

## SUPPLEMENTARY MATERIALS

# General, Practical and Selective Oxidation Protocol for CF<sub>3</sub>S into CF<sub>3</sub>S(O) group

Liubov V. Sokolenko<sup>1</sup>, Raisa K. Orlova<sup>1</sup>, Andrey A. Filatov<sup>1</sup>, Yurii L. Yagupolskii<sup>1,3,\*</sup>, Emmanuel Magnier<sup>2,\*</sup>, Bruce Pégot<sup>2</sup>, Patrick Diter<sup>2</sup>

<sup>1</sup> Institute of Organic Chemistry, National Academy of Sciences of Ukraine, Murmans'ka Str. 5, 02094 Kyiv, Ukraine; yagupolskii@ioch.kiev.ua

<sup>2</sup> Bâtiment Lavoisier, Université de Versailles-Saint-Quentin, 45 avenue des Etats-Unis, 78035 Versailles, France; emmanuel.magnier@uvsq.fr

<sup>3</sup> Enamine Ltd, A. Matrosova str. 23, Kiev 01103, Ukraine

\* Correspondence: yagupolskii@ioch.kiev.ua (Y.Y.); emmanuel.magnier@uvsq.fr (E.M.)

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### Measurement of the H<sub>2</sub>O<sub>2</sub> solution concentration by densimetry

Measurements of density were performed using set of hydrometers (notably, hydrometer with measurement range 1.000 to 1.060 g/cm<sup>3</sup>) “AOH-1” (Minpribor USSR, Production Association “Khimlaborpribor”, 1991 model year).

Table. Densities of H<sub>2</sub>O<sub>2</sub> solutions at 25°C.

| % H <sub>2</sub> O <sub>2</sub> (w/w) | density g/cm <sup>3</sup> | % H <sub>2</sub> O <sub>2</sub> (w/w) | density g/cm <sup>3</sup> |
|---------------------------------------|---------------------------|---------------------------------------|---------------------------|
| 0.0                                   | (0.9970)                  | 49.88                                 | 1.1909                    |
| 1.91                                  | 1.0036                    | 53.48                                 | 1.2067                    |
| 5.99                                  | 1.0179                    | 55.08                                 | 1.2143                    |
| 9.23                                  | 1.0295                    | 59.68                                 | 1.2353                    |
| 13.47                                 | 1.0452                    | 62.55                                 | 1.2490                    |
| 17.44                                 | 1.0597                    | 64.88                                 | 1.2593                    |
| 21.14                                 | 1.0737                    | 68.97                                 | 1.2790                    |
| 24.58                                 | 1.0868                    | 73.15                                 | 1.2996                    |
| 27.96                                 | 1.0996                    | 73.66                                 | 1.3024                    |
| 29.99                                 | 1.1078                    | 76.66                                 | 1.3166                    |
| 34.23                                 | 1.1244                    | 80.64                                 | 1.3378                    |
| 39.12                                 | 1.1450                    | 84.97                                 | 1.3595                    |
| 40.67                                 | 1.1515                    | 89.68                                 | 1.3848                    |
| 42.97                                 | 1.1610                    | 89.78                                 | 1.3855                    |
| 47.02                                 | 1.1785                    | 89.89                                 | 1.3855                    |

Reference:

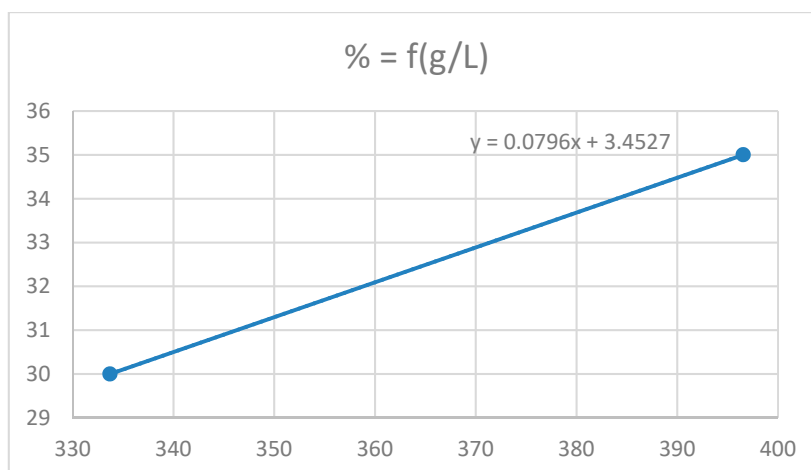
Easton, M.F.; Mitchell, A.G.; Wynne-Jones, W.F.K. The behaviour of mixtures of hydrogen peroxide and water. Part 1.-Determination of the densities of mixtures of hydrogen peroxide and water. *Trans. Faraday. Soc.* **1952**, 48, 796-801. DOI: 10.1039/TF9524800796

**Measurement of the H<sub>2</sub>O<sub>2</sub> solution concentration by titration.** Hydrogen peroxide was quantitatively oxidized by titration with a potassium permanganate solution of known strength under acidic conditions.

The initial solution is diluted to a hundredth (1mL of the solution of hydrogen peroxide in a 100 mL volumetric flask). Then 10 mL of this diluted solution was mixed with 10 mL of sulfuric acid (at 20%) and 10 mL of water. This resulting mixture was titrated twice with a solution of potassium permanganate ( $c = 2.001 \cdot 10^{-2}$  mol/L) until the first appearance of a faint pink color that persists for 30 seconds. An equivalent volume of 20.5 mL was obtained for both experiments giving a concentration of 10.255 mol/L or 348.67g/L

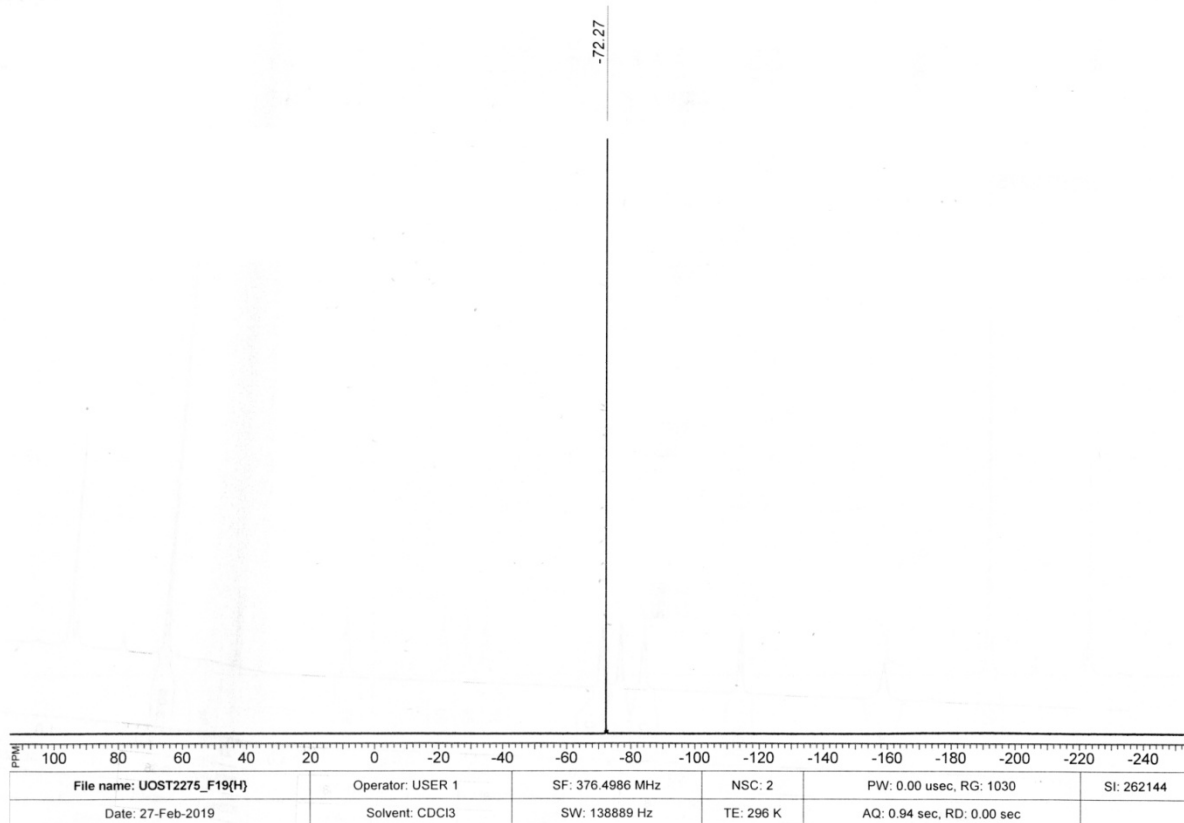
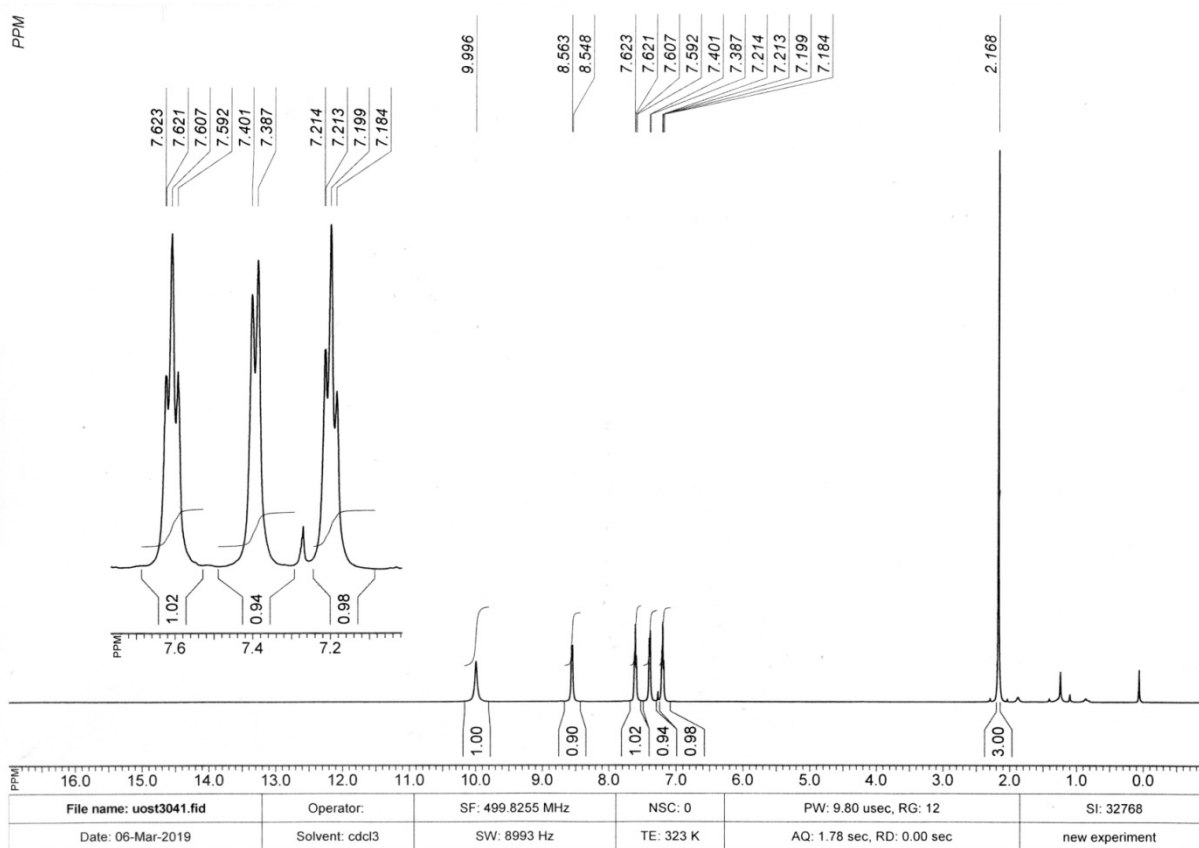
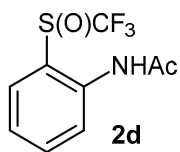
$$C_{H_2O_2} = 5/2 (C_{KMnO_4} * V_{eq}/V_{H_2O_2})$$

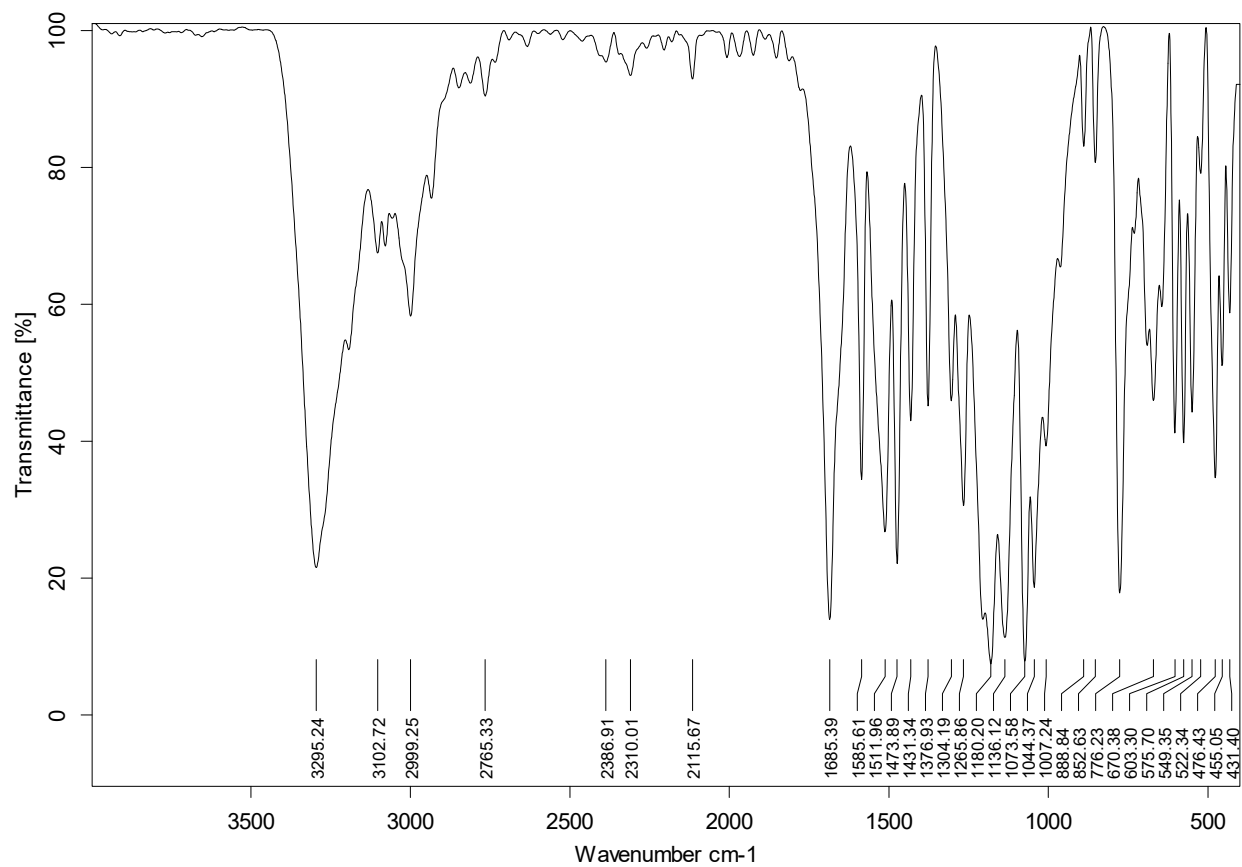
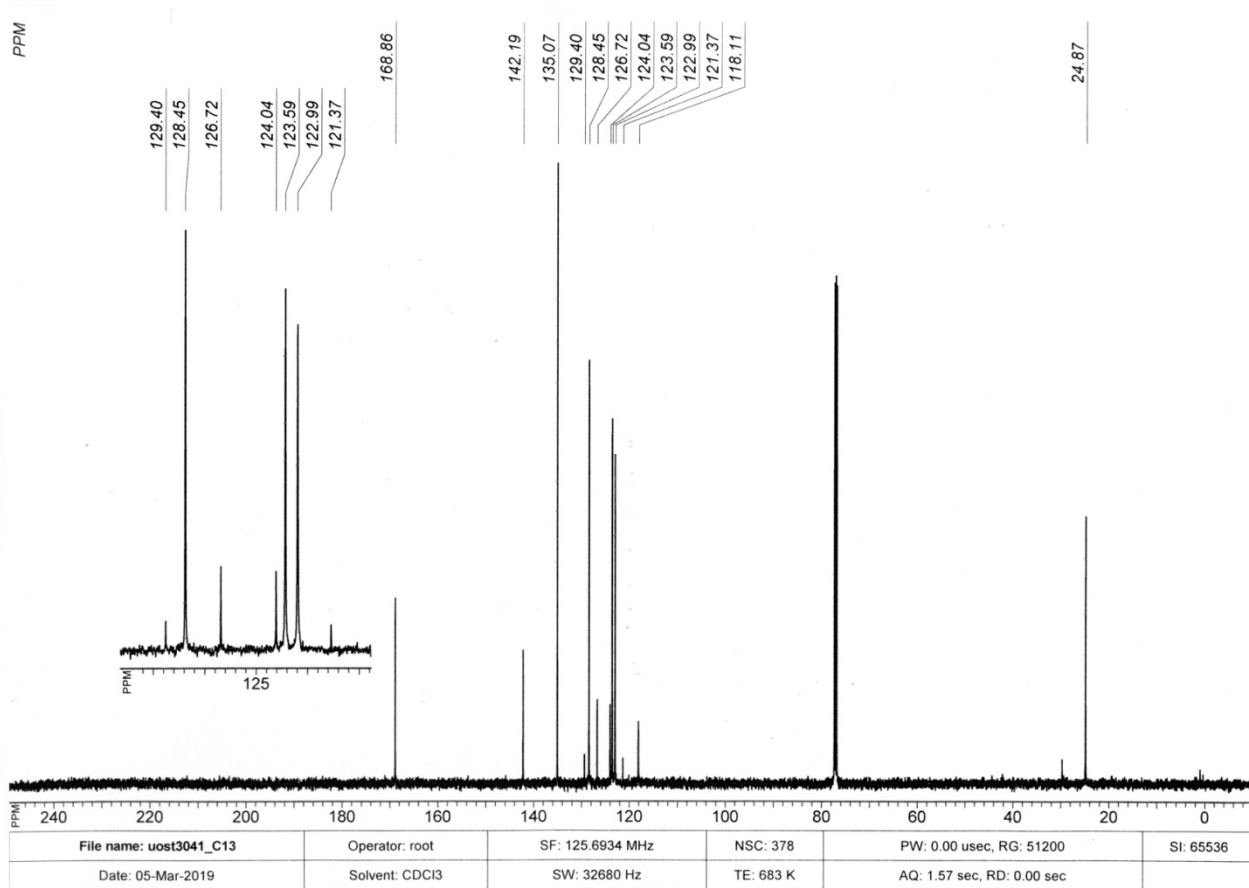
With the table of concentration in percent we deduced a concentration of 31.2% for the initial solution.



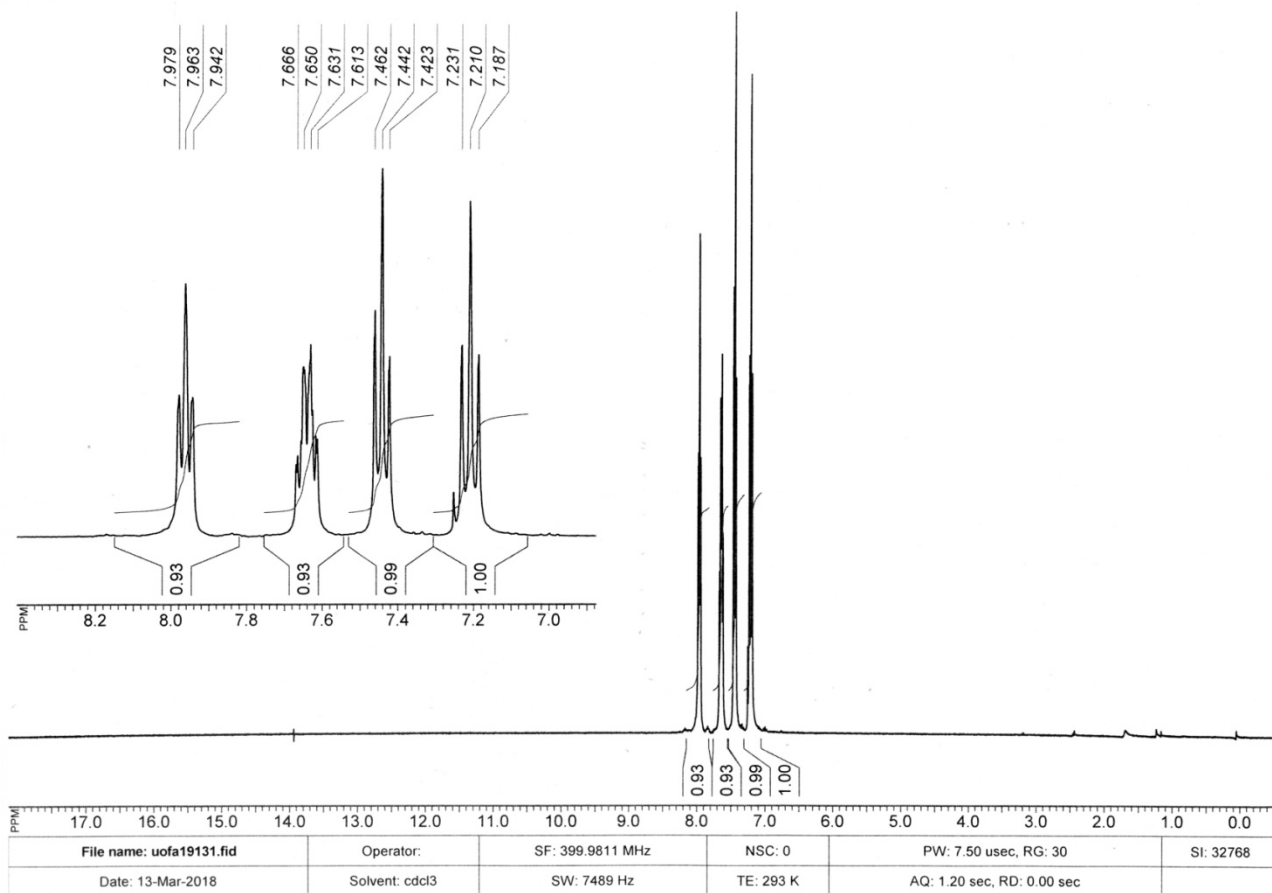
# Spectra of new products

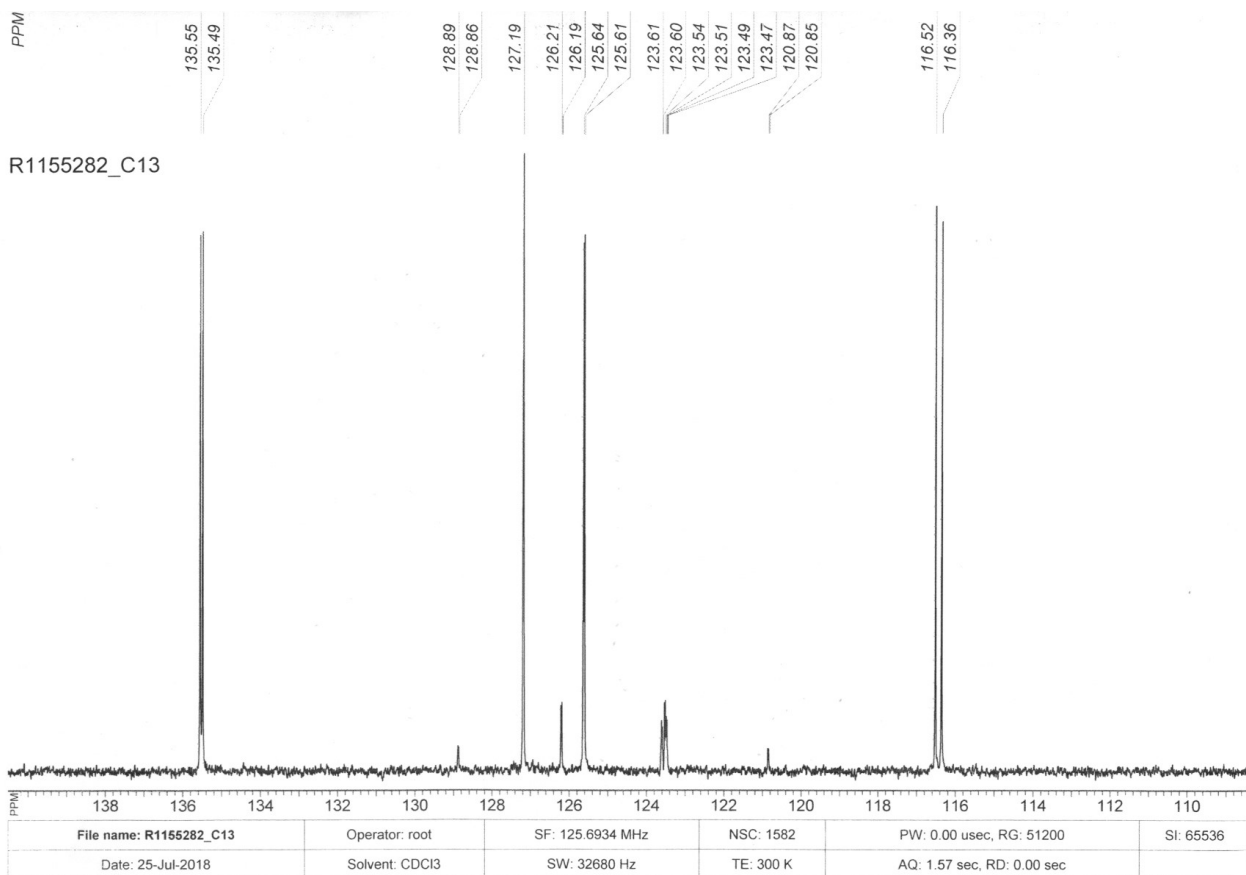
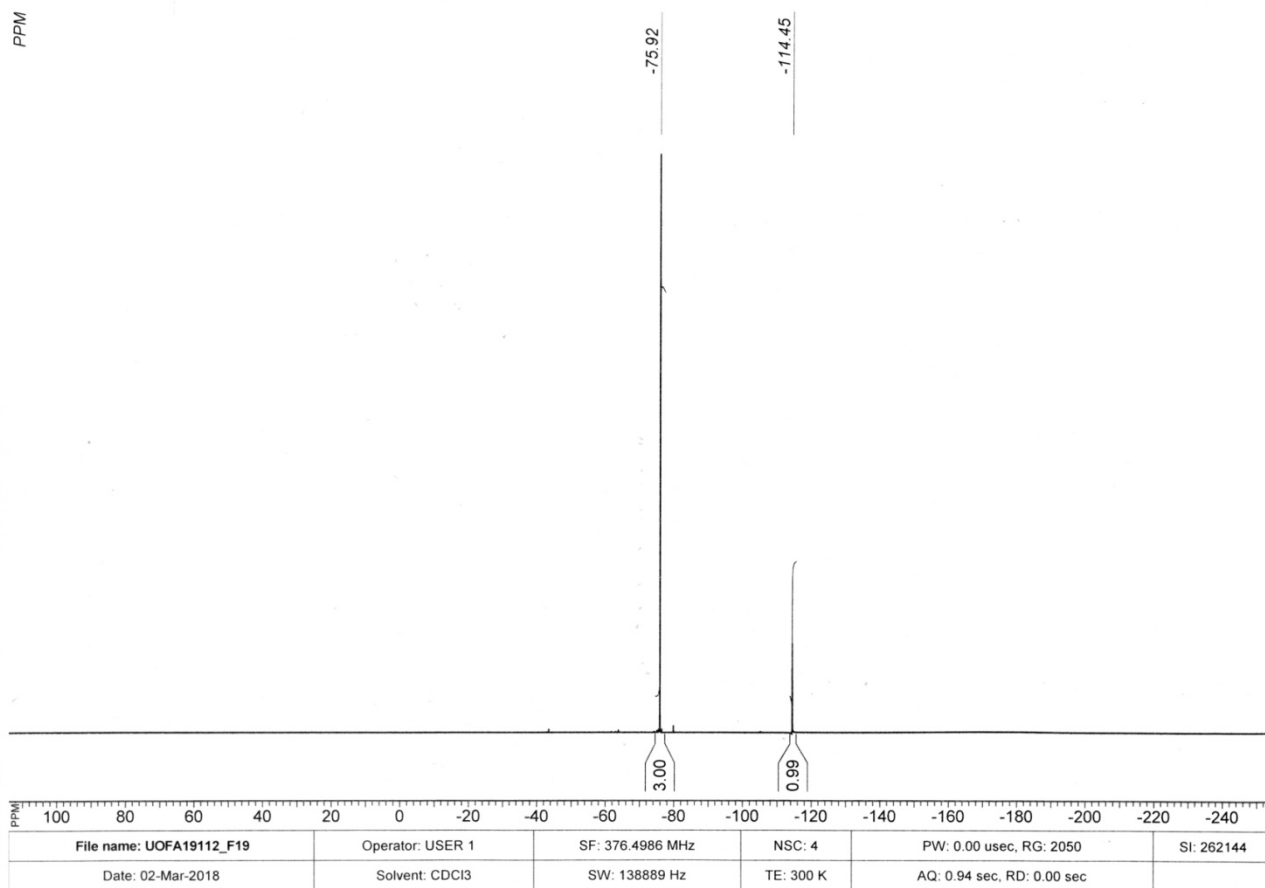
## N-(2-((Trifluoromethyl)sulfinyl)phenyl)acetamide.

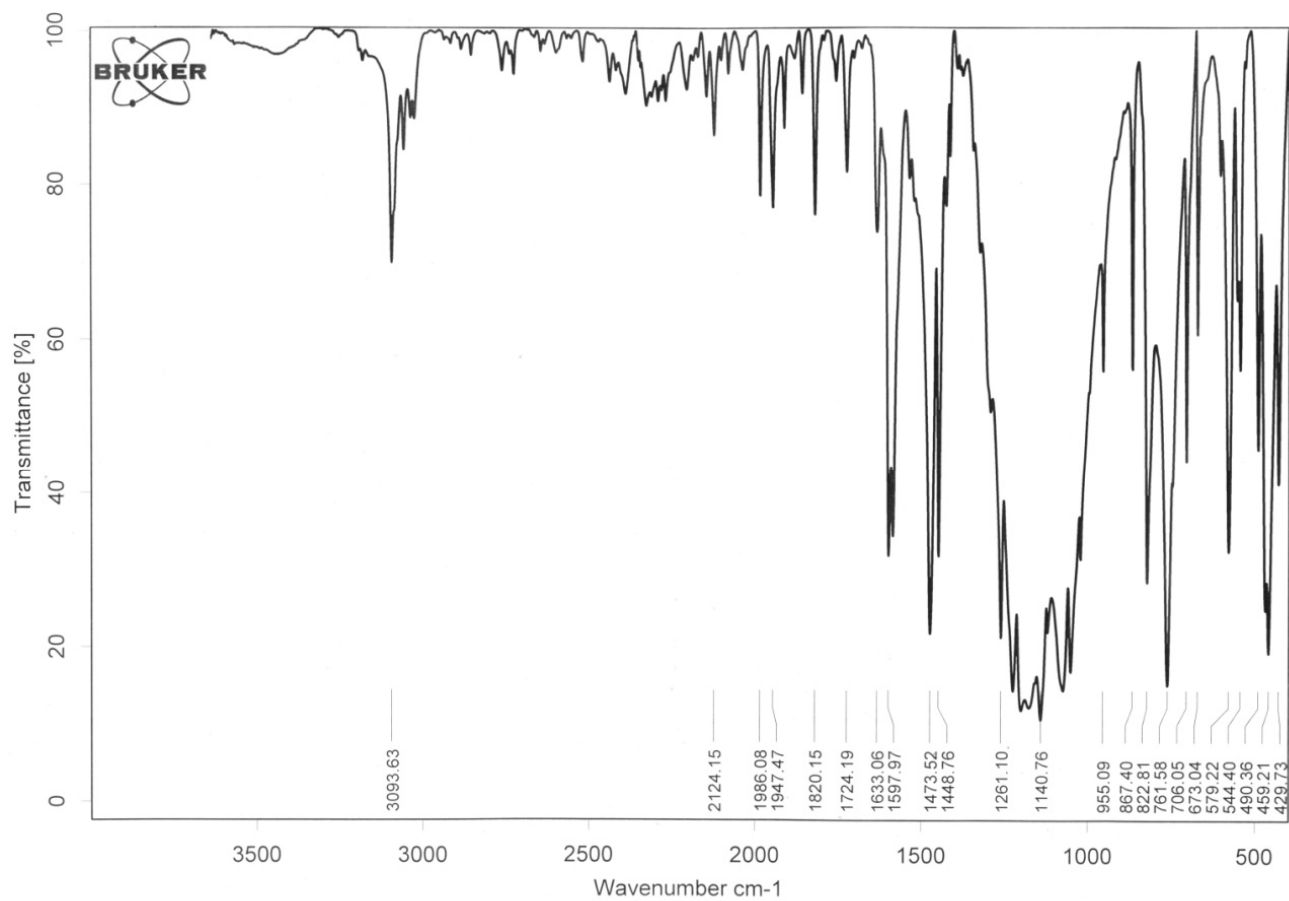
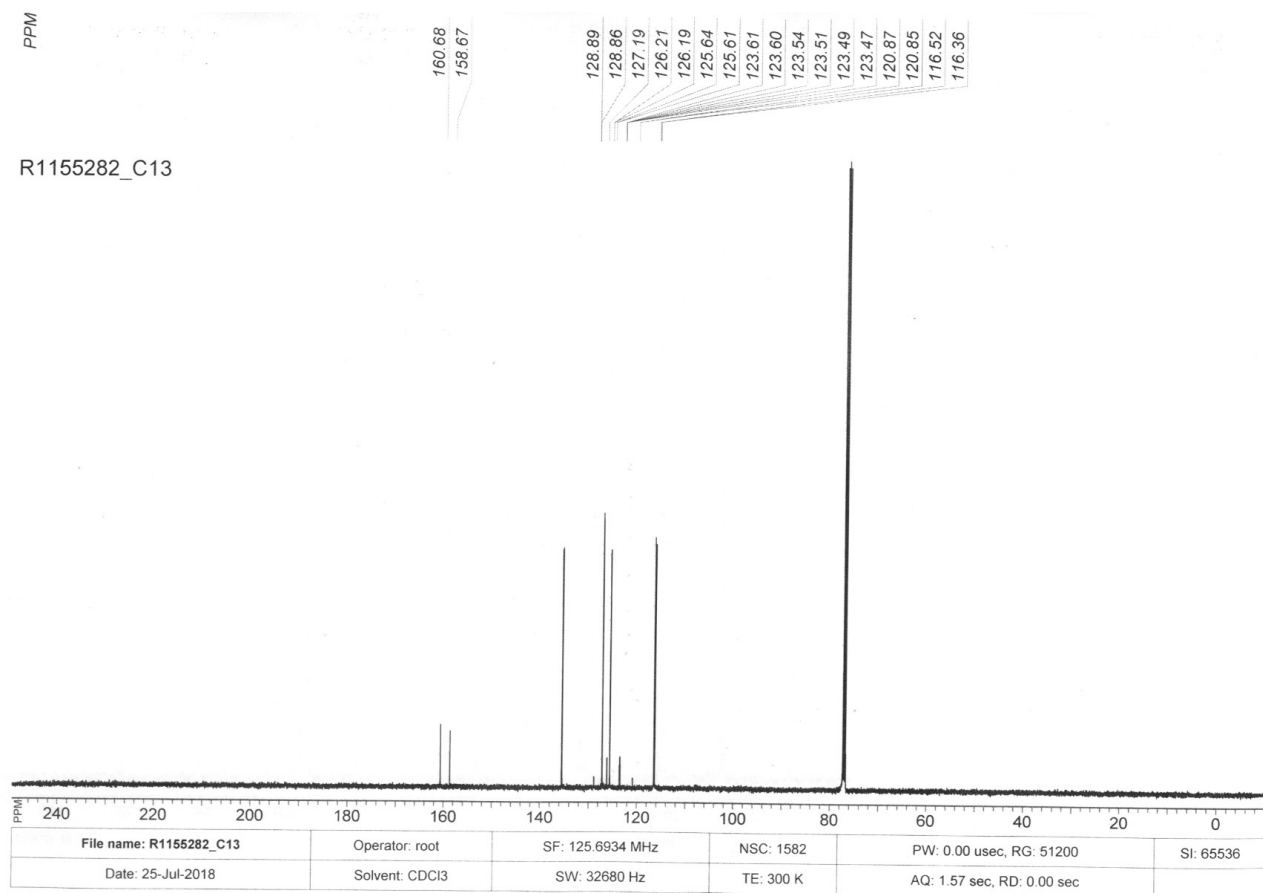




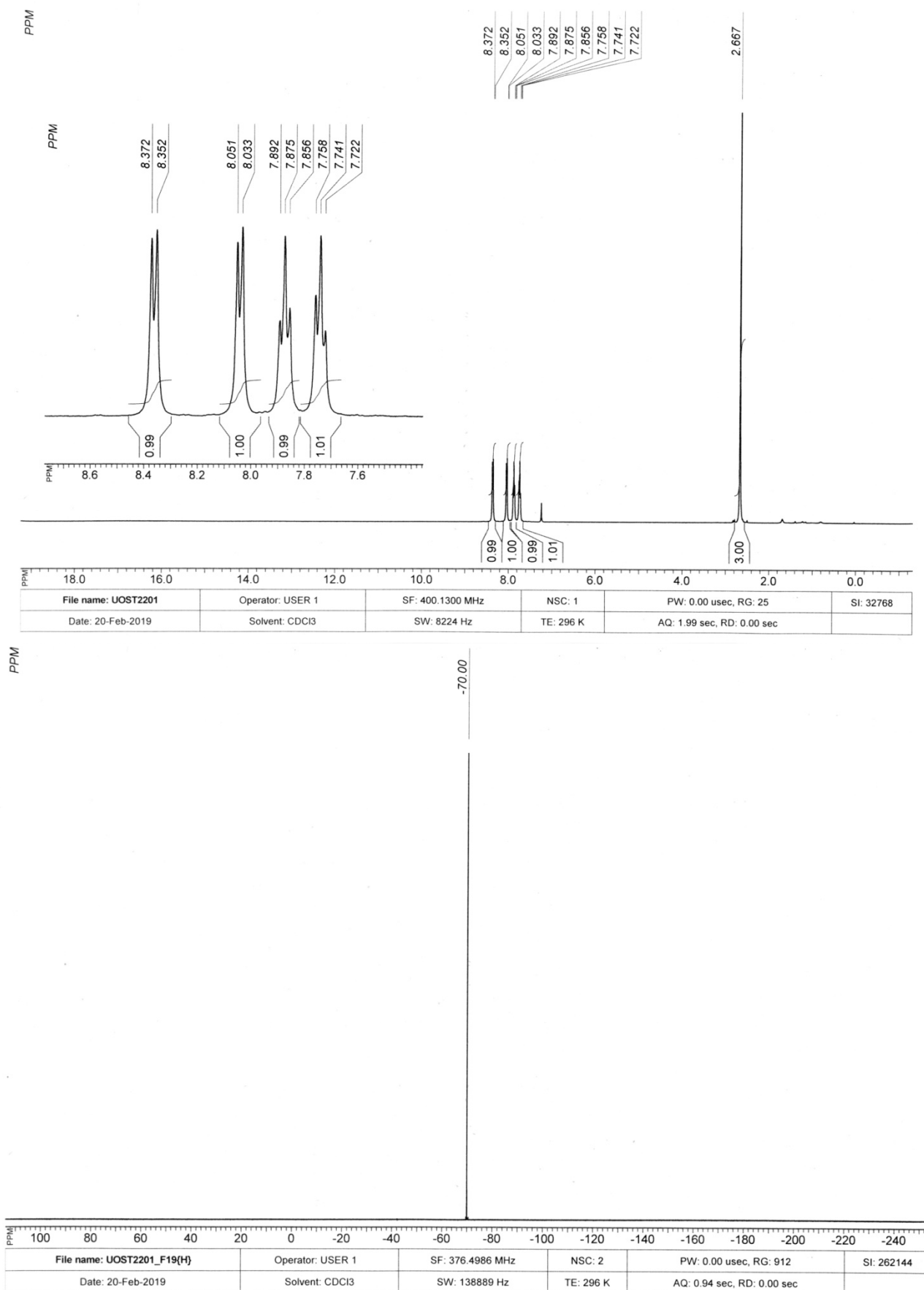
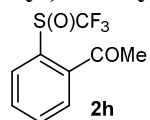


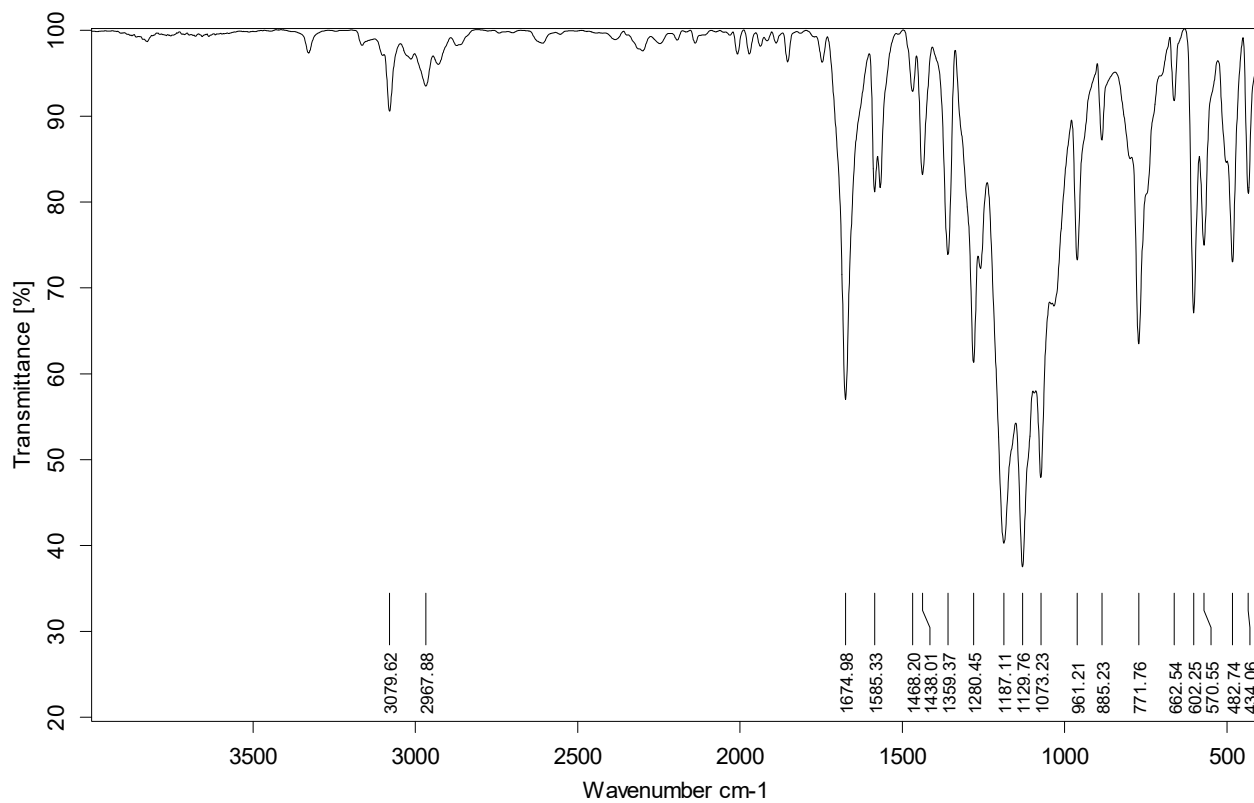
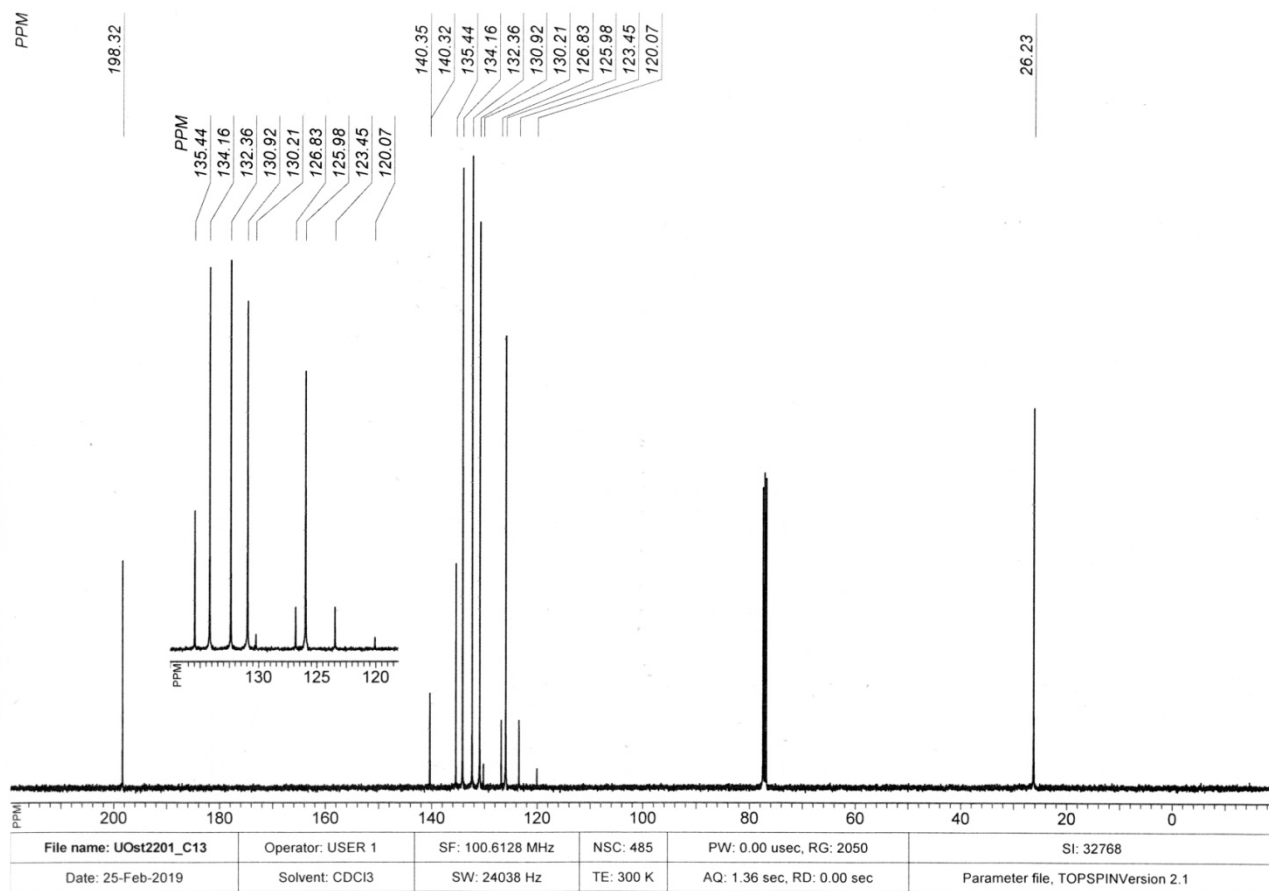
**1-Fluoro-2-((trifluoromethyl)sulfinyl)benzene.**





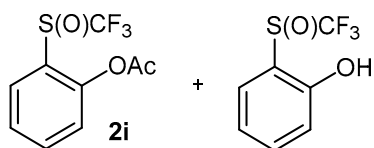
# 2-((Trifluoromethyl)sulfinyl)-acetophenone.



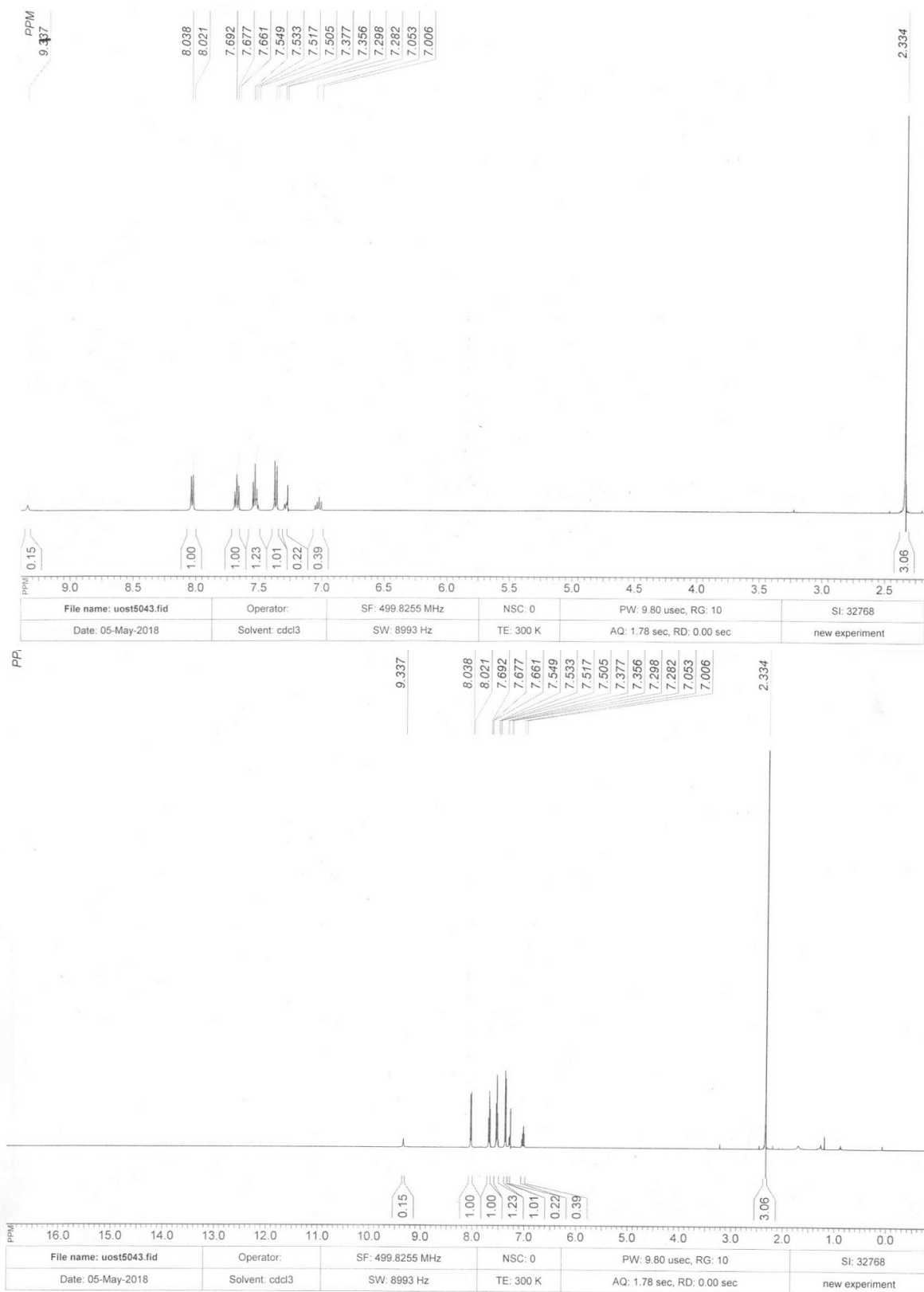


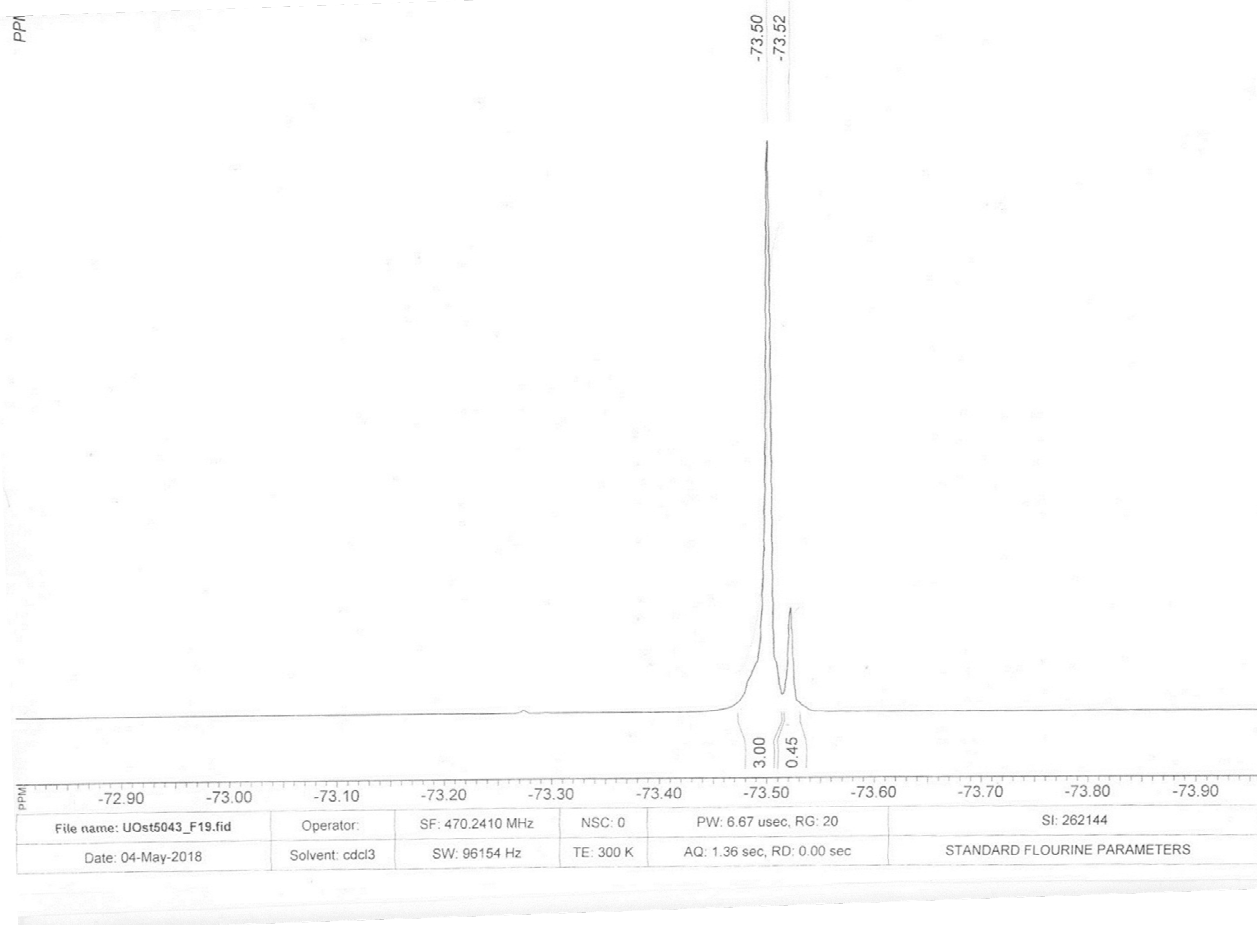
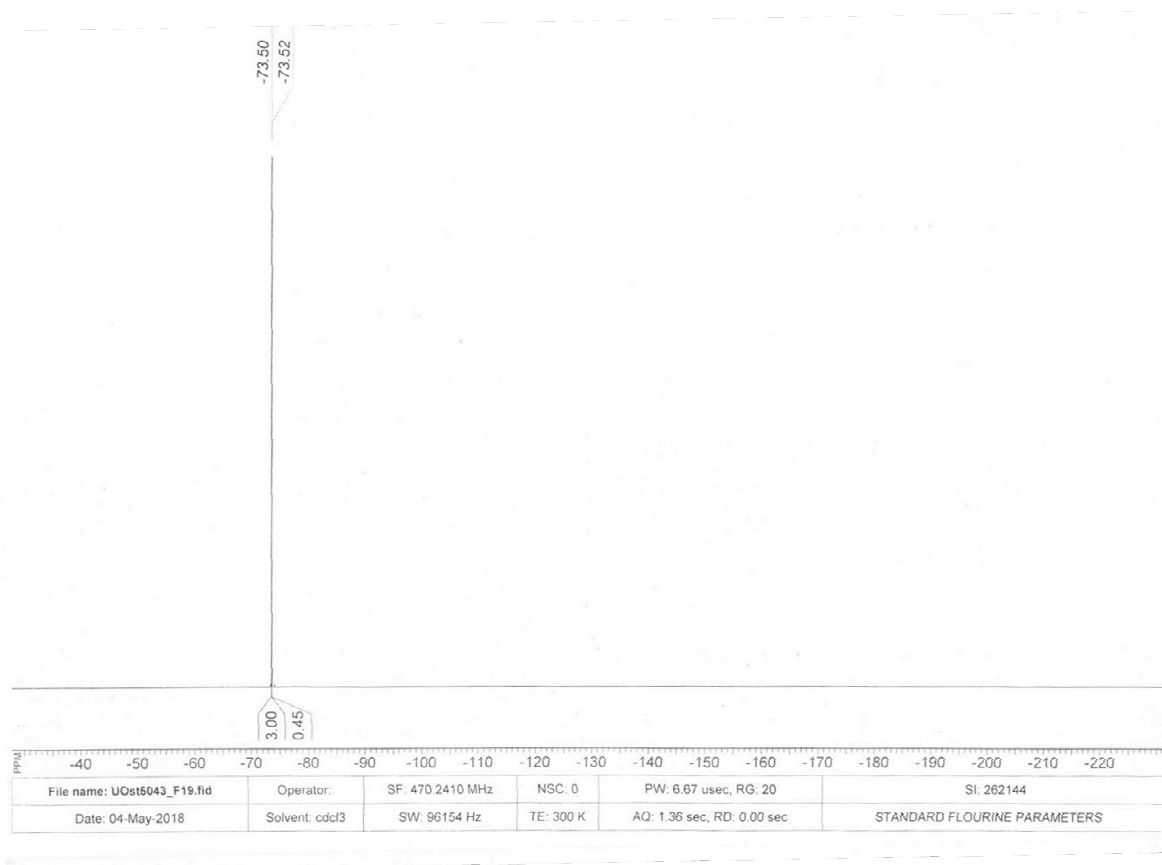
**2-((Trifluoromethyl)sulfinyl)phenyl acetate **2i**.**

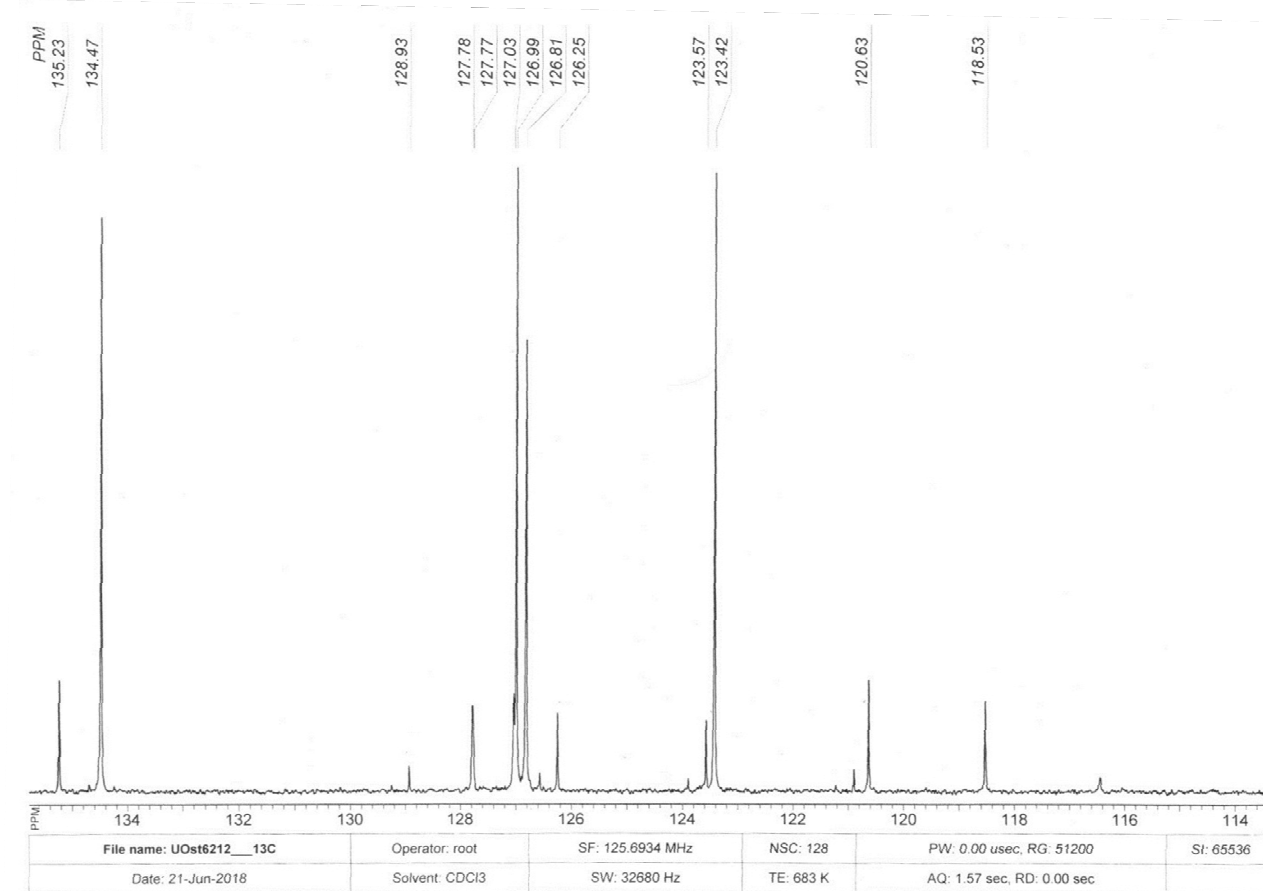
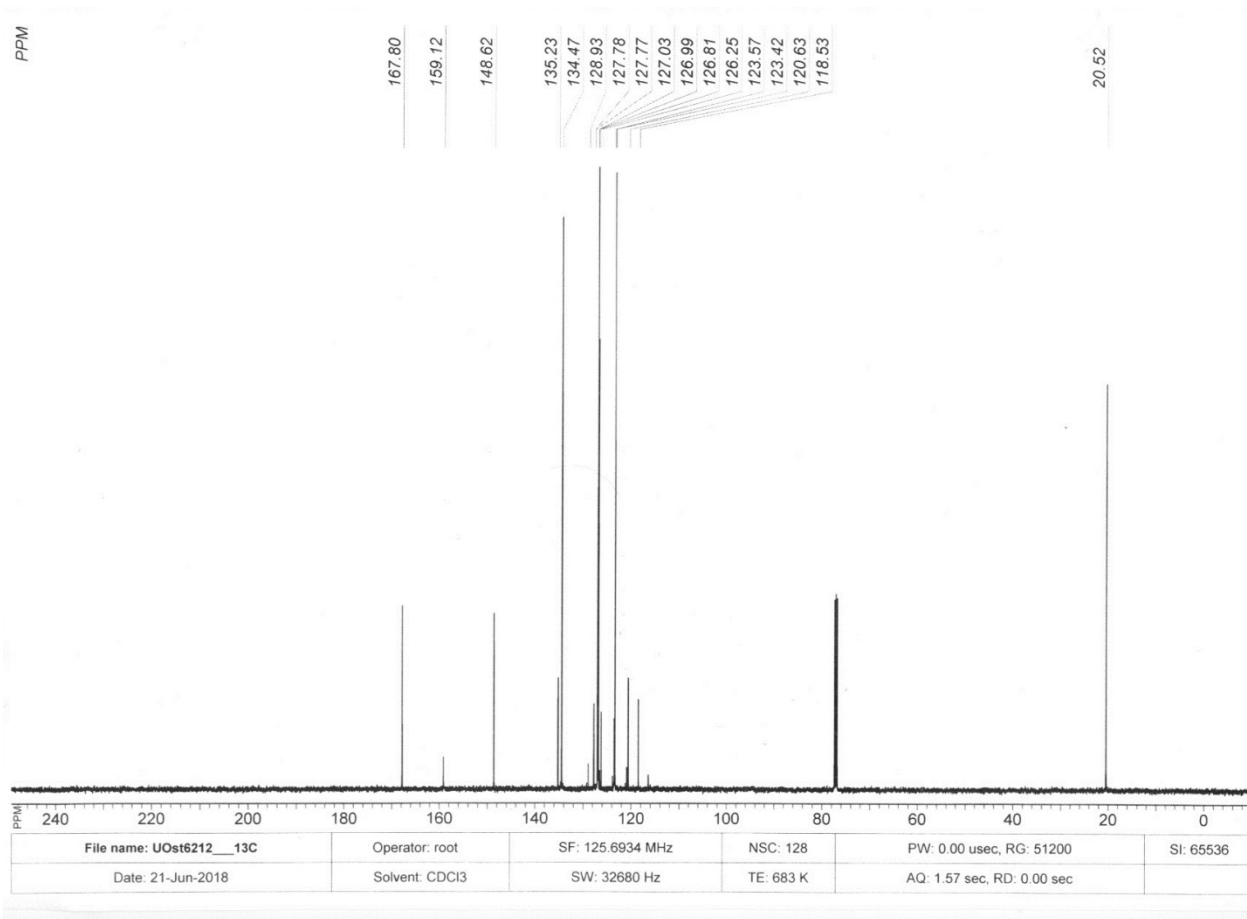
Product after column chromatography. Contains ~15 % of corresponding phenol.



85:15

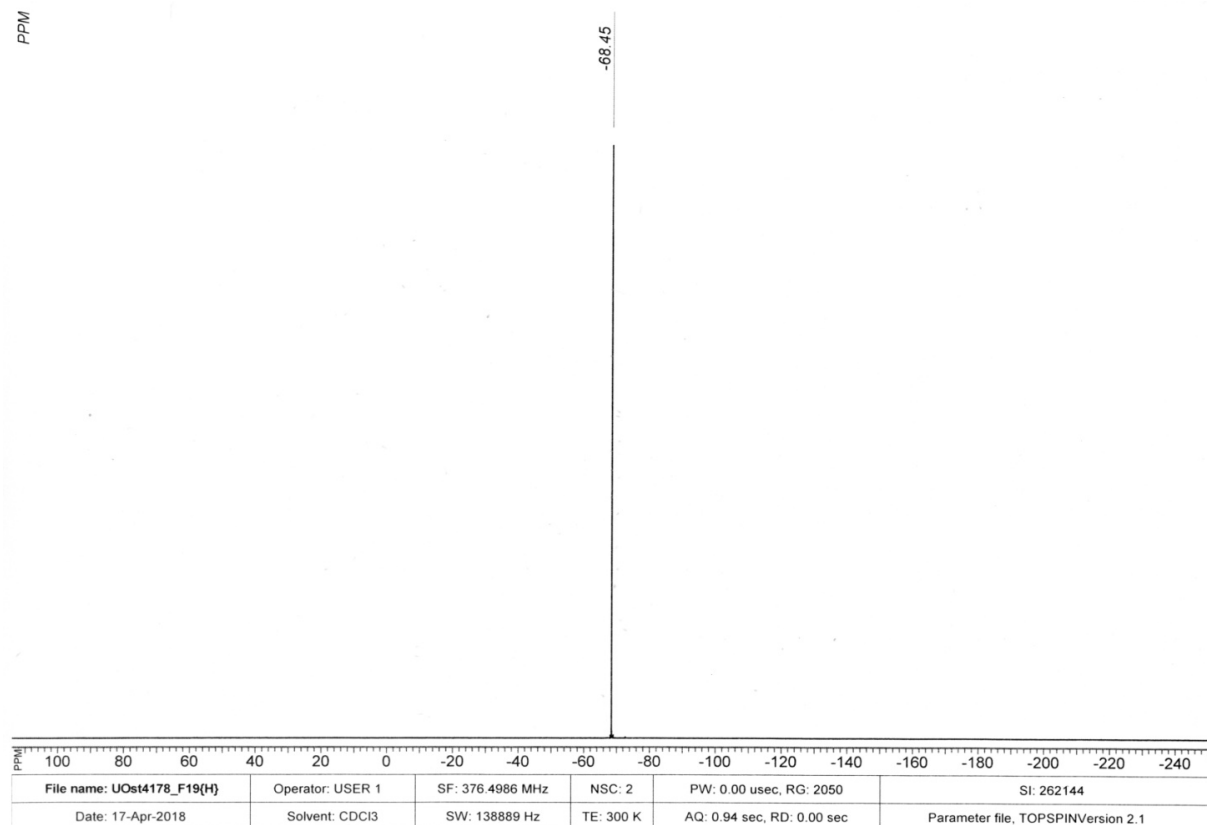
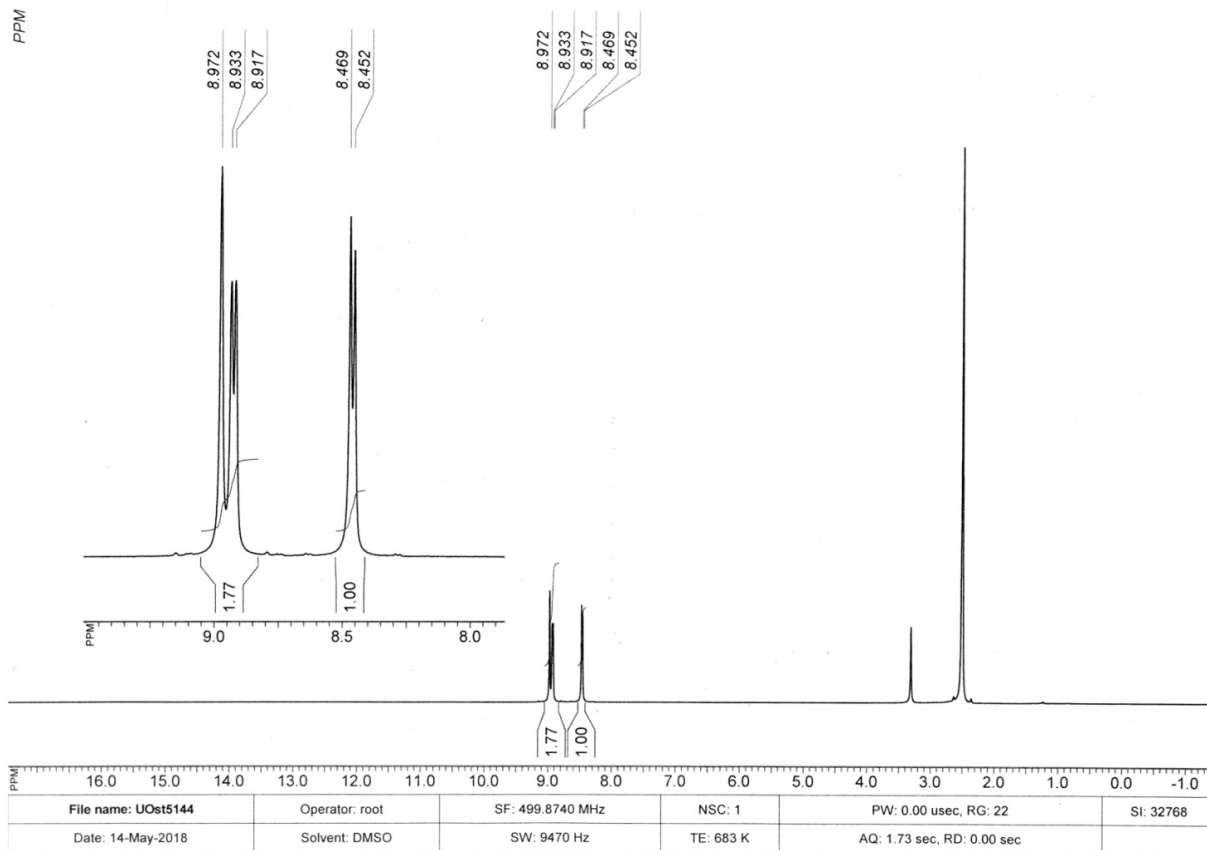
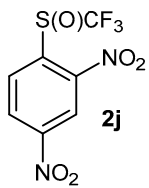


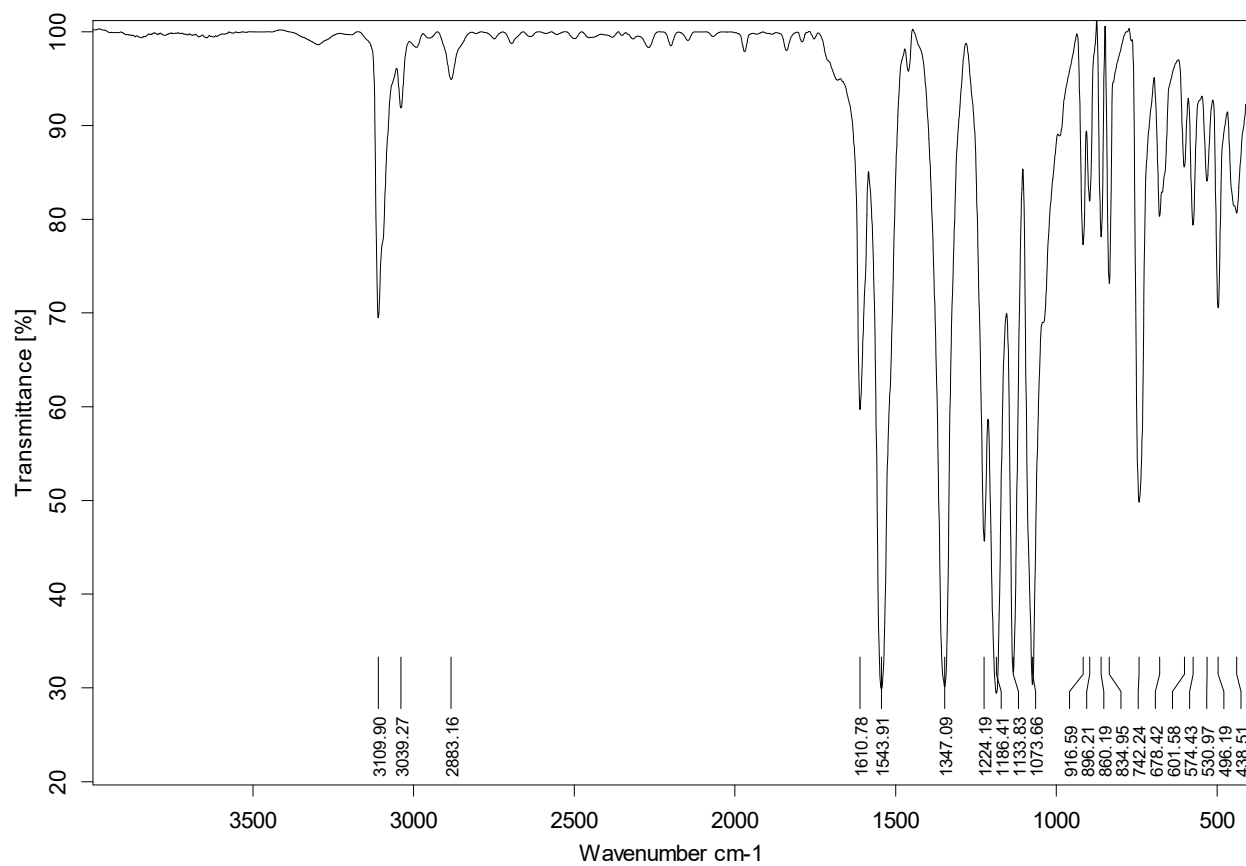
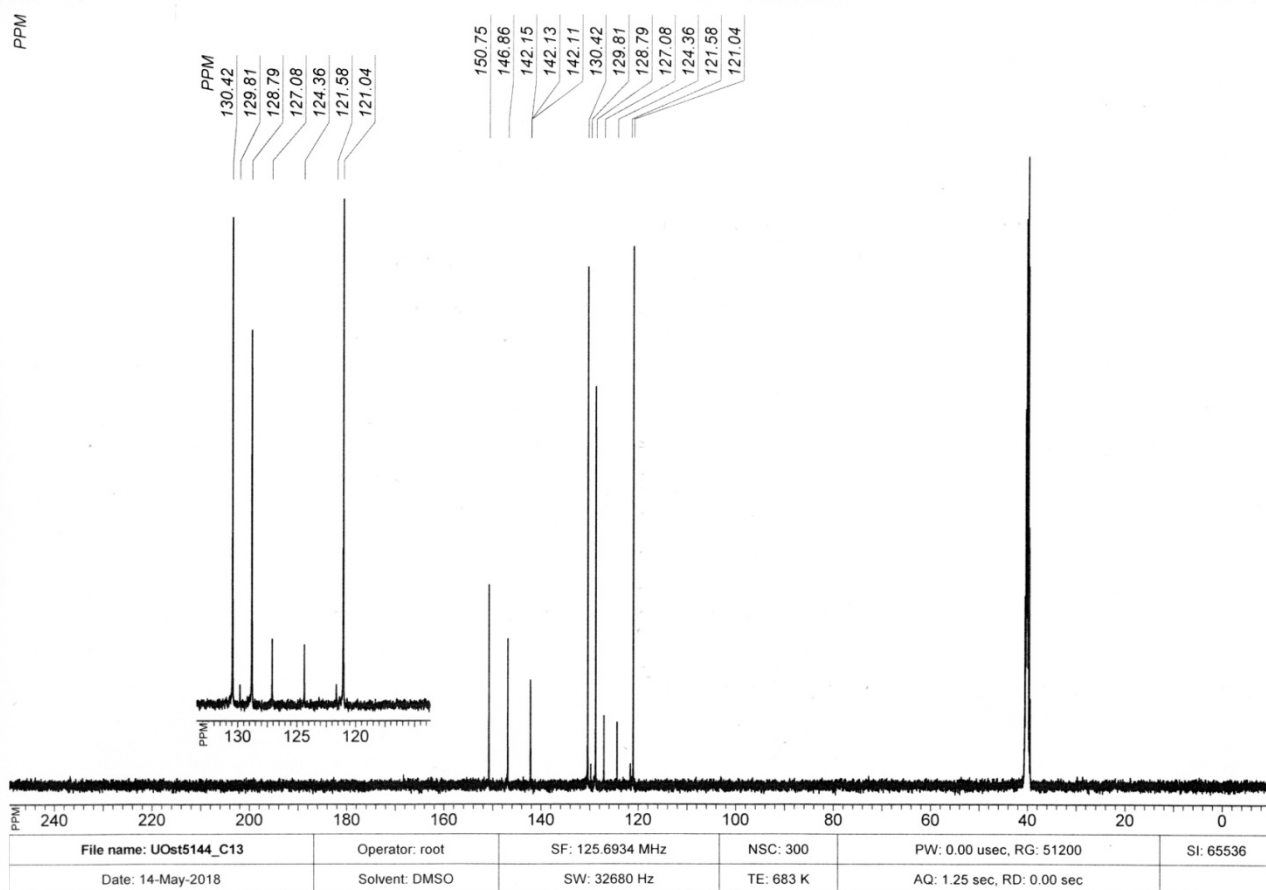


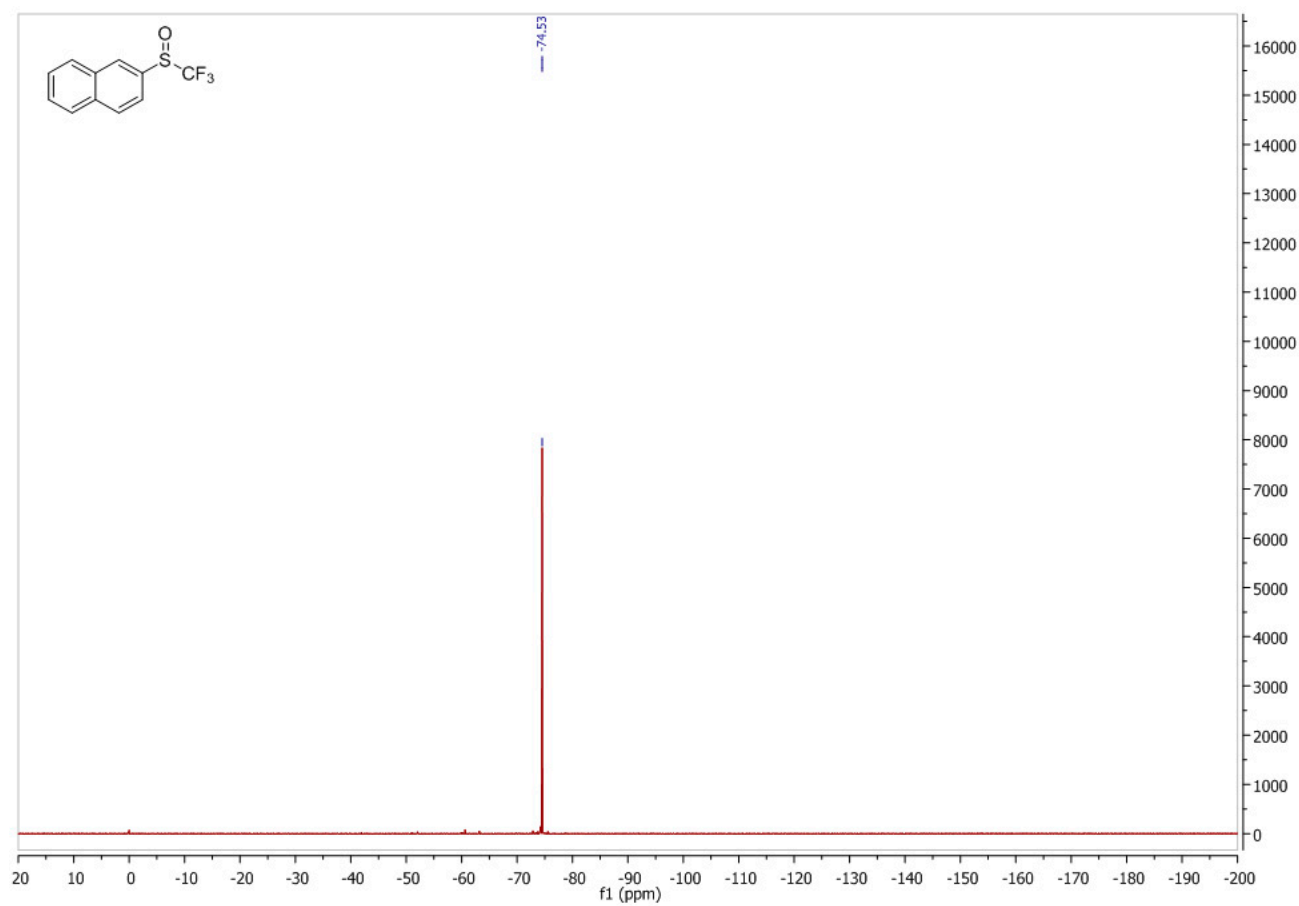
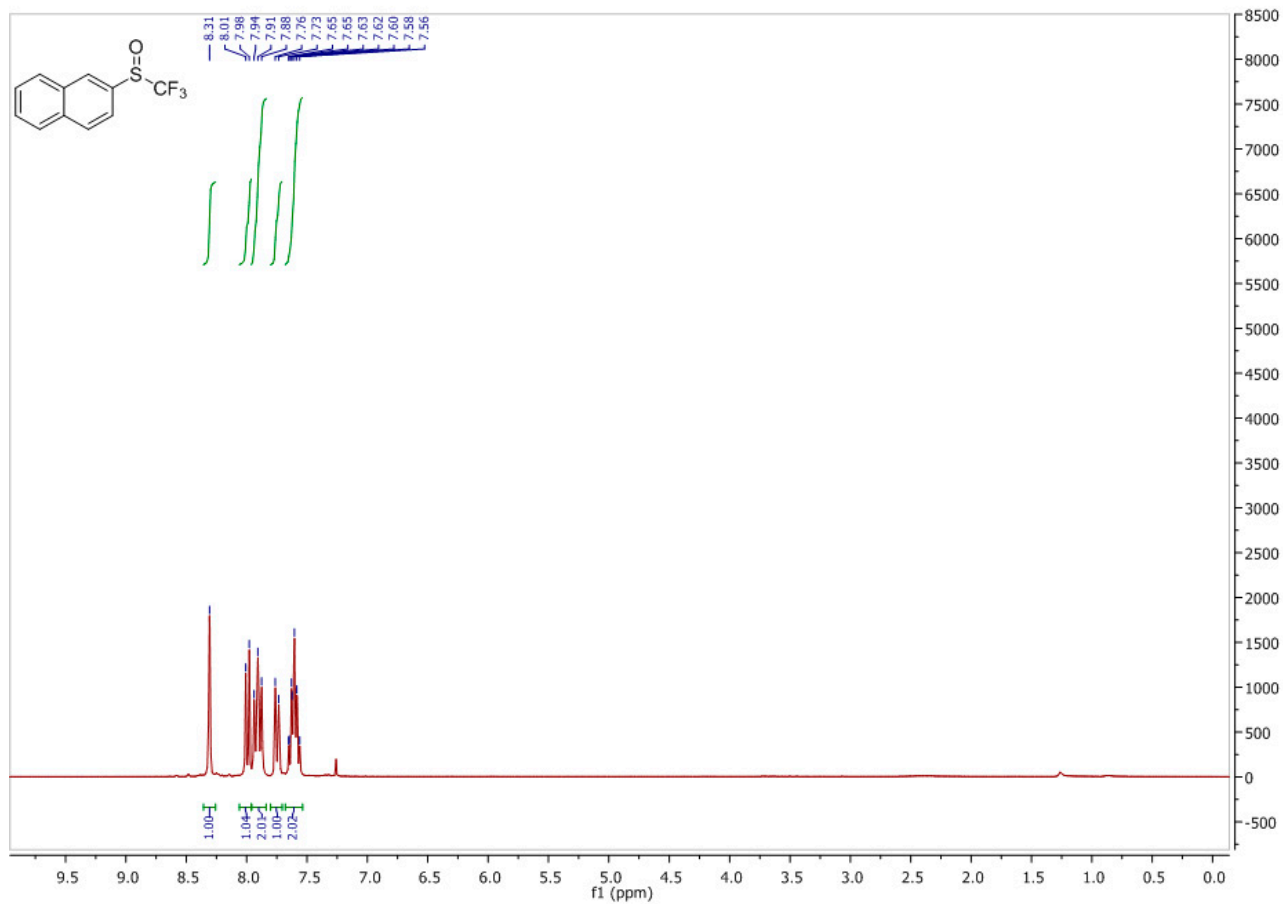


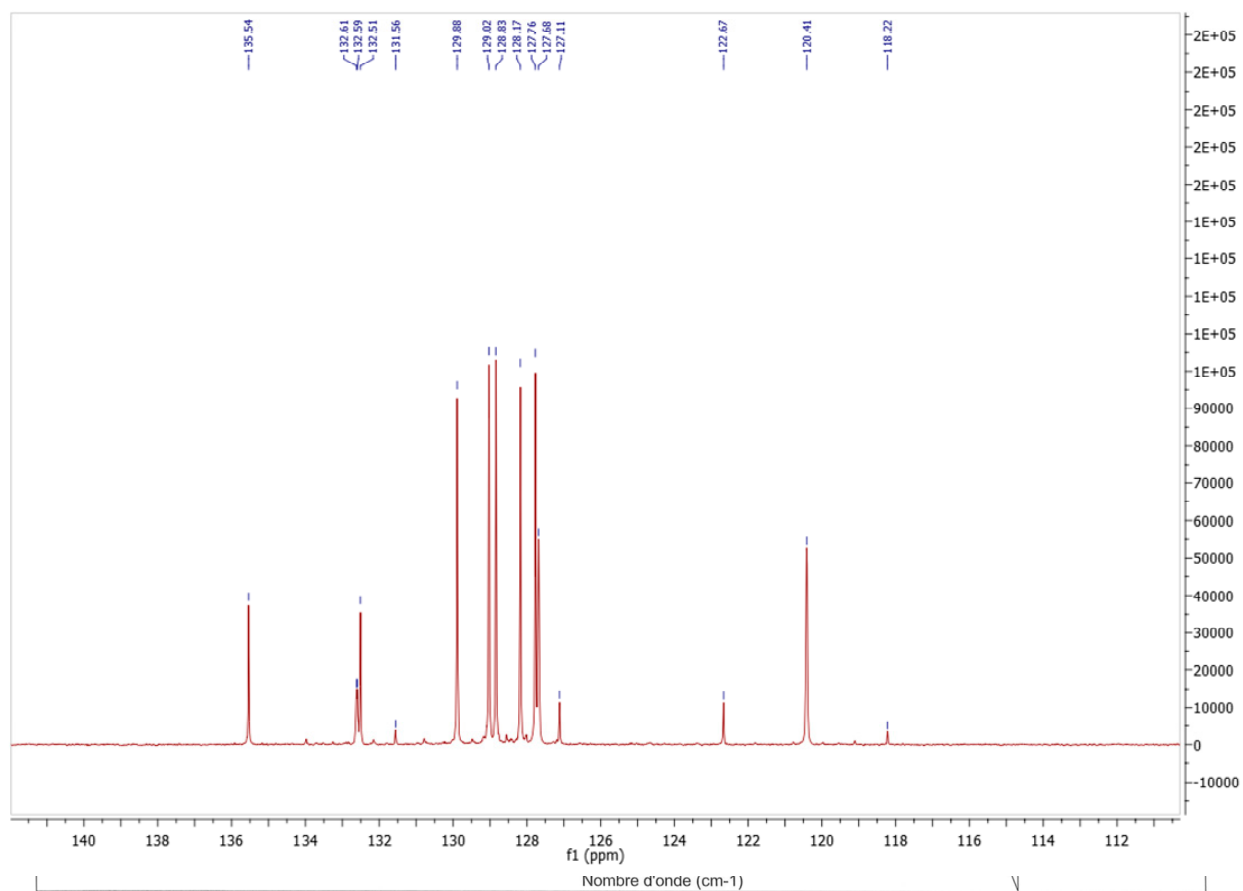
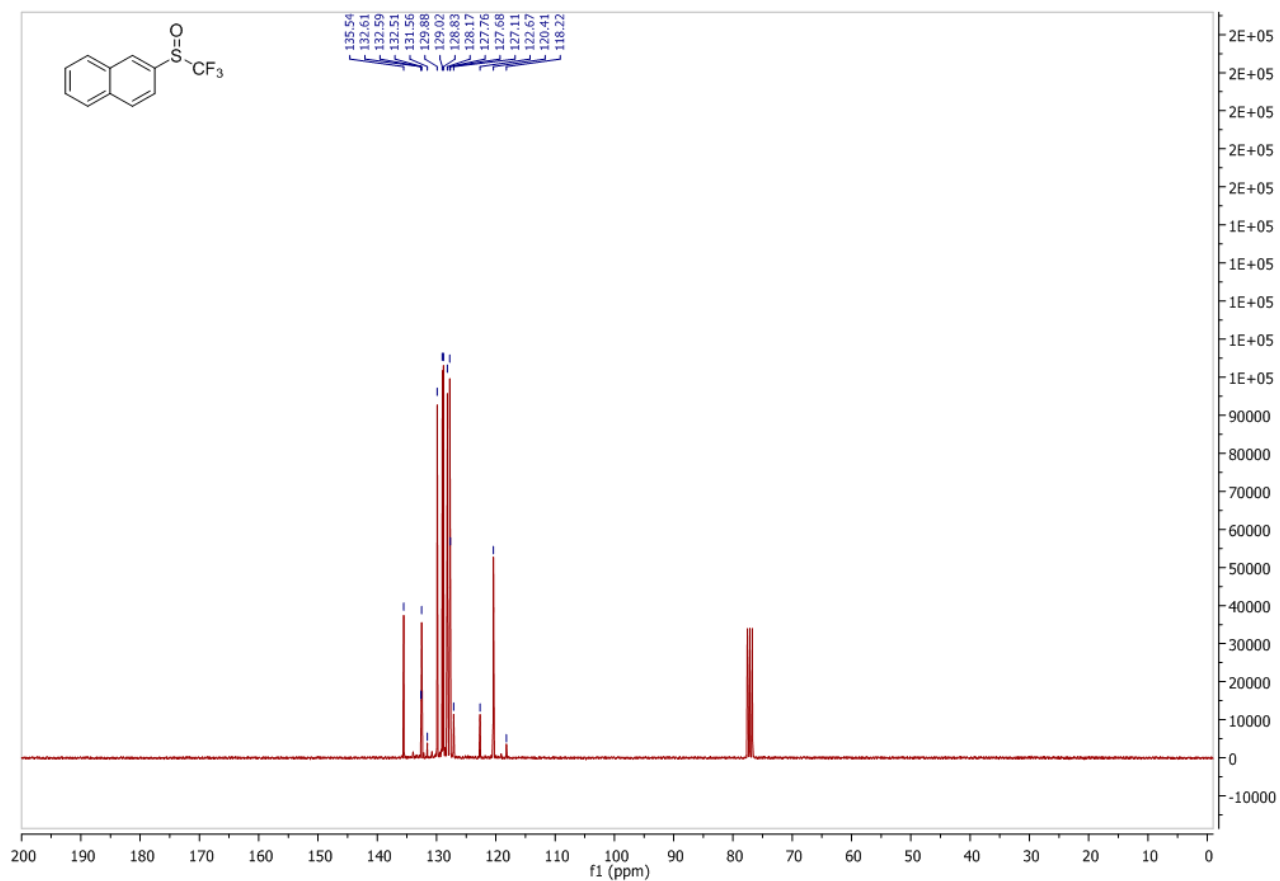


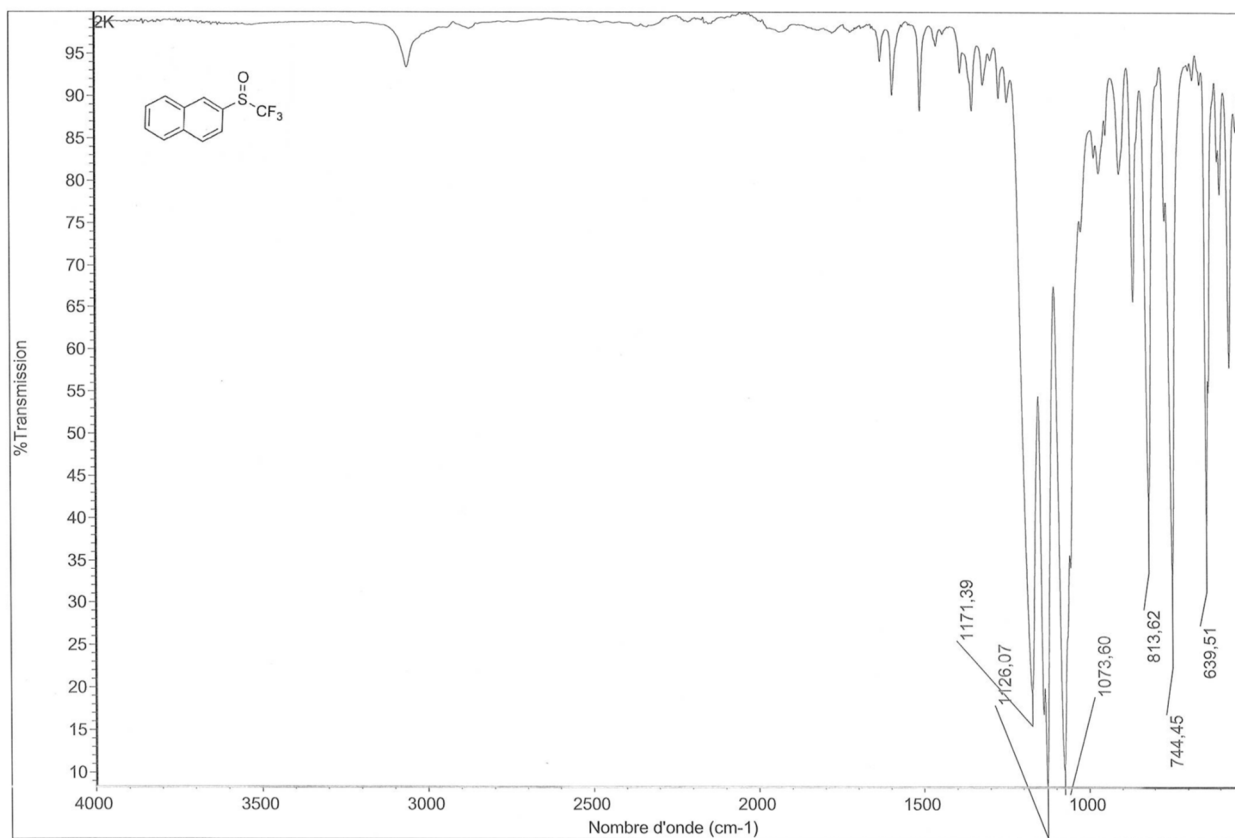
**2,4-Dinitro-1-((trifluoromethyl)sulfinyl)benzene.**





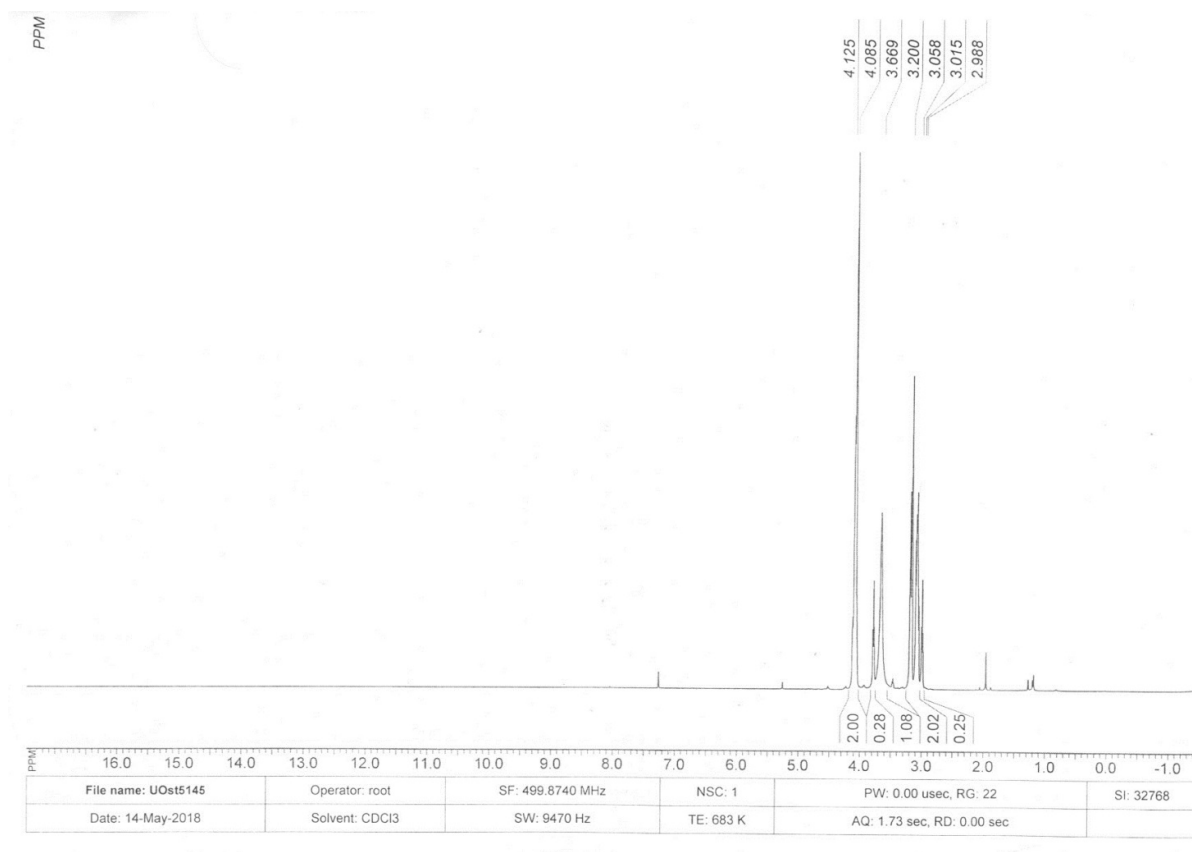
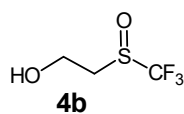
**2-((Trifluoromethyl)sulfinyl)naphthalene 2k.**

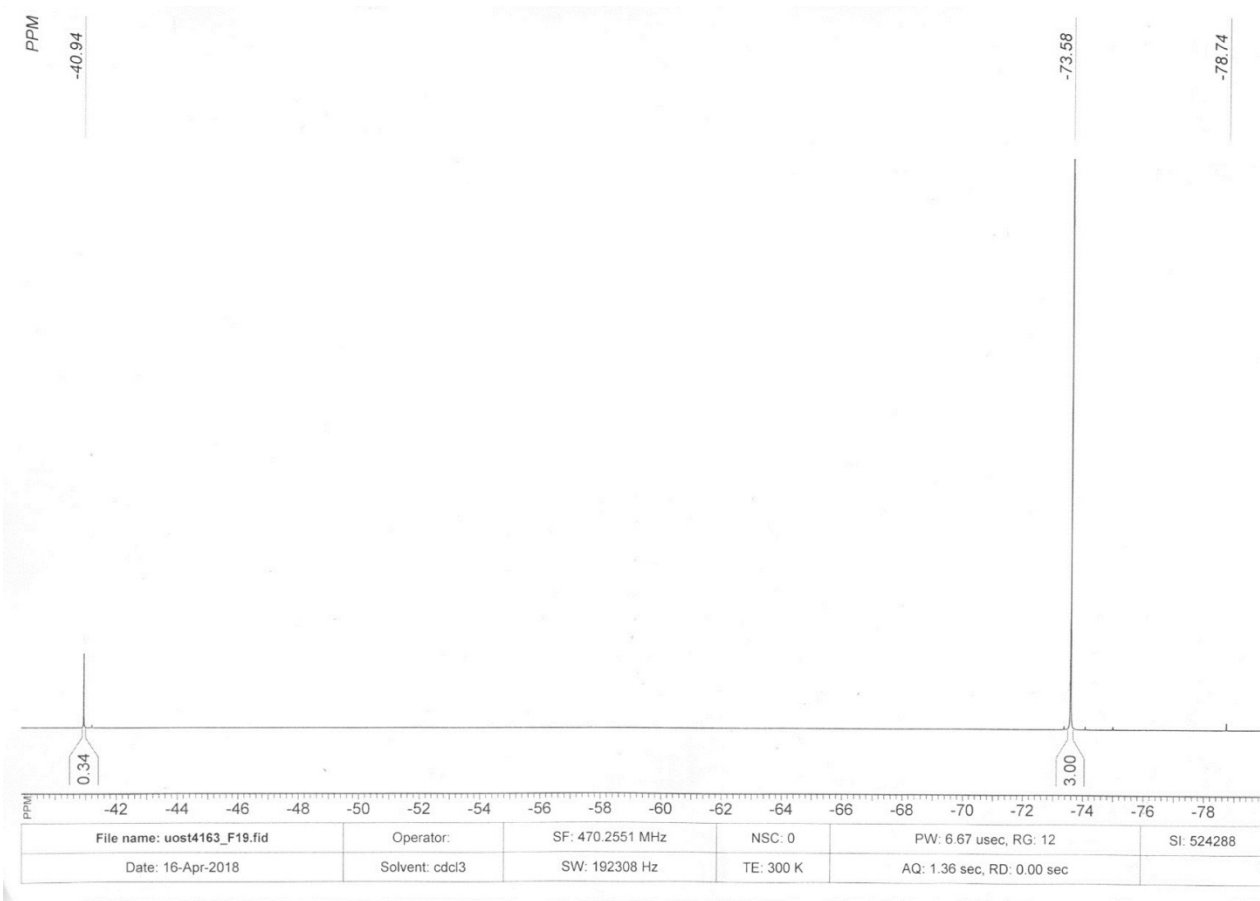
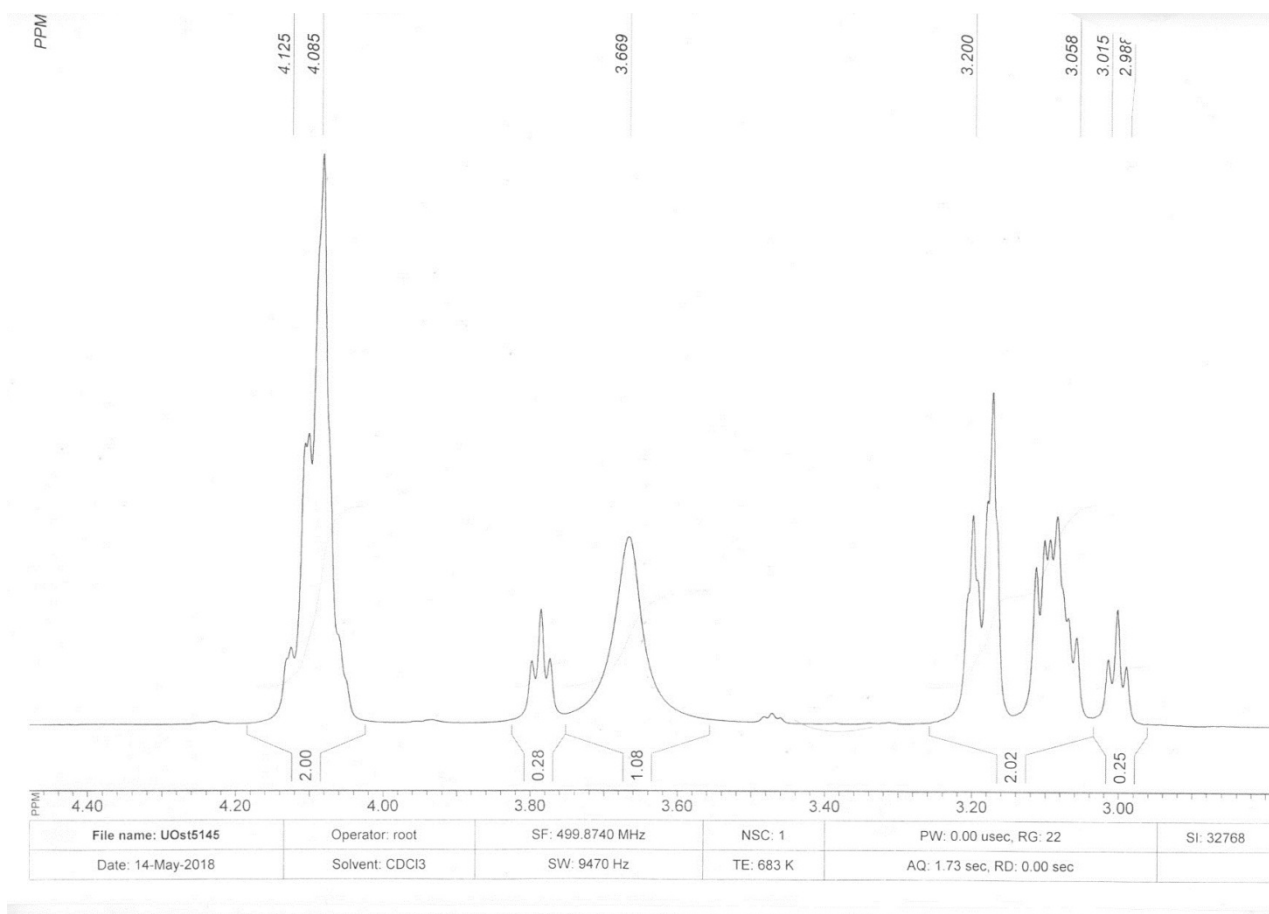


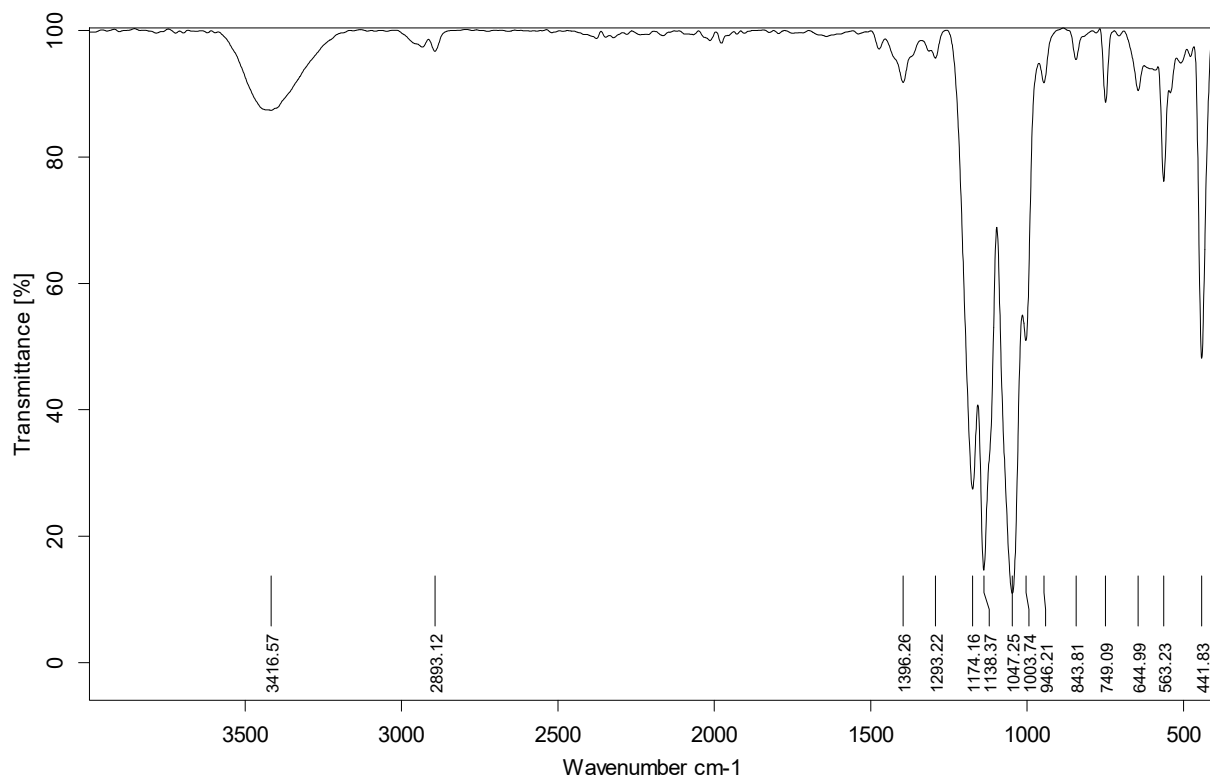
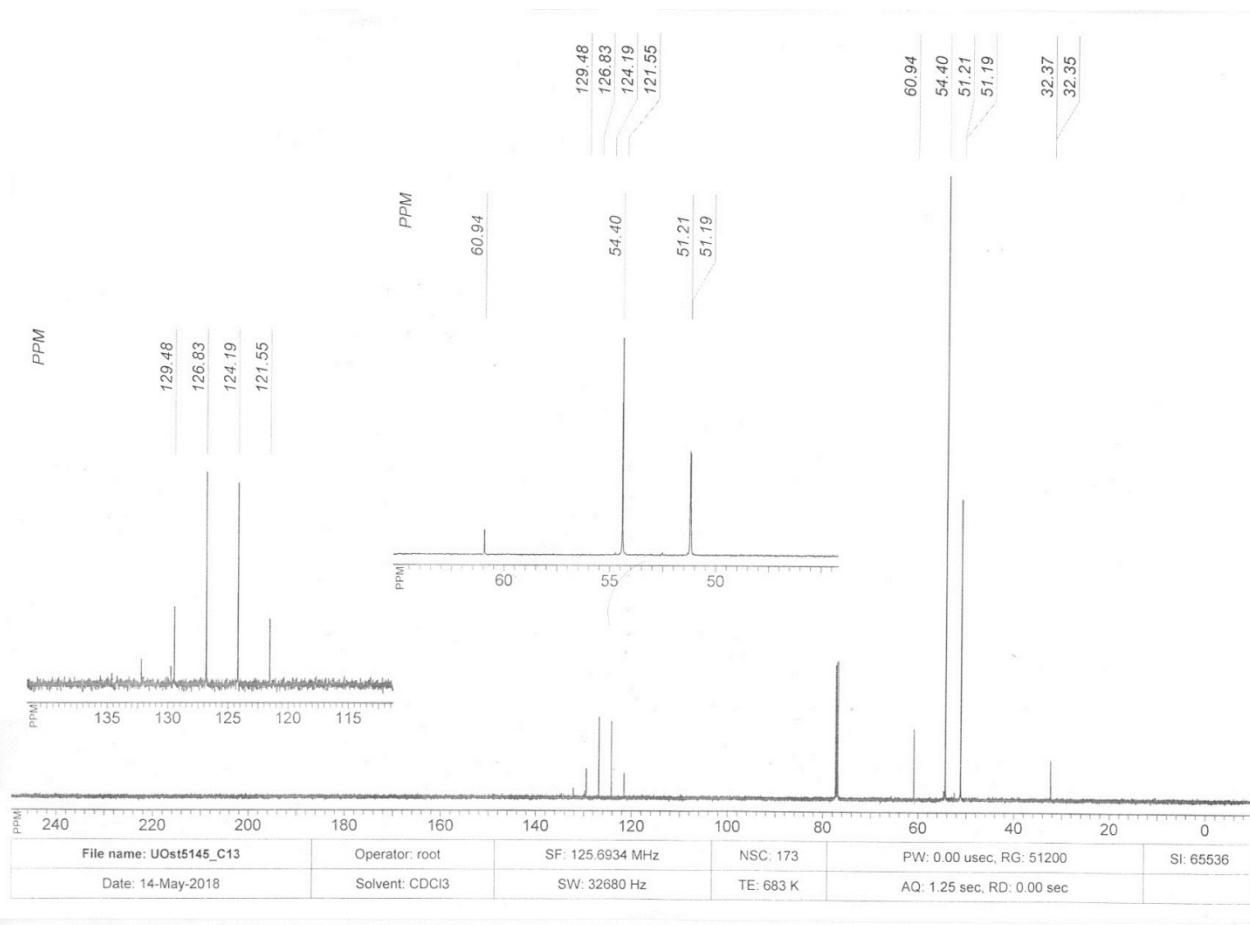


### 2-(Trifluoromethyl)sulfinyl-ethanol.

Contain ~15 % of starting sulfide.

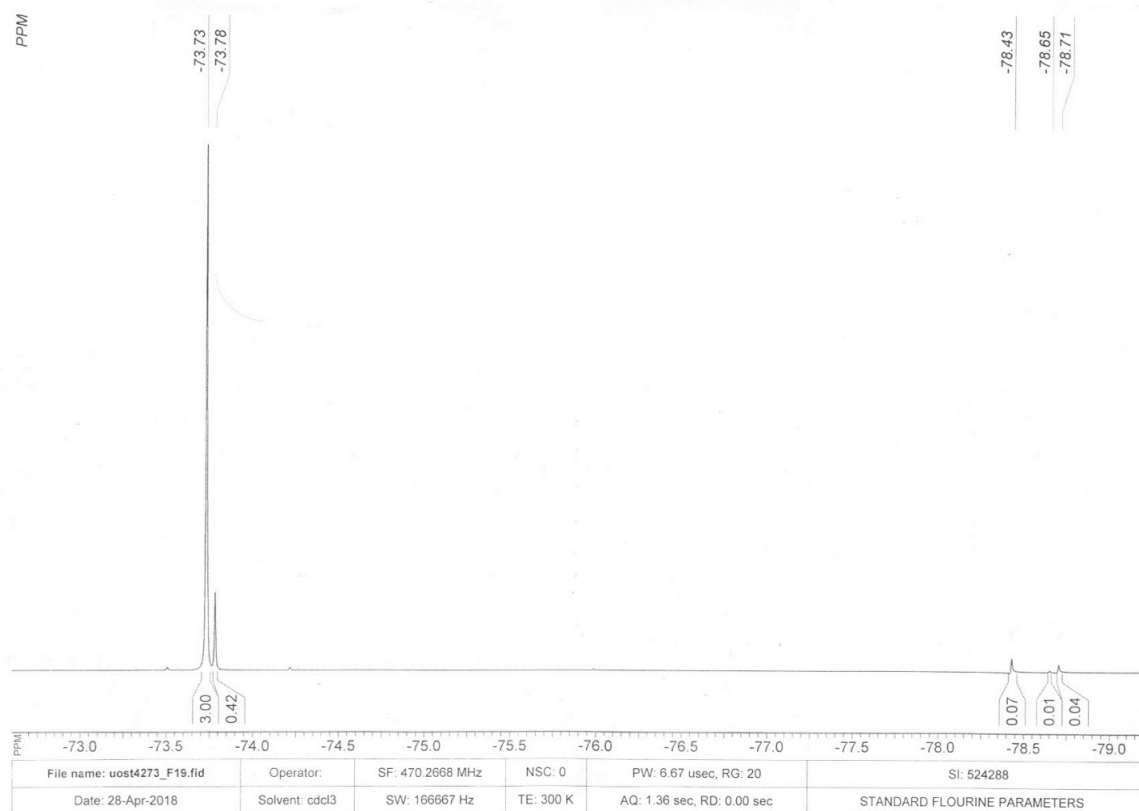
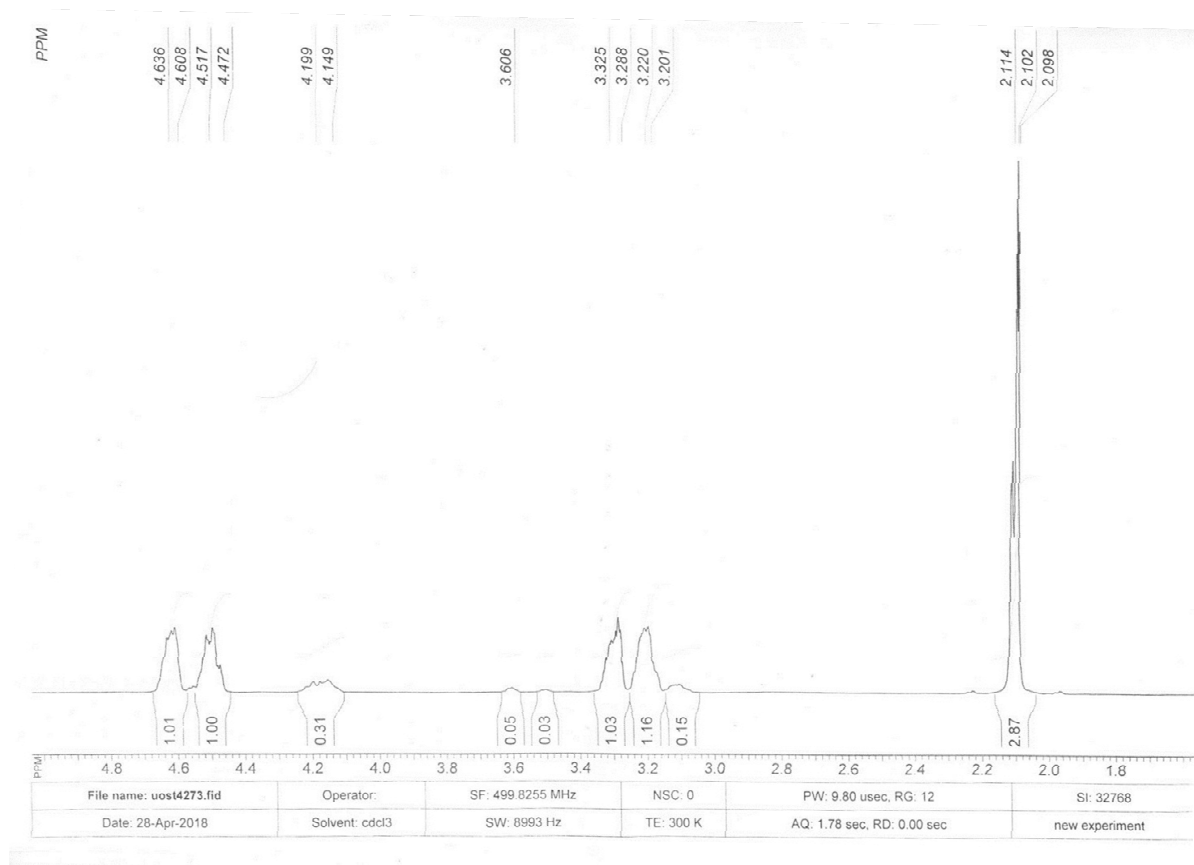
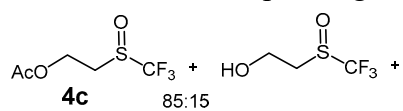




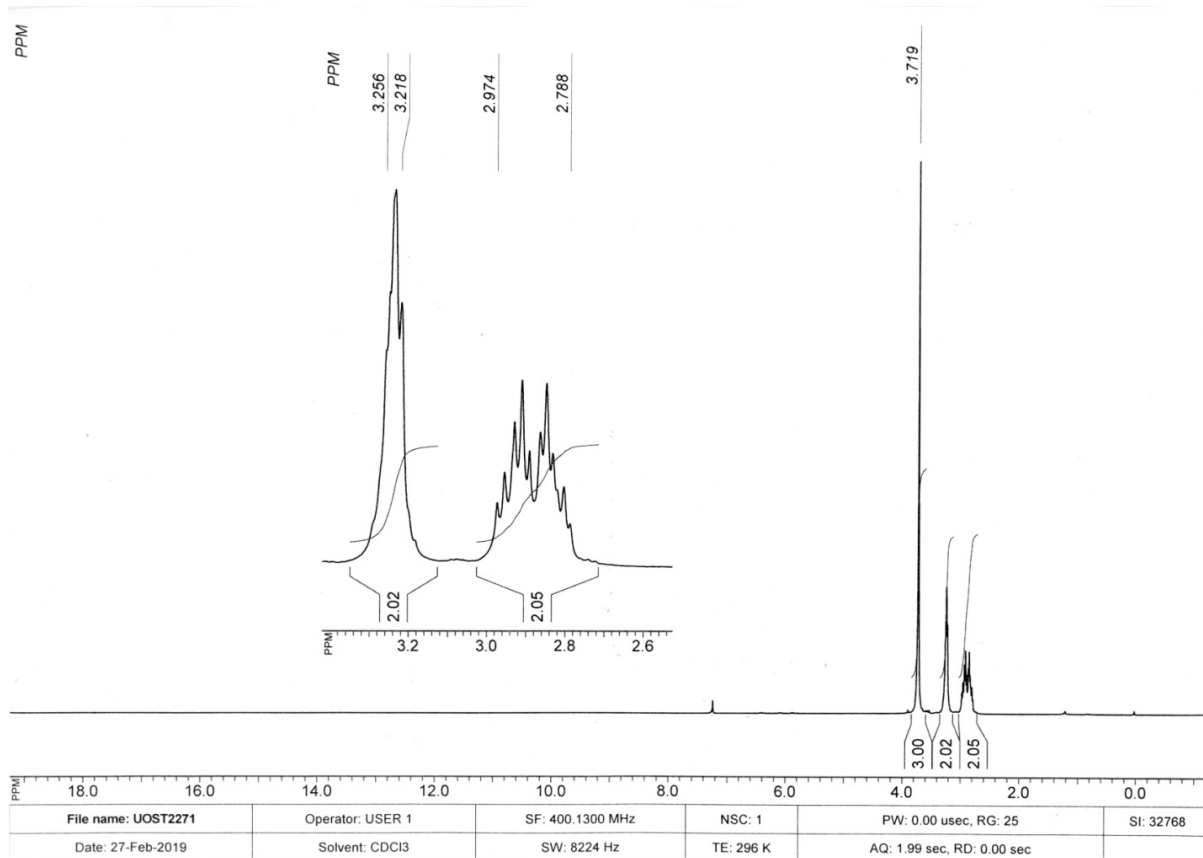


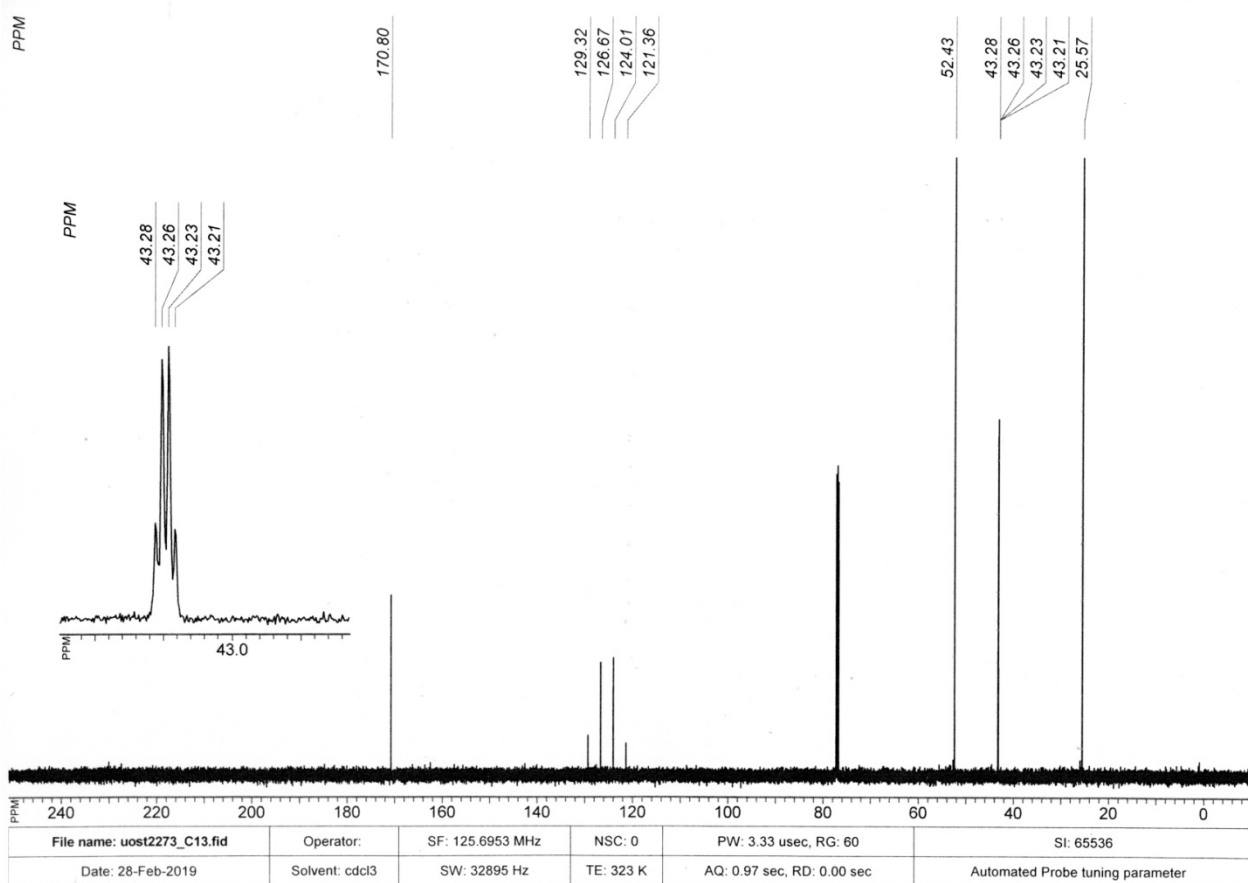
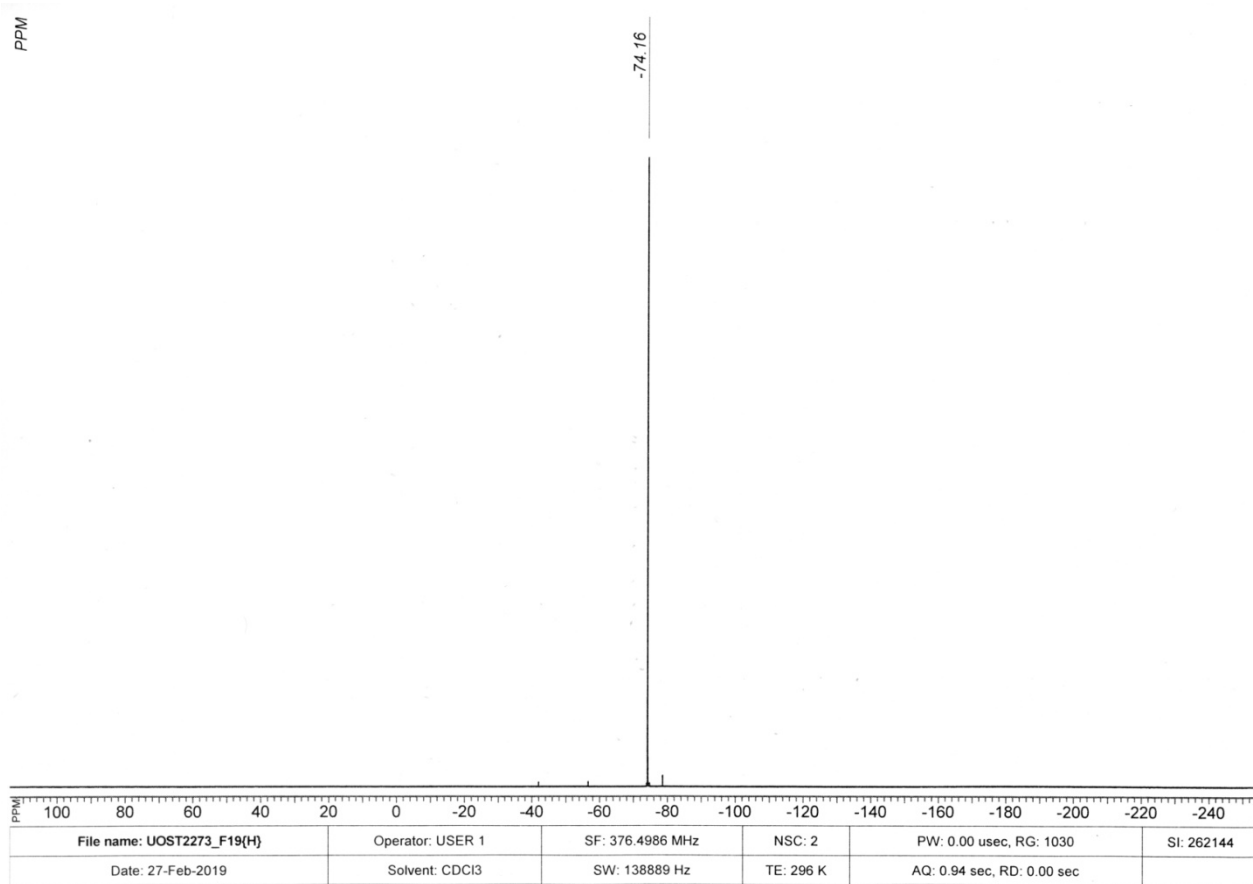
# 2-((Trifluoromethyl)sulfinyl)ethyl acetate.

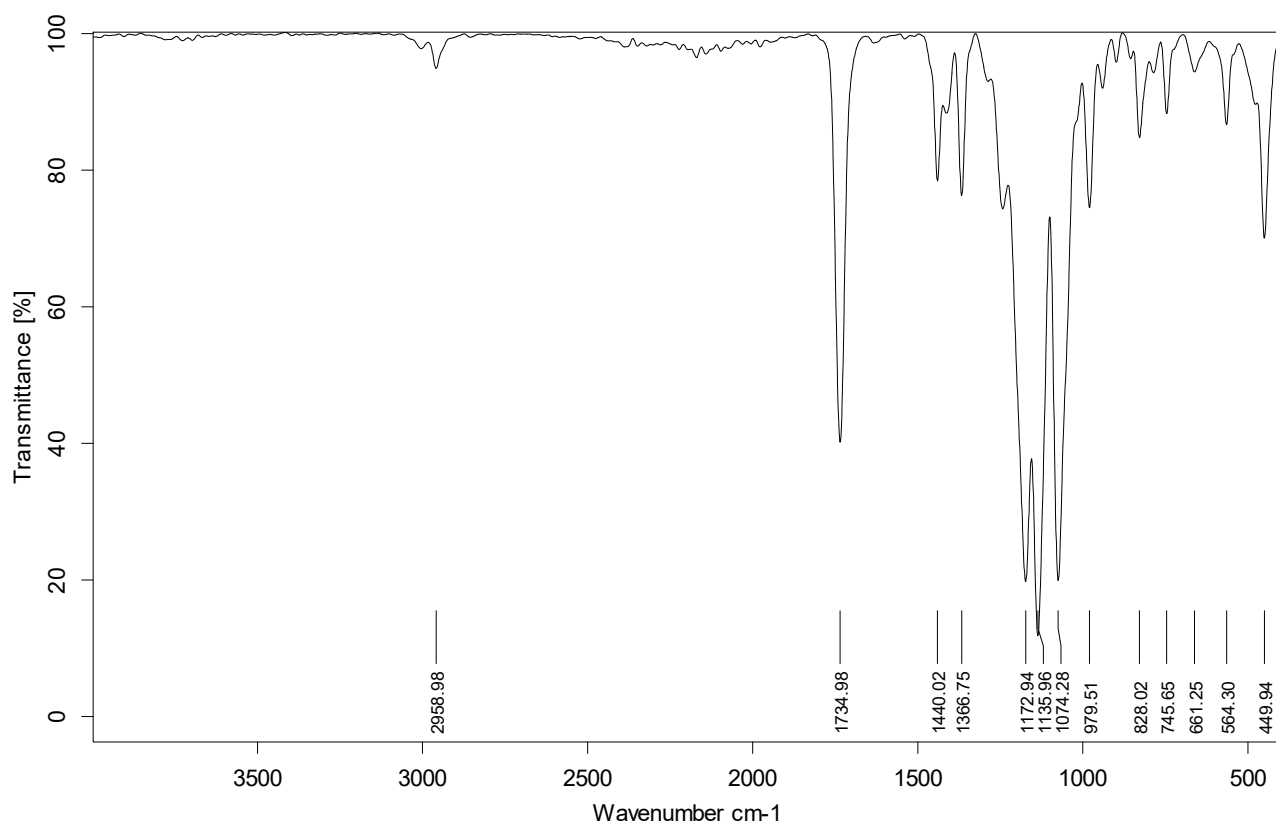
Product after distillation. Contains ~15 % of corresponding alcohol.



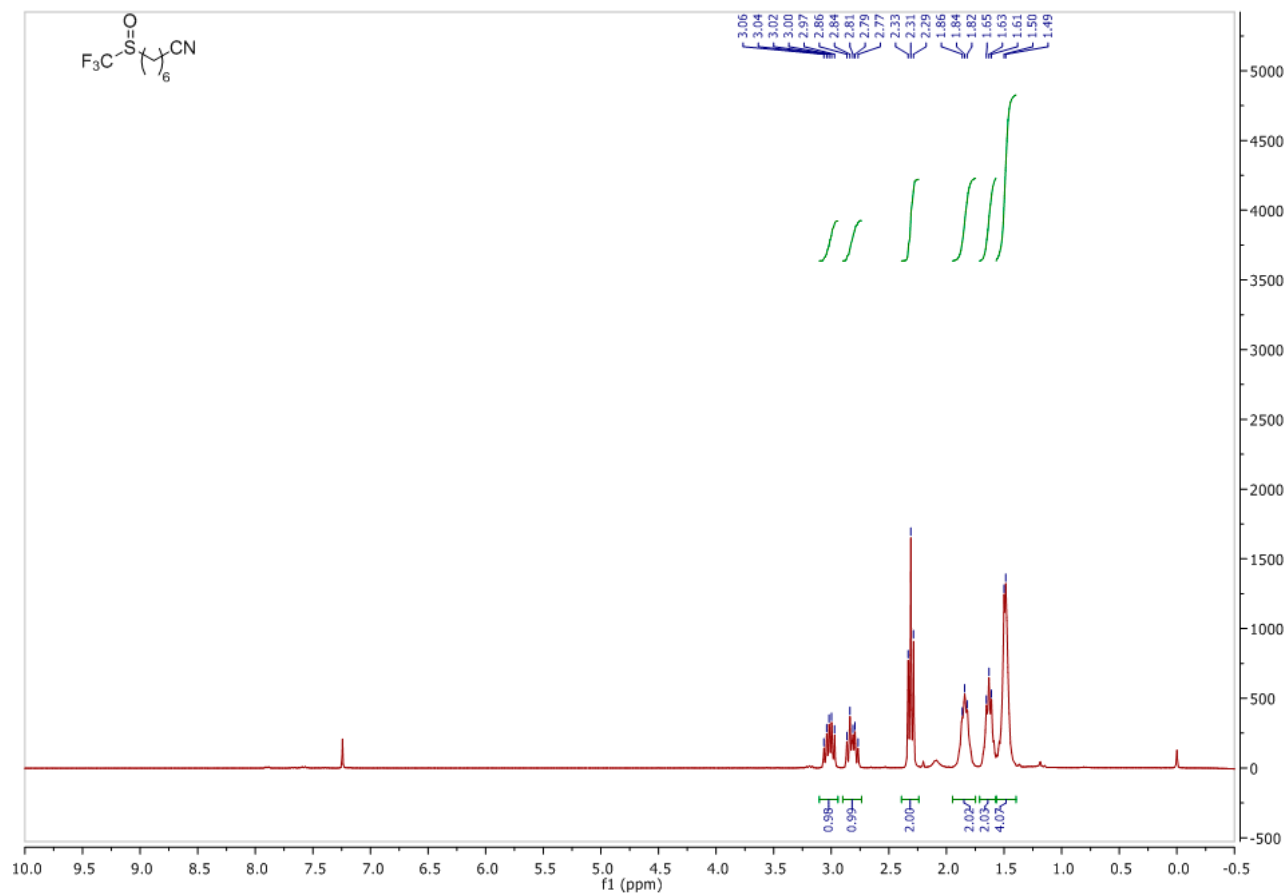


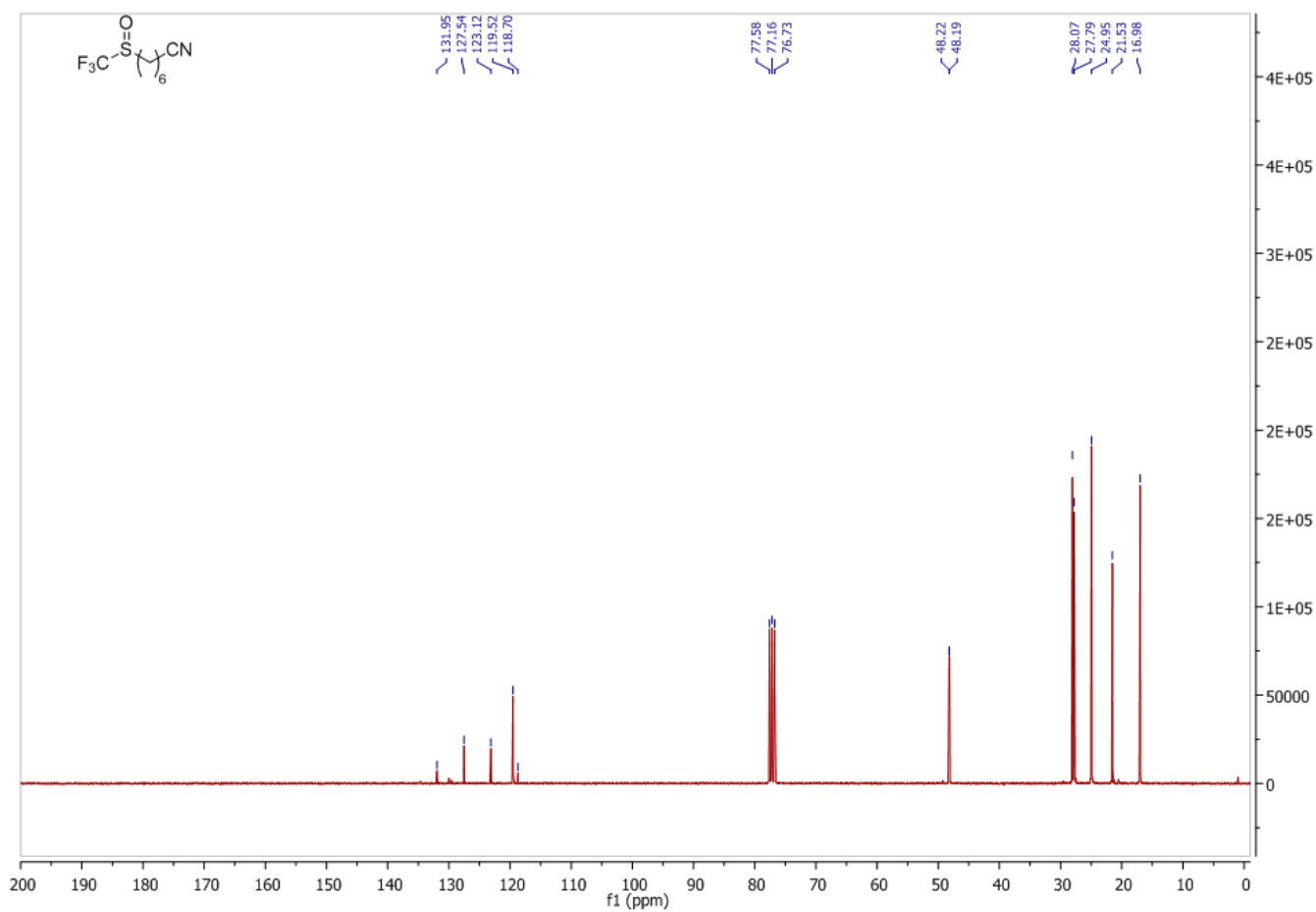
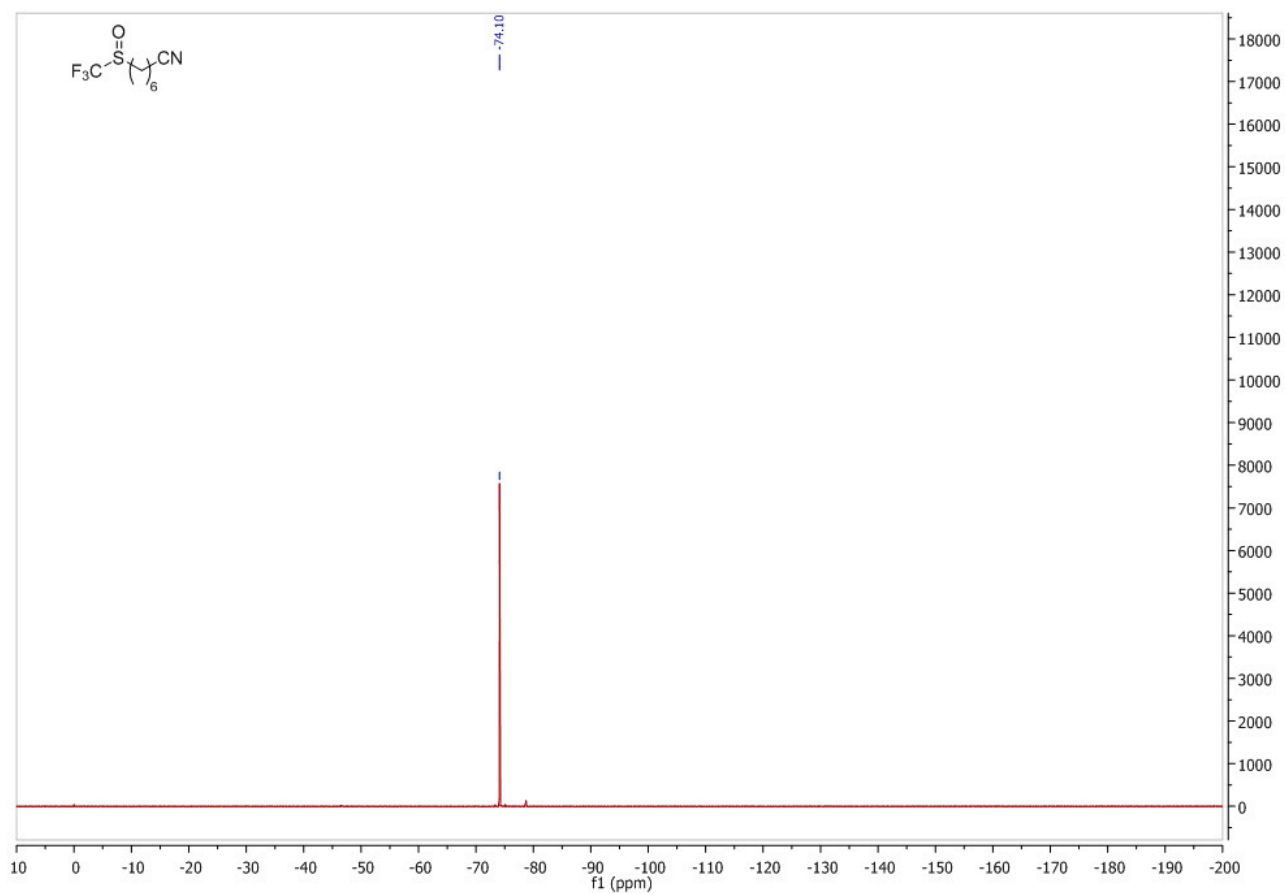
COC(=O)CCS(=O)C(F)(F)F  
**4e**

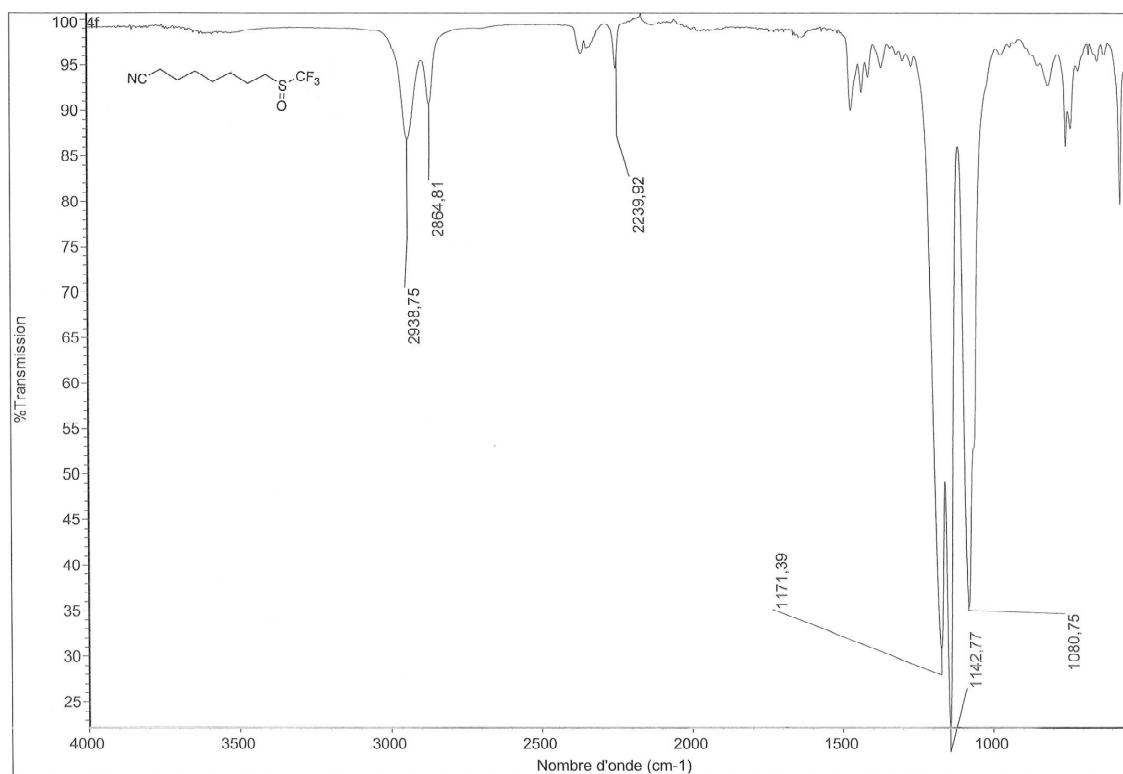




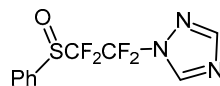
**7-((Trifluoromethyl)sulfinyl)heptanenitrile 4f.**



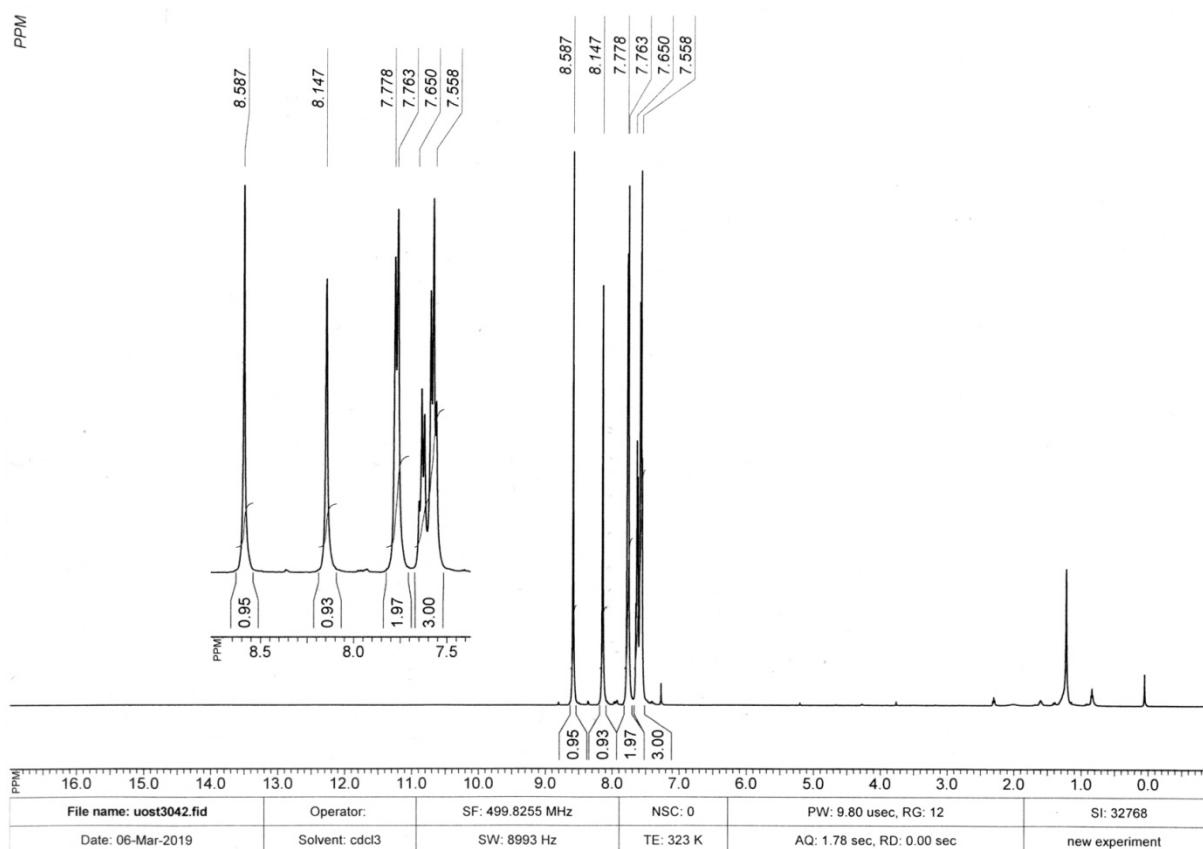


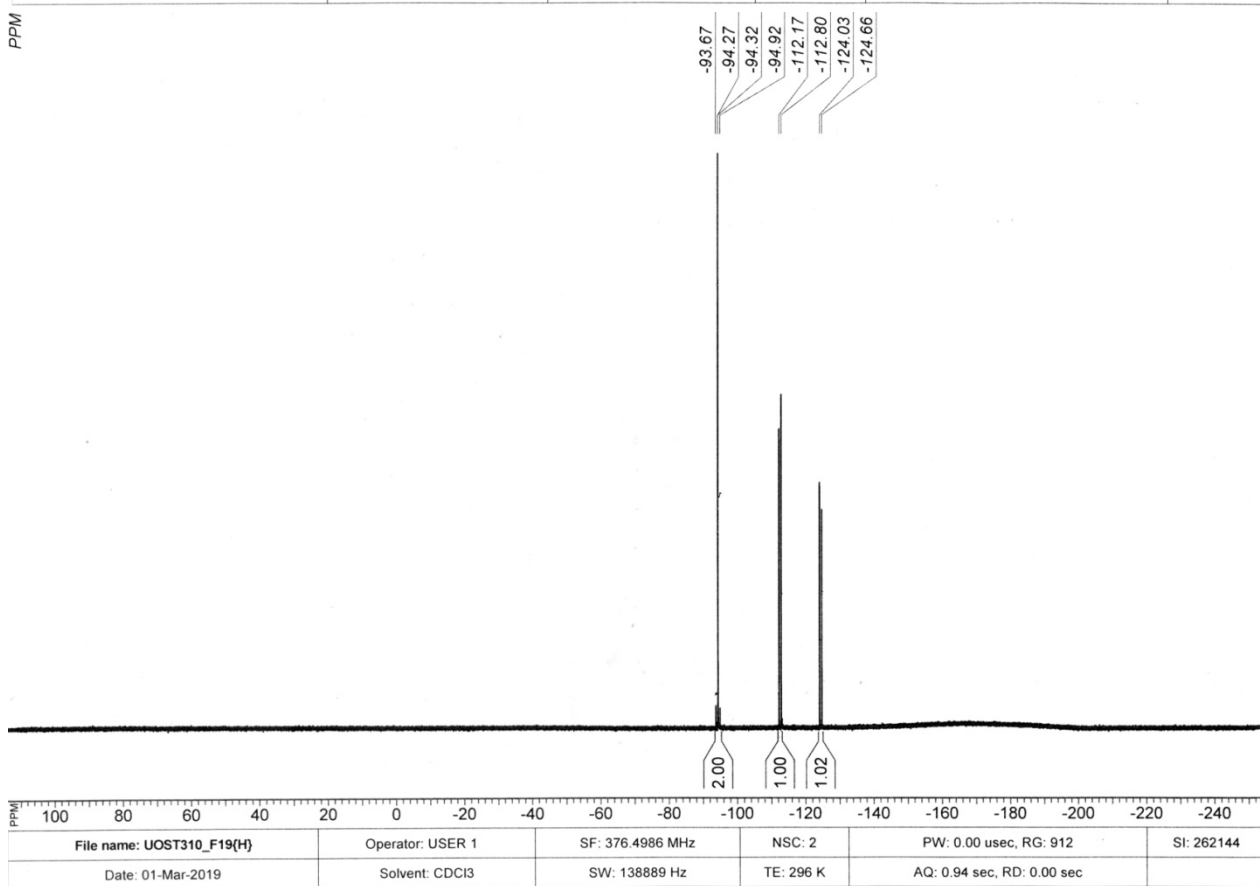
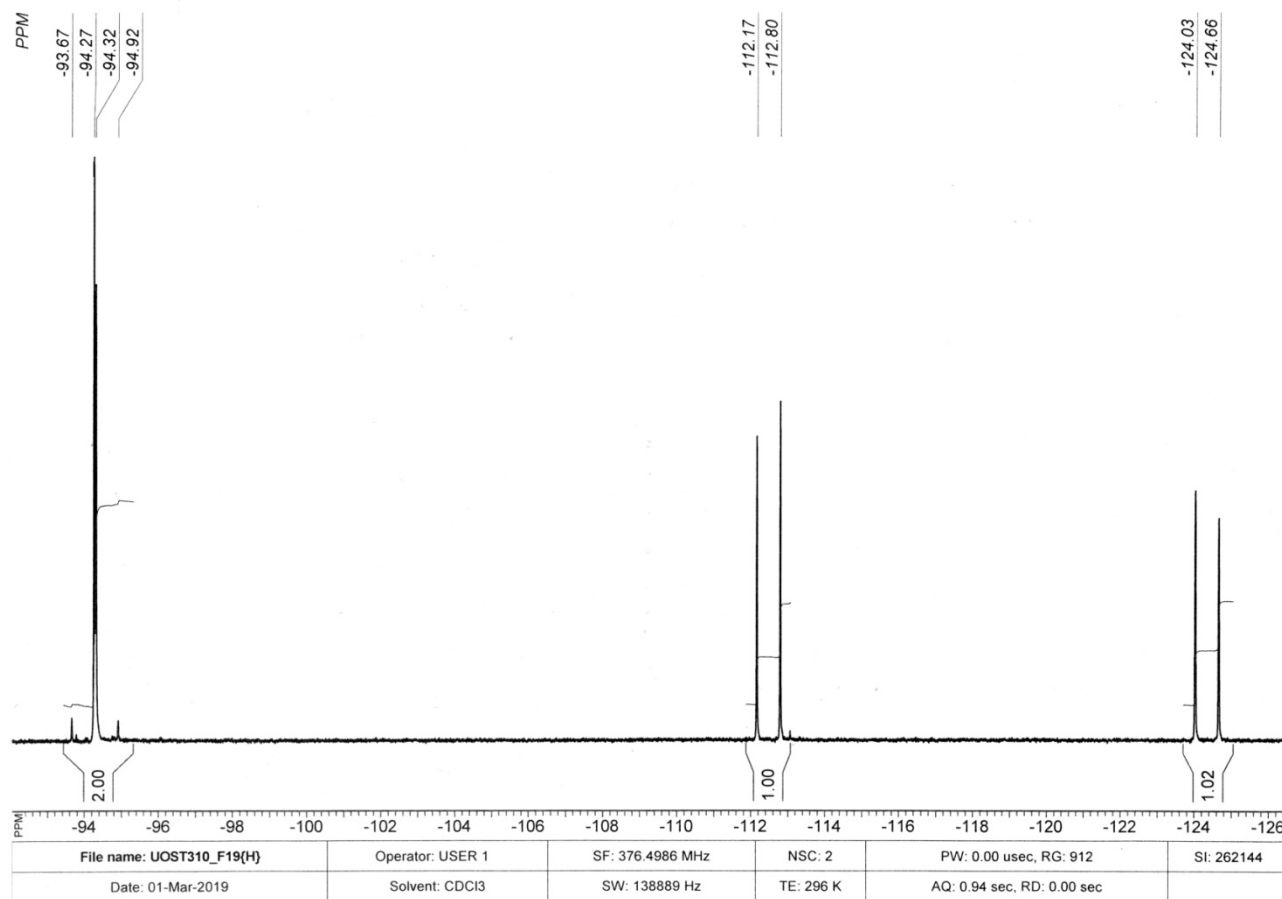


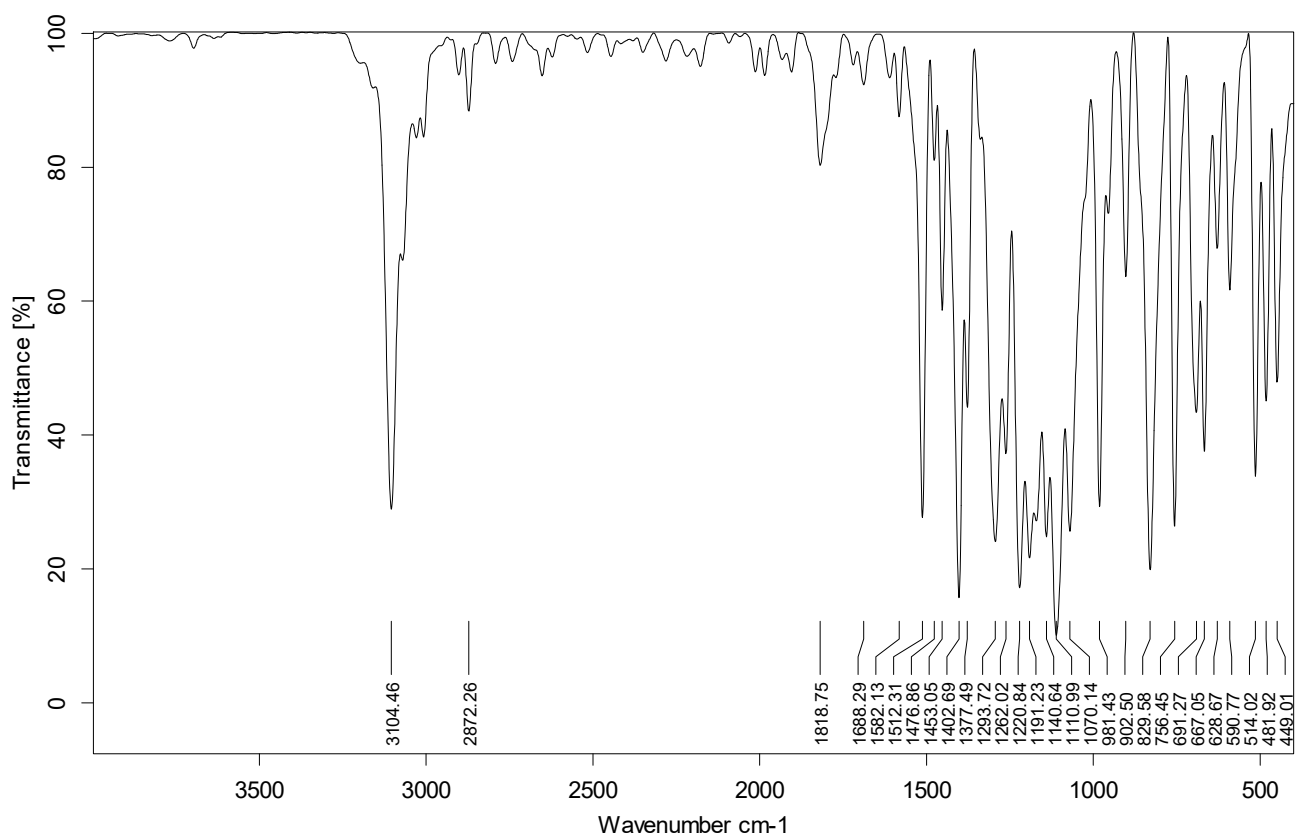
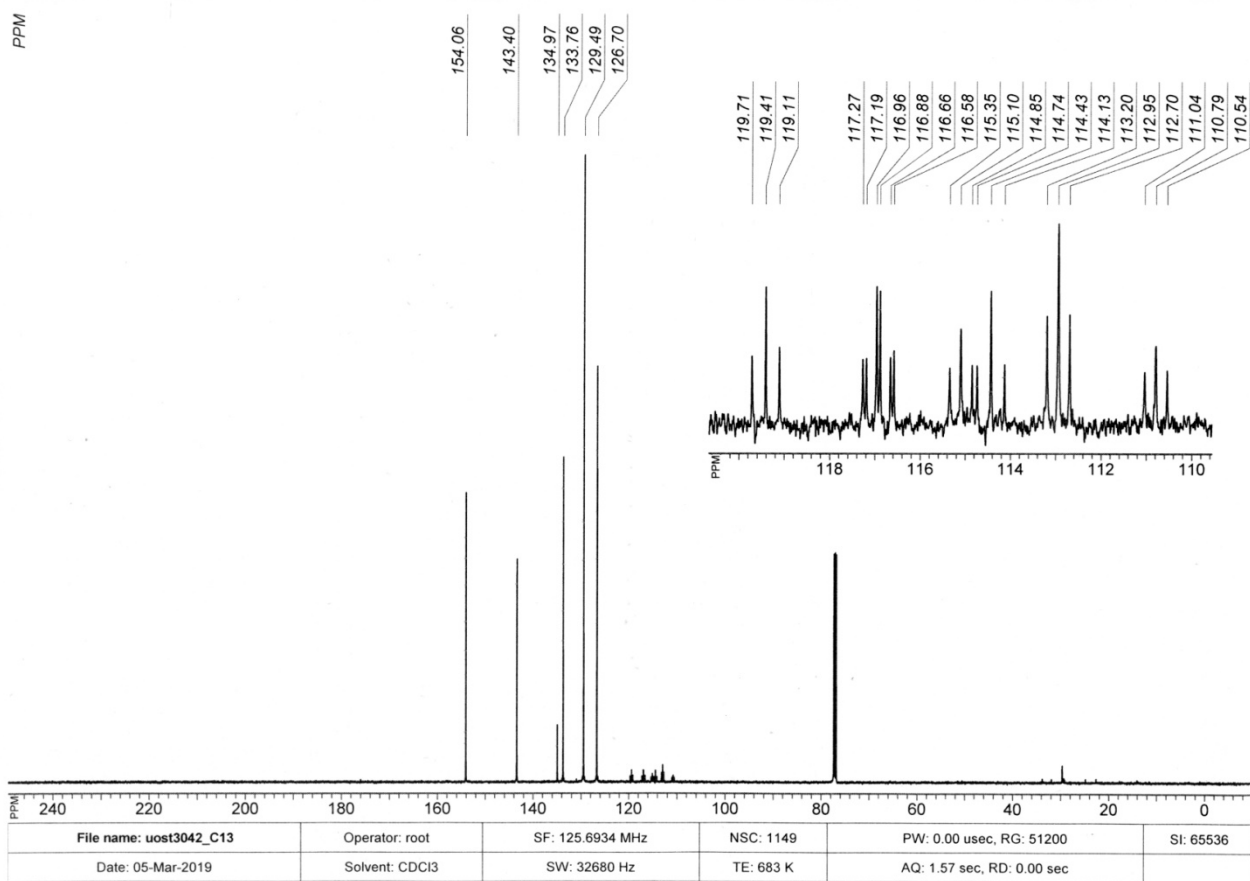
(1,1,2,2-Tetrafluoro-2-((1,2,4-triazol)-1-yl)-ethyl)-sulfinylbenzene 6d.



6d

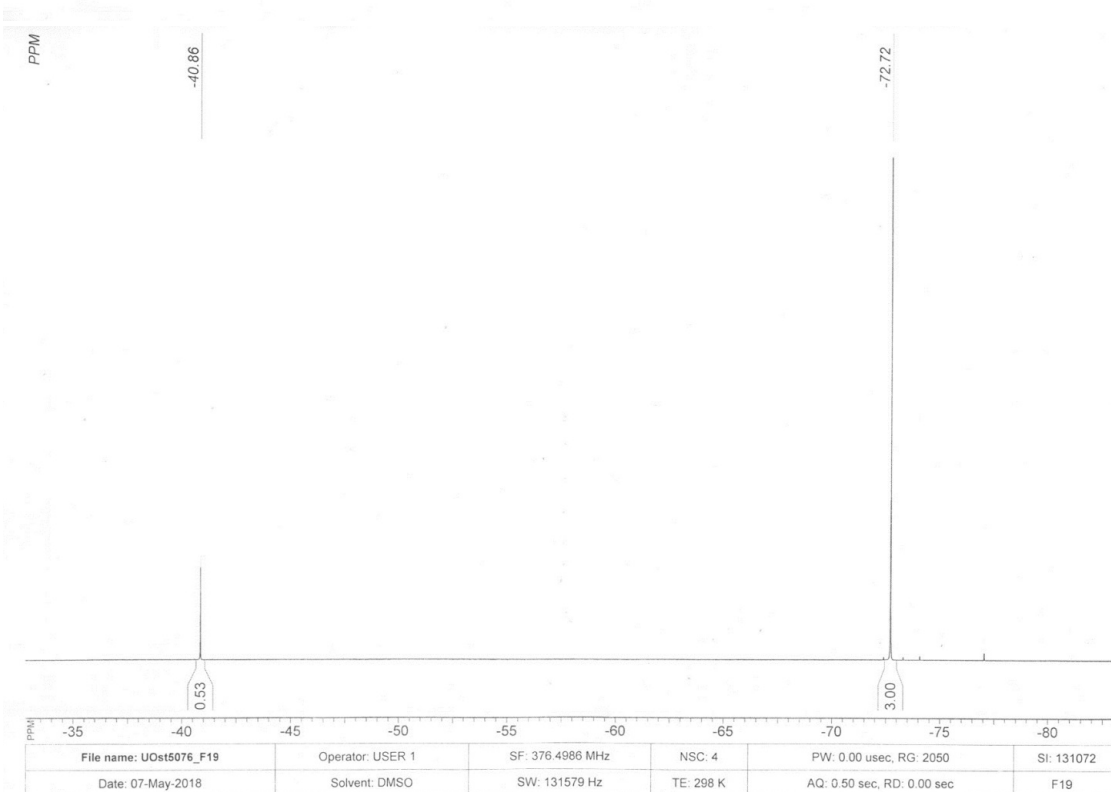
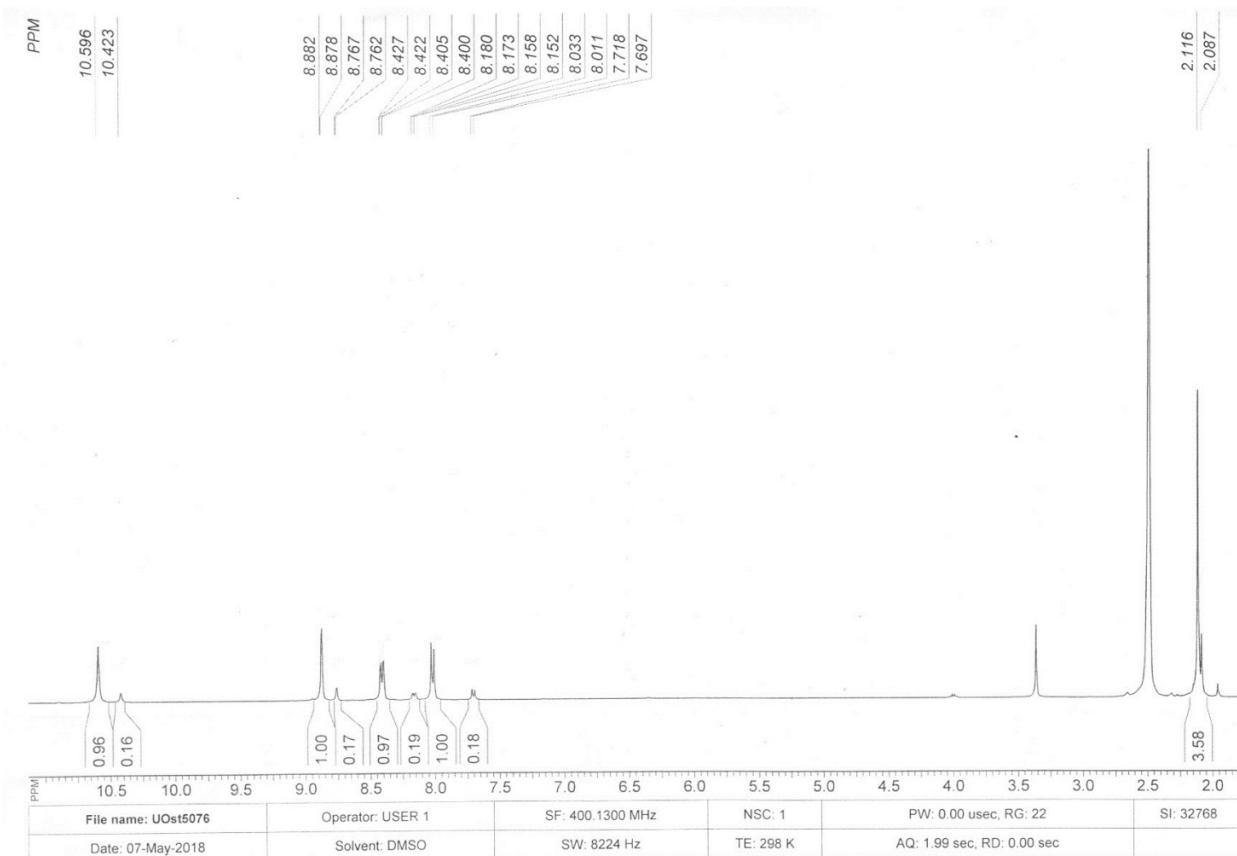
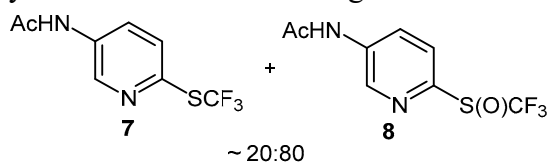




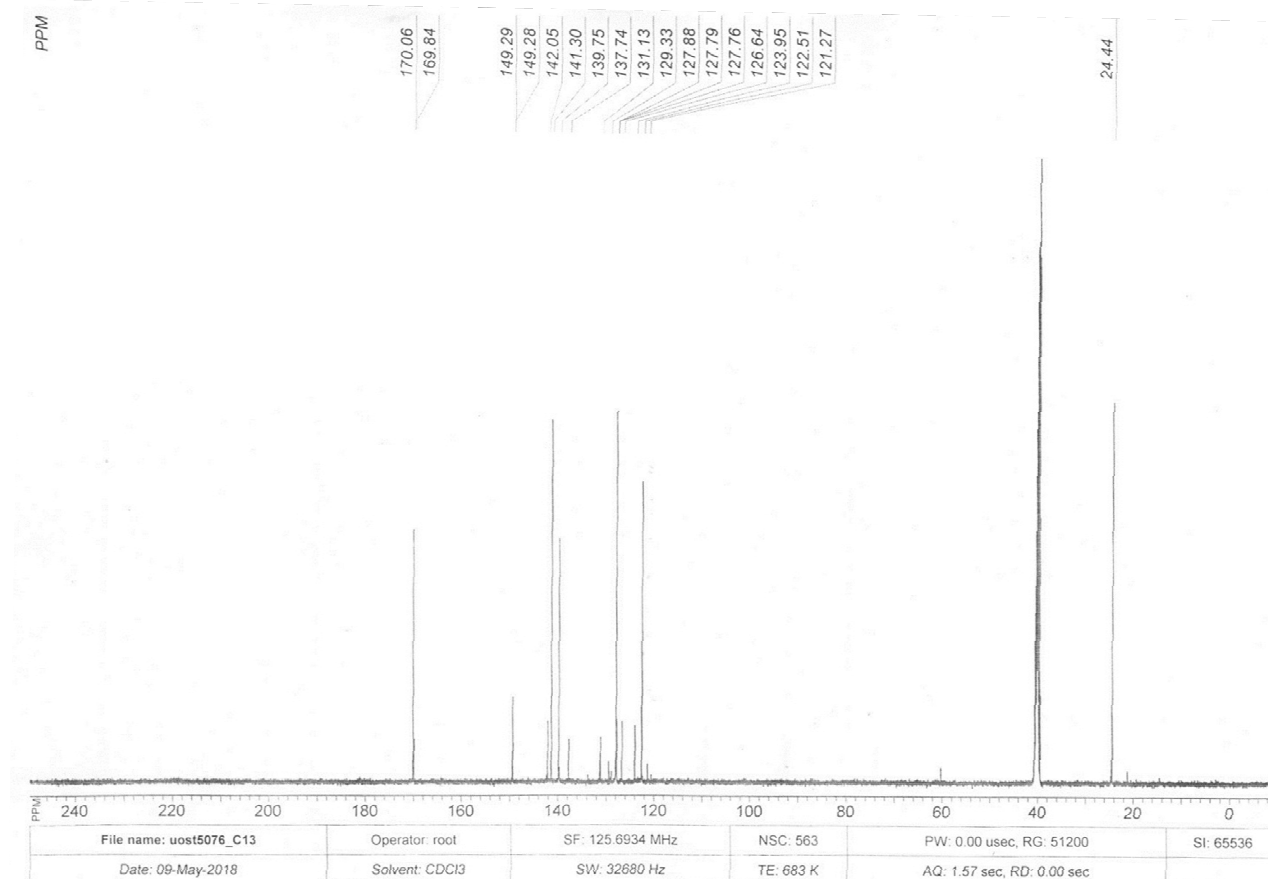
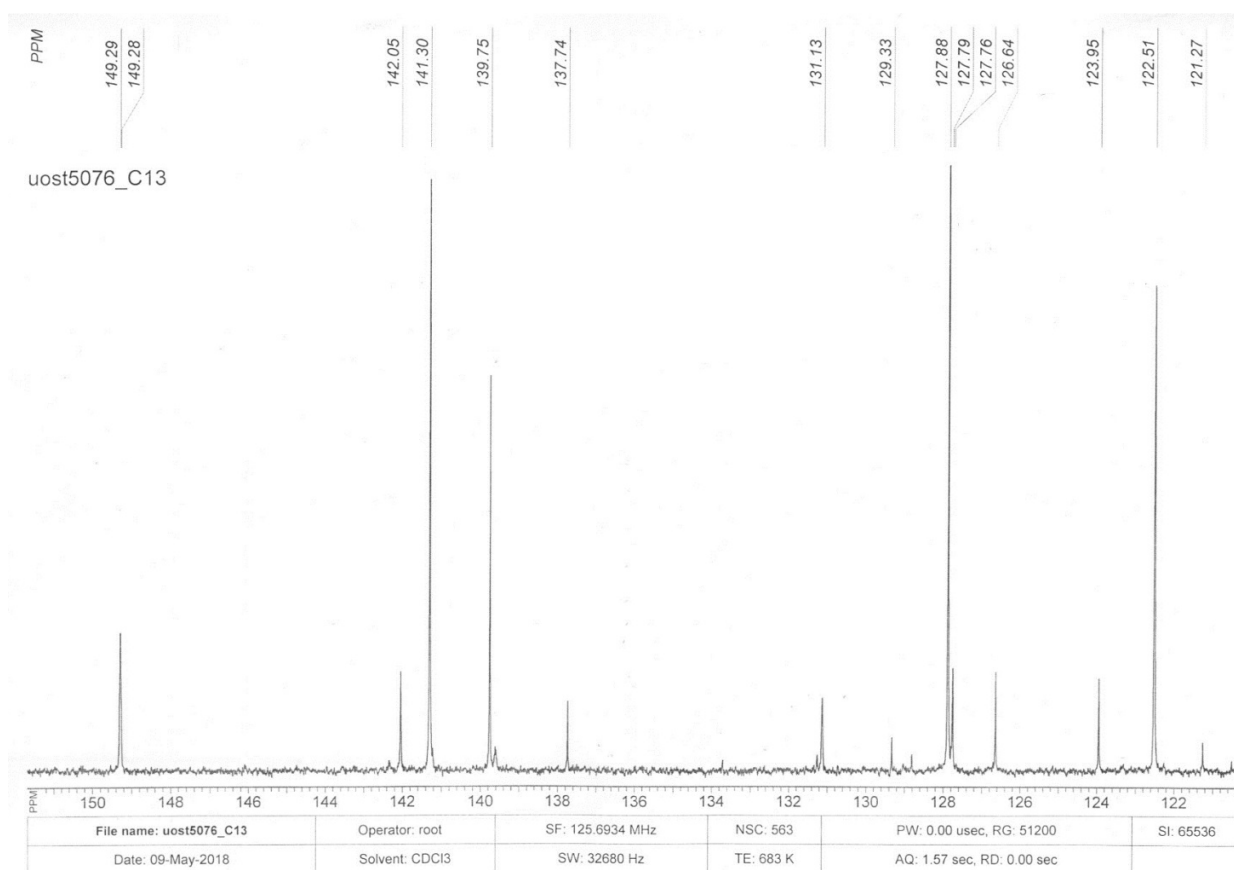


**N-(6-((Trifluoromethyl)sulfinyl)pyridin-3-yl)acetamide 8.**

Product with ~80 % purity. Contain ~20% of starting sulfide.







# Reaction mixture of the oxidation reaction for compound 9.

