

## Supplementary Material

### Synthesis and anti-cancer activity of diverse oxa-carbocycle fused isoflavones using the olefin metathesis

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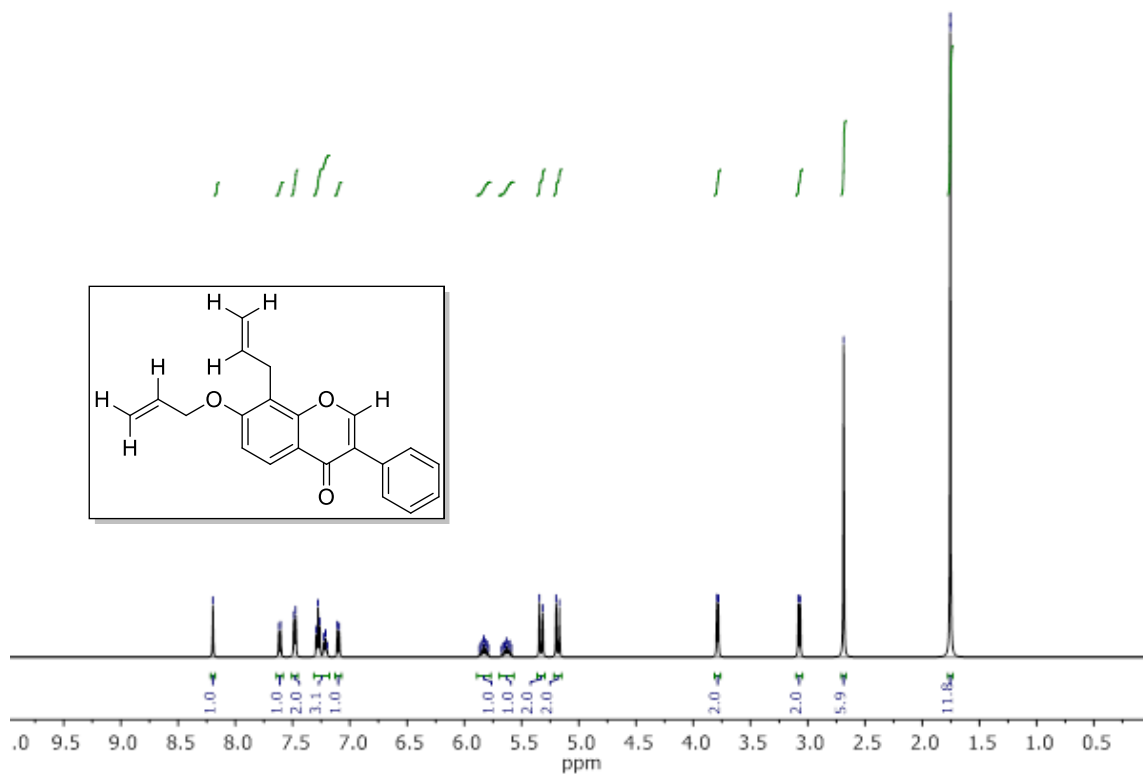
Email: [yjpr\\_19@yahoo.com](mailto:yjpr_19@yahoo.com)

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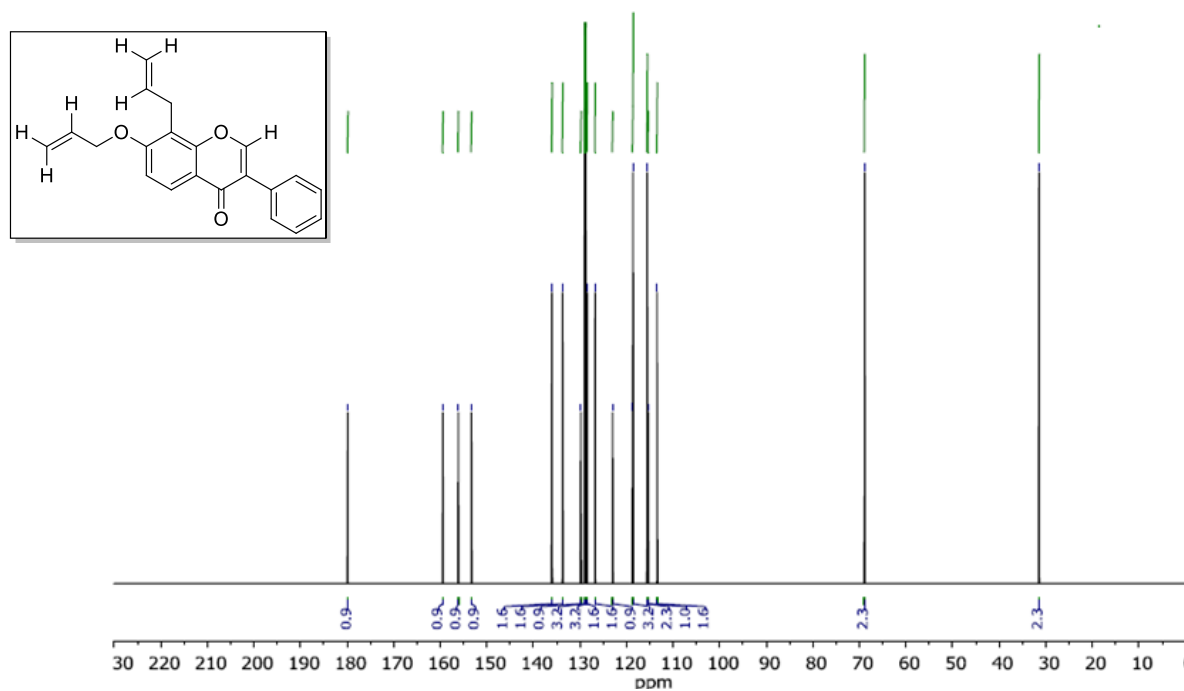
<sup>1</sup>H-NMR, <sup>13</sup>C-NMR and HRMS spectra of compounds

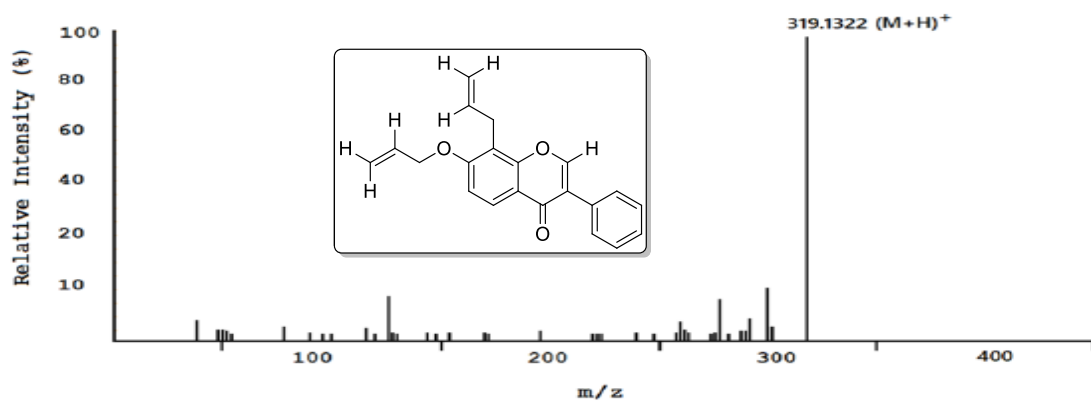
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$^{13}\text{C-NMR}$  Spectrum (DMSO- $d_6$ , 101 MHz) of 8-allyl-7-(allyloxy)-3-phenyl-4H-chromen-4-one (**4a**)



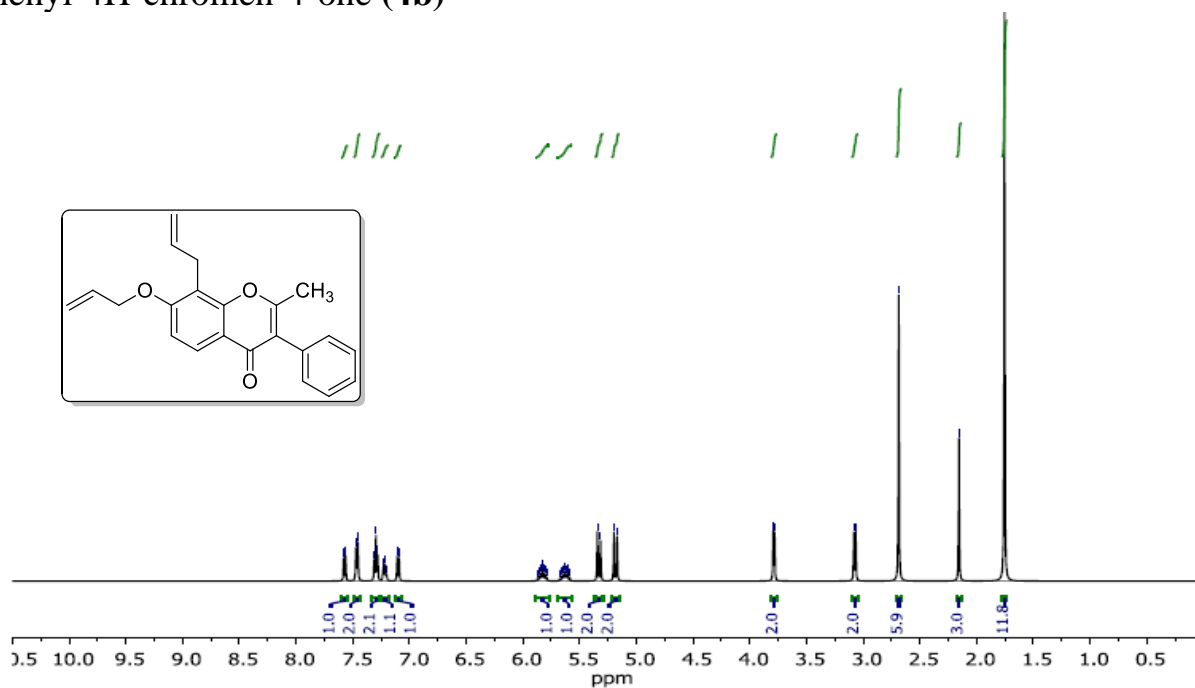
HRMS Spectrum of 8-allyl-7-(allyloxy)-3-phenyl-4H-chromen-4-one (**4a**)

HRMS (ESI) (m/z), of (C<sub>21</sub>H<sub>18</sub>O<sub>3</sub>)

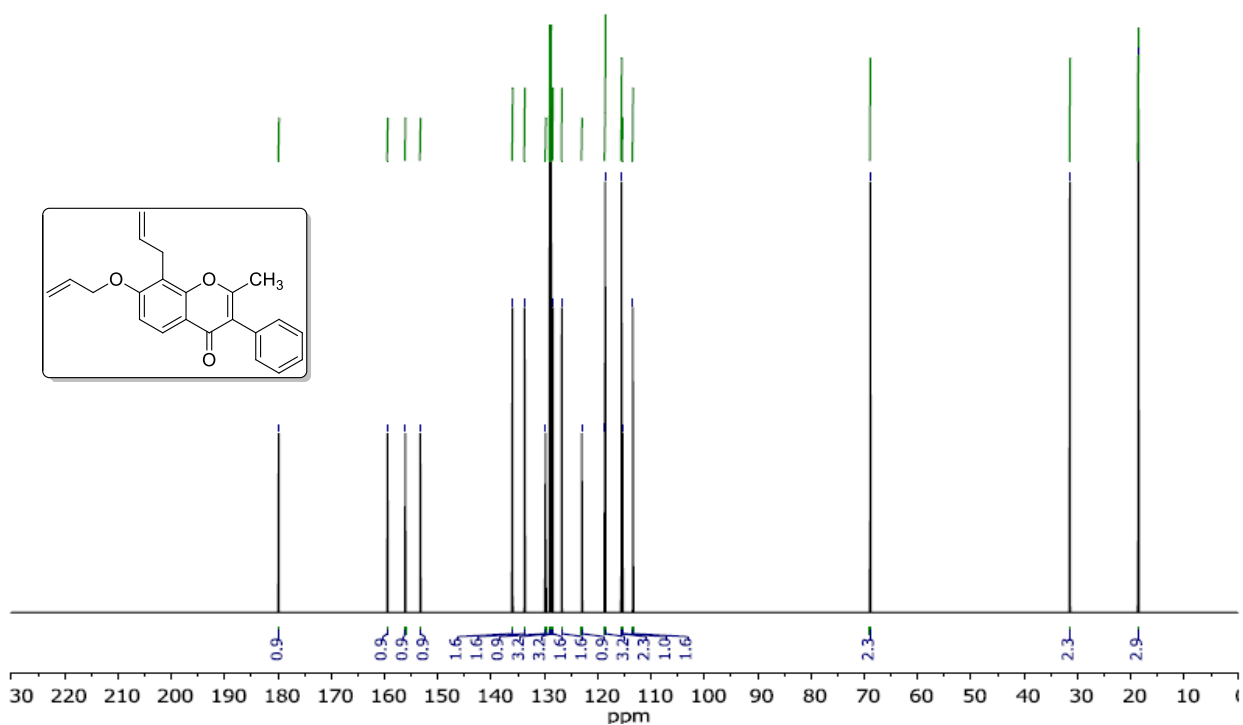
Calcd: 319.1328 [M+H]<sup>+</sup>

Found: 319.1322 [M+H]<sup>+</sup>

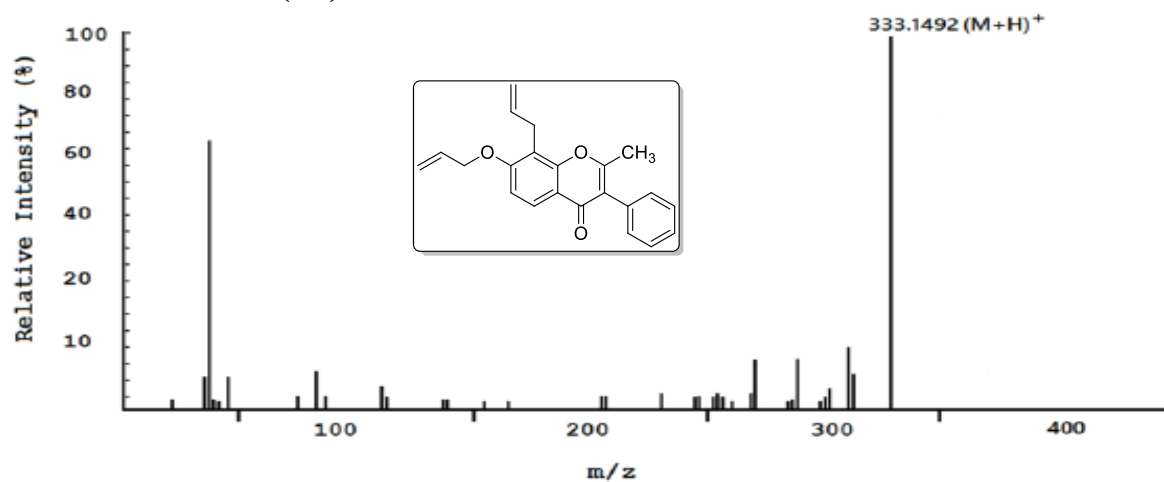
$^1\text{H-NMR}$  Spectrum ( $\text{DMSO-}d_6$ , 400 MHz) of 8-allyl-7-(allyloxy)-2-methyl-3-phenyl-4H-chromen-4-one (**4b**)



$^{13}\text{C-NMR}$  Spectrum ( $\text{DMSO-}d_6$ , 400 MHz) of 8-allyl-7-(allyloxy)-2-methyl-3-phenyl-4H-chromen-4-one (**4b**)



HRMS Spectrum (DMSO-*d*<sub>6</sub>, 400 MHz) of 8-allyl-7-(allyloxy)-2-methyl-3-phenyl-4H-chromen-4-one (**4b**)

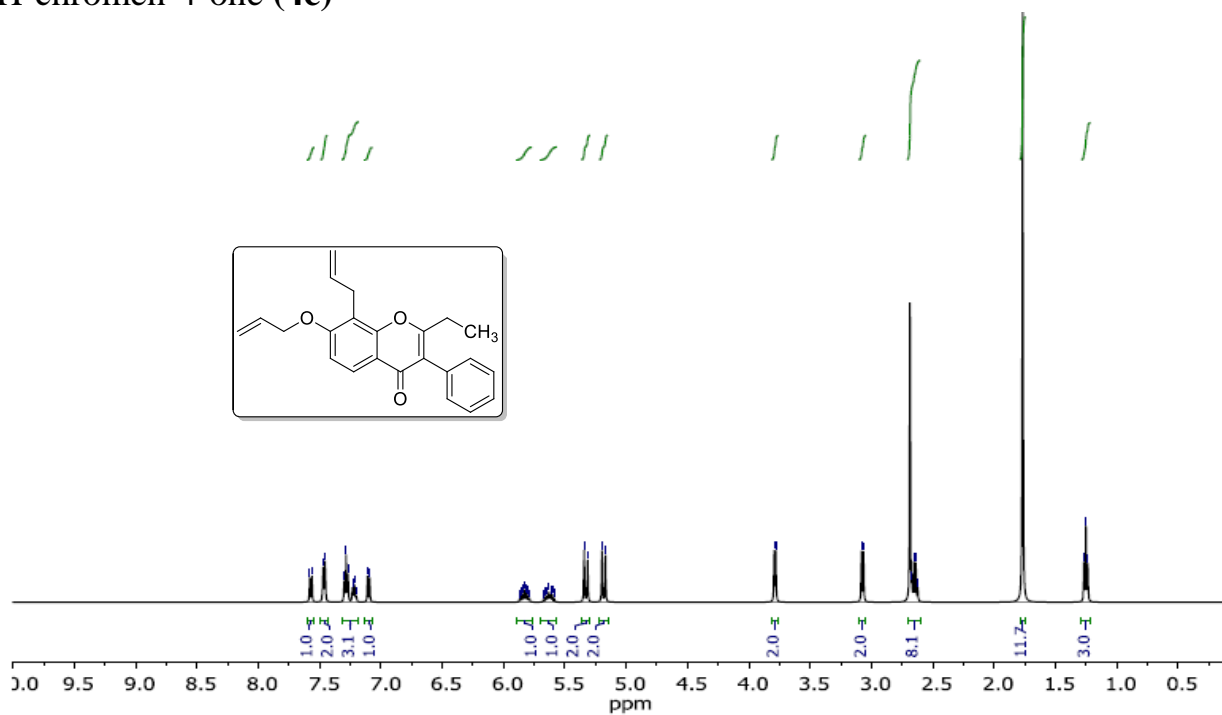


HRMS (ESI) (m/z), of (C<sub>22</sub>H<sub>20</sub>O<sub>3</sub>)

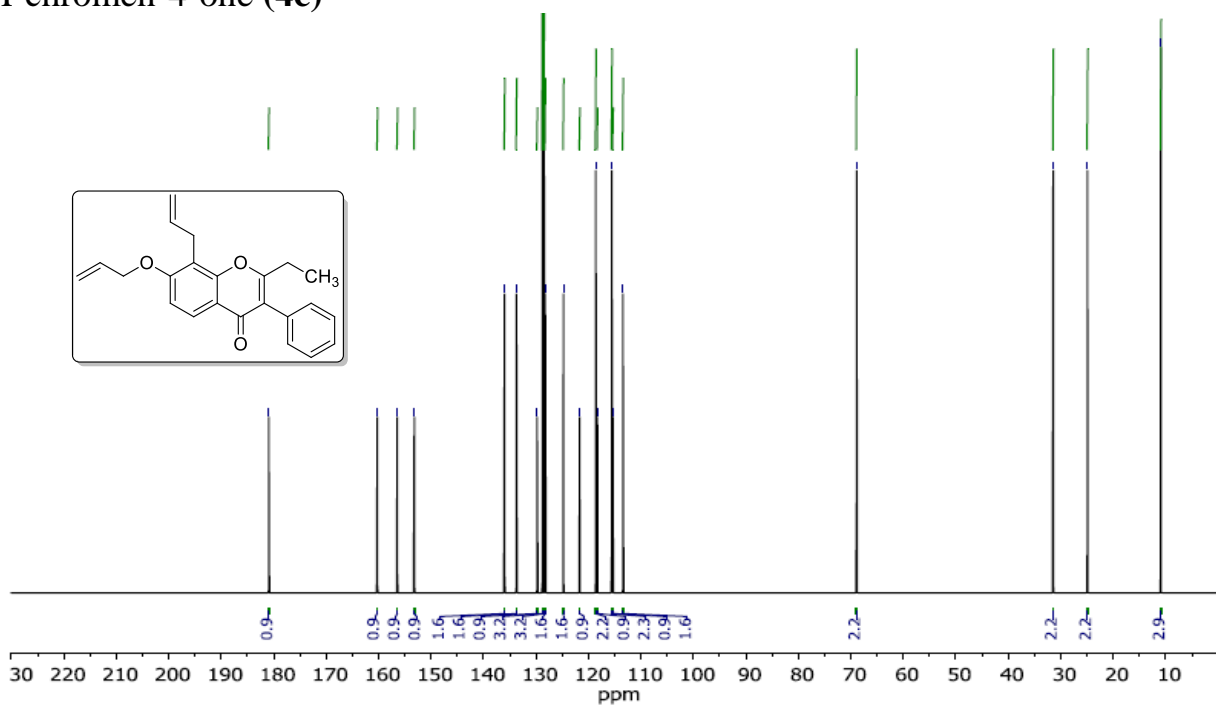
Calcd: 333.1485 [M+H]<sup>+</sup>

Found: 333.1492 [M+H]<sup>+</sup>

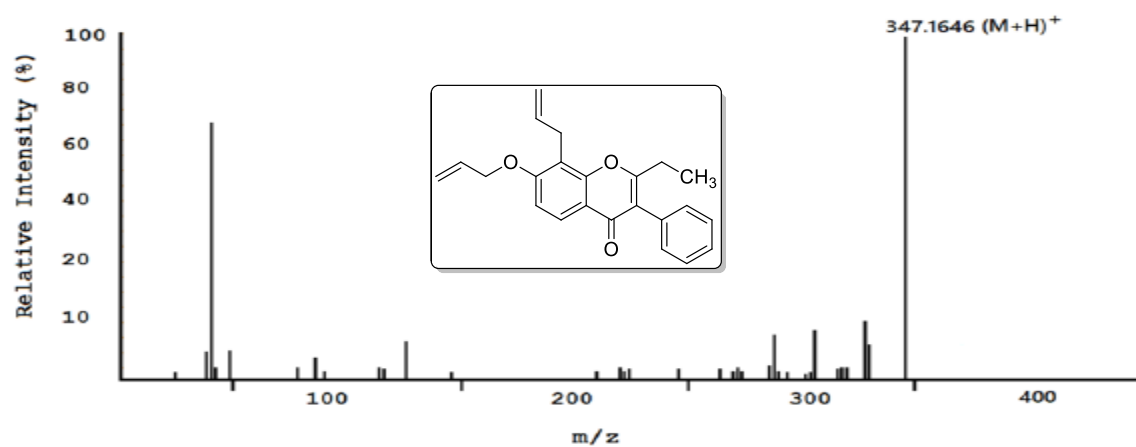
<sup>1</sup>H-NMR Spectrum (DMSO-*d*<sub>6</sub>, 400 MHz) 8-allyl-7-(allyloxy)-2-ethyl-3-phenyl-4H-chromen-4-one (**4c**)



<sup>13</sup>C-NMR Spectrum (DMSO-*d*<sub>6</sub>, 400 MHz) 8-allyl-7-(allyloxy)-2-ethyl-3-phenyl-4H-chromen-4-one (**4c**)



HRMS Spectrum (DMSO-*d*<sub>6</sub>, 400 MHz) 8-allyl-7-(allyloxy)-2-ethyl-3-phenyl-4H-chromen-4-one (**4c**)

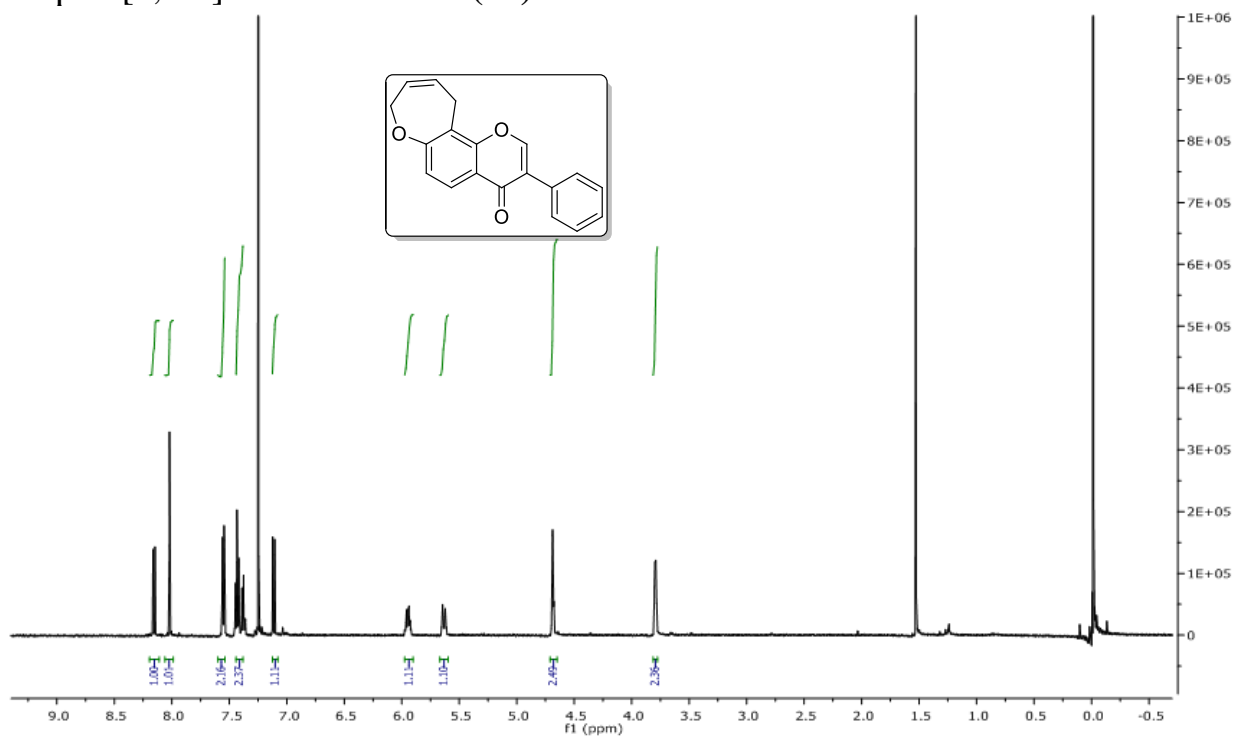


HRMS (ESI) (m/z), of (C<sub>23</sub>H<sub>22</sub>O<sub>3</sub>)

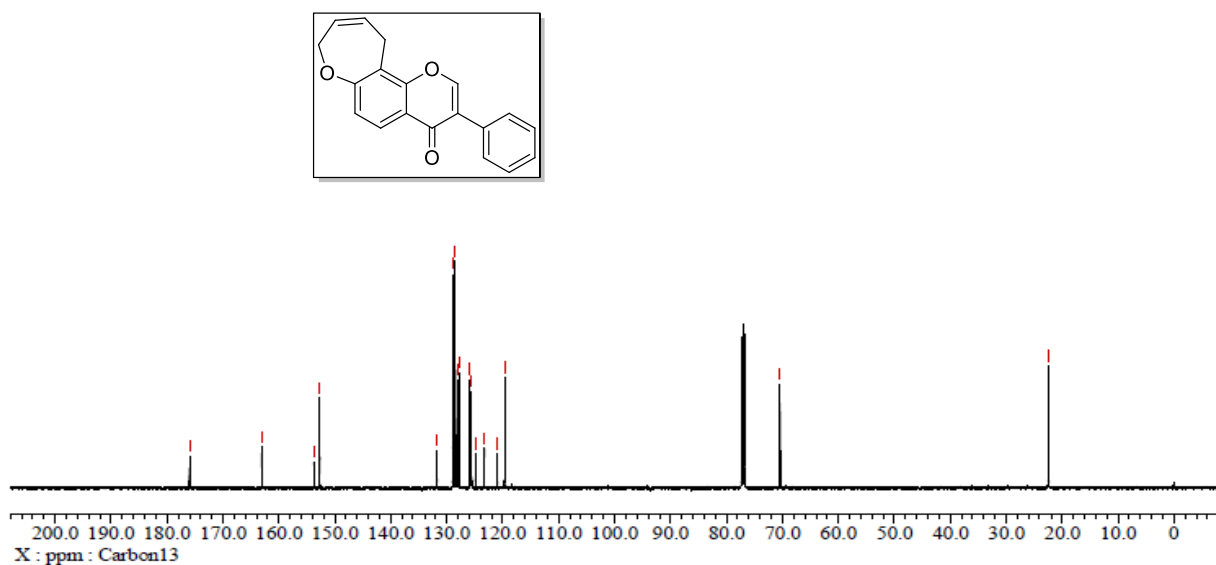
Calcd: 347.1641 [M+H]<sup>+</sup>

Found: 347.1646 [M+H]<sup>+</sup>

<sup>1</sup>H-NMR Spectrum (DMSO-*d*<sub>6</sub>, 400 MHz) of 3-phenyl-8,11-dihydro-4H-oxepino[2,3-*h*]chromen-4-one (**5a**)

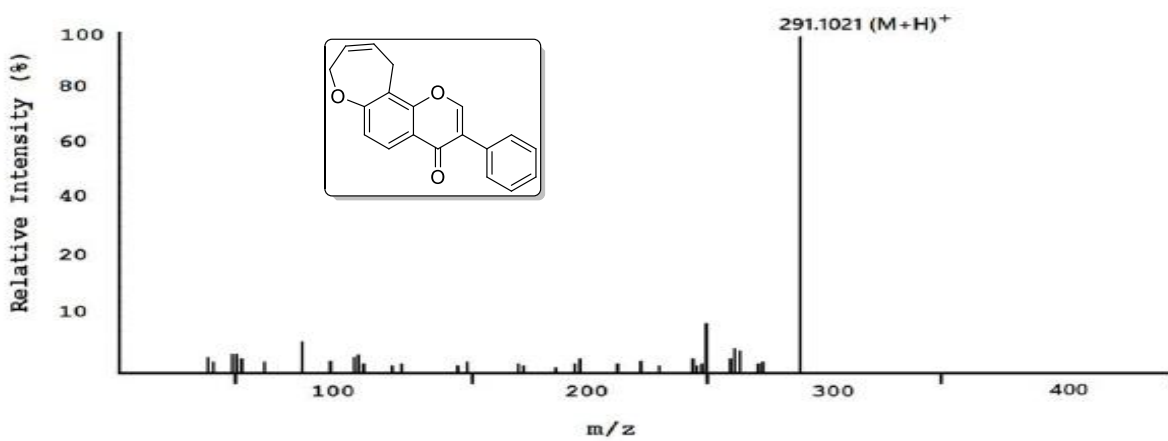


<sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>, 101 MHz) Spectrum of 3-phenyl-8,11-dihydro-4H-oxepino[2,3-*h*]chromen-4-one (**5a**)





## HRMS Spectrum of 3-phenyl-8,11-dihydro-4H-oxepino[2,3-H] chromen-4-one (5a)

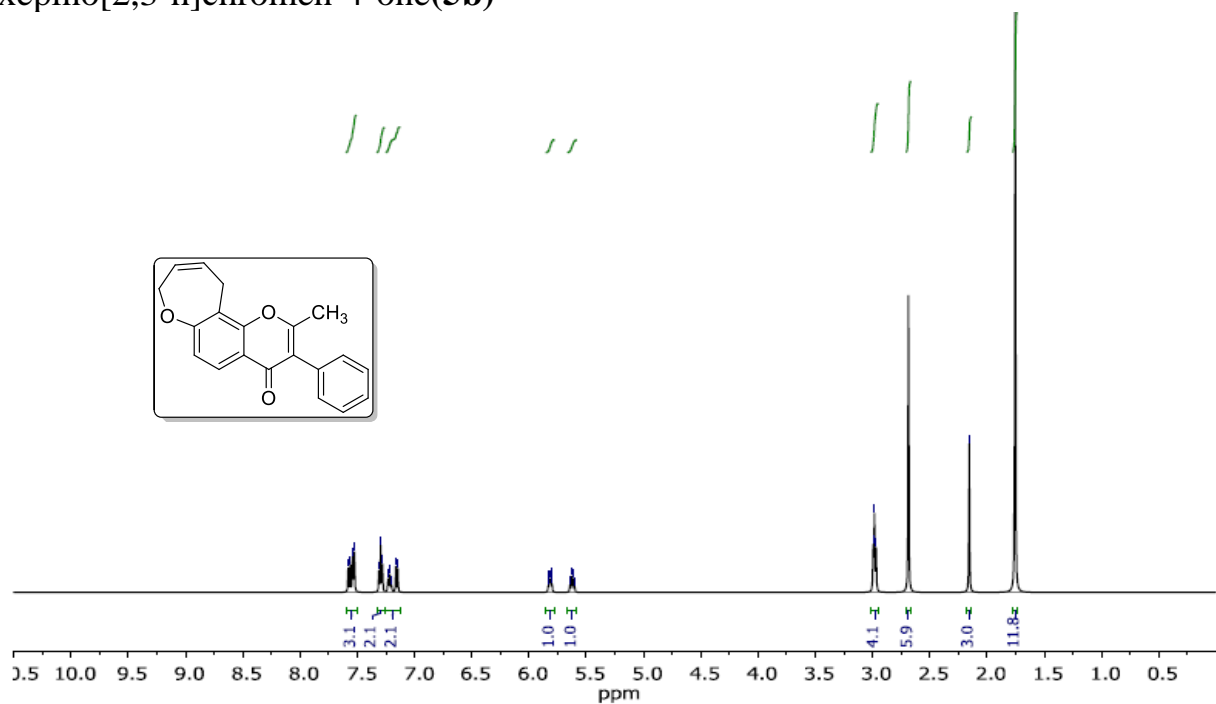


HRMS (ESI) (m/z), of (C<sub>19</sub>H<sub>14</sub>O<sub>3</sub>)

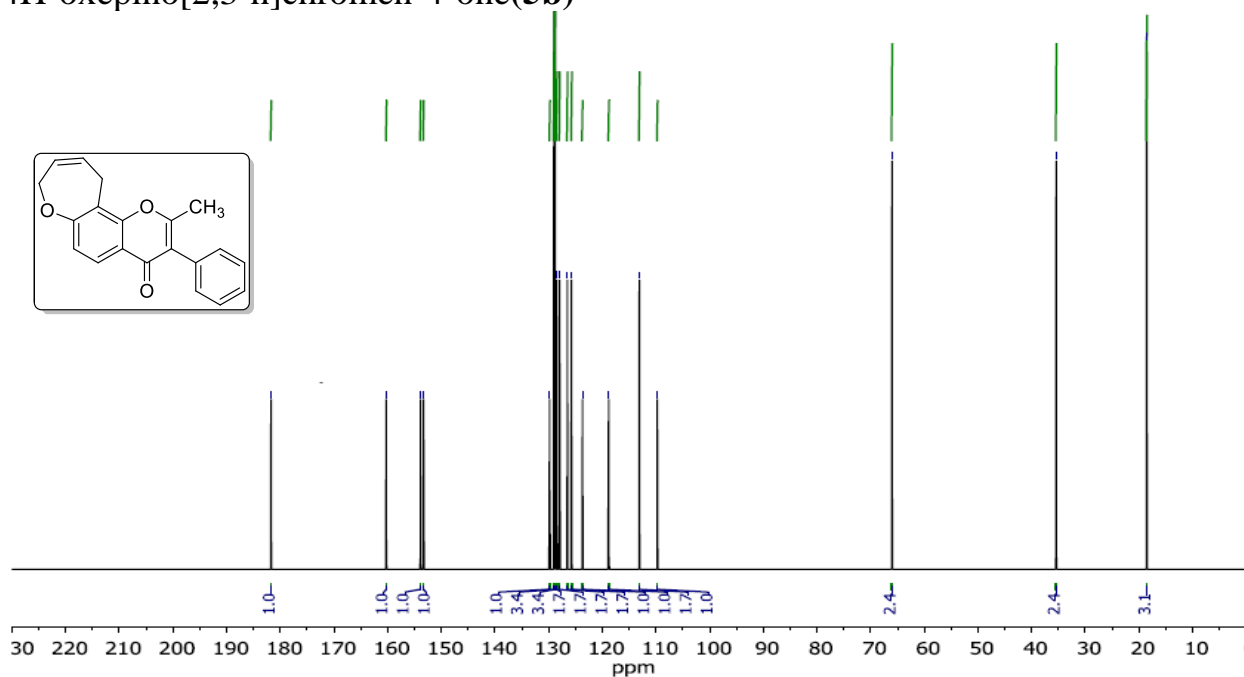
Calcd: 291.1015 [M+H]<sup>+</sup>

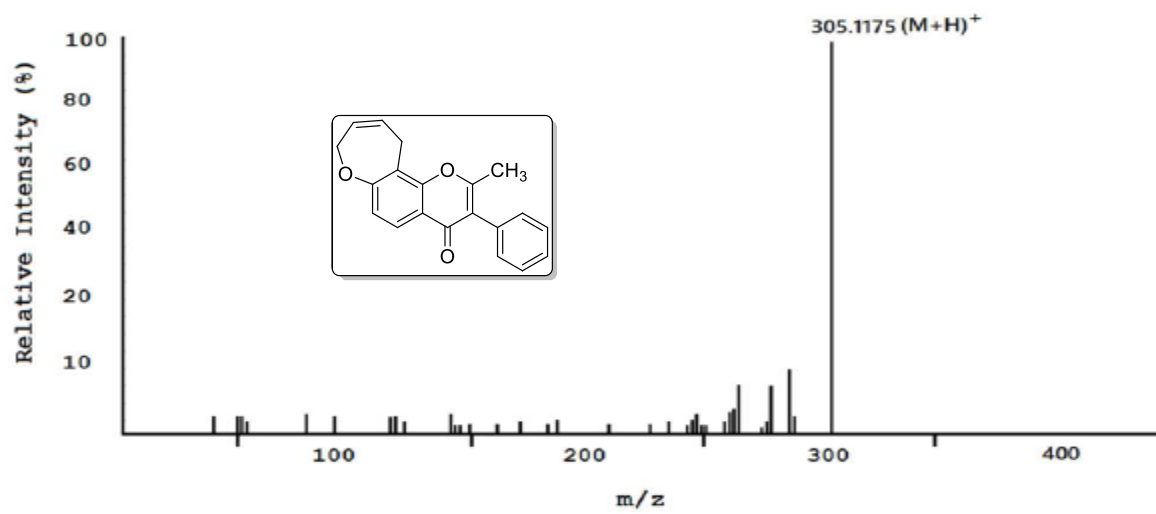
Found: 291.1021 [M+H]<sup>+</sup>

$^1\text{H-NMR}$  Spectrum (DMSO- $d_6$ , 400 MHz) of 2-methyl-3-phenyl-8,11-dihydro-4H-oxepino[2,3-h]chromen-4-one(**5b**)



$^{13}\text{C-NMR}$  Spectrum (DMSO- $d_6$ , 101 MHz) of 2-methyl-3-phenyl-8,11-dihydro-4H-oxepino[2,3-h]chromen-4-one(**5b**)



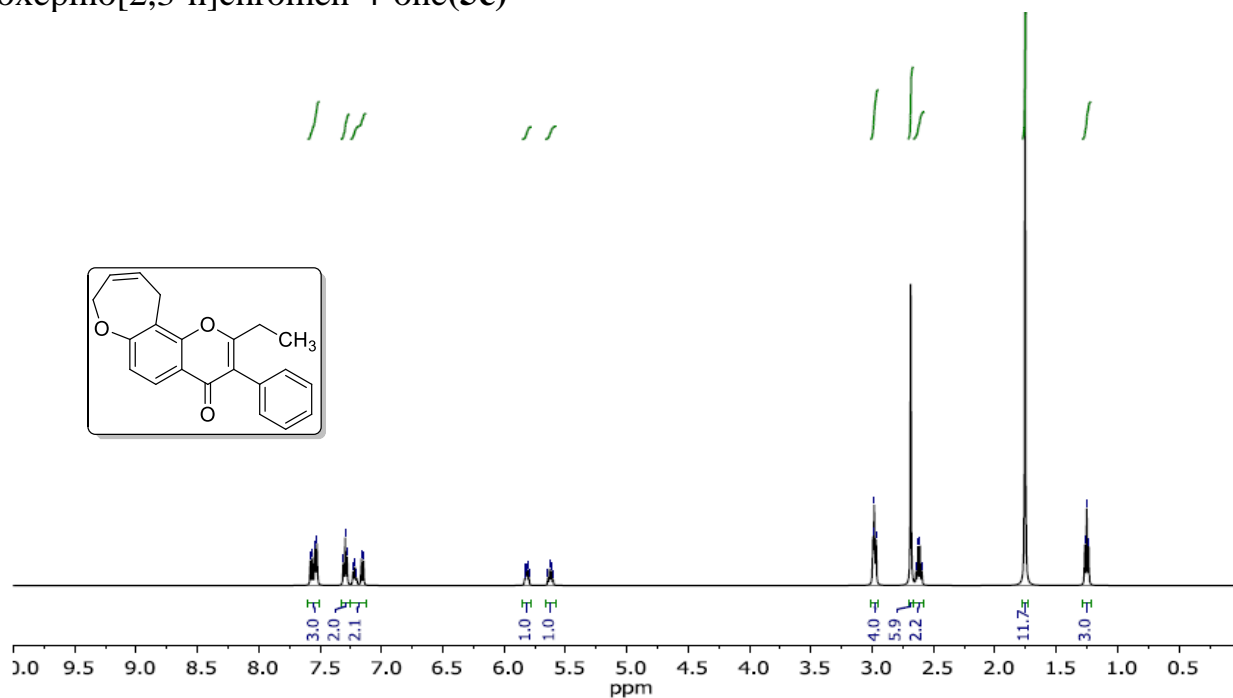
HRMS Spectrum of 2-methyl-3-phenyl-8,11-dihydro-4H-oxepino[2,3-h]chromen-4-one (**5b**)

HRMS (ESI) (m/z), of (C<sub>20</sub>H<sub>16</sub>O<sub>3</sub>)

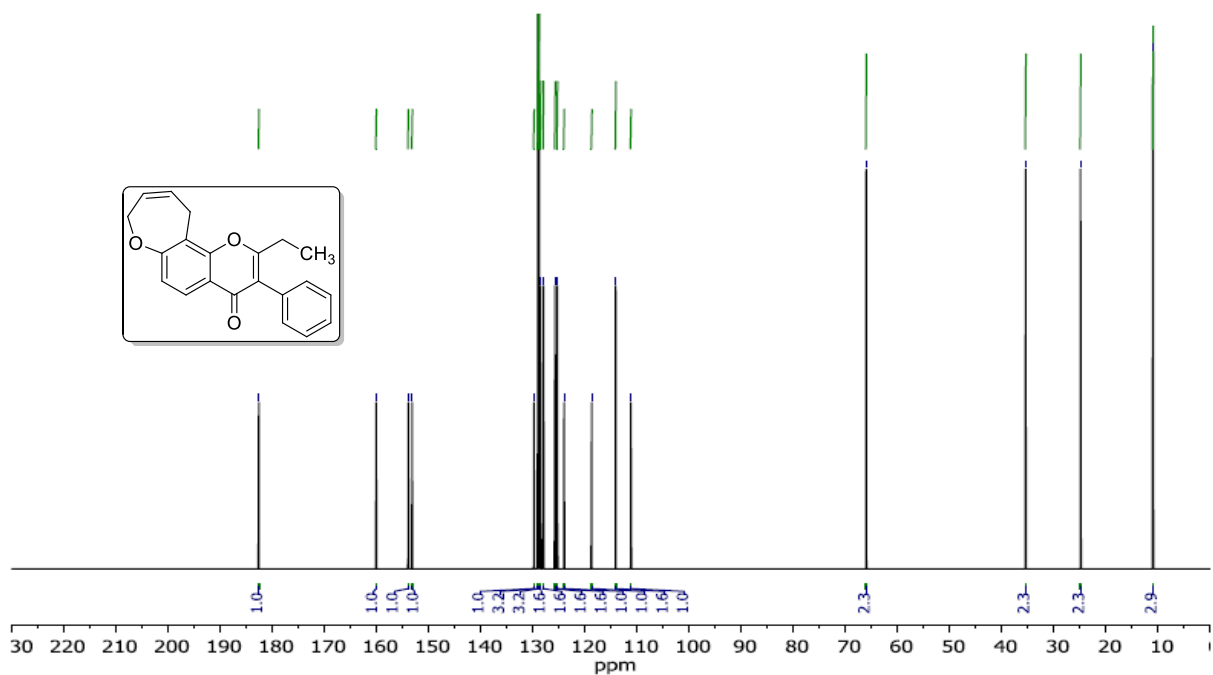
Calcd: 305.1172 [M+H]<sup>+</sup>

Found: 305.1175 [M+H]<sup>+</sup>

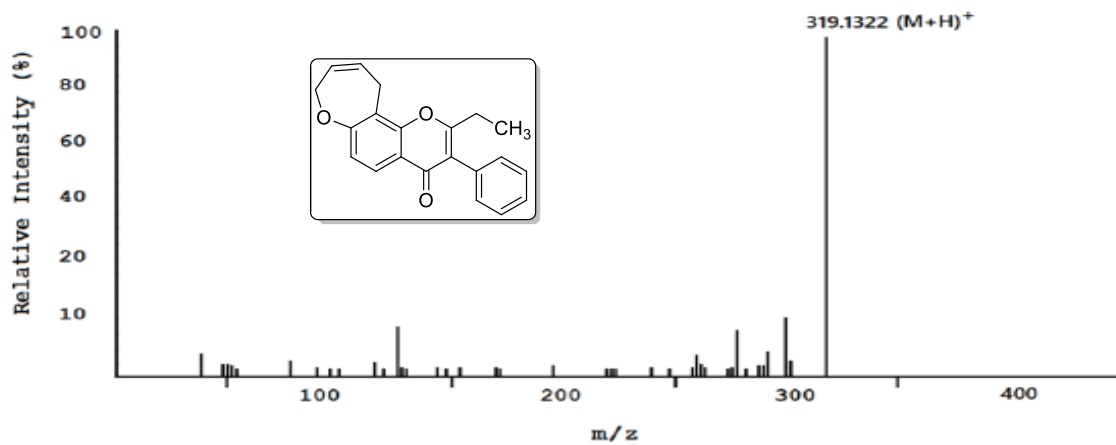
$^1\text{H-NMR}$  Spectrum (DMSO- $d_6$ , 400 MHz) of 2-ethyl-3-phenyl-8,11-dihydro-4H-oxepino[2,3-h]chromen-4-one(**5c**)



$^{13}\text{C-NMR}$  Spectrum (DMSO- $d_6$ , 101 MHz) of 2-ethyl-3-phenyl-8,11-dihydro-4H-oxepino[2,3-h]chromen-4-one(**5c**)



**ig.19** : HRMS Spectrum of 2-ethyl-3-phenyl-8,11-dihydro-4H-oxepino[2,3-h]chromen-4-one (**5c**)

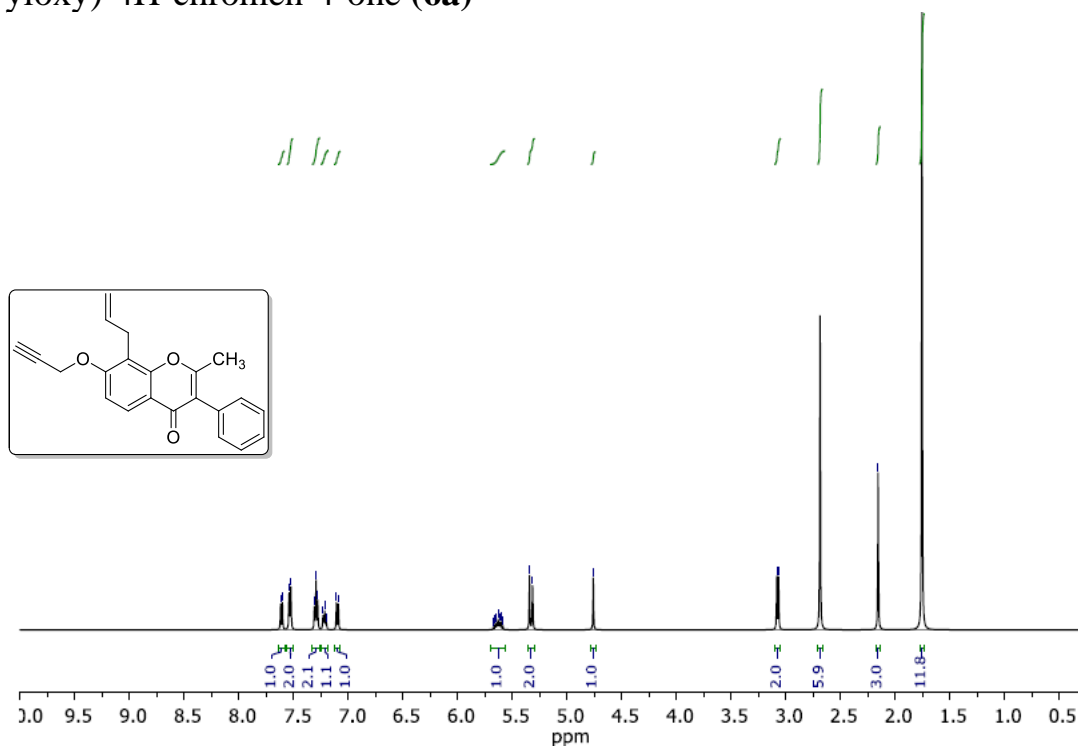


HRMS (ESI) (m/z), of (C<sub>21</sub>H<sub>18</sub>O<sub>3</sub>)

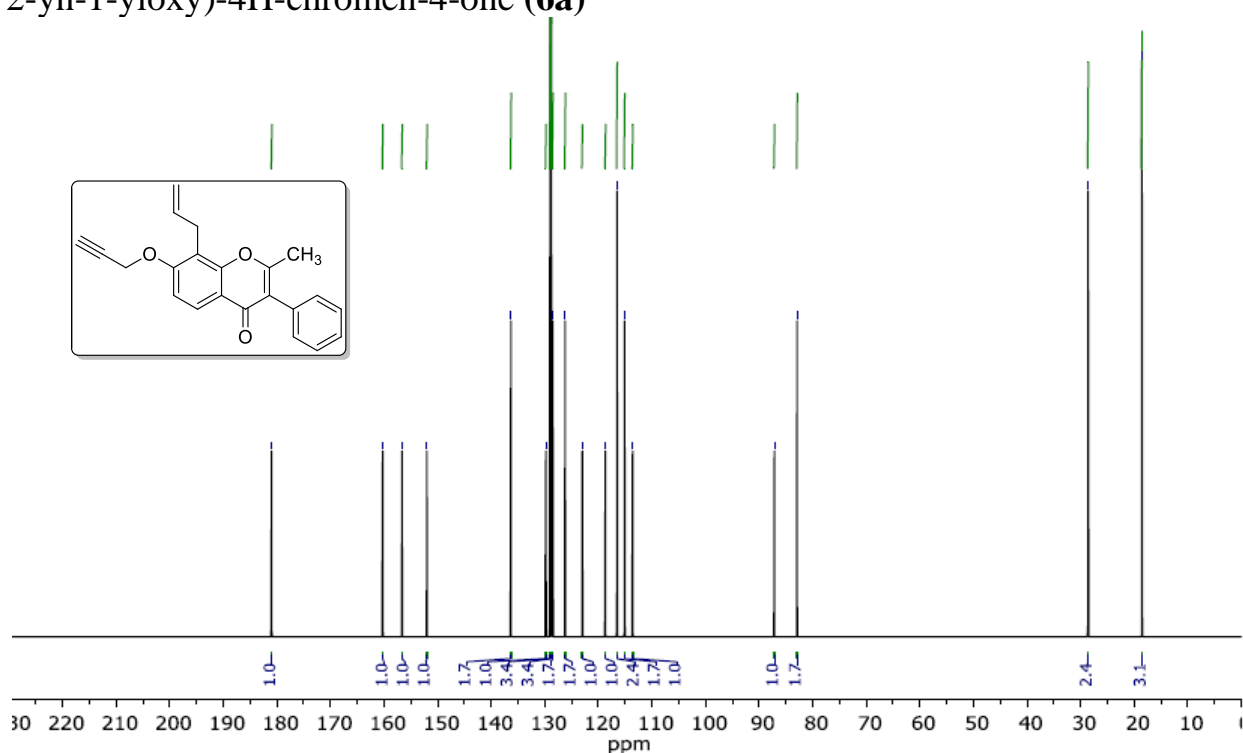
Calcd: 319.1328 [M+H]<sup>+</sup>

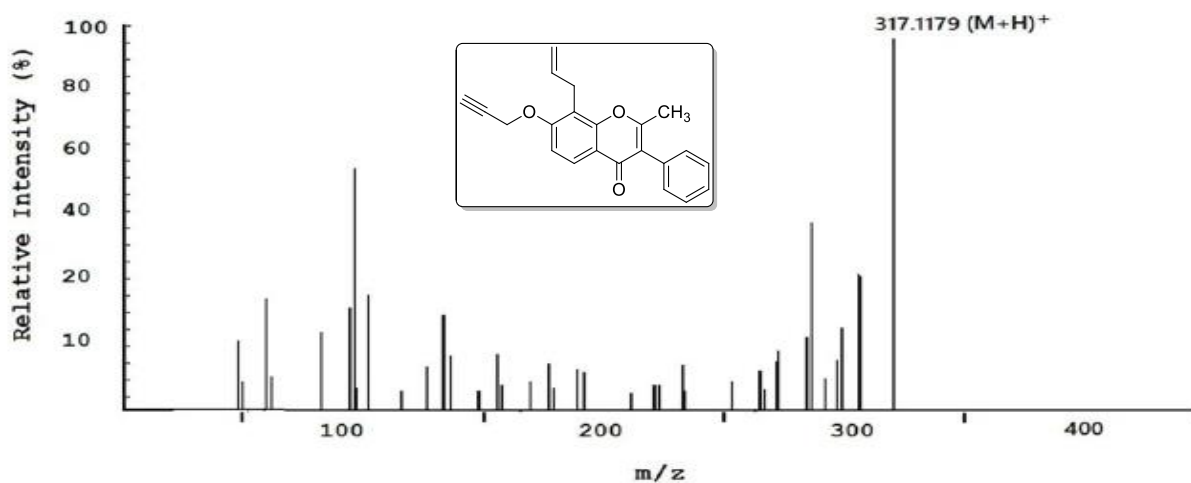
Found: 319.1322 [M+H]<sup>+</sup>

$^1\text{H-NMR}$  Spectrum (DMSO- $d_6$ , 400 MHz) of 8-allyl-2-methyl-3-phenyl-7-(prop-2-yn-1-yloxy)-4H-chromen-4-one (**6a**)



$^{13}\text{C-NMR}$  Spectrum (DMSO- $d_6$ , 101 MHz) of 8-allyl-2-methyl-3-phenyl-7-(prop-2-yn-1-yloxy)-4H-chromen-4-one (**6a**)



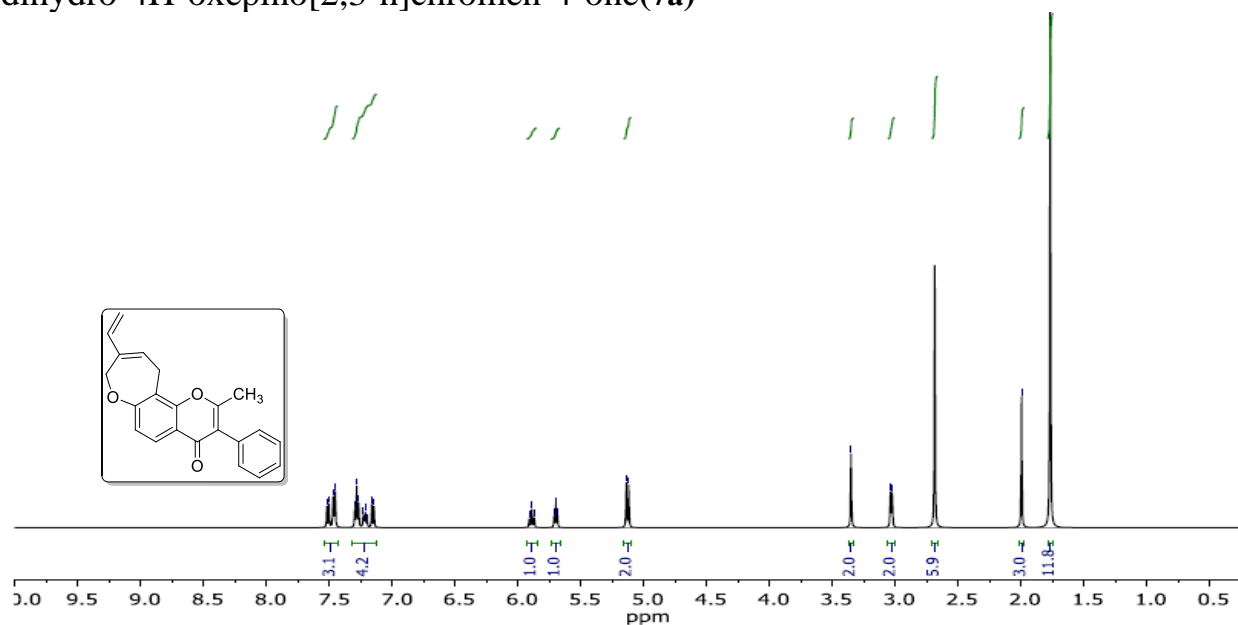
HRMS Spectrum of 8-allyl-2-methyl-3-phenyl-7-(prop-2-yn-1-yloxy)-4H-chromen-4-one (**6a**)

HRMS (ESI) ( $m/z$ ) of ( $C_{21}H_{16}O_3$ )

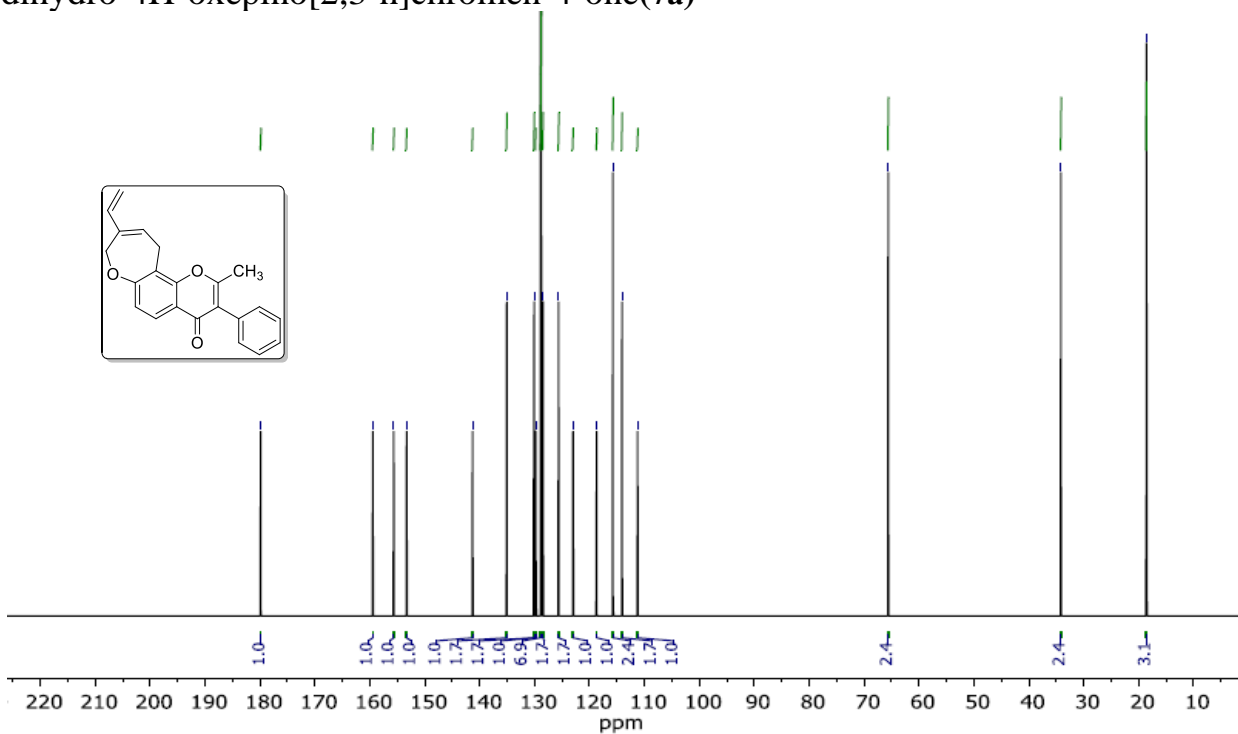
Calcd: 317.1172  $[M+H]^+$

Found: 317.1179  $[M+H]^+$

<sup>1</sup>H-NMR Spectrum (DMSO-*d*<sub>6</sub>, 400 MHz) of 2-methyl-3-phenyl-9-vinyl-8,11-dihydro-4H-oxepino[2,3-h]chromen-4-one (**7a**)

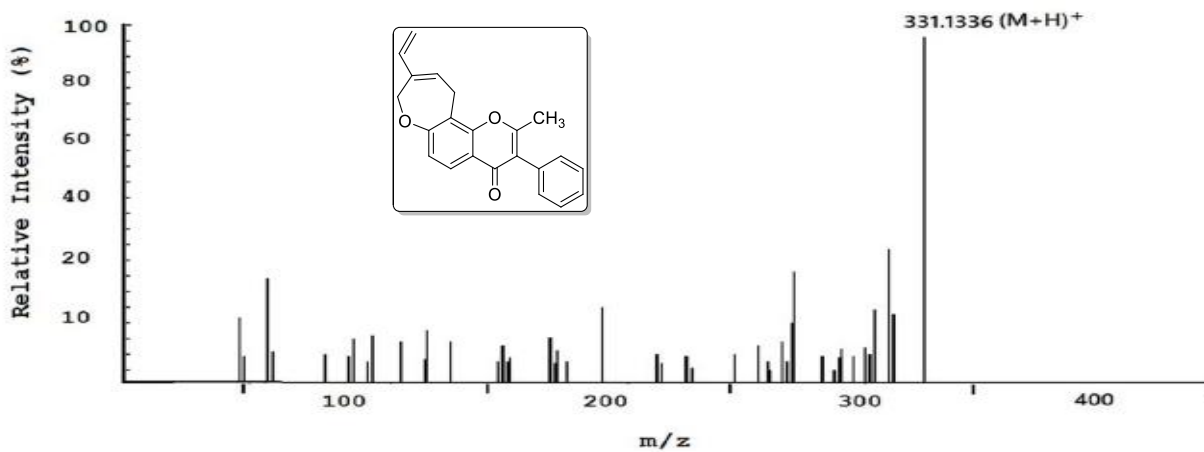


<sup>13</sup>C-NMR Spectrum (DMSO-*d*<sub>6</sub>, 101 MHz) of 2-methyl-3-phenyl-9-vinyl-8,11-dihydro-4H-oxepino[2,3-h]chromen-4-one (**7a**)



HRMS Spectrum of 2-methyl-3-phenyl-9-vinyl-8,11-dihydro-4H-oxepino[2,3-h]chromen-4-one (**7a**)



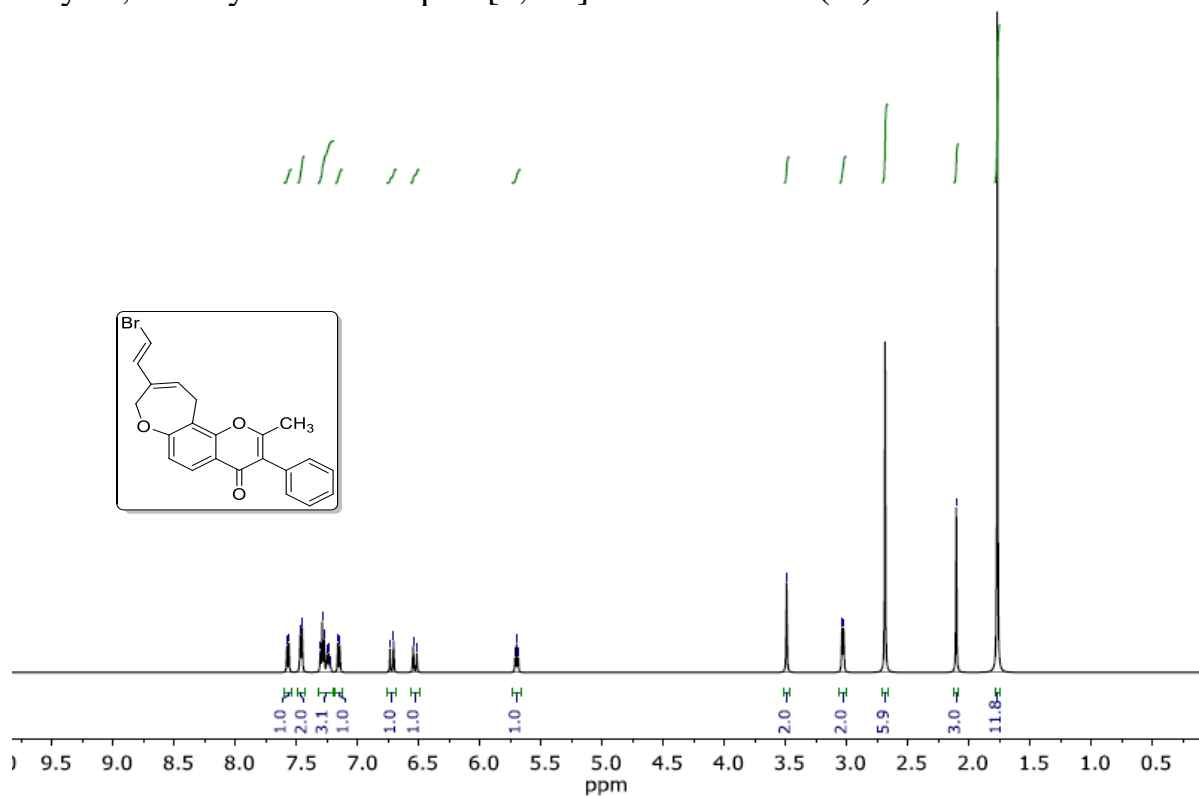


HRMS (ESI) (m/z) of (C<sub>22</sub>H<sub>18</sub>O<sub>3</sub>)

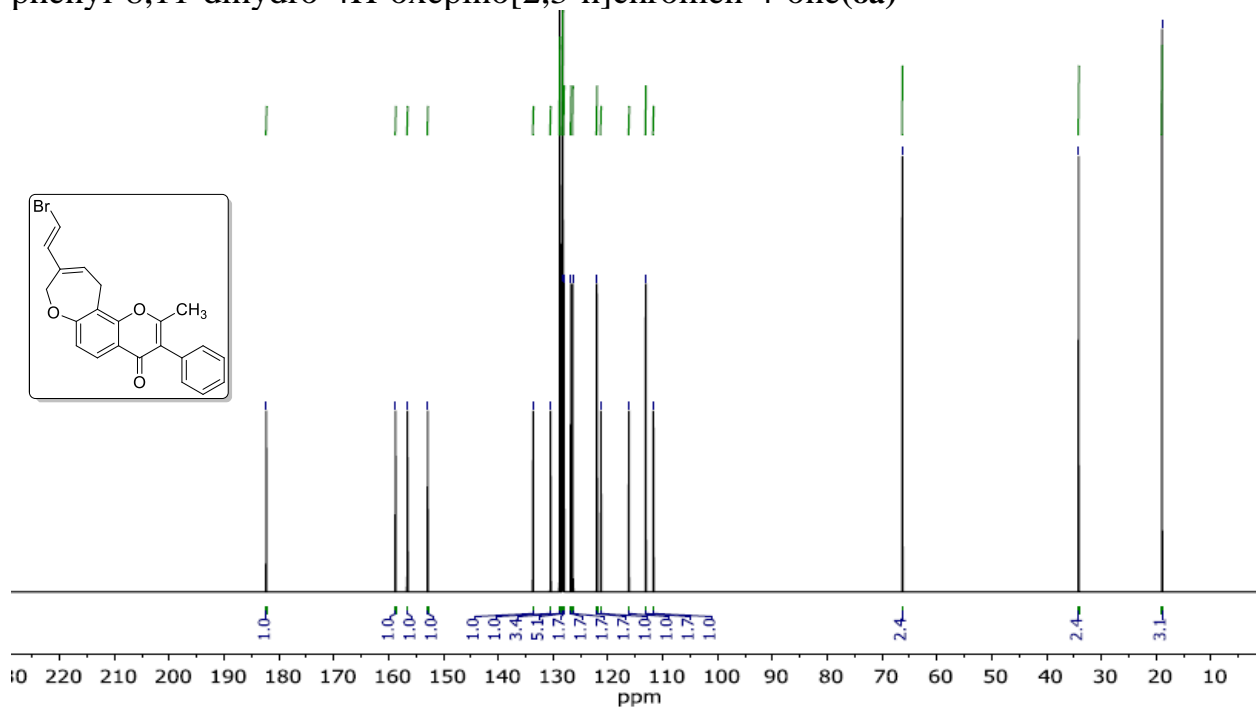
Calcd: 331.1328 [M+H]<sup>+</sup>

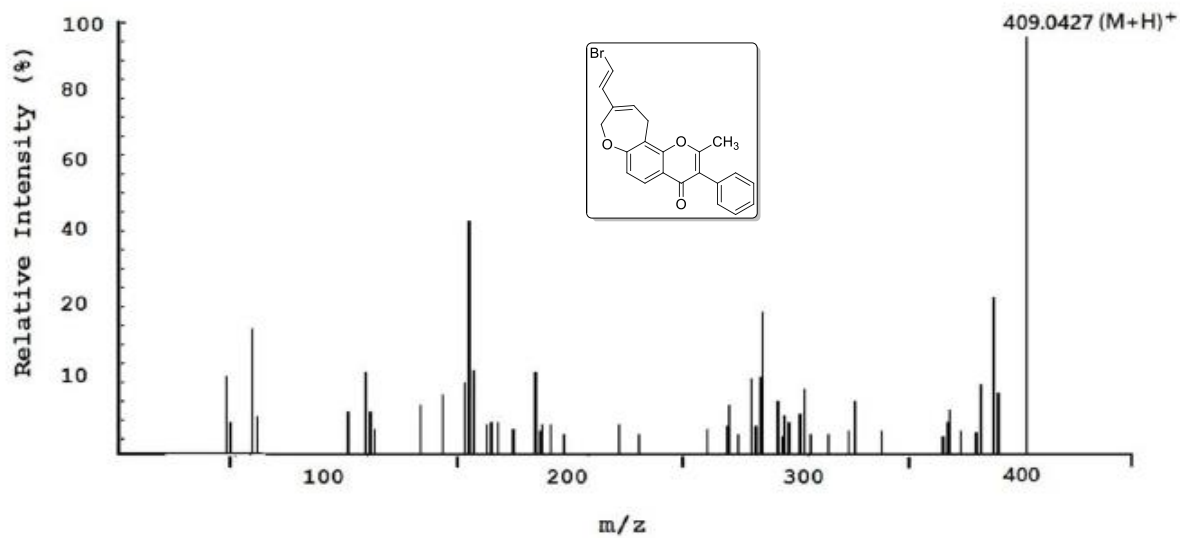
Found: 331.1336[M+H]<sup>+</sup>

H-NMR Spectrum (DMSO-*d*<sub>6</sub>, 400 MHz) of (E)-9-(2-bromovinyl)-2-methyl-3-phenyl-8,11-dihydro-4H-oxepino[2,3-h]chromen-4-one(**8a**)



<sup>13</sup>C-NMR Spectrum (DMSO-*d*<sub>6</sub>, 101 MHz) of (E)-9-(2-bromovinyl)-2-methyl-3-phenyl-8,11-dihydro-4H-oxepino[2,3-h]chromen-4-one(**8a**)



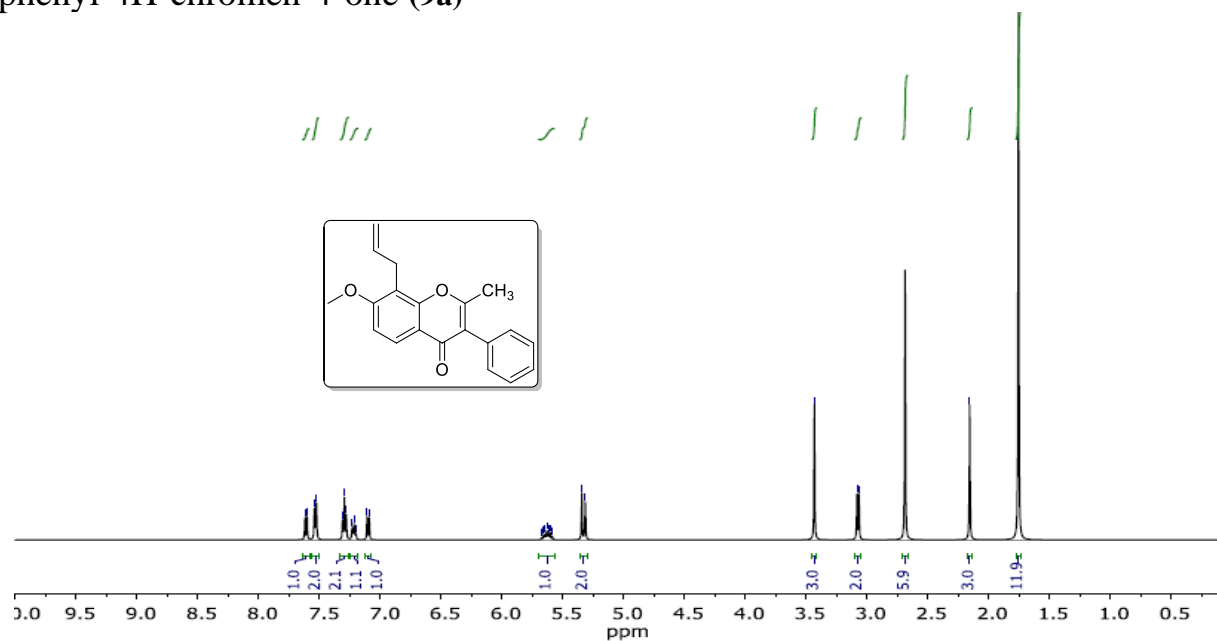
HRMS Spectrum of (E)-9-(2-bromovinyl)-2-methyl-3-phenyl-8,11-dihydro-4H-oxepino[2,3-h]chromen-4-one (**8a**)

HRMS (ESI) (m/z) of (C<sub>22</sub>H<sub>17</sub>BrO<sub>3</sub>)

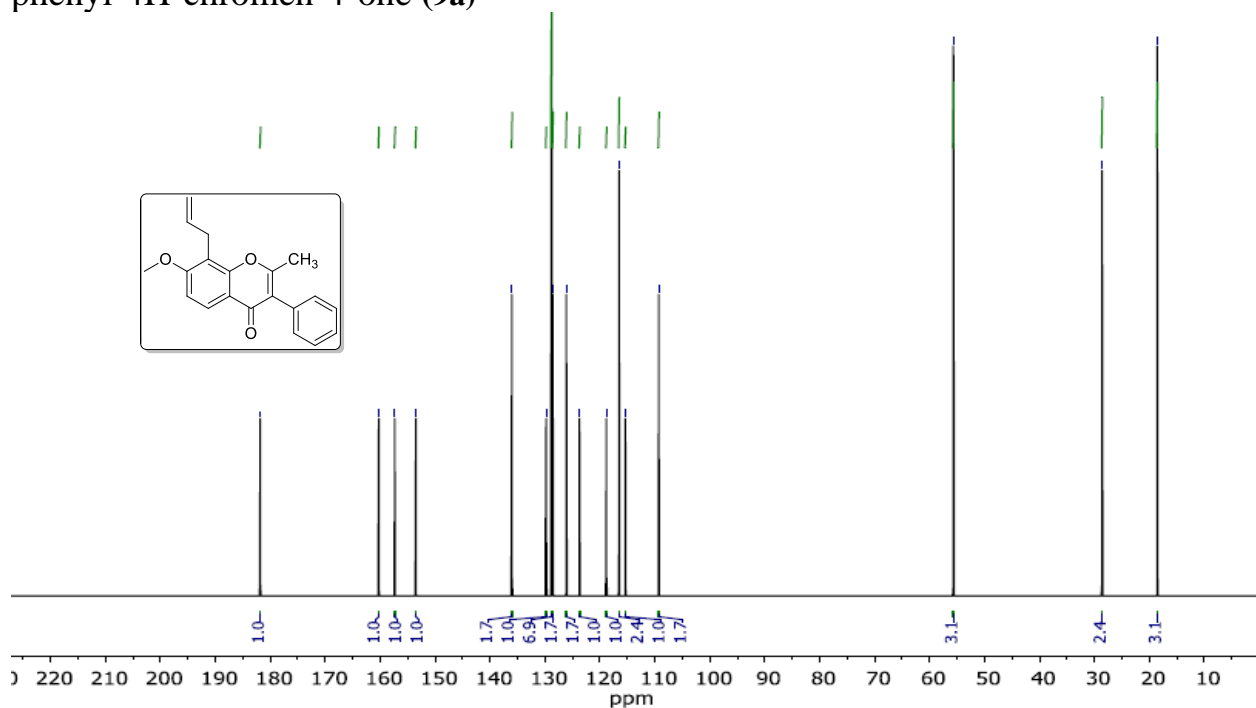
Calcd: 409.0433 [M+H]<sup>+</sup>

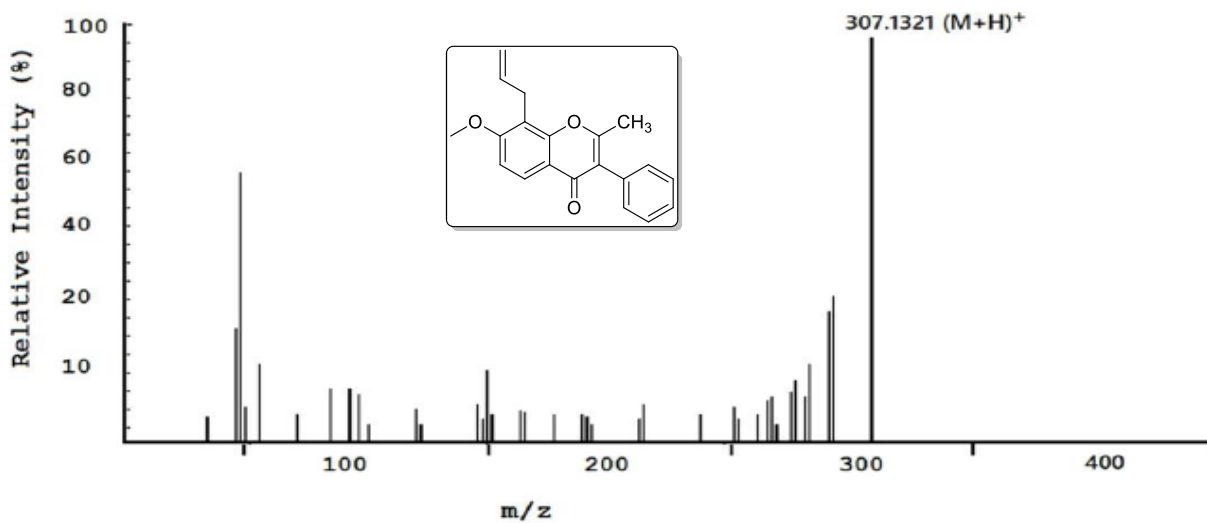
Found: 409.0427 [M+H]<sup>+</sup>

<sup>1</sup>H-NMR Spectrum (DMSO-*d*<sub>6</sub>, 400 MHz) of 8-allyl-7-methoxy-2-methyl-3-phenyl-4H-chromen-4-one (**9a**)



<sup>13</sup>C-NMR Spectrum (DMSO-*d*<sub>6</sub>, 101 MHz) of 8-allyl-7-methoxy-2-methyl-3-phenyl-4H-chromen-4-one (**9a**)



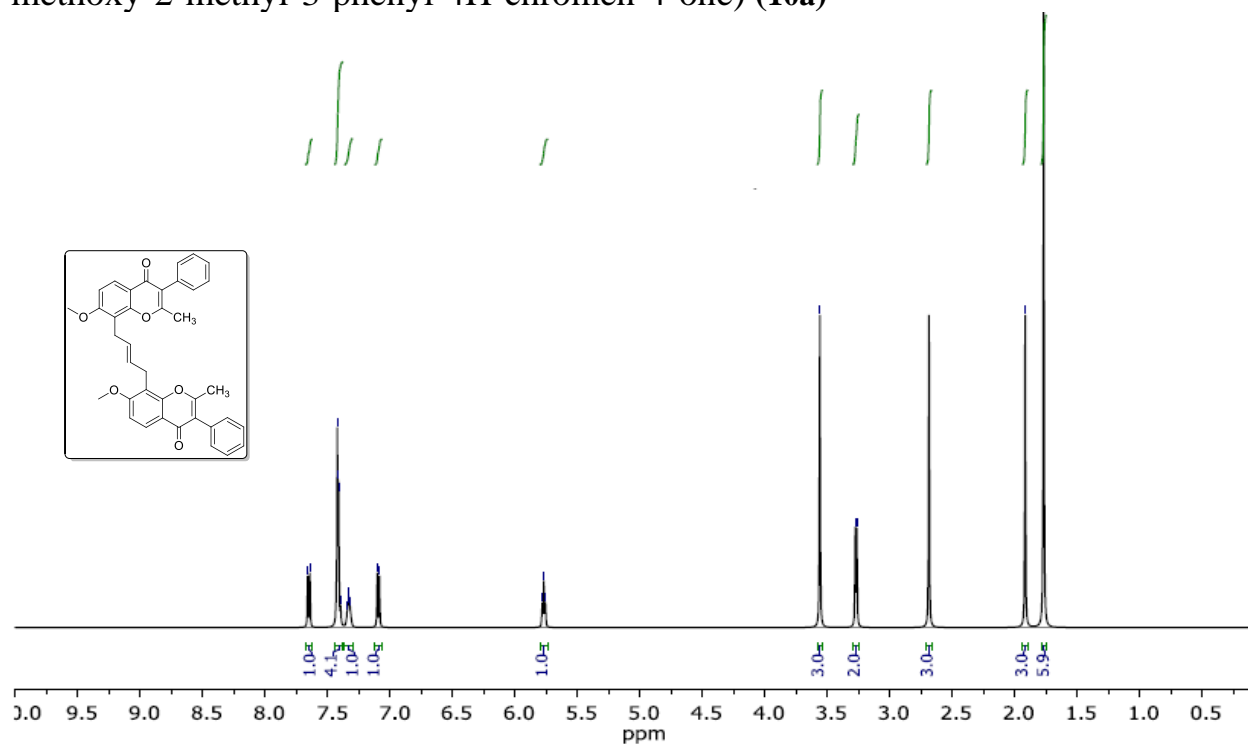
HRMS Spectrum of 8-allyl-7-methoxy-2-methyl-3-phenyl-4H-chromen-4-one (**9a**)

HRMS (ESI) (m/z) of (C<sub>20</sub>H<sub>18</sub>O<sub>3</sub>)

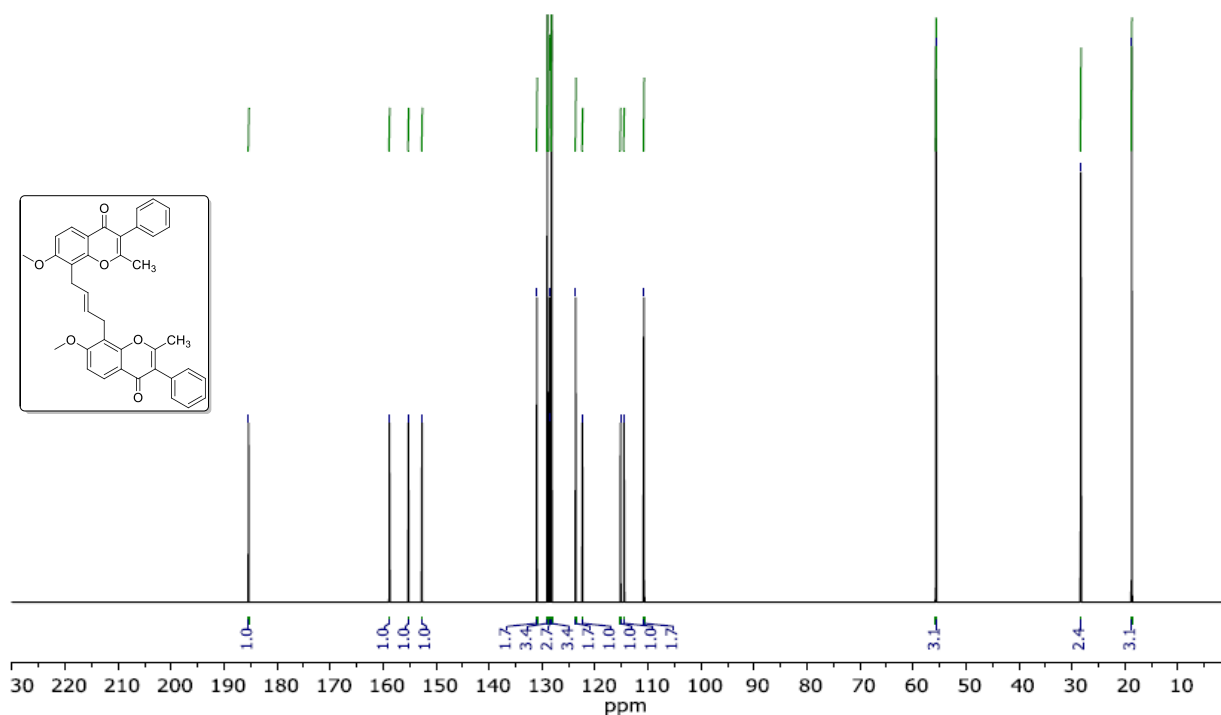
Calcd: 307.1328 [M+H]<sup>+</sup>

Found: 307.1321 [M+H]<sup>+</sup>

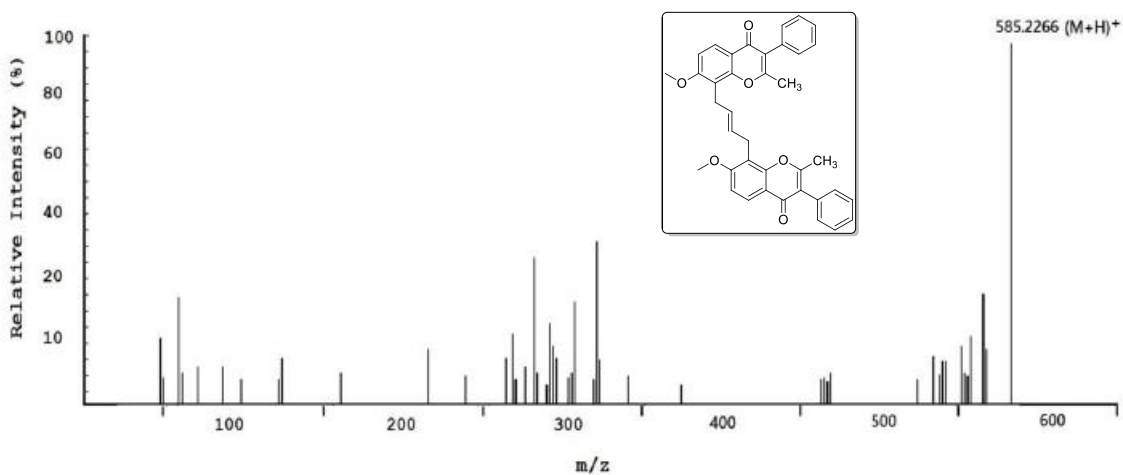
$^1\text{H-NMR}$  Spectrum (DMSO- $d_6$ , 400 MHz) of (E)-8,8'-(but-2-ene-1,4-diyl)bis(7-methoxy-2-methyl-3-phenyl-4H-chromen-4-one) (**10a**)



$^{13}\text{C-NMR}$  Spectrum (DMSO- $d_6$ , 101 MHz) of (E)-8,8'-(but-2-ene-1,4-diyl)bis(7-methoxy-2-methyl-3-phenyl-4H-chromen-4-one) (**10a**)



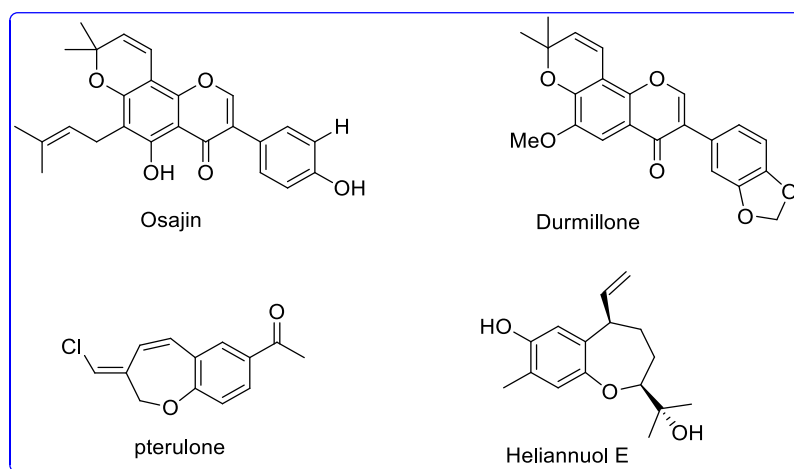
HRMS Spectrum of (E)-8,8'-(but-2-ene-1,4-diyl)bis(7-methoxy-2-methyl-3-phenyl-4H-chromen-4-one)(10a)



HRMS (ESI) (m/z) of (C<sub>38</sub>H<sub>32</sub>O<sub>6</sub>)

Calcd: 585.2271[M+H]<sup>+</sup>

Found: 585.2266 [M+H]<sup>+</sup>

**Figure 1.** Some Biologically active isoflavones andbenzoxepines.**Table 1.** IC<sub>50</sub> values of the tested compounds against human cancer HeLa cell line

S.No	Compound	IC <sub>50</sub> (μM)
1	<b>5a</b>	101.1±2.2
2	<b>5b</b>	111.7±1.0
3	<b>5c</b>	147.5±4.8
4	<b>7a</b>	94.1±1.4
5	<b>7b</b>	95.4±1.5
6	<b>8a</b>	64.5±0.1
7	<b>8b</b>	89.2±3.5
8	<b>10a</b>	80.1±0.5
9	<b>10b</b>	80.4±0.6
10	Cisplatin	7.8±0.1