Supporting Information

Biological activity evaluation and action mechanism of chalcone derivatives containing thiophene sulfonate

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Content

1. Antibacterial activity in vitro

Antibacterial activities of the title compounds **2a-2v** against *Xanthomonas axonopodispv. citri* (Xac), *Xanthomonas oryzaepv. oryzae* (Xoo) and *Ralstonia solanacearum* (Rs) were evaluated by using the turbidimeter test in vitro, commercial agricultural antibacterial Bismerthiazol and Thiodiazole-Copper were used as control. The test compounds were dissolved in 150 μL of dimethylformamide and diluted with 0.1 % (v/v)Tween-20 to prepare two concentrations of 200 and 100 μg/mL. 1 mL of the liquid sample was added to the non-toxic nutrient broth (NB: 1.5 g of beef extract, 2.5 g of peptone, 0.5 g of yeast powder, 5.0 g of glucose and 500 mL of distilled water, pH 7.0–7.2) liquid medium in 4 mL tubes. Then, 40 μL of NB containing Xac was added to 5 mL of solvent NB containing the test compounds or bismerthiazol. The inoculated test tubes were incubated at (30±1) °C under continuous shaking at 180/min for 48 h. The culture growth was monitored spectrophotometrically by measuring the optical density at 595 nm (OD_{595}) and expressed as corrected turbidity. The relative inhibitory rate (*I* %) compared with a blank assay was calculated as follows: $I\ \% = (C_{tur}–T_{tur})/C_{tur} \times 100\%$. C_{tur}: the corrected turbidity value of bacterial growth on untreated NB; T_{tur}: the corrected turbidity value of bacterial growth on treated NB.

Similarly, the solvent of Xoo and Rs were SM (10.0 g of peptone, 5.0 g of glucose, 1.0 g of casein acid hydrolysate, 1000 mL of distilled water, pH 7.0–7.2). Several of the target compounds were tested against Xoo and Xac at five double-declining concentrations (100, 50, 25, 12.5 and 6.25 μg/mL), and their corresponding EC_{50} values were obtained via software SPSS 17.0. Each experiment was computed at least three times.

2. Antiviral activities in vivo

Curative activity of the title compounds against TMV in vivo

Growing N. tabacum L. leaves of the same age were selected. The leaves were inoculated with TMV (concentration of 6×10^{-3} mg/mL) by dipping and brushing the whole leaves, which had previously been scattered with silicon carbide. The leaves were then washed with water after inoculation for 0.5 h. The compound solution was smeared on the left side of the leaves, and the solvent was smeared on the right side as the control. The number of local lesions was counted and recorded 3–4 d after inoculation[38-40]. Three replicates were set up for each.

Protection activity of the title compounds against TMV in vivo

The compound solutions were smeared on the left side of the *N. tabacum* L. leaves, and the solvents were smeared on the right side as the control sample for growing N. tabacum L. leaves. After 12 h, crude TMV (concentration of 6×10^{-3} mg/mL) was inoculated on whole leaves at the same concentration on each side of the leaves, which were previously scattered with silicon carbide. After 0.5 h, the leaves were washed with water and then dried. The number of local lesions was recorded 3–4 d after inoculation. Three replicates were used for each compound[38-40]. The inhibitory rate (*I* %) of the compound was calculated according to the following formula: $(I\ \%) = (C_{num} - T_{num})/ C_{num} \times 100\%$. C_{num}: average local lesion number of control(not treated with compounds); T_{num}: average local lesion number smeared with drugs.

Inactivation activity of the title compounds against TMV in vivo

The virus was inhibited after it was mixed with a compound solution of the same volume for 30 min. The right side of the N. tabacum L. leaves was then inoculated with the solvent and virus mixture for control. All of the leaves were previously scattered with silicon carbide. The number of local lesions was recorded three to four days after the inoculation. Three replications were reproduced for each compound. The inhibition rates *(I* %) of the compounds were calculated according to the following formula: $(I\ \%) = (C_{num} - T_{num})/ C_{num} \times 100\%$. C_{num}: average local lesion number of control(not

treated with compounds); T_{num}: average local lesion number smeared with compounds.

3. Scanning electron microscopy

In this assay, 1.5 mL *Xanthomonas axonopodispv. citri* (Xac) cells incubated at the logarithmic phase were centrifuged and washed with PBS (pH = 7.1), and re-suspended in 1.5 mL of PBS buffer (pH = 7.1). After that, bacteria *Xanthomonas axonopodispv. citri* (Xac) was incubated with compound **2l** at concentration of 50.0 μg/mL, 100.0 μg/mL, and an equivalent volume of DMSO (solvent control) for 4 h at room temperature. After incubation, these samples were washed 3 times with PBS (pH = 7.1). Subsequently, the bacterial cells were fixed for 8 h at 4 °C with 2.5 % glutaraldehyde, and then dehydrated with graded ethanol series and pure tert-butanol (2 times with 10 min/time). Following dehydration, samples were freezing dried and coated with gold, and visualized using Nova Nano SEM 450.

4.Interaction studies between 2e, 2h, 2n and ningnanmycin with TMV-CP

The binding was calculated for MST Monolith NT. 115. A range of ligands from 0 μM to 5 μM were incubated with 0.5 μM of purified recombinant proteins for 5 min with a NT-647 dye and was used in the thermophoresis experiment at a final concentration of 20 nM. A 16 point dilution series was made for selected compounds in DMSO. Each compound dilution series was subsequently transferred to protein solutions in 10 mM Tris-HCl and 100 mM sodium chloride pH 7.5, 0.05% Tween-20. After a 15 min incubation of the labeled TMV-CP with each dilution point (1:1 mix) at room temperature, samples were filled into standard capillaries. Measurements were taken on a Monolith NT.115 microscale thermophoresis system under a setting of 20% LED and 40% IR laser. Laser on time was set at 30 s, and laser-off time was set at 5 min. The Kd values were calculated from the duplicate reads of three separate experiments using the mass action equation in the Nano Temper software.

5.Molecular Docking study

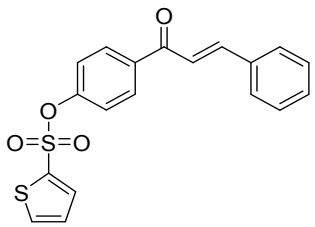
Molecule docking study were obtained by using DS-CDoking implemented in Discovery Studio (version 4.5). Through the UniProt database, we searching the coat protein subunit amino acid sequence of TMV. Using the protein BLAST server to search the template protein and homologies of TMV-CP sequence were aligned. Homology modeling of TMV-CP was constructed using Create Homology Models, which is a model integrated in Discovery Studio. Using Ramachandran plots evaluate the obtained models. The 3D structures of the compounds were carried out using the Sketching module and optimized by the Full Minimization module. During the docking process all parameters were default.

6.The physical properties of compounds 2a-2v

Table 1 The physical properties of compounds **2a**-**2v**

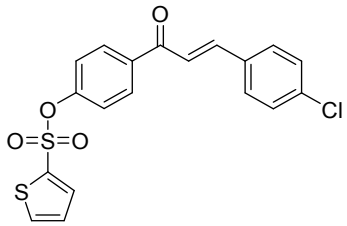
Compounds	R	Appearance	Yield /%	m.p./^{o}C
2a	Ph	Yellow solid	65	99.2-100.7
2b	4-Cl-Ph	Yellow solid	65	88.3-89.4
2c	2-Cl-Ph	Yellow solid	72	98.6-99.8
2d	3-Cl-Ph	Yellow solid	68	95.2-96.5
2e	2-F-Ph	Yellow solid	68	90.3-91.6
2f	3-F-Ph	Yellow solid	66	81.2-82.8
2g	4-F-Ph	Yellow solid	62	115.1-116.6
2h	2-Br-Ph	Yellow solid	71	94.2-95.7
2i	3-Br-Ph	Yellow solid	74	94.2-95.4
2j	4-Br-Ph	Yellow solid	63	95.1-96.2
2k	2-Py	White solid	64	105.4-106.6
2l	3-NO_2-Ph	Yellow solid	63	86.2-87.7
2m	3-CH_3-Ph	White solid	56	87.2-88.0
2n	4-CH_3-Ph	Yellow solid	68	90.1-91.5
2o	3,4-di-OCH_3-Ph	Yellow solid	63	98.1-99.8
2p	2,4-di-Cl-Ph	Yellow solid	71	101.2-102.9
2q	3,4-di-Cl-Ph	Yellow solid	67	96.5-97.4
2r	C_3H_7-Ph	White solid	63	86.1-87.6
2s	2-Th	Yellow solid	72	105.2-106.4
2t	4-Py	Yellow solid	76	88.2-89.8
2u	3,4-di-CH_3-Ph	Yellow solid	58	98.1-99.9
2v	2-OCH_3-Ph	Yellow solid	75	87.2-88.7

7.The data of title compounds 2a–2v



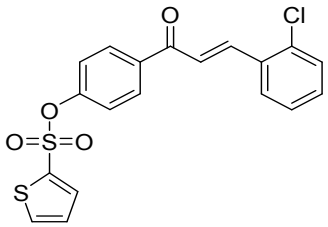
Data for

4-cinnamoylphenyl thiophene-2-sulfonate(**2a**): Yellow solid, m.p. 99.2-100.7 °C, yield 65%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.26 (dd, *J* = 5.0, 1.4 Hz, 1H, Ph-CH=), 8.23 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-2,6-H), 7.95 (dd, *J* = 14.6, 3.6 Hz, 1H, Ph-C=CH), 7.92-7.89 (m, 2H, Ph-2,6-H), 7.88 (dd, *J* = 3.9, 1.3 Hz, 1H, Th-5-H), 7.78 (d, *J* = 15.6 Hz, 1H, Ph-3-H), 7.50-7.46 (m, 3H, Ph-5-H, Ph-4-H, Th-3-H), 7.32 (dd, *J* = 4.9, 3.9 Hz, 1H, Ar(4-O)-3-H), 7.29 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-5-H, Th-4-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 188.38, 152.62, 145.08, 138.14, 137.37, 137.08, 135.00, 133.02, 131.29, 131.19, 129.50, 129.41, 129.12, 122.82, 122.14. HRMS (m/z): Calcd. For $C_{19}H_{14}O_4S_2$ [M + H]$^+$ 371.0406, meas. 371.0399.



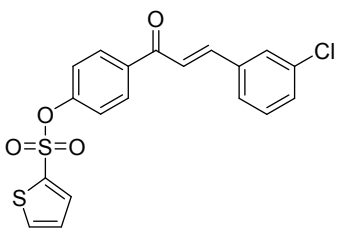
Data for

(E)-4-(3-(4-chlorophenyl)acryloyl)phenyl thiophene-2-sulfonate(**2b**): Yellow solid, m.p. 88.3-89.4 °C, yield 65%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.27 (dd, *J* = 5.0, 1.4 Hz, 1H, Ar-CH=), 8.23 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-2,6-H), 8.01-7.95 (m, 2H, Ar(4-Cl)-2,6-H), 7.94 (s, 1H, Ar(4-Cl)-3-H), 7.87 (dd, *J* = 3.9, 1.4 Hz, 1H, Ar(4-Cl)-5-H), 7.75 (d, *J* = 15.6 Hz, 1H, Ar-C=CH), 7.54 (d, *J* = 8.5 Hz, 2H, Th-5-H, Th-3-H), 7.32 (dd, *J* = 4.9, 3.9 Hz, 1H, Ar(4-O)-3-H), 7.28 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-5-H, Th-4-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 188.26, 152.66, 143.58, 138.19, 137.40, 136.95, 135.77, 133.98, 132.97, 131.24, 131.21, 129.45, 129.14, 122.84. HRMS (m/z): Calcd. For $C_{19}H_{13}ClO_4S_2$ [M + H]$^+$ 405.0016, meas. 405.0006.



Data for

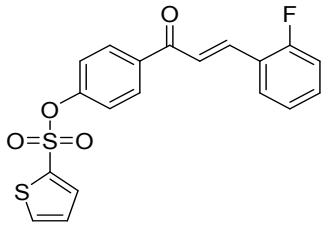
(E)-4-(3-(2-chlorophenyl)acryloyl)phenyl thiophene-2-sulfonate(**2c**): Yellow solid, m.p. 98.6-99.8 °C, yield 72%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.27 (dd, *J* = 5.0, 1.3 Hz, 1H, Ar-CH=), 8.26-8.23 (m, 2H, Ar(4-O)-2,6-H), 8.23 (d, *J* = 2.2 Hz, 1H, Th-5-H), 8.07 (d, *J* = 15.6 Hz, 1H, Ar(2-Cl)-3-H), 8.02-7.97 (m, 1H, Ar-C=CH), 7.89 (dd, *J* = 3.9, 1.4 Hz, 1H, Ar(2-Cl)-6-H), 7.60-7.56 (m, 1H, Ar(2-Cl)-5-H), 7.52-7.44 (m, 2H, Th-3-H, Ar(2-Cl)-4-H), 7.34-7.32 (m, 1H, Ar(4-O)-3-H), 7.30 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-3-H,). ^{13}C NMR (101 MHz, DMSO-d_6) δ 188.19, 152.77, 139.45, 138.13, 137.36, 136.76, 134.97, 133.02, 132.63, 132.57, 131.32, 130.51, 129.10, 128.13, 124.79, 122.86. HRMS (m/z): Calcd. For $C_{19}H_{13}ClO_4S_2$ [M + H]$^+$ 405.0016, meas. 405.0007.



Data for

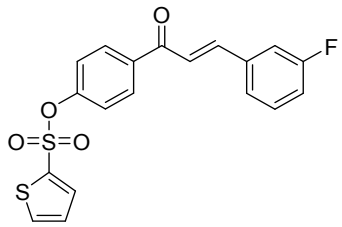
(E)-4-(3-(3-chlorophenyl)acryloyl)phenyl thiophene-2-sulfonate(**2d**): Yellow solid, m.p. 95.2-96.5 °C, yield 68%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.28-8.25 (m, 2H, Ar-CH=, Ar(4-O)-2-H), 8.24 (s, 1H, Ar(4-O)-6-H), 8.11 (s, 1H, Ar-C=CH), 8.04 (d, *J* = 15.6 Hz, 1H, Th-5-H),

7.88 (dd, *J* = 3.9, 1.4 Hz, 1H, Ar(3-Cl)-6-H), 7.84 (d, *J* = 7.1 Hz, 1H, Ar(3-Cl)-5-H), 7.74 (d, *J* = 15.6 Hz, 1H, Ar(3-Cl)-3-H), 7.51 (dd, *J* = 6.5, 4.5 Hz, 2H, Ar(3-Cl)-2-H, Th-3-H), 7.32 (dd, *J* = 5.0, 3.9 Hz, 1H, Ar(4-O)-3-H), 7.29 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-5-H, Th-4-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 188.46, 152.98, 143.54, 138.40, 137.63, 137.51, 137.11, 134.54, 133.26, 131.56, 131.41, 131.04, 129.37, 128.81, 128.74, 123.85, 123.07. HRMS (m/z): Calcd. For $C_{19}H_{13}ClO_4S_2$ [M + H]$^+$ 405.0016, meas. 405.0009.



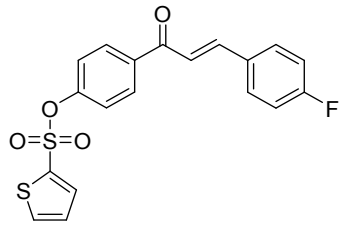
Data for

(E)-4-(3-(2-fluorophenyl)acryloyl)phenyl thiophene-2-sulfonate(**2e**): Yellow solid, m.p. 90.3-91.6 °C, yield 68%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.27 (dd, *J* = 5.0, 1.4 Hz, 1H, Ar-CH=), 8.22 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-2,6-H), 8.17-8.10 (m, 1H, Th-5-H), 7.99 (d, *J* = 15.7 Hz, 1H, Ar-C=CH), 7.90-7.87 (m, 2H, Ar(2-F)-6,3-H), 7.54 (tdd, *J* = 7.2, 5.5, 1.7 Hz, 1H, Ar(2-F)-4-H), 7.37-7.34 (m, 1H, Ar(2-F)-5-H), 7.33-7.31 (m, 2H, Th-3-H, Ar(4-O)-3-H), 7.30 (d, *J* = 8.9 Hz, 2H, Ar(4-O)-5-H, Th-4-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 188.21, 162.68, 160.18, 152.73, 138.13, 137.36, 136.81, 136.09, 136.04, 133.38, 133.29, 133.02, 131.24, 129.61, 129.59, 129.10, 125.44, 125.41, 124.18, 124.14, 122.87, 122.68, 122.57, 116.68, 116.46. ^{19}F NMR (376 MHz, DMSO-d_6) δ -116.10. HRMS (m/z): Calcd. For $C_{19}H_{13}FO_4S_2$ [M + H]$^+$ 389.0312, meas. 389.0307.



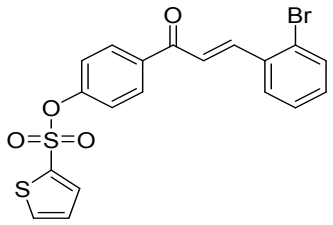
Data for

(E)-4-(3-(3-fluorophenyl)acryloyl)phenyl thiophene-2-sulfonate(**2f**): Yellow solid, m.p. 81.2-82.8 °C, yield 66%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.26 (s, 2H, Ar-CH=, Ar(4-O)-2-H), 8.24 (s, 1H, Ar(4-O)-6-H), 8.02 (d, *J* = 15.6 Hz, 1H, Ar-C=CH), 7.89 (d, *J* = 1.4 Hz, 1H, Th-5-H), 7.88 (dd, *J* = 3.9, 1.4 Hz, 1H, Ar(3-F)-6-H), 7.77 (d, *J* = 15.6 Hz, 1H, Ar(3-F)-5-H), 7.72 (d, *J* = 7.8 Hz, 1H, Th-3-H), 7.55-7.48 (m, 1H, Ar(4-O)-3-H), 7.34-7.31 (m, 2H, Ar(4-O)-5-H, Th-4-H), 7.29 (d, *J* = 8.8 Hz, 2H, Ar(3-F)-4-H, Ar(3-F)-2-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 188.26, 164.16, 161.74, 152.72, 143.55, 143.52, 138.13, 137.61, 137.53, 137.37, 136.88, 133.02, 131.81, 131.37, 131.28, 129.11, 126.24, 126.22, 123.54, 122.83, 118.03, 117.82, 115.31, 115.09. ^{19}F NMR (376 MHz, DMSO-d_6) δ -112.93. HRMS (m/z): Calcd. For $C_{19}H_{13}FO_4S_2$ [M + H]$^+$ 389.0312, meas. 389.0305.



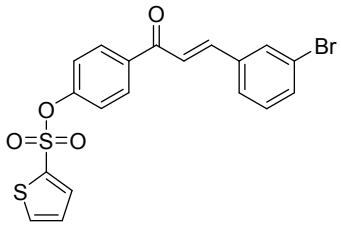
Data for

(E) -4-(3-(4-fluorophenyl)acryloyl)phenyl thiophene-2-sulfonate(**2g**): Yellow solid, m.p. 115.1-116.6 °C, yield 62%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.26 (dd, *J* = 5.0, 1.4 Hz, 1H, Ar-CH=), 8.22 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-2,6-H), 8.02-7.97 (m, 2H, Ar(4-F)-2,6-H), 7.94-7.89 (m, 1H, Ar-C=CH), 7.87 (dd, *J* = 3.9, 1.4 Hz, 1H, Th-5-H), 7.77 (d, *J* = 15.6 Hz, 1H, Ar(4-F)-3-H), 7.35-7.31 (m, 2H, Ar(4-F)-5-H, Th-3-H), 7.30 (d, *J* = 1.9 Hz, 1H, Ar(4-O)-3-H), 7.28 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-5-H, Th-4-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 188.28, 165.23, 162.76, 152.62, 143.84, 138.14, 137.37, 137.05, 133.01, 131.94, 131.85, 131.72, 131.69, 131.19, 129.12, 122.81, 122.02, 122.00, 116.56, 116.34. ^{19}F NMR (376 MHz, DMSO-d_6) δ -109.62. HRMS (m/z): Calcd. For $C_{19}H_{13}FO_4S_2$ [M + H]$^+$ 389.0312, meas. 389.0305.



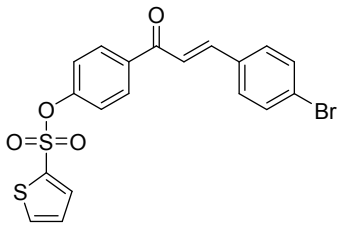
Data for

(E)-4-(3-(2-bromophenyl)acryloyl)phenyl thiophene-2-sulfonate(**2h**): Yellow solid, m.p. 94.2-95.7 °C, yield 62%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.27 (dd, *J* = 5.0, 1.4 Hz, 1H, Ar-CH=), 8.26-8.23 (m, 2H, Ar(4-O)-2,6-H), 8.21 (dd, *J* = 7.9, 1.5 Hz, 1H, Th-5-H), 8.01-7.93 (m, 2H, Ar(2-Br)-3-H, Ar-C=CH), 7.88 (dd, *J* = 3.9, 1.4 Hz, 1H, Ar(2-Br)-5-H), 7.77-7.73 (m, 1H, Ar(2-Br)-4-H), 7.53-7.48 (m, 1H, Ar(2-Br)-6-H), 7.43-7.38 (m, 1H, Th-3-H), 7.33 (dd, *J* = 4.0, 2.9 Hz, 1H, Ar(4-O)-3-H), 7.30 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-5-H, Th-4-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 188.19, 152.77, 142.22, 138.16, 137.38, 136.76, 134.23, 133.79, 133.00, 132.82, 131.33, 129.30, 129.12, 128.69, 126.01, 124.97, 122.87. HRMS (m/z): Calcd. For $C_{19}H_{13}BrO_4S_2$ $[M + H]^+$ 448.9511, meas. 448.9506.



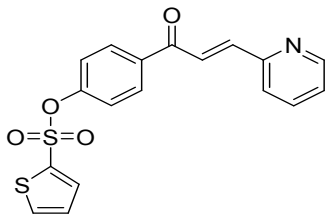
Data for

(E)-4-(3-(3-bromophenyl)acryloyl)phenyl thiophene-2-sulfonate(**2i**): Yellow solid, m.p. 94.2-95.4 °C, yield 74%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (t, *J* = 7.6 Hz, 1H, Ar-CH=), 8.00 (d, *J* = 8.7 Hz, 1H, Ar(4-O)-2-H), 7.82-7.69 (m, 3H, Ar(4-O)-6-H, Ar-C=CH, Th-5-H), 7.62 (dd, *J* = 3.7, 1.1 Hz, 1H, Ar(3-Br)-6-H), 7.57-7.50 (m, 2H, Ar(3-Br)-2-H, Ar(3-Br)-4-H), 7.49-7.36 (m, 2H, Ar(3-Br)-5-H, Th-3-H), 7.30 (td, *J* = 7.9, 2.6 Hz, 1H, Ar(4-O)-3-H), 7.20 (d, *J* = 8.7 Hz, 1H, Ar(4-O)-5-H), 7.15-7.10 (m, 1H, Th-4-H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.59, 154.34, 152.78, 143.75, 143.38, 135.83, 135.11, 130.91, 130.58, 130.56, 130.34, 127.78, 127.42, 127.38, 122.60, 122.51, 122.02. HRMS (m/z): Calcd. For $C_{19}H_{13}BrO_4S_2$ $[M + H]^+$ 448.9511, meas. 448.9508.



Data for

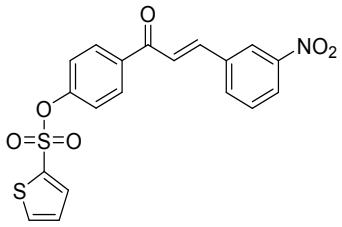
(E)-4-(3-(4-bromophenyl)acryloyl)phenyl thiophene-2-sulfonate(**2j**): Yellow solid, m.p. 95.1-96.2 °C, yield 63%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 (dd, *J* = 5.0, 1.4 Hz, 1H, Ar-CH=), 8.21 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-2,6-H), 7.97 (d, *J* = 15.6 Hz, 1H, Ar(4-Br)-3-H), 7.88-7.85 (m, 3H, Ar(4-Br)-5-H, Ar(4-Br)-2,6-H), 7.73 (d, *J* = 15.7 Hz, 1H, Ar-C=CH), 7.68 (d, *J* = 8.5 Hz, 2H, Th-5-H, Th-3-H), 7.31 (dd, *J* = 5.0, 3.9 Hz, 1H, Ar(4-O)-3-H), 7.28 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-5-H, Th-4-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 187.27, 151.59, 142.63, 137.05, 136.31, 135.87, 133.20, 131.89, 131.32, 130.31, 130.16, 128.08, 123.63, 121.81, 121.77. HRMS (m/z): Calcd. For $C_{19}H_{13}BrO_4S_2$ $[M + H]^+$ 448.9511, meas. 448.9506.



Data for

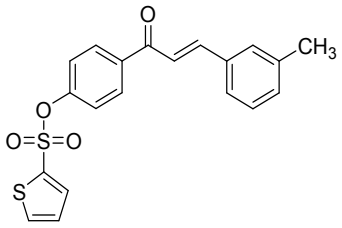
(E)-4-(3-(pyridin-2-yl)acryloyl)phenyl thiophene-2-sulfonate(**2k**): White solid, m.p. 105.4-106.6 °C, yield 64%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.70 (dd, *J* = 5.9, 2.5 Hz, 1H, Py-3-H), 8.27 (dd, *J* = 5.0, 1.4

Hz, 1H, Py-C=CH), 8.17 (d, *J* = 8.8 Hz, 2H, Py-CH=, Ar(4-O)-2-H), 8.13 (d, *J* = 15.4 Hz, 1H, Ar(4-O)-6-H), 7.93 (dd, *J* = 6.5, 1.4 Hz, 2H, Th-5-H, Py-6-H), 7.90-7.87 (m, 1H, Py-5-H), 7.74 (d, *J* = 15.4 Hz, 1H, Py-4-H), 7.46 (ddd, *J* = 6.5, 4.8, 2.5 Hz, 1H, Th-3-H), 7.33 (dd, *J* = 3.6, 2.5 Hz, 1H, Ar(4-O)-3-H), 7.30 (d, *J* = 8.9 Hz, 2H, Ar(4-O)-5-H, Th-4-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 188.77, 153.07, 152.71, 150.53, 144.04, 138.16, 137.70, 137.38, 136.84, 133.01, 131.20, 129.12, 125.58, 125.45, 125.26, 122.95. HRMS (m/z): Calcd. For $C_{18}H_{13}NO_4S_2$ $[M + H]^+$ 372.0359, meas. 372.0352.



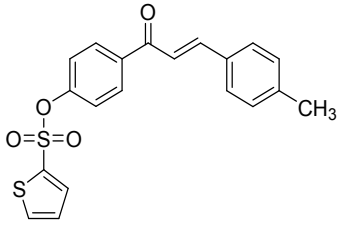
Data for

(E)-4-(3-(3-nitrophenyl)acryloyl)phenyl thiophene-2-sulfonate(**2l**): Yellow solid, m.p. 86.2-87.7 °C, yield 63%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.81 (s, 1H, Ar(3-NO_2)-2-H), 8.34 (d, *J* = 7.8 Hz, 1H, Ar-CH=), 8.28 (d, *J* = 1.9 Hz, 1H, Ar(3-NO_2)-4-H), 8.27 (dd, *J* = 4.6, 1.7 Hz, 3H, Ar(4-O)-2,6-H, Ar(3-NO_2)-6-H), 8.17 (d, *J* = 15.7 Hz, 1H, Ar-C=CH), 7.90-7.85 (m, 2H, Ar(3-NO_2)-5-H, Th-5-H), 7.76 (t, *J* = 7.9 Hz, 1H, Th-3-H), 7.32 (dt, *J* = 5.1, 2.5 Hz, 1H, Ar(4-O)-3-H), 7.29 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-5-H, Th-4-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 188.24, 152.80, 148.87, 142.46, 138.17, 137.39, 136.90, 136.74, 135.76, 133.00, 131.41, 130.84, 129.13, 125.31, 124.83, 123.55, 122.84. HRMS (m/z): Calcd. For $C_{19}H_{13}NO_6S_2$ $[M + H]^+$ 416.0272, meas. 416.0257.



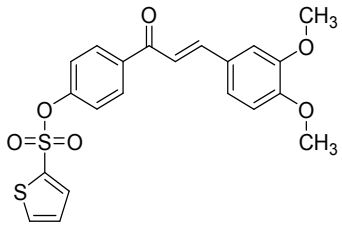
Data for

(E)-4-(3-(m-tolyl)acryloyl)phenyl thiophene-2-sulfonate(**2m**): White solid, m.p. 87.2-88.0 °C, yield 56%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.26 (dd, *J* = 5.0, 1.4 Hz, 1H, Ar-CH=), 8.22 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-2,6-H), 7.92 (d, *J* = 15.6 Hz, 1H, Ar-C=CH), 7.87 (dd, *J* = 3.9, 1.4 Hz, 1H, Th-5-H), 7.77-7.70 (m, 2H, Ar(3-CH_3)-6-H, Ar(3-CH_3)-2-H), 7.67 (d, *J* = 7.5 Hz, 1H, Ar(3-CH_3)-5-H), 7.38-7.33 (m, 1H, Th-3-H), 7.33-7.29 (m, 2H, Ar(4-O)-3,5-H), 7.29-7.26 (m, 2H, Th-4-H, Ar(3-CH_3)-4-H), 2.36 (s, 3H, CH_3). ^{13}C NMR (101 MHz, DMSO-d_6) δ 187.27, 151.53, 144.15, 137.59, 137.08, 136.31, 136.04, 133.85, 131.95, 130.96, 130.10, 128.65, 128.22, 128.05, 125.91, 121.73, 120.84, 20.27. HRMS (m/z): Calcd. For $C_{20}H_{16}O_4S_2$ $[M + H]^+$ 385.0563, meas. 385.0554.



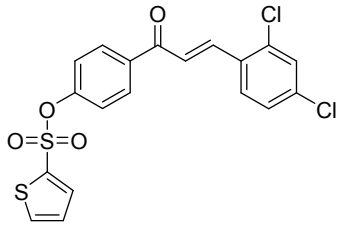
Data for

(E)-4-(3-(p-tolyl)acryloyl)phenyl thiophene-2-sulfonate(**2n**): Yellow solid, m.p. 90.1-91.5 °C, yield 68%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.26 (dd, *J* = 5.0, 1.4 Hz, 1H, Ar-CH=), 8.22 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-2,6-H), 7.89 (dd, *J* = 10.4, 2.9 Hz, 1H, Ar-C=CH), 7.87 (d, *J* = 1.4 Hz, 1H, Ar(4-CH_3)-2-H), 7.80 (d, *J* = 8.1 Hz, 2H, Ar(4-CH_3)-6-H, Th-5-H), 7.74 (d, *J* = 15.5 Hz, 1H, Ar(4-CH_3)-3-H), 7.33-7.29 (m, 2H, Ar(4-CH_3)-5-H, Th-3-H), 7.29-7.27 (m, 2H, Ar(4-O)-3,5-H), 7.26 (d, *J* = 2.0 Hz, 1H, Th-4-H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 187.24, 151.49, 144.10, 140.37, 137.06, 136.30, 136.14, 131.98, 131.24, 130.06, 128.98, 128.49, 128.05, 121.72, 120.00, 20.53. HRMS (m/z): Calcd. For $C_{20}H_{16}O_4S_2$ $[M + H]^+$ 385.0563, meas. 385.0553.



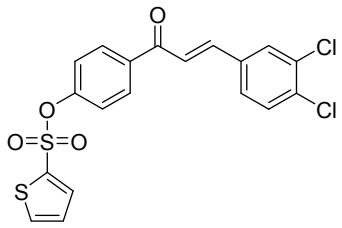
Data for

(E)-4-(3-(3,4-dimethoxyphenyl)acryloyl)phenyl thiophene-2-sulfonate(**2o**): Yellow solid, m.p. 98.1-99.8 °C, yield 63%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.26 (dd, J = 5.0, 1.3 Hz, 1H, Ar-CH=), 8.22 (d, J = 8.8 Hz, 2H, Ar(4-O)-2,6-H), 7.87 (dd, J = 3.8, 1.3 Hz, 1H, Ar-C=CH), 7.83 (d, J = 15.5 Hz, 1H, Th-5-H), 7.73 (d, J = 15.5 Hz, 1H, Ar(3,4-di-OCH_3)-2-H), 7.56 (d, J = 1.8 Hz, 1H, Ar(3,4-di-OCH_3)-5-H), 7.40 (dt, J = 6.5, 3.3 Hz, 1H, Th-3-H), 7.32 (dd, J = 4.9, 3.9 Hz, 1H, Ar(3,4-di-OCH_3)-6-H), 7.28 (d, J = 8.7 Hz, 2H, Ar(4-O)-3,5-H), 7.03 (d, J = 8.4 Hz, 1H, Th-4-H), 3.85 (d, J = 16.2 Hz, 6H, OCH_3). ^{13}C NMR (101 MHz, DMSO-d_6) δ 187.09, 151.41, 150.87, 148.41, 144.59, 137.07, 136.34, 136.30, 131.98, 129.99, 128.06, 126.76, 123.76, 121.68, 118.53, 110.88, 110.05, 55.13, 55.00. HRMS (m/z): Calcd. For $C_{21}H_{18}O_6S_2$ $[M + H]^+$ 431.0618, meas. 431.0610.



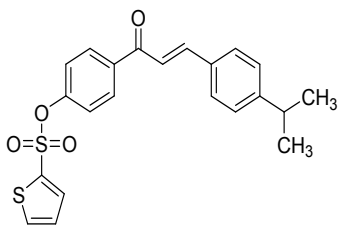
Data for

(E)-4-(3-(2,4-dichlorophenyl)acryloyl)phenyl thiophene-2-sulfonate(**2p**): Yellow solid, m.p. 101.2-102.9 °C, yield 71%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.27 (d, J = 1.5 Hz, 1H, Ar-CH=), 8.25 (s, 2H, Ar(4-O)-2,6-H), 8.23 (s, 1H, Ar(2,4-di-Cl)-3-H), 8.05-8.00 (m, 1H, Ar(2,4-di-Cl)-6-H), 7.96 (d, J = 15.6 Hz, 1H, Th-5-H), 7.88 (dd, J = 3.9, 1.4 Hz, 1H, Ar(2,4-di-Cl)-5-H), 7.74 (d, J = 2.1 Hz, 1H, Ar-C=CH), 7.55 (dd, J = 8.5, 2.0 Hz, 1H, Th-3-H), 7.32 (dd, J = 5.0, 3.9 Hz, 1H, Ar(4-O)-3-H), 7.29 (d, J = 8.8 Hz, 2H, Ar(4-O)-5-H, Th-4-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 186.96, 151.77, 137.10, 136.32, 135.60, 135.24, 134.69, 131.97, 130.58, 130.30, 129.27, 128.93, 128.06, 127.35, 124.24, 121.81. HRMS (m/z): Calcd. For $C_{19}H_{12}Cl_2O_4S_2$ $[M + H]^+$ 438.9627, meas. 438.9617.



Data for

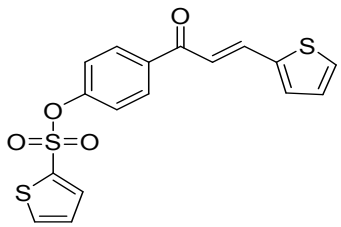
(E)-4-(3-(3,4-dichlorophenyl)acryloyl)phenyl thiophene-2-sulfonate(**2q**): Yellow solid, m.p. 96.5-97.4 °C, yield 67%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.31 (d, J = 1.9 Hz, 1H, Ar-CH=), 8.28-8.24 (m, 2H, Ar(4-O)-2,6-H), 8.24-8.22 (m, 1H, Ar-C=CH), 8.06 (d, J = 15.6 Hz, 1H, Ar(3,4-di-Cl)-6-H), 7.91 – 7.86 (m, 2H, Th-5-H, Ar(3,4-di-Cl)-5-H), 7.7-7.70 (m, 2H, Ar(3,4-di-Cl)-2-H, Th-3-H), 7.31 (dd, J = 5.0, 3.9 Hz, 1H, Ar(4-O)-3-H), 7.28 (d, J = 8.8 Hz, 2H, Ar(4-O)-5-H, Th-4-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 187.06, 151.69, 141.12, 137.10, 136.32, 135.72, 134.83, 132.30, 131.92, 131.23, 130.42, 130.26, 129.63, 128.73, 128.06, 123.05, 121.77. HRMS (m/z): Calcd. For $C_{19}H_{12}Cl_2O_4S_2$ $[M + H]^+$ 438.9627, meas. 438.9622.



Data for

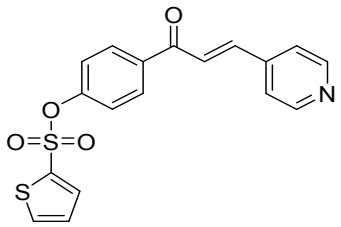
(E)-4-(3-(4-isopropylphenyl)acryloyl)phenyl thiophene-2-sulfonate(**2r**): Wtite solid, m.p. 86.1-87.6 °C, yield 63%. ^{1}H NMR

(400 MHz, DMSO-d_6) δ 8.27 (dd, *J* = 5.0, 1.4 Hz, 1H, Ar-CH=), 8.23 (s, 1H, Ar(4-O)-2-H), 8.21 (s, 1H, Ar(4-O)-6-H), 7.88 (dt, *J* = 5.2, 1.9 Hz, 2H, Ar(4-C_3H_7)-2,6-H), 7.82 (d, *J* = 8.2 Hz, 2H, Ar-C=CH, Th-5-H), 7.75 (d, *J* = 15.6 Hz, 1H, Ar(4-C_3H_7)-3-H), 7.35 (s, 1H, Ar(4-C_3H_7)-5-H), 7.33 (s, 1H, Th-3-H), 7.32-7.31 (m, 1H, Ar(4-O)-3-H), 7.28 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-5-H, Th-4-H), 2.93 (dt, *J* = 13.8, 6.9 Hz, 1H, -CH=), 1.22 (d, *J* = 6.9 Hz, 6H, CH_3). ^{13}C NMR (101 MHz, DMSO-d_6) δ 187.27, 151.51, 151.11, 144.12, 137.07, 136.30, 136.15, 132.00, 131.67, 130.07, 128.62, 128.05, 126.34, 121.74, 120.11, 32.88, 23.01. HRMS (m/z): Calcd. For $C_{22}H_{20}O_4S_2$ $[M + H]^+$ 413.0876, meas. 413.0867.



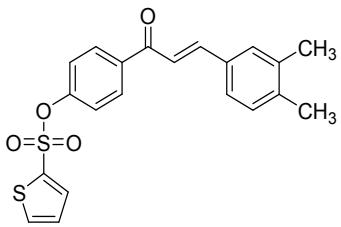
Data for

(E)-4-(3-(thiophen-2-yl)acryloyl)phenyl thiophene-2-sulfonate(**2s**): Yellow solid, m.p. 105.2-106.4 °C, yield 72%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 (dd, *J* = 5.0, 1.4 Hz, 1H, Ar(4-O)-2-H), 8.16 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-6-H, Th-CH=), 7.93 (d, *J* = 15.3 Hz, 1H, Th-5-H), 7.86 (dd, *J* = 3.9, 1.4 Hz, 1H, Th-3-H), 7.82 (d, *J* = 5.0 Hz, 1H, Th-C=CH), 7.72 (d, *J* = 3.5 Hz, 1H, Th-5-H), 7.56 (d, *J* = 15.3 Hz, 1H, Th-4-H), 7.31 (dd, *J* = 5.0, 3.9 Hz, 1H, Th-3-H), 7.26 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-3,5-H), 7.21 (dd, *J* = 5.0, 3.6 Hz, 1H, Th-4-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 186.79, 151.46, 138.99, 137.07, 136.72, 136.30, 135.95, 132.69, 131.93, 130.33, 129.97, 128.18, 128.05, 121.73, 119.31. HRMS (m/z): Calcd. For $C_{17}H_{12}O_4S_3$ $[M + H]^+$ 376.9971, meas. 376.9961.



Data for

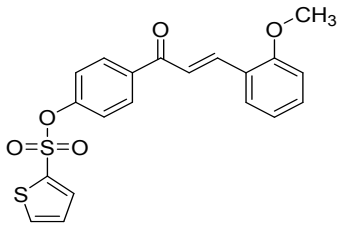
(E)-4-(3-(pyridin-4-yl)acryloyl)phenyl thiophene-2-sulfonate(**2t**): Yellow solid, m.p. 88.2-89.8 °C, yield 76%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.69 (d, *J* = 5.6 Hz, 2H, Py-2,6-H), 8.26 (dt, *J* = 3.2, 1.6 Hz, 2H, Ar(4-O)-2,6-H), 8.24 (d, *J* = 1.9 Hz, 1H, Py-CH=), 8.16 (d, *J* = 15.7 Hz, 1H, Py-C=CH), 7.88 (dd, *J* = 3.9, 1.4 Hz, 1H, Th-5-H), 7.85 (d, *J* = 6.0 Hz, 2H, Py-3,5-H), 7.71 (d, *J* = 15.7 Hz, 1H, Th-3-H), 7.32 (dd, *J* = 3.4, 2.5 Hz, 1H, Ar(4-O)-3-H), 7.30 (dd, *J* = 7.1, 1.7 Hz, 2H, Ar(4-O)-5-H, Th-4-H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 187.30, 151.79, 149.79, 141.03, 140.97, 137.12, 136.34, 135.52, 131.92, 130.35, 128.07, 125.39, 121.98, 121.85. HRMS (m/z): Calcd. For $C_{18}H_{13}NO_4S_2$ $[M + H]^+$ 372.0359, meas. 372.0352.



Data for

(E)-4-(3-(3,4-dimethylphenyl)acryloyl)phenyl thiophene-2-sulfonate(**2u**): Yellow solid, m.p. 98.1-99.9 °C, yield 58%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.26 (dd, *J* = 5.0, 1.4 Hz, 1H, Ar-CH=), 8.21 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-2,6-H), 7.87 (ddd, *J* = 10.8, 7.4, 3.5 Hz, 2H, Ar-C=CH, Th-5-H), 7.73-7.67 (m, 2H, Ar(3,4-di-CH_3)-5,6-H), 7.60 (dd, *J* = 7.9, 1.3 Hz, 1H, Ar(3,4-di-CH_3)-2-H), 7.31 (dd, *J* = 5.0, 3.9 Hz, 1H, Th-3-H), 7.27 (d, *J* = 8.8 Hz, 2H, Ar(4-O)-3,5-H), 7.23 (d, *J* = 7.8 Hz, 1H, Th-4-H), 2.27 (d, *J* = 2.9 Hz, 6H, CH_3). ^{13}C NMR (101 MHz, DMSO-d_6) δ 187.19, 151.47, 144.32, 139.27, 137.07, 136.32, 136.30, 136.17, 131.97, 131.54, 130.03, 129.45,

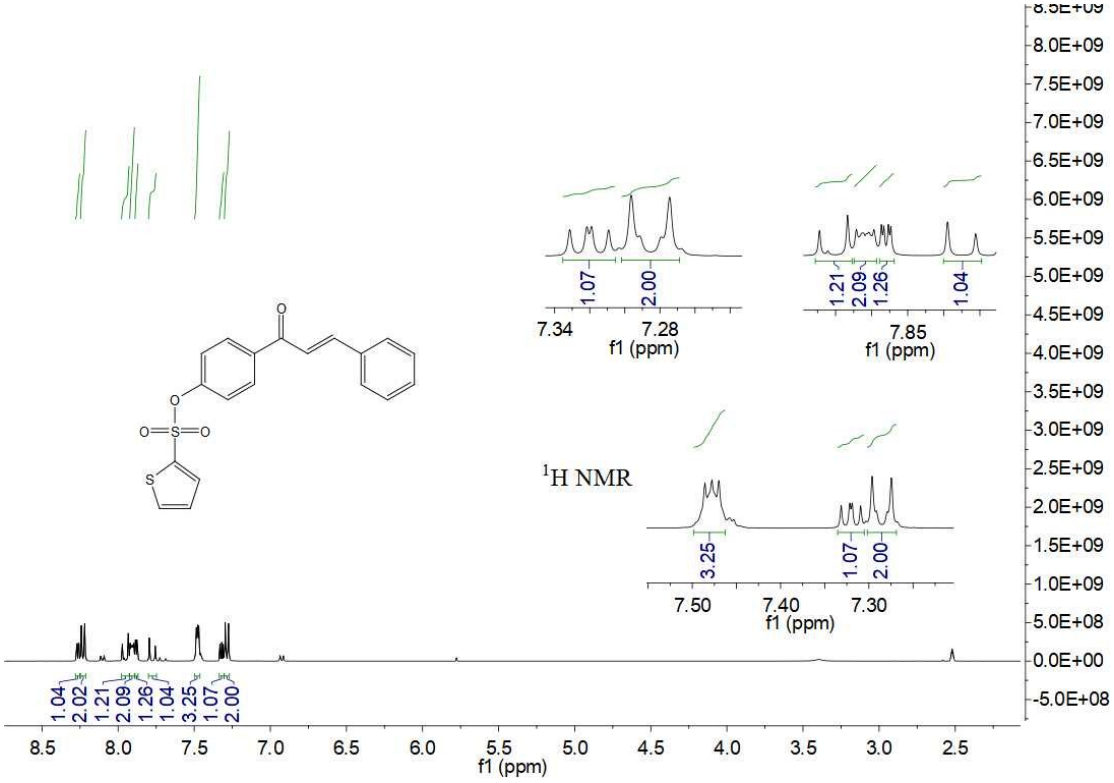
129.20, 128.05, 126.34, 121.71, 119.75, 18.91, 18.69. HRMS (m/z): Calcd. For $C_{21}H_{18}O_4S_2$ $[M + H]^+$ 399.0720, meas. 399.0714.



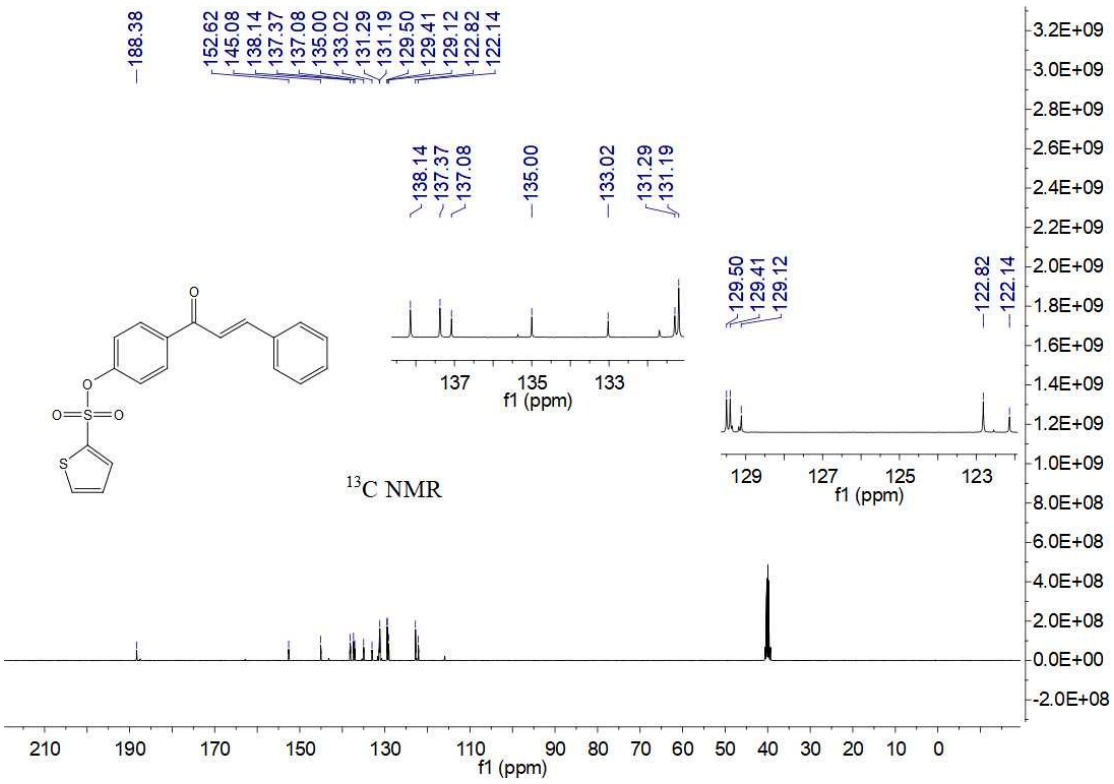
Data for

(E)-4-(3-(2-methoxyphenyl)acryloyl)phenyl thiophene-2-sulfonate(**2v**): Yellow solid, m.p. 87.2-88.7 °C, yield 75%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.26 (dd, J = 5.0, 1.4 Hz, 1H, Ar-CH=), 8.19 (d, J = 6.8 Hz, 2H, Ar(4-O)-2,6-H), 8.08 (d, J = 15.8 Hz, 1H, Ar(2-OCH_3)-6-H), 7.99 (dd, J = 7.8, 1.5 Hz, 1H, Th-5-H), 7.91-7.86 (m, 2H, Ar(2-OCH_3)-4-H, Ar-C=CH), 7.50-7.44 (m, 1H, Th-3-H), 7.32 (dd, J = 5.0, 3.9 Hz, 1H, Ar(2-OCH_3)-3-H), 7.28 (d, J = 8.8 Hz, 2H, Ar(2-OCH_3)-5-H, Ar(4-O)-3-H), 7.13 (d, J = 7.9 Hz, 1H, Ar(4-O)-5-H), 7.05 (dd, J = 9.8, 5.1 Hz, 1H, Th-4-H), 3.91 (s, 3H, CH_3). ^{13}C NMR (101 MHz, DMSO-d_6) δ 187.41, 157.75, 151.47, 138.47, 137.07, 136.30, 136.19, 131.99, 130.02, 128.05, 127.99, 122.15, 121.75, 120.78, 120.11, 114.83, 111.22, 55.14. HRMS (m/z): Calcd. For $C_{20}H_{16}O_5S_2$ $[M + H]^+$ 399.0720, meas. 399.0714.

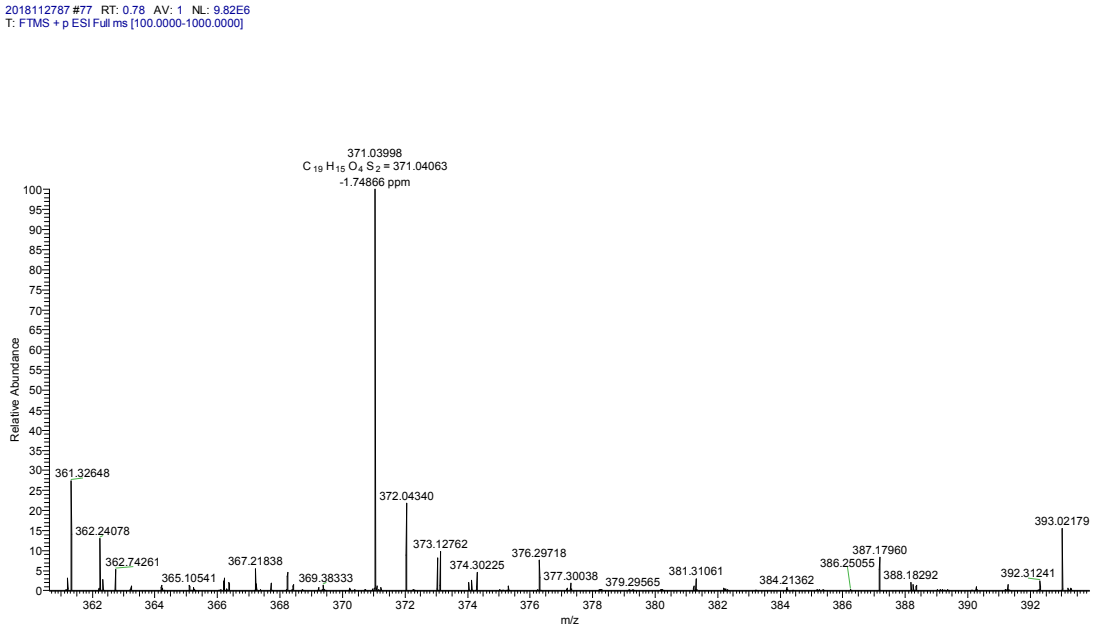
8.Spectrogram of title compounds 2a-2v



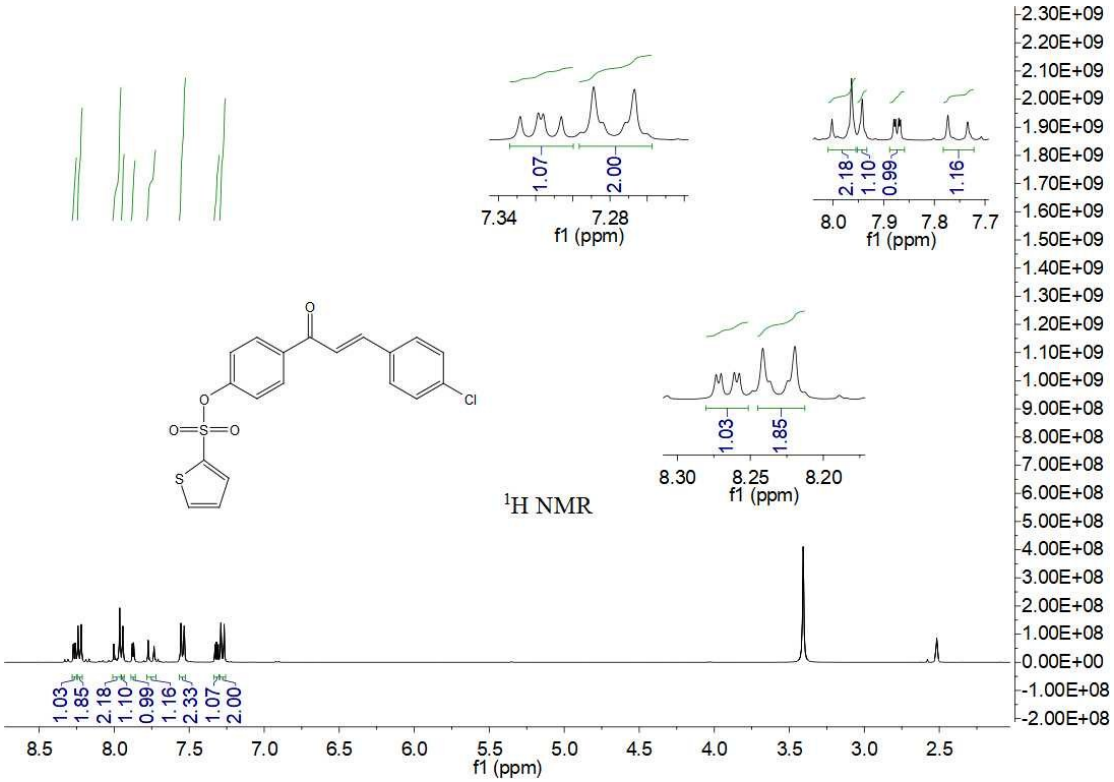
^{1}H NMR spectrum of compound **2a**



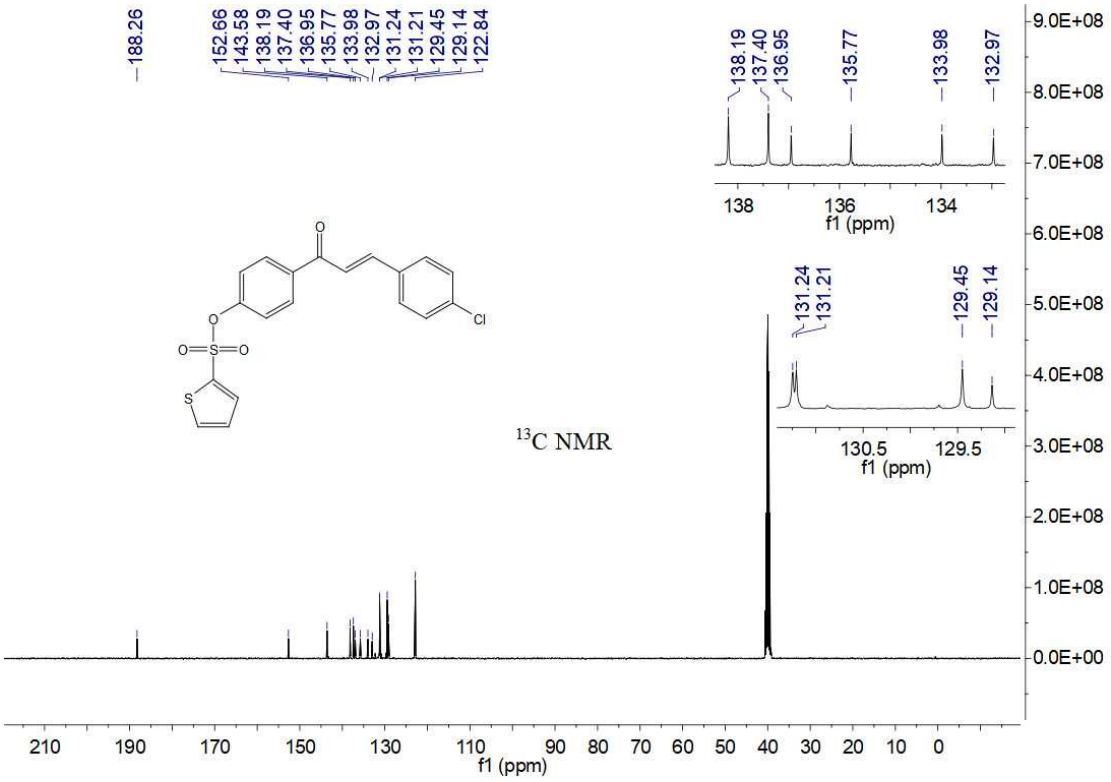
^{13}C NMR spectrum of compound **2a**



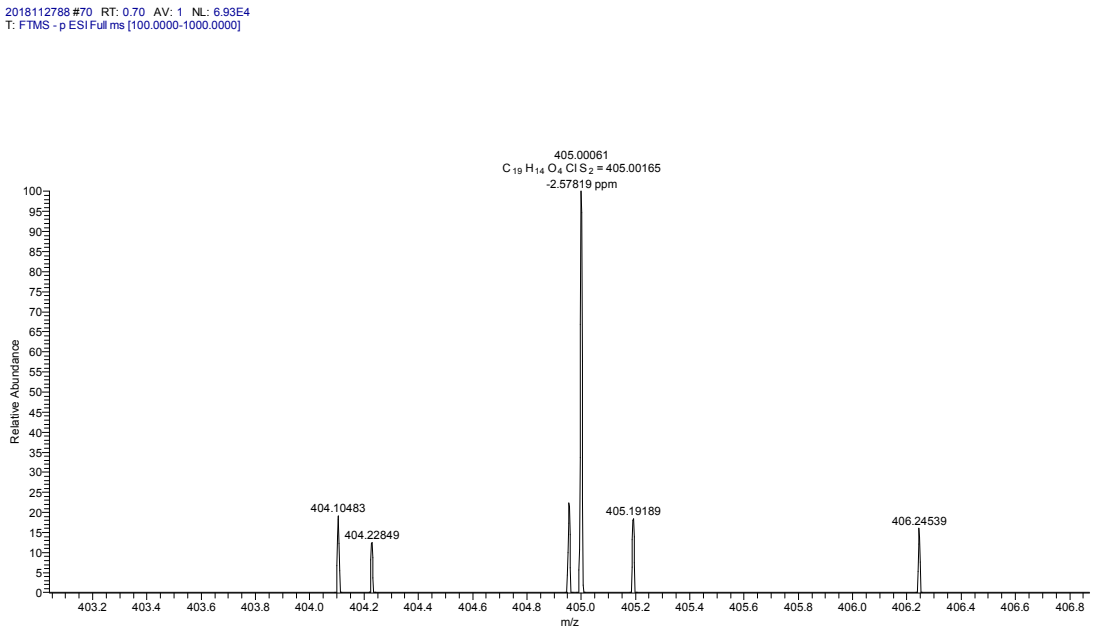
HRMS spectrum of compound **2a**



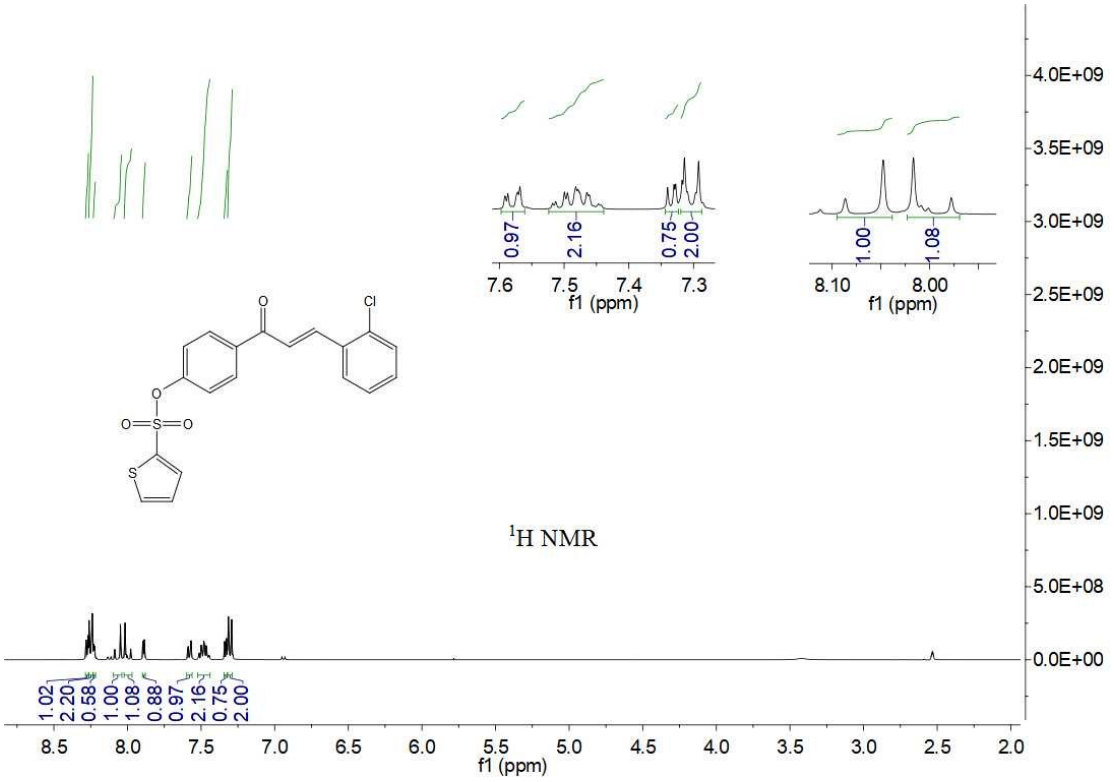
^{1}H NMR spectrum of compound **2b**



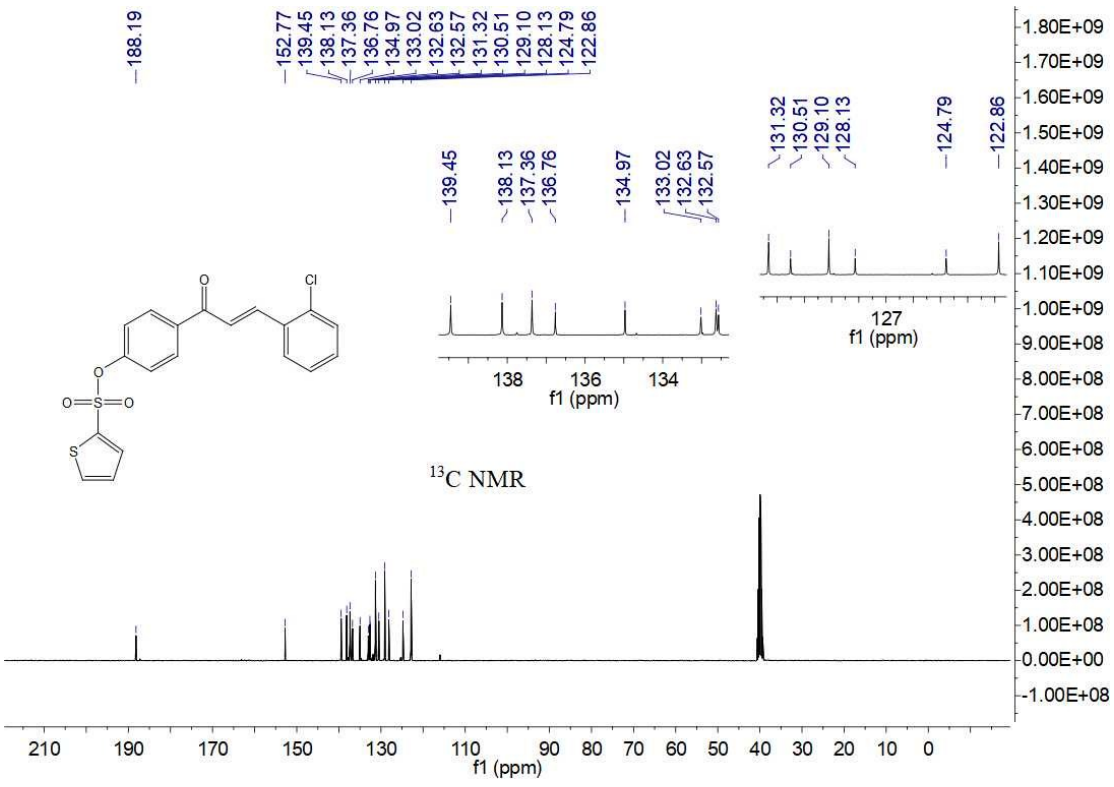
^{13}C NMR spectrum of compound **2b**



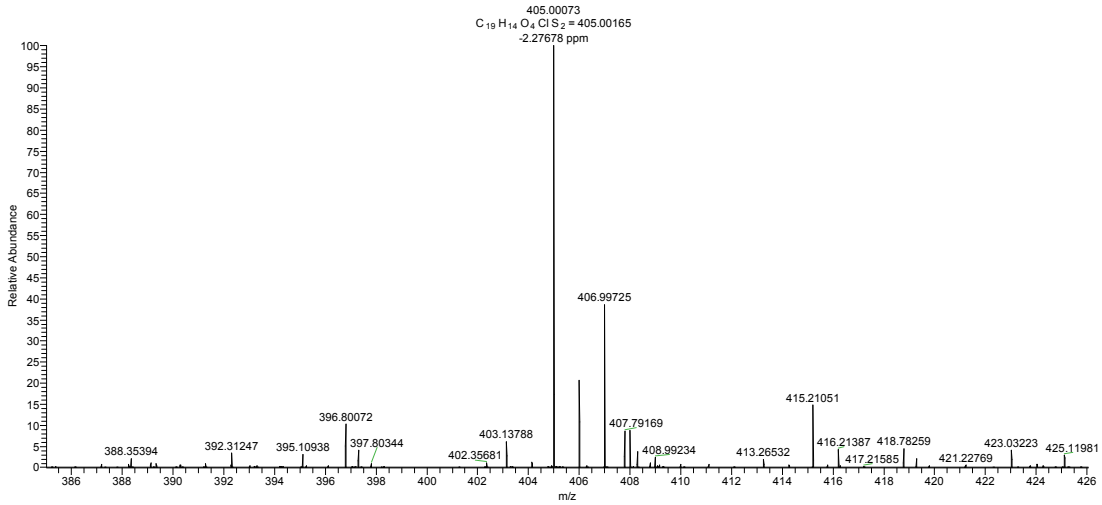
HRMS spectrum of compound **2b**



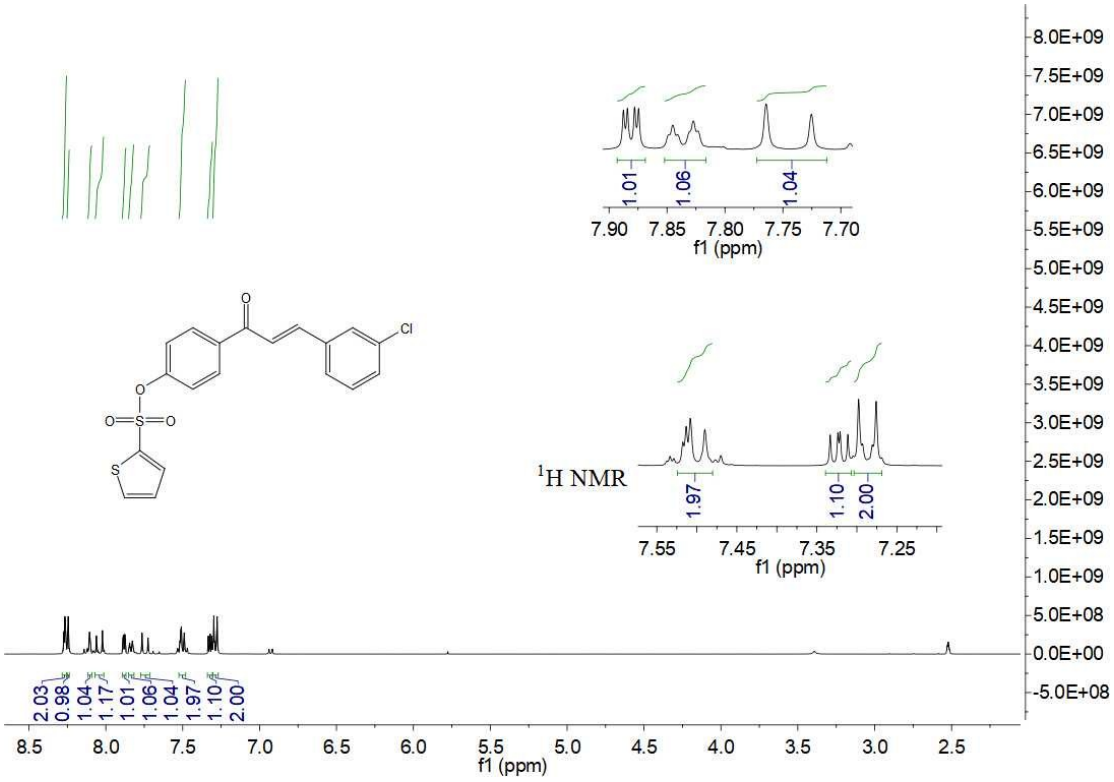
^{1}H NMR spectrum of compound **2c**



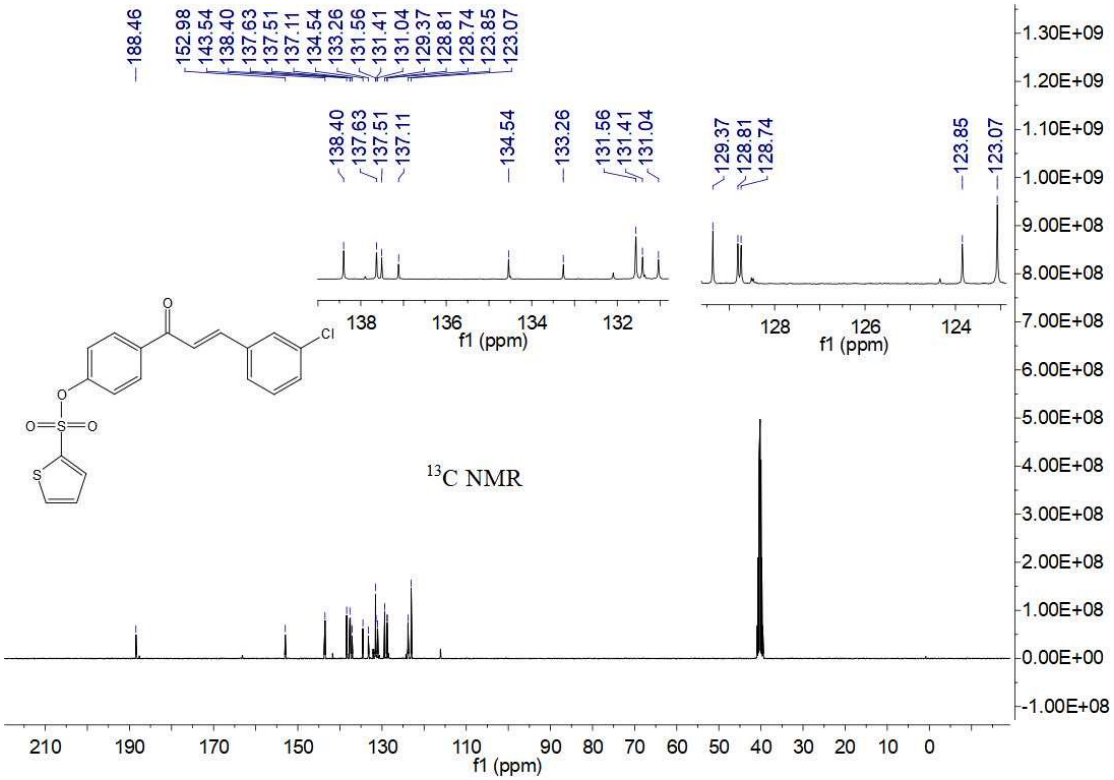
^{13}C NMR spectrum of compound **2c**



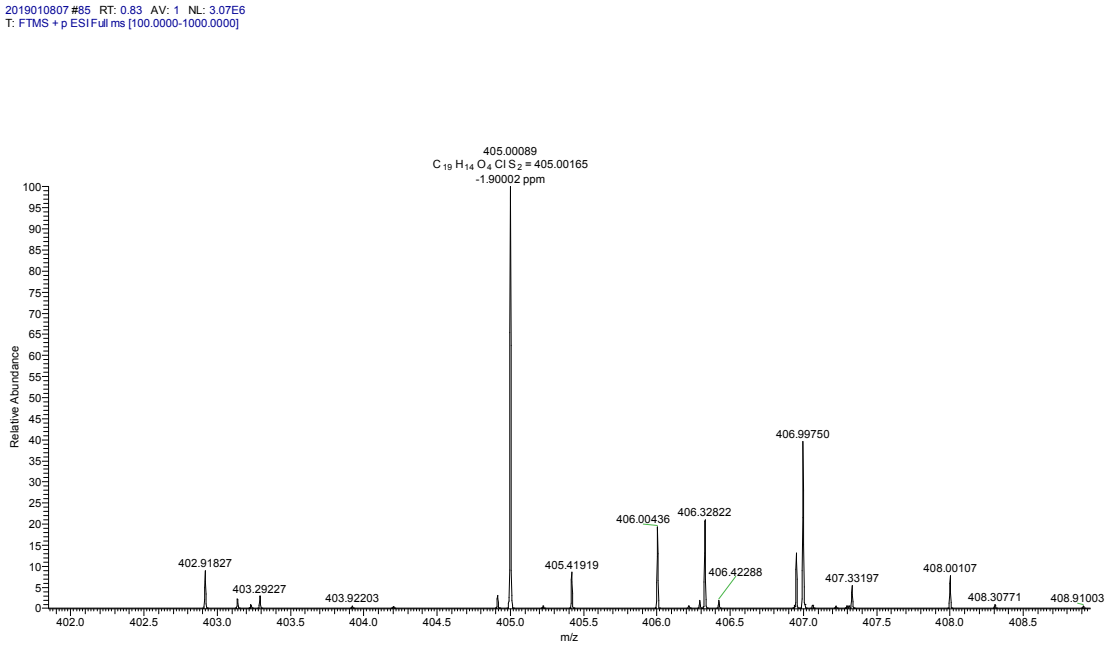
HRMS spectrum of compound **2c**



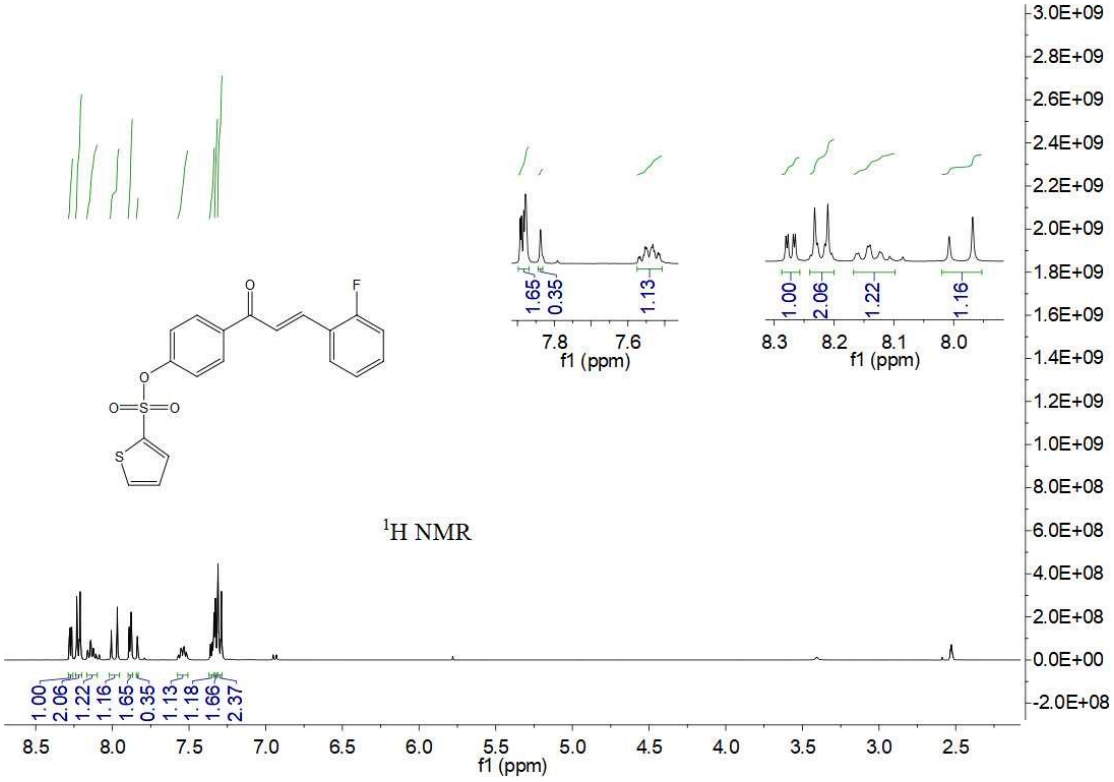
^{1}H NMR spectrum of compound **2d**



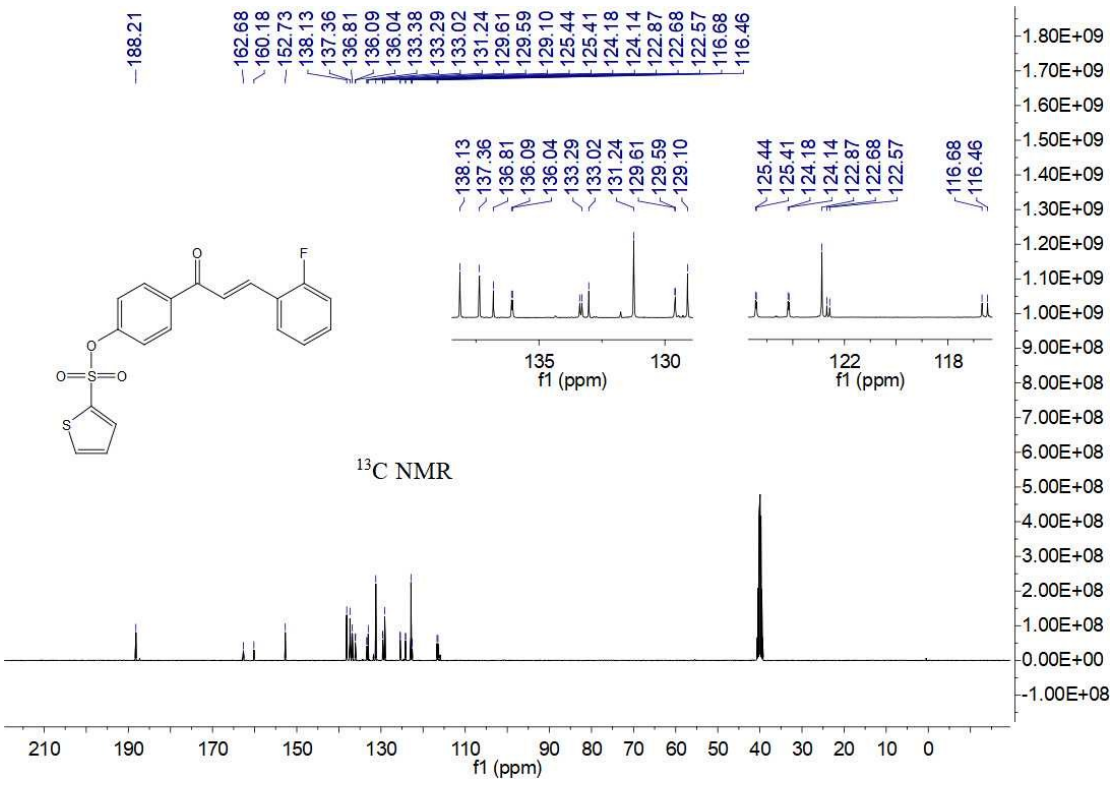
^{13}C NMR spectrum of compound **2d**



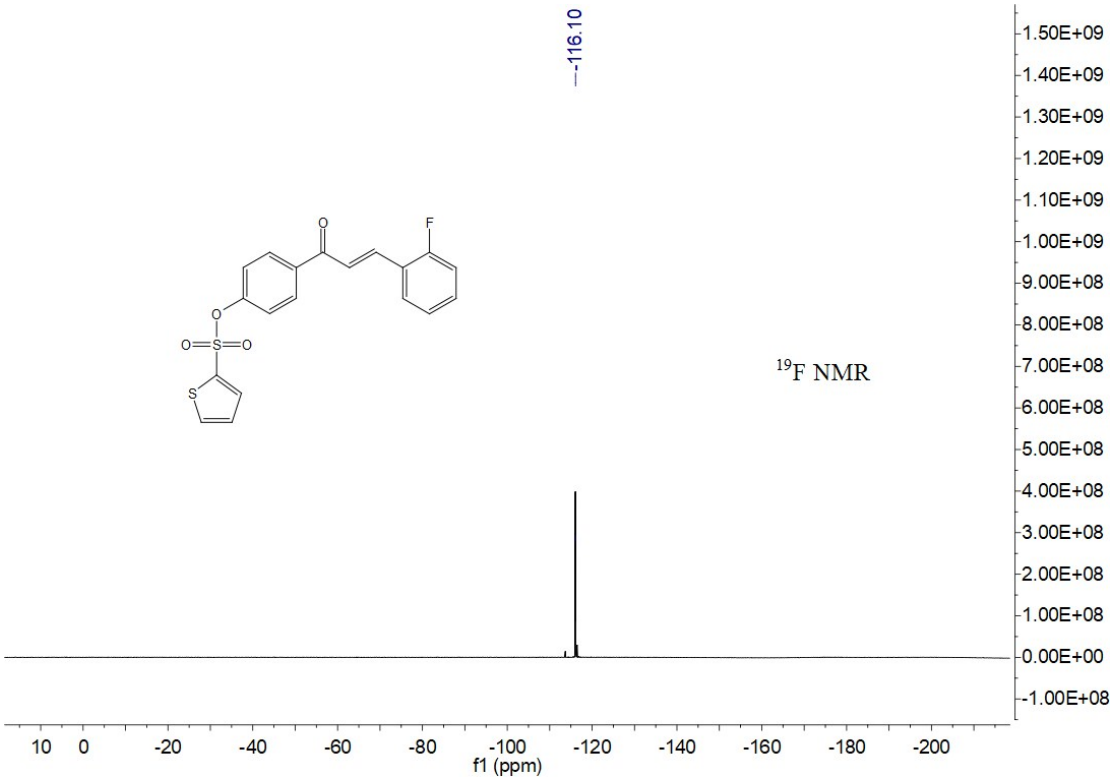
HRMS spectrum of compound **2d**



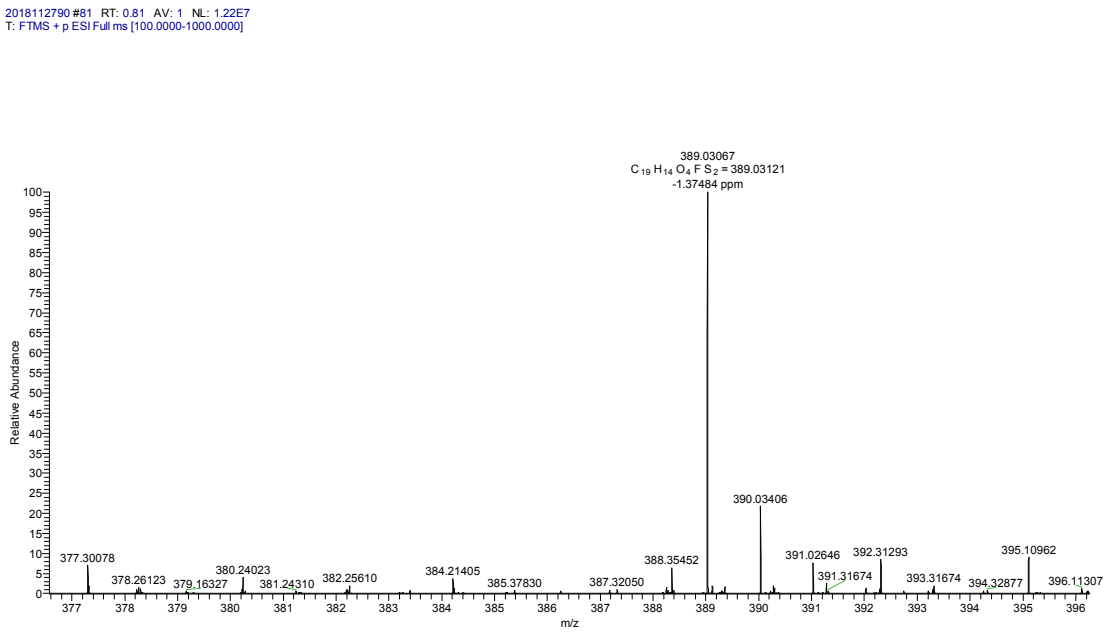
^{1}H NMR spectrum of compound **2e**



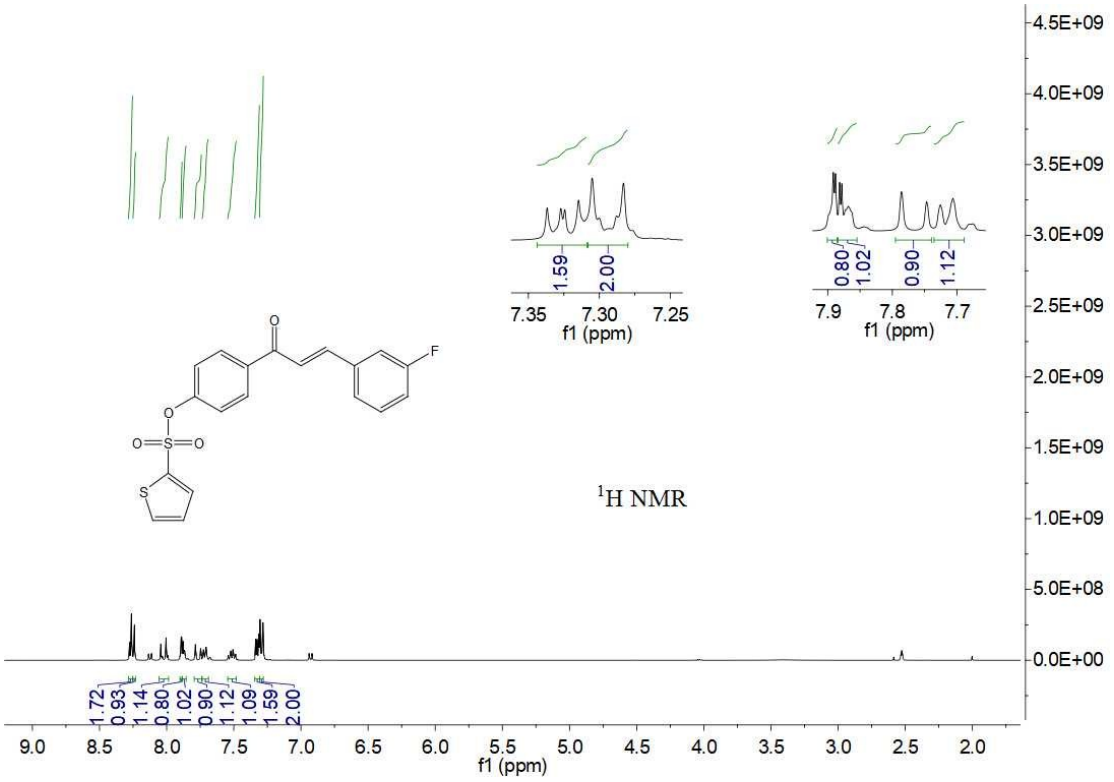
^{13}C NMR spectrum of compound **2e**



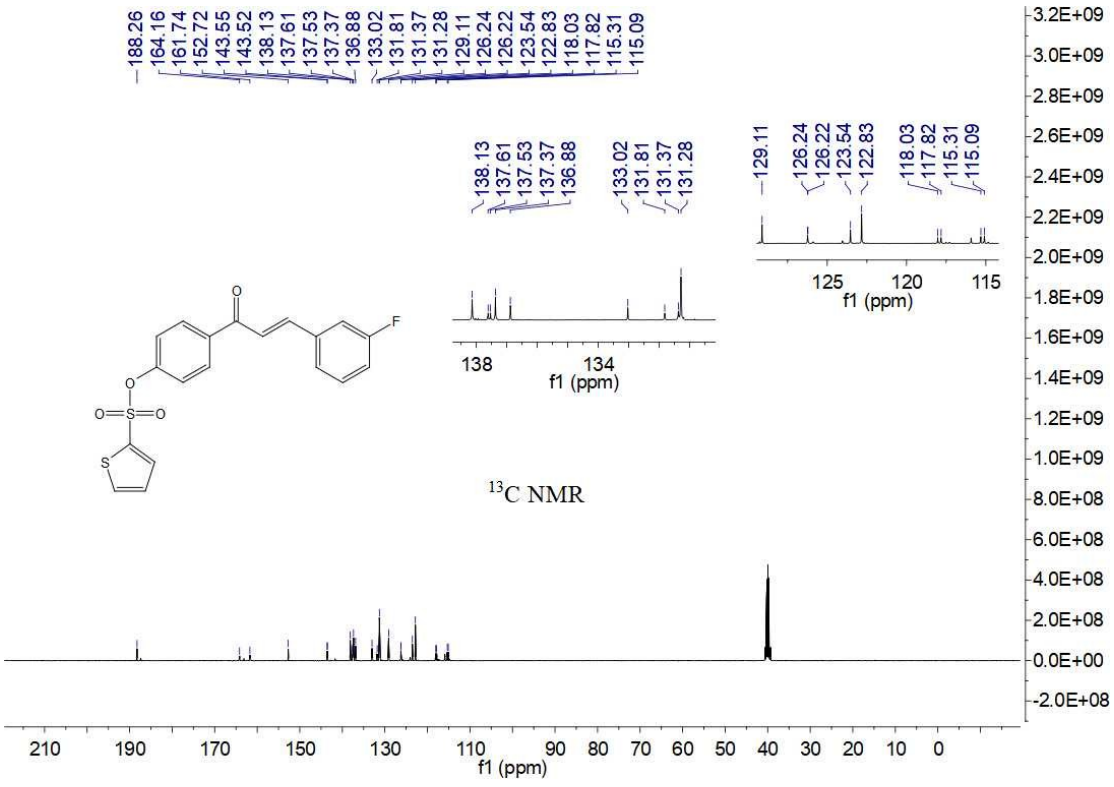
^{19}F NMR spectrum of compound **2e**



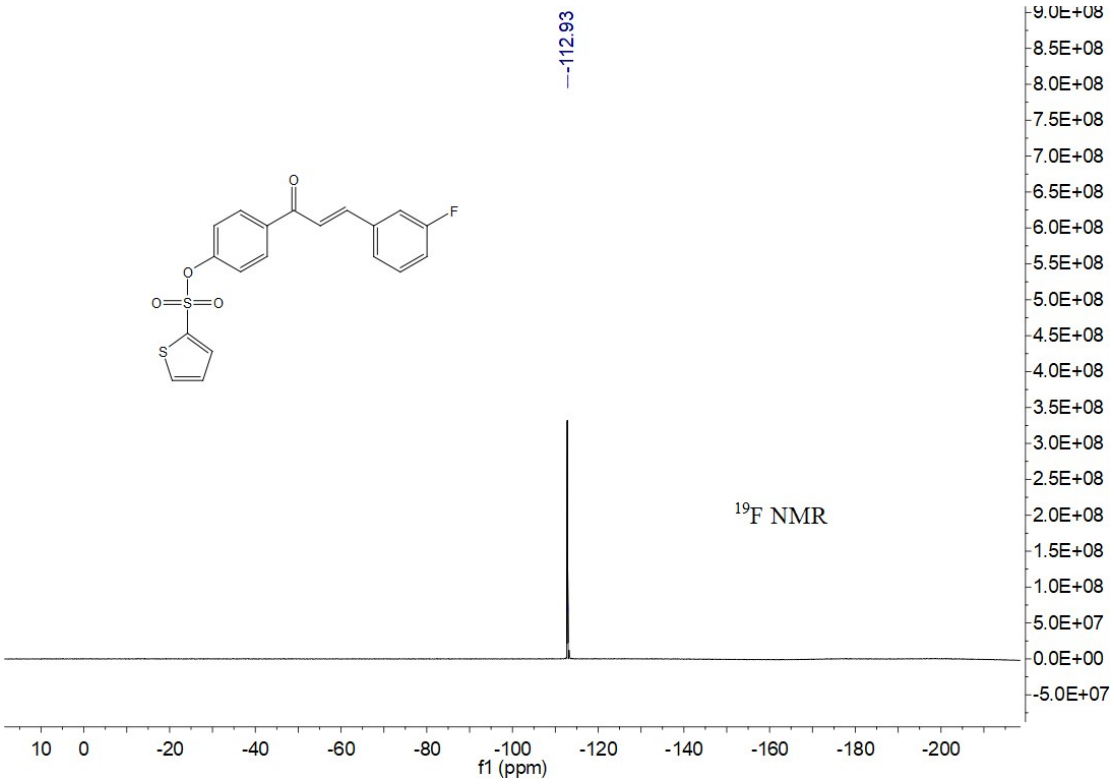
HRMS spectrum of compound **2e**



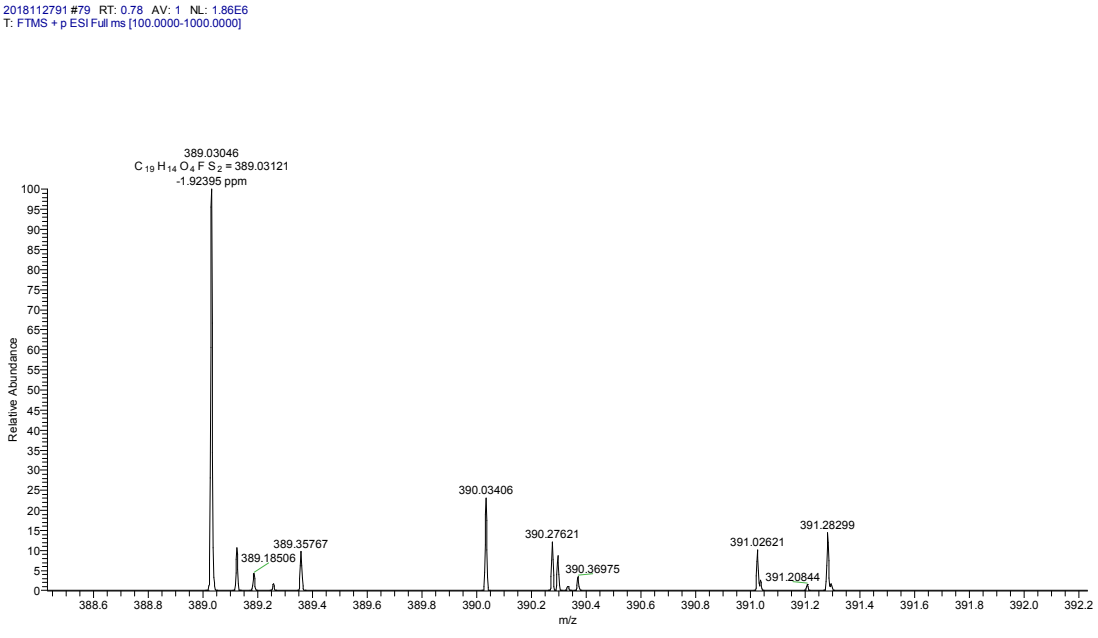
^{1}H NMR spectrum of compound **2f**



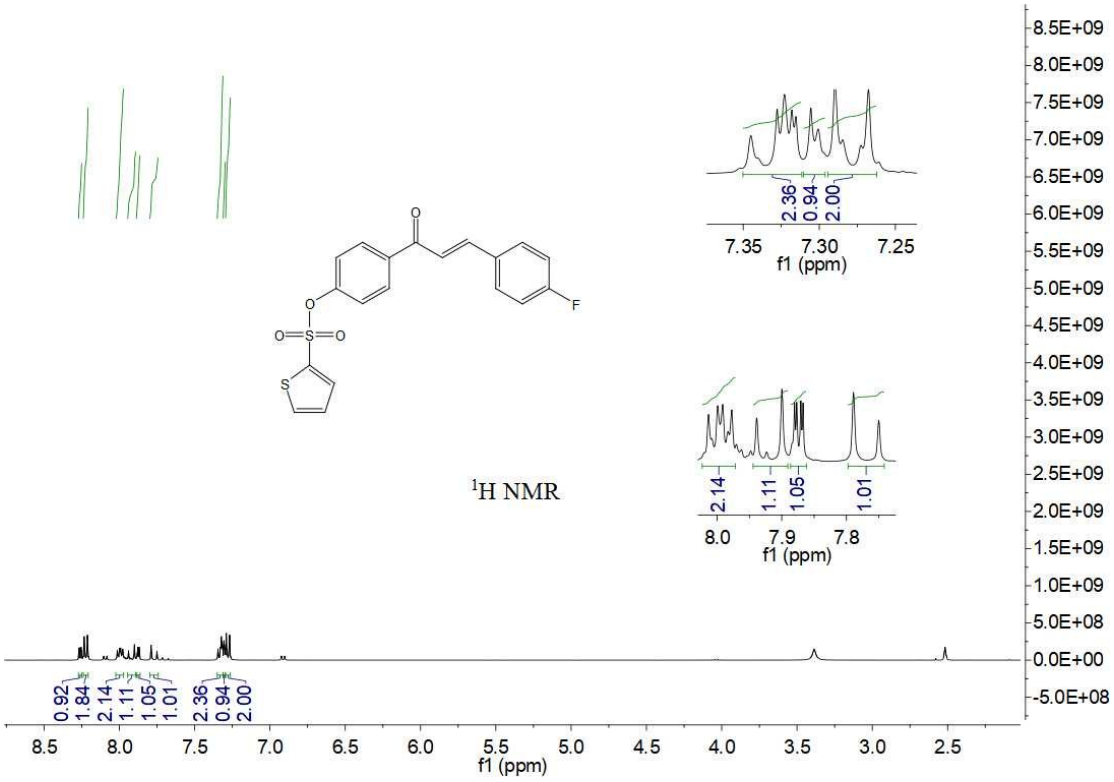
^{13}C NMR spectrum of compound **2f**



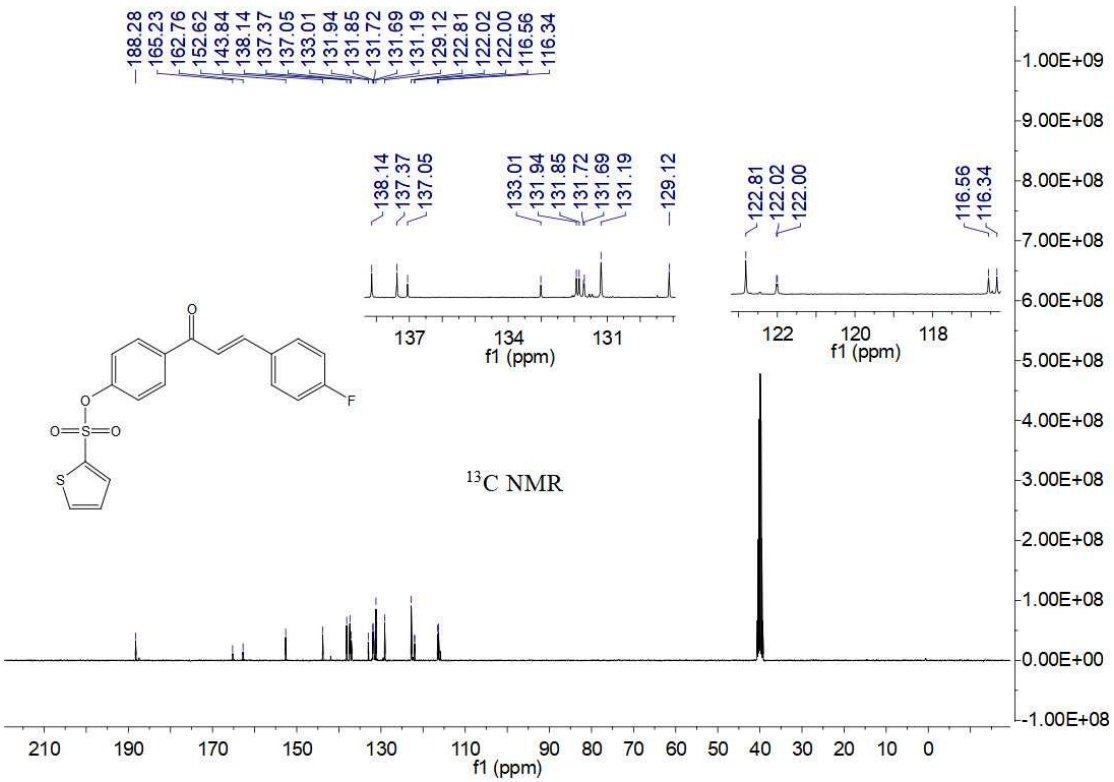
^{19}F NMR spectrum of compound **2f**



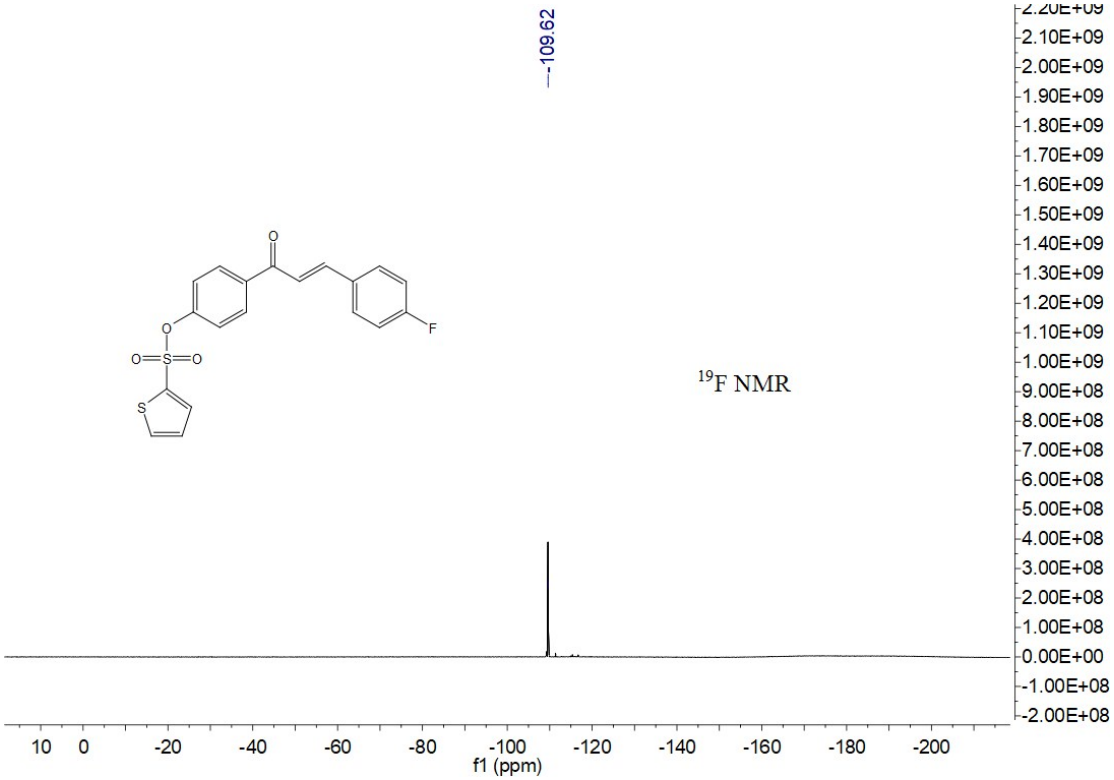
HRMS spectrum of compound **2f**



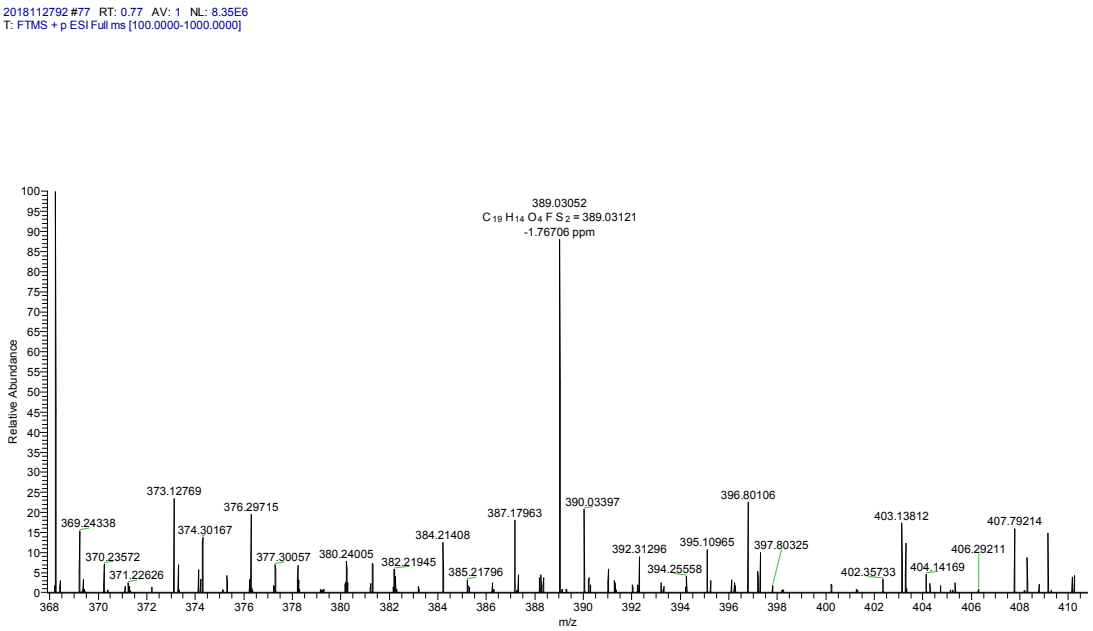
^{1}H NMR spectrum of compound **2g**



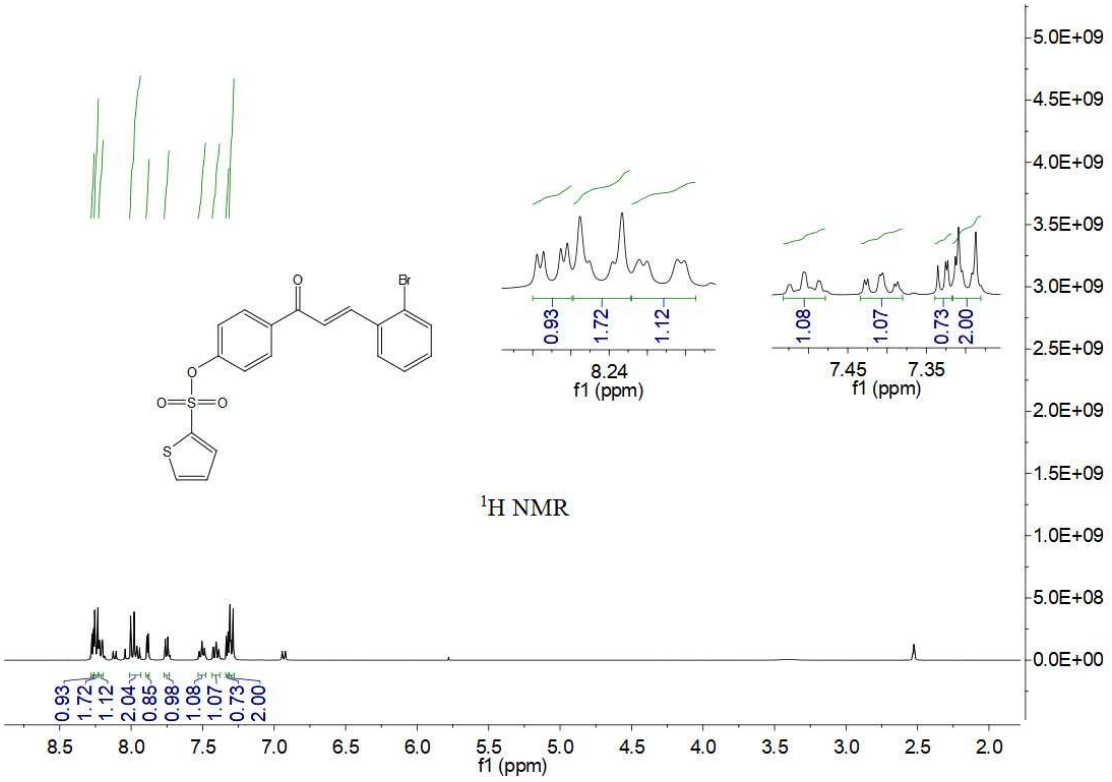
^{13}C NMR spectrum of compound **2g**



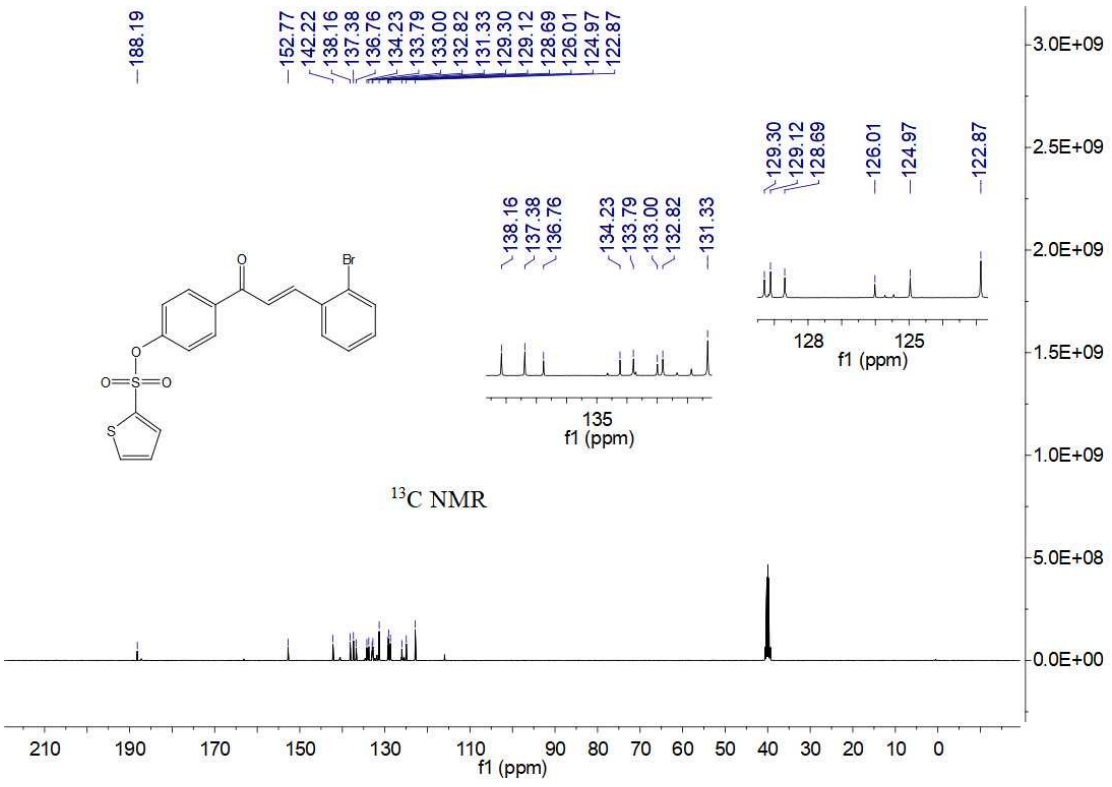
^{19}F NMR spectrum of compound **2g**



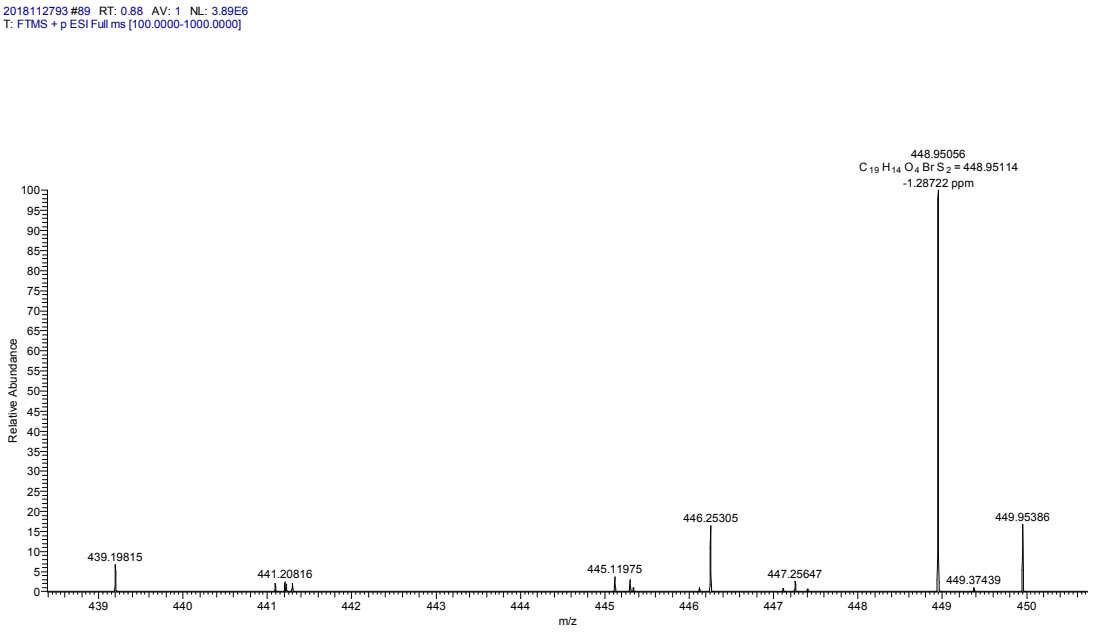
HRMS spectrum of compound **2g**



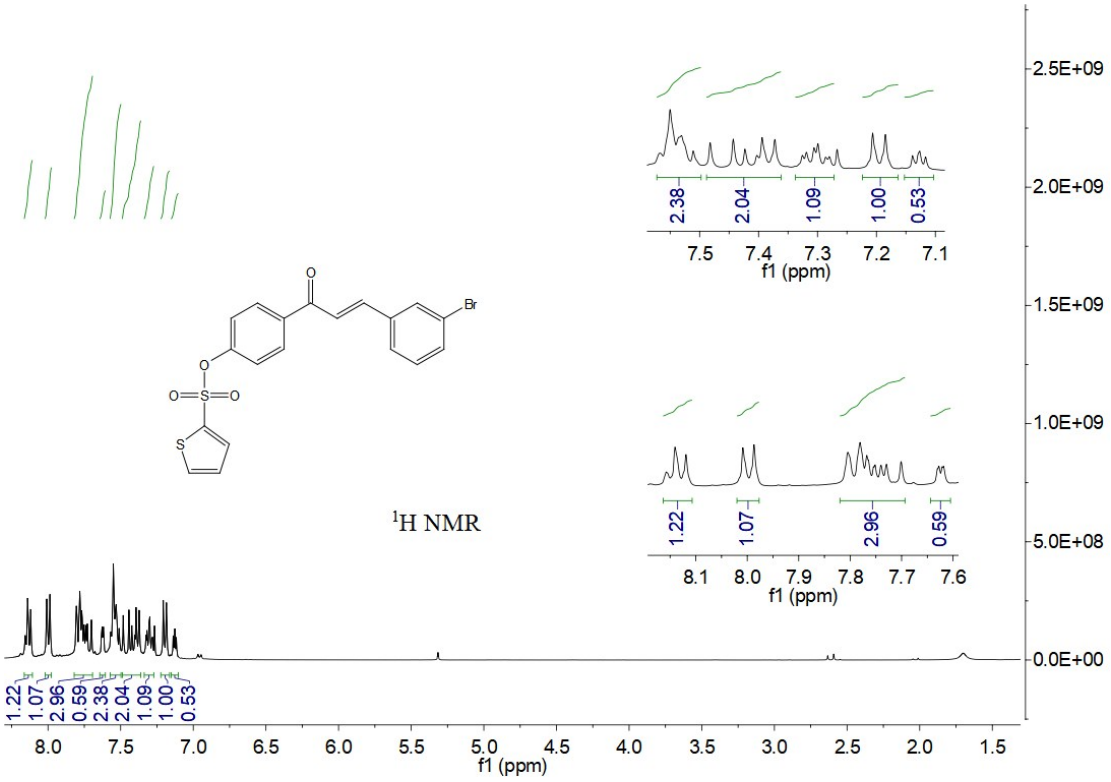
^{1}H NMR spectrum of compound **2h**



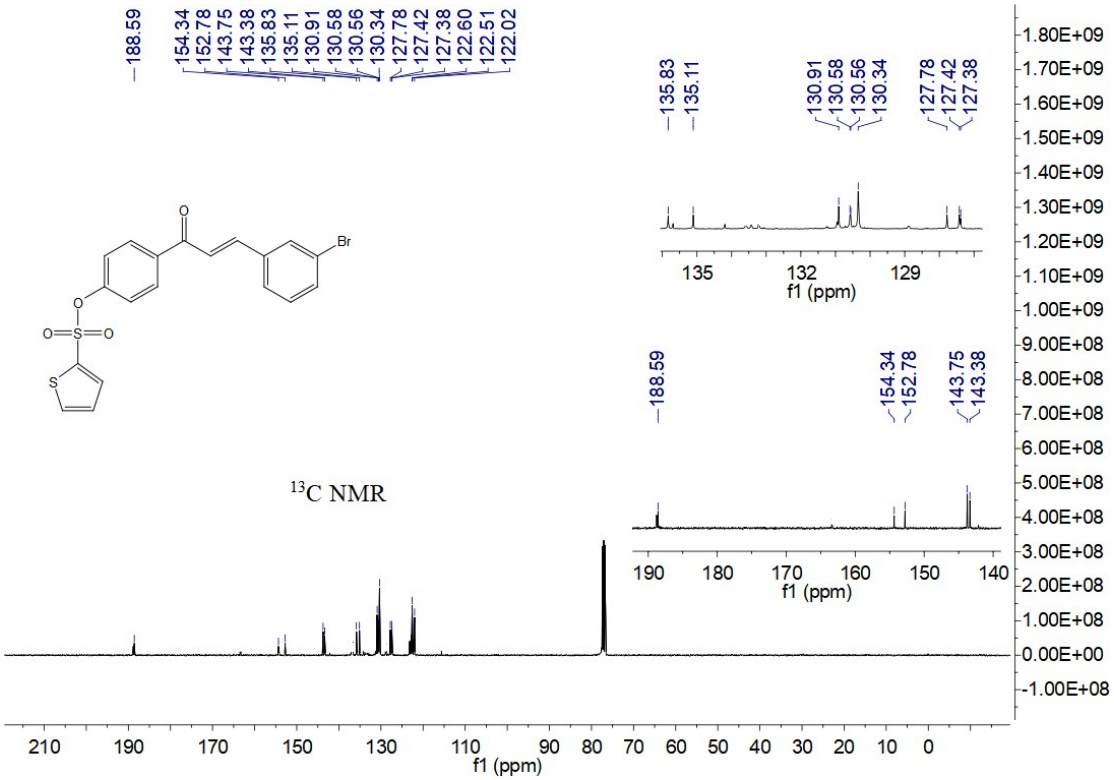
^{13}C NMR spectrum of compound **2h**



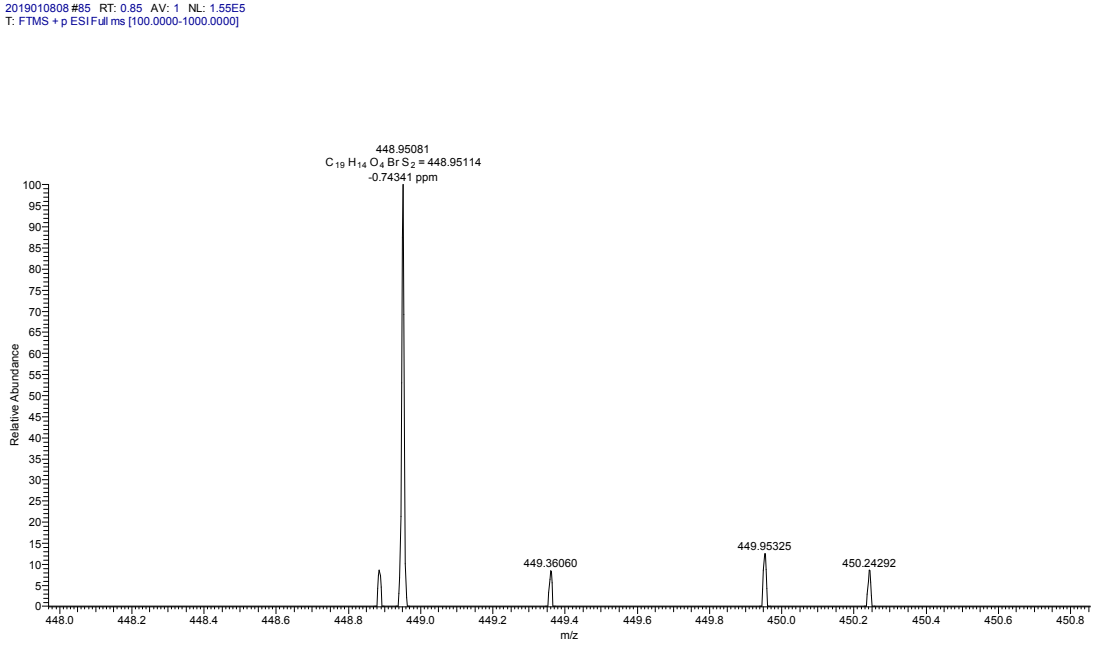
HRMS spectrum of compound **2h**



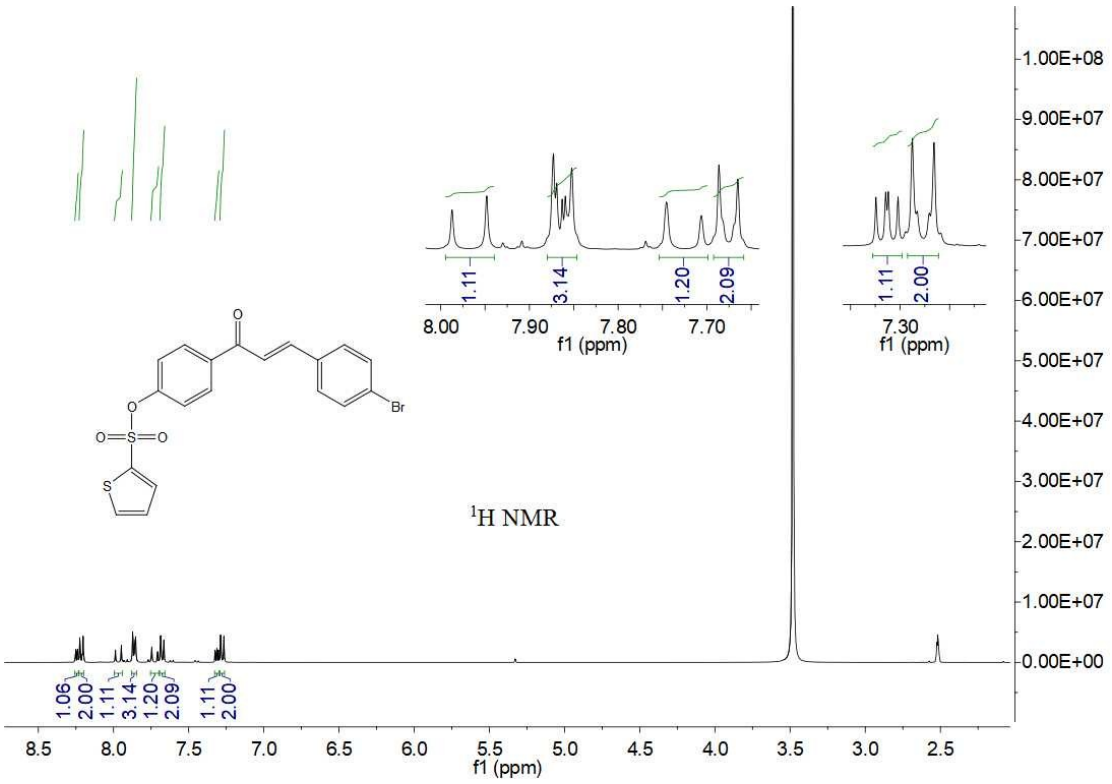
^{1}H NMR spectrum of compound **2i**



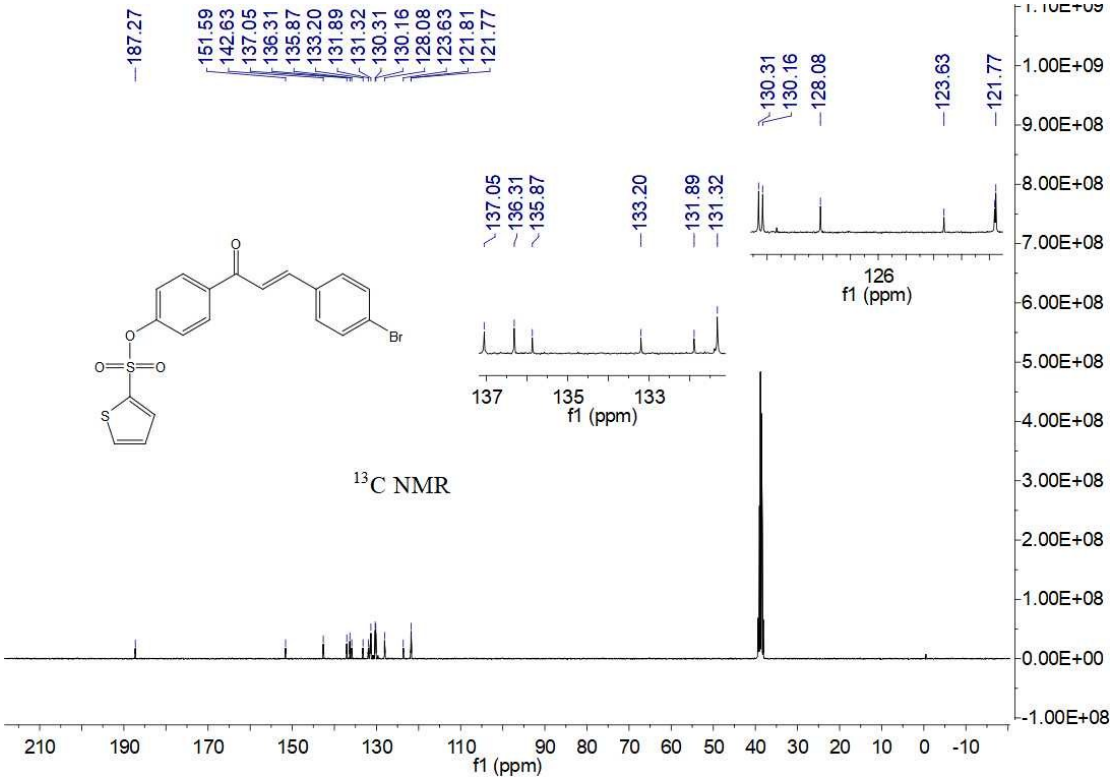
^{13}C NMR spectrum of compound **2i**



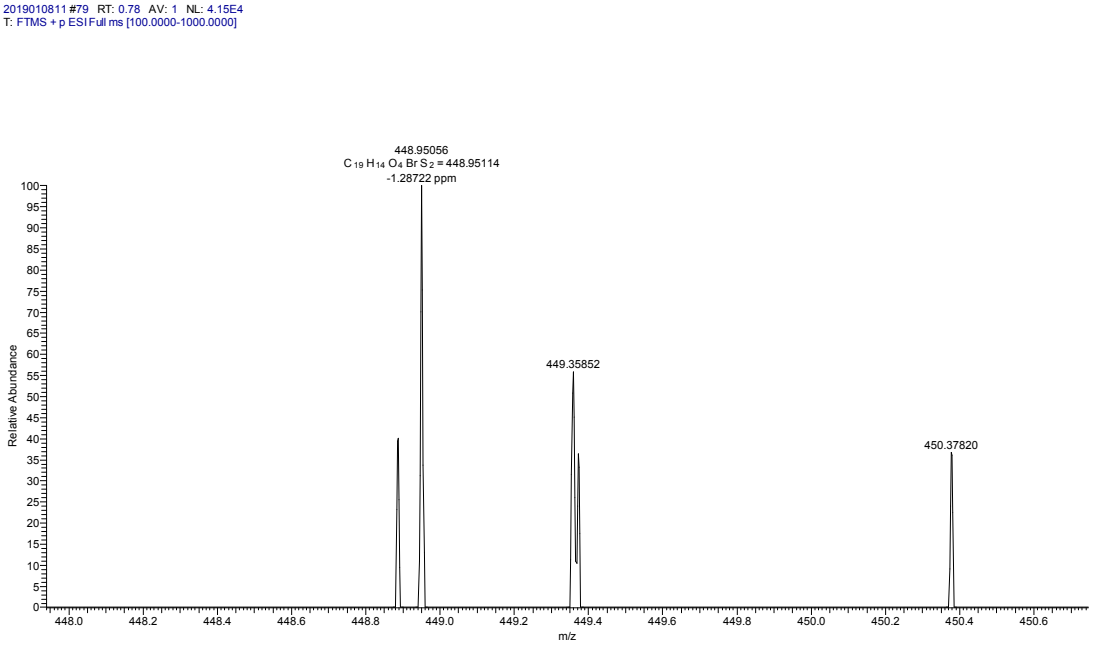
HRMS spectrum of compound **2i**



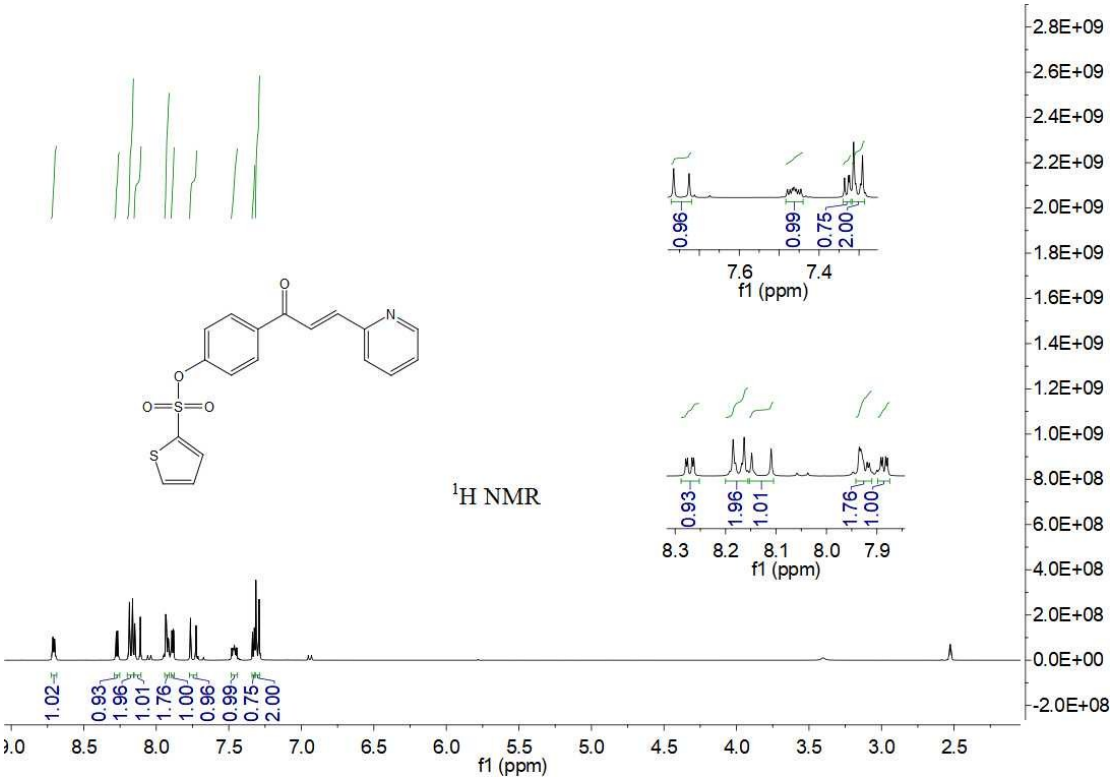
^{1}H NMR spectrum of compound **2j**



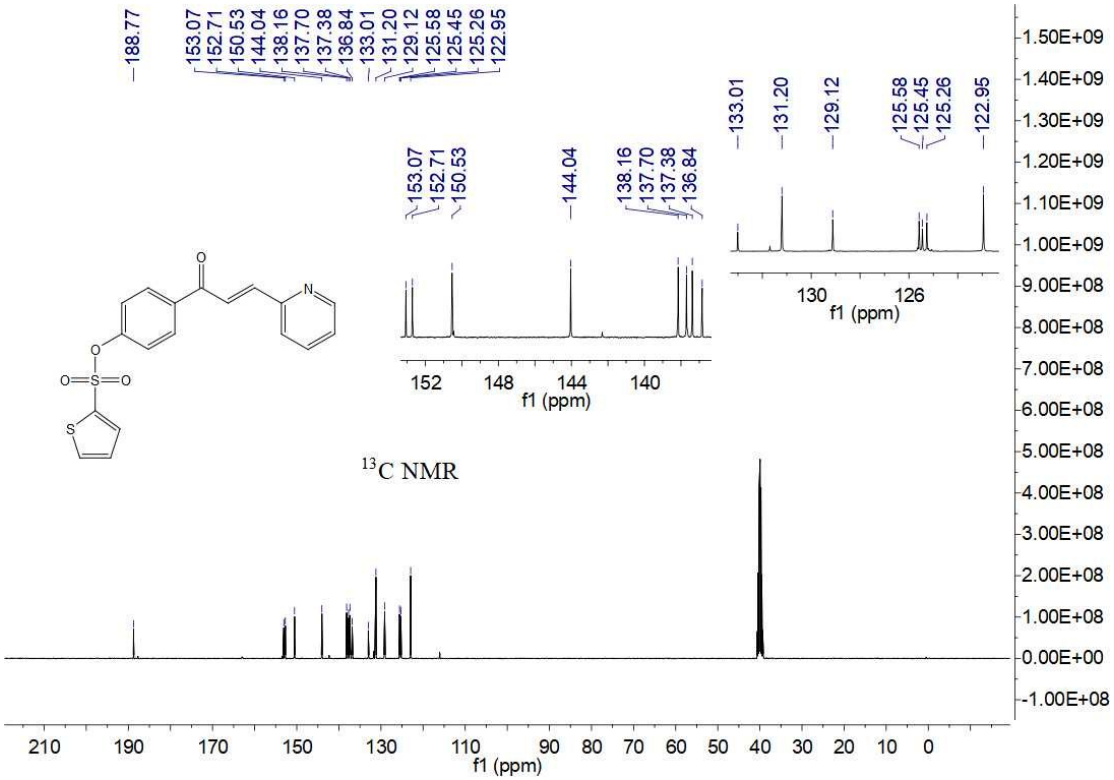
^{13}C NMR spectrum of compound **2j**



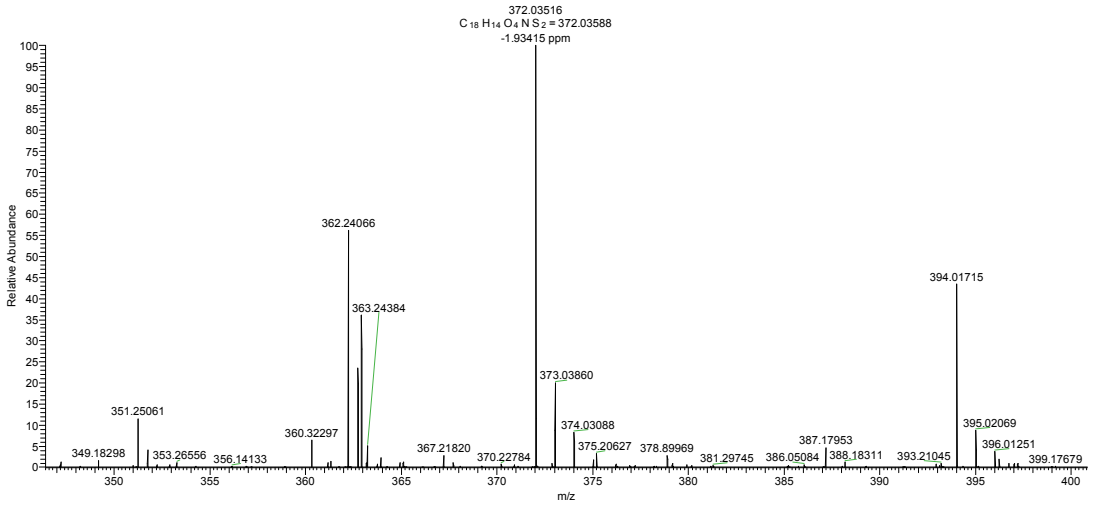
HRMS spectrum of compound **2j**



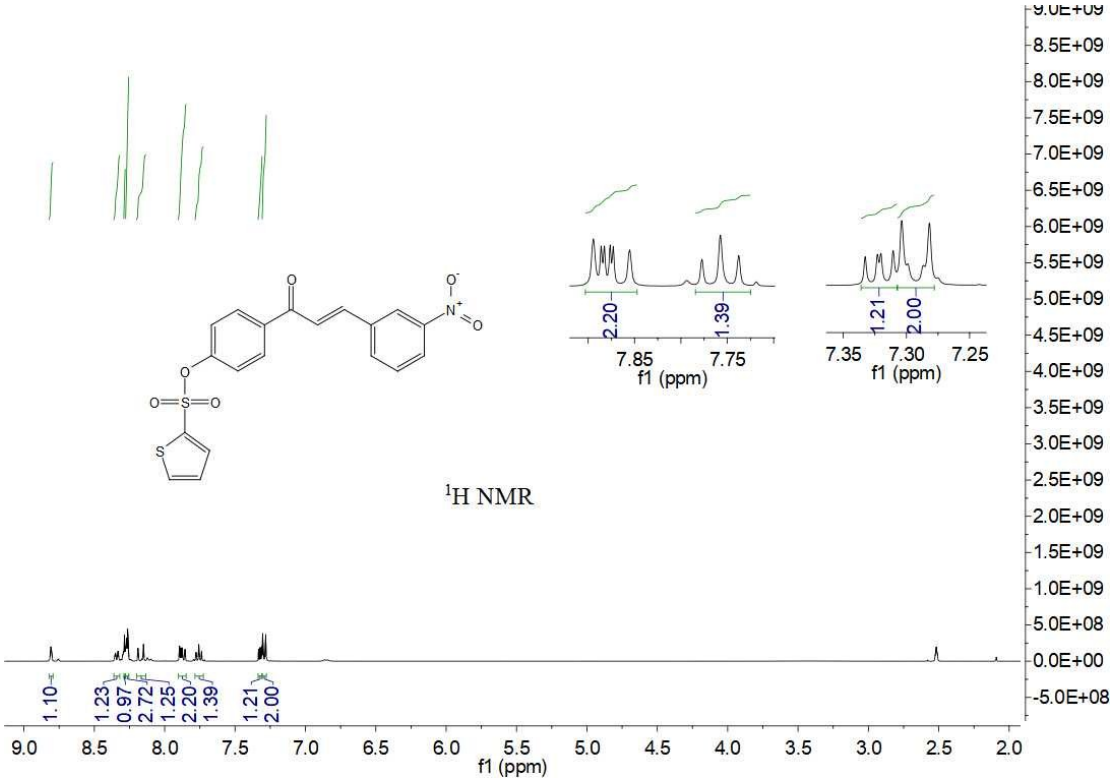
^{1}H NMR spectrum of compound **2k**



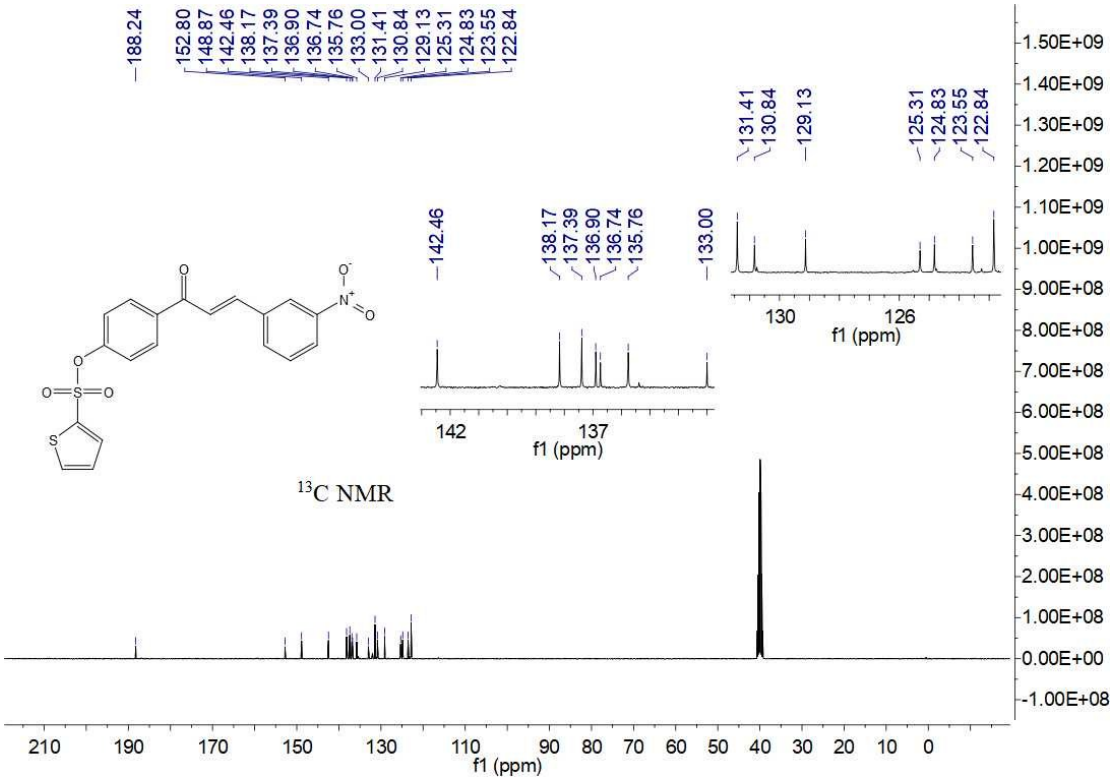
^{13}C NMR spectrum of compound **2k**



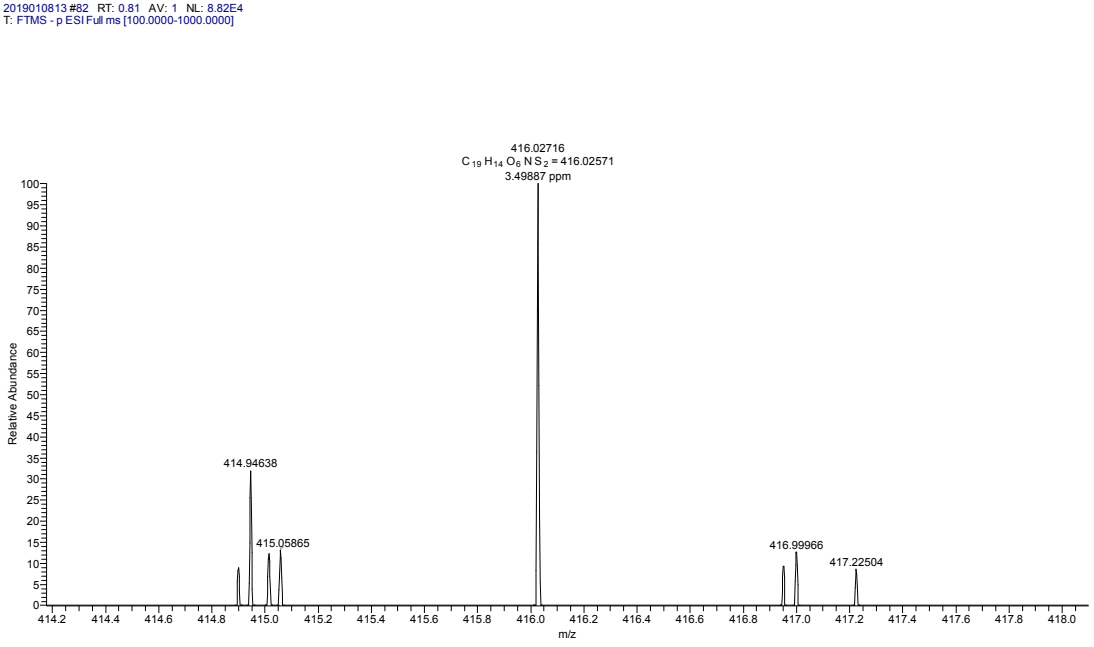
HRMS spectrum of compound **2k**



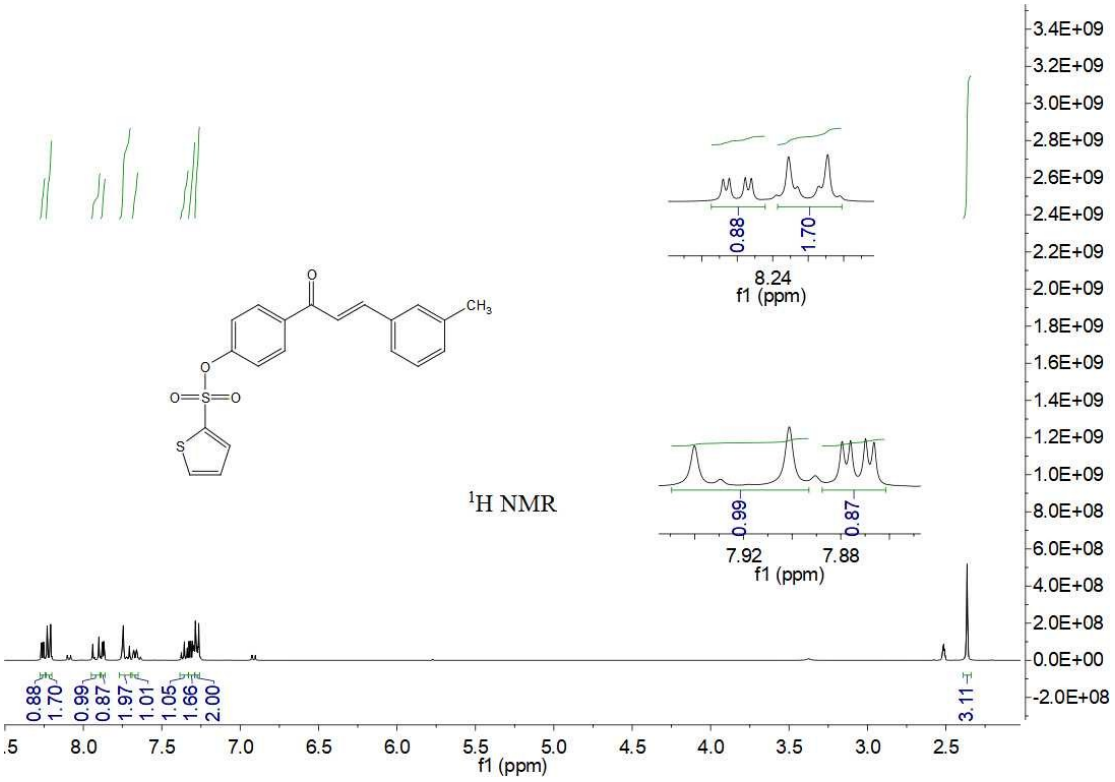
^{1}H NMR spectrum of compound **2l**



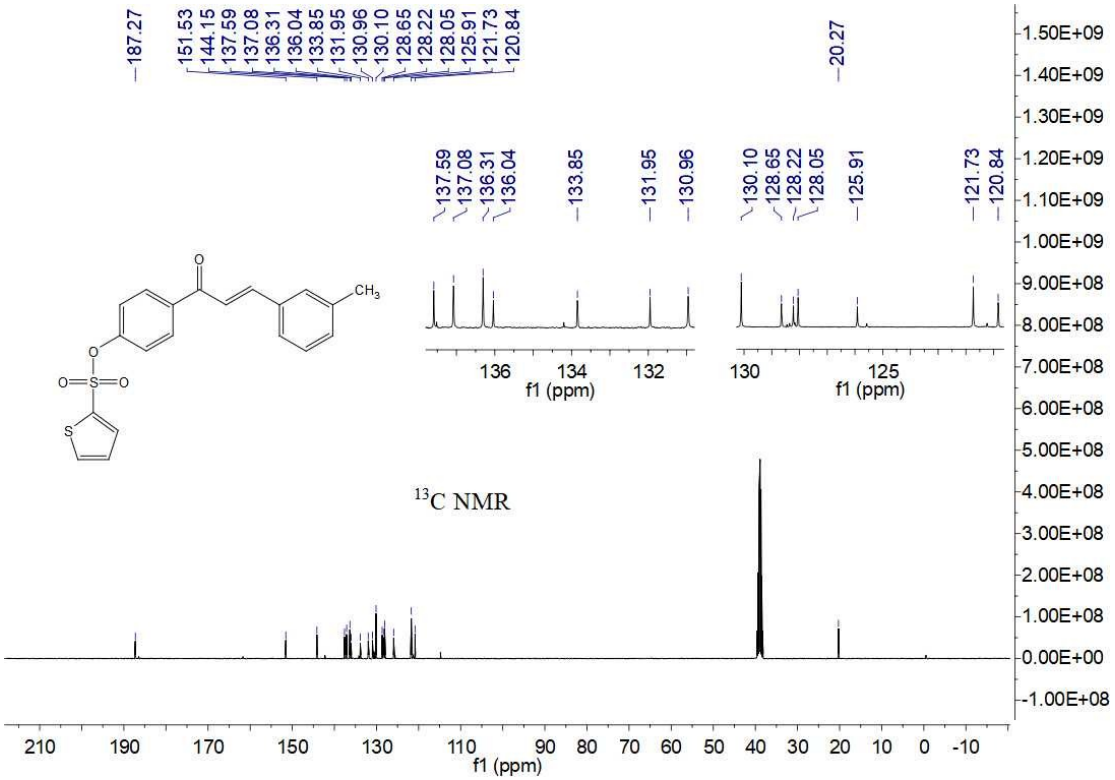
^{13}C NMR spectrum of compound **2l**



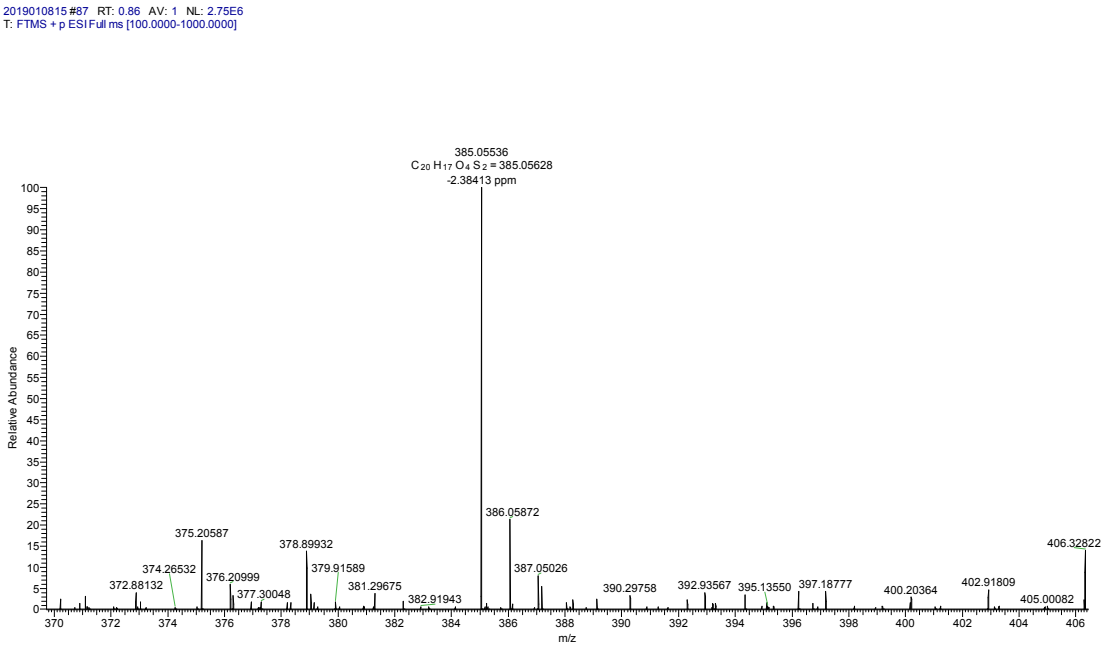
HRMS spectrum of compound **2l**



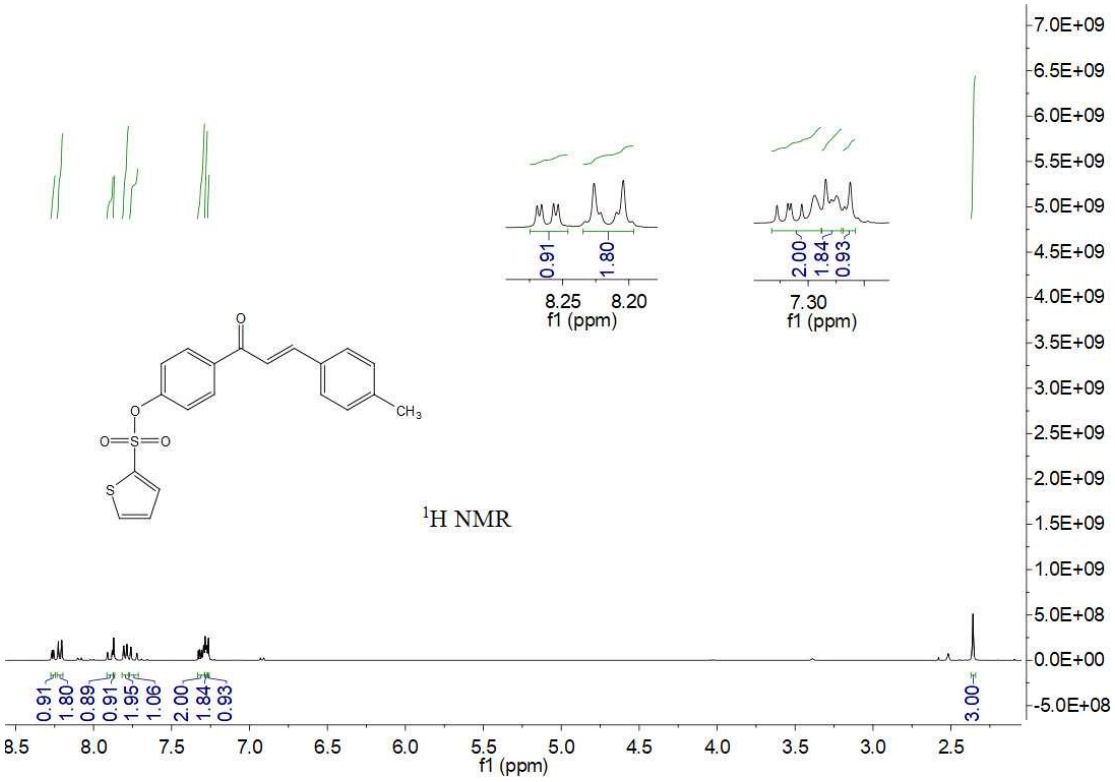
^{1}H NMR spectrum of compound **2m**



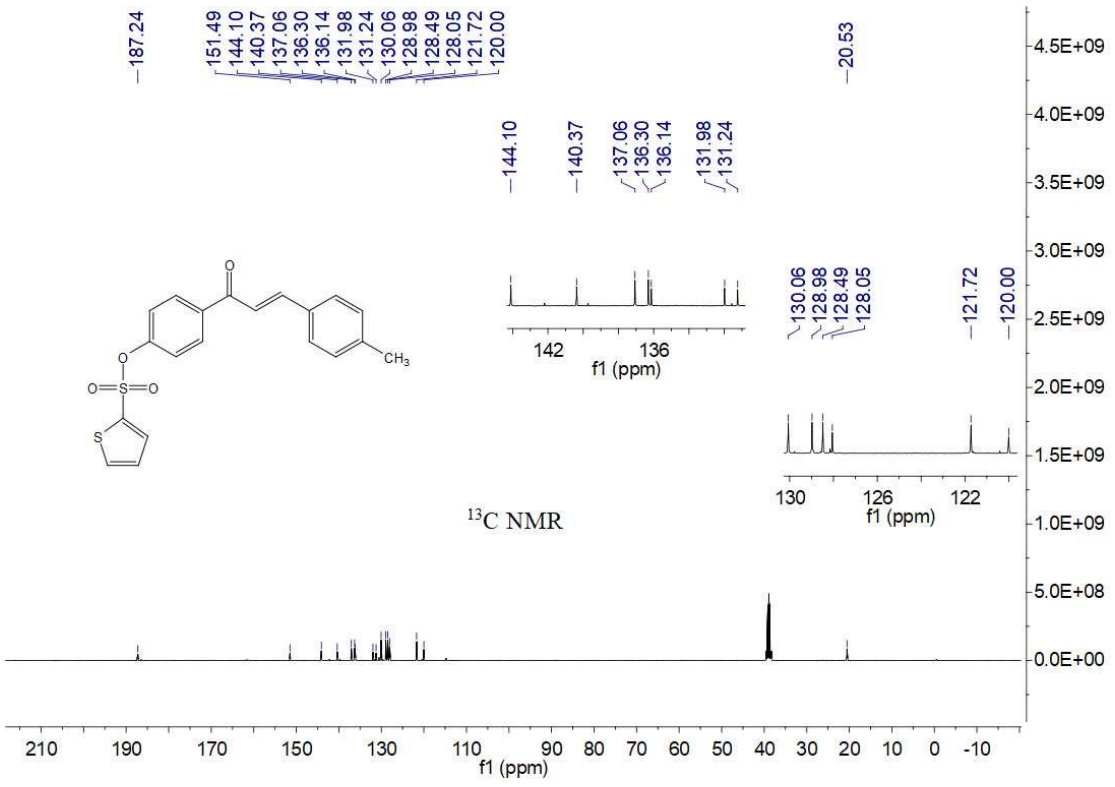
^{13}C NMR spectrum of compound **2m**



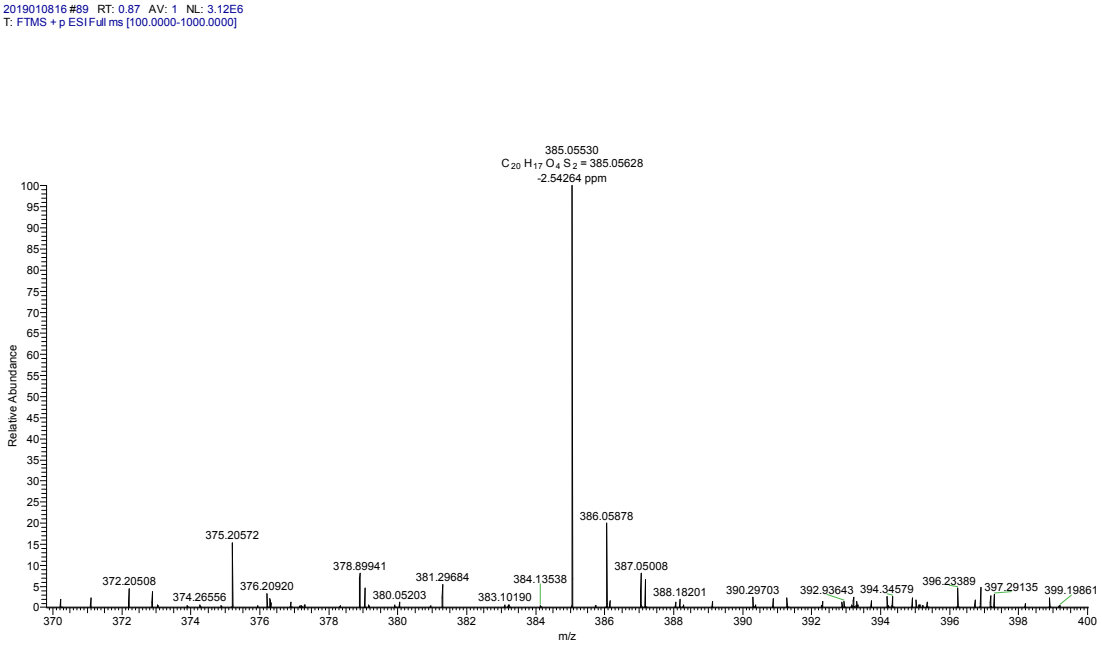
HRMS spectrum of compound **2m**



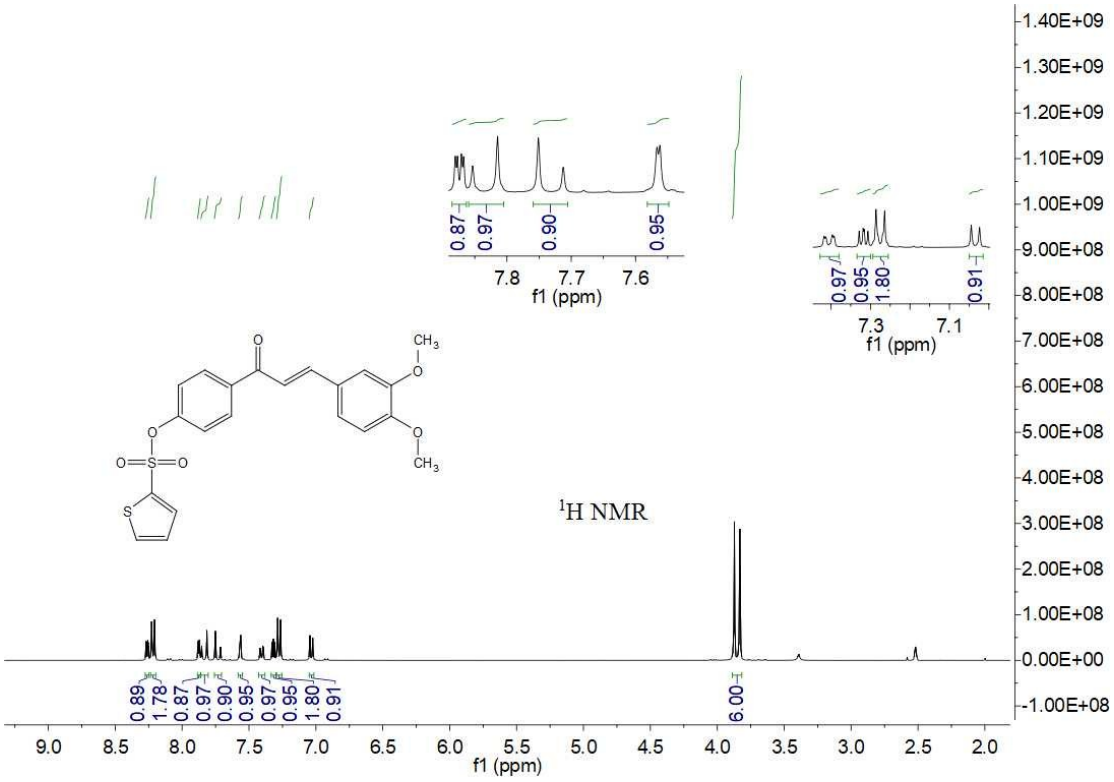
^{1}H NMR spectrum of compound **2n**



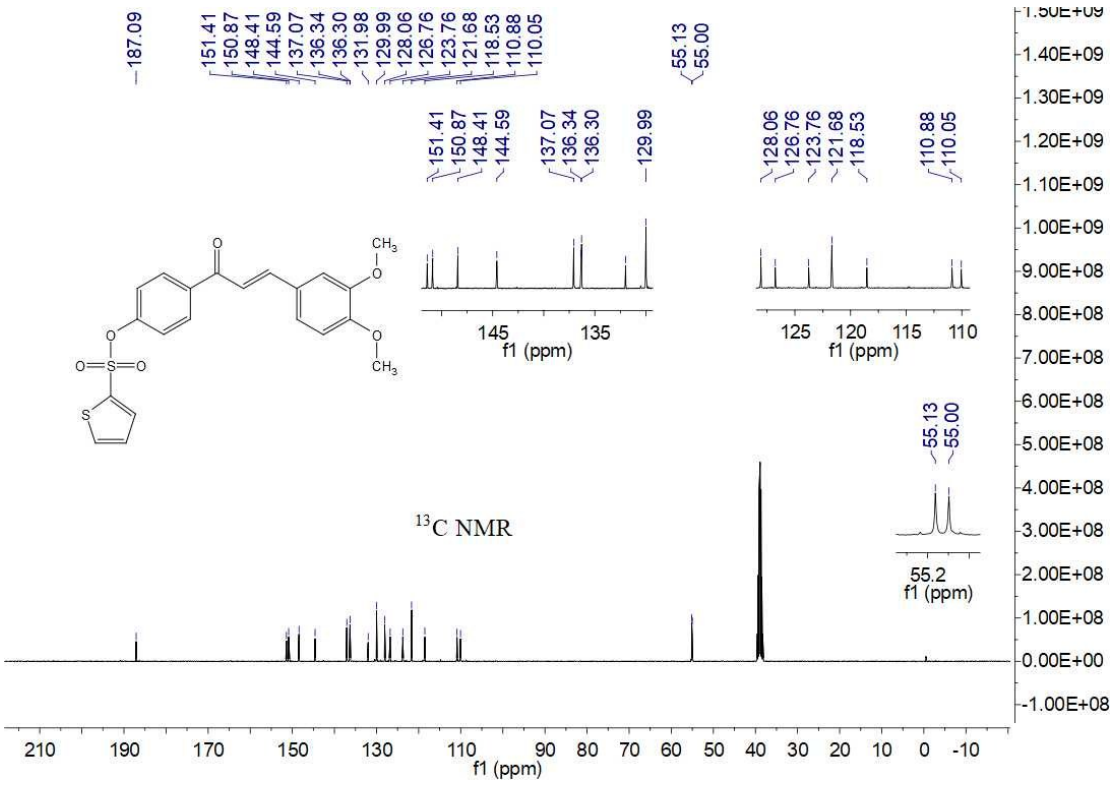
^{13}C NMR spectrum of compound **2n**



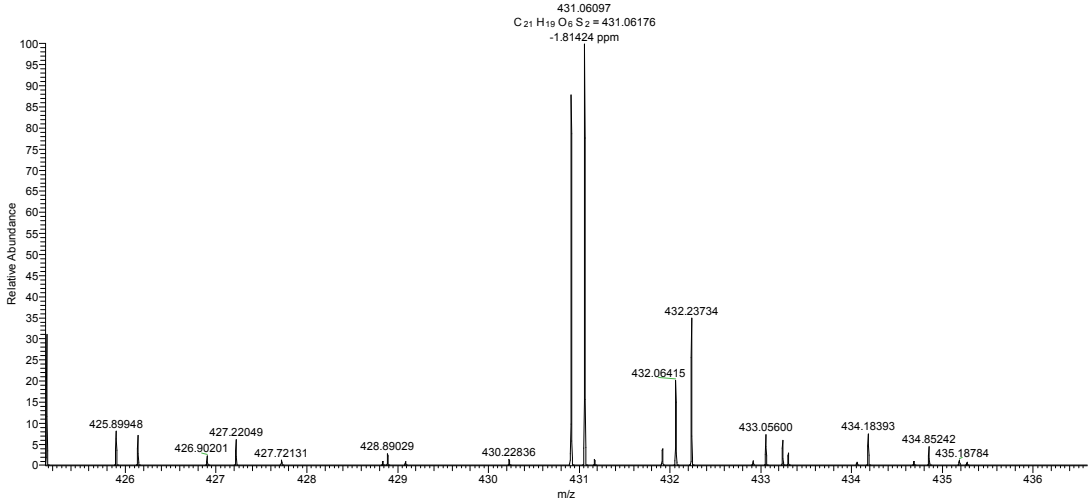
HRMS spectrum of compound **2n**



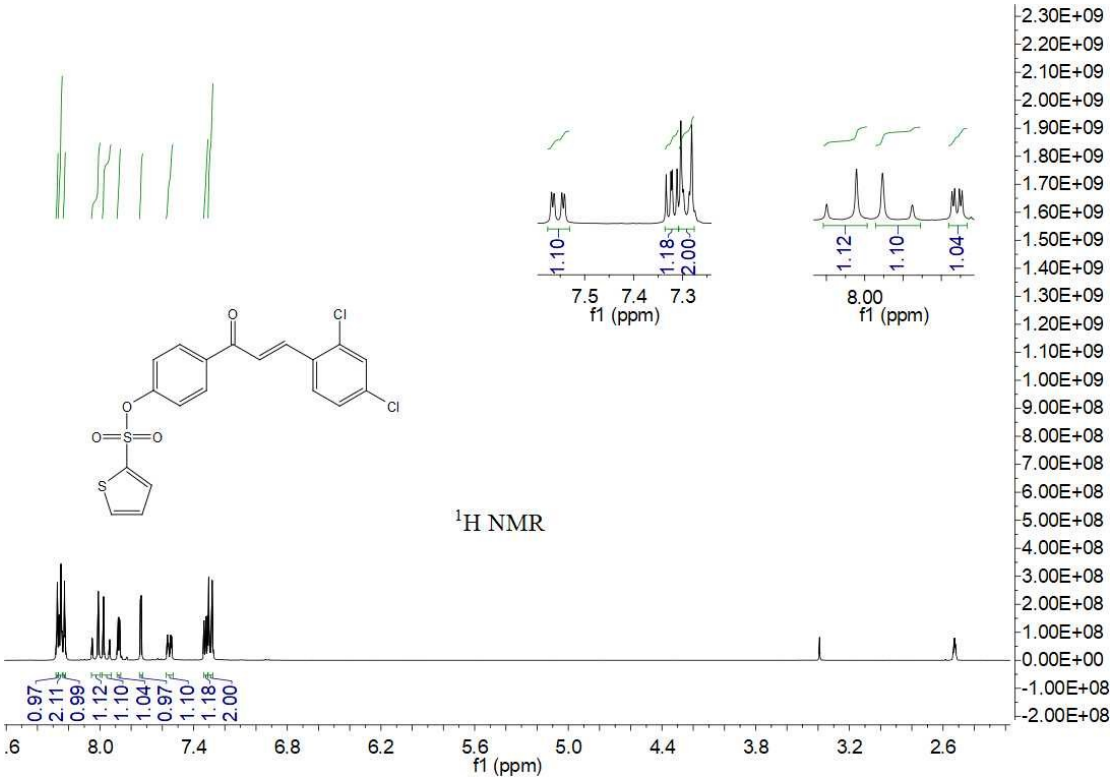
^{1}H NMR spectrum of compound **2o**



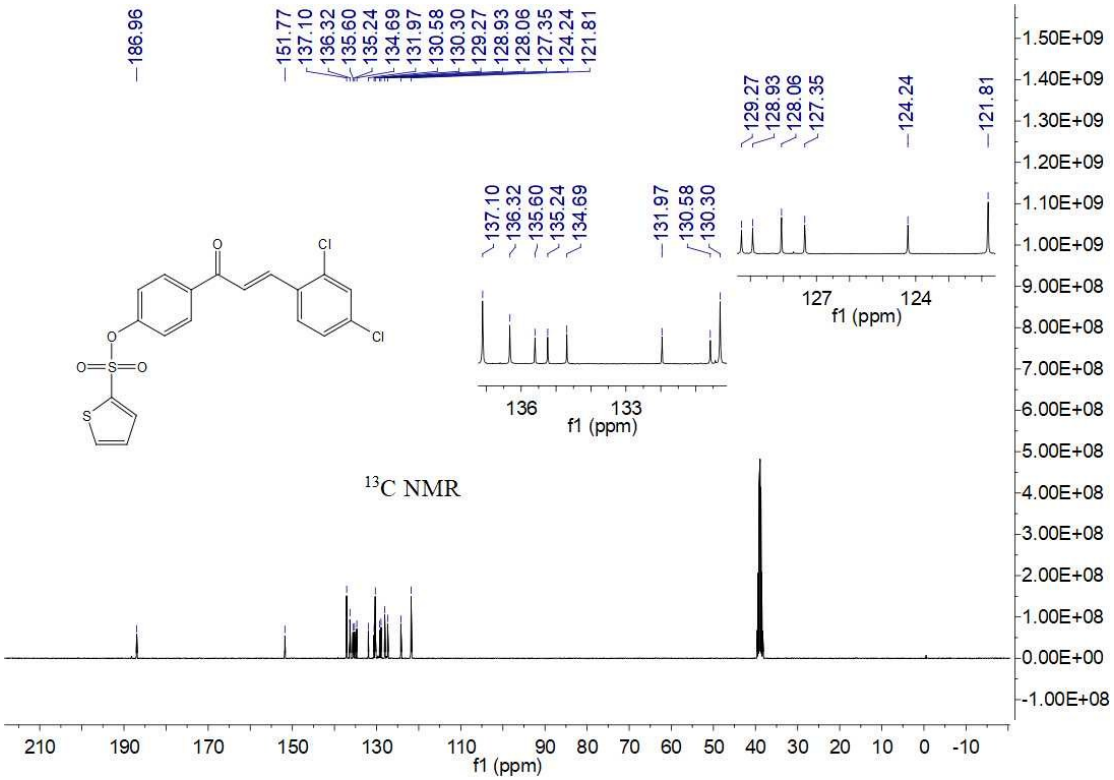
^{13}C NMR spectrum of compound **2o**



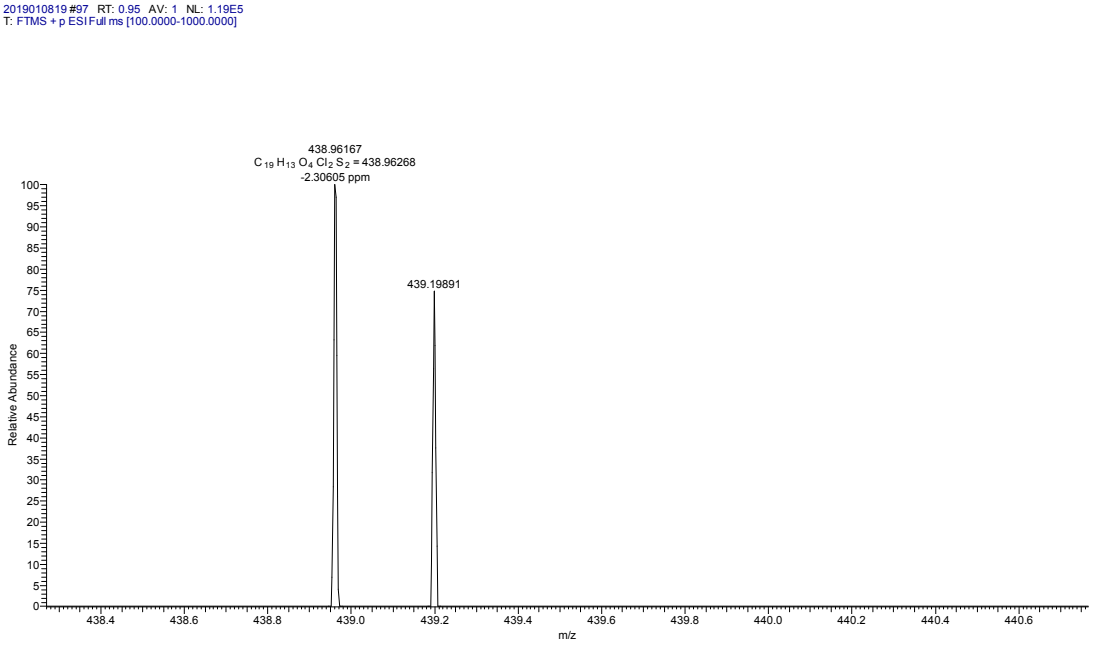
HRMS spectrum of compound **2o**



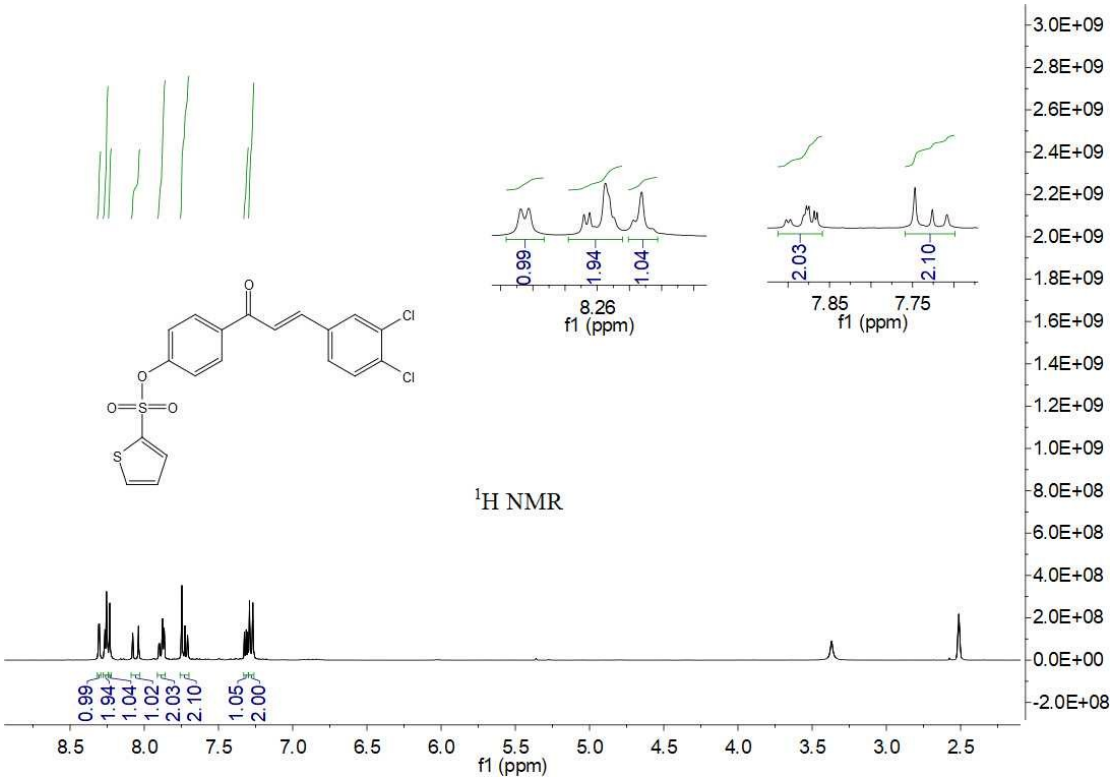
^{1}H NMR spectrum of compound **2p**



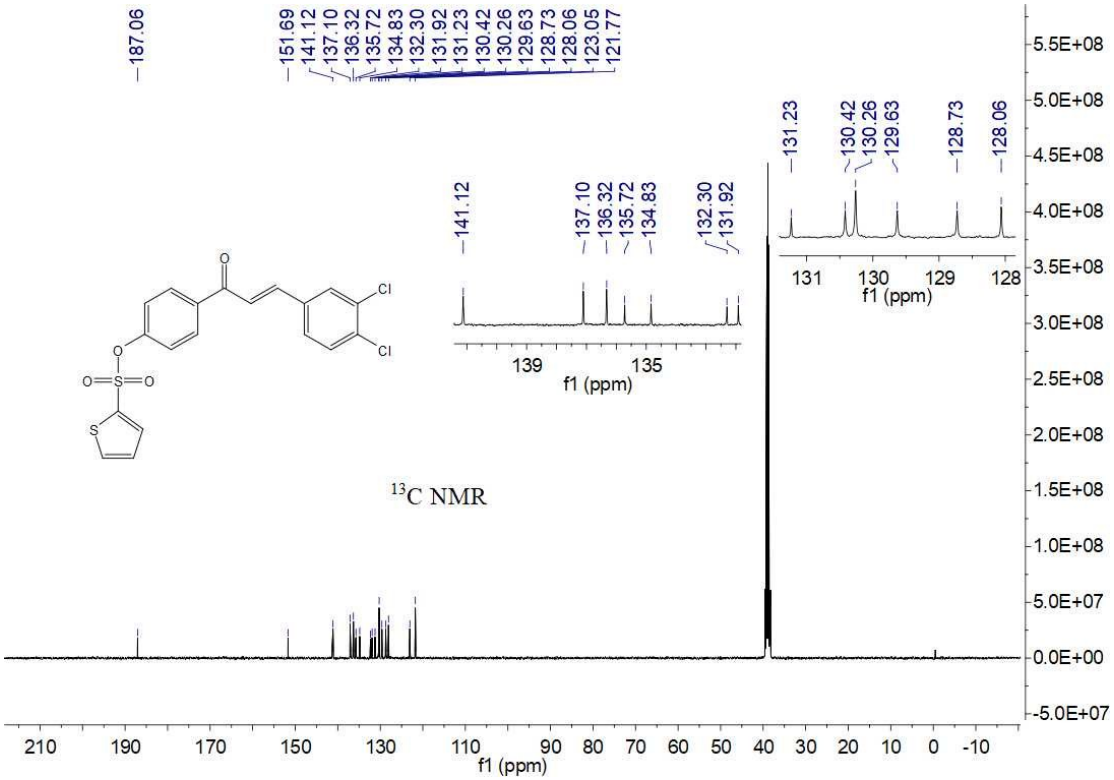
^{13}C NMR spectrum of compound **2p**



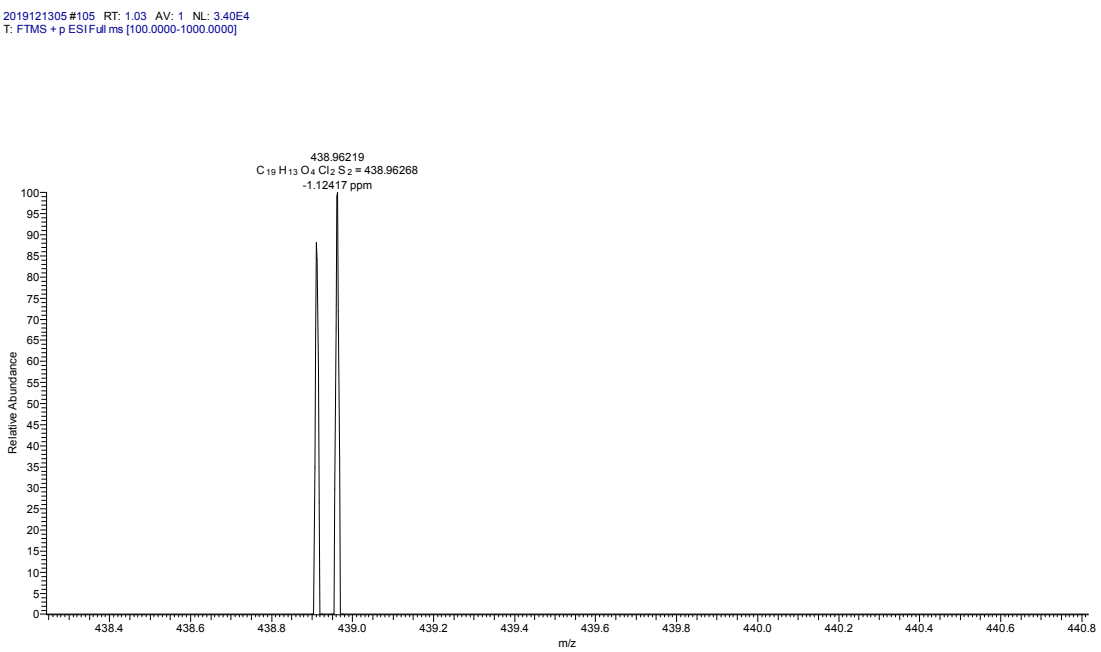
HRMS spectrum of compound **2p**



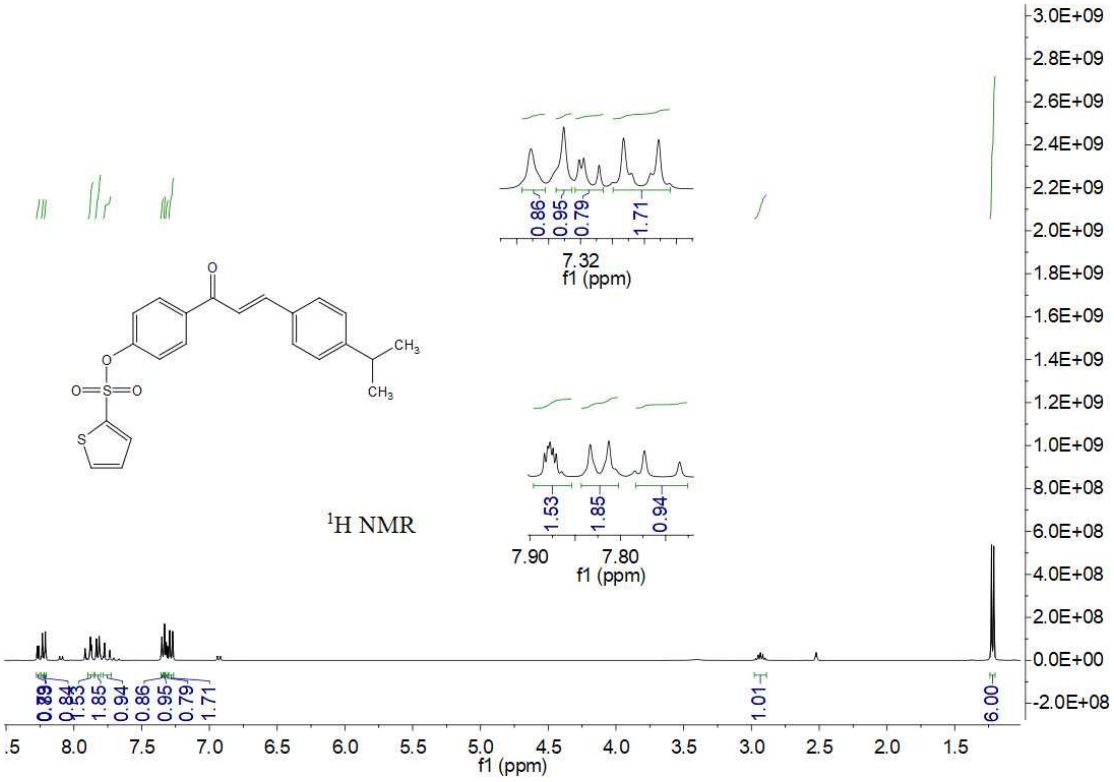
^{1}H NMR spectrum of compound **2q**



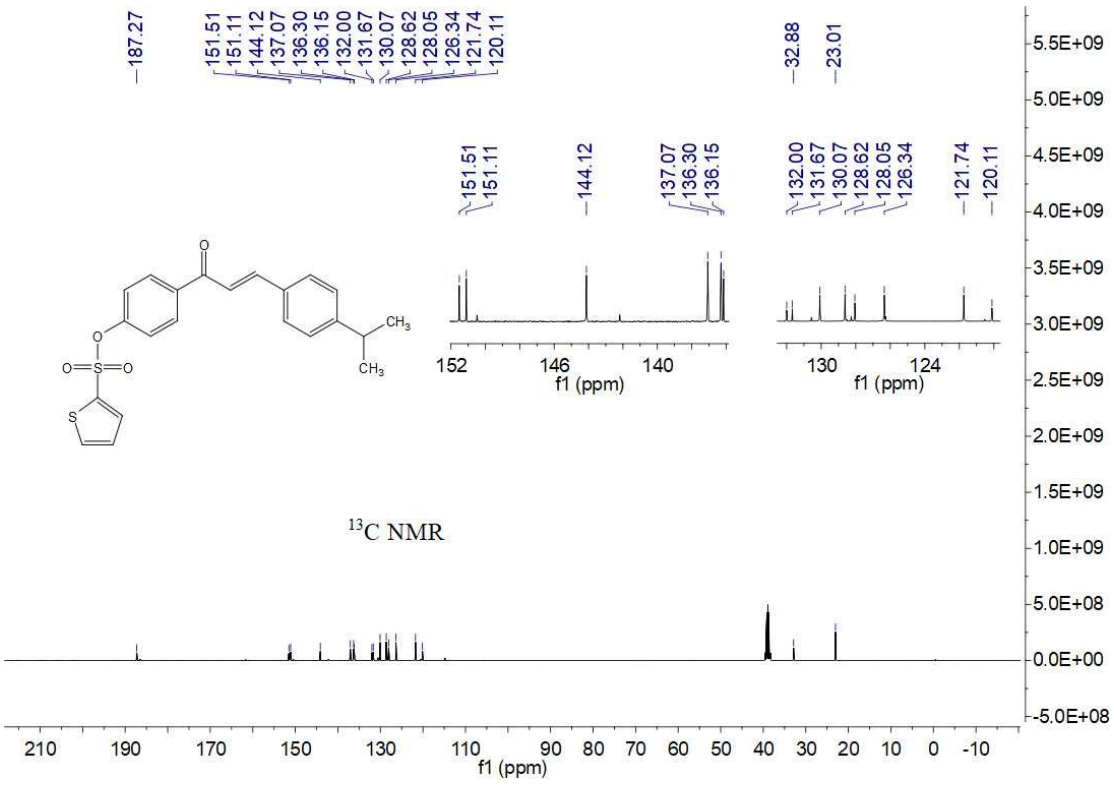
^{13}C NMR spectrum of compound **2q**



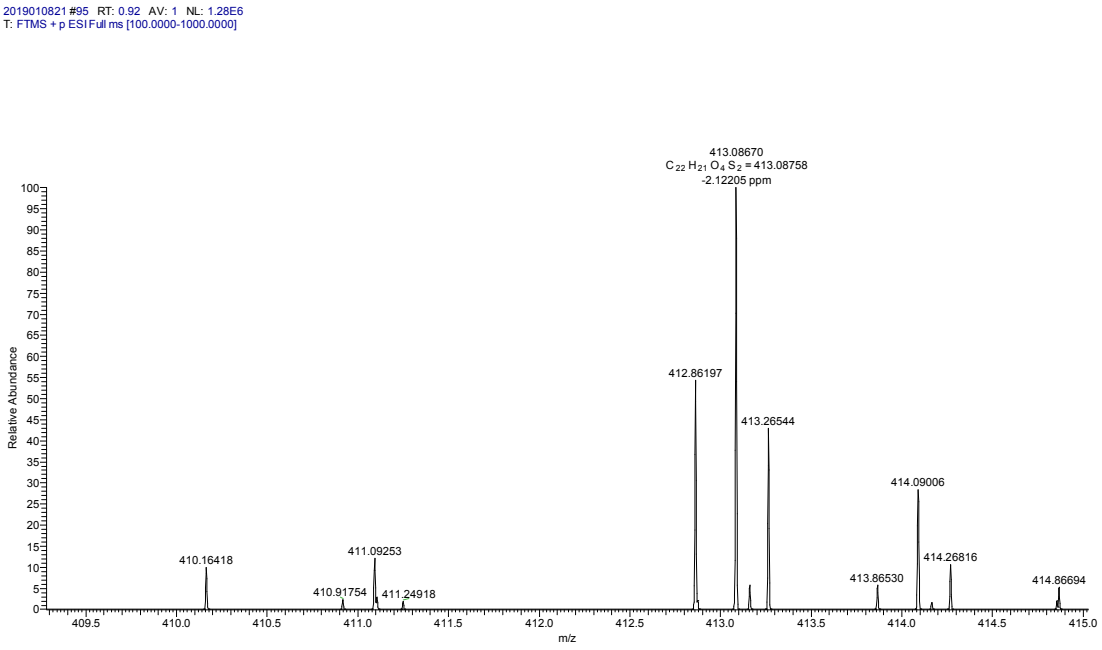
HRMS spectrum of compound **2q**



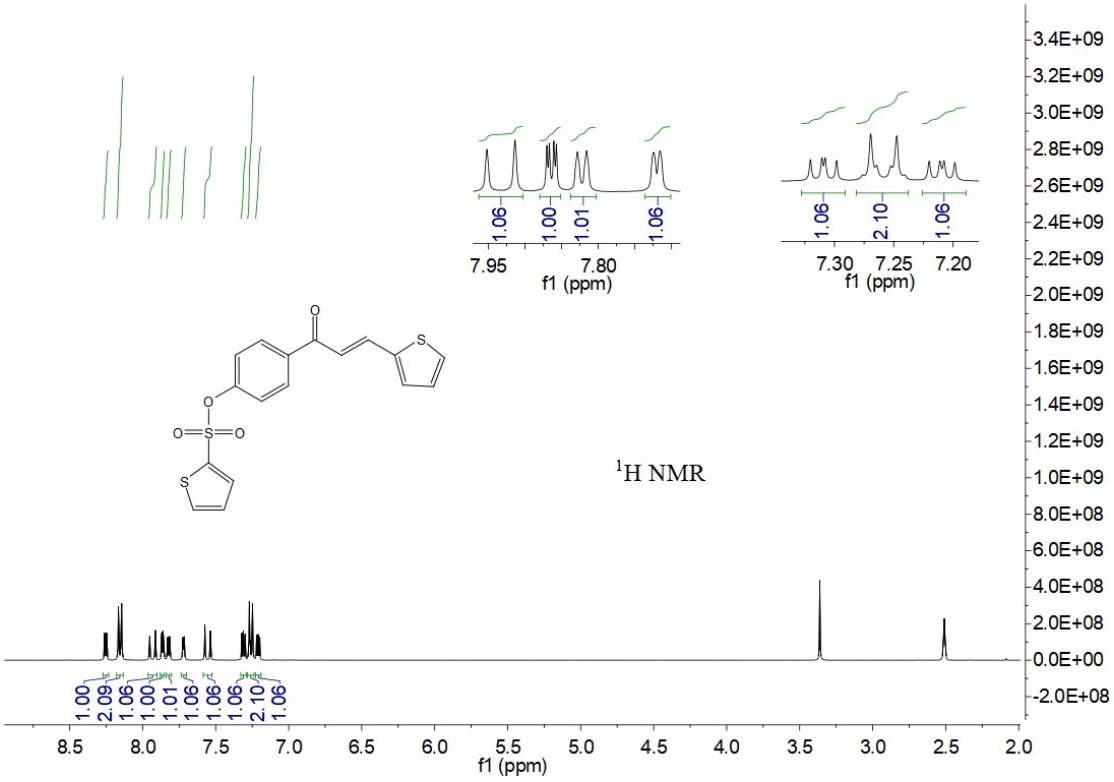
^{1}H NMR spectrum of compound **2r**



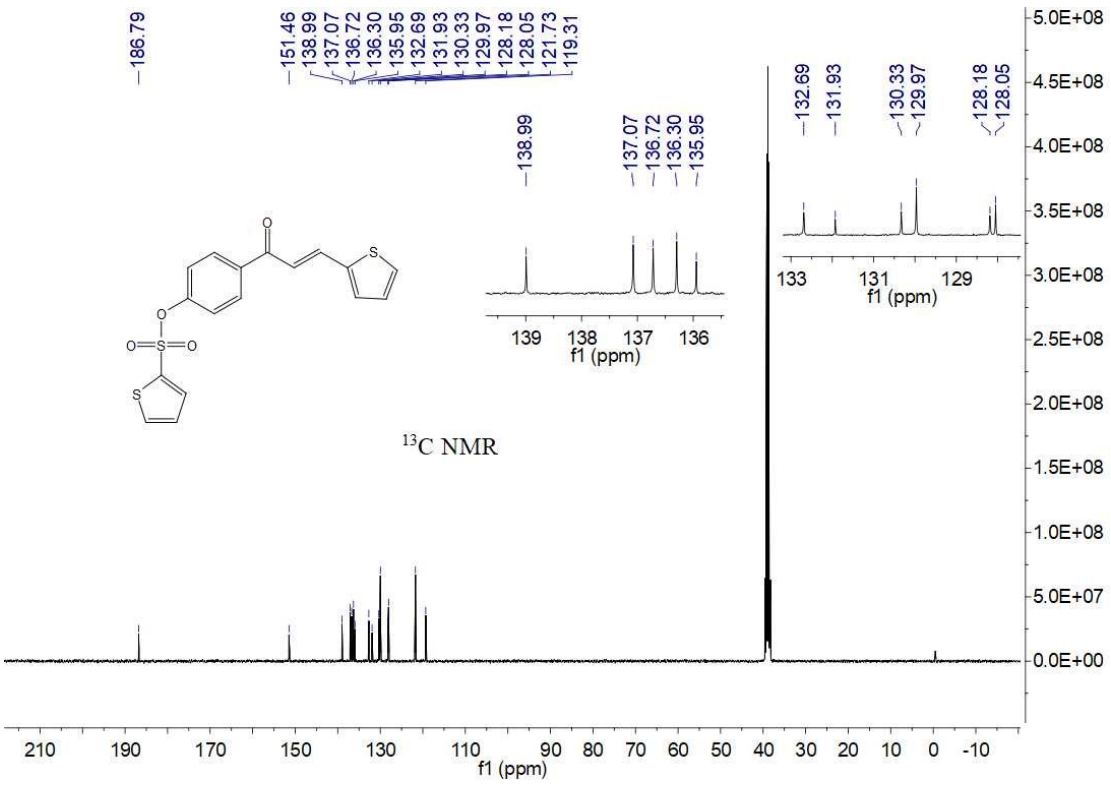
^{13}C NMR spectrum of compound **2r**



HRMS spectrum of compound **2r**

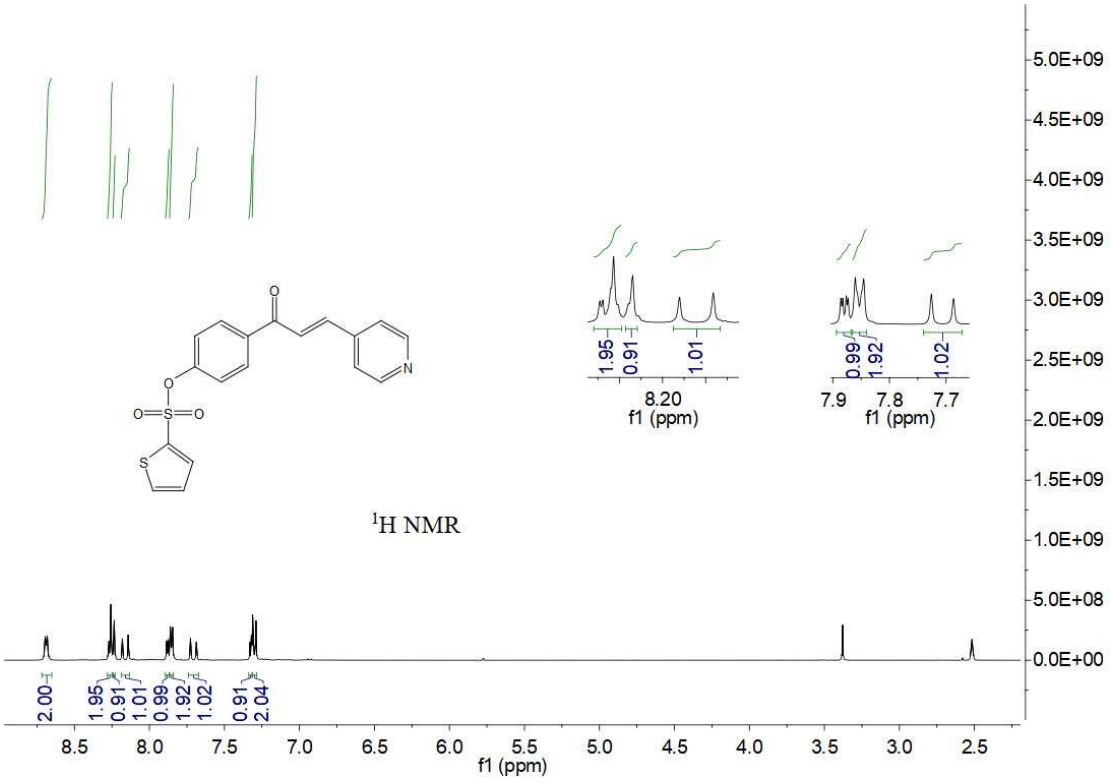


^{1}H NMR spectrum of compound **2s**

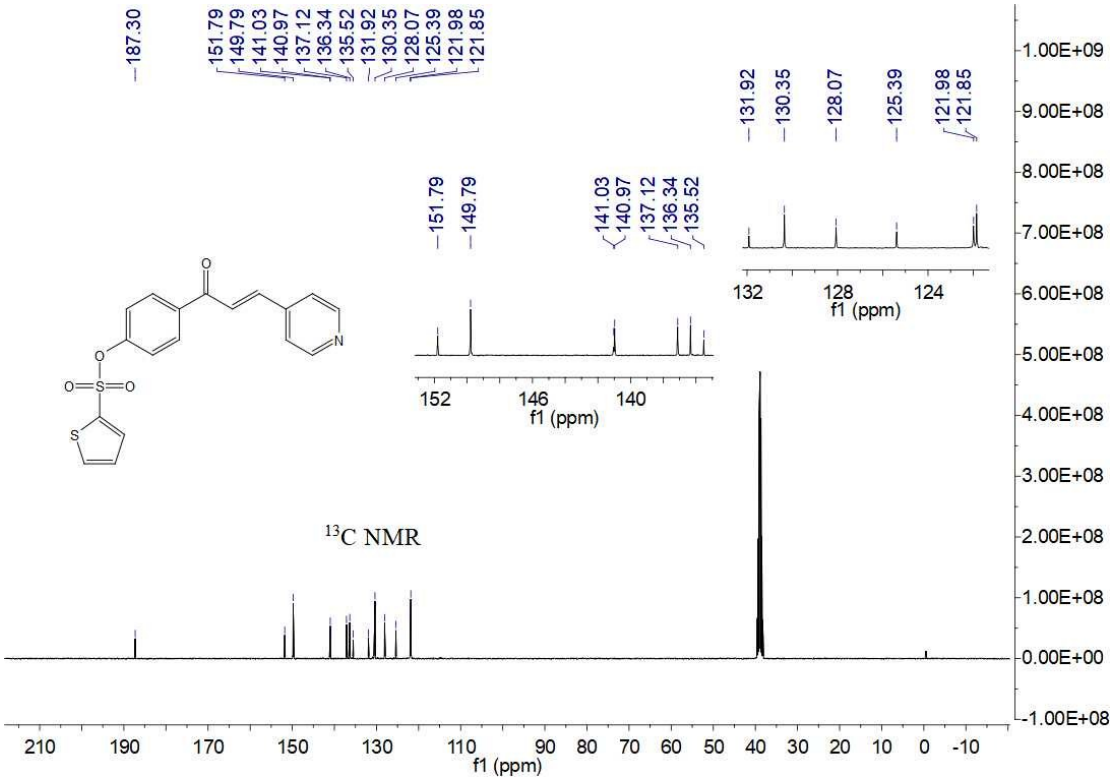


^{13}C NMR spectrum of compound **2s**

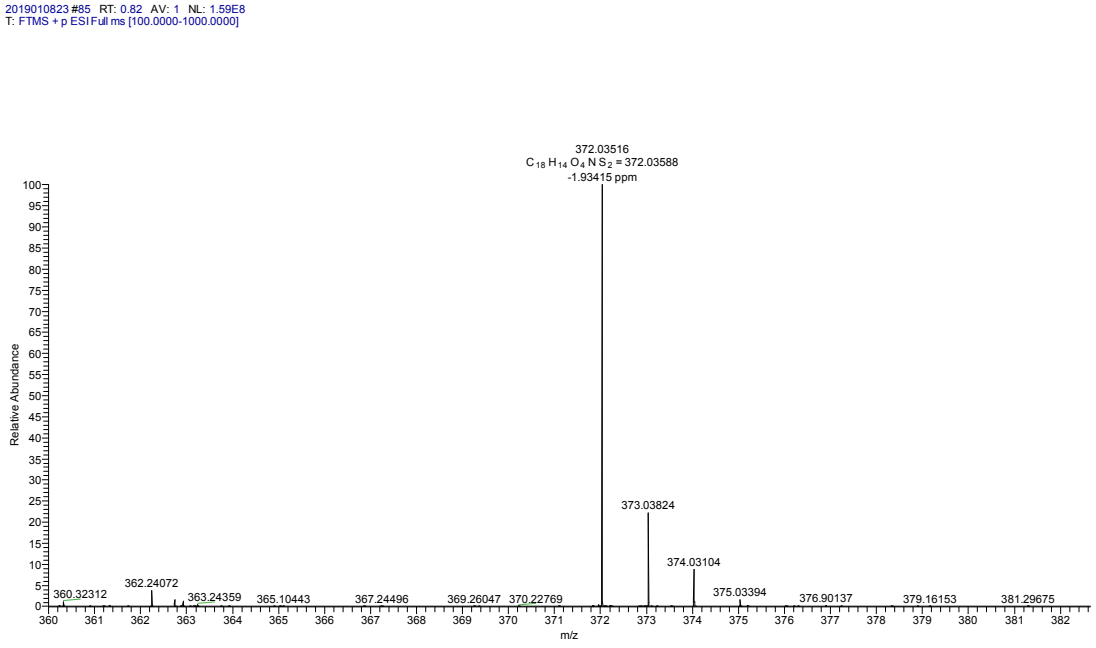
HRMS spectrum of compound **2s**



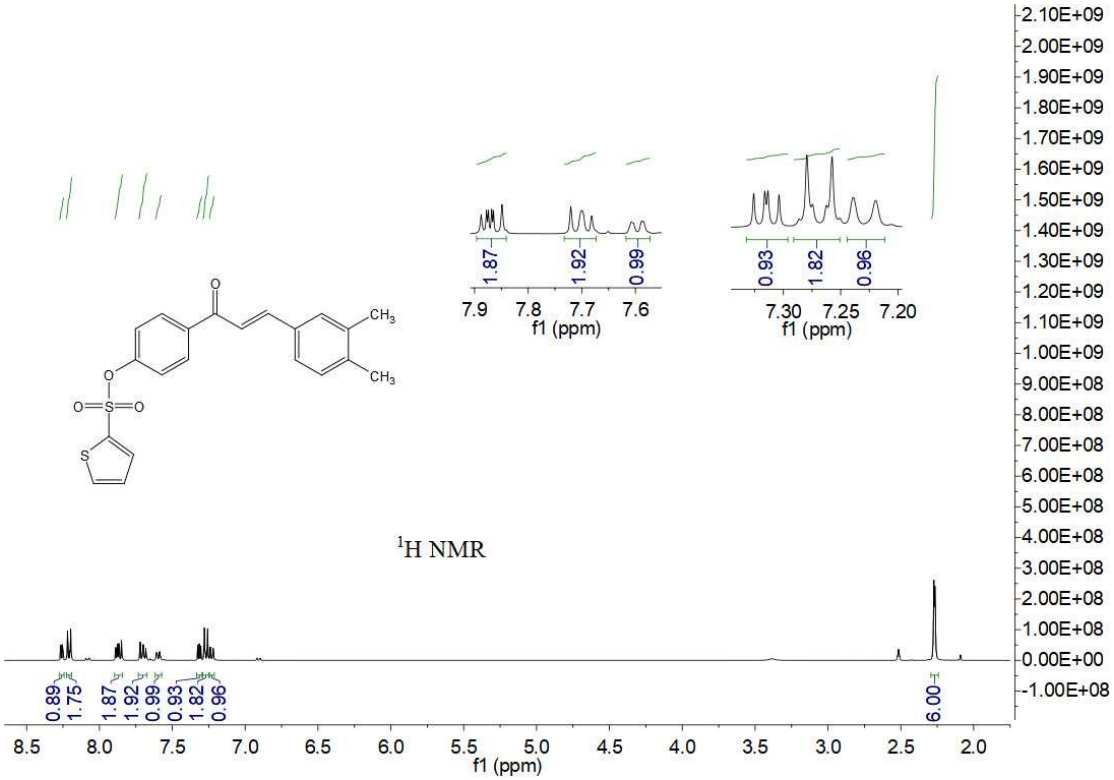
^{1}H NMR spectrum of compound **2t**



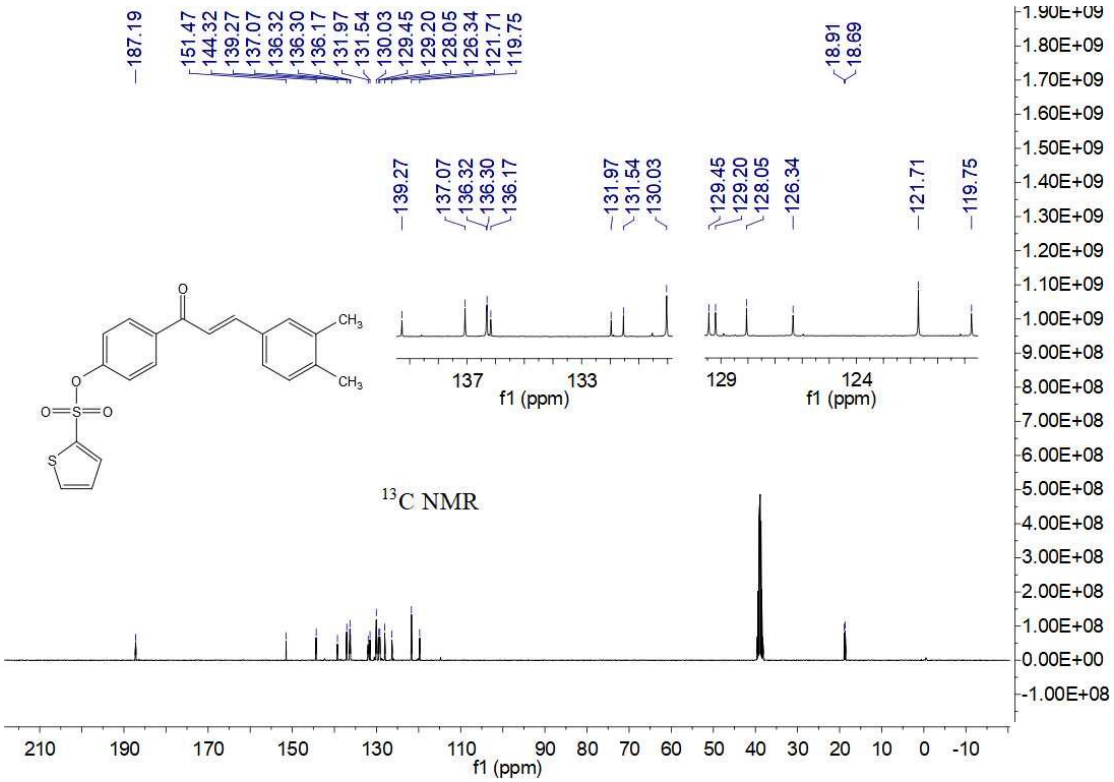
^{13}C NMR spectrum of compound **2t**



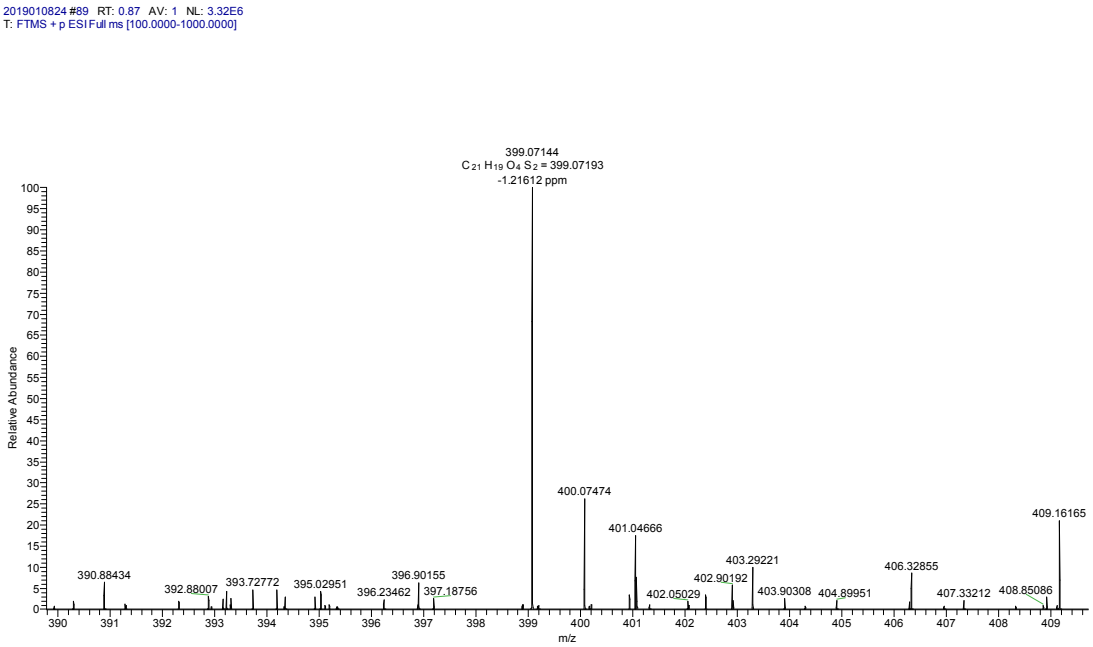
HRMS spectrum of compound **2t**



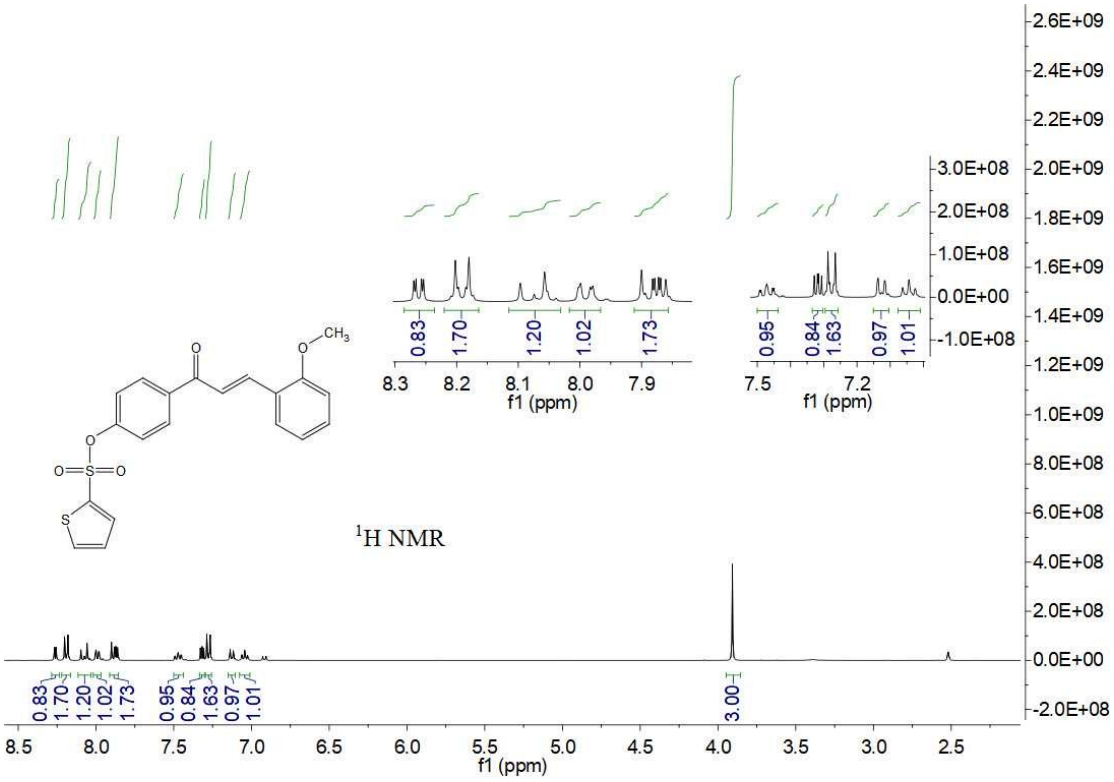
^{1}H NMR spectrum of compound **2u**



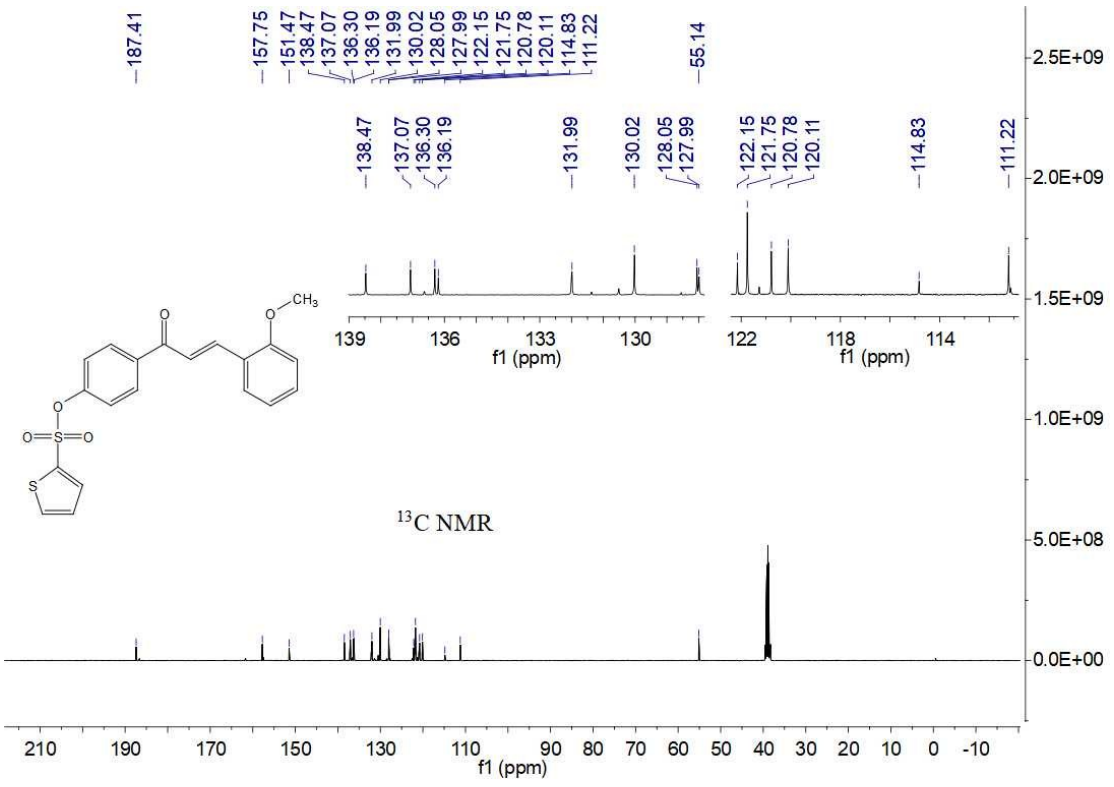
^{13}C NMR spectrum of compound **2u**



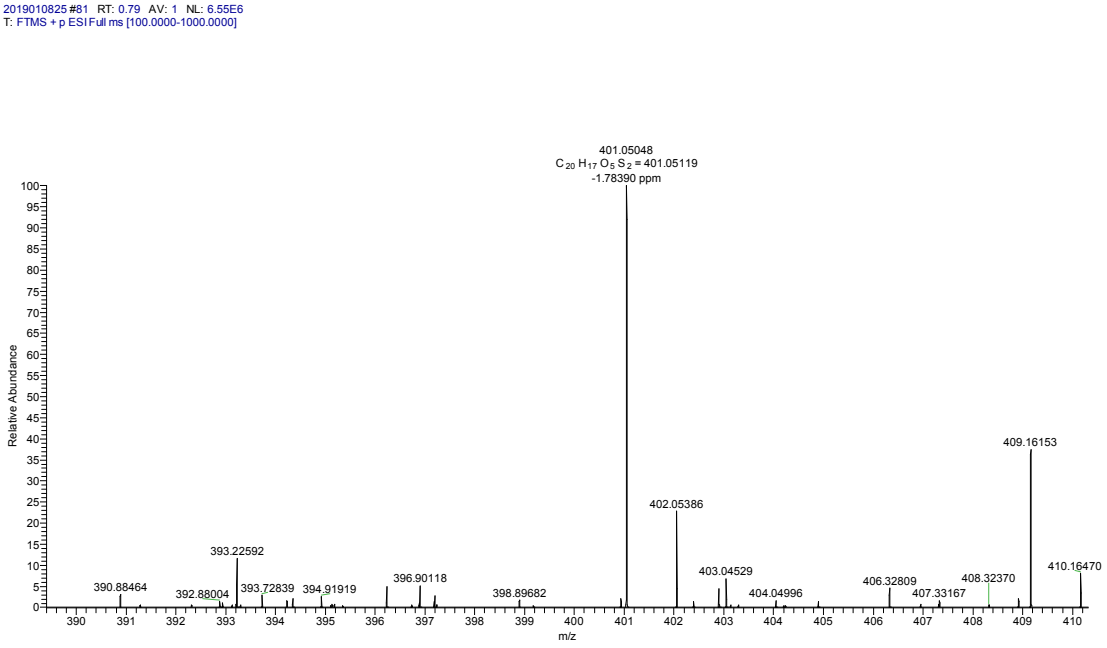
HRMS spectrum of compound **2u**



^{1}H NMR spectrum of compound **2v**



^{13}C NMR spectrum of compound **2v**



HRMS spectrum of compound **2v**