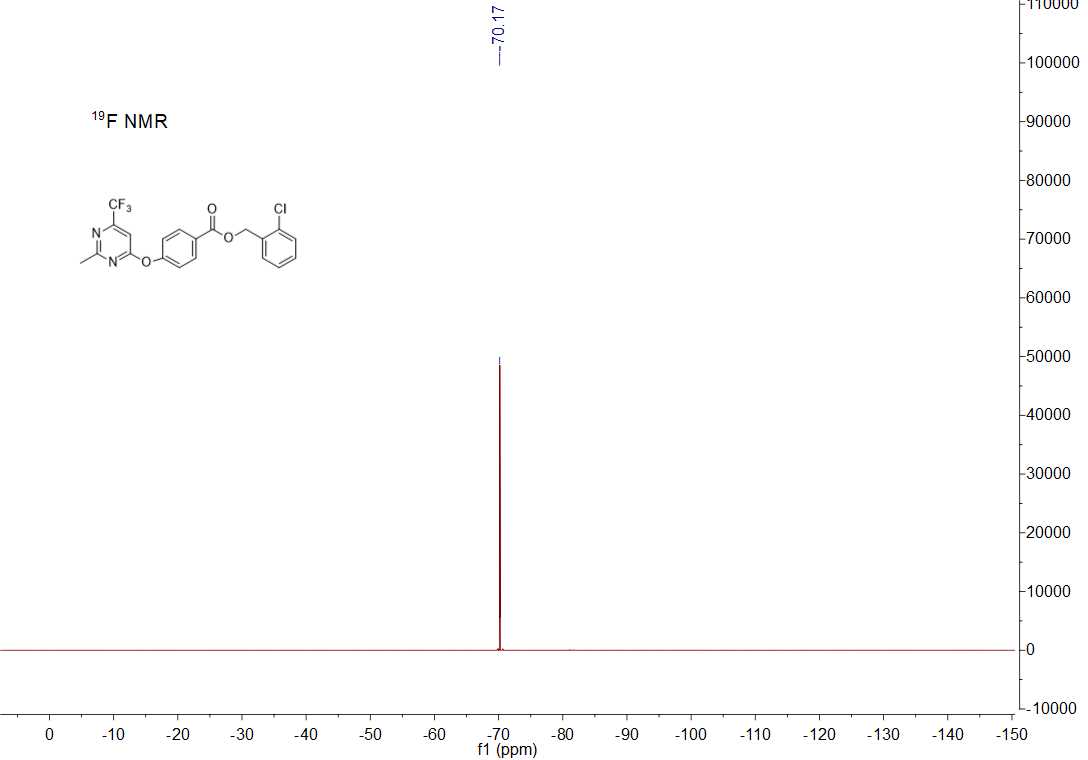
HRMS (ESI) spectrum of compound **5c**



1H NMR spectrum of compound **5d**



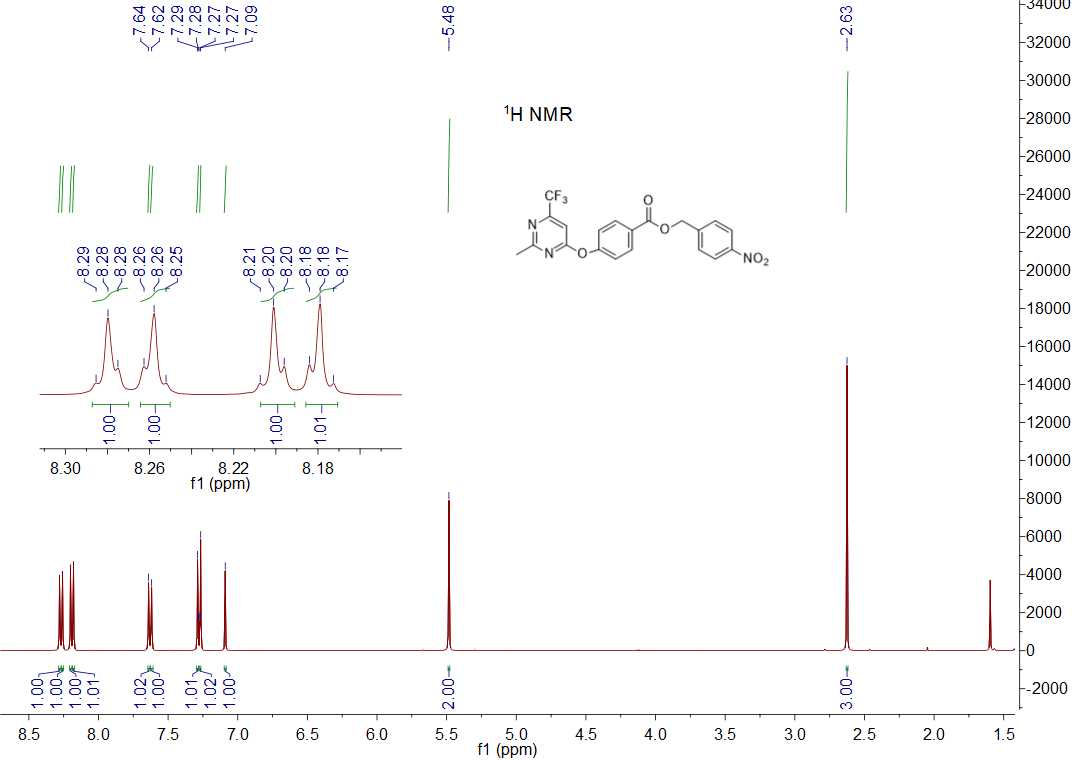
13C NMR spectrum of compound **5d**



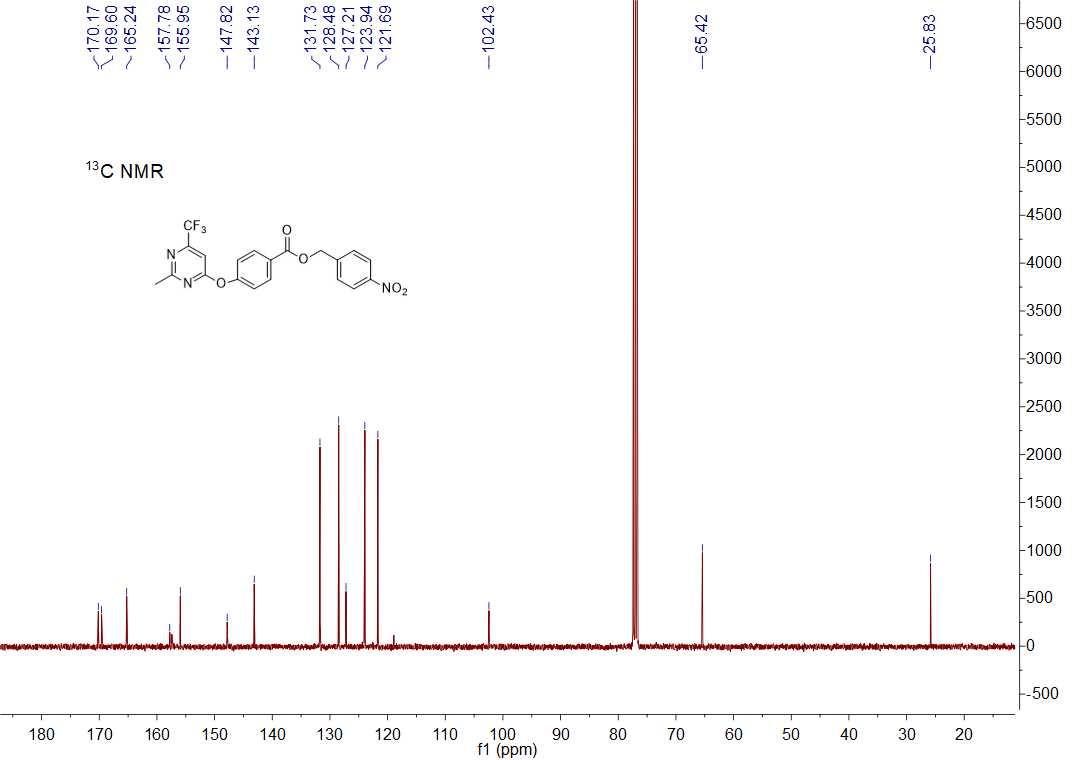
19F NMR spectrum of compound **5d**



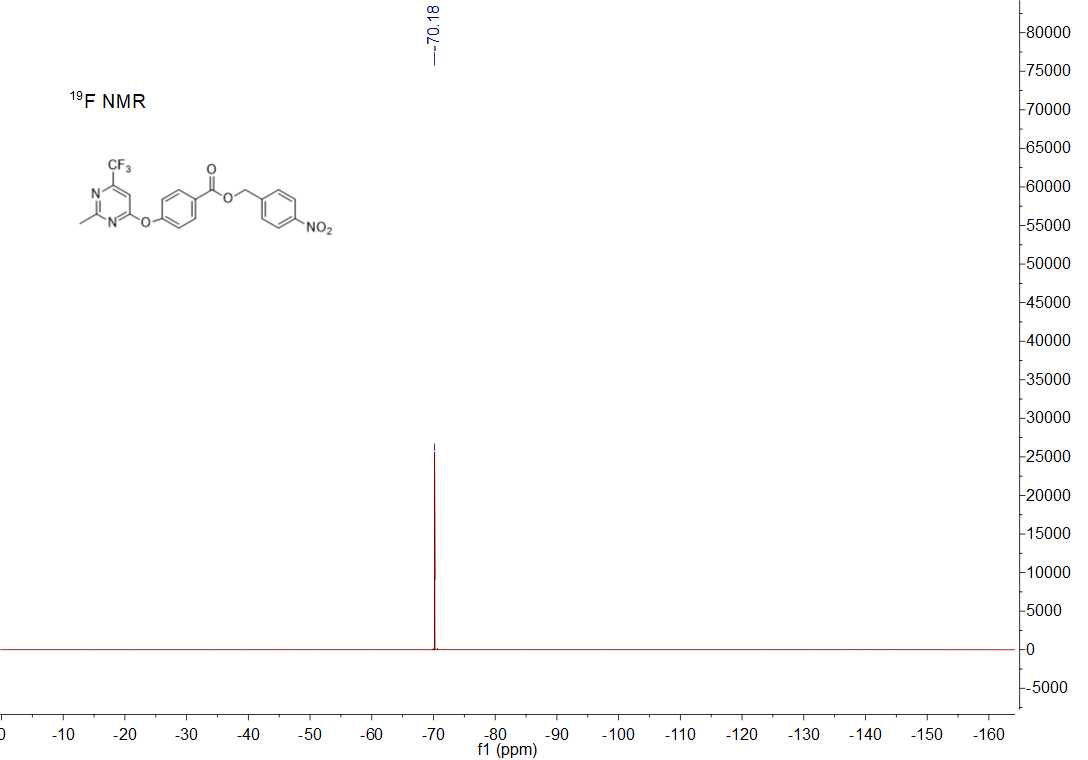
HRMS (ESI) spectrum of compound **5d**



1H NMR spectrum of compound **5e**



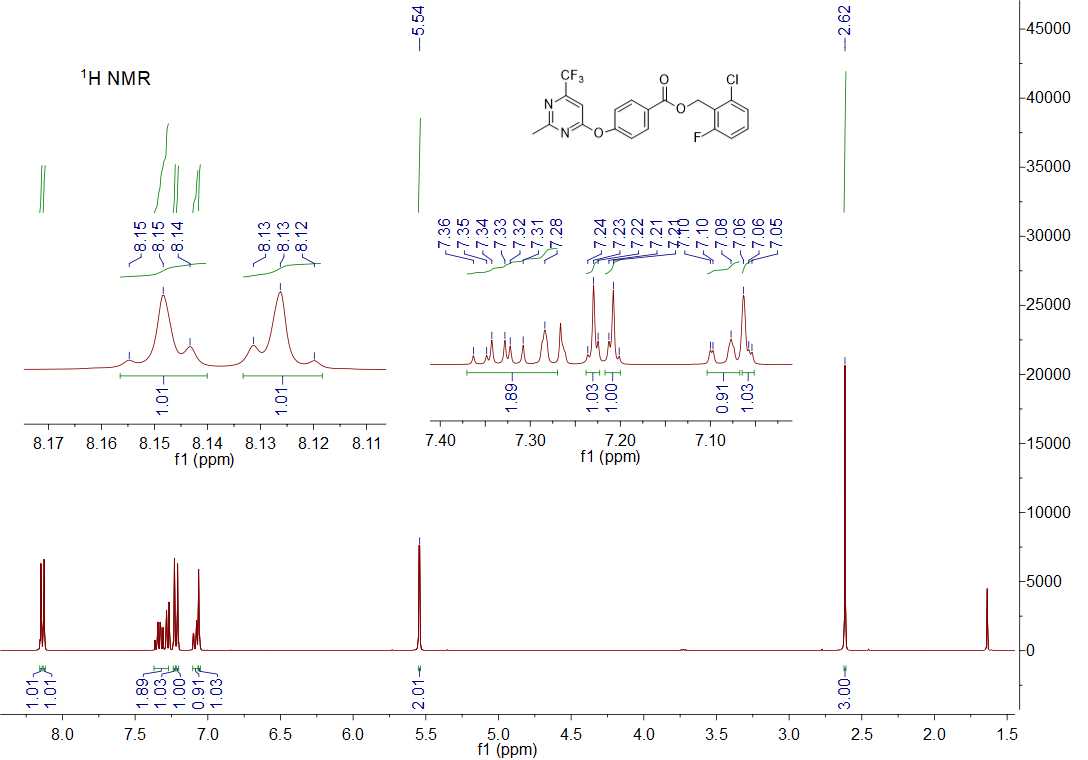
13C NMR spectrum of compound **5e**



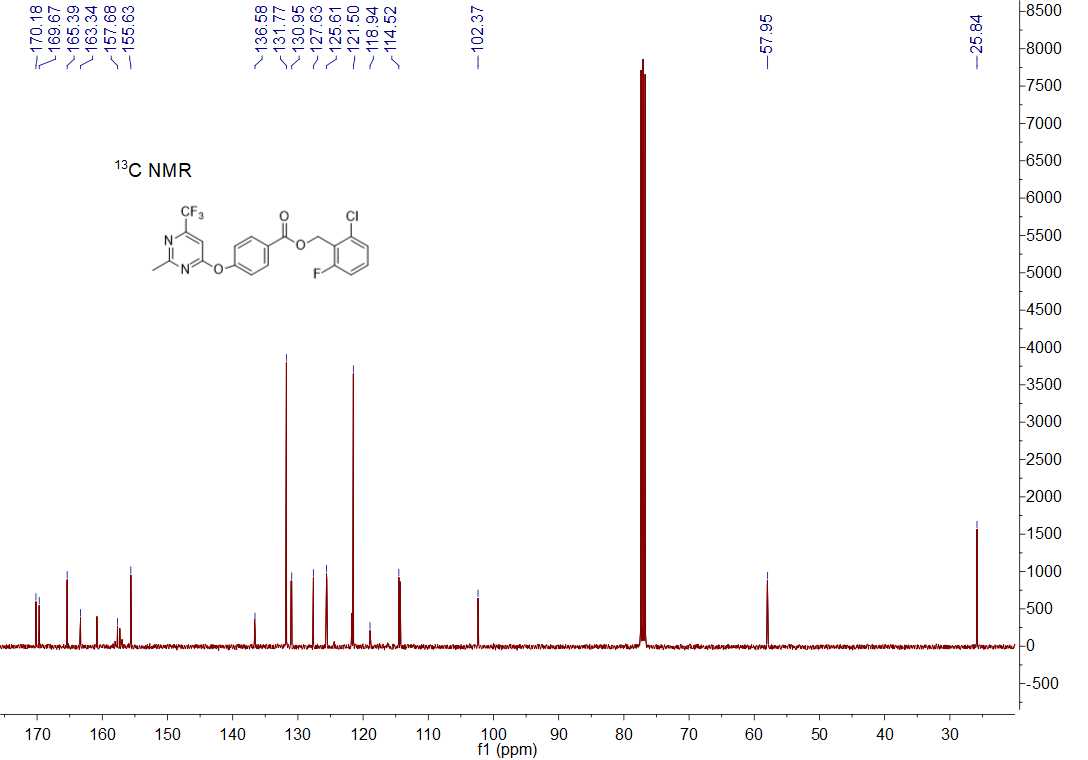
19F NMR spectrum of compound **5e**



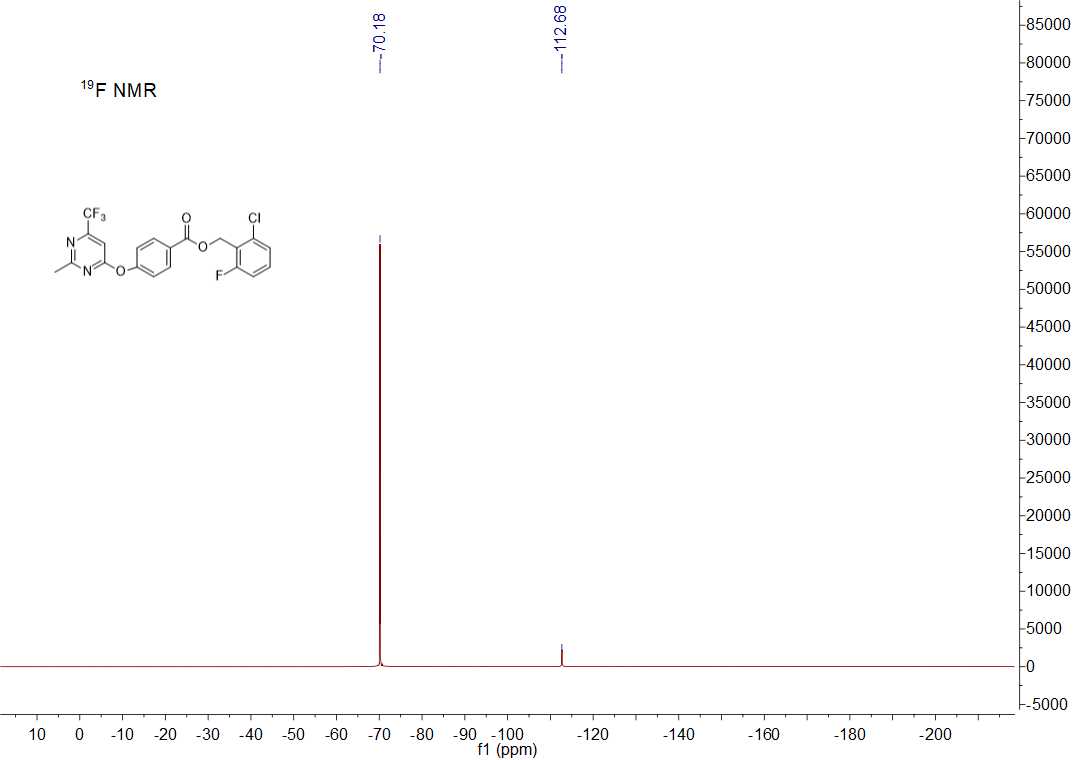
HRMS (ESI) spectrum of compound **5e**



1H NMR spectrum of compound **5f**



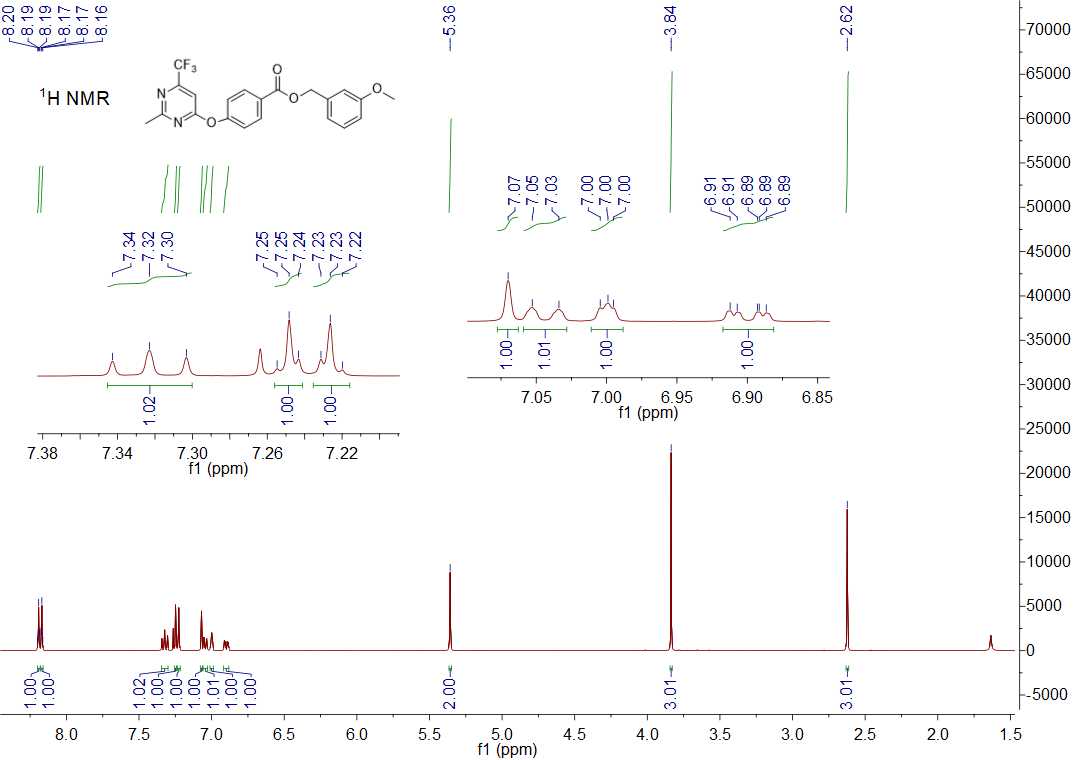
13C NMR spectrum of compound **5f**



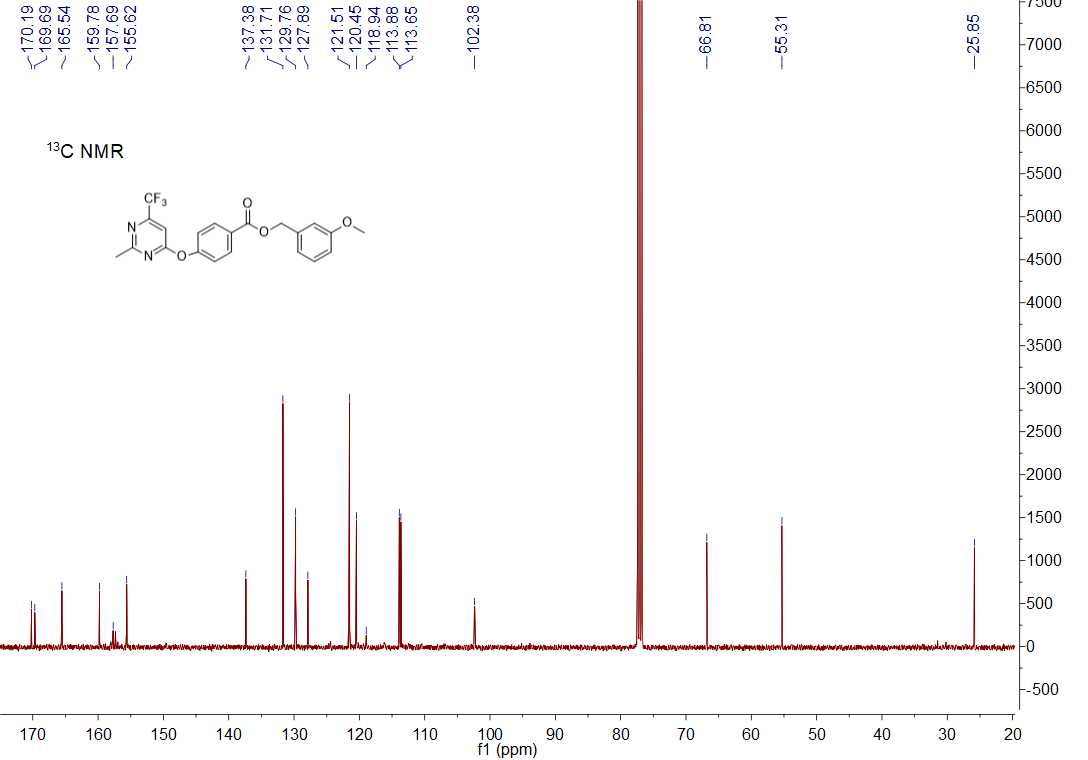
19F NMR spectrum of compound **5f**



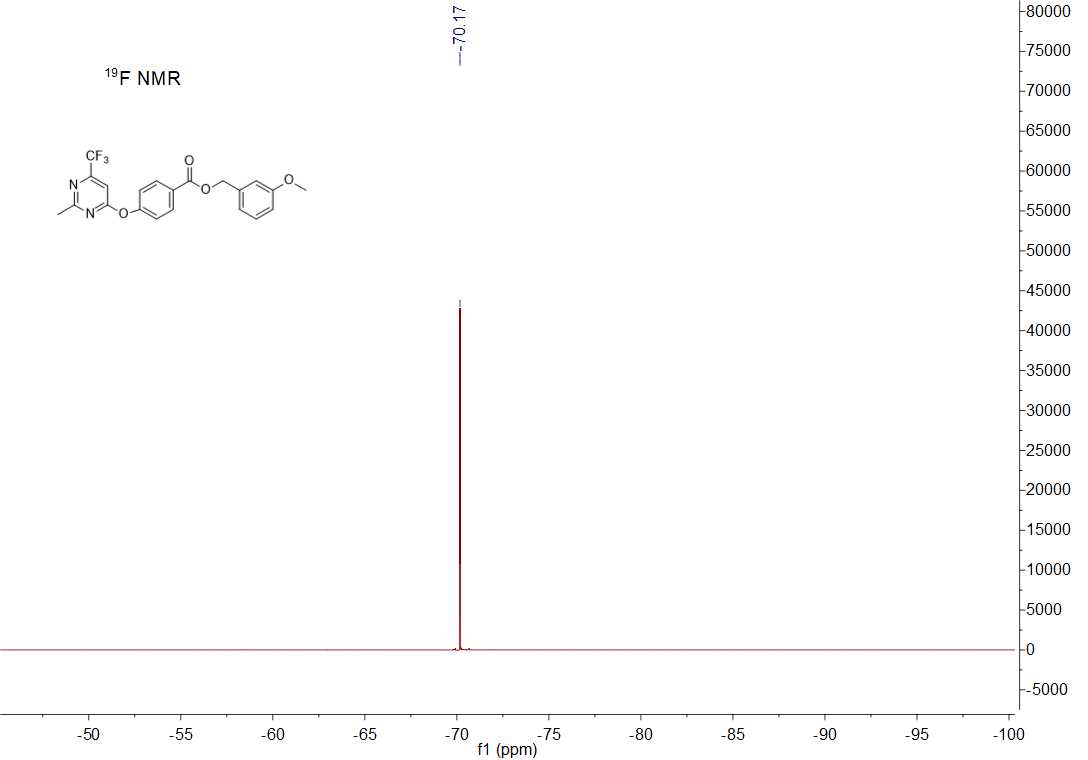
HRMS (ESI) spectrum of compound **5f**



1H NMR spectrum of compound **5g**



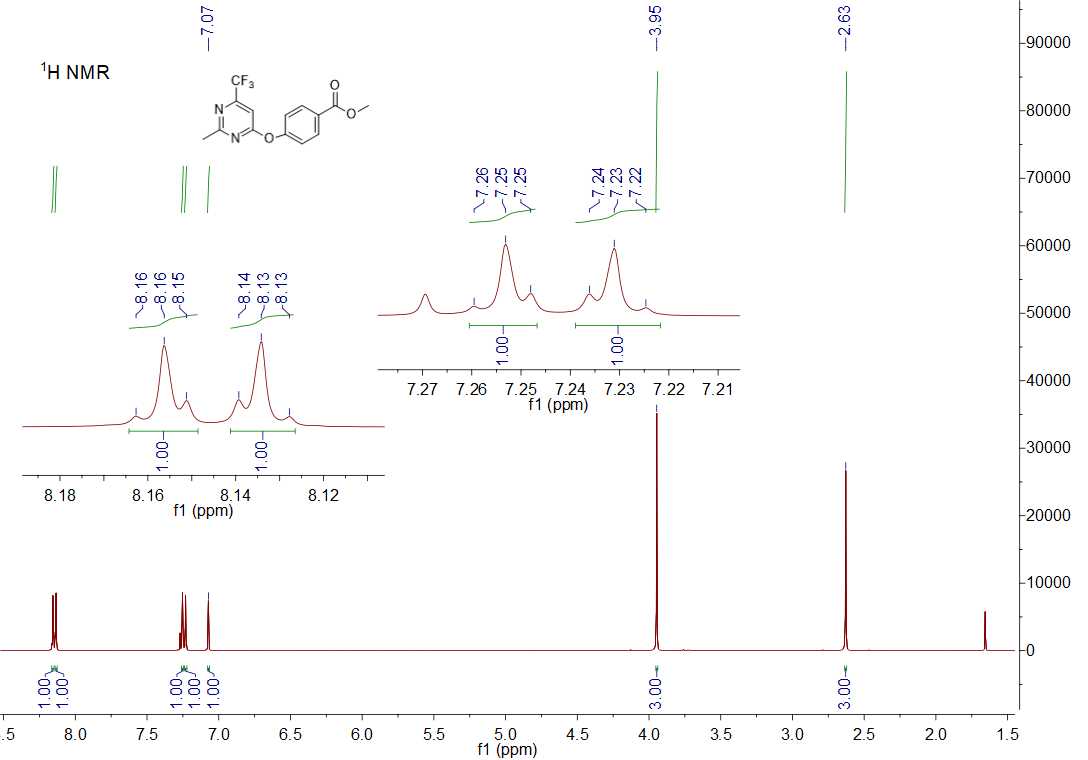
13C NMR spectrum of compound **5g**



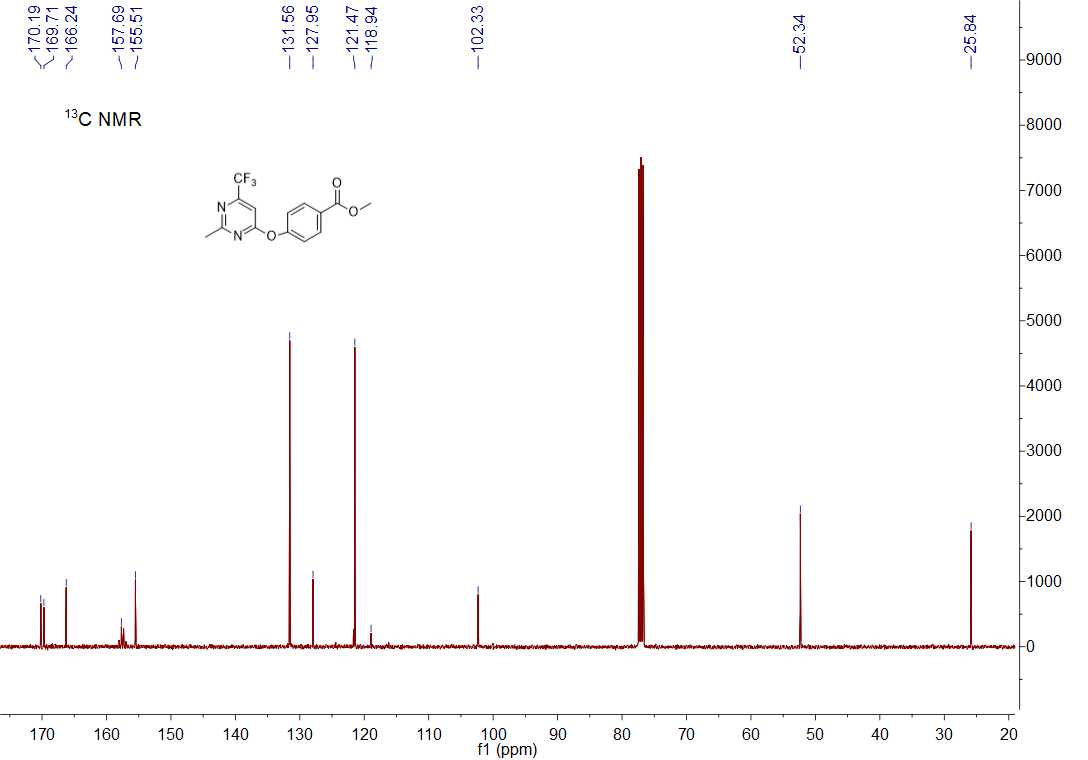
19F NMR spectrum of compound **5g**



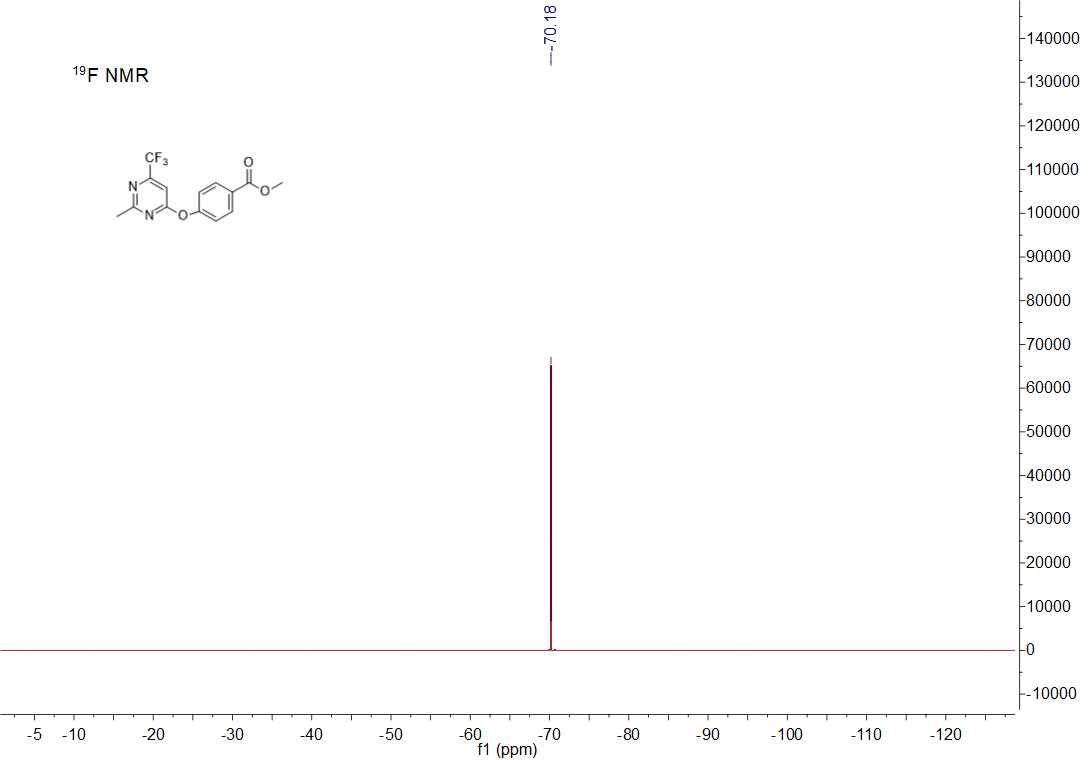
HRMS (ESI) spectrum of compound **5g**



1H NMR spectrum of compound **5h**



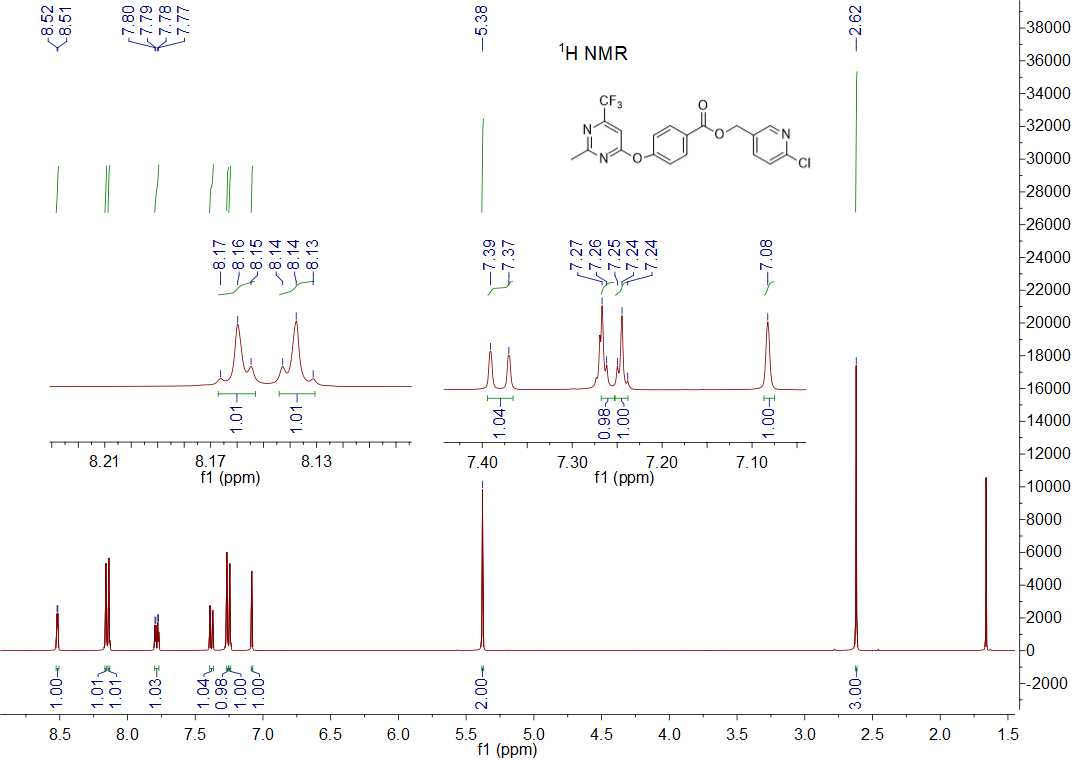
13C NMR spectrum of compound **5h**



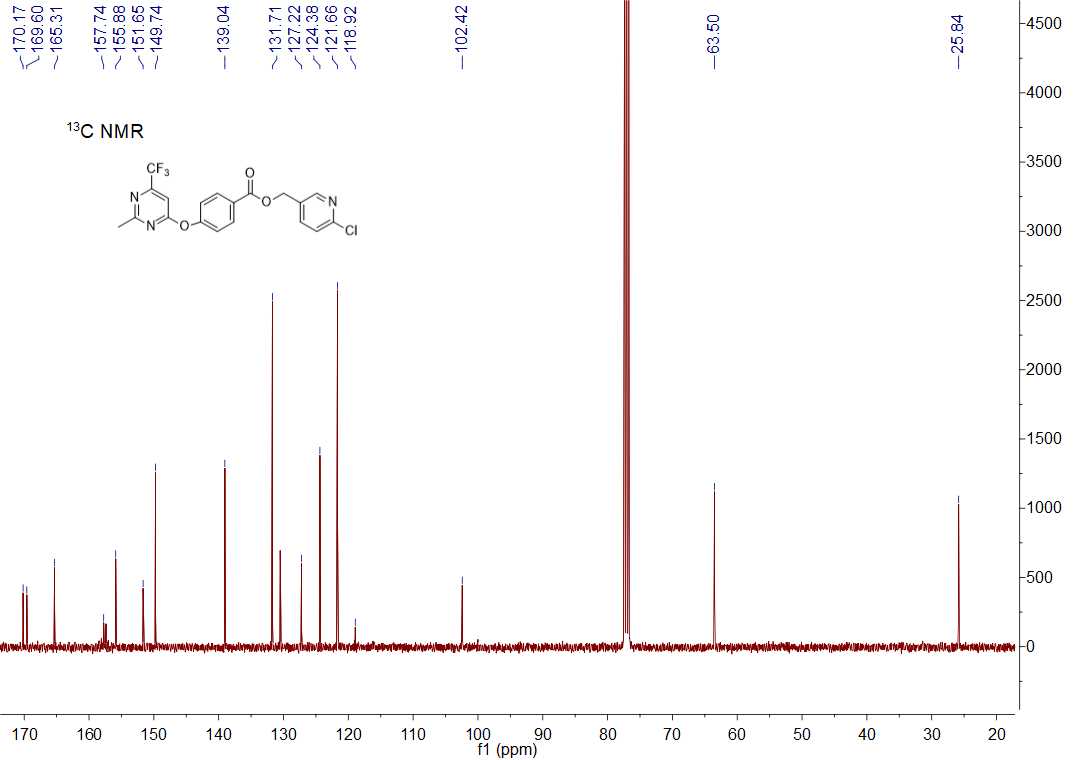
19F NMR spectrum of compound **5h**



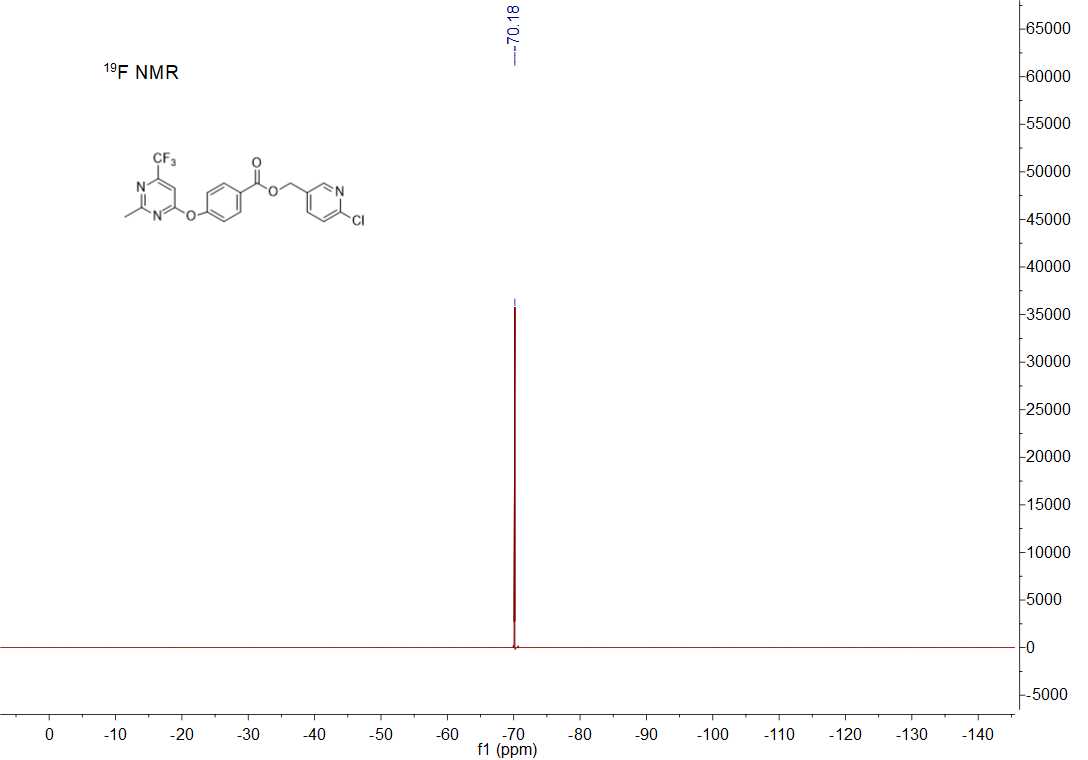
HRMS (ESI) spectrum of compound **5h**



1H NMR spectrum of compound **5i**



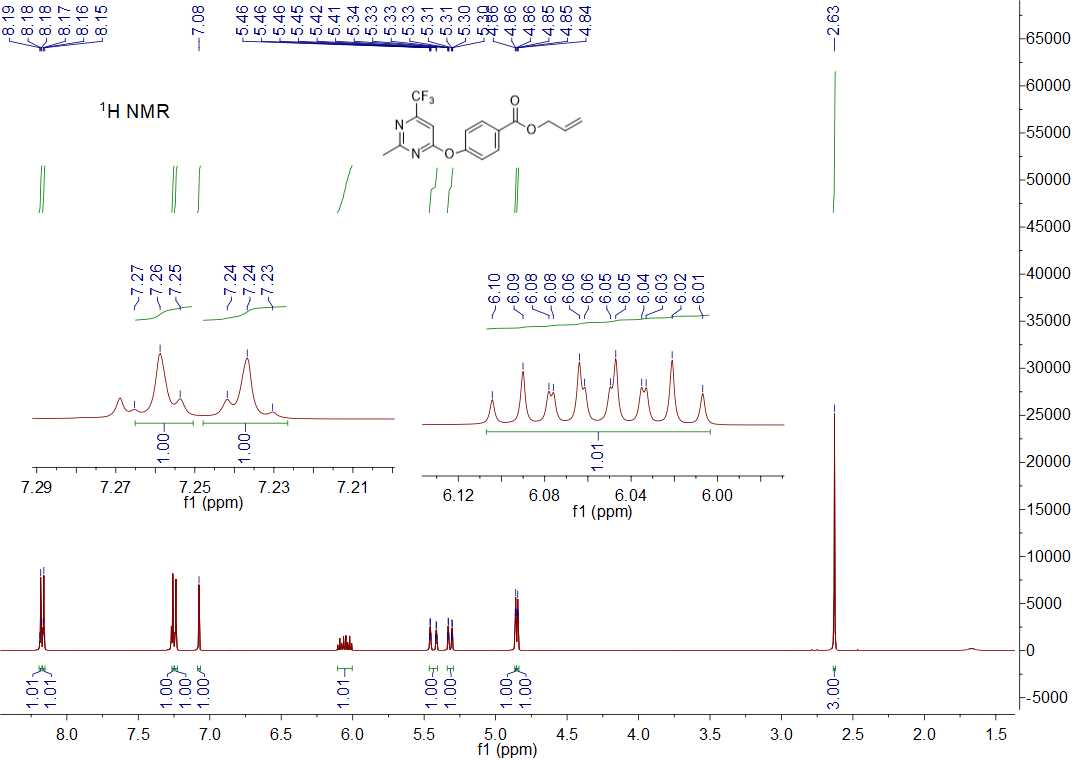
13C NMR spectrum of compound **5i**



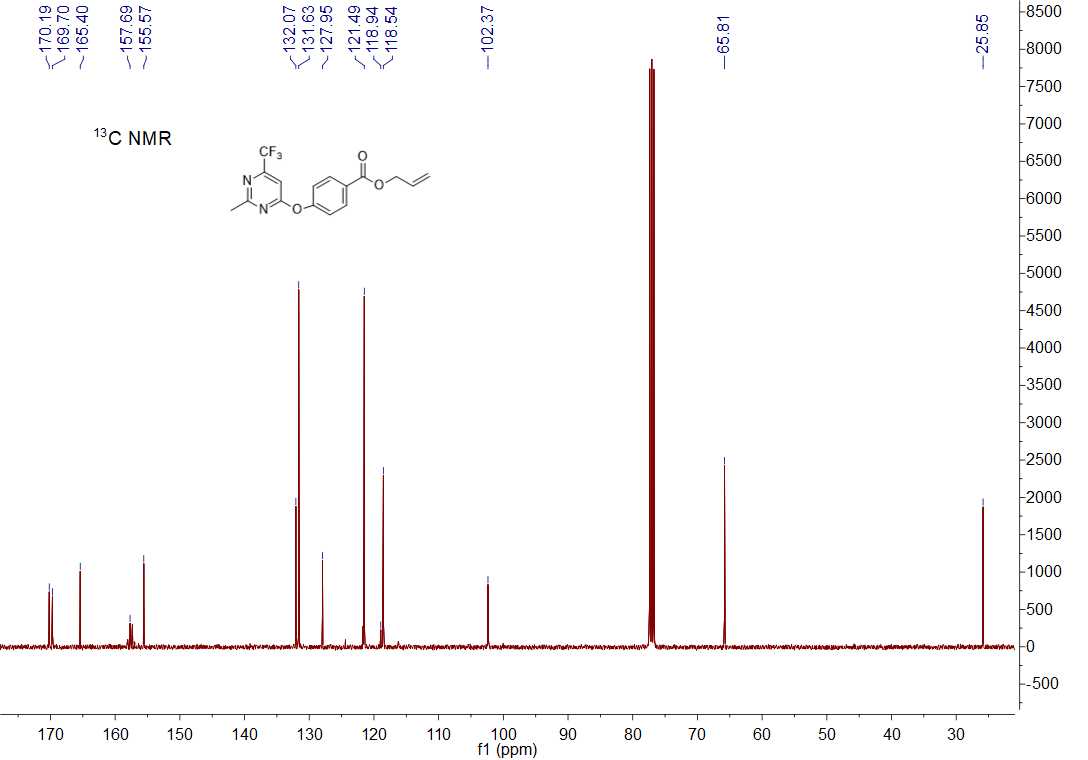
19F NMR spectrum of compound **5i**



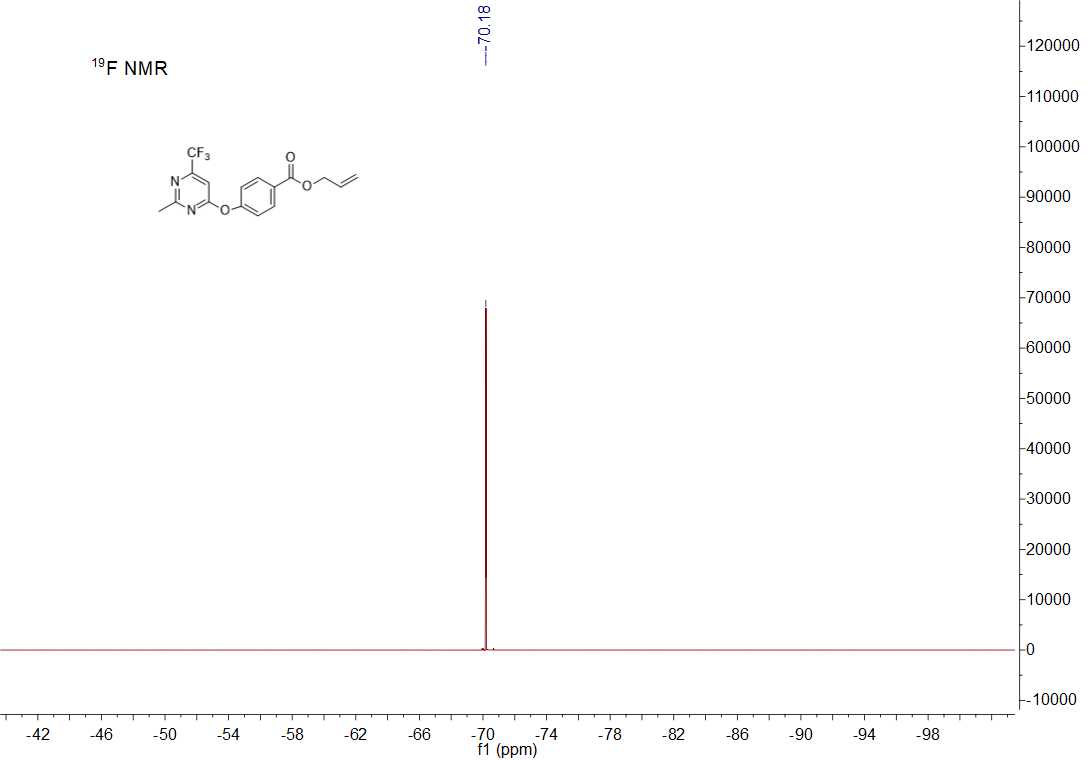
HRMS (ESI) spectrum of compound **5i**



1H NMR spectrum of compound **5j**



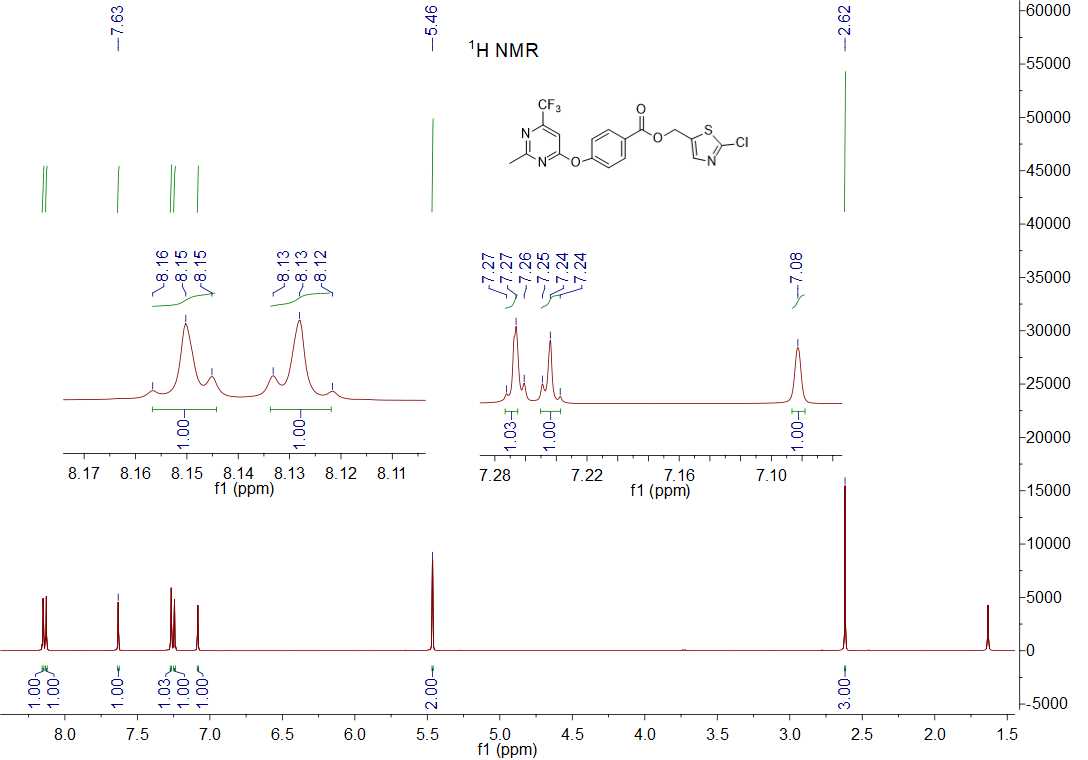
13C NMR spectrum of compound **5j**



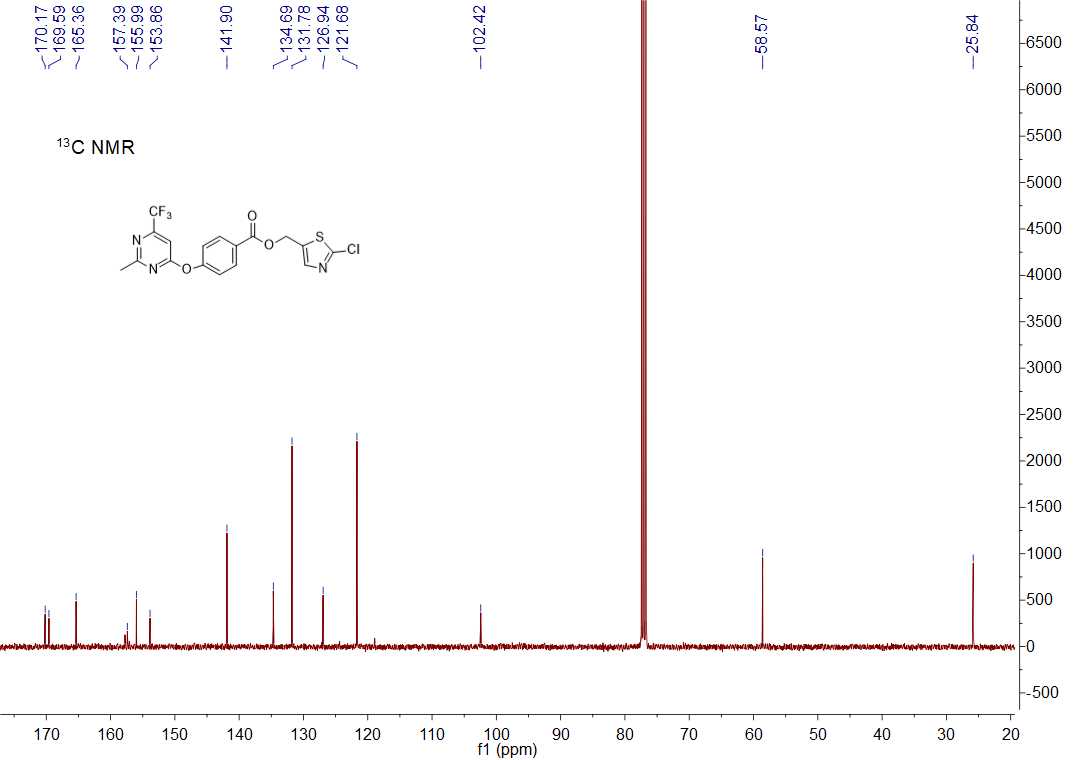
19F NMR spectrum of compound **5j**



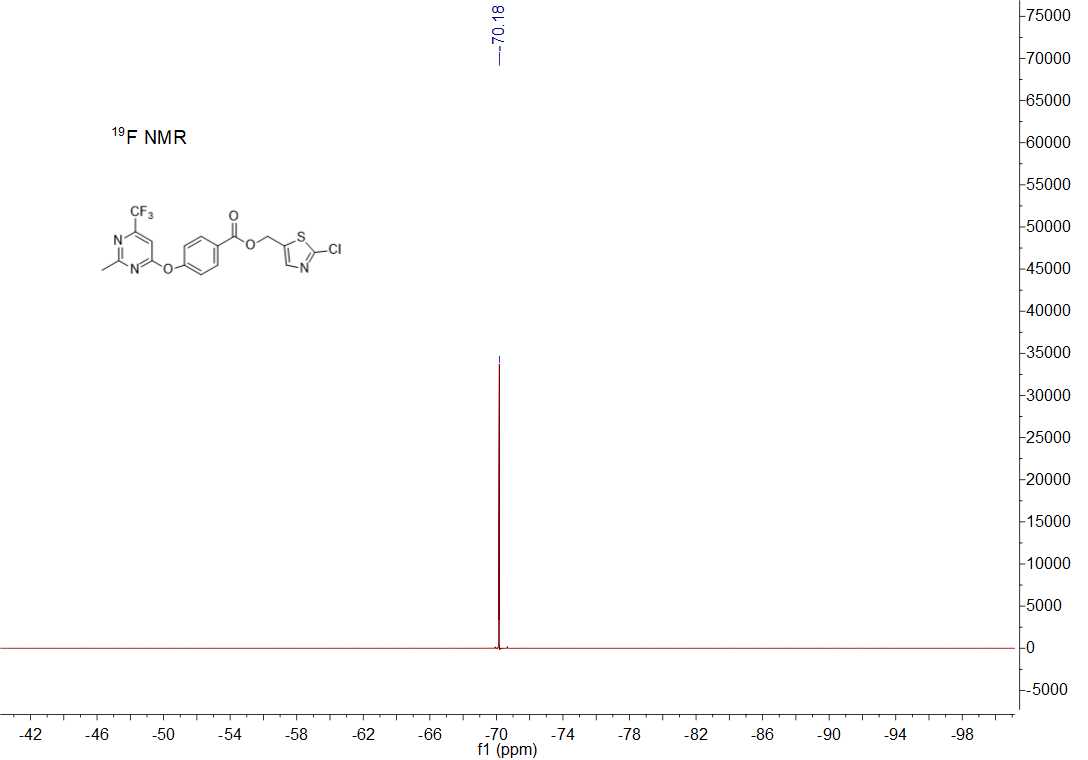
HRMS (ESI) spectrum of compound **5j**



1H NMR spectrum of compound **5k**



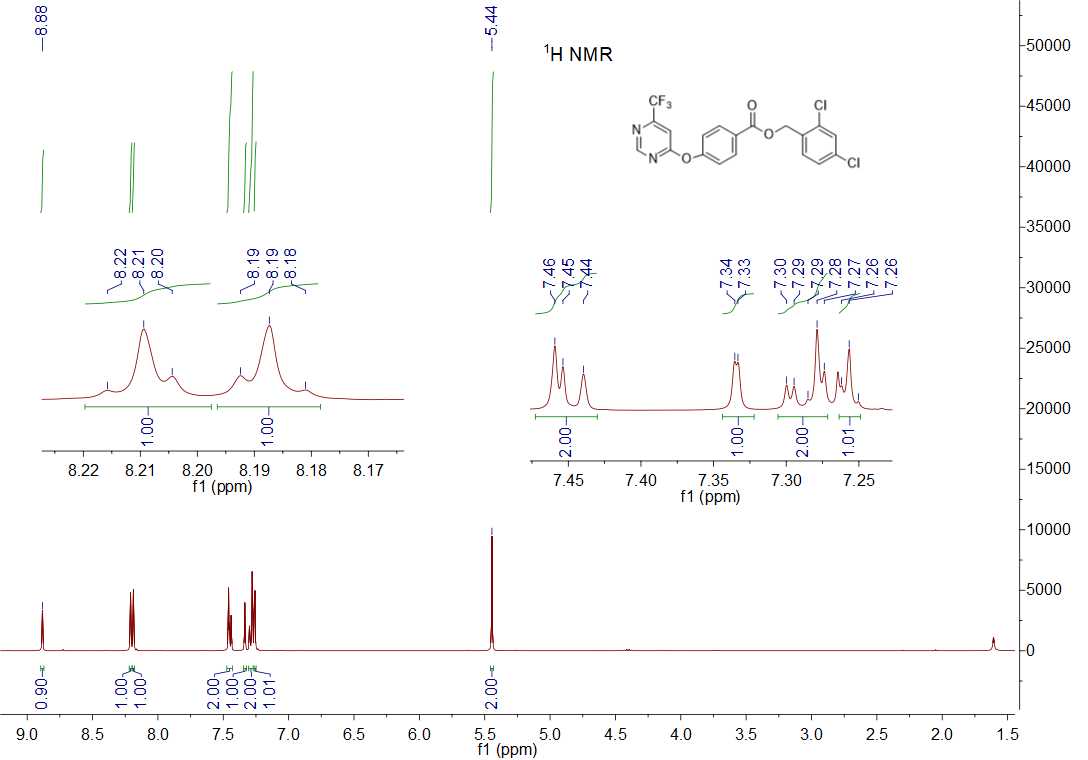
13C NMR spectrum of compound **5k**



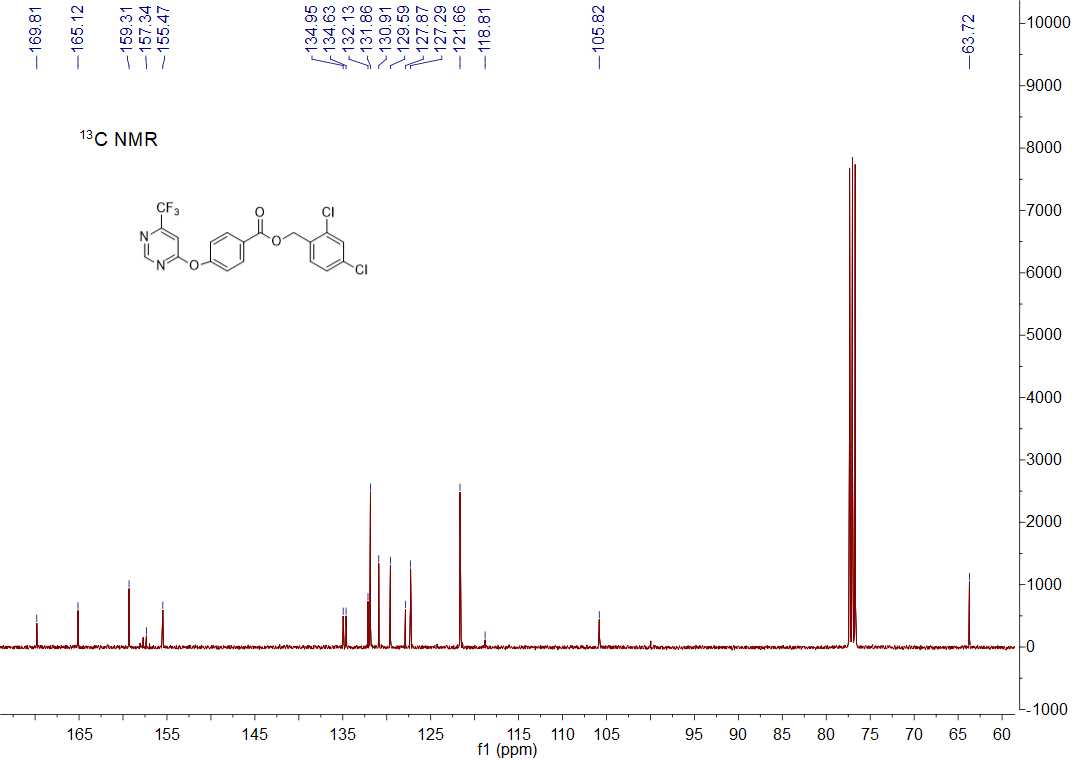
19F NMR spectrum of compound **5k**



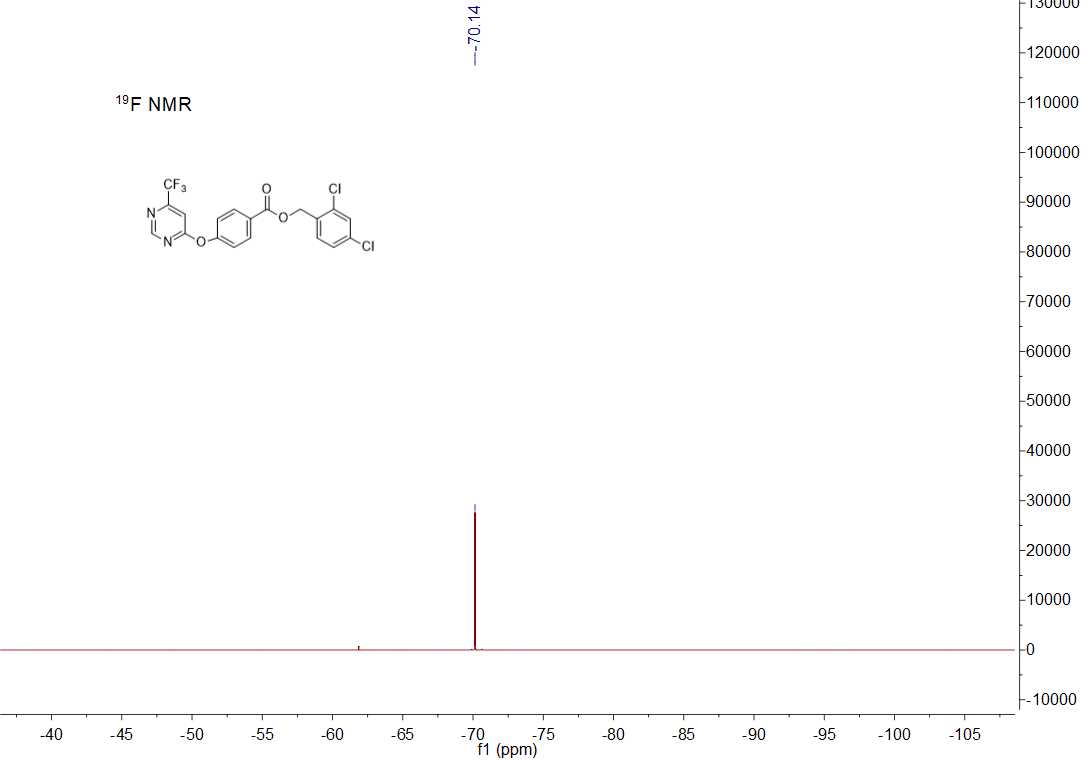
HRMS (ESI) spectrum of compound **5k**



1H NMR spectrum of compound **5l**



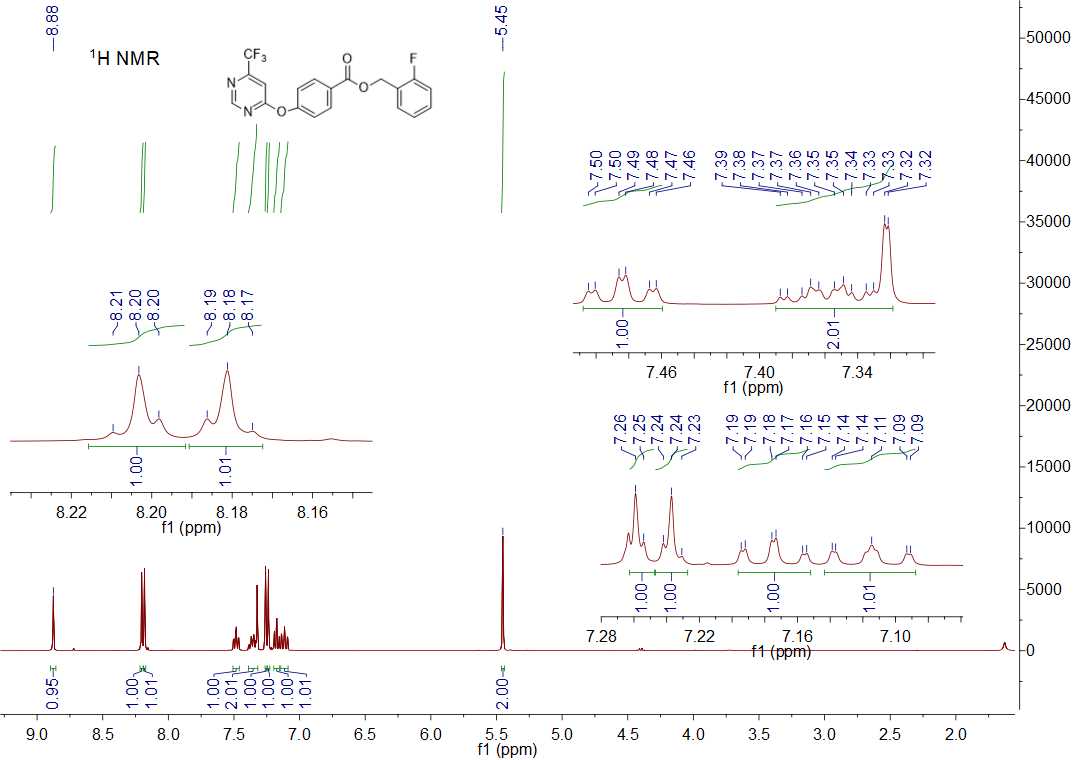
13C NMR spectrum of compound **5l**



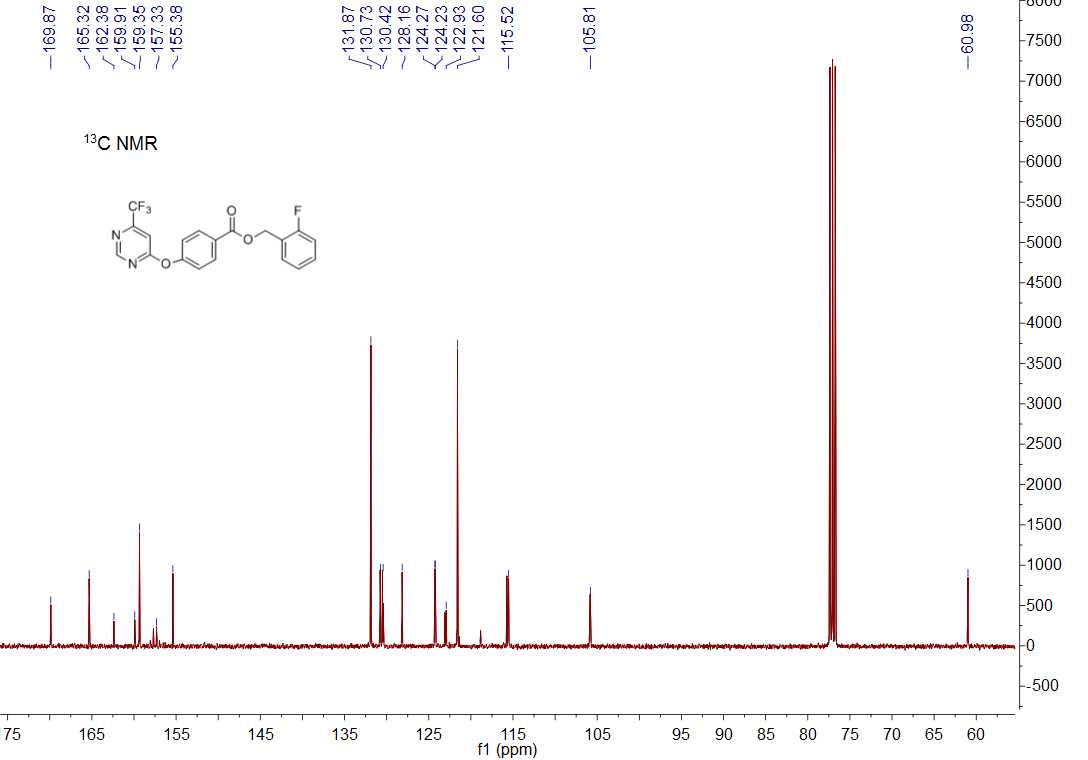
19F NMR spectrum of compound **5l**



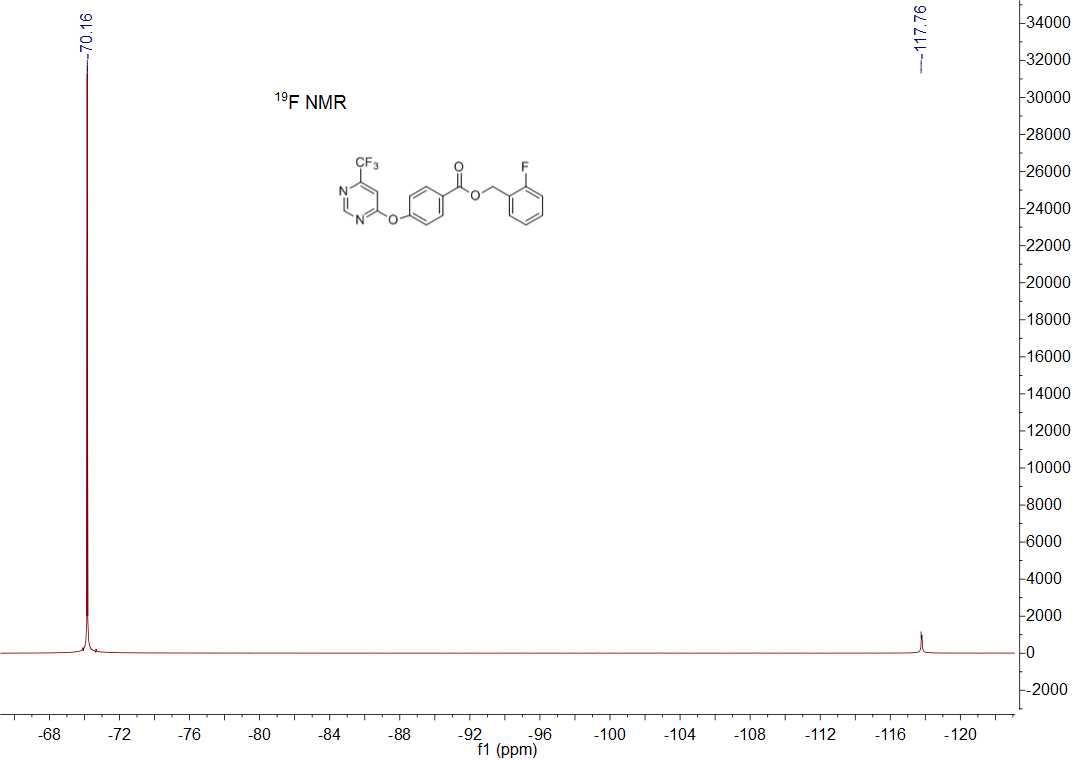
HRMS (ESI) spectrum of compound **5l**



1H NMR spectrum of compound **5m**



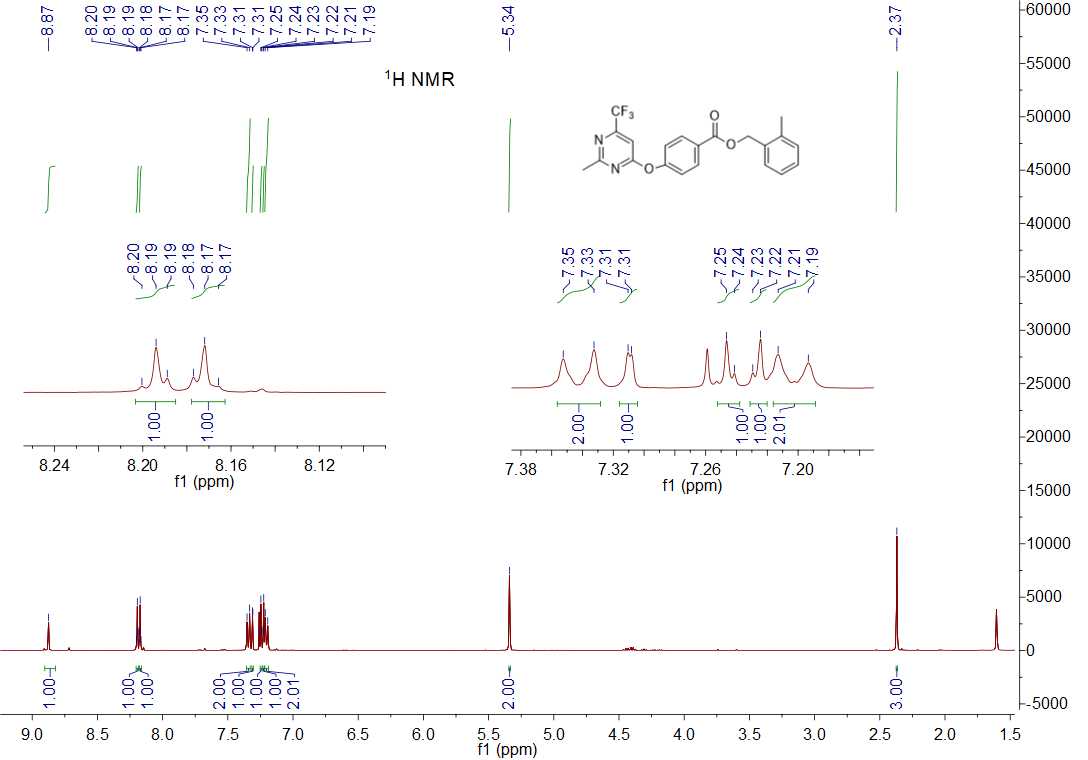
13C NMR spectrum of compound **5m**



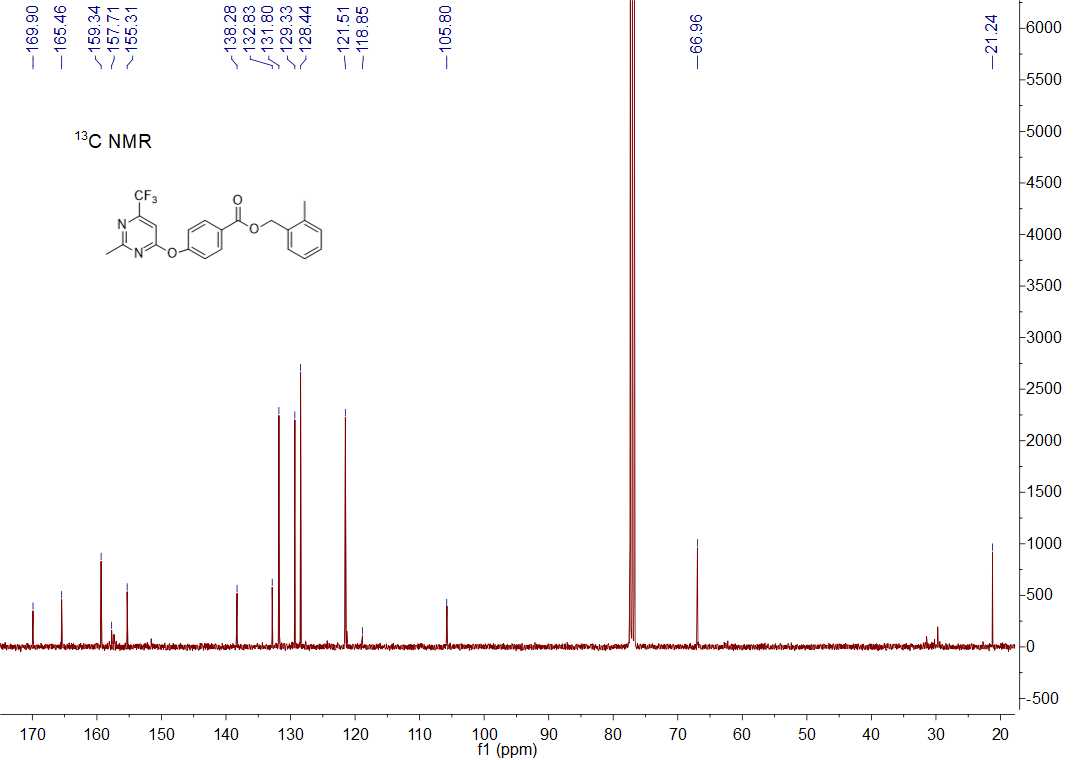
19F NMR spectrum of compound **5m**



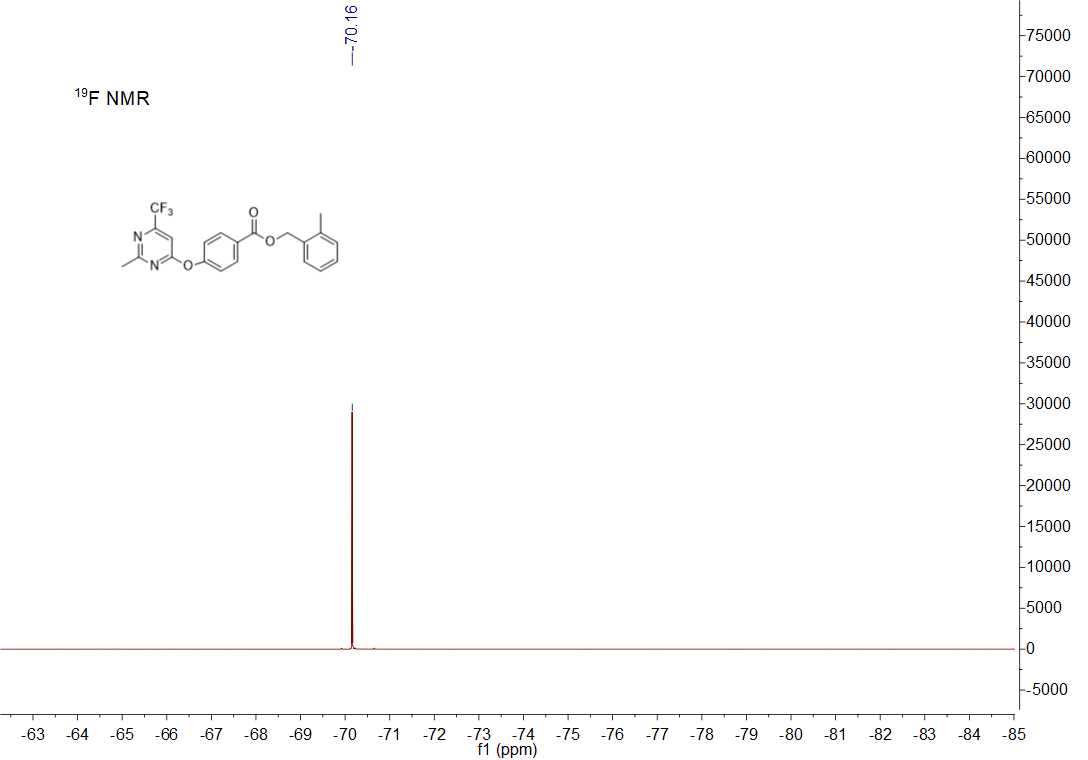
HRMS (ESI) spectrum of compound **5m**



1H NMR spectrum of compound **5n**



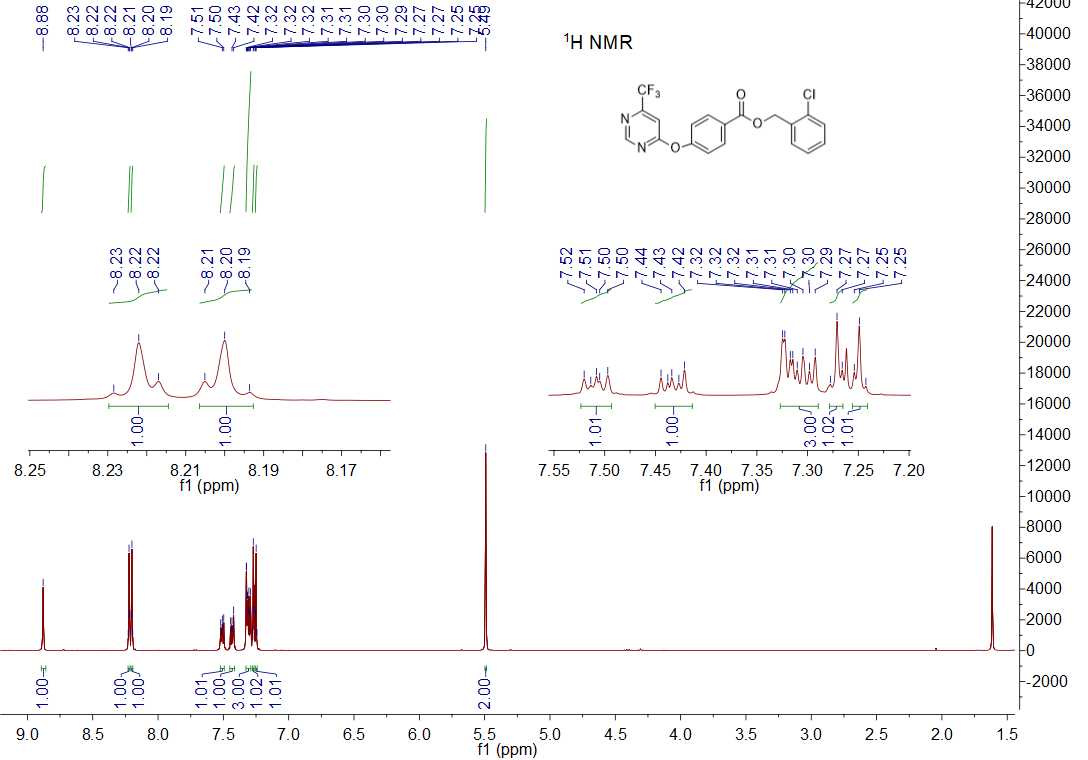
13C NMR spectrum of compound **5n**



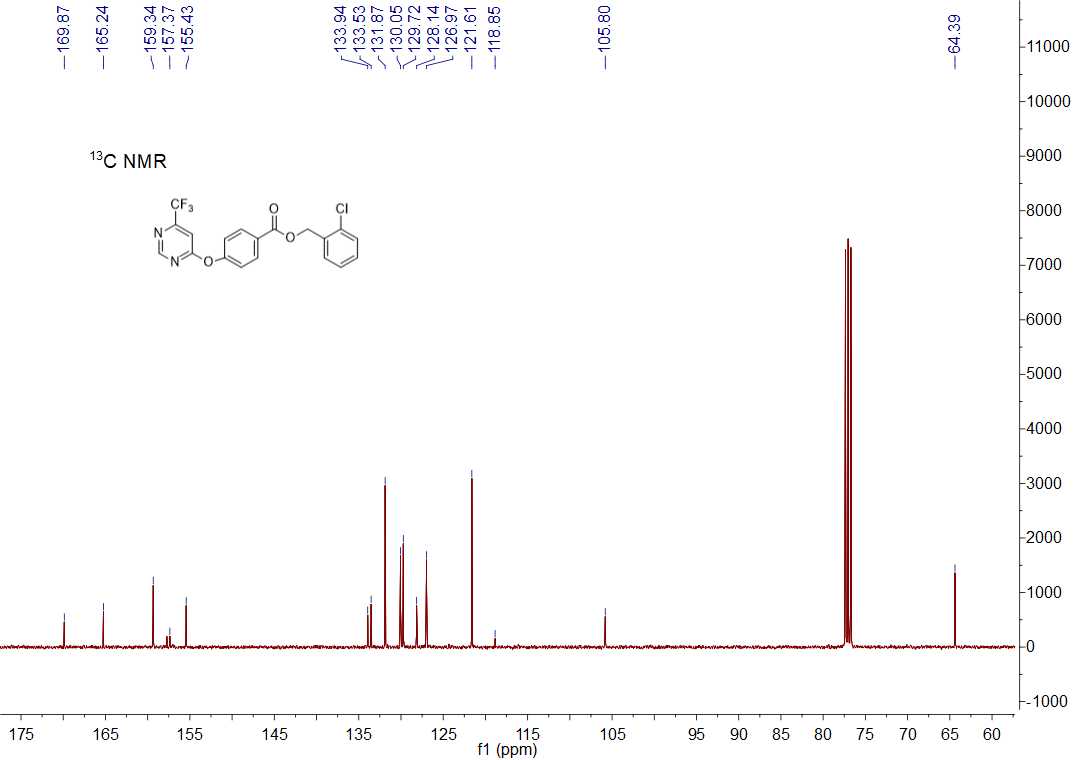
19F NMR spectrum of compound **5n**



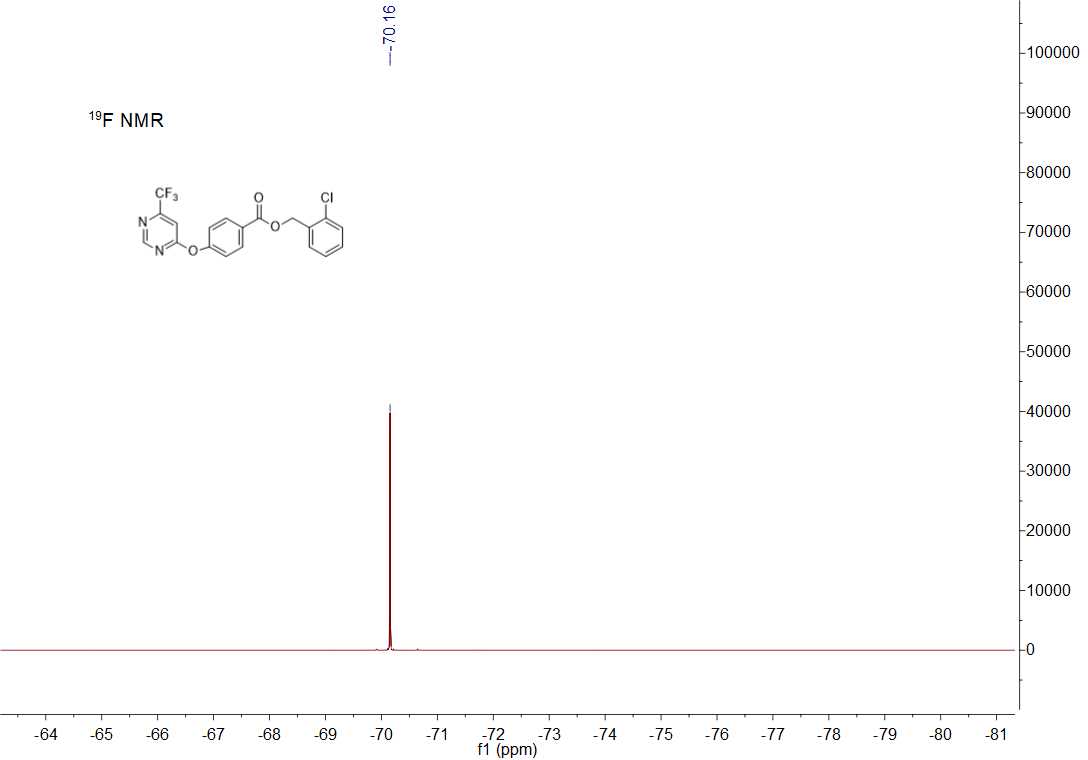
HRMS (ESI) spectrum of compound **5n**



1H NMR spectrum of compound **5o**



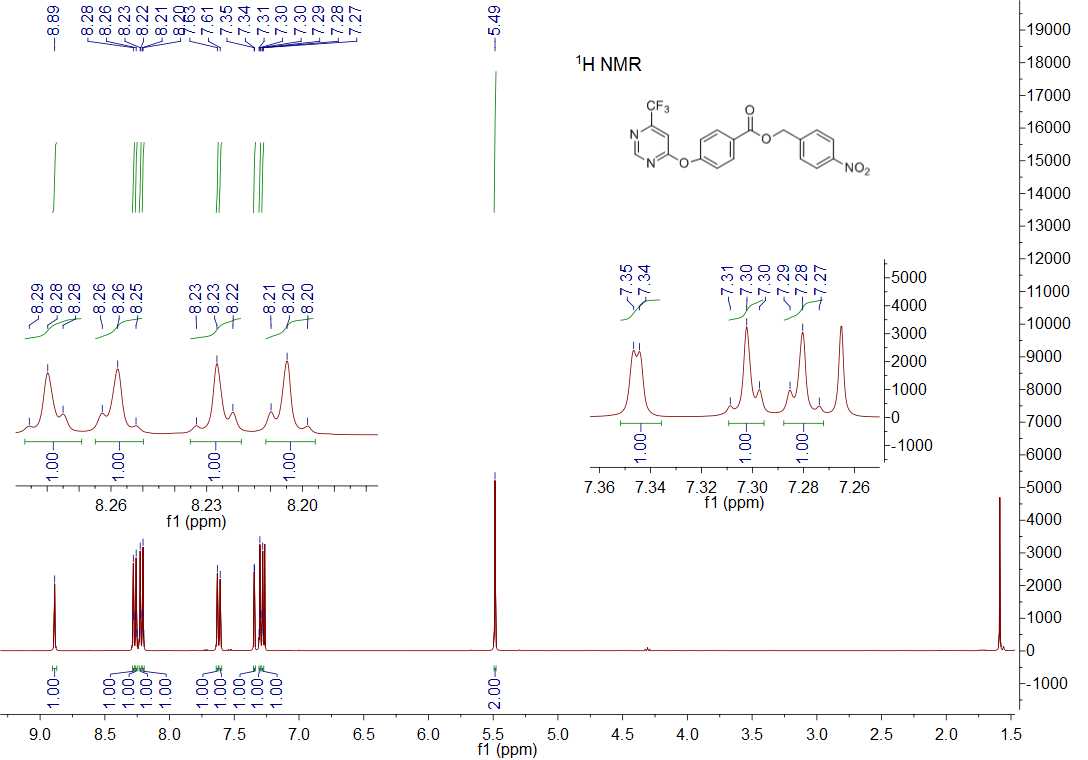
13C NMR spectrum of compound **5o**



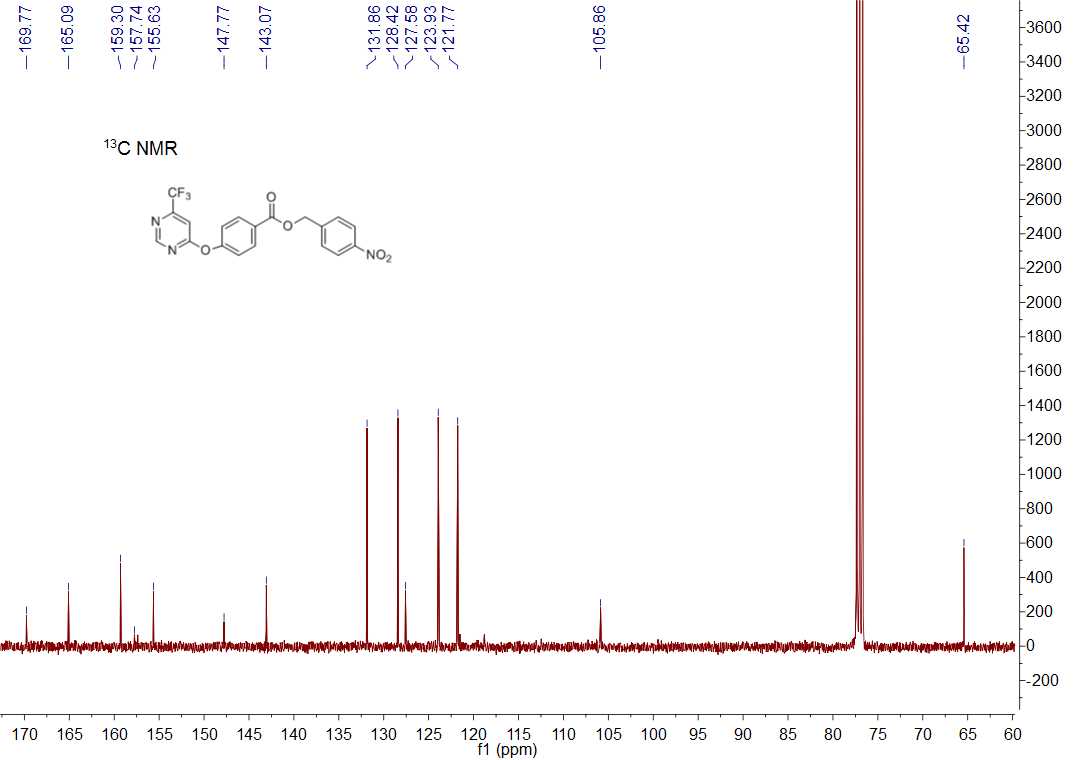
19F NMR spectrum of compound **5o**



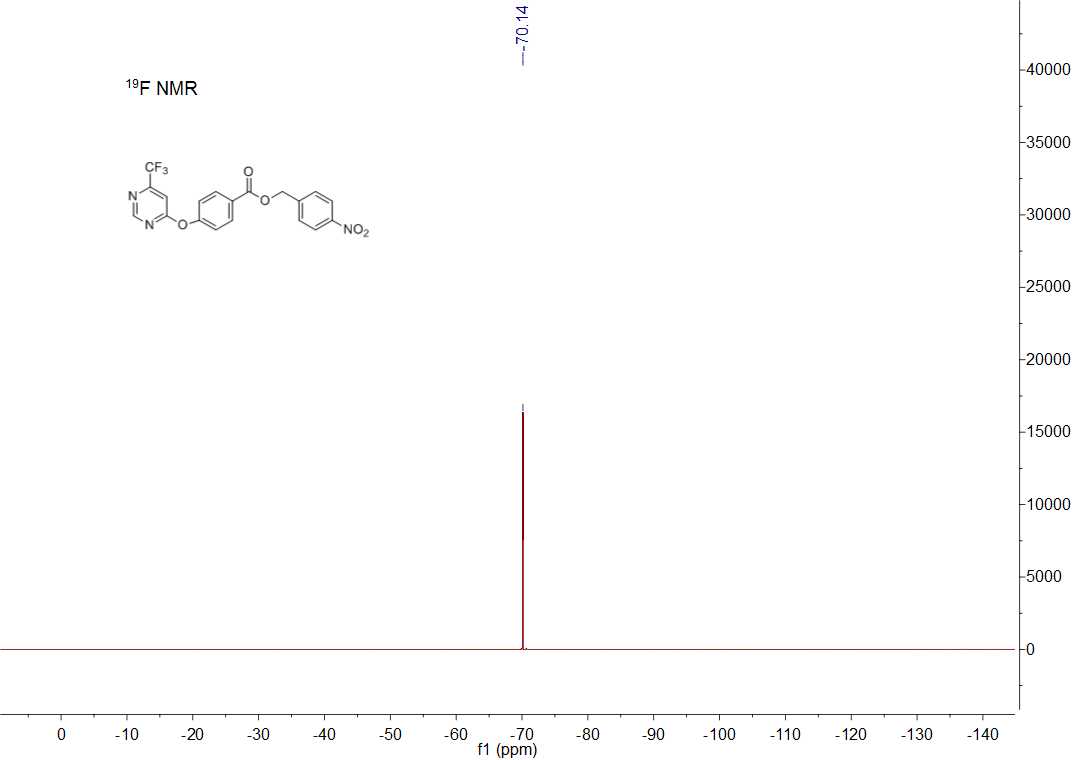
HRMS (ESI) spectrum of compound **5o**



1H NMR spectrum of compound **5p**



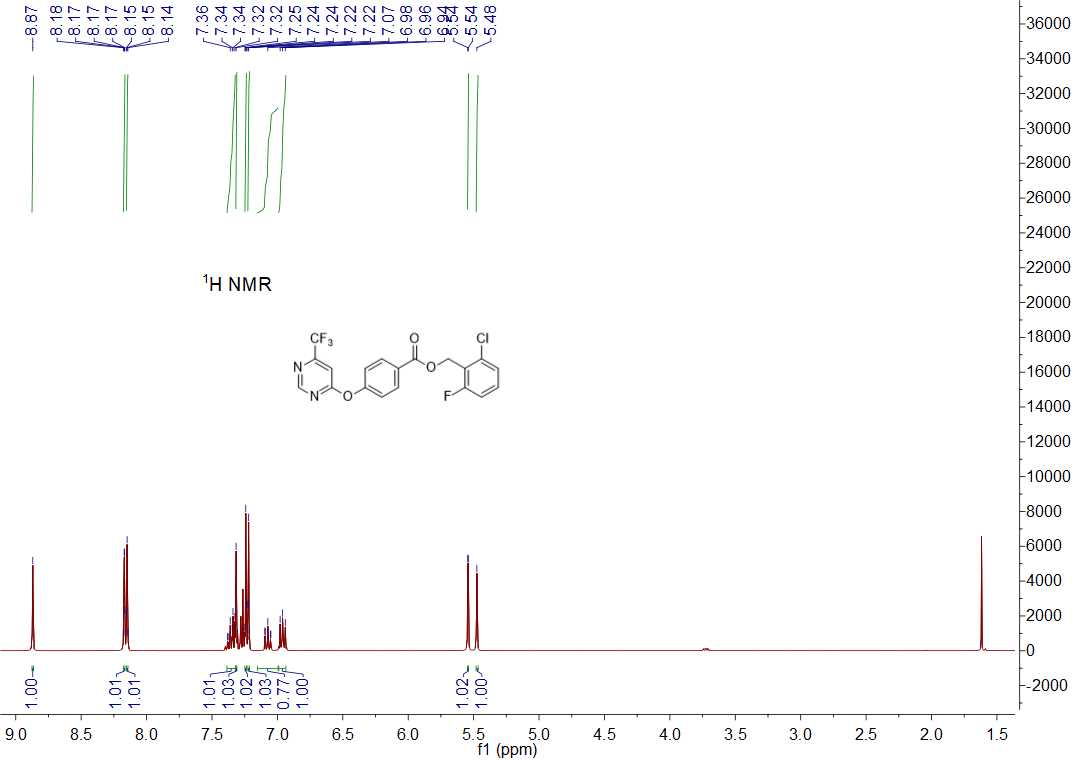
13C NMR spectrum of compound **5p**



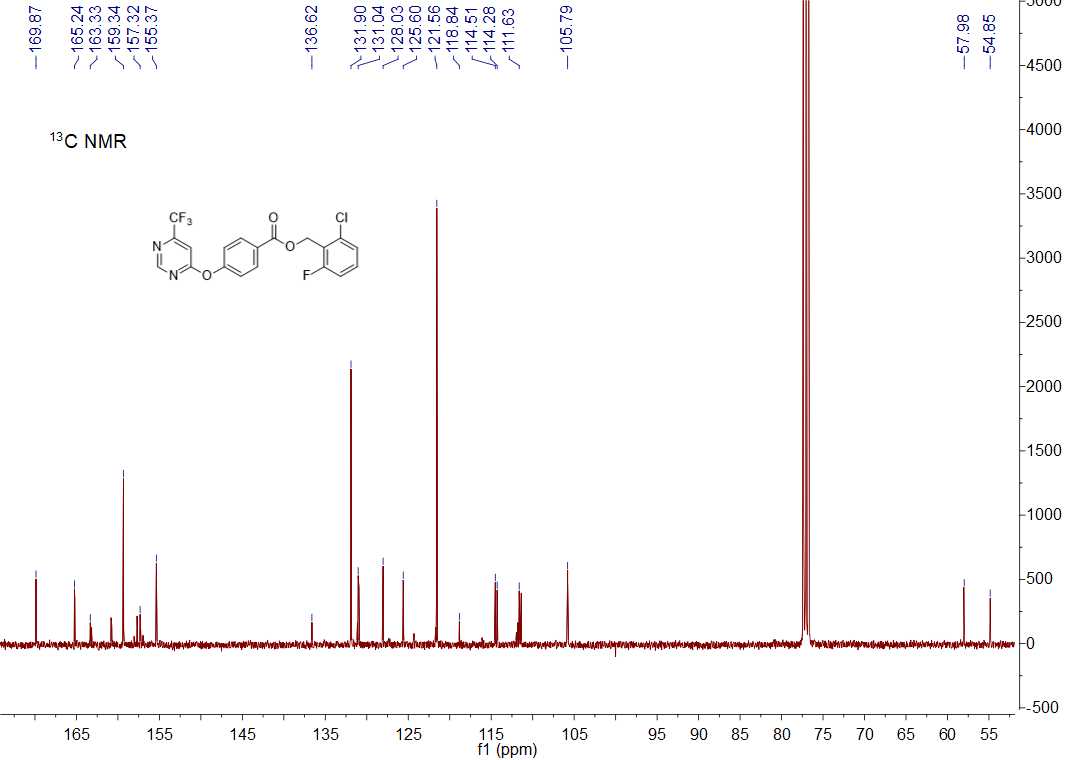
19F NMR spectrum of compound **5p**



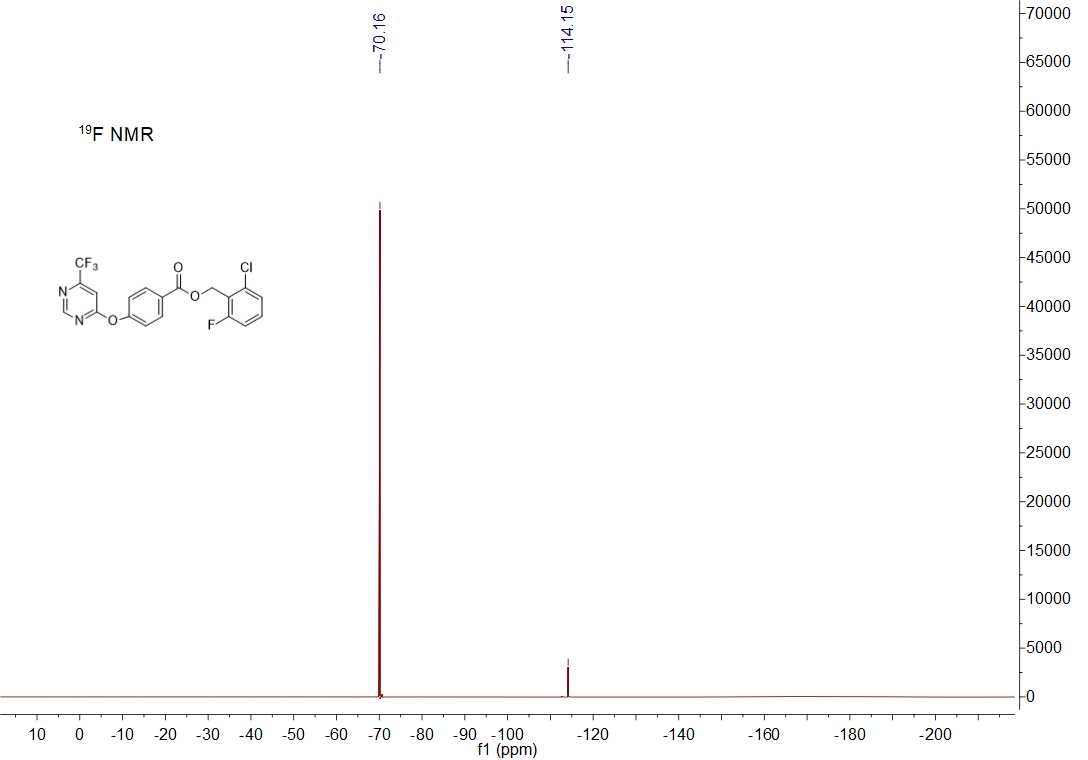
HRMS (ESI) spectrum of compound **5p**



1H NMR spectrum of compound **5q**



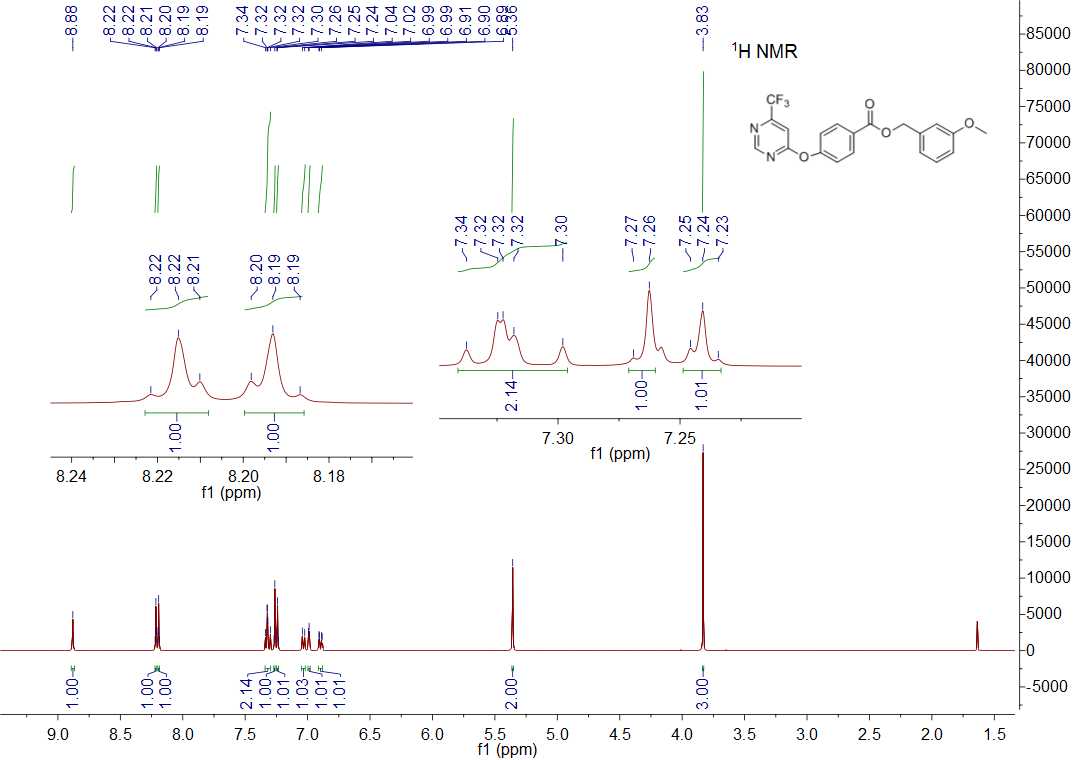
13C NMR spectrum of compound **5q**



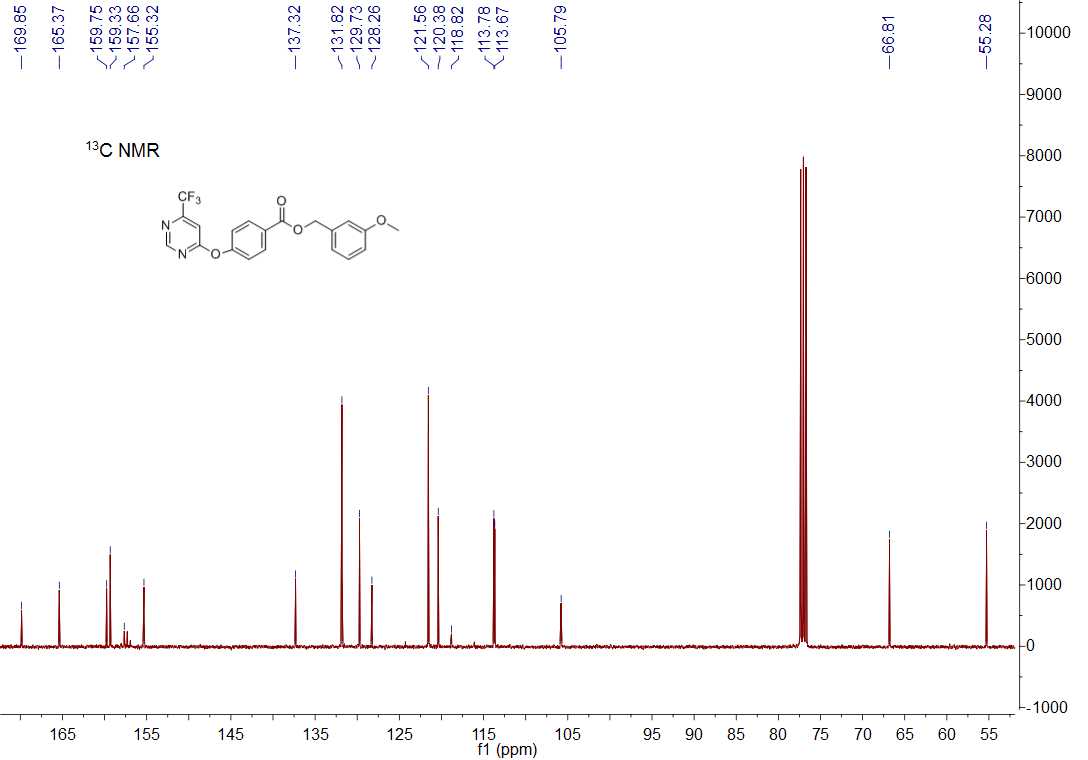
19F NMR spectrum of compound **5q**



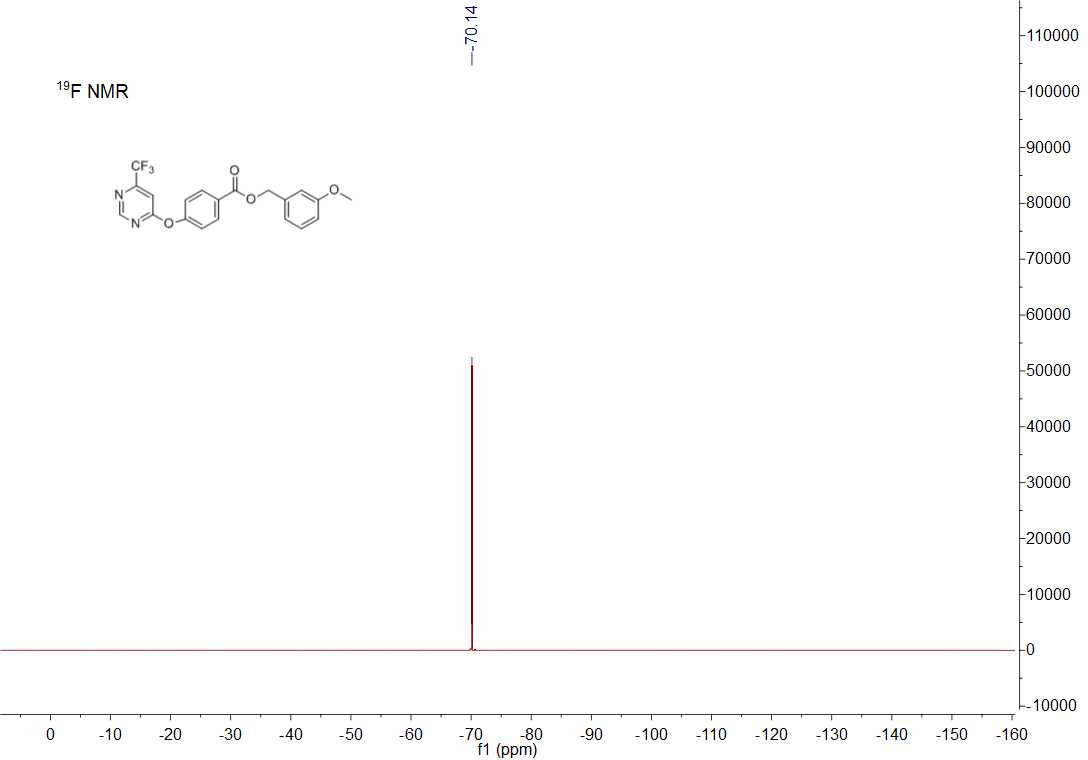
HRMS (ESI) spectrum of compound **5q**



1H NMR spectrum of compound **5r**



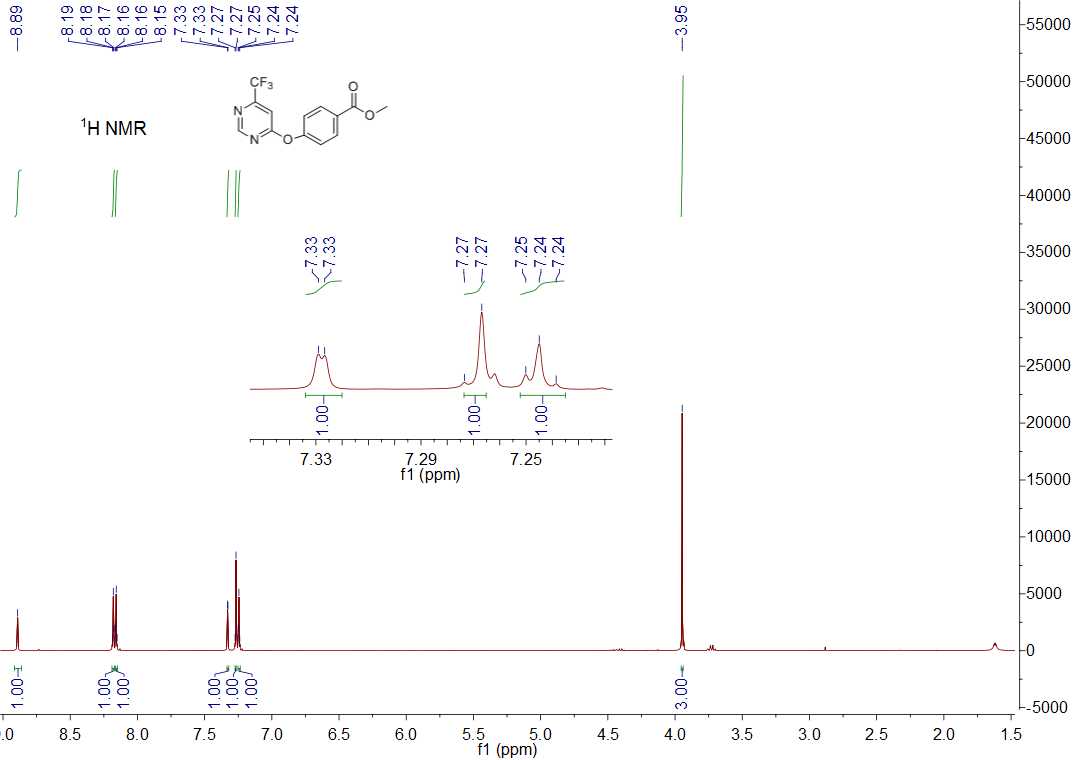
13C NMR spectrum of compound **5r**



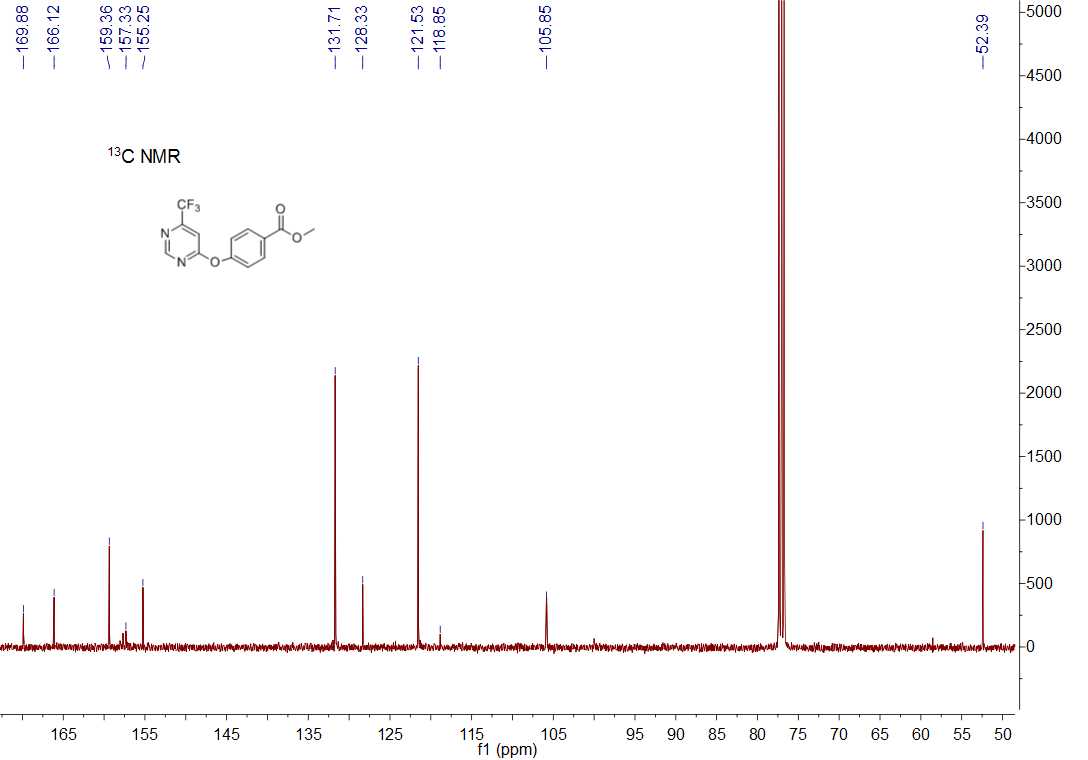
19F NMR spectrum of compound **5r**



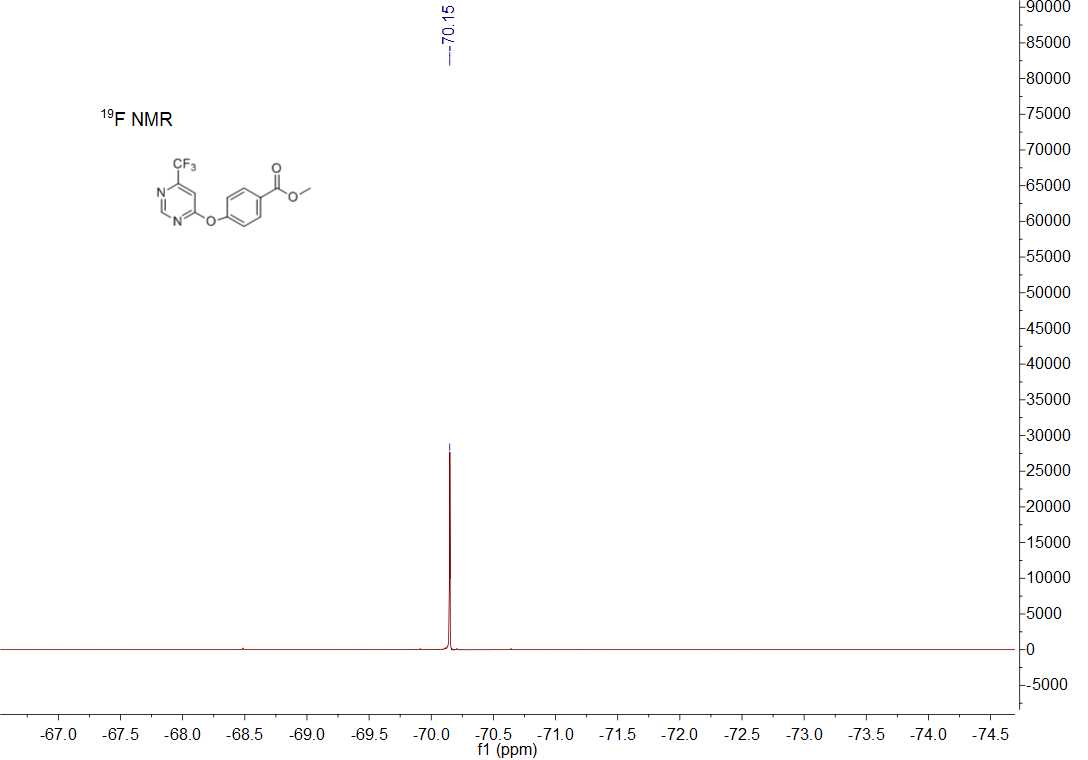
HRMS (ESI) spectrum of compound **5r**



1H NMR spectrum of compound **5s**



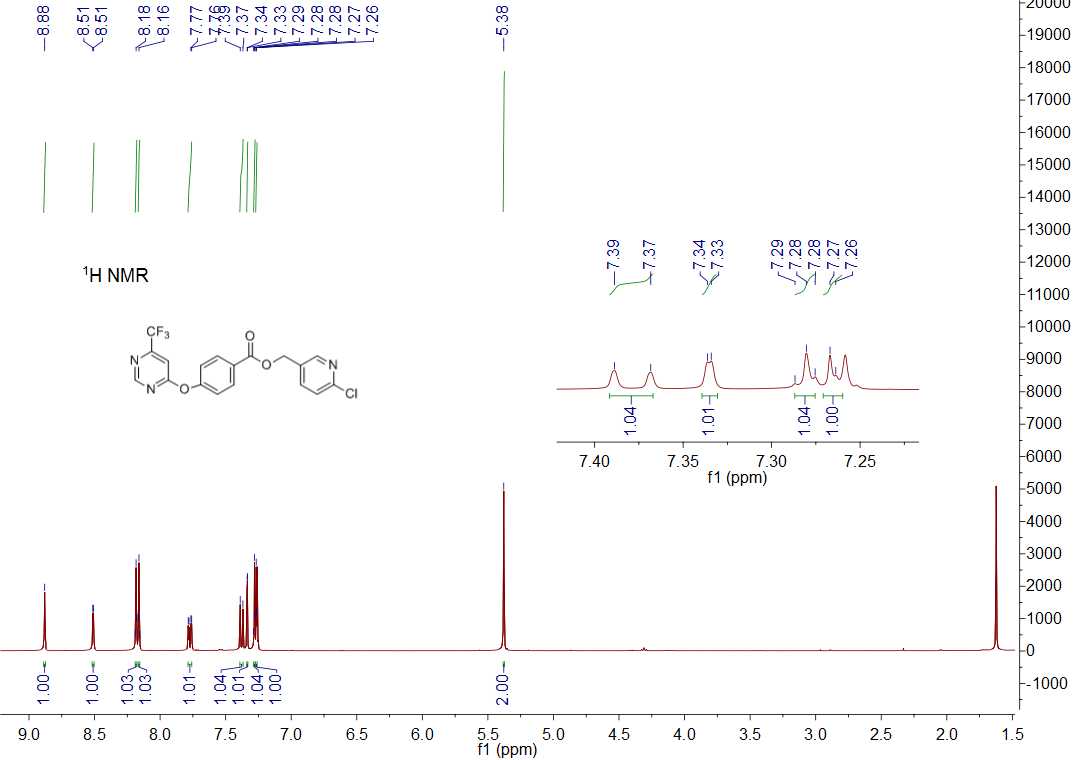
13C NMR spectrum of compound **5s**



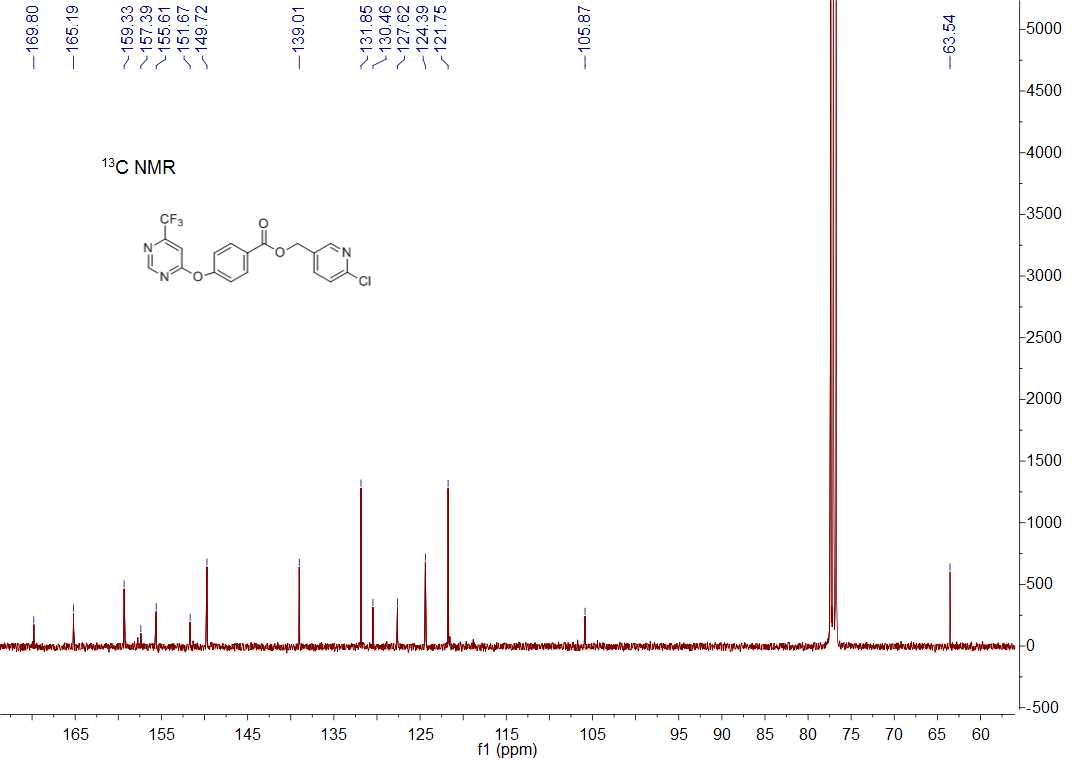
19F NMR spectrum of compound **5s**



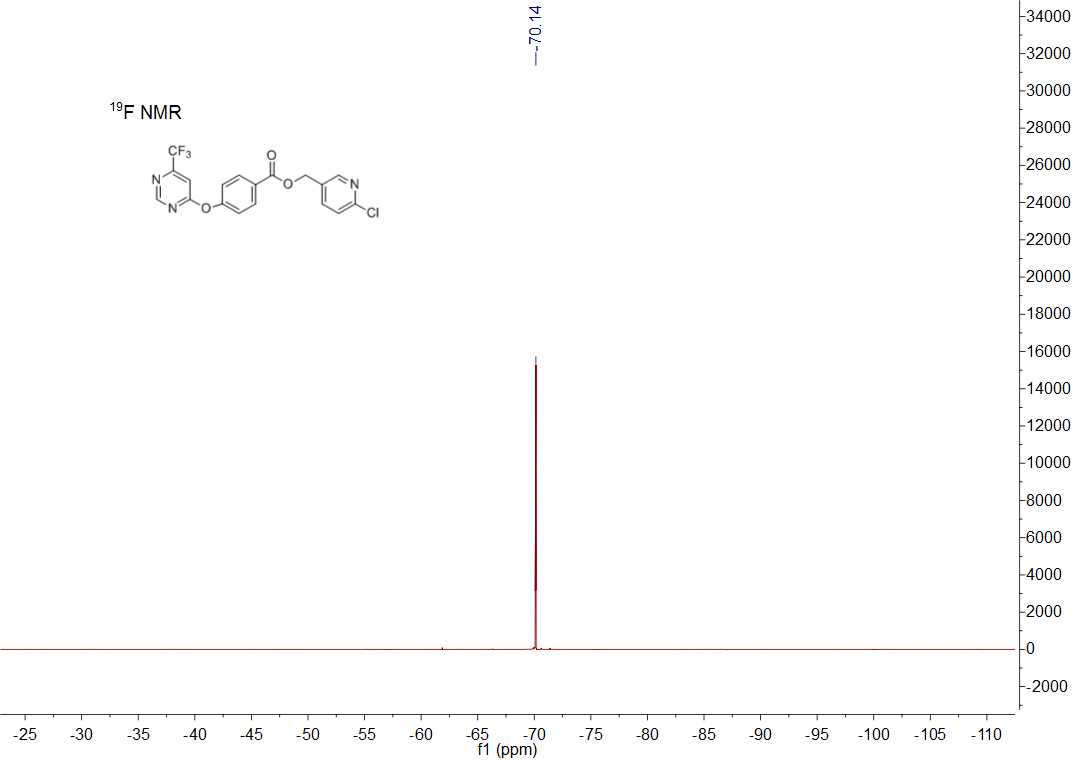
HRMS (ESI) spectrum of compound **5s**



1H NMR spectrum of compound **5t**



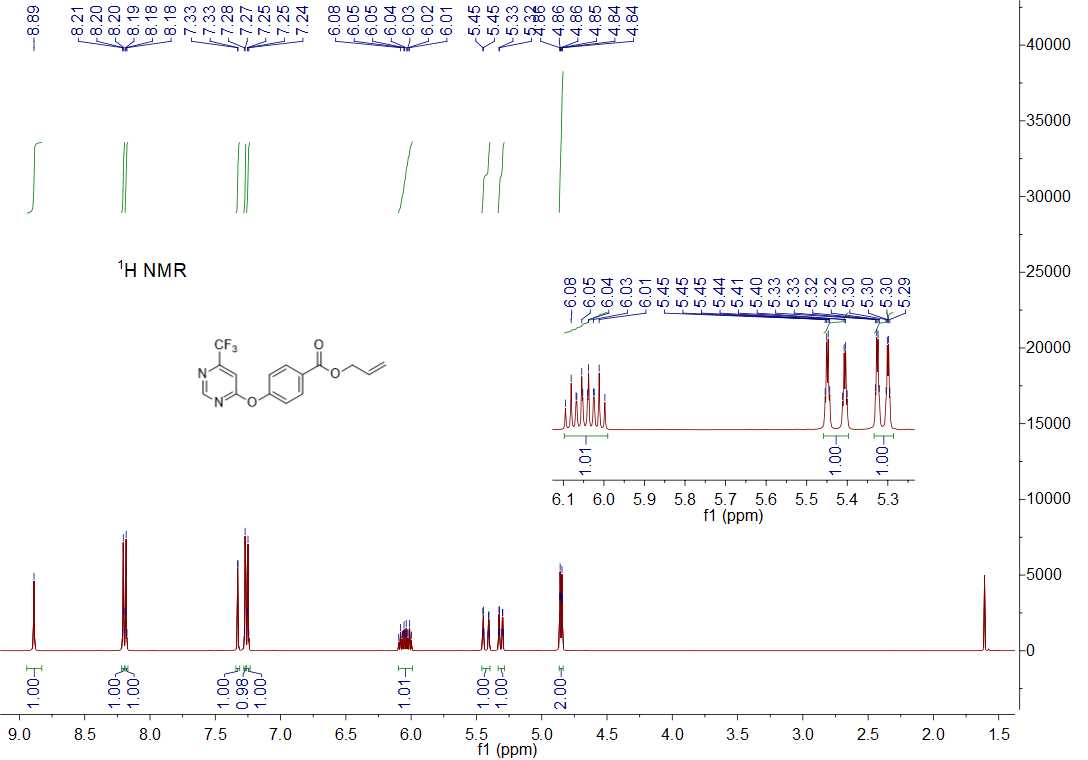
13C NMR spectrum of compound **5t**



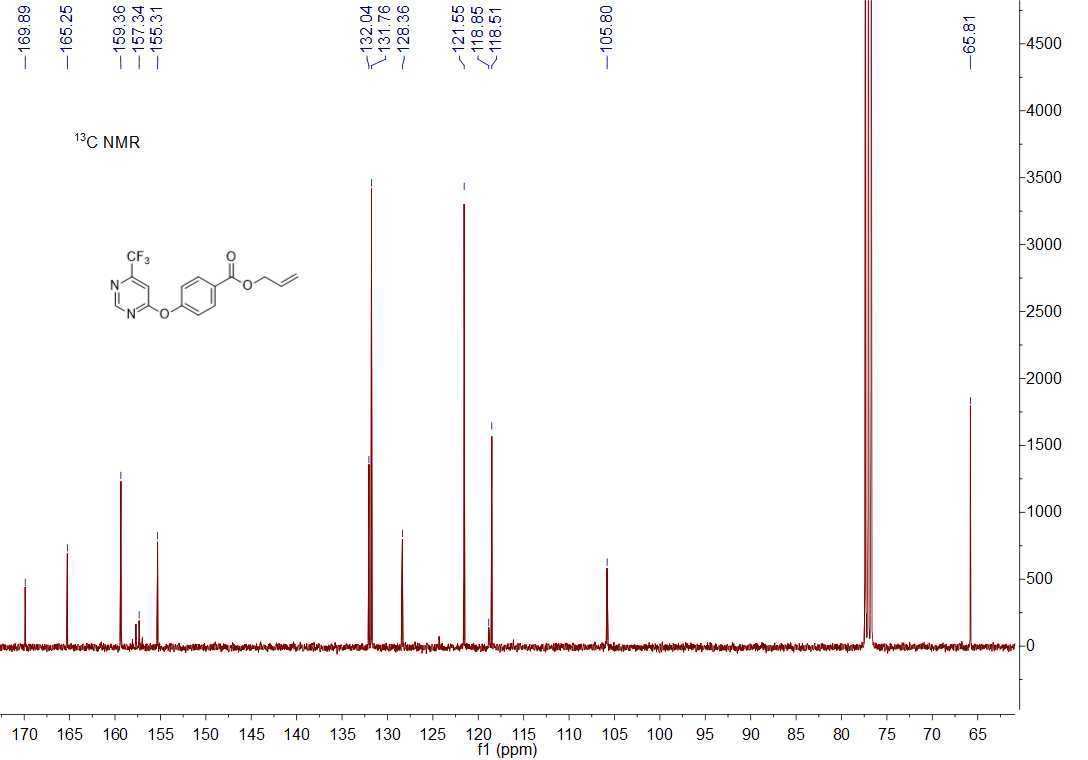
19F NMR spectrum of compound **5t**



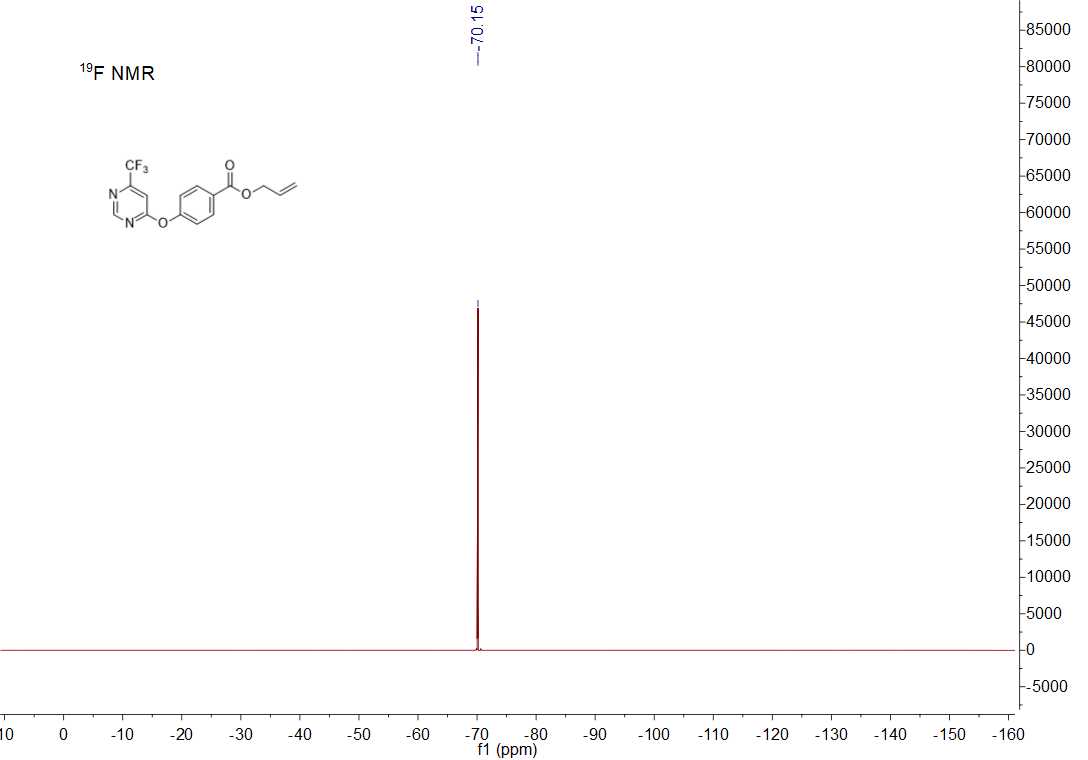
HRMS (ESI) spectrum of compound **5t**



1H NMR spectrum of compound **5u**



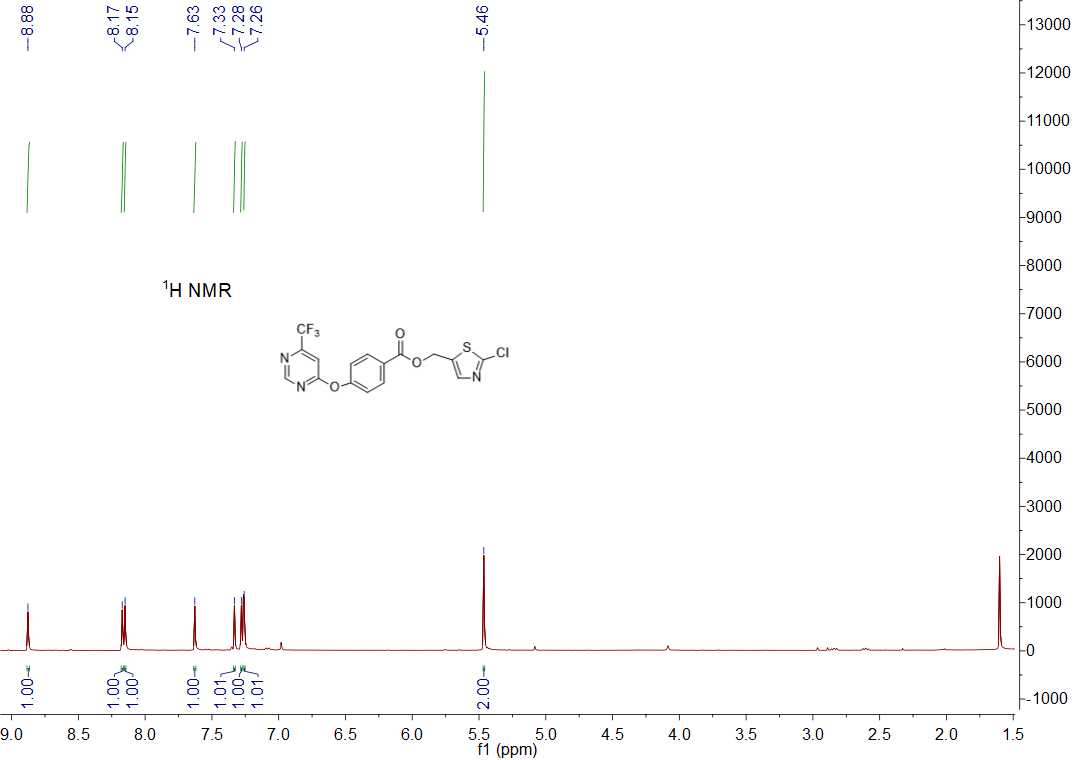
13C NMR spectrum of compound **5u**



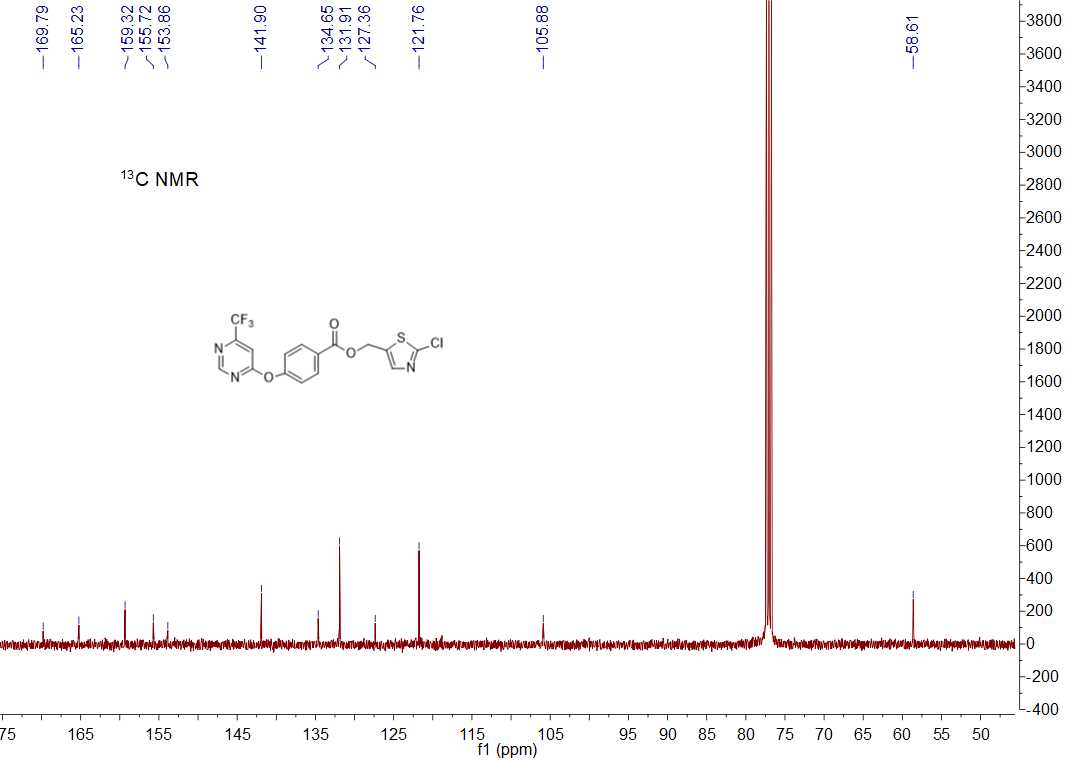
19F NMR spectrum of compound **5u**



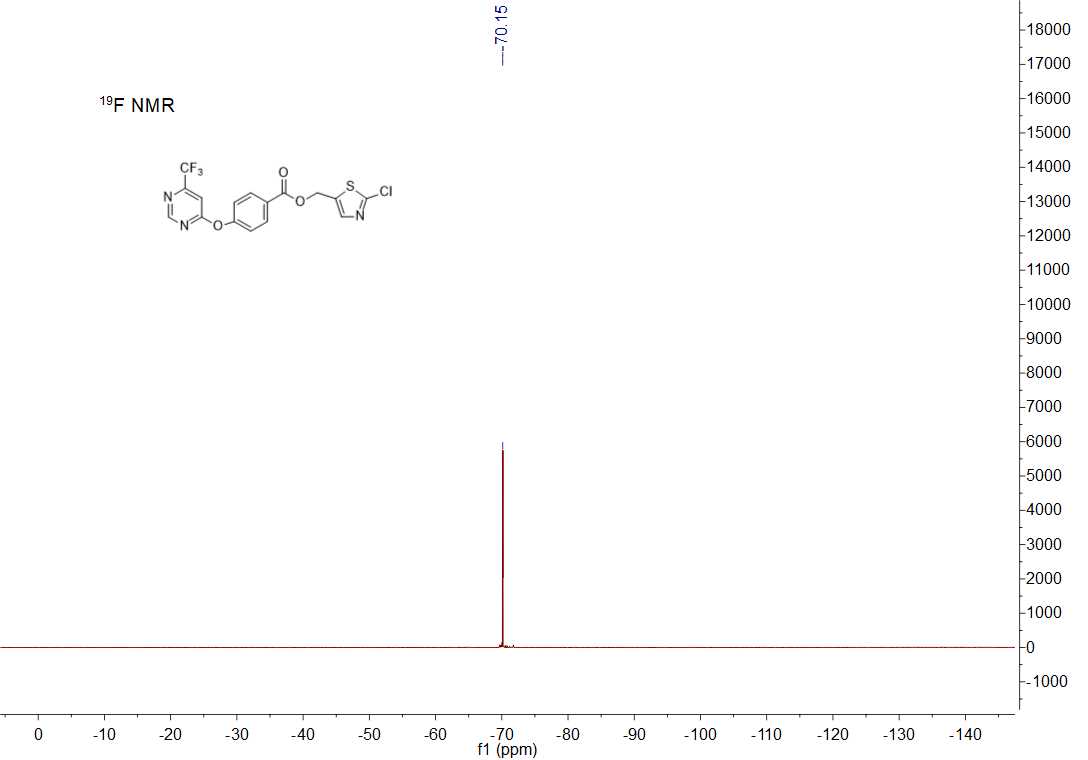
HRMS (ESI) spectrum of compound **5u**



1H NMR spectrum of compound **5v**



13C NMR spectrum of compound **5v**



19F NMR spectrum of compound **5v**



HRMS (ESI) spectrum of compound **5v**