

## Supplementary Materials

### Privileged scaffolds hybridization in the design of carbonic anhydrase inhibitors

Daniela Secci <sup>1</sup>, Erica Sanna <sup>1</sup>, Simona Distinto <sup>1</sup>, Alessia Onali <sup>1</sup>, Antonio Lupia <sup>1,2</sup>, Laura Demuru <sup>1</sup>, Giulia Atzeni <sup>1</sup>, Rita Meleddu <sup>1\*</sup>, Filippo Cottiglia <sup>1</sup>, Andrea Angeli <sup>3</sup>, Claudiu T. Supuran <sup>3\*</sup> and Elias Maccioni <sup>1</sup>

<sup>1</sup>Department of Life and Environmental Sciences, University of Cagliari, Cittadella Universitaria di Monserrato, Monserrato, 09042 Cagliari, Italy

<sup>2</sup>Net4Science S.r.l, Università degli Studi “Magna Græcia” di Catanzaro, Catanzaro, 88100, Italy

<sup>3</sup>Dipartimento NEUROFARBA, Sezione di Scienze Farmaceutiche, Università degli Studi di Firenze, Sesto Fiorentino, Florence, Italy.

\*Correspondence: R.Meleddu, rita.meleddu@unica.it; C.T.Supuran, claudiu.supuran@unifi.it

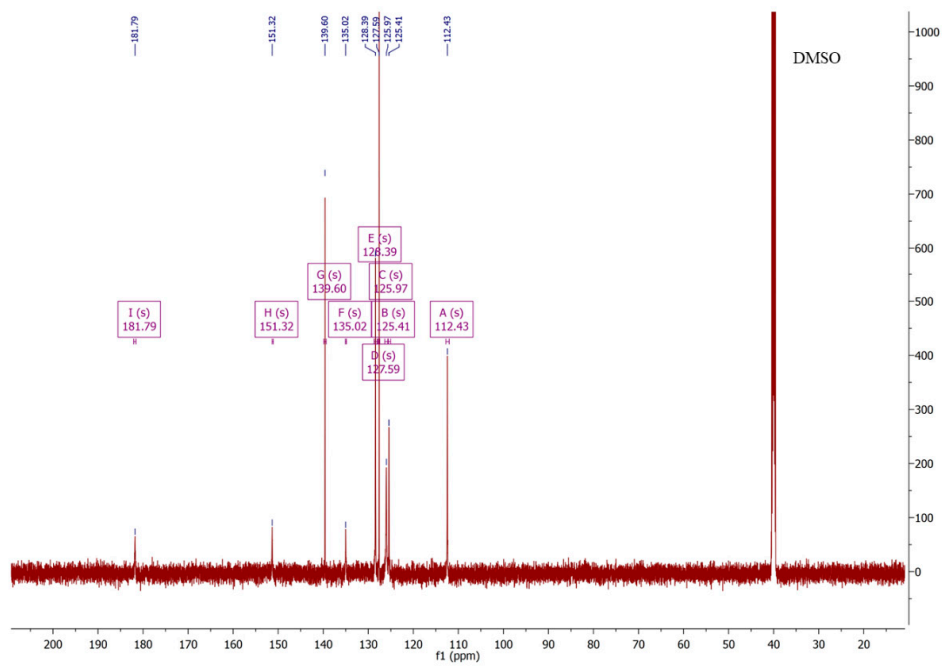
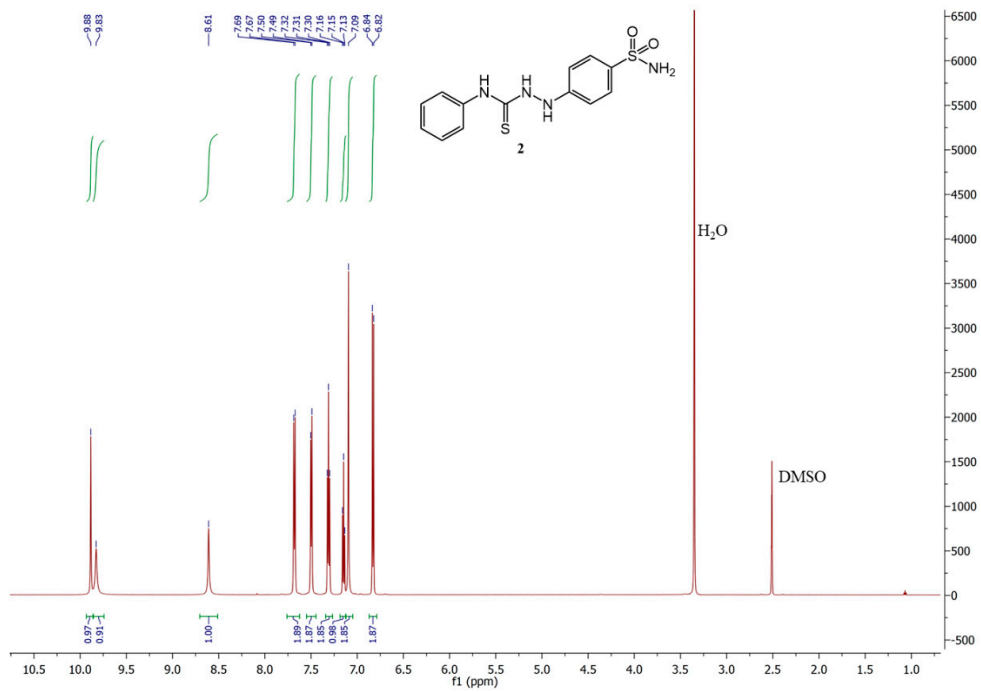
### Table of contents

<sup>1</sup> H NMR and <sup>13</sup> C NMR of <b>2-5a-i</b> compounds .....	3
<sup>1</sup> H NMR and <sup>13</sup> C NMR of compound <b>2</b> .....	3
<sup>1</sup> H NMR and <sup>13</sup> C NMR of compound <b>3</b> .....	4
<sup>1</sup> H NMR and <sup>13</sup> C NMR of compound <b>4</b> .....	5
<sup>1</sup> H NMR and <sup>13</sup> C NMR of compound <b>5a</b> .....	6
<sup>1</sup> H NMR and <sup>13</sup> C NMR of compound <b>5b</b> .....	7
<sup>1</sup> H NMR and <sup>13</sup> C NMR of compound <b>5c</b> .....	8
<sup>1</sup> H NMR and <sup>13</sup> C NMR of compound <b>5d</b> .....	9
<sup>1</sup> H NMR and <sup>13</sup> C NMR of compound <b>5e</b> .....	10
<sup>1</sup> H NMR and <sup>13</sup> C NMR of compound <b>5f</b> .....	11
<sup>1</sup> H NMR and <sup>13</sup> C NMR of compound <b>5g</b> .....	12
<sup>1</sup> H NMR and <sup>13</sup> C NMR of compound <b>5h</b> .....	13
<sup>1</sup> H NMR and <sup>13</sup> C NMR of compound <b>5i</b> .....	14
ESI-HRMS spectra of <b>5a-i</b> compounds ([M-H] <sup>-</sup> ) .....	15
MS spectrum of compound <b>5a</b> .....	15
MS spectrum of compound <b>5b</b> .....	15
MS spectrum of compound <b>5c</b> .....	16
MS spectrum of compound <b>5d</b> .....	16
MS spectrum of compound <b>5e</b> .....	17
MS spectrum of compound <b>5f</b> .....	17
MS spectrum of compound <b>5g</b> .....	18

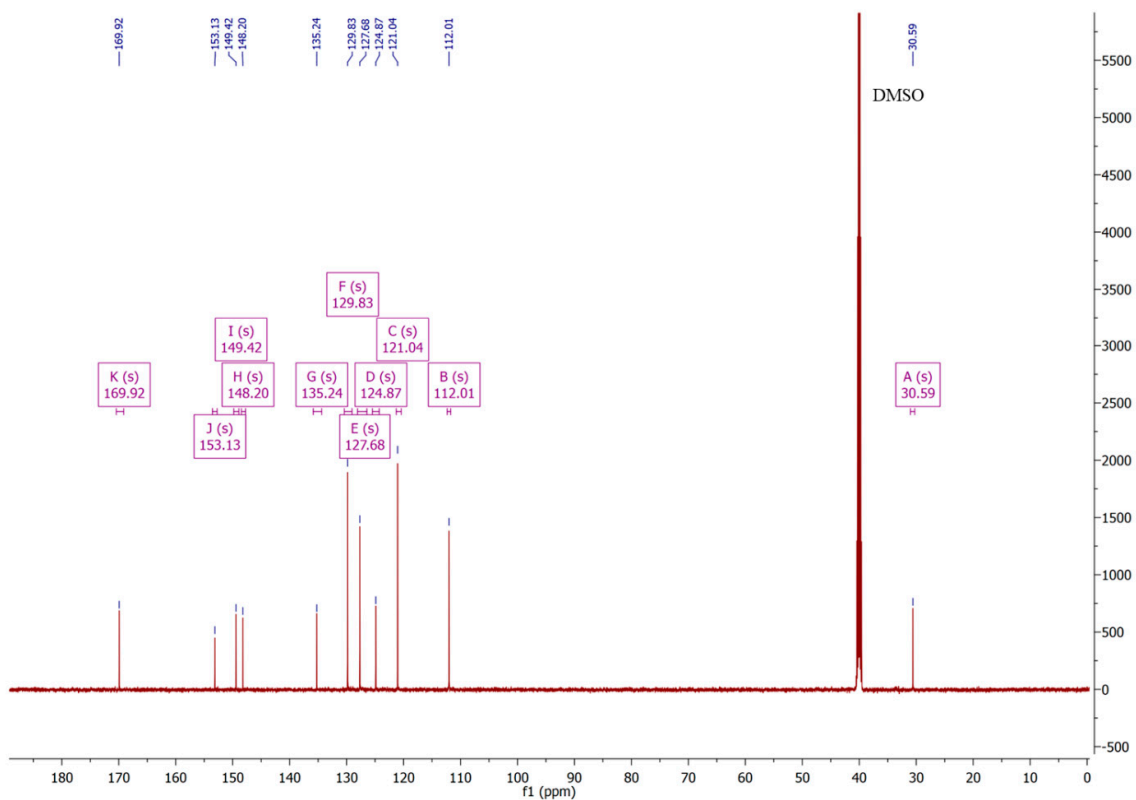
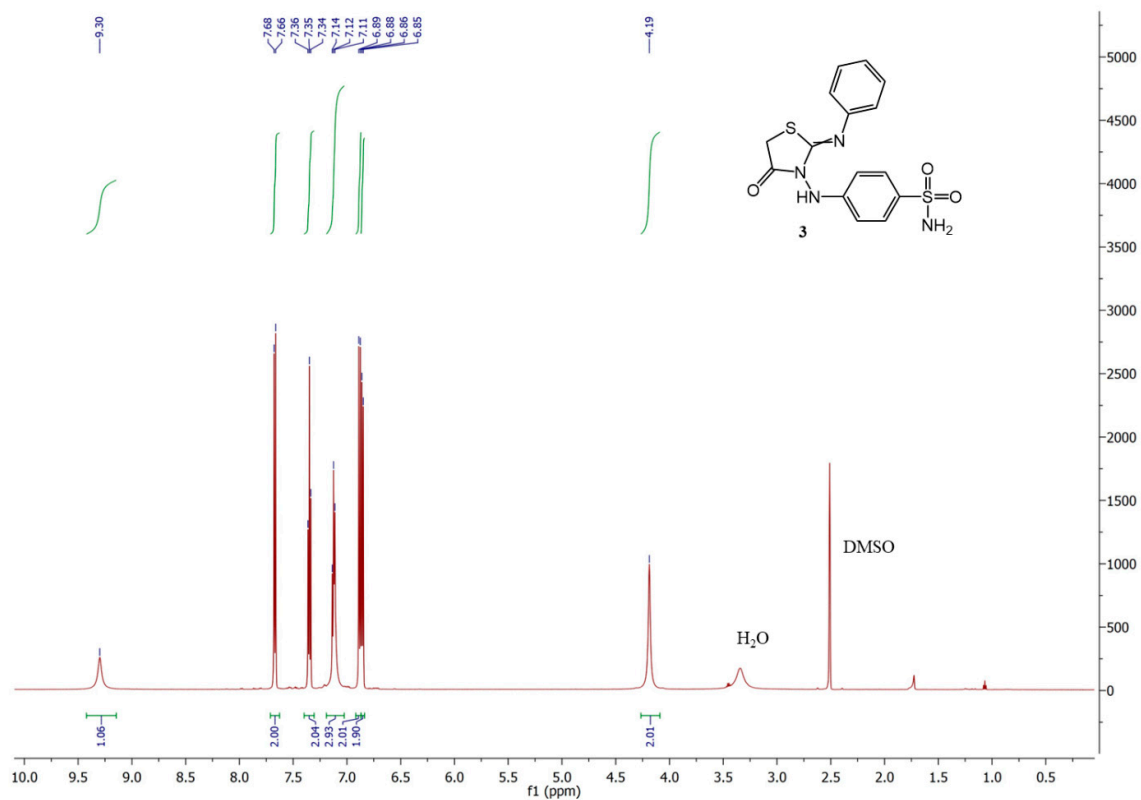
MS spectrum of compound <b>5h</b> .....	18
MS spectrum of compound <b>5i</b> .....	19

$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR of **2-5a-i** compounds

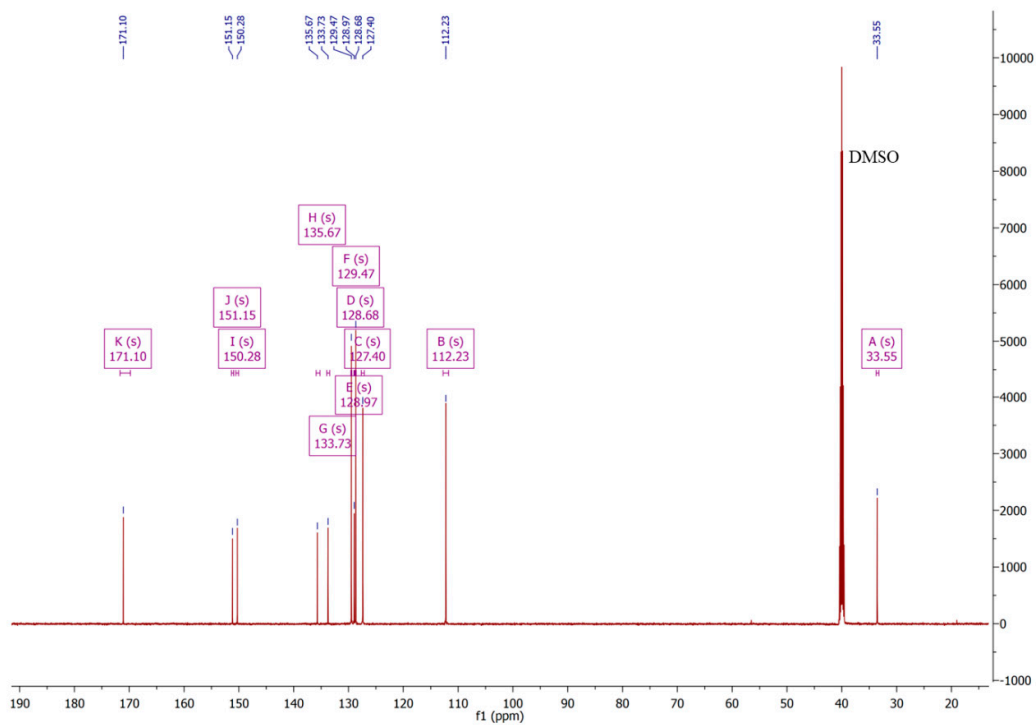
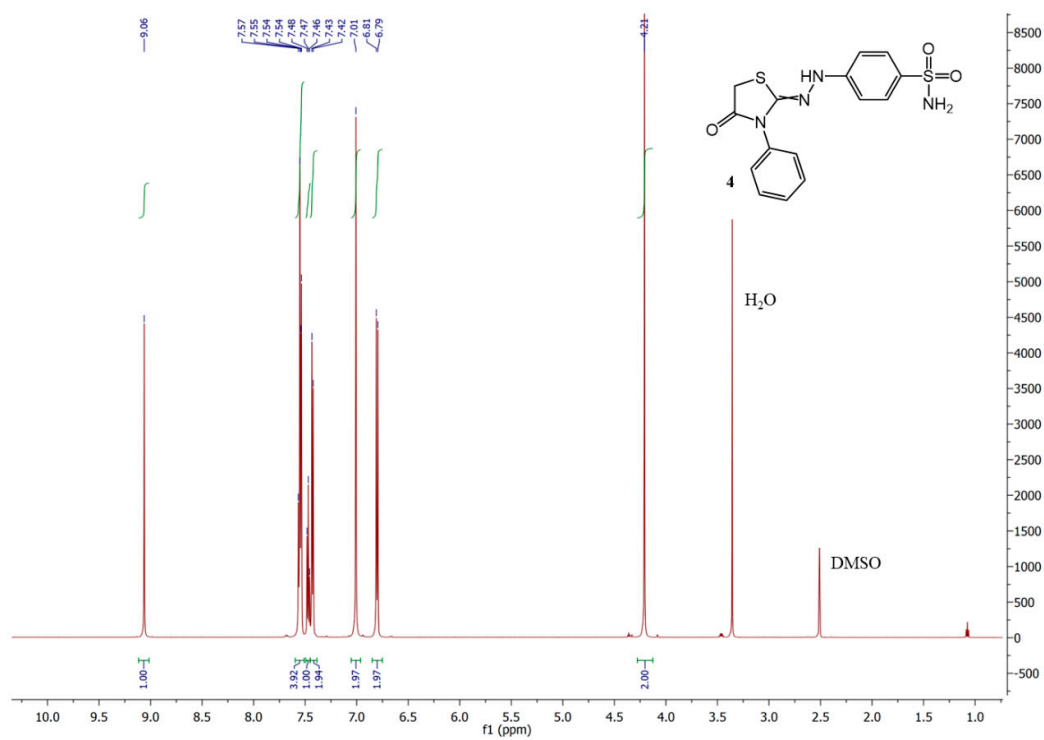
$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR of compound **2**



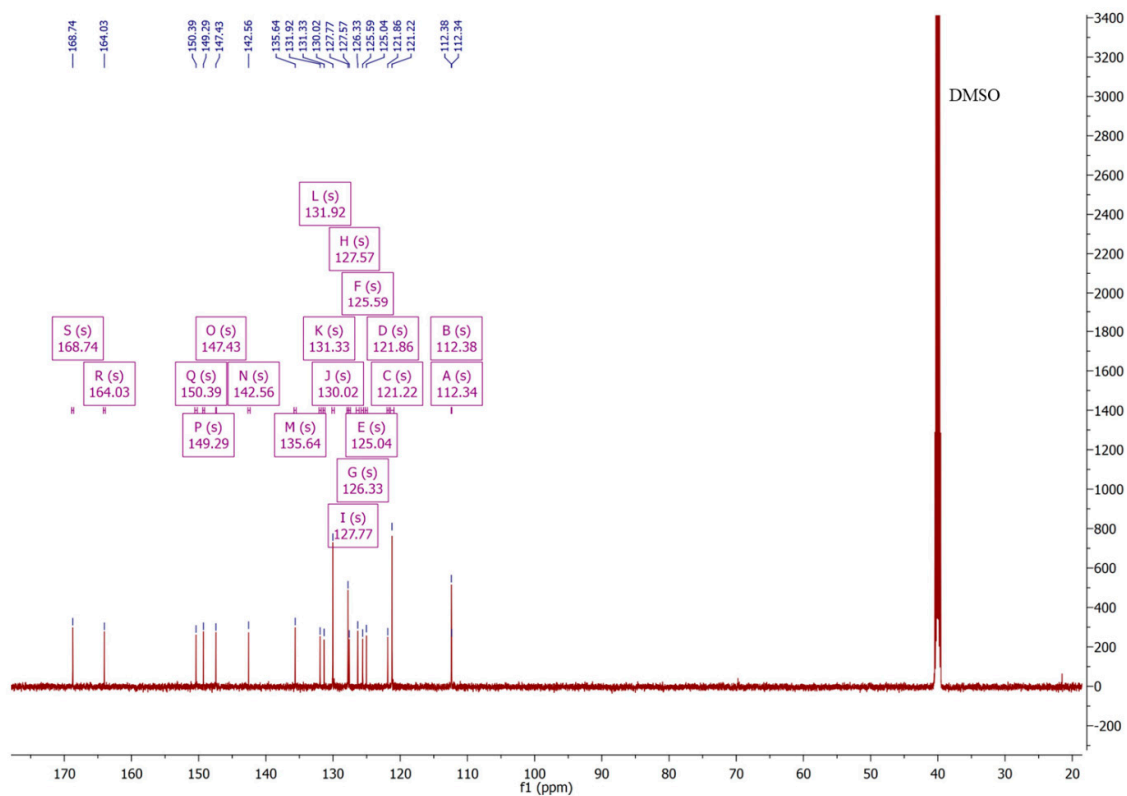
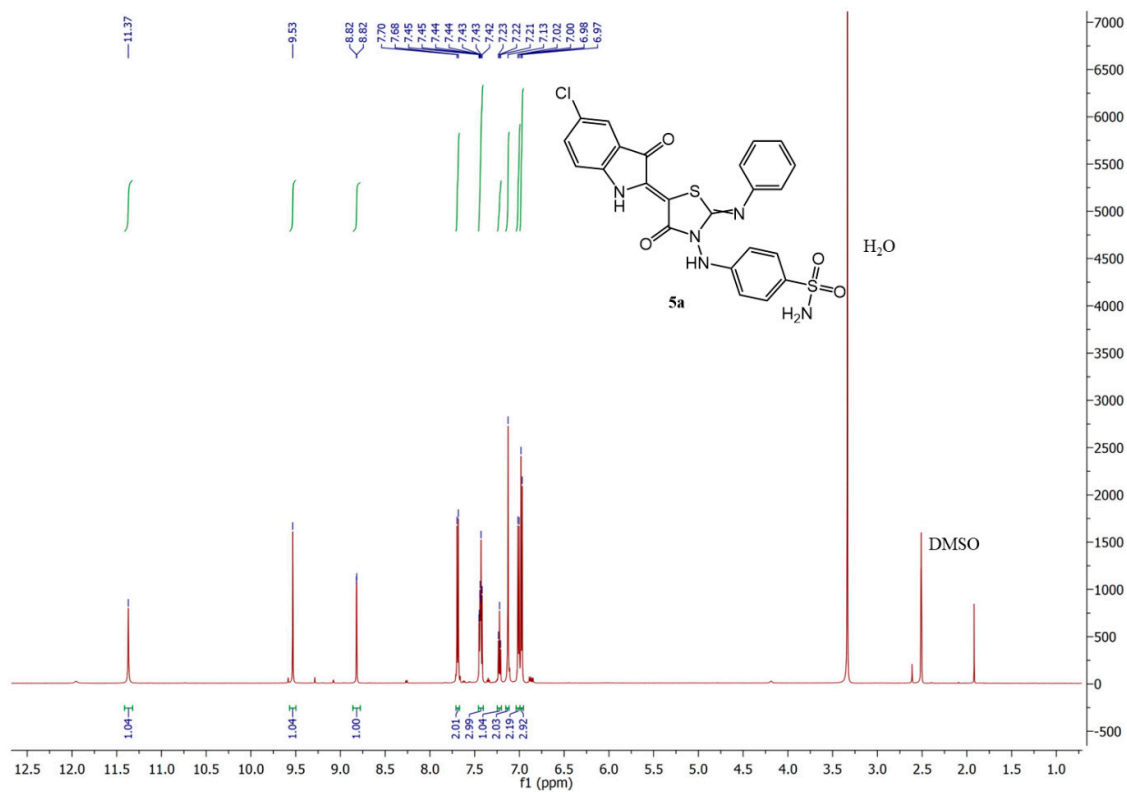
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of compound **3**



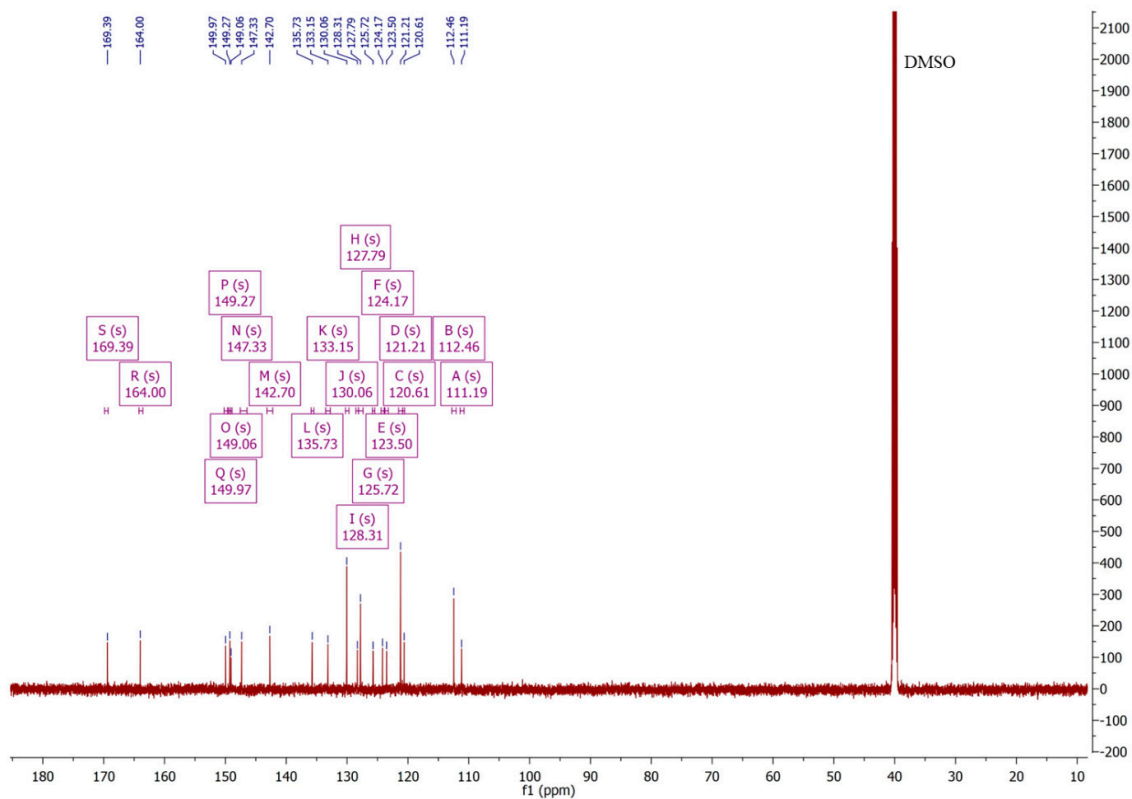
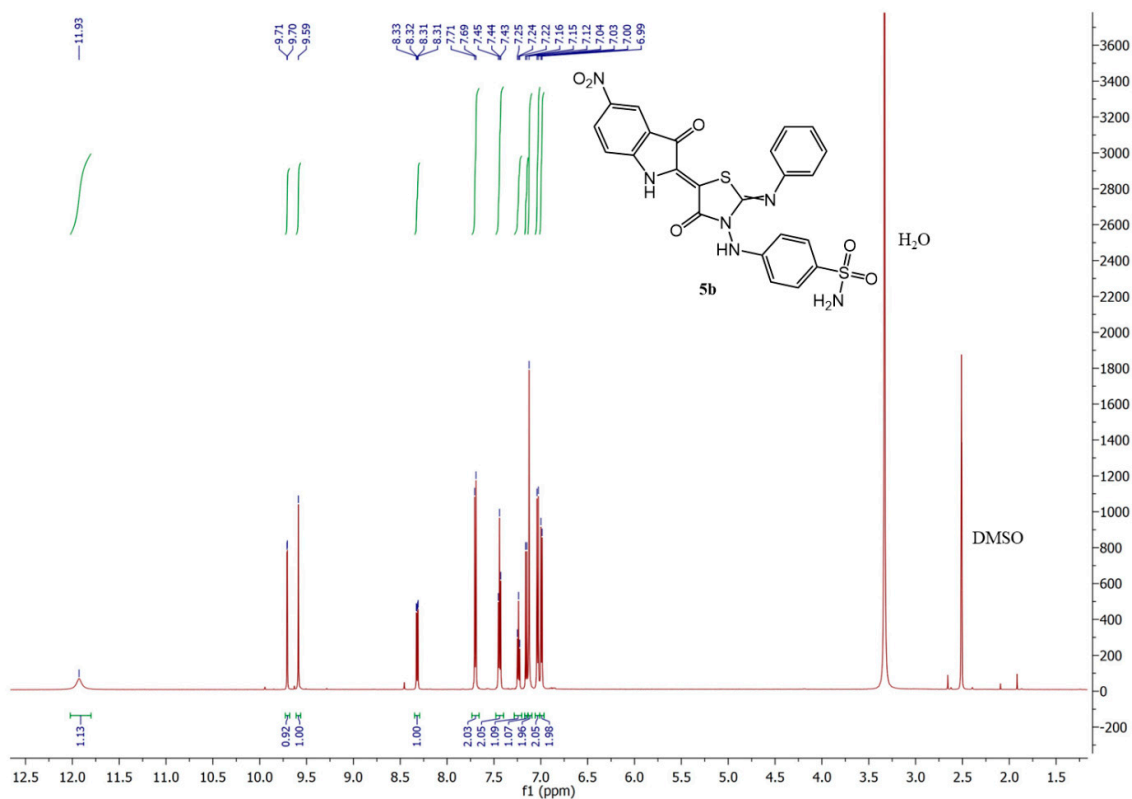
$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR of compound **4**



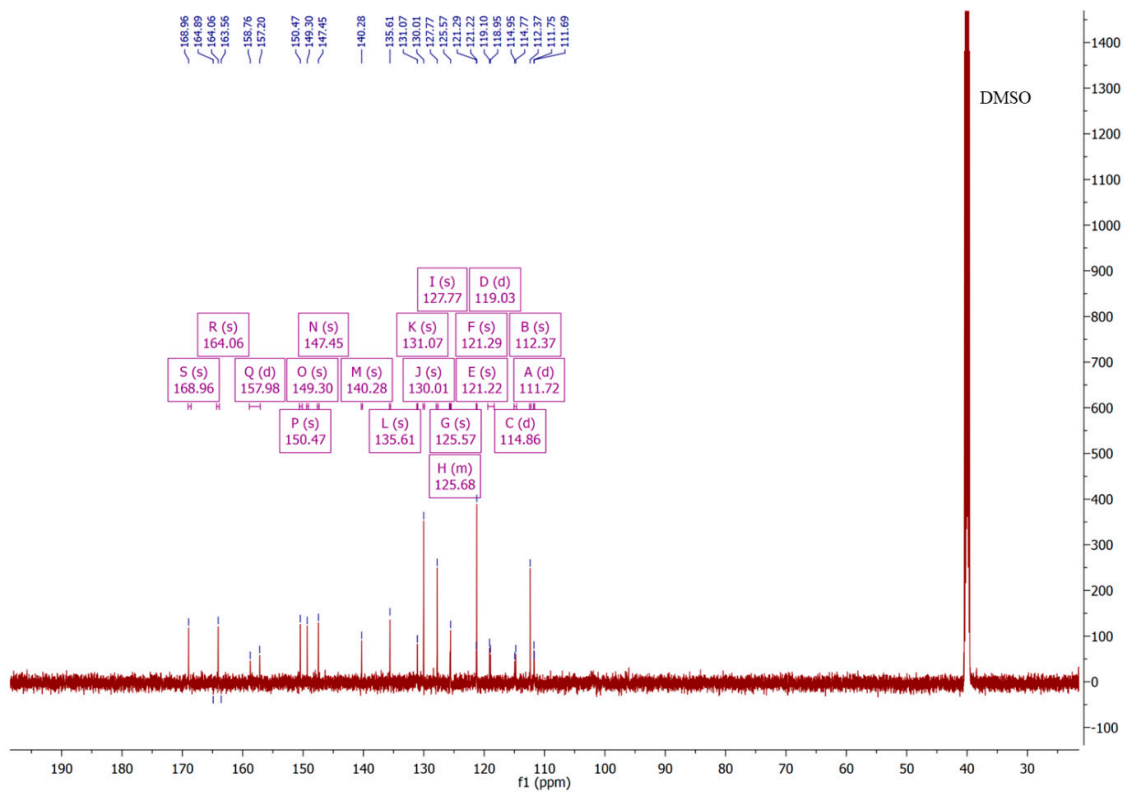
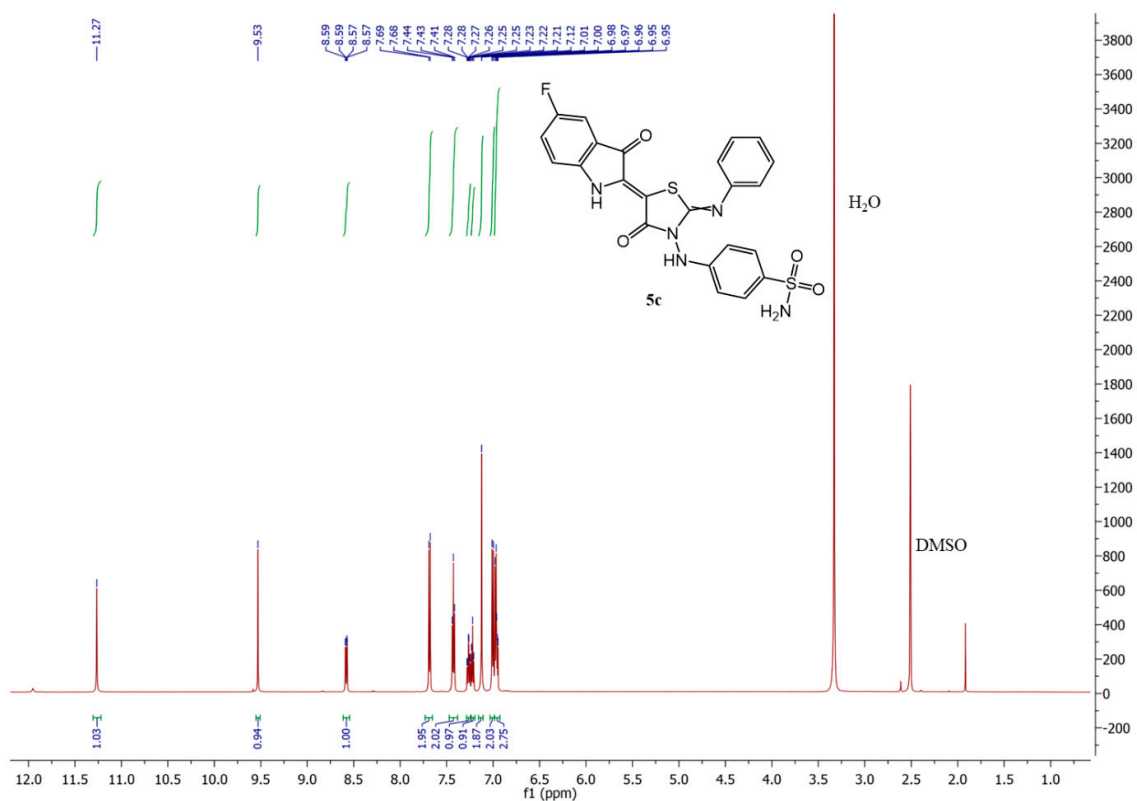
$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR of compound **5a**



# <sup>1</sup>H NMR and <sup>13</sup>C NMR of compound **5b**

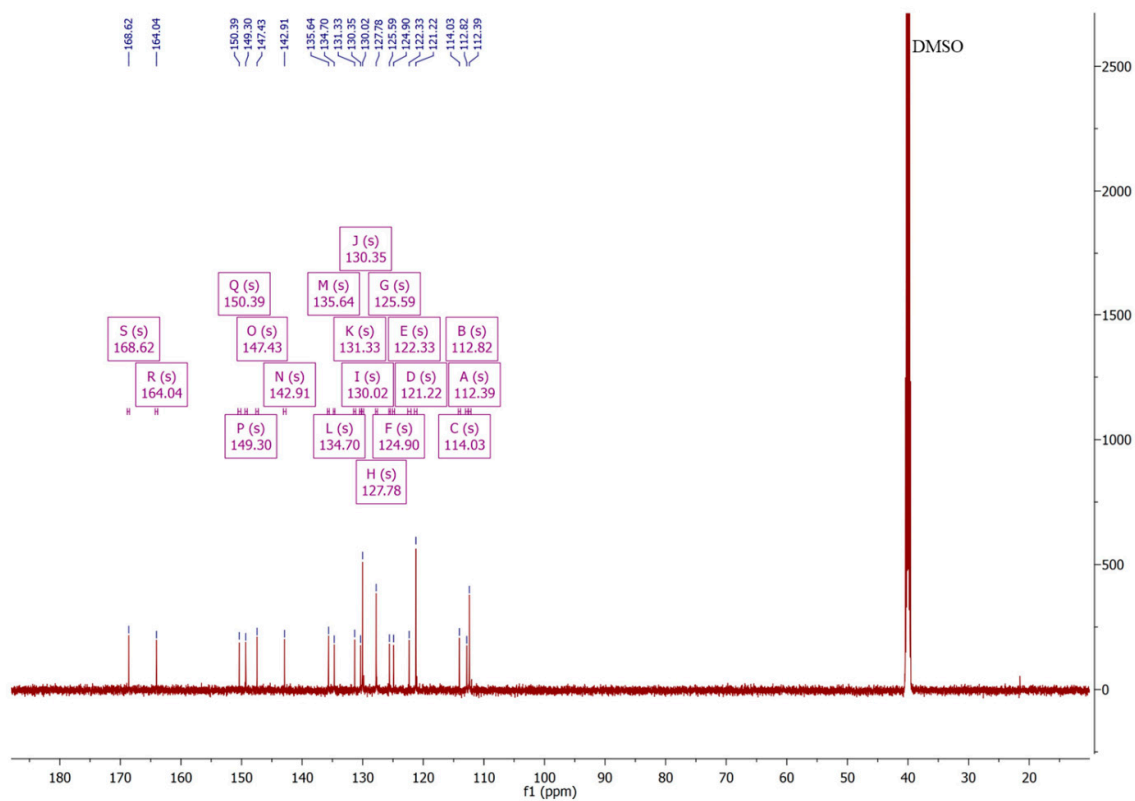
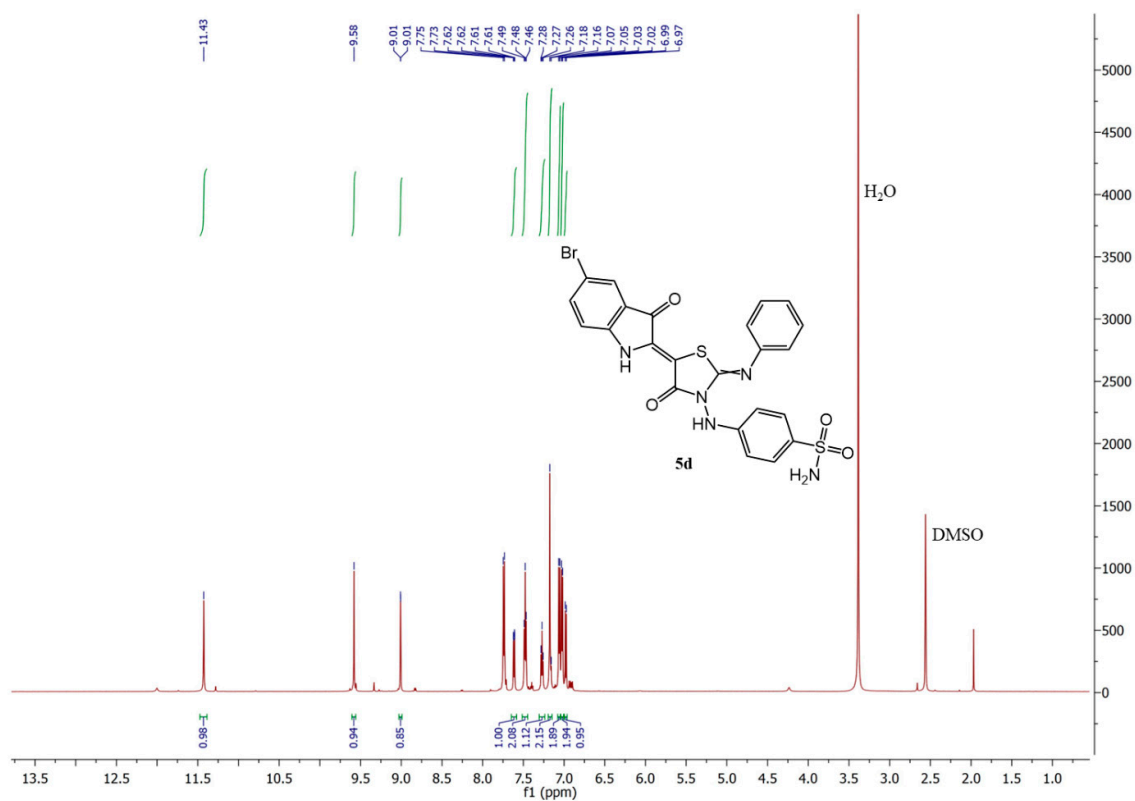


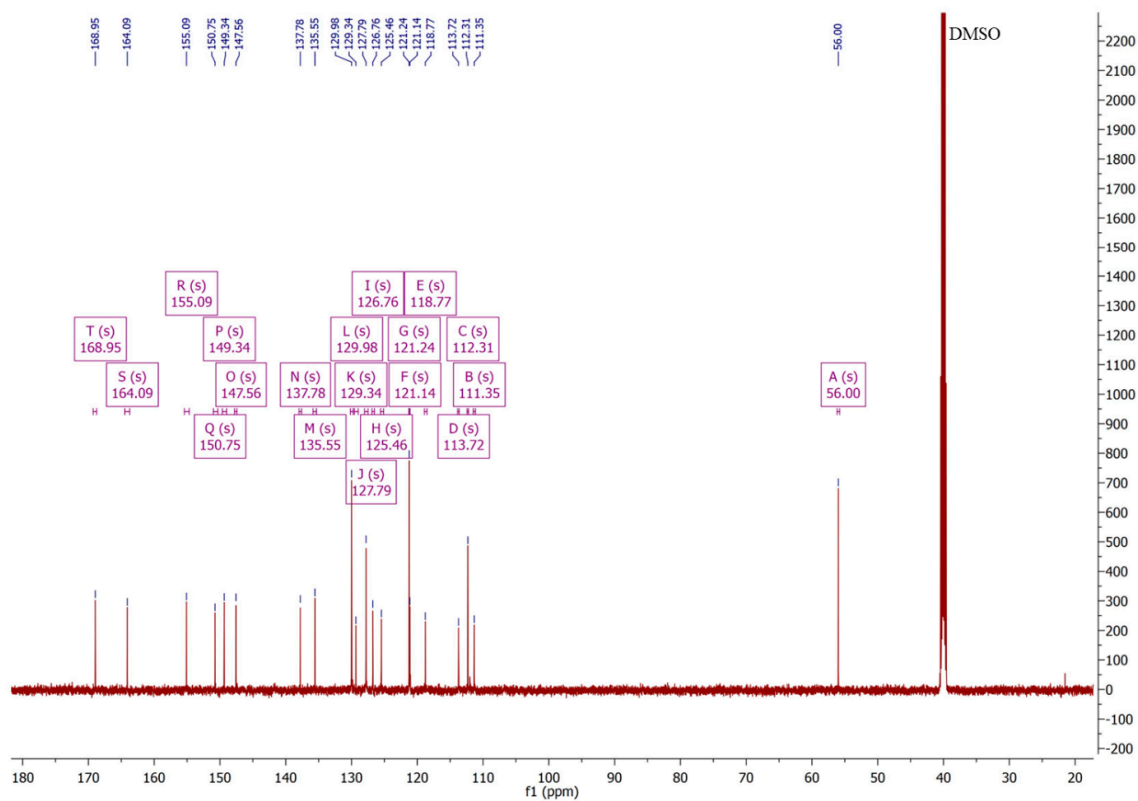
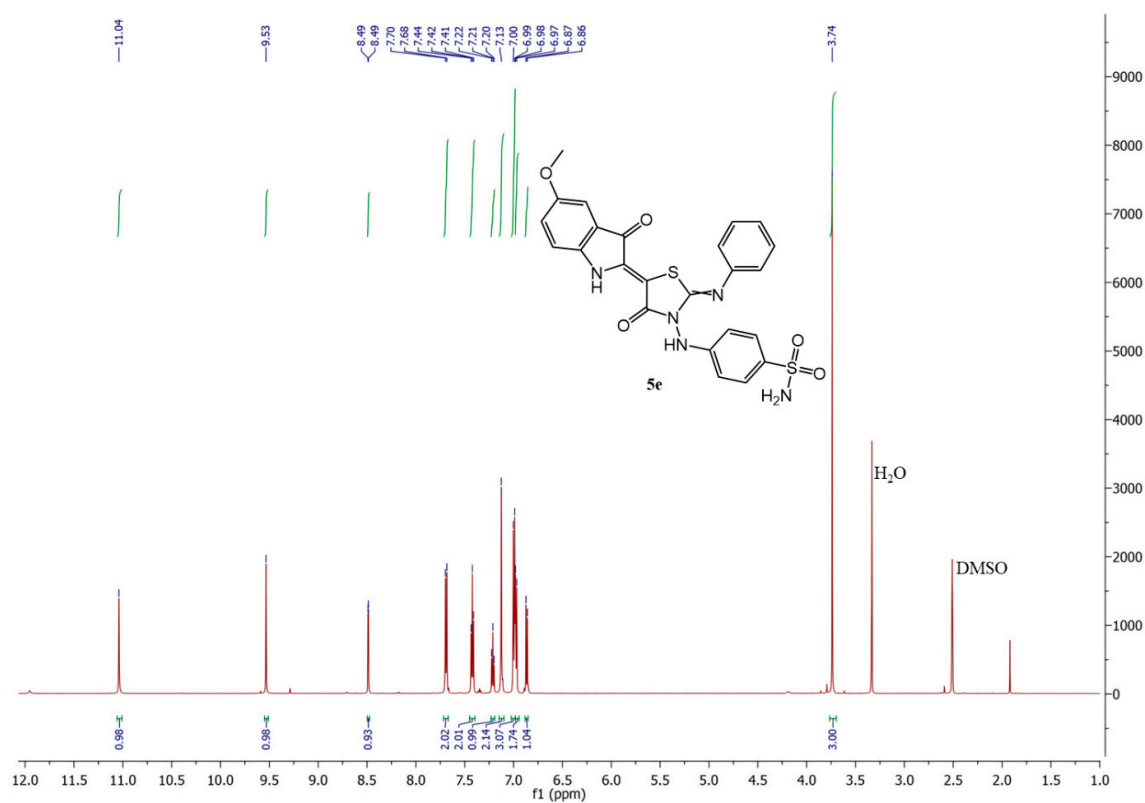
$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR of compound **5c**



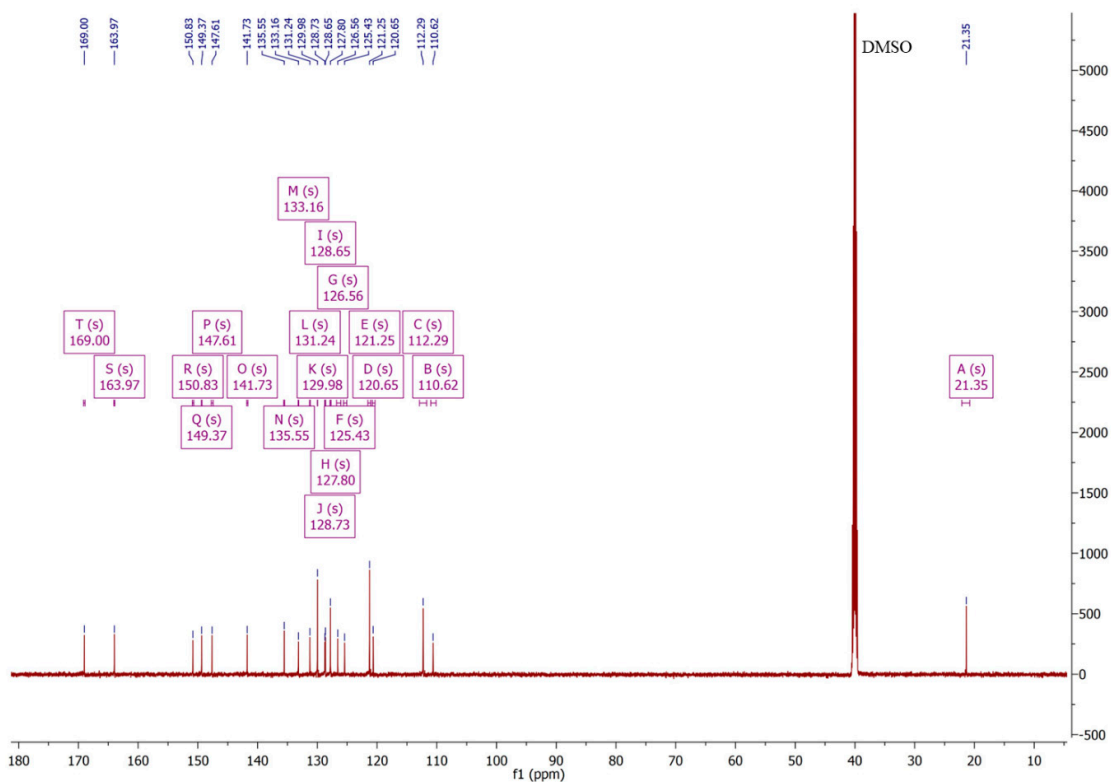
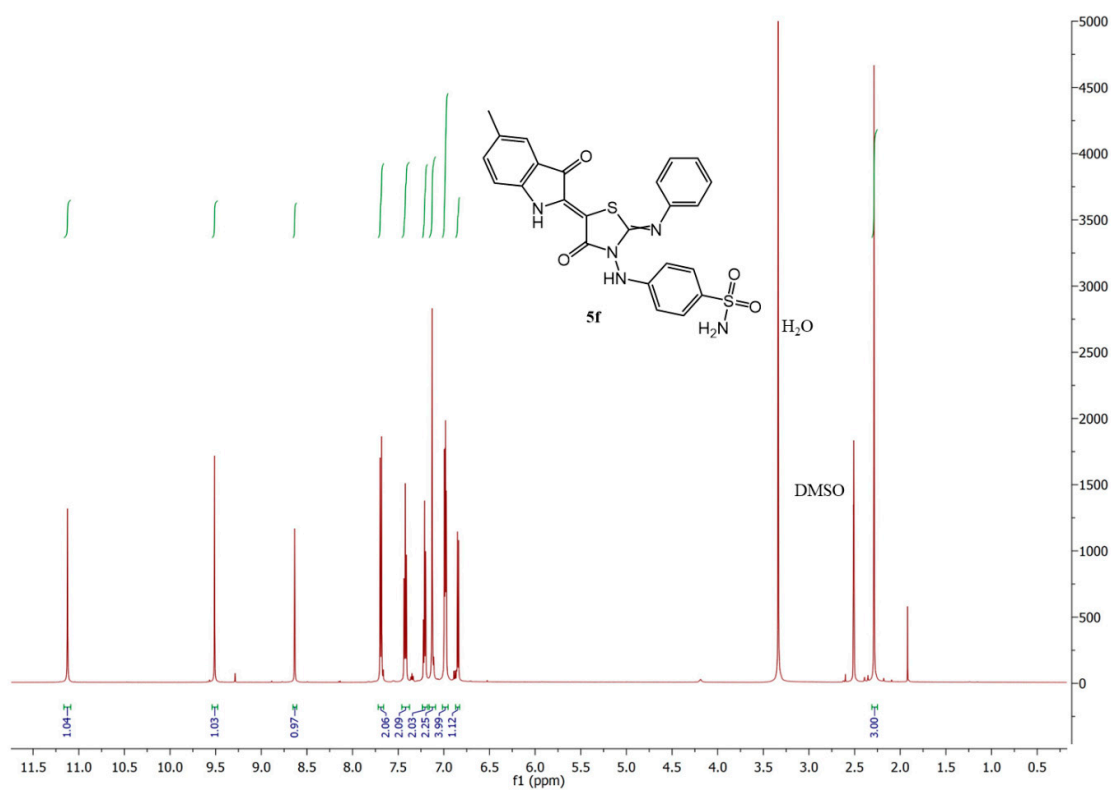


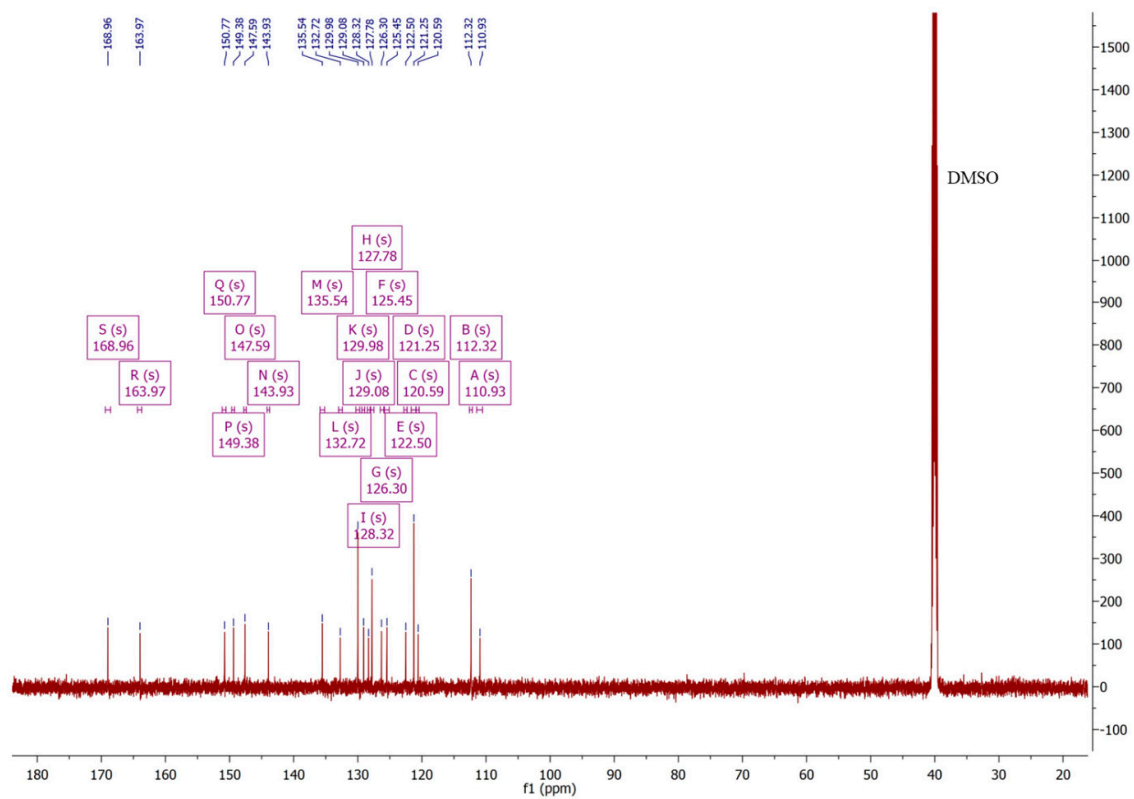
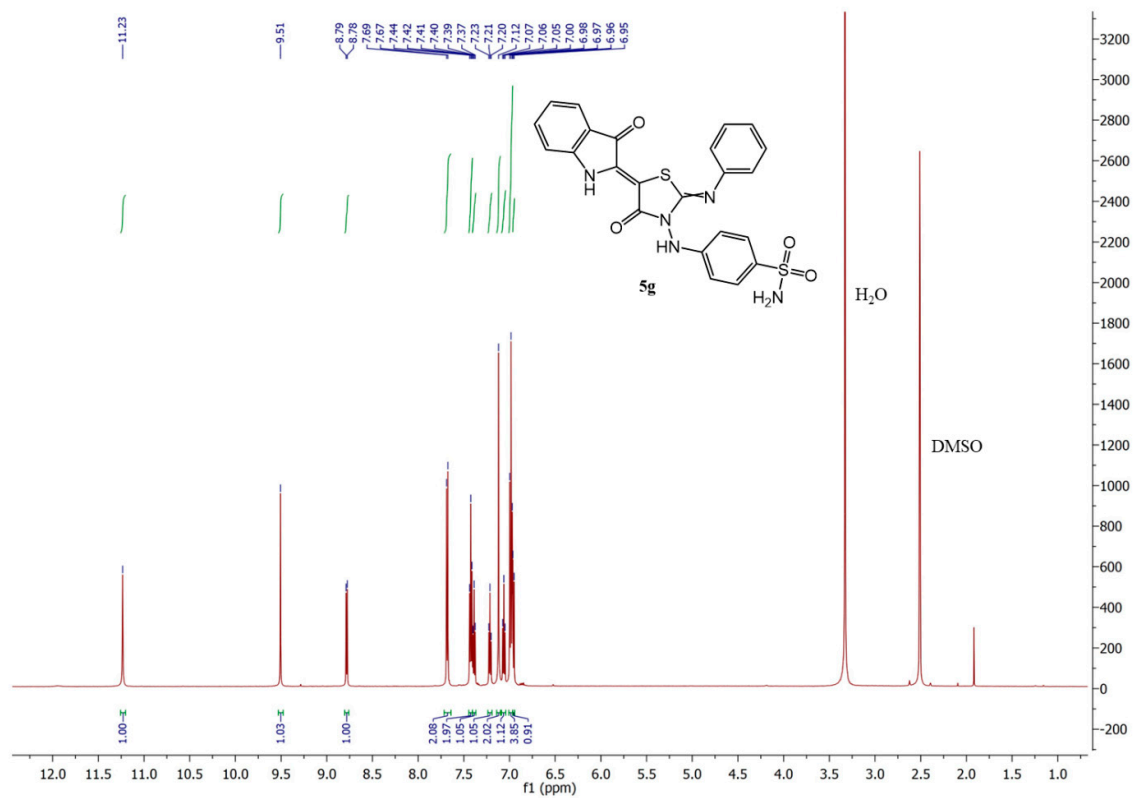
$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR of compound **5d**



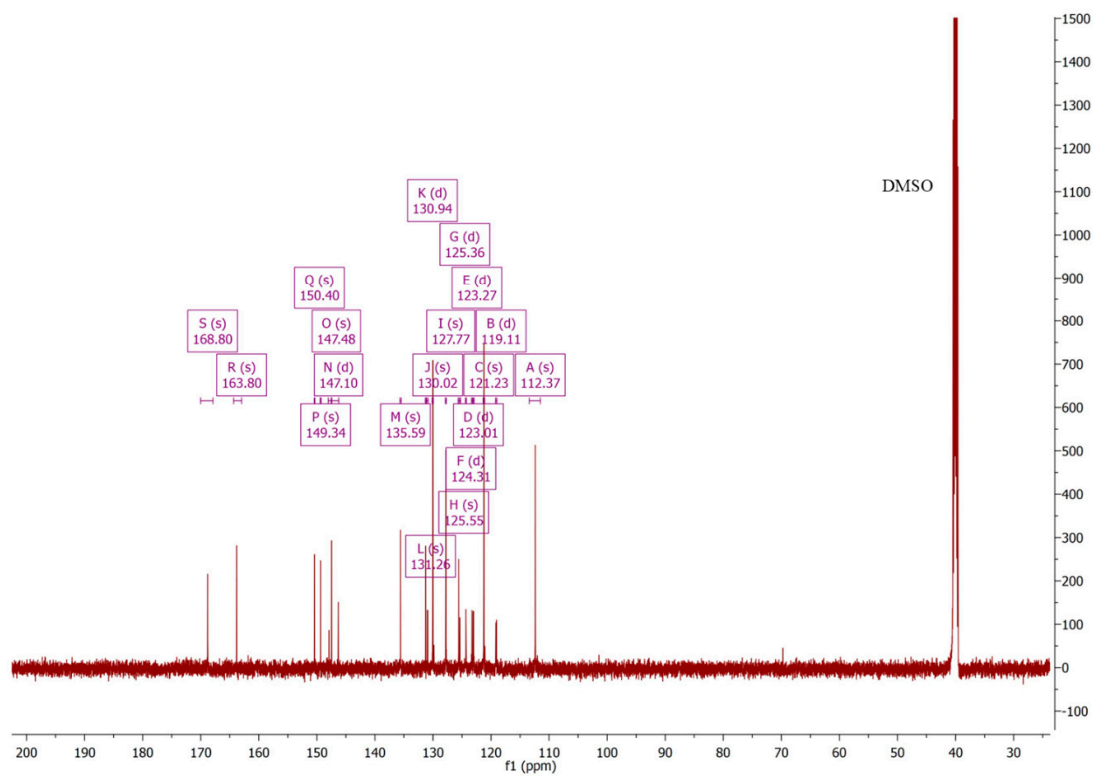
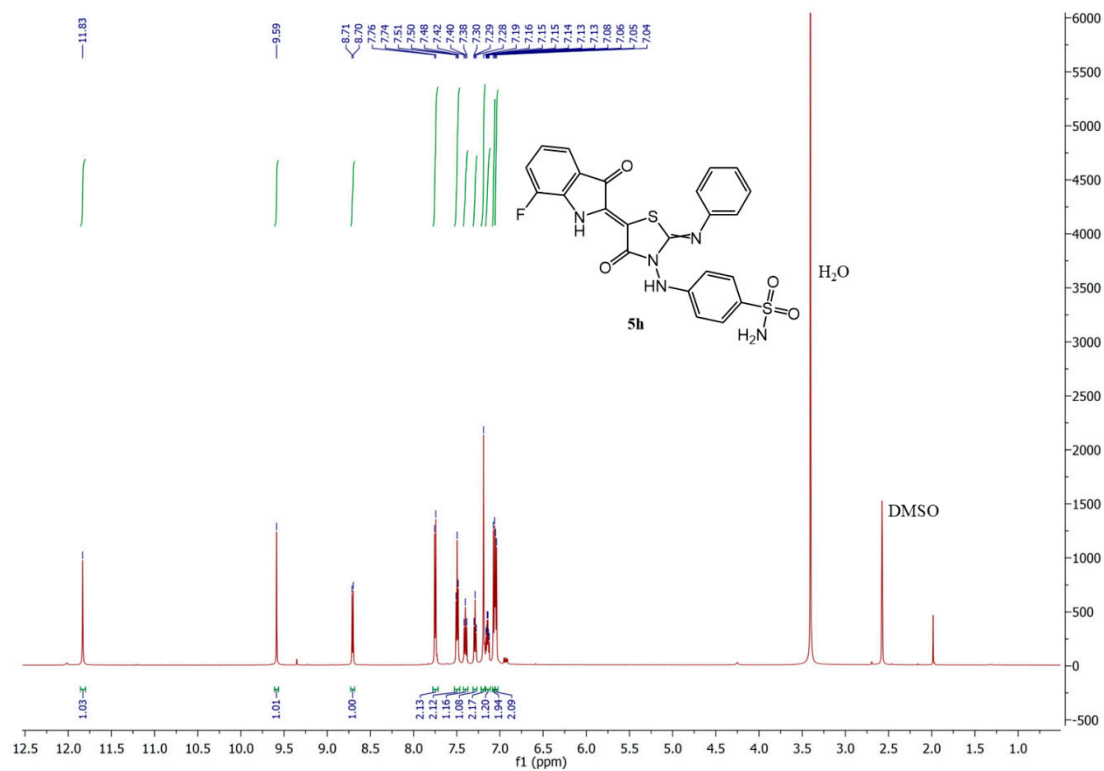
<sup>1</sup>H NMR and <sup>13</sup>C NMR of compound **5e**

$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR of compound **5f**

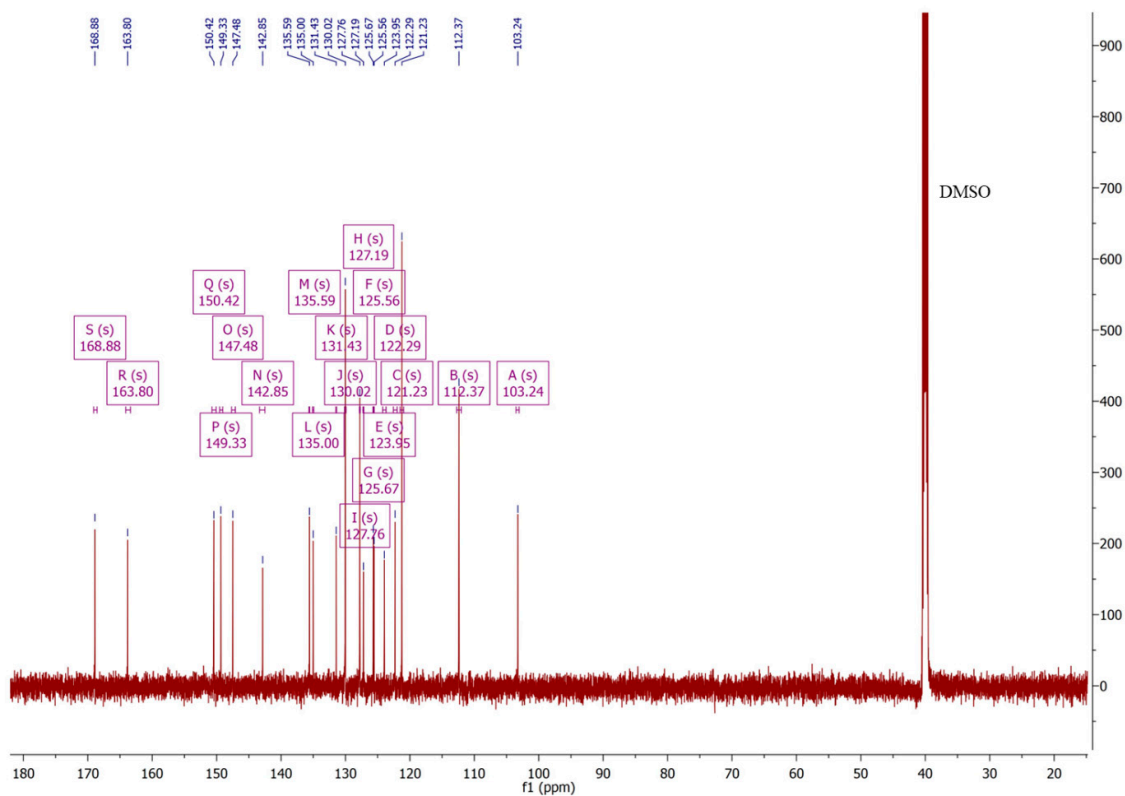
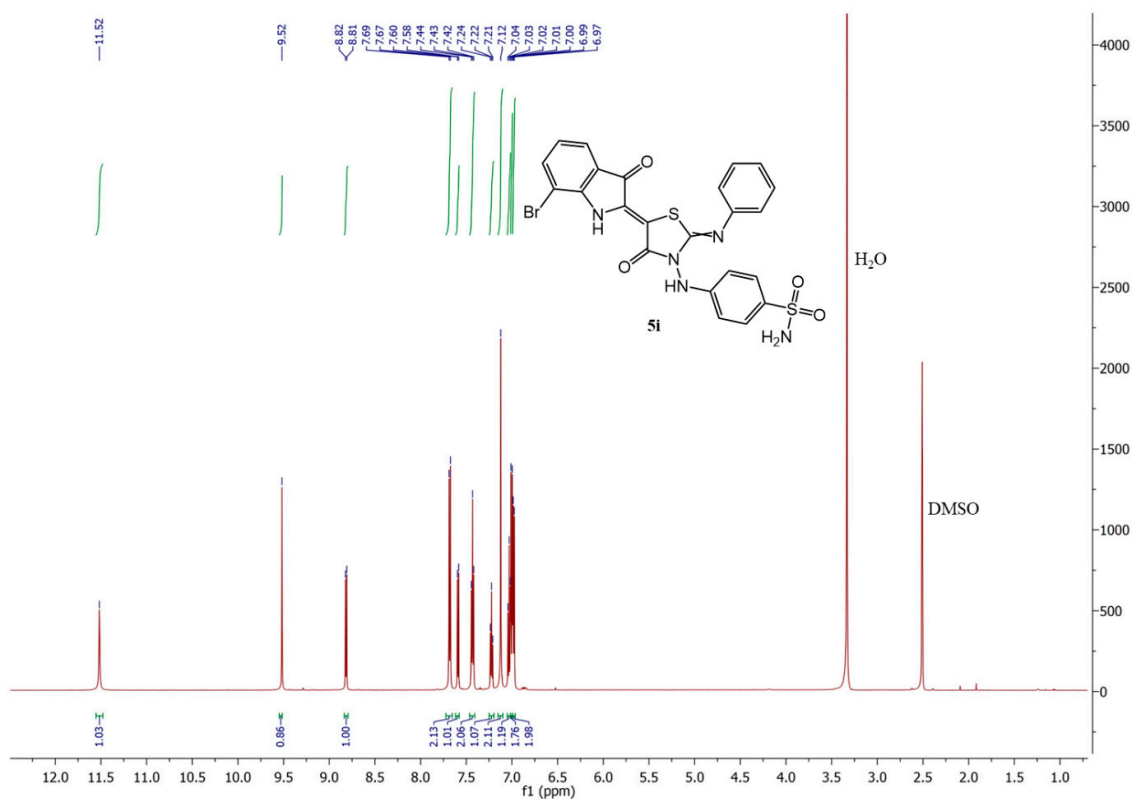


<sup>1</sup>H NMR and <sup>13</sup>C NMR of compound **5g**

$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR of compound **5h**

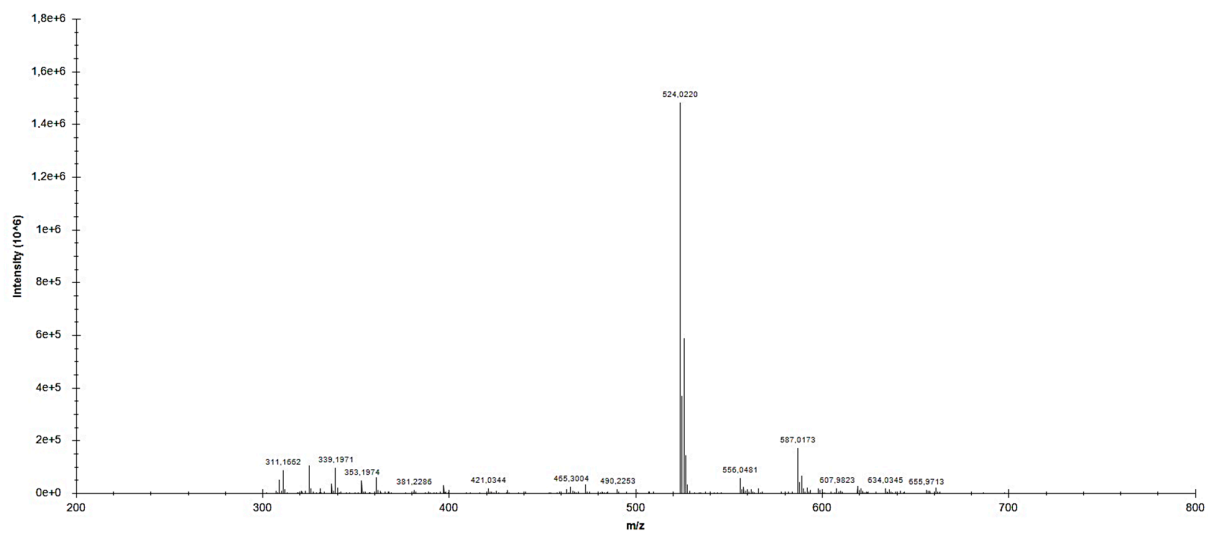


# <sup>1</sup>H NMR and <sup>13</sup>CNMR of compound **5i**

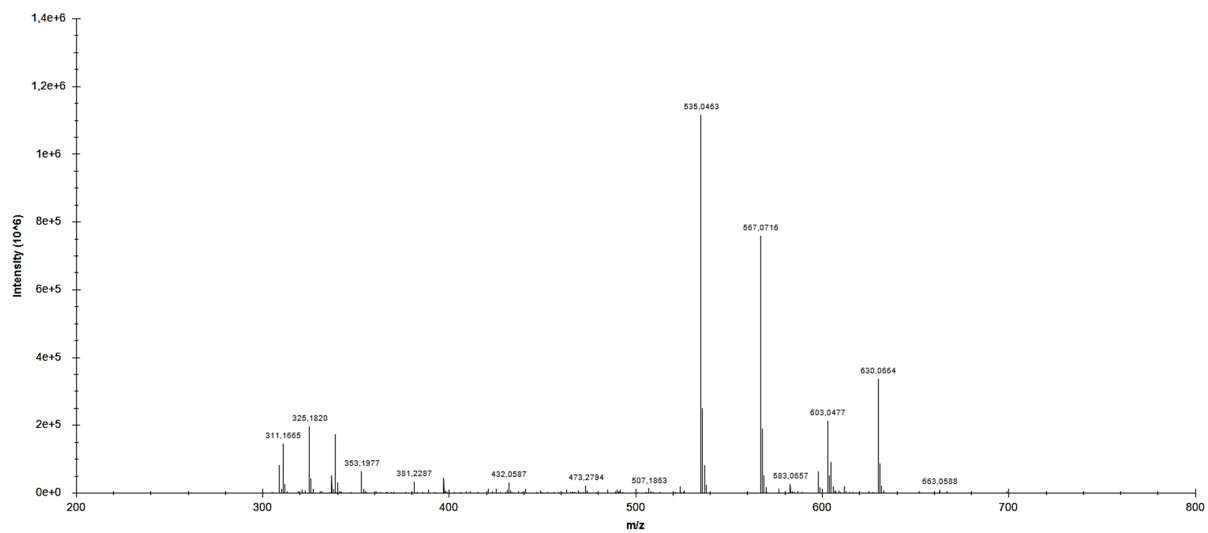


## ESI-HRMS spectra of **5a-i** compounds ( $[M-H]^-$ )

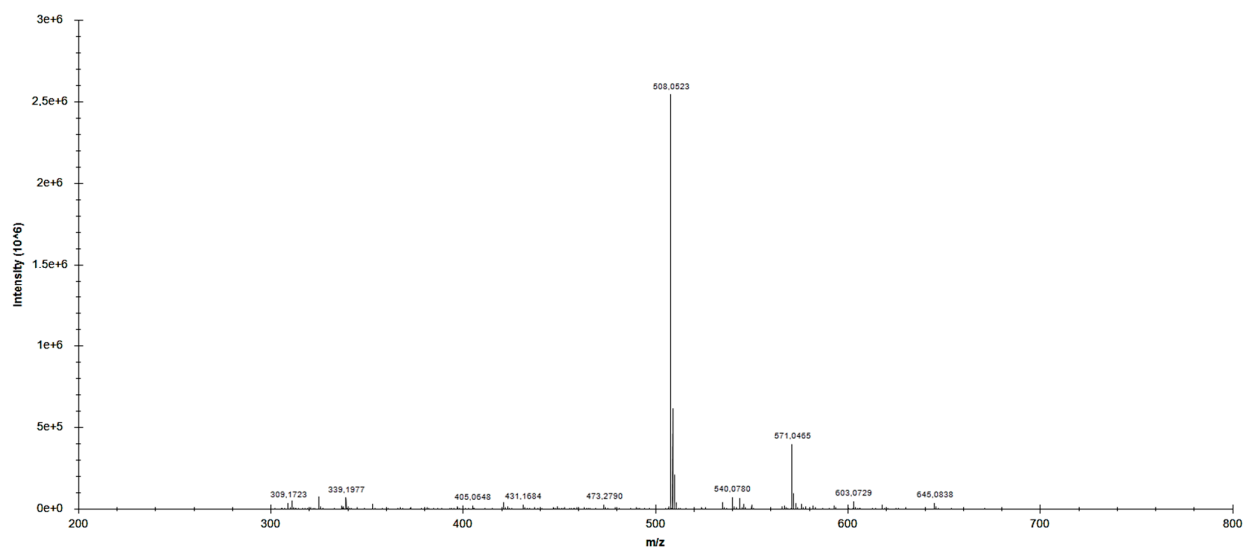
### MS spectrum of compound **5a**



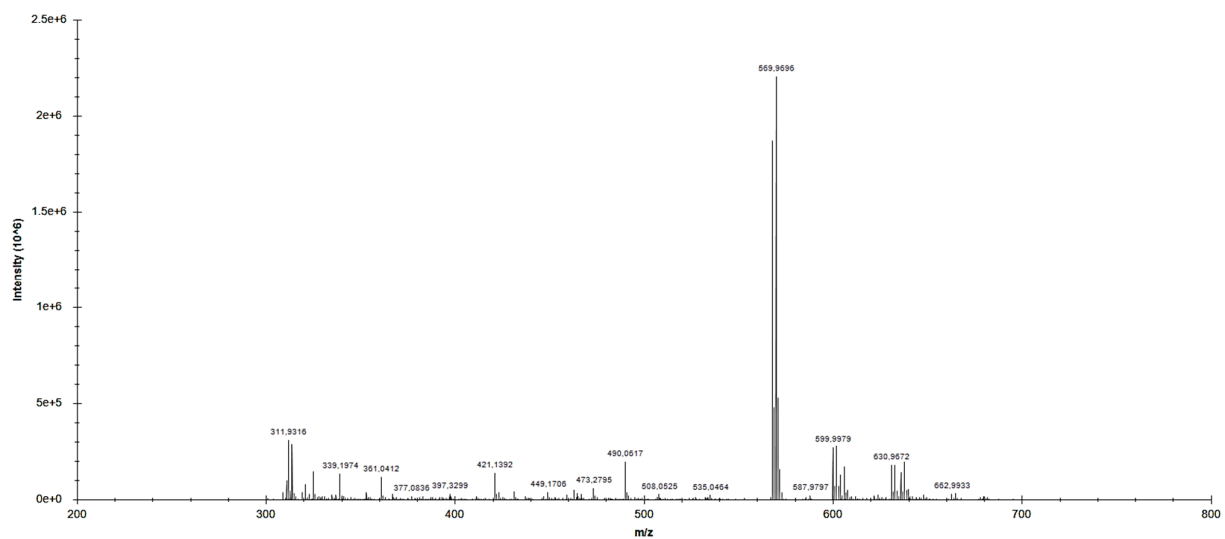
### MS spectrum of compound **5b**



### MS spectrum of compound **5c**

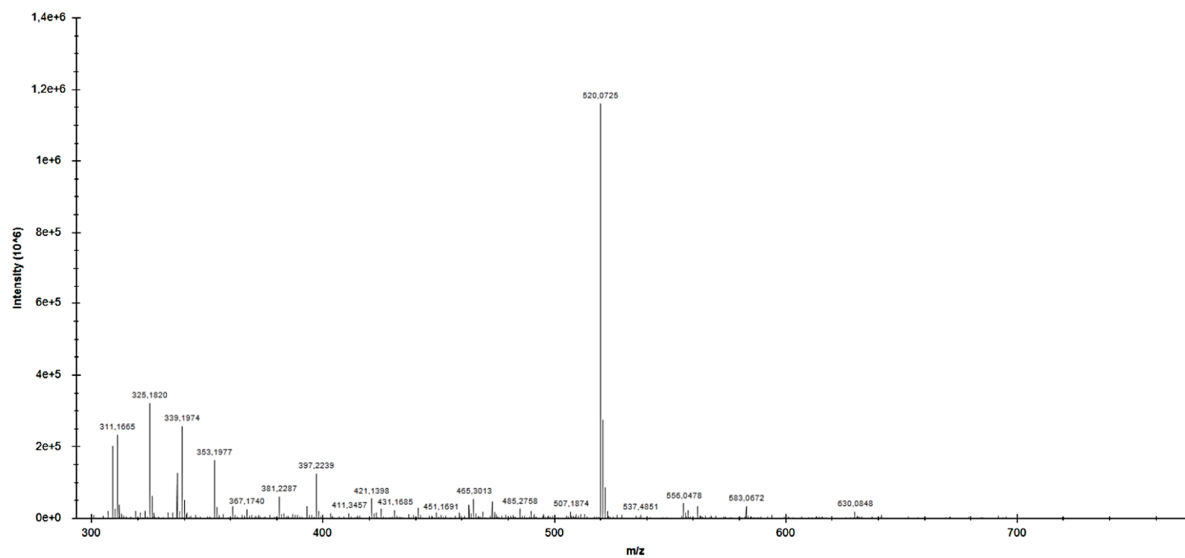


### MS spectrum of compound **5d**

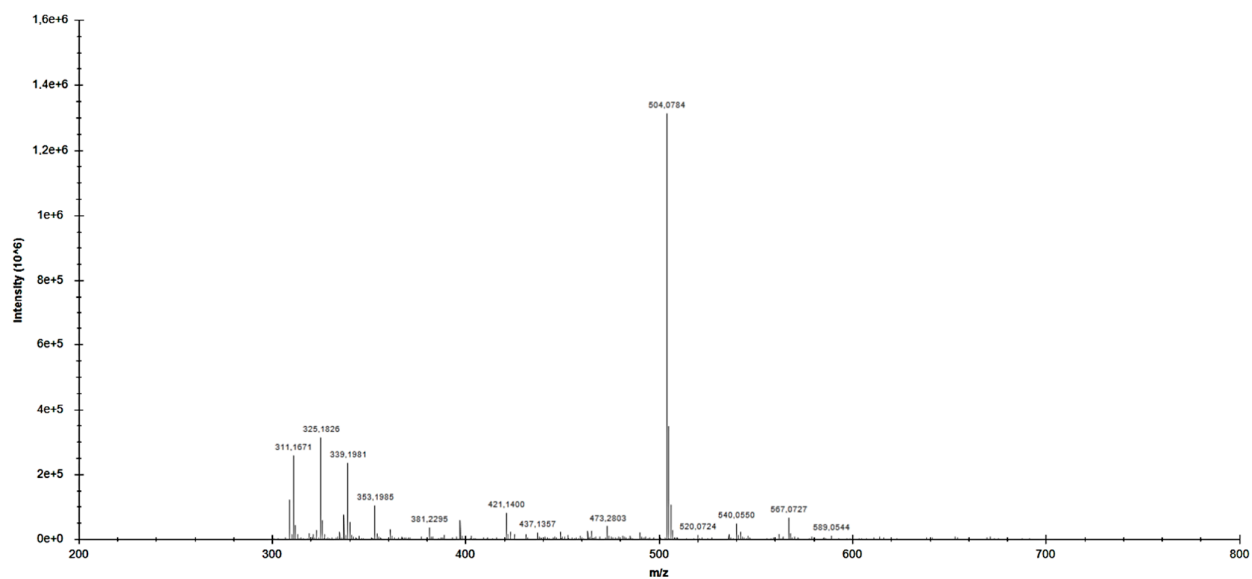




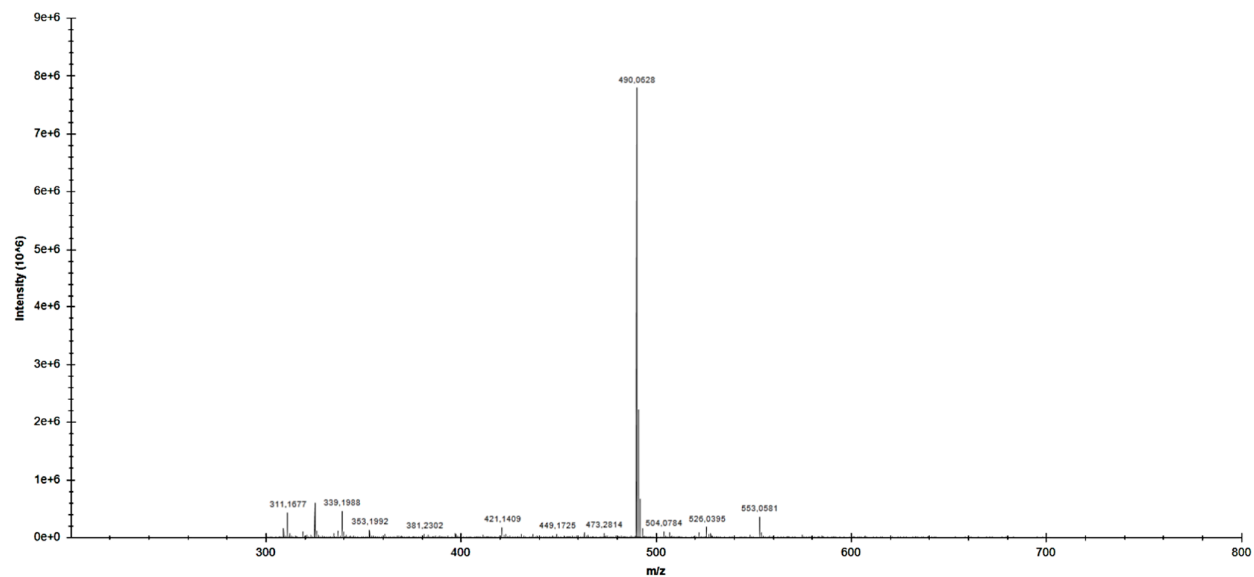
### MS spectrum of compound **5e**



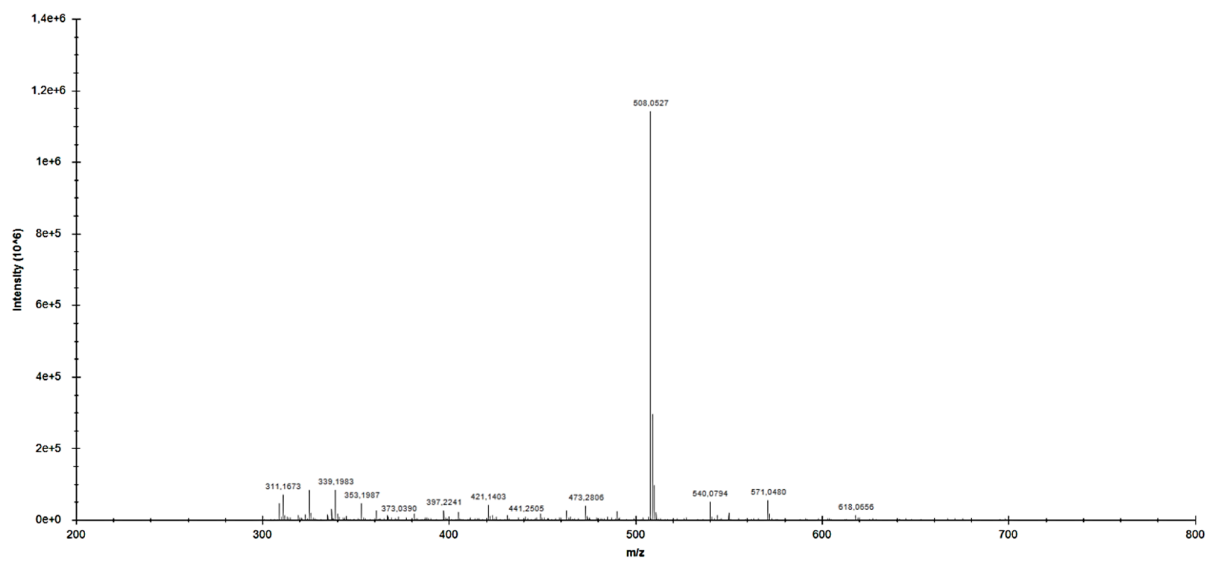
### MS spectrum of compound **5f**



### MS spectrum of compound **5g**



### MS spectrum of compound **5h**



# MS spectrum of compound **5i**

