Supporting Information

Photocatalyst-free H_2O-regulated and regiodivergent multicomponent hydrogenation/bifunctional sulfonylation of alkynes

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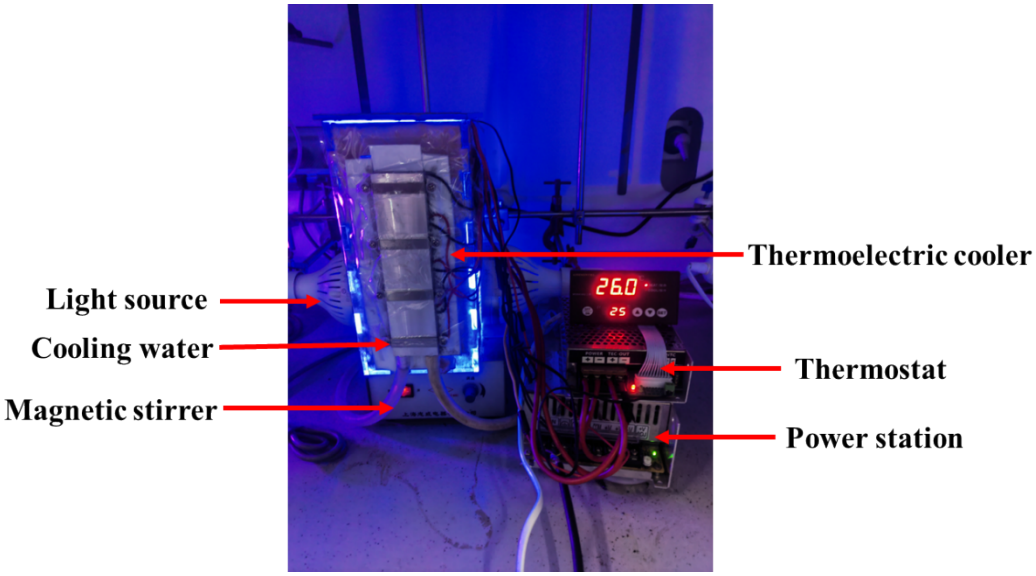
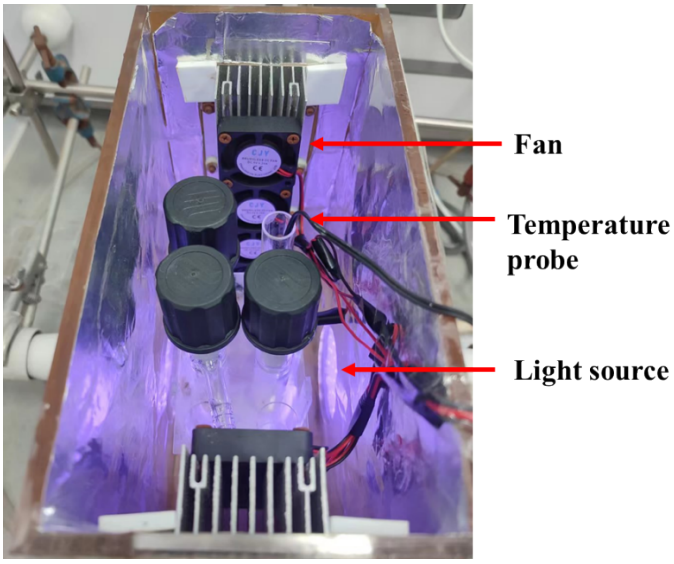
1. General information.

Unless otherwise specified, all reagents are obtained from commercial sources and can be used without further purification (including acetonitrile (AR, moisture ≤ 3000 ppm and moisture ≤ 30 ppm) and dimethyl sulfoxide (AR, moisture ≤ 1000 ppm and moisture ⩽ 50 ppm)). Chromatographic purification of products was performed by flash column chromatography on silica gel (200−300 meshes). Thin-layer chromatography (TLC) was carried out on silica plates (TLC Silica GF254). Visualization of the compounds was accomplished by projecting UV light onto the developed plates. The experiments were conducted in sealed 10 mL or 100 mL Schlenk tube for gram-scale synthesis. The experiments under 460-465 nm light irradiation were performed using two 25 W JG LED lamps from Xuzhou Ai Jia Electronic Technology Co., Ltd. The distance from the light source to the irradiation vessel was approximate 2-3 cm, and no filter was used in our study. A fan was employed to ensure reactions remained at or near room temperature when using LED. ^{1}H NMR (400/600 MHz), ^{13}C NMR (100/150 MHz) and ^{19}F NMR (376/565 MHz) spectra were recorded on a Varian spectrometer in $CDCl_3$ or DMSO-d_6 using tetramethylsilane (TMS) as internal standards. Data are reported as follows: Chemical shift (number of protons, multiplicity, coupling constants). Coupling constants were quoted to the nearest 0.1 Hz and multiplicity reported according to the following convention: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, td = triplet of doublets, ddd = doublet of doublet of doublets, brs = broad singlet. HRMS spectra were recorded on a Bruker Impact II UHR-QTOF spectrometer using ESI on a TOF mass analyze. UV-visible absorption experiments were performed on UV-2250 spectrophotometer. Fluorescence quenching experiments were performed on Hitachi F7000 FL Spectrophotometer. The cyclic voltammetry measurements were detected by using a CHI 600E electrochemical workstation.

2. Light-promoted reaction equipment.

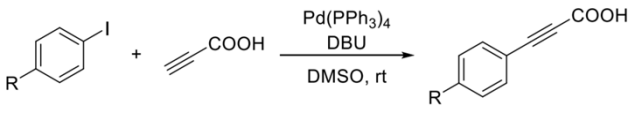




Light source details: The experiments under 460-465 nm light irradiation were performed using two 25 W JG LED lamps from Xuzhou Ai Jia Electronic Technology Co., Ltd. The distance between the light source and the irradiation glass vessel is 2-3 cm, and no filter was used in our study. A fan was employed to ensure reactions remained at or near room temperature when using LEDs.

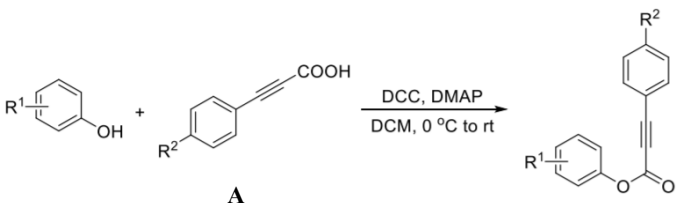
3. General Procedure for Synthesis of Products 1、2、2'、3 and 4.

(1) General Procedure for the Synthesis of 1. [1]



A

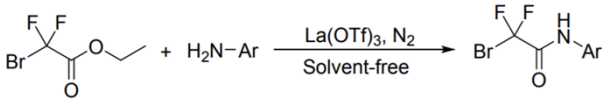
Arylpropiolic acids were prepared using a modified procedure according to the reported literature.[1] To a solution of aryl iodide (5.0 mmol) in DMSO (6 mL) was added $Pd(PPh_3)_4$ (144 mg, 2.5 mol%) and DBU (1.83 g, 12 mmol, 2.4 equiv.). The solution of propiolic acid (420 mg, 6.0 mmol, 1.2 equiv.) in DMSO (6 mL) was poured into the flask. The mixture was stirred at room temperature for 12 h before ethyl acetate (20 mL) was poured into the reaction mixture. The reaction mixture was extracted with saturated aqueous $NaHCO_3$ solution. The aqueous layer was separated, acidified to pH 2.0 by addition of cold HCl (1 N), and extracted with DCM. The combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the desired product **A**.



A **1**

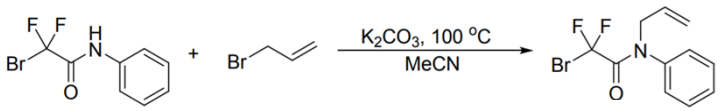
To a solution of the relative phenol **A** (3.0 mmol, 1.0 equiv.) in DCM (30 mL) was added arylpropiolic acid (3.3 mmol, 1.1 equiv.) at 0 ℃, then a mixture of DCC (929 mg, 4.5 mmol, 1.5 equiv.) and DMAP (37 mg, 0.3 mmol, 0.1 equiv.) in CH_2Cl_2 (15 mL) was added dropwise. The mixture was stirred at room temperature for 12 h. Then, the crude mixture was filtered and washed with DCM and concentrated. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the desired product **1**.

(2) General Procedure for the Synthesis of 2. [2]



B

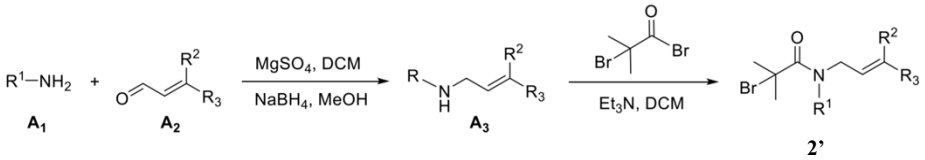
A 10 mL Schlenk bomb was charged with lanthanum trifluoromethanesulfonate $La(OTf)_3$, 0.25 mmol, 5 mol%), ethyl bromodifluoroaceate (6.0 mmol) and amine (5.0 mmol) in an atmosphere of N_2 at the room temperature. The mixture was monitored by TLC. After the amine was exhausted, purification by chromatography on silica gel afforded the target amides **B**.



B **2**

To a solution of the 2-bromo-2,2-difluoro-*N*-phenylacetamide **B** (1.25 g, 5.0 mmol) in CH_3CN (25 mL), K_2CO_3 (2.07 g, 15 mmol) and 3-bromopropene (1.21 g, 10 mmol) were added. The reaction mixture was stirred at 100 °C and monitored by TLC. After the amide was exhausted, the mixture was purified by silica gel column chromatography to give the desired product **2**.

(3) General Procedure for the Synthesis of 2'. [3]



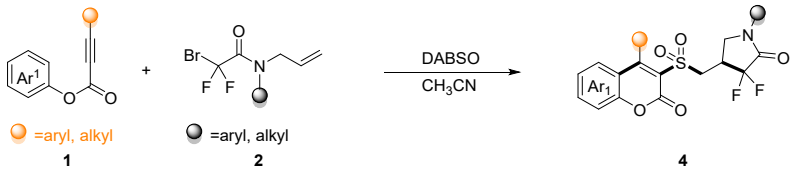
A1 **A2** **A3** **2'**

Appropriate amine $\mathbf{A_1}$ (10 mmol, 1.0 equiv.), magnesium sulfate (1.81 g, 15.0 mmol) and 3-methyl-2-butenal $\mathbf{A_2}$ (1.38 g, 10.0 mmol, 1.0 equiv.) suspended in DCM stirred 4 hours at room temperature. Filtered the mixture and concentrated the filtrate by evaporation. The residue was dissolved in methanol (10.00 mL) and cooled to 0 °C. Slowly added the sodium borohydride (0.19 g, 5.0 mmol), stirred reaction mixture at room temperature for 2 hours. Then, quenched the reaction system with saturated NH_4Cl aqueous solution, extracted with EtOAc, washed with brine, and dried over Na_2SO_4. Final, the organic layer was evaporated under reduced pressure and residue was purified by column chromatography on silica to afford the $\mathbf{A_3}$ (10/1 petroleum ether/EtOAc).

$\mathbf{A_3}$ and Et_3N (1.40 mL, 10.0 mmol, 2.0 equiv.) were suspended in DCM (20.00 mL) and cooled to 0 °C, subsequently, dropwise added 2-bromo-2-methylpropanoyl bromide (0.67 mL, 5.5 mmol, 1.1 equiv.) and stirred the reaction system at room temperature for 12 h. After that, NH_4Cl aqueous solution was added, extracted with dichloromethane washed with saturated sodium bicarbonate,

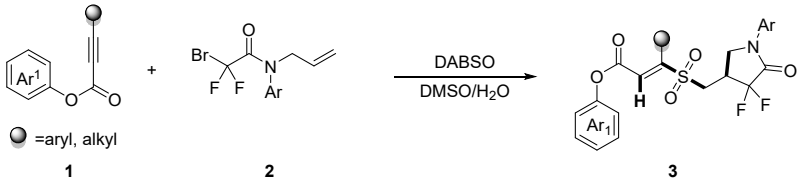
dried with Na_2SO_4. Evaporated the organic layer and purified by column chromatography (10-20% EtOAc in petroleum ether) gave the **2'**

(4) General Procedure for the Synthesis of 4.



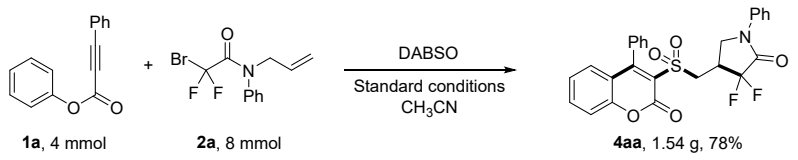
To a 10 mL schlenk-tube was charged with **1** (0.2 mmol, 1.0 equiv.), **2** (0.4 mmol, 2.0 equiv.), DABCO·$(SO_2)_2$ (0.4 mmol, 2.0 equiv.) in dry CH_3CN (2 mL, moisture ≤ 30 ppm) under nitrogen atmosphere. The mixture was irradiated with 25 W blue LEDs under vigorous stirring at room temperature for 12-16 h. After the reaction completed, the reaction mixture was diluted with H_2O (15 mL) and extracted with CH_2Cl_2 (20 mL × 4). The combined organic layers were washed with brine (30 mL), dried over anhydrous Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the desired product **3**.

(5) General Procedure for the Synthesis of 3.



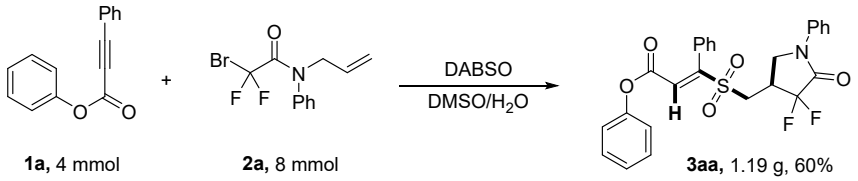
To a 10 mL schlenk-tube was charged with **1** (0.2 mmol, 1.0 equiv.), **2** (0.4 mmol, 2.0 equiv.), DABCO·$(SO_2)_2$ (0.4 mmol, 2.0 equiv.) in DMSO/H_2O (2 mL (v/v = 39:1)) under nitrogen atmosphere. The mixture was irradiated with 25 W blue LEDs under vigorous stirring at room temperature for 12-24 h. After the reaction completed, the reaction mixture was diluted with H_2O (15 mL) and extracted with CH_2Cl_2 (20 mL × 4). The combined organic layers were washed with brine (30 mL), dried over anhydrous Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the desired product **4**.

(6) Gram Procedure for the Synthesis of 4aa and 3aa.



To a 100 mL schlenk-tube was charged with **1a** (4 mmol, 1.0 equiv.), **2a** (8 mmol, 2.0 equiv.), DABCO·$(SO_2)_2$ (8 mmol, 2.0 equiv.) in dry CH_3CN (40 mL, moisture ≤ 30 ppm) under nitrogen

atmosphere. The mixture was irradiated with 25 W blue LEDs under vigorous stirring at room temperature for 30 h. After the reaction completed, the reaction mixture was diluted with H_2O (50 mL) and extracted with CH_2Cl_2 (40 mL × 4). The combined organic layers were washed with brine (40 mL), dried over anhydrous Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (5:1) to afford the desired product **4aa**.

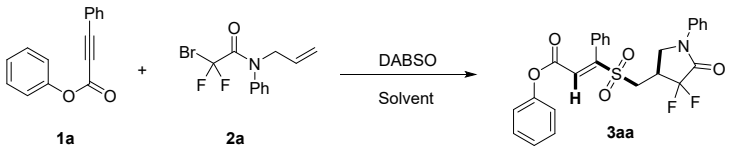


1a, 4 mmol **2a,** 8 mmol **3aa,** 1.19 g, 60%

To a 100 mL schlenk-tube was charged with **1a** (4 mmol, 1.0 equiv.), **2a** (8 mmol, 2.0 equiv.), DABCO·$(SO_2)_2$ (8 mmol, 2.0 equiv.) in DMSO/H_2O (40 mL (v/v = 39:1)) under nitrogen atmosphere. The mixture was irradiated with 25 W blue LEDs under vigorous stirring at room temperature for 30 h. After the reaction completed, the reaction mixture was diluted with H_2O (50 mL) and extracted with CH_2Cl_2 (40 mL × 4). The combined organic layers were washed with brine (40 mL× 3), dried over anhydrous Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (10:1) to afford the desired product **3aa**.

4. Optimization of reaction conditions.

4.1 Effect of solvent ratio on reaction. [a]



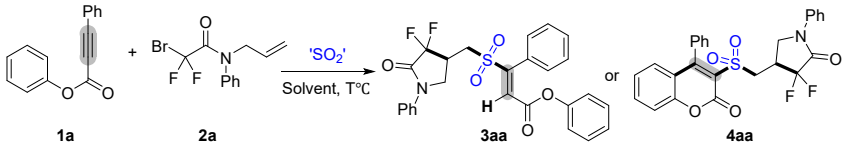
1a **2a** **3aa**

Entry	Solvent	4aa/Yield (%) [b]
1	DMSO (2 mL)	0
2[c]	DMSO (2 mL)	14
3	DMSO/H_2O (2 mL, v/v=199:1)	27
4	DMSO/H_2O (2 mL, v/v=99:1)	35
5	DMSO/H_2O (2 mL, v/v=197:3)	48
6	DMSO/H_2O (2 mL, v/v=49:1)	66
7	*DMSO/H_2O (2 mL, v/v=39:1)*	*76*
8	DMSO/H_2O (2 mL, v/v=97:3)	68
9	DMSO/H_2O (2 mL, v/v=19:1)	47
10	DMSO/H_2O (2 mL, v/v=1:1)	0

[a]Reaction conditions: **1** (0.2 mmol, 1.0 equiv.), **2** (0.4 mmol, 2.0 equiv.), DABSO (0.4 mmol, 2.0

equiv.), solvent (2 mL, (dry DMSO, moisture ≤50 ppm)), room temperature under N_2, irradiation with blue LEDs (25W × 2, 460-465nm) for 12 h. [b]Isolated yields. [c]Solvent (2 mL, moisture ≤1000 ppm).

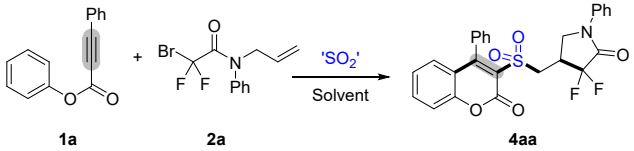
4.2 Effect of temperature on reaction. [a]



Entry	T/°C	Solvent	3aa/Yield (%) [b]	4aa/Yield (%) [b]
1	**25**	**DMSO/H_2O**	**76**	**<10**
2	20	DMSO/H_2O	trace	N.D.
3	30	DMSO/H_2O	72	<15
4	**25**	**CH_3CN**	**N.D.**	**90**
5	20	CH_3CN	N.D.	30
6	30	CH_3CN	N.D.	82

[a]Reaction conditions: **1a** (0.2 mmol, 1.0 equiv.), **2a** (0.4 mmol, 2.0 equiv.), DABSO (0.4 mmol, 2.0 equiv.), degassed solvent (2 mL, (CH_3CN (moisture ≤ 30 ppm) and DMSO (moisture ≤ 1000 ppm)), room temperature under N_2, irradiation with blue LEDs (25W × 2, 460-465nm) for 12-24 h. [b]Isolated yields.

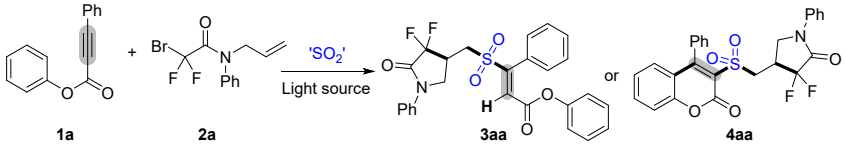
4.3 Effect of solvent on reaction.[4] [a]



Entry	Solvent	4aa/Yield (%) [b]
1	**CH_3CN**	**90**
2	MeOH	31
3	2-Methyltetrahydrofuran	49
4	Ethyl acetate	18
5	Acetone	74
6	*N*-Methylpyrrolidone	N.D.
7	DCE	45

[a]Reaction conditions: **1a** (0.2 mmol, 1.0 equiv.), **2a** (0.4 mmol, 2.0 equiv.), DABSO (0.4 mmol, 2.0 equiv.), degassed solvent (2 mL), room temperature under N_2, irradiation with blue LEDs (25W × 2, 460-465nm) for 12-31 h. [b]Isolated yields.

4.4 Effect of light sources on reaction. [a]

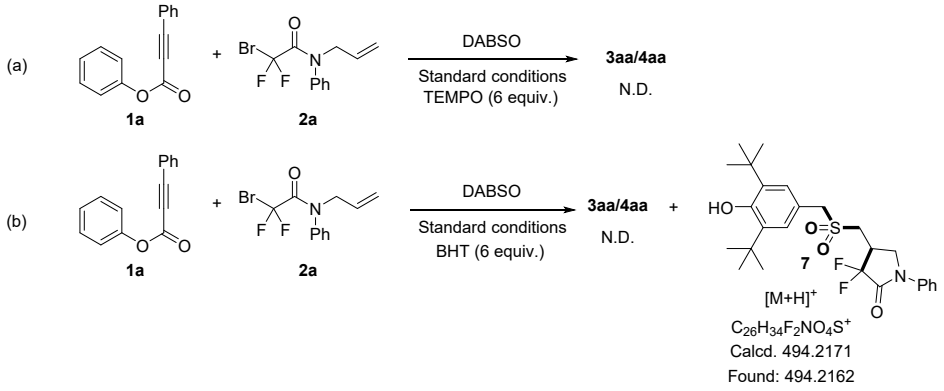


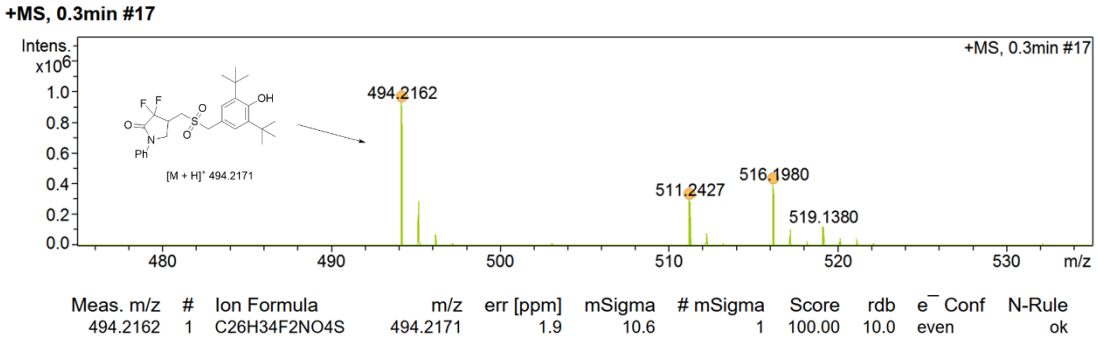
Entry	Solvent	Light source	3aa/Yield (%) [b]	4aa/Yield (%) [b]
1	**DMSO/H_2O**	**blue LEDs (460-465 nm)**	**76**	**<10**
2	DMSO/H_2O	green LEDs (520-530 nm)	trace	N.D.
3	DMSO/H_2O	violet LEDs (390-400 nm)	61	<5
4	DMSO/H_2O	white LEDs (400-800 nm)	24	trace
5	**CH_3CN**	**blue LEDs (460-465 nm)**	**N.D.**	**90**
6	CH_3CN	green LEDs (520-530 nm)	N.D.	24
7	CH_3CN	violet LEDs (390-400 nm)	N.D.	78
8	CH_3CN	white LEDs (400-800 nm)	N.D.	43

[a]Reaction conditions: **1a** (0.2 mmol, 1.0 equiv.), **2a** (0.4 mmol, 2.0 equiv.), DABSO (0.4 mmol, 2.0 equiv.), degassed solvent (2 mL, (CH_3CN (moisture ≤ 30 ppm) and DMSO (moisture ≤ 1000 ppm)), room temperature under N_2, irradiation with light sources (25W × 2) for 12-16 h. [b]Isolated yields.

5. Mechanistic Studies.

(1) Radical trapping Experiment.

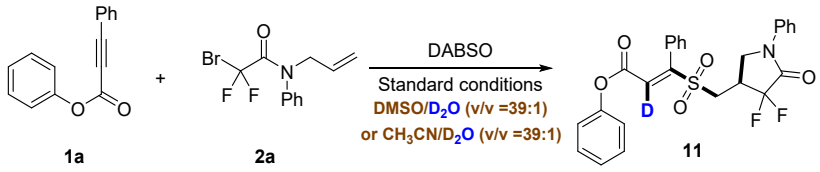




The radical trapping experiments were conducted with **1a** and **2a** under the standard conditions with two different trapping agents (TEMPO or BHT) to capture the radical intermediates. No desired product **3aa/4aa** were detected in the above two controlled experiments, indicating that the reaction was completely inhibited. Meanwhile, a trapping product **7** was detected by the HRMS.

HRMS-ESI (m/z): calcd for $C_{26}H_{34}F_2NO_4S^+$ $[M + H]^+$ 494.2171, found 494.2162.

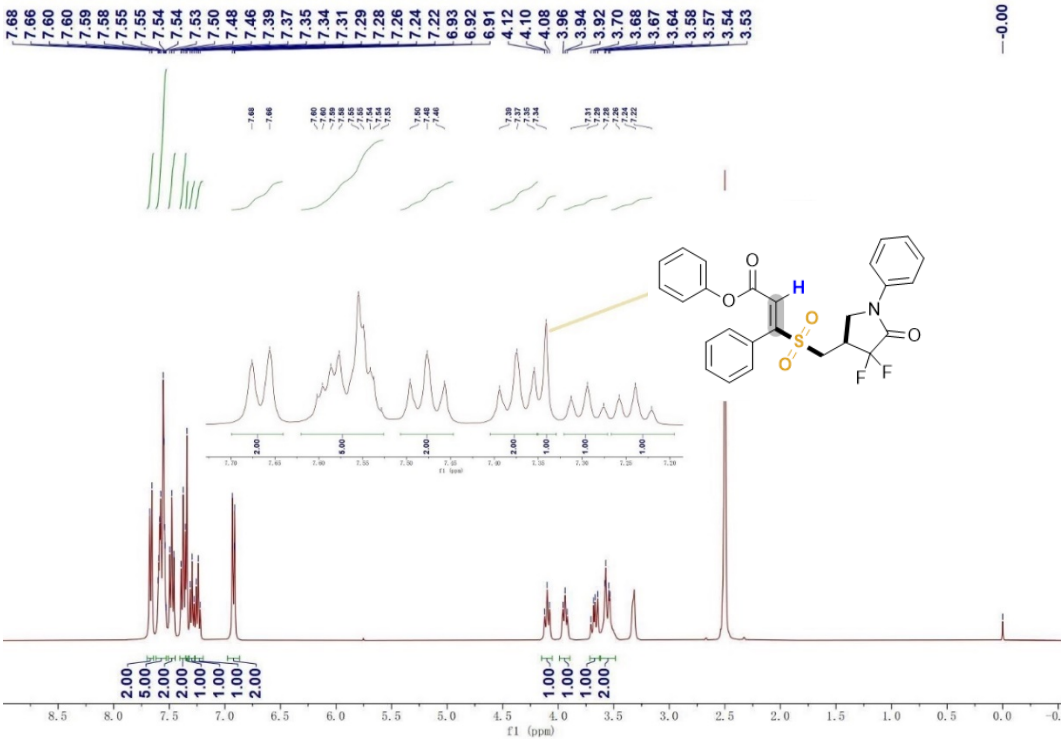
(2) Deuterium Experiment.

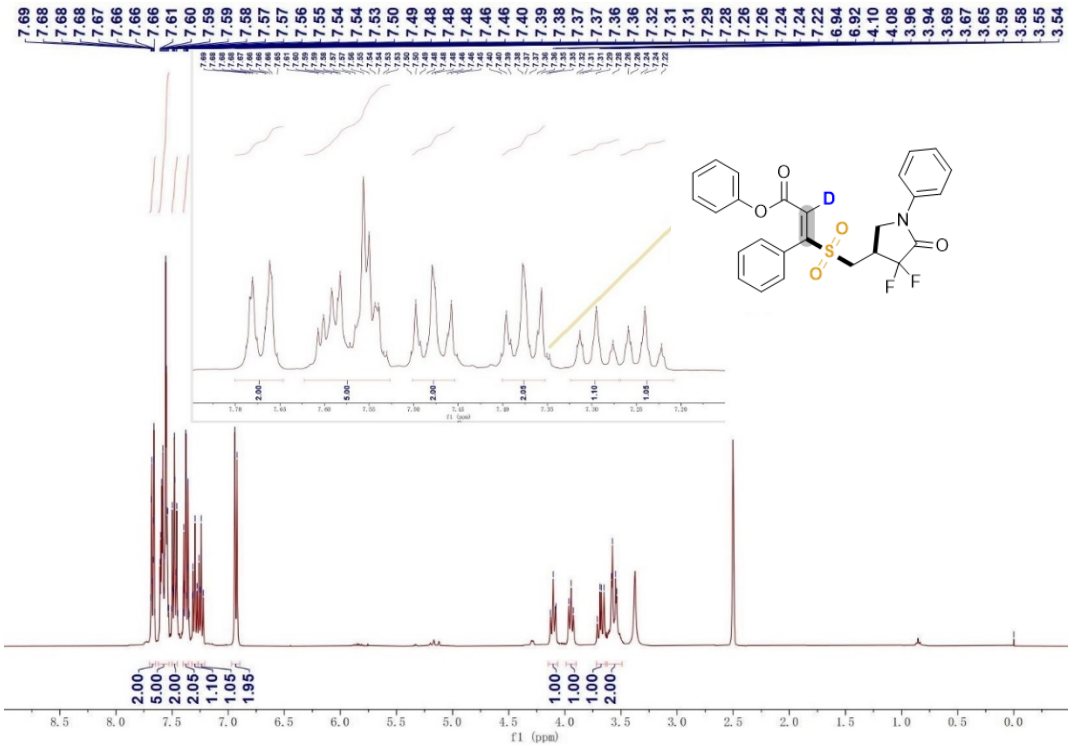


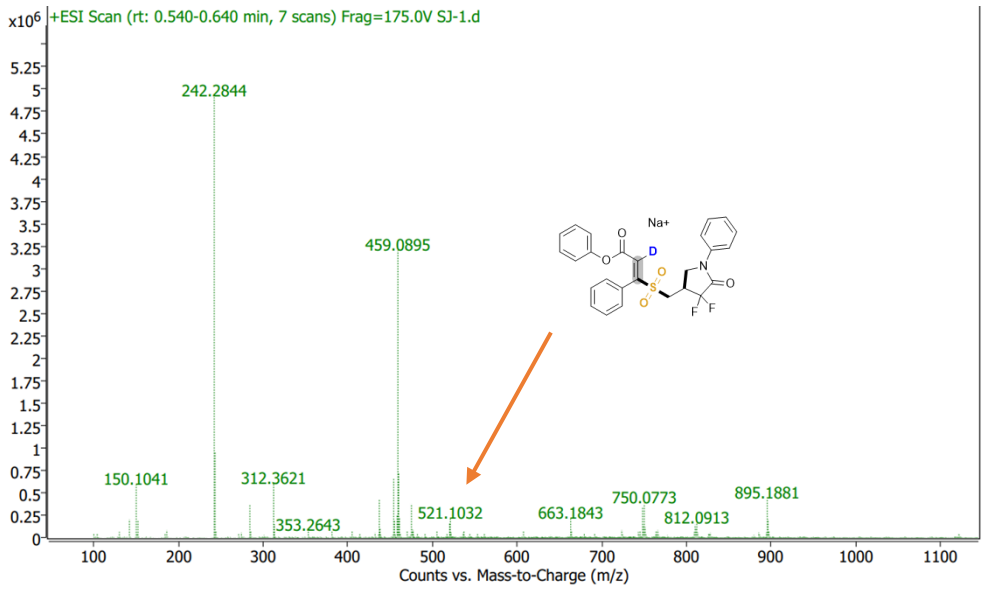
To a 10 mL schlenk-tube was charged with **1** (0.2 mmol, 1.0 equiv.), **2** (0.4 mmol, 2.0 equiv.), DABCO·$(SO_2)_2$ (0.4 mmol, 2.0 equiv.) in DMSO/D_2O or CH_3CN/D_2O (2 mL, v/v =39:1) under nitrogen atmosphere. The mixture was irradiated with 25 W blue LEDs under vigorous stirring at room temperature for 12 h. After the reaction completed, the reaction mixture was diluted with H_2O (15 mL) and extracted with CH_2Cl_2 (20 mL × 4). The combined organic layers were washed with brine (30 mL), dried over anhydrous Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the desired product **11**.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.7–7.6 (m, 2H), 7.6–7.5 (m, 5H), 7.5–7.4 (m, 2H), 7.4–7.3 (m, 2H), 7.3 (t, J = 7.5 Hz, 1H), 7.2 (t, J = 7.4 Hz, 1H), 6.9 (d, J = 7.5 Hz, 2H), 4.1 (t, J = 10.0 Hz, 1H), 3.9 (t, J = 7.7 Hz, 1H), 3.7–3.6 (m, 1H), 3.6–3.5 (m, 2H).

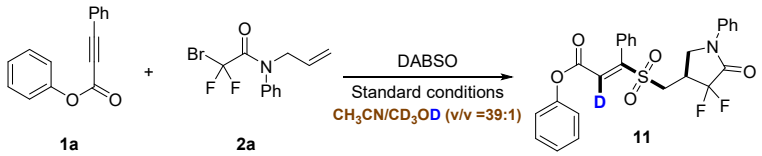
HRMS-ESI (m/z): calcd for $C_{26}H_{20}DF_2NNaO_5S^+$ $[M+Na]^+$ 521.1063, found 521.1032.



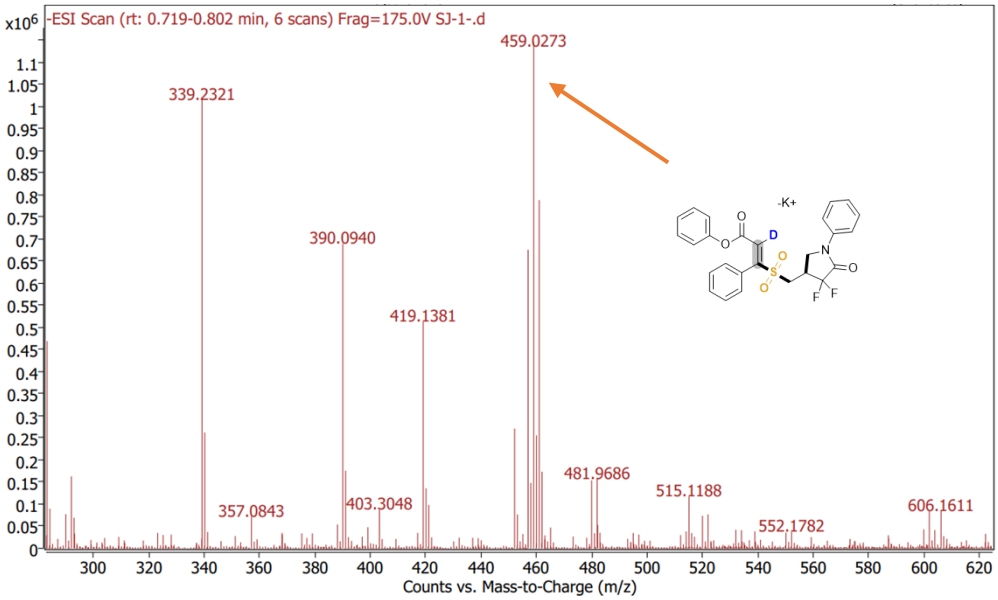




To a 10 mL schlenk-tube was charged with **1** (0.2 mmol, 1.0 equiv.), **2** (0.4 mmol, 2.0 equiv.), DABCO·$(SO_2)_2$ (0.4 mmol, 2.0 equiv.) in CH_3CN/CD_3OD (2 mL, v/v =39:1) under nitrogen atmosphere. The mixture was irradiated with 25 W blue LEDs under vigorous stirring at room temperature for 12 h. After the reaction completed, the reaction mixture was diluted with H_2O (15 mL) and extracted with CH_2Cl_2 (20 mL × 4). The combined organic layers were washed with brine (30 mL), dried over anhydrous Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the desired product **11**.

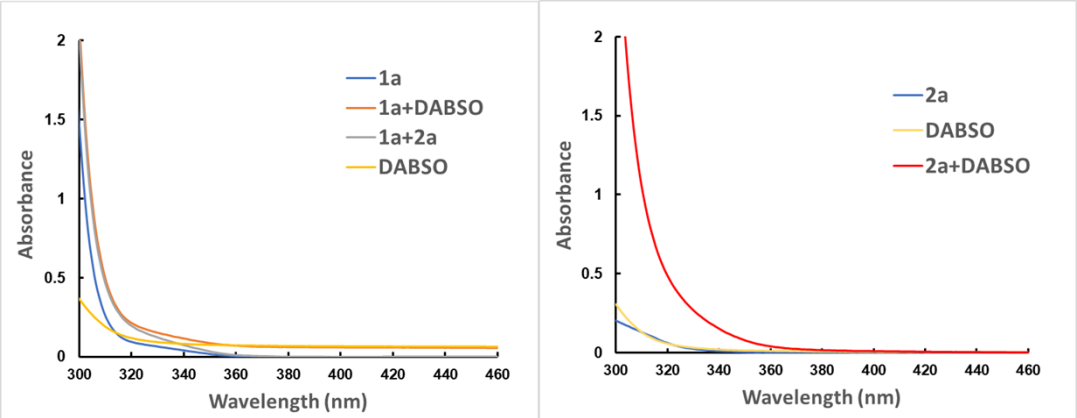


HRMS-ESI (m/z): calcd for $[C_{26}H_{20}DF_2NO_5S\text{-}K]^+$ [M-K] $^+$ 459.0271 found 459.0273.



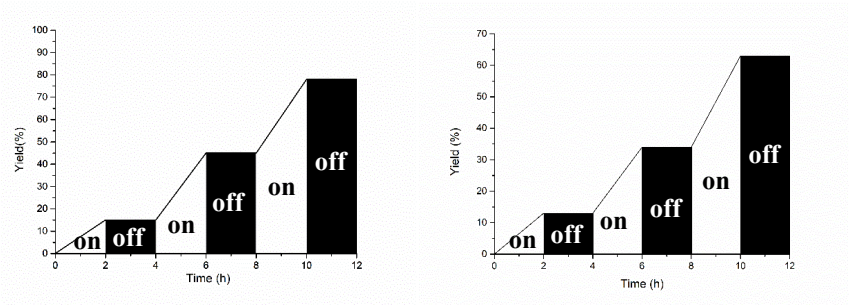
(3) UV-vis absorption spectra.

UV/vis absorption spectra between **1a** (0.01 M), **2a** (0.01 M) and DABCO·$(SO_2)_2$ (0.01 M) in 10 mL CH_3CN were recorded in 1 cm path quartz cuvettes using a Shimadzu UV-2550 UV-vis spectrophotometer.

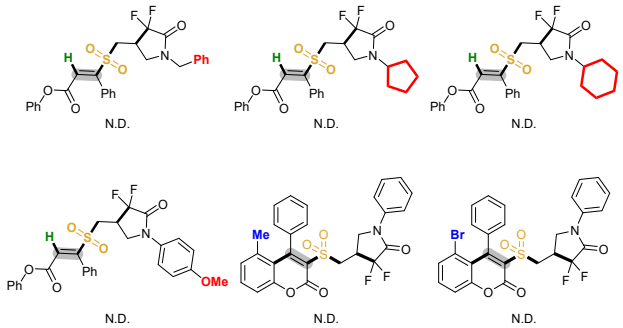


(4) On/off light experiments.

On/off experiments of model reaction in CH_3CN (left) and DMSO/H_2O (right).



(5) Results for other substrates.



6. References.

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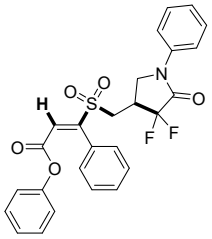
2. K. Sun, S. N. Wang, R. R. Feng, Y. X. Zhang, X. Wang, Z. G. Zhang, B. Zhang, *Org. Lett.*, **2019**, 21, 2052-2055.
3. X. Y. Gou, Y. Li, Y. Y. Luan, W. Y. Shi, Y. M. Liang, *ACS Catal*., **2021**, 11, 4263-427.
4. (a) P. G. Jessop, *Green Chem.*, 2011, **13**, 1391-1398. (b) S. U. Hong, Y. Wang, L. S. Soh and W. F. Yong, *Green Chem.*, 2023, **25**, 4501-4512. (c) J. Pawlas, B. Antonic, M. Lundqvist, T. Svensson, J. Finnman and J. H. Rasmussen, *Green Chem.*, 2019, **21**, 2594-2600.

7. Characterization data for the products.

(*E*)-phenyl-2-(((4,4-difluoro-5-oxo-1-phenylpyrrolidin-3-yl)methyl)sulfonyl)-3-phenylacrylate (3aa).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 230.3-233.1 ℃; 76% yield;

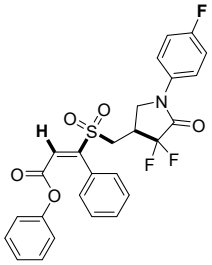
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.67 (d, J = 8.0 Hz, 2H), 7.63 – 7.50 (m, 5H), 7.48 (t, J = 7.8 Hz, 2H), 7.37 (t, J = 8.0 Hz, 2H), 7.34 (s, 1H), 7.29 (t, J = 7.4 Hz, 1H), 7.24 (t, J = 7.4 Hz, 1H), 6.92 (d, J = 8.2 Hz, 2H), 4.10 (t, J = 8.8 Hz, 1H), 3.94 (t, J = 7.8 Hz, 1H), 3.67 (dd, J = 14.8, 9.4 Hz, 1H), 3.61 – 3.52 (m, 2H).

^{13}C NMR (101 MHz, DMSO) δ 161.8, 160.5 (t, $J_{C\text{-}F}$= 32.2 Hz), 151.0, 149.6, 137.5, 130.3, 129.5, 129.4, 129.4, 129.2, 129.1, 128.6, 126.2, 126.1, 121.1, 120.2, 116.9 (t, $J_{C\text{-}F}$= 249.4 Hz), 47.4 (d, $J_{C\text{-}F}$= 5.9 Hz), 47.2 (d, $J_{C\text{-}F}$= 7.0 Hz), 33.2 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.73 (d, J = 262.9 Hz, 1F), -112.34 (d, J = 262.9 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{22}F_2NO_5S^+$ [M+H] $^+$ 498.1181, found 498.1178.

(*E*)-phenyl-2-(((4,4-difluoro-1-(4-fluorophenyl)-5-oxopyrrolidin-3-yl)methyl)sulfonyl)-3-phenyl-acrylate (3ab).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 168.1-169.7 ℃; 54% yield;

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.78 – 7.65 (m, 2H), 7.61 – 7.53 (m, 5H), 7.44 – 7.29 (m, 5H), 7.24 (t, J = 7.4 Hz, 1H), 6.92 (dd, J = 7.7, 1.6 Hz, 2H), 4.08 (t, J = 8.7 Hz, 1H), 3.93 (ddd, J = 9.7, 7.2, 2.1 Hz, 1H), 3.72 – 3.43 (m, 3H).

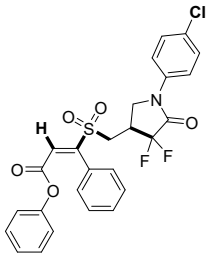
^{13}C NMR (101 MHz, DMSO) δ 161.8, 160.4 (t, $J_{C\text{-}F}$= 31.2 Hz), 158.5, 151.0, 149.5, 133.9 (d, $J_{C\text{-}F}$= 2.9 Hz), 130.3, 129.5, 129.4 (d, $J_{C\text{-}F}$= 5.6 Hz), 129.2, 128.6, 126.2, 122.6, 122.5, 121.1, 116.7 (t,

$J_{C\text{-}F}$= 252.5 Hz), 115.9 (d, $J_{C\text{-}F}$= 22.7 Hz), 47.7 (d, $J_{C\text{-}F}$= 5.0 Hz), 47.2 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.2 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.73 (d, J = 263.0 Hz, 1F), -112.26 (d, J = 263.1 Hz, 1F), -115.44(s, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{21}F_3NO_5S^+$ [M+H] $^+$ 516.1087, found 516.1081.

(*E*)-phenyl-2-(((1-(4-chlorophenyl)-4,4-difluoro-5-oxopyrrolidin-3-yl)methyl)sulfonyl)-3-phenyl-acrylate (3ac).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 179.0-180.7 ℃; 58% yield;

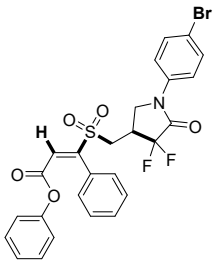
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.71 (d, J = 7.0 Hz, 2H), 7.60 – 7.52 (m, 7H), 7.37 (q, J = 7.0, 6.2 Hz, 3H), 7.24 (t, J = 7.4 Hz, 1H), 6.92 (d, J = 7.0 Hz, 2H), 4.09 (t, J = 8.6 Hz, 1H), 3.93 (t, J = 8.4 Hz, 1H), 3.73 – 3.44 (m, 3H).

^{13}C NMR (101 MHz, DMSO) δ 161.8, 160.5 (t, $J_{C\text{-}F}$= 31.2 Hz), 151.0, 149.5, 136.4, 130.3, 130.0, 129.5, 129.4, 129.4, 129.2, 129.0, 128.6, 126.2, 121.8, 121.1, 116.8 (t, $J_{C\text{-}F}$= 250.4 Hz), 47.4 (d, $J_{C\text{-}F}$= 5.0 Hz), 47.2 (d, $J_{C\text{-}F}$= 7.0 Hz), 33.1 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.77 (d, J = 263.2 Hz, 1F), -112.20 (d, J = 263.2 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{21}ClF_2NO_5S^+$ [M+H] $^+$ 532.0792, found 532.0788.

(*E*)-phenyl-2-(((1-(4-bromophenyl)-4,4-difluoro-5-oxopyrrolidin-3-yl)methyl)sulfonyl)-3-phenyl-acrylate (3ad).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 173.2-175.9 ℃; 67% yield;

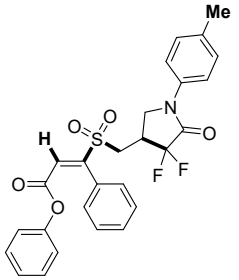
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.71 – 7.62 (m, 4H), 7.63 – 7.50 (m, 5H), 7.37 (dd, J = 15.4, 7.2 Hz, 3H), 7.24 (t, J = 7.4 Hz, 1H), 6.92 (d, J = 7.6 Hz, 2H), 4.10 (t, J = 9.0 Hz, 1H), 3.93 (t, J = 7.4 Hz, 1H), 3.78 – 3.46 (m, 3H).

^{13}C NMR (101 MHz, DMSO) δ 161.8, 160.6 (t, $J_{C\text{-}F}$= 32.2 Hz), 151.0, 149.5, 136.8, 131.9, 130.3, 129.5, 129.4, 129.4, 129.2, 128.6, 126.2, 122.1, 121.1, 118.3, 116.7 (t, $J_{C\text{-}F}$= 250.4 Hz), 47.3 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.2 (d, $J_{C\text{-}F}$= 7.0 Hz), 33.1 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.78 (d, J = 262.9 Hz, 1F), -112.19 (d, J = 262.9 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{21}BrF_2NO_5S^+$ [M+H] $^+$ 576.0286, found 576.0280.

(*E*)-phenyl-3-(((4,4-difluoro-5-oxo-1-(p-tolyl)pyrrolidin-3-yl)methyl)sulfonyl)-3-phenylacrylate (3ae).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 183.0-185.1 ℃; 61% yield;

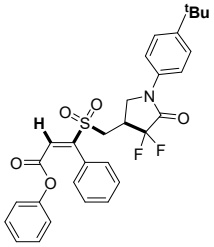
^{1}H NMR (600 MHz, DMSO-d_6) δ 7.6 (dd, J = 7.0, 2.7 Hz, 2H), 7.5 (d, J = 7.9 Hz, 5H), 7.4 (t, J = 8.0 Hz, 2H), 7.3 (s, 1H), 7.3 (d, J = 8.2 Hz, 2H), 7.2 (t, J = 7.4 Hz, 1H), 6.9 (d, J = 8.0 Hz, 2H), 4.1 (t, J = 9.2 Hz, 1H), 3.9 (t, J = 9.6 Hz, 1H), 3.7 (dd, J = 14.8, 9.3 Hz, 1H), 3.5 (dd, J = 14.9, 4.0 Hz, 2H), 2.3 (s, 3H).

^{13}C NMR (151 MHz, DMSO) δ 161.8, 160.4 (t, $J_{C\text{-}F}$= 31.2 Hz), 151.0, 149.6, 135.5, 135.1, 130.3, 129.5, 129.4, 129.4, 129.2, 128.6, 126.2, 121.1, 120.1, 117.0 (t, $J_{C\text{-}F}$= 249.5 Hz), 47.4 (d, $J_{C\text{-}F}$= 5.0 Hz), 47.3 (d, $J_{C\text{-}F}$= 6.8 Hz), 33.2 (t, $J_{C\text{-}F}$= 21.2 Hz), 20.4.

^{19}F NMR (565 MHz, DMSO-d_6) δ -107.64 (d, J = 262.8 Hz, 1F), -112.18 (d, J = 262.4 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{27}H_{24}F_2NO_5S^+$ [M+H] $^+$ 512.1338, found 512.1331.

(*E*)-phenyl-2-(((1-(4-(tert-butyl)phenyl)-4,4-difluoro-5-oxopyrrolidin-3-yl)methyl)sulfonyl)-3-phenylacrylate (3af).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 193.4-194.7 ℃; 59% yield;

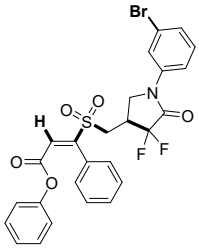
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.63 – 7.50 (m, 7H), 7.48 (d, J = 8.8 Hz, 2H), 7.40 – 7.32 (m, 3H), 7.27 – 7.21 (m, 1H), 6.92 (d, J = 7.4 Hz, 2H), 4.08 (t, J = 9.8 Hz, 1H), 3.91 (ddd, J = 9.0, 6.9, 1.9 Hz, 1H), 3.67 (dd, J = 14.8, 9.3 Hz, 1H), 3.55 (dd, J = 14.9, 4.0 Hz, 2H), 1.29 (s, 9H).

^{13}C NMR (101 MHz, DMSO) δ 161.7, 160.3 (t, $J_{C\text{-}F}$= 31.2 Hz), 151.0, 149.5, 148.7, 135.0, 130.2, 129.5, 129.4, 129.4, 129.2, 128.6, 126.2, 125.7, 121.1, 120.0, 116.9 (t, $J_{C\text{-}F}$= 249.4 Hz), 47.4 (d, $J_{C\text{-}F}$= 5.9 Hz), 47.3 (d, $J_{C\text{-}F}$= 7.0 Hz), 34.2, 33.3 (t, $J_{C\text{-}F}$= 20.2 Hz), 31.0.

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.69 (d, J = 262.9 Hz, 1F), -112.35 (d, J = 262.8 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{30}H_{30}F_2NO_5S^+$ [M+H] $^+$ 554.1807, found 554.1800.

(*E*)-phenyl-2-(((1-(3-bromophenyl)-4,4-difluoro-5-oxopyrrolidin-3-yl)methyl)sulfonyl)-3-phenyl-acrylate (3ag).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 160.7-164.3 ℃; 70% yield;

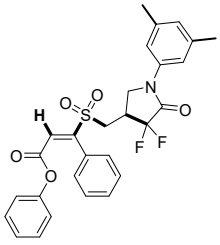
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.9 (s, 1H), 7.6 (d, J = 8.2 Hz, 1H), 7.6 – 7.5 (m, 6H), 7.4 (t, J = 8.1 Hz, 1H), 7.4 (t, J = 7.7 Hz, 2H), 7.3 (s, 1H), 7.2 (t, J = 7.5 Hz, 1H), 6.9 (d, J = 7.9 Hz, 2H), 4.1 (t, J = 9.3 Hz, 1H), 3.9 (t, J = 8.9 Hz, 1H), 3.7 – 3.4 (m, 3H).

^{13}C NMR (101 MHz, DMSO) δ 161.8, 160.8 (t, $J_{C\text{-}F}$= 33.2 Hz), 150.9, 149.6, 148.5, 139.0, 131.1, 130.3, 129.6, 129.5, 129.2, 128.9, 128.7, 126.3, 122.8, 121.7, 121.1, 119.1, 117.0 (t, $J_{C\text{-}F}$= 249.5 Hz), 47.4, 47.1, 33.2 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.9 (d, J = 263.2 Hz, 1F), -112.3 (d, J = 263.1 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{21}BrF_2NO_5S^+$ [M+H] $^+$ 576.0286, found 576.0280.

(*E*)-phenyl-2-(((1-(3,5-dimethylphenyl)-4,4-difluoro-5-oxopyrrolidin-3-yl)methyl)sulfonyl)-3-phenylacrylate (3ah).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 145.2-148.1 ℃; 74% yield;

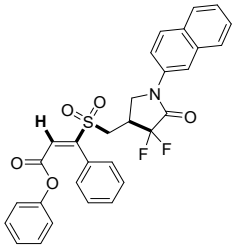
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.6 – 7.5 (m, 5H), 7.4 (t, J = 7.7 Hz, 2H), 7.3 (d, J = 3.6 Hz, 1H), 7.3 (s, 2H), 7.2 (t, J = 8.0 Hz, 1H), 6.9 (d, J = 8.4 Hz, 3H), 4.1 (t, J = 9.5 Hz, 1H), 3.9 (t, J = 8.9 Hz, 1H), 3.7 – 3.6 (m, 1H), 3.6 – 3.5 (m, 2H), 2.3 (s, 6H).

^{13}C NMR (101 MHz, DMSO) δ 161.8, 160.4 (t, $J_{C\text{-}F}$= 31.2 Hz), 151.0, 149.6, 147.1, 138.3, 137.5, 130.3, 129.6, 129.5, 129.3, 128.7, 127.6, 126.3, 121.2, 118.0, 117.0 (t, $J_{C\text{-}F}$= 254.5 Hz), 47.6 (d, $J_{C\text{-}F}$= 5.9 Hz), 47.2 (d, $J_{C\text{-}F}$= 7.0 Hz), 33.2 (t, $J_{C\text{-}F}$= 20.2 Hz), 21.0.

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.8 (d, J = 262.3 Hz, 1F), -112.4 (d, J = 262.5 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{28}H_{26}F_2NO_5S^+$ [M+H] $^+$ 526.1494, found 526.1488.

(*E*)-phenyl2-(((4,4-difluoro-1-(naphthalen-2-yl)-5-oxopyrrolidin-3-yl)methyl)sulfonyl)-3-phenyl-acrylate (3ai).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 167.3-169.0 ℃; 47% yield;

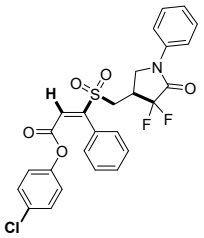
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.1 (s, 1H), 8.1 – 7.9 (m, 4H), 7.7 – 7.5 (m, 7H), 7.4 – 7.3 (m, 3H), 7.2 (t, J = 7.4 Hz, 1H), 6.9 (d, J = 7.9 Hz, 2H), 4.2 (t, J = 9.1 Hz, 1H), 4.1 (t, J = 8.8 Hz, 1H), 3.8 – 3.7 (m, 1H), 3.6 (d, J = 11.9 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 161.8, 160.7 (t, J_{C-F}= 31.2 Hz), 151.0, 149.6, 135.3, 133.9, 132.8, 130.9, 130.3, 129.6, 129.5, 129.3, 128.8, 128.7, 127.9, 127.5, 126.9, 126.3, 126.1, 121.2, 119.4, 117.7, 117.0 (t, J_{C-F}= 247.5 Hz), 47.7 (d, J_{C-F}= 6.1 Hz), 47.3 (d, J_{C-F}= 7.1 Hz), 33.3 (t, J_{C-F}= 19.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.7 (d, J = 262.9 Hz, 1F), -112.1 (d, J = 262.8 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{30}H_{24}F_2NO_5S^+$ [M+H] $^+$ 548.1338, found 548.1332.

(*E*)-4-chlorophenyl-2-(((4,4-difluoro-5-oxo-1-phenylpyrrolidin-3-yl)methyl)sulfonyl)-3-phenyl-acrylate (3ba).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 71.2-174.0 ℃; 61% yield;

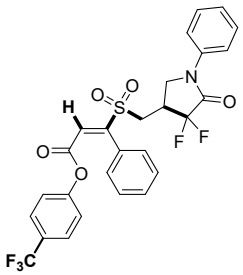
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.7 (d, J = 8.0 Hz, 2H), 7.6 – 7.5 (m, 5H), 7.5 – 7.4 (m, 4H), 7.3 (d, J = 6.3 Hz, 2H), 7.0 (d, J = 8.3 Hz, 2H), 4.1 (t, J = 9.1 Hz, 1H), 3.9 (t, J = 8.6 Hz, 1H), 3.7 (dd, J = 14.9, 9.4 Hz, 1H), 3.6 – 3.5 (m, 2H).

^{13}C NMR (101 MHz, DMSO) δ 161.6, 160.5 (t, J_{C-F}= 30.2 Hz), 151.3, 148.3, 137.6, 130.5, 130.4, 130.0, 129.5, 129.5, 129.2, 129.1, 128.7, 126.2, 123.1, 120.2, 116.9 (t, J_{C-F}= 248.5 Hz), 47.4 (d, J_{C-F}= 7.1 Hz), 47.2 (d, J_{C-F}= 6.0 Hz), 33.2 (t, J_{C-F}= 21.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.8 (d, J = 262.5 Hz, 1F), -112.3 (d, J = 262.8 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{21}ClF_2NO_5S^+$ [M+H] $^+$ 532.0792, found 532.0788.

(*E*)-4-(trifluoromethyl)phenyl-2-(((4,4-difluoro-5-oxo-1-phenylpyrrolidin-3-yl)methyl)sulfonyl)-3-phenylacrylate (3ca).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 273.8-276.3 ℃; 53% yield;

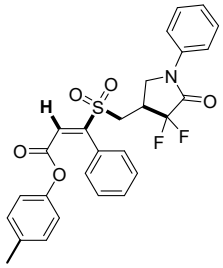
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (d, J = 8.3 Hz, 2H), 7.7 (d, J = 8.0 Hz, 2H), 7.6 – 7.5 (m, 5H), 7.5 (t, J = 7.8 Hz, 2H), 7.4 – 7.3 (m, 2H), 7.2 (d, J = 8.3 Hz, 2H), 4.1 (t, J = 9.2 Hz, 1H), 3.9 (t, J = 8.5 Hz, 1H), 3.7 (dd, J = 14.9, 9.5 Hz, 2H), 3.5 (d, J = 15.0 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 161.3, 160.5 (t, $J_{C\text{-}F}$= 30.2 Hz), 152.5, 151.6, 137.6, 130.4, 129.5, 129.1, 129.0, 128.7, 127.1, 127.1, 126.2, 122.3, 120.2, 116.9 (t, $J_{C\text{-}F}$= 257.5 Hz), 47.4 (d, $J_{C\text{-}F}$= 6.1 Hz), 47.2 (d, $J_{C\text{-}F}$= 7.1 Hz), 33.2 (t, $J_{C\text{-}F}$= 21.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -60.8 (s, 3F), -107.8 (d, J = 262.7 Hz, 1F), -112.3 (d, J = 262.7 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{27}H_{21}F_5NO_5S^+$ $[M+H]^+$ 566.1055, found 566.1051.

(*E*)-*p*-tolyl-2-(((4,4-difluoro-5-oxo-1-phenylpyrrolidin-3-yl)methyl)sulfonyl)-3-phenylacrylate (3da).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 251.9-254.5 ℃; 48% yield;

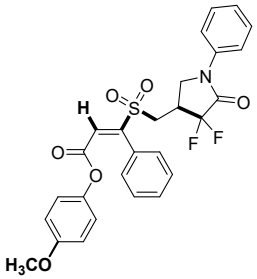
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.7 (d, J = 8.1 Hz, 2H), 7.6 (d, J = 8.3 Hz, 5H), 7.5 (t, J = 7.9 Hz, 2H), 7.3 (dd, J = 14.7, 5.4 Hz, 2H), 7.2 (d, J = 8.0 Hz, 2H), 6.8 (d, J = 8.3 Hz, 2H), 4.1 (t, J = 9.1 Hz, 1H), 3.9 (t, J = 8.6 Hz, 1H), 3.7 (dd, J = 14.9, 9.5 Hz, 1H), 3.5 (d, J = 14.9 Hz, 2H), 2.3 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 162.0, 160.5 (t, $J_{C\text{-}F}$= 31.2 Hz), 150.8, 147.4, 137.6, 135.6, 130.3, 129.9, 129.6, 129.5, 129.3, 129.1, 128.7, 126.2, 120.8, 120.2, 116.9 (t, $J_{C\text{-}F}$= 254.5 Hz), 47.4 (d, $J_{C\text{-}F}$= 5.6 Hz), 47.2 (d, $J_{C\text{-}F}$= 7.1 Hz), 33.2 (t, $J_{C\text{-}F}$= 20.2 Hz), 20.3.

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.8 (d, J = 262.3 Hz, 1F), -112.3 (d, J = 262.3 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{27}H_{24}F_2NO_5S^+$ [M+H] $^+$ 512.1338, found 512.1331.

(*E*)-4-methoxyphenyl-2-(((4,4-difluoro-5-oxo-1-phenylpyrrolidin-3-yl)methyl)sulfonyl)-3-phenyl-acrylate (3ea).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 179.7-181.1 ℃; 49% yield;

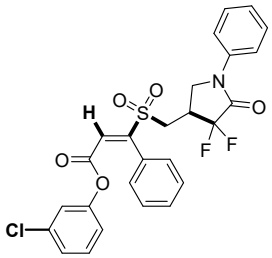
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.7 (d, J = 7.6 Hz, 2H), 7.6 – 7.5 (m, 5H), 7.5 (m, 2H), 7.3 – 7.3 (m, 2H), 6.9 (d, J = 9.2 Hz, 2H), 6.8 (d, J = 9.1 Hz, 2H), 4.1 (ddd, J = 9.9, 8.2, 1.8 Hz, 1H), 3.9 (td, J = 7.6, 3.8 Hz, 1H), 3.7 (s, 3H), 3.7 – 3.6 (m, 1H), 3.6 – 3.5 (m, 2H).

^{13}C NMR (101 MHz, DMSO) δ 162.2, 160.5 (t, $J_{C\text{-}F}$= 30.2 Hz), 157.1, 150.7, 142.9, 137.6, 130.3, 129.6, 129.5, 129.3, 129.1, 128.7, 126.2, 122.0, 120.2, 117.0 (t, $J_{C\text{-}F}$= 249.5 Hz), 114.5, 55.4, 47.4 (d, $J_{C\text{-}F}$= 6.6 Hz), 47.2 (d, $J_{C\text{-}F}$= 7.4 Hz), 33.2 (t, $J_{C\text{-}F}$= 21.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.8 (d, J = 262.8 Hz, 1F), -112.3 (d, J = 262.8 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{27}H_{24}F_2NO_6S^+$ [M+H] $^+$ 528.1287, found 528.1283.

(*E*)-3-chlorophenyl-2-(((4,4-difluoro-5-oxo-1-phenylpyrrolidin-3-yl)methyl)sulfonyl)-3-phenyl-acrylate (3fa).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). White solid; m.p.: 152.1-154.5 ℃; 60% yield;

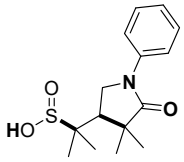
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.7 (d, J = 8.0 Hz, 2H), 7.6 – 7.5 (m, 5H), 7.5 (t, J = 7.7 Hz, 2H), 7.4 (t, J = 8.3 Hz, 1H), 7.4 – 7.2 (m, 3H), 7.1 (s, 1H), 6.9 (d, J = 8.1 Hz, 1H), 4.1 (t, J = 9.2 Hz, 1H), 3.9 (t, J = 8.6 Hz, 1H), 3.7 (dd, J = 14.9, 9.4 Hz, 1H), 3.6 (d, J = 14.8 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 161.5, 160.5 (t, $J_{C\text{-}F}$= 29.2 Hz), 151.5, 150.2, 137.6, 133.3, 131.1, 130.4, 129.5, 129.2, 129.1, 129.0, 128.7, 126.5, 126.2, 122.4, 121.6, 120.2, 116.9 (t, $J_{C\text{-}F}$= 249.5 Hz), 47.4 (d, $J_{C\text{-}F}$= 6.1 Hz), 47.2 (d, $J_{C\text{-}F}$= 7.1 Hz), 33.2 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.7 (d, J = 262.8 Hz, 1F), -112.3 (d, J = 262.4 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{21}ClF_2NO_5S^+$ [M+H] $^+$ 532.0792, found 532.0788.

4-(2-hydrosulfonylpropan-2-yl)-3,3-dimethyl-1-phenylpyrrolidin-2-one (3ap).



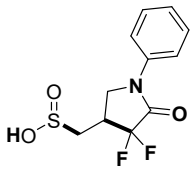
The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). Yellow solid; m.p.: 89.9-92.7 ℃; 35% yield;

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.7 – 7.7 (m, 2H), 7.4 (dd, J = 8.6, 7.3 Hz, 2H), 7.2 – 7.1 (m, 1H), 3.8 (t, J = 9.9 Hz, 1H), 3.7 (dd, J = 9.7, 7.9 Hz, 1H), 2.1 (dd, J = 10.2, 7.9 Hz, 1H), 1.3 (d, J = 6.2 Hz, 6H), 1.2 (s, 3H), 1.1 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 178.4, 139.8, 128.6, 123.8, 119.3, 69.7, 51.7, 46.3, 44.7, 30.3, 29.0, 26.5, 20.4.

HRMS-ESI (m/z): calcd for $C_{15}H_{22}NO_3S^+$ [M+H] $^+$ 296.1315, found 296.1310.

3,3-difluoro-4-(hydrosulfonylmethyl)-1-phenylpyrrolidin-2-one (3ma).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (12:1). Light yellow oil; 43% yield;

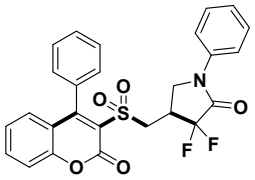
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.7 (dd, J = 8.7, 1.2 Hz, 2H), 7.6 – 7.4 (m, 2H), 7.4 – 7.3 (m, 1H), 4.7 (ddd, J = 15.2, 5.8, 4.5 Hz, 1H), 4.5 (dt, J = 15.6, 8.1 Hz, 1H), 4.1 (ddd, J = 10.3, 8.6, 2.0 Hz, 1H), 3.9 (ddd, J = 10.0, 7.7, 2.4 Hz, 1H), 3.7 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 160.5 (t, $J_{C\text{-}F}$= 30.2 Hz), 137.5, 129.2, 126.3, 120.3, 116.6 (t, $J_{C\text{-}F}$= 250.5 Hz), 46.9 (d, $J_{C\text{-}F}$= 6.3 Hz), 46.2 (dd, $J_{C\text{-}F}$= 16.8, 9.1 Hz), 34.2 (t, $J_{C\text{-}F}$= 19.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.6 (dd, J = 264.5, 3.4 Hz, 1F), -112.5 (dd, J = 264.5, 4.3 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{11}H_{12}F_2NO_3S^+$ [M+H] $^+$ 276.0500, found 276.0496.

3,3-difluoro-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)-1-phenylpyrrolidin-2-one (4aa).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 203.0-206.7 ℃; 90% yield;

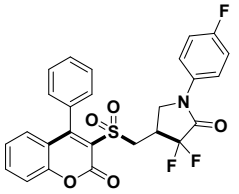
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (t, J = 7.0 Hz, 1H), 7.6 (d, J = 7.7 Hz, 3H), 7.6 – 7.4 (m, 5H), 7.4 – 7.3 (m, 3H), 7.3 (t, J = 7.4 Hz, 1H), 6.9 (d, J = 8.2 Hz, 1H), 4.2 (dd, J = 14.6, 4.2 Hz, 1H), 3.9 (t, J = 8.4 Hz, 1H), 3.9 – 3.8 (m, 2H), 3.7 – 3.5 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 160.6 (t, $J_{C\text{-}F}$= 30.3 Hz), 160.5, 156.5, 153.2, 137.5, 135.2, 132.2, 129.3, 129.1, 128.9, 128.0, 127.8, 127.6, 127.0, 126.2, 125.2, 123.2, 120.2, 120.2, 117.1 (t, $J_{C\text{-}F}$= 256.5 Hz), 116.7, 50.7 (d, $J_{C\text{-}F}$= 6.0 Hz), 47.6 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.6 (t, $J_{C\text{-}F}$= 21.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.3 (d, J = 261.8 Hz, 1F), -112.8 (d, J = 261.8 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{20}F_2NO_5S^+$ [M+H] $^+$ 496.1025, found 496.1020.

3,3-difluoro-1-(4-fluorophenyl)-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)pyroli-din-2-one (4ab).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 224.2-226.8 ℃; 60% yield;

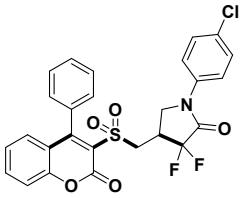
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (ddd, J = 8.6, 7.3, 1.6 Hz, 1H), 7.7 – 7.6 (m, 3H), 7.6 – 7.4 (m, 3H), 7.4 – 7.3 (m, 5H), 6.9 (dd, J = 8.1, 1.5 Hz, 1H), 4.2 (dd, J = 14.6, 4.2 Hz, 1H), 4.0 – 3.8 (m, 3H), 3.7 – 3.5 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 160.9, 160.5 (t, $J_{C\text{-}F}$= 29.3 Hz), 160.5, 158.5, 156.4, 153.2, 133.9 (d, $J_{C\text{-}F}$= 3.0 Hz), 133.7 (d, $J_{C\text{-}F}$= 311.1 Hz), 129.3, 128.8, 127.9, 127.8, 127.6, 127.0, 125.2, 123.2, 122.7 (d, $J_{C\text{-}F}$= 8.1 Hz), 120.1, 117.0 (t, $J_{C\text{-}F}$= 246.4 Hz), 116.6, 115.8 (d, $J_{C\text{-}F}$= 23.2 Hz), 50.7 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.9 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.6 (t, $J_{C\text{-}F}$= 21.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.3 (d, J = 261.9 Hz, 1F), -112.7 (d, J = 262.1 Hz, 1F), -115.4 (s, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{19}F_3NO_5S^+$ [M+H] $^+$ 514.0931, found 514.0928.

1-(4-chlorophenyl)-3,3-difluoro-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)pyrrolidin-2-one (4ac).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 261.7-263.8 ℃; 71% yield;

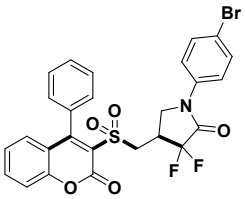
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (ddd, J = 8.6, 7.3, 1.6 Hz, 1H), 7.7 – 7.6 (m, 3H), 7.6 – 7.4 (m, 5H), 7.4 – 7.3 (m, 3H), 6.9 (dd, J = 8.2, 1.5 Hz, 1H), 4.2 (dd, J = 14.6, 4.2 Hz, 1H), 4.0 – 3.7 (m, 3H), 3.7 – 3.5 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 160.6 (t, $J_{C\text{-}F}$= 30.3 Hz), 160.5, 156.4, 153.2, 136.4, 135.2, 132.1, 130.0, 129.3, 129.0, 128.8, 127.9, 127.8, 127.6, 127.0, 125.2, 123.2, 121.8, 120.1, 117.1 (t, $J_{C\text{-}F}$= 255.4 Hz), 116.6, 50.6 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.5 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.4 (t, $J_{C\text{-}F}$= 21.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.3 (d, J = 262.3 Hz, 1F), -112.7 (d, J = 262.2 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{19}ClF_2NO_5S^+$ [M+H] $^+$ 530.0635, found 530.0633.

1-(4-bromophenyl)-3,3-difluoro-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)pyrrolidin-2-one (4ad).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 245.3-248.0 ℃; 78% yield;

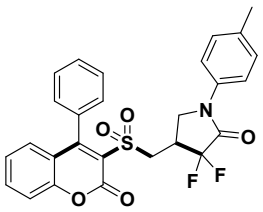
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (t, J = 7.0 Hz, 1H), 7.7 (d, J = 8.9 Hz, 2H), 7.6 (t, J = 7.9 Hz, 3H), 7.6 – 7.5 (m, 3H), 7.4 – 7.3 (m, 3H), 6.9 (dd, J = 8.1, 1.6 Hz, 1H), 4.2 (dd, J = 14.5, 4.1 Hz, 1H), 4.0 – 3.8 (m, 3H), 3.7 – 3.5 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 160.6 (t, $J_{C\text{-}F}$= 31.3 Hz), 160.5, 156.4, 153.2, 136.8, 135.2, 132.1, 131.9, 129.3, 128.8, 127.9, 127.8, 127.6, 127.0, 125.2, 123.2, 122.0, 120.1, 118.3, 117.0 (t, $J_{C\text{-}F}$= 250.4 Hz), 116.6, 50.6 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.4 (d, $J_{C\text{-}F}$= 5.0 Hz), 33.4 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.3 (d, J = 262.4 Hz, 1F), -112.7 (d, J = 262.3 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{19}BrF_2NO_5S^+$ [M+H] $^+$ 574.0130, found 574.0126.

3,3-difluoro-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)-1-(p-tolyl)pyrrolidin-2-one (4ae).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 205.1-206.7 ℃; 68% yield;

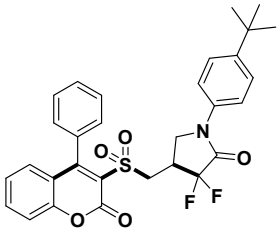
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (t, J = 7.9 Hz, 1H), 7.6 (d, J = 8.3 Hz, 1H), 7.5 (dd, J = 11.8, 6.4 Hz, 5H), 7.4 (d, J = 6.9 Hz, 3H), 7.3 (d, J = 8.1 Hz, 2H), 6.9 (d, J = 8.1 Hz, 1H), 4.2 (dd, J = 14.5, 3.9 Hz, 1H), 4.0 – 3.7 (m, 3H), 3.6 – 3.5 (m, 1H), 2.3 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 160.6, 160.4 (t, $J_{C\text{-}F}$= 31.3 Hz), 156.5, 153.2, 135.5, 135.3, 135.1, 132.2, 129.5, 129.3, 128.9, 128.0, 127.8, 127.7, 127.0, 125.3, 123.1, 120.2, 120.1, 117.2 (t, $J_{C\text{-}F}$= 256.4 Hz), 116.7, 50.6 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.6 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.5 (t, $J_{C\text{-}F}$= 21.2 Hz), 20.5.

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.3 (d, J = 261.6 Hz, 1F), -112.7 (d, J = 261.6 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{27}H_{22}F_2NO_5S^+$ [M+H] $^+$ 510.1181, found 510.1178.

1-(4-(tert-butyl)phenyl)-3,3-difluoro-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl) pyrrolidin-2-one (4af).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 230.3-232.3 ℃; 66% yield;

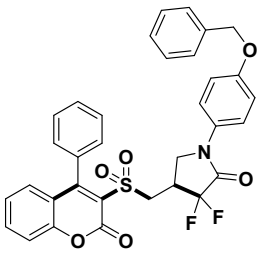
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (ddd, J = 8.7, 7.3, 1.6 Hz, 1H), 7.6 (dd, J = 8.4, 1.1 Hz, 1H), 7.6 – 7.5 (m, 7H), 7.4 – 7.3 (m, 3H), 6.9 (dd, J = 8.2, 1.5 Hz, 1H), 4.2 (dd, J = 14.5, 4.2 Hz, 1H), 3.9 (t, J = 9.3 Hz, 1H), 3.9 – 3.8 (m, 2H), 3.7 – 3.5 (m, 1H), 1.3 (s, 9H).

^{13}C NMR (101 MHz, DMSO) δ 160.5, 160.4 (t, $J_{C\text{-}F}$= 30.3 Hz), 156.4, 153.2, 148.7, 135.2, 135.0, 132.1, 129.3, 128.8, 127.9, 127.8, 127.6, 127.0, 125.7, 125.2, 123.2, 120.1, 120.0, 117.1 (t, $J_{C\text{-}F}$= 249.4 Hz), 116.6, 50.7 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.6 (d, $J_{C\text{-}F}$= 6.0 Hz), 34.2, 33.3 (t, $J_{C\text{-}F}$= 20.2 Hz), 31.0.

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.2 (d, J = 261.8 Hz, 1F), -112.7 (d, J = 262.1 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{30}H_{28}F_2NO_5S^+$ [M+H] $^+$ 552.1651, found 552.1647.

1-(4-(benzyloxy)phenyl)-3,3-difluoro-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl) pyrrolidin-2-one (4ag).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (10:1). White solid; m.p.: 200.1-202.0 ℃; 61% yield;

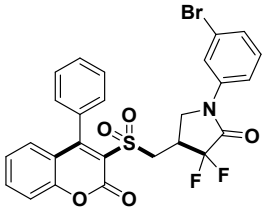
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (t, J = 7.8 Hz, 1H), 7.6 (d, J = 8.4 Hz, 1H), 7.5 (d, J = 7.5 Hz, 4H), 7.5 (d, J = 7.2 Hz, 3H), 7.4 – 7.3 (m, 6H), 7.1 (d, J = 8.5 Hz, 2H), 6.9 (d, J = 8.3 Hz, 1H), 5.1 (s, 2H), 4.2 – 4.0 (m, 1H), 3.9 – 3.7 (m, 2H), 3.6 – 3.4 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 160.6, 160.5 (t, $J_{C\text{-}F}$= 30.3 Hz), 156.5, 156.3, 153.2, 136.8, 135.3, 132.2, 130.7, 129.4, 128.9, 128.4, 128.0, 127.9, 127.8, 127.7, 127.7, 127.0, 125.2, 123.2, 122.1, 120.2, 117.3 (t, $J_{C\text{-}F}$= 251.4 Hz), 116.7, 115.2, 69.4, 50.7, 47.9, 33.6 (t, $J_{C\text{-}F}$= 21.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.2 (d, J = 261.6 Hz, 1F), -112.6 (d, J = 261.7 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{33}H_{26}F_2NO_6S^+$ [M+H] $^+$ 602.1443, found 602.1440.

1-(3-bromophenyl)-3,3-difluoro-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)pyrrolidin-2-one (4ah).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 265.7-268.2 ℃; 55% yield;

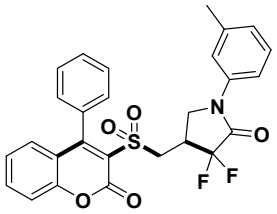
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.9 (s, 1H), 7.8 (t, J = 7.9 Hz, 1H), 7.6 (t, J = 8.2 Hz, 2H), 7.5 – 7.4 (m, 5H), 7.4 (d, J = 6.8 Hz, 3H), 6.9 (d, J = 8.1 Hz, 1H), 4.2 (dd, J = 14.6, 4.2 Hz, 1H), 3.9 (ddd, J = 33.2, 14.4, 9.3 Hz, 3H), 3.7 – 3.5 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 160.9 (t, $J_{C\text{-}F}$= 29.3 Hz), 160.6, 156.5, 153.2, 139.0, 135.3, 132.2, 131.1, 129.4, 128.9, 128.9, 128.0, 127.9, 127.7, 127.1, 125.3, 123.2, 122.8, 121.8, 120.2, 119.1, 117.0 (t, $J_{C\text{-}F}$= 258.4 Hz), 116.7, 50.6 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.5 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.5 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.4 (d, J = 262.3 Hz, 1F), -112.8 (d, J = 262.3 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{19}BrF_2NO_5S^+$ [M+H] $^+$ 574.0130, found 574.0126.

3,3-difluoro-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)-1-(*m*-tolyl)pyrrolidin-2-one (4ai).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (6:1). White solid; m.p.: 210.1-212.8 ℃; 68% yield;

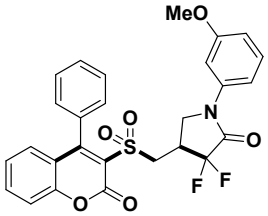
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (t, J = 7.9 Hz, 1H), 7.6 (d, J = 8.3 Hz, 1H), 7.5 (t, J = 4.2 Hz, 2H), 7.5 – 7.3 (m, 7H), 7.1 (d, J = 7.5 Hz, 1H), 6.9 (d, J = 8.1 Hz, 1H), 4.2 (dd, J = 14.6, 4.1 Hz, 1H), 4.0 – 3.7 (m, 3H), 3.7 – 3.5 (m, 1H), 2.3 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 160.6, 160.6 (t, $J_{C\text{-}F}$= 30.3 Hz), 156.5, 153.2, 138.6, 137.5, 135.3, 132.2, 129.4, 129.0, 128.9, 128.1, 127.8, 127.7, 127.0, 126.9, 125.3, 123.2, 120.7, 120.2, 117.5 (t, $J_{C\text{-}F}$= 256.4 Hz), 117.2, 116.7, 50.6 (d, $J_{C\text{-}F}$= 6.0 Hz), 47.7 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.6 (t, $J_{C\text{-}F}$= 21.2 Hz), 21.1.

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.4 (d, J = 261.6 Hz, 1F), -112.9 (d, J = 261.7 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{27}H_{22}F_2NO_5S^+$ [M+H] $^+$ 510.1181, found 510.1178.

3,3-difluoro-1-(3-methoxyphenyl)-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl) pyrrolidin-2-one (4aj).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 254.1-255.2 ℃; 86% yield;

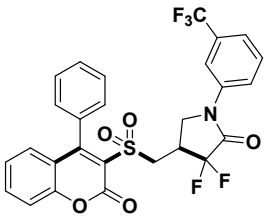
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (t, J = 7.9 Hz, 1H), 7.6 (d, J = 8.3 Hz, 1H), 7.5 – 7.4 (m, 3H), 7.3 (d, J = 7.7 Hz, 4H), 7.2 (s, 1H), 7.1 (d, J = 8.2 Hz, 1H), 6.9 (dd, J = 14.9, 8.3 Hz, 2H), 4.2 (dd, J = 14.8, 4.2 Hz, 1H), 3.9 – 3.8 (m, 3H), 3.7 (s, 3H), 3.6 – 3.4 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 160.7 (t, $J_{C\text{-}F}$= 31.3 Hz), 160.6, 159.6, 156.5, 153.2, 138.7, 135.3, 132.2, 130.0, 129.4, 128.9, 128.0, 127.8, 127.7, 127.1, 125.3, 123.2, 120.2, 117.1 (t, $J_{C\text{-}F}$= 256.4 Hz), 116.7, 112.3, 111.6, 106.4, 55.3, 50.6 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.7 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.5 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.3 (d, J = 261.8 Hz, 1F), -112.8 (d, J = 261.7 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{27}H_{22}F_2NO_6S^+$ [M+H] $^+$ 526.1130, found 526.1125.

3,3-difluoro-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)-1-(3-(trifluoromethyl) phenyl)pyrrolidin-2-one (4ak).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 232.8-236.7 ℃; 62% yield;

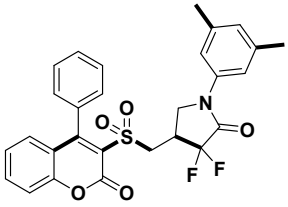
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.0 (s, 1H), 7.9 – 7.8 (m, 2H), 7.7 (t, J = 8.0 Hz, 1H), 7.7 (d, J = 7.8 Hz, 1H), 7.6 (dd, J = 8.4, 1.1 Hz, 1H), 7.6 – 7.5 (m, 2H), 7.5 – 7.4 (m, 1H), 7.4 – 7.3 (m, 3H), 6.9 (dd, J = 8.1, 1.5 Hz, 1H), 4.2 (dd, J = 14.6, 4.3 Hz, 1H), 4.0 – 3.9 (m, 2H), 3.8 (dd, J = 14.6, 9.4 Hz, 1H), 3.7 – 3.5 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 161.1 (t, $J_{C\text{-}F}$= 30.3 Hz), 160.6, 156.5, 153.2, 138.2, 135.3, 132.2, 130.5, 129.5 (q, $J_{C\text{-}F}$= 32.3 Hz), 129.4, 128.9, 128.0, 127.8, 127.6, 127.1, 125.3, 125.2, 124.0, 123.2, 122.6 (q, $J_{C\text{-}F}$= 4.0 Hz), 122.4, 120.2, 117.0 (t, $J_{C\text{-}F}$= 246.4 Hz), 116.7 (q, $J_{C\text{-}F}$= 4.0 Hz), 50.6(d, $J_{C\text{-}F}$= 7.0 Hz), 47.6(d, $J_{C\text{-}F}$= 6.0 Hz), 33.6 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -61.3 (s, 3F), -108.4 (d, J = 262.3 Hz, 1F), -112.8 (d, J = 262.6 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{27}H_{19}F_5NO_5S^+$ [M+H] $^+$ 564.0899, found 564.0893.

1-(3,5-dimethylphenyl)-3,3-difluoro-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl) pyrrolidin-2-one (4al).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 198.9-201.6 ℃; 87% yield;

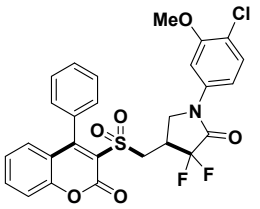
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (t, J = 7.8 Hz, 1H), 7.6 (d, J = 8.2 Hz, 1H), 7.5 (t, J = 4.2 Hz, 2H), 7.5 (d, J = 6.3 Hz, 1H), 7.4 (dd, J = 7.5, 4.4 Hz, 3H), 7.2 (s, 2H), 7.0 – 6.9 (m, 2H), 4.2 (dd, J = 14.6, 4.2 Hz, 1H), 3.9 (t, J = 9.4 Hz, 1H), 3.8 – 3.7 (m, 3H), 2.3 (s, 6H).

^{13}C NMR (101 MHz, DMSO) δ 161.1, 160.8 (t, $J_{C\text{-}F}$= 30.3 Hz), 156.9, 153.5, 138.7, 137.7, 135.7, 132.4, 129.7, 129.3, 128.3, 128.2, 128.1, 128.0, 127.3, 125.6, 123.3, 120.4, 118.3, 117.5 (t, $J_{C\text{-}F}$= 251.4 Hz), 117.0, 50.9 (d, $J_{C\text{-}F}$= 7.0 Hz), 48.0 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.7 (t, $J_{C\text{-}F}$= 20.2 Hz), 21.3.

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.3 (d, J = 261.6 Hz, 1F), -112.9 (d, J = 261.6 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{28}H_{24}F_2NO_5S^+$ [M+H] $^+$ 524.1338, found 524.1334.

1-(4-chloro-3-methoxyphenyl)-3,3-difluoro-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl) methyl)pyrrolidin-2-one (4am).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 281.2-283.0 ℃; 64% yield;

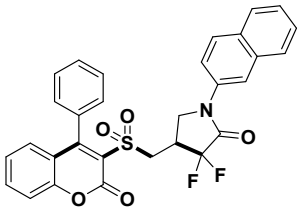
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.6 (ddd, *J* = 8.6, 7.2, 1.6 Hz, 1H), 7.5 (d, *J* = 2.5 Hz, 1H), 7.5 – 7.4 (m, 3H), 7.4 (d, *J* = 8.4 Hz, 1H), 7.3 (dd, *J* = 8.1, 4.3 Hz, 2H), 7.2 – 7.2 (m, 2H), 7.0 (dd, *J* = 8.2, 1.6 Hz, 1H), 6.8 (dd, *J* = 8.6, 2.5 Hz, 1H), 4.0 (t, *J* = 3.3 Hz,, 1H), 4.0 (dd, *J* = 14.0, 3.3 Hz, 1H), 3.8 (s, 3H), 3.8 – 3.7 (m, 2H), 3.3 – 3.1 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.4, 160.8 (t, $J_{C\text{-}F}$= 30.3 Hz), 156.7, 155.2, 153.7, 137.1, 135.6, 131.4, 130.1, 130.1, 129.7, 128.3, 128.1, 128.0, 127.0, 125.4, 123.7, 120.1, 119.7, 117.1, 116.4 (t, $J_{C\text{-}F}$= 251.4 Hz), 111.8, 104.7, 56.3, 51.8 (d, $J_{C\text{-}F}$= 7.0 Hz), 48.0 (d, $J_{C\text{-}F}$= 6.0 Hz), 34.5 (t, $J_{C\text{-}F}$= 21.2 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -109.9 (d, *J* = 266.4 Hz, 1F), -114.5 (d, *J* = 266.4 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{27}H_{21}ClF_2NO_6S^+$ $[M+H]^+$ 560.0741, found 560.0738.

3,3-difluoro-1-(naphthalen-2-yl)-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl) pyrrolidin-2-one (4an).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 259.6-261.4 ℃; 47% yield;

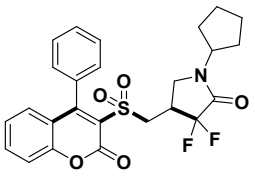
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.0 (d, *J* = 7.2 Hz, 2H), 8.0 (t, *J* = 8.4 Hz, 2H), 7.9 (d, *J* = 9.2 Hz, 1H), 7.8 (t, *J* = 7.9 Hz, 1H), 7.6 (d, *J* = 8.4 Hz, 1H), 7.5 (dd, *J* = 15.4, 7.2 Hz, 4H), 7.5 (d, *J* = 4.1 Hz, 1H), 7.4 (t, *J* = 6.7 Hz, 2H), 6.9 (d, *J* = 8.1 Hz, 2H), 4.2 (dd, *J* = 14.5, 4.0 Hz, 1H), 4.1 (t, *J* = 9.4 Hz, 1H), 4.0 (t, *J* = 9.0 Hz, 1H), 3.9 (dd, *J* = 14.5, 9.6 Hz, 1H), 3.7 – 3.6 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 161.1, 160.6, 156.5, 153.2, 135.3, 135.3, 132.8, 132.2, 130.9, 129.4, 128.9, 128.9, 128.0, 127.9, 127.8, 127.7, 127.6, 127.1, 127.0, 126.2, 125.3, 123.2, 120.2, 119.4, 117.8, 117.3 (t, $J_{C\text{-}F}$= 258.4 Hz), 116.7, 50.6, 47.9, 33.4 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.2 (d, *J* = 261.8 Hz, 1F), -112.6 (d, *J* = 261.8 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{30}H_{22}F_2NO_5S^+$ $[M+H]^+$ 546.1181, found 546.1177.

1-cyclopentyl-3,3-difluoro-4-(((2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)pyrrolidin-2-one (4ao).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 192.1-193.4 ℃; 51% yield;

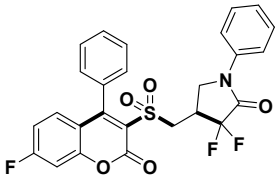
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (t, J = 7.8 Hz, 1H), 7.6 (d, J = 8.3 Hz, 1H), 7.5 (d, J = 4.6 Hz, 3H), 7.4 (t, J = 6.7 Hz, 3H), 6.9 (d, J = 8.1 Hz, 1H), 4.3 (t, J = 7.5 Hz, 1H), 4.1 (d, J = 14.4 Hz, 1H), 3.7 (dd, J = 14.6, 9.2 Hz, 1H), 3.4 (d, J = 7.7 Hz, 2H), 3.3 (d, J = 6.9 Hz, 1H), 1.9 – 1.7 (m, 2H), 1.7 – 1.4 (m, 6H).

^{13}C NMR (101 MHz, DMSO) δ 161.1 (t, $J_{C\text{-}F}$= 30.3 Hz), 160.7, 156.5, 153.2, 135.2, 132.3, 129.4, 128.8, 128.1, 127.8, 127.5, 126.8, 125.2, 122.9, 120.3, 117.7 (t, $J_{C\text{-}F}$= 255.4 Hz), 116.7, 52.7, 50.5, (d, $J_{C\text{-}F}$= 7.0 Hz), 42.7 (d, $J_{C\text{-}F}$= 7.0 Hz), 34.0 (t, $J_{C\text{-}F}$= 21.2 Hz), 28.4, 28.3, 24.2, 24.1.

^{19}F NMR (376 MHz, DMSO-d_6) δ -110.1 (d, J = 260.7 Hz, 1F), -113.5 (d, J = 260.3 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{25}H_{24}F_2NO_5S^+$ [M+H] $^+$ 488.1338, found 488.1335.

3,3-difluoro-4-(((7-fluoro-2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)-1-phenylpyrrolidin-2-one (4ba).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1). White solid; m.p.: 293.7-297.0 ℃; 52% yield;

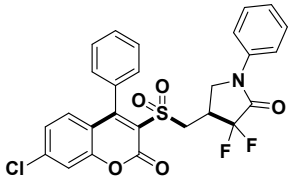
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.7 (d, J = 8.0 Hz, 1H), 7.6 (s, 1H), 7.5 (t, J = 7.6 Hz, 1H), 7.3 – 7.3 (m, 1H), 7.2 (t, J = 8.8 Hz, 1H), 7.0 – 6.9 (m, 1H), 4.1 (t, J = 8.9 Hz, 1H), 3.9 (t, J = 8.4 Hz, 1H), 3.7 (dd, J = 14.8, 9.4 Hz, 1H), 3.5 (d, J = 14.2 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 162.3, 161.5, 151.6, 146.1 (d, $J_{C\text{-}F}$= 2.0 Hz), 139.9, 138.0, 130.8, 129.9, 129.7, 129.7, 129.6, 129.2, 126.6, 123.6, 123.5, 120.7, 117.4 (t, $J_{C\text{-}F}$= 255.5 Hz), 116.9, 116.6, 47.9, 47.6, 33.9 (t, $J_{C\text{-}F}$= 21.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.8 (d, J = 263.0 Hz, 1F), -112.3 (d, J = 262.6 Hz, 1F), -116.4 (s, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{19}F_3NO_5S^+$ [M+H] $^+$ 514.0931, found 514.0928.

4-(((7-chloro-2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)-3,3-difluoro-1-phenylpyrrolidin-2-one (4ca).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 259.1-261.3 ℃; 65% yield;

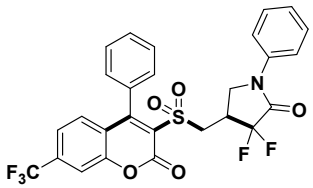
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.9 (s, 1H), 7.6 (d, J = 8.1 Hz, 2H), 7.6 – 7.4 (m, 6H), 7.4 (s, 2H), 7.3 (t, J = 7.5 Hz, 1H), 6.9 (d, J = 8.7 Hz, 1H), 4.2 (dd, J = 14.5, 4.1 Hz, 1H), 3.9 (ddd, J = 23.0, 14.9, 9.6 Hz, 3H), 3.7 – 3.4 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 160.6 (t, $J_{C\text{-}F}$= 31.3 Hz), 159.9, 156.2, 153.5, 139.6, 137.5, 131.9, 130.7, 129.1, 129.0, 128.0, 127.9, 127.8, 127.0, 126.2, 125.6, 123.3, 120.2, 119.4, 117.1 (t, $J_{C\text{-}F}$= 256.5 Hz), 116.8, 50.7 (d, $J_{C\text{-}F}$= 6.0 Hz), 47.6 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.5 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.2 (d, J = 262.0 Hz, 1F), -112.8 (d, J = 261.8 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{19}ClF_2NO_5S^+$ [M+H] $^+$ 530.0635, found 530.0633.

3,3-difluoro-4-(((2-oxo-4-phenyl-7-(trifluoromethyl)-2*H*-chromen-3-yl)sulfonyl)methyl)-1-phenylpyrrolidin-2-one (4da).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 203.7-206.4 ℃; 69% yield;

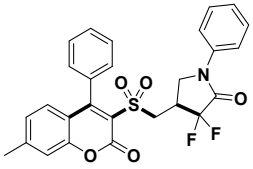
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.1 (s, 1H), 7.7 (d, J = 8.6 Hz, 1H), 7.6 (d, J = 8.1 Hz, 2H), 7.6 – 7.4 (m, 5H), 7.4 (d, J = 7.7 Hz, 2H), 7.3 (t, J = 7.5 Hz, 1H), 7.1 (d, J = 8.4 Hz, 1H), 4.2 (dd, J = 14.7, 4.1 Hz, 1H), 4.0 – 3.8 (m, 3H), 3.7 – 3.5 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 160.6 (t, $J_{C\text{-}F}$= 29.3 Hz), 159.2, 156.1, 153.0, 137.5, 133.8 (q, $J_{C\text{-}F}$= 33.3 Hz), 131.7, 130.7, 129.2, 129.1, 128.1, 128.0, 127.9, 127.1, 126.2, 125.4, 124.4, 123.6, 121.4, 120.2, 117.1 (t, $J_{C\text{-}F}$= 241.5 Hz), 114.2, 50.7 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.5 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.5 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -61.6 (s, 3F), -108.2 (d, J = 262.2 Hz, 1F), -112.8 (d, J = 261.9 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{27}H_{19}F_5NO_5S^+$ [M+H] $^+$ 564.0899, found 564.0893.

3,3-difluoro-4-(((7-methyl-2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)-1-phenylpyrrolidin-2-one (4ea).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 261.4-261.7 ℃; 87% yield;

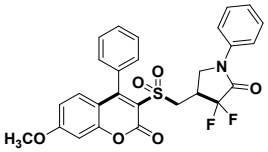
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.6 (d, J = 8.1 Hz, 2H), 7.5 – 7.4 (m, 6H), 7.3 (d, J = 6.7 Hz, 2H), 7.3 (t, J = 7.5 Hz, 1H), 7.2 (d, J = 8.4 Hz, 1H), 6.8 (d, J = 8.3 Hz, 1H), 4.2 (dd, J = 14.5, 3.9 Hz, 1H), 3.9 (ddd, J = 29.6, 21.5, 12.3 Hz, 3H), 3.7 – 3.4 (m, 1H), 2.4 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ160.6, 160.6 (t, $J_{C\text{-}F}$= 31.3 Hz), 156.7, 153.3, 147.0, 137.6, 132.3, 129.1, 129.1, 128.8, 128.0, 127.8, 127.6, 127.0, 126.4, 126.2, 121.9, 120.2, 117.8, 117.2 (t, $J_{C\text{-}F}$= 252.5 Hz), 116.6, 50.6 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.6 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.6 (t, $J_{C\text{-}F}$= 20.2 Hz), 21.3.

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.3 (d, J = 261.9 Hz, 1F), -112.8 (d, J = 261.8 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{27}H_{22}F_2NO_5S^+$ [M+H] $^+$ 510.1181, found 510.1178.

3,3-difluoro-4-(((7-methoxy-2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)-1-phenylpyrrolidin-2-one (4fa).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 248.3-251.8 ℃; 80% yield;

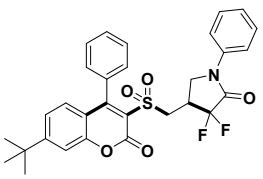
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.6 (d, J = 7.4 Hz, 1H), 7.5 (m, 5H), 7.4 – 7.3 (m, 2H), 7.3 (t, J = 7.4 Hz, 1H), 7.2 (d, J = 2.5 Hz, 1H), 7.0 (dd, J = 9.1, 2.5 Hz, 1H), 6.8 (d, J = 9.1 Hz, 1H), 4.2 (dd, J = 14.5, 4.2 Hz, 1H), 3.9 (s, 3H), 3.9 – 3.7 (m, 2H), 3.6 – 3.4 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 165.2, 160.8, 160.6 (t, $J_{C\text{-}F}$= 30.3 Hz), 156.9, 155.6, 137.6, 132.6, 130.7, 129.1, 128.8, 127.9, 127.8, 127.6, 127.0, 126.1, 120.2, 119.4, 117.2 (t, $J_{C\text{-}F}$= 249.5 Hz), 113.8, 113.5, 100.6, 56.5, 50.4 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.6 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.7 (t, $J_{C\text{-}F}$= 21.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.4 (d, J = 261.8 Hz, 1F), -112.8 (d, J = 261.9 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{27}H_{22}F_2NO_6S^+$ [M+H] $^+$ 526.1130, found 526.1125.

4-(((7-(tert-butyl)-2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)-3,3-difluoro-1-phenylpyrrolidin-2-one (4ga).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 263.8-265.3 ℃; 88% yield;

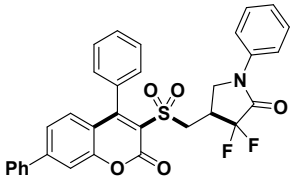
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.6 (d, J = 8.5 Hz, 3H), 7.5 – 7.4 (m, 6H), 7.4 (d, J = 7.6 Hz, 2H), 7.3 (t, J = 7.4 Hz, 1H), 6.8 (d, J = 8.5 Hz, 1H), 4.2 (dd, J = 14.6, 4.0 Hz, 1H), 3.8 (ddd, J = 34.4, 14.9, 9.3 Hz, 3H), 3.7 – 3.4 (m, 1H), 1.3 (s, 9H).

^{13}C NMR (101 MHz, DMSO) δ 160.6, 160.6 (t, J_{C-F}= 30.3 Hz), 159.6, 156.7, 153.3, 137.6, 132.4, 129.1, 129.0, 128.8, 128.0, 127.8, 127.6, 126.9, 126.1, 122.8, 122.0, 120.2, 117.8, 117.1 (t, J_{C-F}= 253.5 Hz), 113.4, 50.5 (d, J_{C-F}= 7.0 Hz), 47.6 (d, J_{C-F}= 6.0 Hz), 35.3, 33.7 (t, J_{C-F}= 21.2 Hz), 30.5.

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.4 (d, J = 261.7 Hz, 1F), -112.9 (d, J = 261.8 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{30}H_{28}F_2NO_5S^+$ [M+H] $^+$ 552.1651, found 552.1647.

3,3-difluoro-4-(((2-oxo-4,7-diphenyl-2*H*-chromen-3-yl)sulfonyl)methyl)-1-phenylpyrrolidin-2-one (4ha).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 305.2-306.7 ℃; 51% yield;

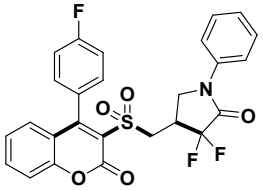
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.0 (s, 1H), 7.8 (d, J = 7.4 Hz, 2H), 7.7 (d, J = 8.6 Hz, 1H), 7.6 (d, J = 8.1 Hz, 2H), 7.6 – 7.4 (m, 8H), 7.4 (d, J = 6.8 Hz, 2H), 7.3 (t, J = 7.5 Hz, 1H), 7.0 (d, J = 8.4 Hz, 1H), 4.2 (dd, J = 14.6, 4.0 Hz, 1H), 3.9 (ddd, J = 24.5, 16.1, 9.4 Hz, 3H), 3.7 – 3.5 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 160.6 (t, J_{C-F}= 30.3 Hz), 160.4, 156.7, 153.8, 146.7, 137.6, 137.4, 132.3, 129.9, 129.4, 129.2, 129.1, 128.9, 128.0, 127.9, 127.7, 127.3, 127.0, 126.2, 123.5, 122.5, 120.2, 119.2, 117.1 (t, J_{C-F}= 253.5 Hz), 114.1, 50.6 (d, J_{C-F}= 7.0 Hz), 47.6 (d, J_{C-F}= 6.0 Hz), 33.6 (t, J_{C-F}= 21.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.3 (d, J = 262.0 Hz, 1F), -112.8 (d, J = 261.9 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{32}H_{24}F_2NO_5S^+$ [M+H] $^+$ 572.1338, found 572.1338.

3,3-difluoro-4-(((4-(4-fluorophenyl)-2-oxo-2*H*-chromen-3-yl)sulfonyl)methyl)-1-phenylpyrrolidin-2-one (4ia).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (6:1). White solid; m.p.: 188.1-190.6 ℃; 66% yield;

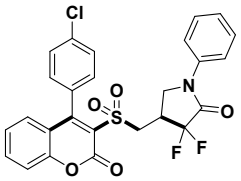
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (t, J = 7.9 Hz, 1H), 7.6 (d, J = 8.1 Hz, 3H), 7.5 – 7.2 (m, 8H), 7.0 (d, J = 8.1 Hz, 1H), 4.2 (dd, J = 14.6, 4.1 Hz, 1H), 3.9 (ddd, J = 21.4, 17.2, 9.9 Hz, 3H), 3.7 – 3.4 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 163.6, 161.2, 160.6 (t, $J_{C\text{-}F}$= 30.2 Hz), 159.8, 156.5, 153.2, 137.6, 135.3, 130.4 (d, $J_{C\text{-}F}$ = 8.6 Hz), 129.5 (d, $J_{C\text{-}F}$ = 8.3 Hz), 129.4, 129.3, 129.1, 128.4 (d, $J_{C\text{-}F}$ = 3.2 Hz), 126.2, 125.3, 123.6, 120.2, 120.2, 117.2 (t, $J_{C\text{-}F}$= 249.5 Hz), 116.7, 115.0 (dd, $J_{C\text{-}F}$= 22.0, 11.9 Hz), 50.6 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.6 (d, $J_{C\text{-}F}$ = 6.3 Hz), 33.5 (t, $J_{C\text{-}F}$= 21.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.1 (d, J = 262.0 Hz, 1F), -112.7 (d, J = 261.7 Hz, 1F), -112.8(s, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{19}F_3NO_5S^+$ [M+H] $^+$ 514.0931, found 514.0928.

4-(((4-(4-chlorophenyl)-2-oxo-2*H*-chromen-3-yl)sulfonyl)methyl)-3,3-difluoro-1-phenylpyrrolidin-2-one (4ja).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (6:1). White solid; m.p.: 297.3-299.9 ℃; 65% yield;

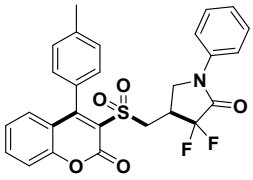
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.8 (t, J = 7.9 Hz, 1H), 7.6 (d, J = 7.9 Hz, 4H), 7.5 (d, J = 8.4 Hz, 1H), 7.5 (t, J = 7.8 Hz, 2H), 7.4 (d, J = 8.1 Hz, 2H), 7.4 (d, J = 7.7 Hz, 1H), 7.3 (t, J = 7.5 Hz, 1H), 7.0 (d, J = 8.1 Hz, 1H), 4.2 (dd, J = 14.6, 4.2 Hz, 1H), 4.0 – 3.8 (m, 3H), 3.7 – 3.5 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 160.6 (t, $J_{C\text{-}F}$= 30.2 Hz), 159.5, 156.4, 153.2, 137.5, 135.4, 133.8, 131.1, 130.0, 129.3, 129.1, 129.1, 128.0, 127.9, 126.2, 125.4, 123.5, 120.2, 120.0, 117.1 (t, $J_{C\text{-}F}$= 253.5 Hz), 116.7, 50.6 (d, $J_{C\text{-}F}$= 7.1 Hz), 47.6 (d, $J_{C\text{-}F}$= 6.0 Hz), 33.5 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.1 (d, J = 261.6 Hz, 1F), -112.7 (d, J = 261.9 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{19}ClF_2NO_5S^+$ [M+H] $^+$ 530.0635, found 530.0633.

3,3-difluoro-4-(((2-oxo-4-(p-tolyl)-2*H*-chromen-3-yl)sulfonyl)methyl)-1-phenylpyrrolidin-2-one (4ka).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 210.2-212.7 ℃; 48% yield;

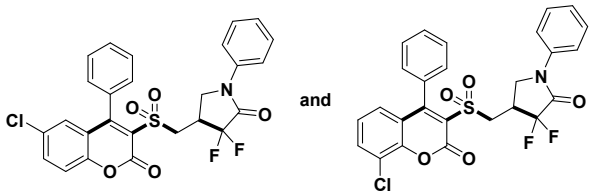
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.6 (d, J = 8.0 Hz, 2H), 7.5 (dd, J = 15.6, 6.7 Hz, 6H), 7.3 (d, J = 6.7 Hz, 2H), 7.3 (t, J = 7.5 Hz, 1H), 7.2 (d, J = 8.4 Hz, 1H), 6.8 (d, J = 8.2 Hz, 1H), 4.2 (dd, J = 14.6, 4.1 Hz, 1H), 3.9 (t, J = 9.4 Hz, 1H), 3.8 (dd, J = 14.4, 9.0 Hz, 1H), 3.8 (d, J = 10.3 Hz, 1H), 3.6 – 3.4 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 161.4, 161.1, 157.2, 153.8, 147.5, 138.1, 132.8, 129.6, 129.6, 129.3, 128.3 (t, $J_{C\text{-}F}$= 19.2 Hz), 127.5, 126.9, 126.7, 122.4, 120.7, 118.3, 117.7 (t, $J_{C\text{-}F}$= 246.4 Hz), 117.1, 51.0 (d, $J_{C\text{-}F}$= 7.0 Hz), 48.1 (d, $J_{C\text{-}F}$= 6.3 Hz), 34.1 (t, $J_{C\text{-}F}$= 20.2 Hz), 21.8.

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.3 (d, J = 261.6 Hz, 1F), -112.8 (d, J = 261.9 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{27}H_{22}F_2NO_5S^+$ [M+H] $^+$ 510.1181, found 510.1178.

4-(((6-chloro-2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)-3,3-difluoro-1-phenylpyrrolidin-2-one (4la) and 4-(((8-chloro-2-oxo-4-phenyl-2*H*-chromen-3-yl)sulfonyl)methyl)-3,3-difluoro-1-phenylpyrrolidin-2-one (4l'a).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (8:1). White solid; m.p.: 211.9-213.4 ℃; 75% yield;

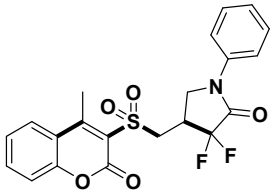
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.0 (d, J = 8.0 Hz, 0.27H), 7.9 (d, J = 9.0 Hz, 0.73H), 7.7 (d, J = 8.9 Hz, 1H), 7.6 (d, J = 8.1 Hz, 2H), 7.6 – 7.4 (m, 5H), 7.4 (d, J = 6.7 Hz, 2H), 7.3 (t, J = 7.5 Hz, 1H), 6.9 (d, J = 8.2 Hz, 0.27H), 6.8 (d, J = 2.4 Hz, 0.73H), 4.2 (dd, J = 14.8, 4.5 Hz, 1H), 4.0 – 3.8 (m, 3H), 3.7 – 3.5 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 160.6 (t, $J_{C\text{-}F}$= 31.3 Hz), 160.2, 159.2, 156.2, 155.8, 151.9, 148.7, 137.5, 134.8, 134.7, 132.0, 131.6, 129.2, 129.1, 129.1, 129.0, 128.4, 128.0, 127.9, 127.7, 127.1, 127.0, 126.2, 125.5, 124.4, 124.0, 122.0, 121.8, 120.2, 119.0, 117.1 (t, $J_{C\text{-}F}$= 253.5 Hz), 50.7 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.6 (d, $J_{C\text{-}F}$= 5.0 Hz), 33.5 (t, $J_{C\text{-}F}$= 20.2 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -108.2 (d, J = 261.6 Hz, 1F), -112.8 (d, J = 261.9 Hz, 1F).

HRMS-ESI (m/z): calcd for $C_{26}H_{19}ClF_2NO_5S^+$ [M+H] $^+$ 530.0635, found 530.0633.

3,3-difluoro-4-(((4-methyl-2-oxo-2*H*-chromen-3-yl)sulfonyl)methyl)-1-phenylpyrrolidin-2-one (4ma).



The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (10:1). White solid; m.p.: 197.1-199.5 ℃; 33% yield;

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.1 (dd, J = 8.1, 1.5 Hz, 1H), 7.8 (ddd, J = 8.6, 7.2, 1.5 Hz, 1H), 7.7 (d, J = 7.6 Hz, 2H), 7.5 (d, J = 8.6 Hz, 1H), 7.5 (t, J = 8.0 Hz, 2H), 7.3 (t, J = 7.4 Hz, 1H), 4.2 (dd, J = 14.6, 5.0 Hz, 1H), 4.1 (ddd, J = 10.2, 8.6, 1.7 Hz, 1H), 4.0 – 4.0 (m, 1H), 3.9 (dd, J = 14.6, 8.4 Hz, 1H), 3.7 – 3.5 (m, 1H), 3.0 (s, 3H).

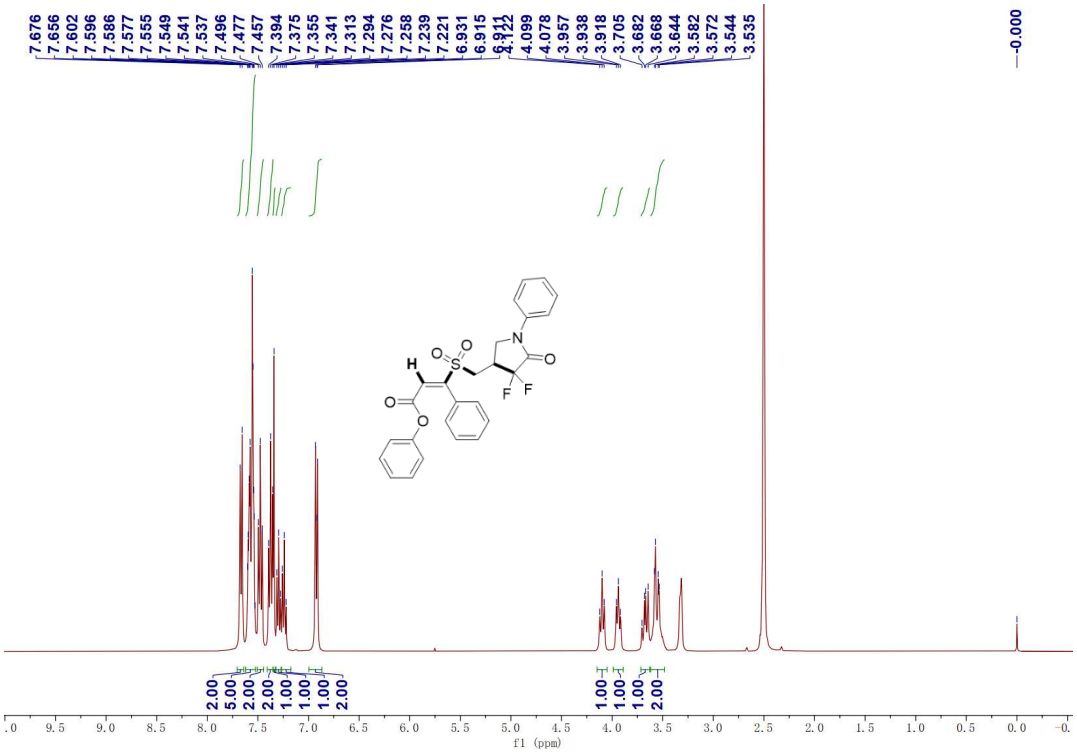
^{13}C NMR (101 MHz, DMSO) δ 160.9, 160.7 (t, $J_{C\text{-}F}$= 30.2 Hz), 156.2, 152.6, 137.6, 135.2, 129.1, 127.6, 126.2, 125.3, 123.1, 120.3, 119.5, 117.2 (t, $J_{C\text{-}F}$= 249.5 Hz), 116.7, 51.1 (d, $J_{C\text{-}F}$= 7.0 Hz), 47.6 (d, $J_{C\text{-}F}$= 7.0 Hz), 33.7 (t, $J_{C\text{-}F}$= 21.2 Hz), 14.7.

^{19}F NMR (376 MHz, DMSO-d_6) δ -107.8 (d, J = 262.3 Hz, 1F), -112.6 (d, J = 262.2 Hz, 1F).

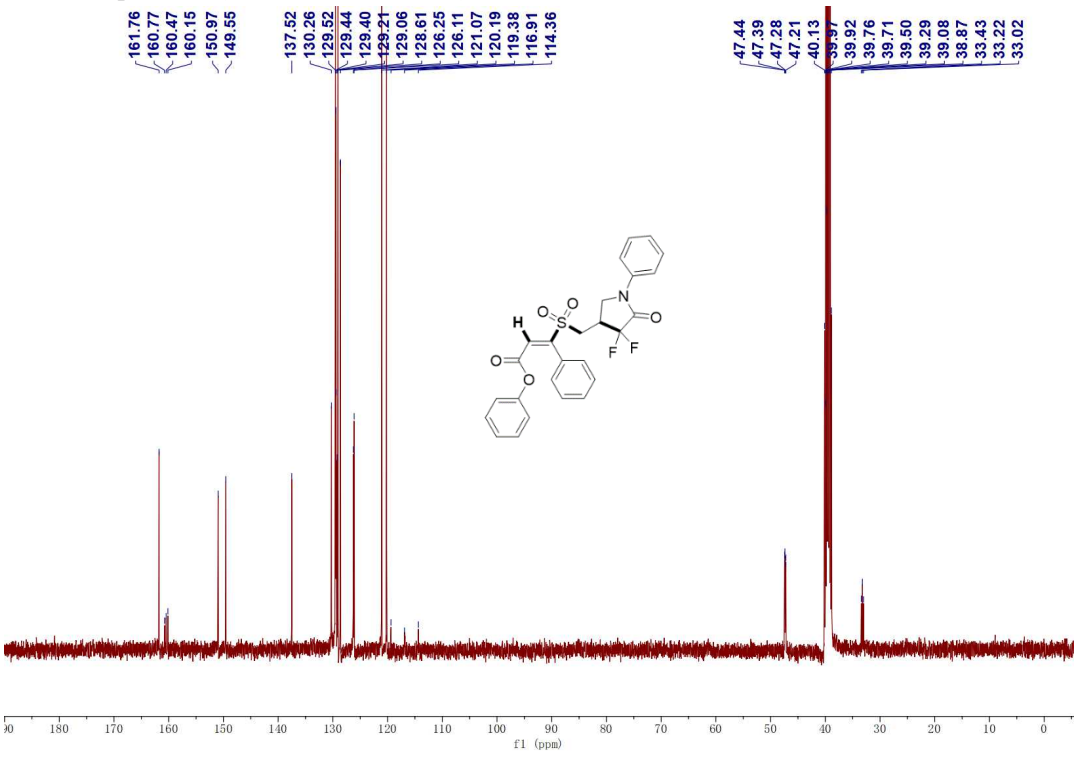
HRMS-ESI (m/z): calcd for $C_{21}H_{18}F_2NO_5S^+$ $[M+H]^+$ 434.0868, found 434.0864.

8. ^{1}H, ^{13}C and ^{19}F NMR spectra for products.

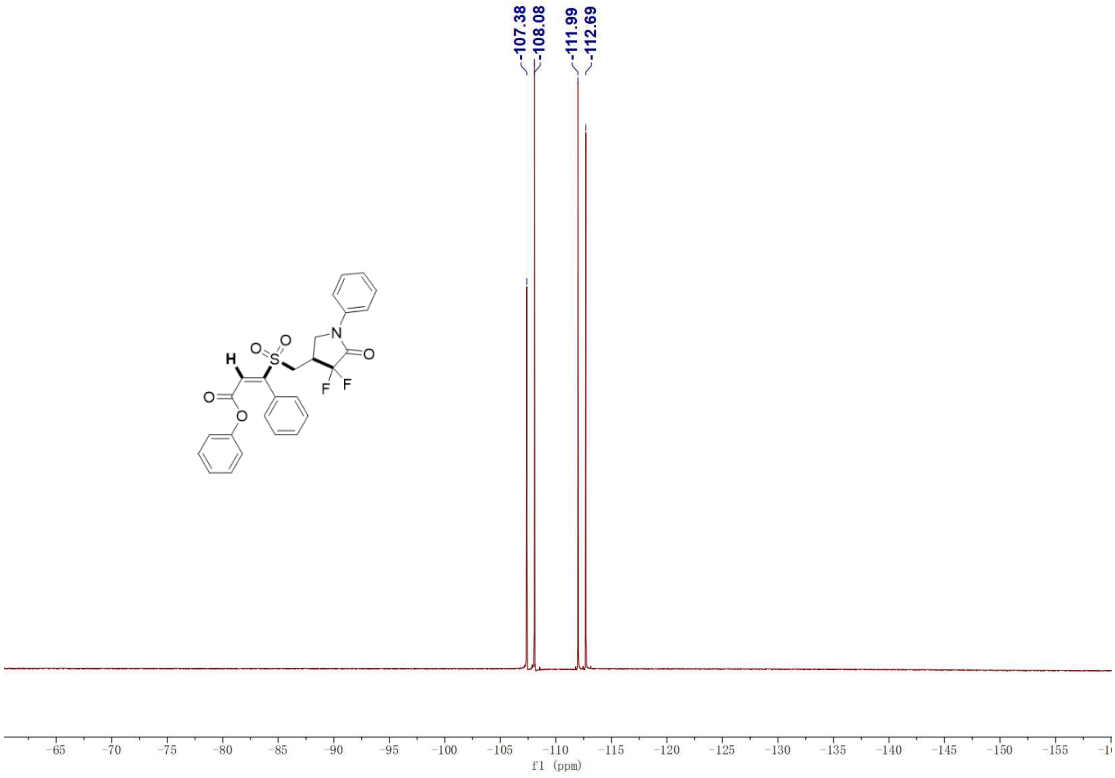
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3aa**



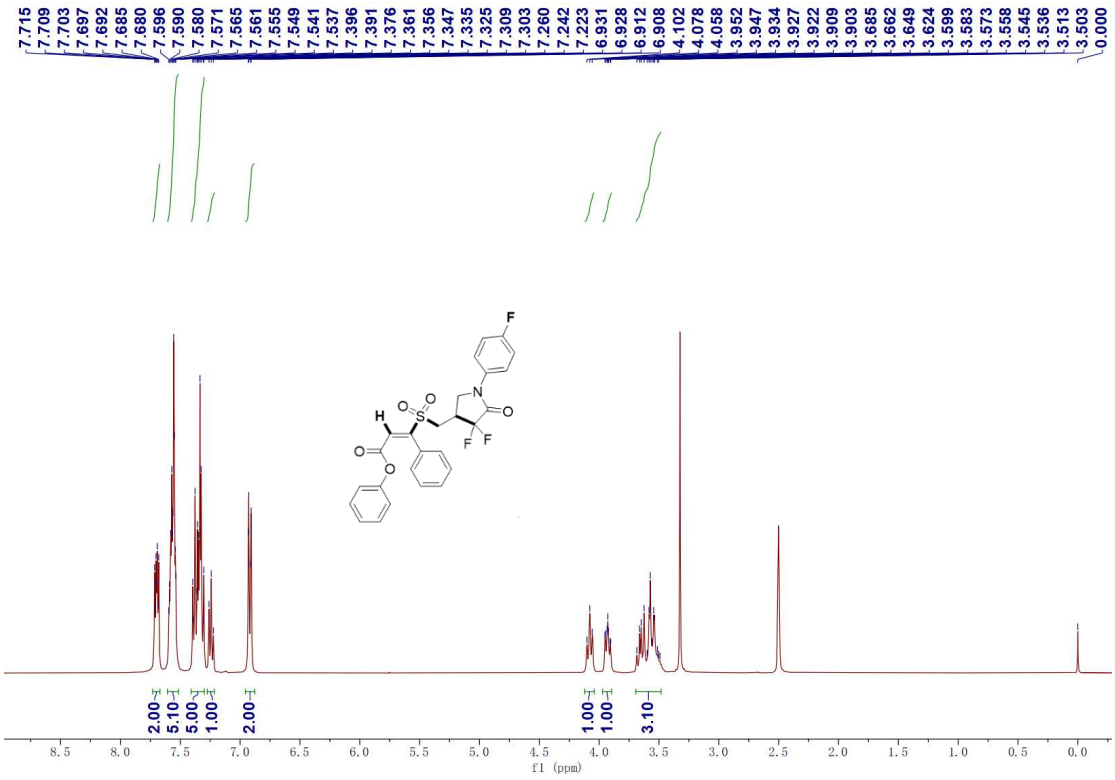
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3aa**



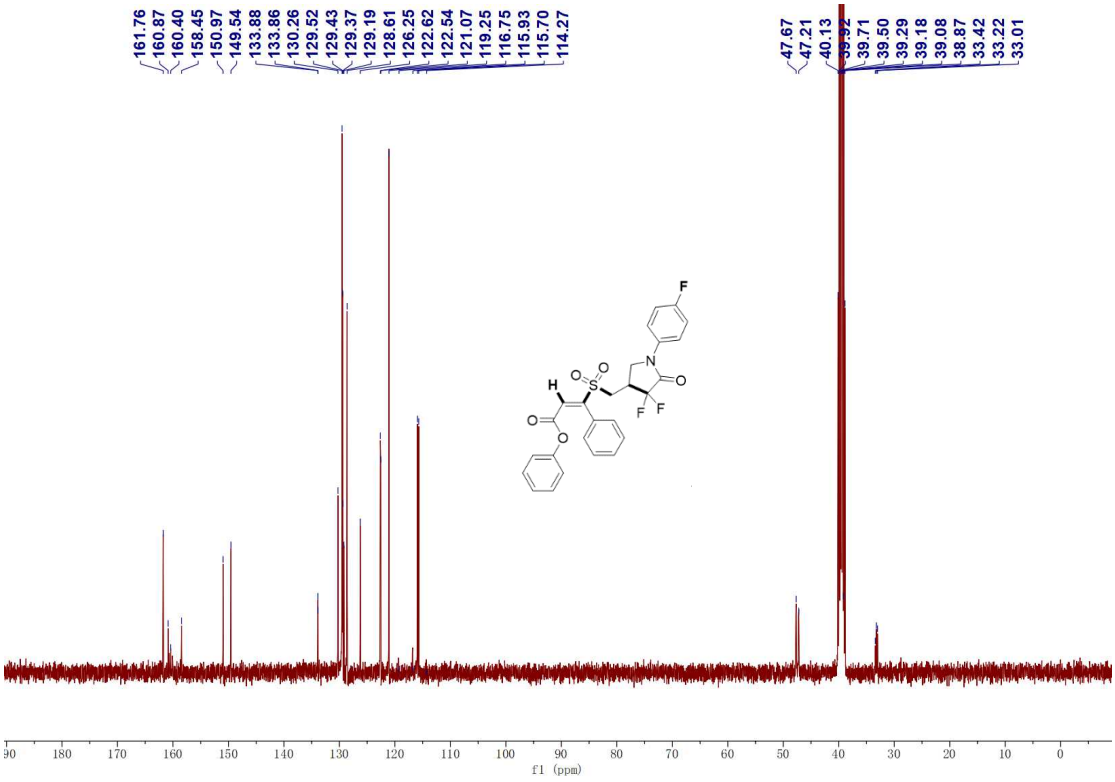
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **3aa**



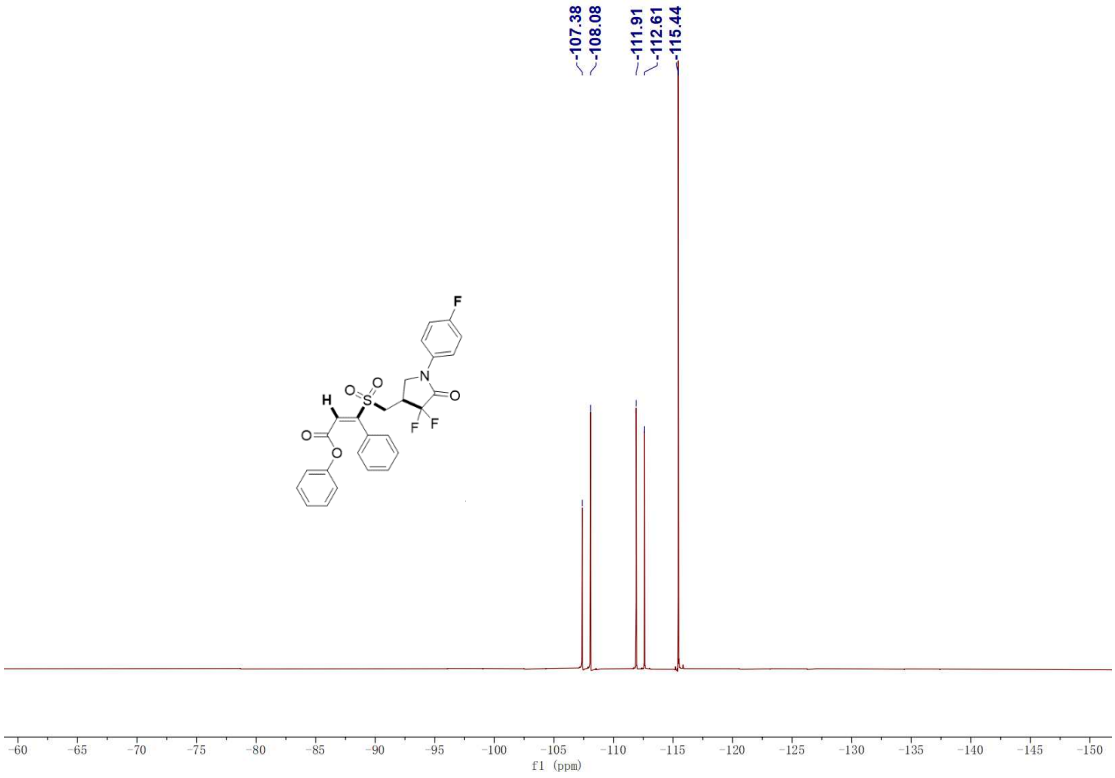
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3ab**



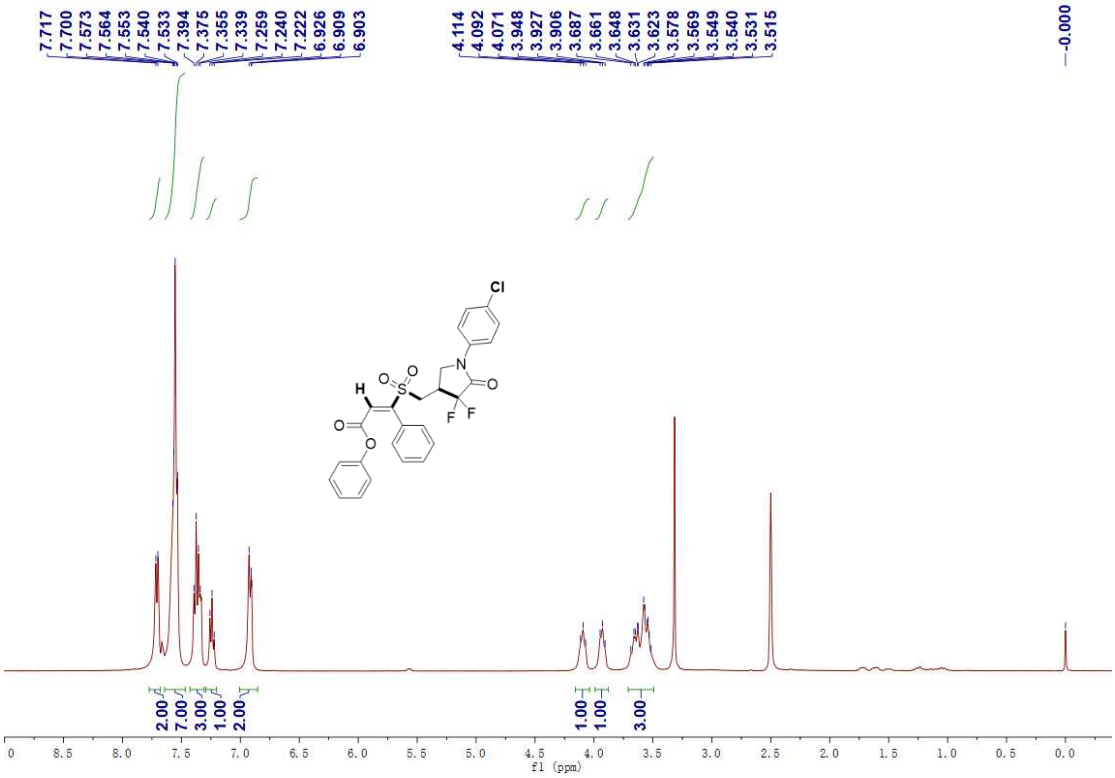
^{13}C NMR-spectrum (101MHz, DMSO-d_6) of **3ab**



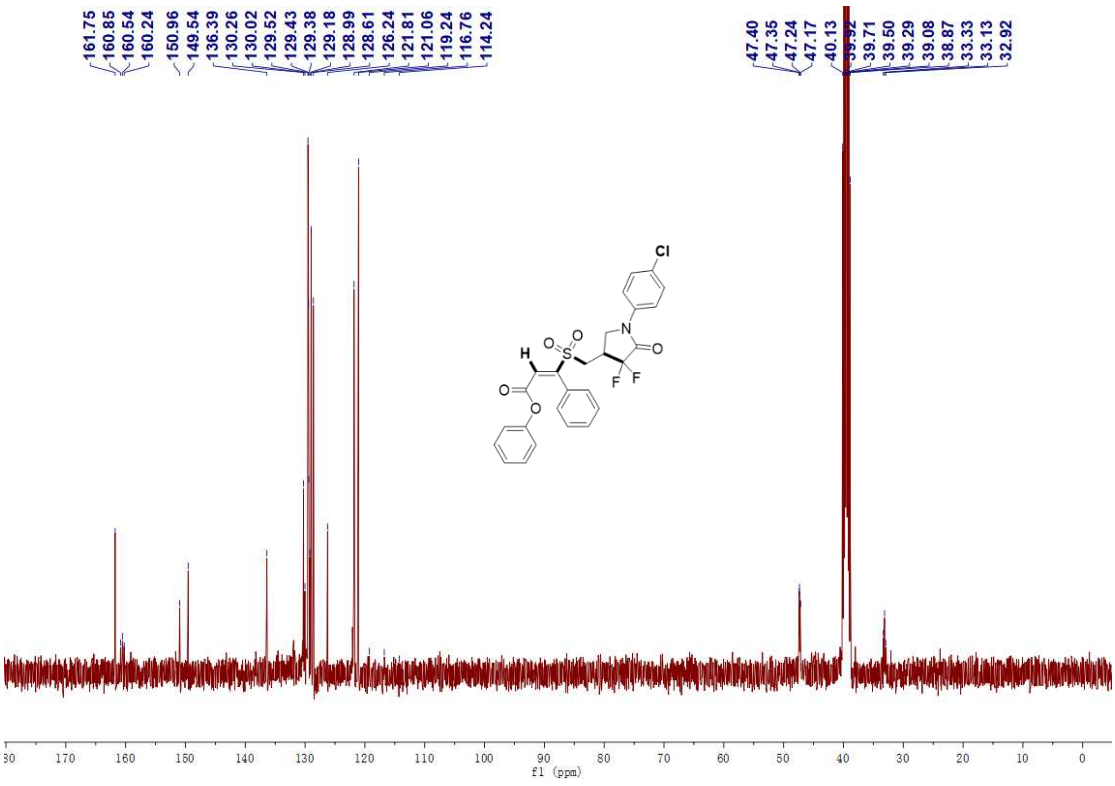
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **3ab**



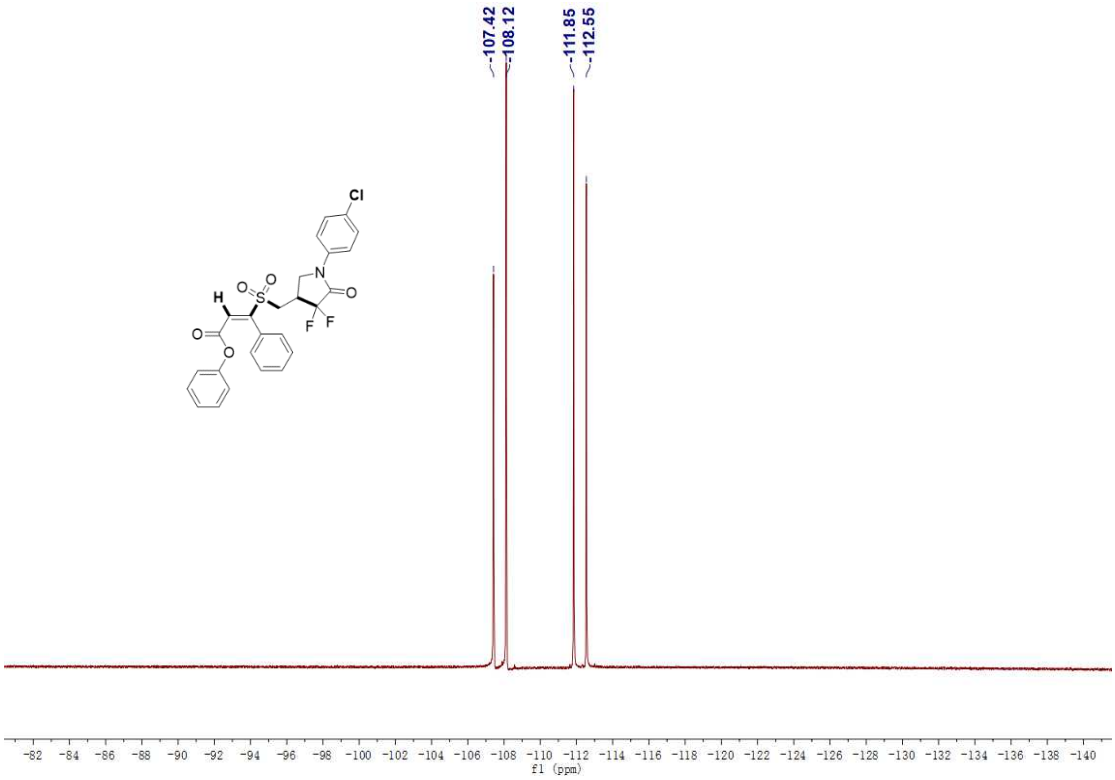
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3ac**



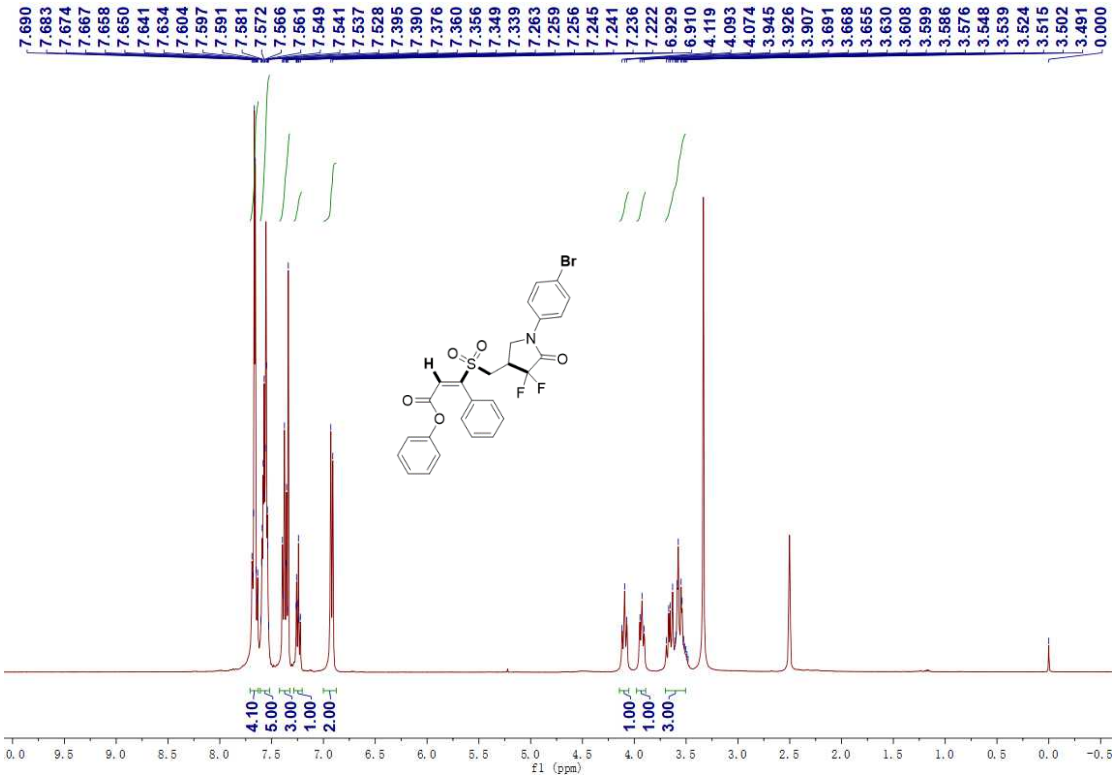
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3ac**



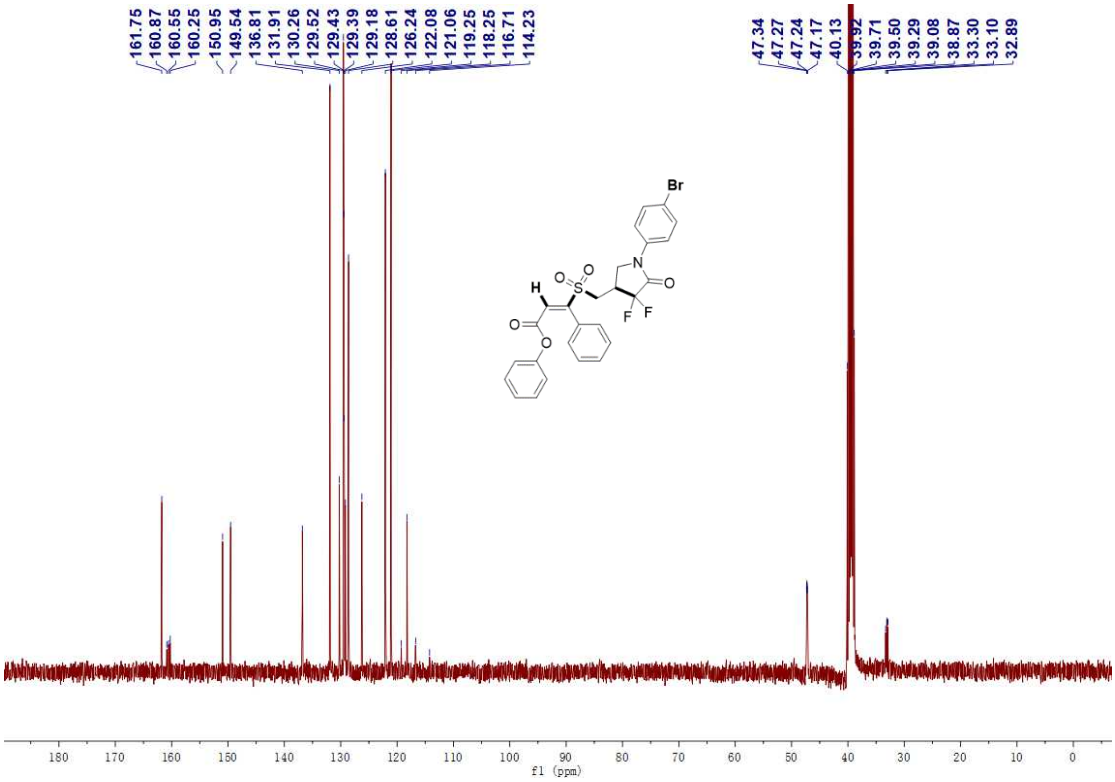
[19]F NMR-spectrum (376 MHz, DMSO-d_6) of **3ac**



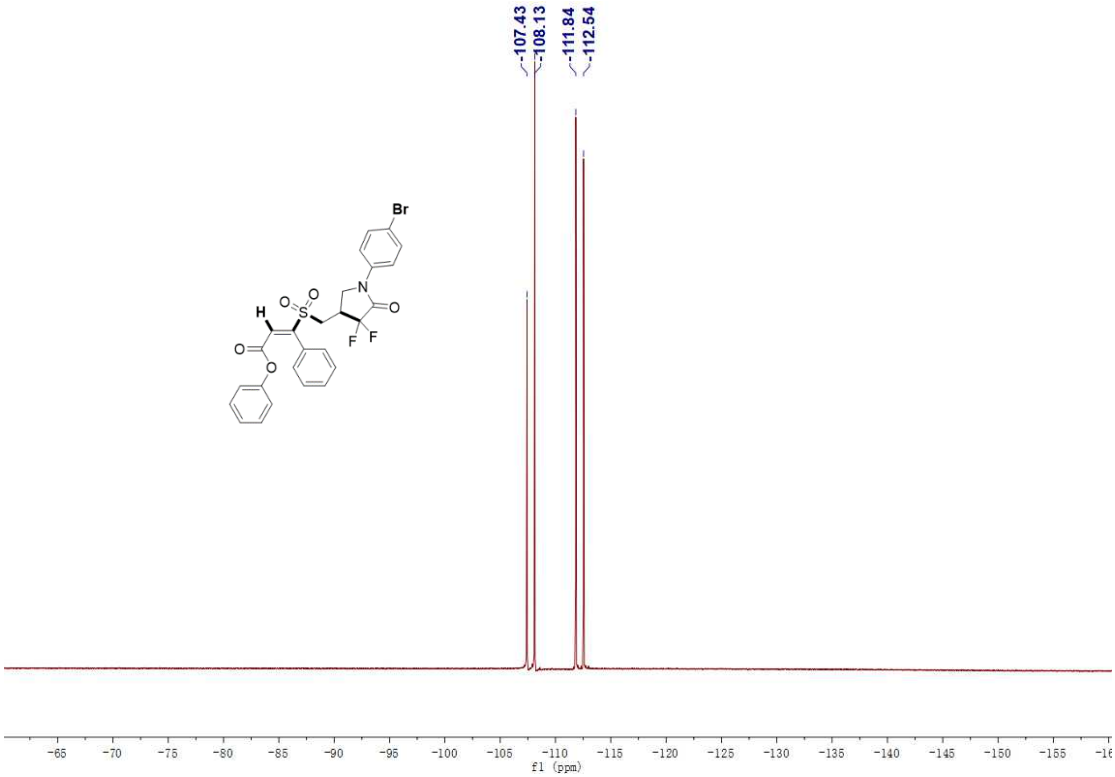
[1]H NMR-spectrum (400 MHz, DMSO-d_6) of **3ad**



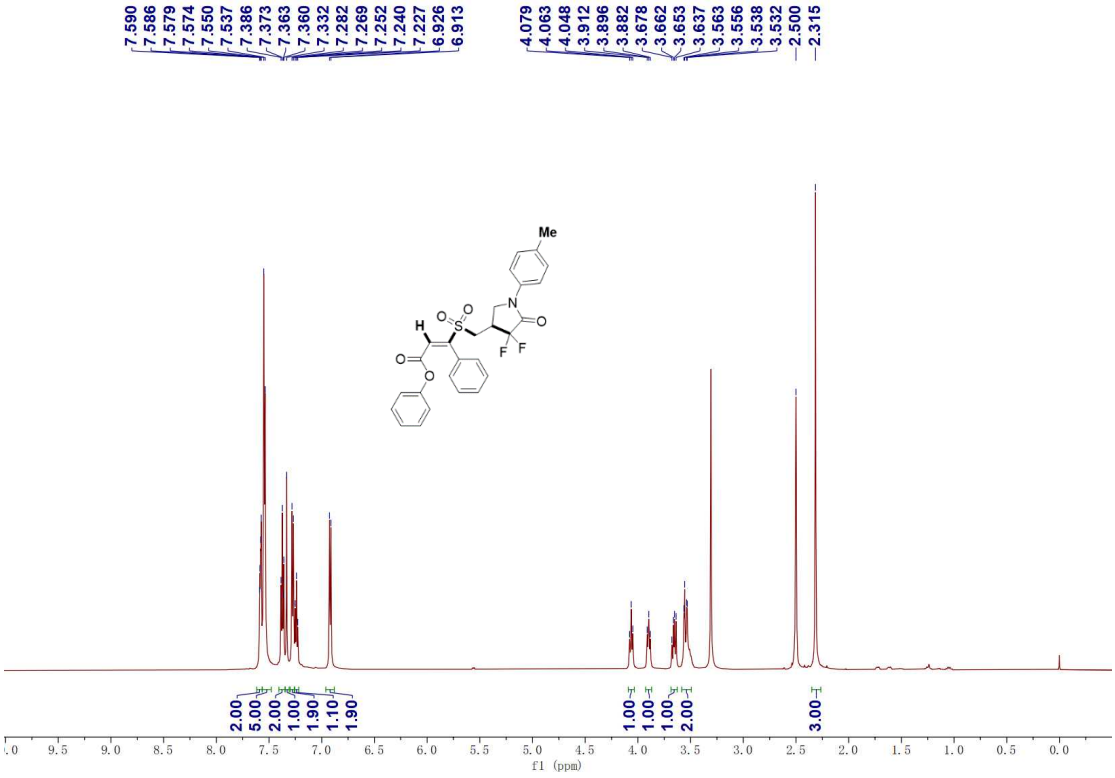
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3ad**



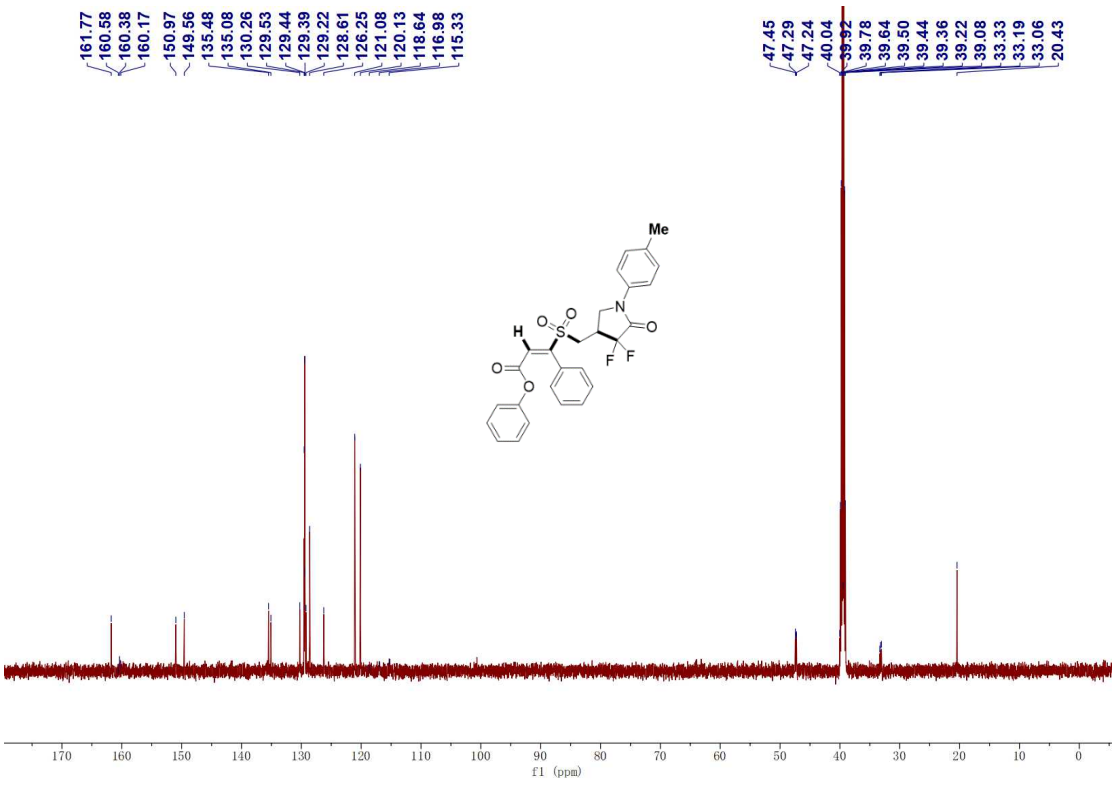
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **3ad**



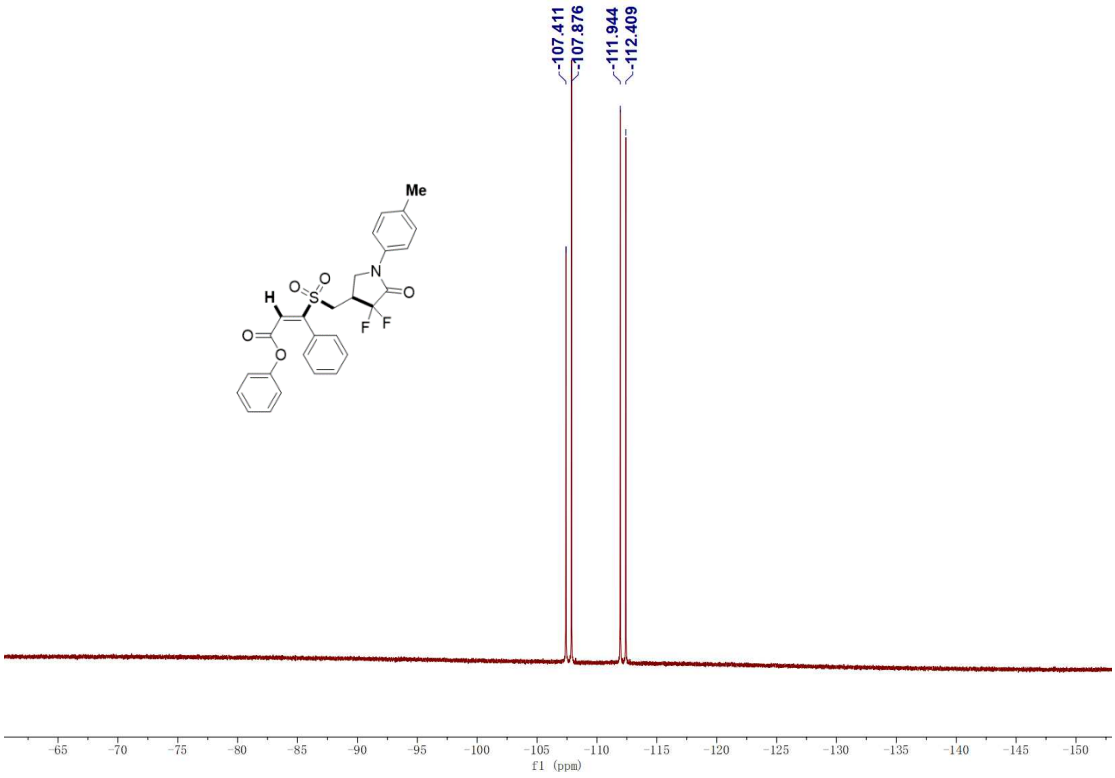
[1]H NMR-spectrum (600 MHz, DMSO-d_6) of **3ae**



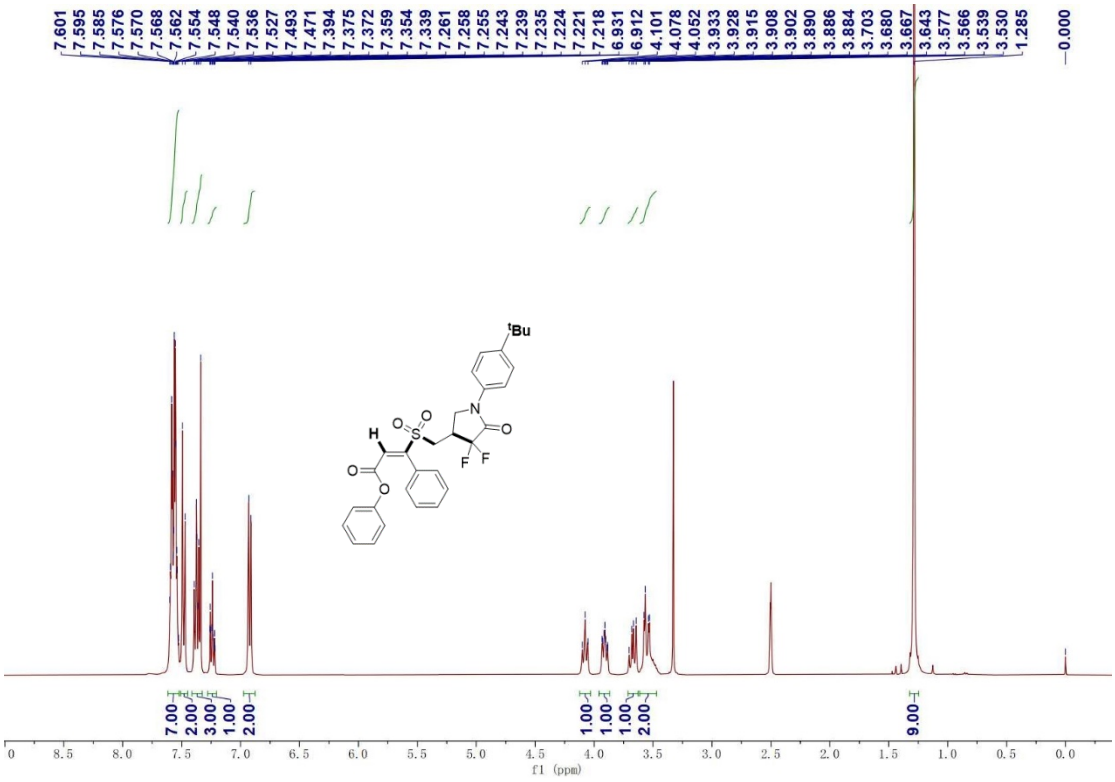
[13]C NMR-spectrum (151 MHz, DMSO-d_6) of **3ae**



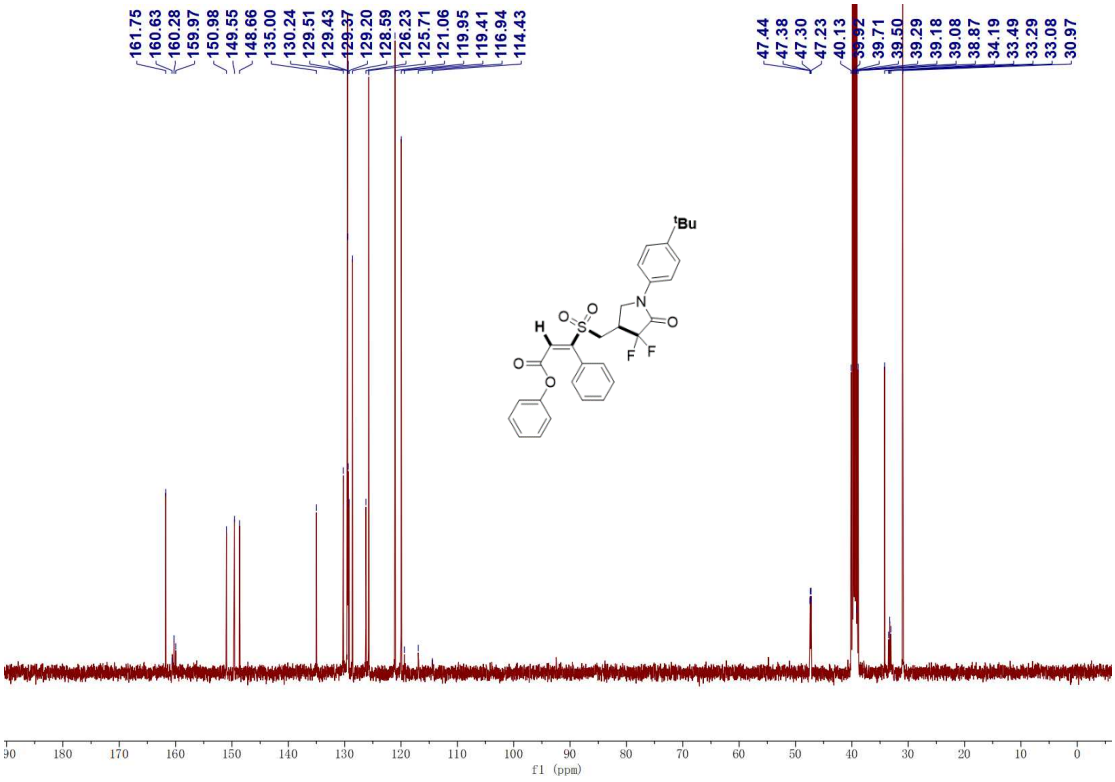
^{19}F NMR-spectrum (565 MHz, DMSO-d_6) of **3ae**



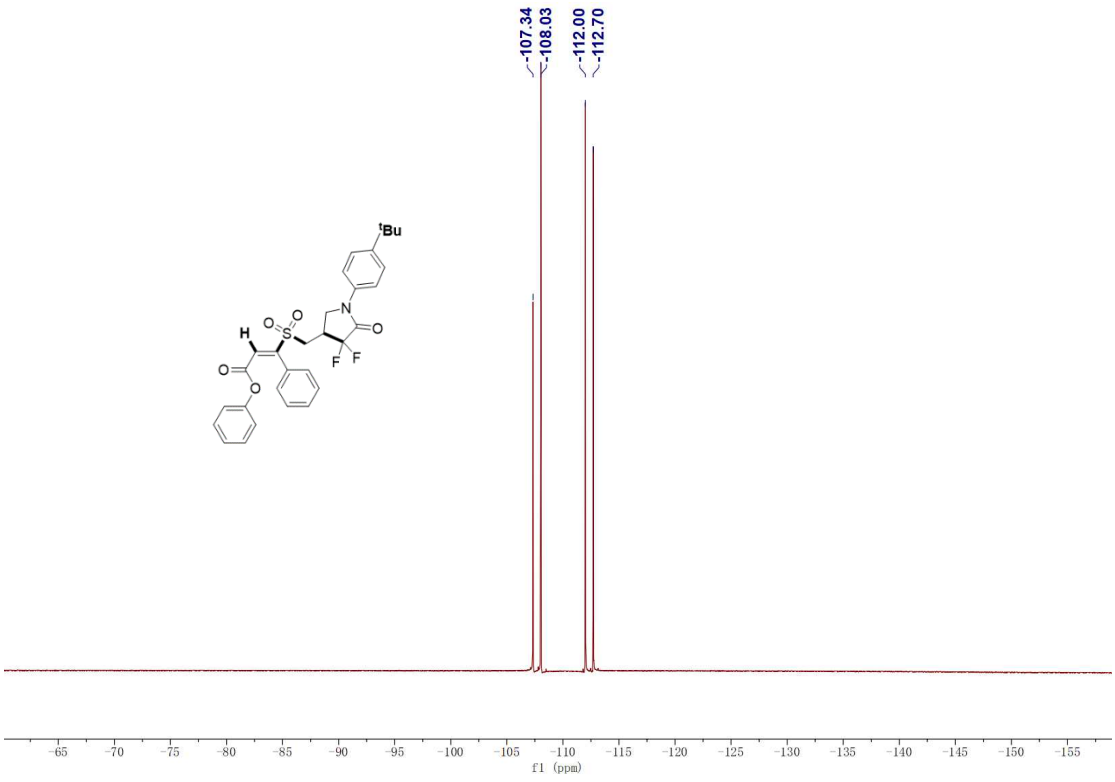
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3af**



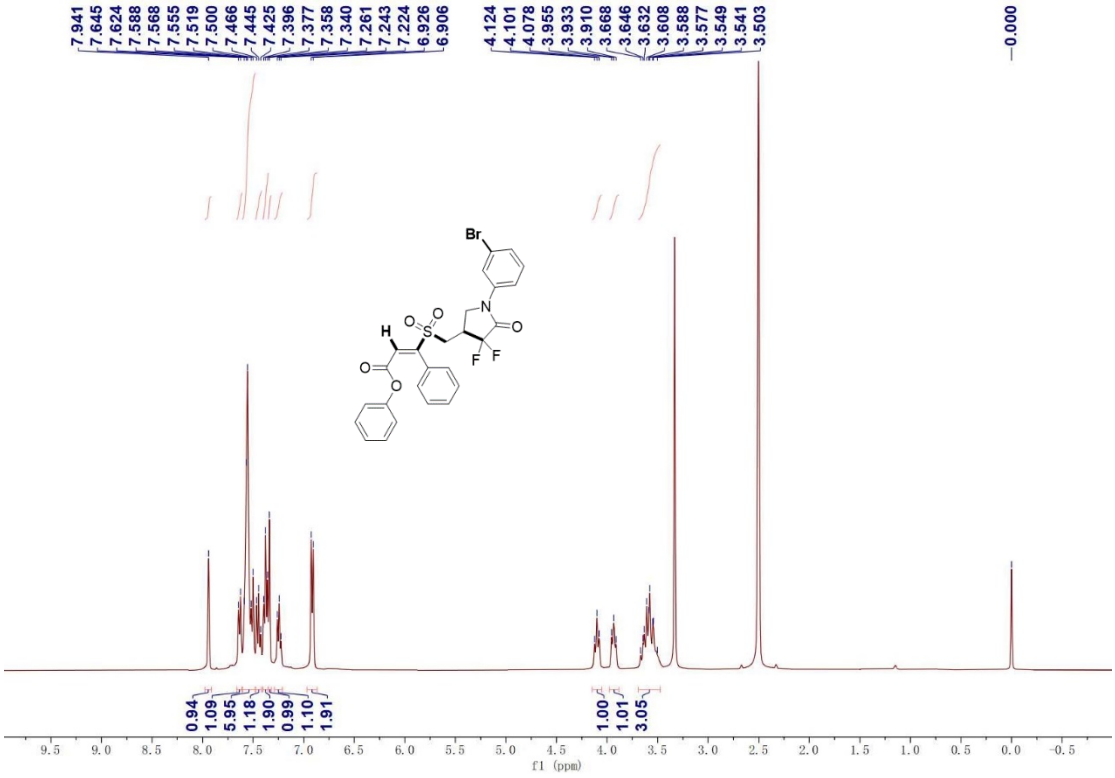
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3af**



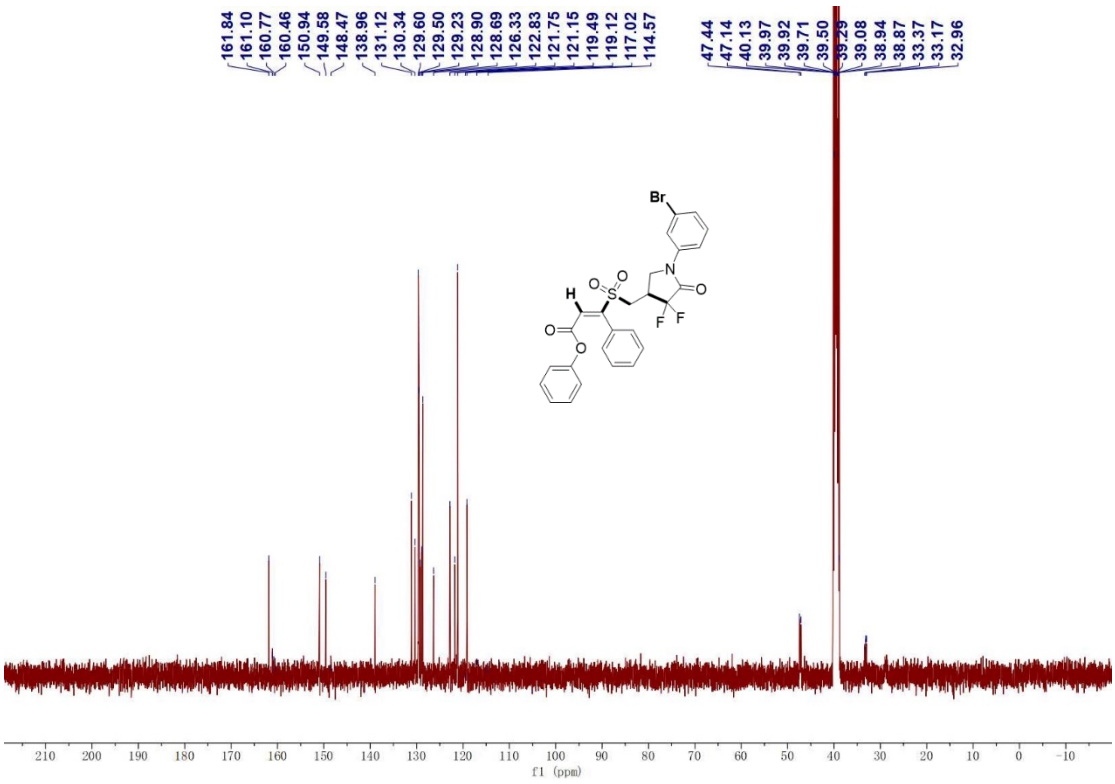
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **3af**



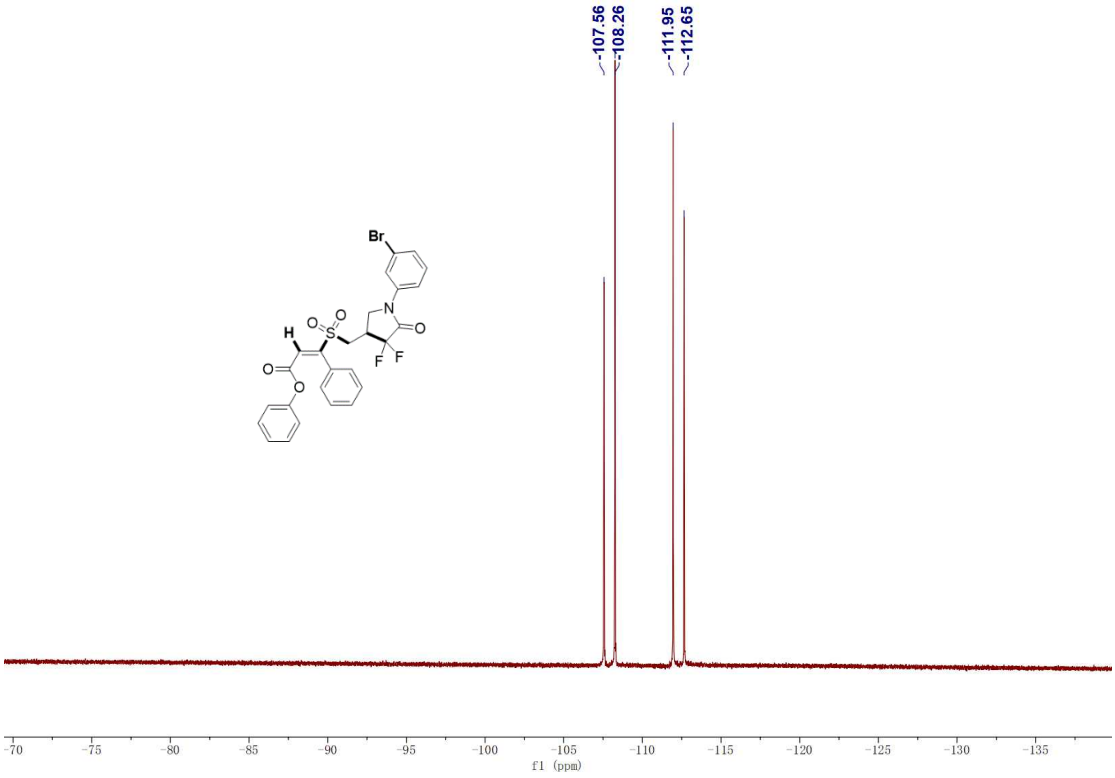
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3ag**



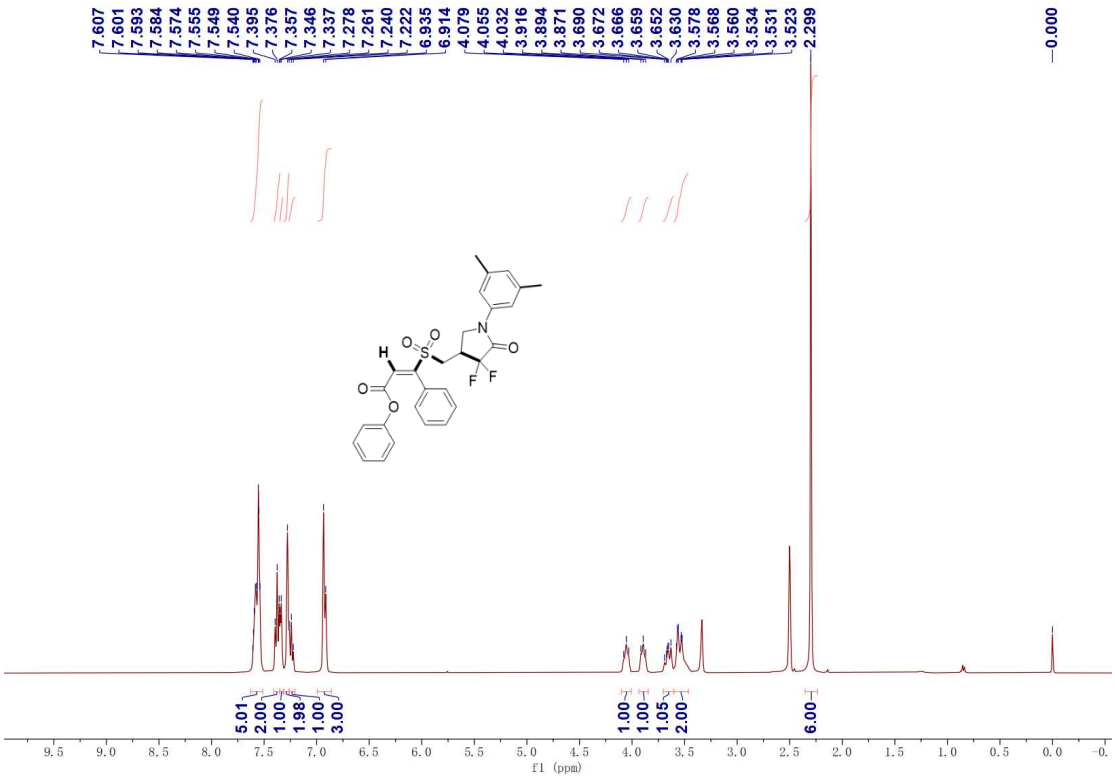
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3ag**



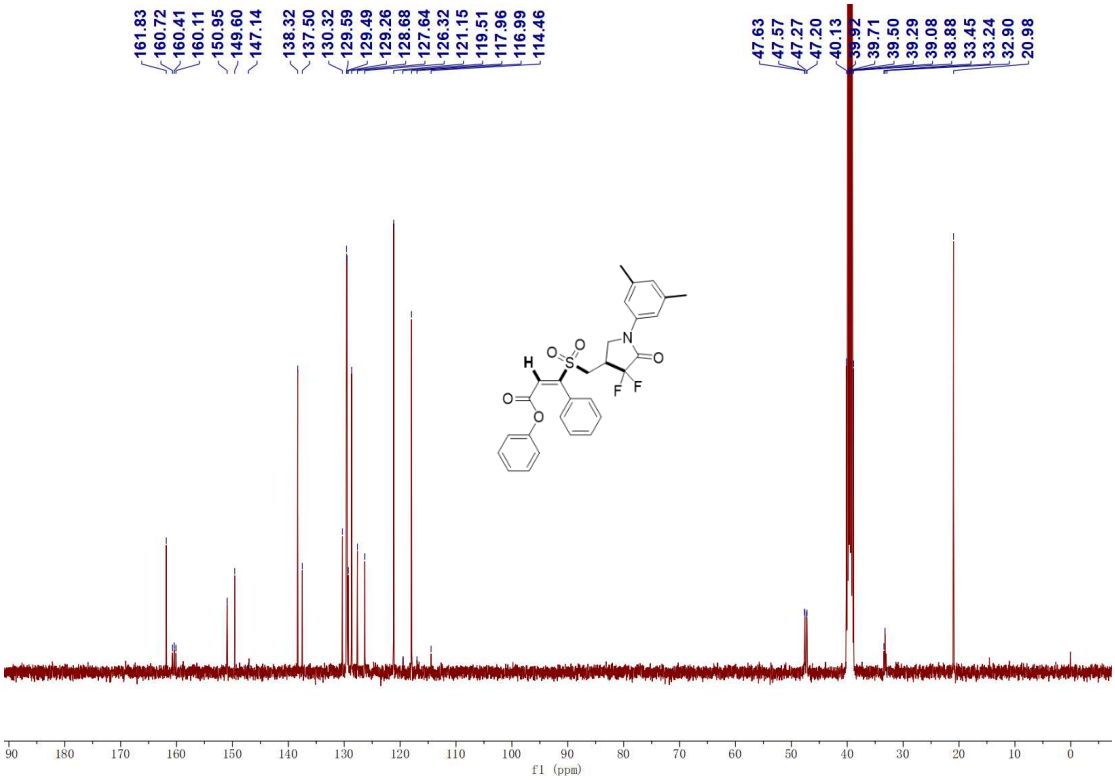
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **3ag**



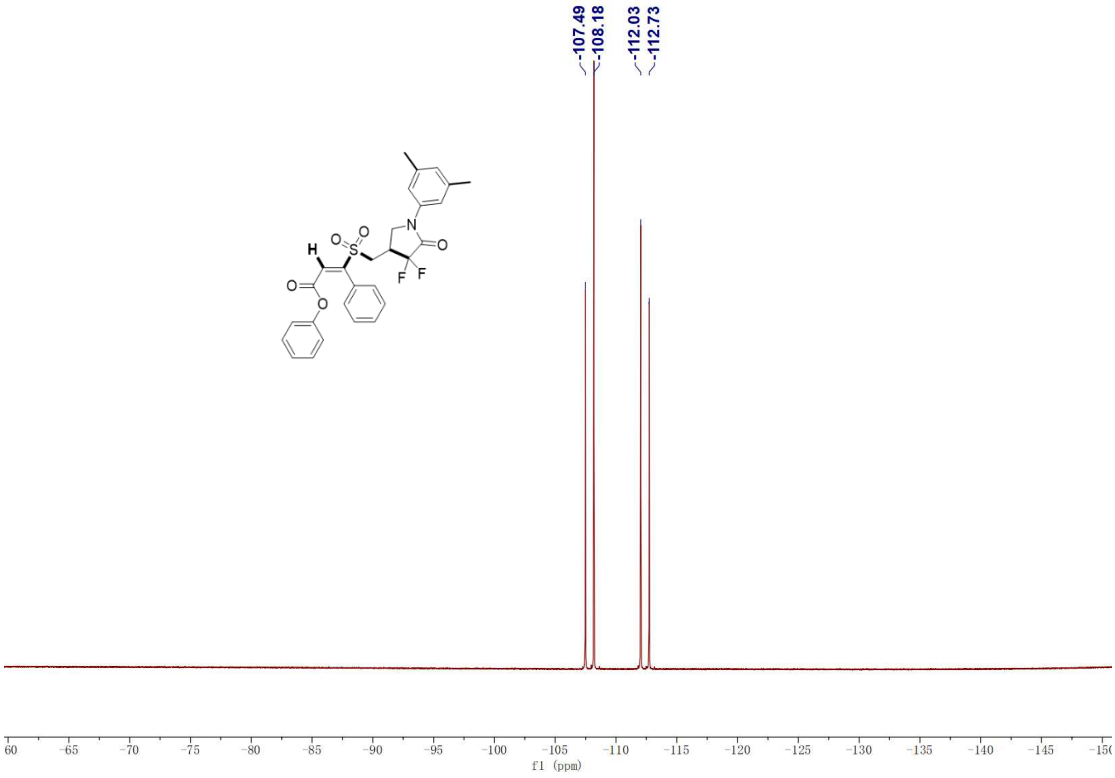
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3ah**



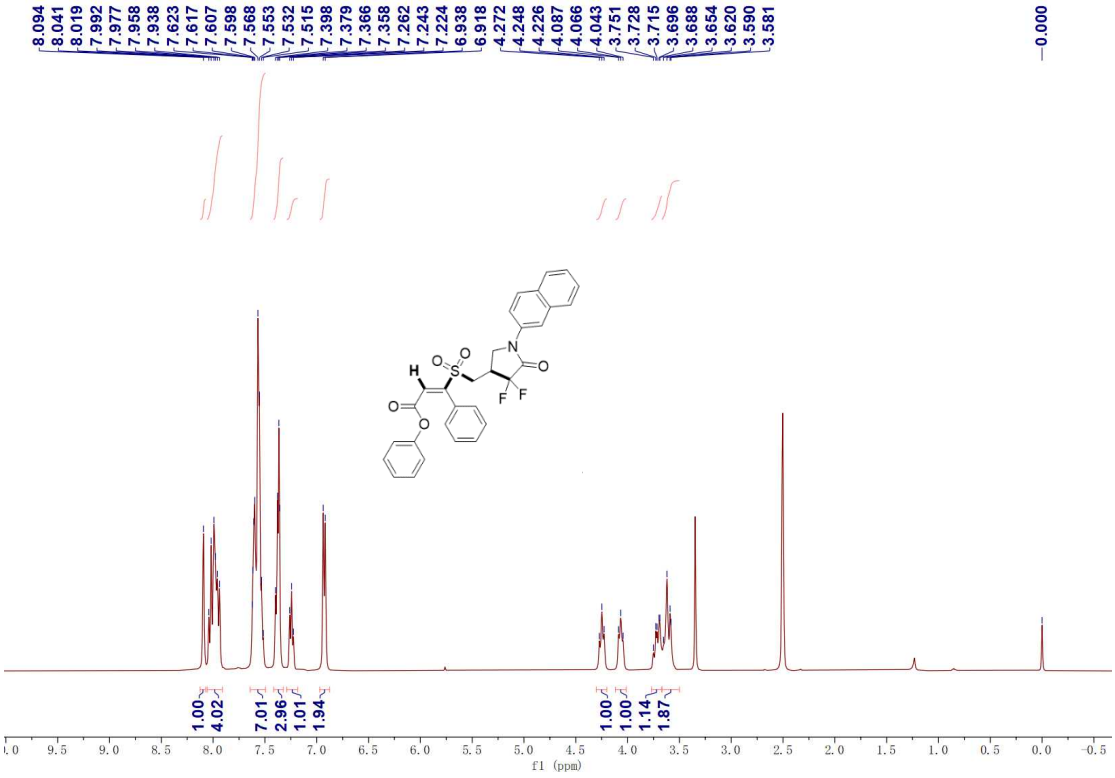
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3ah**



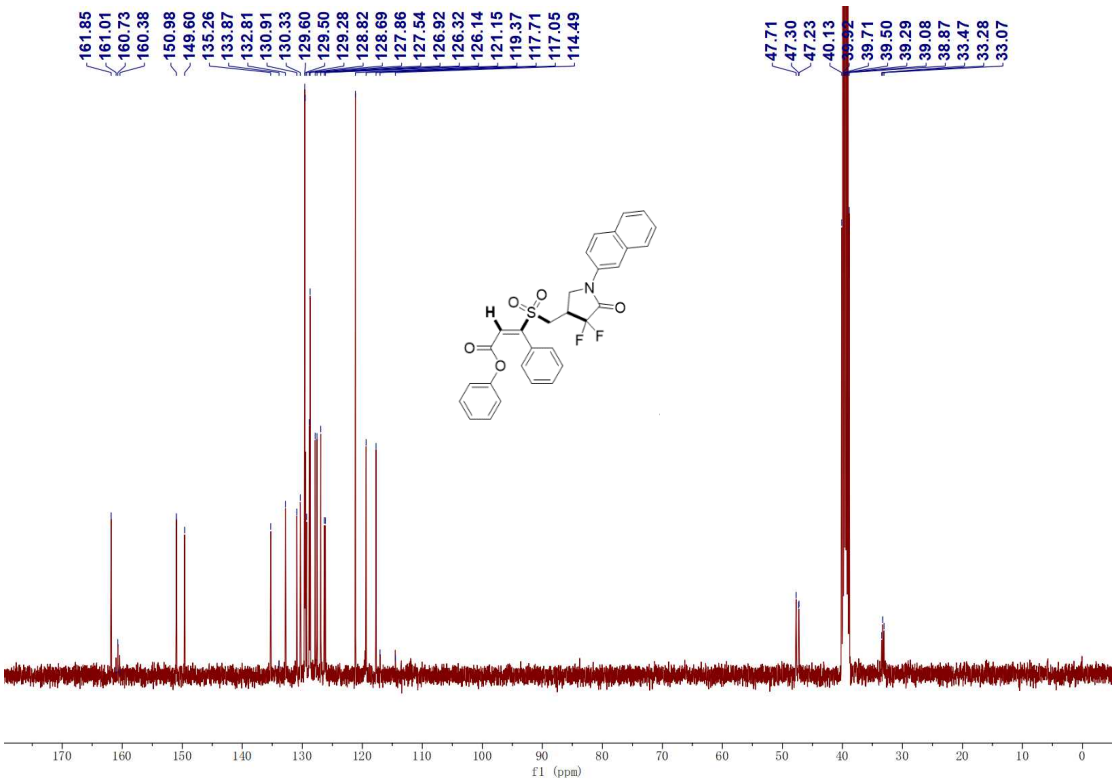
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **3ah**



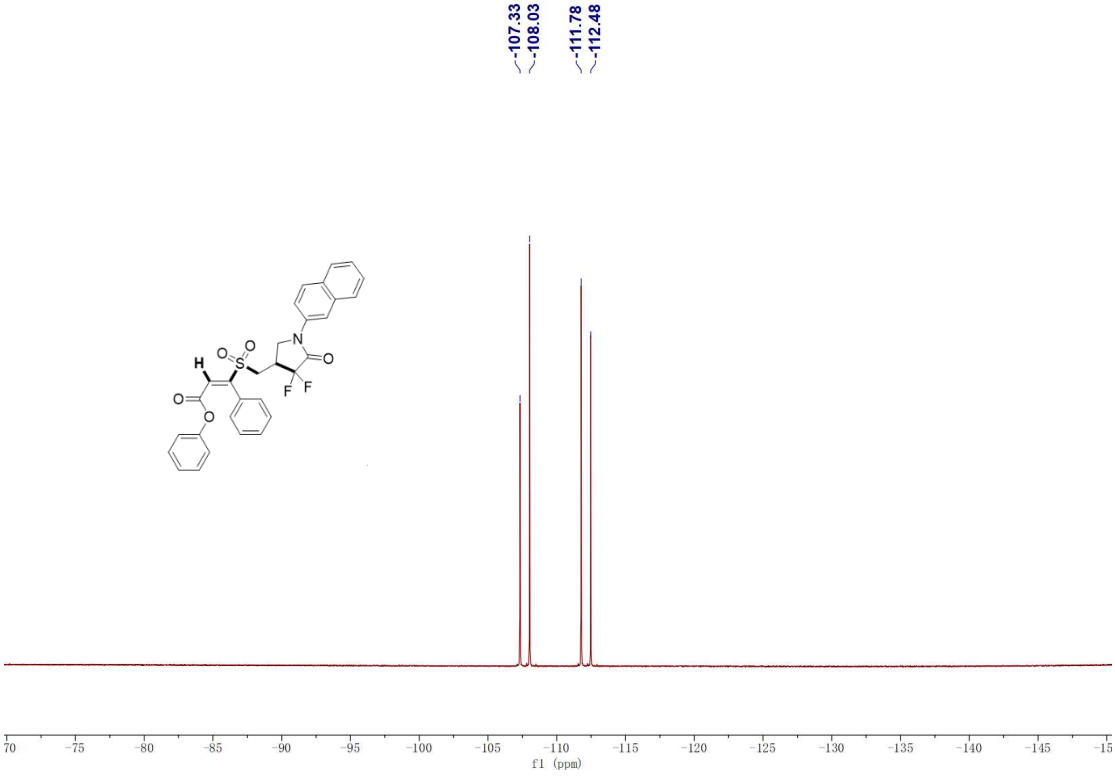
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3ai**



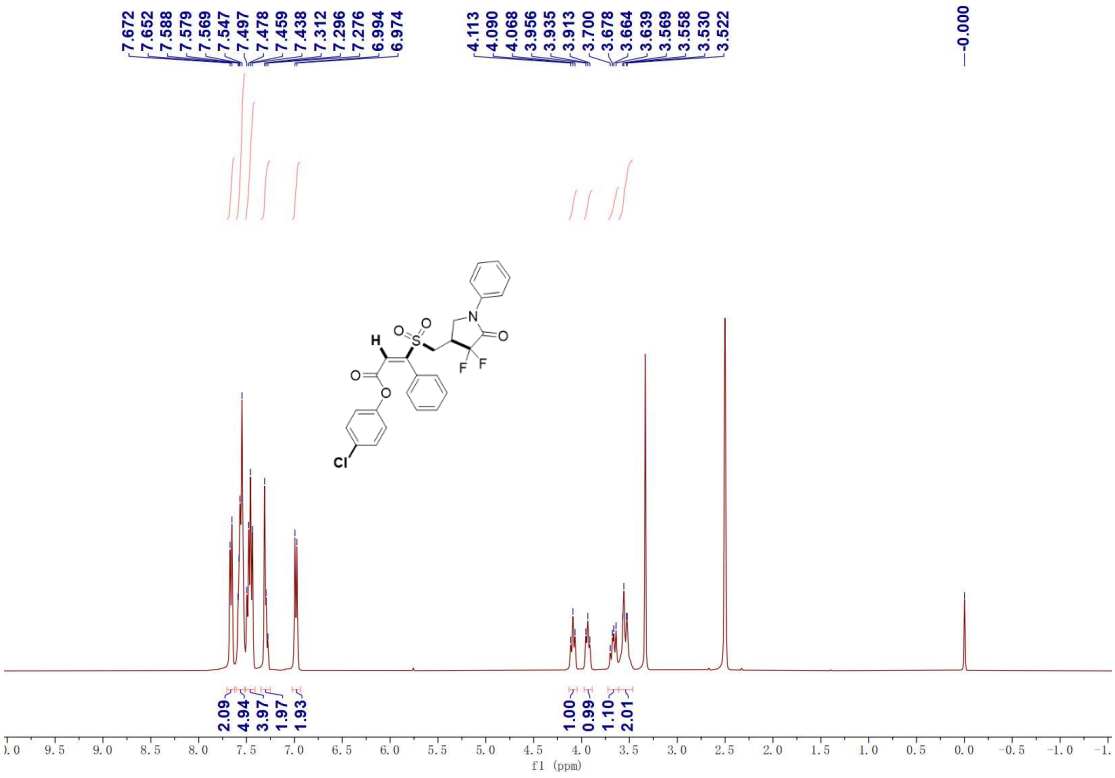
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3ai**



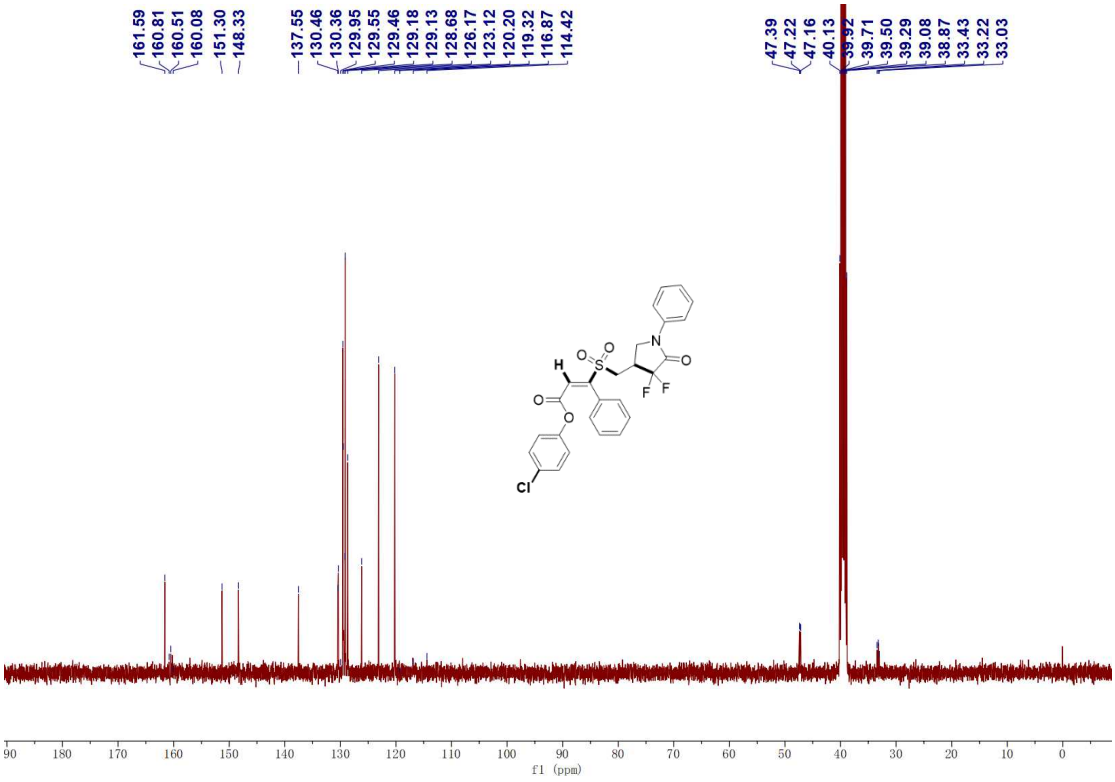
^{19}F NMR-spectrum (101 MHz, DMSO-d_6) of **3ai**



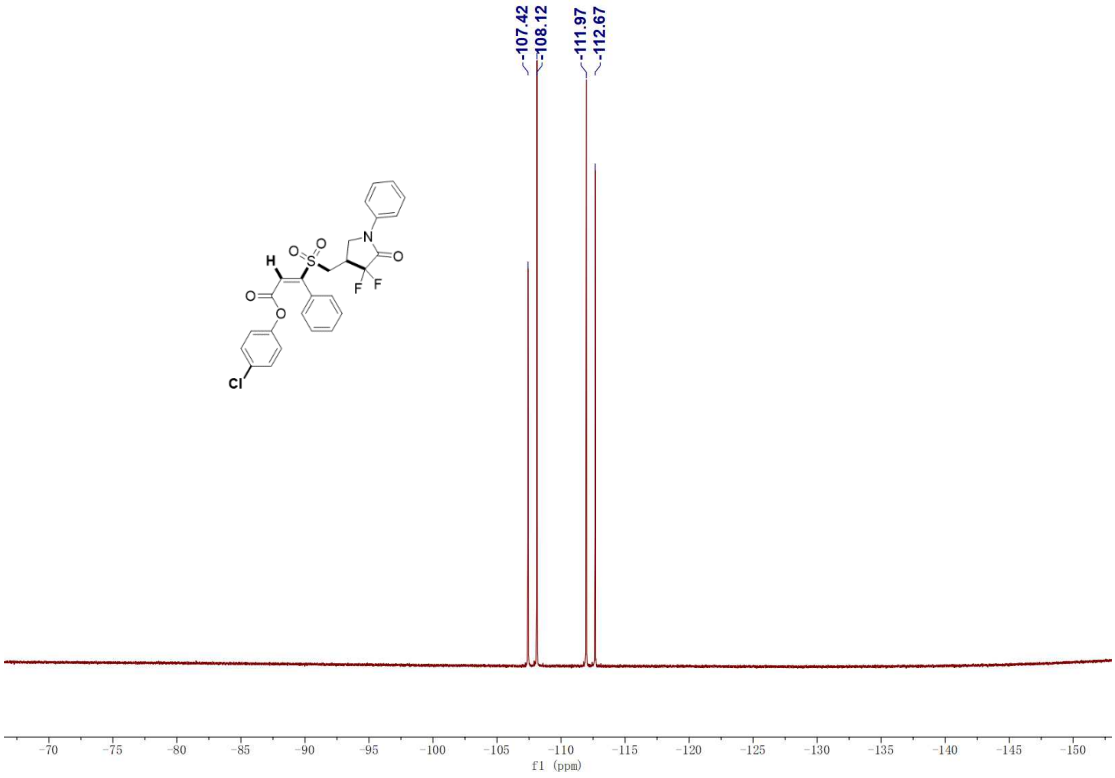
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3ba**



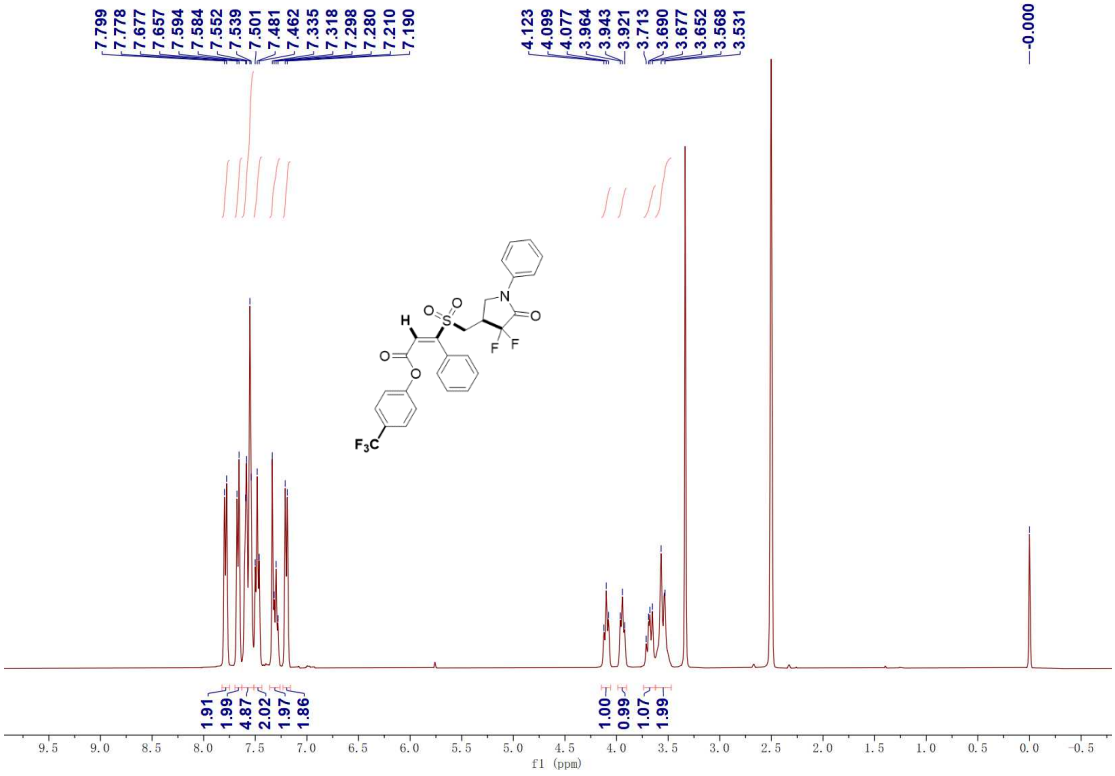
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3ba**



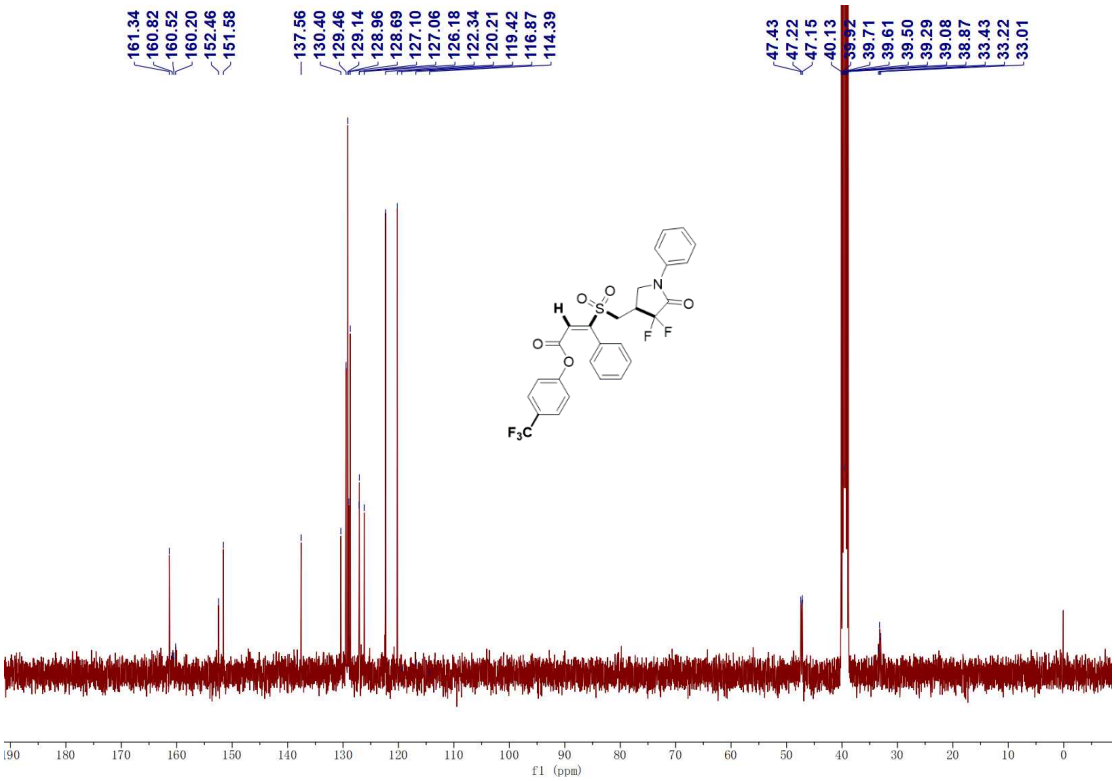
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **3ba**



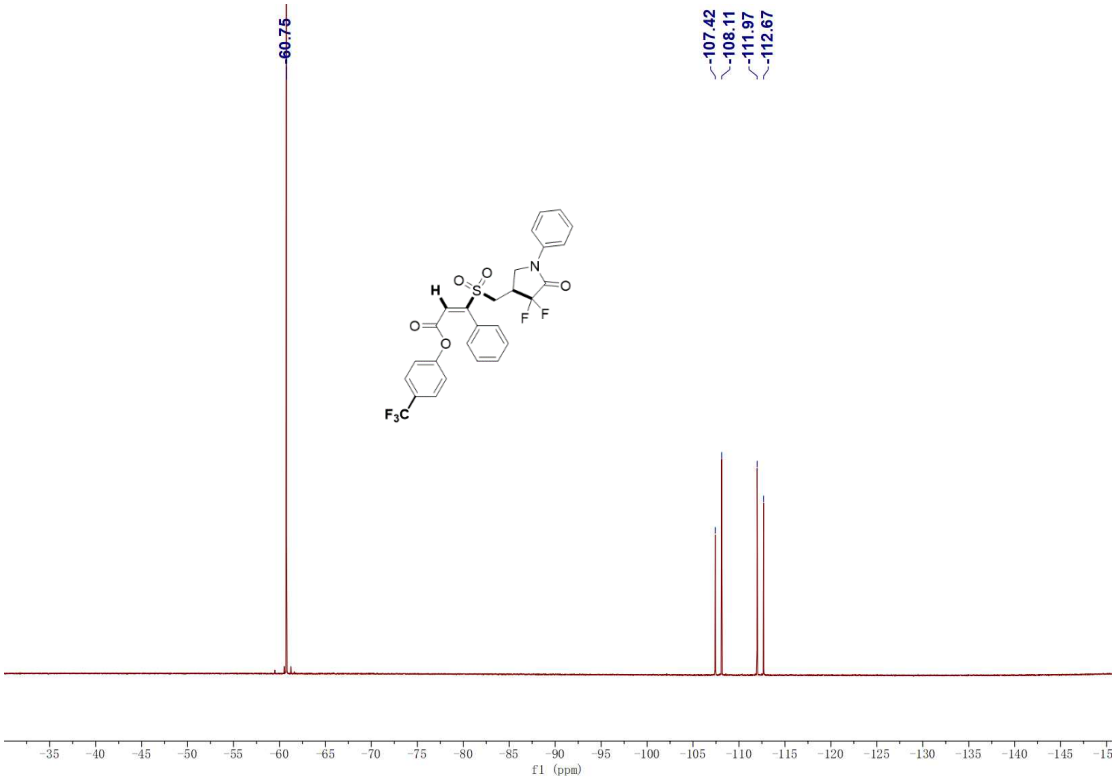
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3ca**



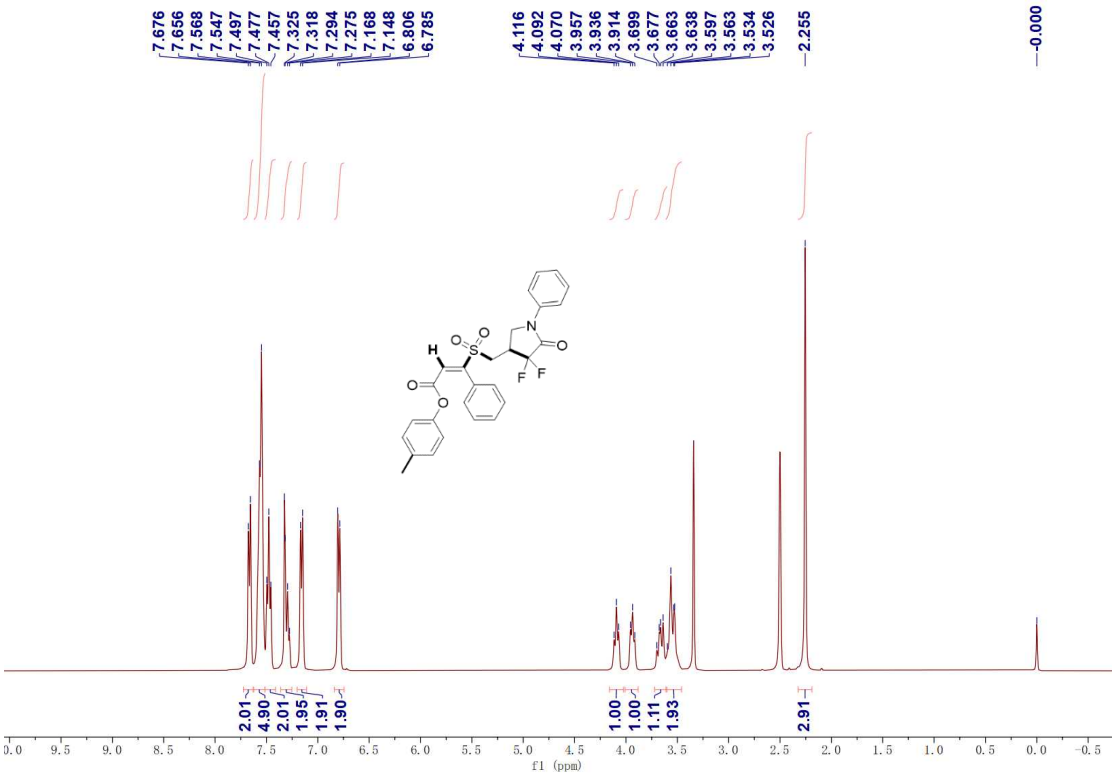
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3ca**



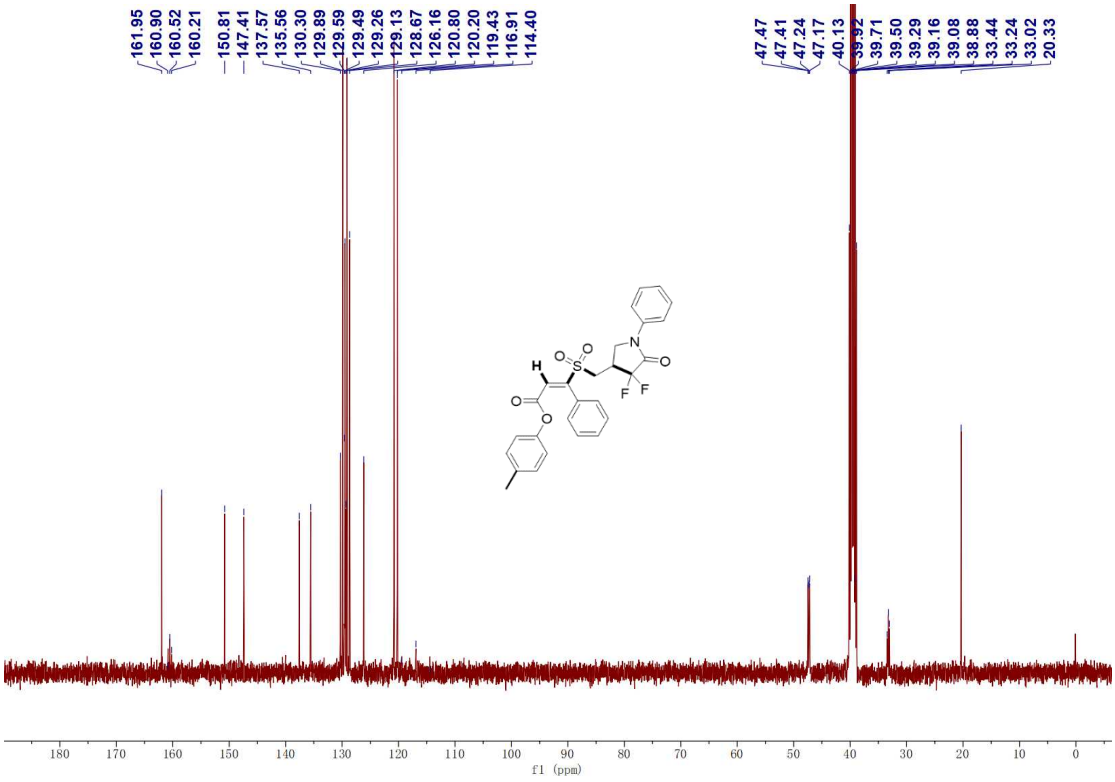
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **3ca**



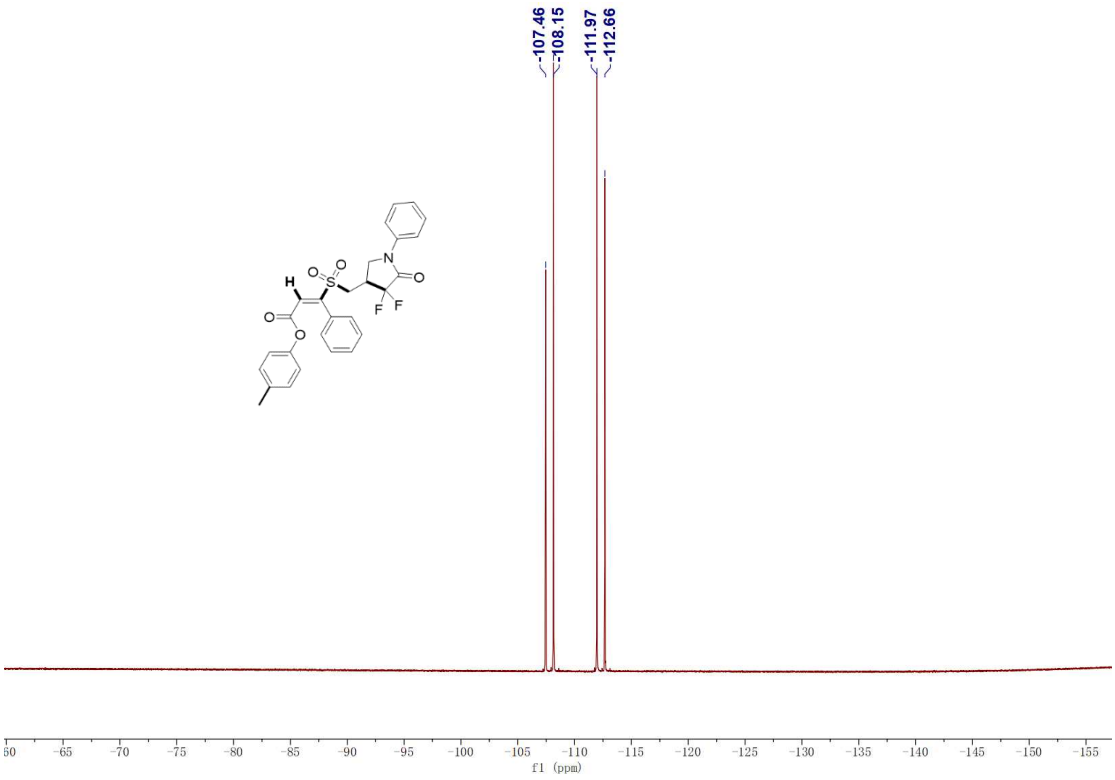
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3da**



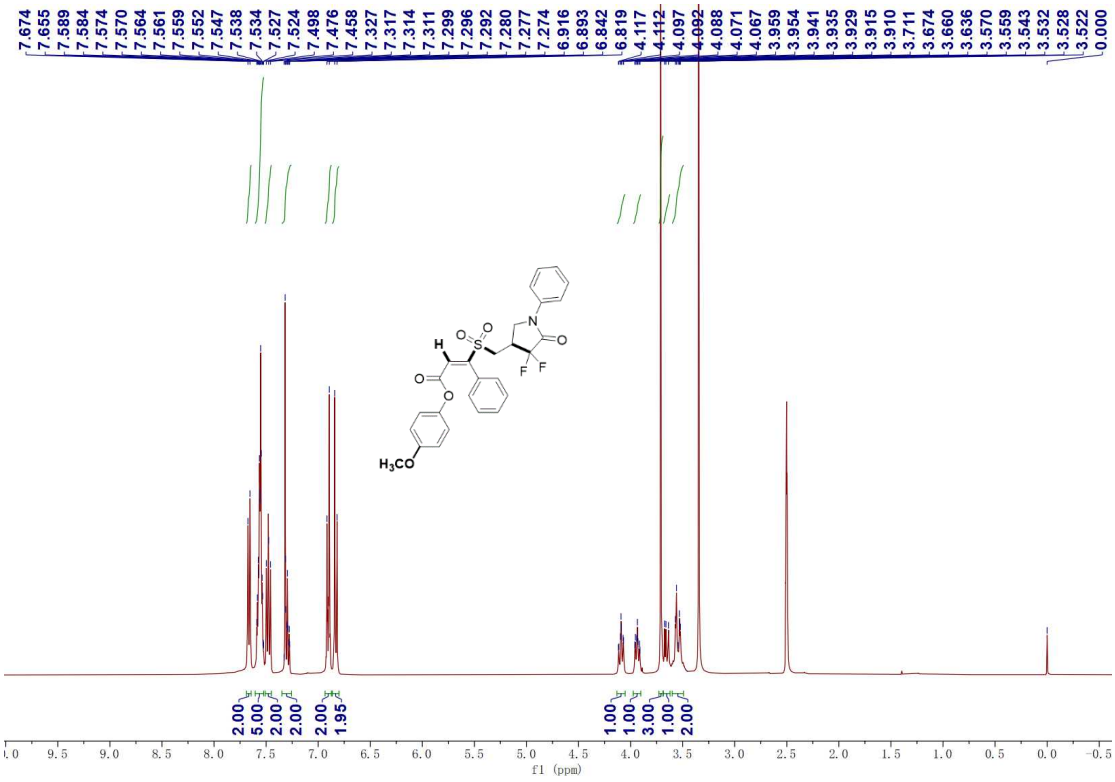
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3da**



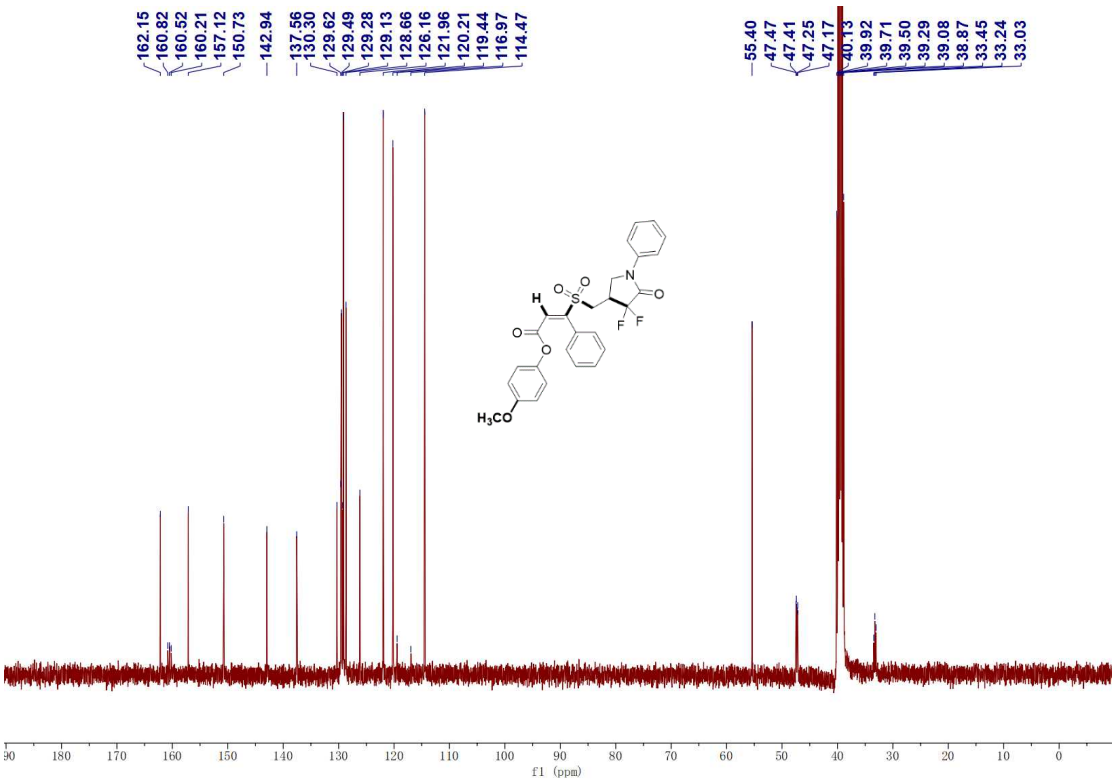
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **3da**



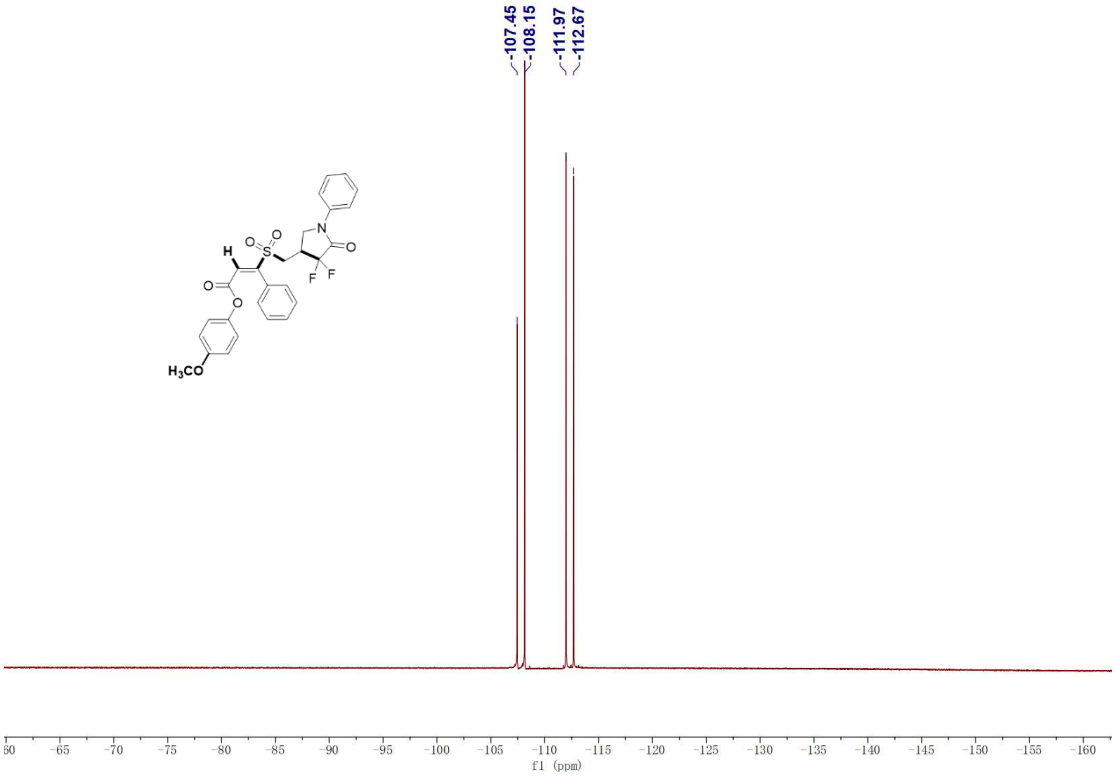
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3ea**



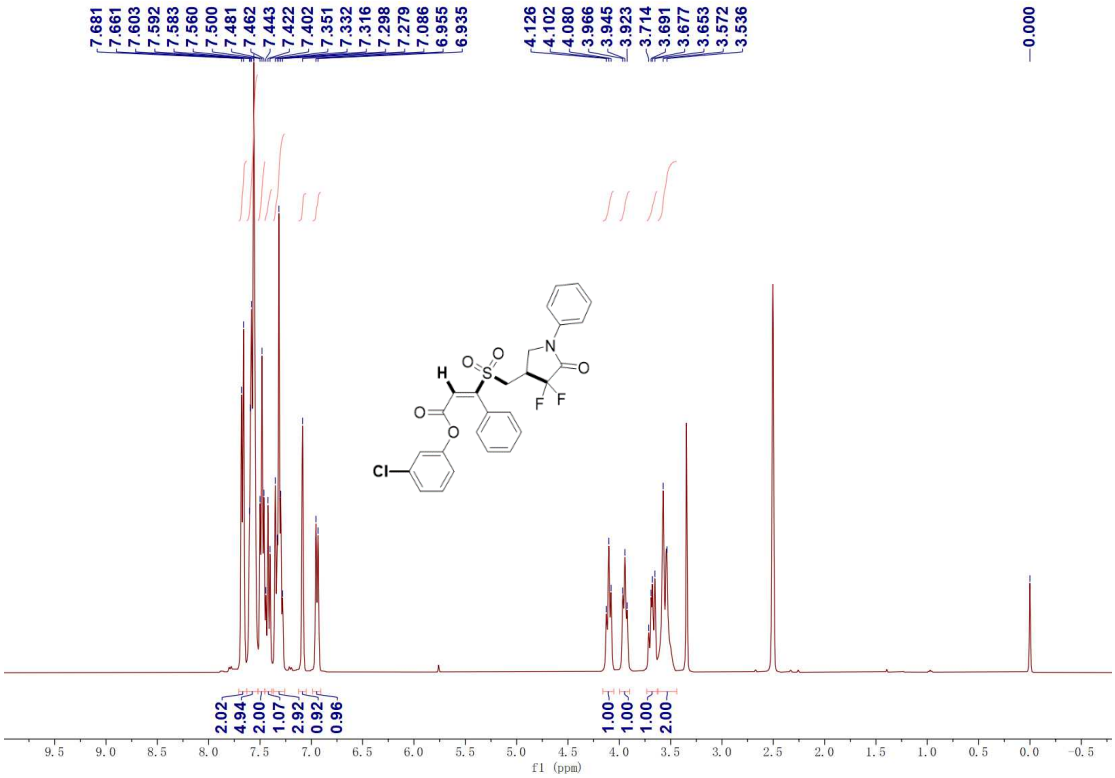
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3ea**



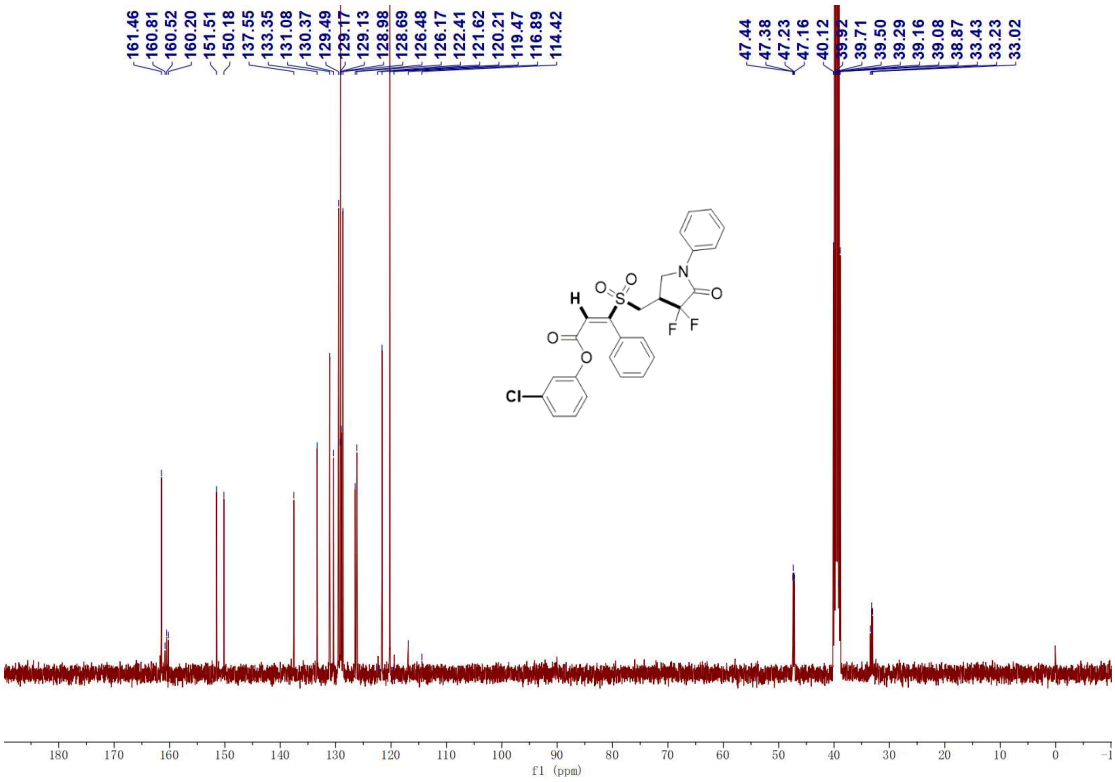
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **3ea**



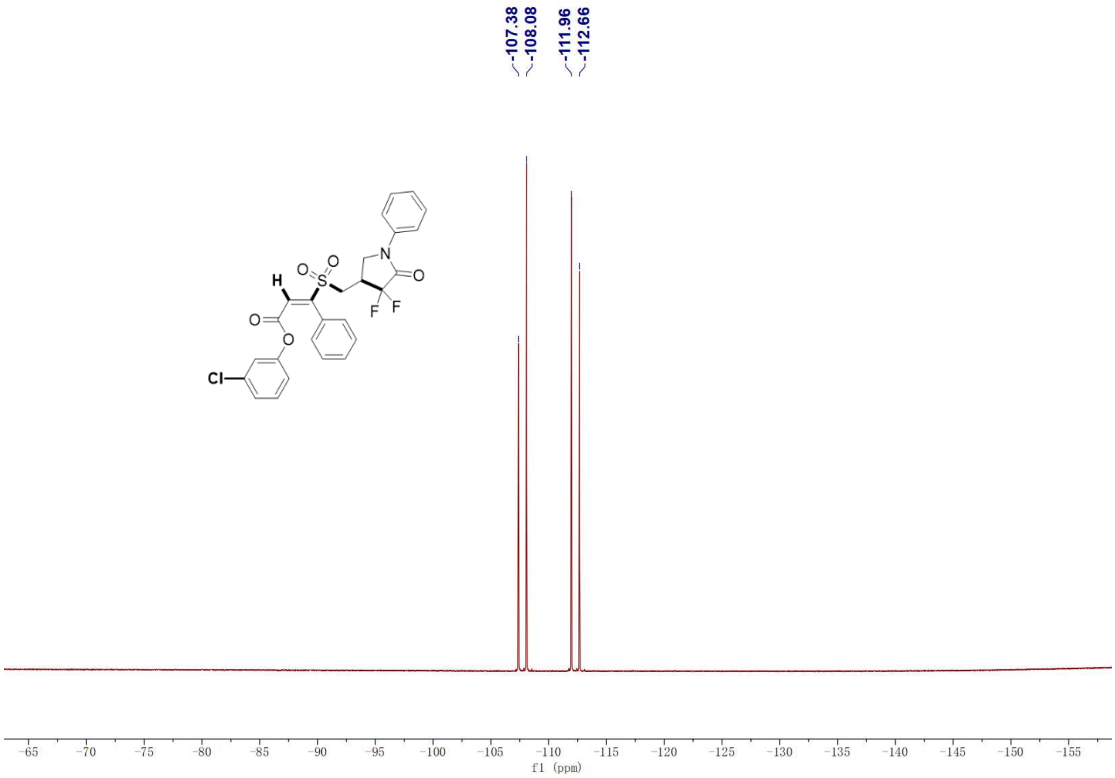
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3fa**



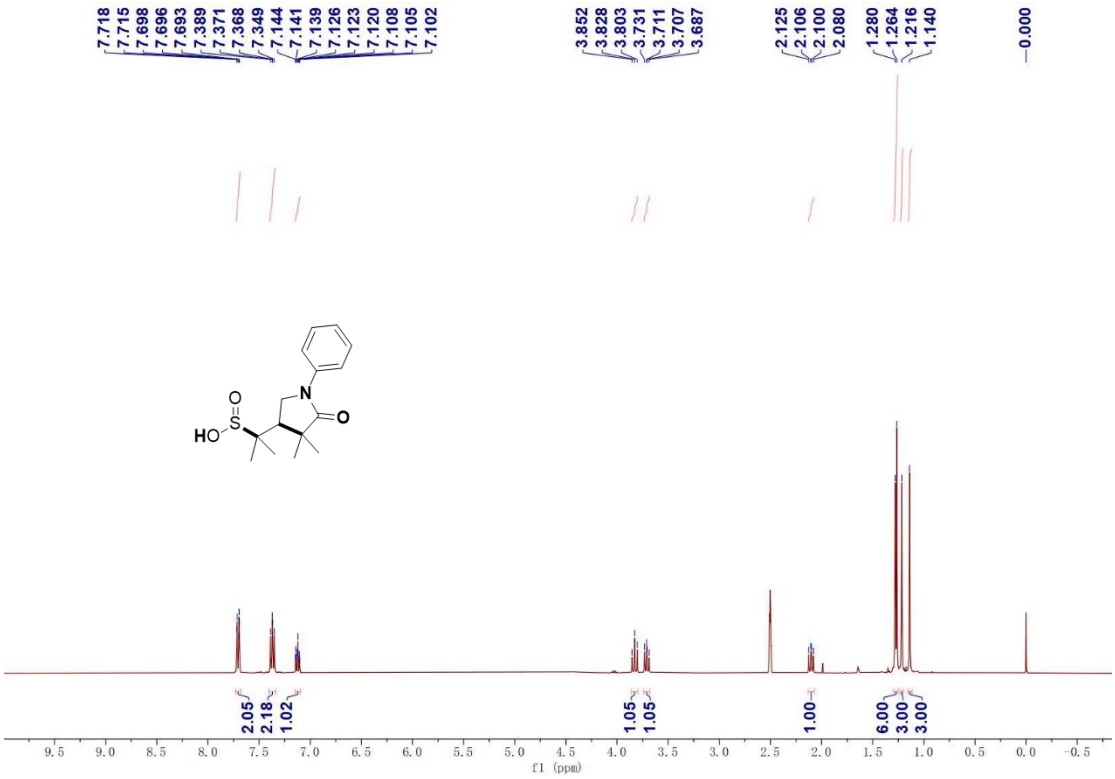
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3fa**



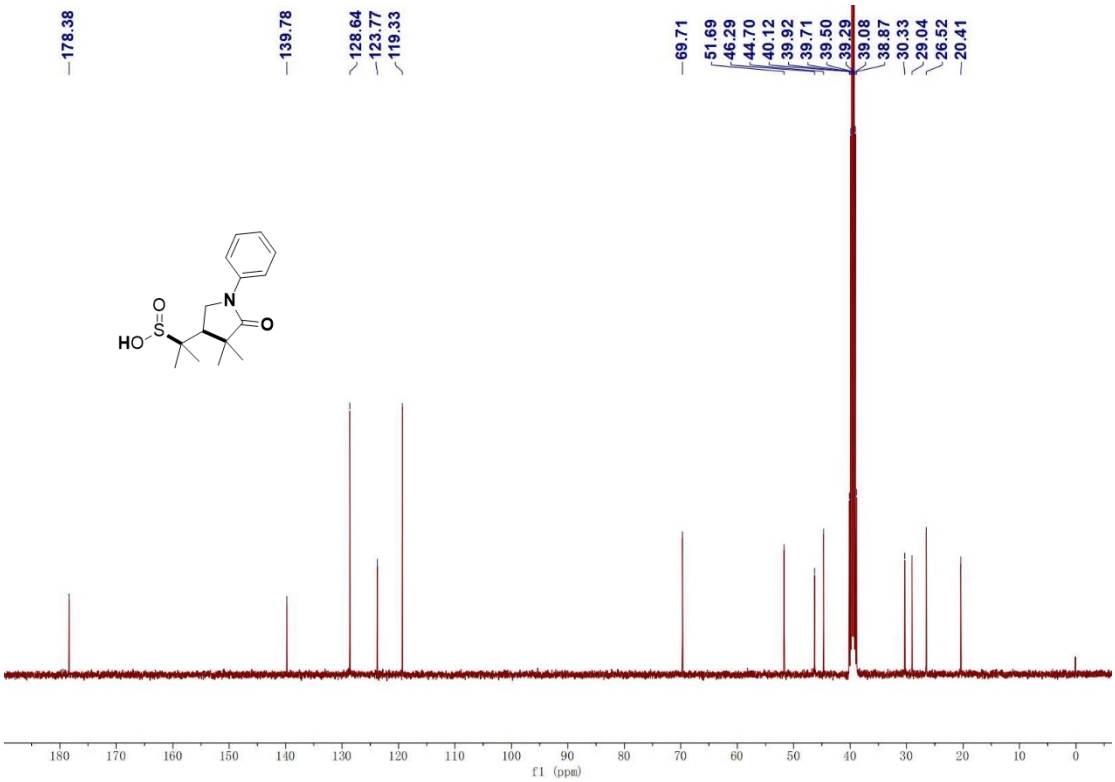
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **3fa**



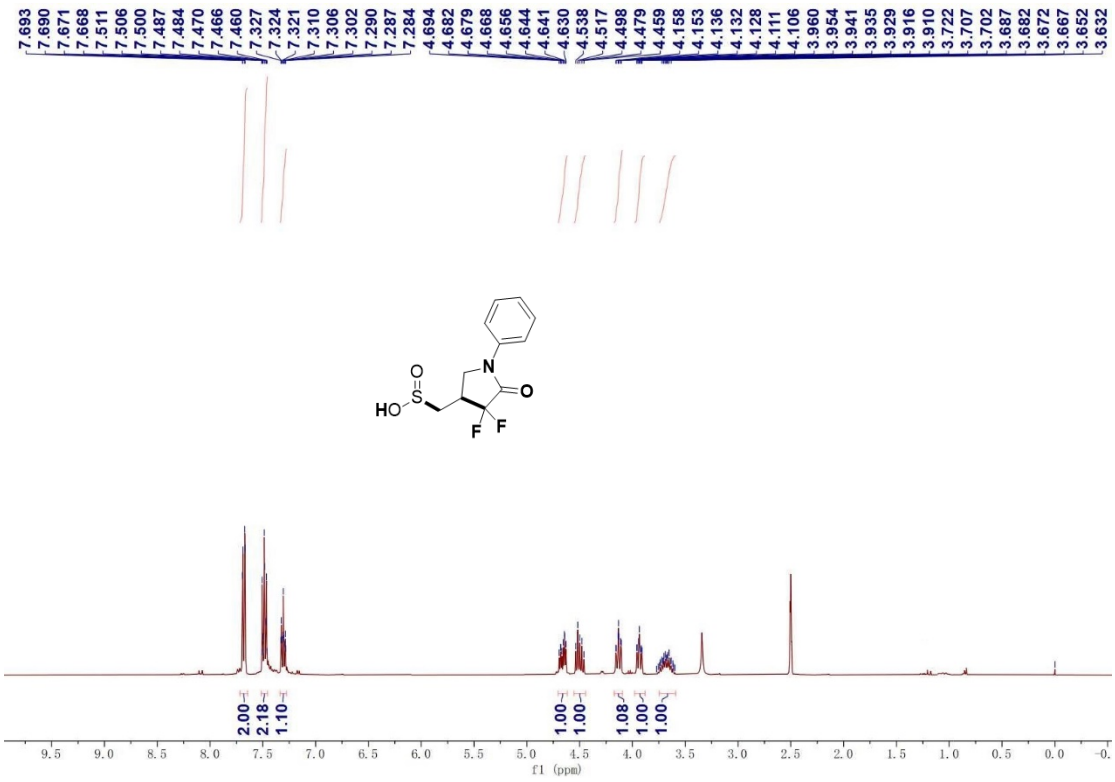
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3ap**



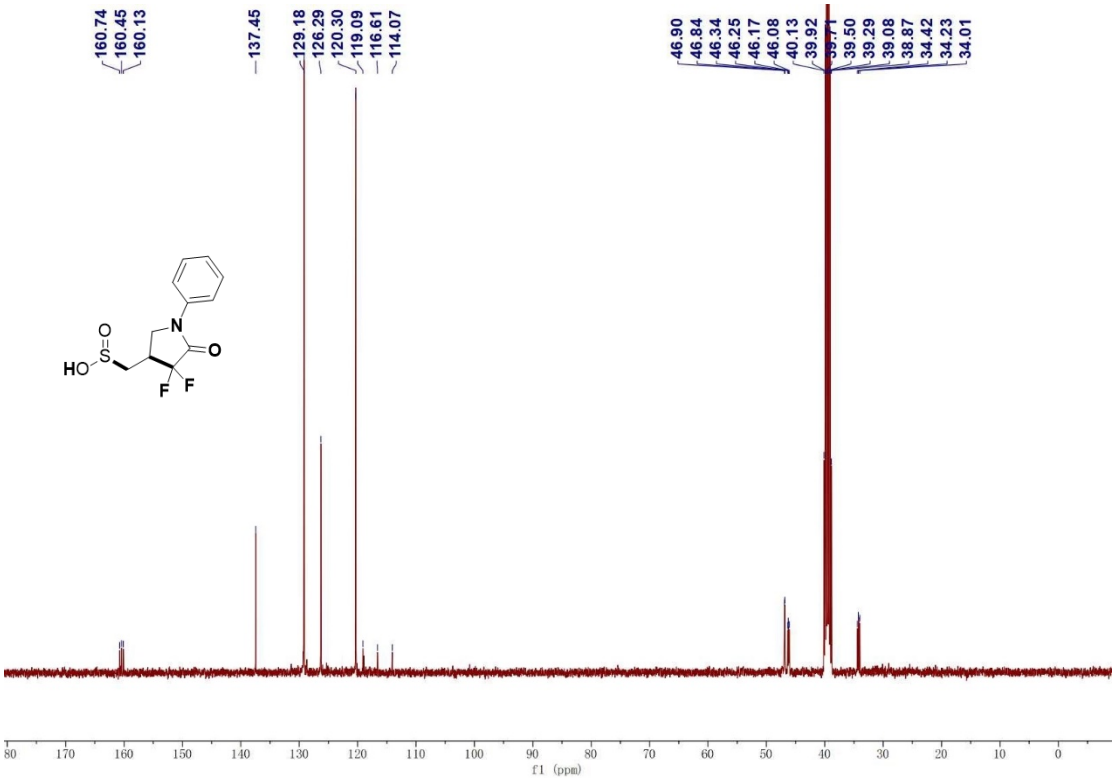
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3ap**



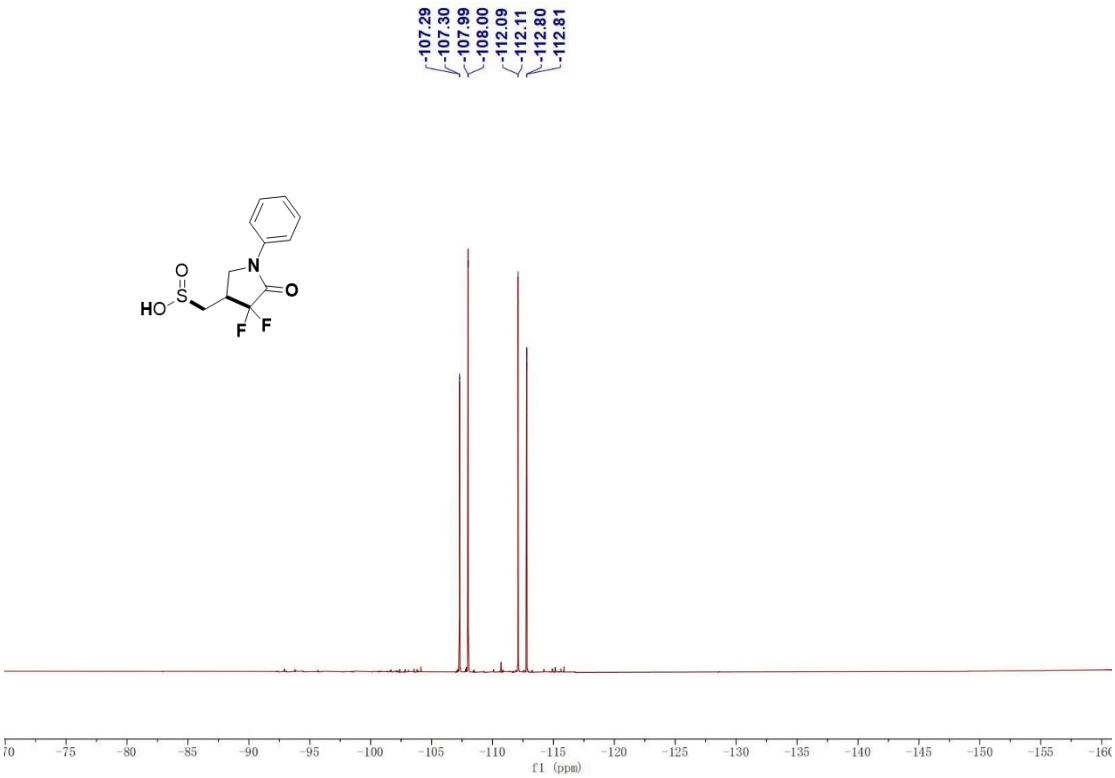
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **3ma**



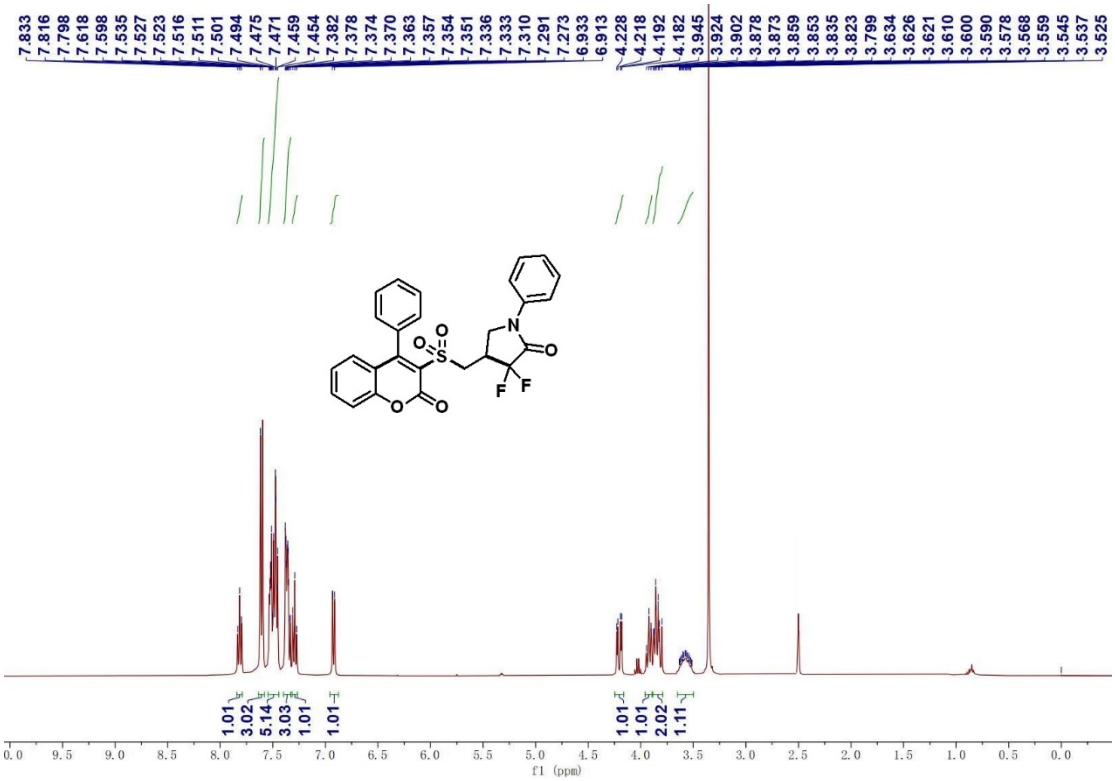
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **3ma**



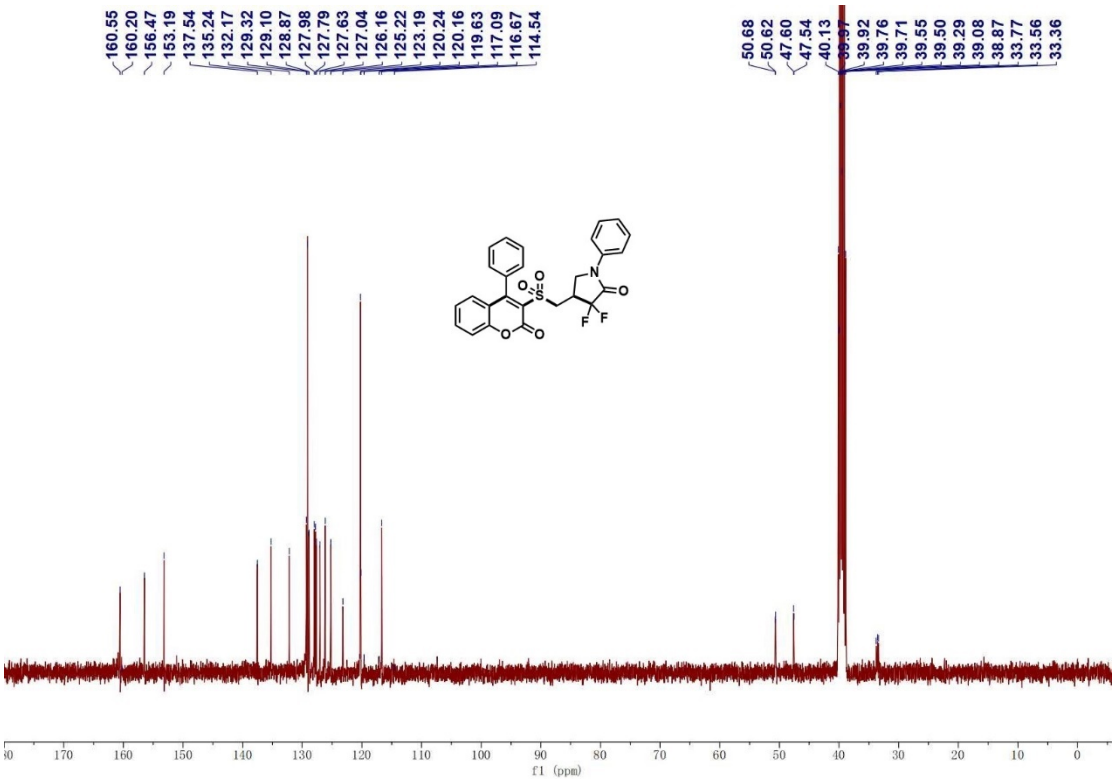
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **3ma**



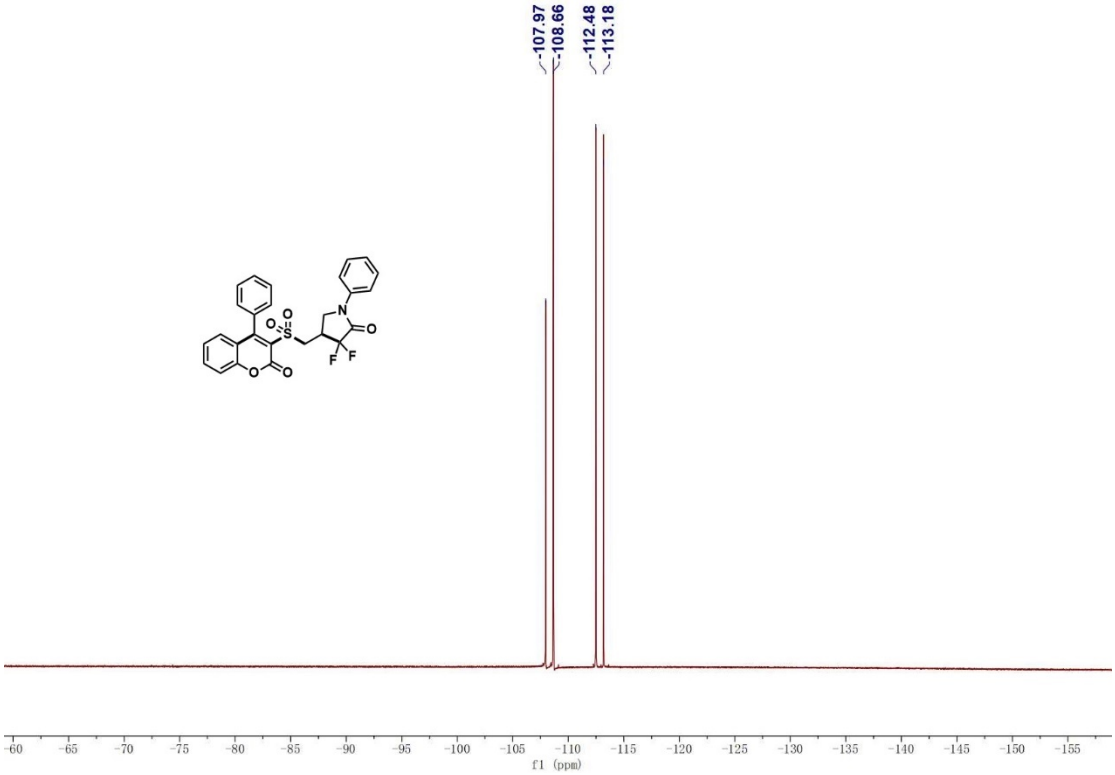
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4aa**



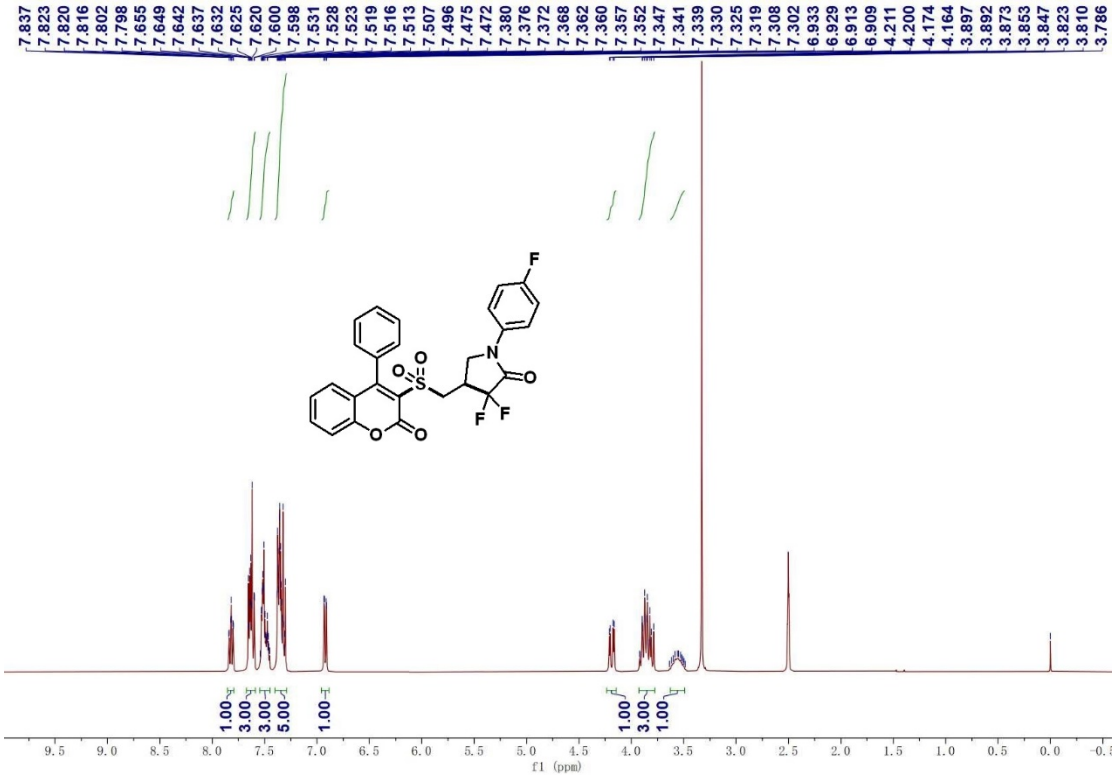
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4aa**



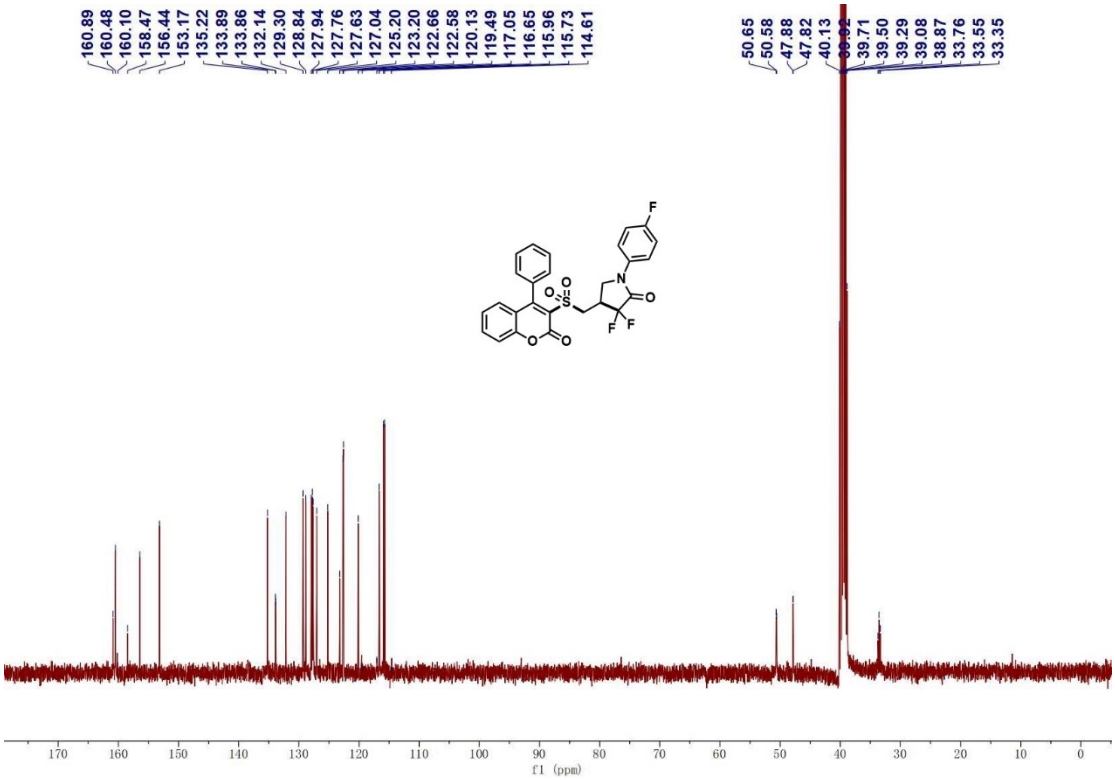
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4aa**



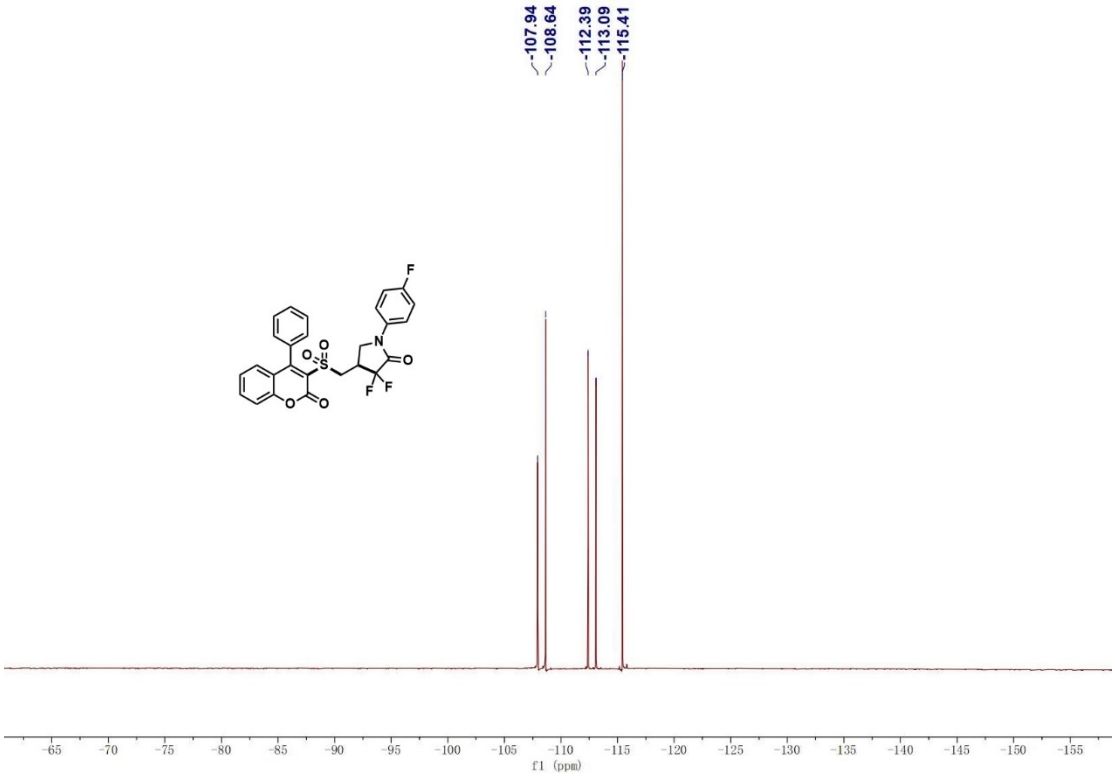
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ab**



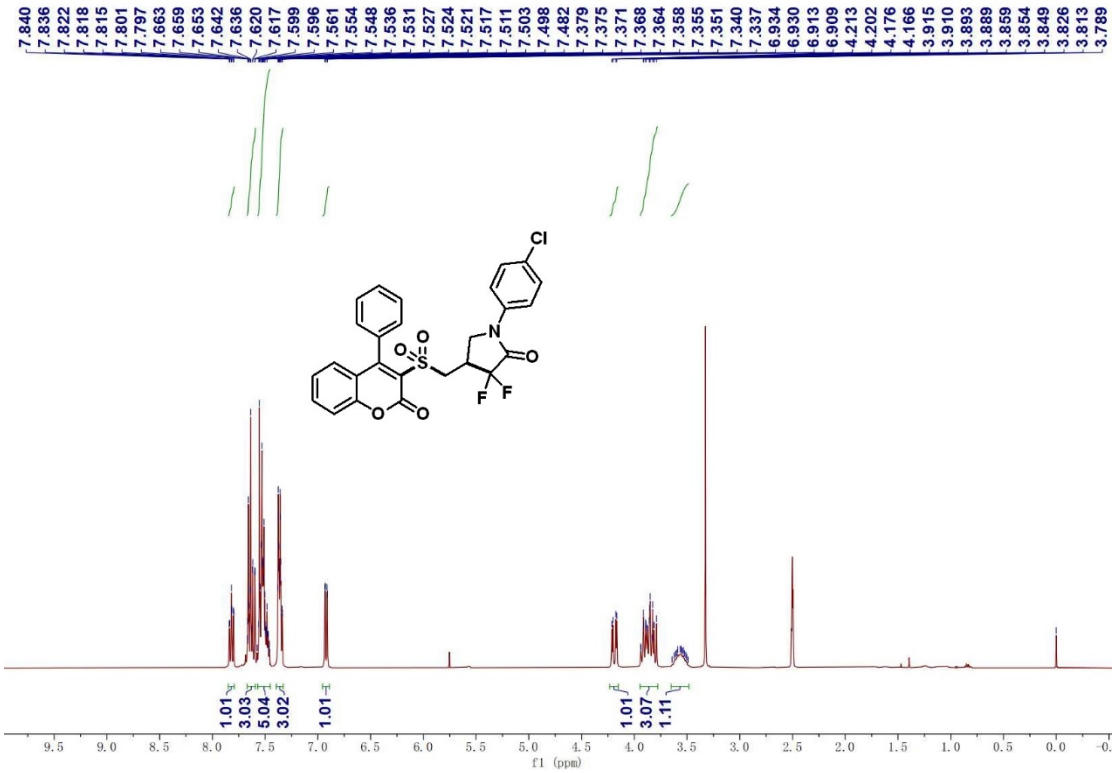
^{13}C NMR-spectrum (101MHz, DMSO-d_6) of **4ab**



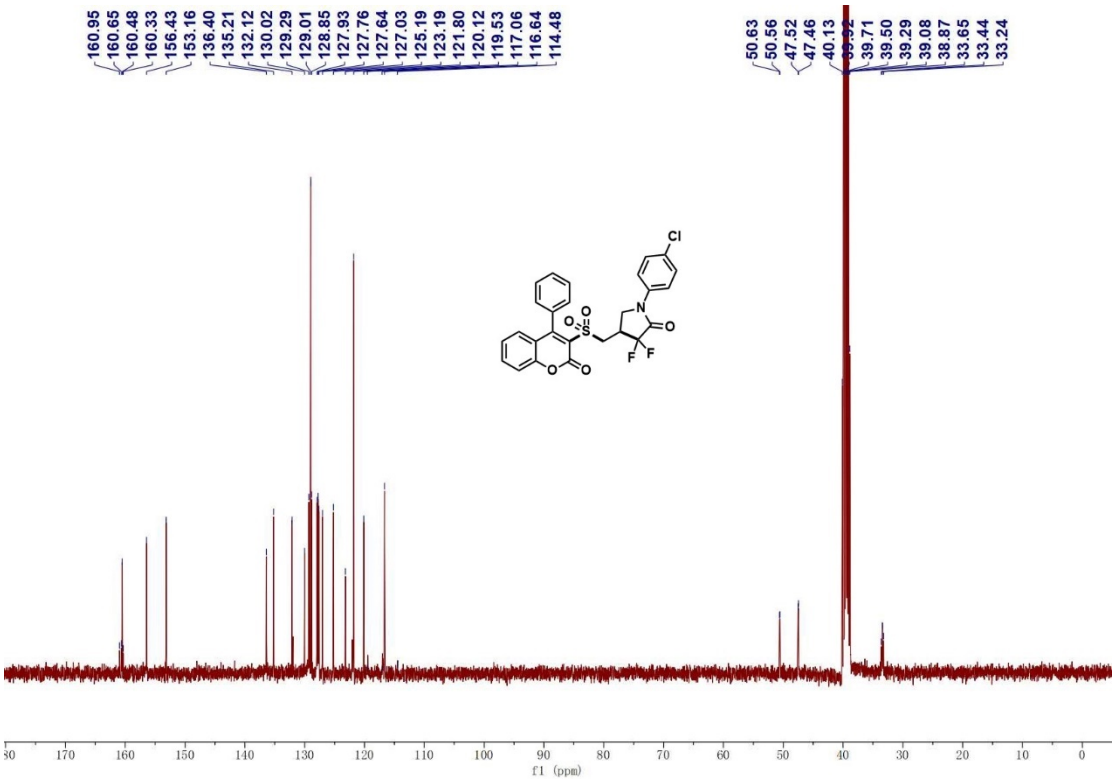
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ab**



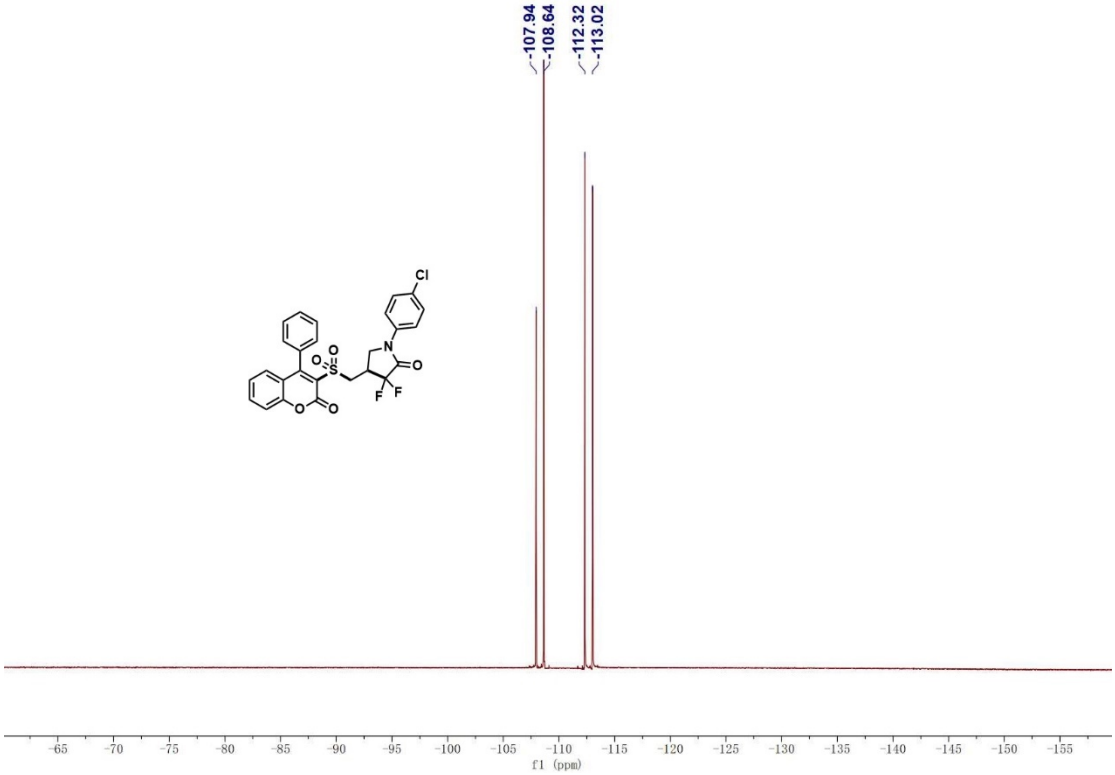
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ac**



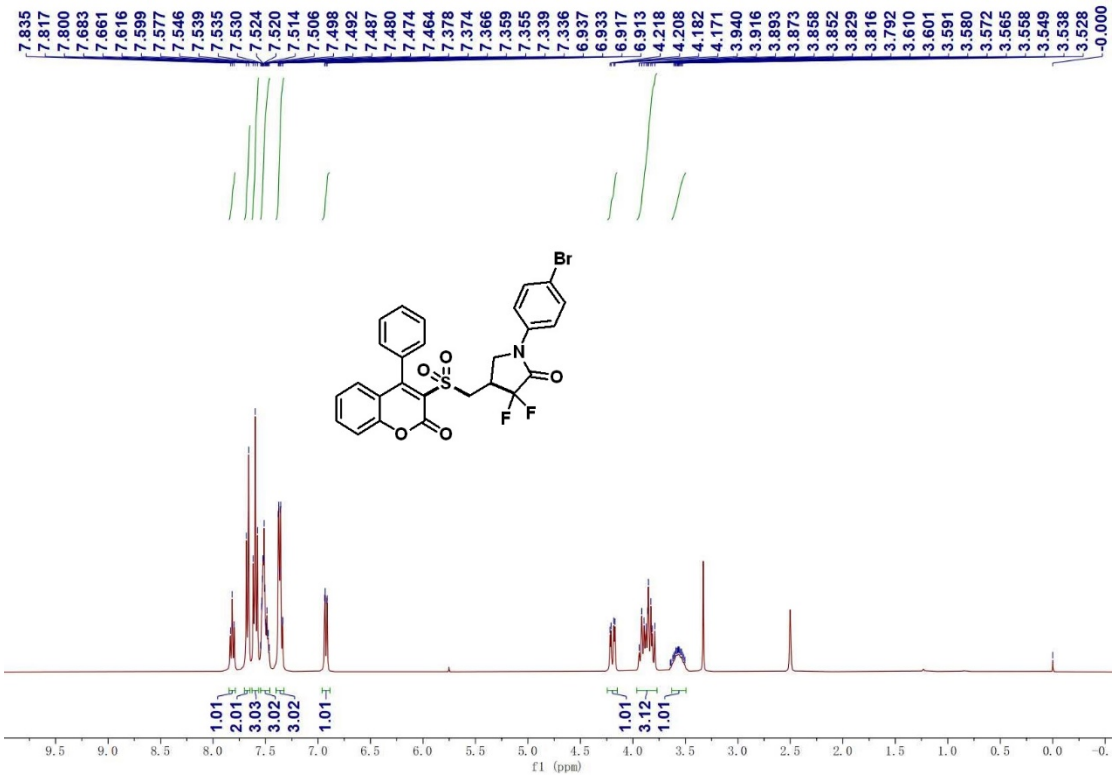
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ac**



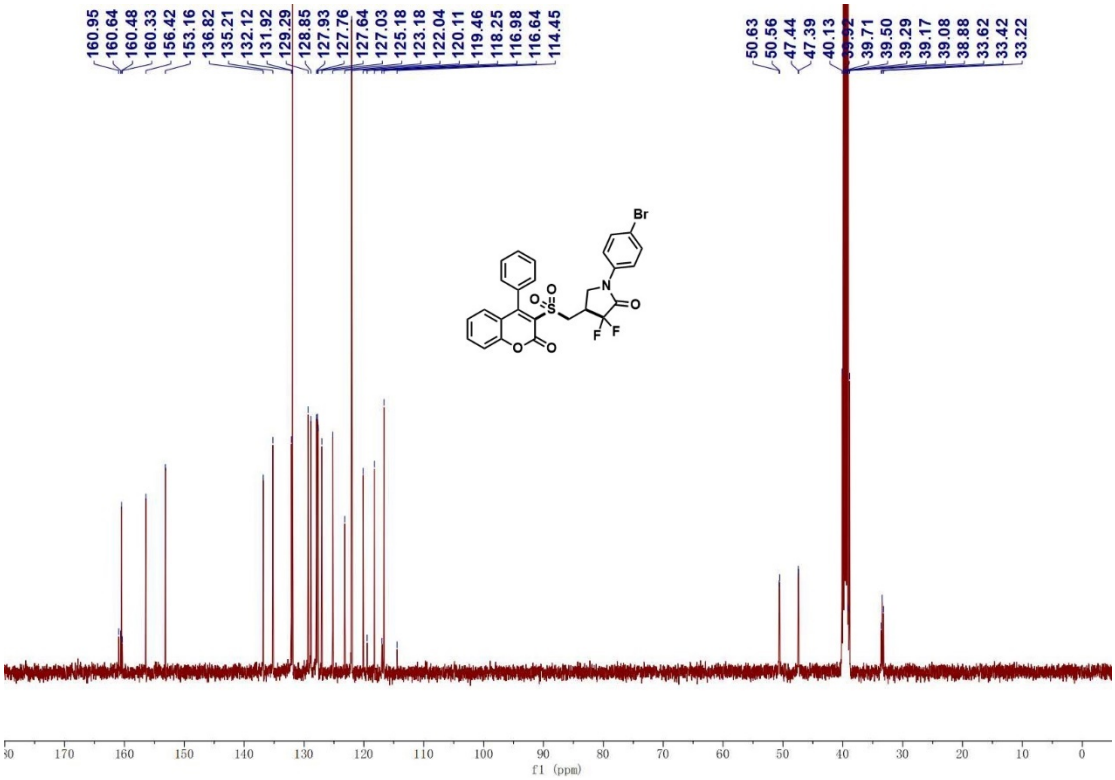
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ac**



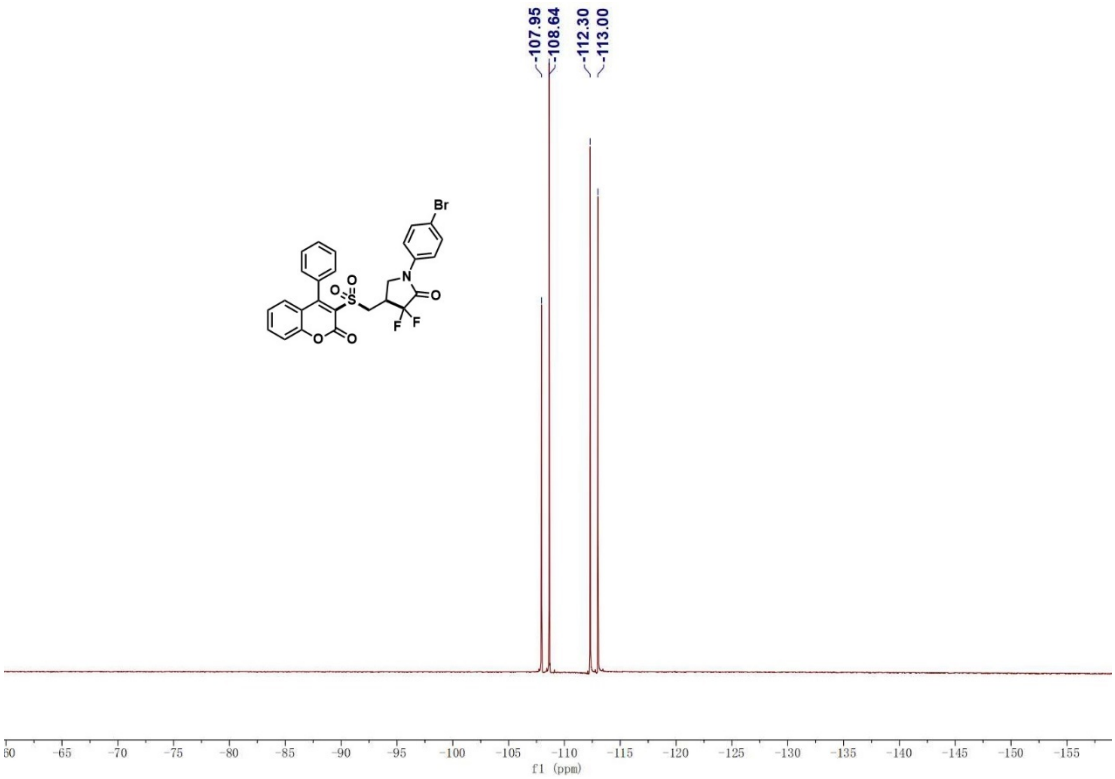
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ad**



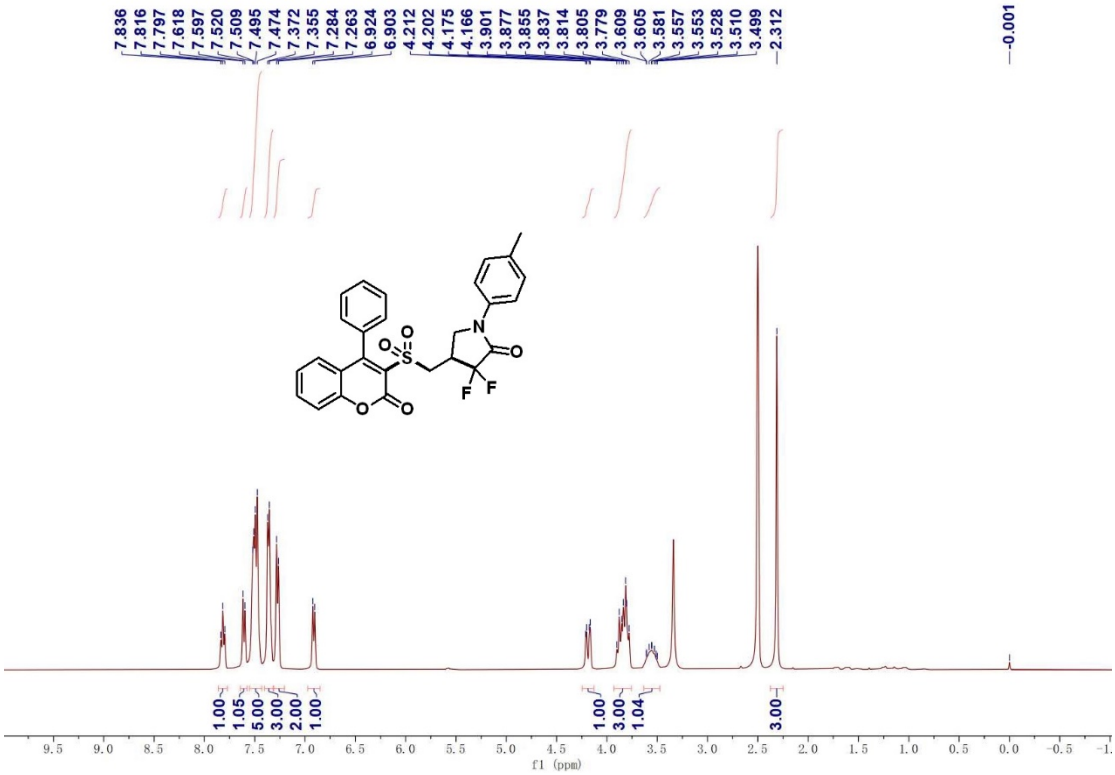
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ad**



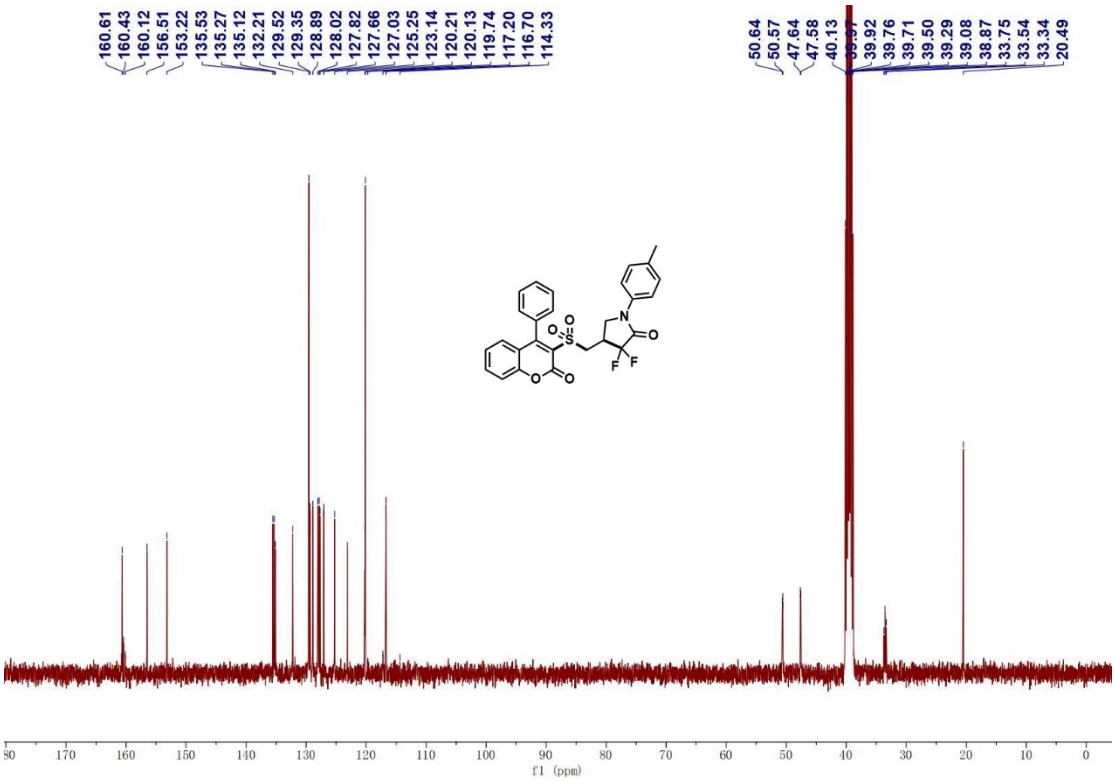
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ad**



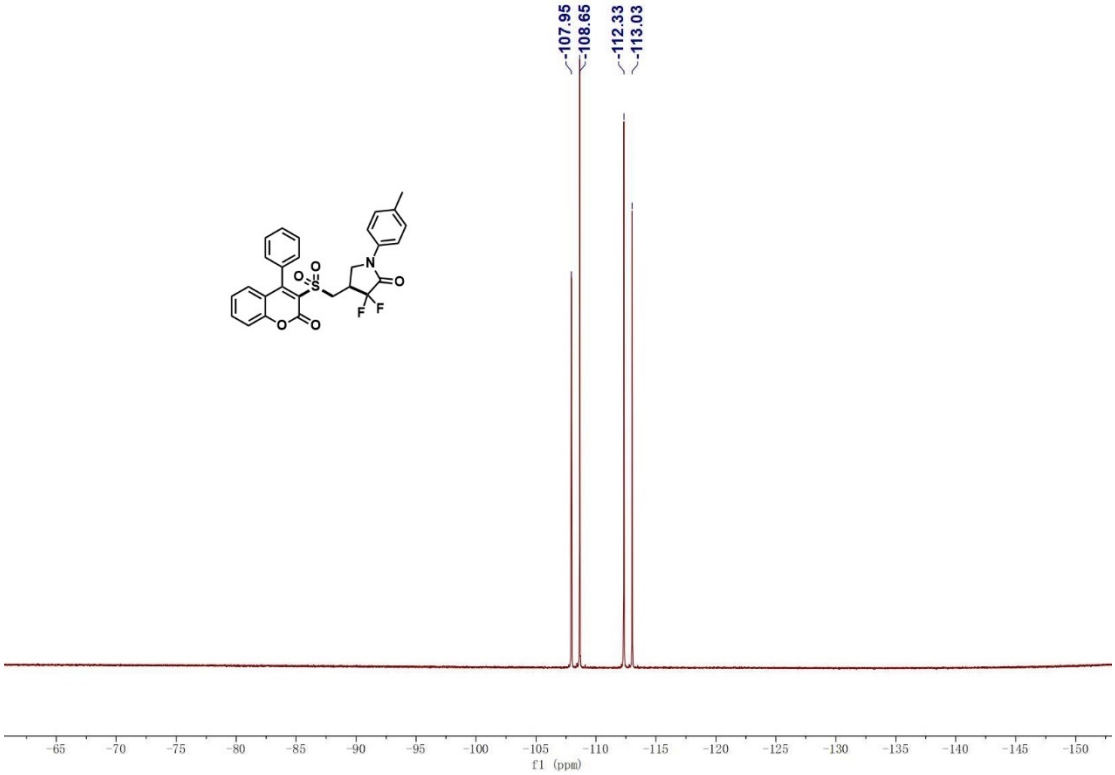
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ae**



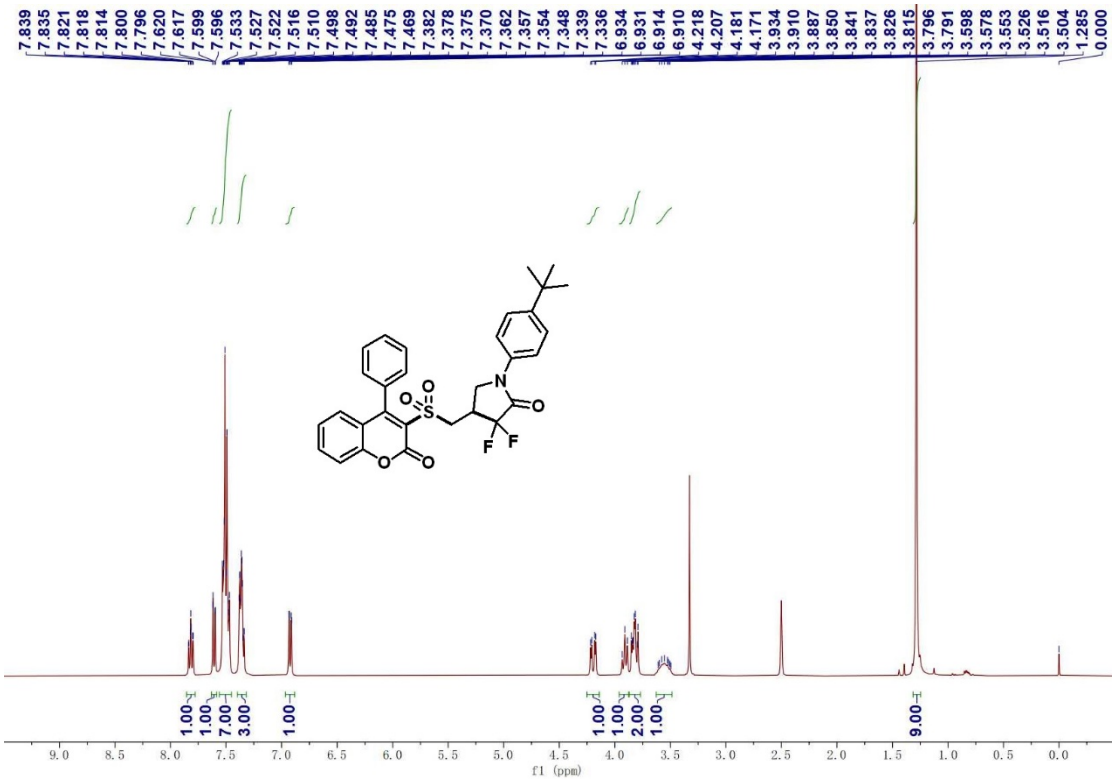
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ae**



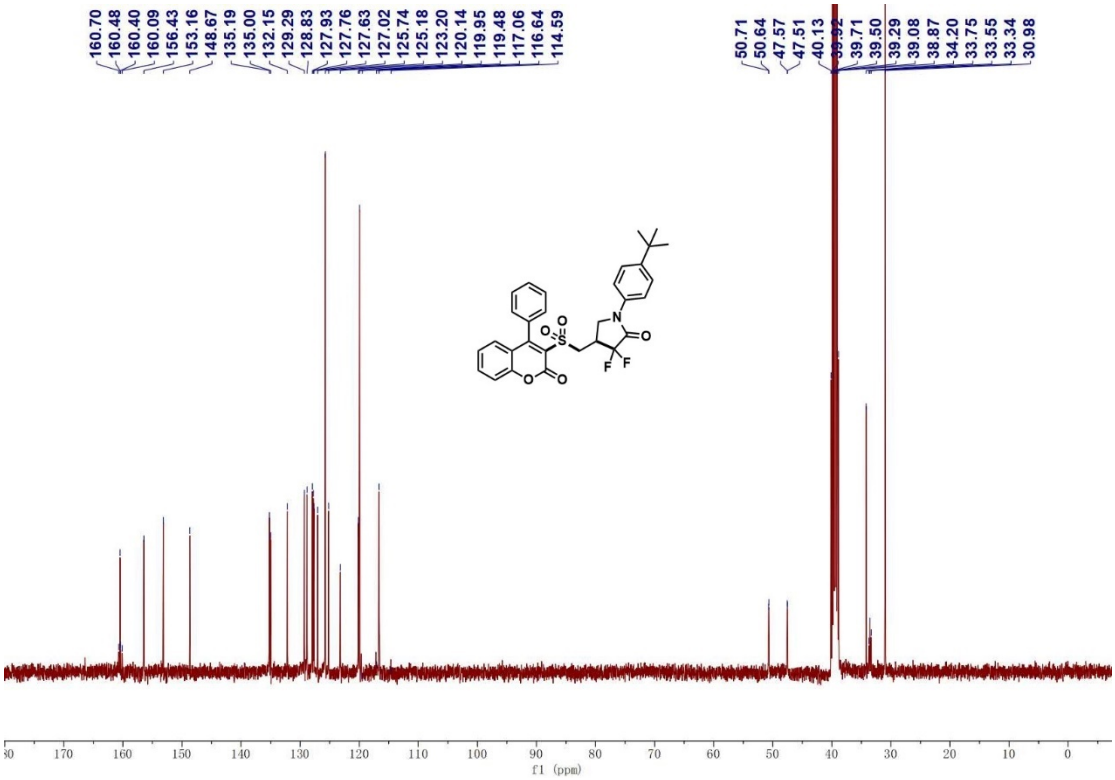
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ae**



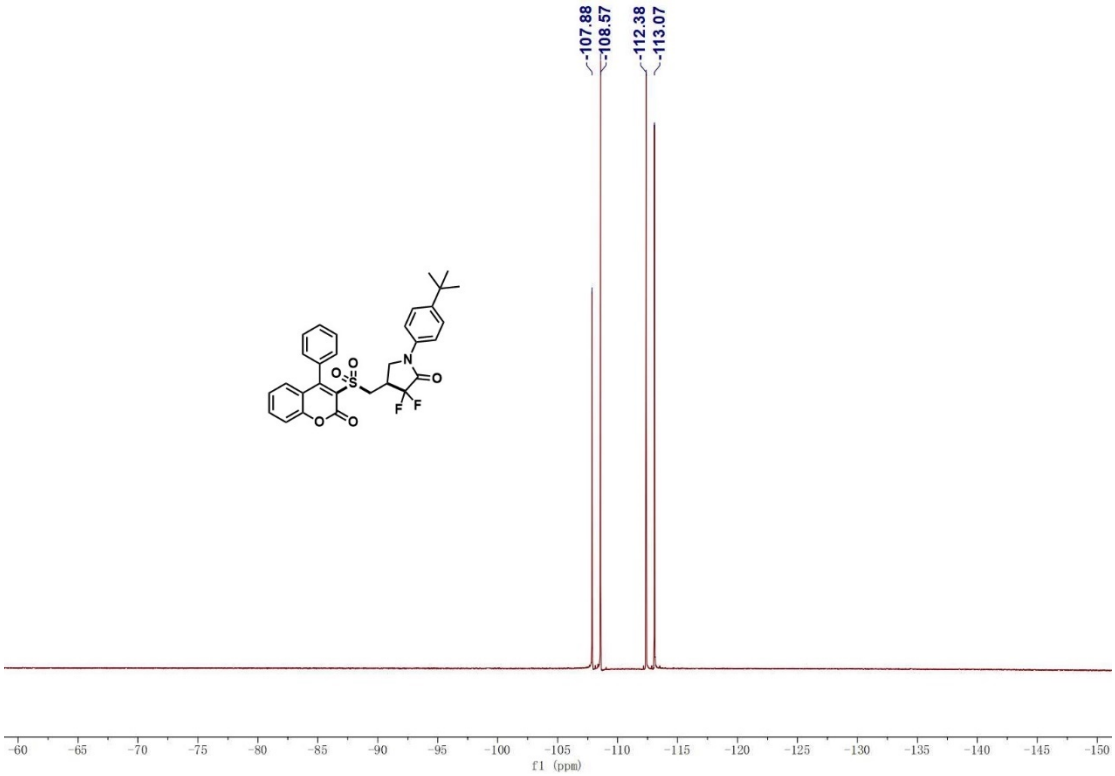
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4af**



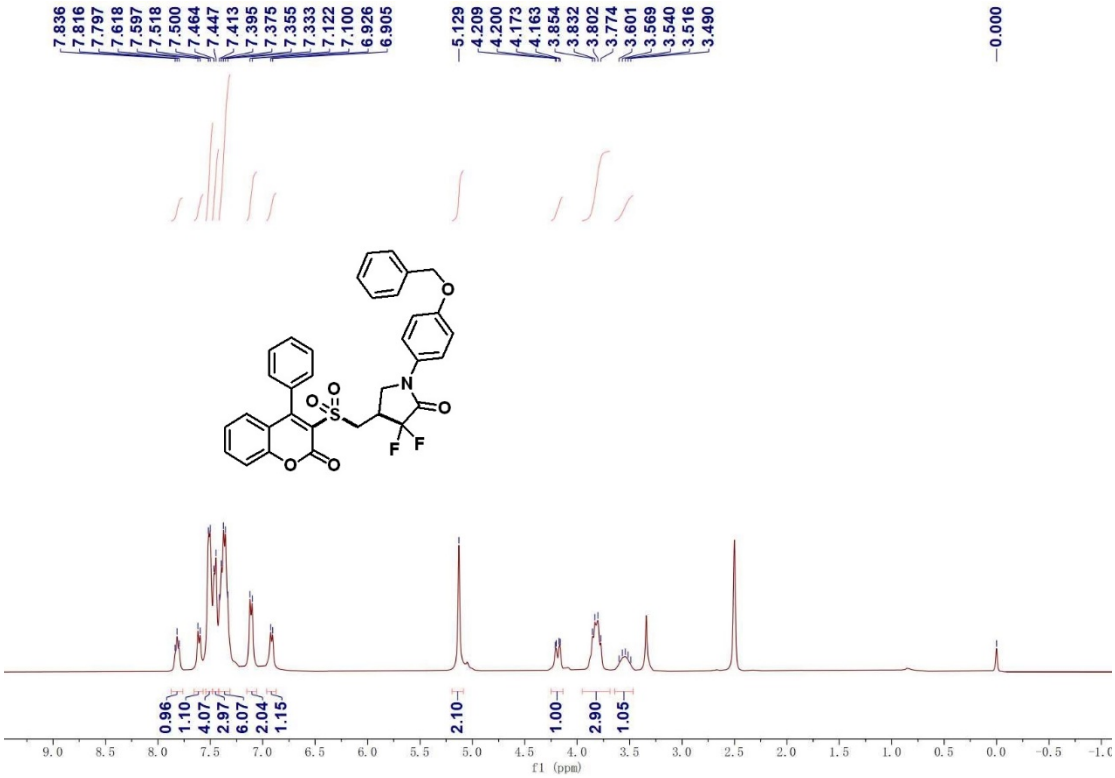
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4af**



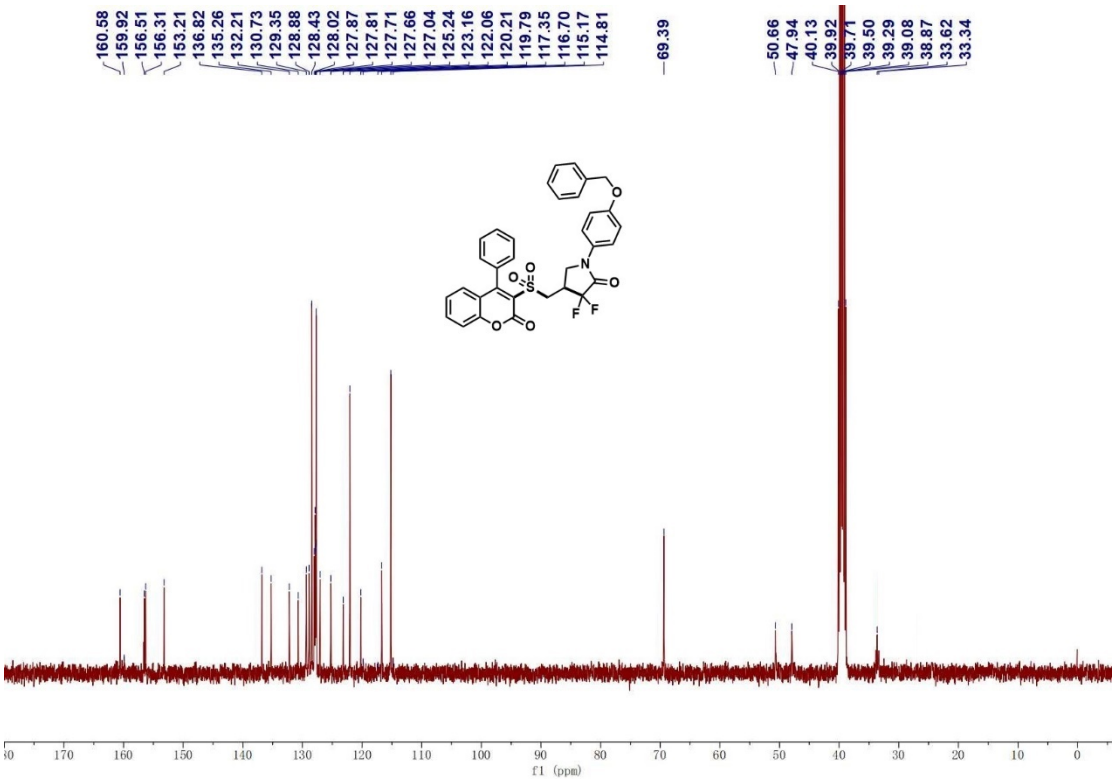
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4af**



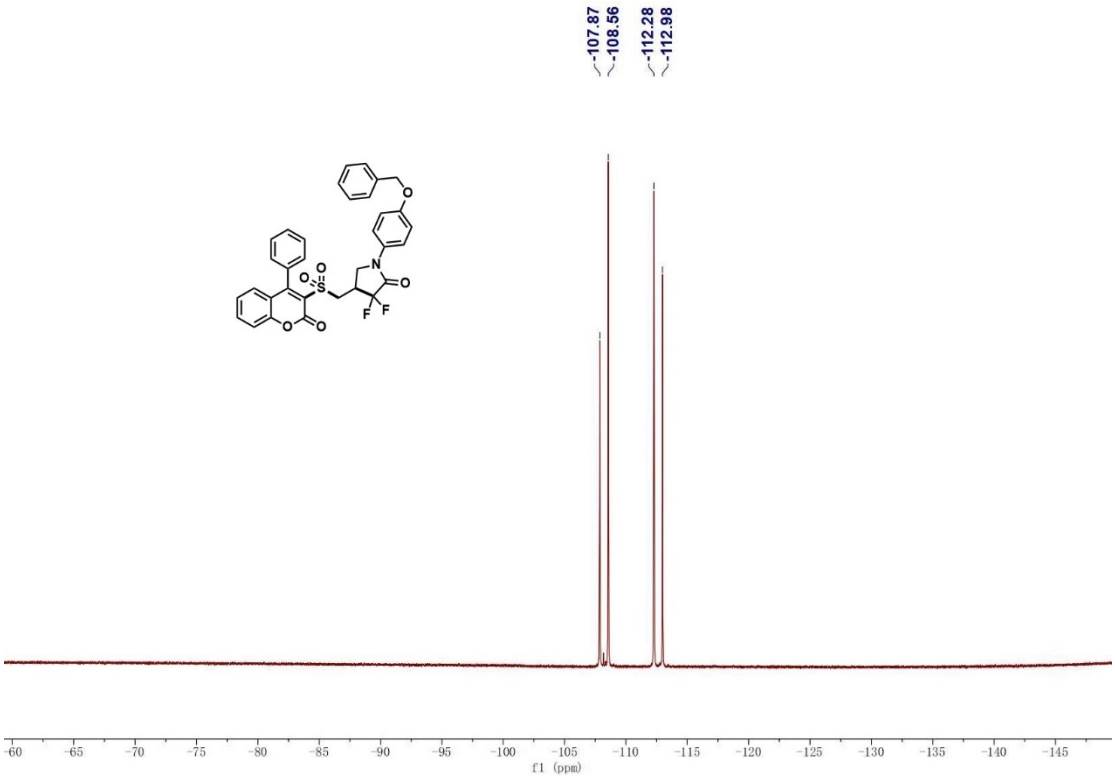
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ag**



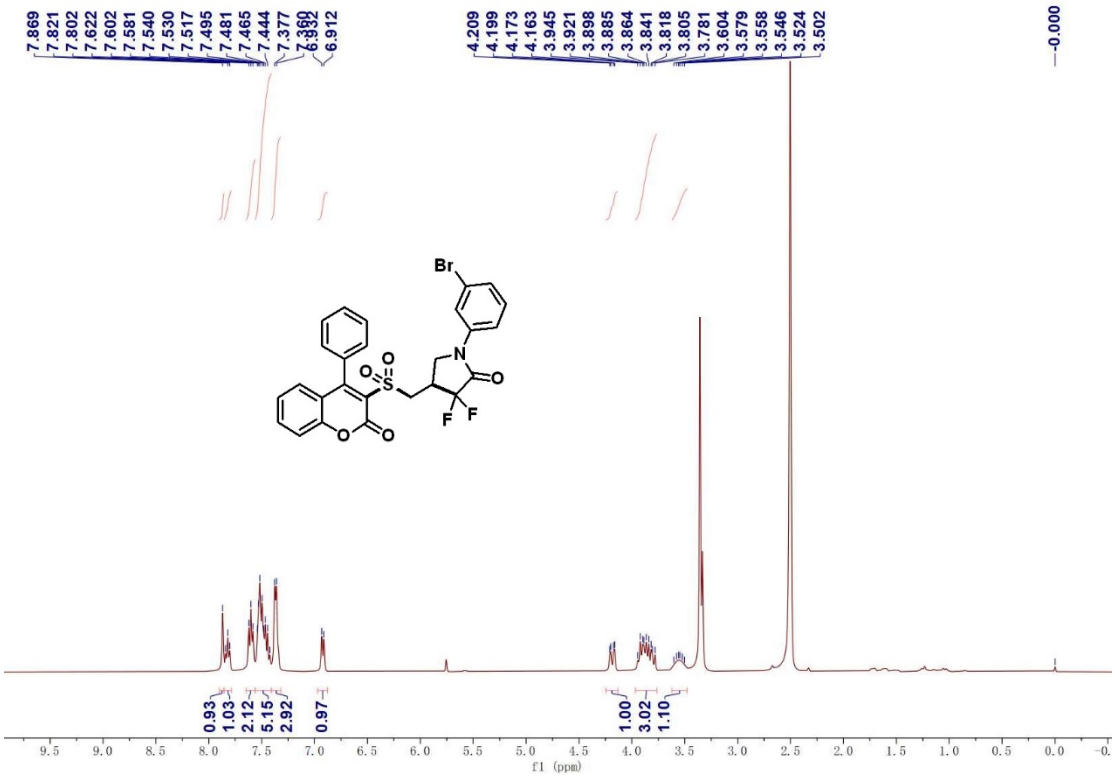
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ag**



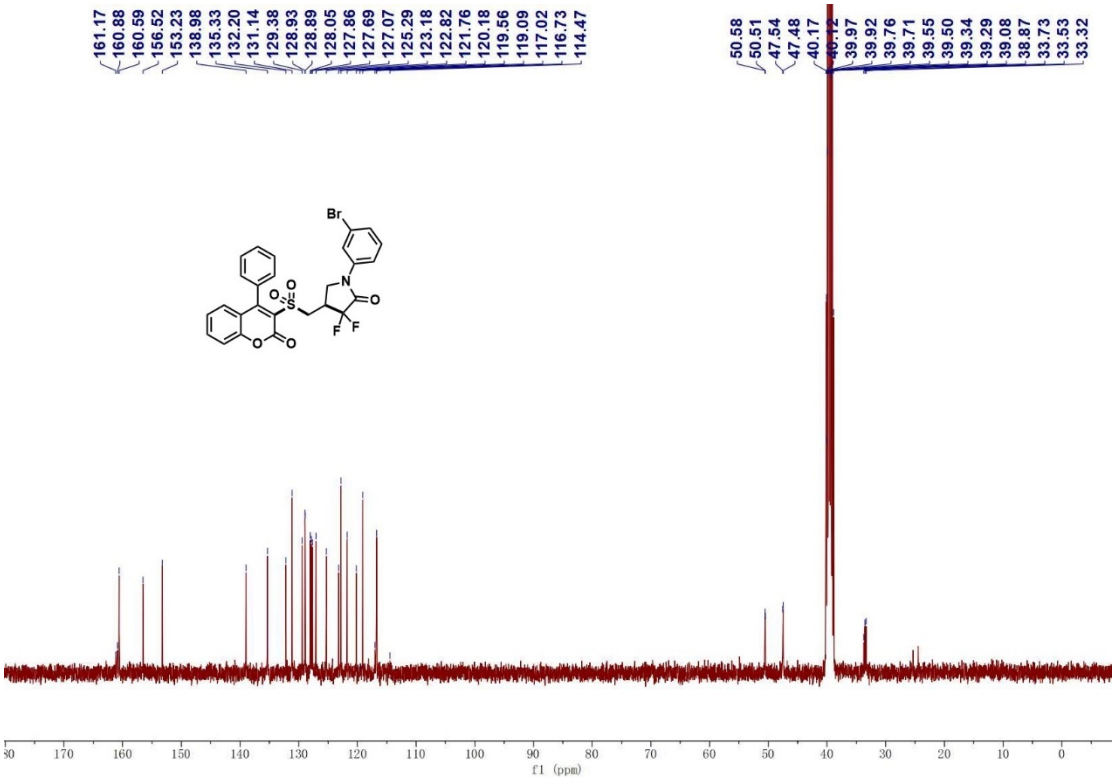
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ag**



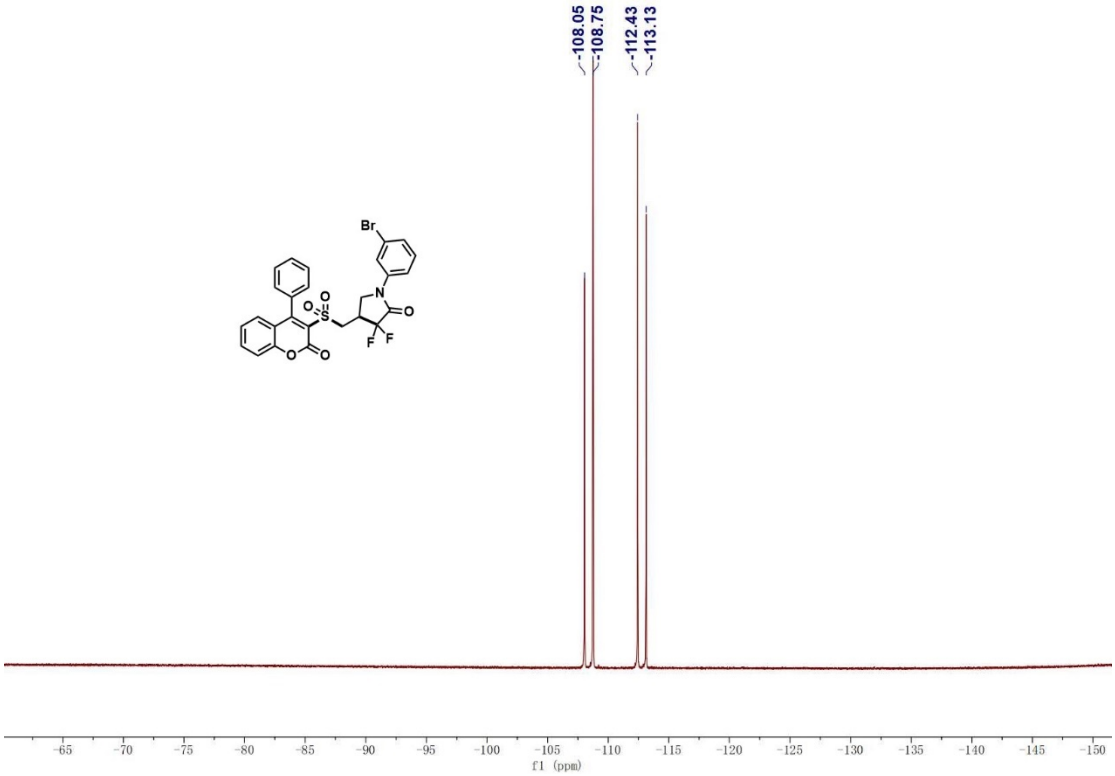
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ah**



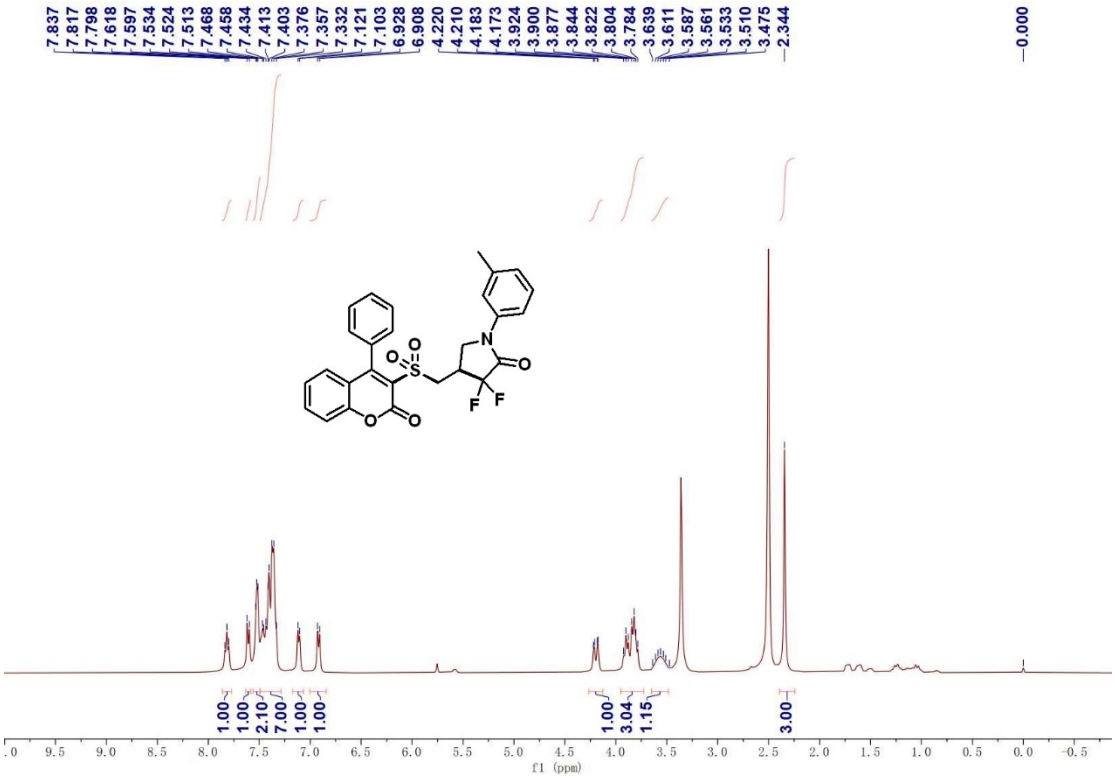
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ah**



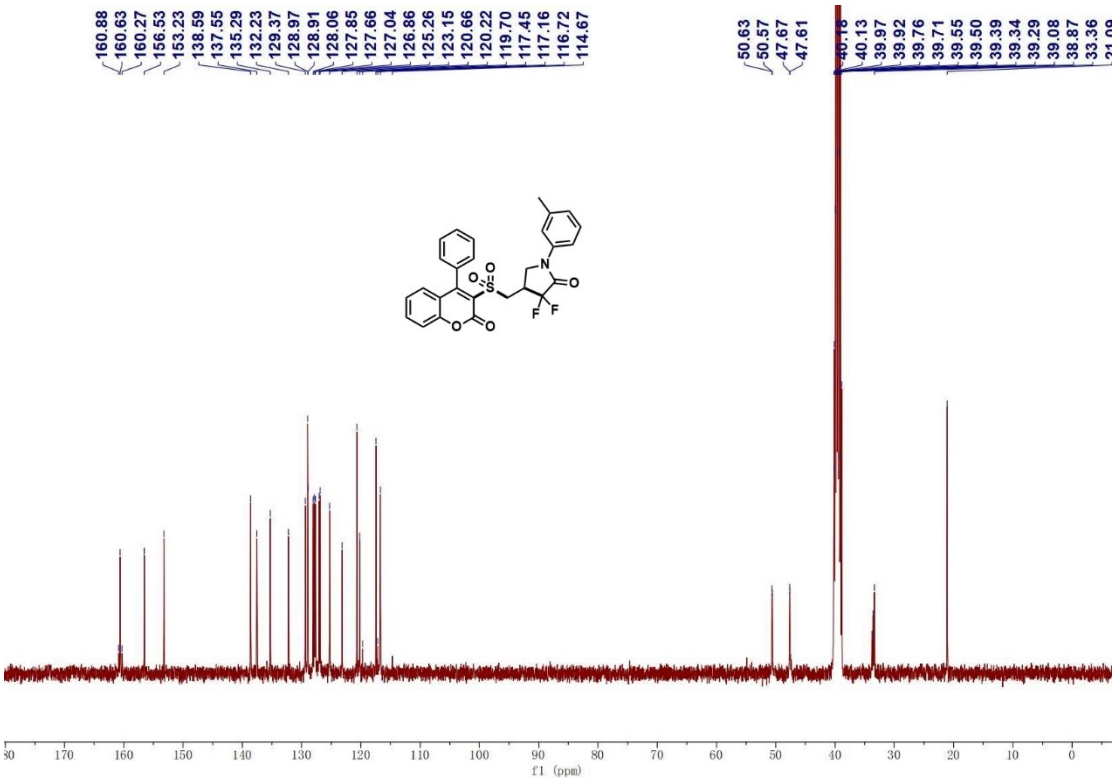
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ah**



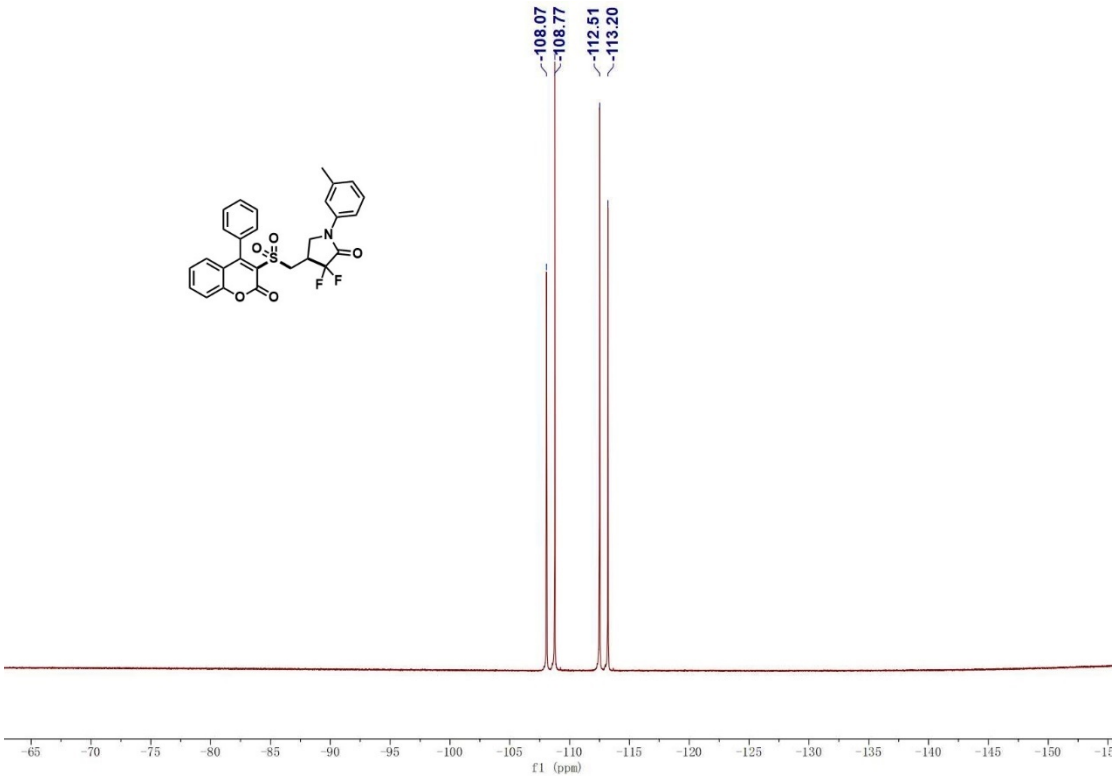
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ai**



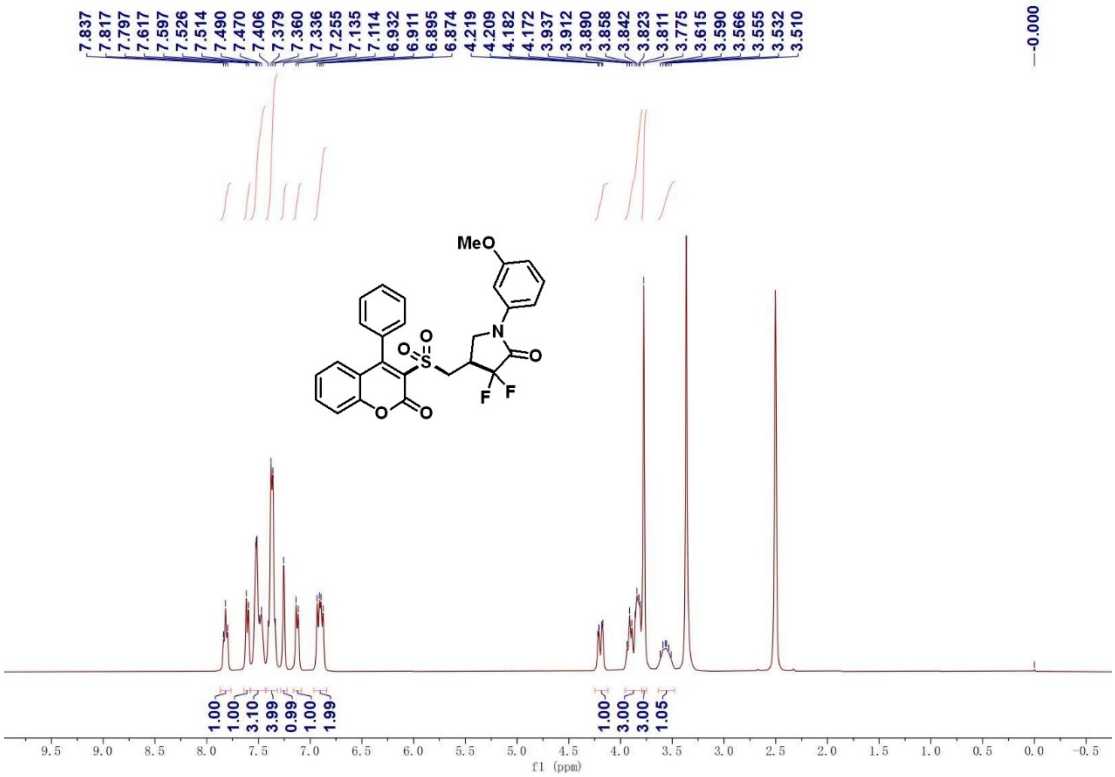
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ai**



^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ai**



^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4aj**



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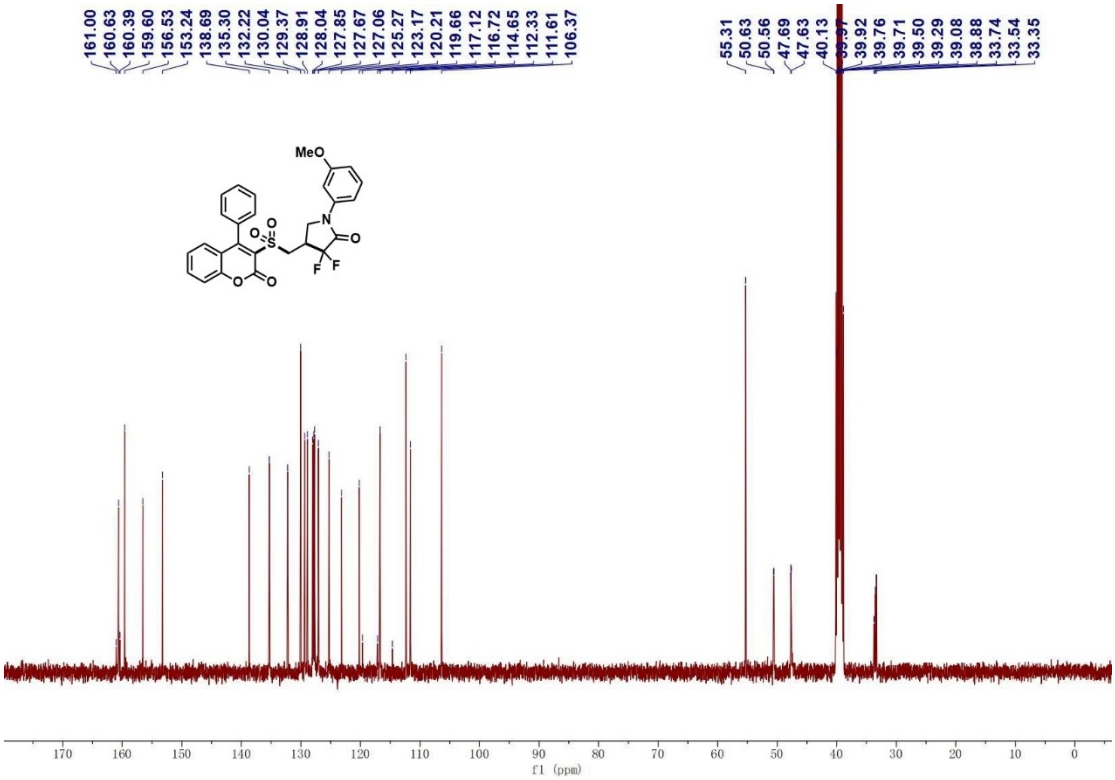
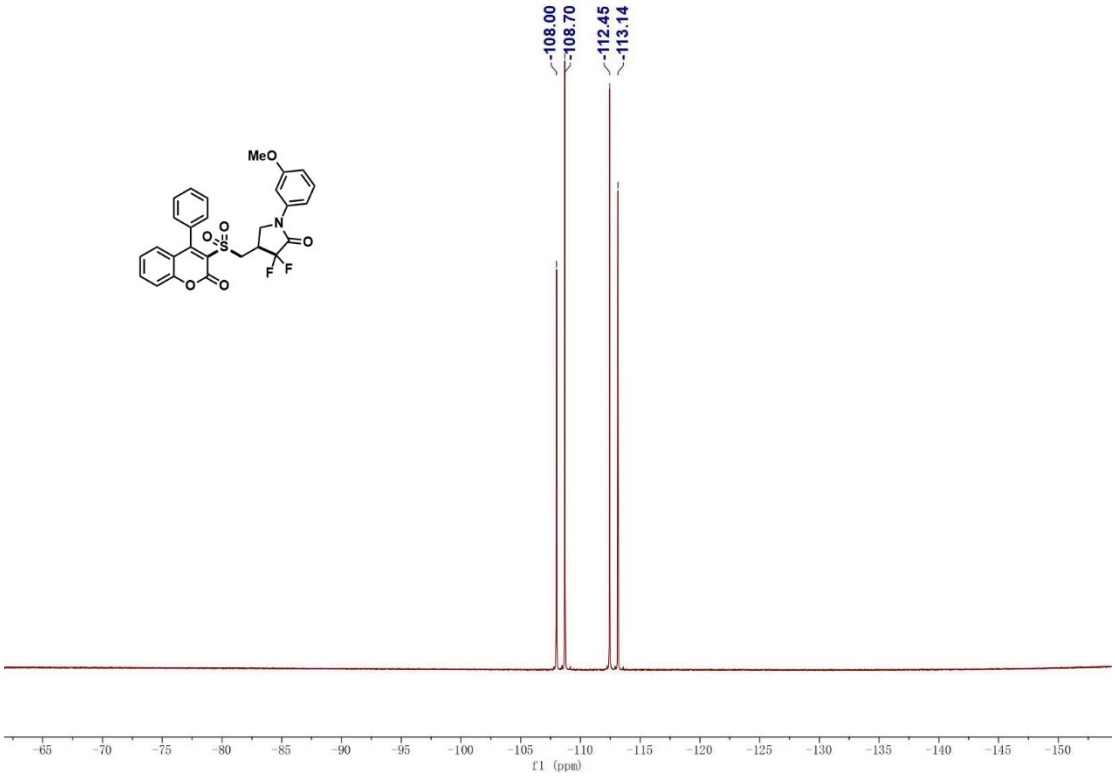
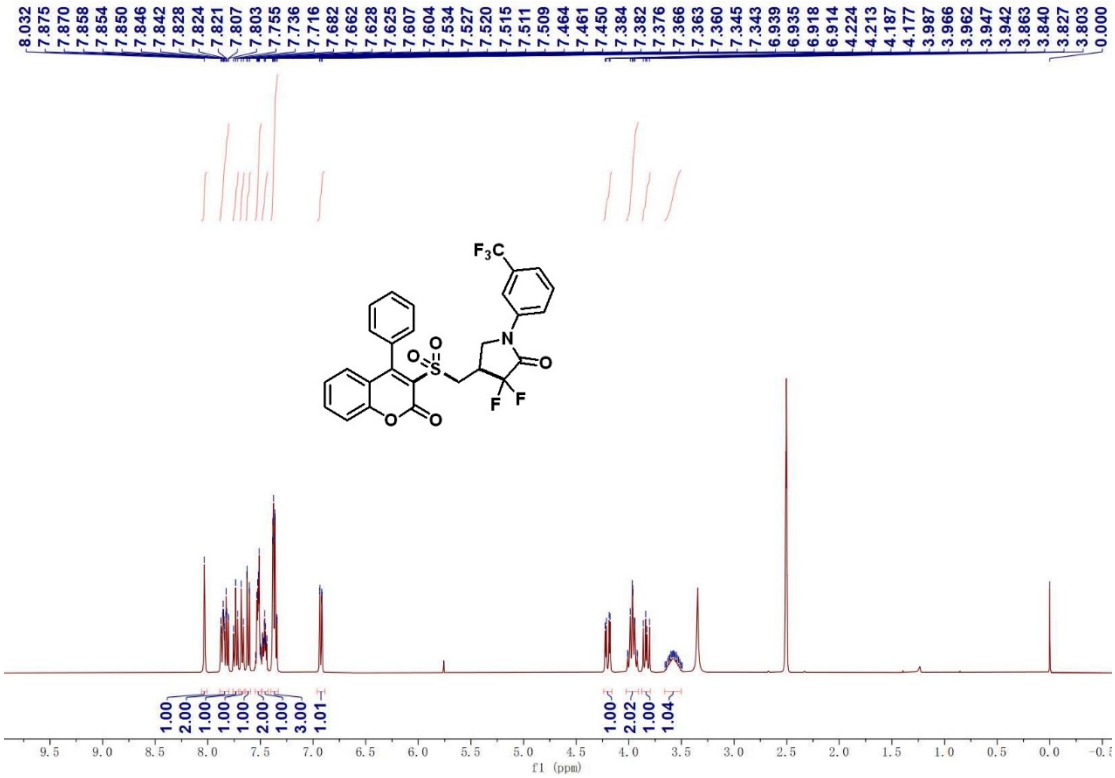


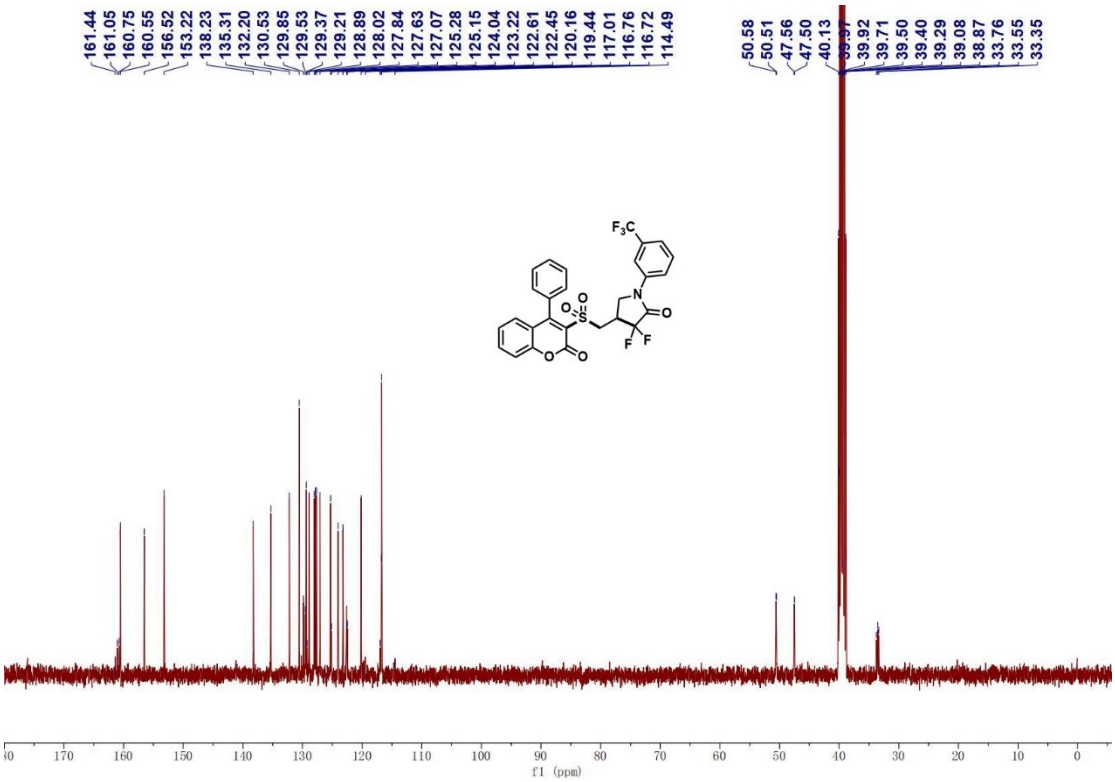
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4aj**



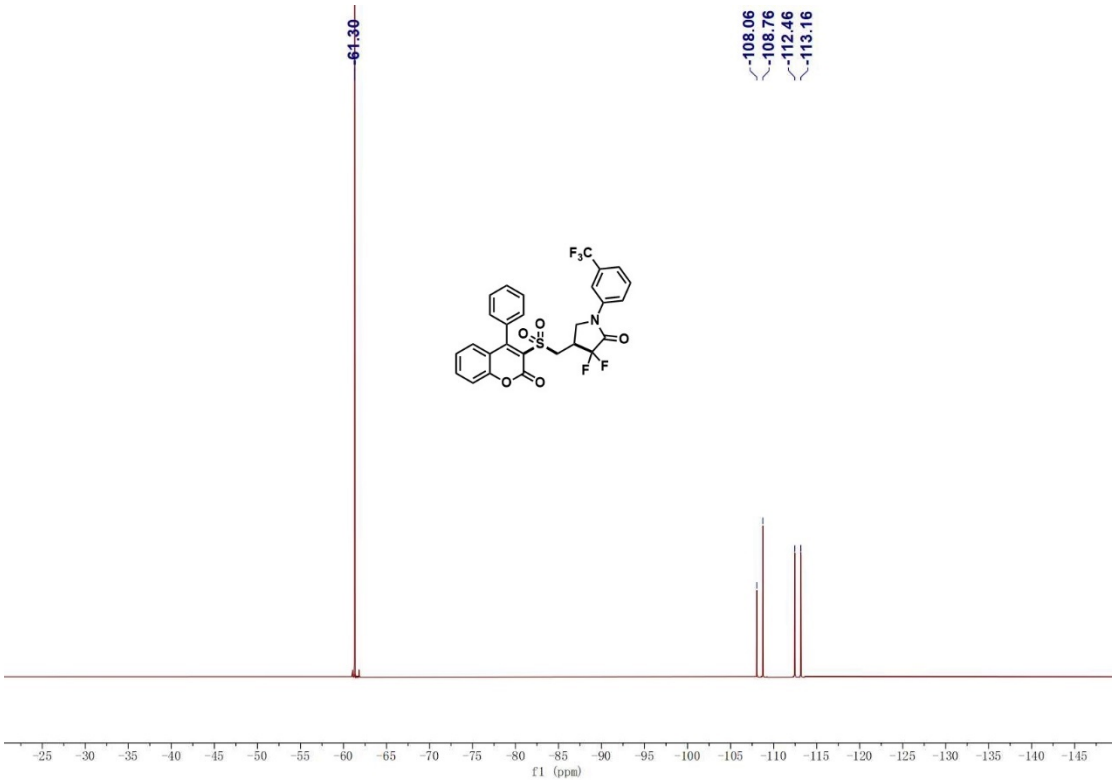
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ak**



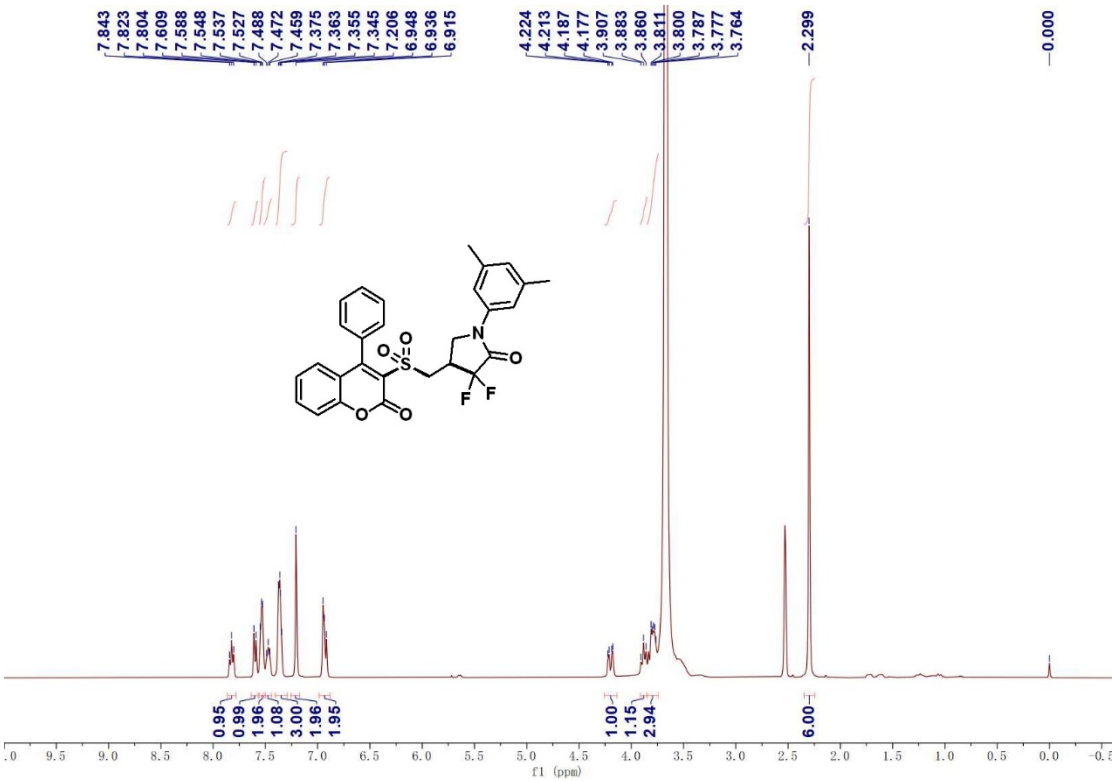
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ak**



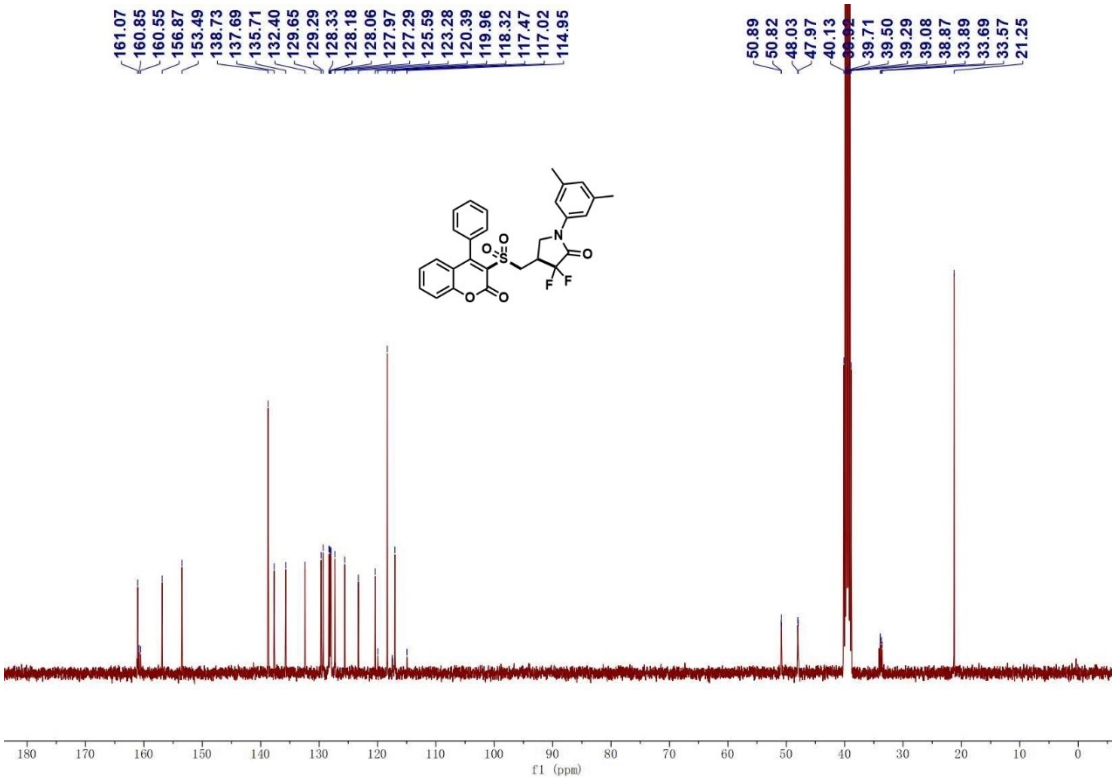
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ak**



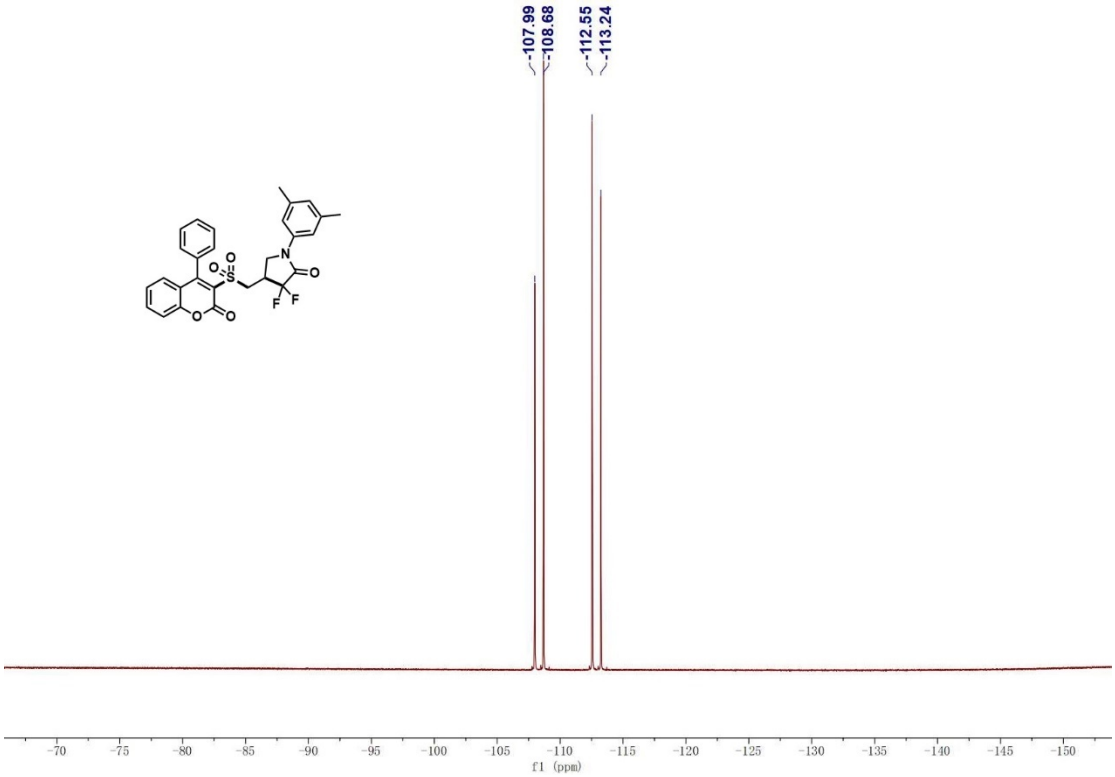
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4al**



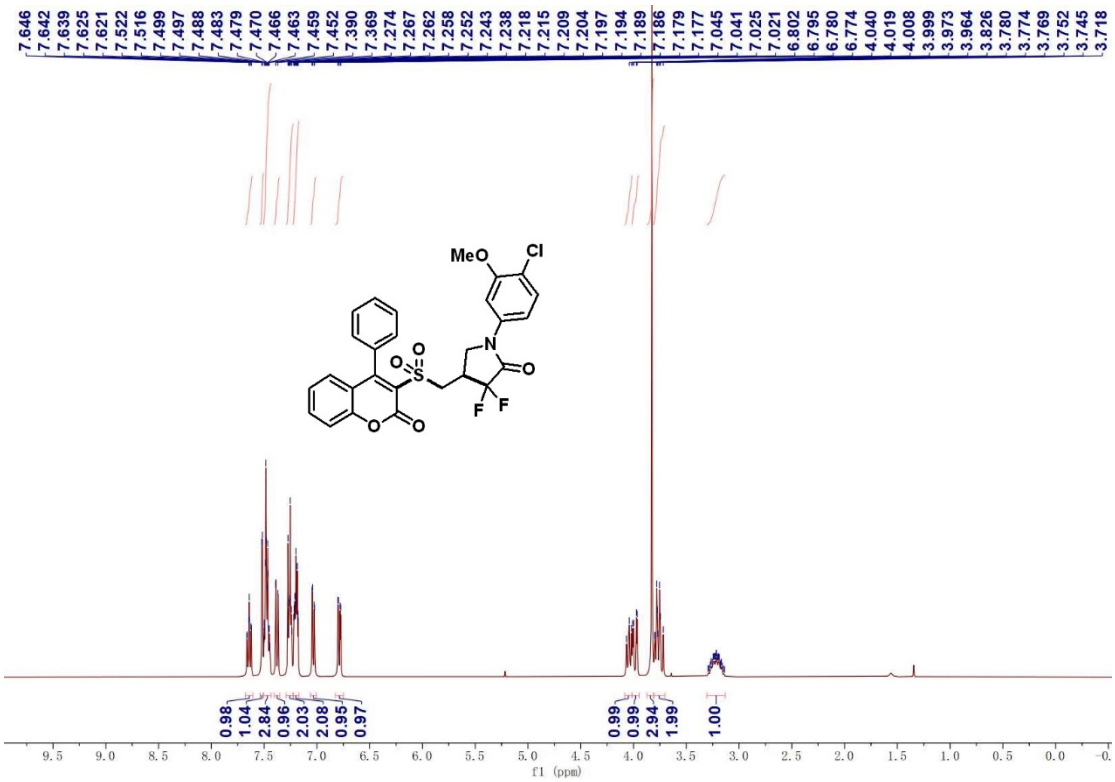
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4al**



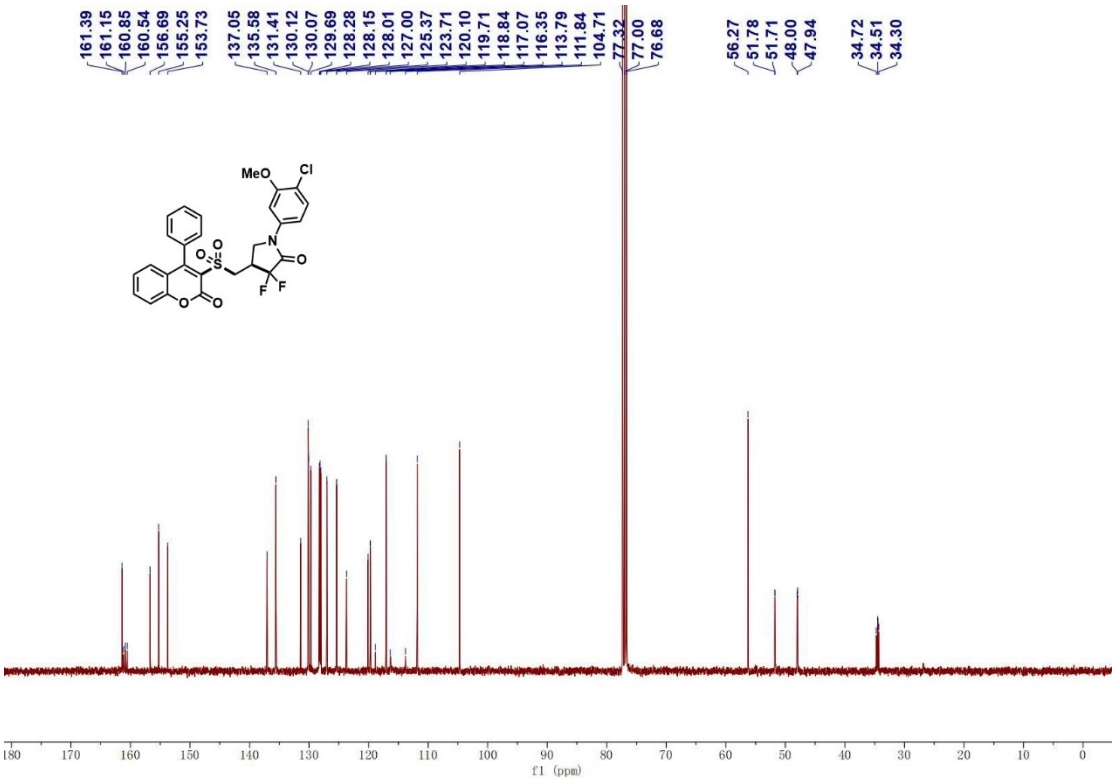
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4al**



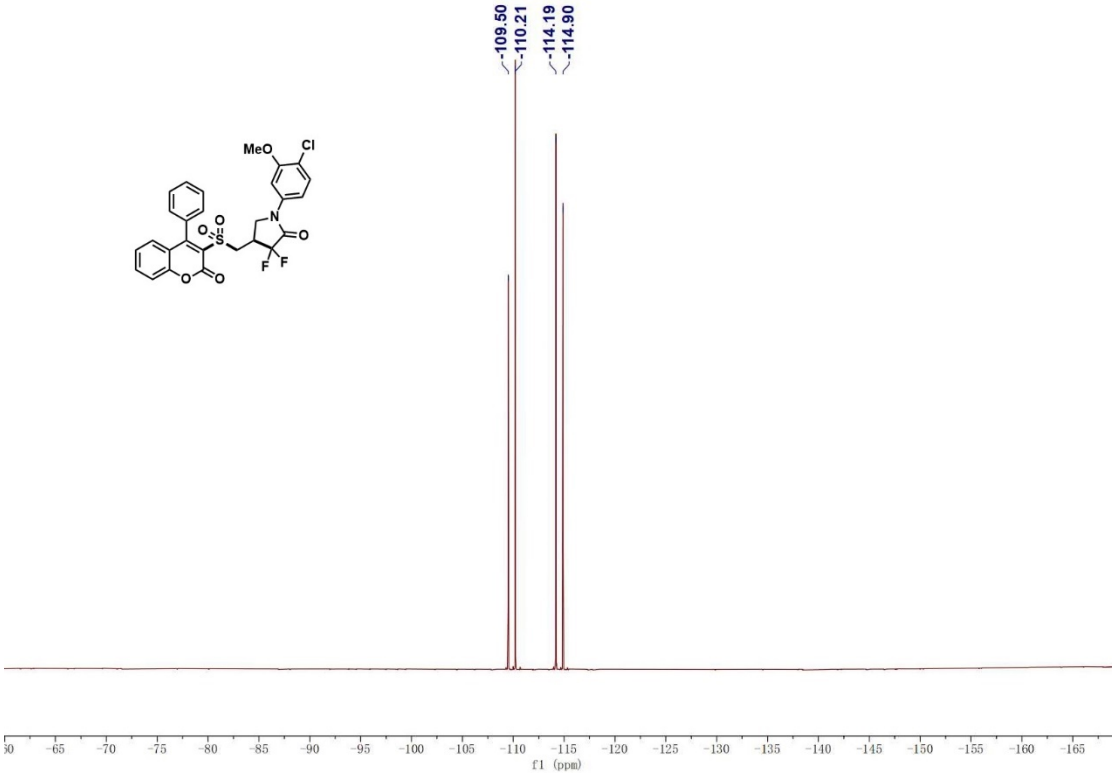
^{1}H NMR-spectrum (400 MHz, $CDCl_3$) of **4am**



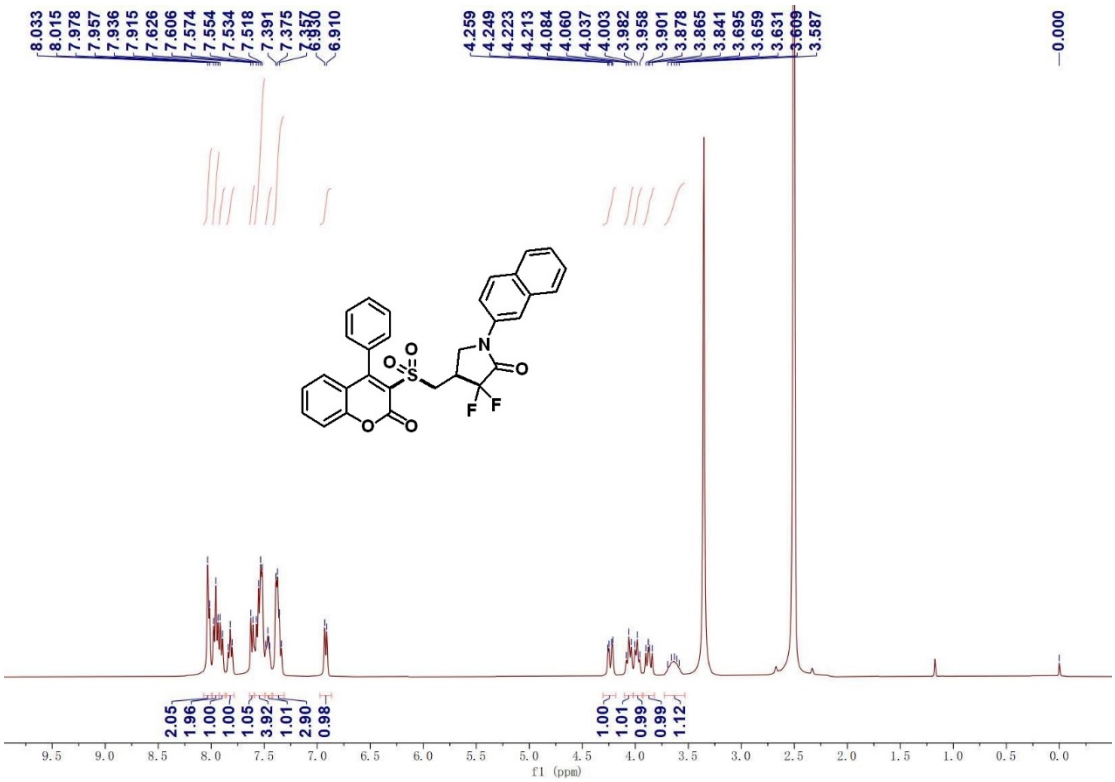
^{13}C NMR-spectrum (101 MHz, $CDCl_3$) of **4am**



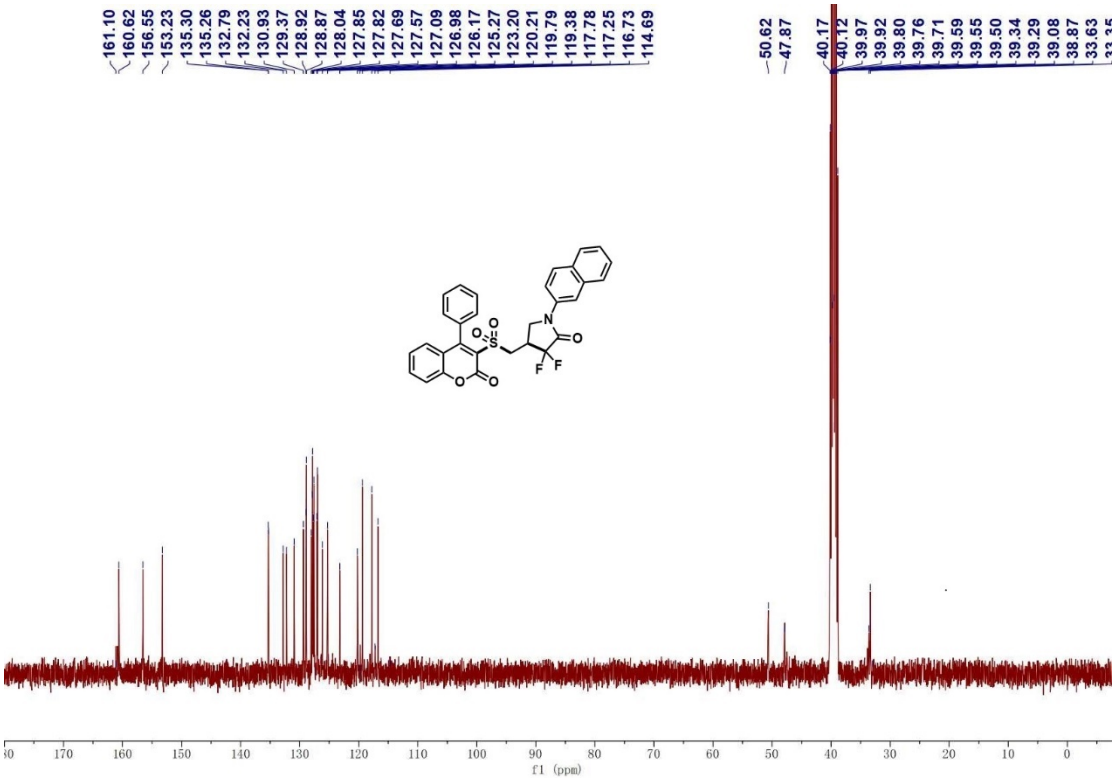
^{19}F NMR-spectrum (376 MHz, $CDCl_3$) of **4am**



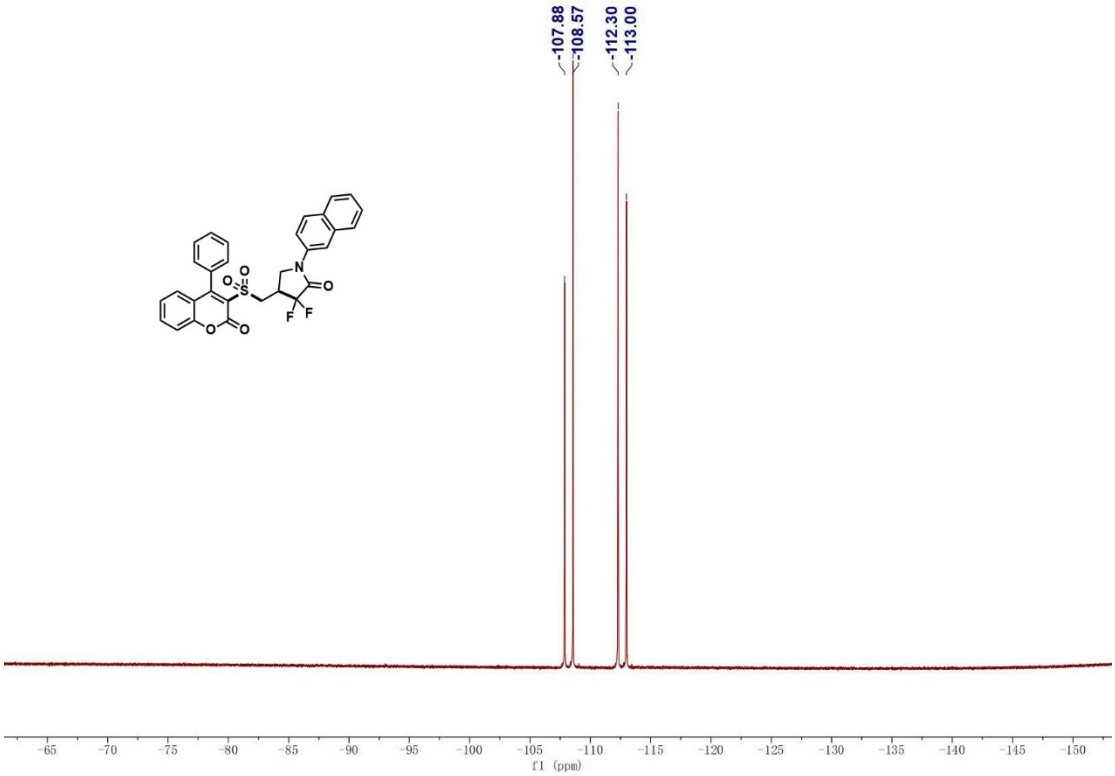
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4an**



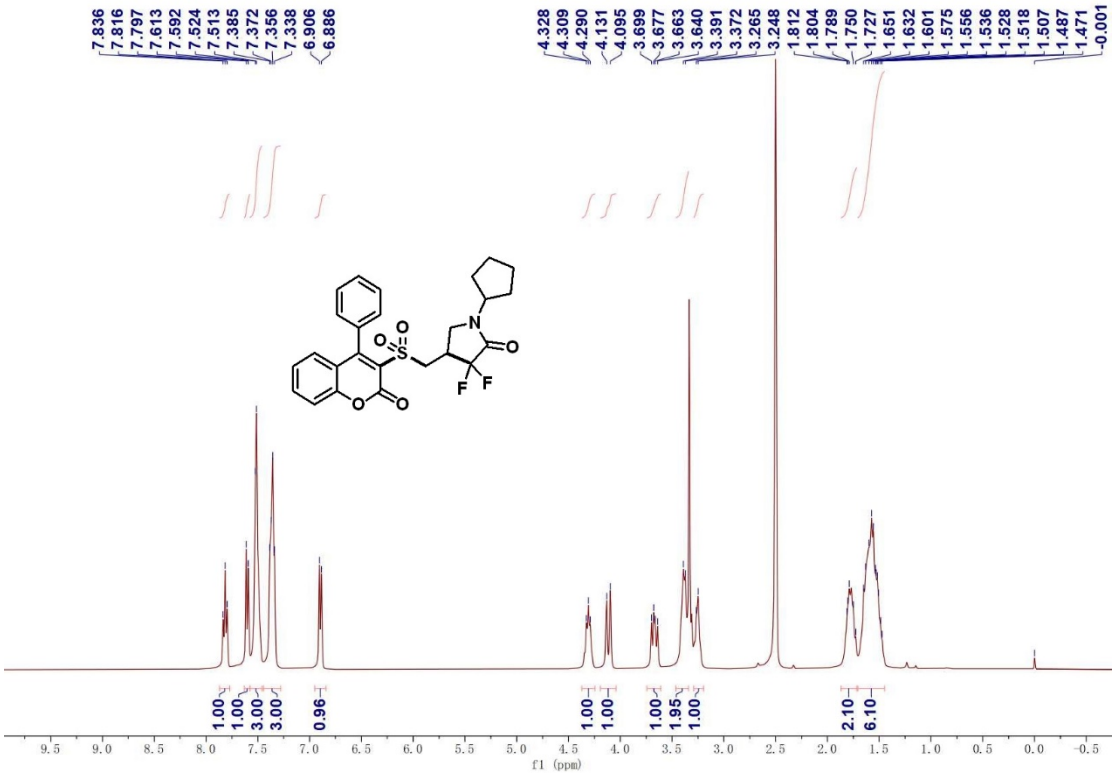
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4an**



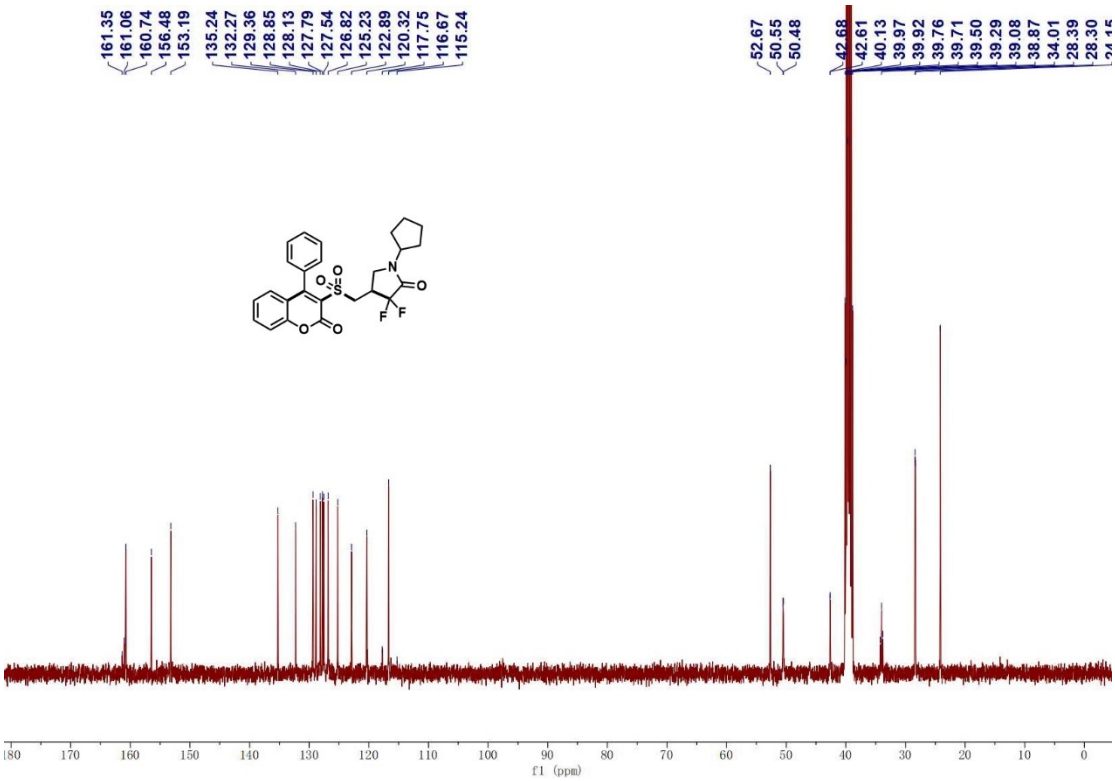
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4an**



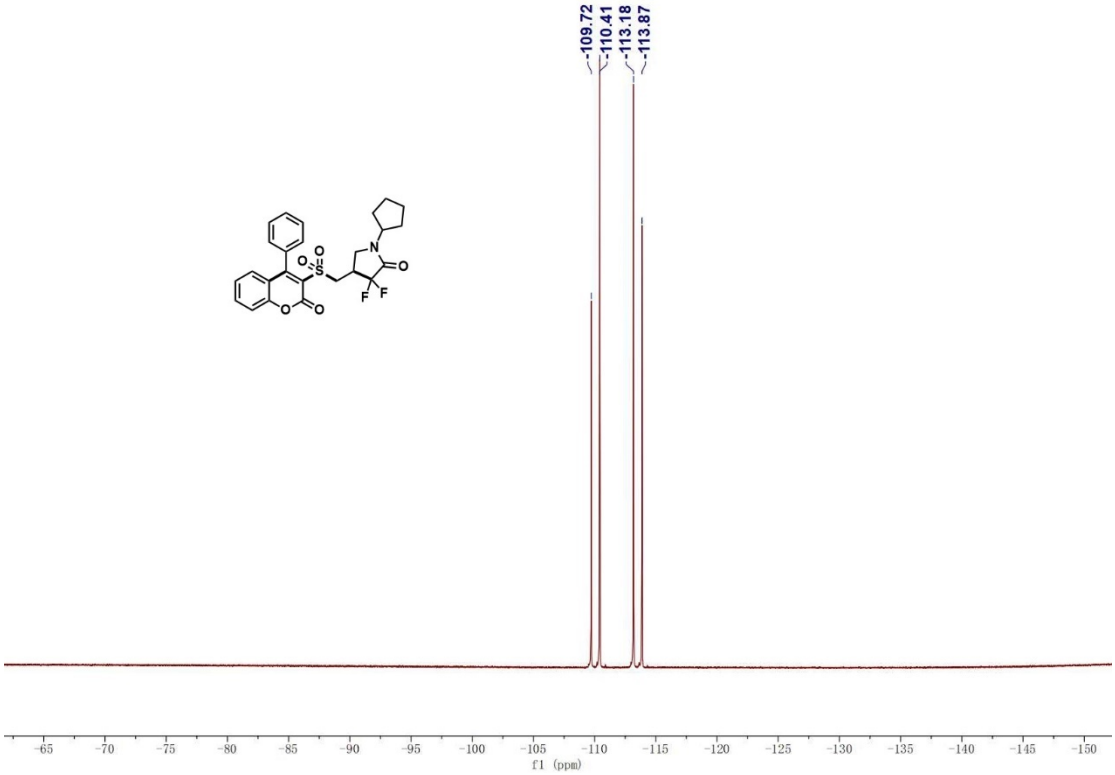
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ao**



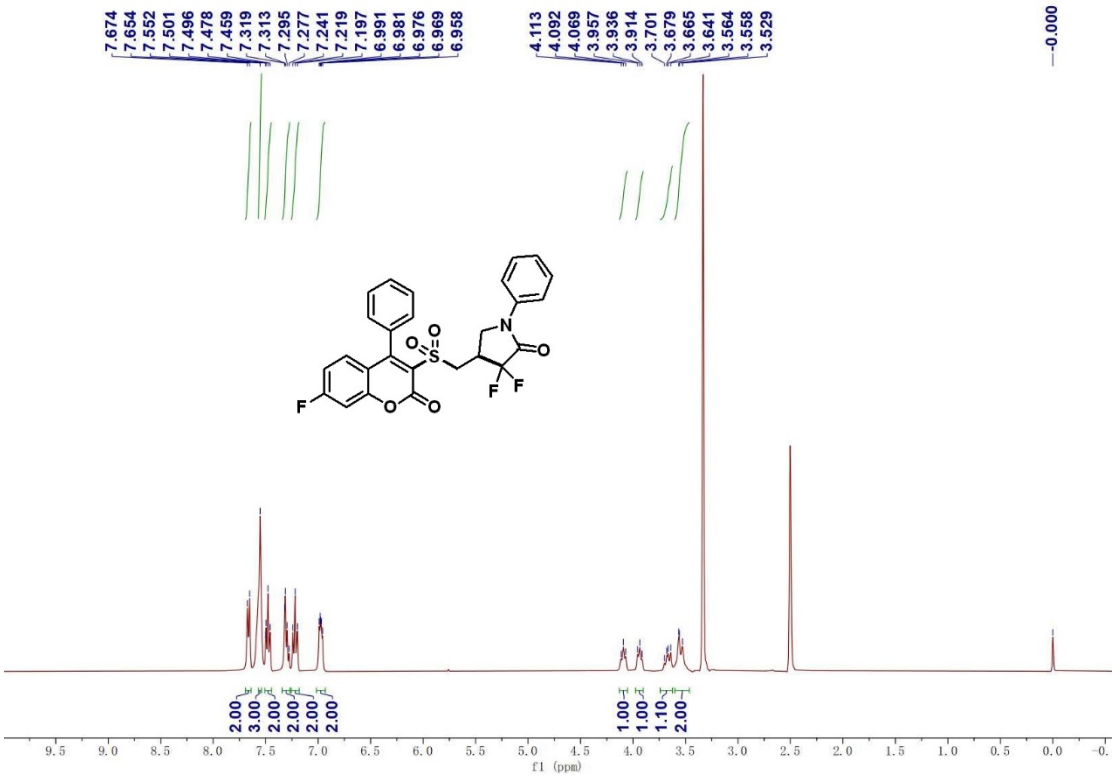
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ao**



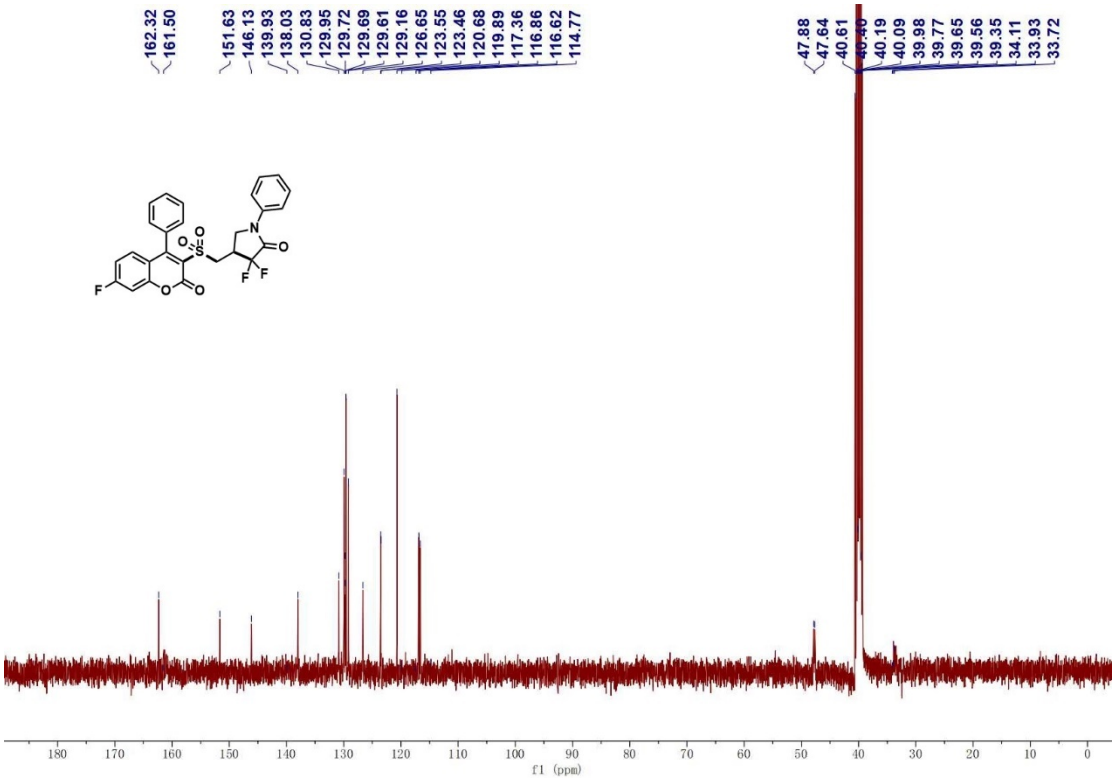
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ao**



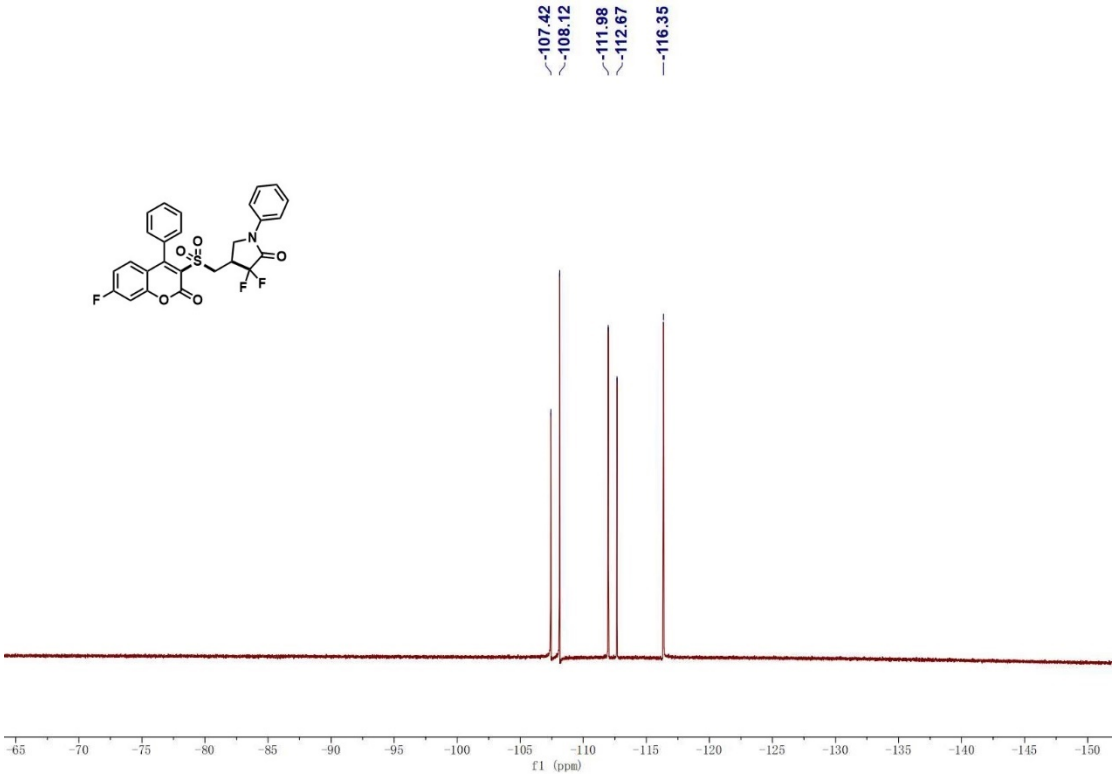
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ba**



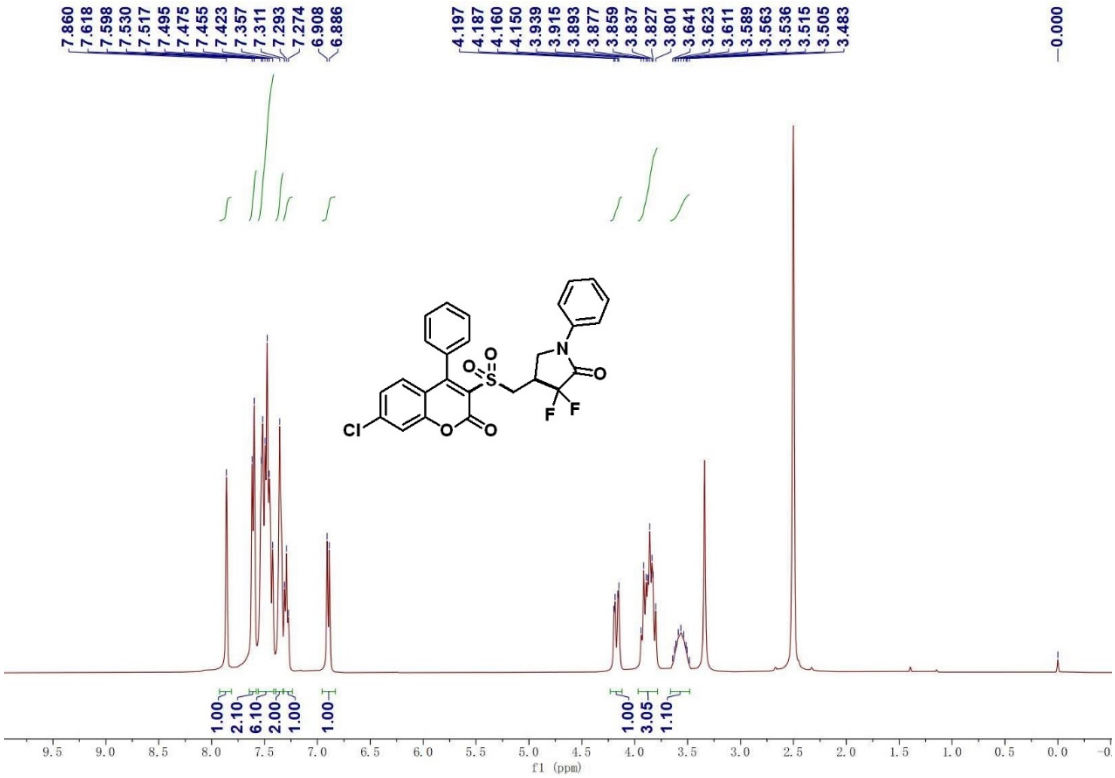
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ba**



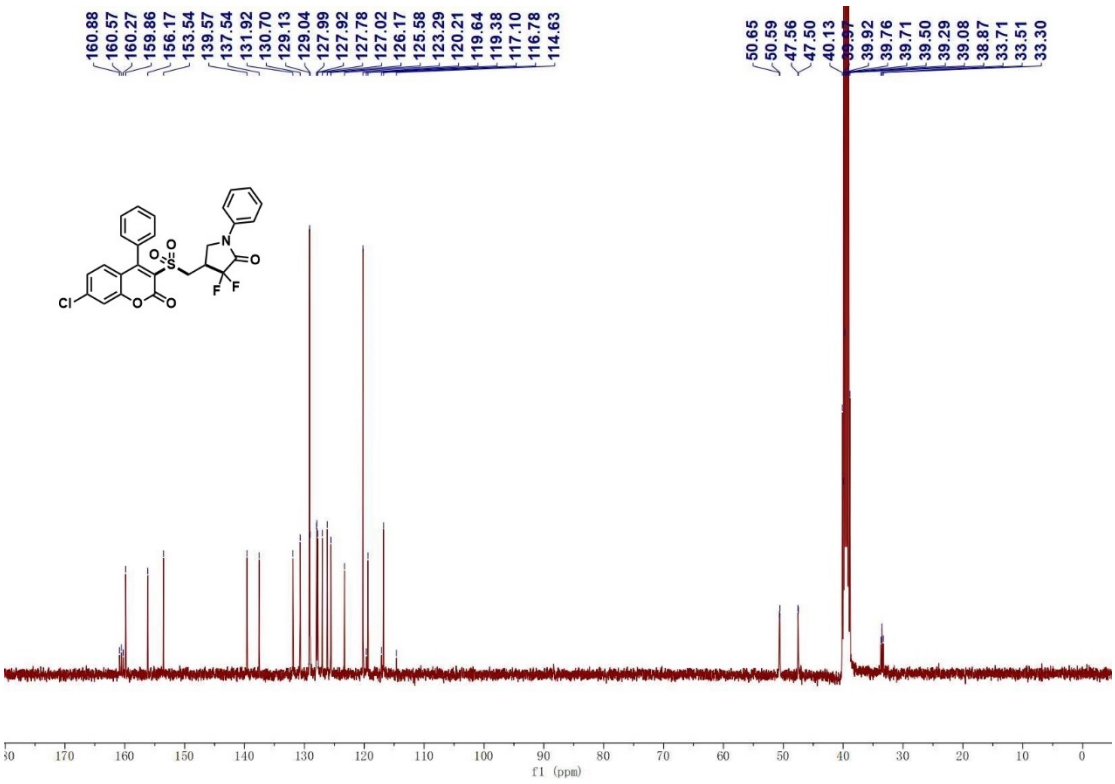
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ba**



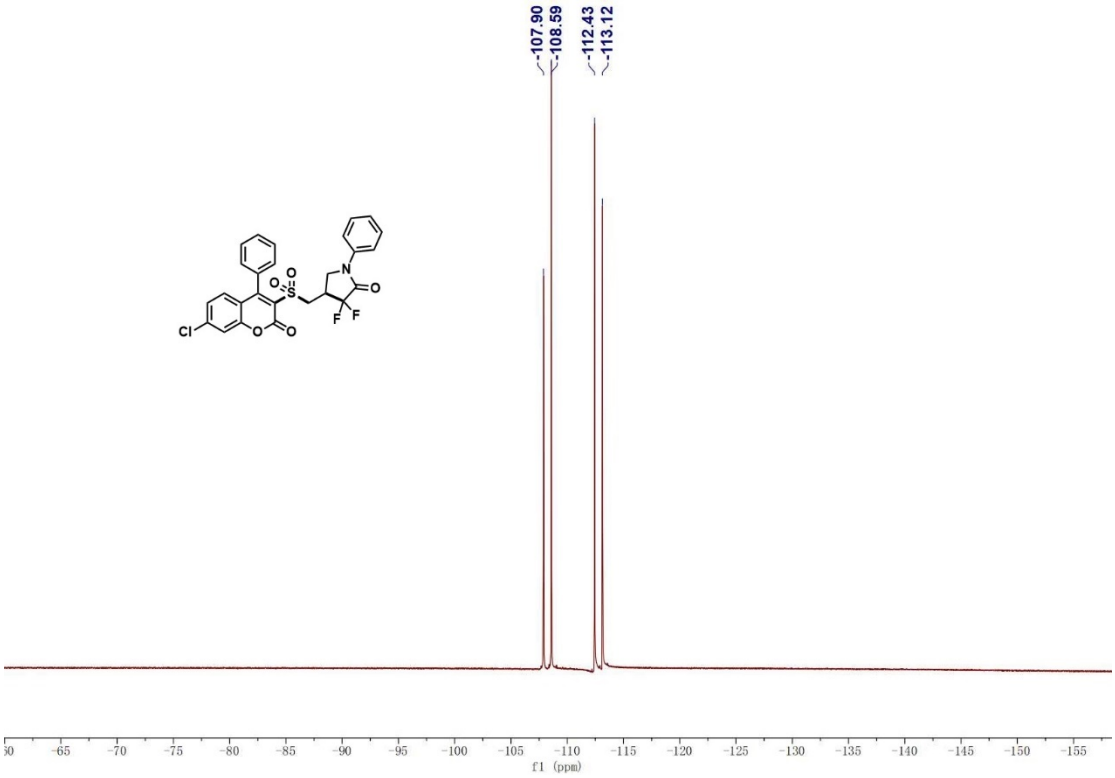
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ca**



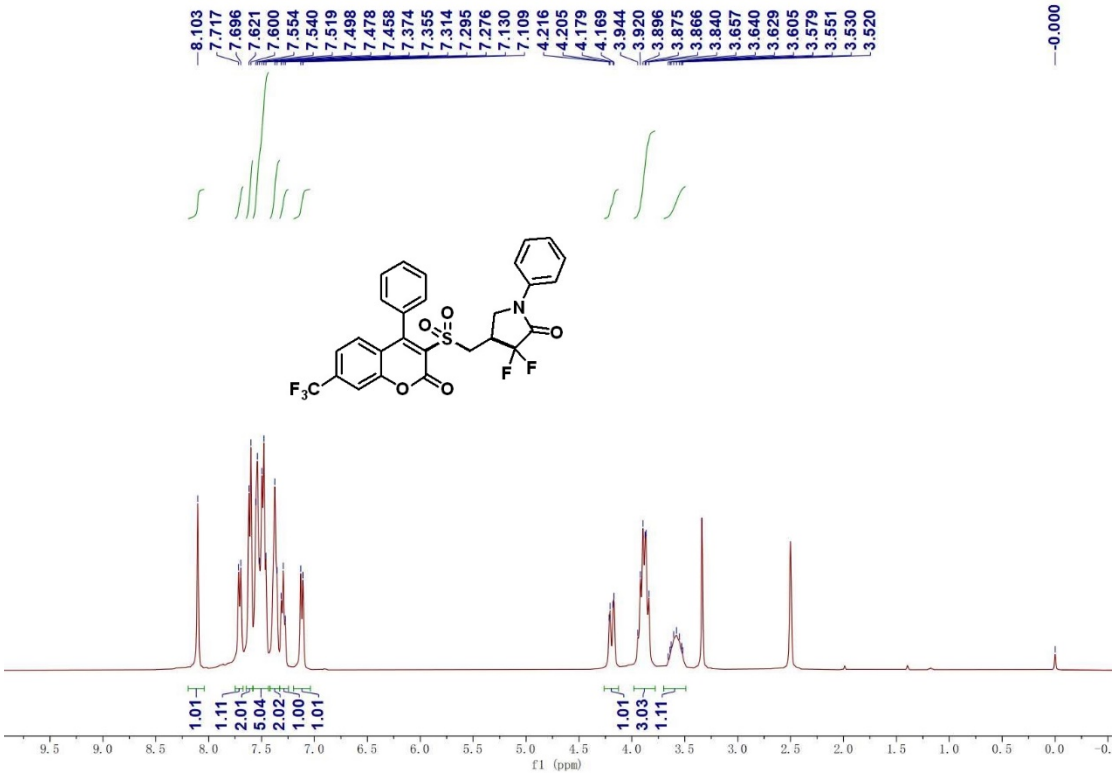
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ca**



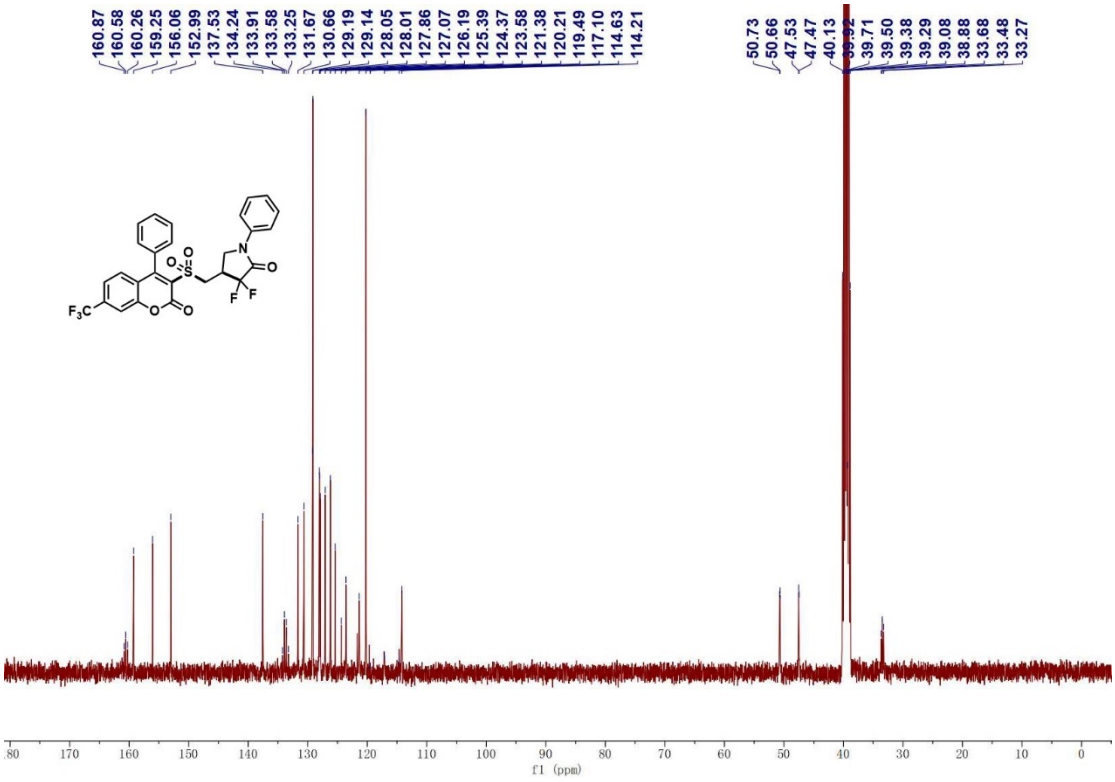
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ca**



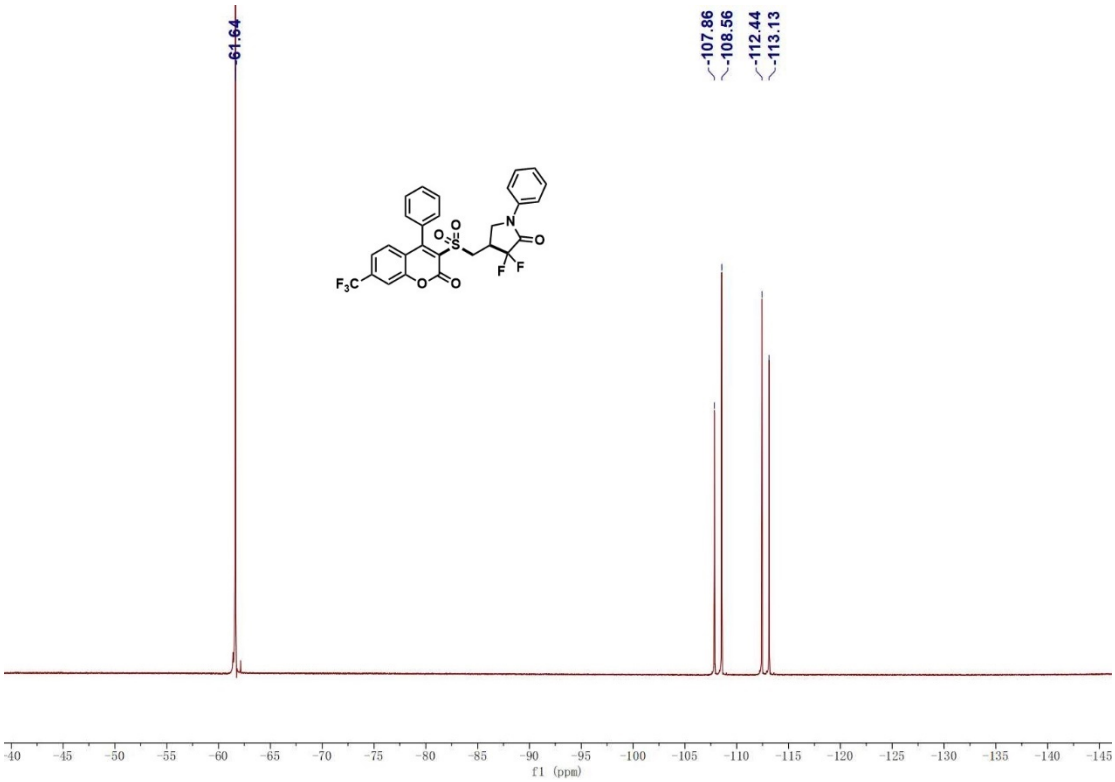
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4da**



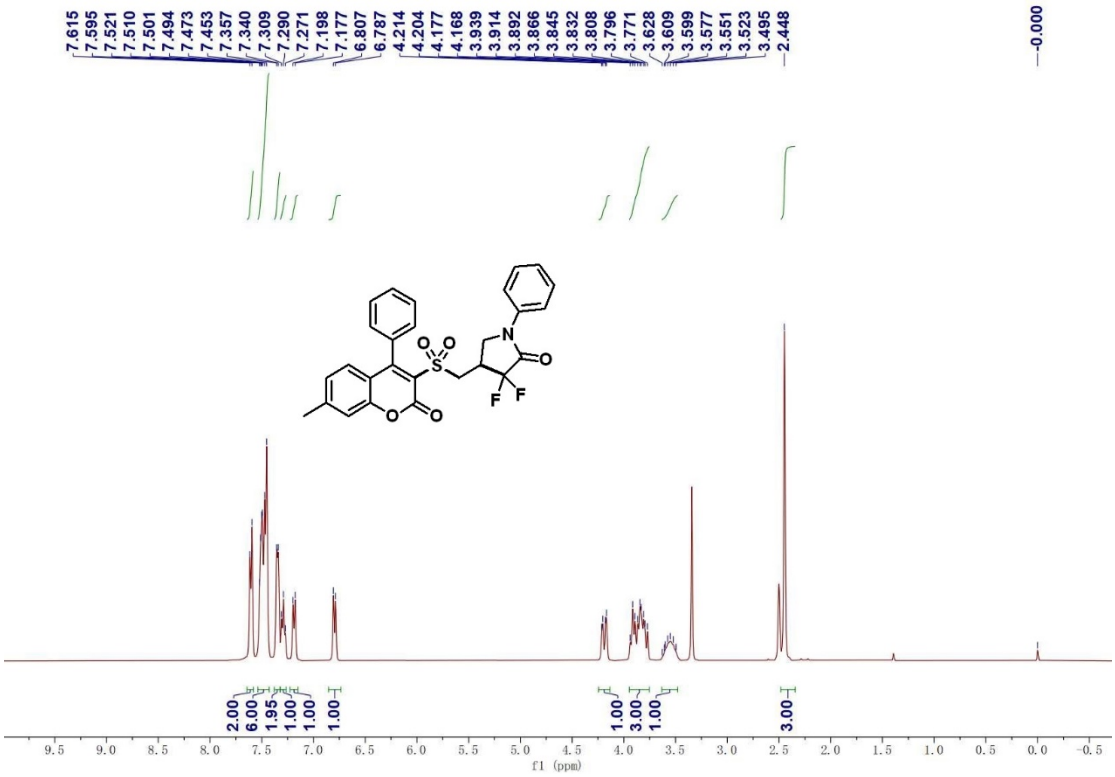
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4da**



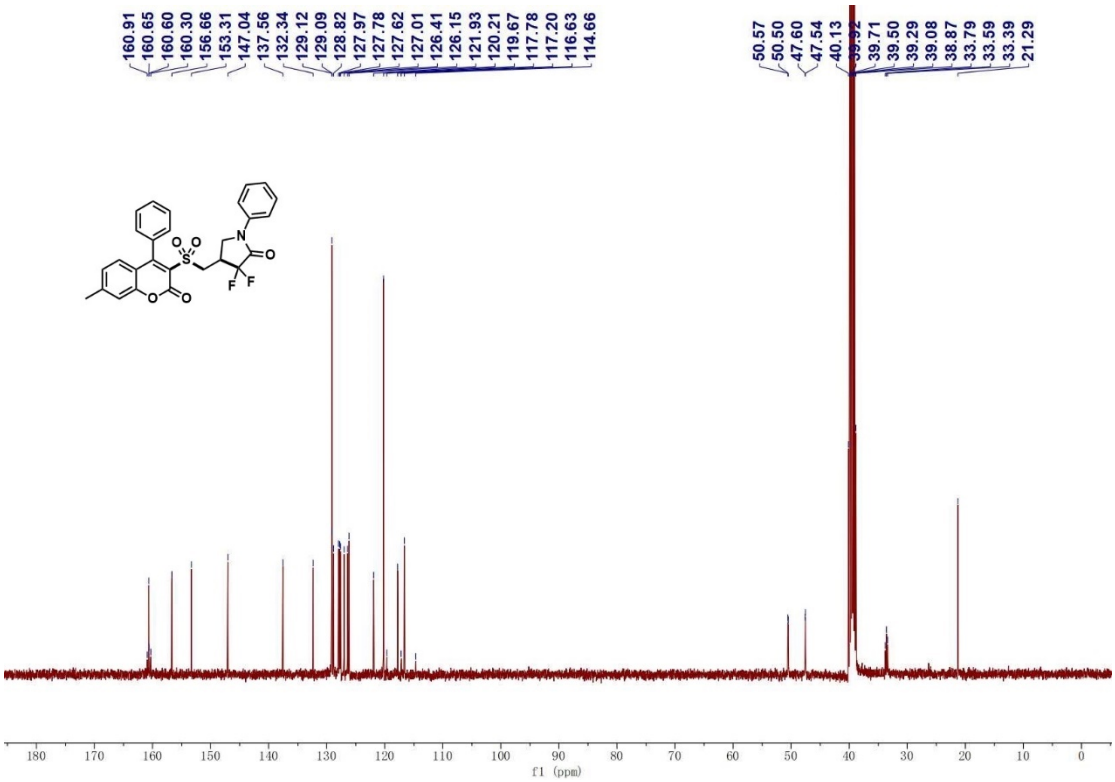
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4da**



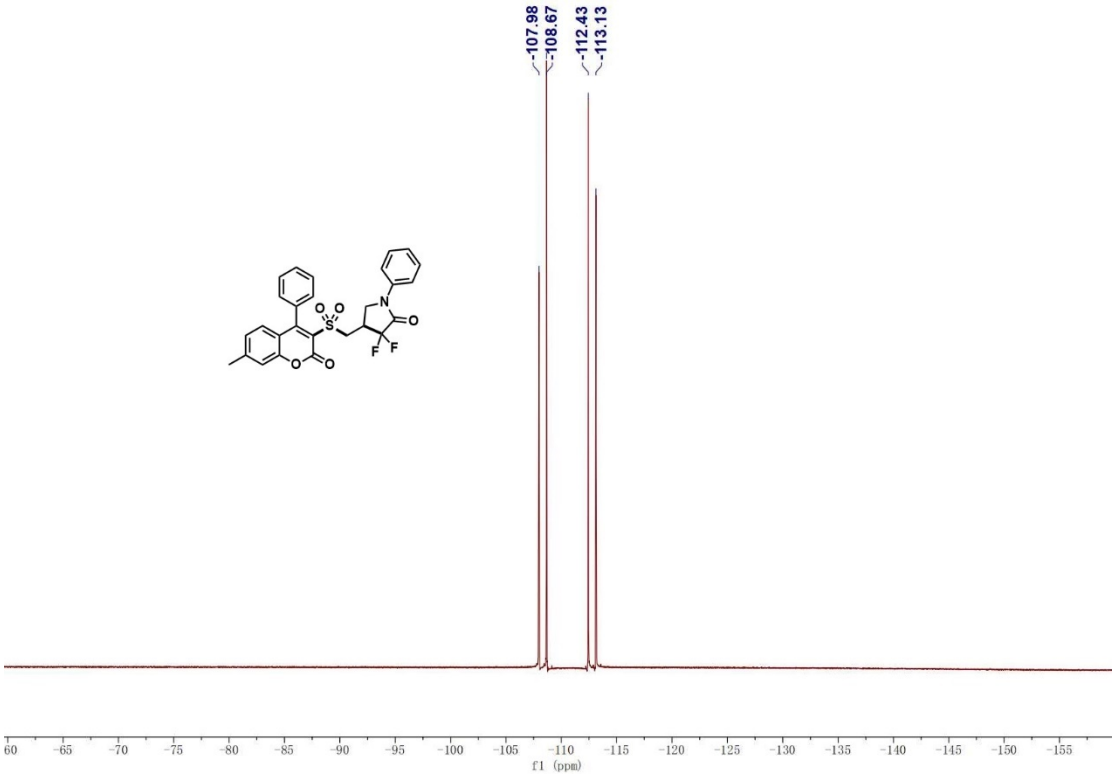
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ea**



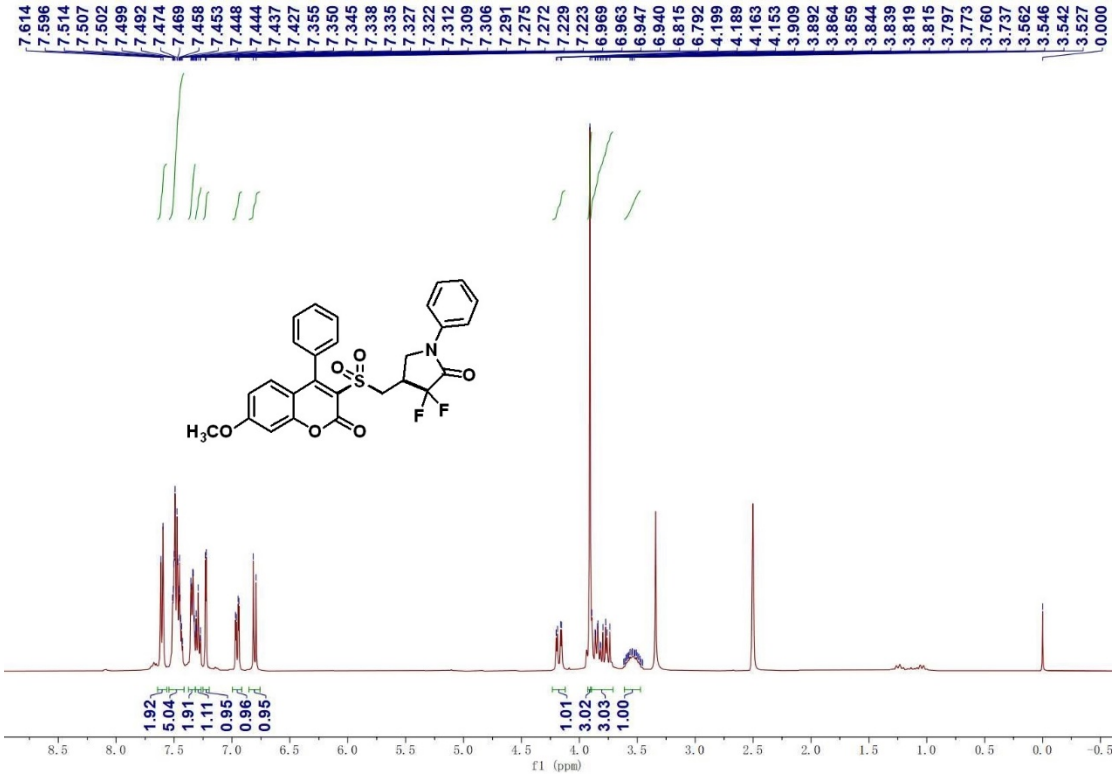
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ea**



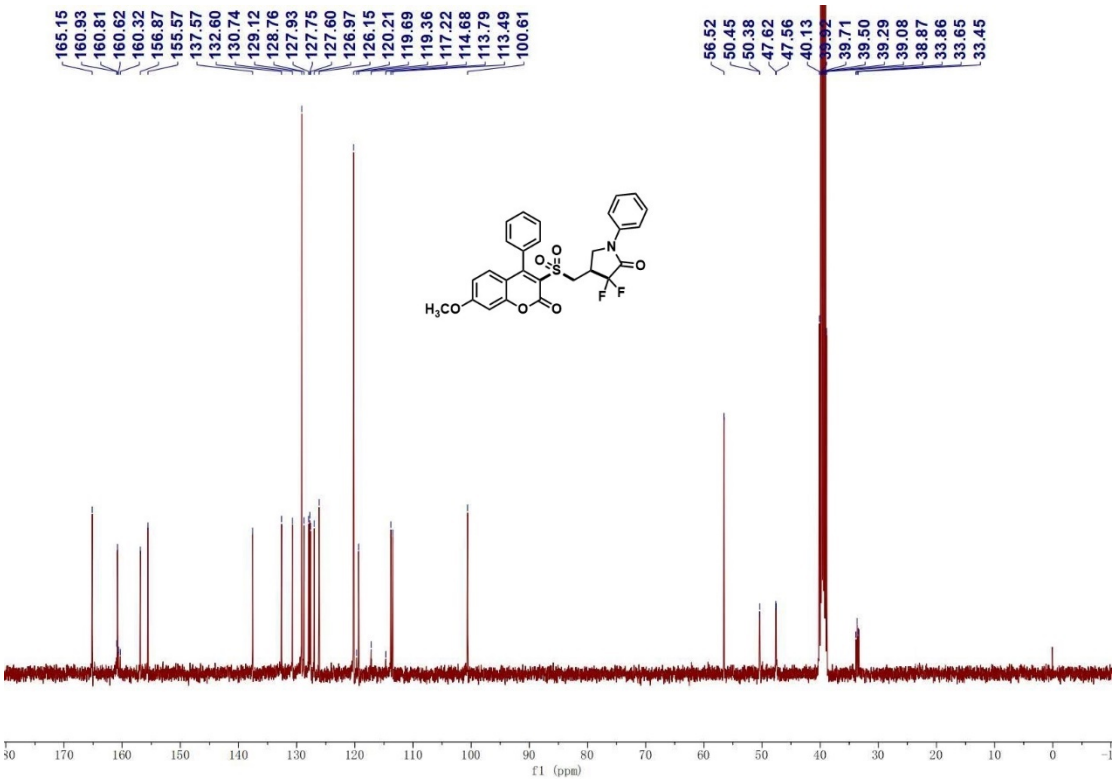
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ea**



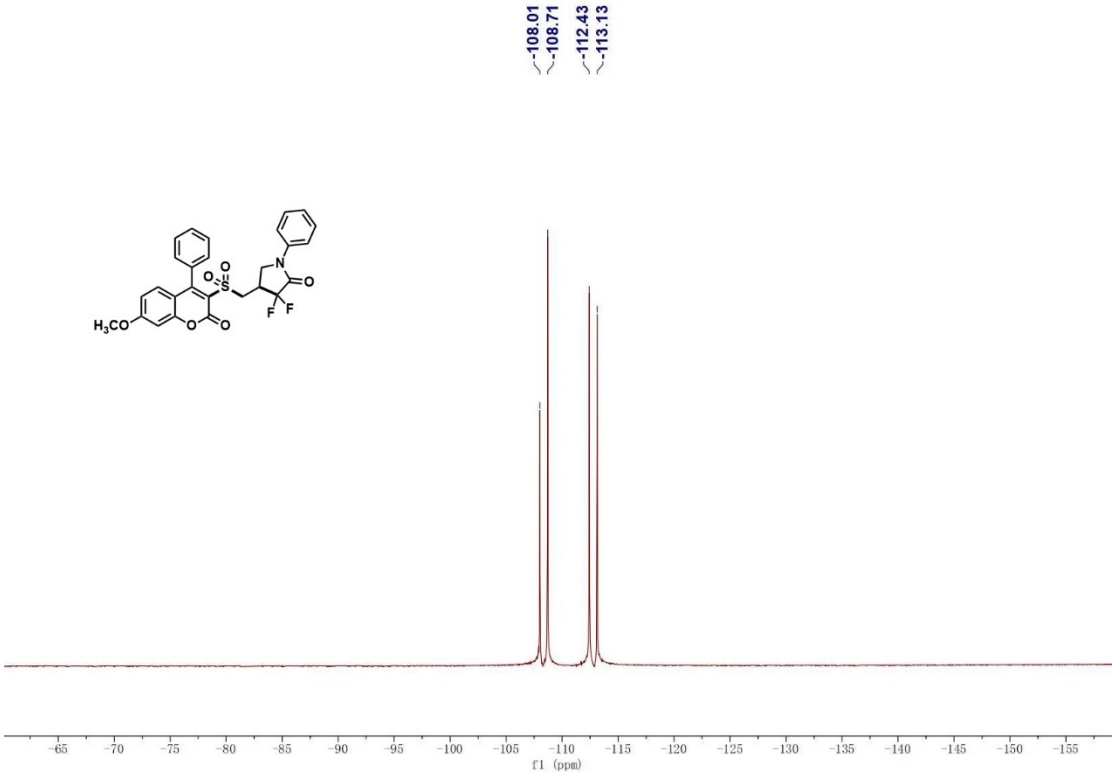
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4fa**



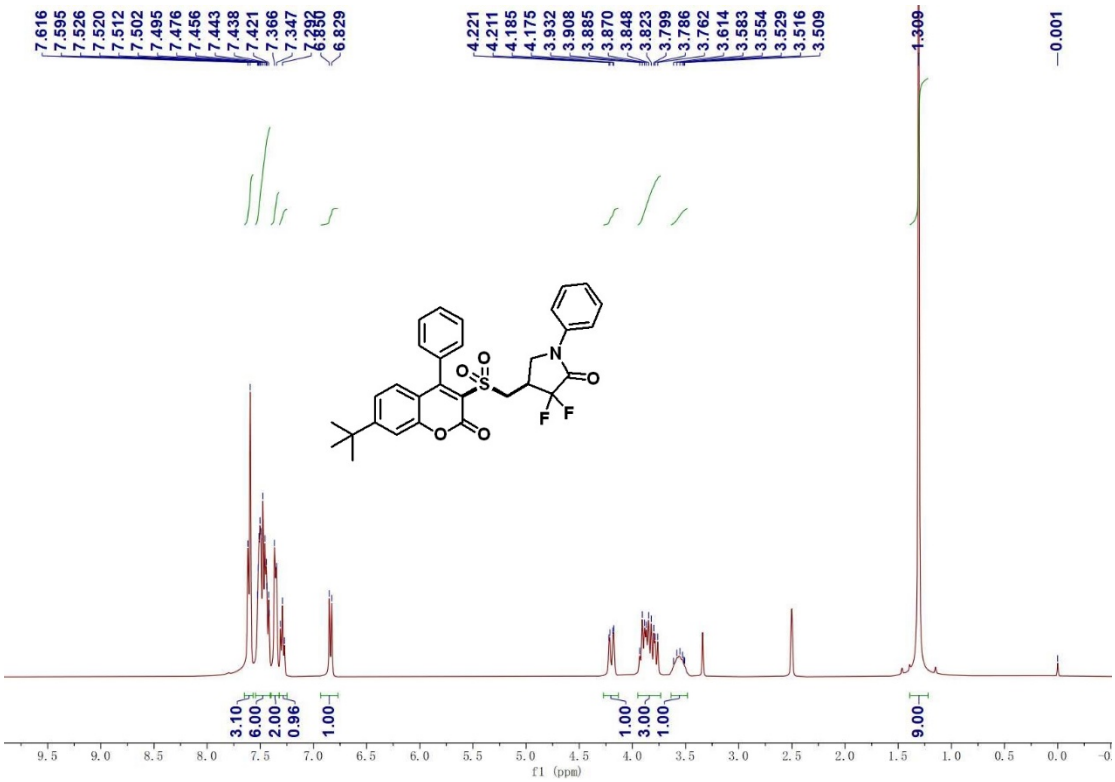
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4fa**



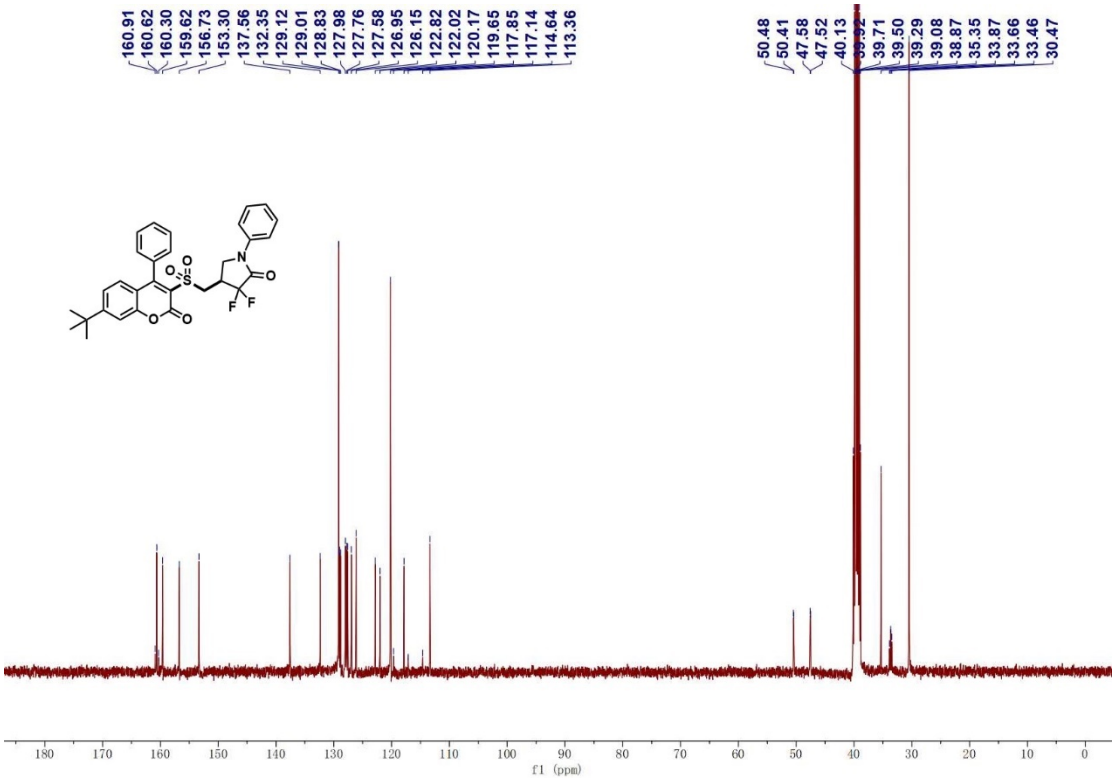
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4fa**



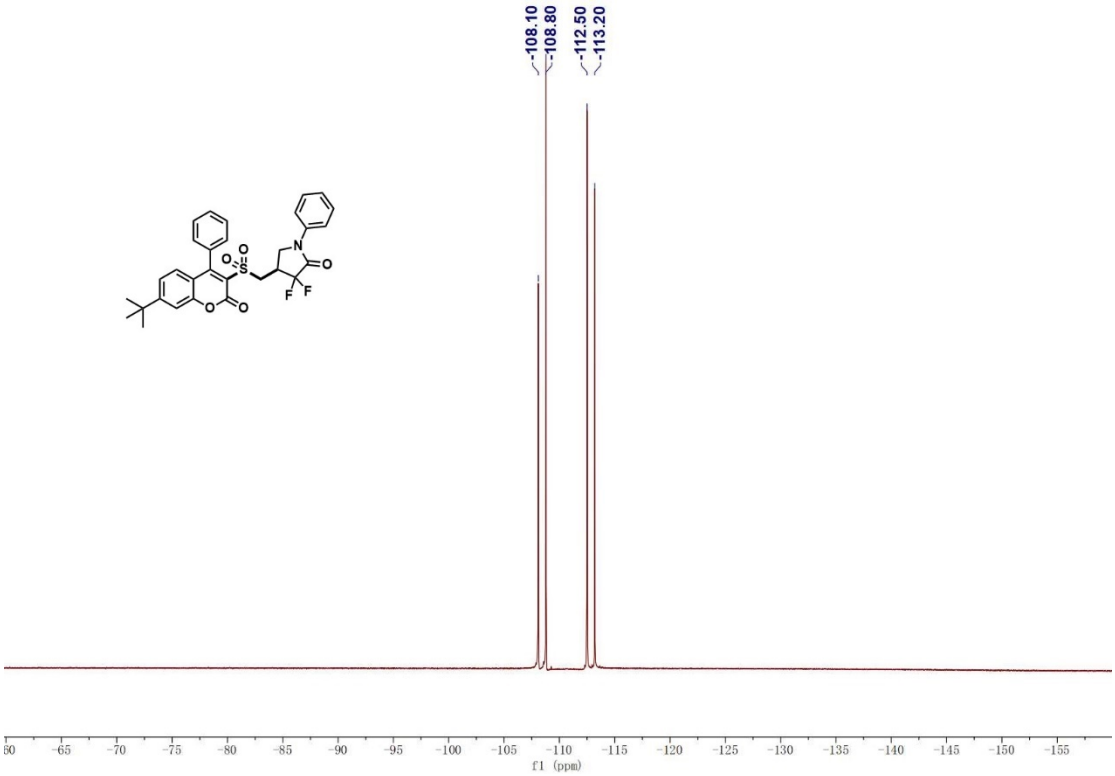
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ga**



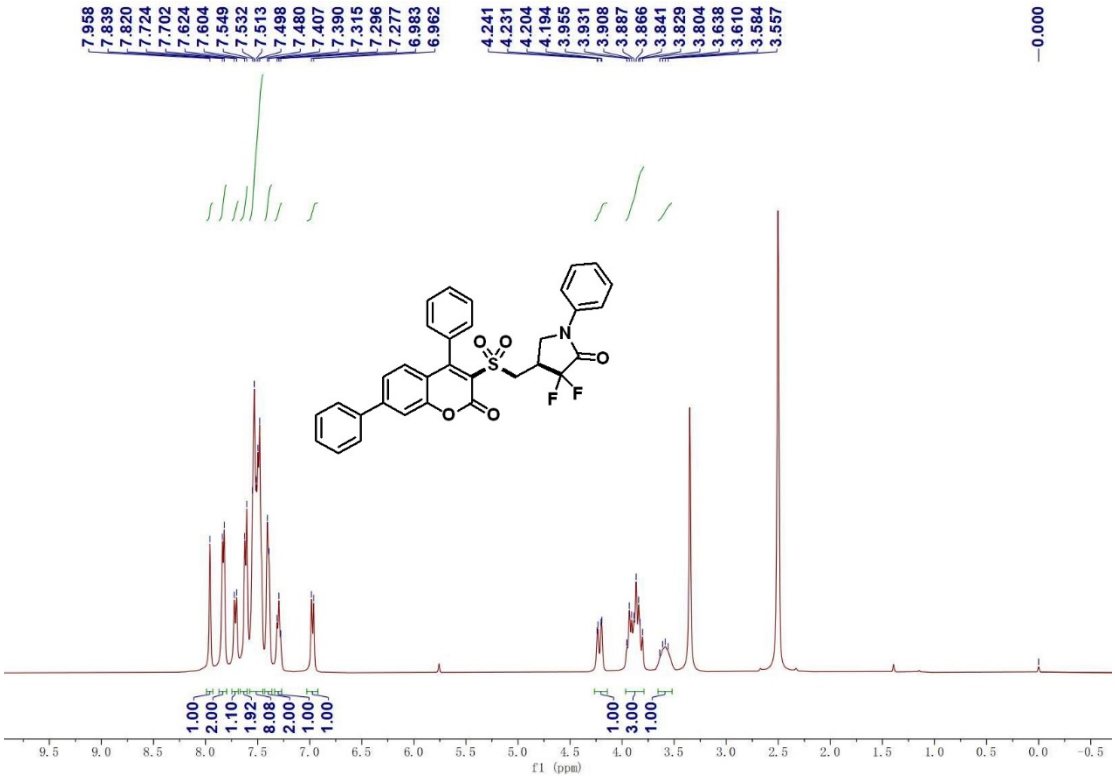
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ga**



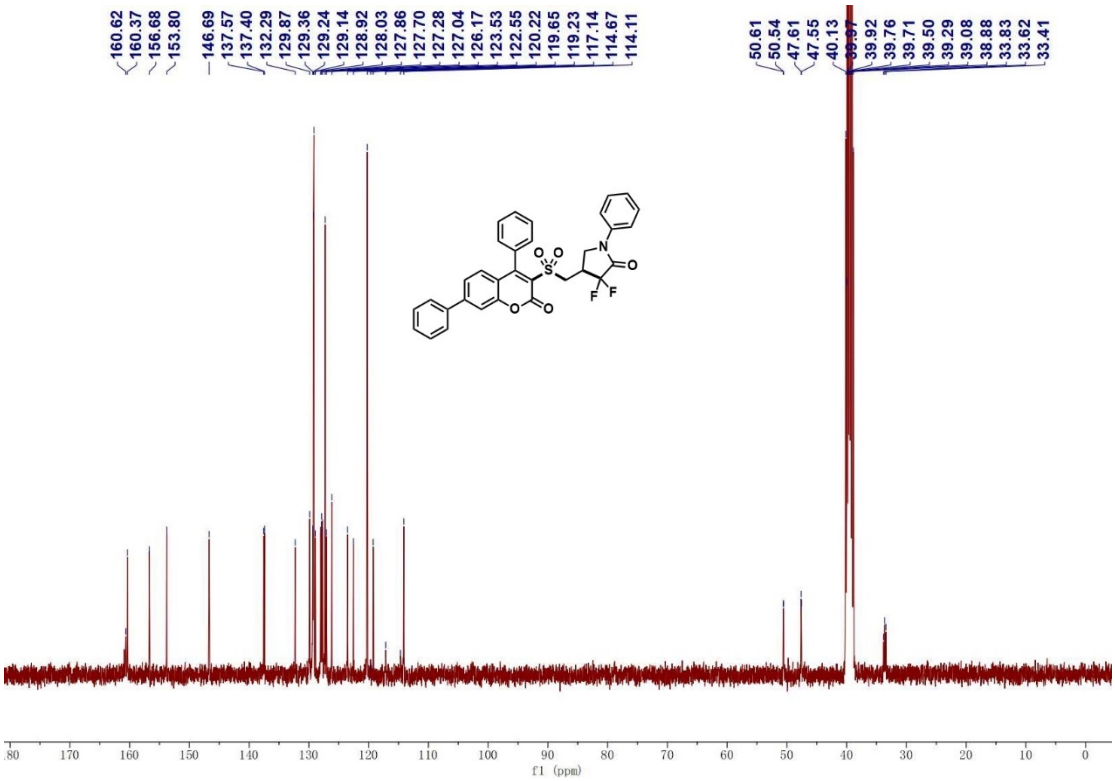
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ga**



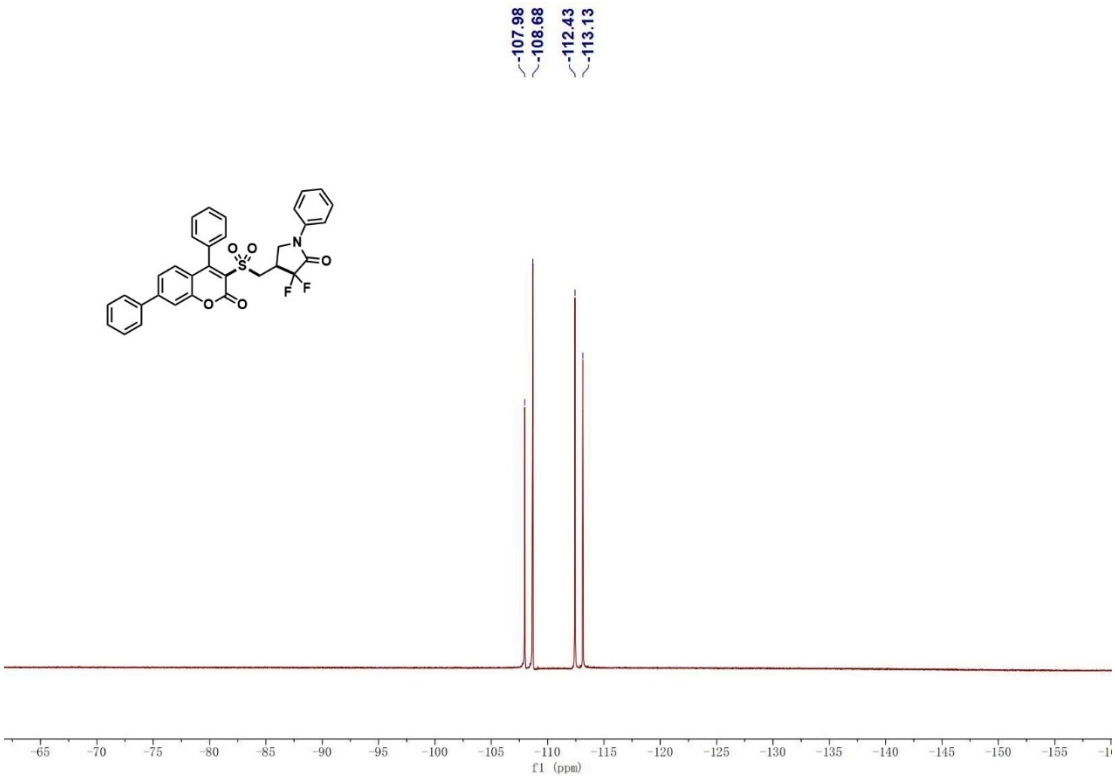
[1]H NMR-spectrum (400 MHz, DMSO-d_6) of **4ha**



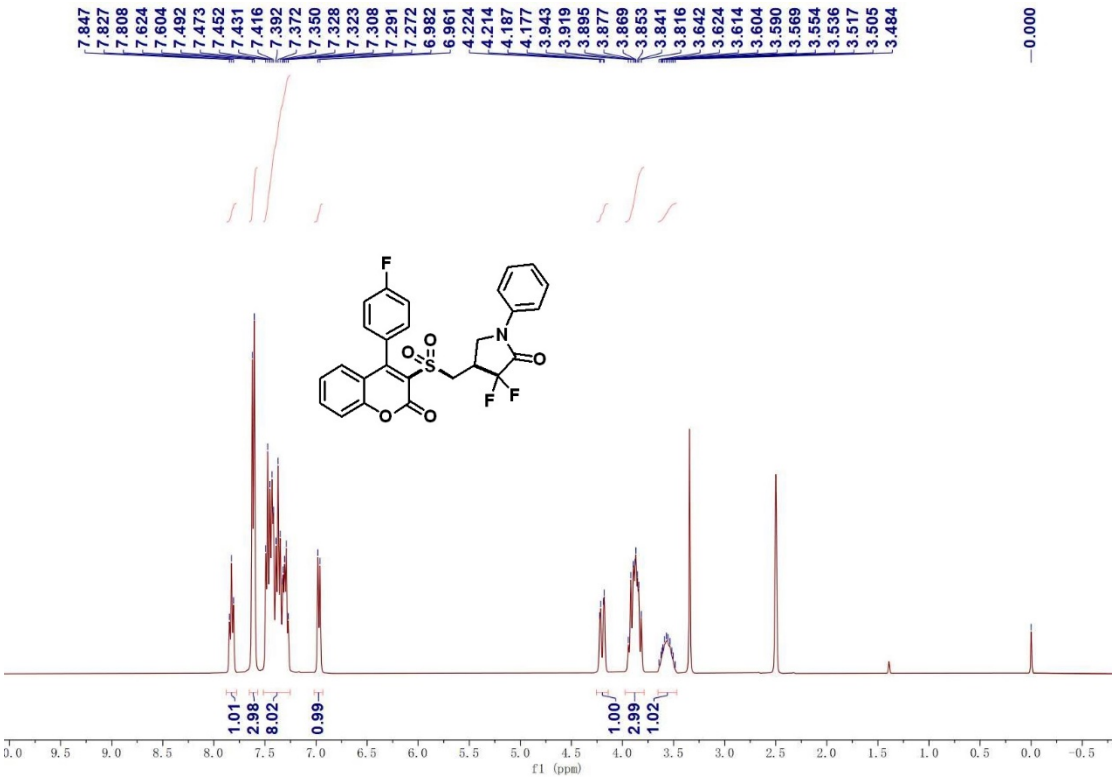
[13]C NMR-spectrum (101 MHz, DMSO-d_6) of **4ha**



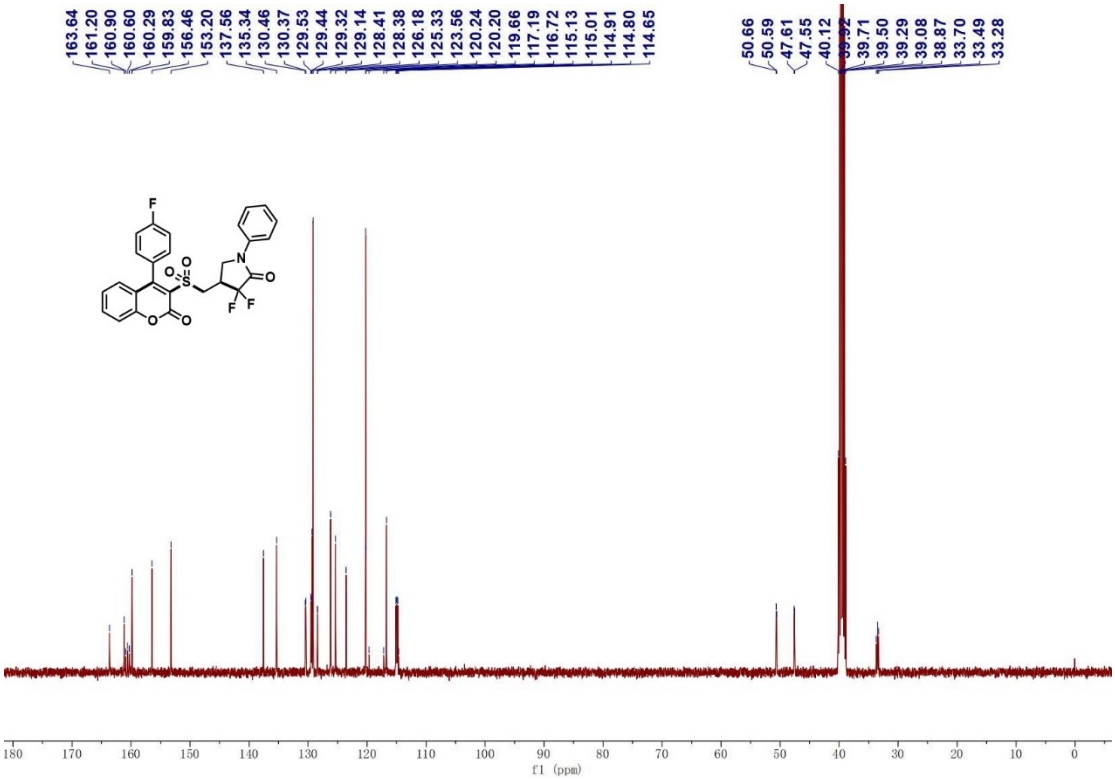
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ha**



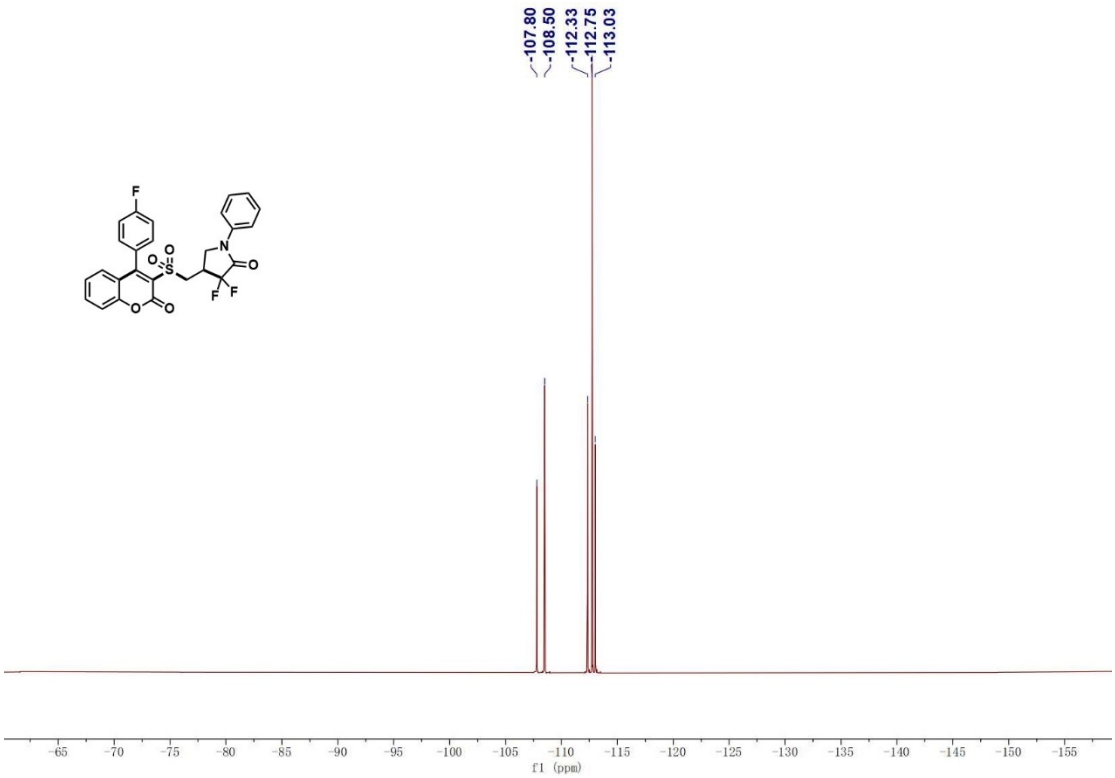
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ia**



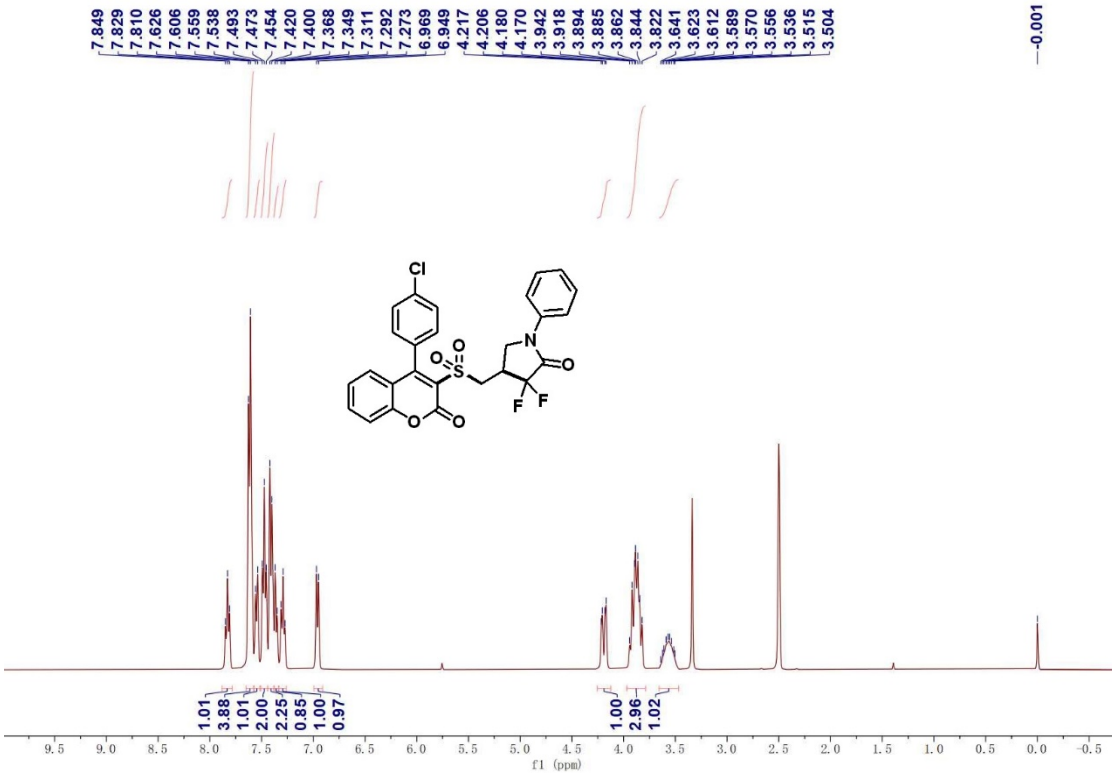
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ia**



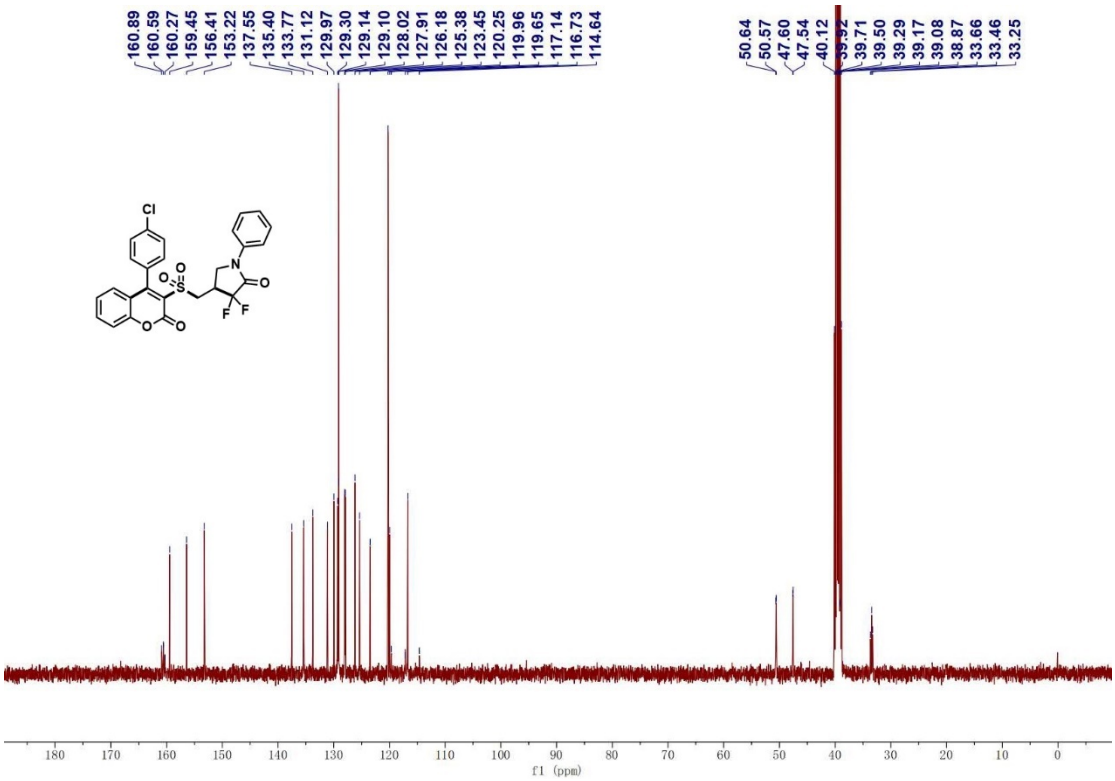
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ia**



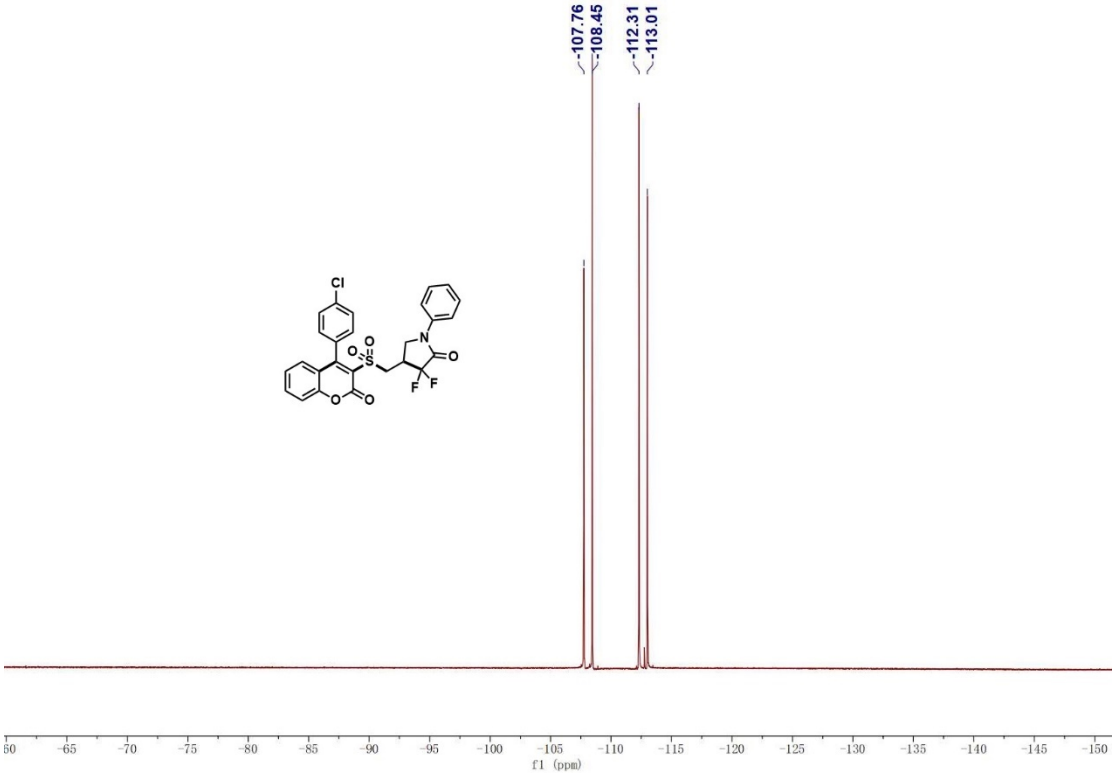
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ja**



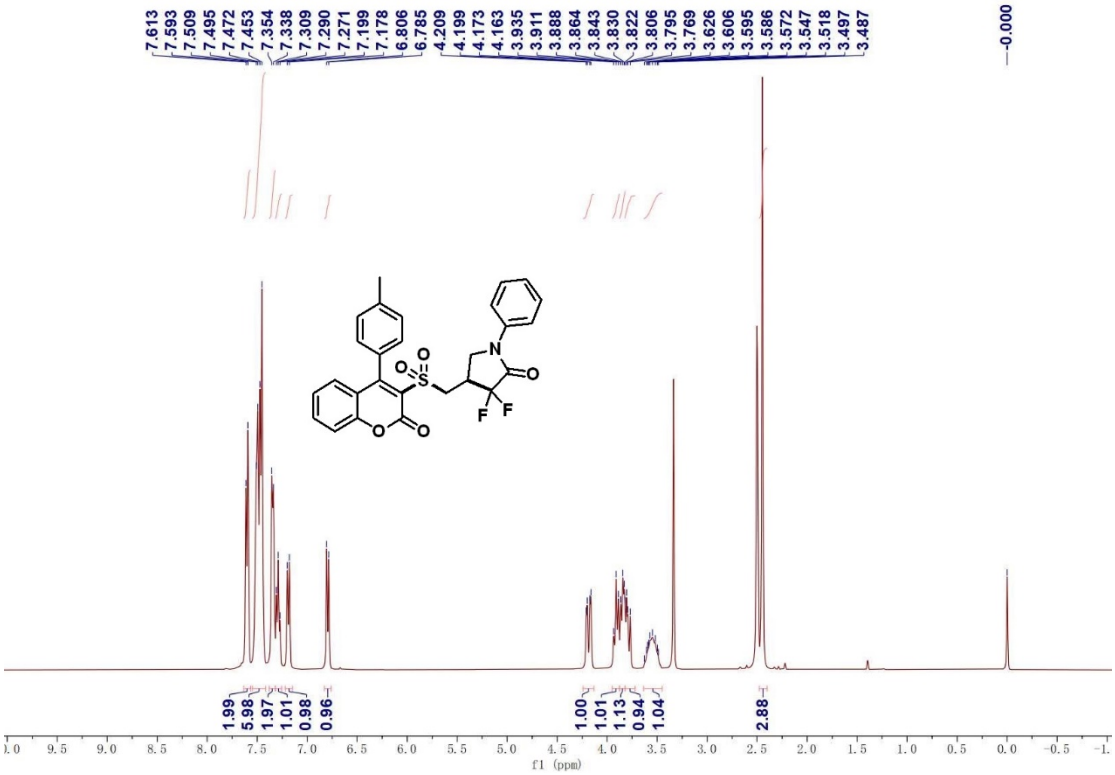
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ja**



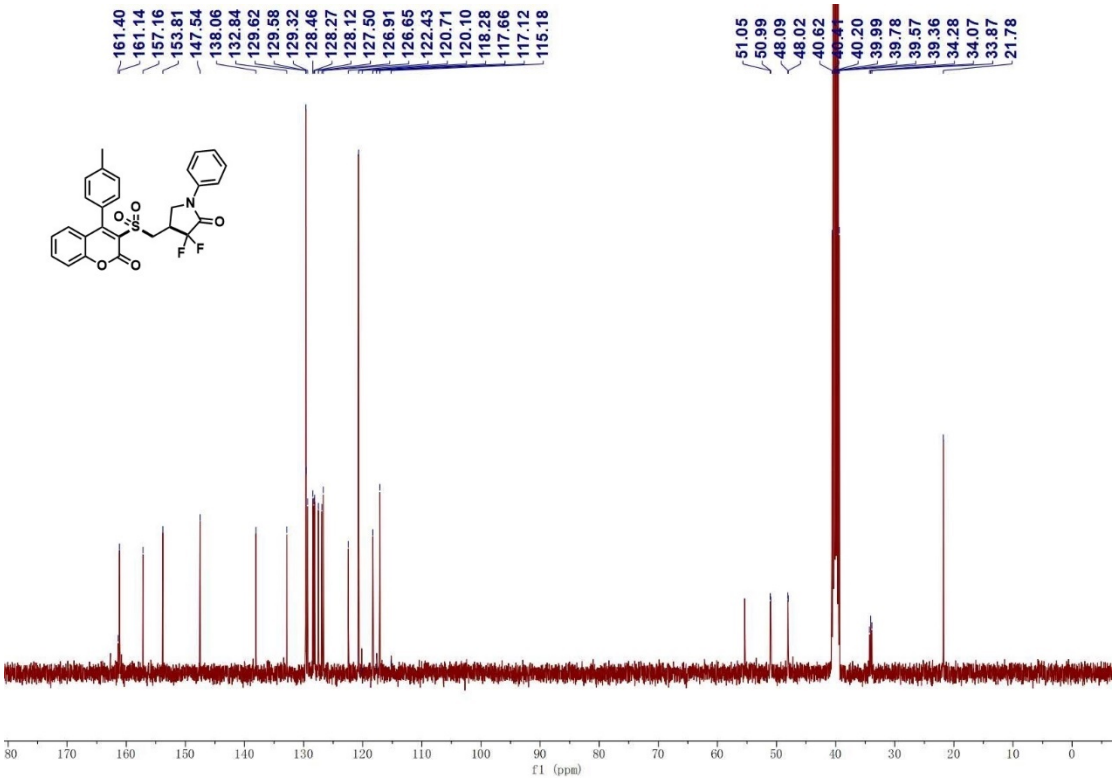
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ja**



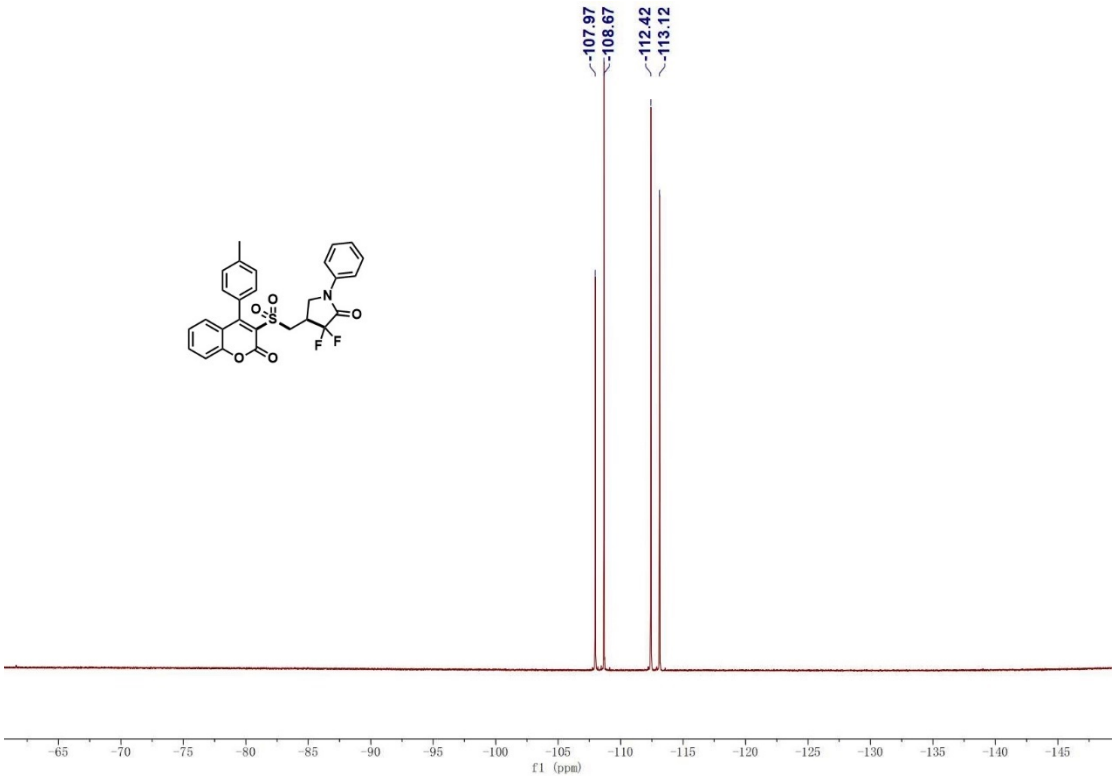
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ka**



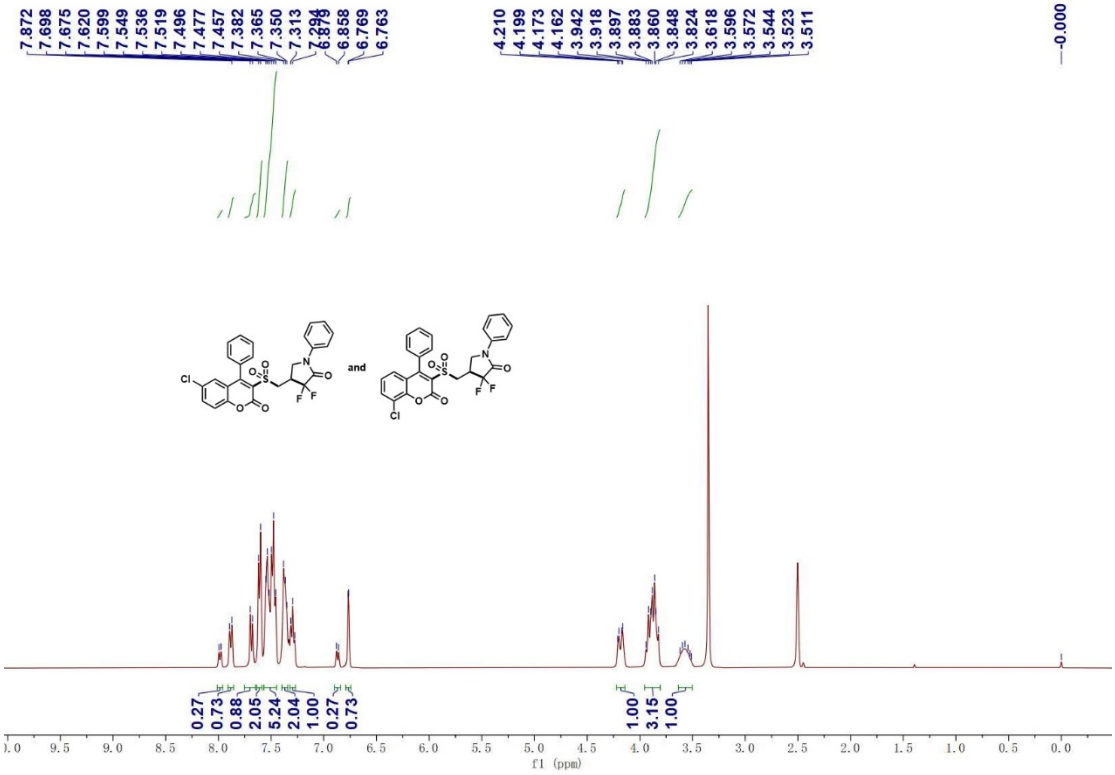
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ka**



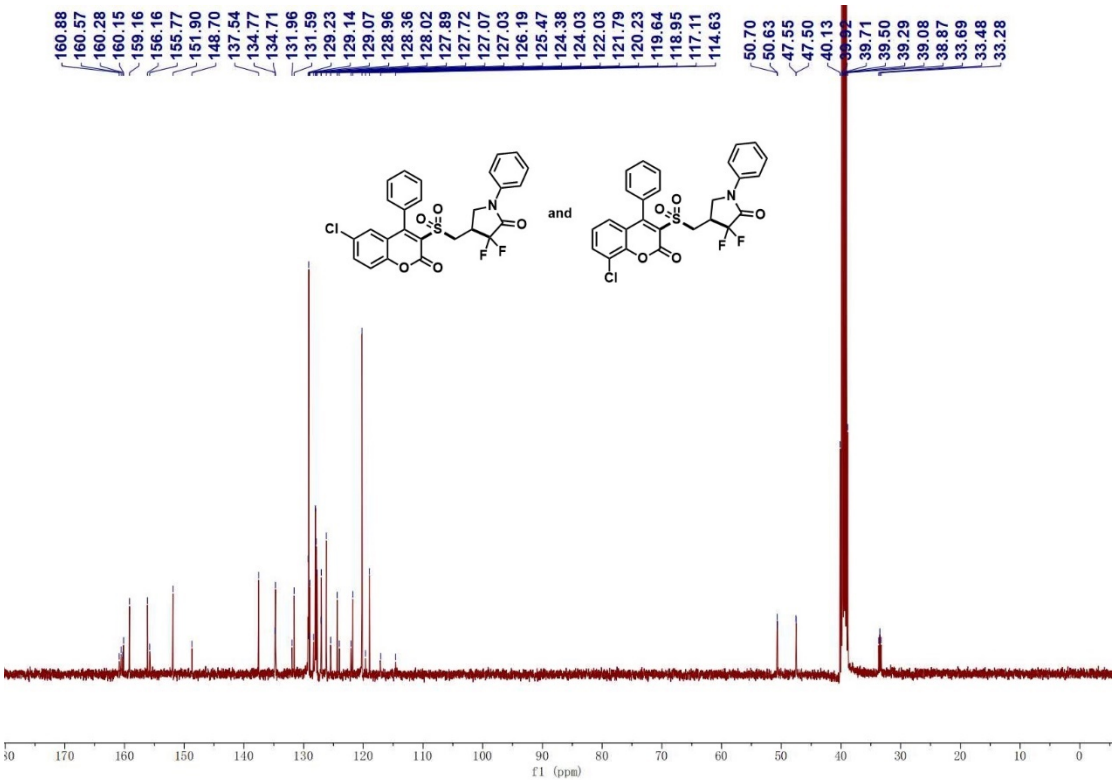
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ka**



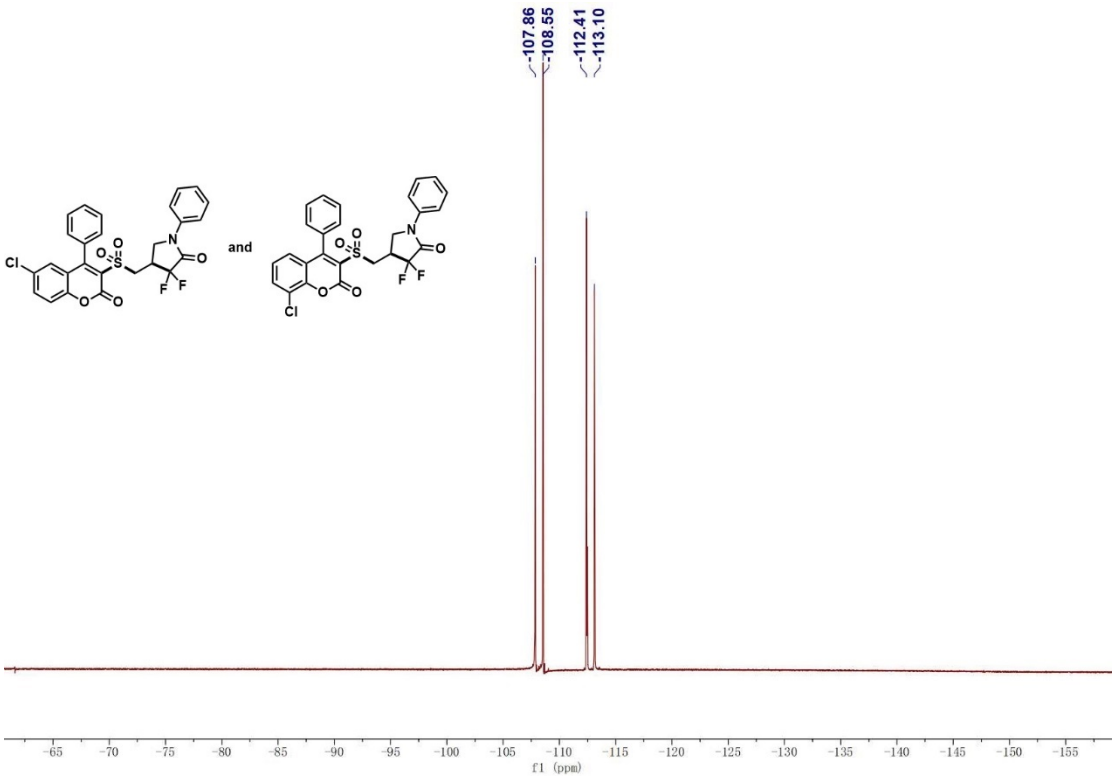
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4la and 4l'a**



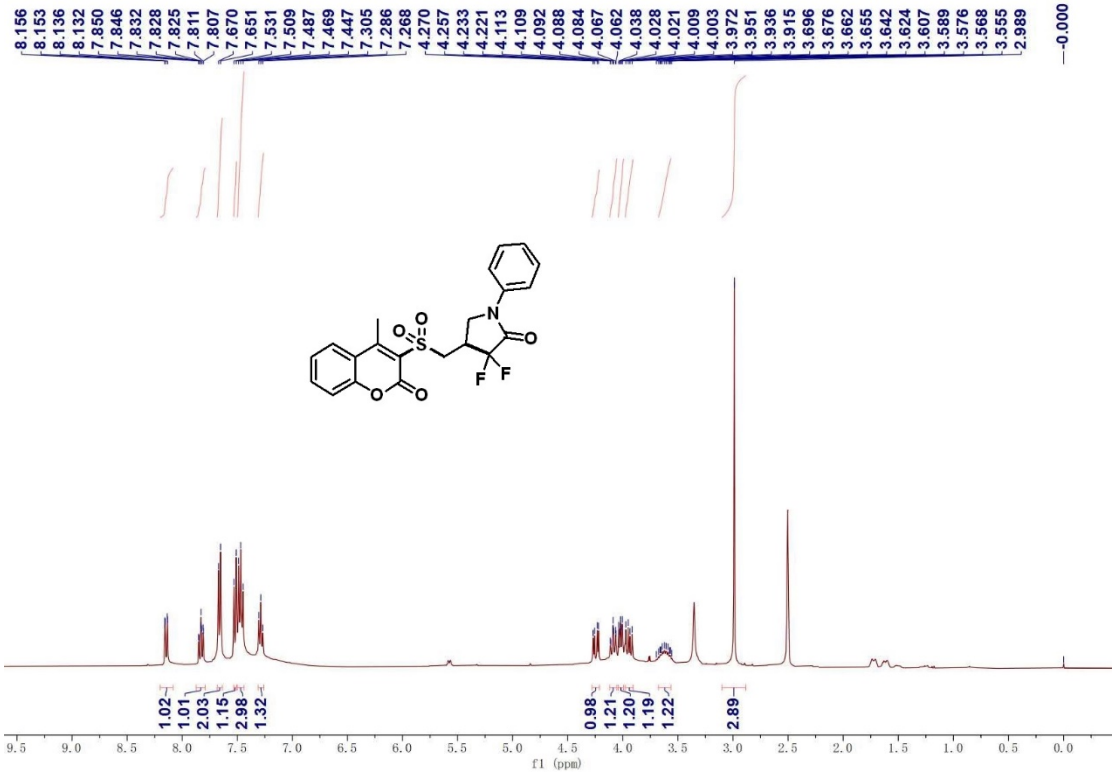
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4la and 4l'a**



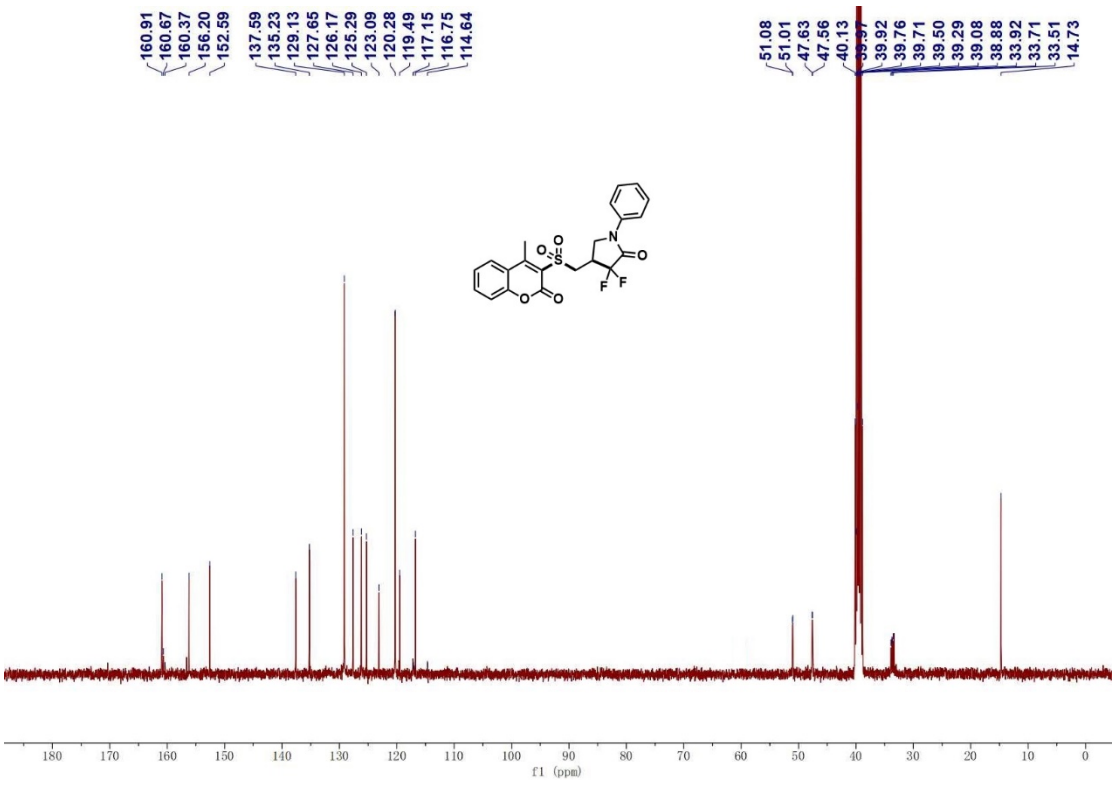
^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4la and 4l'a**



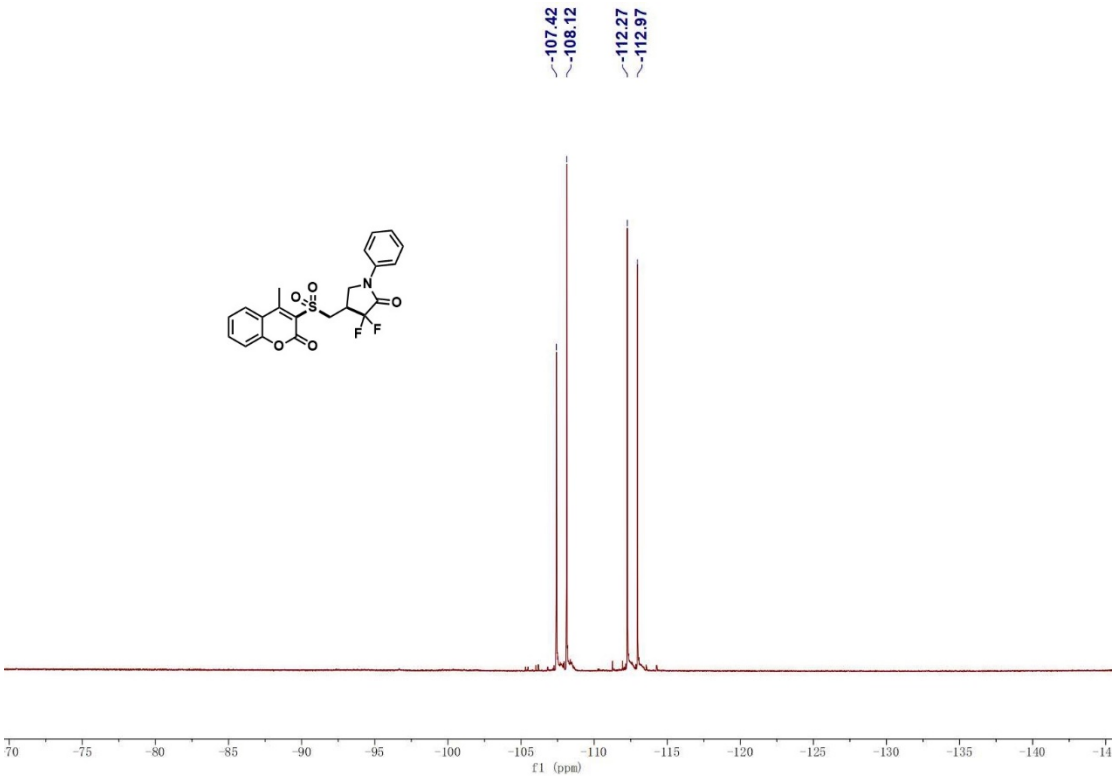
^{1}H NMR-spectrum (400 MHz, DMSO-d_6) of **4ma**



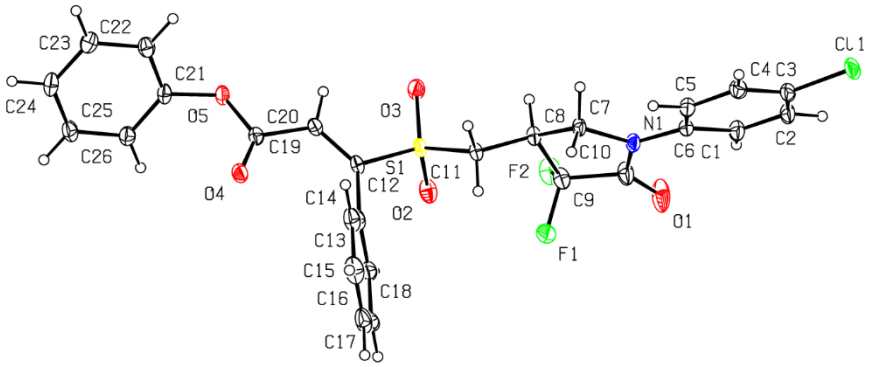
^{13}C NMR-spectrum (101 MHz, DMSO-d_6) of **4ma**



^{19}F NMR-spectrum (376 MHz, DMSO-d_6) of **4ma**



9.1 X-ray crystallography date of 3ac.



Crystal structure determination of 3ac.

Crystal Data for $C_{26}H_{20}ClF_2NO_5S$ (M =531.94 g/mol): triclinic, space group P-1 (no. 2), a = 6.3919(4) Å, b = 10.6731(6) Å, c = 18.7577(11) Å, α = 73.689(2)°, β = 87.428(2)°, γ = 75.023(2)°, V = 1185.92(12) Å^3, Z = 2, T = 170.00 K, μ(GaKα) = 1.799 mm^{-1}, $Dcalc$ = 1.490 g/cm^3, 37998 reflections measured (7.752° ≤ 2Θ ≤ 114.212°), 4772 unique (R_{int} = 0.0554, R_{sigma} = 0.0415) which

were used in all calculations. The final R_1 was 0.0798 (I > 2σ(I)) and wR_2 was 0.2236 (all data).

Table 1 Crystal data and structure refinement for 3ac.

Identification code	3ac
Empirical formula	$C_{26}H_{20}ClF_2NO_5S$
Formula weight	531.94
Temperature/K	170.00
Crystal system	triclinic
Space group	P-1
a/Å	6.3919(4)
b/Å	10.6731(6)
c/Å	18.7577(11)
α/°	73.689(2)
β/°	87.428(2)
γ/°	75.023(2)
Volume/Å^3	1185.92(12)
Z	2
ρ_{calc}g/cm^3	1.490
μ/mm^{-1}	1.799
F(000)	548.0
Crystal size/mm^3	0.2 × 0.03 × 0.02
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	7.752 to 114.212
Index ranges	-7 ≤ h ≤ 7, -13 ≤ k ≤ 13, -23 ≤ l ≤ 23
Reflections collected	37998
Independent reflections	4772 [R_{int} = 0.0554, R_{sigma} = 0.0415]
Data/restraints/parameters	4772/0/325
Goodness-of-fit on F^2	1.125
Final R indexes [I>=2σ (I)]	R_1 = 0.0798, wR_2 = 0.2190
Final R indexes [all data]	R_1 = 0.0859, wR_2 = 0.2236
Largest diff. peak/hole / e Å^{-3}	1.54/-0.52

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3ac. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	-1142.0(18)	9783.9(9)	7618.8(5)	45.8(3)
S1	4539.8(13)	5374.5(8)	3097.4(4)	25.4(2)
F1	-535(4)	7536(3)	3387.0(12)	42.0(6)
O1	-2901(5)	7259(5)	4781(2)	71.7(12)
N1	420(4)	7589(3)	5008.1(16)	27.1(6)
C1	-1845(6)	8048(4)	6043(2)	34.8(8)
F2	-332(4)	5482(3)	4048.8(14)	47.4(6)
O2	2566(4)	5384(3)	2768.9(15)	39.3(6)
C2	-2183(7)	8576(4)	6648(2)	39.3(9)
O3	5682(5)	4151(3)	3627.2(15)	40.8(7)
C3	-713(7)	9184(4)	6830(2)	36.3(8)
O4	9744(4)	5952(2)	1221.0(13)	33.1(6)
C4	1093(6)	9305(4)	6411(2)	35.4(8)
O5	11074(4)	3747(2)	1836.1(13)	28.9(5)
C5	1422(6)	8801(4)	5795(2)	31.4(7)

C6	-26(5)	8166(3)	5610.2(18)	27.9(7)
C7	2556(5)	7424(4)	4670.3(18)	25.8(7)
C8	2583(5)	6440(4)	4203.0(19)	27.4(7)
C9	220(6)	6629(4)	4058(2)	34.2(8)
C10	-993(6)	7189(5)	4668(2)	39.7(9)
C11	4025(5)	6705(3)	3530.9(17)	25.3(7)
C12	6321(5)	5858(3)	2360.9(17)	25.0(7)
C13	5509(6)	7223(3)	1837.7(18)	27.3(7)
C14	6736(7)	8166(4)	1751(2)	39.0(9)
C15	5992(9)	9445(4)	1274(3)	50.9(12)
C16	4068(9)	9793(4)	885(2)	54.6(13)
C17	2832(8)	8884(4)	966(2)	47.0(11)
C18	3548(6)	7588(4)	1444.5(19)	34.5(8)
C19	8150(5)	4915(3)	2351.9(18)	26.0(7)
C20	9699(5)	4990(3)	1733.7(18)	26.2(7)
C21	12755(6)	3582(3)	1330.2(19)	27.5(7)
C22	14842(6)	3265(4)	1606(2)	31.6(8)
C23	16558(6)	3020(4)	1137(2)	33.9(8)
C24	16149(6)	3092(4)	406(2)	36.2(8)
C25	14038(6)	3411(4)	140(2)	35.3(8)
C26	12313(6)	3655(4)	605(2)	31.1(7)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 3ac. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	71.2(7)	34.2(5)	24.8(4)	-14.0(4)	9.5(4)	4.2(4)
S1	31.0(5)	24.4(4)	21.8(4)	-8.5(3)	8.3(3)	-8.0(3)
F1	35.7(12)	56.7(14)	32.8(11)	-16.3(10)	-3.1(9)	-5.6(10)
O1	29.7(16)	149(4)	68(2)	-69(2)	21.8(15)	-39(2)
N1	20.9(13)	35.8(15)	26.4(14)	-11.8(12)	7.4(11)	-8.0(11)
C1	31.4(18)	40(2)	32.3(18)	-12.0(16)	10.6(14)	-7.6(15)
F2	49.1(14)	55.4(15)	55.5(15)	-28.3(12)	13.3(11)	-32.4(12)
O2	40.3(15)	51.6(16)	37.6(14)	-22.0(13)	12.7(11)	-23.6(13)
C2	41(2)	39(2)	29.1(18)	-5.9(16)	15.5(15)	-1.0(16)
O3	49.0(16)	27.6(13)	33.0(14)	1.0(11)	16.1(12)	-0.3(11)
C3	47(2)	29.4(18)	24.7(17)	-8.7(14)	6.0(15)	4.8(15)
O4	39.9(14)	30.2(13)	25.1(12)	-5.5(10)	9.1(10)	-5.5(10)
C4	43(2)	30.7(18)	30.8(18)	-11.8(15)	1.9(15)	-3.5(15)
O5	33.2(13)	27.4(12)	26.7(12)	-10.6(10)	10.8(9)	-6.8(10)
C5	30.4(18)	33.2(18)	29.7(17)	-11.2(14)	6.8(13)	-5.0(14)
C6	28.3(17)	29.2(17)	22.0(15)	-6.5(13)	4.5(12)	-1.6(13)
C7	19.9(15)	36.2(18)	25.4(16)	-13.6(14)	7.1(12)	-9.9(13)
C8	27.4(17)	32.6(17)	25.8(16)	-12.5(13)	7.9(13)	-10.2(13)
C9	34.1(19)	46(2)	30.8(18)	-17.6(16)	7.4(14)	-18.3(16)
C10	30.4(19)	63(3)	35(2)	-24.5(19)	10.8(15)	-18.6(18)
C11	27.6(16)	31.0(17)	20.8(15)	-11.6(13)	6.6(12)	-9.9(13)
C12	32.0(17)	27.8(16)	19.5(14)	-11.2(12)	7.2(12)	-11.2(13)
C13	37.1(18)	25.8(16)	20.7(15)	-11.7(13)	11.4(13)	-7.3(13)
C14	55(2)	34.2(19)	34.5(19)	-16.5(16)	16.8(17)	-17.2(17)
C15	79(3)	30(2)	46(2)	-12.6(18)	26(2)	-20(2)
C16	91(4)	25.6(19)	34(2)	-5.5(16)	25(2)	1(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 3ac. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C17	66(3)	37(2)	22.5(17)	-7.2(15)	4.5(17)	11.1(19)
C18	42(2)	32.9(18)	25.1(17)	-10.6(14)	6.2(14)	-2.6(15)
C19	30.6(17)	27.7(16)	20.4(15)	-7.4(12)	4.6(12)	-8.5(13)
C20	27.8(17)	29.5(16)	24.1(16)	-11.7(13)	3.7(12)	-7.9(13)
C21	32.0(18)	24.0(16)	29.5(17)	-12.2(13)	11.6(13)	-9.2(13)
C22	37.6(19)	29.9(17)	31.4(18)	-13.5(14)	6.2(14)	-11.3(14)
C23	29.5(18)	32.8(18)	43(2)	-15.2(16)	7.0(15)	-10.0(14)
C24	38(2)	32.8(19)	42(2)	-19.0(16)	17.9(16)	-10.9(15)
C25	45(2)	35.7(19)	28.9(18)	-16.1(15)	9.1(15)	-9.9(16)
C26	32.3(18)	30.5(18)	31.2(18)	-11.8(14)	5.5(14)	-6.4(14)

Table 4 Bond Lengths for 3ac.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C3	1.756(4)	C7	C8	1.541(5)
S1	O2	1.426(3)	C8	C9	1.498(5)
S1	O3	1.438(3)	C8	C11	1.533(4)
S1	C11	1.780(3)	C9	C10	1.528(5)
S1	C12	1.798(3)	C12	C13	1.486(5)
F1	C9	1.372(4)	C12	C19	1.334(5)
O1	C10	1.215(5)	C13	C14	1.399(5)
N1	C6	1.417(4)	C13	C18	1.391(5)
N1	C7	1.469(4)	C14	C15	1.381(6)
N1	C10	1.345(5)	C15	C16	1.370(8)
C1	C2	1.389(5)	C16	C17	1.376(7)
C1	C6	1.400(5)	C17	C18	1.393(5)
F2	C9	1.363(4)	C19	C20	1.489(4)
C2	C3	1.374(6)	C21	C22	1.376(5)
C3	C4	1.380(6)	C21	C26	1.379(5)
O4	C20	1.199(4)	C22	C23	1.392(5)
C4	C5	1.391(5)	C23	C24	1.385(6)
O5	C20	1.356(4)	C24	C25	1.383(6)
O5	C21	1.411(4)	C25	C26	1.392(5)
C5	C6	1.386(5)			

Table 5 Bond Angles for 3ac.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	S1	O3	118.11(18)	C8	C9	C10	106.6(3)
O2	S1	C11	108.77(16)	O1	C10	N1	129.5(4)
O2	S1	C12	108.00(15)	O1	C10	C9	123.3(4)
O3	S1	C11	108.15(16)	N1	C10	C9	107.2(3)
O3	S1	C12	109.11(16)	C8	C11	S1	111.5(2)
C11	S1	C12	103.78(15)	C13	C12	S1	115.5(2)
C6	N1	C7	121.0(3)	C19	C12	S1	114.9(2)
C10	N1	C6	126.1(3)	C19	C12	C13	129.6(3)
C10	N1	C7	112.9(3)	C14	C13	C12	118.9(3)
C2	C1	C6	119.6(4)	C18	C13	C12	121.5(3)

Table 5 Bond Angles for 3ac.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C3	C2	C1	120.0(3)	C18	C13	C14	119.6(3)
C2	C3	Cl1	118.7(3)	C15	C14	C13	119.6(4)
C2	C3	C4	121.1(3)	C16	C15	C14	120.4(4)
C4	C3	Cl1	120.1(3)	C15	C16	C17	120.8(4)
C3	C4	C5	119.2(4)	C16	C17	C18	119.8(4)
C20	O5	C21	118.2(3)	C13	C18	C17	119.7(4)
C6	C5	C4	120.5(3)	C12	C19	C20	124.6(3)
C1	C6	N1	121.1(3)	O4	C20	O5	124.6(3)
C5	C6	N1	119.3(3)	O4	C20	C19	127.6(3)
C5	C6	C1	119.5(3)	O5	C20	C19	107.8(3)
N1	C7	C8	104.5(3)	C22	C21	O5	117.0(3)
C9	C8	C7	102.6(3)	C22	C21	C26	121.9(3)
C9	C8	C11	117.8(3)	C26	C21	O5	121.0(3)
C11	C8	C7	110.8(3)	C21	C22	C23	119.0(3)
F1	C9	C8	113.2(3)	C24	C23	C22	120.0(4)
F1	C9	C10	107.7(3)	C25	C24	C23	120.1(3)
F2	C9	F1	104.9(3)	C24	C25	C26	120.3(3)
F2	C9	C8	114.6(3)	C21	C26	C25	118.7(3)
F2	C9	C10	109.7(3)				

Table 6 Torsion Angles for 3ac.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Cl1	C3	C4	C5	178.8(3)	C7	C8	C11	S1	167.7(2)
S1	C12	C13	C14	121.7(3)	C8	C9	C10	O1	-168.2(5)
S1	C12	C13	C18	-57.3(4)	C8	C9	C10	N1	13.4(4)
S1	C12	C19	C20	169.7(3)	C9	C8	C11	S1	-74.7(3)
F1	C9	C10	O1	70.1(6)	C10	N1	C6	C1	17.5(6)
F1	C9	C10	N1	-108.4(3)	C10	N1	C6	C5	-165.7(4)
N1	C7	C8	C9	23.9(3)	C10	N1	C7	C8	-17.2(4)
N1	C7	C8	C11	150.5(3)	C11	S1	C12	C13	-54.8(3)
C1	C2	C3	Cl1	-177.7(3)	C11	S1	C12	C19	127.3(3)
C1	C2	C3	C4	1.2(6)	C11	C8	C9	F1	-26.5(4)
F2	C9	C10	O1	-43.6(6)	C11	C8	C9	F2	93.8(4)
F2	C9	C10	N1	138.0(3)	C11	C8	C9	C10	-144.7(3)
O2	S1	C11	C8	67.5(3)	C12	S1	C11	C8	-177.7(2)
O2	S1	C12	C13	60.5(3)	C12	C13	C14	C15	-179.2(3)
O2	S1	C12	C19	-117.3(3)	C12	C13	C18	C17	179.3(3)
C2	C1	C6	N1	177.2(3)	C12	C19	C20	O4	12.3(6)
C2	C1	C6	C5	0.4(5)	C12	C19	C20	O5	-166.3(3)
C2	C3	C4	C5	0.0(6)	C13	C12	C19	C20	-7.8(6)
O3	S1	C11	C8	-61.9(3)	C13	C14	C15	C16	-0.2(6)
O3	S1	C12	C13	-169.9(2)	C14	C13	C18	C17	0.3(5)
O3	S1	C12	C19	12.2(3)	C14	C15	C16	C17	0.6(6)
C3	C4	C5	C6	-1.0(5)	C15	C16	C17	C18	-0.4(6)
C4	C5	C6	N1	-176.1(3)	C16	C17	C18	C13	0.0(5)
C4	C5	C6	C1	0.8(5)	C18	C13	C14	C15	-0.2(5)
O5	C21	C22	C23	176.5(3)	C19	C12	C13	C14	-60.9(5)

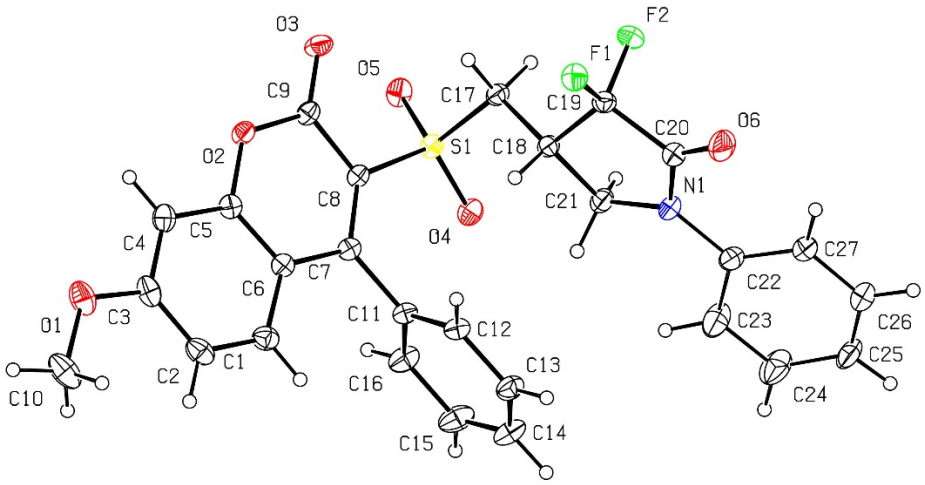
Table 6 Torsion Angles for 3ac.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O5	C21	C26	C25	-176.5(3)	C19	C12	C13	C18	120.2(4)
C6	N1	C7	C8	165.1(3)	C20	O5	C21	C22	114.5(3)
C6	N1	C10	O1	2.0(8)	C20	O5	C21	C26	-69.4(4)
C6	N1	C10	C9	-179.7(3)	C21	O5	C20	O4	3.8(5)
C6	C1	C2	C3	-1.3(6)	C21	O5	C20	C19	-177.6(3)
C7	N1	C6	C1	-165.2(3)	C21	C22	C23	C24	-0.2(5)
C7	N1	C6	C5	11.7(5)	C22	C21	C26	C25	-0.6(5)
C7	N1	C10	O1	-175.6(5)	C22	C23	C24	C25	0.2(5)
C7	N1	C10	C9	2.7(5)	C23	C24	C25	C26	-0.3(6)
C7	C8	C9	F1	95.5(3)	C24	C25	C26	C21	0.5(5)
C7	C8	C9	F2	-144.2(3)	C26	C21	C22	C23	0.4(5)
C7	C8	C9	C10	-22.7(4)					

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3ac.

Atom	*x*	*y*	*z*	U(eq)
H1	-2843.49	7610.57	5922.46	42
H2	-3430.26	8515.76	6937.49	47
H4	2098.41	9727.83	6541.24	42
H5	2648.78	8892.56	5499.33	38
H7A	3729.4	7041.39	5057.29	31
H7B	2735.01	8300.31	4352.06	31
H8	3189.91	5498.15	4521.05	33
H11A	5417.04	6795.64	3693.93	30
H11B	3306.68	7566	3166.16	30
H14	8074.32	7926.48	2018.64	47
H15	6820.68	10087.25	1215.63	61
H16	3579.72	10674.06	555.52	65
H17	1495.08	9138.17	695.74	56
H18	2700.93	6955.42	1502.28	41
H19	8487.3	4139.82	2769.27	31
H22	15109.78	3214.2	2108.7	38
H23	18008.3	2802.91	1318.5	41
H24	17319.85	2922.55	86.41	43
H25	13764.12	3464.2	-362.72	42
H26	10860.55	3867.93	425.83	37

9.2 X-ray crystallography date of 4fa.



Crystal structure determination of 4fa.

Crystal Data for $C_{27}H_{21}F_2NO_6S$ (M =525.51 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 10.2939(4) Å, b = 9.7381(4) Å, c = 25.5602(11) Å, β = 91.730(2)°, V = 2561.06(18) Å^3, Z = 4, T = 170.00 K, μ(MoKα) = 0.183 mm^{-1}, $Dcalc$ = 1.363 g/cm^3, 61885 reflections measured (5.008° ≤ 2Θ ≤ 55.026°), 5903 unique (R_{int} = 0.0797, R_{sigma} = 0.0343) which were used in all calculations. The final R_1 was 0.0441 (I > 2σ(I)) and wR_2 was 0.1095 (all data).

Table 1 Crystal data and structure refinement for 4fa.

Identification code	4af
Empirical formula	$C_{27}H_{21}F_2NO_6S$
Formula weight	525.51
Temperature/K	170.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.2939(4)
b/Å	9.7381(4)
c/Å	25.5602(11)
α/°	90
β/°	91.730(2)

γ/°	90
Volume/Å^3	2561.06(18)
Z	4
ρ_{calc}g/cm^3	1.363
μ/mm^{-1}	0.183
F(000)	1088.0
Crystal size/mm^3	0.4 × 0.23 × 0.16
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.008 to 55.026
Index ranges	-13 ≤ h ≤ 12, -12 ≤ k ≤ 12, -33 ≤ l ≤ 33
Reflections collected	61885
Independent reflections	5903 [R_{int} = 0.0797, R_{sigma} = 0.0343]
Data/restraints/parameters	5903/207/390
Goodness-of-fit on F^2	1.021
Final R indexes [I>=2σ (I)]	R_1 = 0.0441, wR_2 = 0.0998
Final R indexes [all data]	R_1 = 0.0658, wR_2 = 0.1095
Largest diff. peak/hole / e Å^{-3}	0.26/-0.31

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3fa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	8832.0(4)	2251.7(5)	7517.4(2)	26.53(12)
F1	9550.2(10)	6029.7(11)	8688.7(4)	35.4(3)
F2	9107.7(11)	4164.0(12)	9110.2(4)	36.4(3)
O1	11106.9(16)	6836.3(16)	5087.3(6)	46.6(4)
O2	11295.3(11)	4051.7(13)	6561.6(5)	28.7(3)
O3	11572.7(12)	2909.8(14)	7294.9(5)	34.7(3)
O4	7448.7(12)	2113.4(14)	7471.2(5)	32.9(3)
O5	9601.3(13)	1021.0(13)	7512.3(5)	34.2(3)
O6	7280.0(15)	6520.0(18)	9258.7(6)	52.7(4)
N1	6400.1(15)	4910.8(18)	8679.8(6)	33.4(4)
C1	8484.0(19)	5726(2)	5925.8(7)	33.6(4)
C2	9085(2)	6387(2)	5524.2(8)	38.1(5)
C3	10423(2)	6241(2)	5470.9(7)	35.2(4)
C4	11149.9(19)	5441(2)	5820.2(7)	32.7(4)
C5	10523.7(17)	4796.5(18)	6221.0(7)	26.4(4)
C6	9183.9(17)	4902.5(18)	6287.3(7)	26.2(4)
C7	8592.7(16)	4142.8(17)	6701.9(7)	24.8(4)
C8	9380.5(16)	3348.8(17)	7017.2(7)	23.4(3)
C9	10799.3(17)	3393.2(18)	6984.7(7)	26.5(4)
C10	10426(3)	7708(2)	4725.3(9)	53.8(6)
C11	7163.9(16)	4347.5(18)	6768.4(7)	26.2(4)
C12	6765.2(17)	5514.4(19)	7029.6(7)	29.2(4)
C13	5446.2(19)	5743(2)	7101.1(8)	37.1(5)
C14	4539(2)	4830(2)	6900.2(9)	45.0(5)
C15	4934(2)	3699(2)	6624.4(10)	48.2(6)
C16	6244.9(19)	3443(2)	6557.6(9)	38.3(5)
C17	9225.0(17)	3138.1(19)	8111.6(7)	28.0(4)
C18	8299.6(16)	4314.9(18)	8225.6(7)	25.8(4)
C19	8633.0(17)	5046.9(19)	8730.4(7)	28.6(4)
C20	7353.9(19)	5628(2)	8931.0(7)	34.9(4)

C21	6874.1(17)	3904(2)	8300.5(7)	32.2(4)
C22	5070(6)	4932(17)	8828(3)	36.5(13)
C23	4152(6)	4400(7)	8488(3)	52.9(15)
C24	2870(6)	4315(7)	8632(3)	60.1(15)
C25	2495(7)	4756(10)	9108(3)	50.7(15)
C26	3398(4)	5414(6)	9425.6(15)	56.0(11)
C27	4686(3)	5514(6)	9293.1(14)	48.8(10)
C22A	5023(11)	4820(40)	8780(5)	39(2)
C23A	4101(11)	4765(12)	8387(4)	33.7(18)
C24A	2802(11)	4623(12)	8492(4)	37.6(17)
C25A	2441(14)	4550(20)	8994(5)	49(2)
C26A	3360(7)	4456(12)	9411(3)	57.6(18)
C27A	4669(7)	4577(12)	9292(3)	54.4(17)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 3fa. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	26.4(2)	20.9(2)	32.4(2)	2.25(18)	4.15(17)	-0.52(17)
F1	34.9(6)	33.6(6)	37.7(6)	-1.7(5)	2.3(5)	-5.5(5)
F2	38.5(6)	40.2(7)	30.3(6)	9.0(5)	-3.6(5)	5.8(5)
O1	65.9(10)	40.2(9)	34.2(8)	8.4(7)	9.7(7)	-4.7(7)
O2	23.3(6)	29.0(7)	34.0(7)	4.5(5)	4.3(5)	1.5(5)
O3	25.4(7)	34.5(8)	44.1(8)	10.4(6)	-1.5(6)	5.1(6)
O4	27.5(7)	31.1(7)	40.3(7)	0.1(6)	4.9(5)	-6.9(5)
O5	41.9(8)	19.9(7)	41.2(8)	3.9(6)	9.1(6)	5.0(6)
O6	45.7(9)	66.5(11)	45.9(9)	-22.1(8)	4.4(7)	11.5(8)
N1	23.8(8)	43.0(10)	33.7(8)	0.1(7)	5.6(6)	5.6(7)
C1	35.5(10)	30.5(10)	34.5(10)	0.5(8)	-2.9(8)	3.1(8)
C2	52.3(13)	30.5(11)	31.2(10)	3.0(8)	-5.0(9)	1.2(9)
C3	52.4(12)	25.9(10)	27.5(9)	-0.6(8)	6.4(9)	-6.1(9)
C4	37.1(10)	28.6(10)	32.6(10)	-3.9(8)	6.5(8)	-2.7(8)
C5	31.1(9)	19.4(9)	28.8(9)	-1.5(7)	2.0(7)	-0.2(7)
C6	29.2(9)	21.0(9)	28.3(9)	-1.4(7)	0.7(7)	0.1(7)
C7	24.3(9)	19.6(9)	30.3(9)	-5.7(7)	-1.1(7)	-1.2(7)
C8	23.8(8)	17.9(8)	28.7(9)	-1.2(7)	2.3(7)	0.2(7)
C9	26.0(9)	19.7(9)	34.0(9)	0.4(7)	4.2(7)	1.8(7)
C10	85.0(18)	42.2(13)	33.9(11)	8.6(10)	-3.1(11)	-10.6(13)
C11	22.9(9)	23.0(9)	32.6(9)	0.7(7)	-1.8(7)	0.6(7)
C12	25.9(9)	26.1(9)	35.4(10)	0.3(8)	-3.4(7)	1.2(7)
C13	31.6(10)	35.1(11)	44.8(11)	-2.5(9)	0.4(8)	9.5(9)
C14	23.1(10)	46.5(13)	65.2(14)	0.2(11)	0.1(9)	4.9(9)
C15	26.5(10)	43.9(13)	73.5(16)	-6.8(12)	-8.3(10)	-6.9(9)
C16	29.1(10)	30.3(11)	55.2(13)	-9.4(9)	-2.8(9)	-0.4(8)
C17	24.4(9)	29.2(10)	30.4(9)	1.2(7)	1.5(7)	3.4(7)
C18	23.2(9)	26.9(9)	27.5(9)	3.4(7)	2.2(7)	1.8(7)
C19	26.1(9)	30.1(10)	29.6(9)	4.8(7)	-0.9(7)	1.5(7)
C20	31.1(10)	43.8(12)	30.0(10)	1.1(9)	2.3(8)	6.9(9)
C21	24.8(9)	37.2(11)	34.8(10)	-2.1(8)	3.9(8)	1.2(8)
C22	27(2)	44(3)	38(2)	6(2)	2.6(18)	5.4(18)
C23	37(2)	61(4)	61(3)	-22(2)	12(2)	-5(2)
C24	33(2)	72(4)	76(4)	-18(3)	9(3)	-11(2)

C25	27(2)	68(3)	58(3)	7(3)	17(2)	10(2)
C26	35.3(18)	90(3)	43.5(18)	-1(2)	9.6(14)	15(2)
C27	29.7(16)	81(3)	35.4(16)	-5.8(19)	0.3(13)	10.8(19)
C22A	27(3)	56(4)	33(3)	0(3)	8(3)	12(3)
C23A	25(3)	44(4)	31(3)	13(3)	-1(2)	-6(3)
C24A	29(3)	47(4)	37(3)	21(3)	-3(3)	-3(3)
C25A	29(3)	75(5)	45(4)	-4(4)	1(3)	0(3)
C26A	39(3)	97(4)	38(3)	-7(3)	13(3)	-7(4)
C27A	33(3)	93(4)	37(3)	-3(3)	1(2)	0(3)

Table 4 Bond Lengths for 4fa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O4	1.4317(13)	C7	C11	1.499(2)
S1	O5	1.4367(13)	C8	C9	1.466(2)
S1	C8	1.7716(18)	C11	C12	1.386(3)
S1	C17	1.7828(18)	C11	C16	1.389(3)
F1	C19	1.351(2)	C12	C13	1.393(3)
F2	C19	1.375(2)	C13	C14	1.378(3)
O1	C3	1.354(2)	C14	C15	1.376(3)
O1	C10	1.425(3)	C15	C16	1.388(3)
O2	C5	1.369(2)	C17	C18	1.524(2)
O2	C9	1.369(2)	C18	C19	1.505(3)
O3	C9	1.203(2)	C18	C21	1.538(2)
O6	C20	1.211(2)	C19	C20	1.535(3)
N1	C20	1.351(3)	C22	C23	1.366(8)
N1	C21	1.472(2)	C22	C27	1.385(9)
N1	C22	1.431(6)	C23	C24	1.383(6)
N1	C22A	1.451(11)	C24	C25	1.357(7)
C1	C2	1.374(3)	C25	C26	1.375(7)
C1	C6	1.405(3)	C26	C27	1.382(5)
C2	C3	1.396(3)	C22A	C23A	1.362(12)
C3	C4	1.387(3)	C22A	C27A	1.388(14)
C4	C5	1.378(3)	C23A	C24A	1.379(11)
C5	C6	1.399(2)	C24A	C25A	1.347(12)
C6	C7	1.442(2)	C25A	C26A	1.407(13)
C7	C8	1.366(2)	C26A	C27A	1.395(9)

Table 5 Bond Angles for 4fa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	S1	O5	117.90(8)	C16	C11	C7	122.06(16)
O4	S1	C8	109.57(8)	C11	C12	C13	119.86(17)
O4	S1	C17	108.38(8)	C14	C13	C12	120.02(19)
O5	S1	C8	107.98(8)	C15	C14	C13	120.02(19)
O5	S1	C17	107.50(8)	C14	C15	C16	120.7(2)
C8	S1	C17	104.70(9)	C15	C16	C11	119.47(19)
C3	O1	C10	117.95(19)	C18	C17	S1	113.58(12)
C5	O2	C9	121.84(14)	C17	C18	C21	115.62(15)
C20	N1	C21	113.97(15)	C19	C18	C17	113.11(14)
C20	N1	C22	123.6(4)	C19	C18	C21	102.13(14)
C20	N1	C22A	130.4(9)	F1	C19	F2	105.33(14)
C22	N1	C21	121.5(5)	F1	C19	C18	114.20(15)

C22A	N1	C21	114.8(11)	F1	C19	C20	111.95(16)
C2	C1	C6	121.66(19)	F2	C19	C18	112.09(15)
C1	C2	C3	119.55(19)	F2	C19	C20	106.54(14)
O1	C3	C2	124.30(19)	C18	C19	C20	106.57(15)
O1	C3	C4	115.10(19)	O6	C20	N1	129.76(18)
C4	C3	C2	120.60(18)	O6	C20	C19	124.60(18)
C5	C4	C3	118.62(18)	N1	C20	C19	105.62(16)
O2	C5	C4	116.02(16)	N1	C21	C18	104.20(15)
O2	C5	C6	121.16(15)	C23	C22	N1	118.4(6)
C4	C5	C6	122.81(17)	C23	C22	C27	119.4(5)
C1	C6	C7	123.81(17)	C27	C22	N1	122.2(5)
C5	C6	C1	116.76(16)	C22	C23	C24	120.1(6)
C5	C6	C7	119.40(16)	C25	C24	C23	121.3(6)
C6	C7	C11	116.90(15)	C24	C25	C26	118.1(6)
C8	C7	C6	117.89(16)	C25	C26	C27	121.7(4)
C8	C7	C11	125.13(16)	C26	C27	C22	118.8(4)
C7	C8	S1	124.81(13)	C23A	C22A	N1	122.3(10)
C7	C8	C9	121.64(16)	C23A	C22A	C27A	119.5(10)
C9	C8	S1	113.48(12)	C27A	C22A	N1	117.6(11)
O2	C9	C8	117.03(15)	C22A	C23A	C24A	121.2(9)
O3	C9	O2	116.68(16)	C25A	C24A	C23A	119.1(10)
O3	C9	C8	126.29(17)	C24A	C25A	C26A	121.8(11)
C12	C11	C7	117.99(15)	C27A	C26A	C25A	117.4(9)
C12	C11	C16	119.89(17)	C22A	C27A	C26A	120.1(8)

Table 6 Torsion Angles for 4fa.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	C8	C9	O2	170.56(12)	C10	O1	C3	C4	-178.01(18)
S1	C8	C9	O3	-9.7(2)	C11	C7	C8	S1	7.8(3)
S1	C17	C18	C19	179.46(12)	C11	C7	C8	C9	-168.90(16)
S1	C17	C18	C21	62.19(18)	C11	C12	C13	C14	-1.7(3)
F1	C19	C20	O6	-37.3(3)	C12	C11	C16	C15	-1.9(3)
F1	C19	C20	N1	144.53(16)	C12	C13	C14	C15	-0.7(3)
F2	C19	C20	O6	77.3(2)	C13	C14	C15	C16	1.8(4)
F2	C19	C20	N1	-100.82(17)	C14	C15	C16	C11	-0.5(4)
O1	C3	C4	C5	-179.80(17)	C16	C11	C12	C13	3.0(3)
O2	C5	C6	C1	178.09(16)	C17	S1	C8	C7	-104.52(16)
O2	C5	C6	C7	-4.0(3)	C17	S1	C8	C9	72.43(14)
O4	S1	C8	C7	11.54(18)	C17	C18	C19	F1	84.14(19)
O4	S1	C8	C9	-171.51(12)	C17	C18	C19	F2	-35.5(2)
O4	S1	C17	C18	-40.07(15)	C17	C18	C19	C20	-151.72(15)
O5	S1	C8	C7	141.15(15)	C17	C18	C21	N1	148.10(15)
O5	S1	C8	C9	-41.91(15)	C18	C19	C20	O6	-162.8(2)
O5	S1	C17	C18	-168.52(12)	C18	C19	C20	N1	19.0(2)
N1	C22	C23	C24	175.6(8)	C19	C18	C21	N1	24.84(18)
N1	C22	C27	C26	-175.8(9)	C20	N1	C21	C18	-14.6(2)
N1	C22A	C23A	C24A	177.4(18)	C20	N1	C22	C23	167.0(8)
N1	C22A	C27A	C26A	-179.0(16)	C20	N1	C22	C27	-10.7(16)
C1	C2	C3	O1	179.37(18)	C20	N1	C22A	C23A	141.5(19)
C1	C2	C3	C4	-0.2(3)	C20	N1	C22A	C27A	-48(3)
C1	C6	C7	C8	178.09(17)	C21	N1	C20	O6	179.6(2)

C1	C6	C7	C11	-4.9(3)	C21	N1	C20	C19	-2.3(2)
C2	C1	C6	C5	0.5(3)	C21	N1	C22	C23	-24.6(15)
C2	C1	C6	C7	-177.32(18)	C21	N1	C22	C27	157.8(9)
C2	C3	C4	C5	-0.2(3)	C21	N1	C22A	C23A	-50(3)
C3	C4	C5	O2	-178.27(16)	C21	N1	C22A	C27A	121(2)
C3	C4	C5	C6	0.7(3)	C21	C18	C19	F1	-150.92(15)
C4	C5	C6	C1	-0.9(3)	C21	C18	C19	F2	89.40(17)
C4	C5	C6	C7	177.01(17)	C21	C18	C19	C20	-26.78(18)
C5	O2	C9	O3	-171.13(16)	C22	N1	C20	O6	-11.1(8)
C5	O2	C9	C8	8.7(2)	C22	N1	C20	C19	166.9(7)
C5	C6	C7	C8	0.4(2)	C22	N1	C21	C18	175.8(6)
C5	C6	C7	C11	177.33(16)	C22	C23	C24	C25	0.2(12)
C6	C1	C2	C3	0.1(3)	C23	C22	C27	C26	6.6(16)
C6	C7	C8	S1	-175.48(13)	C23	C24	C25	C26	6.3(12)
C6	C7	C8	C9	7.8(2)	C24	C25	C26	C27	-6.3(12)
C6	C7	C11	C12	-79.7(2)	C25	C26	C27	C22	-0.1(11)
C6	C7	C11	C16	97.4(2)	C27	C22	C23	C24	-6.7(17)
C7	C8	C9	O2	-12.4(2)	C22A	N1	C20	O6	-11.3(17)
C7	C8	C9	O3	167.39(18)	C22A	N1	C20	C19	166.7(16)
C7	C11	C12	C13	-179.85(17)	C22A	N1	C21	C18	174.5(12)
C7	C11	C16	C15	-178.90(19)	C22A	C23A	C24A	C25A	1(3)
C8	S1	C17	C18	76.81(14)	C23A	C22A	C27A	C26A	-8(4)
C8	C7	C11	C12	97.1(2)	C23A	C24A	C25A	C26A	-8(3)
C8	C7	C11	C16	-85.8(2)	C24A	C25A	C26A	C27A	6(3)
C9	O2	C5	C4	178.19(16)	C25A	C26A	C27A	C22A	2(2)
C9	O2	C5	C6	-0.8(2)	C27A	C22A	C23A	C24A	7(4)
C10	O1	C3	C2	2.4(3)					