

# Design, Synthesis and Preliminary Biological Evaluation of Novel Benzylsulfone Coumarin Derivatives as Anticancer Agents

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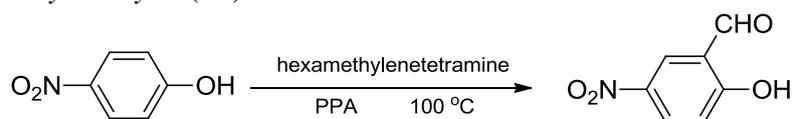
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## Supplementary Materials

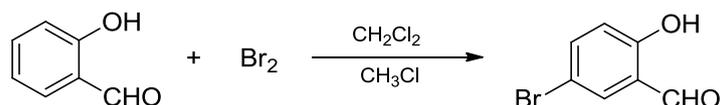
### 1. Synthesis of Intermediates

#### 1.1. 5-nitrosalicylaldehyde (**4b**)



A mixture of 4-nitrophenol (7.5 g, 54 mmol, 1.0 eq.), hexamethylene tetramine (7.5 g, 54 mmol, 1.0 eq.), and 75% PPA (60 mL) was agitated for 5 hours at 100 °C. Subsequently, the mixture was placed in 100 mL of ethyl acetate and 200 mL of water, and agitated until the mixture became completely dissolved. In addition, as a result of additionally adding 100 ml of ethyl acetate to the foregoing solution, the solution separated into 2 phases. The water phase was removed and the remaining solution was washed with saturated brine (50 mL\*2), then the organic layer was dried with anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under vacuum to obtain the desired product **4b** as a yellow solid, yield, 33.0%; m.p. 127-129 °C. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 12.22 (s, 1H, -CHO), 10.30 (s, 1H, -OH), 8.43 (d, 1H, *J* = 2.8 Hz, H-6), 8.35 (d, 1H, *J* = 8.8 Hz, H-4), 7.19 (d, 1H, *J* = 8.8 Hz, H-3).

#### 1.2. 5-Bromosalicylaldehyde (**4c**)



To a solution of salicylaldehyde (3.66 g, 30 mmol, 1.0 eq.) in 20 mL dichloromethane, 5.28 g (33 mmol, 1.1 eq.) bromine in 60 mL chloroform was added dropwisely over a period of 4-5 h. After completion of the reaction (TLC monitoring), the solvent was evaporated to obtain the crude product, which was recrystallized in 90% ethanol to yield the desired product. Yield, 64.2%; white solid, m.p. 105-107 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 10.94 (s, 1H, -CHO); 9.84 (s, 1H, -OH); 7.68 (d, 1H, *J* = 2.4 Hz, H-6); 7.61 (d, 1H, *J* = 8.8 Hz, H-4); 6.92 (d, 1H, *J* = 8.8 Hz, H-3).

#### 1.3. General Procedure for the Preparation of Benzylthioacetic Acids (**2a-2j**).

The following benzylthioacetic acids were synthesized according to the procedure described in the literature and identified by comparing their melting points and properties with the literature data.

**2-(2-Fluorobenzylthio)acetic Acid (2a)**. Condensation of 2-fluorobenzyl chloride **1a** with mercaptoacetic acid yielded the corresponding 2-(2-fluorobenzylthio)acetic

acid. The yield of this reaction was 98.5%, giving a pale yellow oil. It was identified by comparing its physical data with the literature data [1].

*2-(3-Fluorobenzylthio)acetic Acid (2b)*. Condensation of 3-fluorobenzyl chloride **1b** with mercaptoacetic acid yielded the corresponding 2-(3-fluorobenzylthio)acetic acid. The yield of this reaction was 98.1%, giving a pale yellow oil. It was identified by comparing its physical data with the literature data [1].

*2-(4-Fluorobenzylthio)acetic Acid (2c)*. Condensation of 4-fluorobenzyl chloride **1c** with mercaptoacetic acid yielded the corresponding 2-(4-fluorobenzylthio)acetic acid. The yield of this reaction was 94.8%, giving a pale yellow oil. It was identified by comparing its physical data with the literature data [2].

*2-(2-Chlorobenzylthio)acetic Acid (2d)*. Condensation of 2-chlorobenzyl chloride **1d** with mercaptoacetic acid yielded the corresponding 2-(2-chlorobenzylthio)acetic acid. The yield of this reaction was 89.8%, giving a white solid with a melting point of 52-53 °C. It was identified by comparing its physical data with the literature data [3].

*2-(2-Bromobenzylthio)acetic Acid (2e)*. Condensation of 2-bromobenzyl bromide **1e** with mercaptoacetic acid yielded the corresponding 2-(2-bromobenzylthio)acetic acid. The yield of this reaction was 94.6%, giving a white solid with a melting point of 49-51 °C. It was identified by comparing its physical data with the literature data [3].

*2-(3-Bromobenzylthio)acetic Acid (2f)*. Condensation of 3-bromobenzyl bromide **1f** with mercaptoacetic acid yielded the corresponding 2-(3-bromobenzylthio)acetic acid. The yield of this reaction was 91.7%, giving a pale yellow solid with a melting point of 87-89 °C. It was identified by comparing its physical data with the literature data [4].

*2-(4-Bromobenzylthio)acetic Acid (2g)*. Condensation of 4-bromobenzyl bromide **1g** with mercaptoacetic acid yielded the corresponding 2-(4-bromobenzylthio)acetic acid. The yield of this reaction was 91.2%, giving a pale yellow solid with a melting point of 73-76 °C. It was identified by comparing its physical data with the literature data [4].

*2-(3-Methylbenzylthio)acetic Acid (2h)*. Condensation of 3-methylbenzyl chloride **1h** with mercaptoacetic acid yielded the corresponding 2-(3-methylbenzylthio)acetic acid. The yield of this reaction was 91.5%, giving a pale yellow solid with a melting point of 72-74 °C. It was identified by comparing its physical data with the literature data [5].

*2-(4-Methylbenzylthio)acetic Acid (2i)*. Condensation of 4-methylbenzyl chloride **1i** with mercaptoacetic acid yielded the corresponding 2-(4-methylbenzylthio)acetic acid. The yield of this reaction was 78.7%, giving a pale yellow solid with a melting point of 65-67 °C. It was identified by comparing its physical data with the literature data [6].

*2-[2-(Trifluoromethyl)benzylthio]acetic Acid (2j)*. Condensation of 2-(trifluoromethyl)benzyl bromide **1j** with mercaptoacetic acid yielded the corresponding 2-[2-(trifluoromethyl)benzylthio]acetic acid. The yield of this reaction was 94.5%, giving a pale yellow oil. It was identified by comparing its physical data with the

literature data [5].

#### 1.4. General Procedure for the Preparation of Benzylsulfonylacetic Acids (3a-3j).

The following benzylsulfonylacetic acids were synthesized according to the procedure described in the literature and identified by comparing their melting points and properties with the literature data.

2-[(2-Fluorobenzyl)sulfonyl]acetic Acid (3a). Oxidation of 2-(2-fluorobenzylthio)acetic acid **2a** with 30% hydrogen peroxide yielded the corresponding 2-[(2-fluorobenzyl)sulfonyl]acetic acid. The yield of this reaction was 58.9%, giving a white solid with a melting point of 134.5-136 °C. It was identified by comparing its physical data with the literature data [7].

2-[(3-Fluorobenzyl)sulfonyl]acetic Acid (3b). Oxidation of 2-(3-fluorobenzylthio)acetic acid **2b** with 30% hydrogen peroxide yielded the corresponding 2-[(3-fluorobenzyl)sulfonyl]acetic acid. The yield of this reaction was 83.3%, giving a white solid with a melting point of 126-128 °C. It was identified by comparing its physical data with the literature data [7].

2-[(4-Fluorobenzyl)sulfonyl]acetic Acid (3c). Oxidation of 2-(4-fluorobenzylthio)acetic acid **2c** with 30% hydrogen peroxide yielded the corresponding 2-[(4-fluorobenzyl)sulfonyl]acetic acid. The yield of this reaction was 60.5%, giving a white solid with a melting point of 160-164 °C. It was identified by comparing its physical data with the literature data [2].

2-[(2-Chlorobenzyl)sulfonyl]acetic Acid (3d). Oxidation of 2-(2-chlorobenzylthio)acetic acid **2d** with 30% hydrogen peroxide yielded the corresponding 2-[(2-chlorobenzyl)sulfonyl]acetic acid. The yield of this reaction was 70.0%, giving a white solid with a melting point of 162-165°C. It was identified by comparing its physical data with the literature data [8].

2-[(2-Bromobenzyl)sulfonyl]acetic Acid (3e). Oxidation of 2-(2-bromobenzylthio)acetic acid **2e** with 30% hydrogen peroxide yielded the corresponding 2-[(2-bromobenzyl)sulfonyl]acetic acid. The yield of this reaction was 78.7%, giving a white solid with a melting point of 175-177 °C. It was identified by comparing its physical data with the literature data [3].

2-[(3-Bromobenzyl)sulfonyl]acetic Acid (3f). Oxidation of 2-(3-bromobenzylthio)acetic acid **2f** with 30% hydrogen peroxide yielded the corresponding 2-[(3-bromobenzyl)sulfonyl]acetic acid. The yield of this reaction was 85.8%, giving a white solid with a melting point of 179-181 °C. It was identified by comparing its physical data with the literature data [3].

2-[(4-Bromobenzyl)sulfonyl]acetic Acid (3g). Oxidation of 2-(4-bromobenzylthio)acetic acid **2g** with 30% hydrogen peroxide yielded the corresponding 2-[(4-bromobenzyl)sulfonyl]acetic acid. The yield of this reaction was 87.7%, giving a white solid with a melting point of 177-179 °C. It was identified by comparing its physical data with the literature data [9].

2-[(3-Methylbenzyl)sulfonyl]acetic Acid (3h). Oxidation of 2-(3-methylbenzylthio)acetic acid **2h** with 30% hydrogen peroxide yielded the corresponding 2-[(3-methylbenzyl)sulfonyl]acetic acid. The yield of this reaction was

82.8%, giving a white solid with a melting point of 134-136 °C. It was identified by comparing its physical data with the literature data [5].

*2-[(4-Methylbenzyl)sulfonyl]acetic Acid (3i)*. Oxidation of 2-(4-methylbenzylthio)acetic acid **2i** with 30% hydrogen peroxide yielded the corresponding 2-[(4-methylbenzyl)sulfonyl]acetic acid. The yield of this reaction was 43.2%, giving a white solid with a melting point of 145-146 °C. It was identified by comparing its physical data with the literature data [5].

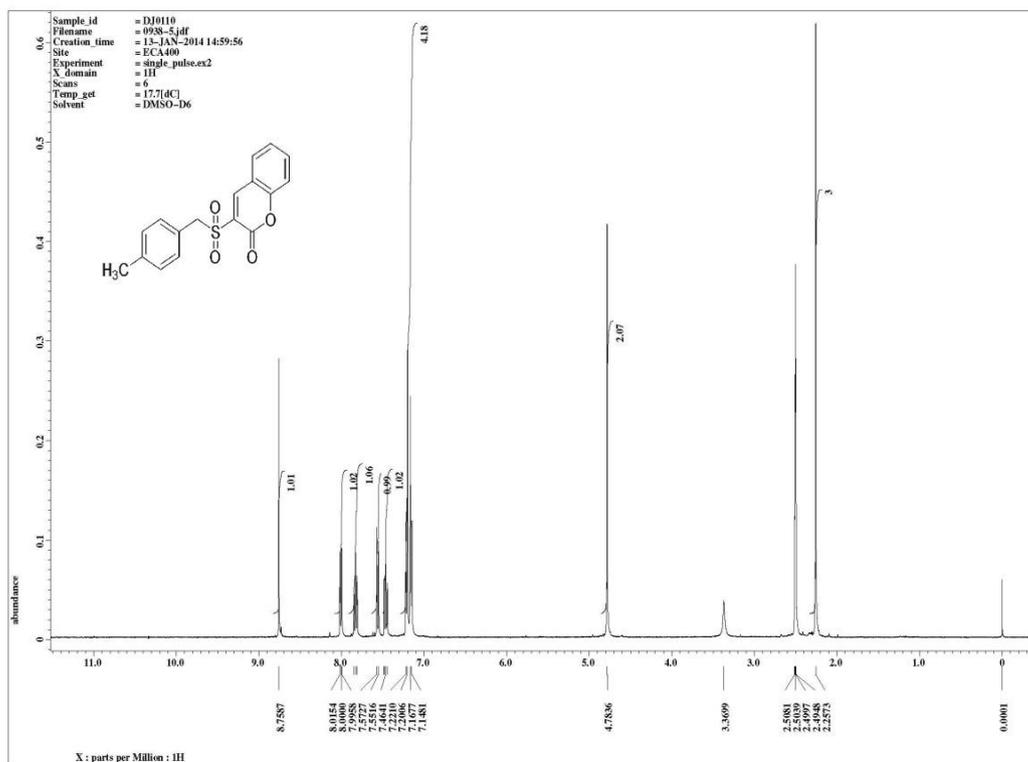
*2-[[2-(Trifluoromethyl)benzyl]sulfonyl]acetic Acid (3j)*. Oxidation of 2-[2-(trifluoromethyl)benzylthio]acetic acid **2j** with 30% hydrogen peroxide yielded the corresponding 2-[[2-(trifluoromethyl)benzyl]sulfonyl]acetic acid. The yield of this reaction was 79.0%, giving a white solid with a melting point of 168-169 °C. It was identified by comparing its physical data with the literature data [8].

## References

- [1] Kojima, K; Koyama, K; Kurata, H; Fukumi, H; Tabata, K; Yasuda, H. Preparation of disubstituted thiophenes and ulcer inhibitors. *Jpn. Kokai Tokkyo Koho*, **1996**, JP 08127581, A 19960521.
- [2] Zhou, N.; Feng, T.; Shen, X.; Cui, J.; Wu, R.; Wang, L.; Chen, H. Synthesis, characterization, and radioprotective activity of  $\alpha,\beta$ -unsaturated aryl sulfone analogs and their Tempol conjugates. *MedChemComm*. **2017**, 8, 1063-1068.
- [3] Janczewski, M.; Ksiezopolski, J. Effect of molecular structure on optical properties of sulfoxide systems, m-Bromobenzylsulfinylacetic acids and some of their derivatives, Part VII. *Pol. J. Chem.* **1984**, 58, 103-106.
- [4] Abraham, D.J.; Kennedy, P.E.; Mehanna, A.S.; Patwa, D.C.; Williams, F.L. Design, synthesis, and testing of potential antisickling agents. 4. structure activity relationships of benzyloxy and phenoxy acids. *J. Med. Chem.* **1984**, 16, 967-981.
- [5] Janczewski, M.; Janowski, W. Effect of molecular structure on optical properties of sulfoxide systems. Optical relations in the group of isomeric o-, m-, and p-methylbenzylsulfinylacetic acids. *Roczniki Chemii*. **1975**, 49, 1961-1962.
- [6] Mccaw, P.G; Buckley N.M.; Eccles K.S.; Lawrence S.E.; Maguire A.R.; Collins S.G. Synthesis of Cyclic  $\alpha$ -Diazo- $\beta$ -keto Sulfoxides in Batch and Continuous Flow. *J. Org. Chem.* **2017**, 82, 3666-3679.
- [7] Bordwell, F.G; Wolfinger, M.D.; O'Dwyer, J.B. Synthesis of dihalomethyl and alpha-haloalkyl sulfones by the halogenative decarboxylation of alpha-aryl- and alpha-alkylsulfonylalkane carboxylic acids. *ChemInform*. 1974, 5, 2516-2519.
- [8] Ning X.L.; Guo Y.; Wang X.W.; Ma X.Y.; Tian C.; Shi X.Q.; Zhu R.Z.; Cheng C.; Du Y.S.; Ma Z.Z.; et al. Design, synthesis, and biological evaluation of (E)-3,4-dihydroxystyryl aralkyl sulfones and sulfoxides as novel multifunctional neuroprotective Agents. *J. Med. Chem.* **2014**, 57, 4302-4312.
- [9] Janczewski, M.; Ksiezopolski, J. Effect of molecular structure on optical properties of sulfoxide systems, p-Bromobenzylsulfinylacetic acids and some of their derivatives, Part III. *Pol. J. Chem.* **1981**, 55, 535-546.

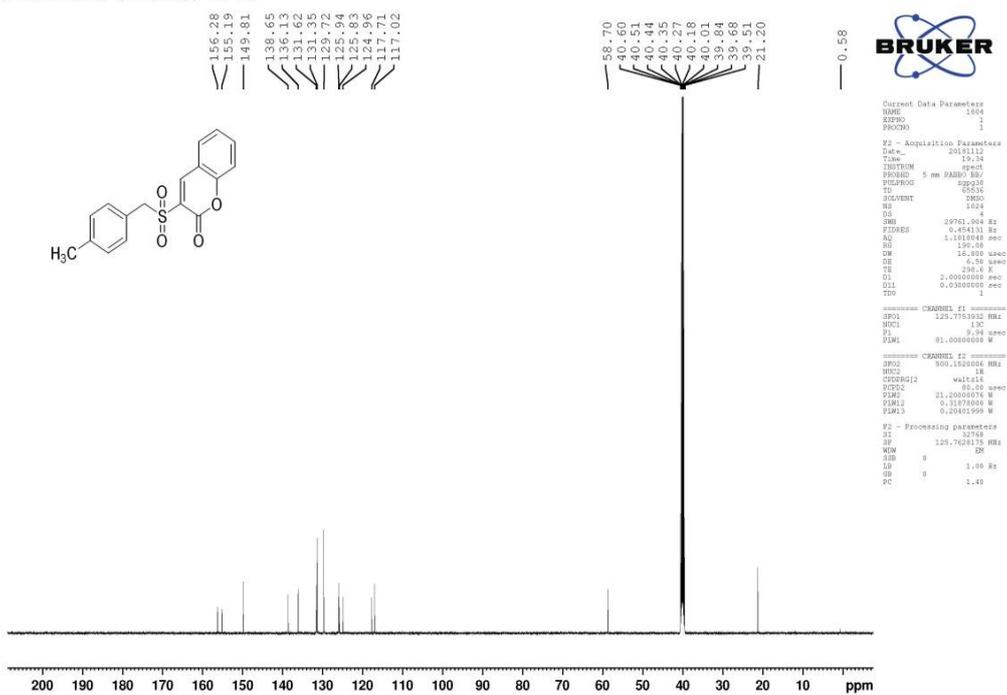
## 2. Copies of $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ for target compounds (5a -5o)

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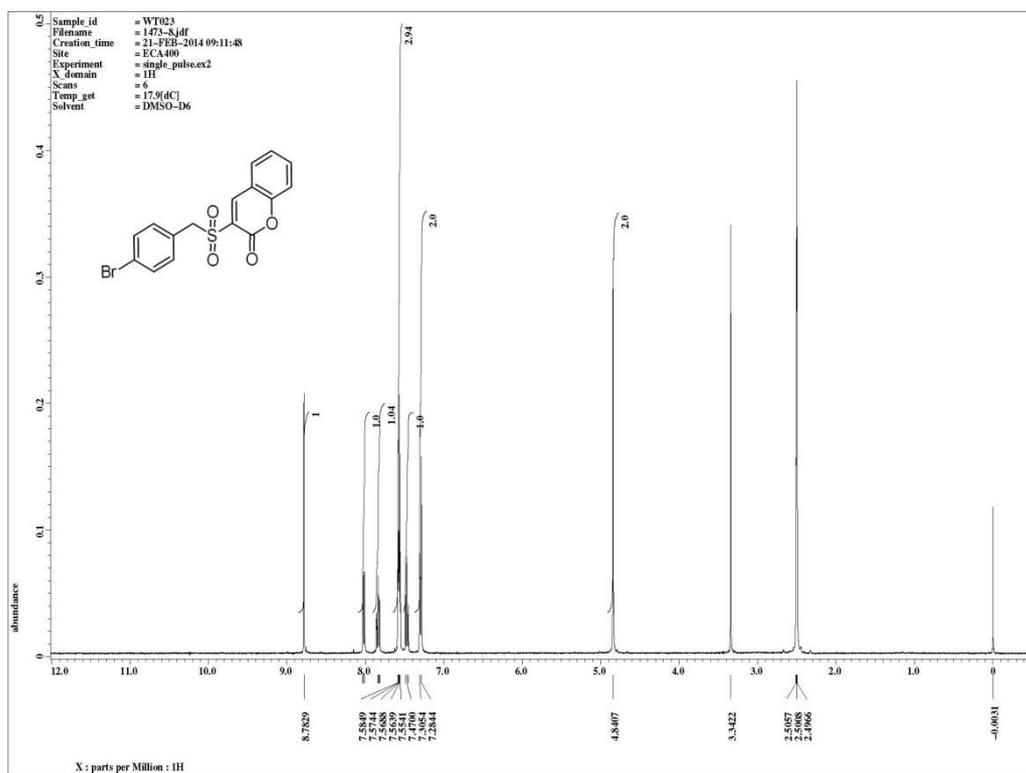


### $^{13}\text{C-NMR}$ of Compound 5a:

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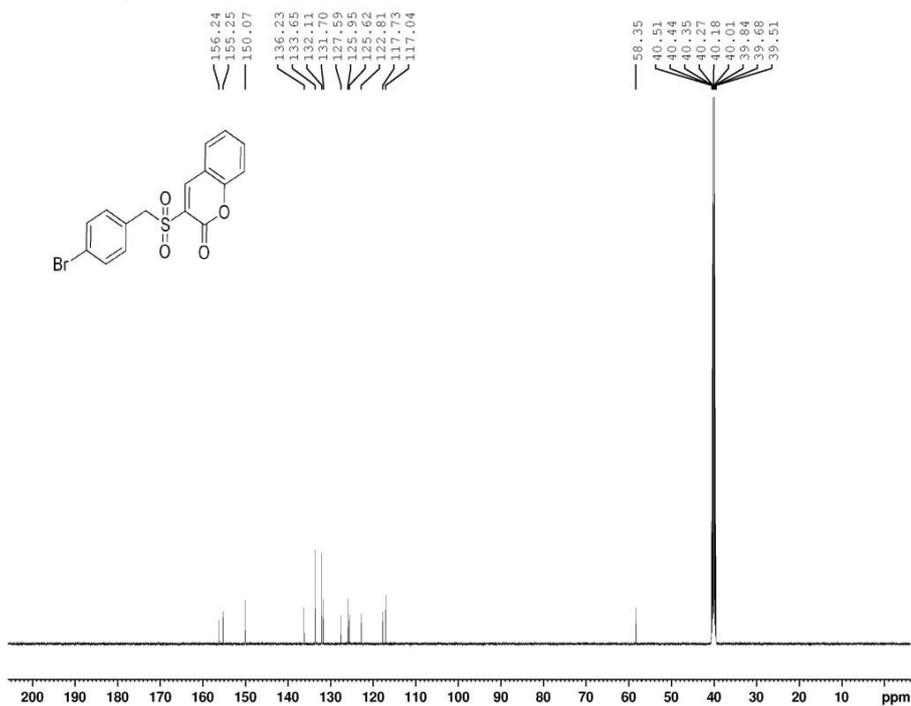


# <sup>1</sup>H-NMR of Compound 5b:



# <sup>13</sup>C-NMR of Compound 5b:

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RG         388.08
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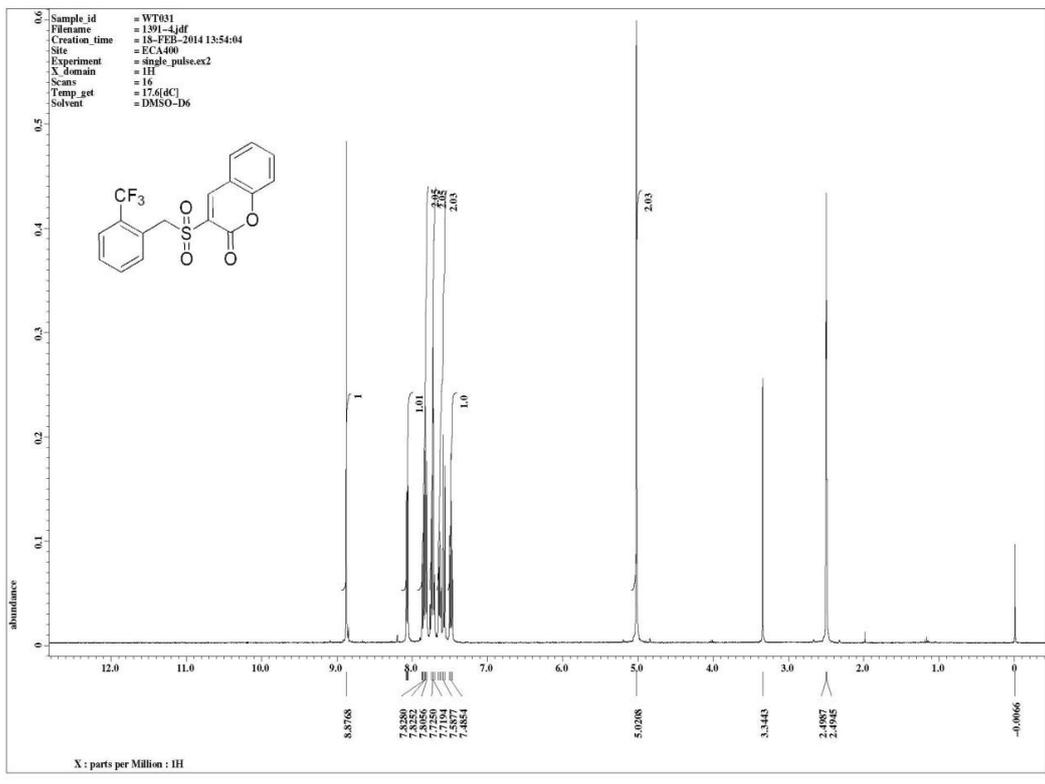
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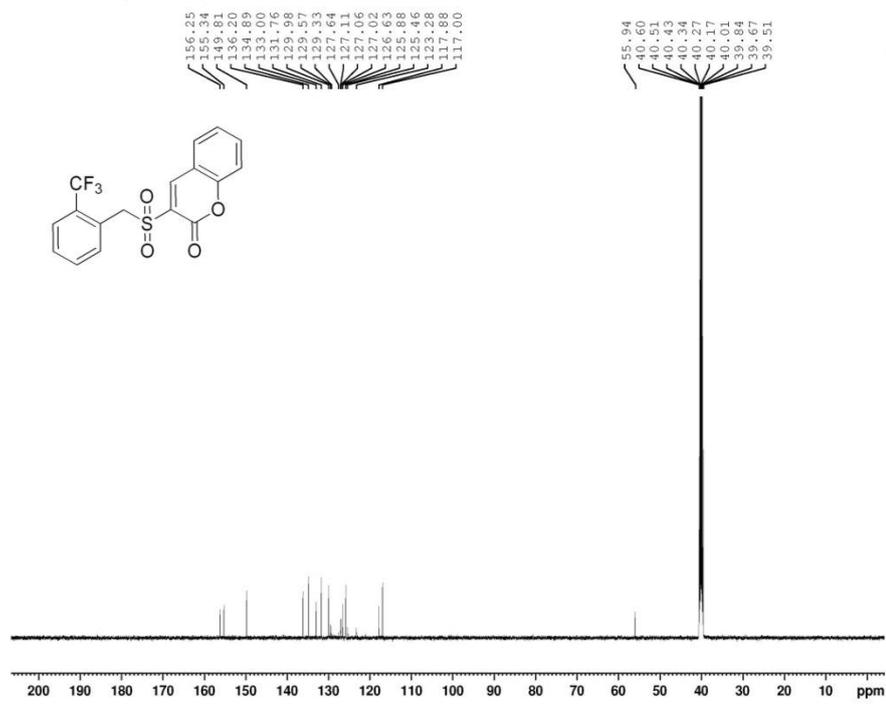
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### <sup>1</sup>H-NMR of Compound 5c:



### <sup>13</sup>C-NMR of Compound 5c:

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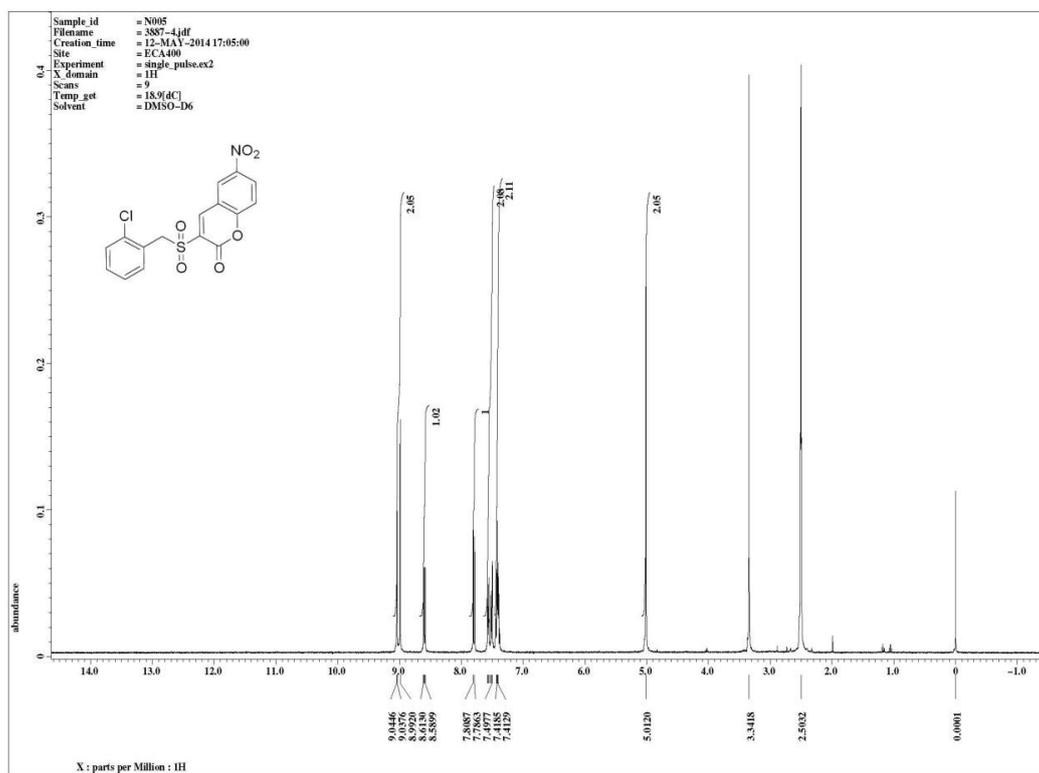
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 TD 1

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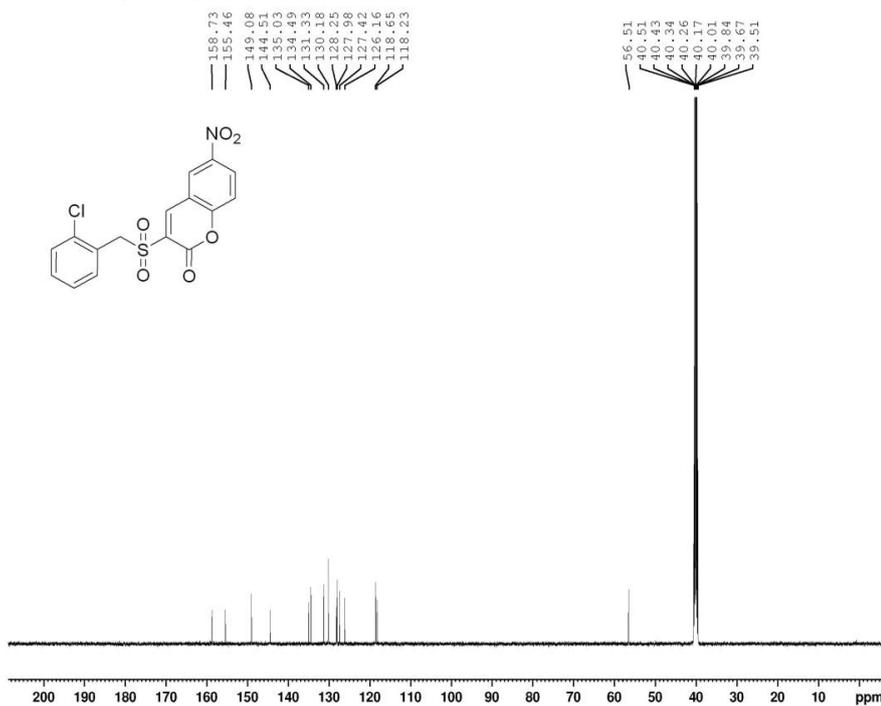
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# <sup>1</sup>H-NMR of Compound 5d:



# <sup>13</sup>C-NMR of Compound 5d:

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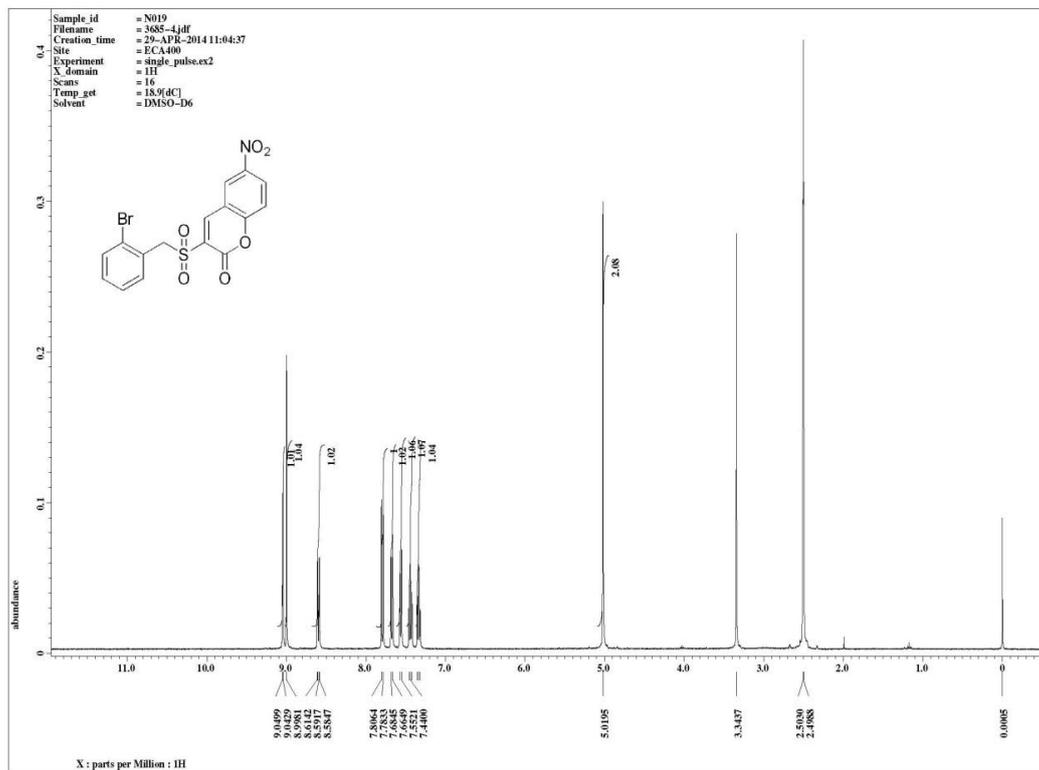
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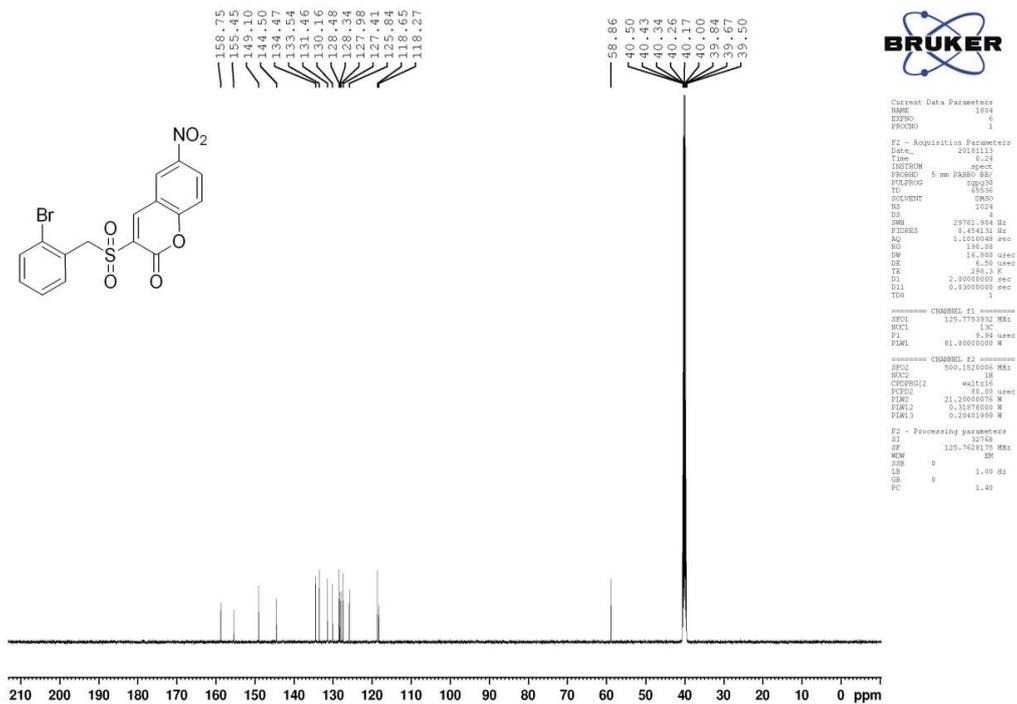
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# <sup>1</sup>H-NMR of Compound 5e:

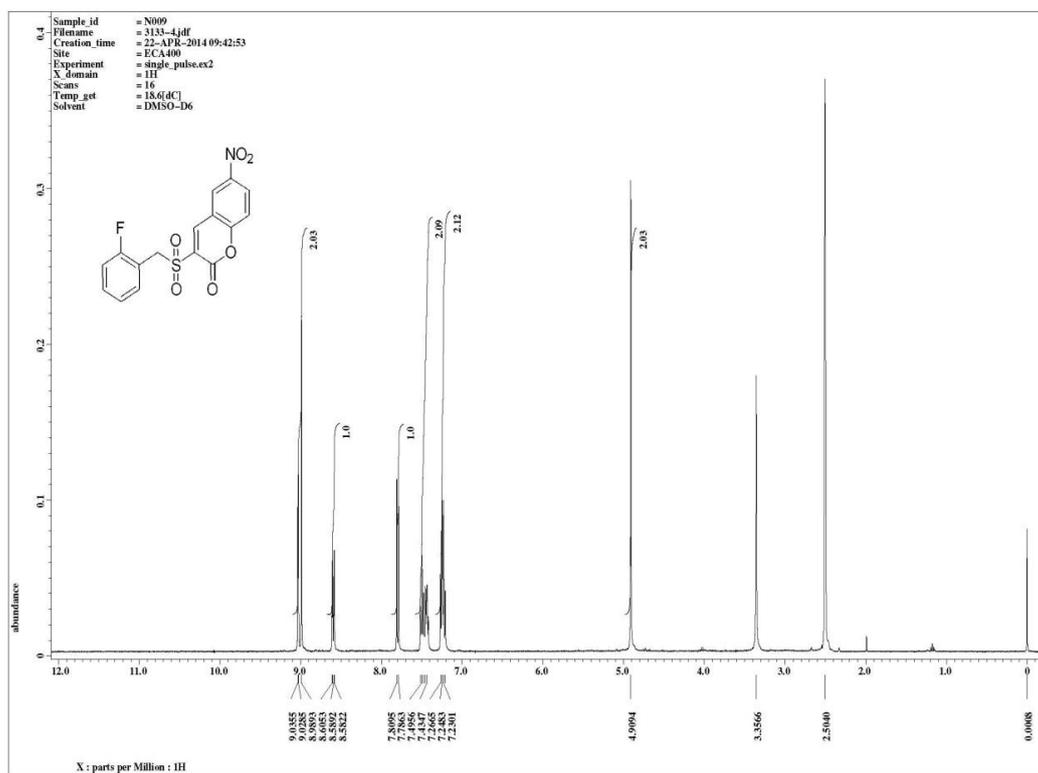


# <sup>13</sup>C-NMR of Compound 5e:

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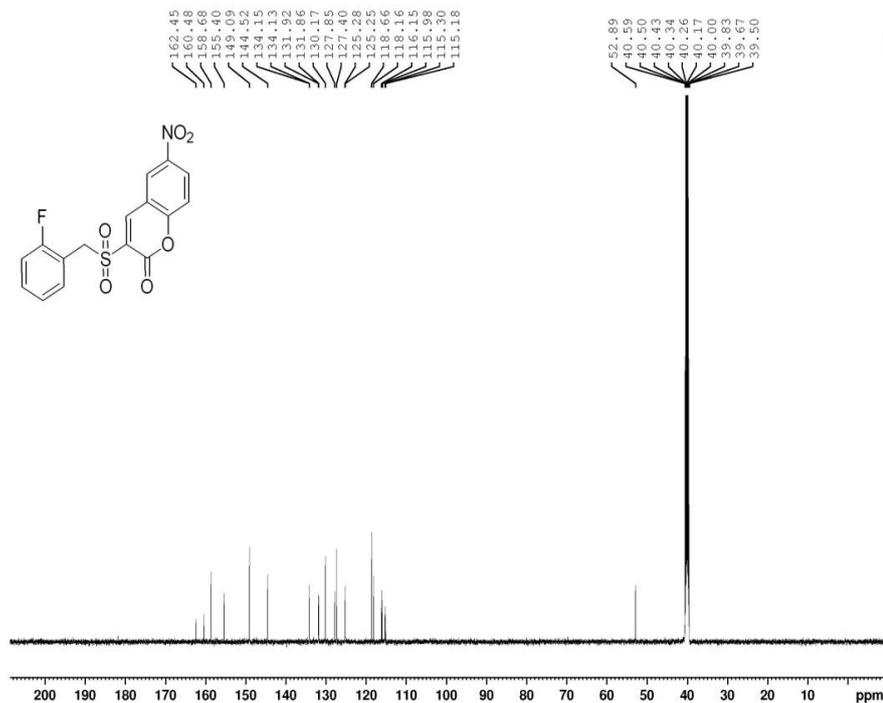


# <sup>1</sup>H-NMR of Compound 5f:



# <sup>13</sup>C-NMR of Compound 5f:

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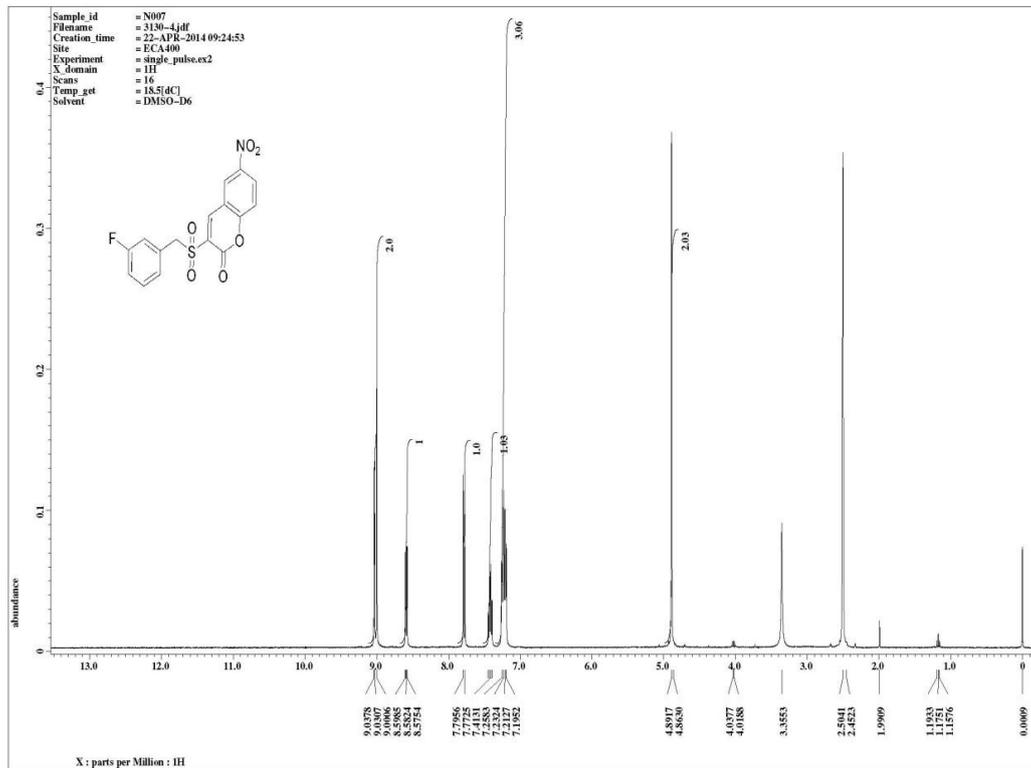
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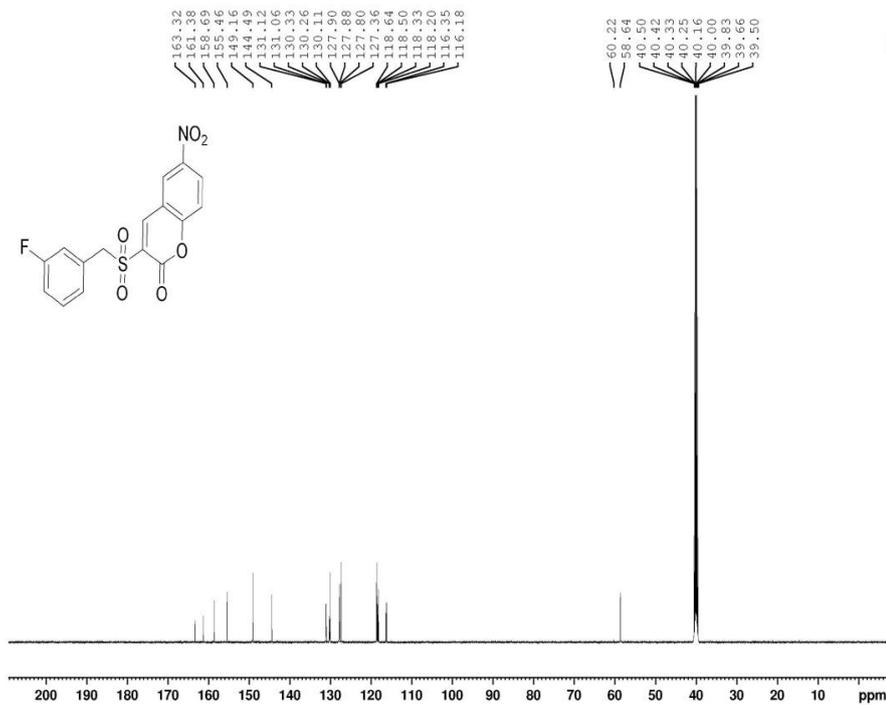
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# <sup>1</sup>H-NMR of Compound 5g:



# <sup>13</sup>C-NMR of Compound 5g:

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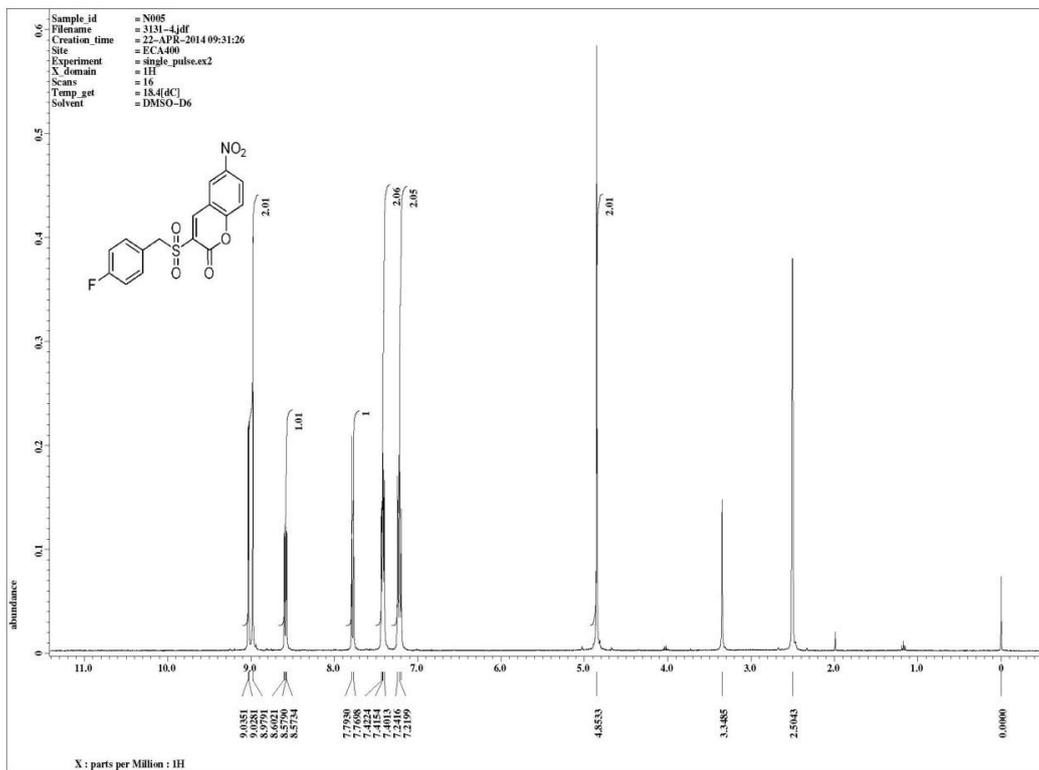
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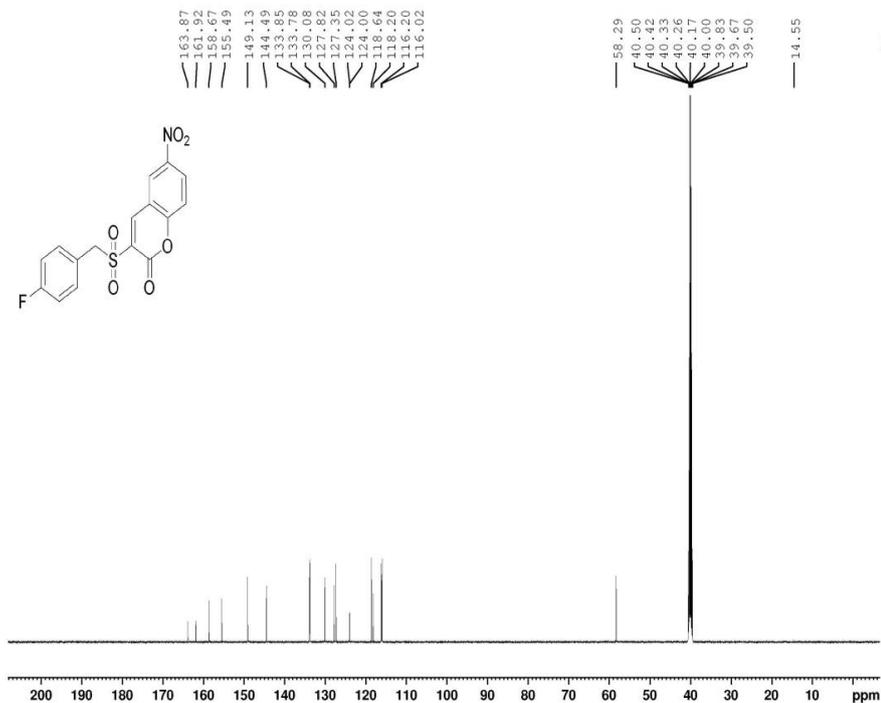
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# <sup>1</sup>H-NMR of Compound 5h:

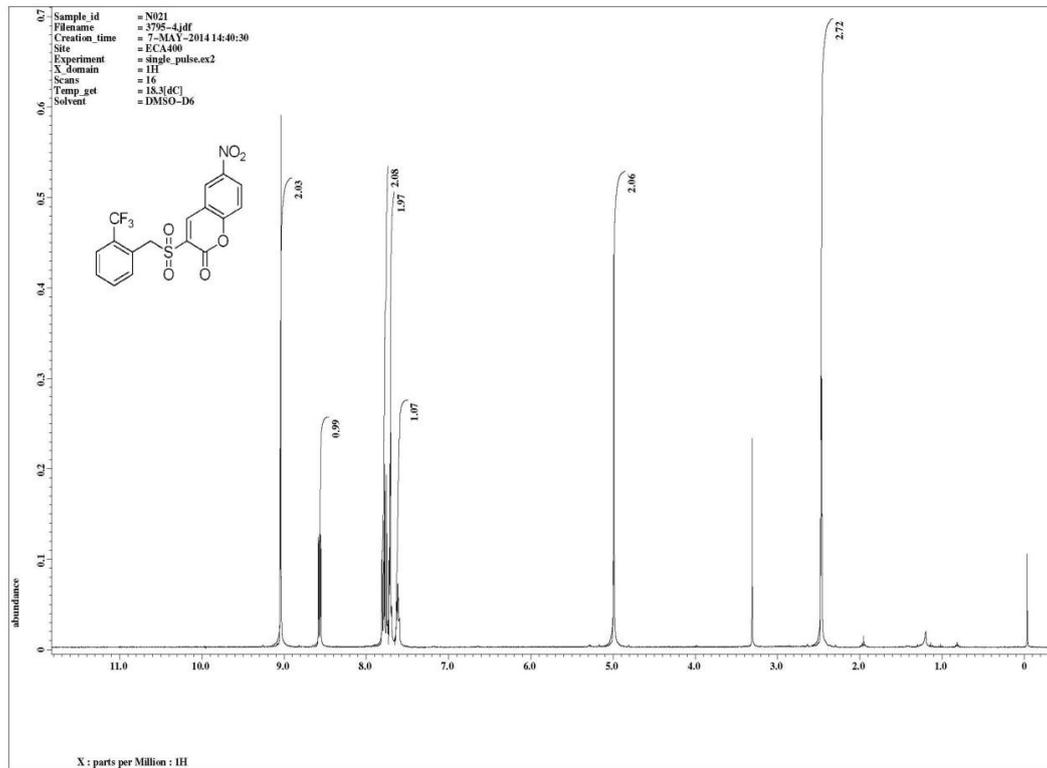


# <sup>13</sup>C-NMR of Compound 5h:

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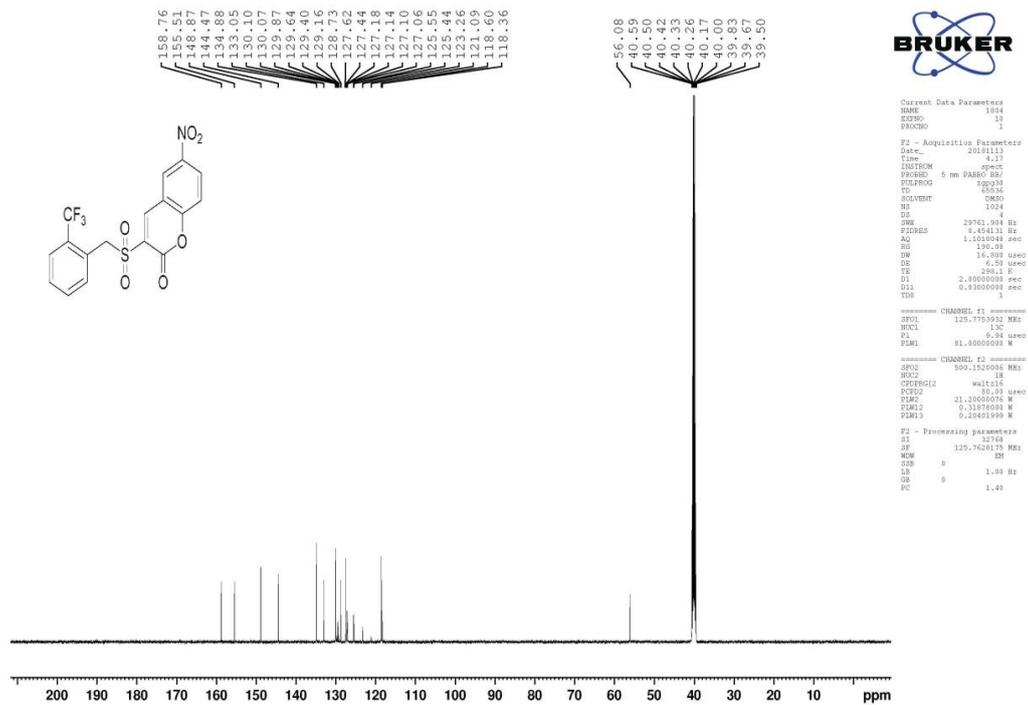


# <sup>1</sup>H-NMR of Compound 5i:

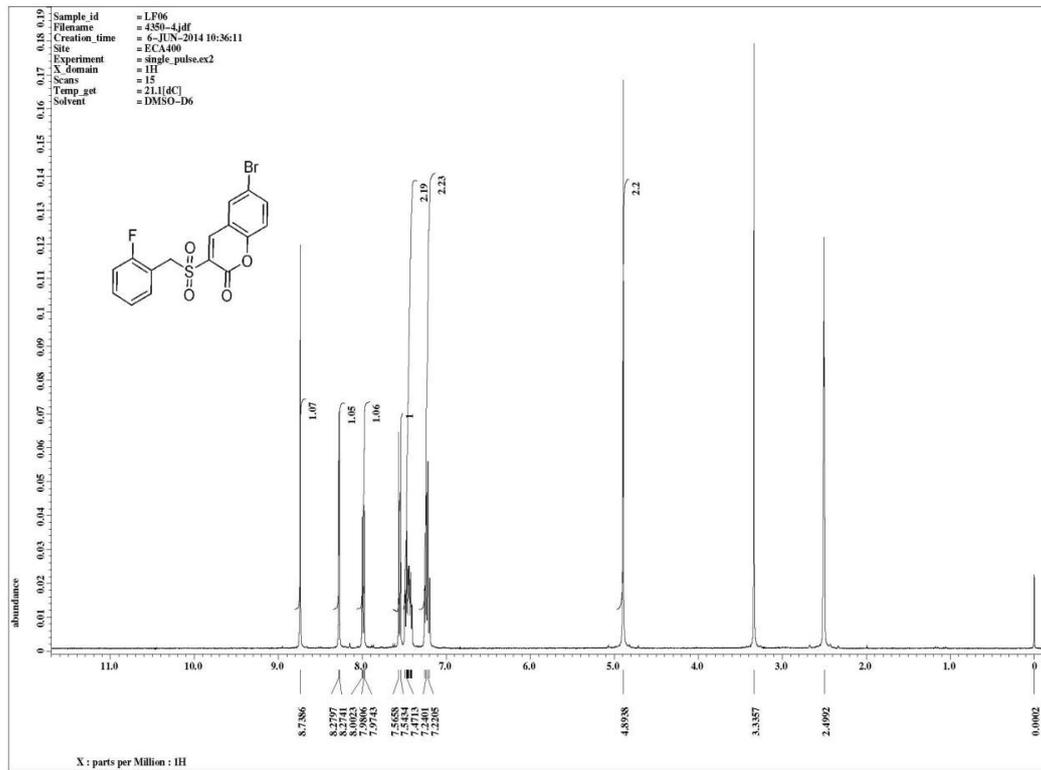


# <sup>13</sup>C-NMR of Compound 5i:

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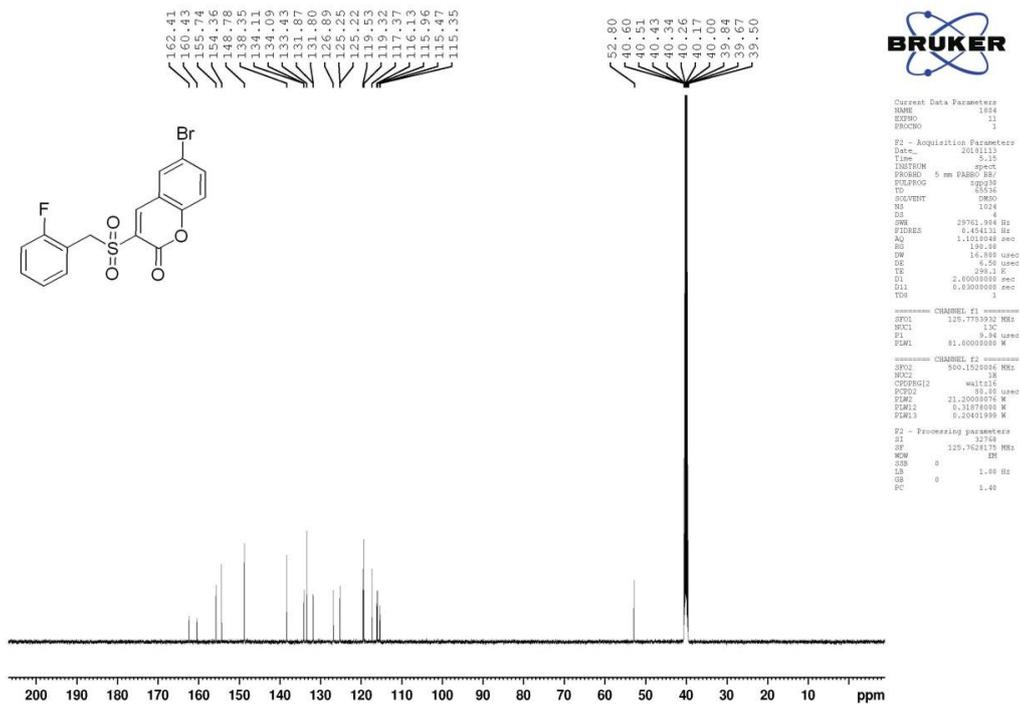


### <sup>1</sup>H-NMR of Compound 5j:

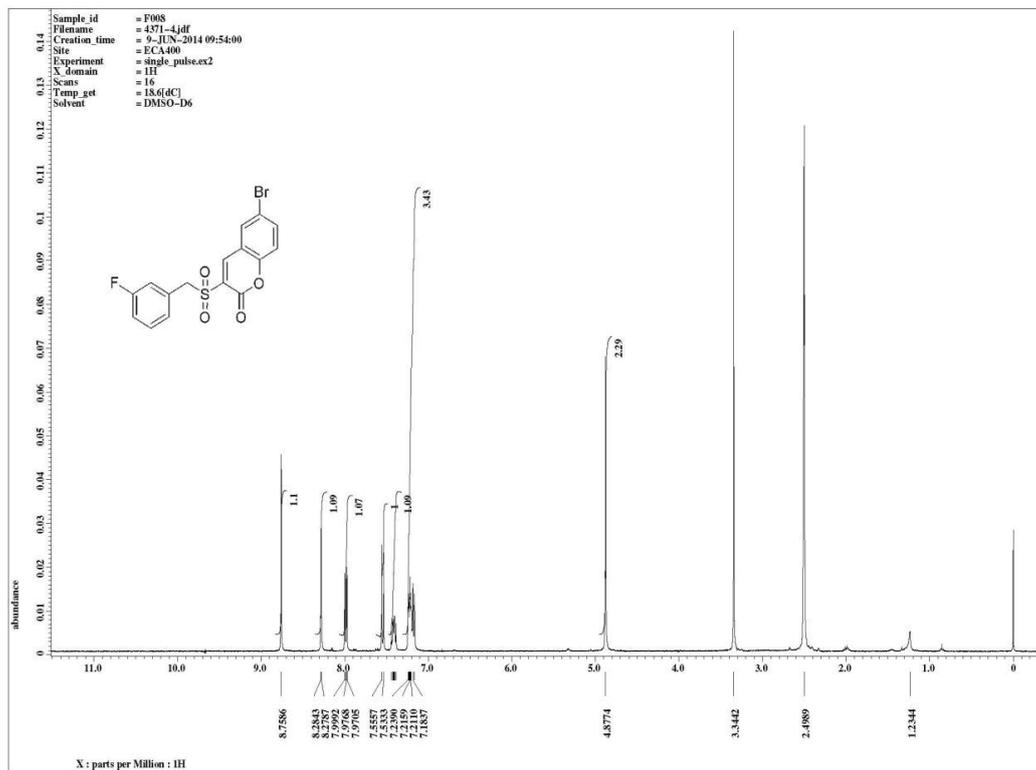


### <sup>13</sup>C-NMR of Compound 5j:

Spectrometer AVIII HD 500MHz  
 operator LLJ  
 B06  
 C13CPD DMSO {E:\data} RL 23

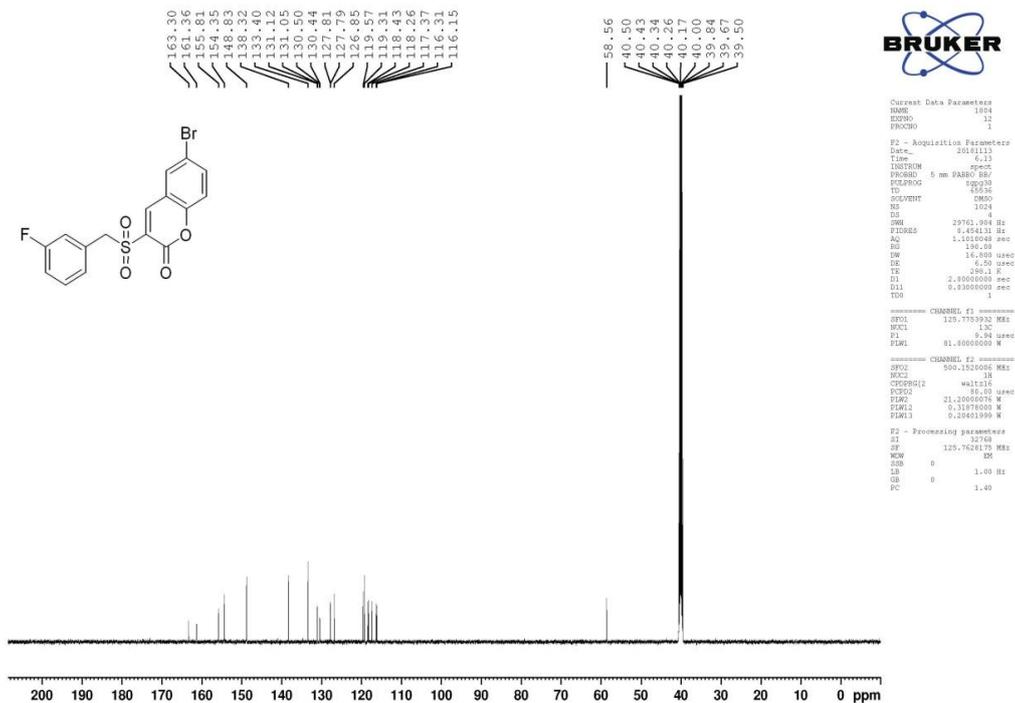


# <sup>1</sup>H-NMR of Compound 5k:

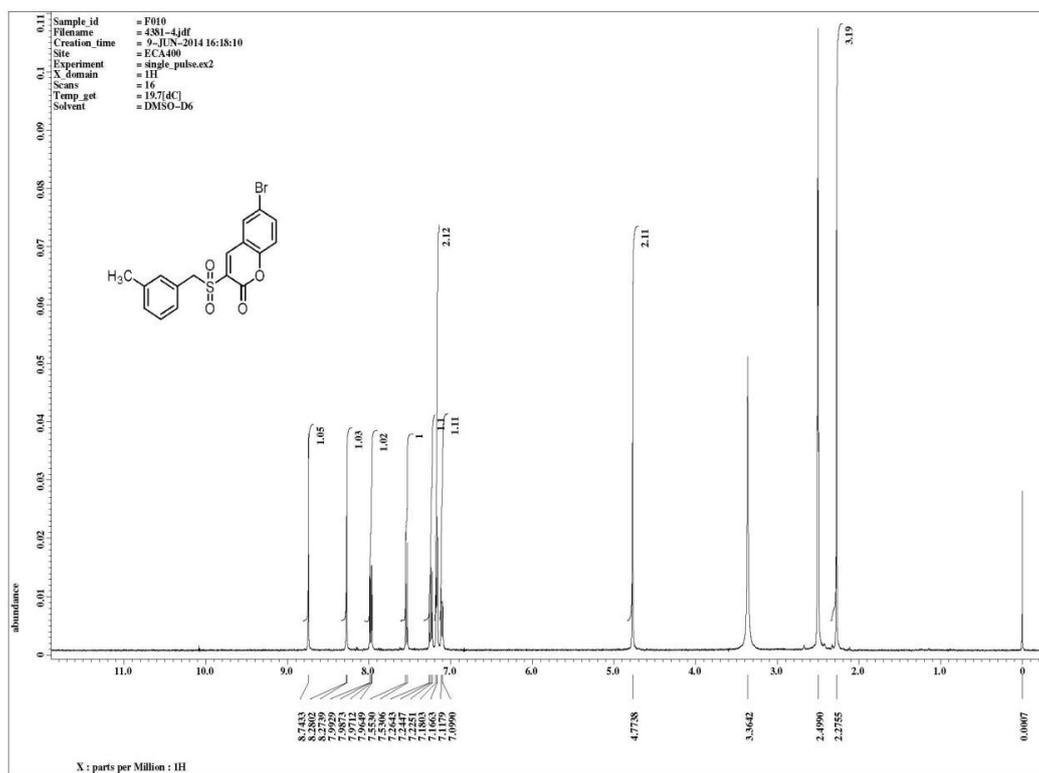


# <sup>13</sup>C-NMR of Compound 5k:

Spectrometer AVIII HD 500MHz  
 operator LLJ  
 B08  
 C13CPD DMSO {E:\data} RL 24

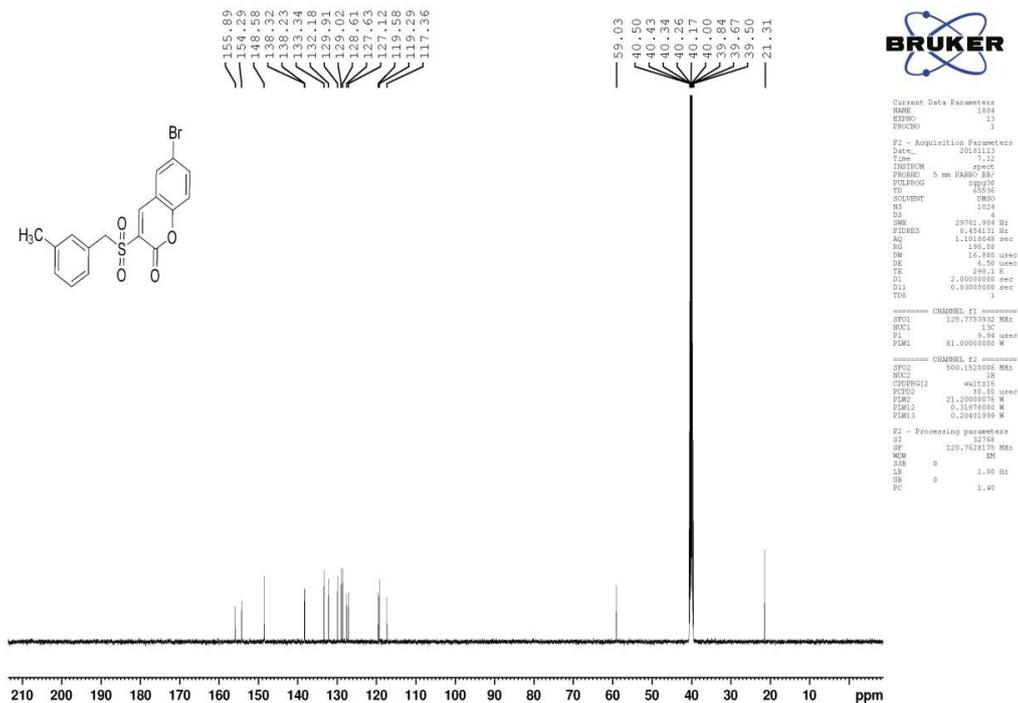


# <sup>1</sup>H-NMR of Compound 51:

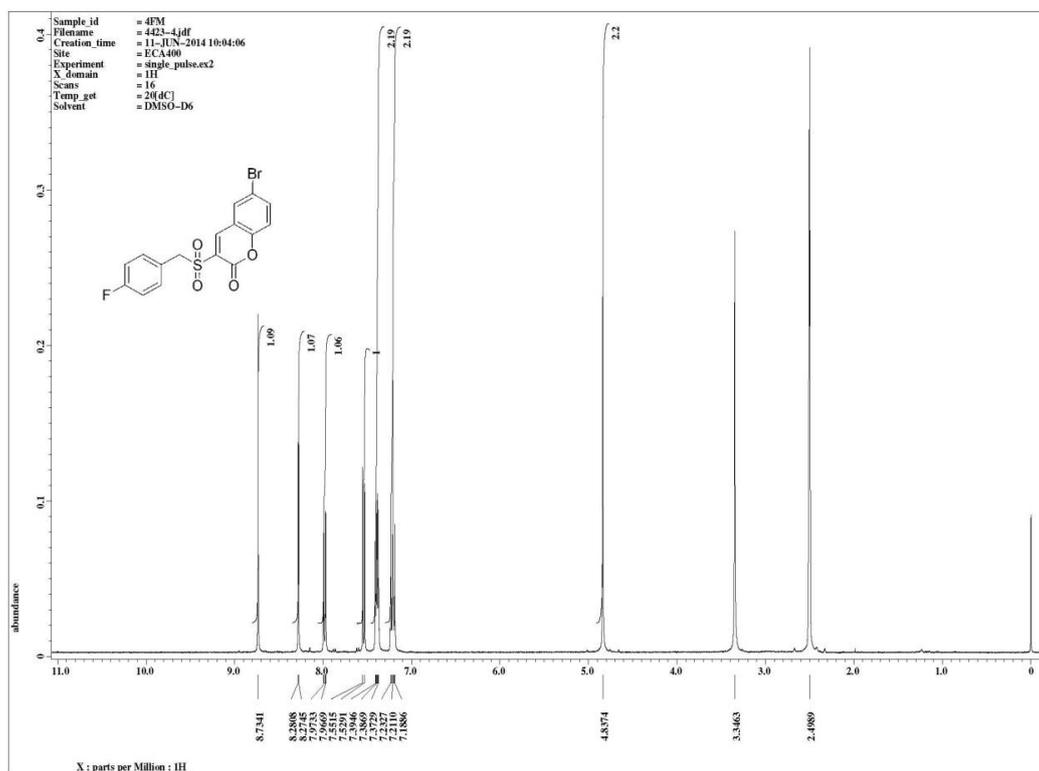


# <sup>13</sup>C-NMR of Compound 51:

Spectrometer AVIII HD 500MHz  
 operator LLJ  
 B10  
 C13CPD DMSO {E:\data} RL 1



# <sup>1</sup>H-NMR of Compound 5m:



# <sup>13</sup>C-NMR of Compound 5m:

Spectrometer AVIII HD 500MHz  
 operator LLJ  
 B12  
 C13CPD DMSO {E:\data} RL 2

