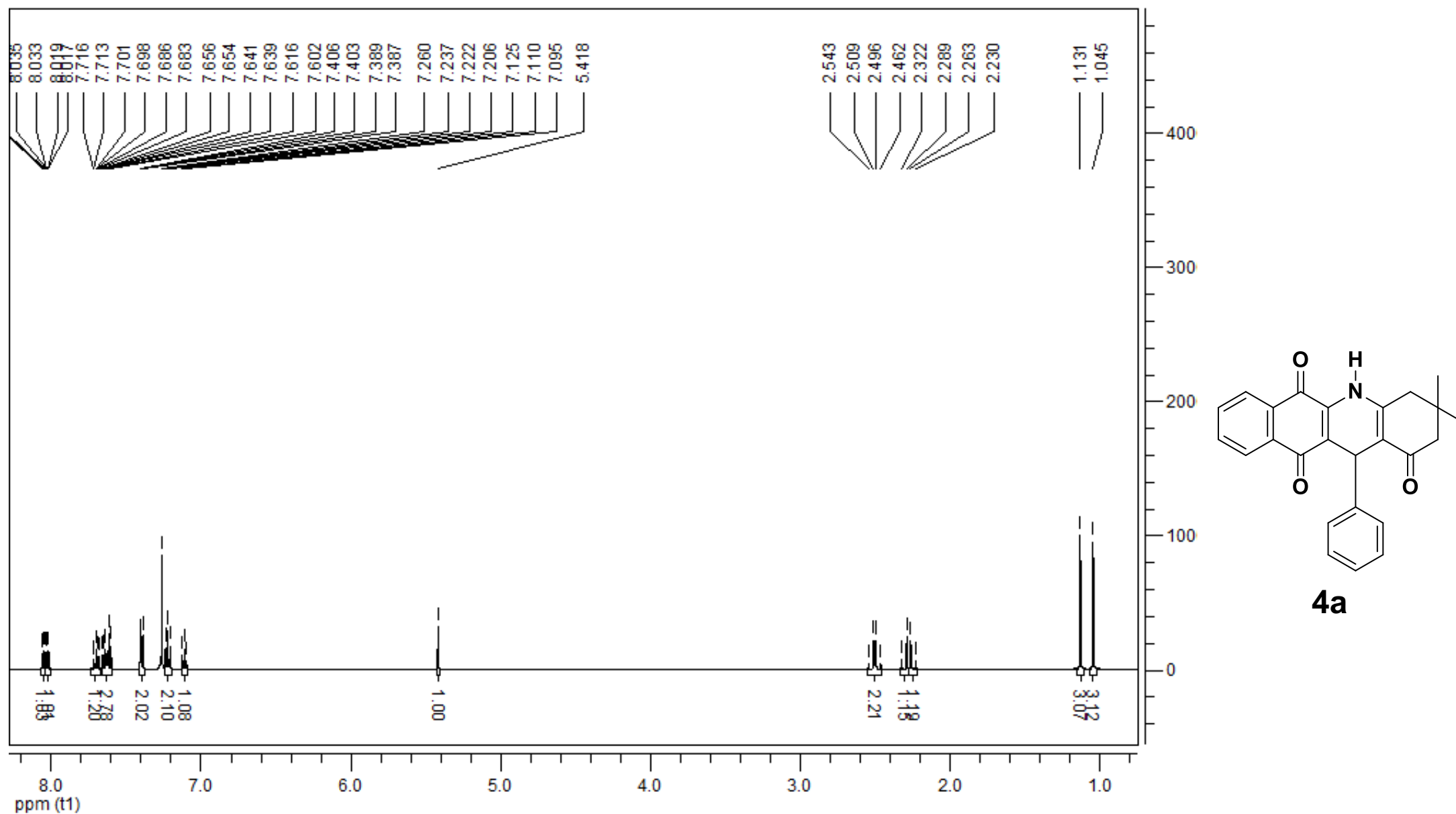
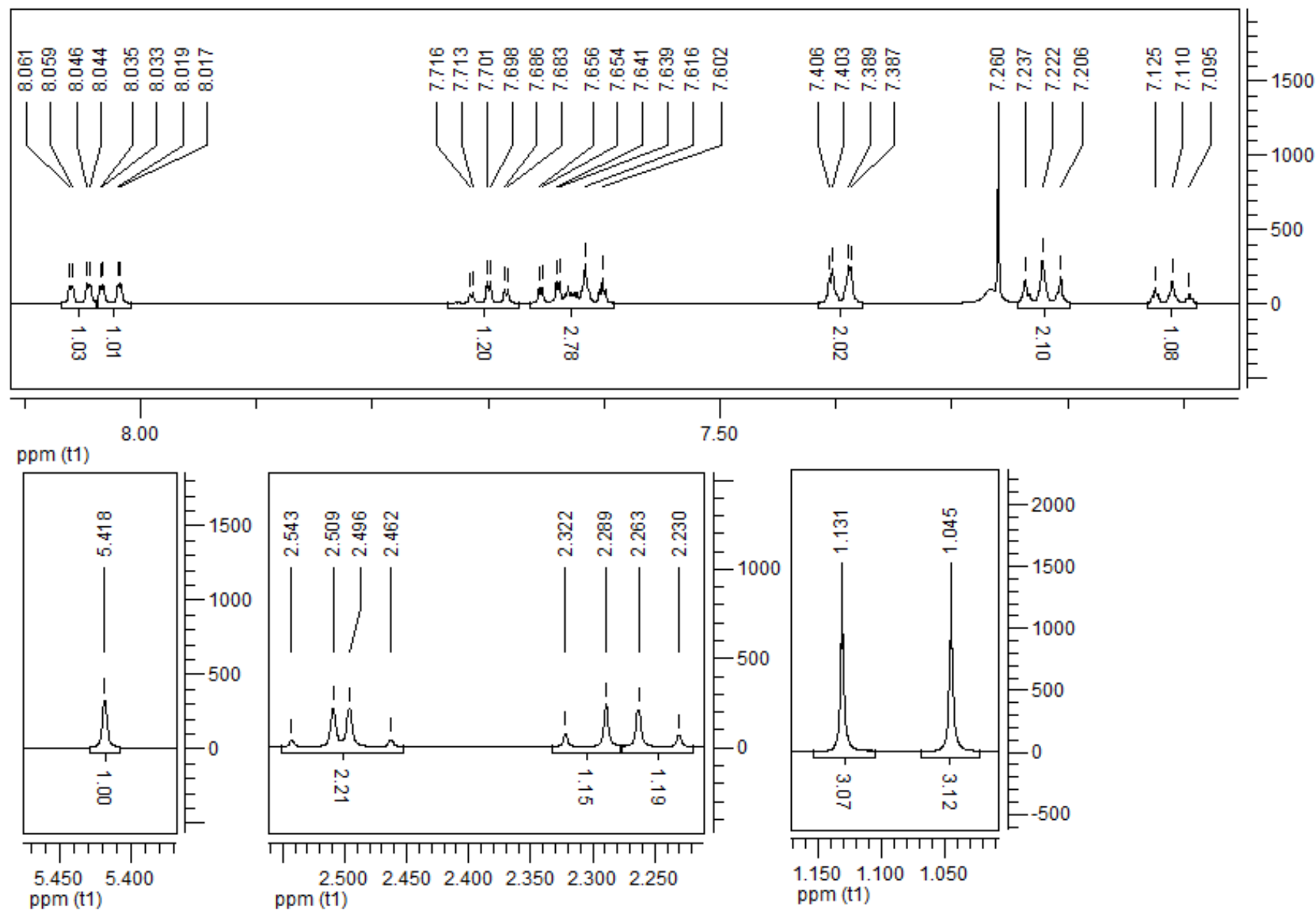


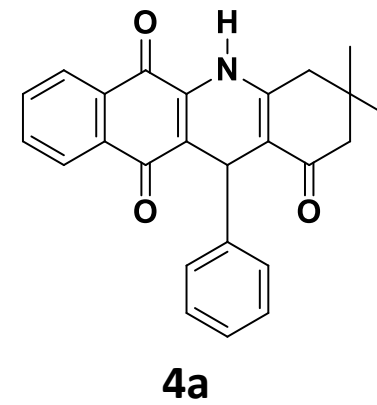
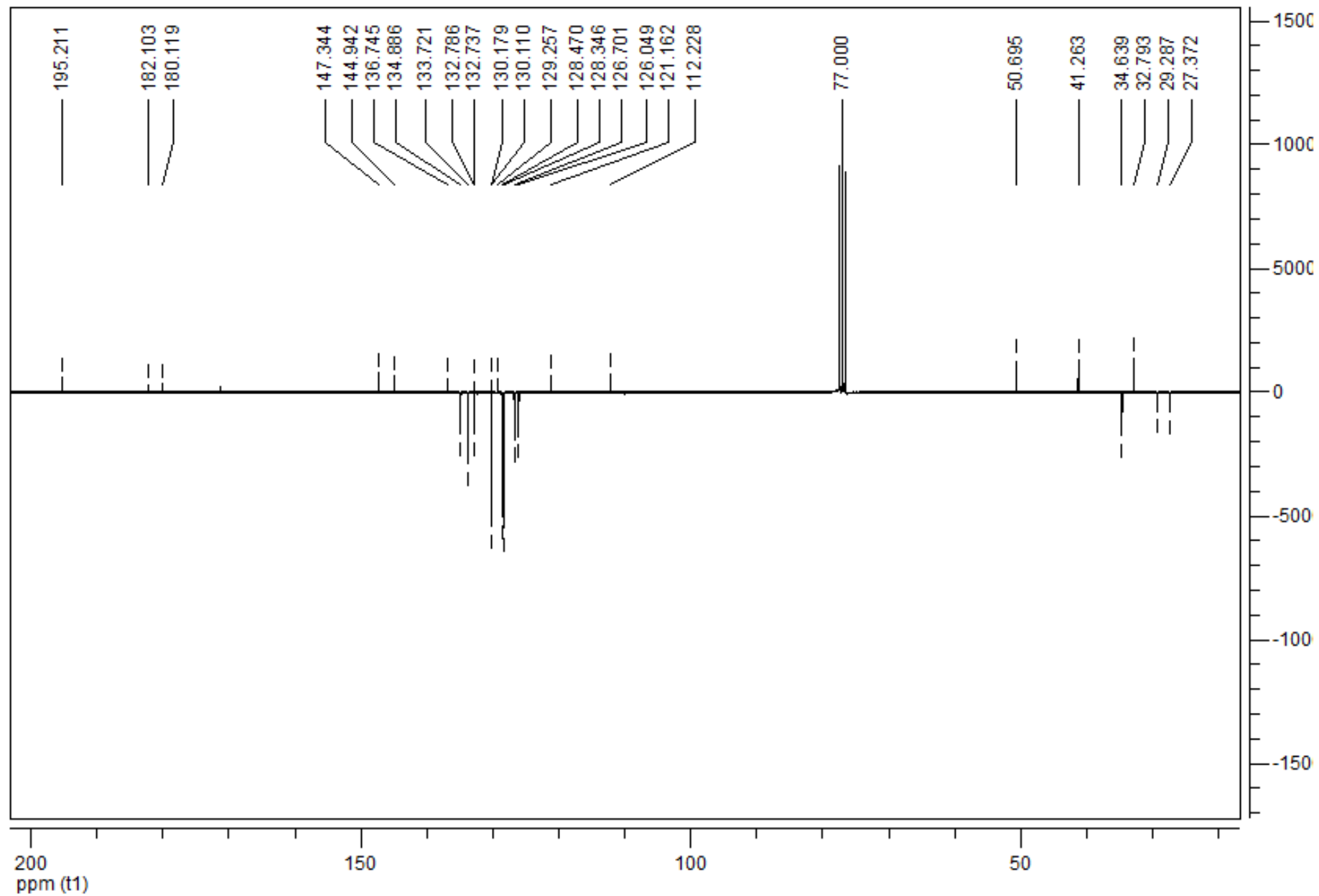
IR spectrum of compound **4a**



$^1\text{H}$  NMR spectrum of compound **4a** (500.00 MHz,  $\text{CDCl}_3$ )

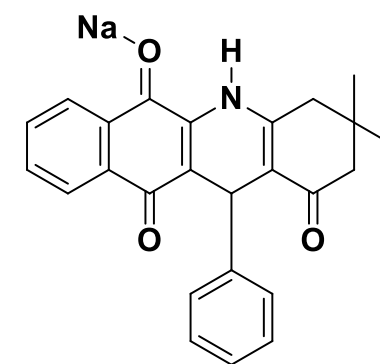
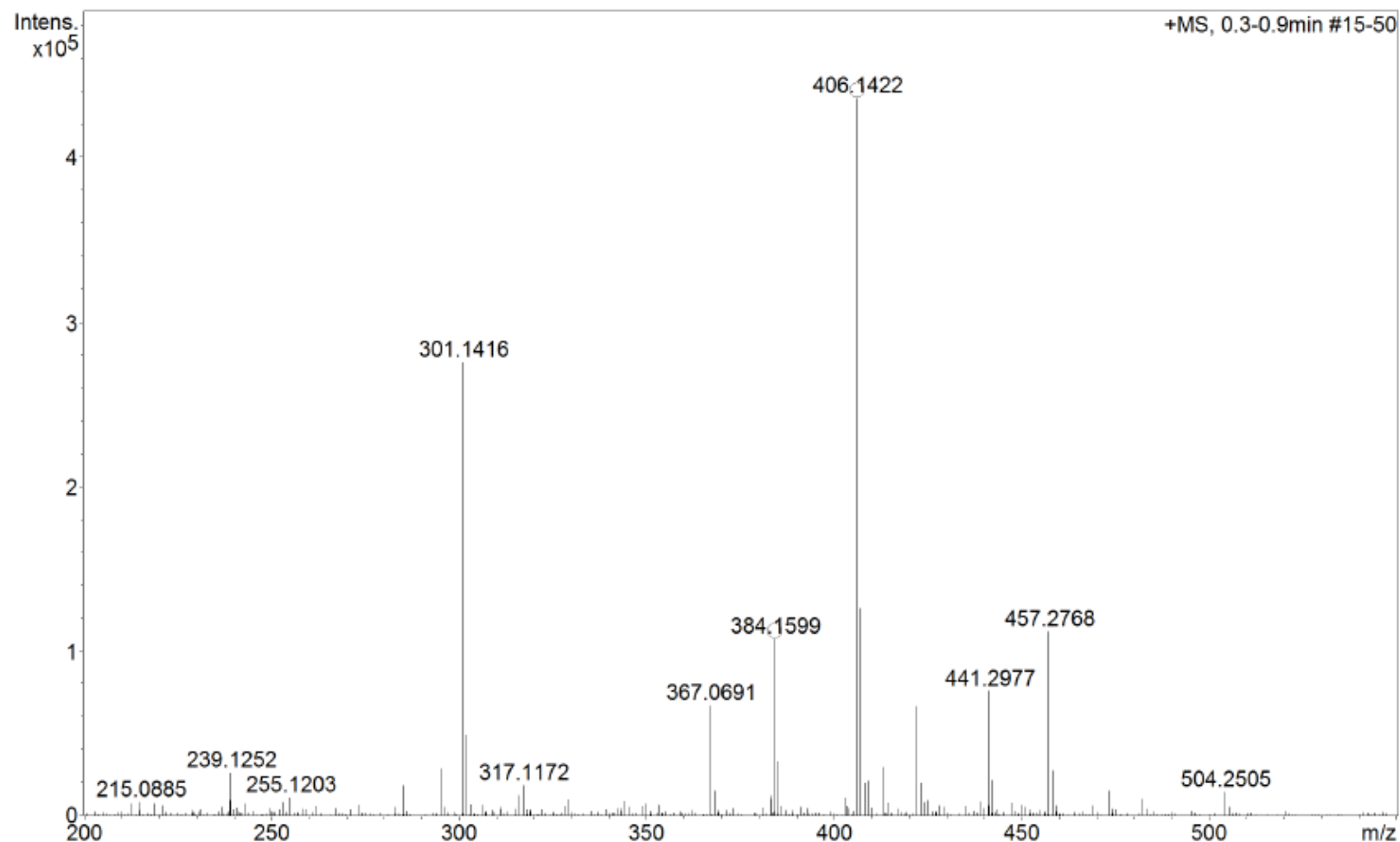


$^1\text{H}$  NMR spectrum of compound **4a** (500.00 MHz,  $\text{CDCl}_3$ )



<sup>13</sup>C NMR spectrum of compound **4a** (75.0 MHz, CDCl<sub>3</sub>)

+MS, 0.3-0.9min #15-50

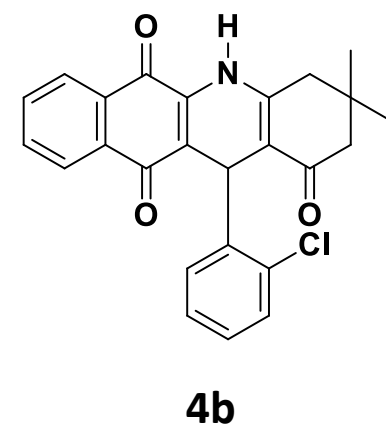
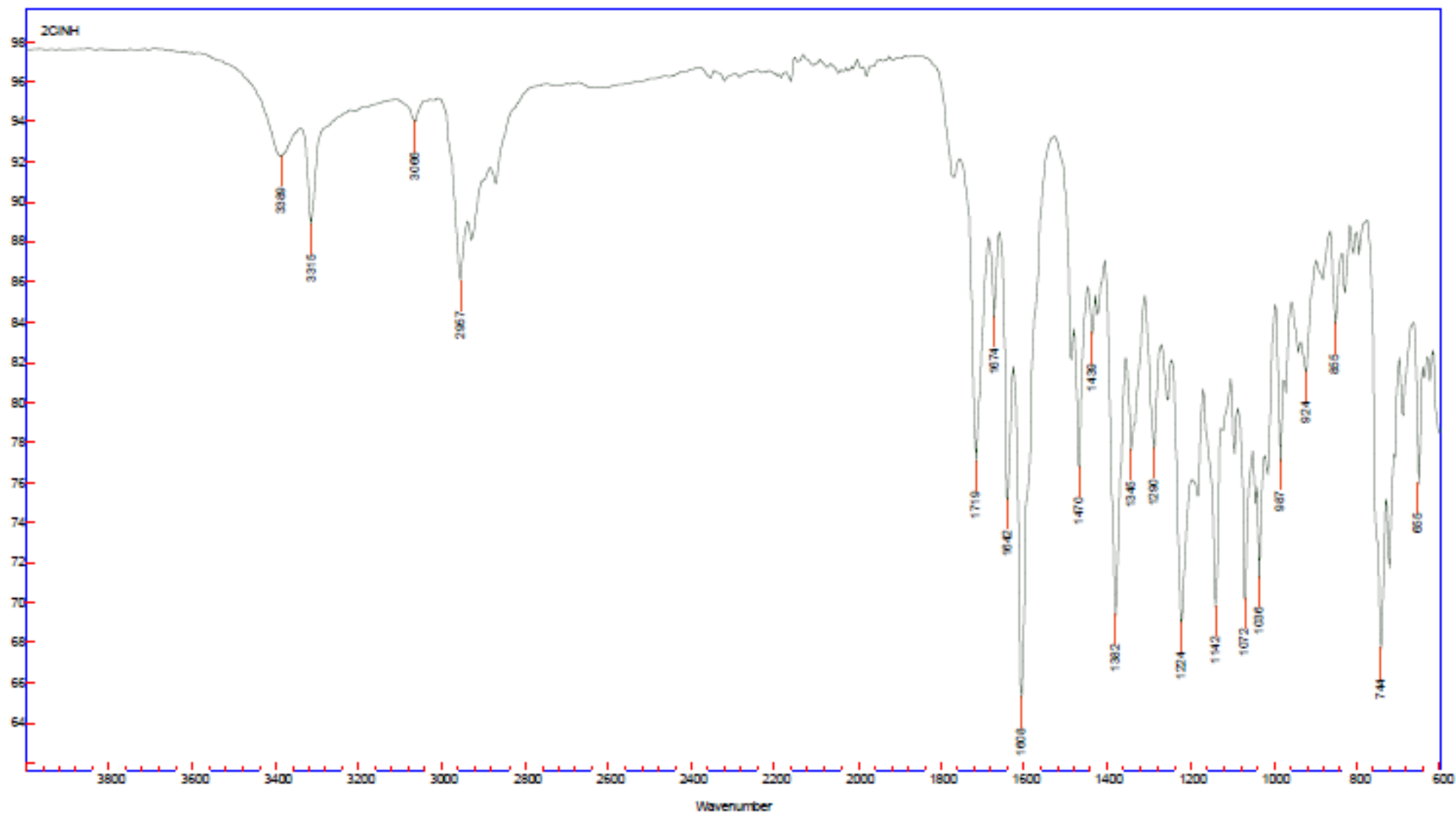


Exact Mass: 406,1419

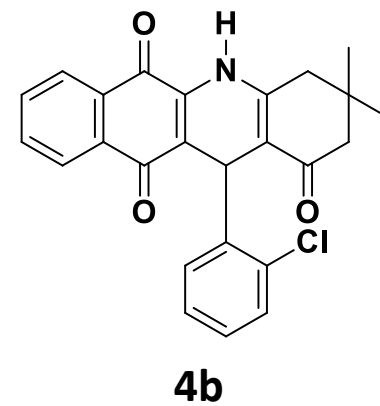
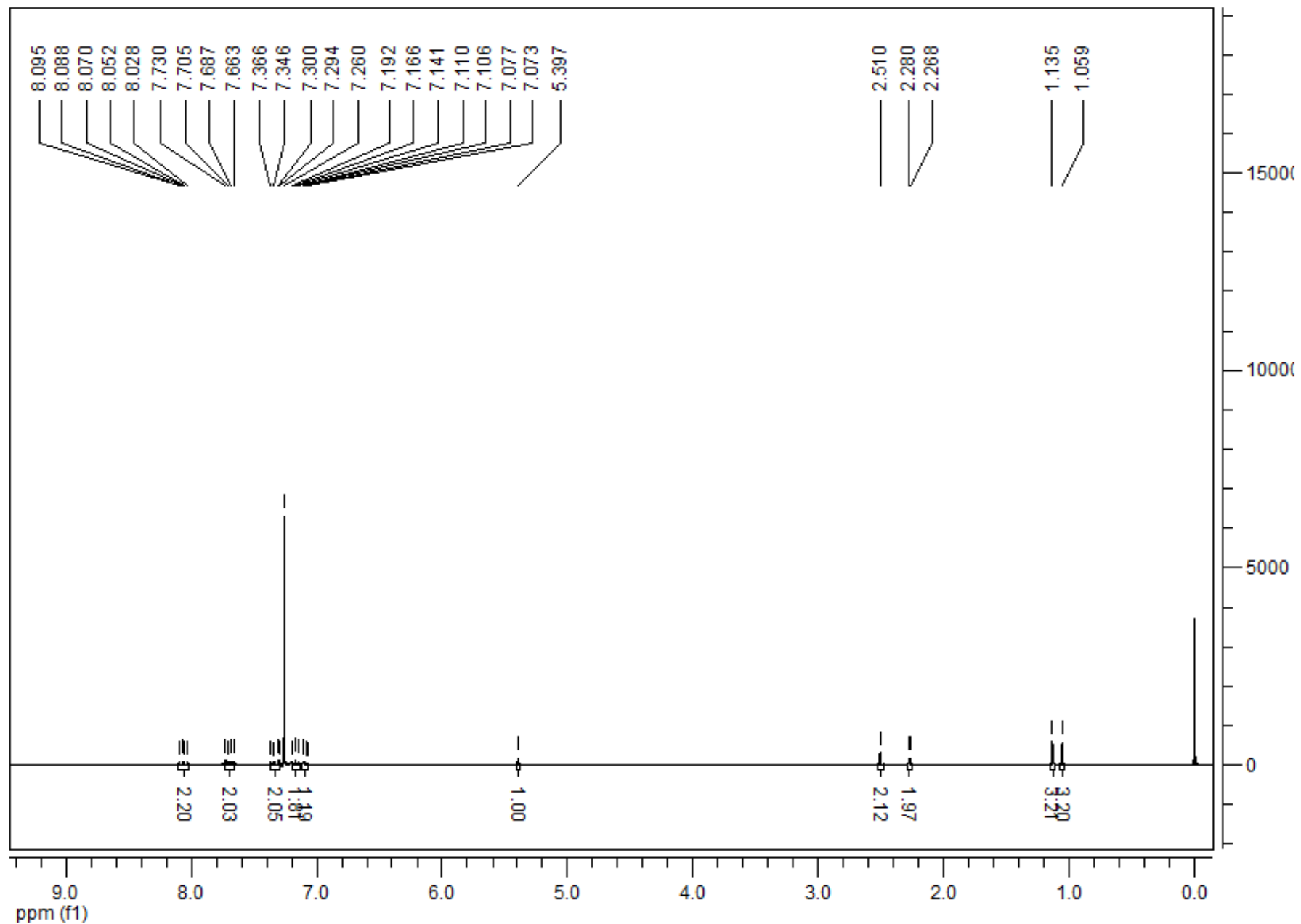
**4a**

Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std	m/z	Diff	Std	Comb	Dev
384.159934	1	C <sub>25</sub> H <sub>22</sub> NO <sub>3</sub>	384.159420	-1.3	0.9	15.5	ok	even		16.7	25.8		n.a.		n.a.		n.a.			n.a.	
	2	C <sub>21</sub> H <sub>18</sub> N <sub>7</sub> O	384.156735	-8.3	-6.9	16.5	ok	even		30.9	49.5		n.a.		n.a.		n.a.			n.a.	
406.142155	1	C <sub>25</sub> H <sub>21</sub> NNaO <sub>3</sub>	406.141364	-1.9	-1.0	15.5	ok	even		7.4	11.1		n.a.		n.a.		n.a.			n.a.	
	2	C <sub>21</sub> H <sub>17</sub> N <sub>7</sub> NaO	406.138679	-8.6	-8.4	16.5	ok	even		21.5	34.6		n.a.		n.a.		n.a.			n.a.	

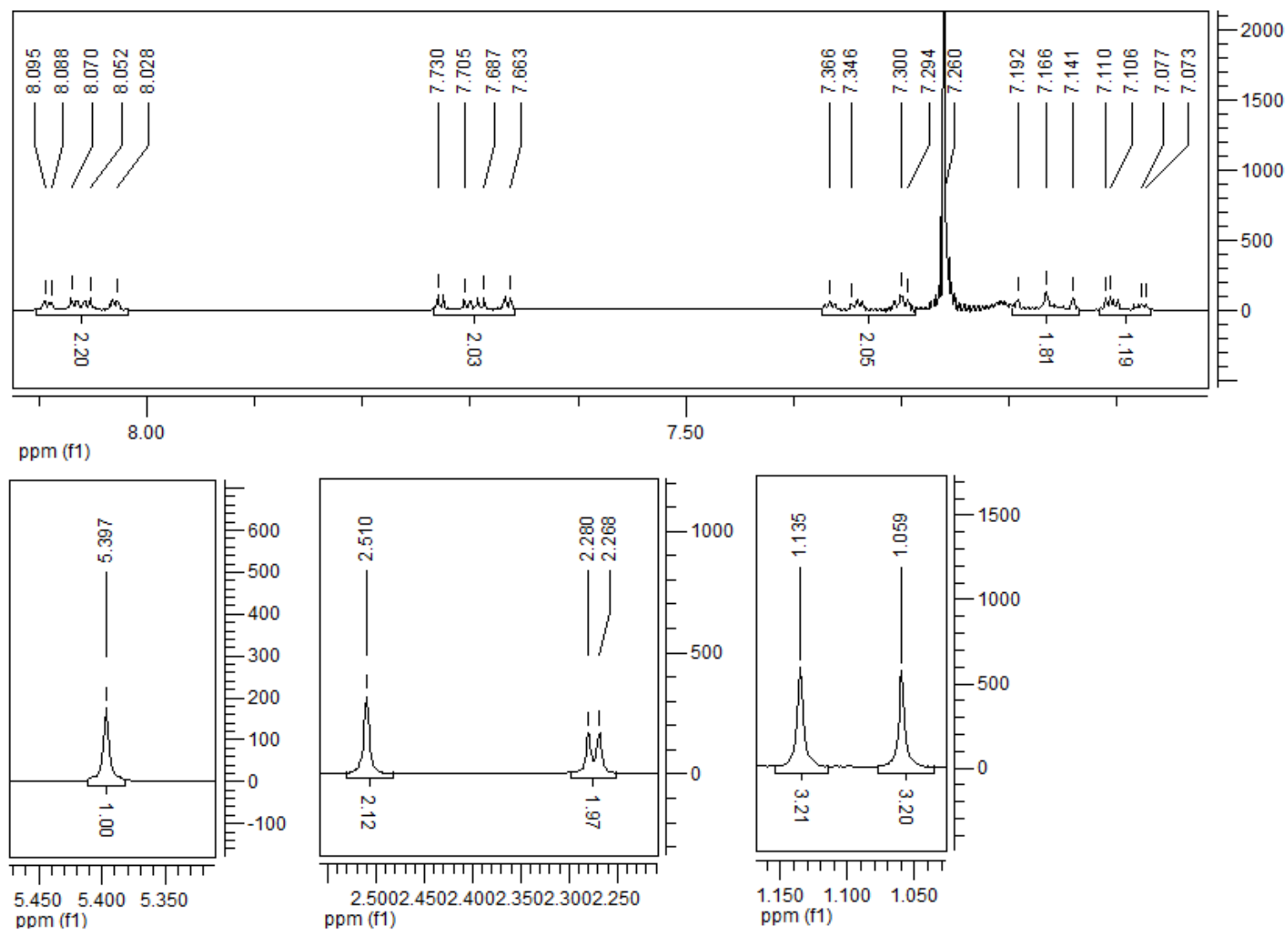
HRMS of compound **4a**



IR spectrum of compound **4b**

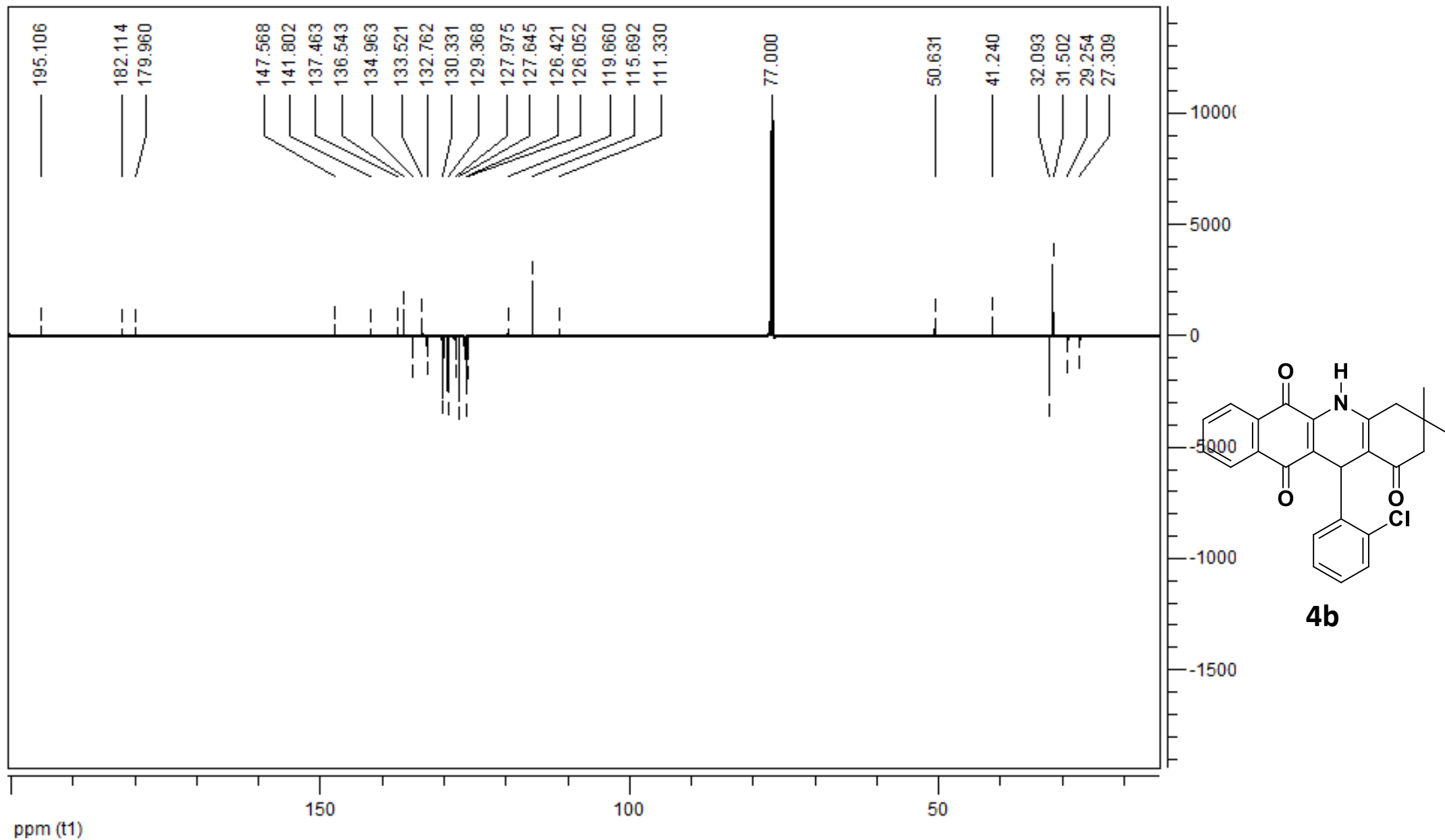


<sup>1</sup>H NMR spectrum of compound **4b** (300.00 MHz, CDCl<sub>3</sub>)



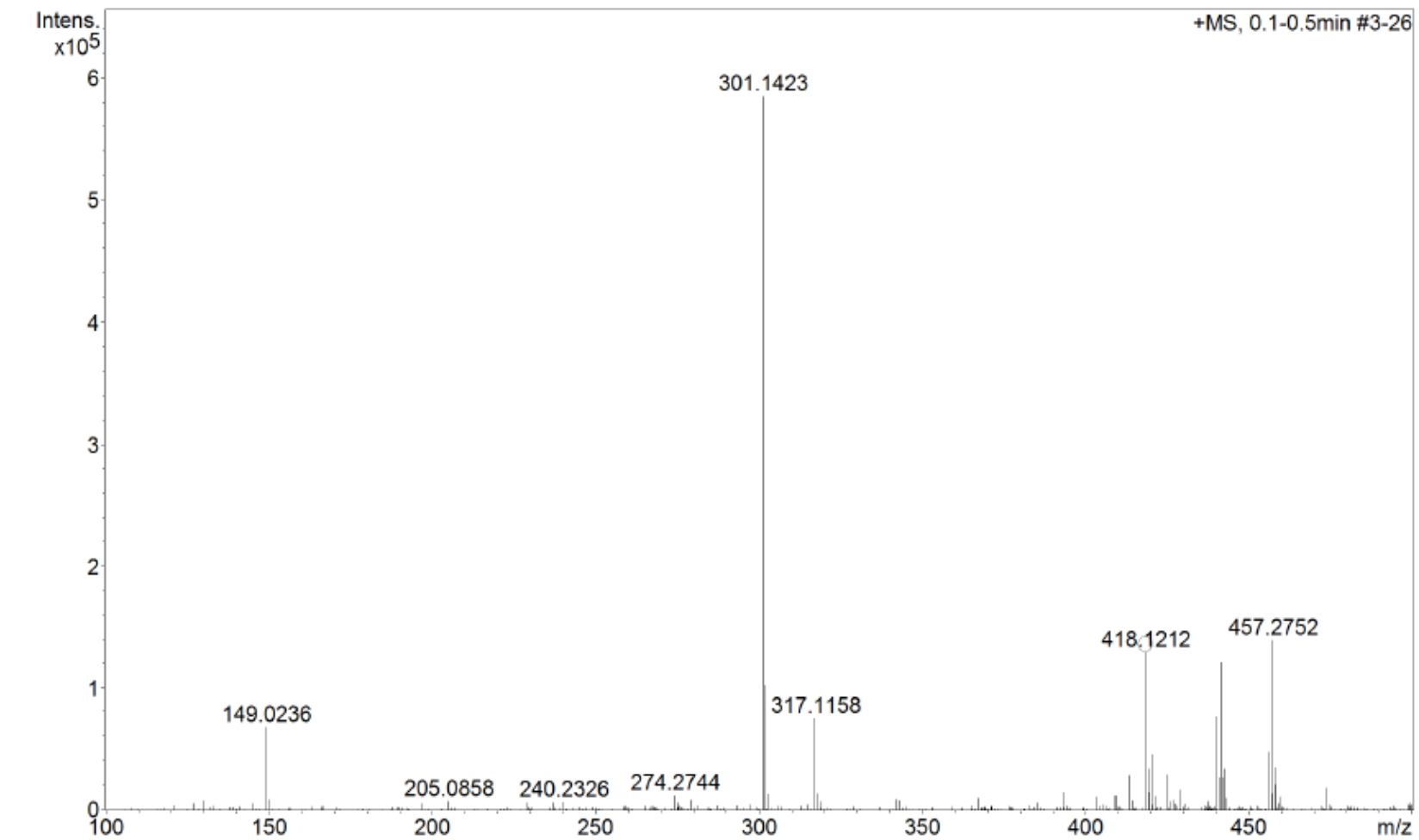
$^1\text{H}$  NMR spectrum of compound **4b** (300.00 MHz,  $\text{CDCl}_3$ )



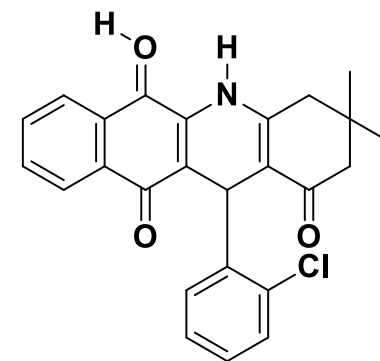


$^{13}\text{C}$  NMR spectrum of compound **4b** (125.0 MHz,  $\text{CDCl}_3$ )

+MS, 0.1-0.5min #3-26



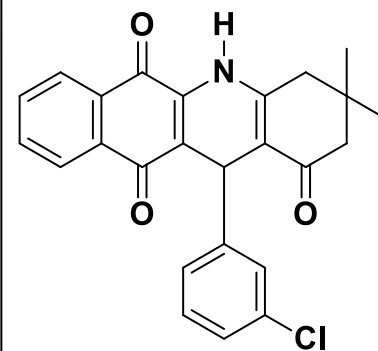
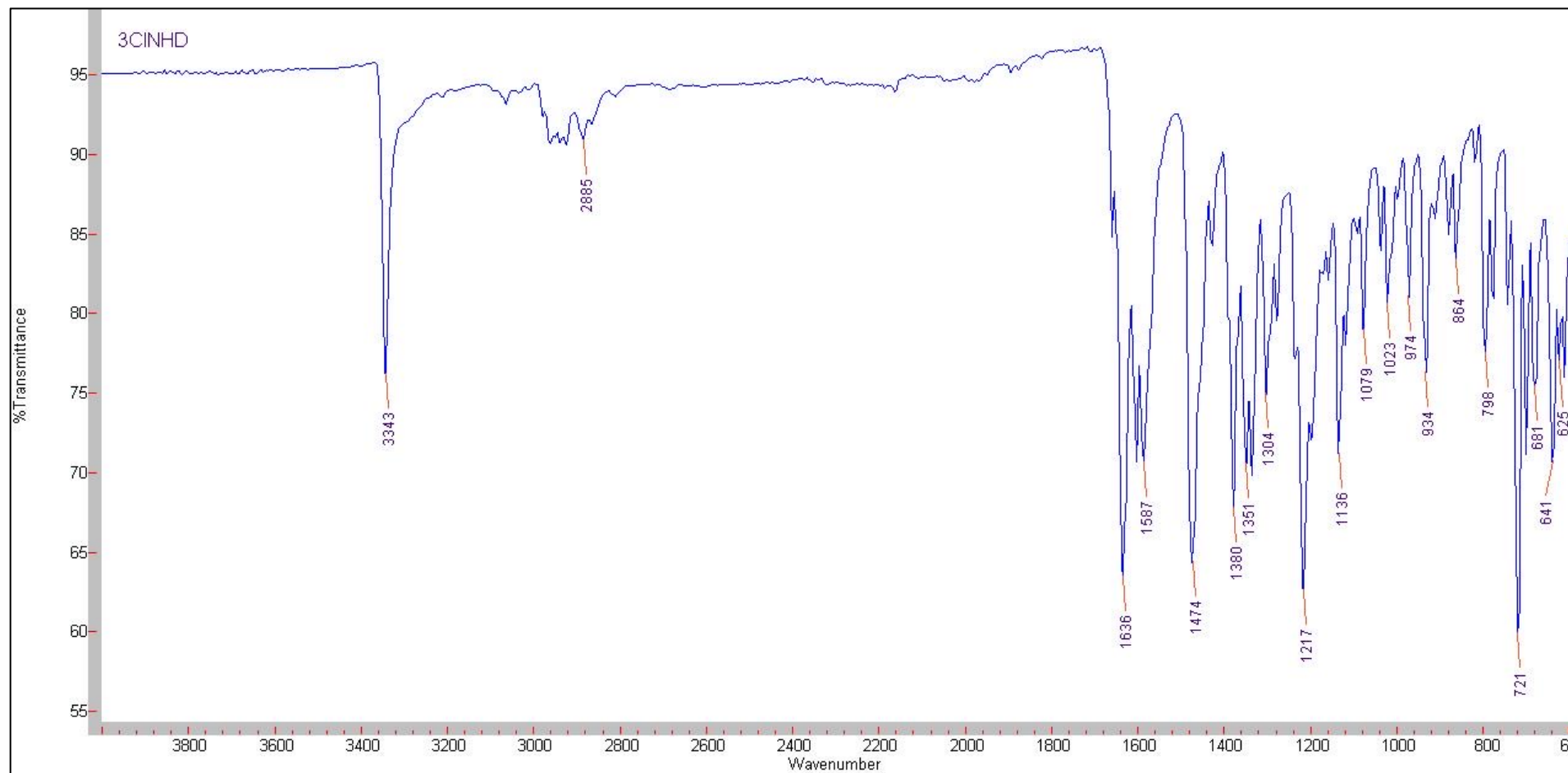
Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
418.121246	1	C <sub>21</sub> H <sub>17</sub> ClN <sub>7</sub> O	418.117762	-8.3	-9.0	16.5	ok	even		3.6	5.7	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
	2	C <sub>25</sub> H <sub>21</sub> ClNO <sub>3</sub>	418.120448	-1.9	-1.6	15.5	ok	even		10.2	14.4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	



Exact Mass: 418,1210

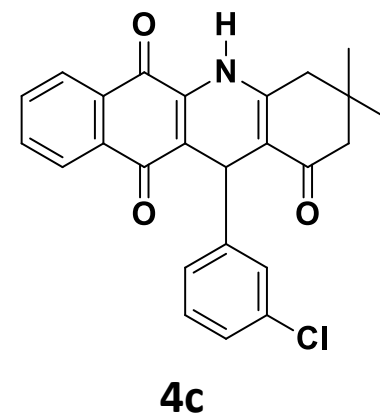
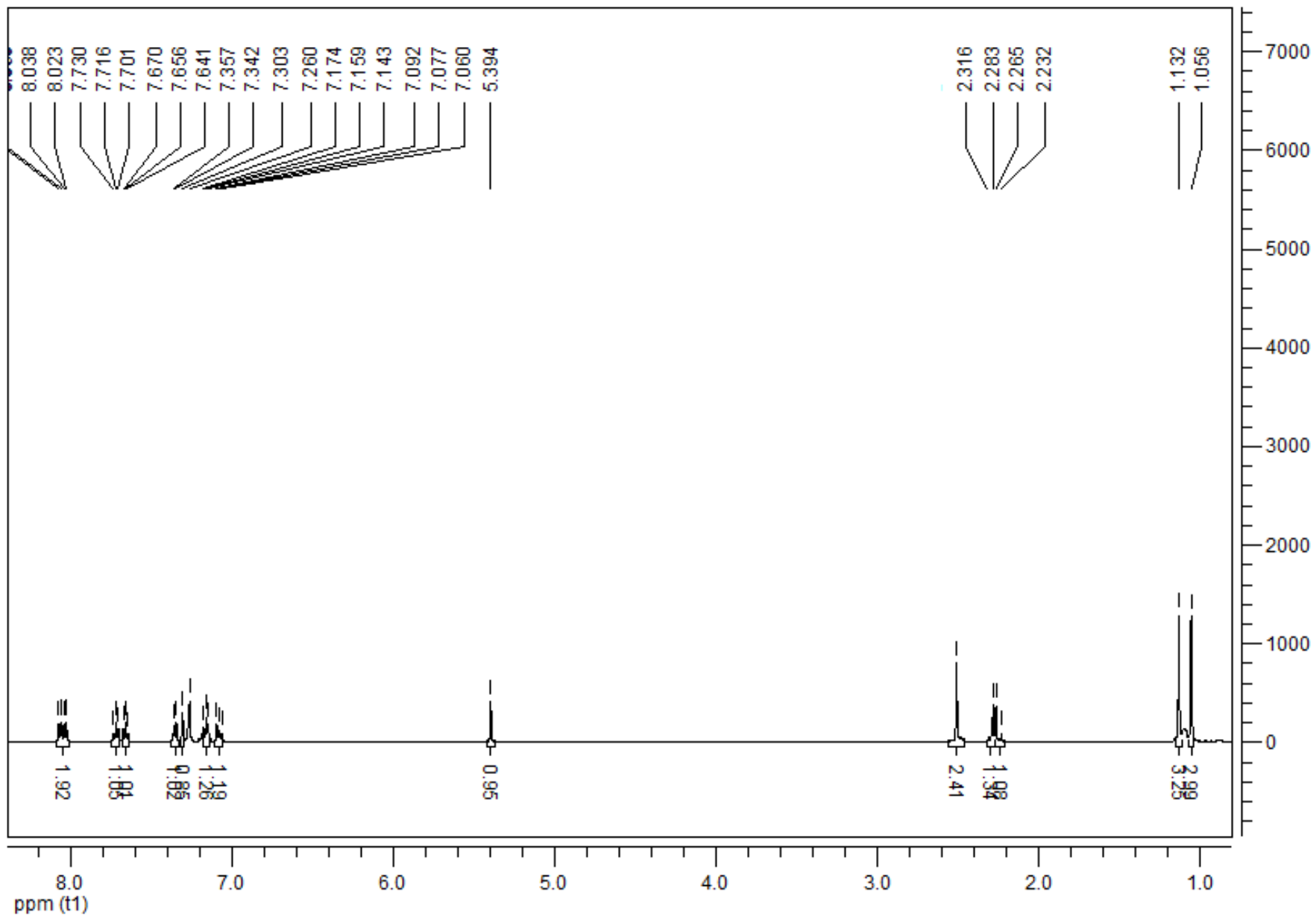
**4b**

HRMS of compound **4b**

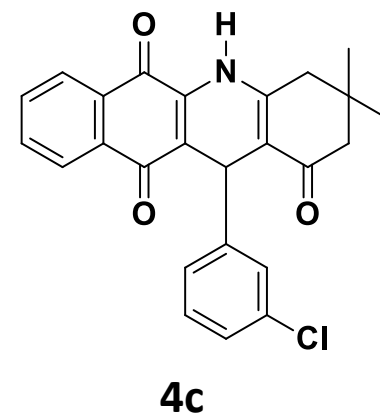
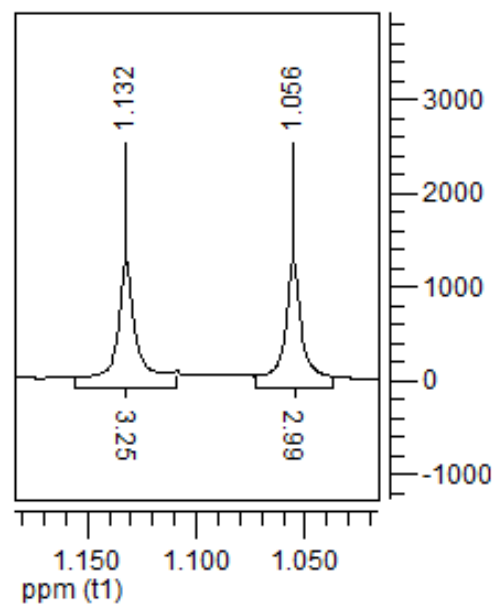
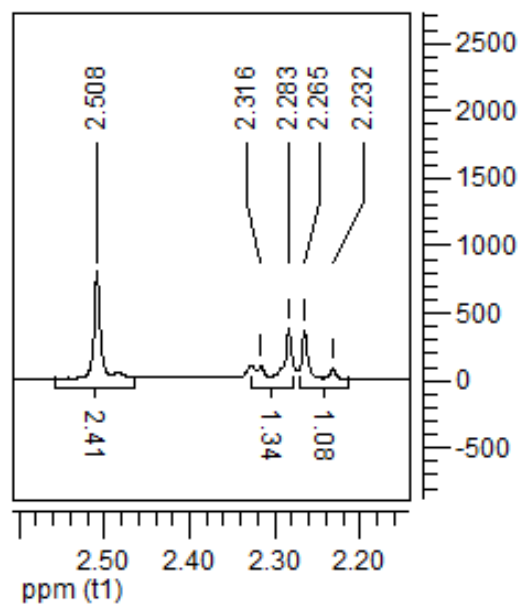
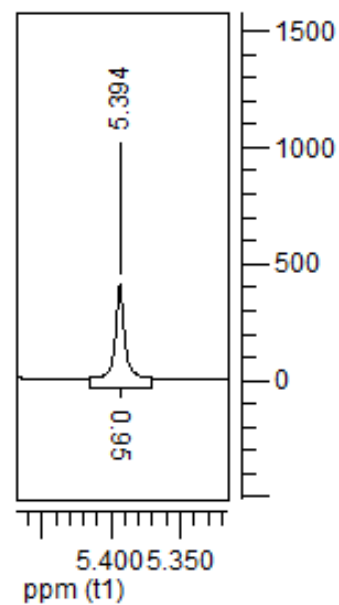
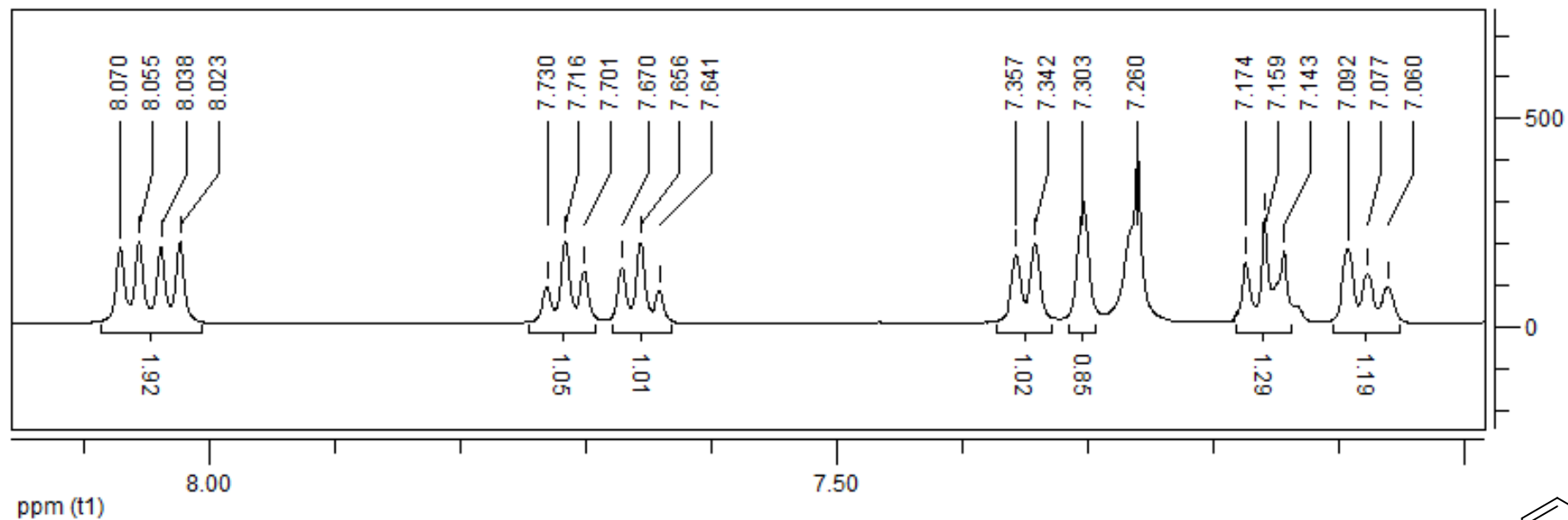


**4c**

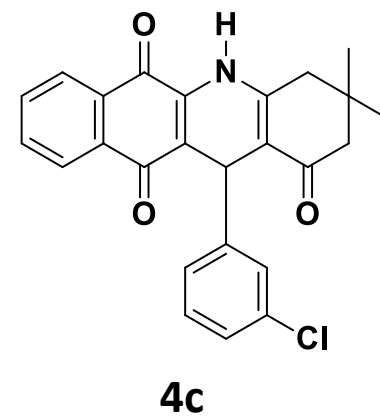
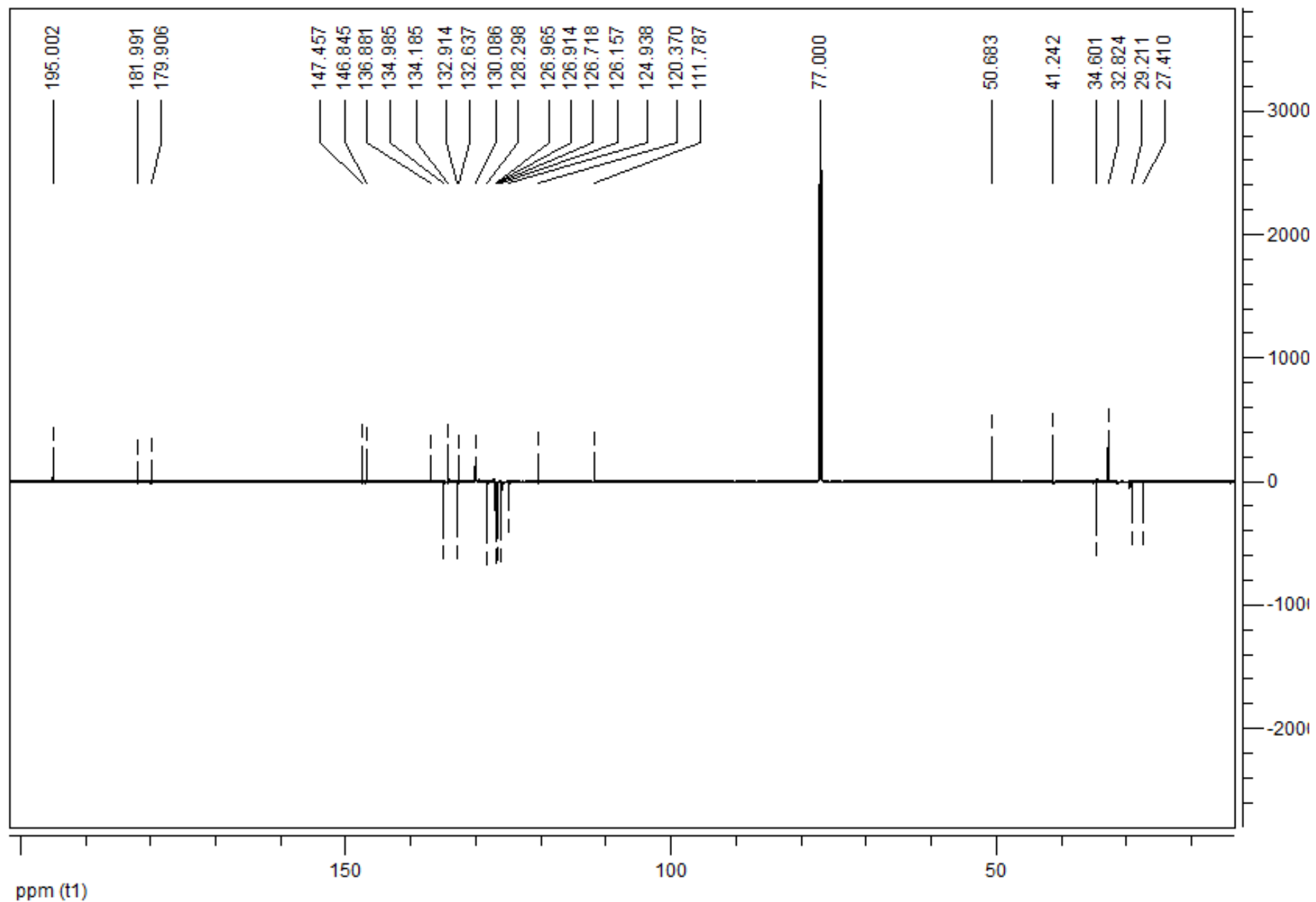
IR spectrum of compound **4c**



<sup>1</sup>H NMR spectrum of compound **4c** (500.00 MHz, CDCl<sub>3</sub>)

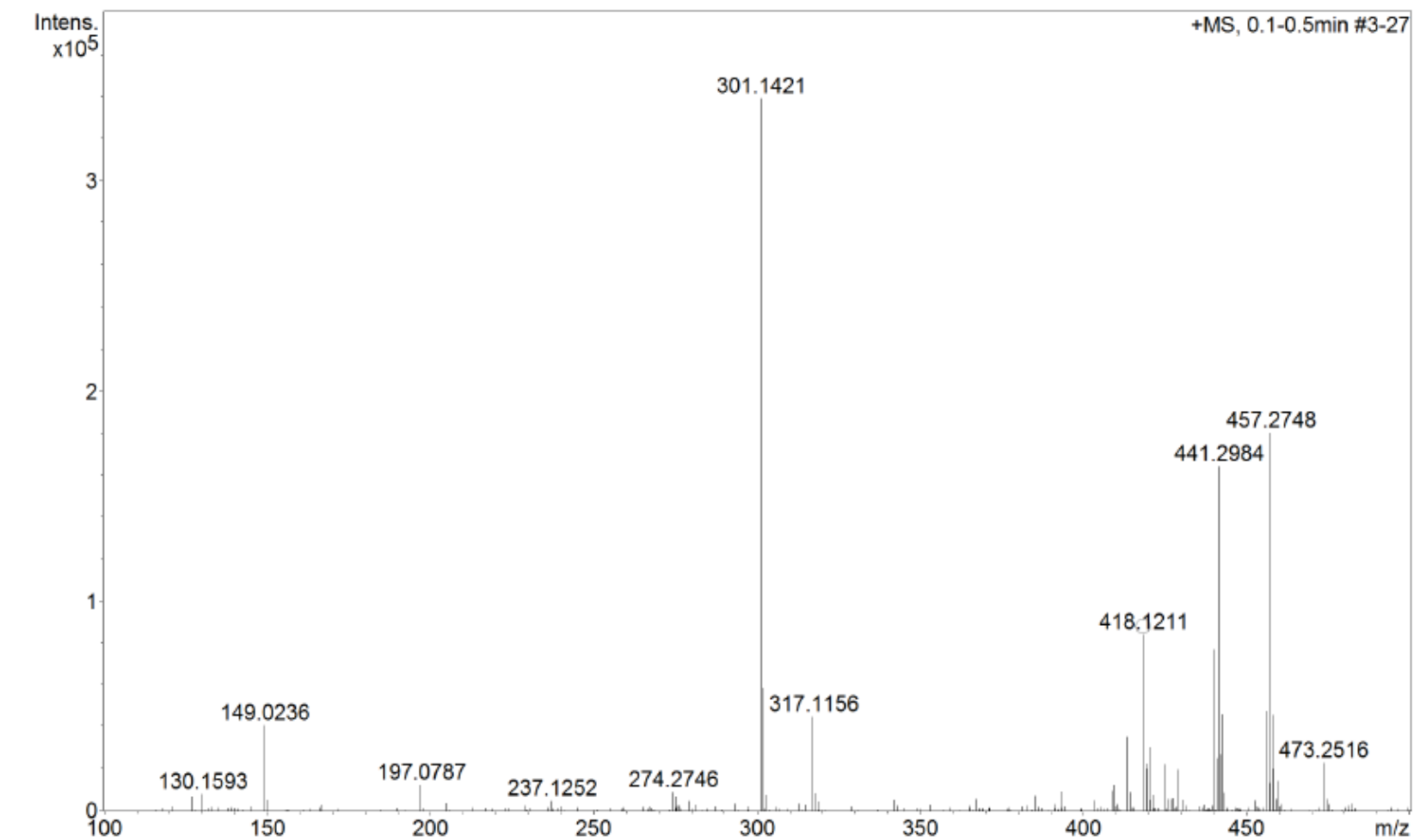


<sup>1</sup>H NMR spectrum of compound **4c** (500.00 MHz, CDCl<sub>3</sub>)

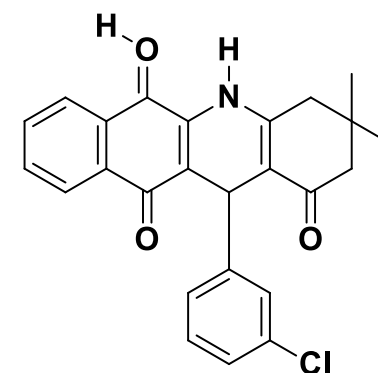


$^{13}\text{C}$  NMR spectrum of compound **4c** (75.0 MHz,  $\text{CDCl}_3$ )

+MS, 0.1-0.5min #3-27



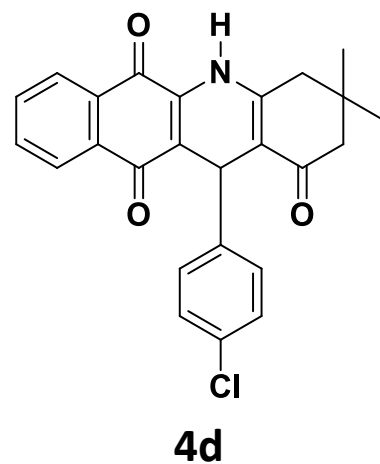
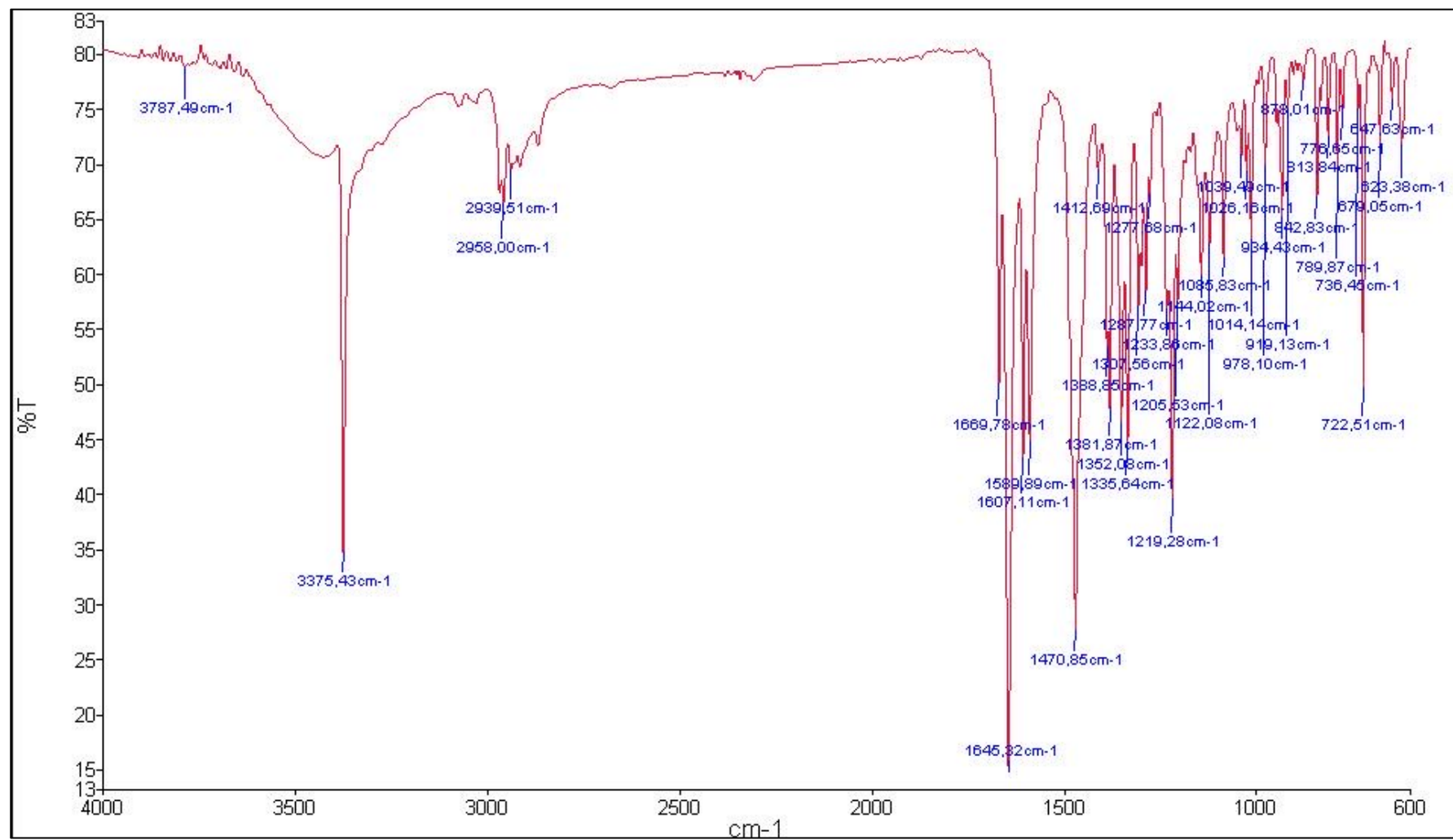
Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
418.121080	1	C <sub>25</sub> H <sub>21</sub> ClNO <sub>3</sub>	418.120448	-1.5	-0.8	15.5	ok	even		5.6	7.7		n.a.		n.a.		n.a.		n.a.
	2	C <sub>21</sub> H <sub>17</sub> ClN <sub>7</sub> O	418.117762	-7.9	-8.2	16.5	ok	even		6.7	11.2		n.a.		n.a.		n.a.		n.a.



Exact Mass: 418,1210

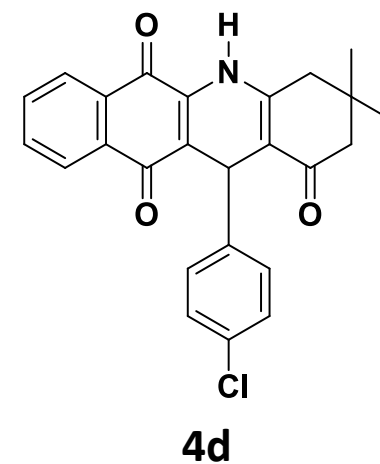
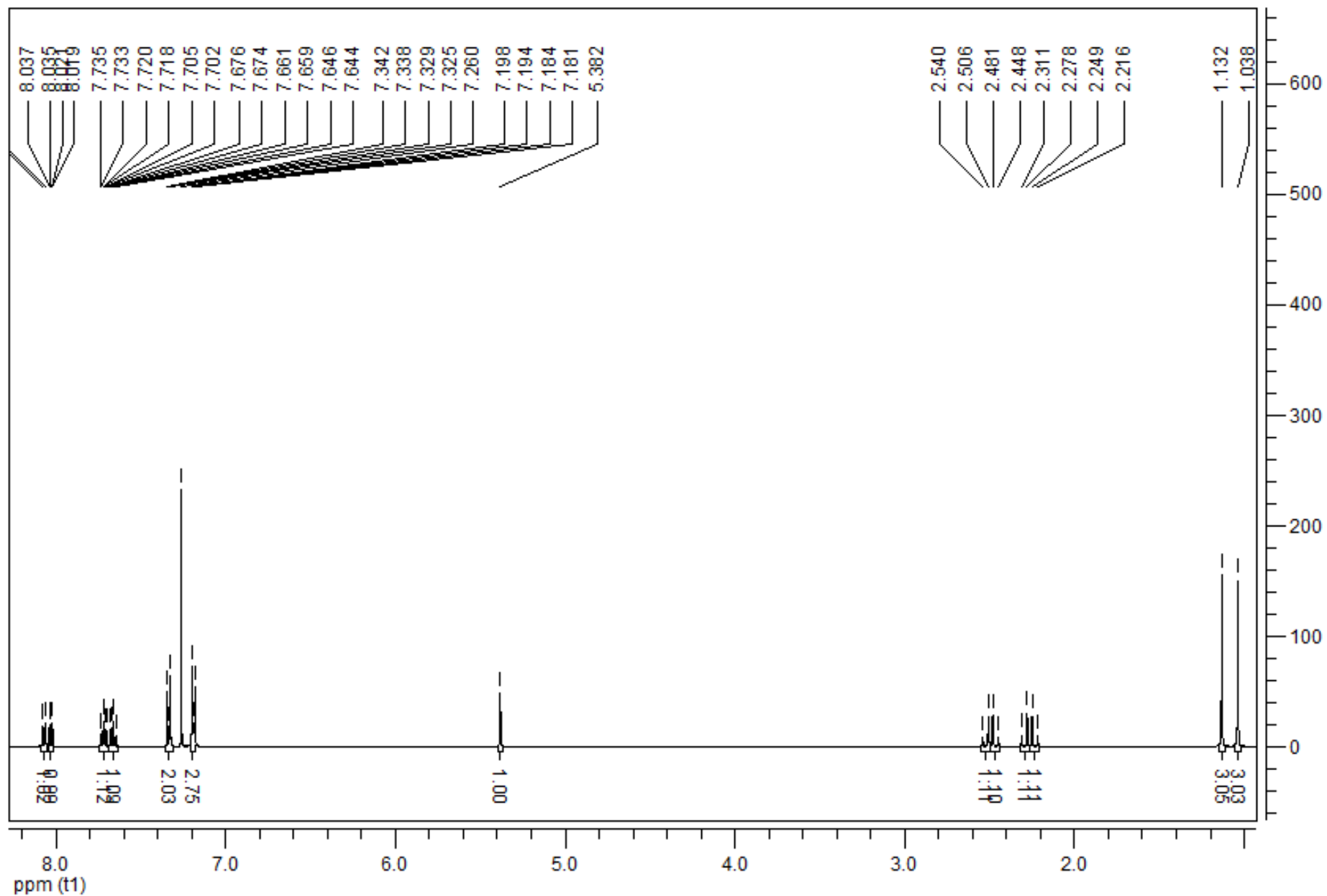
**4c**

HRMS of compound **4c**

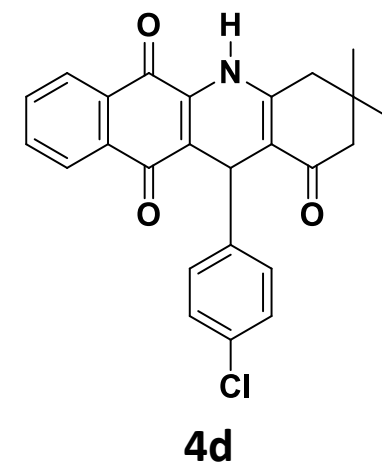
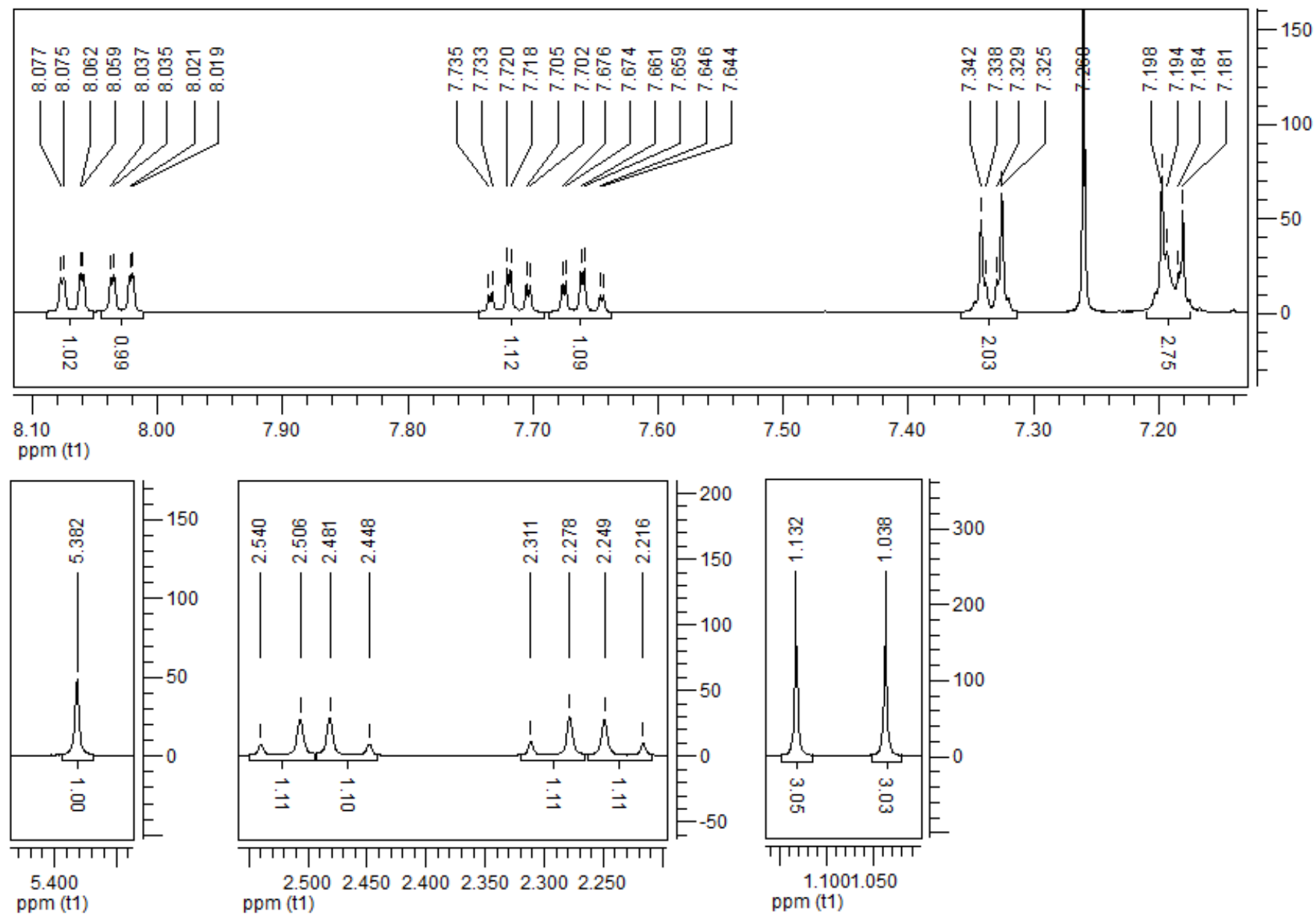


IR spectrum of compound **4d**

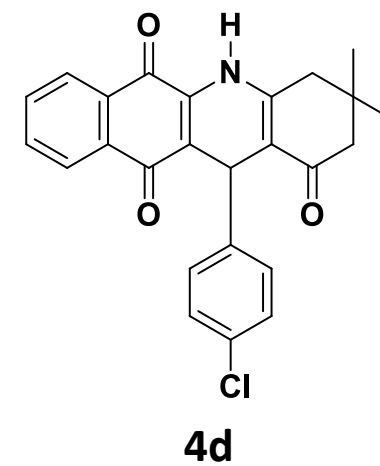
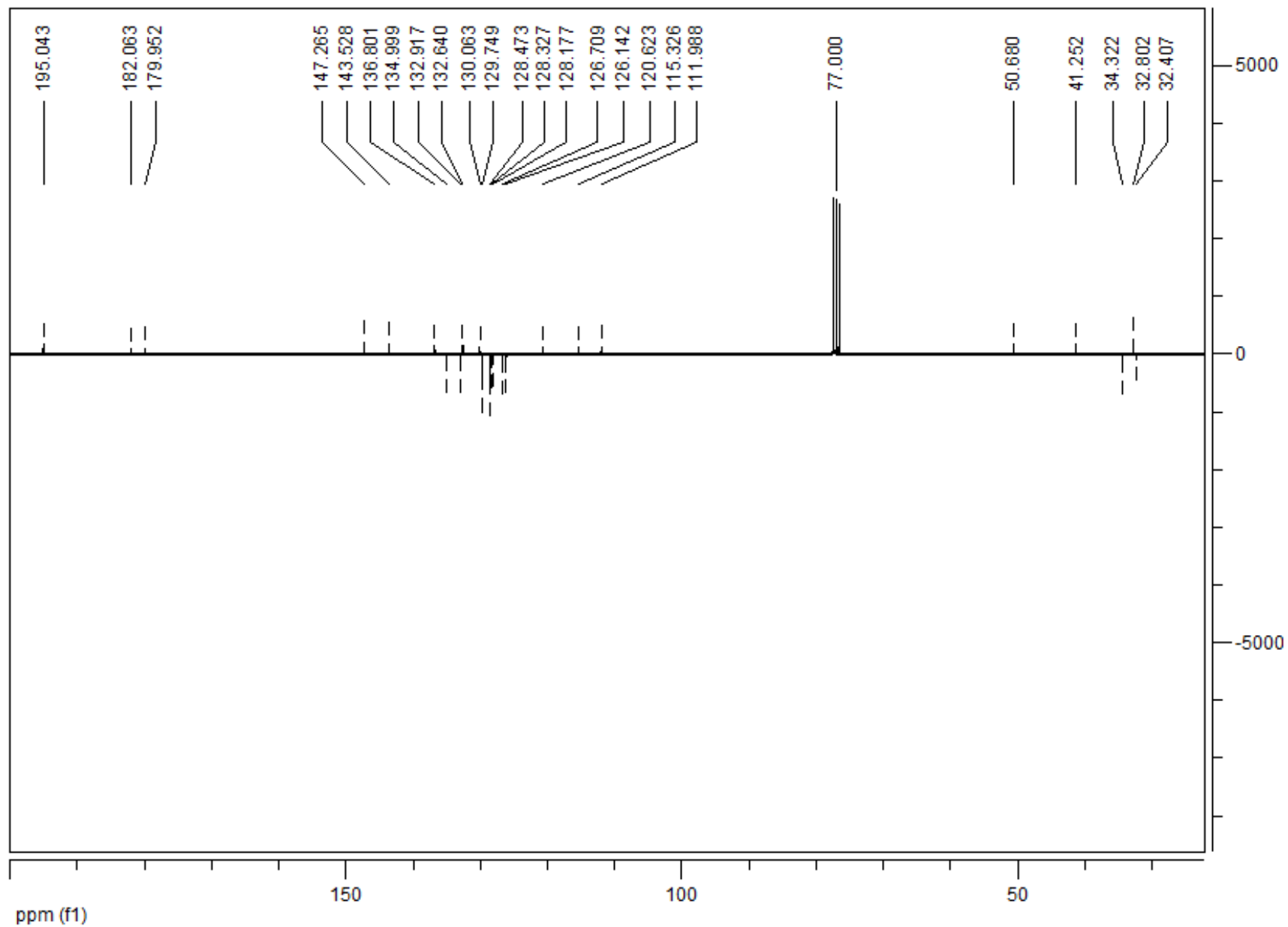




$^1\text{H}$  NMR spectrum of compound **4d** (500.00 MHz,  $\text{CDCl}_3$ )

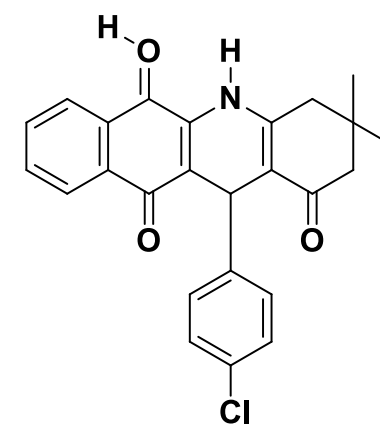
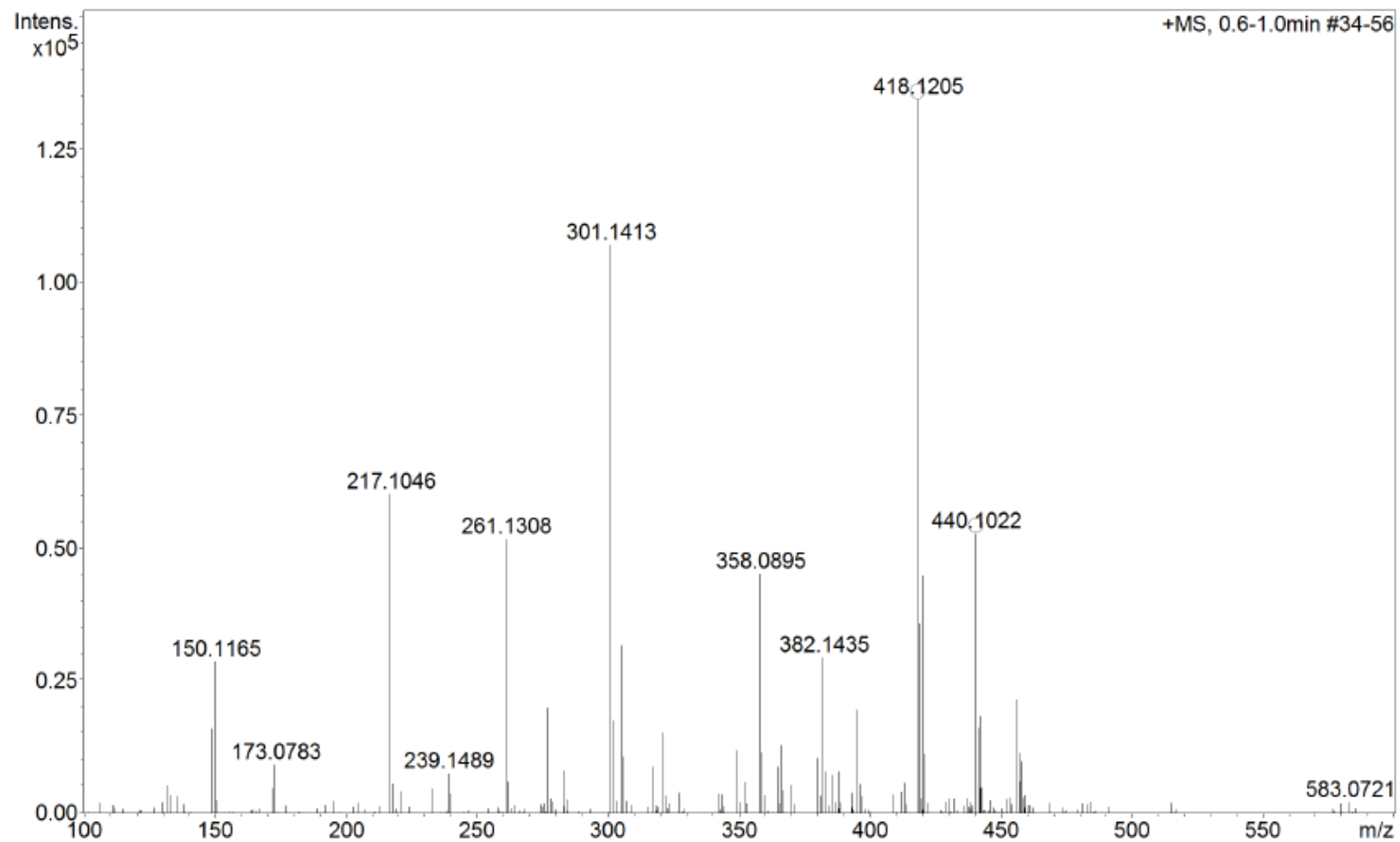


<sup>1</sup>H NMR spectrum of compound **4d** (500.00 MHz, CDCl<sub>3</sub>)



<sup>13</sup>C NMR spectrum of compound **4d** (75.0 MHz, CDCl<sub>3</sub>)

+MS, 0.6-1.0min #34-56

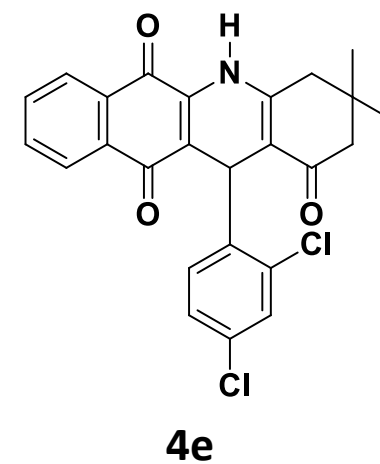
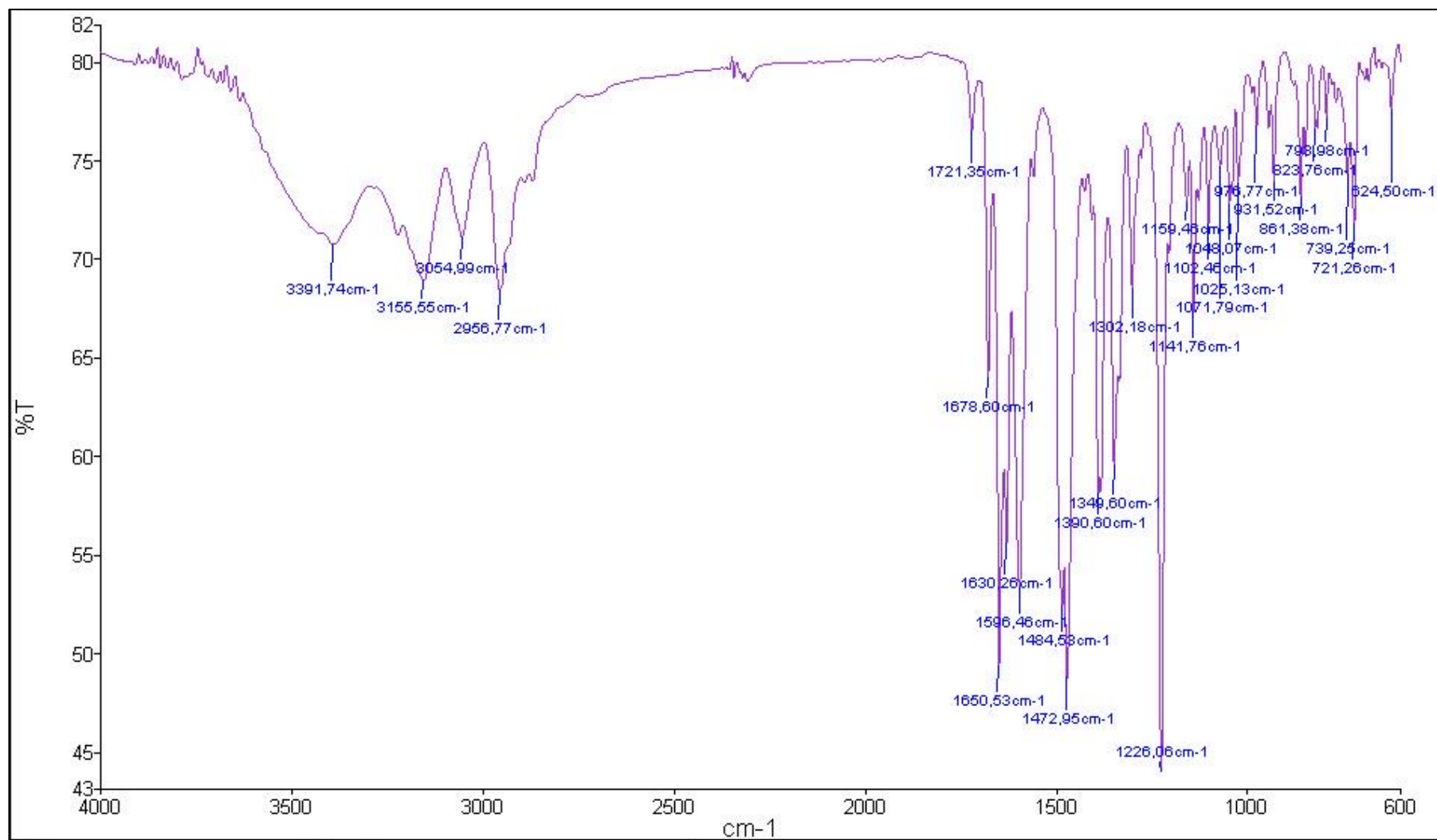


Exact Mass: 418,1210

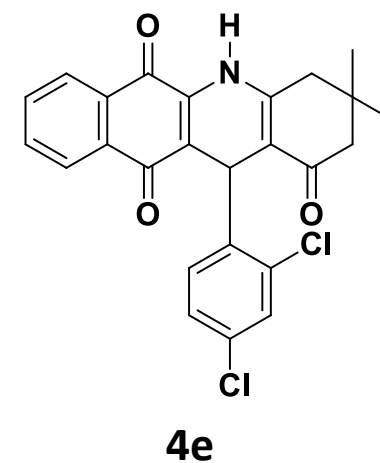
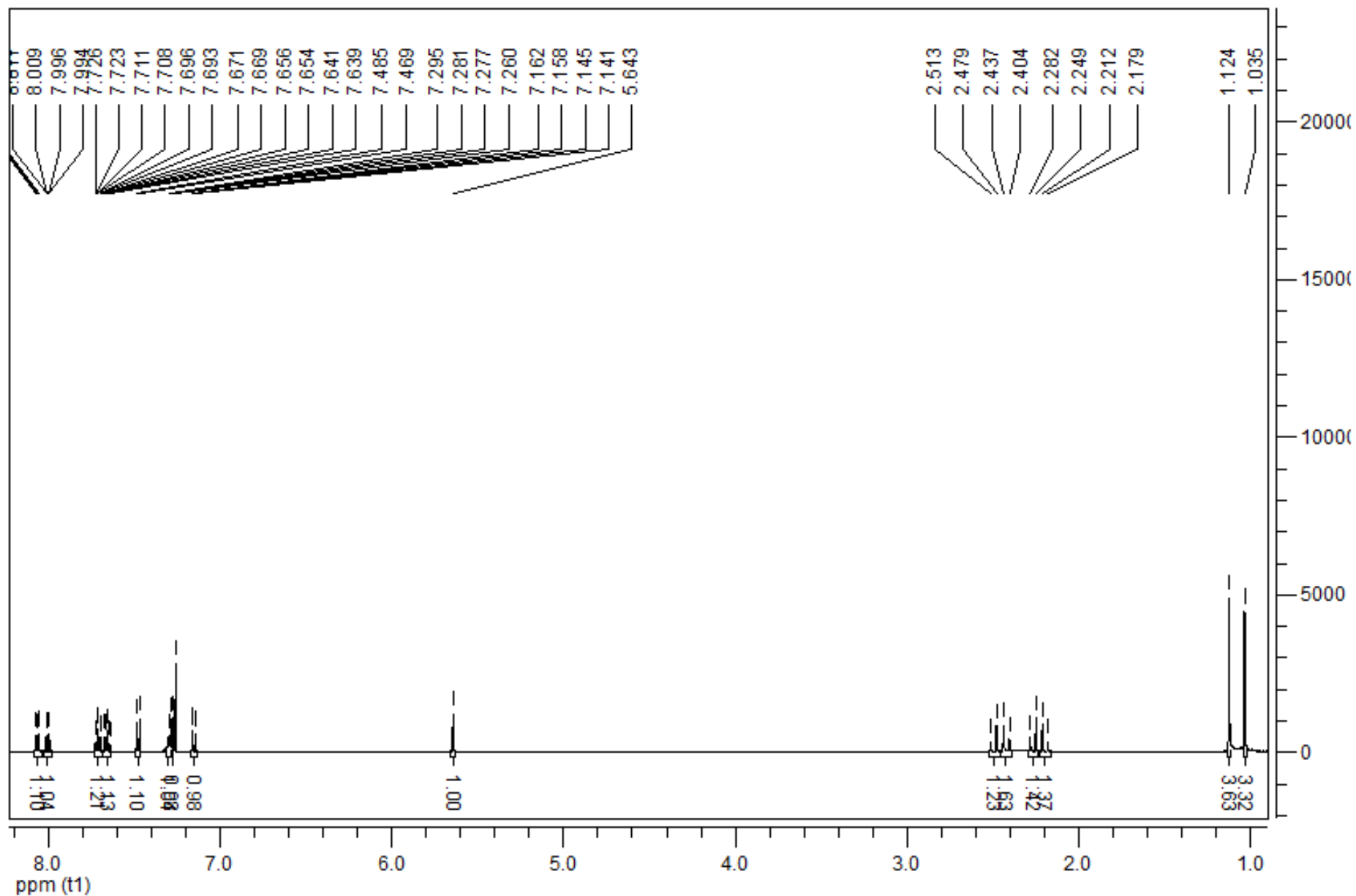
**4d**

Meas. m/z	# Ion	Formula	m/z err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std	m/z Diff	Std	Comb	Dev
418.1205	41	C <sub>25</sub> H <sub>21</sub> ClNO <sub>3</sub>	-0.2	1.1	15.5	ok	even		14.8	21.2		n.a.		n.a.		n.a.		n.a.	
440.1022	237	C <sub>25</sub> H <sub>20</sub> ClNaO <sub>3</sub>	0.4	1.6	15.5	ok	even		13.8	20.5		n.a.		n.a.		n.a.		n.a.	

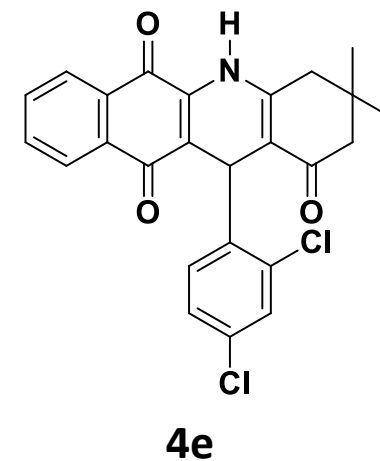
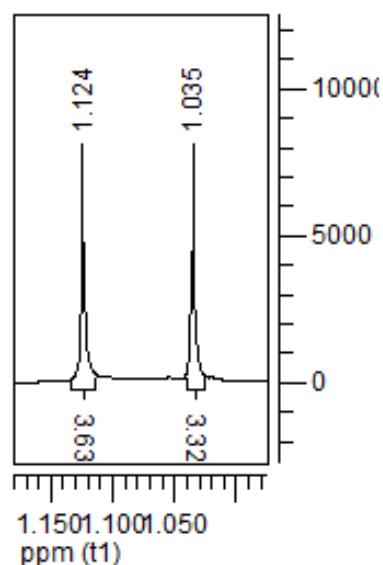
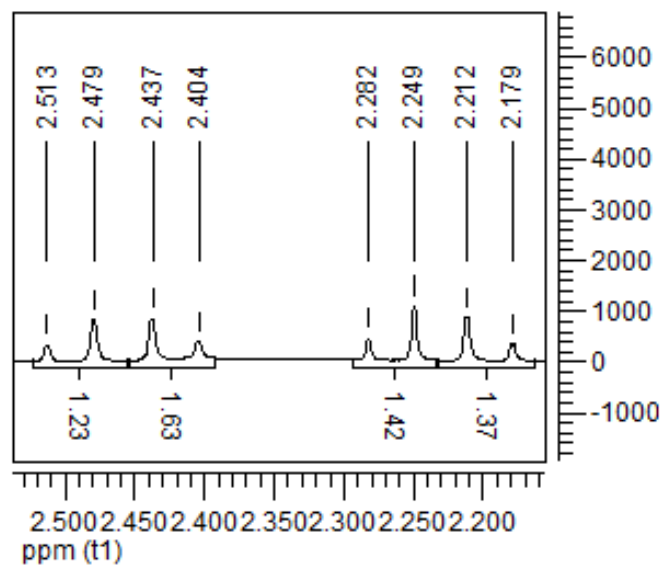
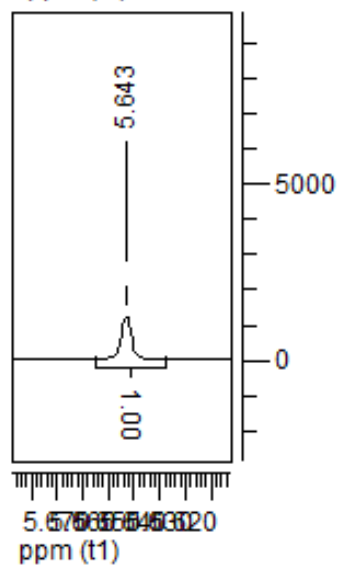
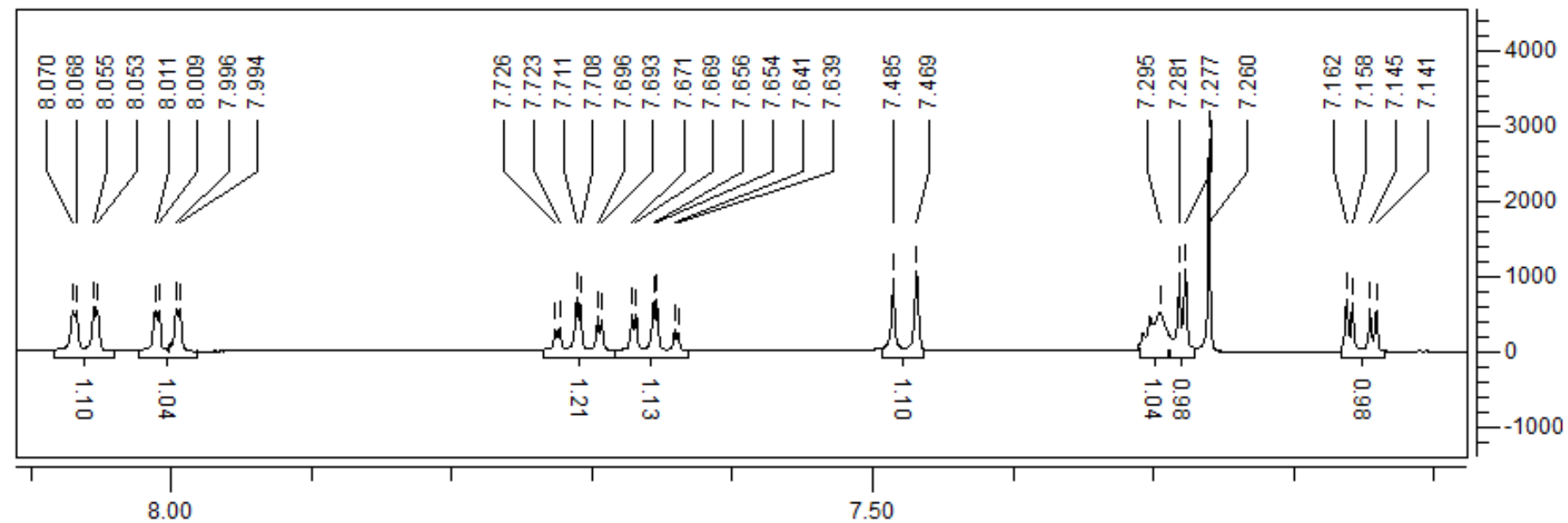
HRMS of compound **4d**



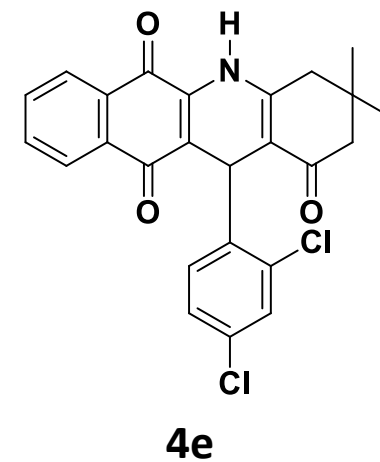
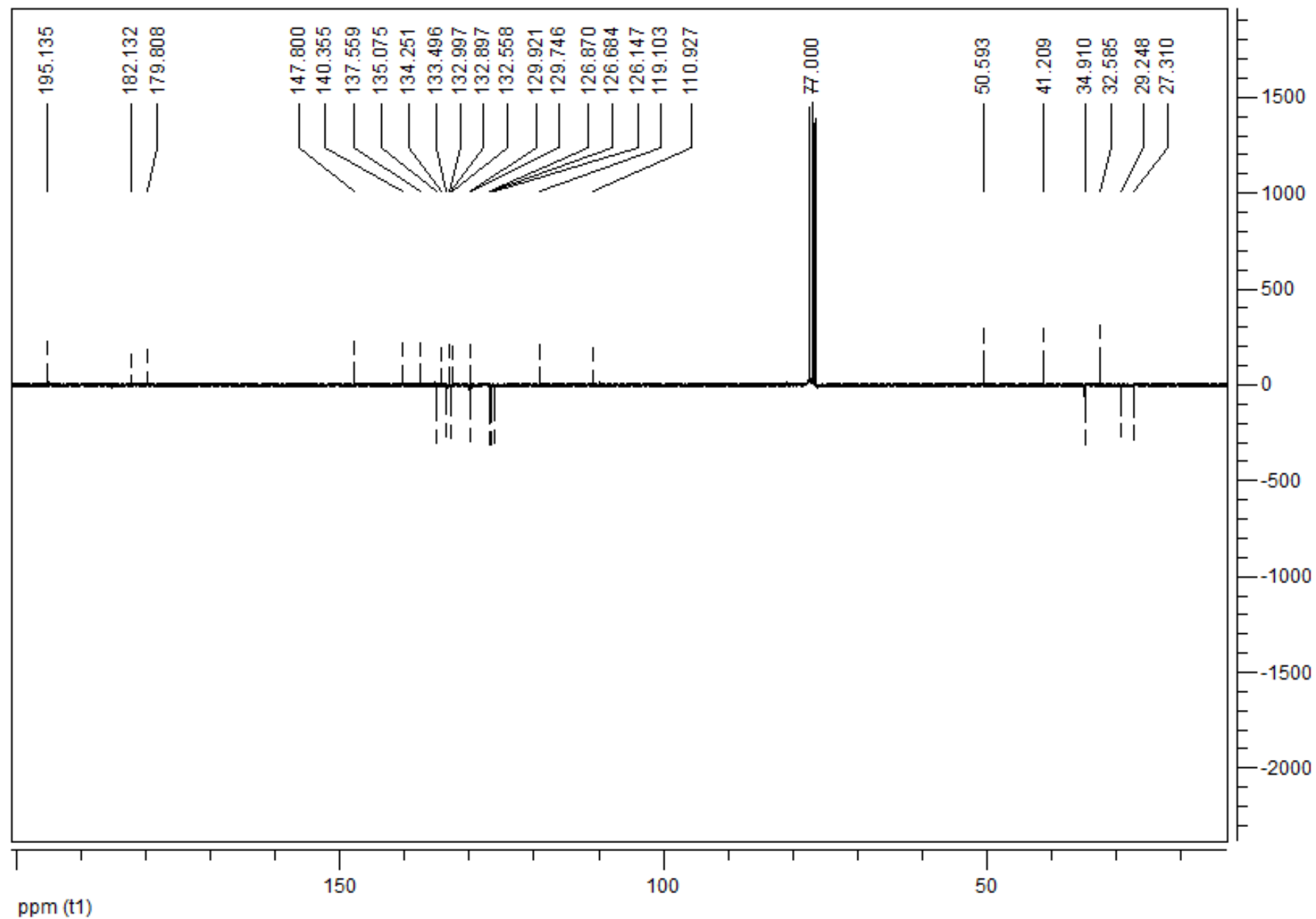
IR spectrum of compound **4e**



$^1\text{H}$  NMR spectrum of compound **4e** (500.00 MHz,  $\text{CDCl}_3$ )



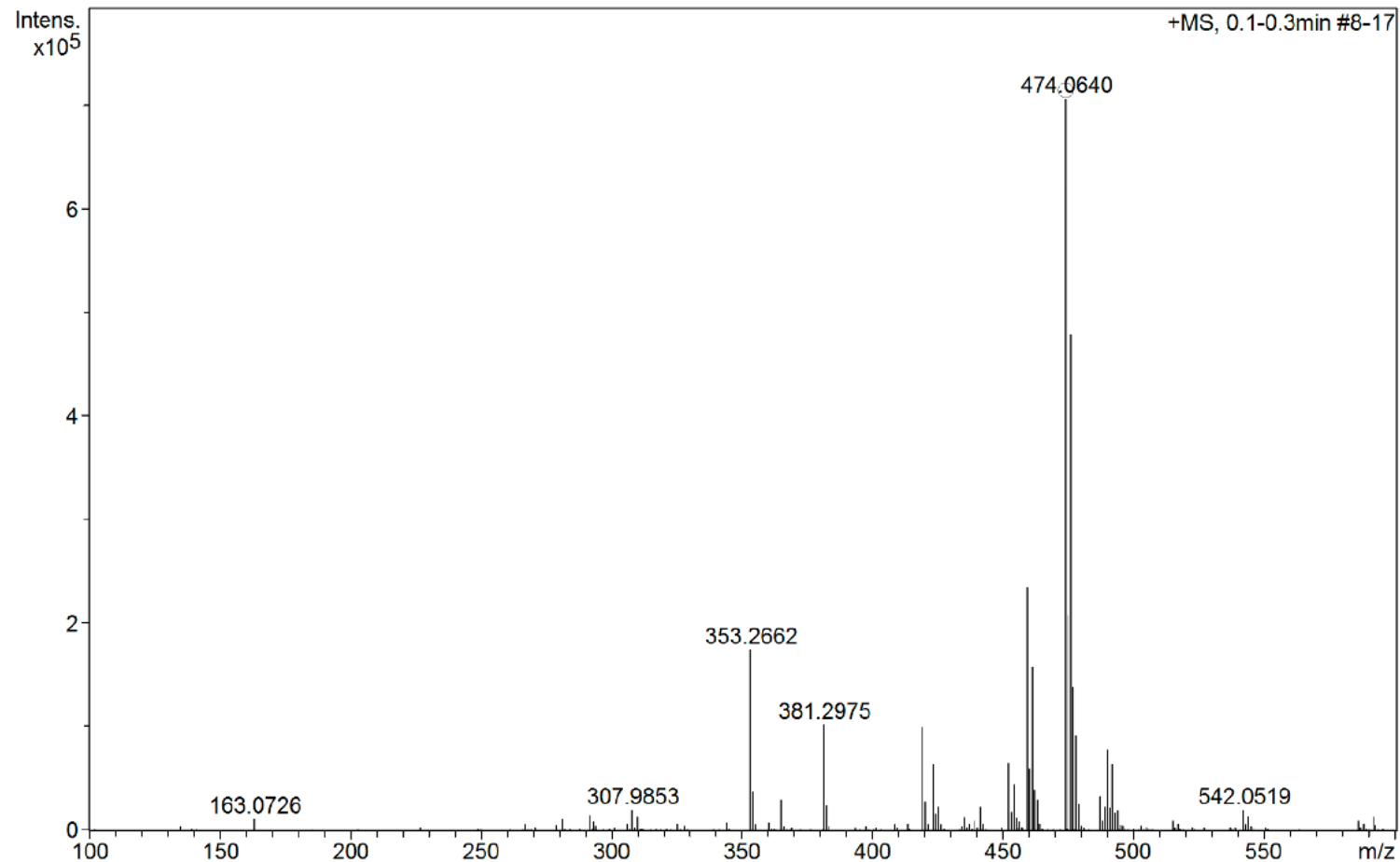
$^1\text{H}$  NMR spectrum of compound **4e** (500.00 MHz,  $\text{CDCl}_3$ )



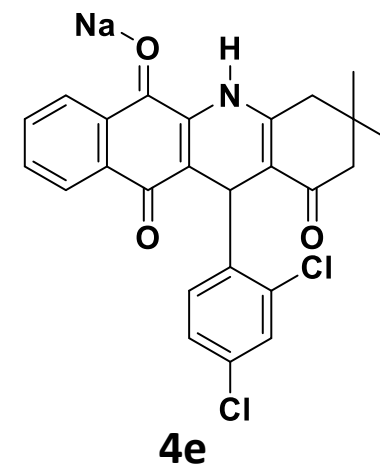
<sup>13</sup>C NMR spectrum of compound **4e** (75.0 MHz, CDCl<sub>3</sub>)



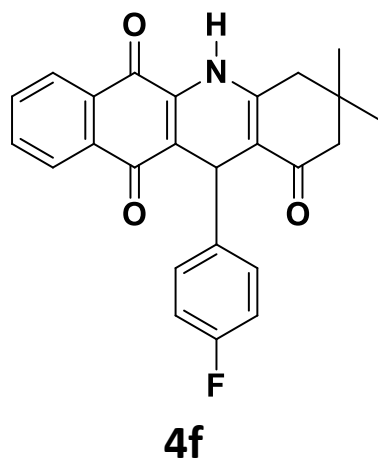
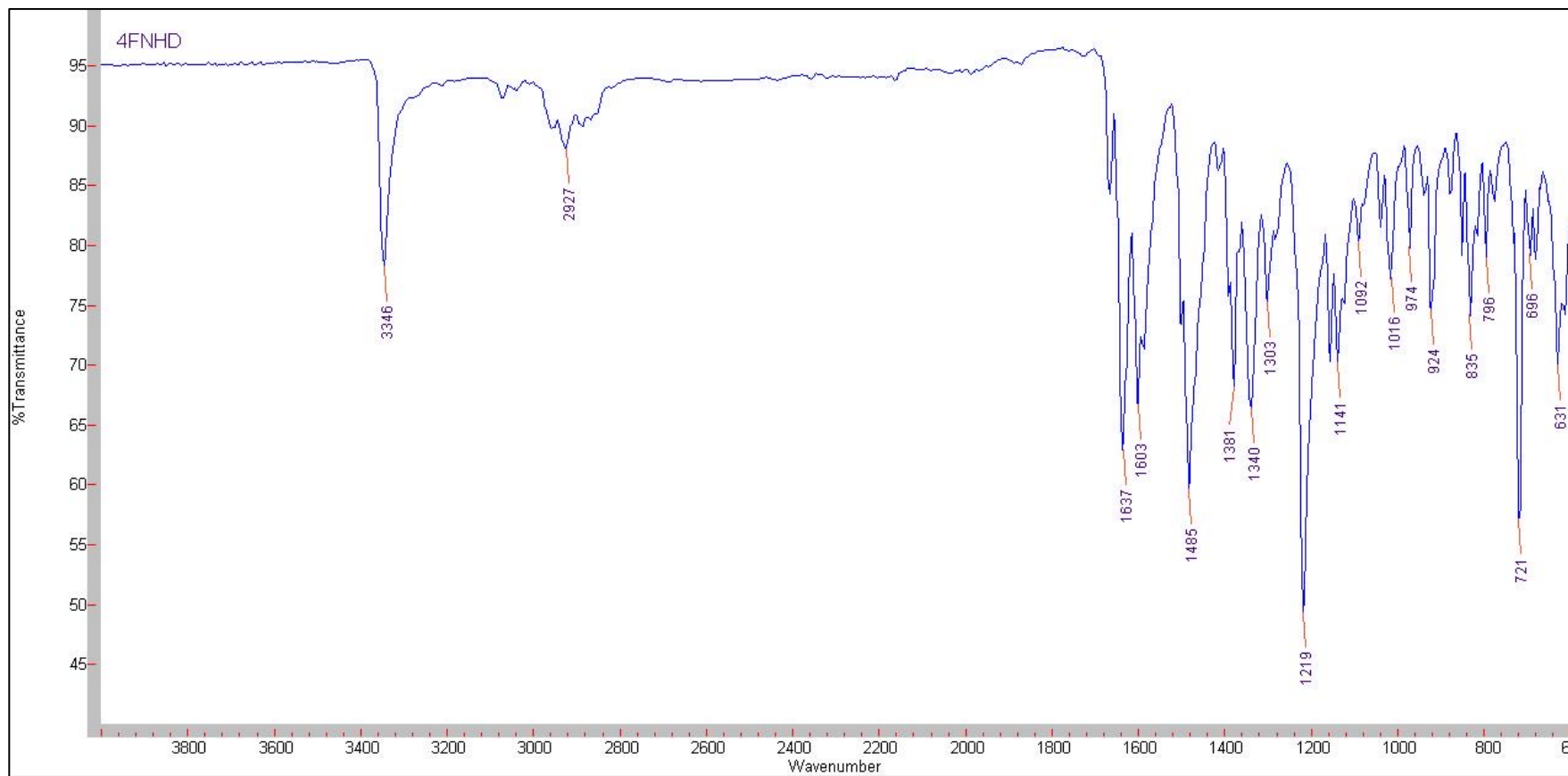
+MS, 0.1-0.3min #8-17



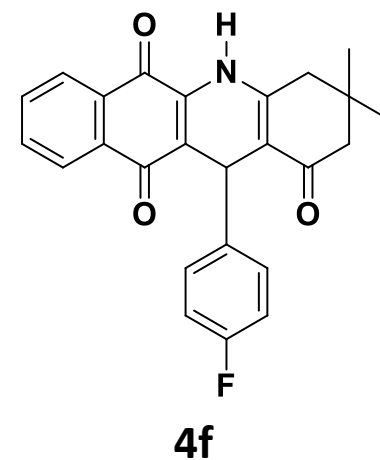
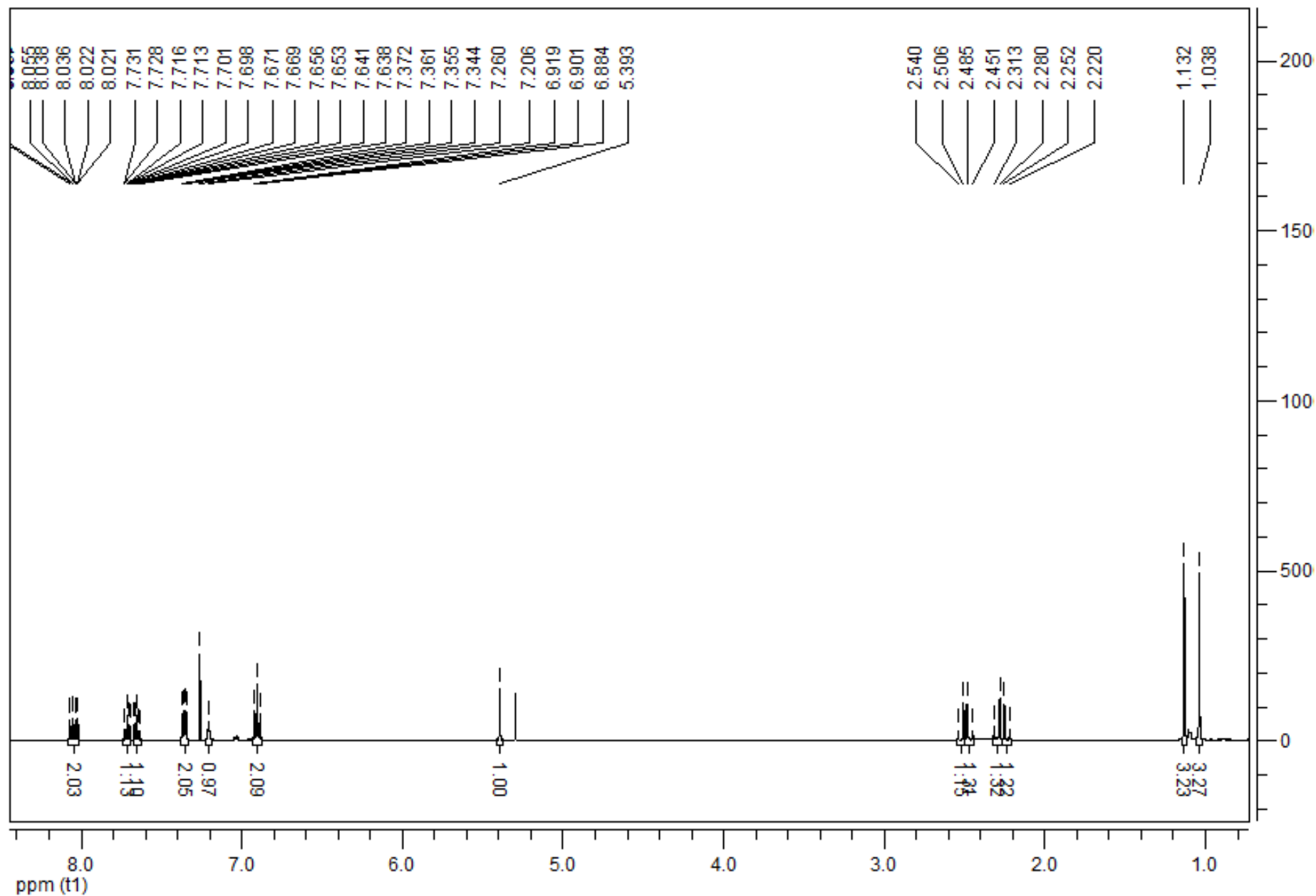
Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
474.063981	1	C <sub>25</sub> H <sub>19</sub> Cl <sub>2</sub> NNaO <sub>3</sub>	474.063420	-1.2	-2.6	15.5	ok	even		9.4	11.3	n.a.	n.a.	n.a.	n.a.



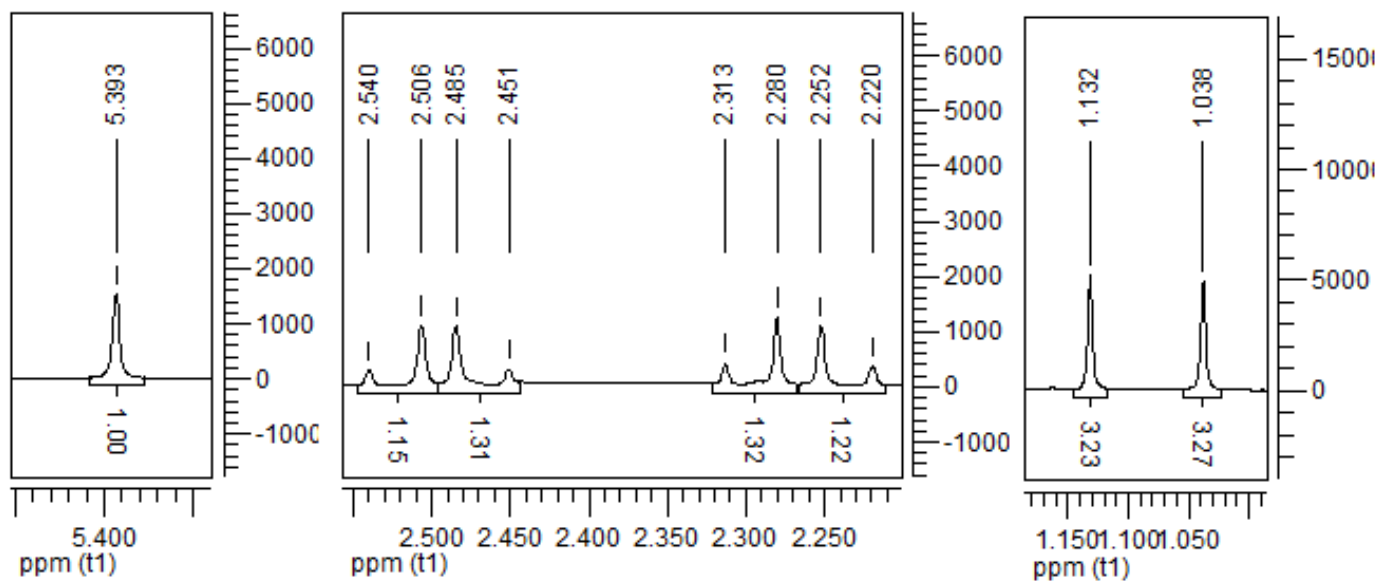
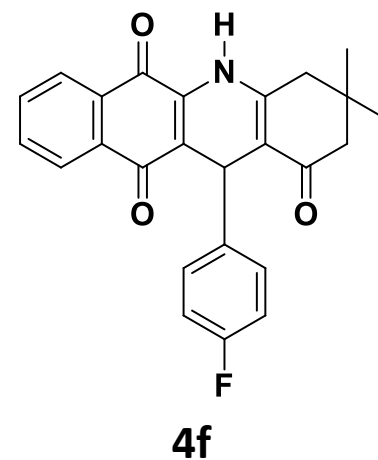
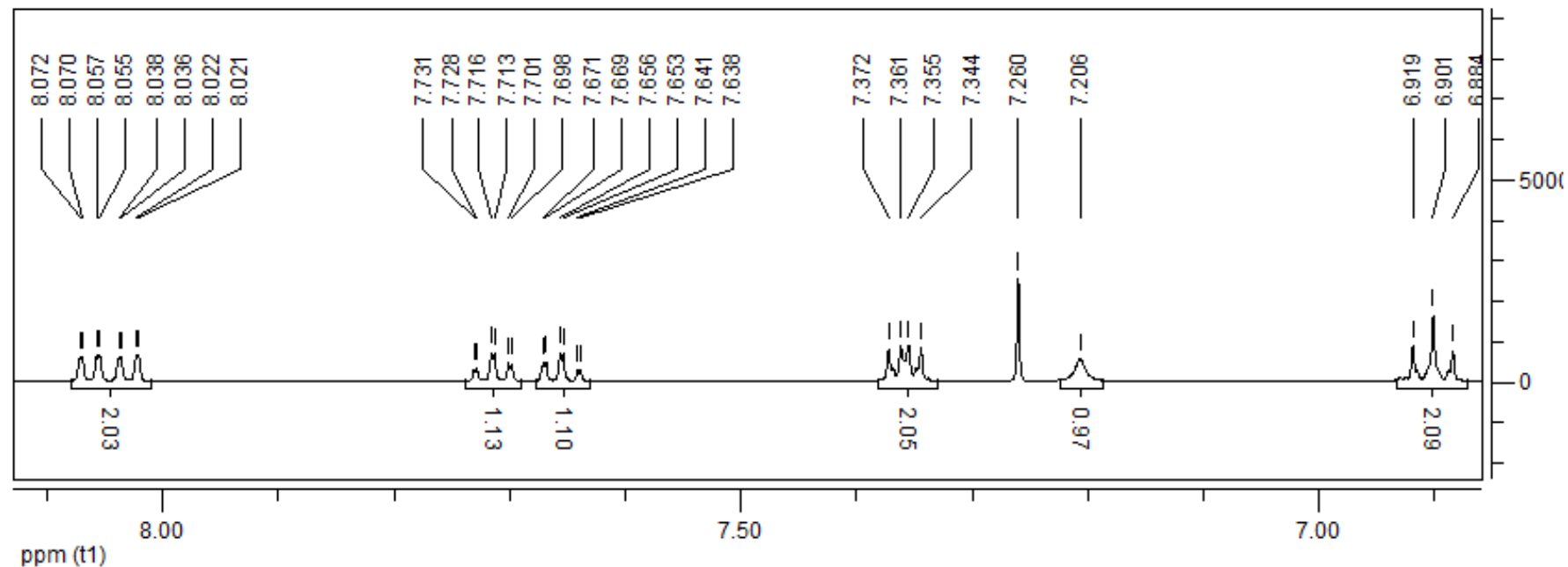
HRMS of compound 4e



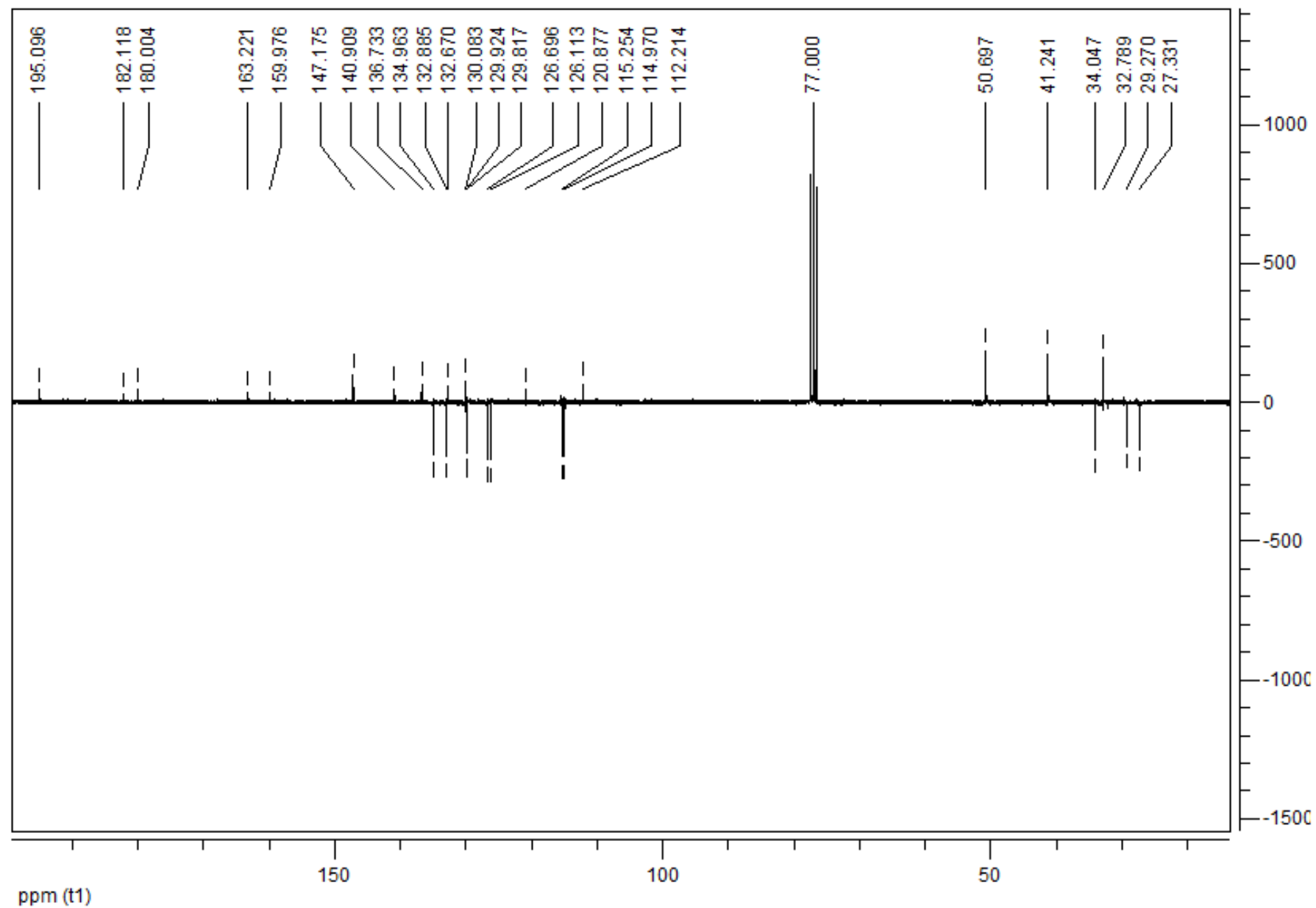
IR spectrum of compound **4f**



<sup>1</sup>H NMR spectrum of compound **4f** (500.00 MHz, CDCl<sub>3</sub>)

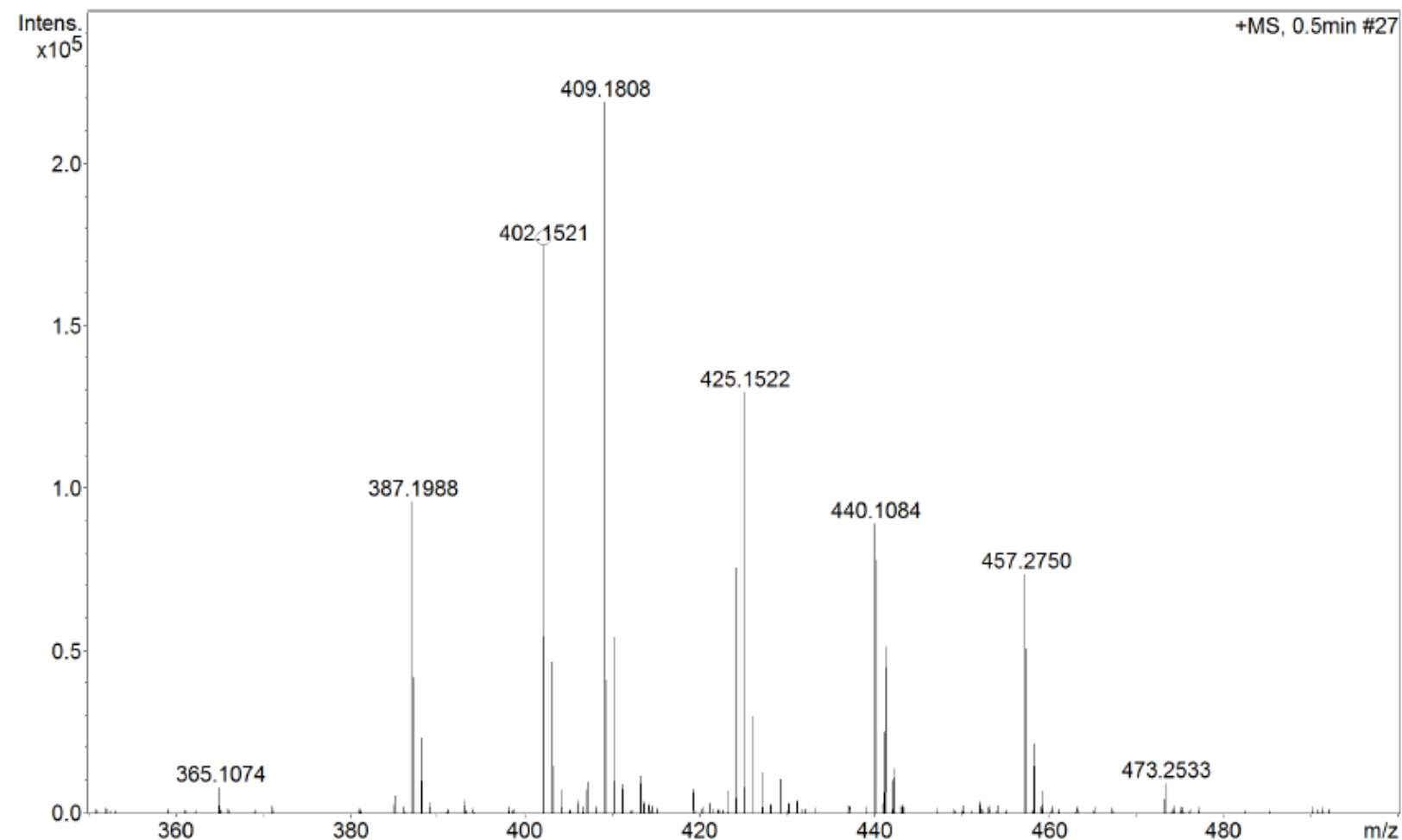


$^1\text{H}$  NMR spectrum of compound **4f** (500.00 MHz,  $\text{CDCl}_3$ )

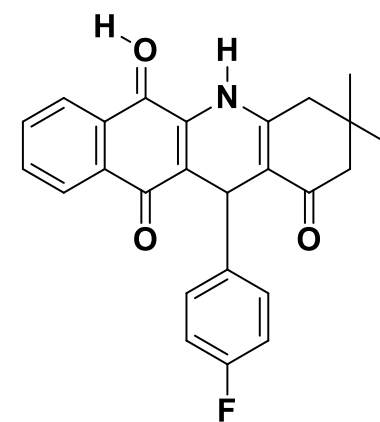


$^{13}\text{C}$  NMR spectrum of compound **4f** (75.0 MHz,  $\text{CDCl}_3$ )

+MS, 0.5min #27



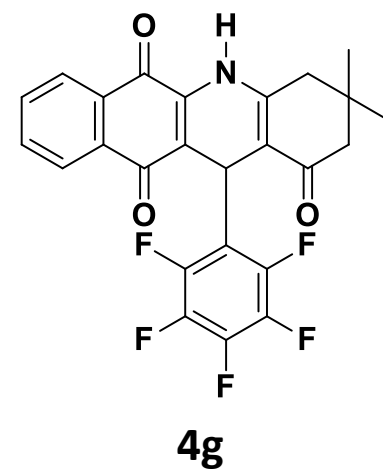
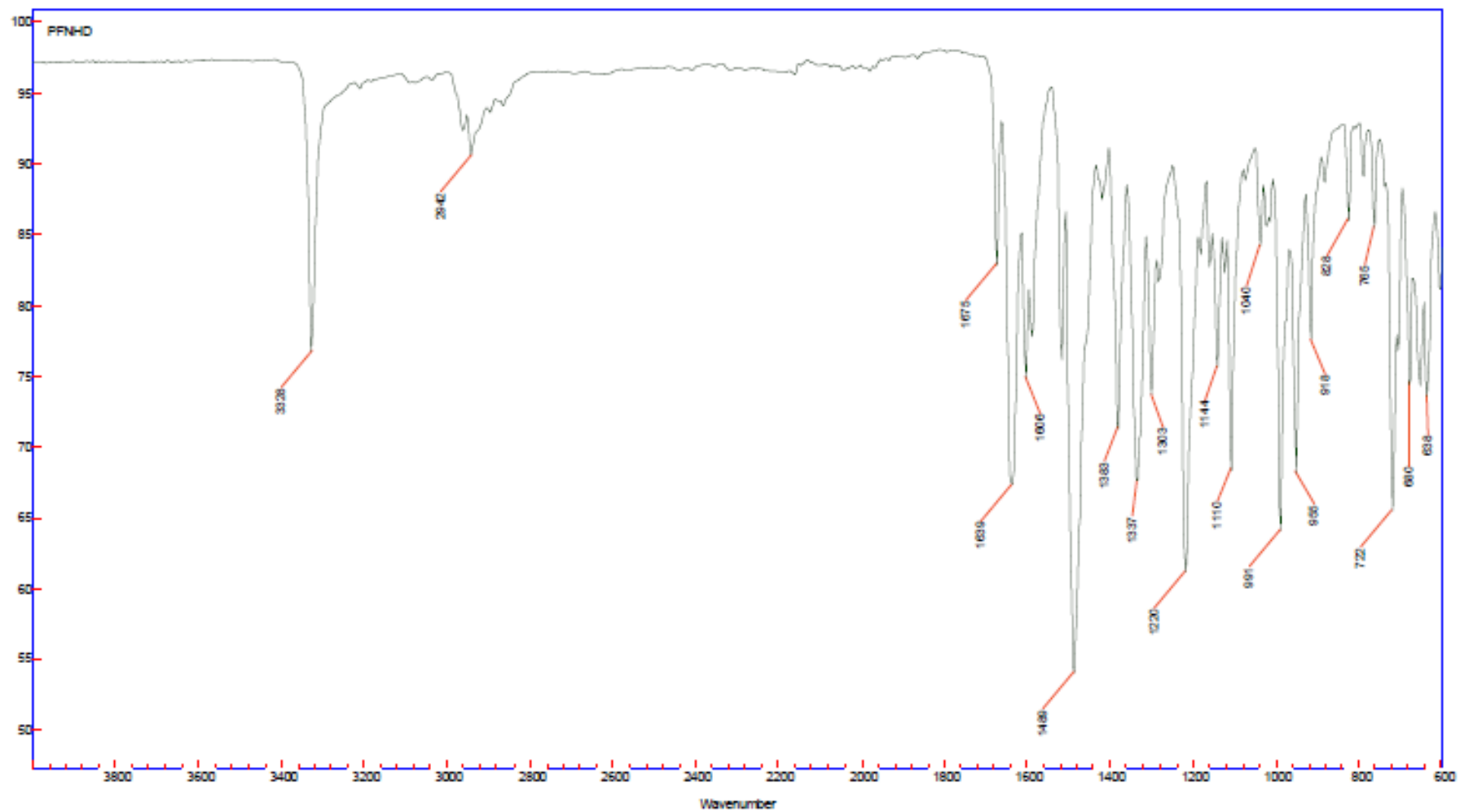
Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
402.1521	1	C <sub>25</sub> H <sub>21</sub> FNO <sub>3</sub>	402.149998	-5.3	-4.4	15.5	ok	even		5.8	8.9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
	2	C <sub>18</sub> H <sub>25</sub> FNO <sub>8</sub>	402.155871	9.3	9.8	6.5	ok	even		36.7	58.1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	



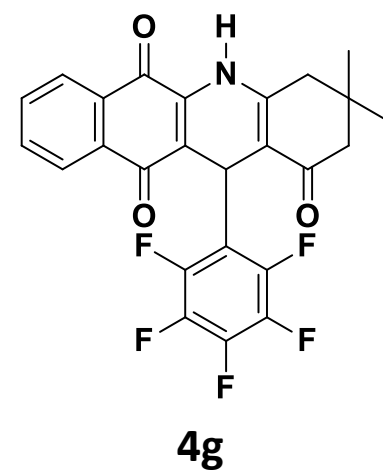
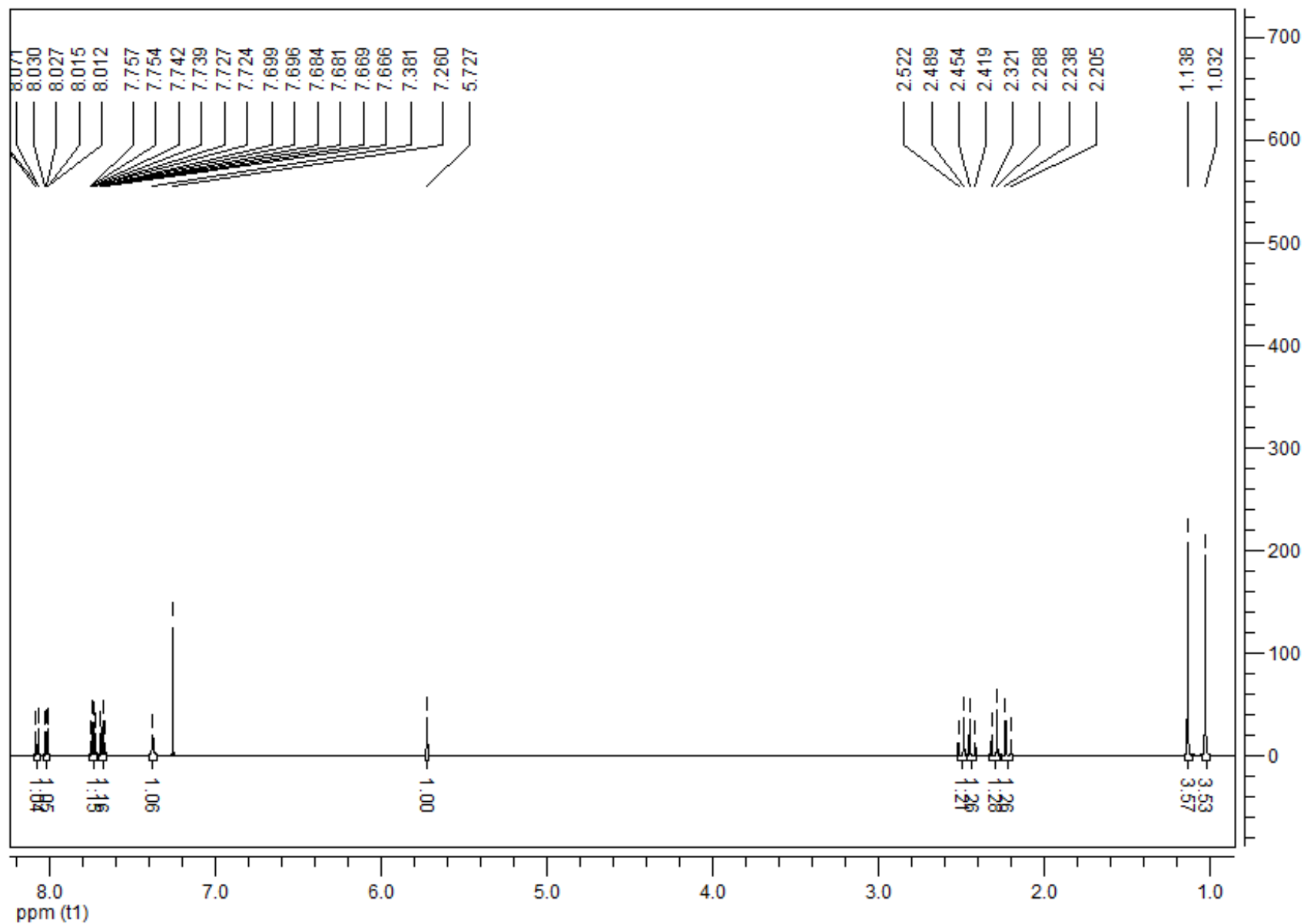
Exact Mass: 402,1505

**4f**

HRMS of compound **4f**

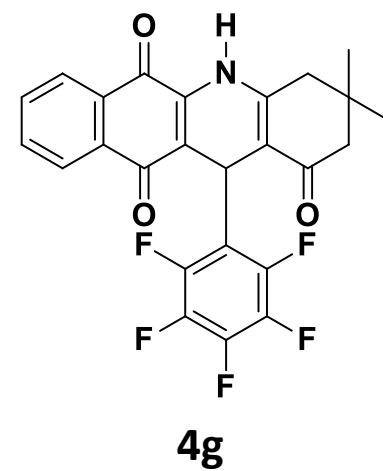
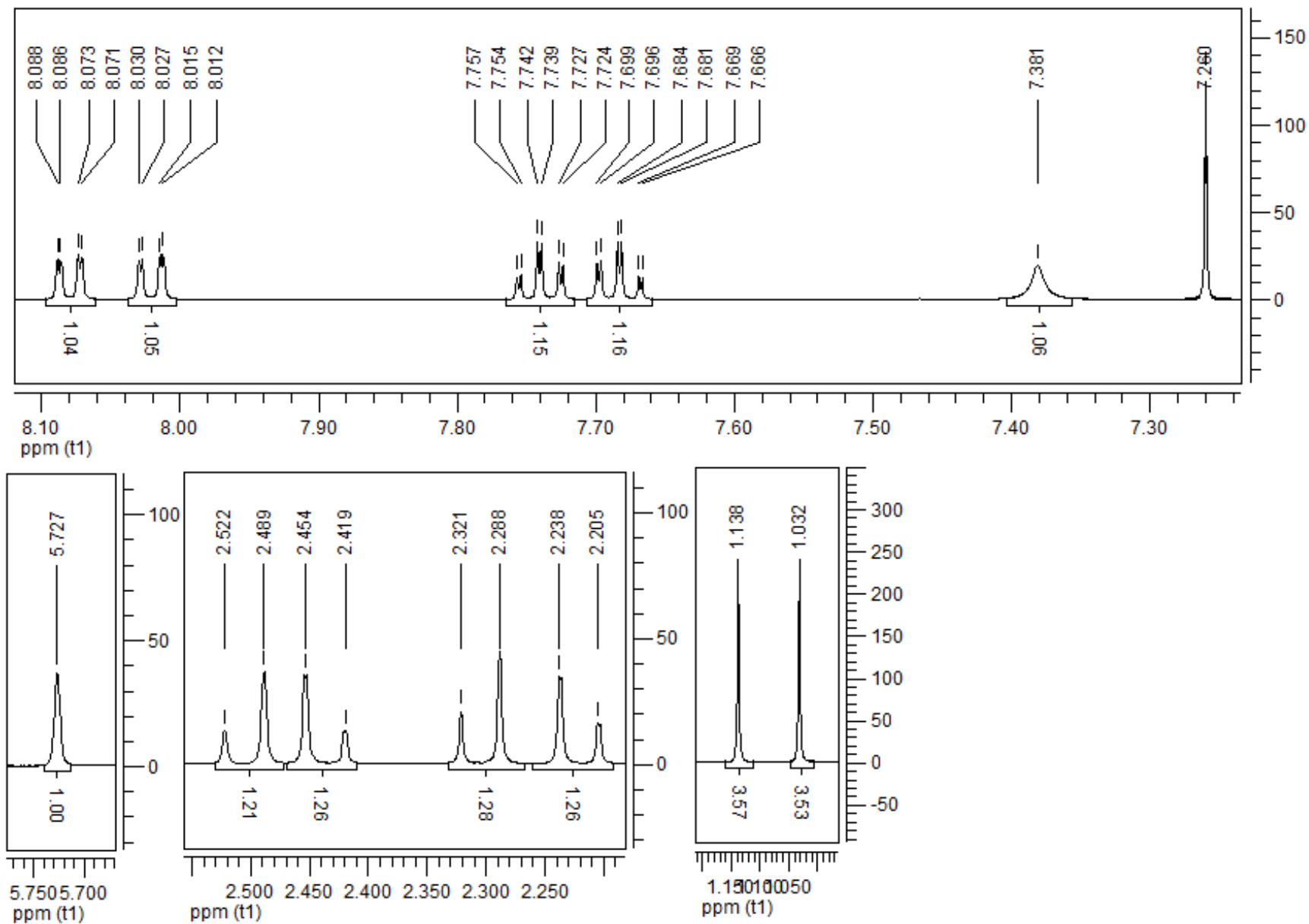


IR spectrum of compound **4g**

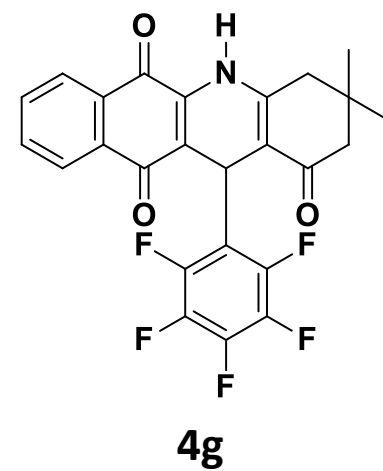
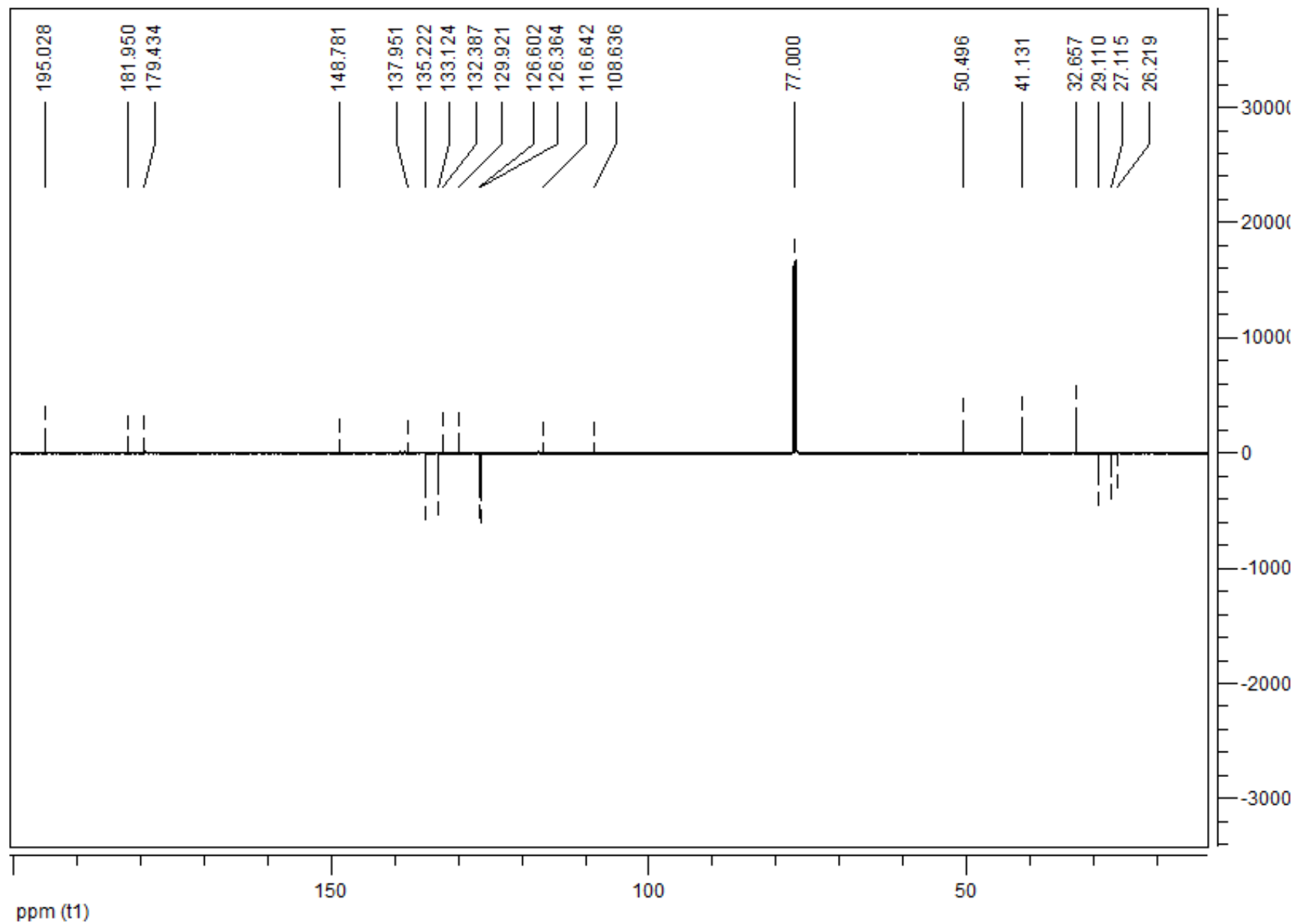


<sup>1</sup>H NMR spectrum of compound **4g** (500.00 MHz, CDCl<sub>3</sub>)



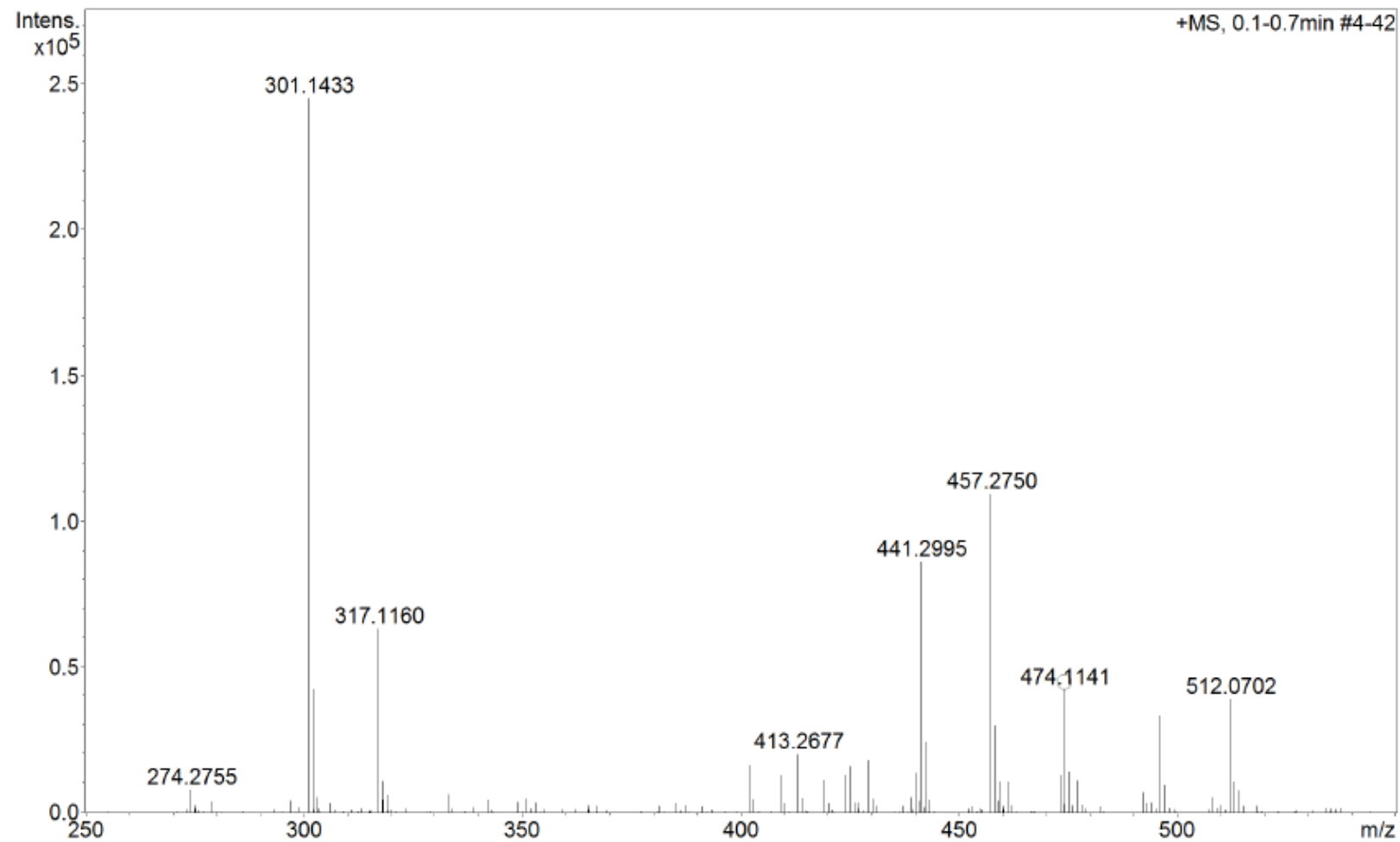


$^1\text{H}$  NMR spectrum of compound **4g** (500.00 MHz,  $\text{CDCl}_3$ )

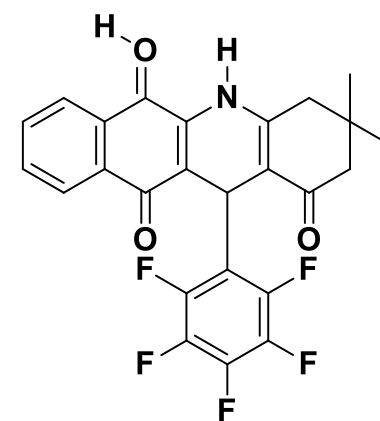


$^{13}\text{C}$  NMR spectrum of compound **4g** (125.0 MHz,  $\text{CDCl}_3$ )

+MS, 0.1-0.7min #4-42



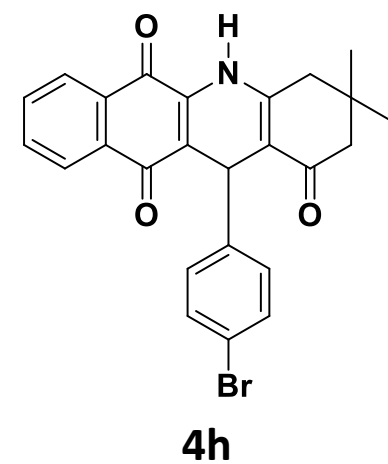
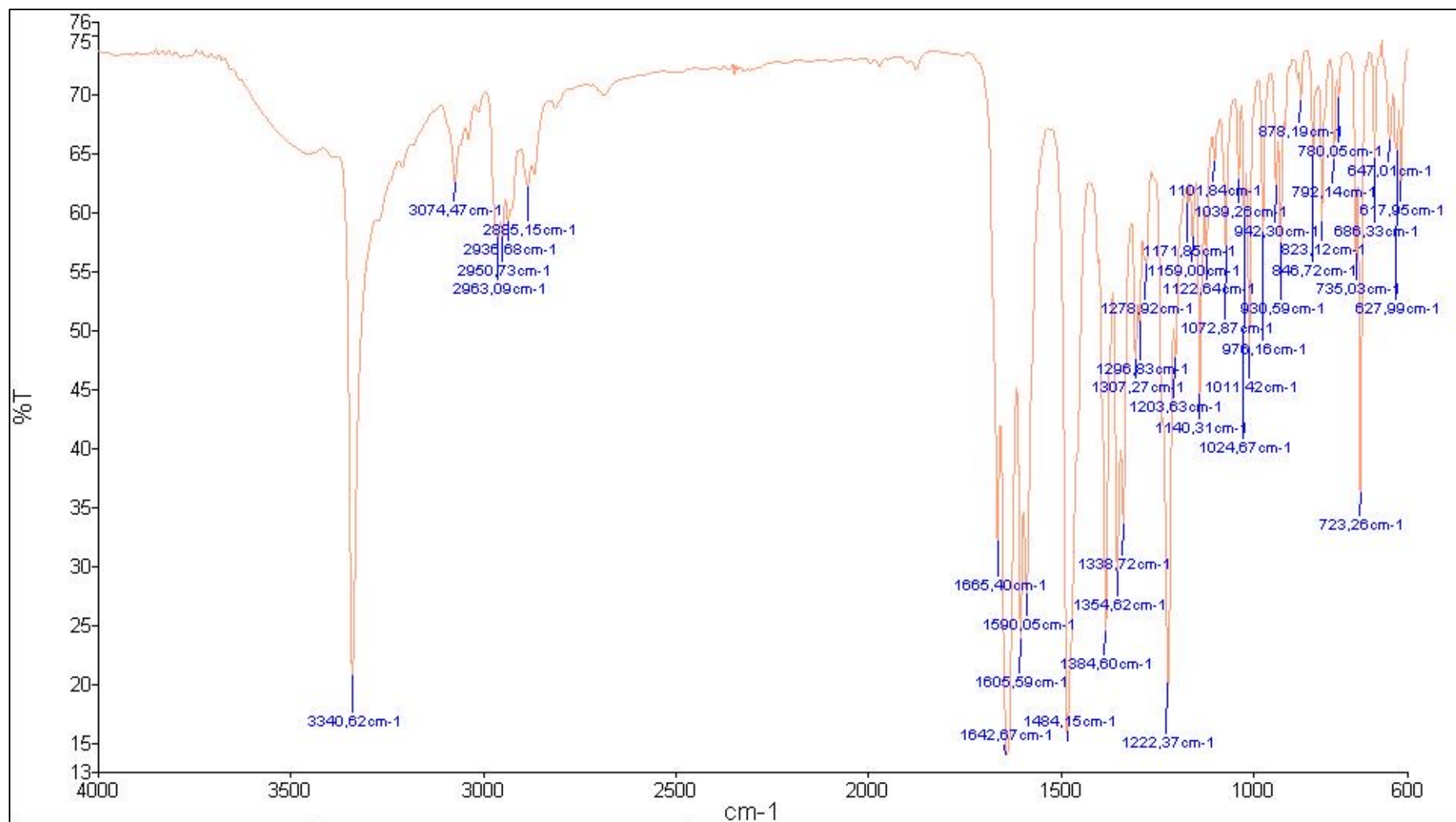
Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
474.114109	1	C <sub>25</sub> H <sub>17</sub> F <sub>5</sub> NO <sub>3</sub>	474.112311	-3.8	-2.1	15.5	ok	even		35.0	52.4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.		



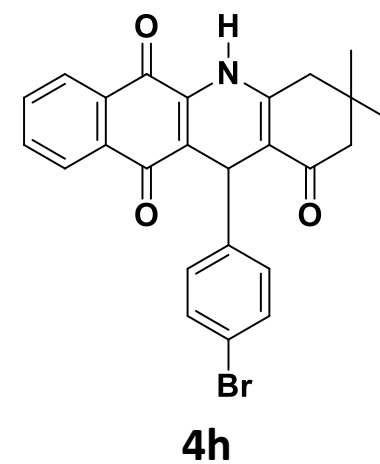
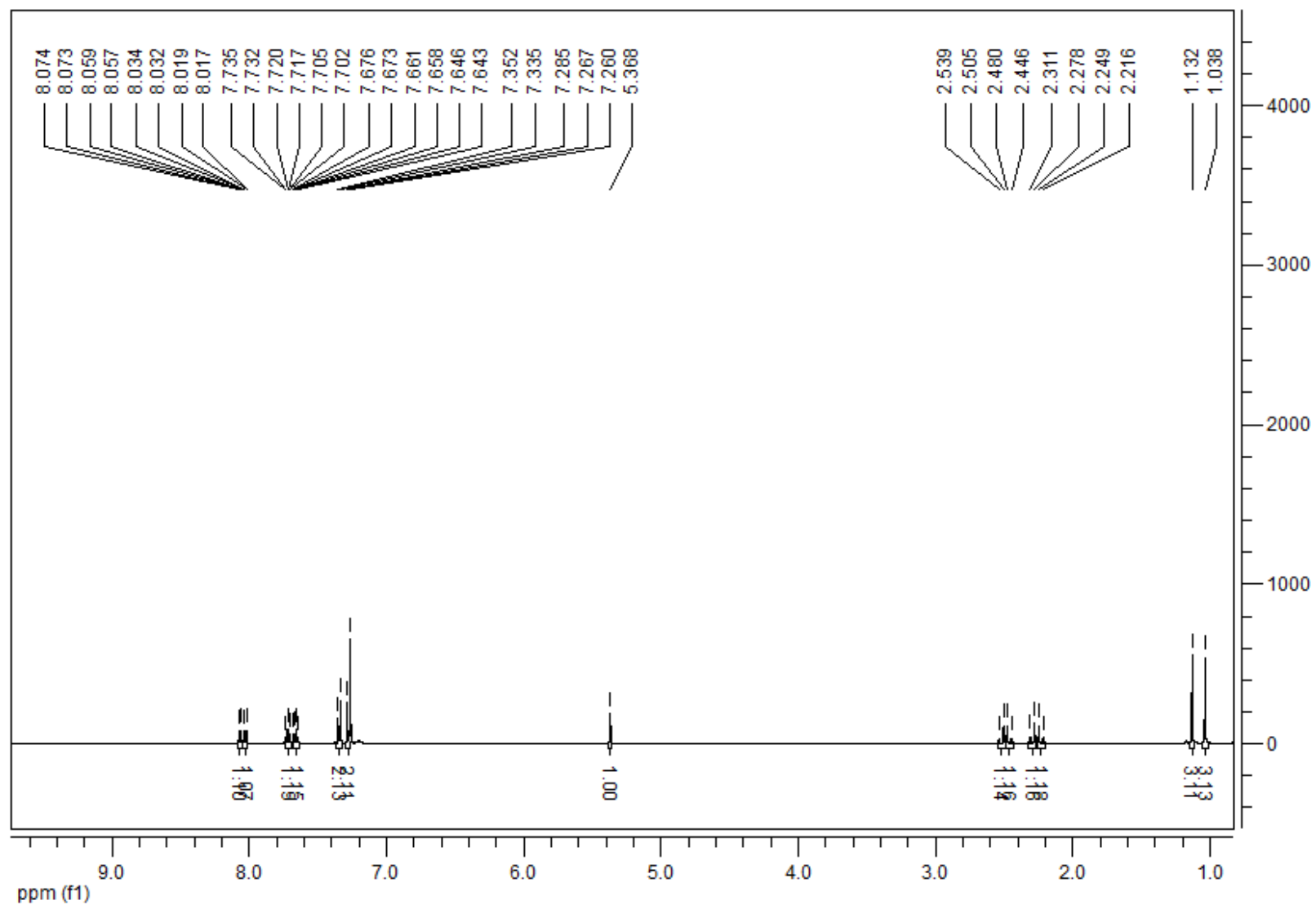
Exact Mass: 474,1129

**4g**

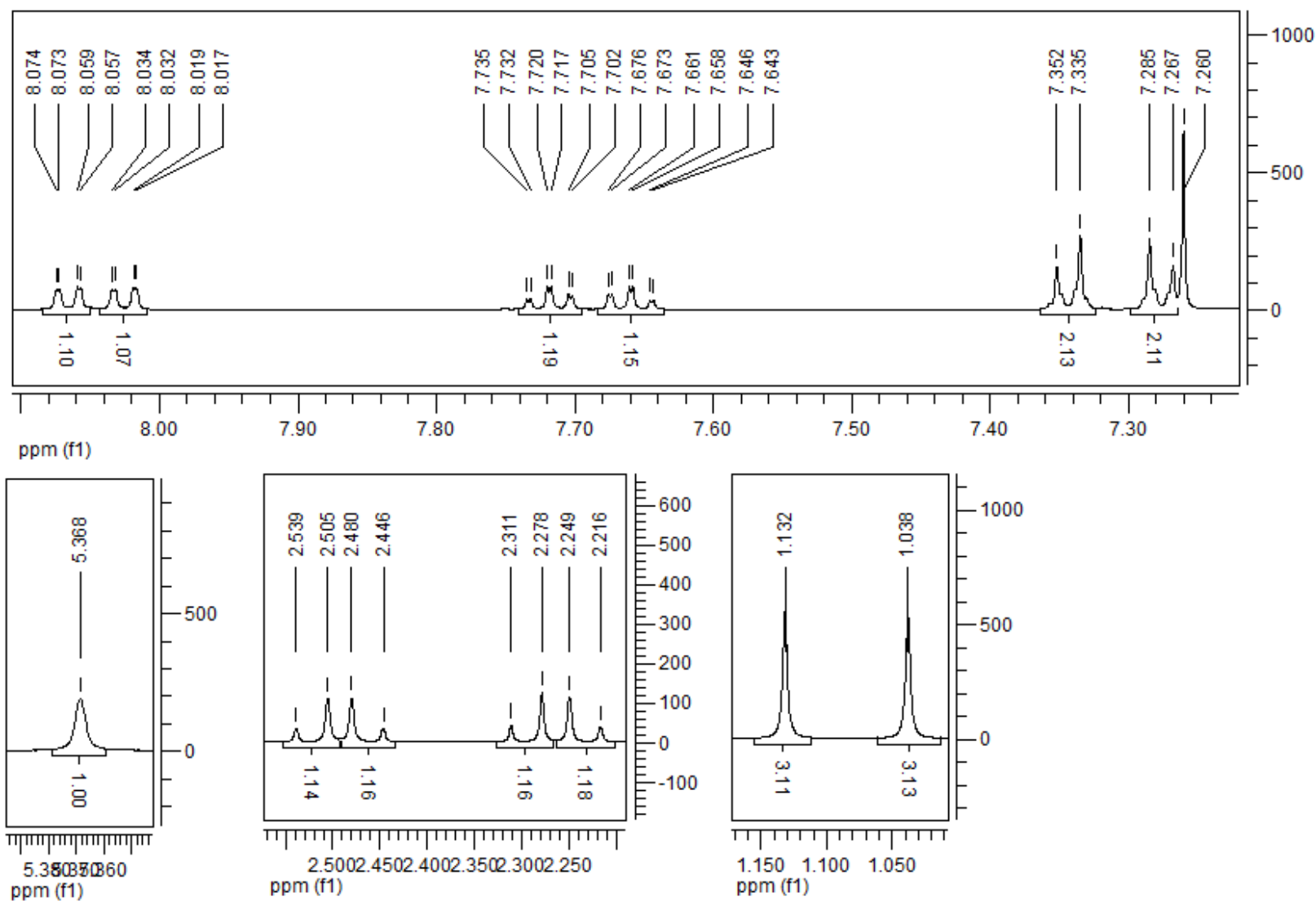
HRMS of compound **4g**



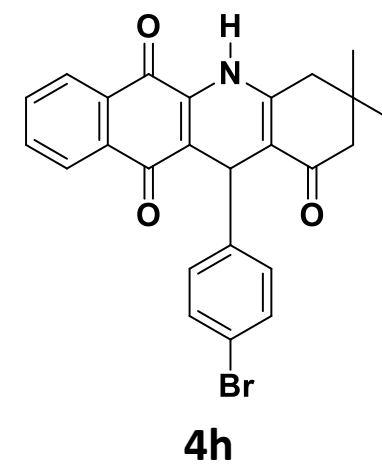
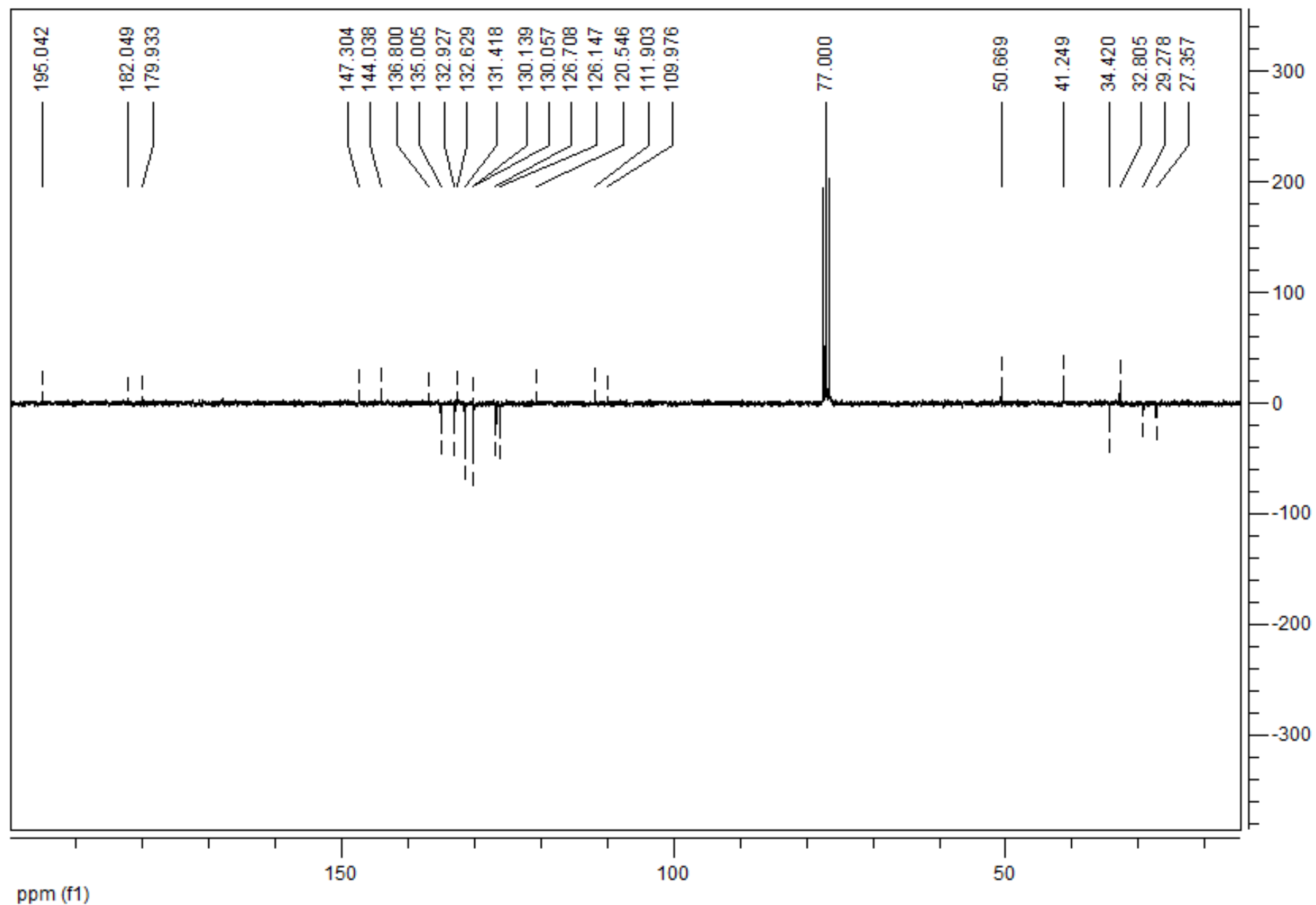
IR spectrum of compound **4h**



<sup>1</sup>H NMR spectrum of compound **4h** (500.00 MHz, CDCl<sub>3</sub>)

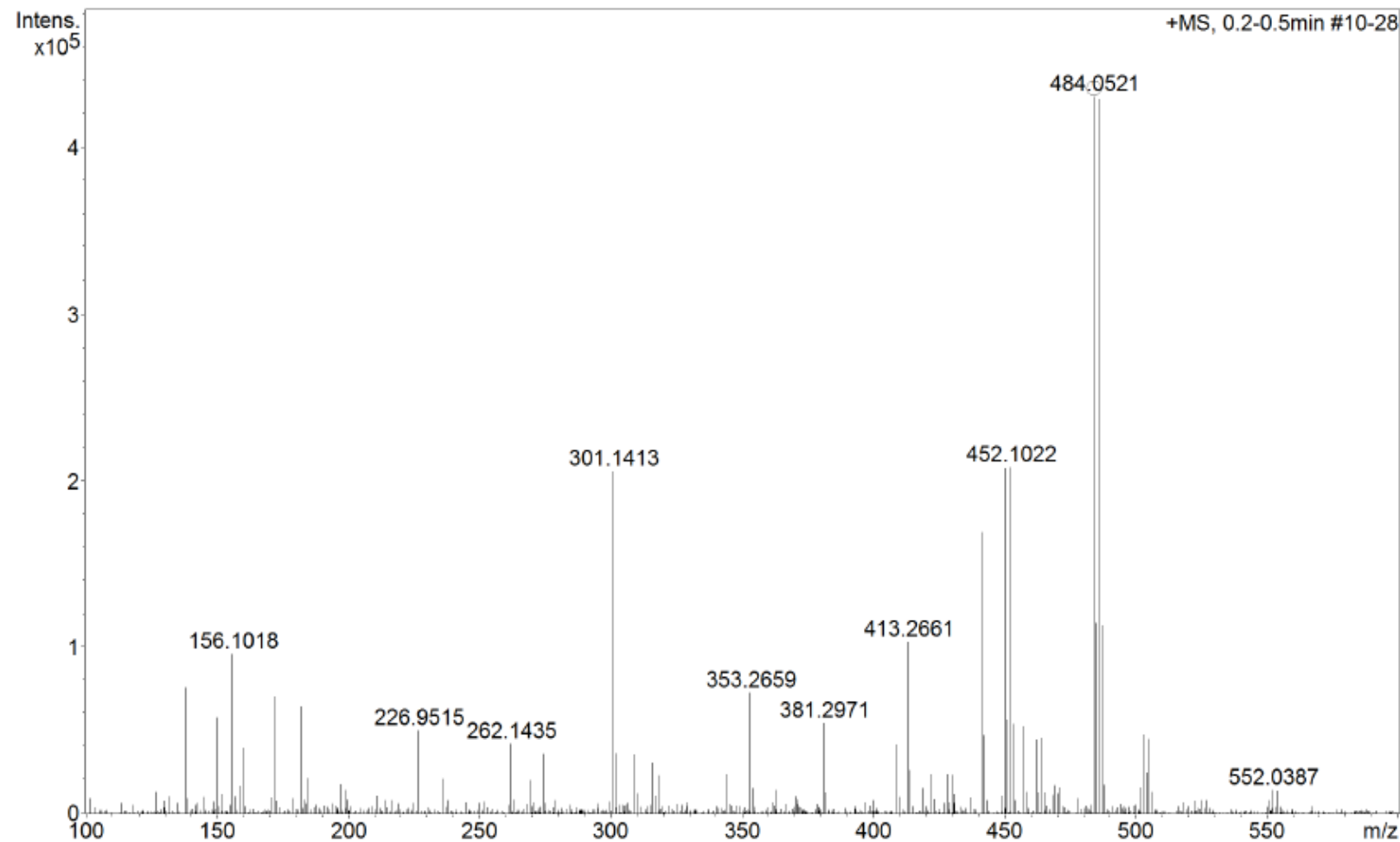


<sup>1</sup>H NMR spectrum of compound **4h** (500.00 MHz, CDCl<sub>3</sub>)

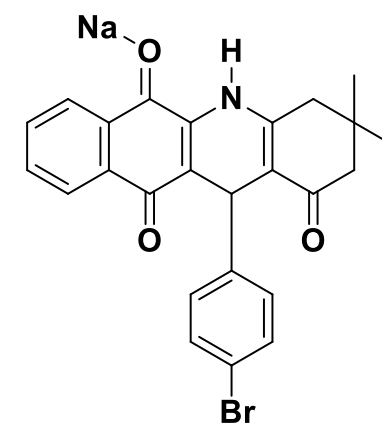


$^{13}\text{C}$  NMR spectrum of compound **4h** (75.0 MHz,  $\text{CDCl}_3$ )

+MS, 0.2-0.5min #10-28



Meas. m/z	# Ion	Formula	m/z err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
484.052074	1	C <sub>25</sub> H <sub>20</sub> BrNNaO <sub>3</sub>	484.051876	-0.4	0.2	15.5	ok	even	8.3	7.4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
	2	C <sub>21</sub> H <sub>16</sub> BrN <sub>7</sub> NaO	484.049191	-6.0	-6.0	16.5	ok	even	10.2	10.5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

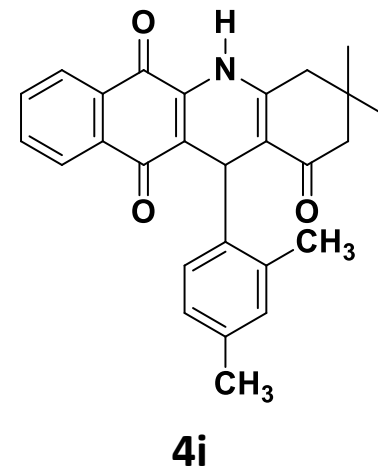
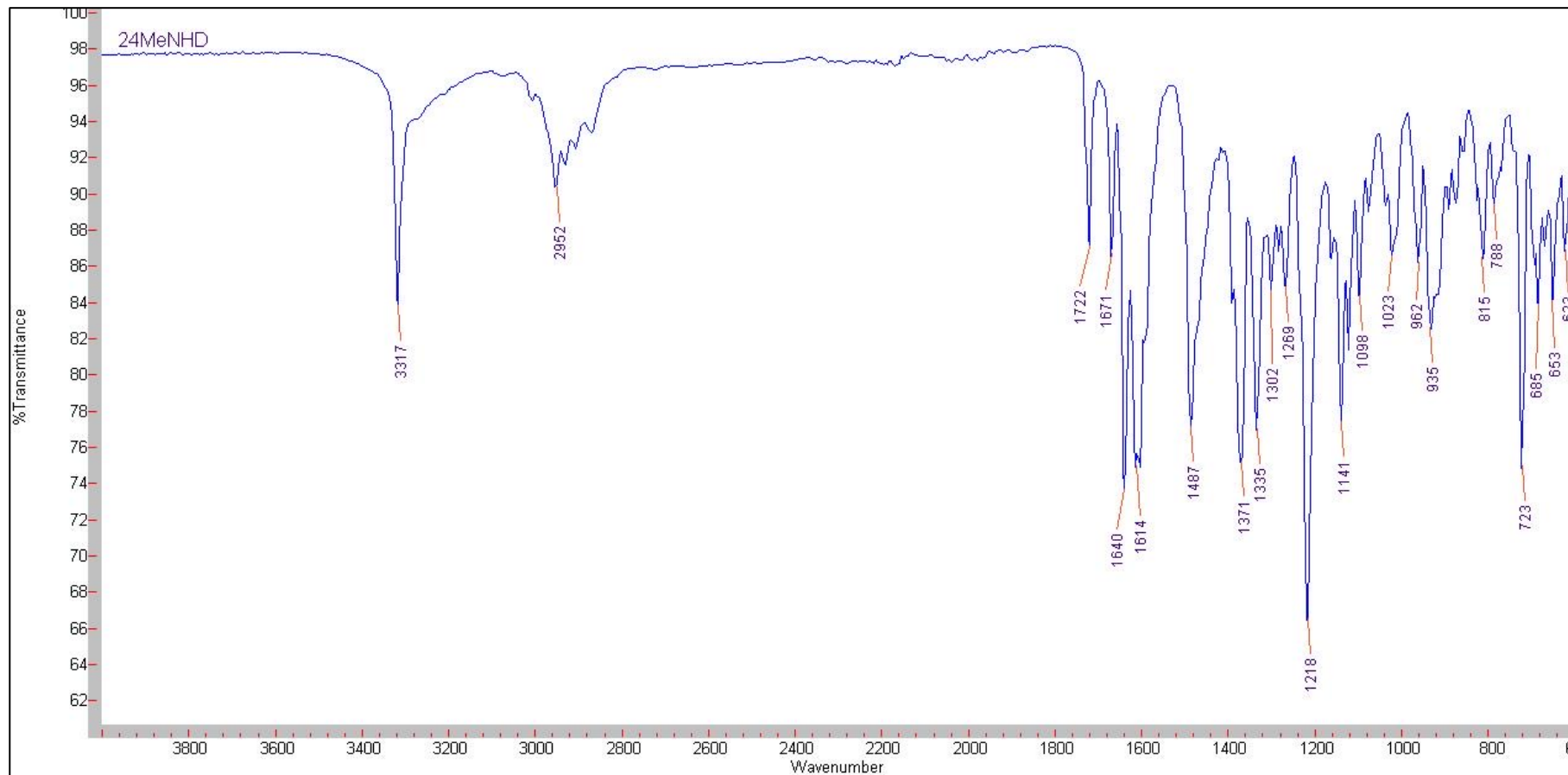


Exact Mass: 484,0524

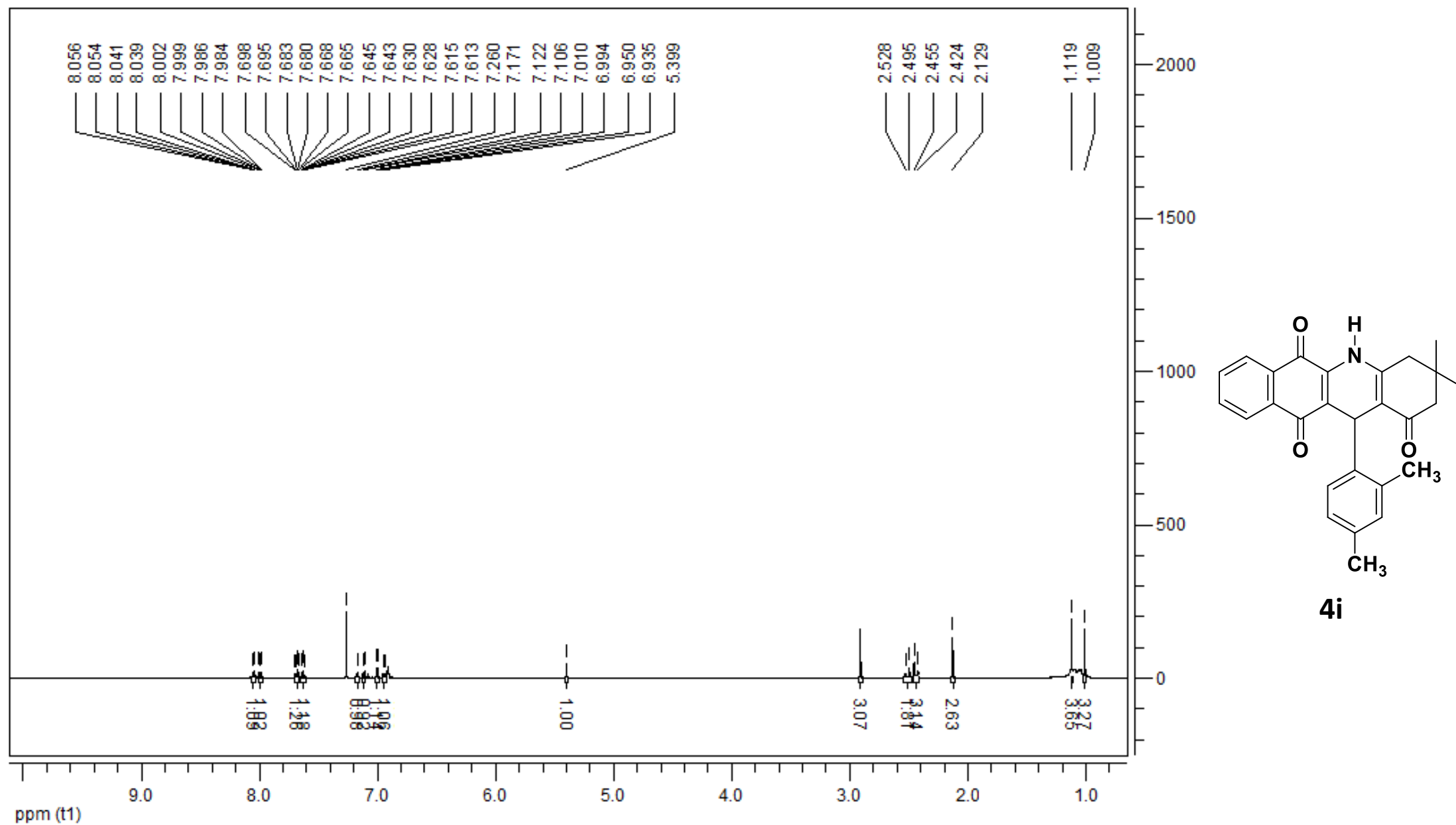
**4h**

HRMS of compound **4h**

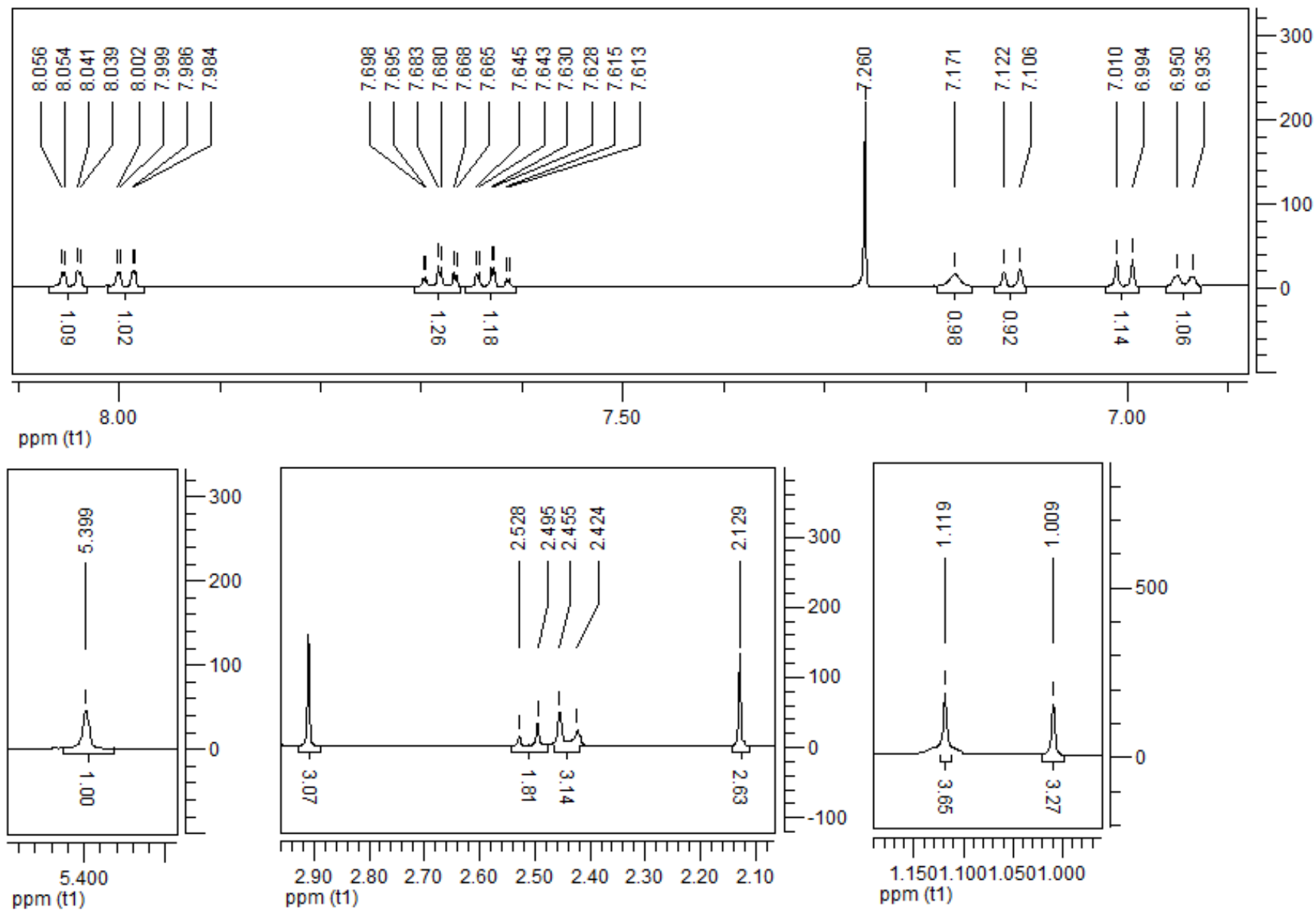




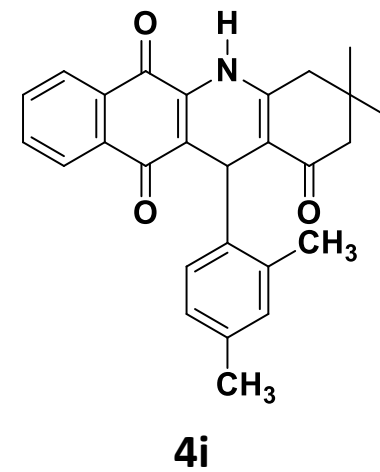
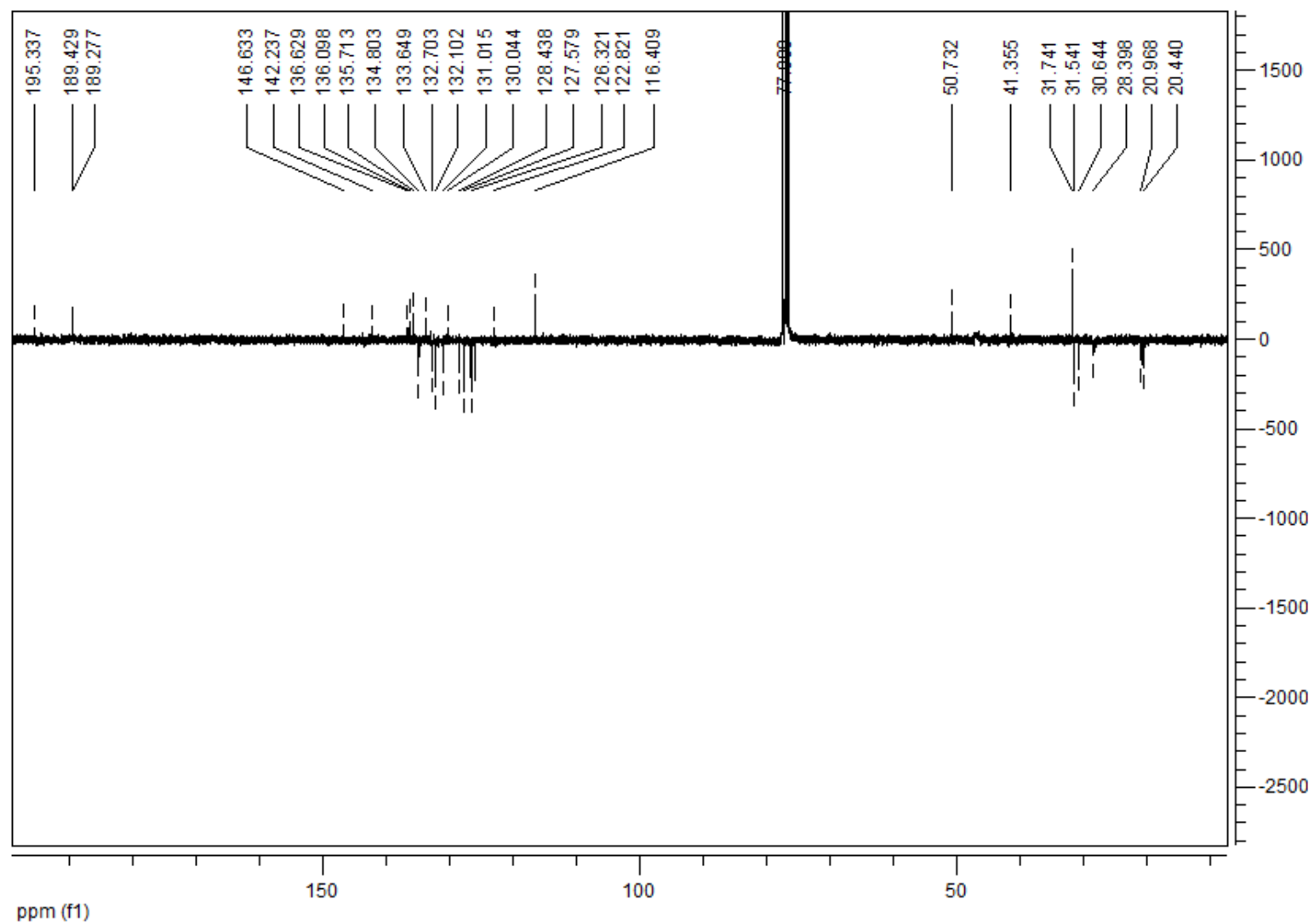
IR spectrum of compound **4i**



$^1\text{H}$  NMR spectrum of compound **4i** (500.00 MHz,  $\text{CDCl}_3$ )

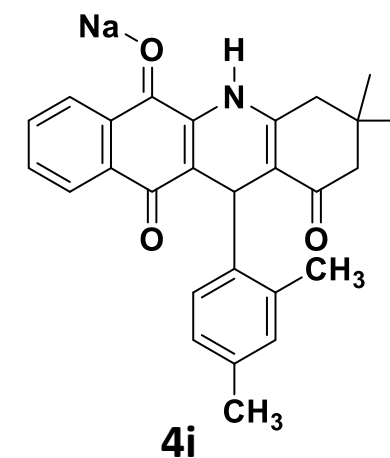
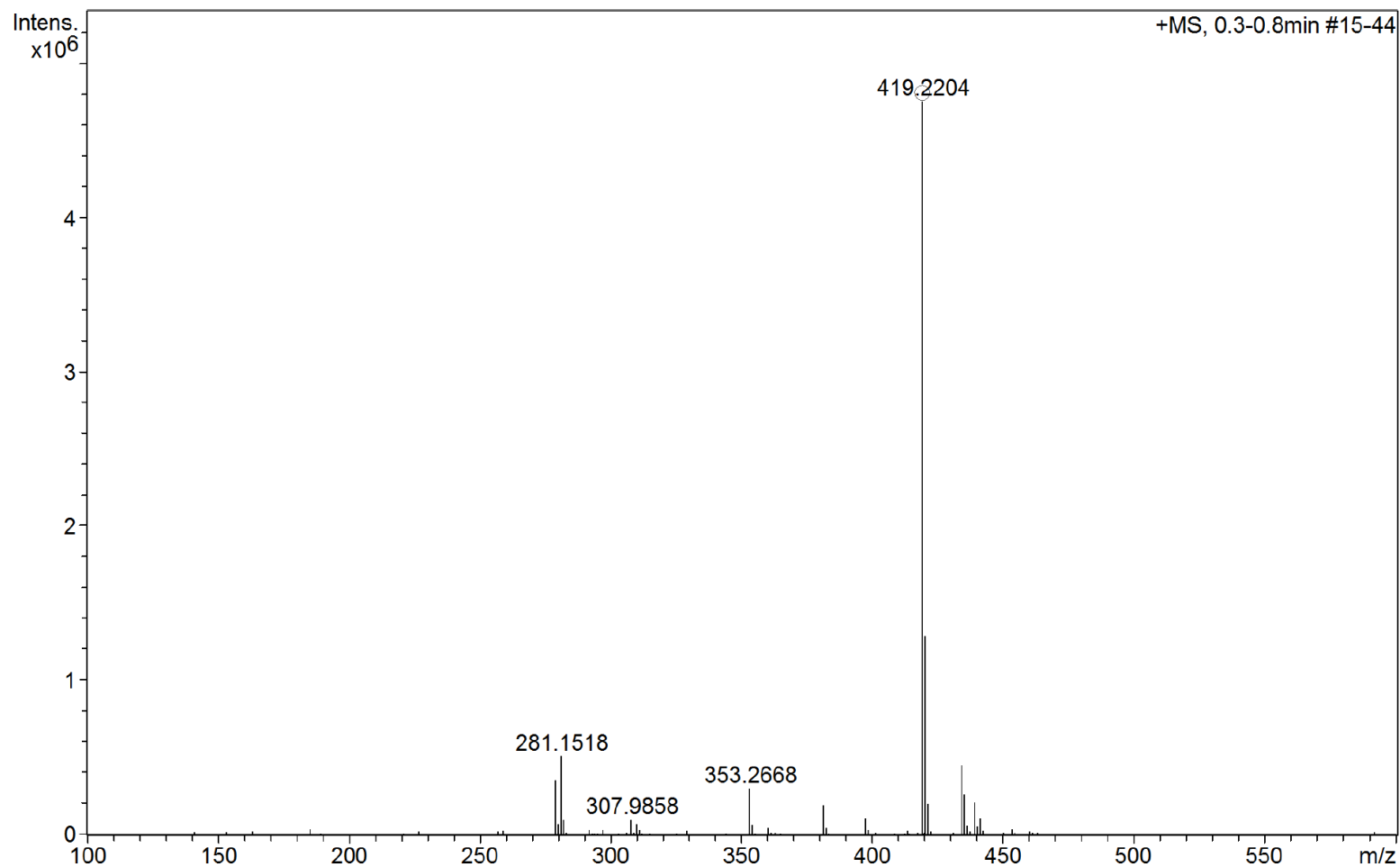


$^1\text{H}$  NMR spectrum of compound **4i** (500.00 MHz,  $\text{CDCl}_3$ )



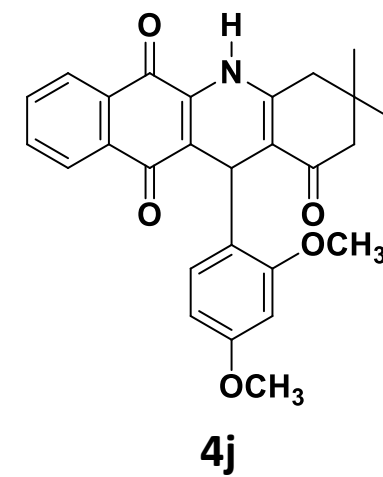
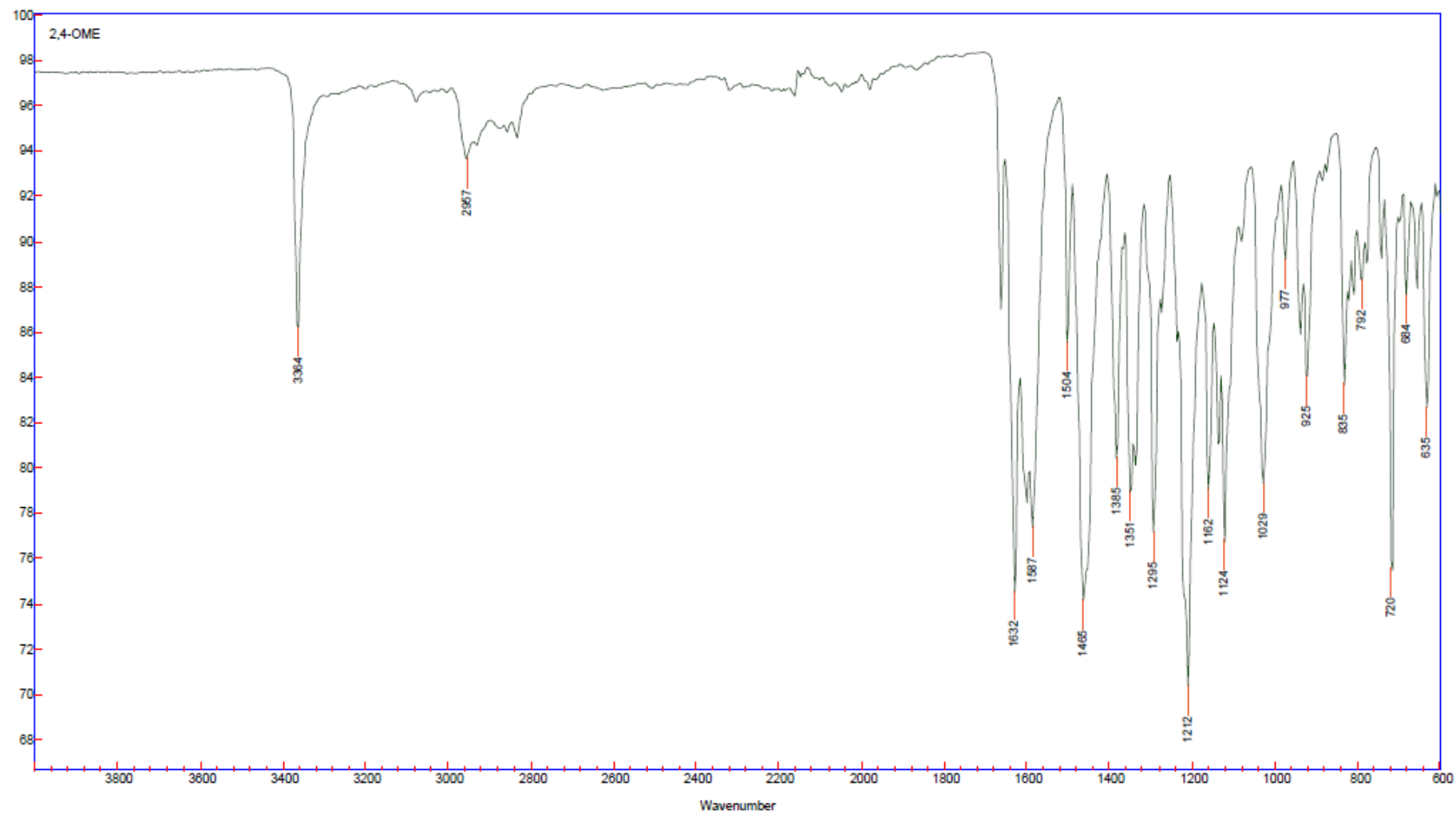
$^{13}\text{C}$  NMR spectrum of compound **4i** (75.0 MHz,  $\text{CDCl}_3$ )

+MS, 0.3-0.8min #15-44

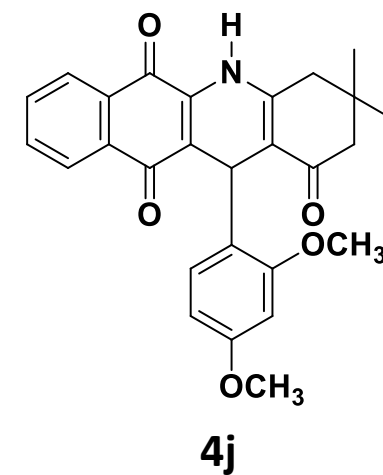
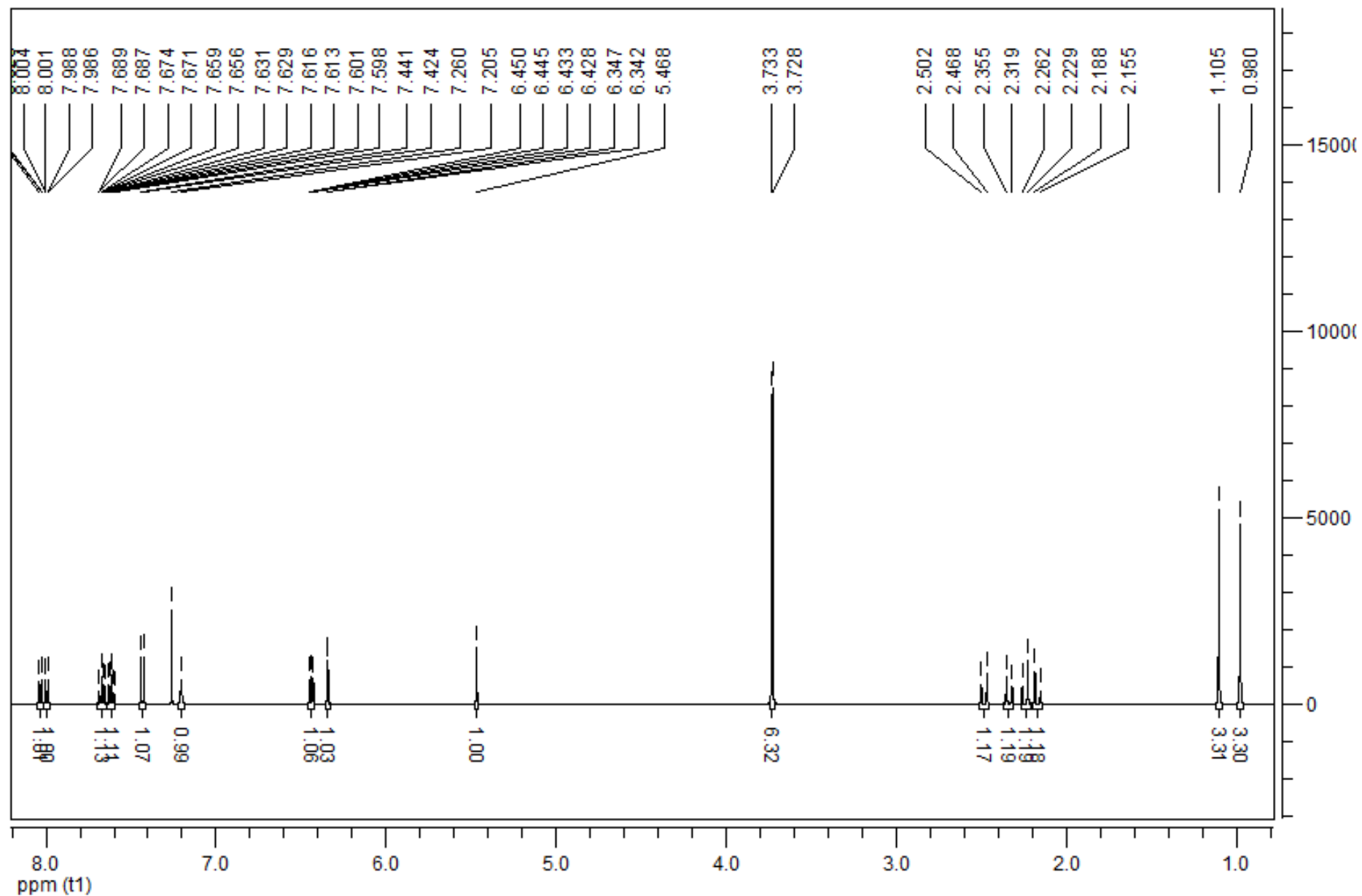


Meas. m/z	# Ion	Formula	m/z err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std	Mean m/z	Std I	VarNorm	Std	m/z Diff	Std	Comb	Dev
419.220360	1	C <sub>23</sub> H <sub>27</sub> N <sub>6</sub> O <sub>2</sub>	419.219001	-3.2	-4.0	13.5	ok	even	2.0	2.5		n.a.		n.a.		n.a.		n.a.	
	2	C <sub>27</sub> H <sub>31</sub> O <sub>4</sub>	419.221686	3.2	3.1	12.5	ok	even	15.7	24.5		n.a.		n.a.		n.a.		n.a.	
	1	C <sub>25</sub> H <sub>32</sub> NaO <sub>4</sub>	419.219280	-2.6	-2.6	9.5	ok	even	2.9	4.9		n.a.		n.a.		n.a.		n.a.	
	2	C <sub>26</sub> H <sub>28</sub> N <sub>4</sub> Na	419.220618	0.6	0.3	14.5	ok	even	15.9	22.9		n.a.		n.a.		n.a.		n.a.	

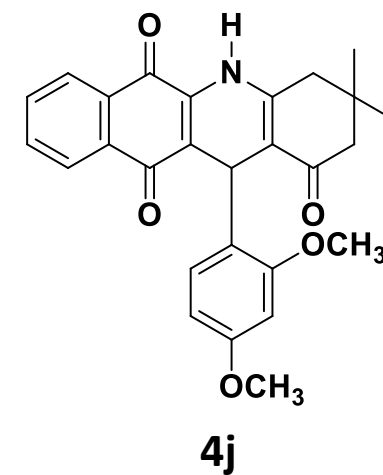
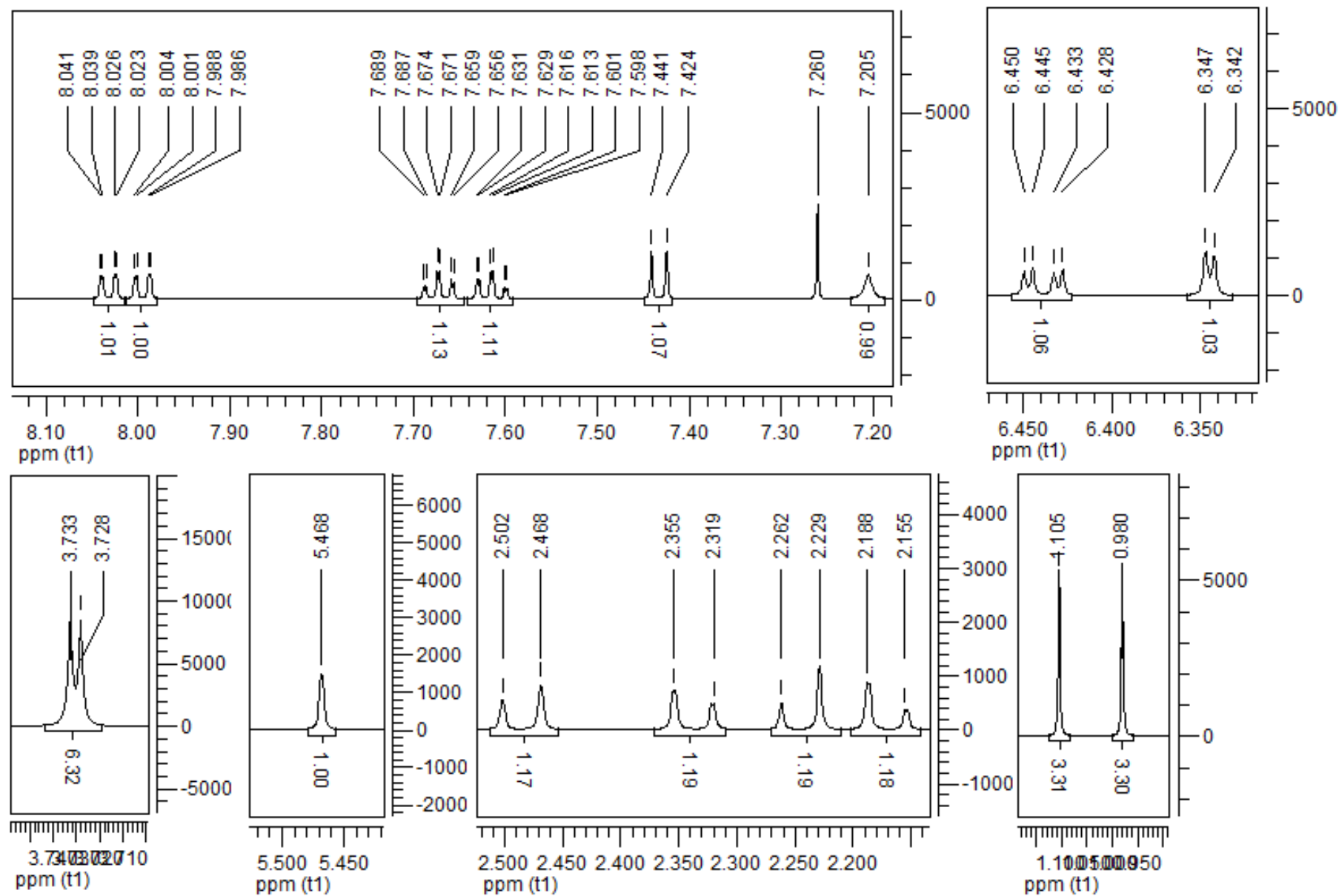
HRMS of compound **4i**



IR spectrum of compound **4j**

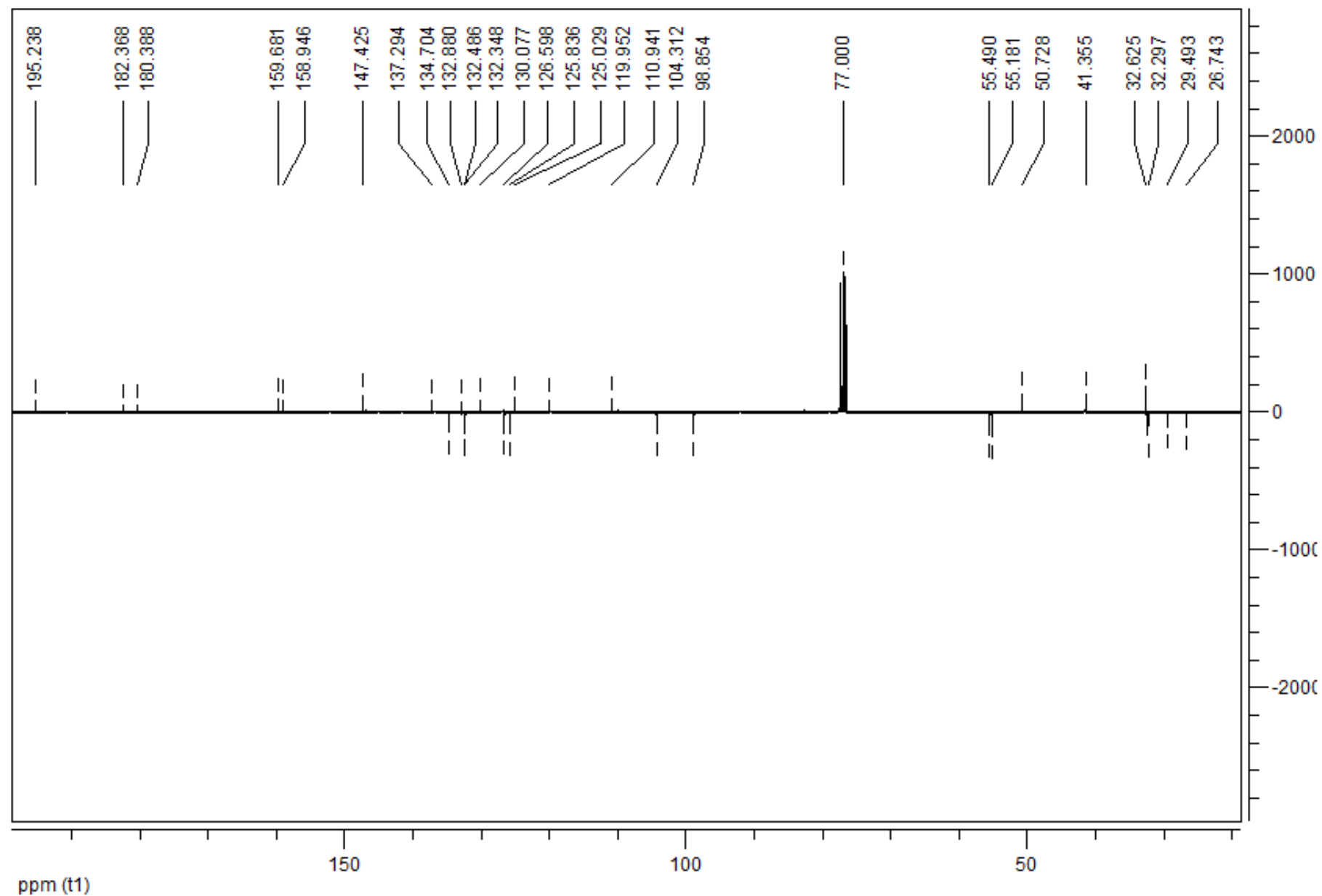


<sup>1</sup>H NMR spectrum of compound **4j** (500.00 MHz, CDCl<sub>3</sub>)

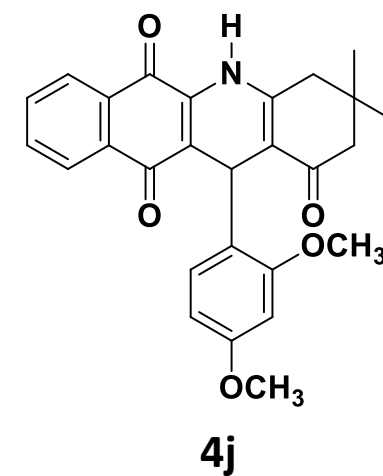


$^1\text{H}$  NMR spectrum of compound **4j** (500.00 MHz,  $\text{CDCl}_3$ )

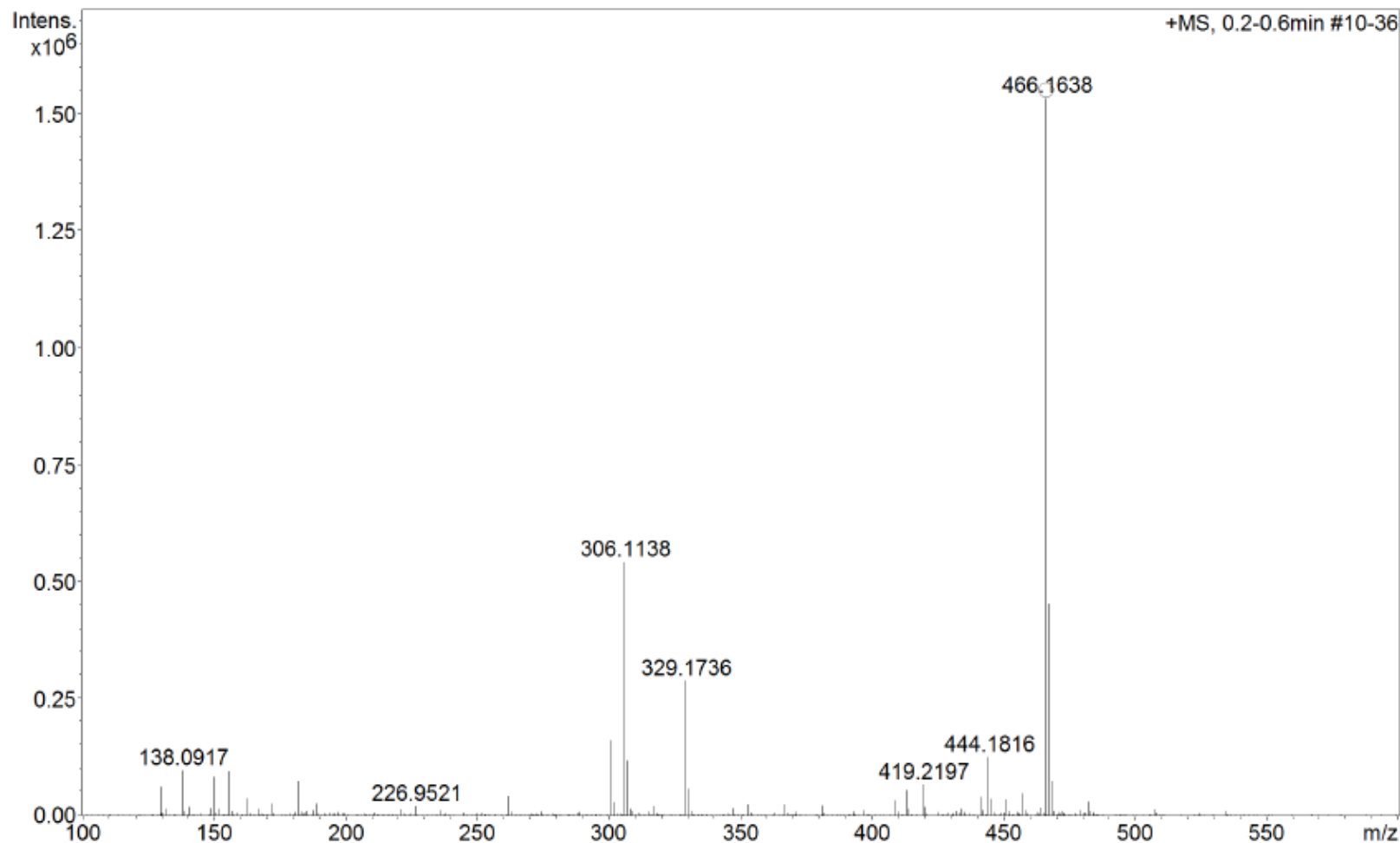




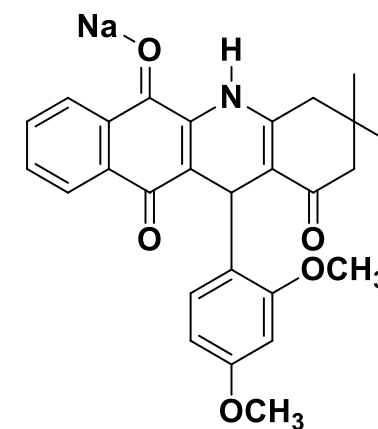
$^{13}\text{C}$  NMR spectrum of compound **4j** (75.0 MHz,  $\text{CDCl}_3$ )



+MS, 0.2-0.6min #10-36



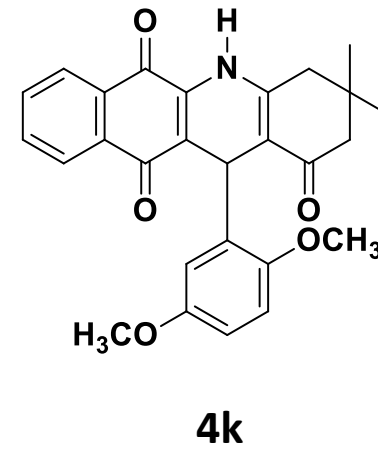
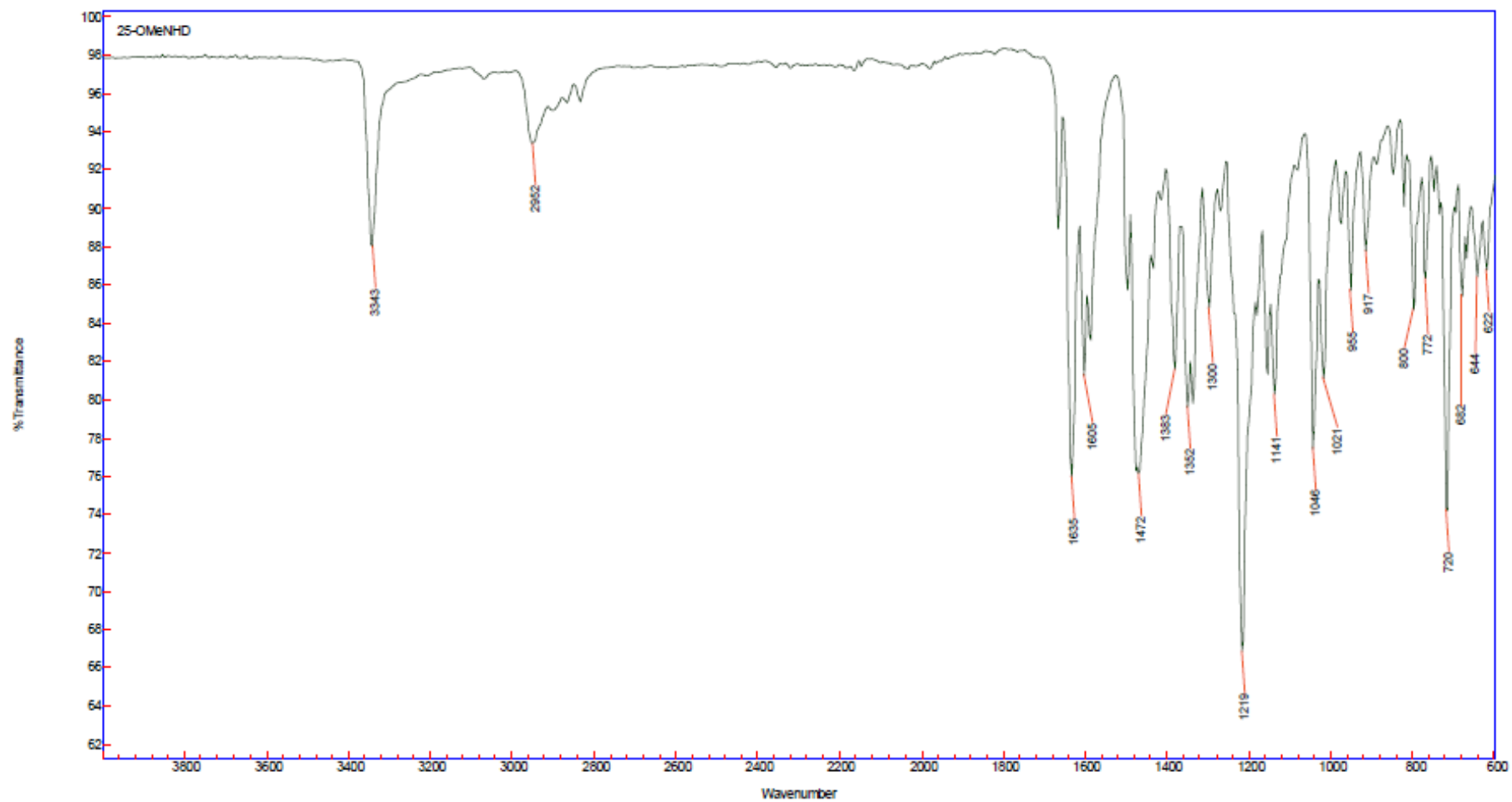
Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
466.163781	1	C <sub>27</sub> H <sub>25</sub> NNaO <sub>5</sub>	466.162494	-2.8	-2.4	15.5	ok	even		3.4	6.8	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
	2	C <sub>28</sub> H <sub>21</sub> N <sub>5</sub> NaO	466.163831	0.1	-0.2	20.5	ok	even		15.8	22.6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.



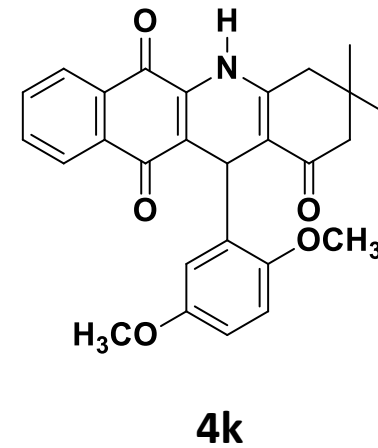
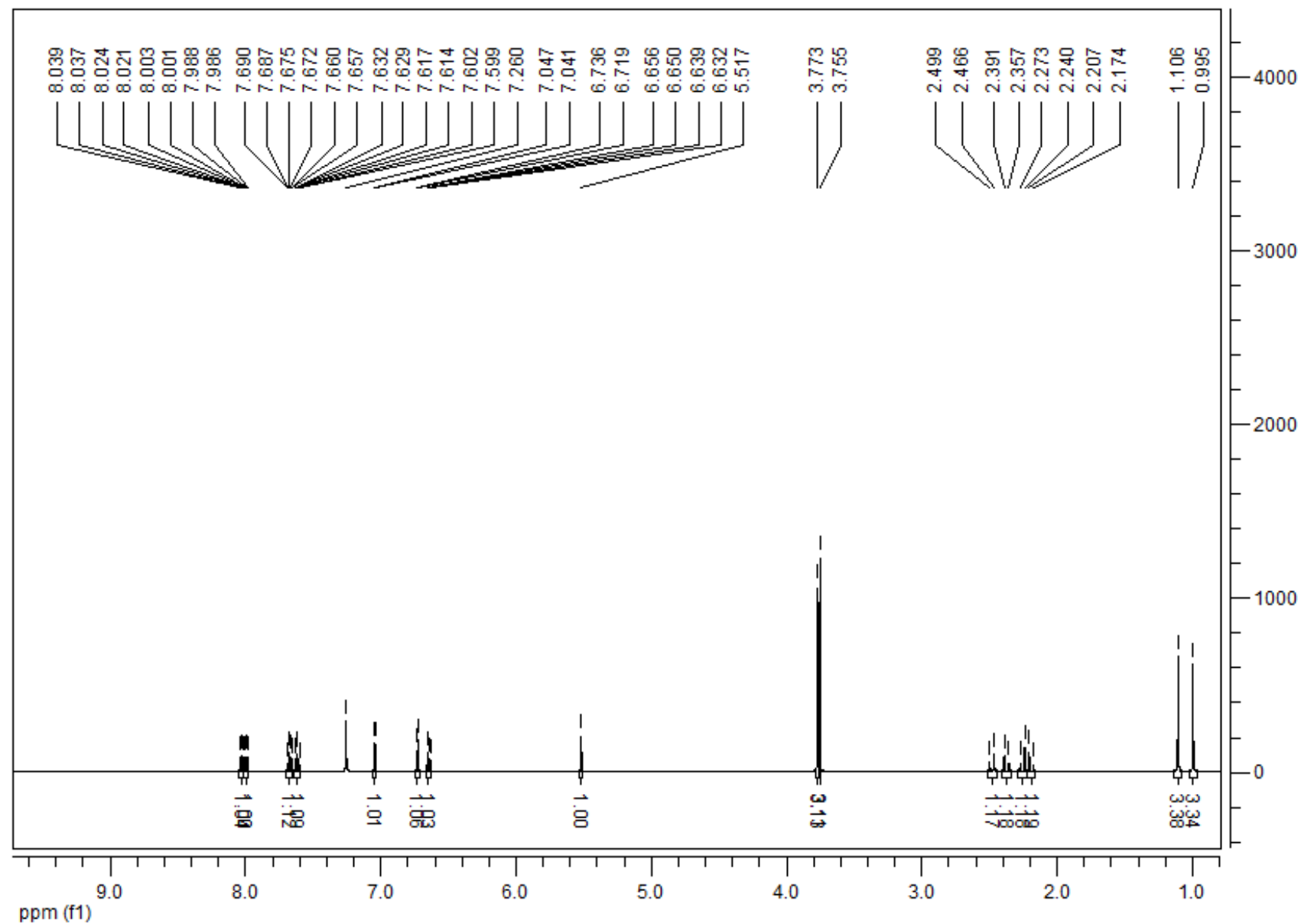
Exact Mass: 466,1630

**4j**

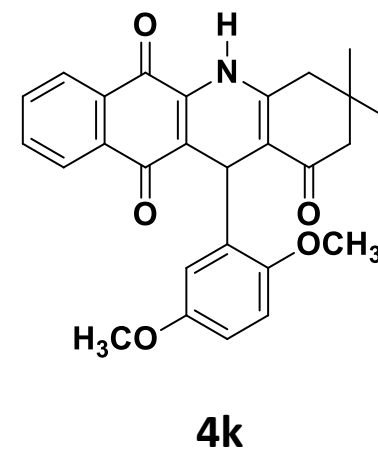
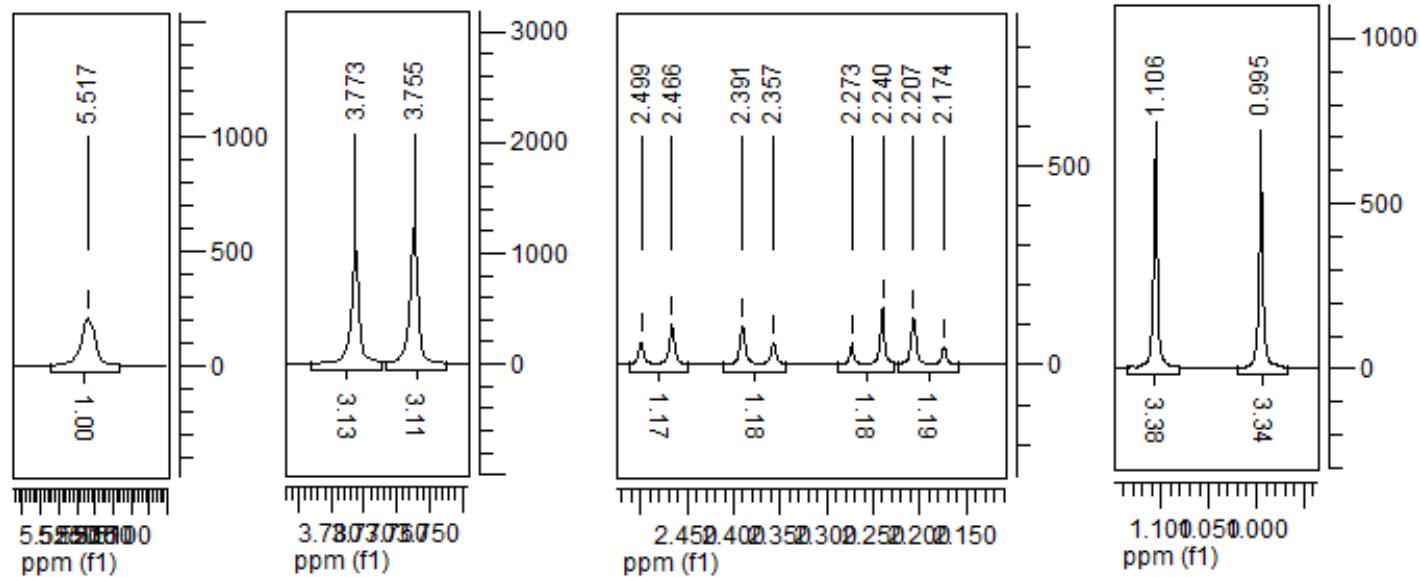
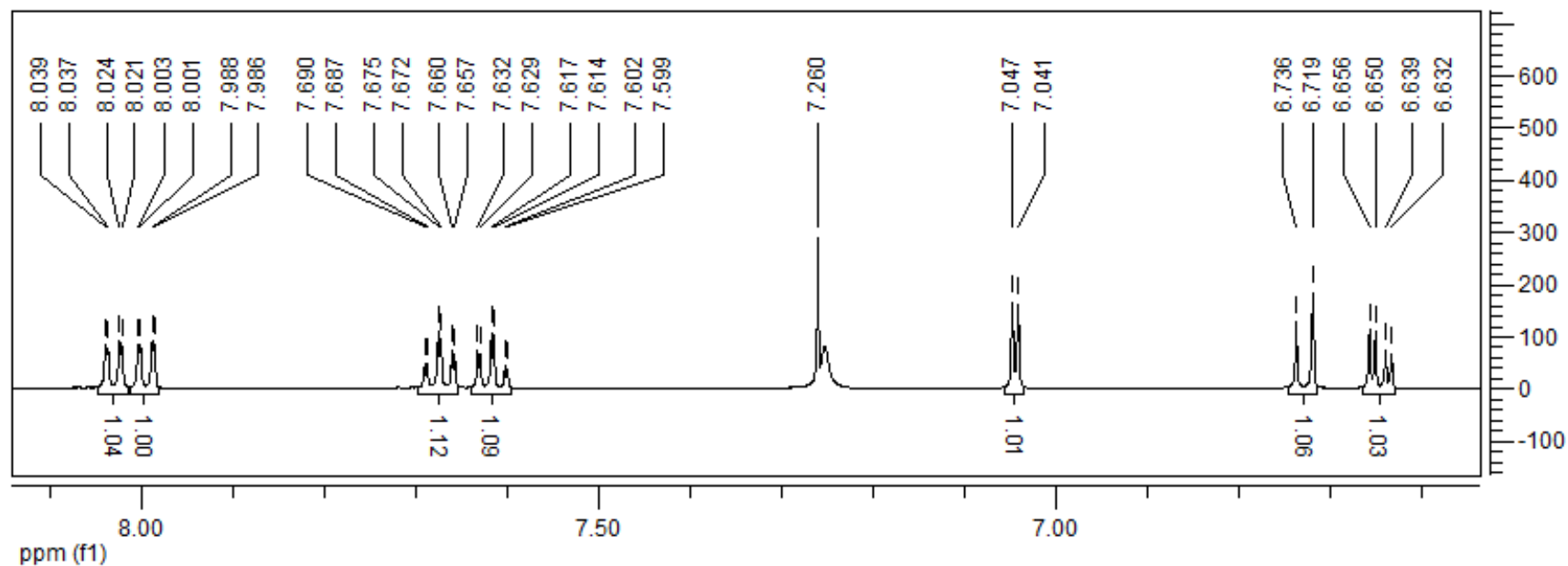
HRMS of compound **4j**



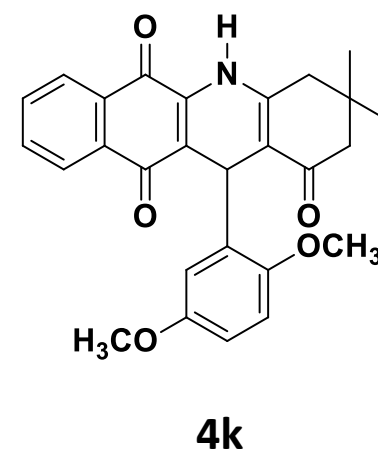
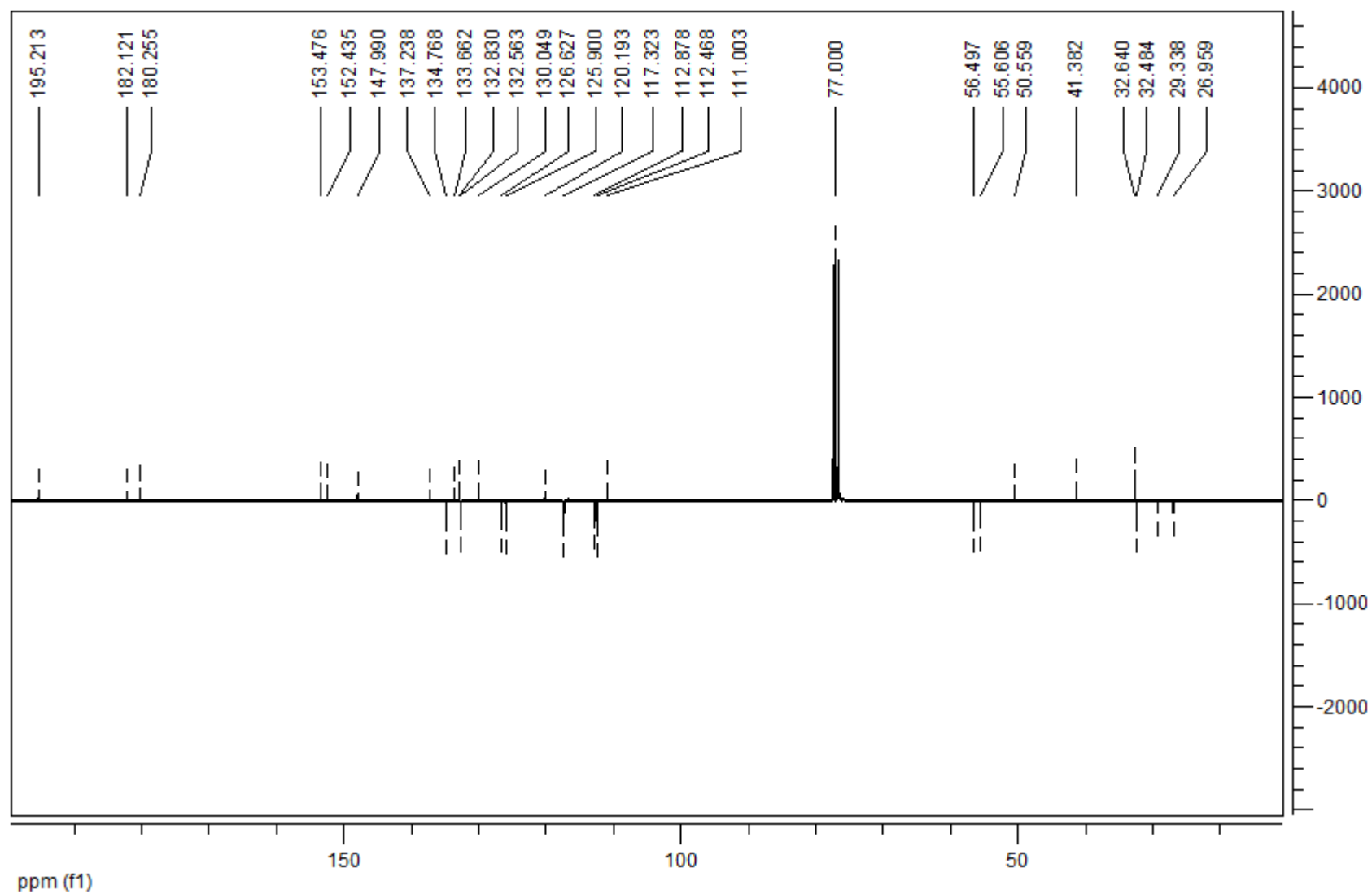
IR spectrum of compound **4k**



<sup>1</sup>H NMR spectrum of compound **4k** (500.00 MHz, CDCl<sub>3</sub>)

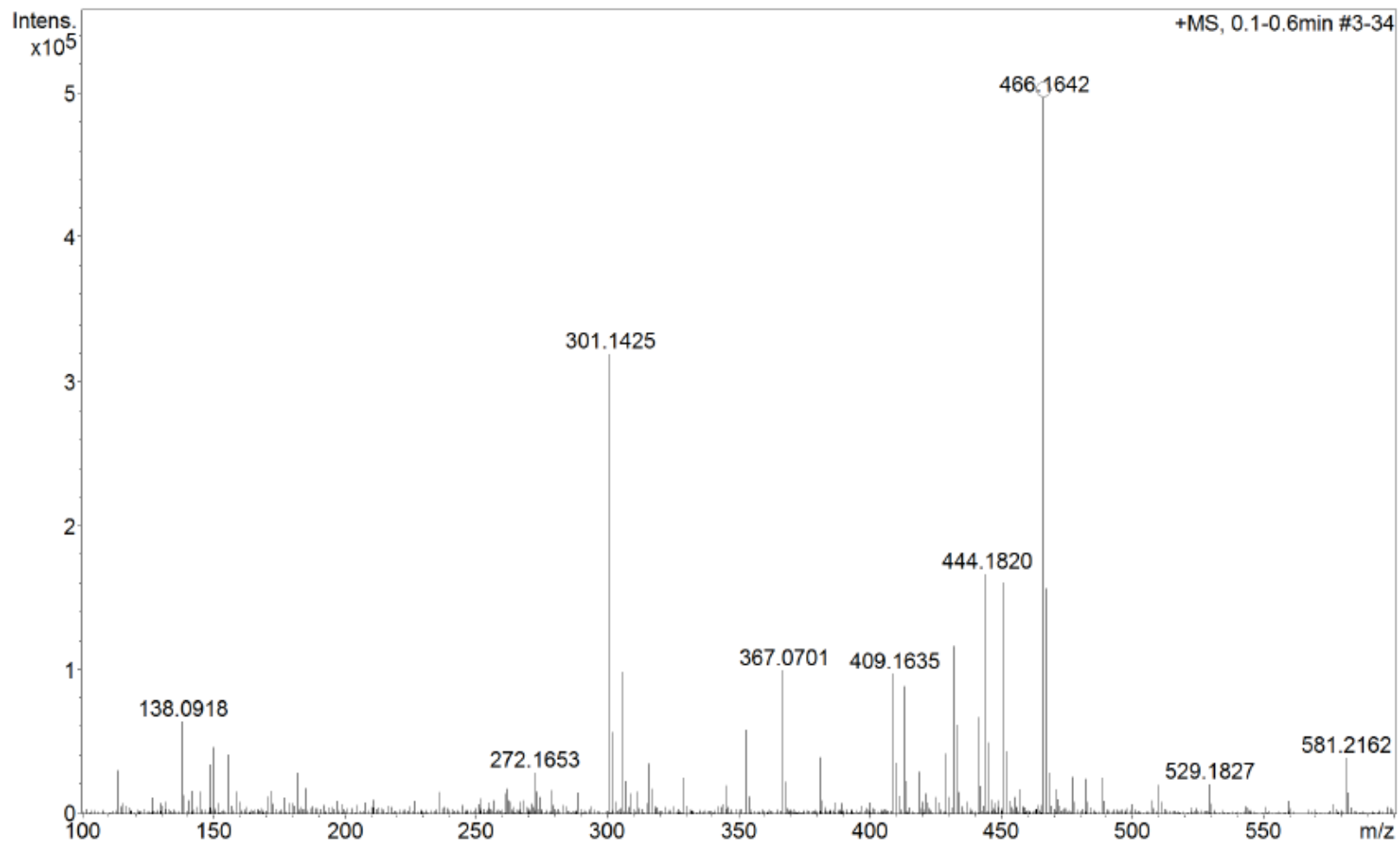


$^1\text{H}$  NMR spectrum of compound **4k** (500.00 MHz,  $\text{CDCl}_3$ )

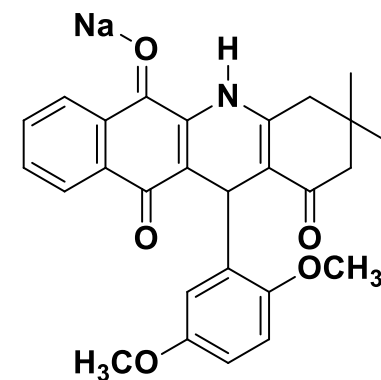


<sup>13</sup>C NMR spectrum of compound **4k** (75.0 MHz, CDCl<sub>3</sub>)

+MS, 0.1-0.6min #3-34



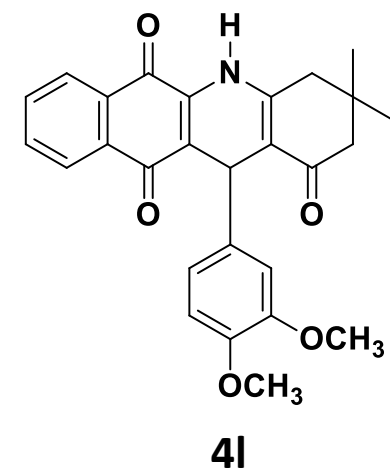
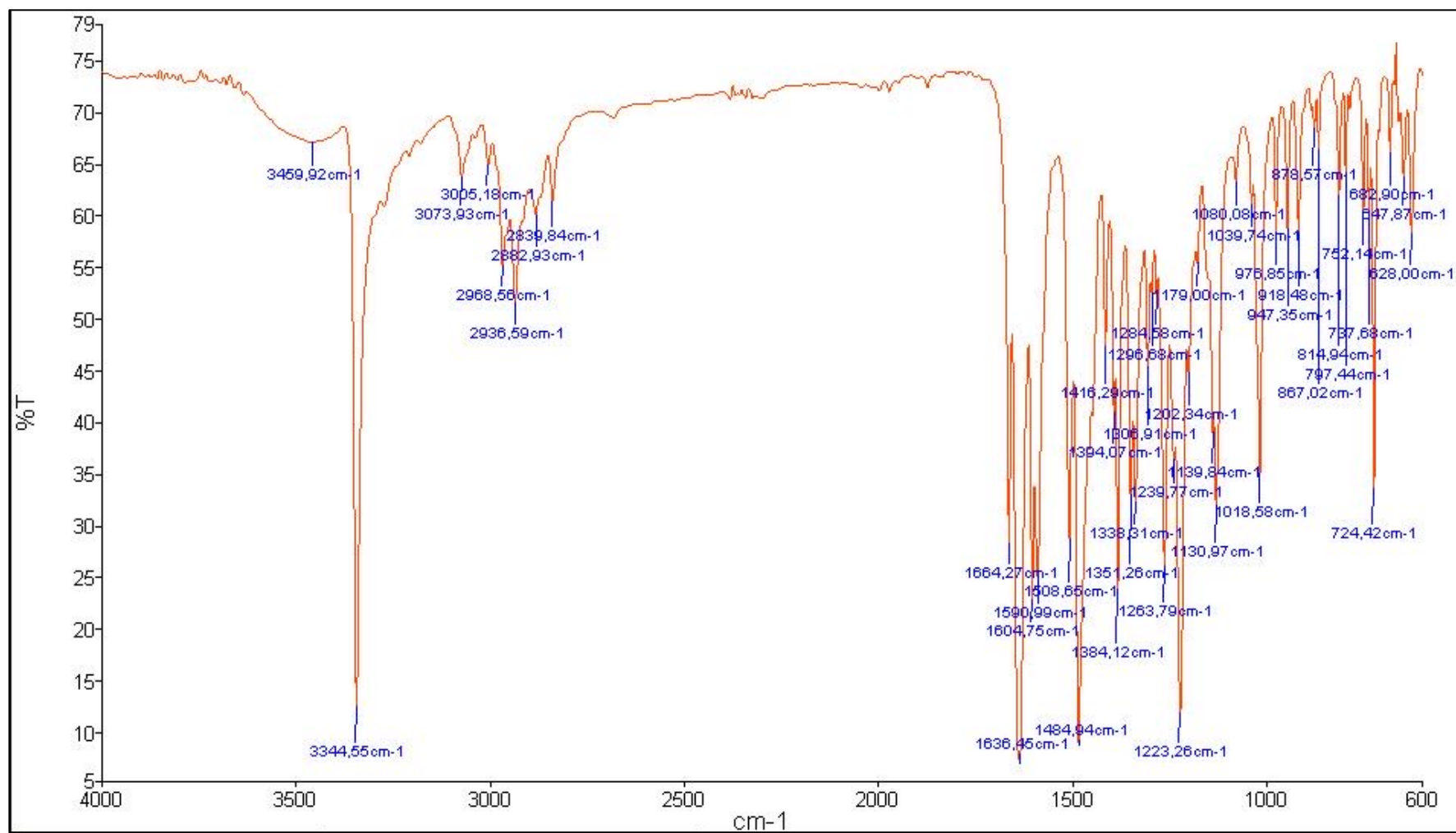
Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
466.164222	1	C <sub>28</sub> H <sub>21</sub> N <sub>5</sub> NaO	466.163831	-0.8	-0.6	20.5	ok	even		4.9	6.0	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
	2	C <sub>27</sub> H <sub>25</sub> NNaO <sub>5</sub>	466.162494	-3.7	-4.4	15.5	ok	even		8.4	15.0	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	



Exact Mass: 466,1630

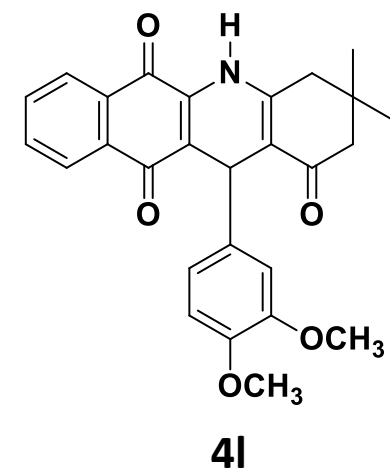
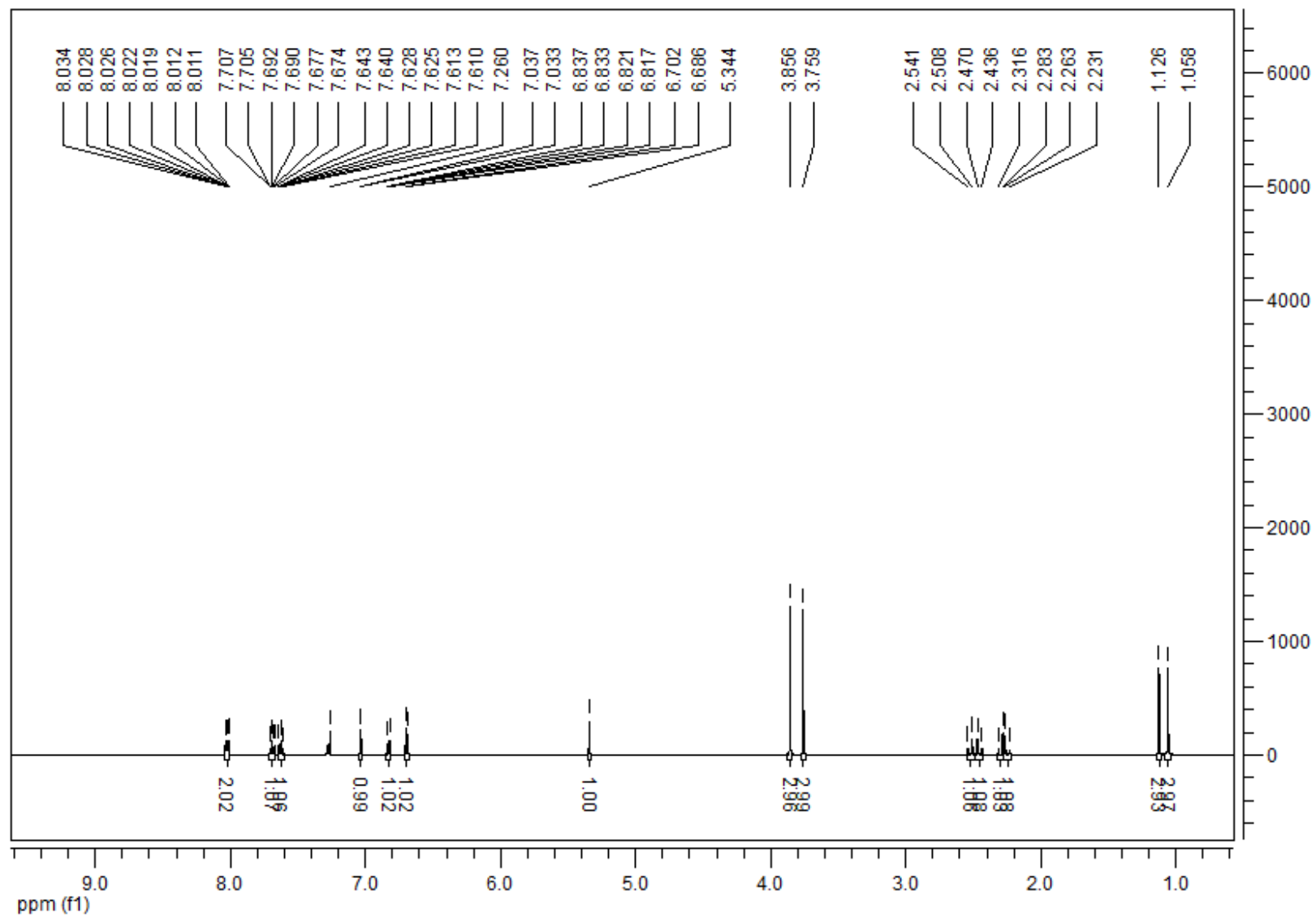
**4k**

HRMS of compound **4k**

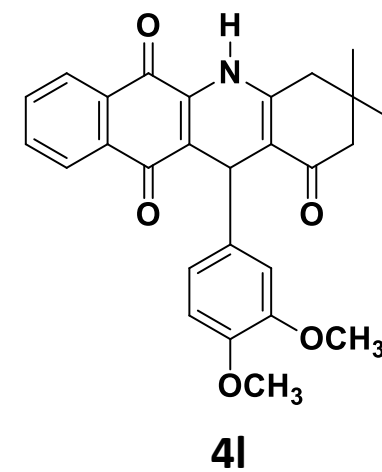
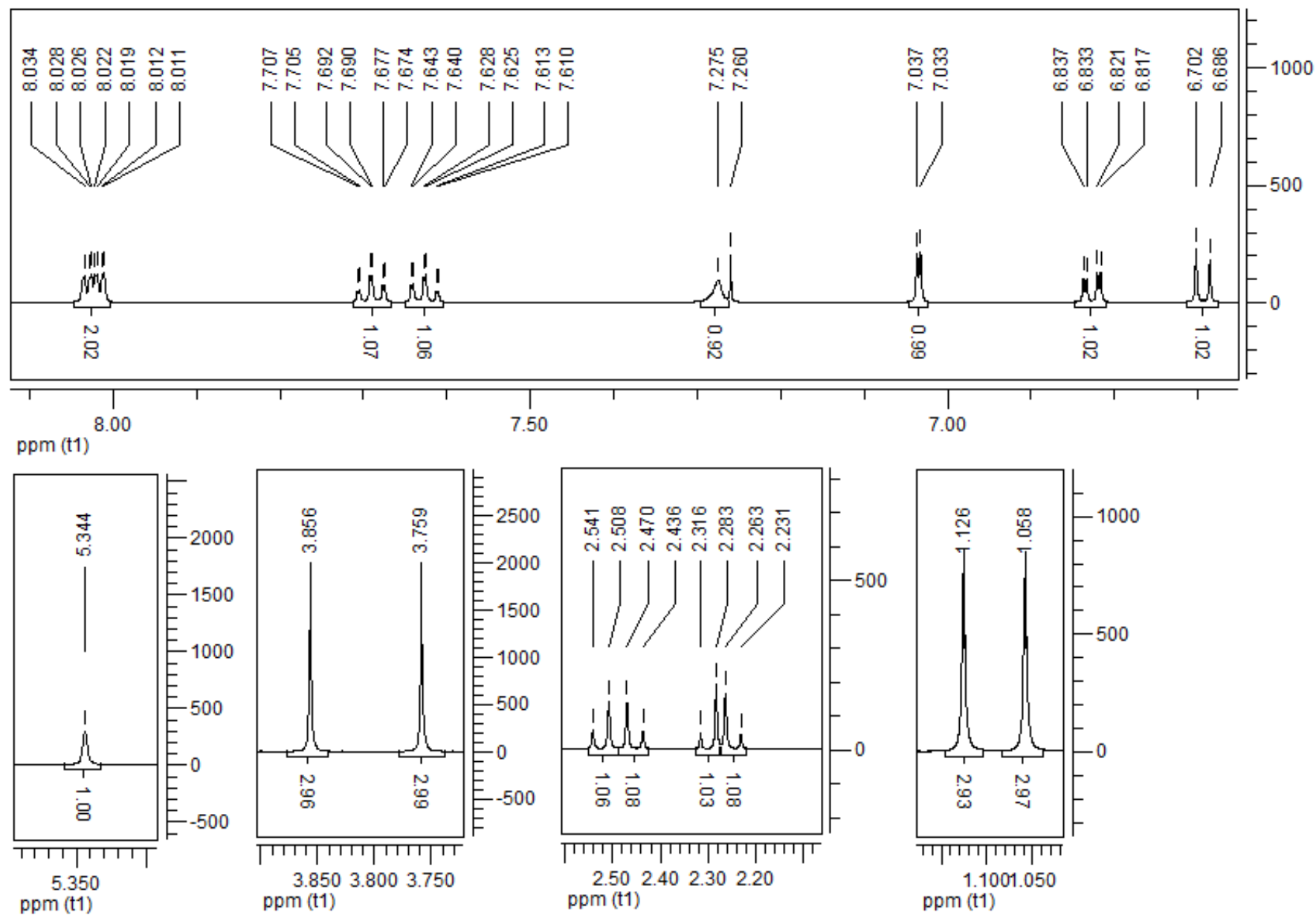


IR spectrum of compound **4l**

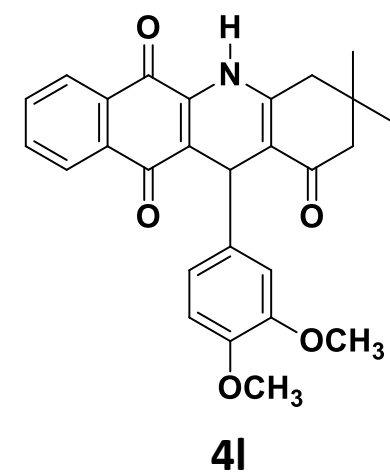
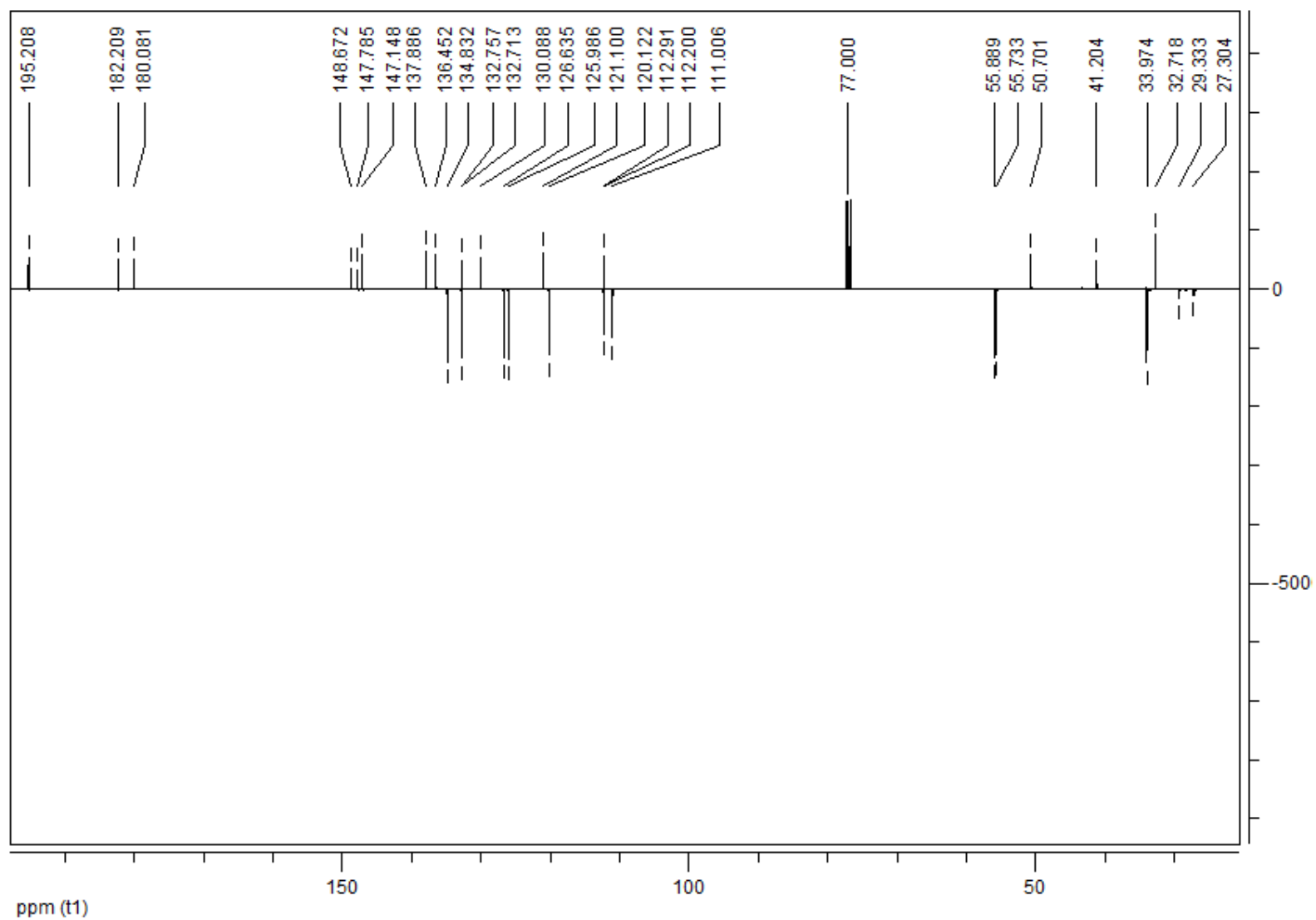




<sup>1</sup>H NMR spectrum of compound **4I** (500.00 MHz, CDCl<sub>3</sub>)

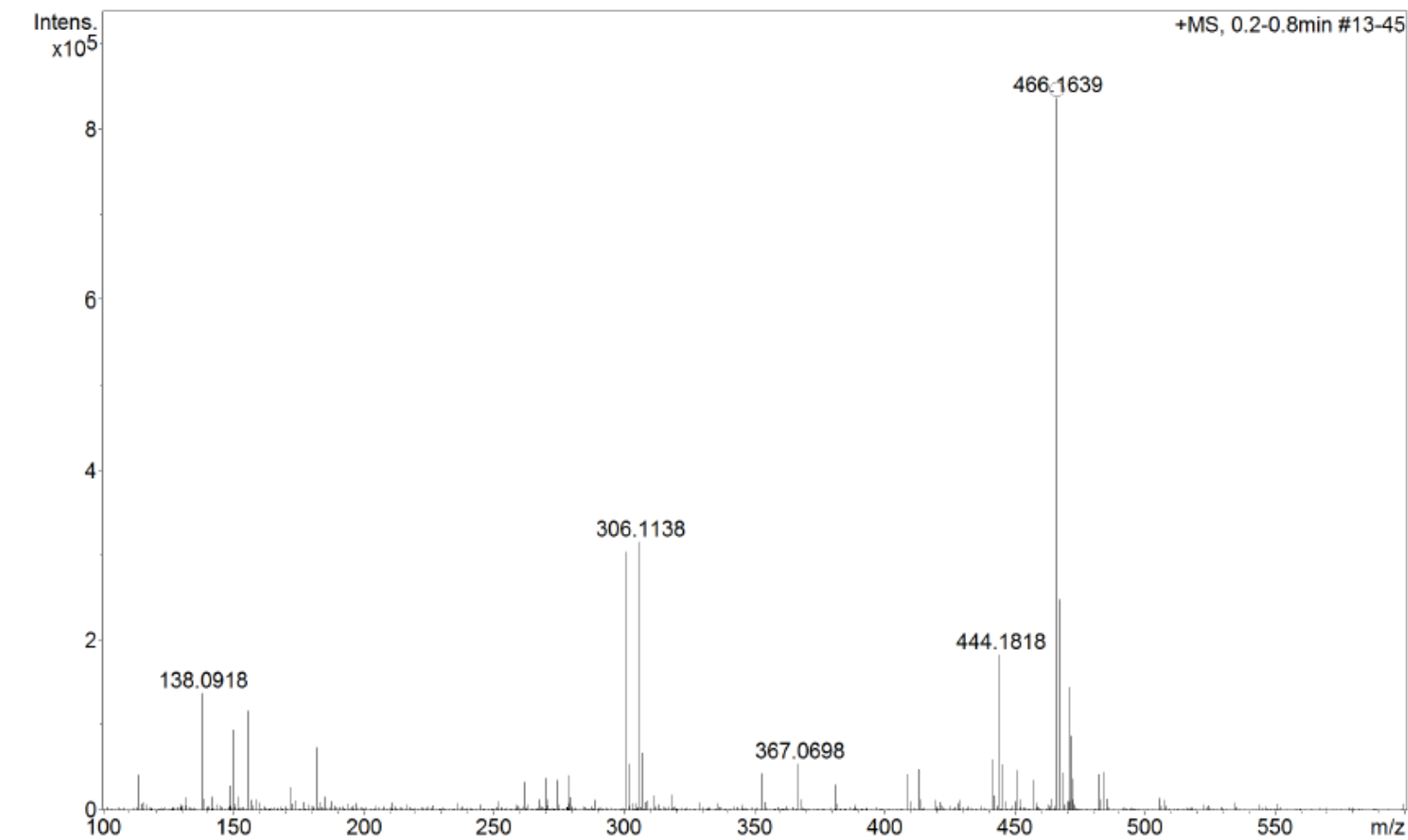


<sup>1</sup>H NMR spectrum of compound **4l** (500.00 MHz, CDCl<sub>3</sub>)

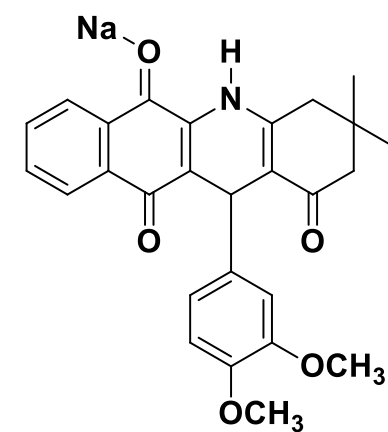


<sup>13</sup>C NMR spectrum of compound **4I** (125.0 MHz, CDCl<sub>3</sub>)

+MS, 0.2-0.8min #13-45



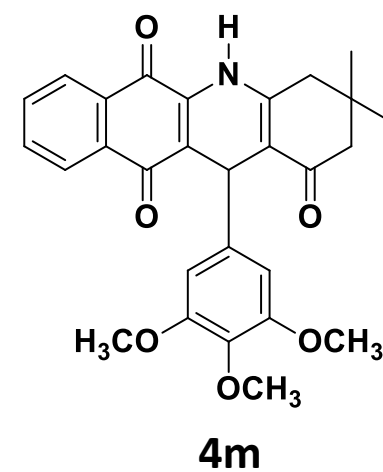
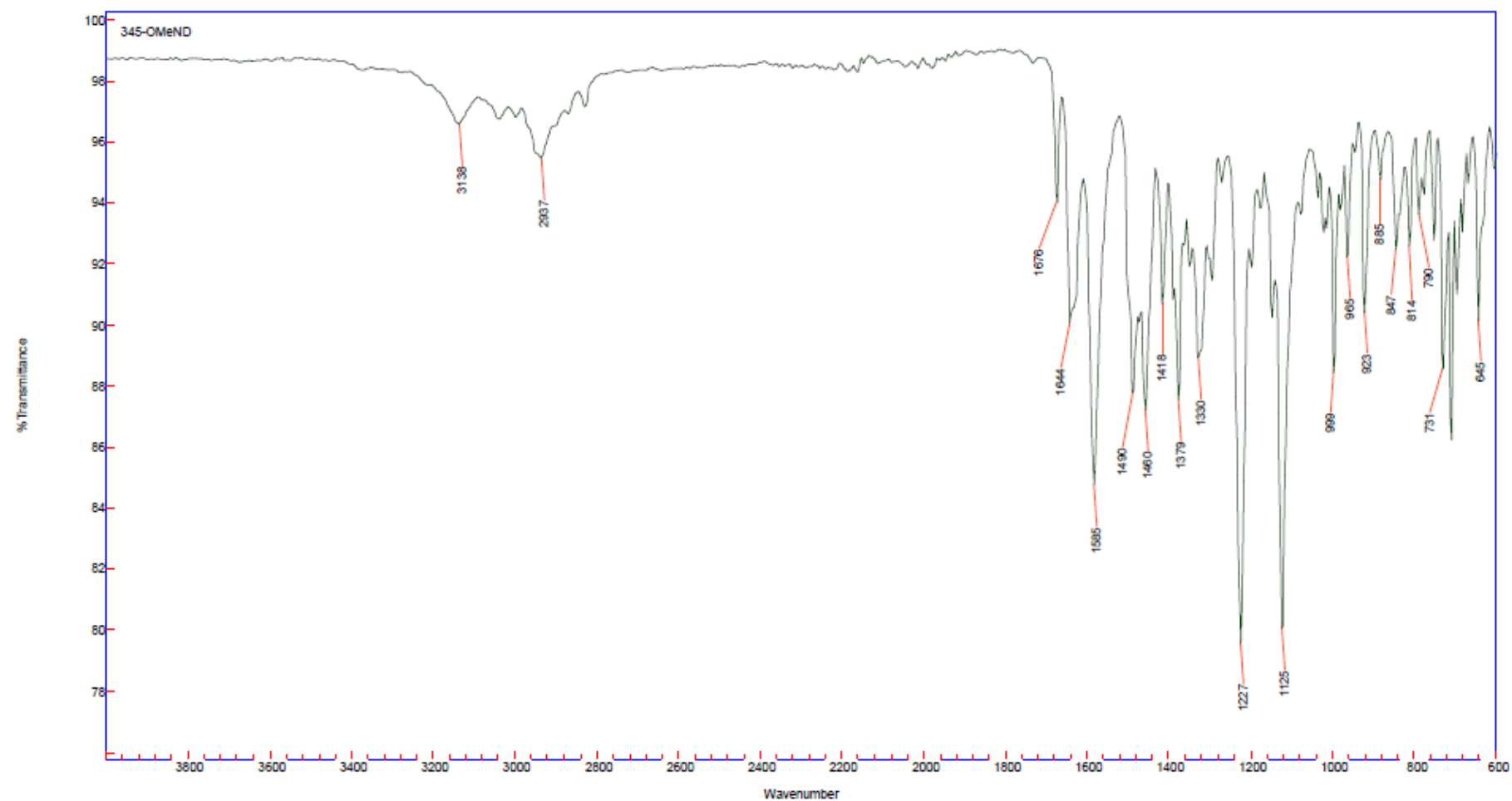
Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
466.1639	1	C <sub>27</sub> H <sub>25</sub> NNaO <sub>5</sub>	466.162494	-3.1	-4.5	15.5	ok	even		1.8	3.0		n.a.		n.a.	n.a.	n.a.	n.a.	
	2	C <sub>28</sub> H <sub>21</sub> N <sub>5</sub> NaO	466.163831	-0.2	-0.9	20.5	ok	even		15.3	20.9		n.a.		n.a.	n.a.	n.a.	n.a.	



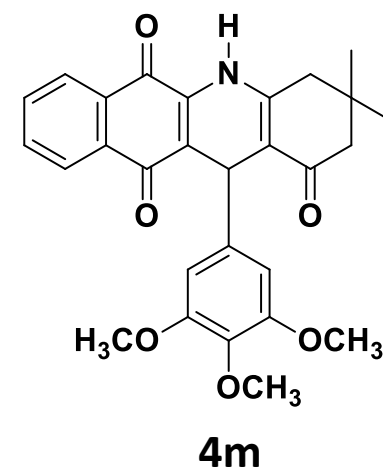
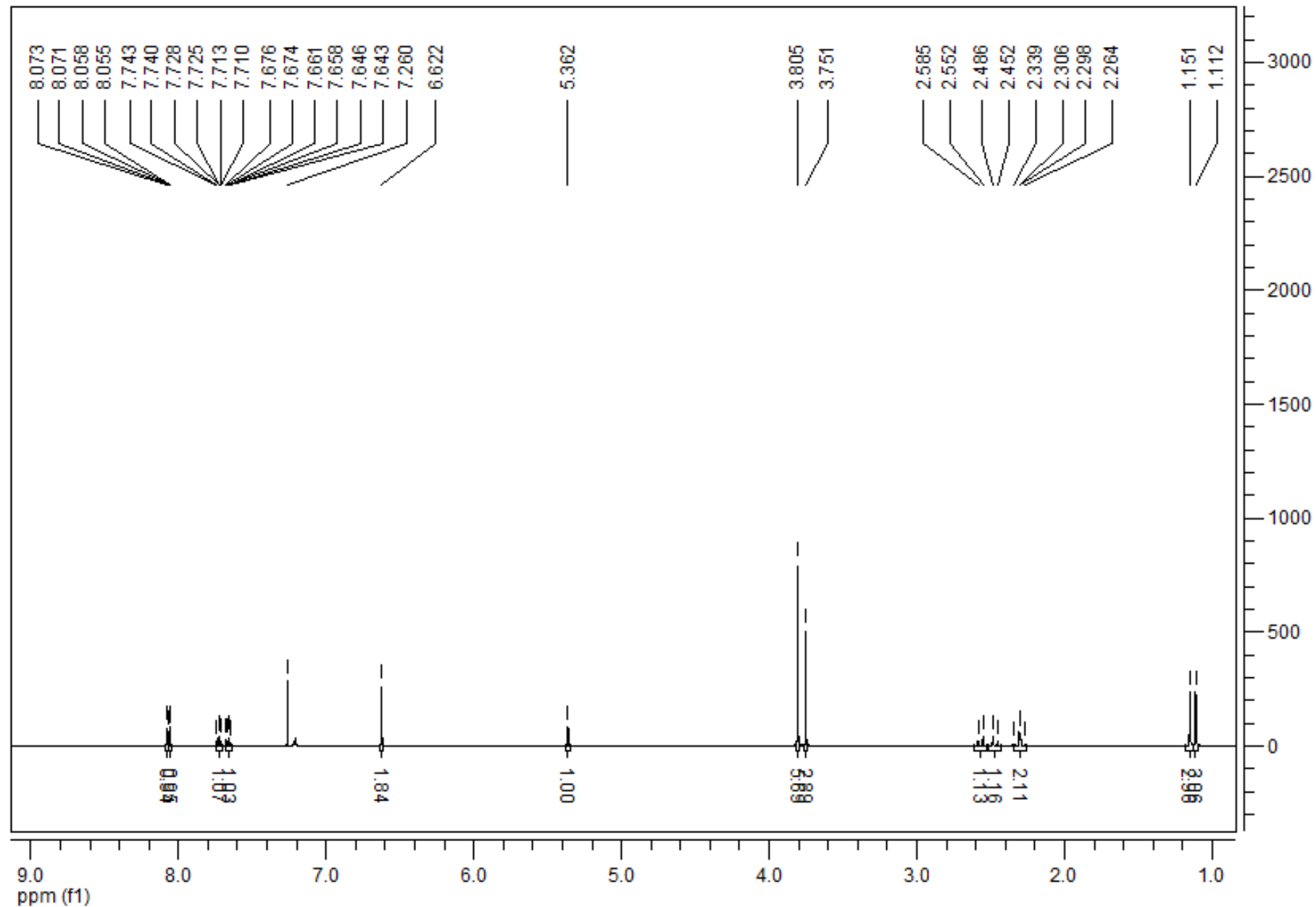
Exact Mass: 466,1630

**4I**

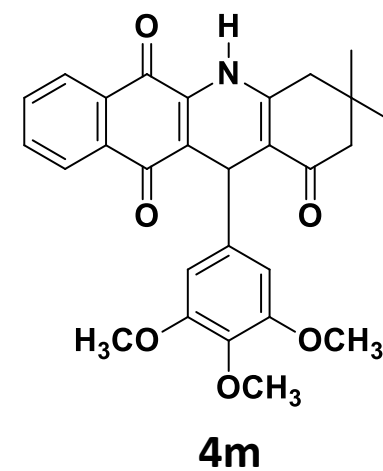
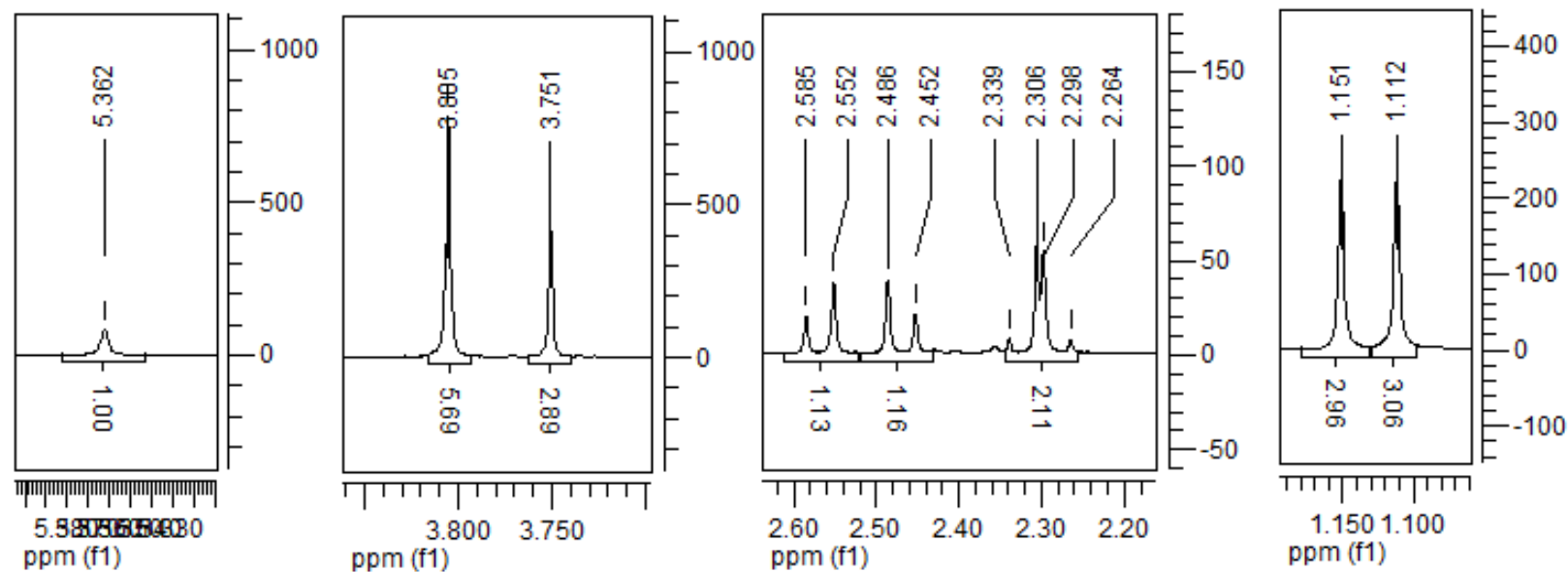
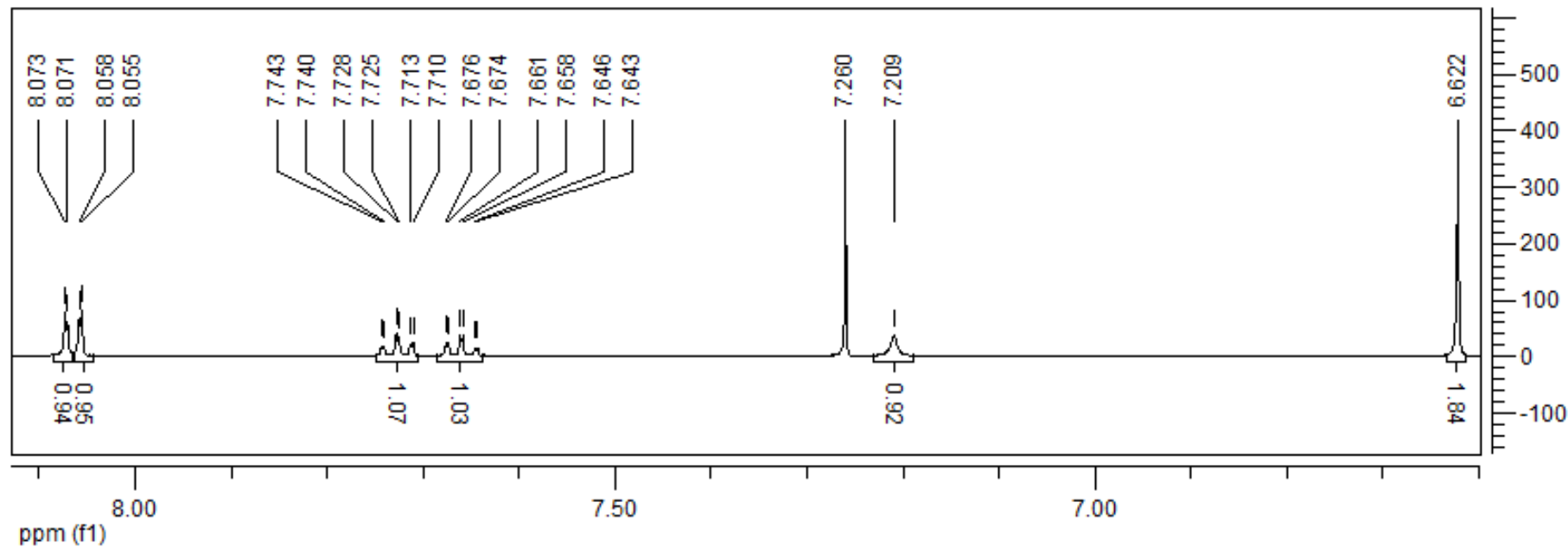
HRMS of compound **4I**



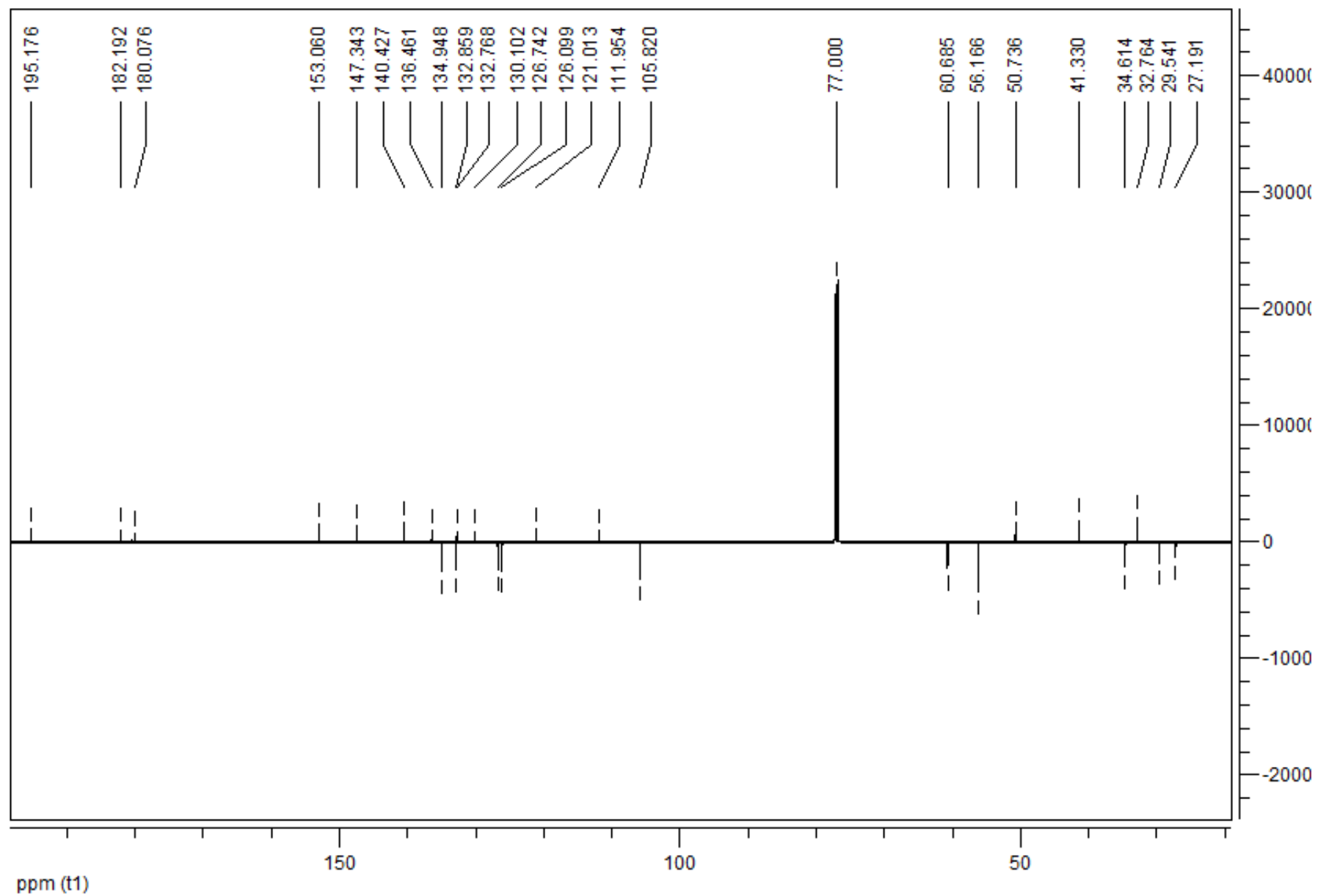
IR spectrum of compound **4m**



<sup>1</sup>H NMR spectrum of compound **4m** (500.00 MHz, CDCl<sub>3</sub>)



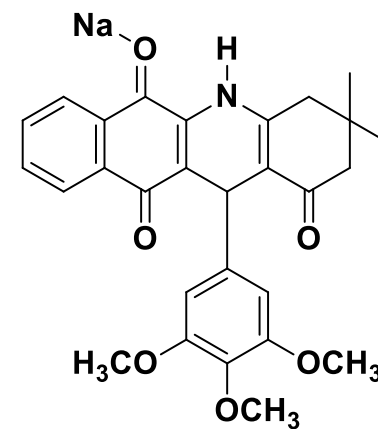
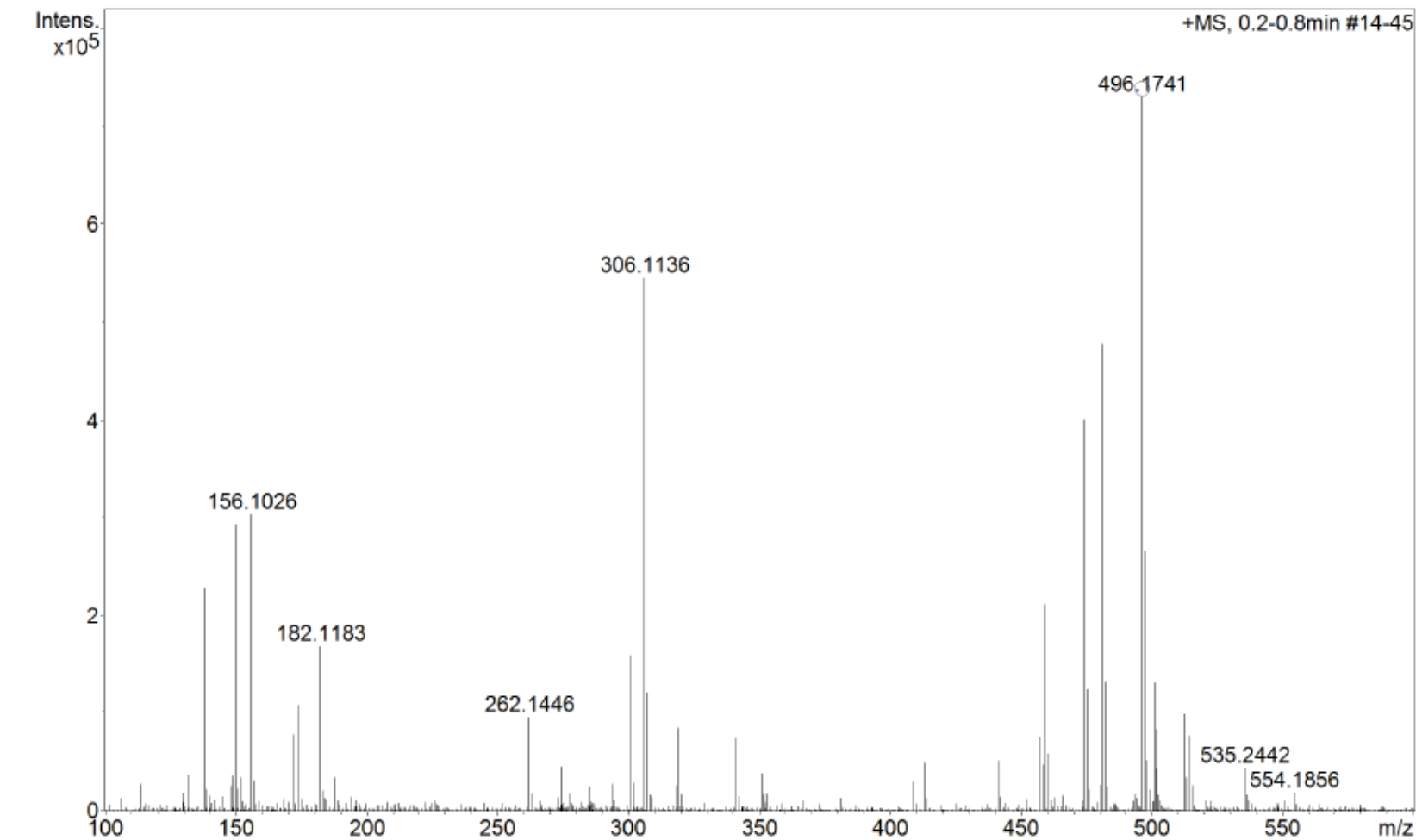
$^1\text{H}$  NMR spectrum of compound **4m** (500.00 MHz,  $\text{CDCl}_3$ )



$^{13}\text{C}$  NMR spectrum of compound **4m** (125.0 MHz,  $\text{CDCl}_3$ )



+MS, 0.2-0.8min #14-45

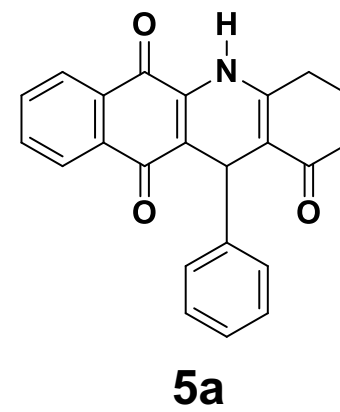
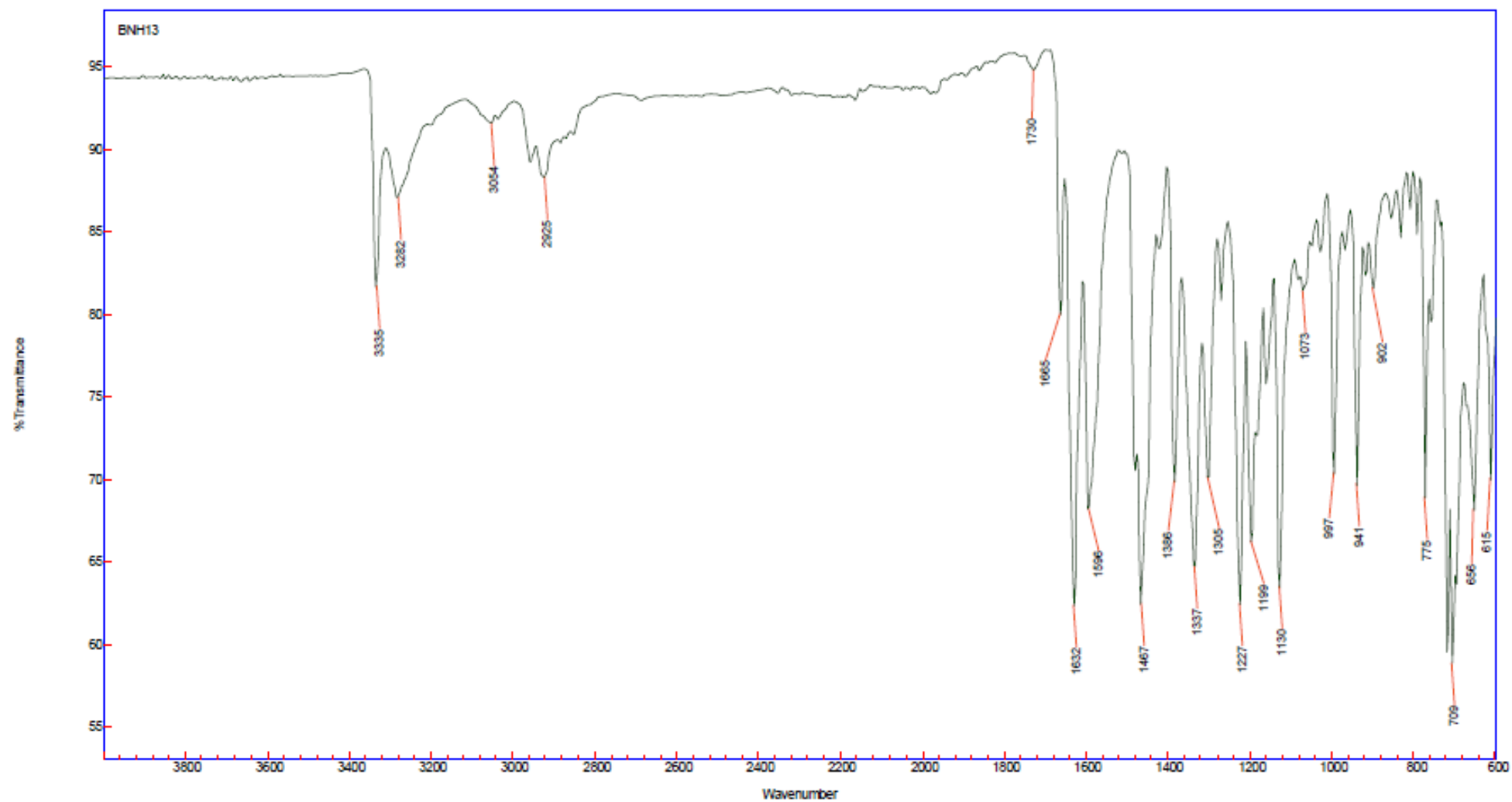


Exact Mass: 496,1736

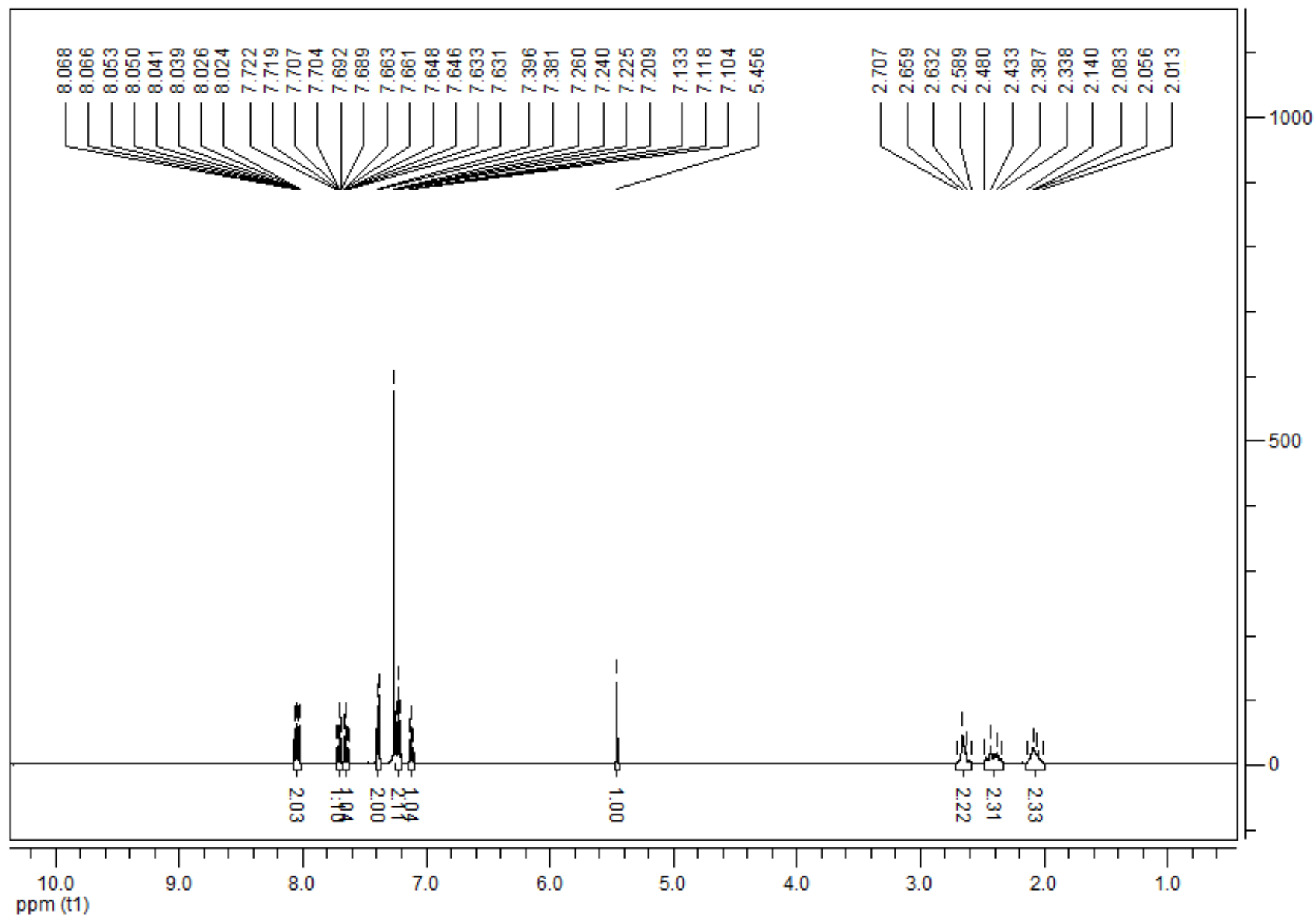
**4m**

Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std	Mean m/z	Std I	VarNorm	Std m/z	Diff	Std	Comb	Dev
496.174090	1	C <sub>29</sub> H <sub>23</sub> N <sub>5</sub> NaO <sub>2</sub>	496.174396	0.6	982.8	20.5	ok	even		16.8	25.1		n.a.		n.a.		n.a.		n.a.	
	2	C <sub>28</sub> H <sub>27</sub> NNaO <sub>6</sub>	496.173058	-2.1	986.9	15.5	ok	even		27.9	41.5		n.a.		n.a.		n.a.		n.a.	

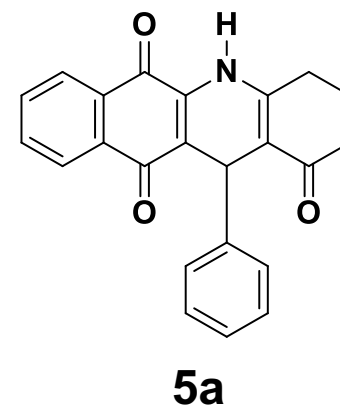
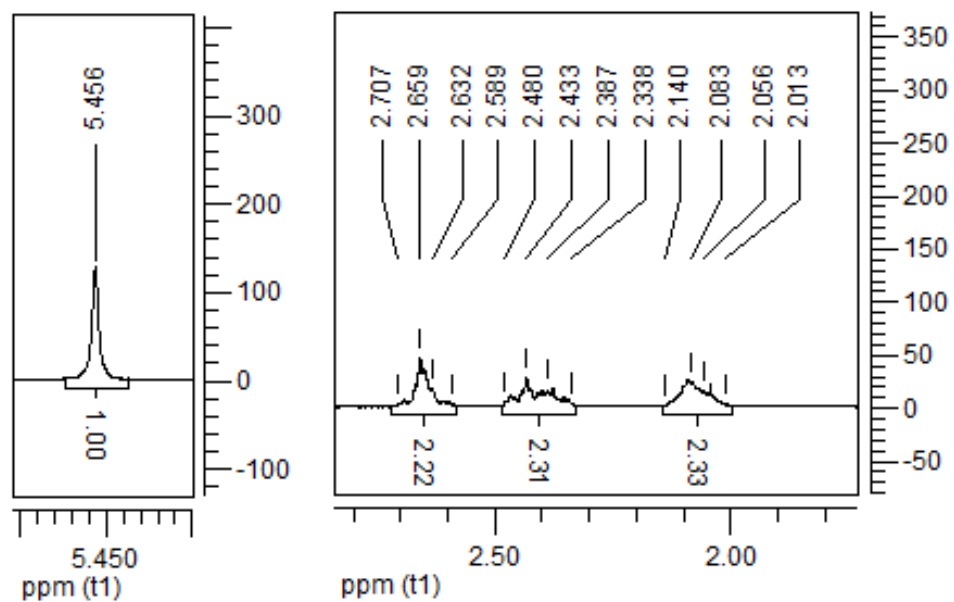
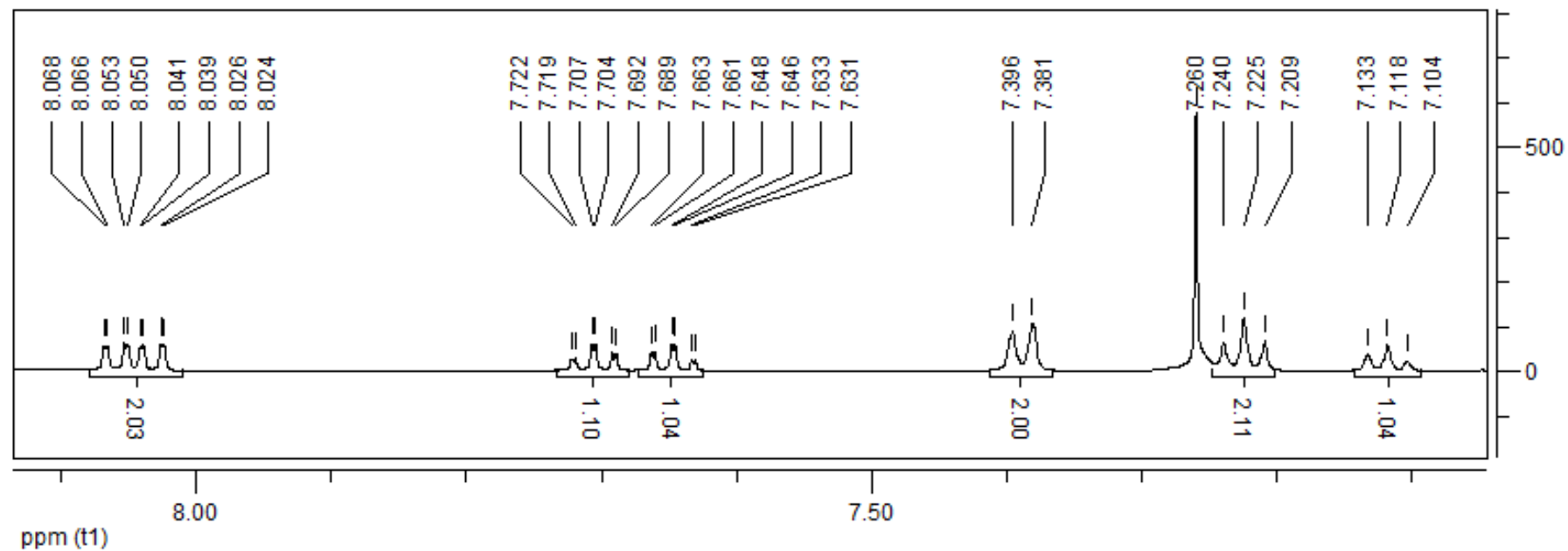
HRMS of compound **4m**



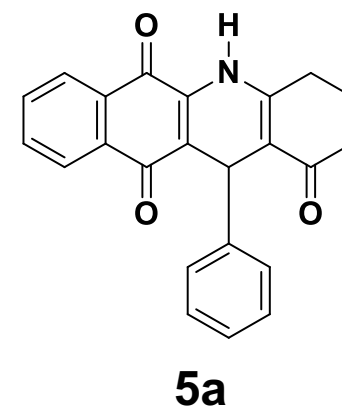
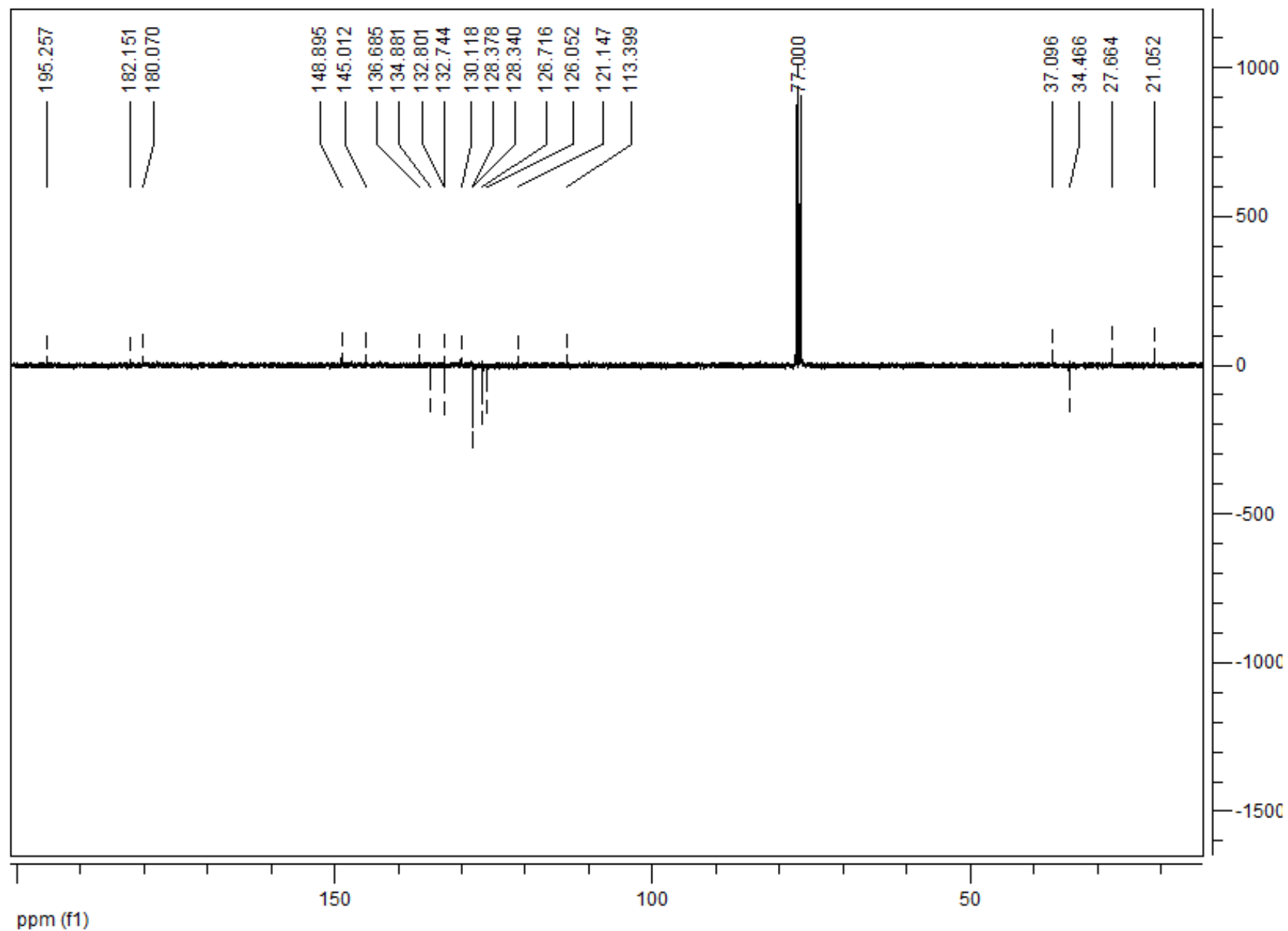
IR spectrum of compound **5a**



$^1\text{H}$  NMR spectrum of compound **5a** (500.00 MHz,  $\text{CDCl}_3$ )

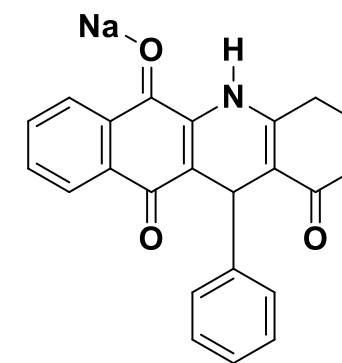
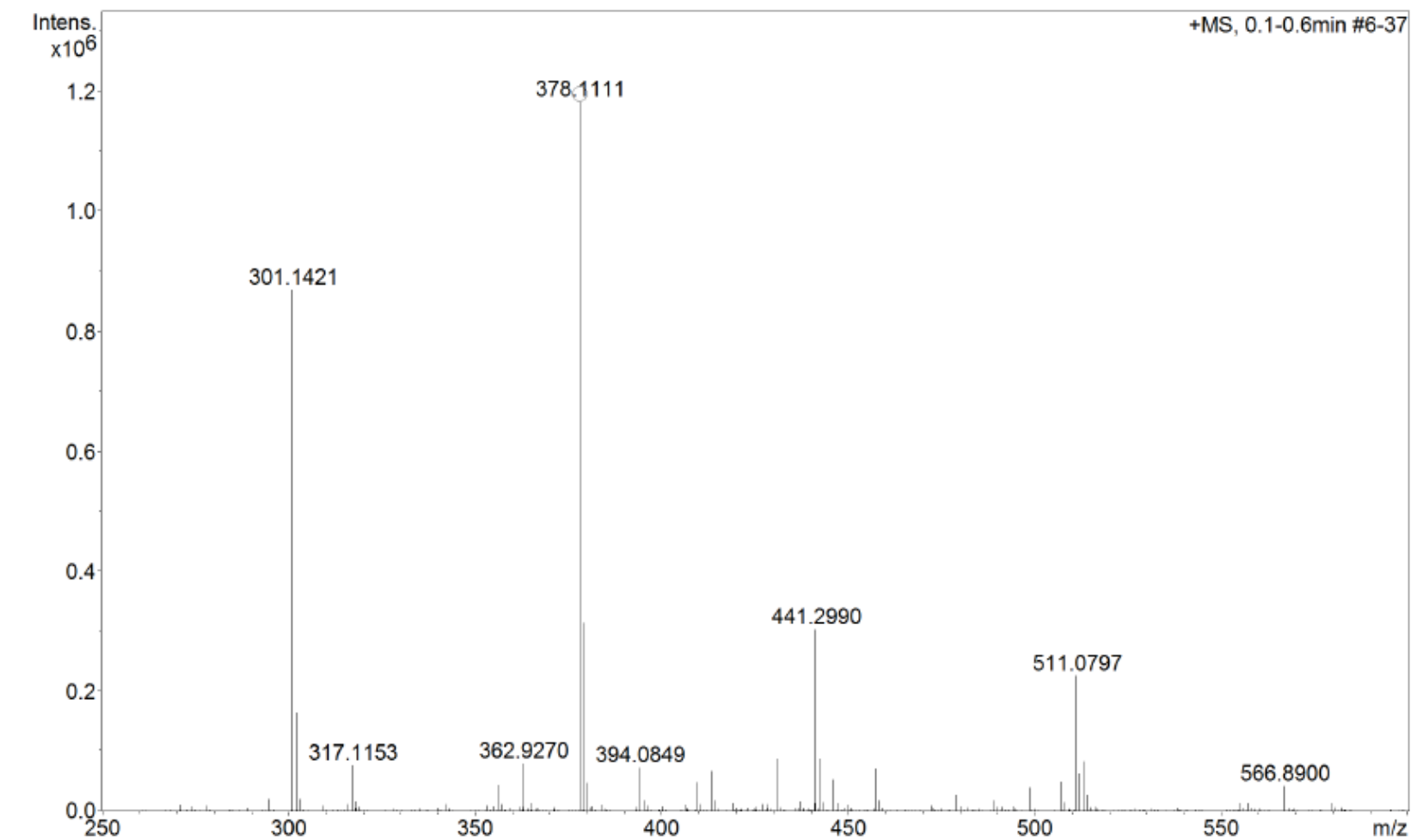


<sup>1</sup>H NMR spectrum of compound **5a** (500.00 MHz, CDCl<sub>3</sub>)



<sup>13</sup>C NMR spectrum of compound **5a** (75.0 MHz, CDCl<sub>3</sub>)

+MS, 0.1-0.6min #6-37

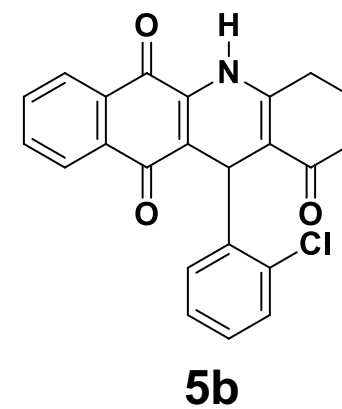
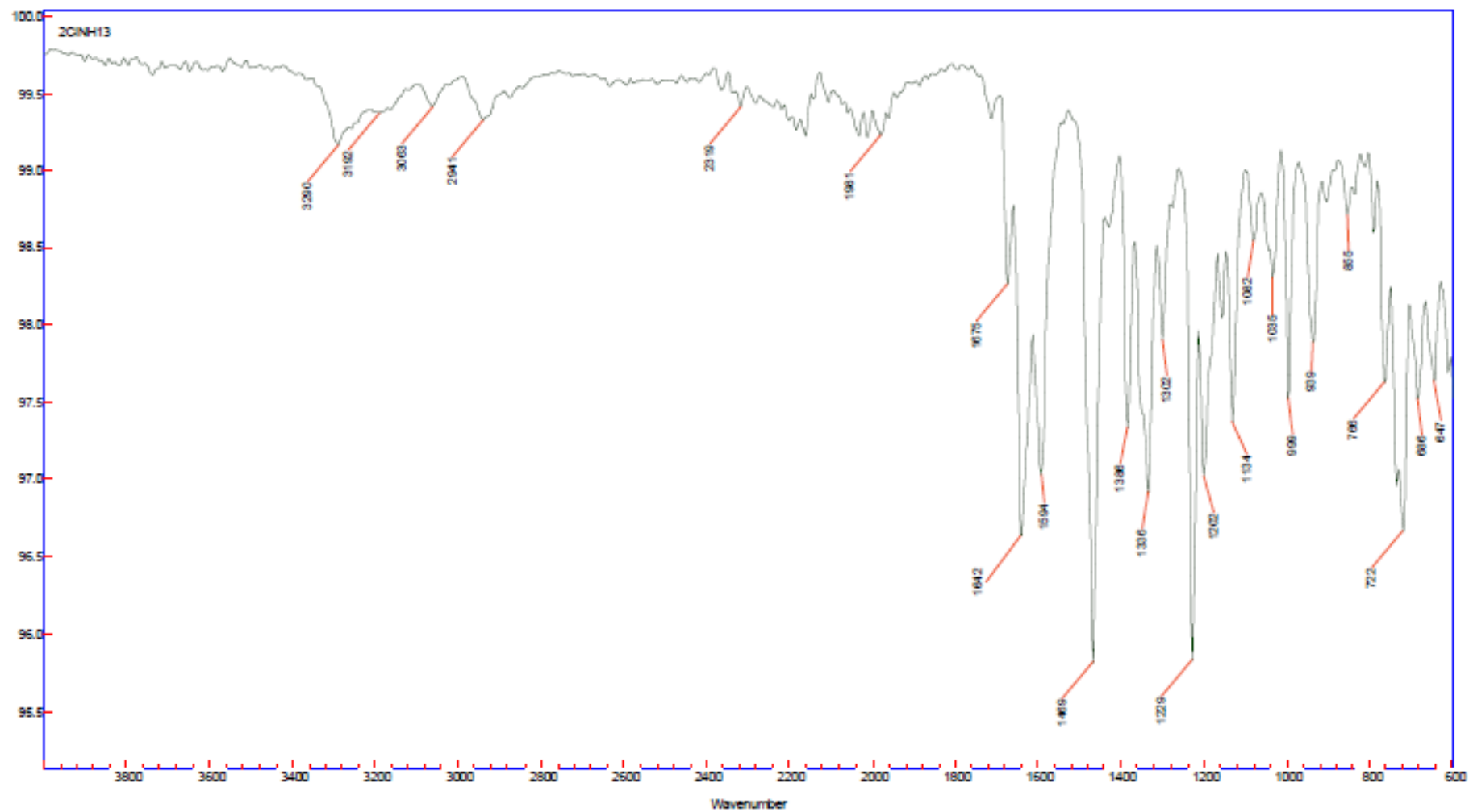


Exact Mass: 378,1106

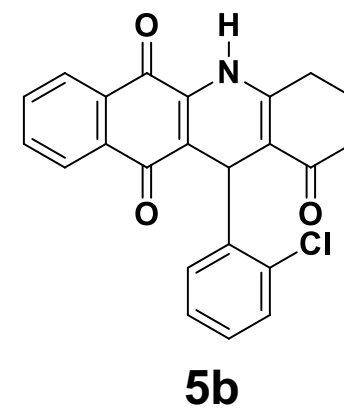
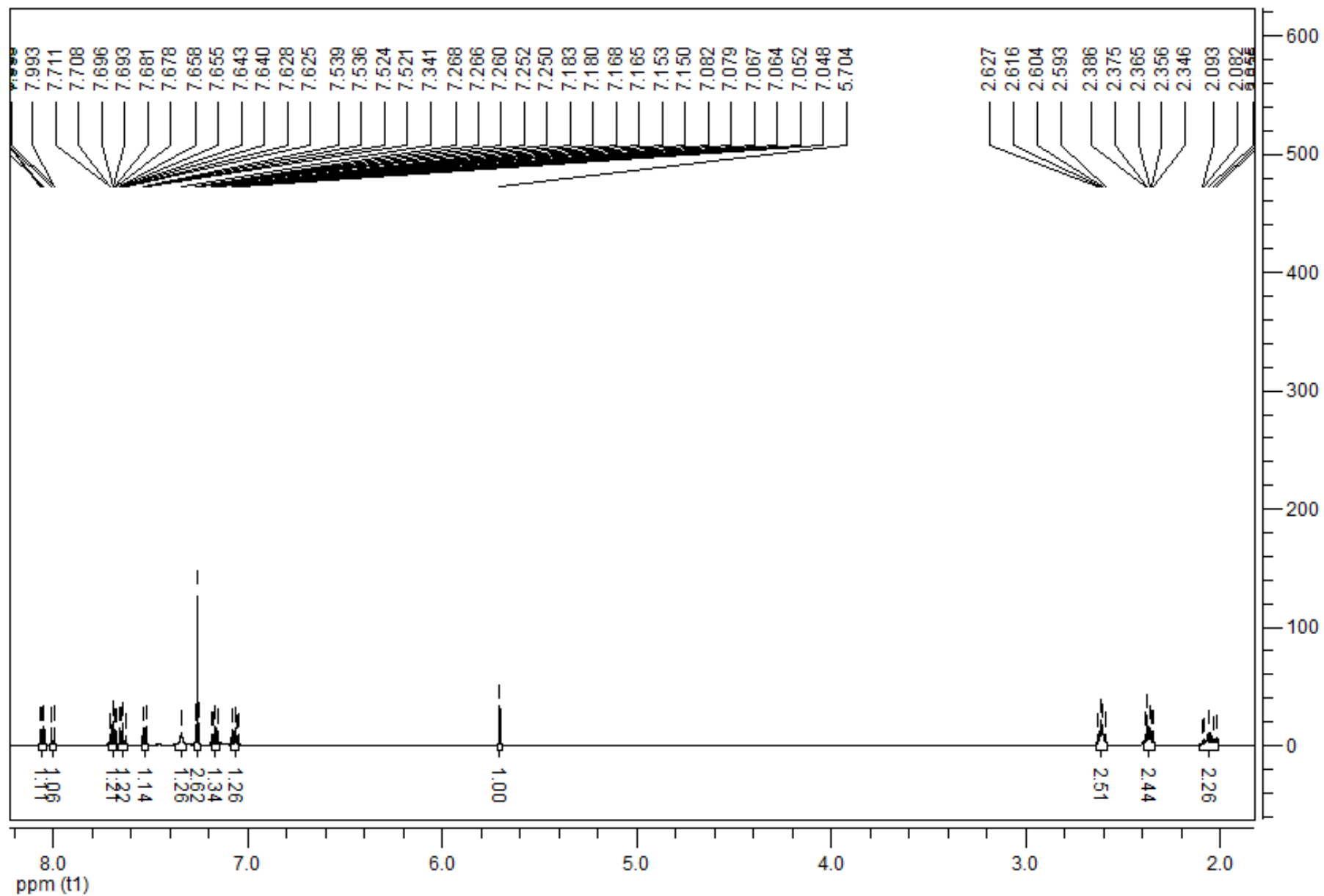
**5a**

Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
378.111144	1	C <sub>23</sub> H <sub>17</sub> NNaO <sub>3</sub>	378.110064	-2.9	-3.4	15.5	ok	even		6.8	10.7	n.a.		n.a.	n.a.	n.a.		n.a.	
	2	C <sub>19</sub> H <sub>13</sub> N <sub>7</sub> NaO	378.107379	-10.0	-11.5	16.5	ok	even		20.9	35.0	n.a.		n.a.	n.a.	n.a.		n.a.	

HRMS of compound **5a**

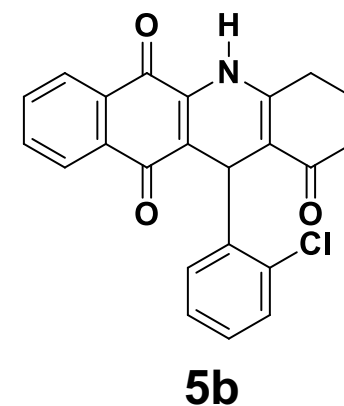
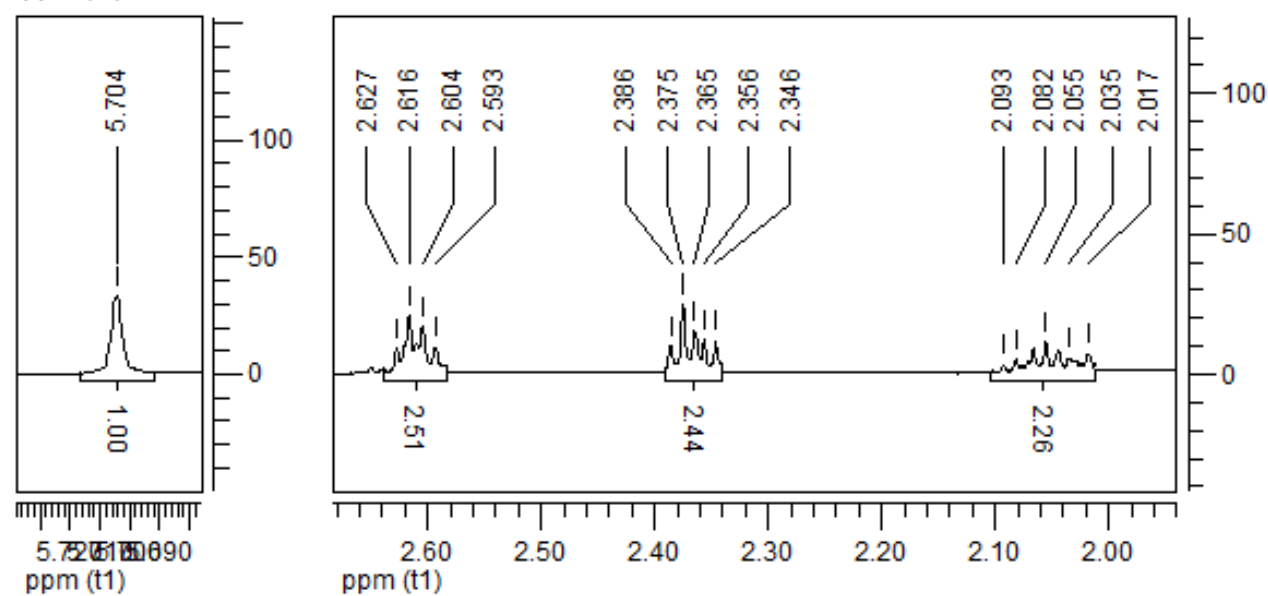
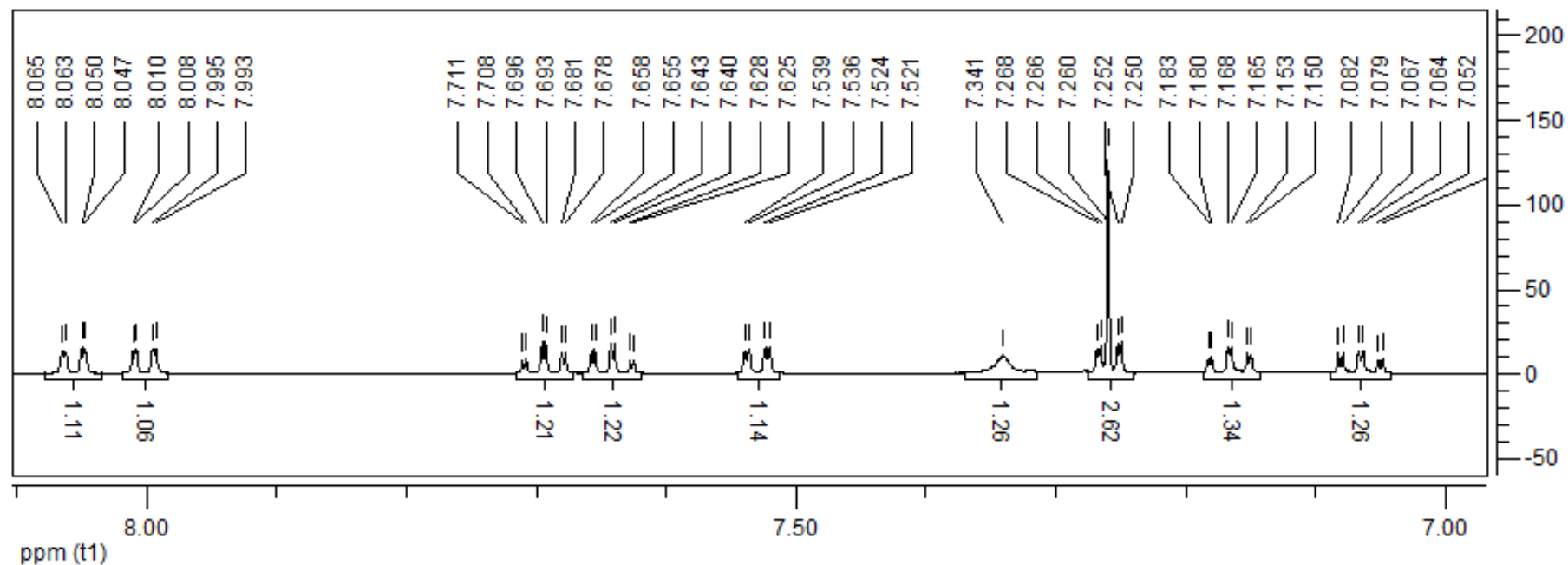


IR spectrum of compound **5b**

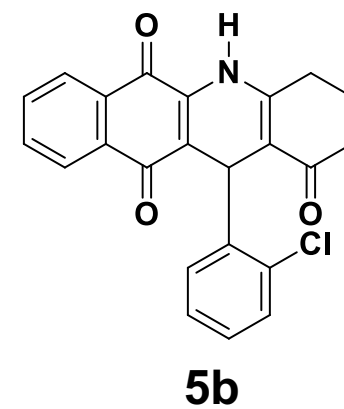
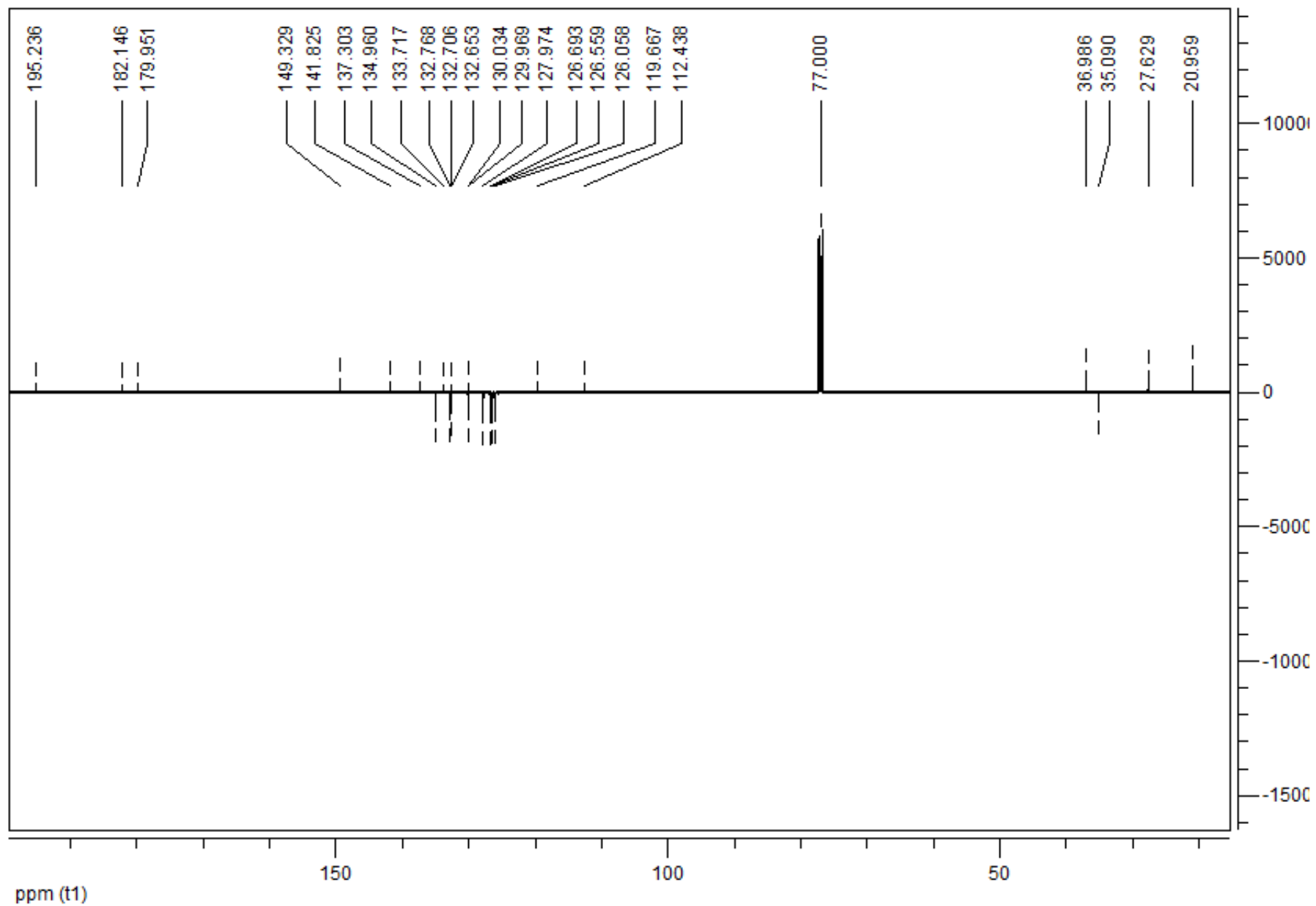


$^1\text{H}$  NMR spectrum of compound **5b** (500.00 MHz,  $\text{CDCl}_3$ )



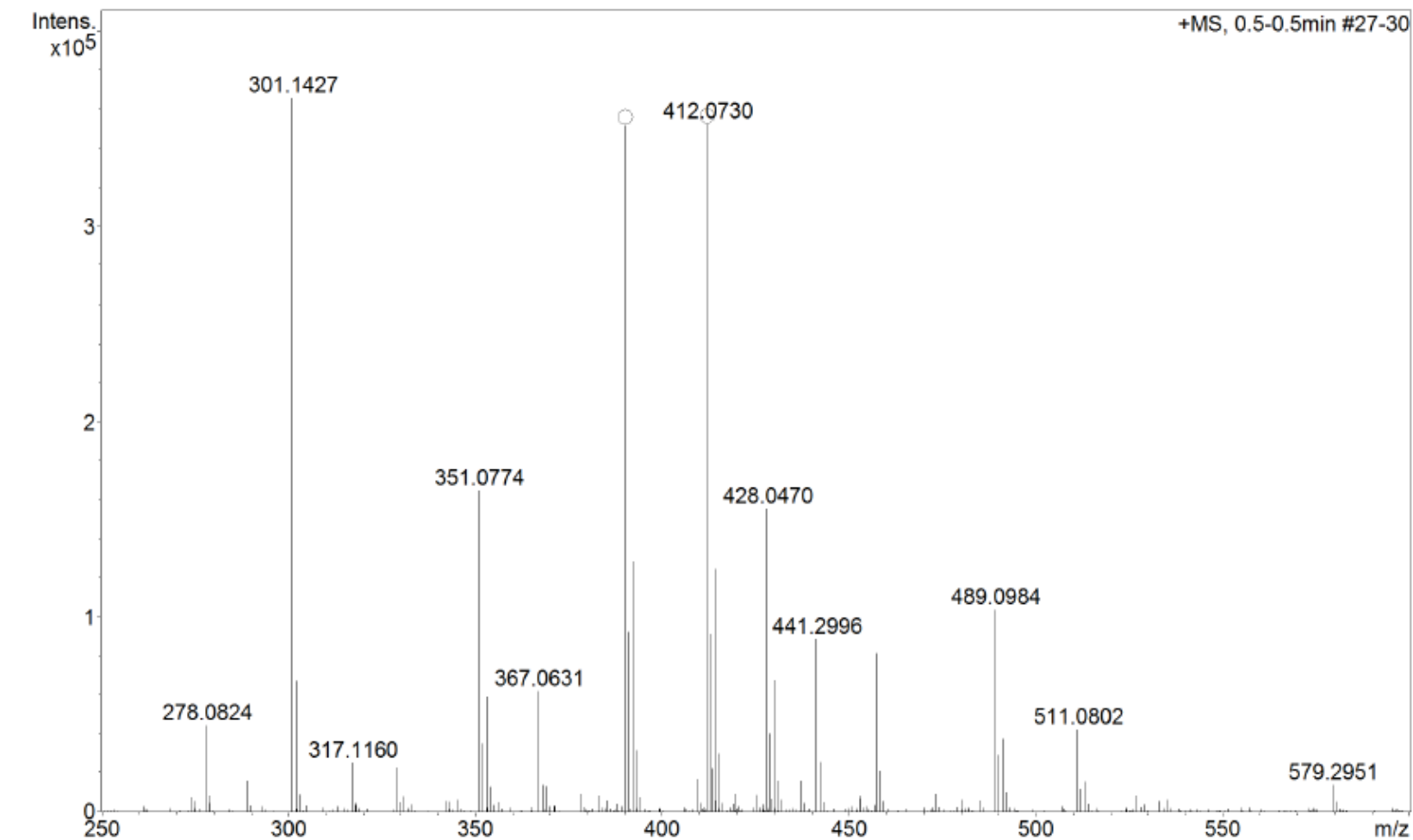


<sup>1</sup>H NMR spectrum of compound **5b** (500.00 MHz, CDCl<sub>3</sub>)

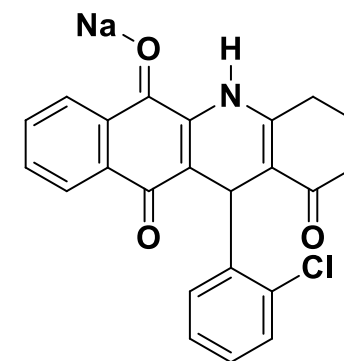


<sup>13</sup>C NMR spectrum of compound **5b** (125.0 MHz, CDCl<sub>3</sub>)

+MS, 0.5-0.5min #27-30



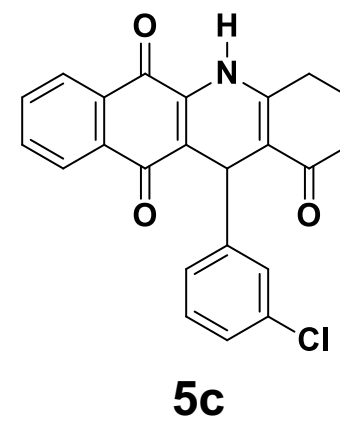
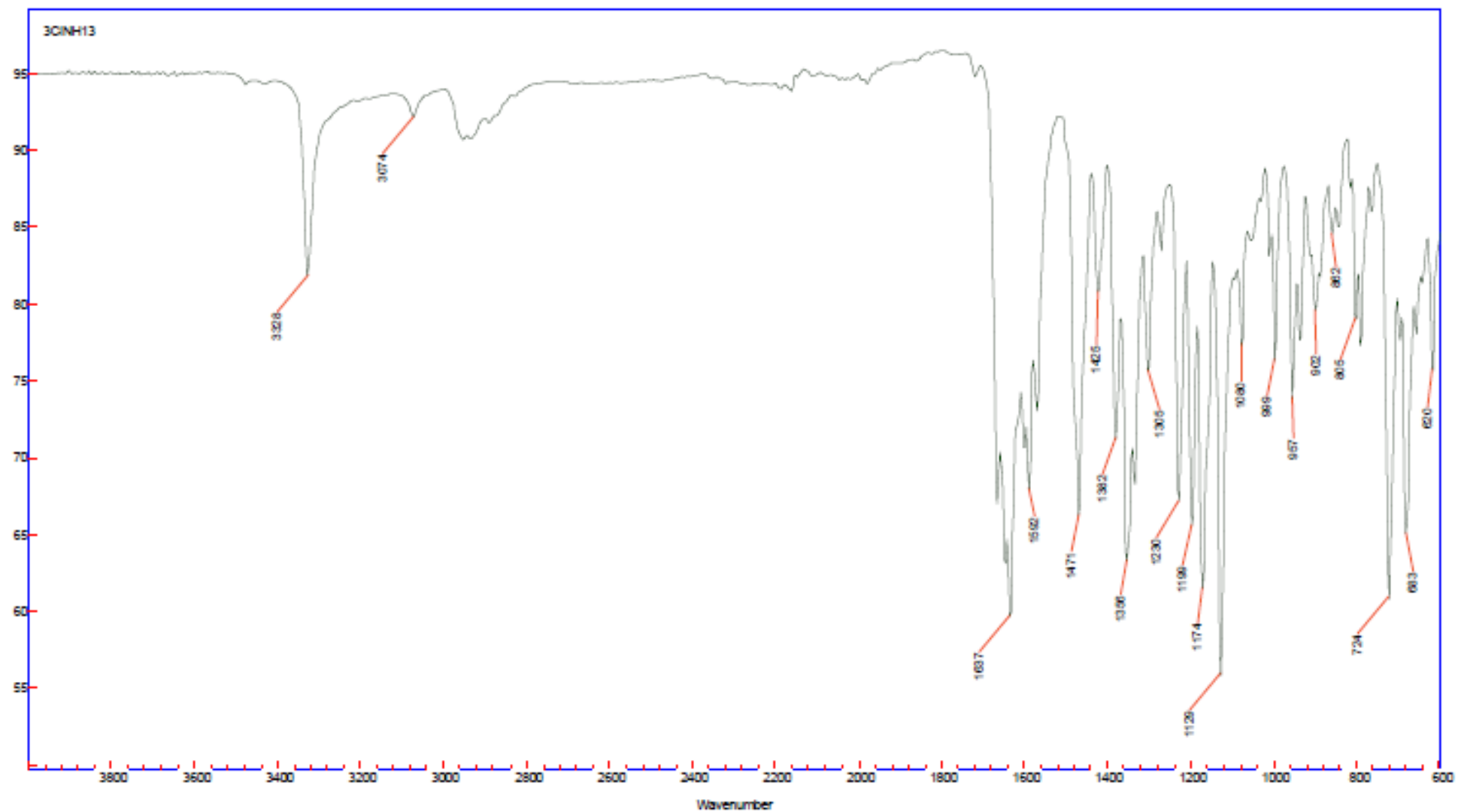
Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std	Mean m/z	Std I	VarNorm	Std	m/z	Diff	Std	Comb	Dev
390.090698	1	C23H17ClNO3	390.089148	-4.0	-3.3	15.5	ok	even		7.0	11.8		n.a.		n.a.		n.a.		n.a.	n.a.	
412.073029	1	C23H16ClNNaO3	412.071092	-4.7	-4.2	15.5	ok	even		2.5	3.3		n.a.		n.a.		n.a.		n.a.	n.a.	



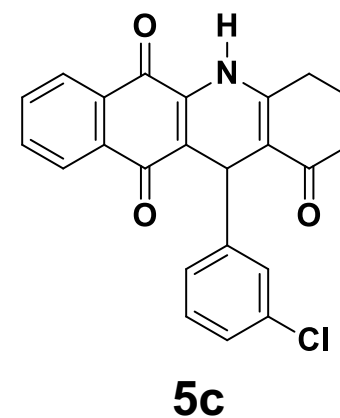
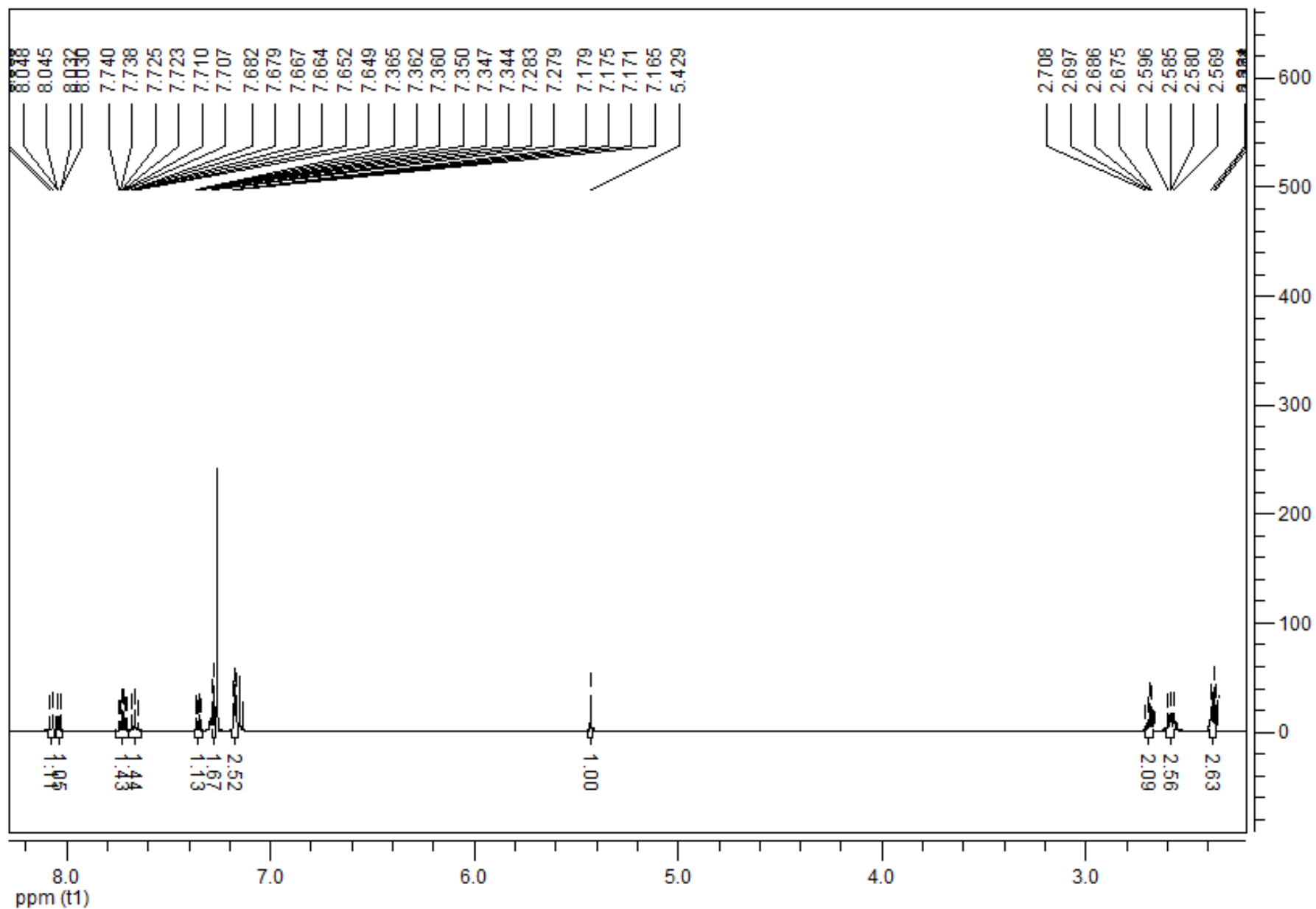
Exact Mass: 412,0716

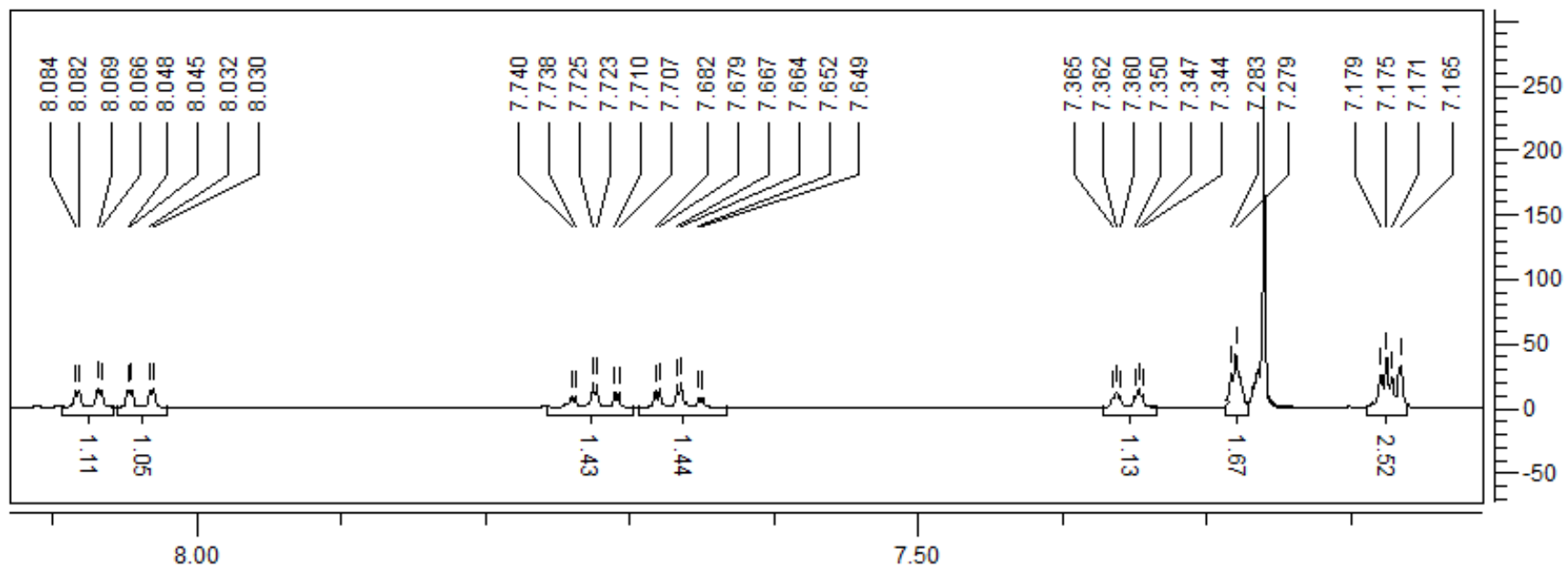
**5b**

HRMS of compound **5b**

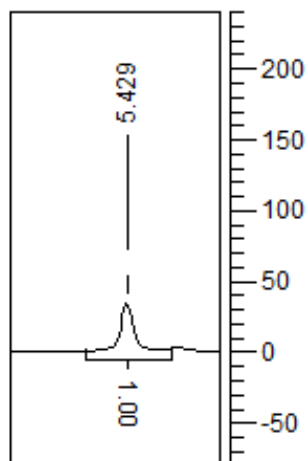


IR spectrum of compound **5c**

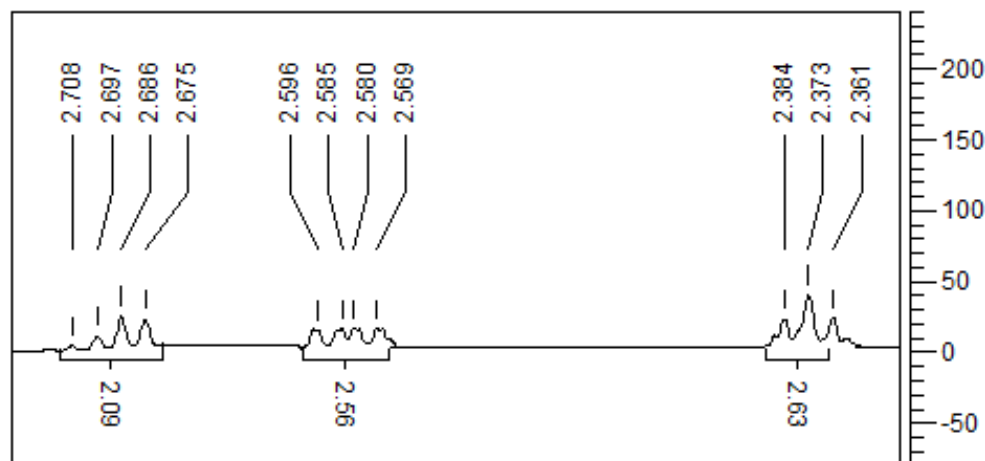




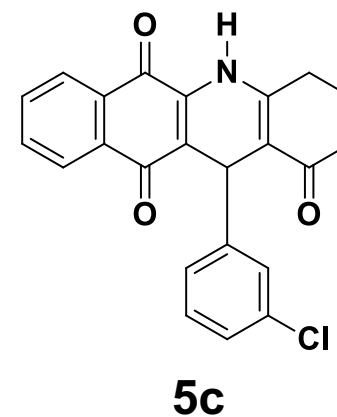
ppm (t1)



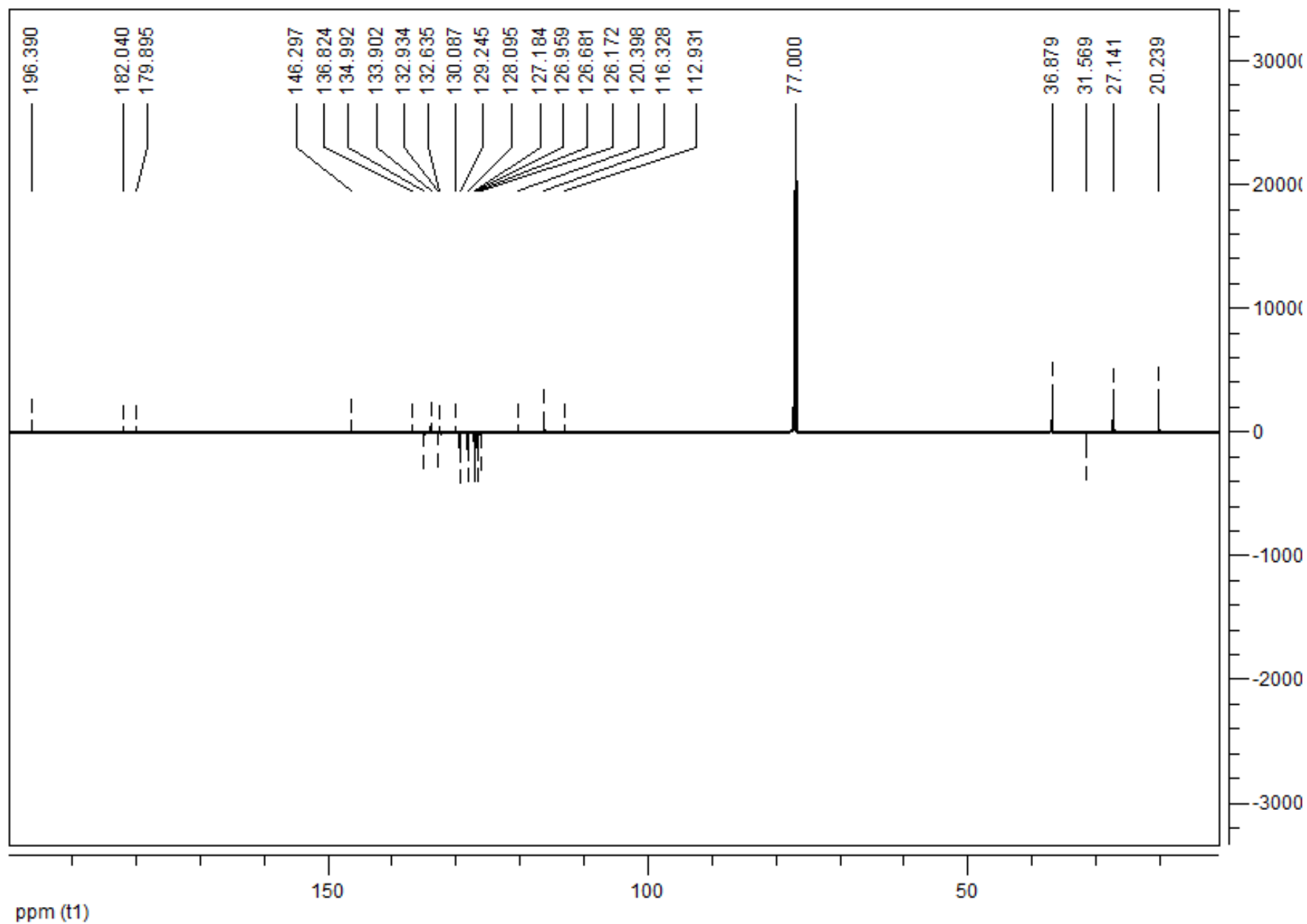
5.450 5.404 5.420  
ppm (t1)



2.700 2.650 2.600 2.550 2.500 2.450 2.400 2.350  
ppm (t1)

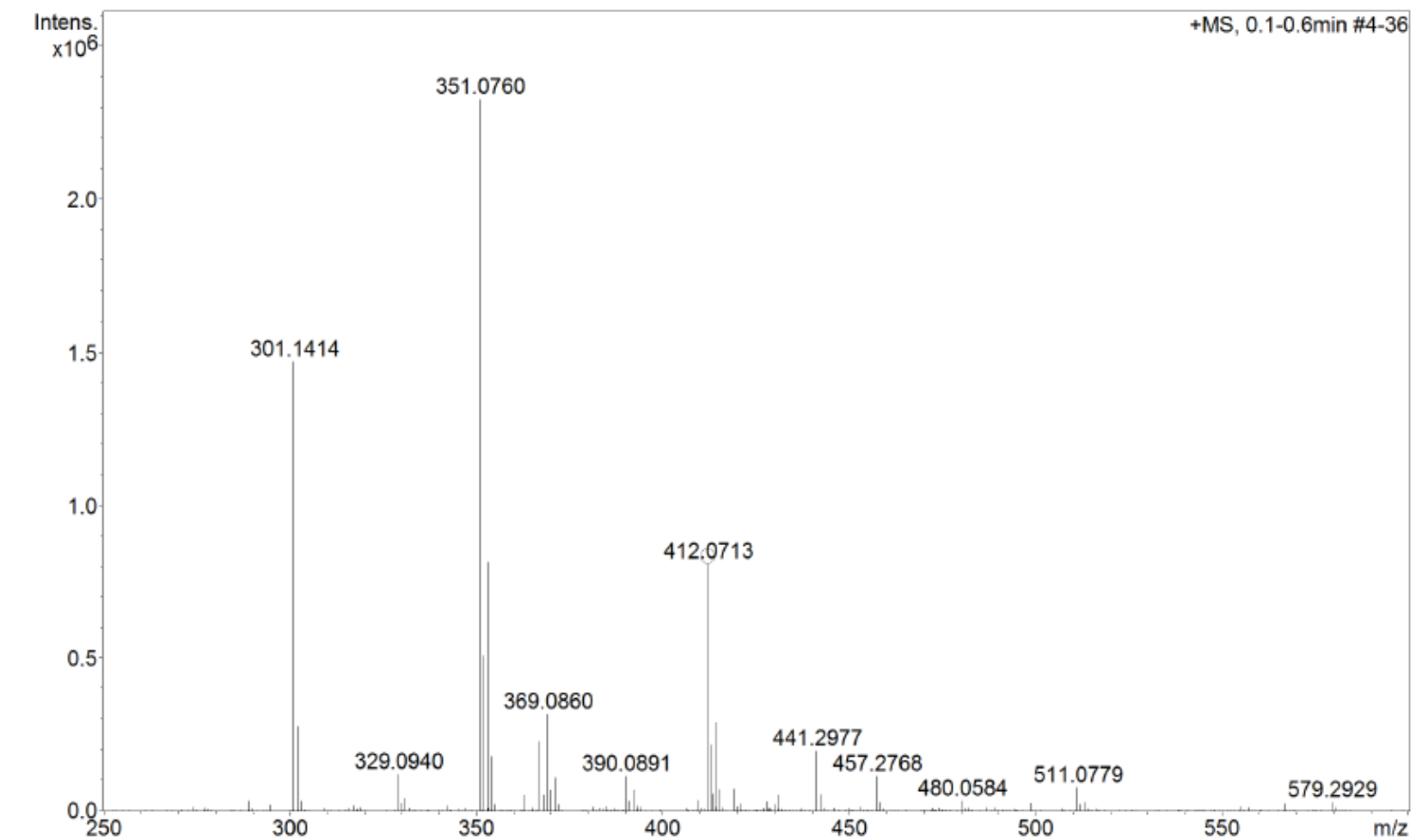


$^1\text{H}$  NMR spectrum of compound **5c** (500.00 MHz,  $\text{CDCl}_3$ )

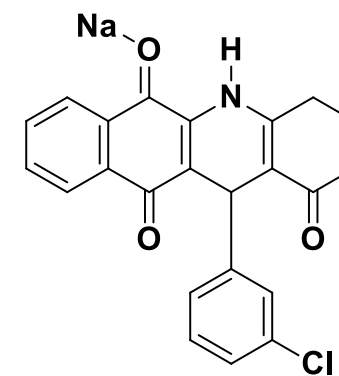


<sup>13</sup>C NMR spectrum of compound **5c** (125.0 MHz, CDCl<sub>3</sub>)

+MS, 0.1-0.6min #4-36



Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std	Mean m/z	Std I	VarNorm	Std	m/z Diff	Std	Comb	Dev
412.071268	1	C <sub>23</sub> H <sub>16</sub> ClNNaO <sub>3</sub>	412.071092	-0.4	0.3	15.5	ok	even		5.1	7.1		n.a.		n.a.		n.a.		n.a.	n.a.
	2	C <sub>19</sub> H <sub>12</sub> ClN <sub>7</sub> NaO	412.068406	-6.9	-7.2	16.5	ok	even		16.6	25.5		n.a.		n.a.		n.a.		n.a.	n.a.

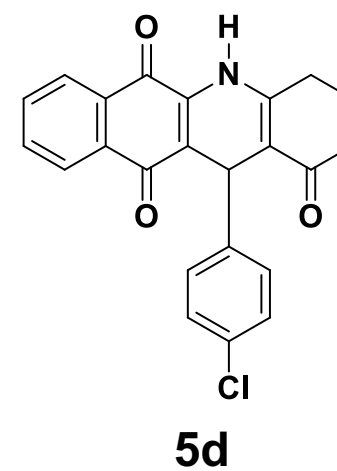
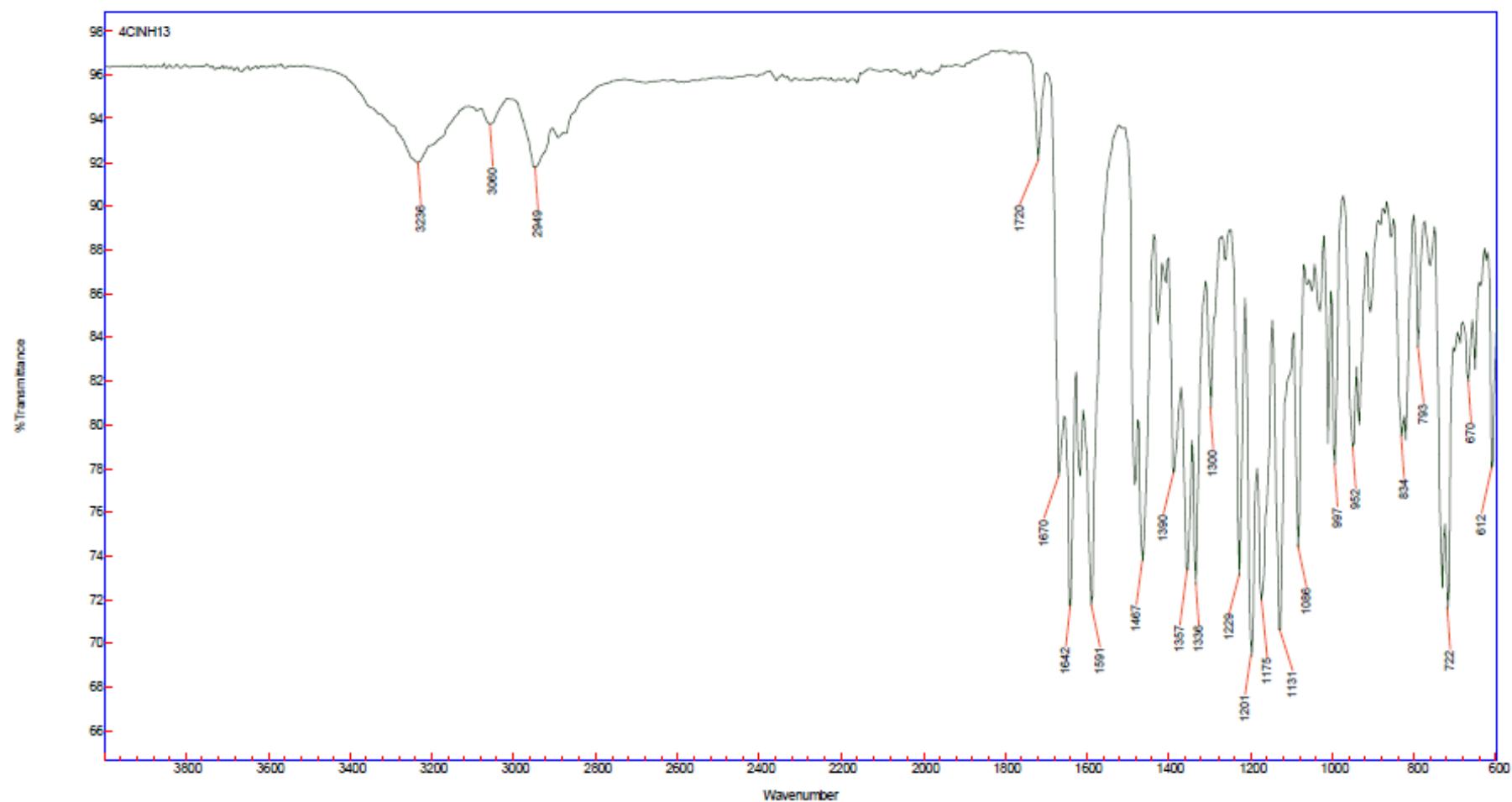


Exact Mass: 412,0716

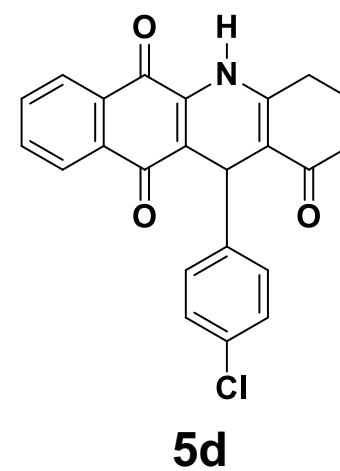
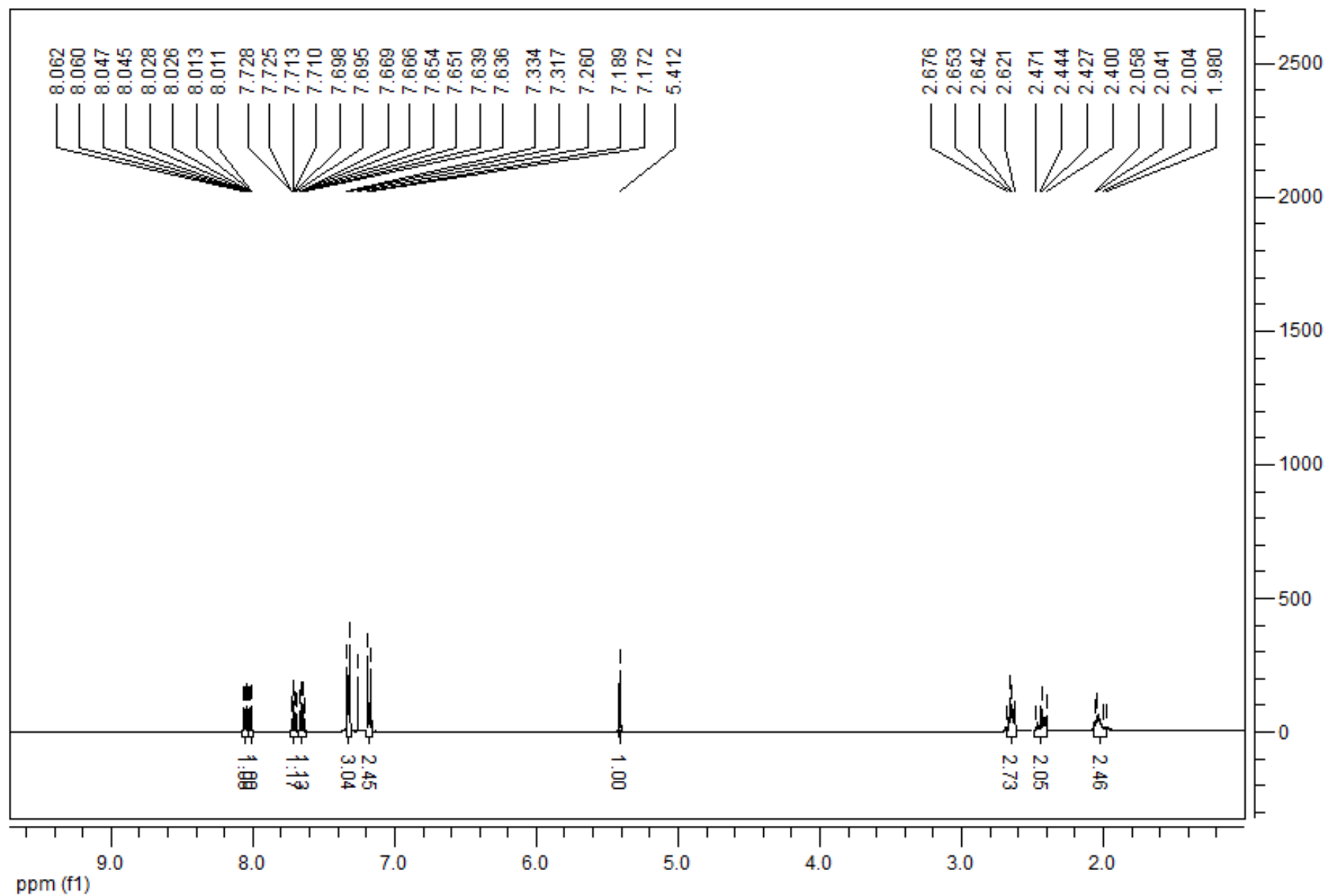
**5c**

HRMS of compound **5c**

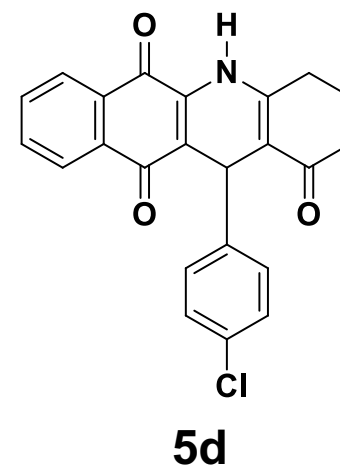
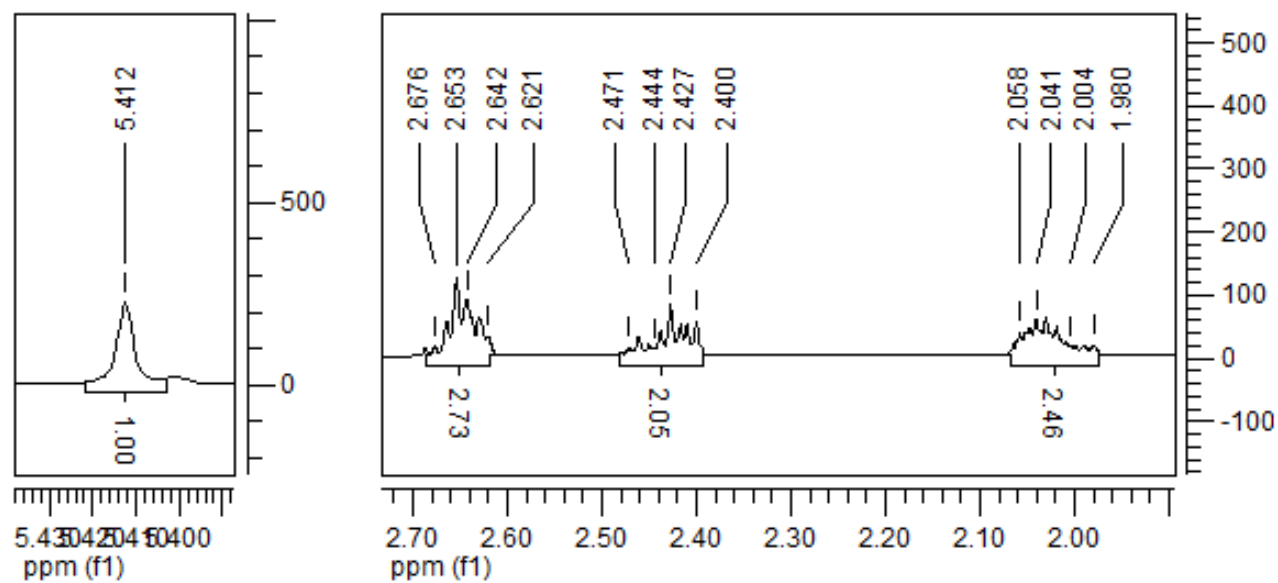
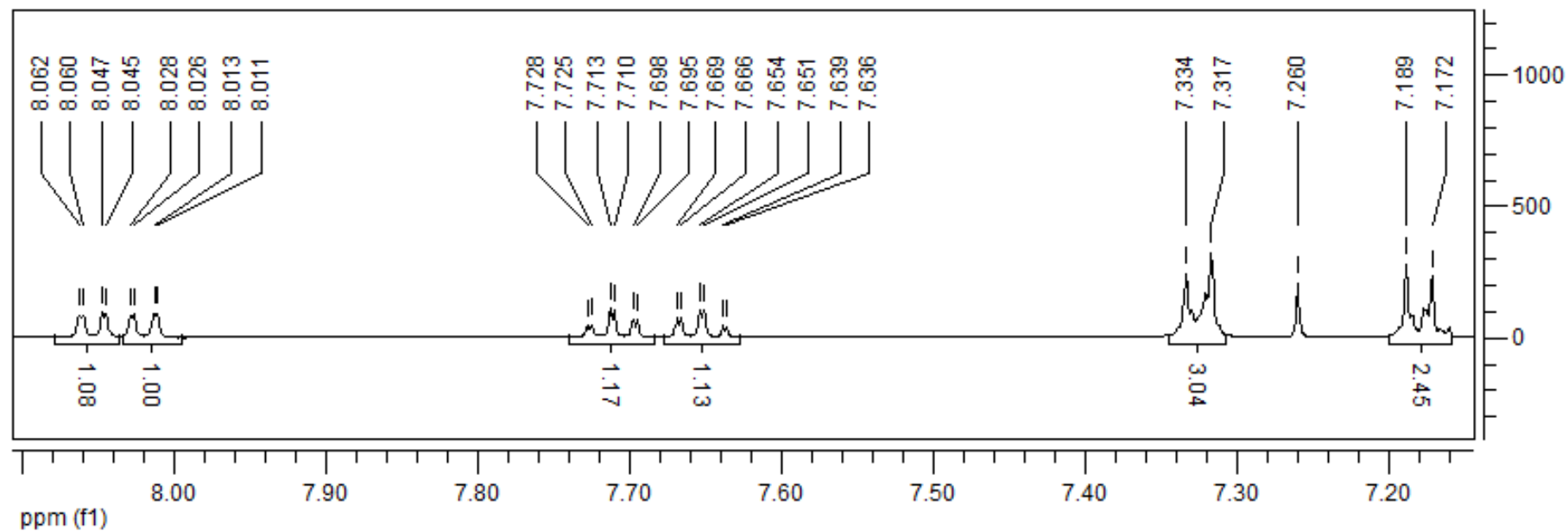




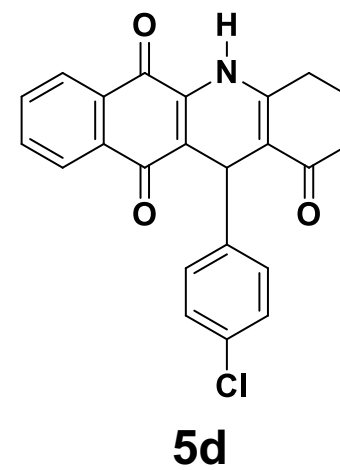
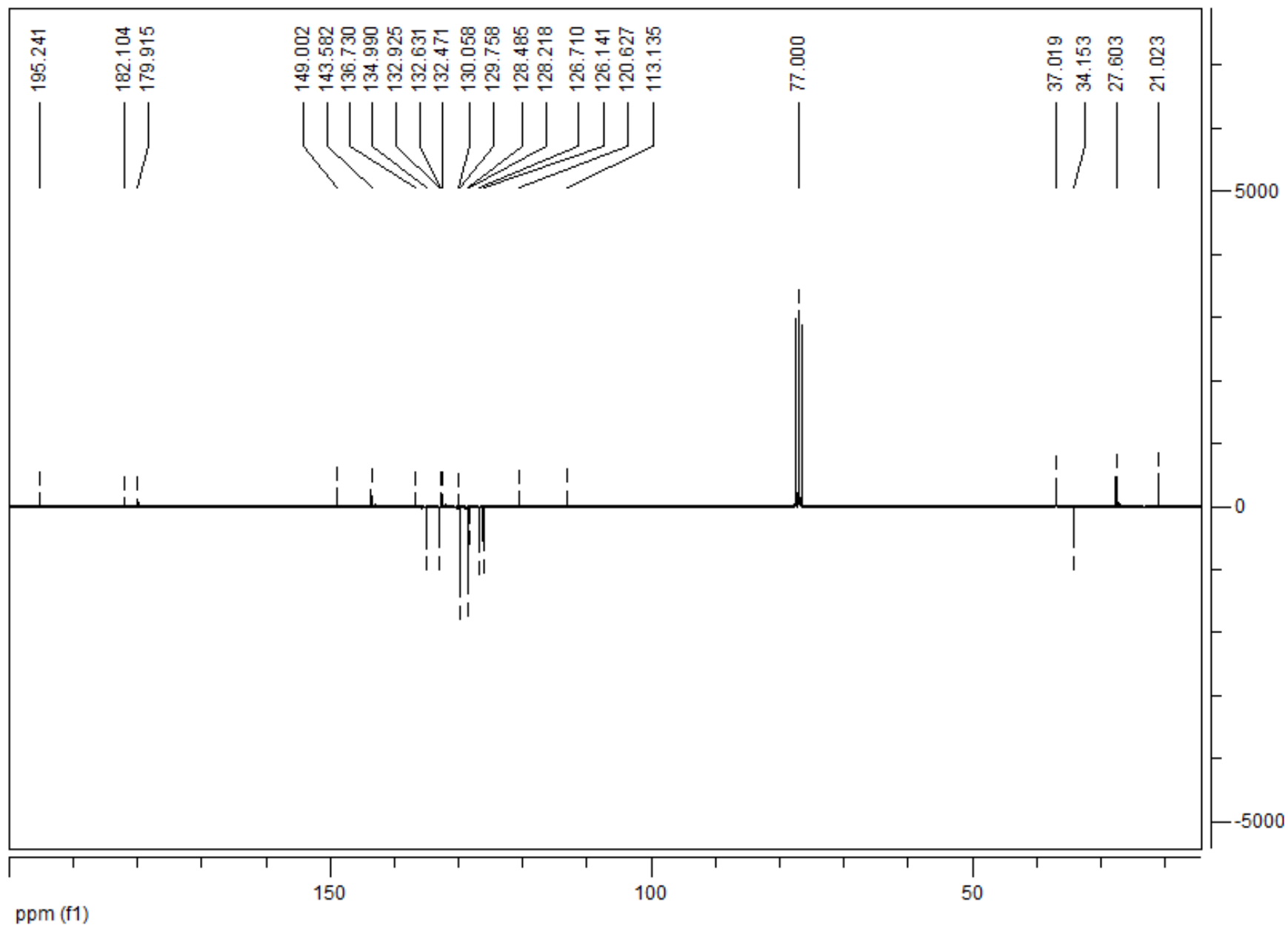
IR spectrum of compound **5d**



<sup>1</sup>H NMR spectrum of compound **5d** (500.00 MHz, CDCl<sub>3</sub>)

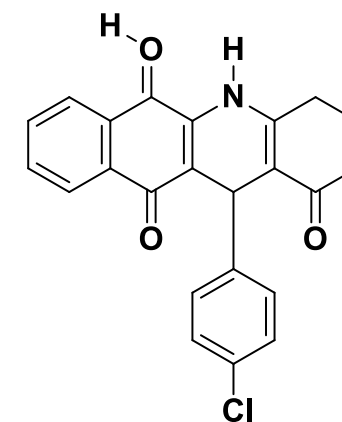
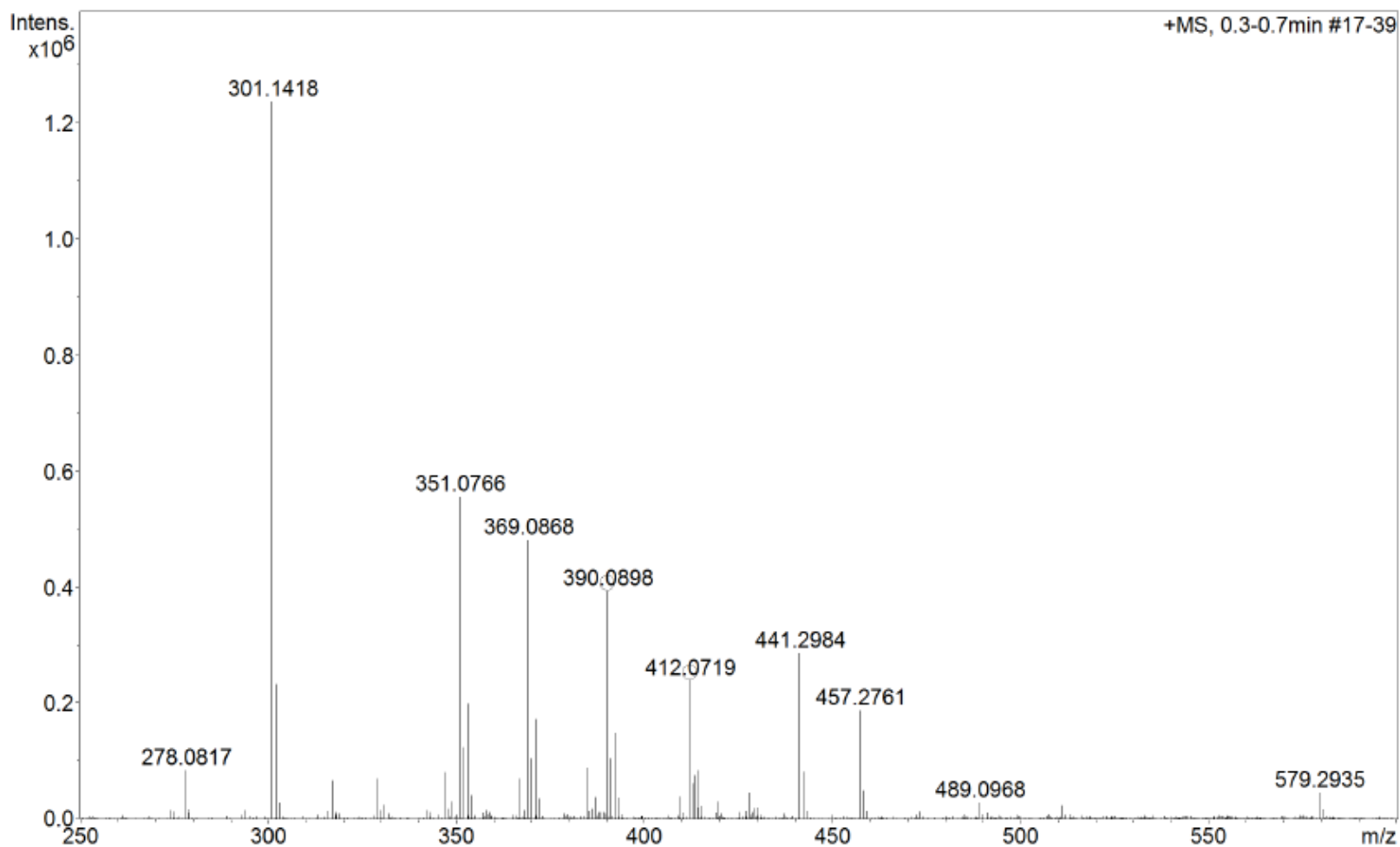


$^1\text{H}$  NMR spectrum of compound **5d** (500.00 MHz,  $\text{CDCl}_3$ )



$^{13}\text{C}$  NMR spectrum of compound **5d** (75.0 MHz,  $\text{CDCl}_3$ )

+MS, 0.3-0.7min #17-39



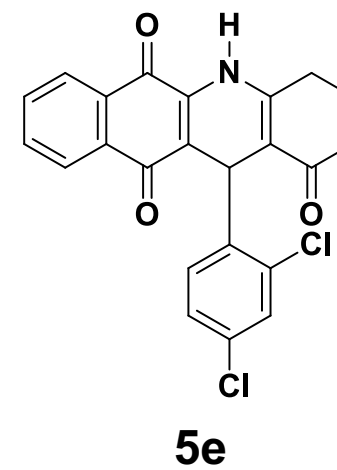
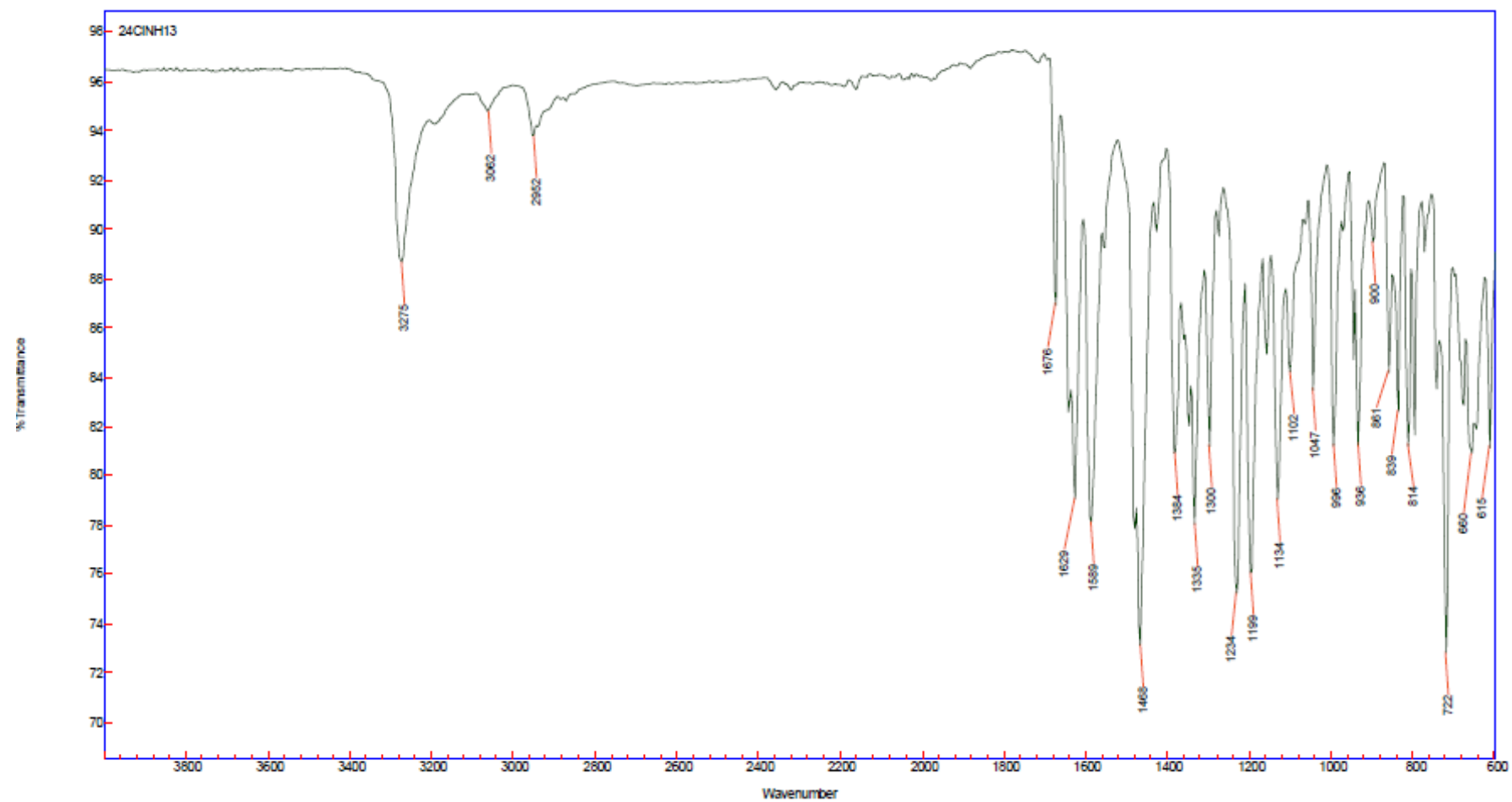
Exact Mass: 390,0897

**5d**

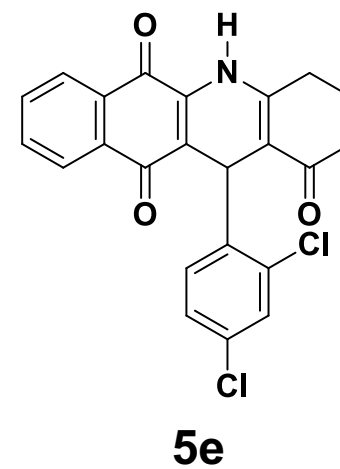
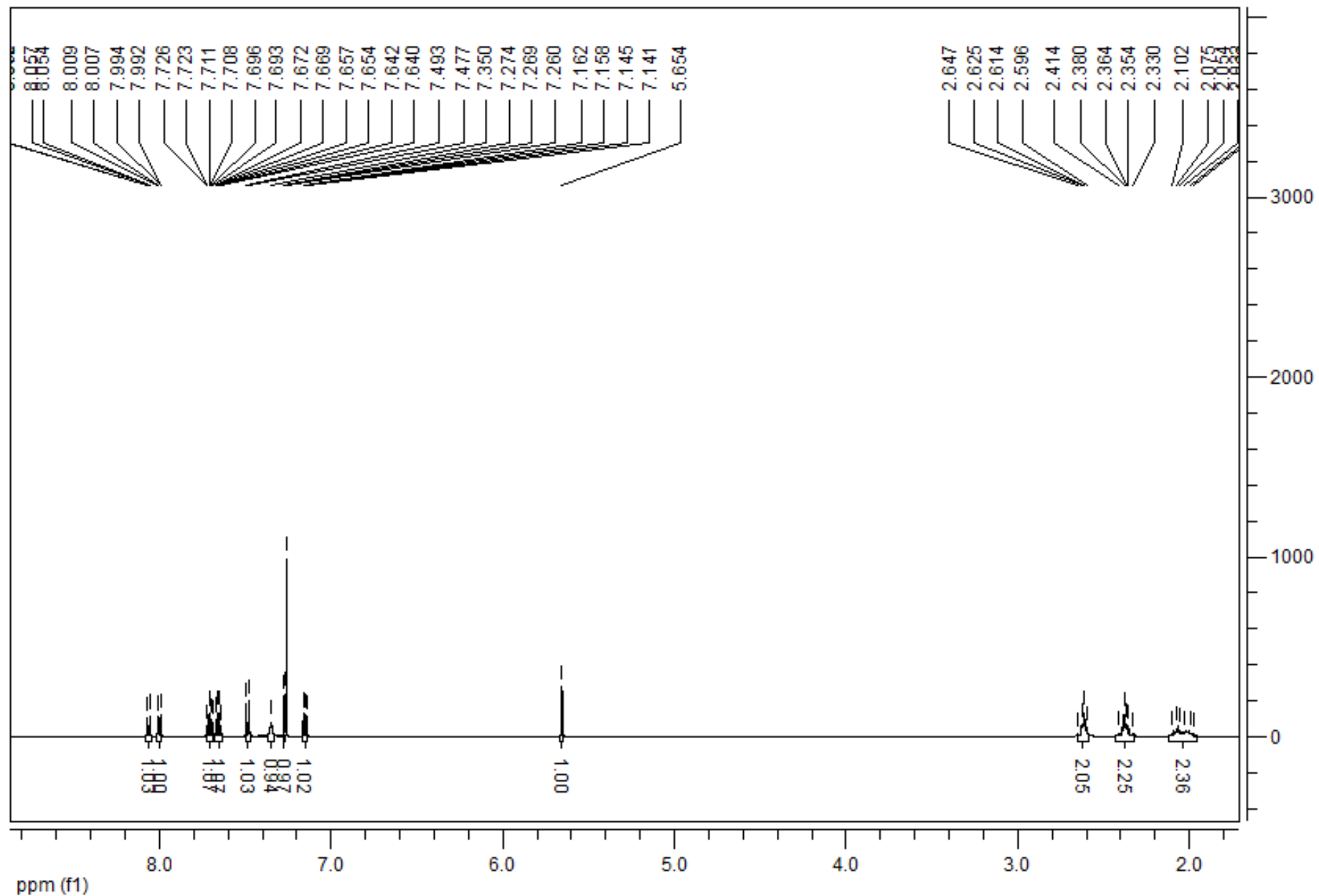
Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std	m/z	Diff	Std	Comb	Dev
390.089822	1	C <sub>23</sub> H <sub>17</sub> ClNO <sub>3</sub>	390.089148	-1.7	-2.0	15.5	ok	even		11.0	17.0		n.a.		n.a.		n.a.			n.a.	
	2	C <sub>19</sub> H <sub>13</sub> ClN <sub>7</sub> O	390.086462	-8.6	-9.9	16.5	ok	even		21.4	34.3		n.a.		n.a.		n.a.			n.a.	
412.071891	1	C <sub>23</sub> H <sub>16</sub> ClNNaO <sub>3</sub>	412.071092	-1.9	-2.1	15.5	ok	even		4.9	6.6		n.a.		n.a.		n.a.			n.a.	
	2	C <sub>19</sub> H <sub>12</sub> ClN <sub>7</sub> NaO	412.068406	-8.5	-9.7	16.5	ok	even		13.0	21.6		n.a.		n.a.		n.a.			n.a.	

HRMS of compound **5d**

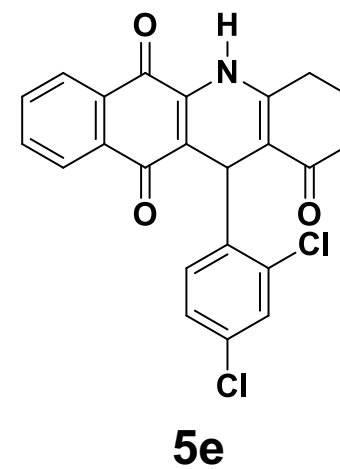
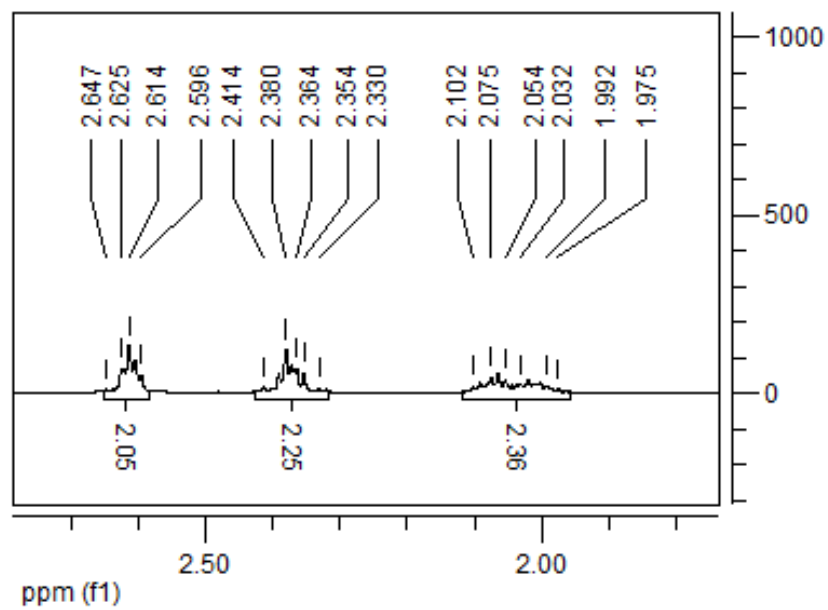
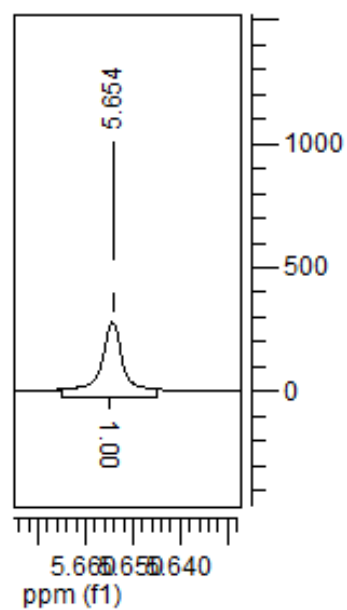
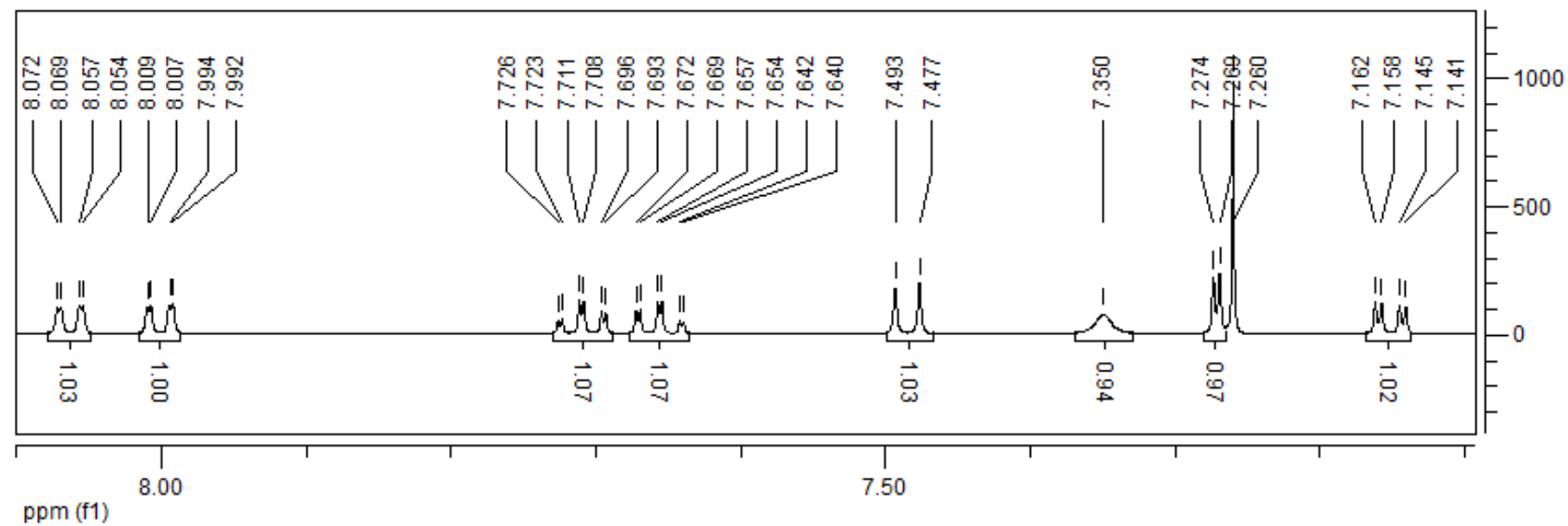
## IR (KBr)



IR spectrum of compound **5e**

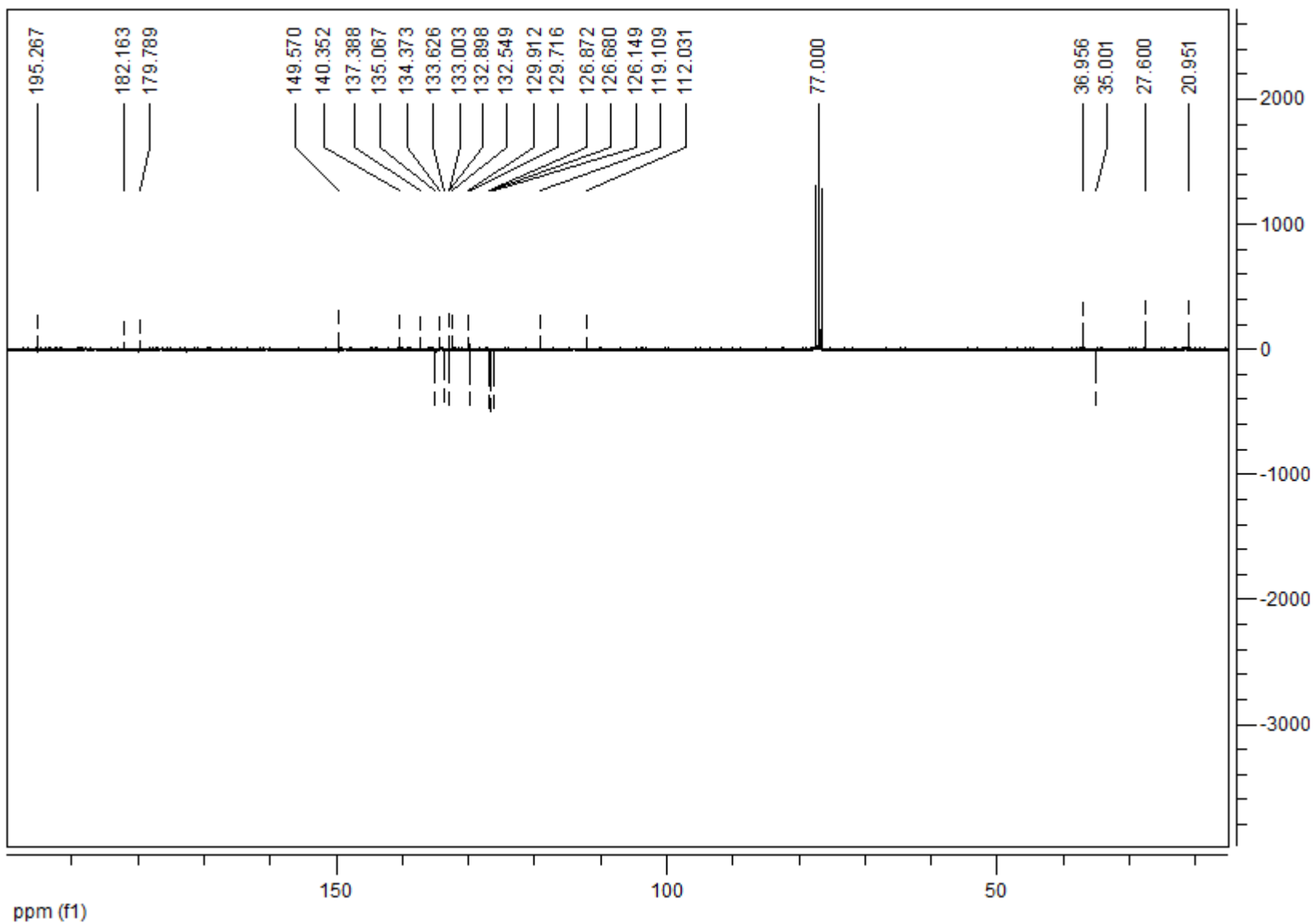


<sup>1</sup>H NMR spectrum of compound **5e** (500.00 MHz, CDCl<sub>3</sub>)



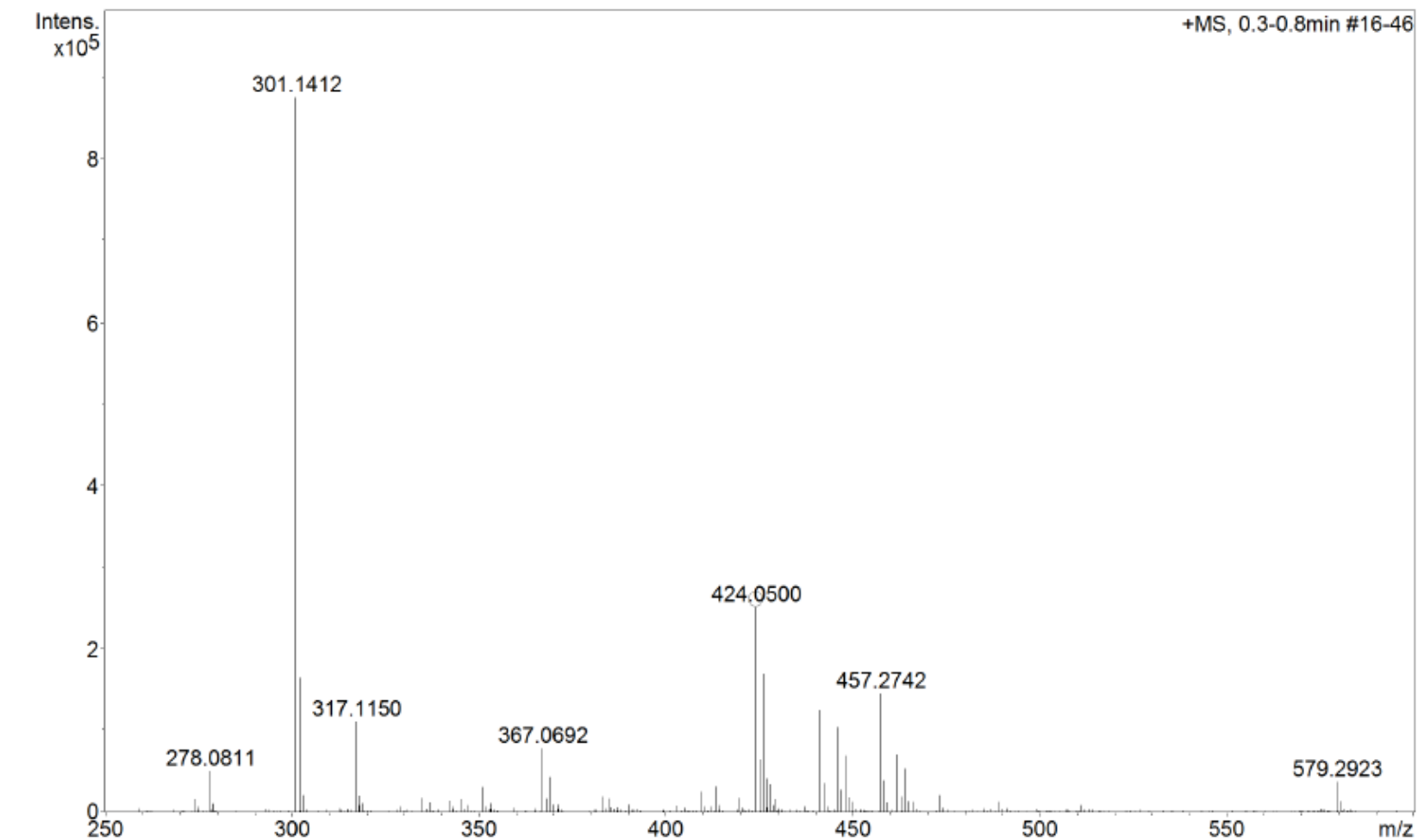
<sup>1</sup>H NMR spectrum of compound **5e** (500.00 MHz, CDCl<sub>3</sub>)



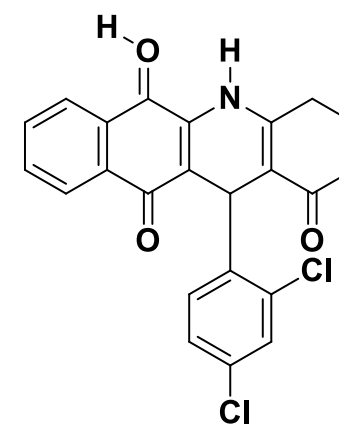


$^{13}\text{C}$  NMR spectrum of compound **5e** (75.0 MHz,  $\text{CDCl}_3$ )

+MS, 0.3-0.8min #16-46



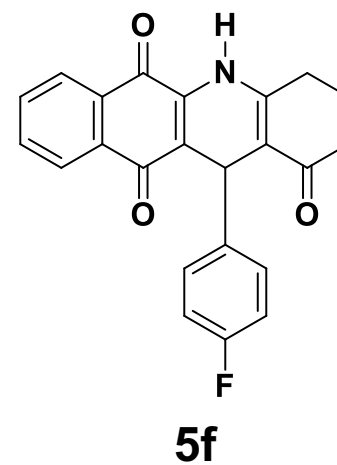
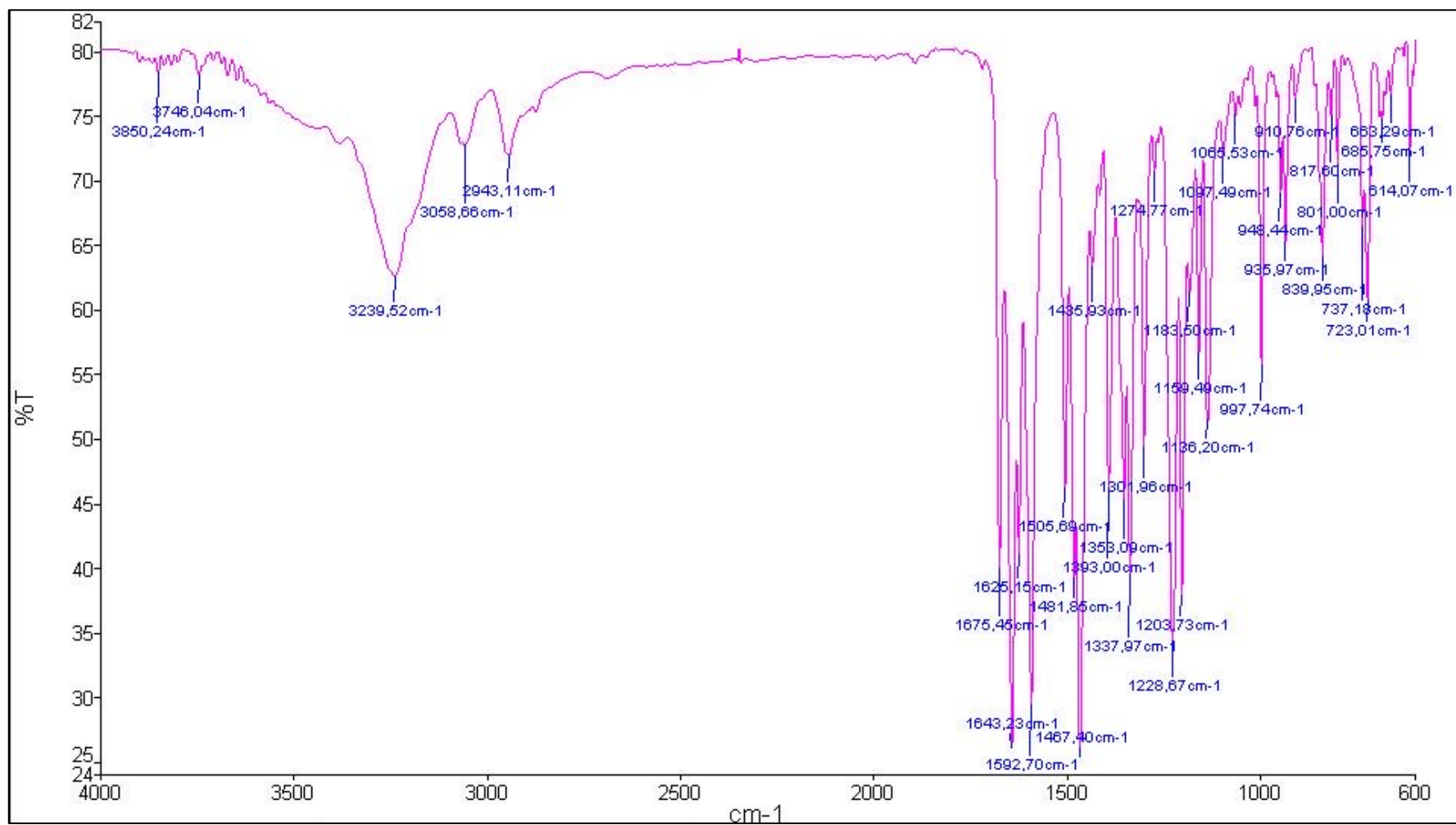
Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std	Mean m/z	Std I	VarNorm	Std	m/z	Diff	Std	Comb	Dev
424.049984	1	C <sub>23</sub> H <sub>16</sub> Cl <sub>2</sub> NO <sub>3</sub>	424.050175	0.5	0.8	15.5	ok	even		4.2	4.6		n.a.		n.a.		n.a.			n.a.	
	2	C <sub>19</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>7</sub> O	424.047490	-5.9	-6.4	16.5	ok	even		12.0	16.3		n.a.		n.a.		n.a.			n.a.	
	3	C <sub>18</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>5</sub>	424.046152	-9.0	-9.1	11.5	ok	even		22.1	29.4		n.a.		n.a.		n.a.			n.a.	



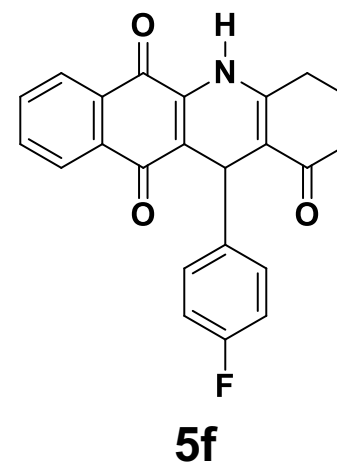
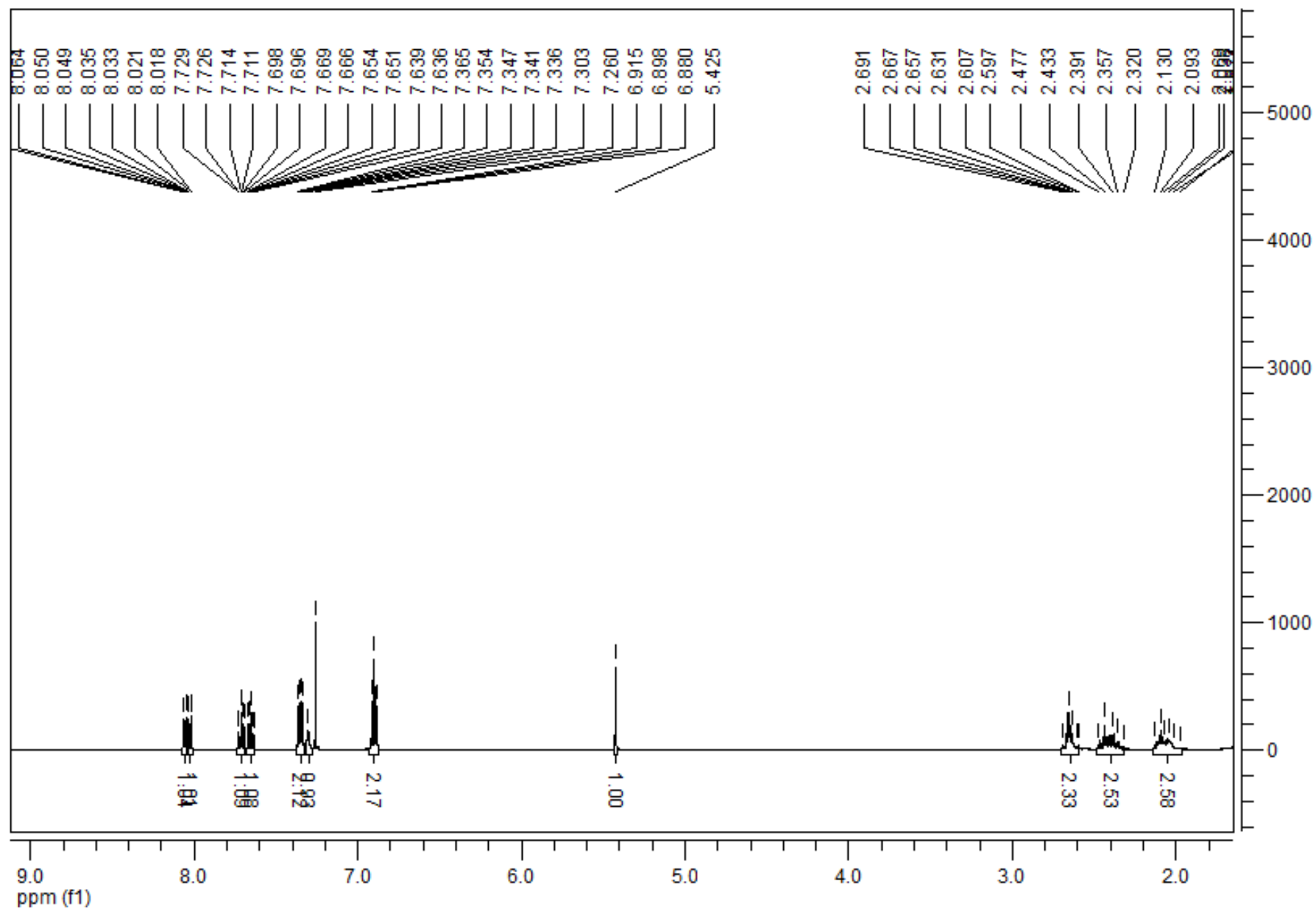
Exact Mass: 424,0507

**5e**

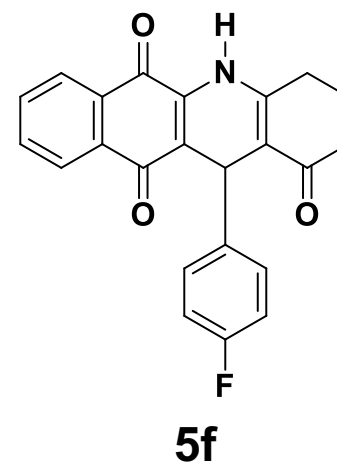
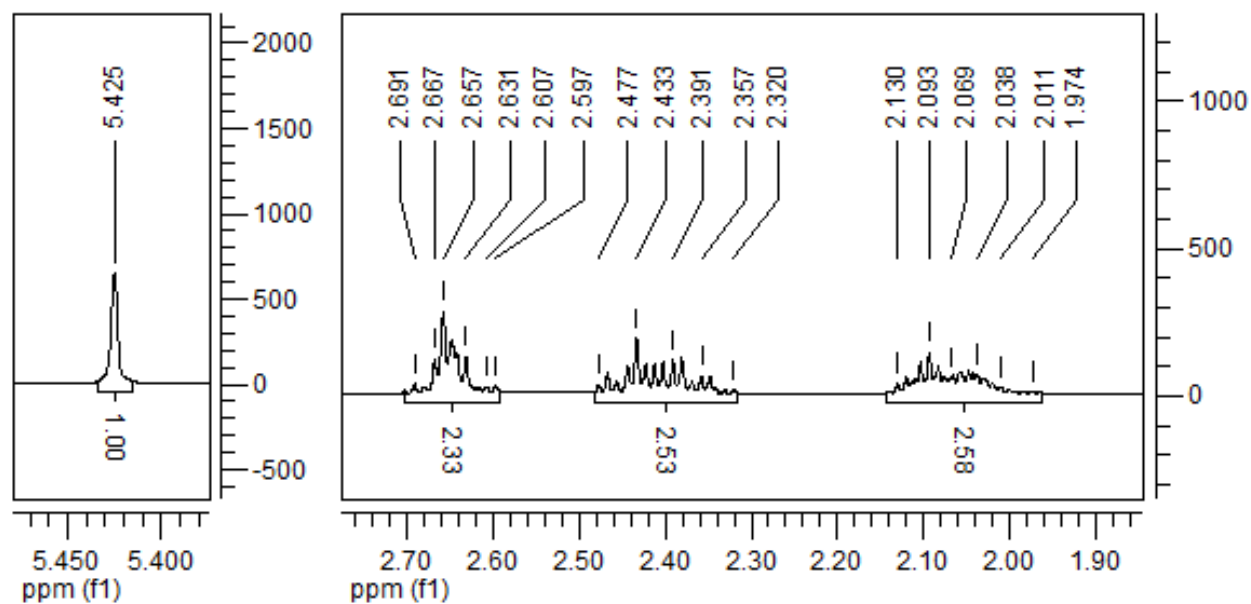
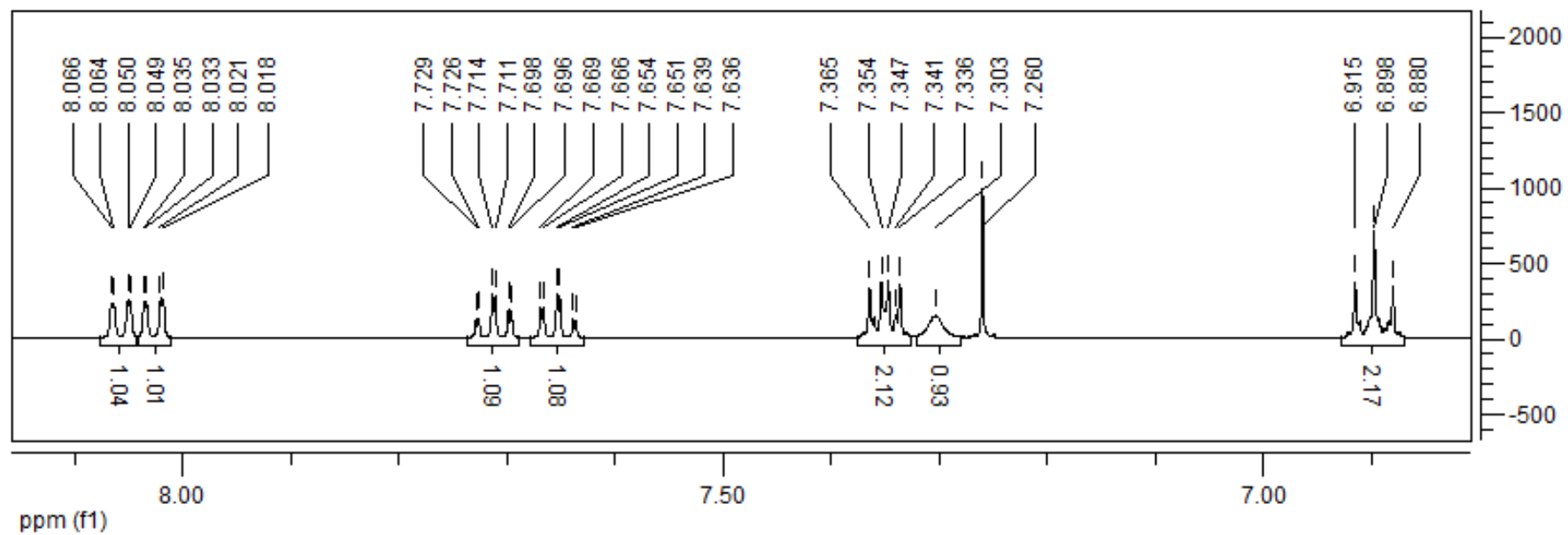
HRMS of compound **5e**



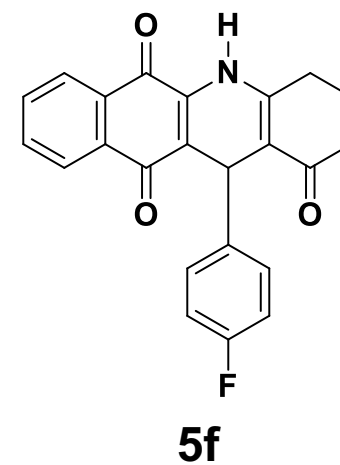
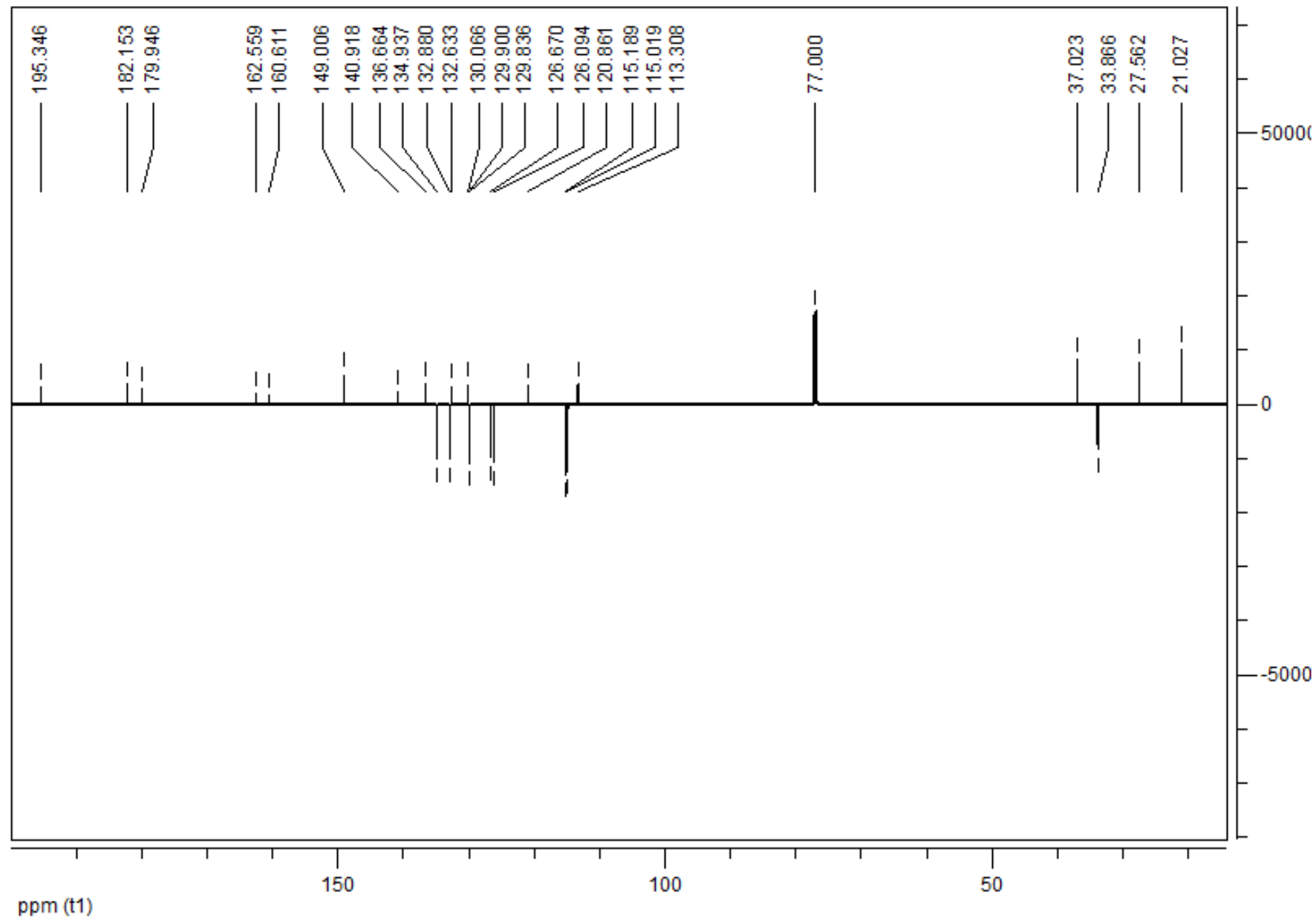
IR spectrum of compound **5f**



<sup>1</sup>H NMR spectrum of compound **5f** (500.00 MHz, CDCl<sub>3</sub>)

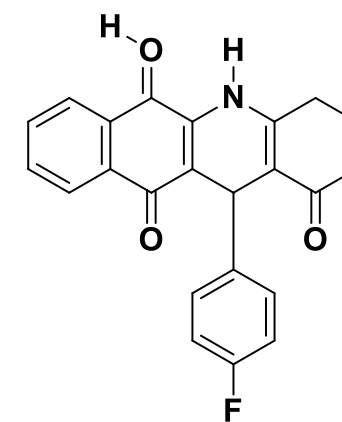
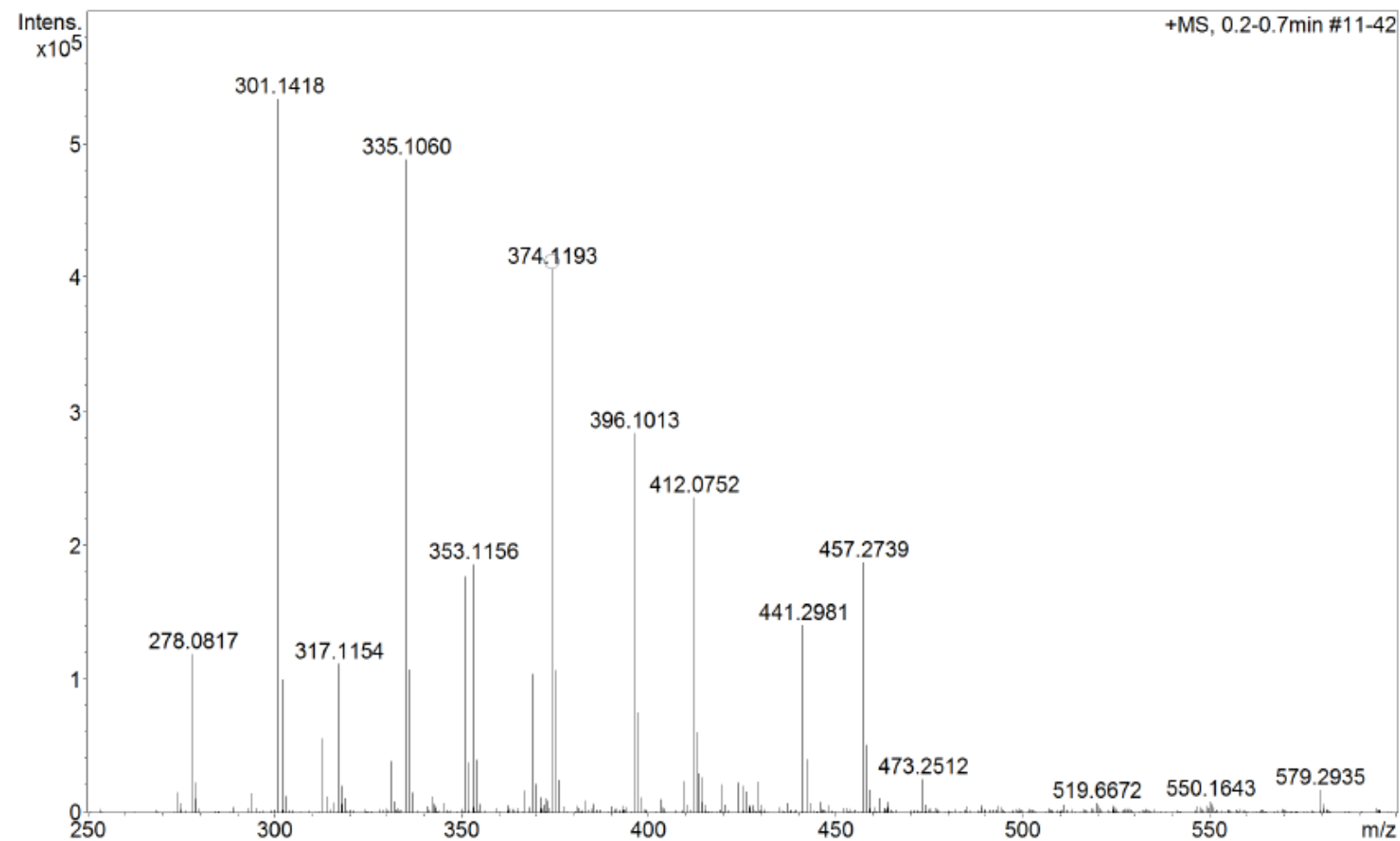


<sup>1</sup>H NMR spectrum of compound **5f** (500.00 MHz, CDCl<sub>3</sub>)



<sup>13</sup>C NMR spectrum of compound **5f** (75.0 MHz, CDCl<sub>3</sub>)

+MS, 0.2-0.7min #11-42

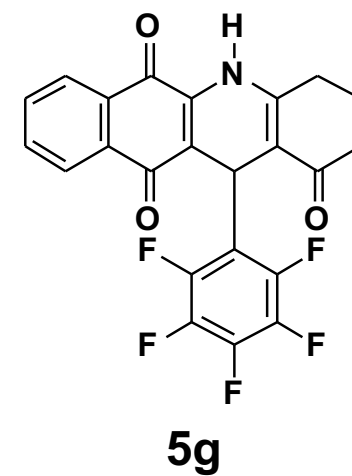
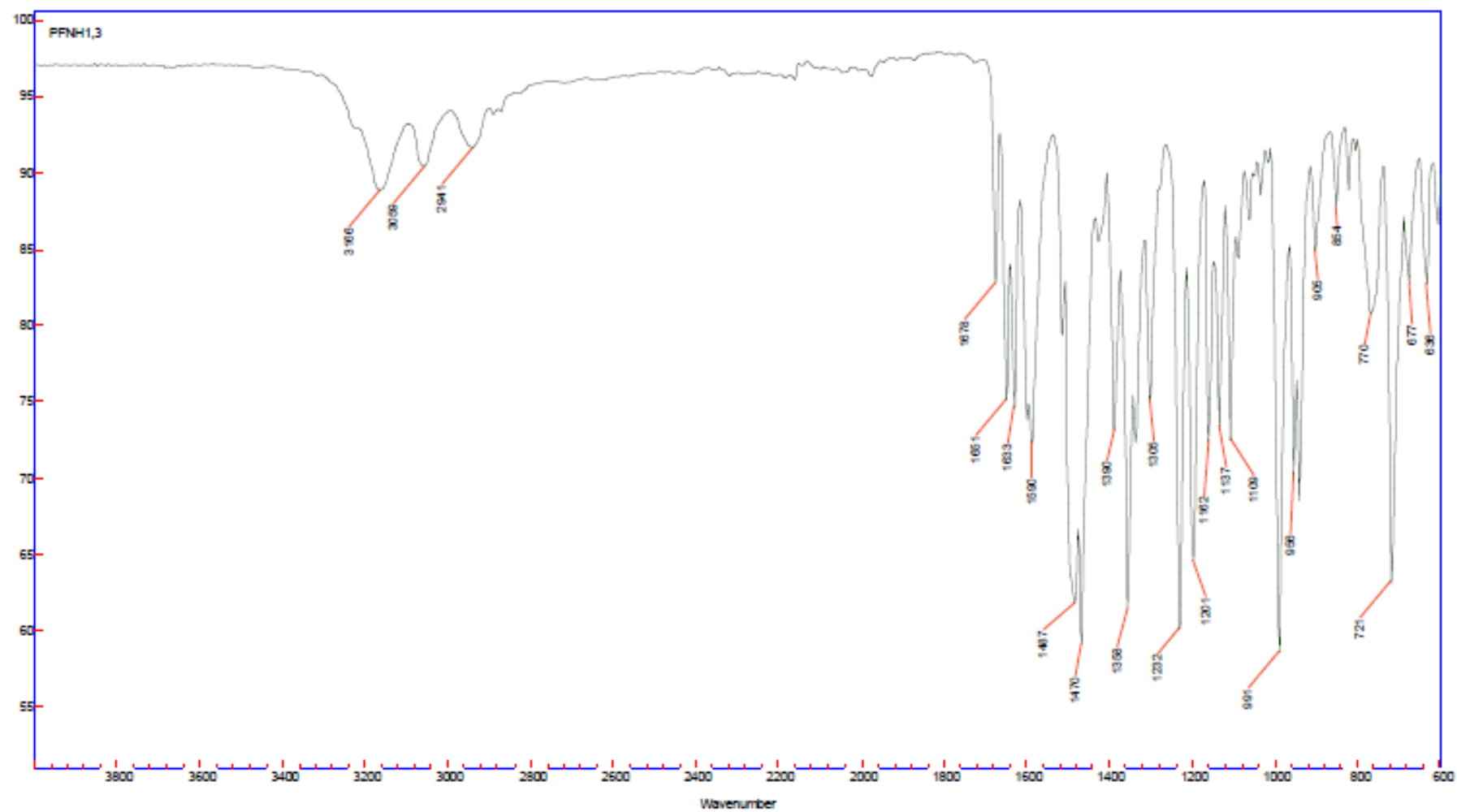


Exact Mass: 374,1192

**5f**

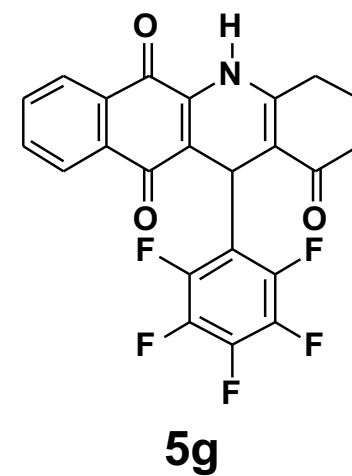
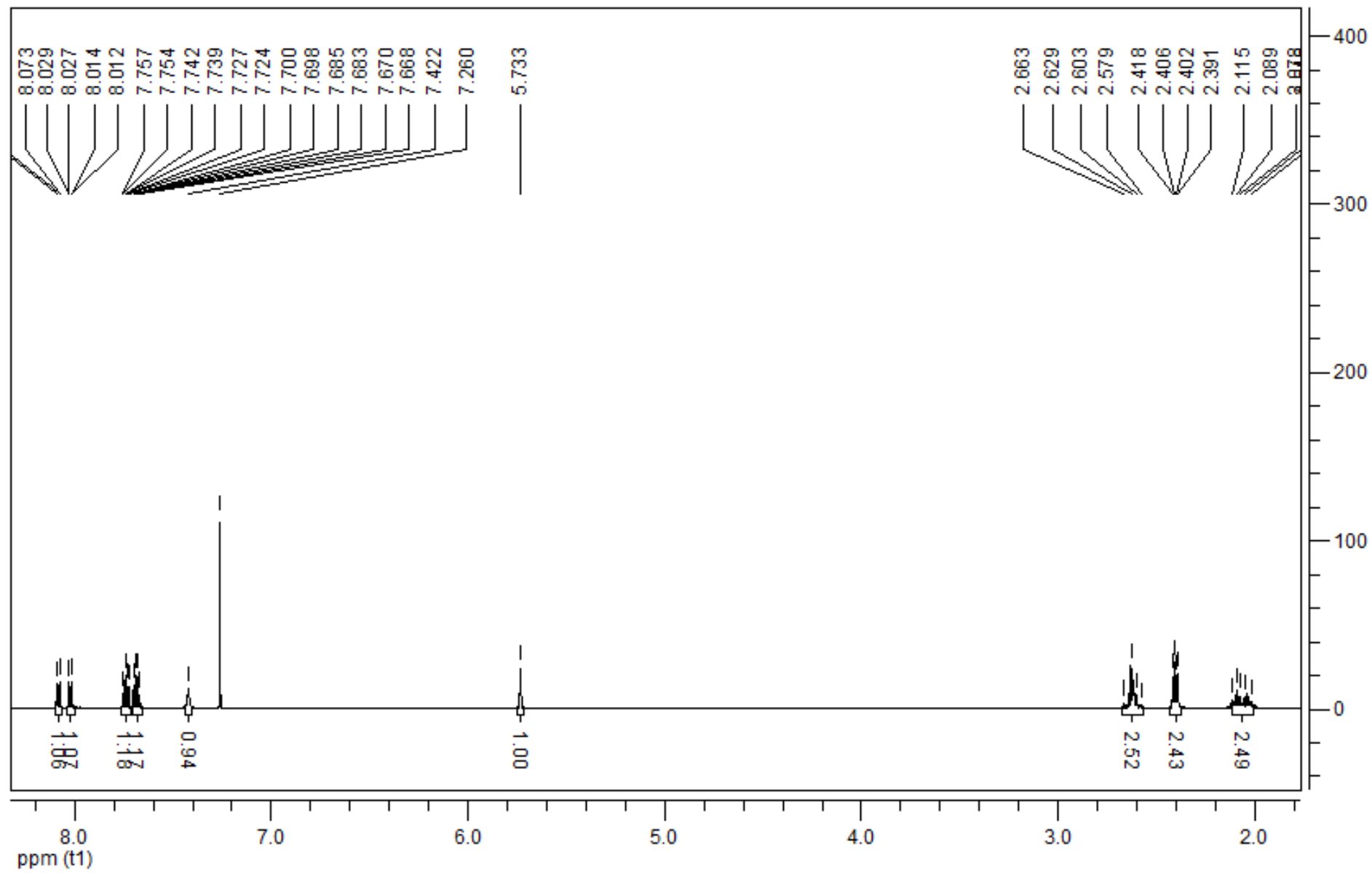
Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
374.119336	1	C <sub>23</sub> H <sub>17</sub> FN <sub>3</sub> O	374.118698	-1.7	-2.8	15.5	ok	even		13.8	24.2		n.a.		n.a.		n.a.		n.a.
	2	C <sub>19</sub> H <sub>13</sub> FN <sub>7</sub> O	374.116013	-8.9	-10.9	16.5	ok	even		25.3	46.0		n.a.		n.a.		n.a.		n.a.

HRMS of compound **5f**

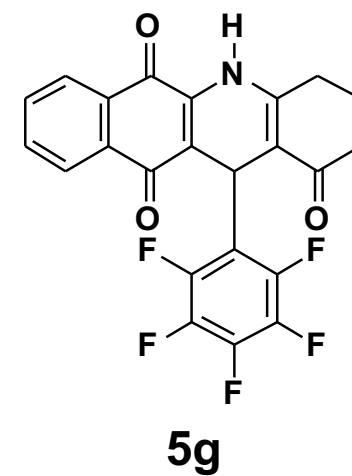
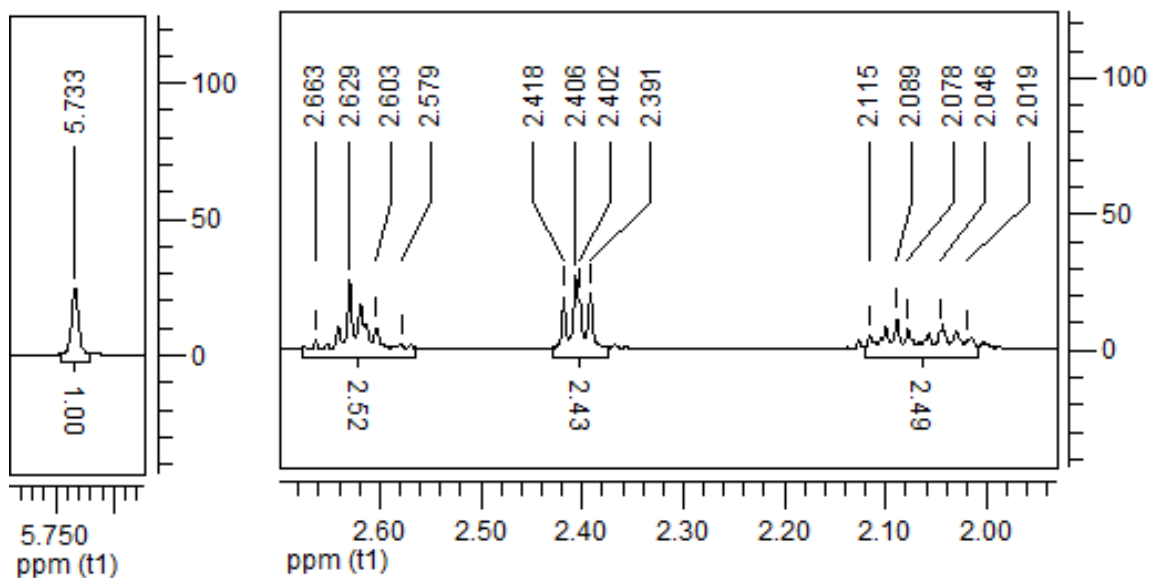
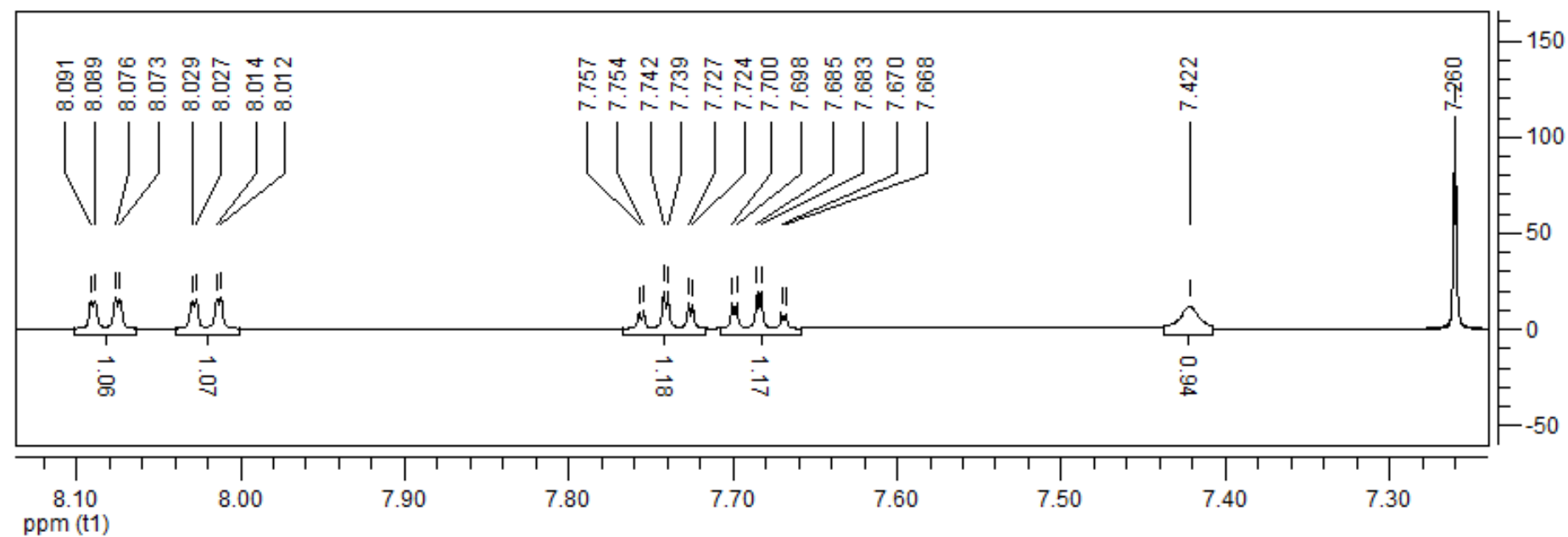


IR spectrum of compound **5g**

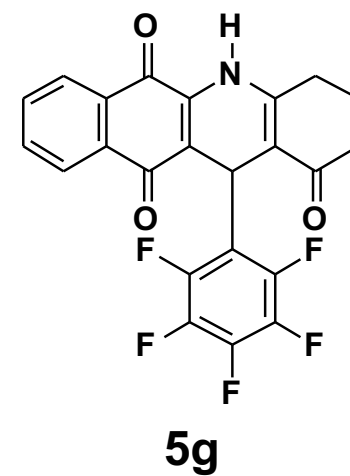
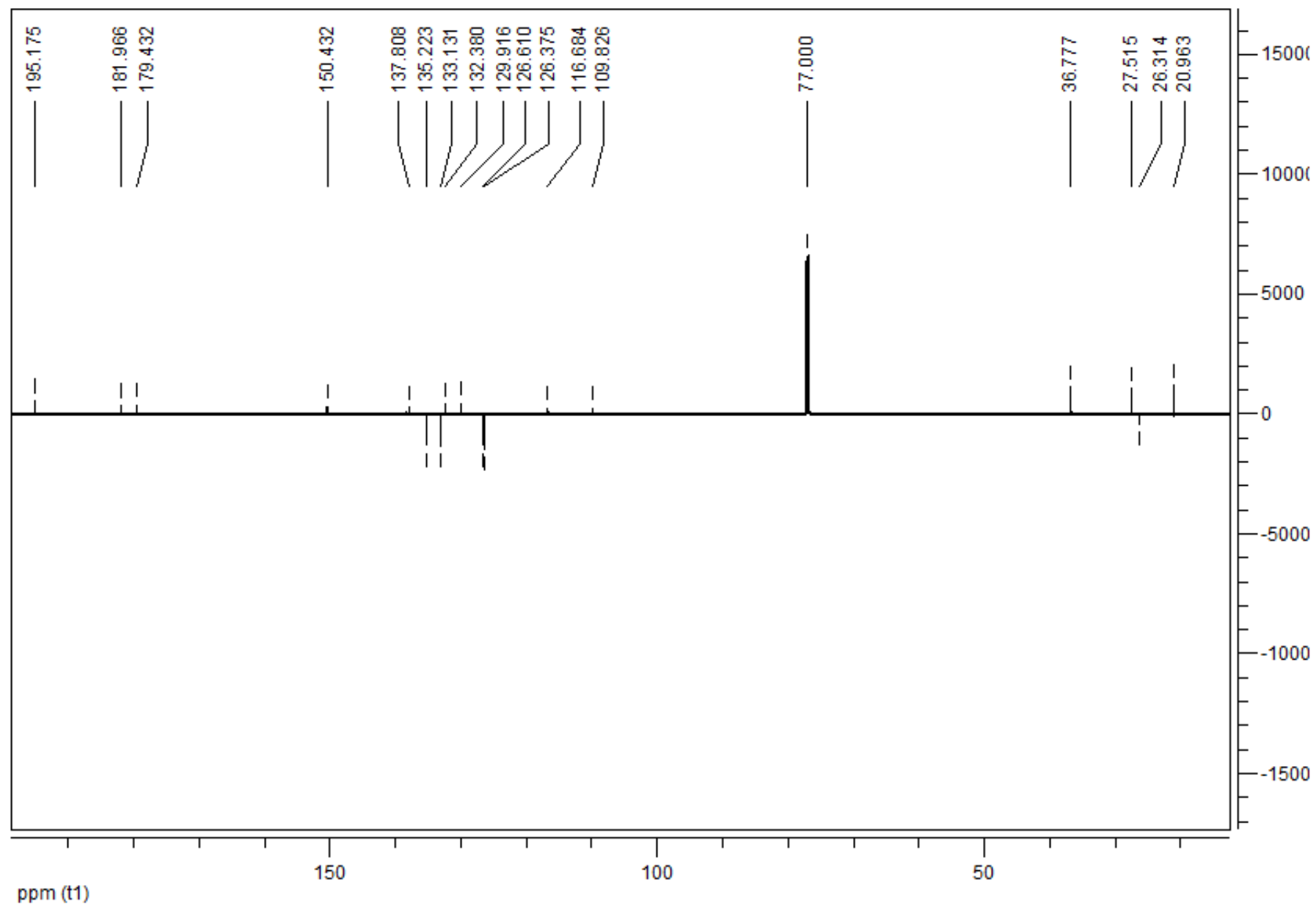




<sup>1</sup>H NMR spectrum of compound **5g** (500.00 MHz, CDCl<sub>3</sub>)

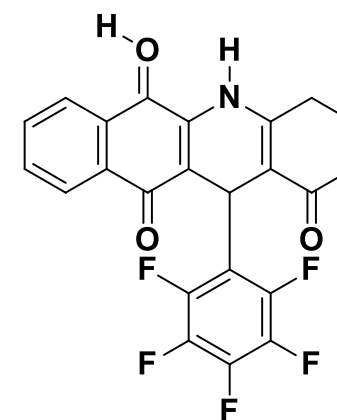
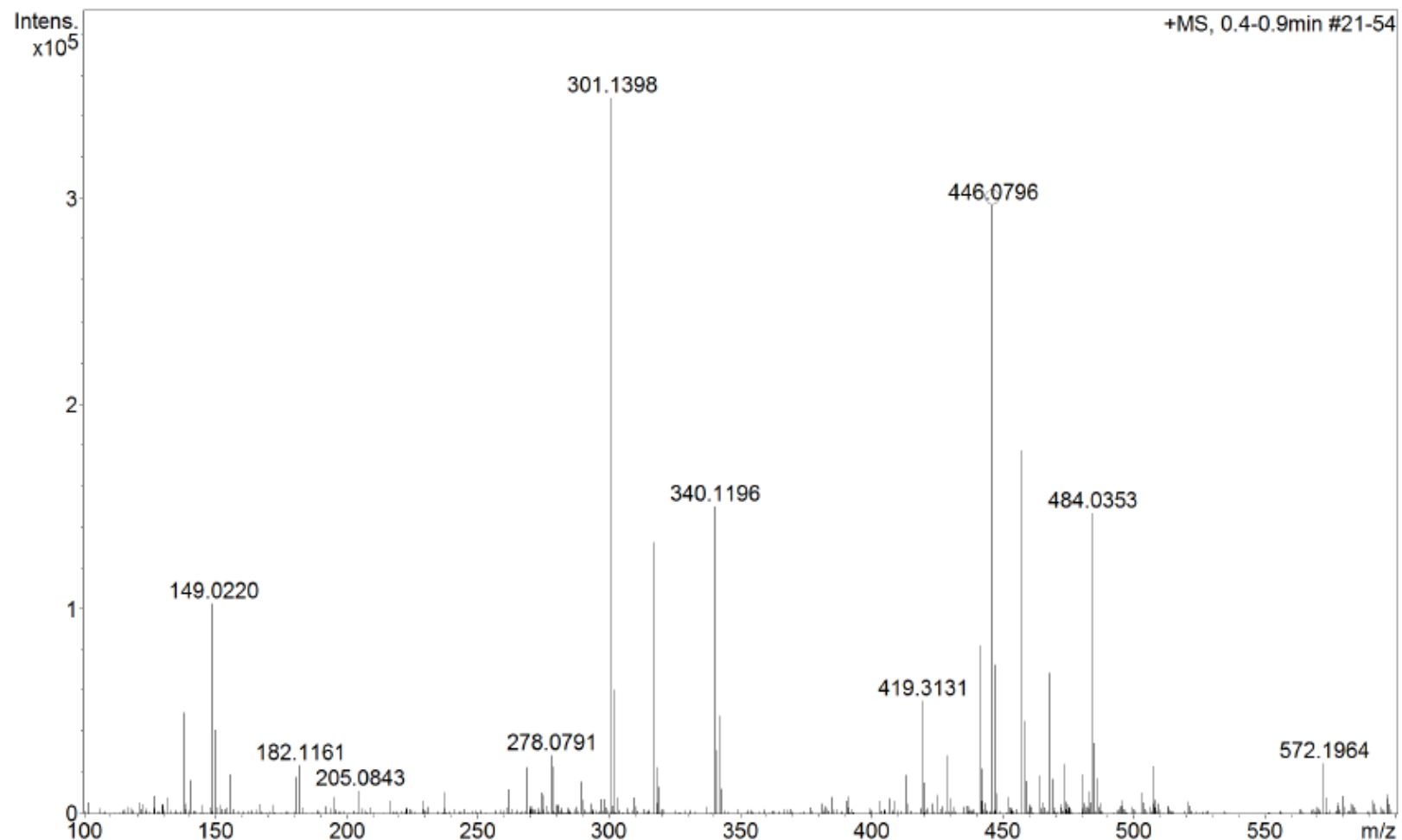


<sup>1</sup>H NMR spectrum of compound **5g** (500.00 MHz, CDCl<sub>3</sub>)



<sup>13</sup>C NMR spectrum of compound **5g** (125.0 MHz, CDCl<sub>3</sub>)

+MS, 0.4-0.9min #21-54

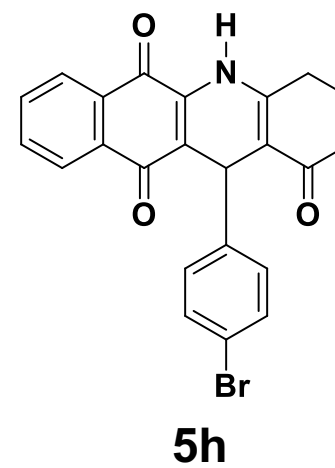
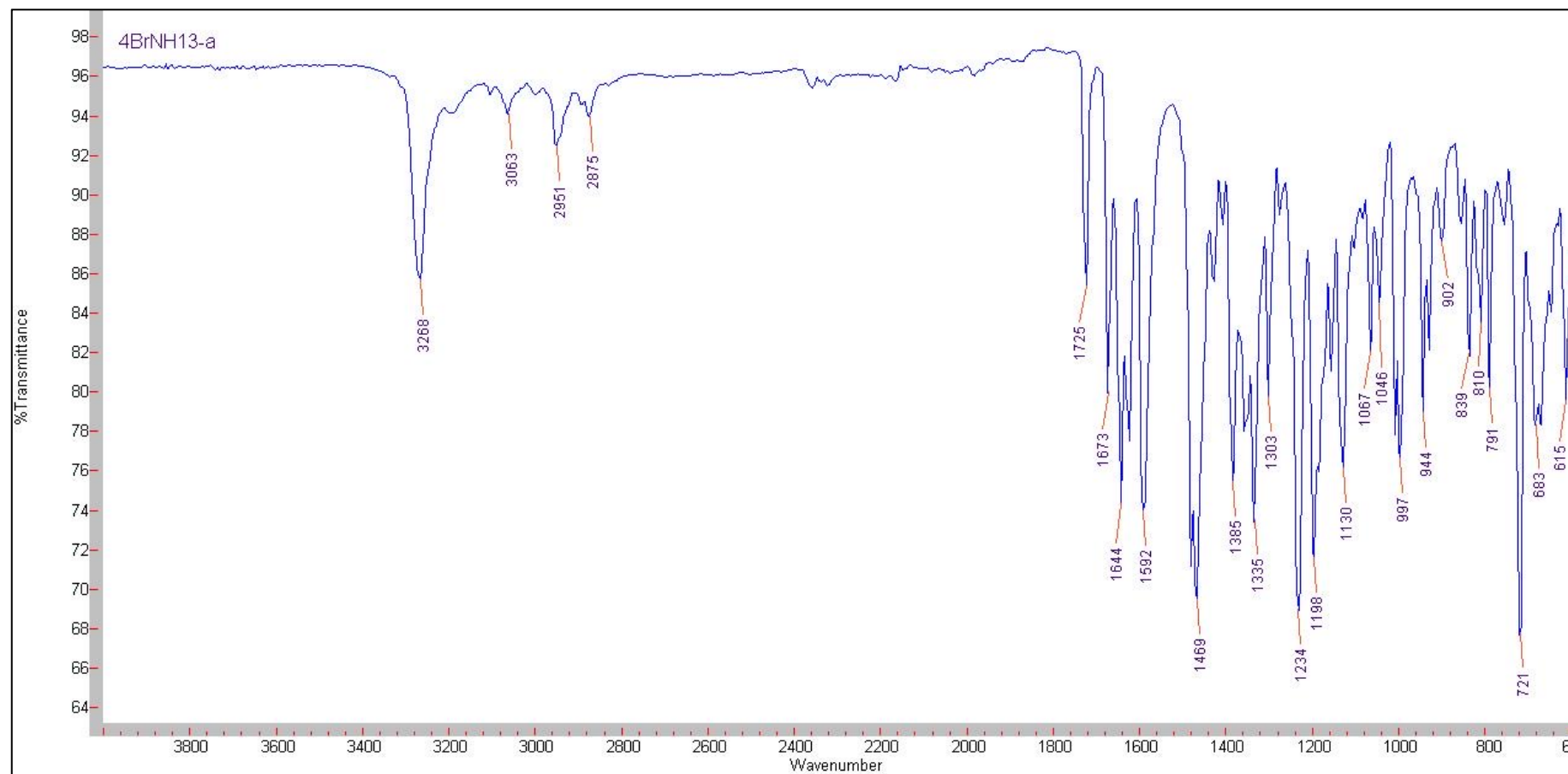


Exact Mass: 446,0816

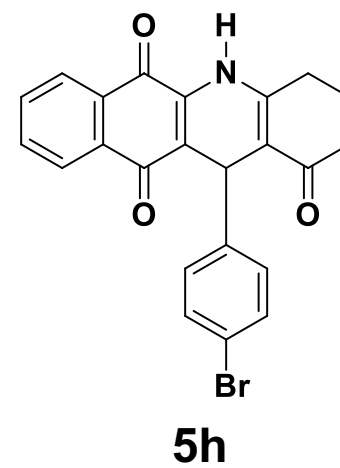
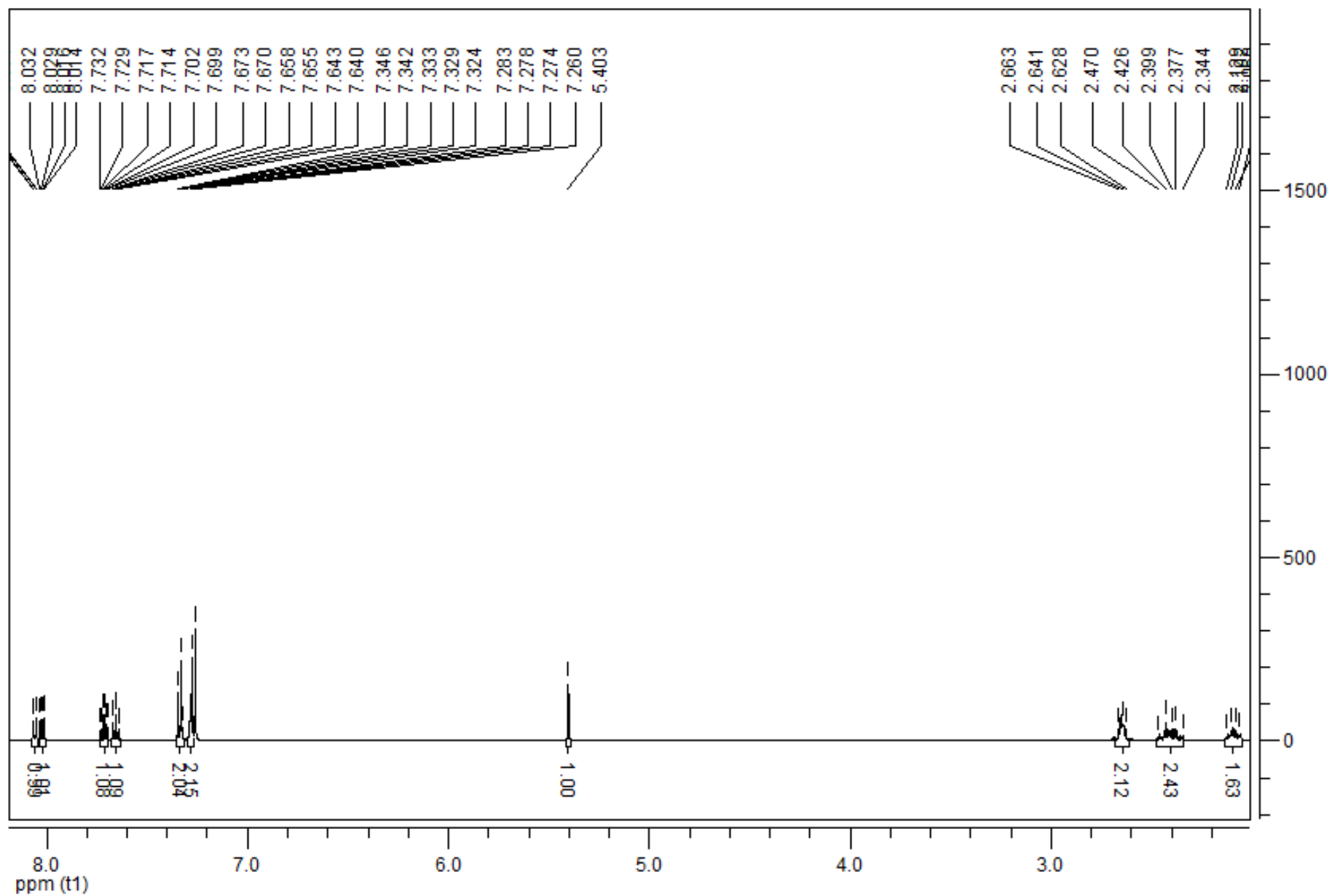
**5g**

Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std	m/z	Diff	Std	Comb	Dev
446.079562	1	C <sub>23</sub> H <sub>13</sub> F <sub>5</sub> NO <sub>3</sub>	446.081011	3.2	4.4	15.5	ok	even		6.3	10.8	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.			n.a.	
	2	C <sub>19</sub> H <sub>9</sub> F <sub>5</sub> N <sub>7</sub> O	446.078325	-2.8	-2.4	16.5	ok	even		7.8	13.7	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.			n.a.	
	3	C <sub>18</sub> H <sub>13</sub> F <sub>5</sub> N <sub>3</sub> O <sub>5</sub>	446.076988	-5.8	-5.1	11.5	ok	even		20.8	33.3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.			n.a.	

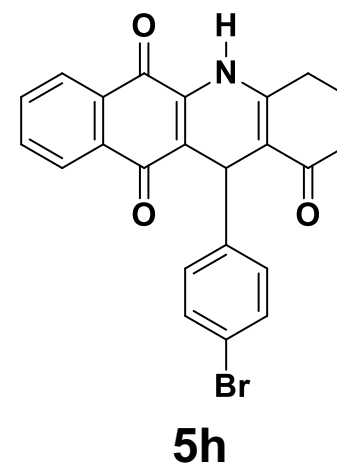
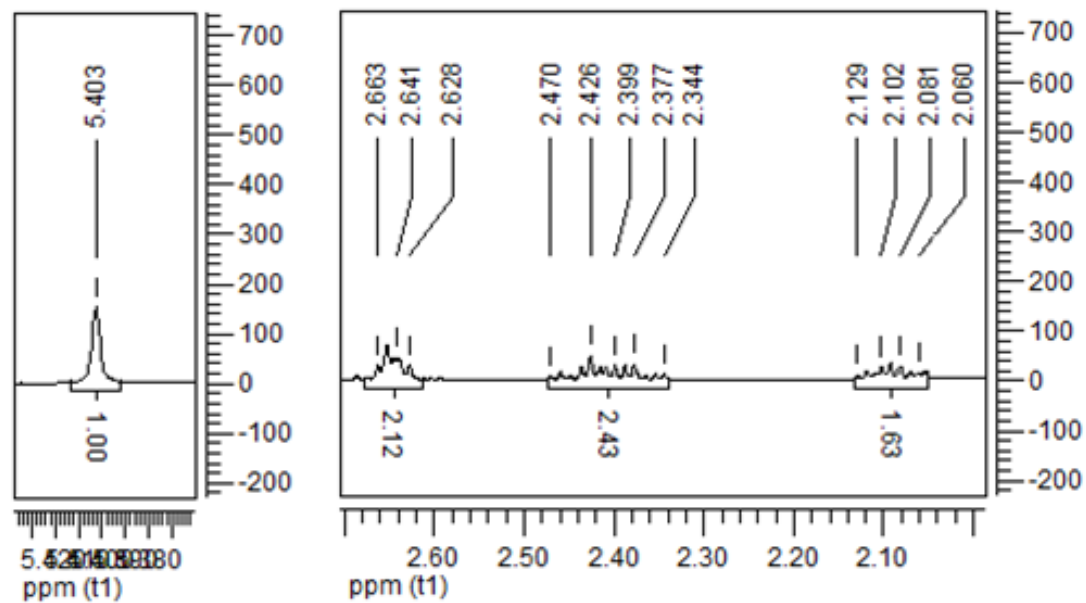
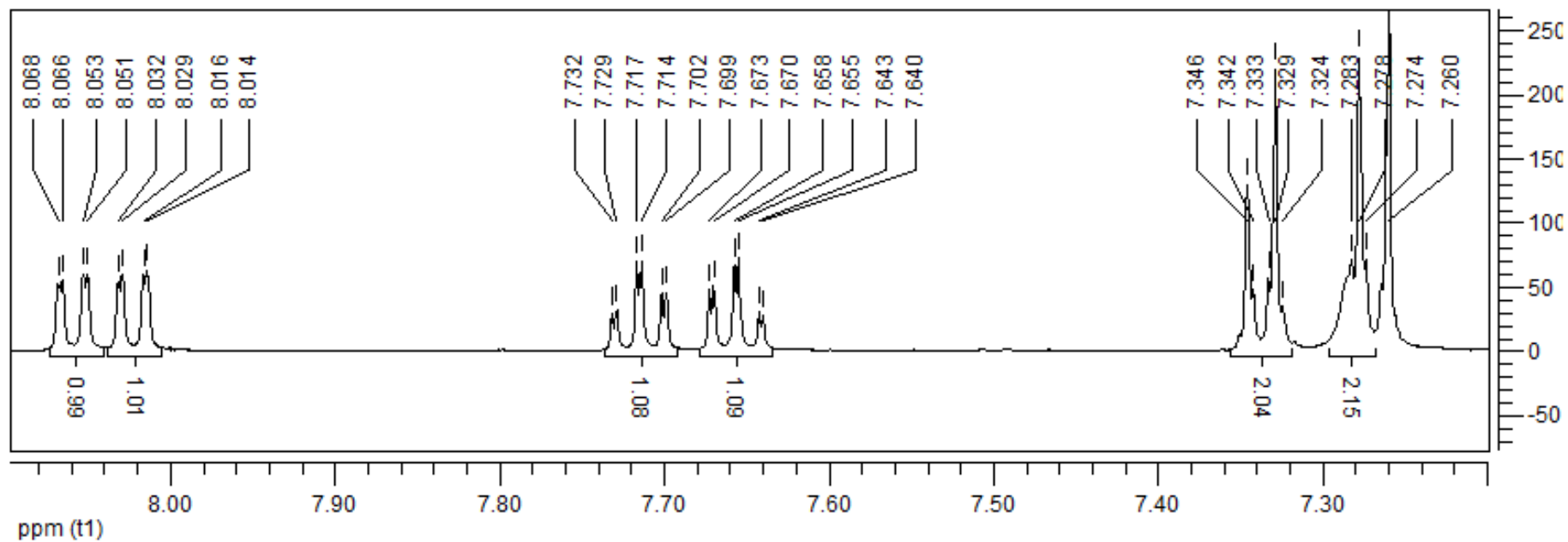
HRMS of compound **5g**



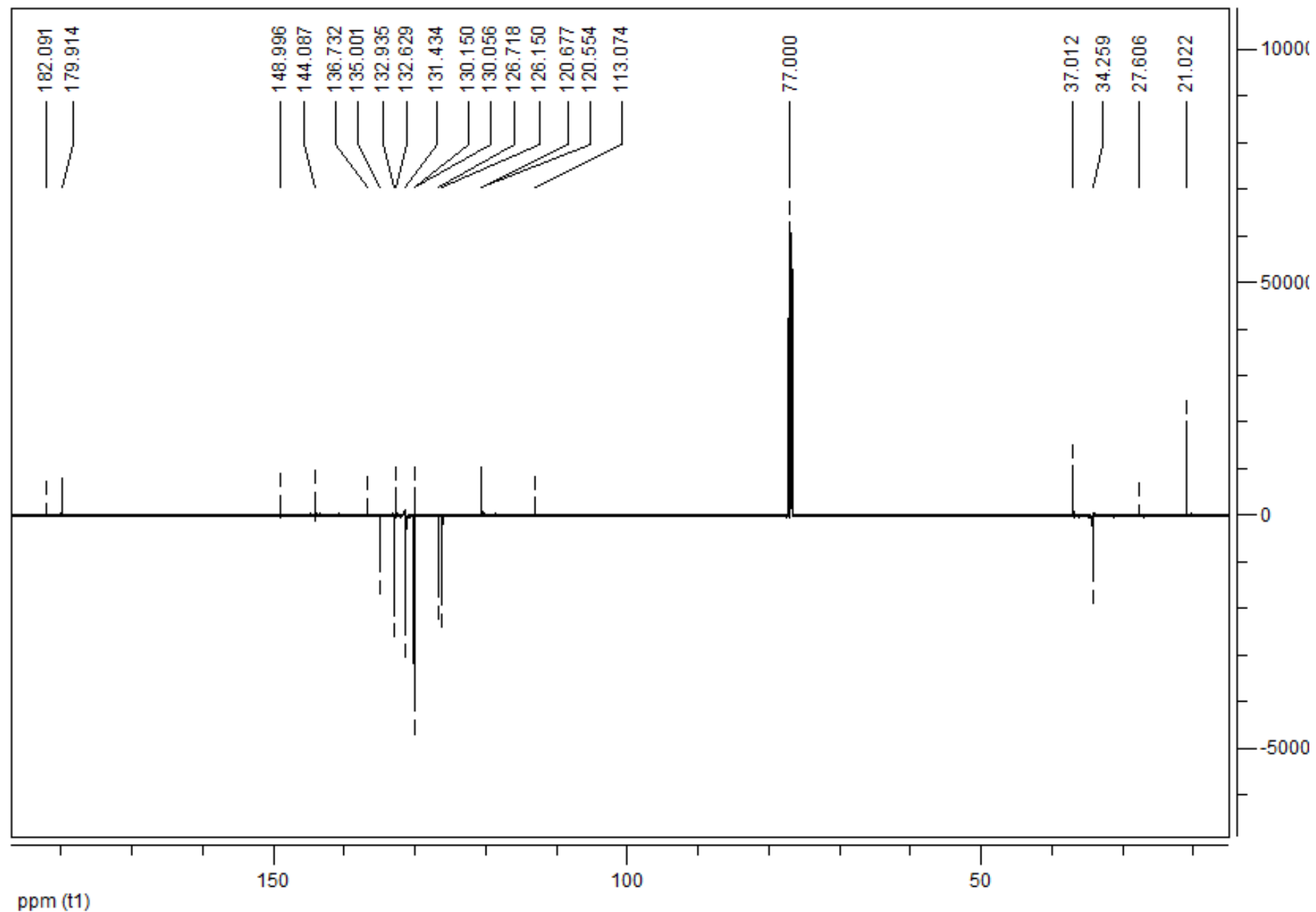
IR spectrum of compound **5h**



<sup>1</sup>H NMR spectrum of compound **5h** (500.00 MHz, CDCl<sub>3</sub>)



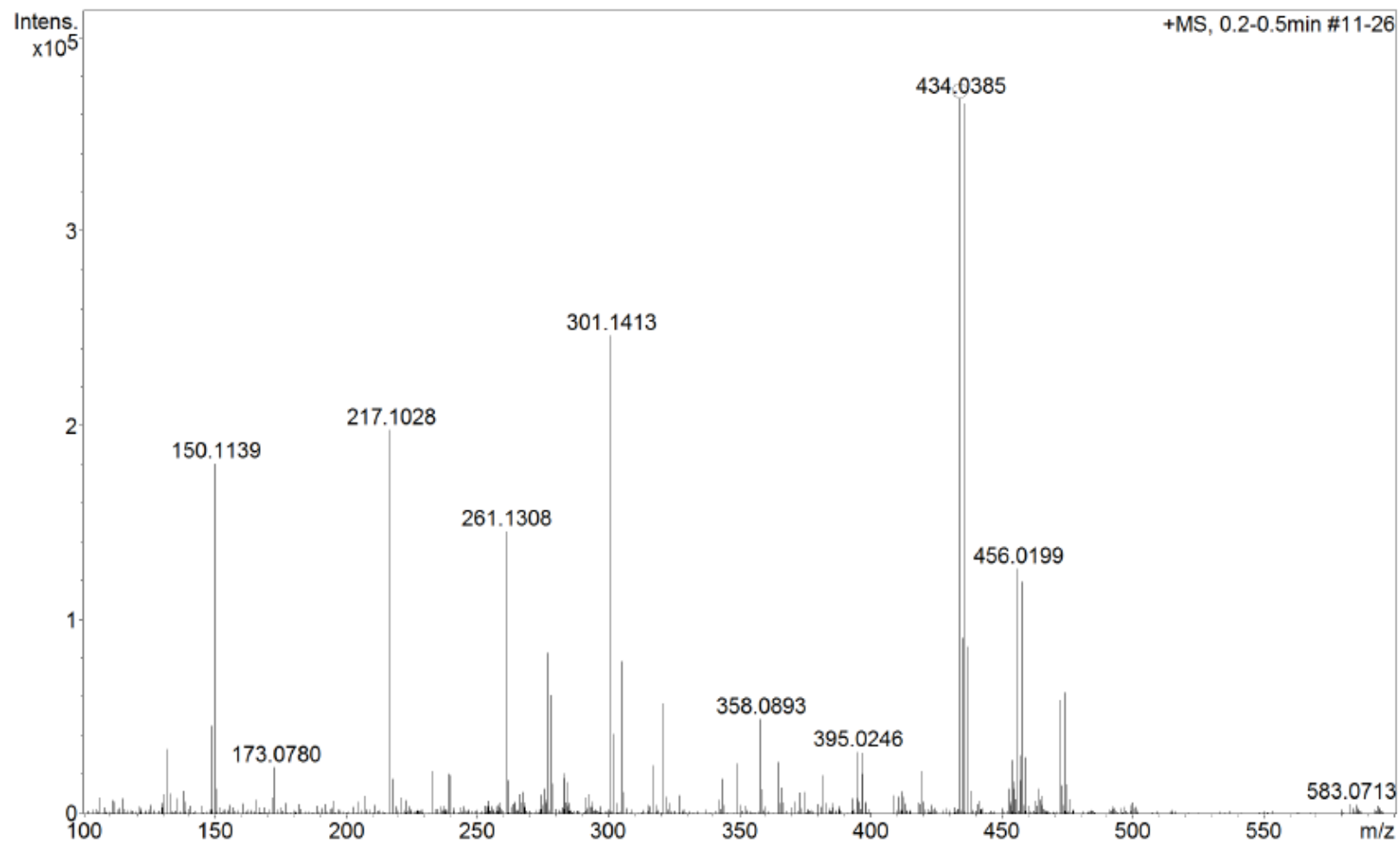
<sup>1</sup>H NMR spectrum of compound **5h** (500.00 MHz, CDCl<sub>3</sub>)



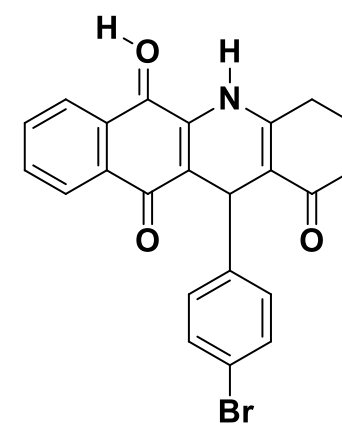
$^{13}\text{C}$  NMR spectrum of compound **5h** (125.0 MHz,  $\text{CDCl}_3$ )



+MS, 0.2-0.5min #11-26



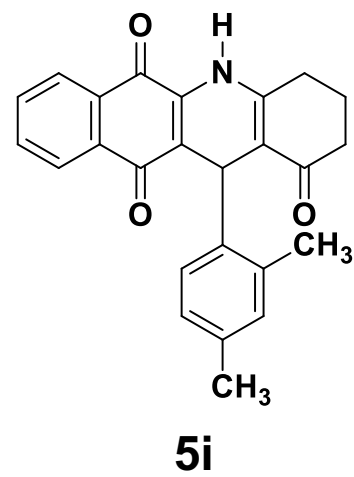
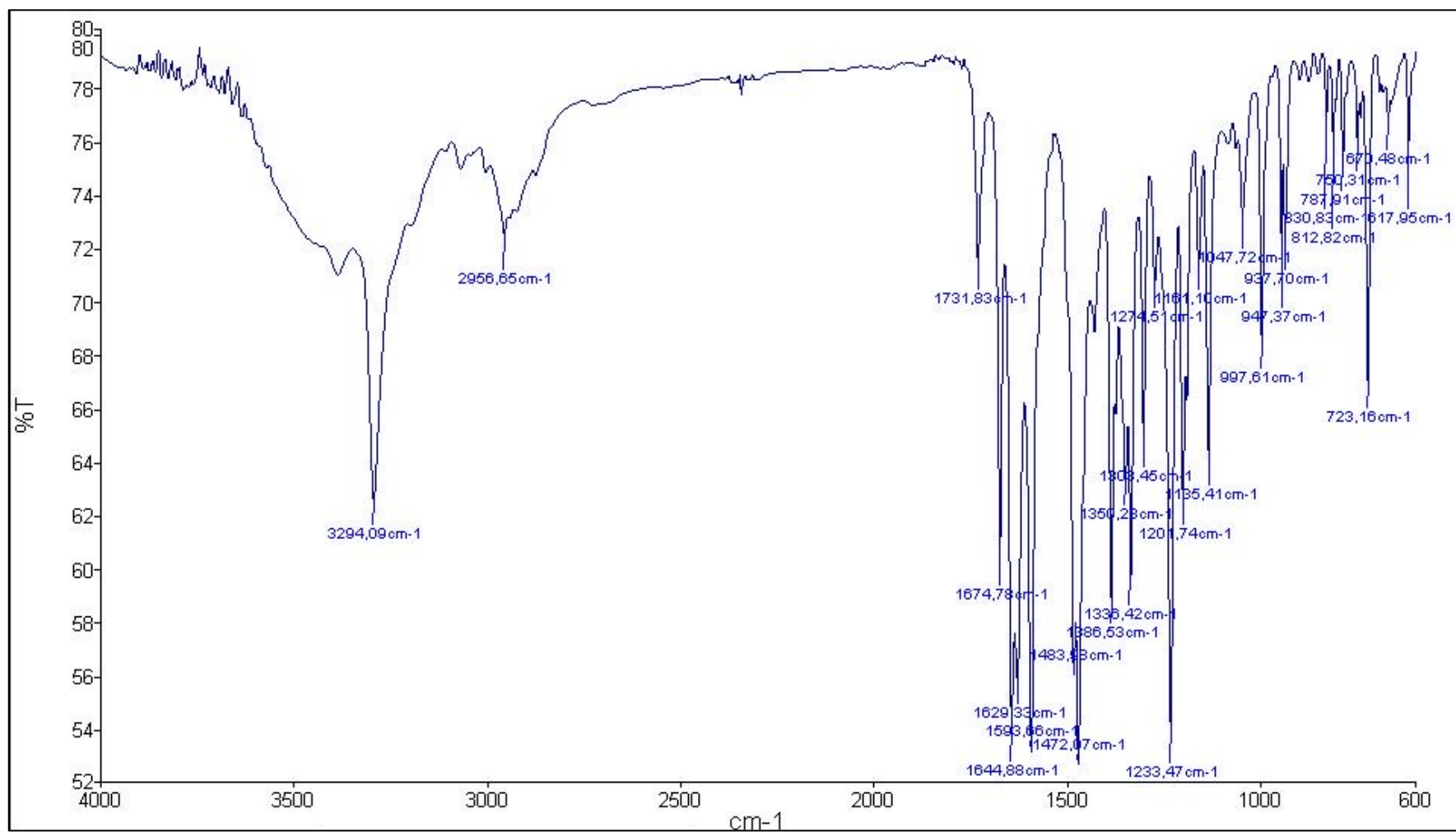
Meas. m/z	# Ion	Formula	m/z err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
434.038533	1	C <sub>23</sub> H <sub>17</sub> BrNO <sub>3</sub>	434.038632	0.2	0.7	15.5	ok	even	9.2	9.2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.



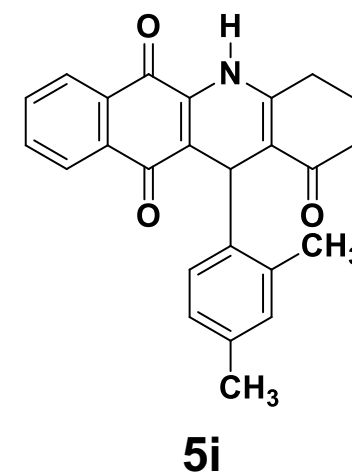
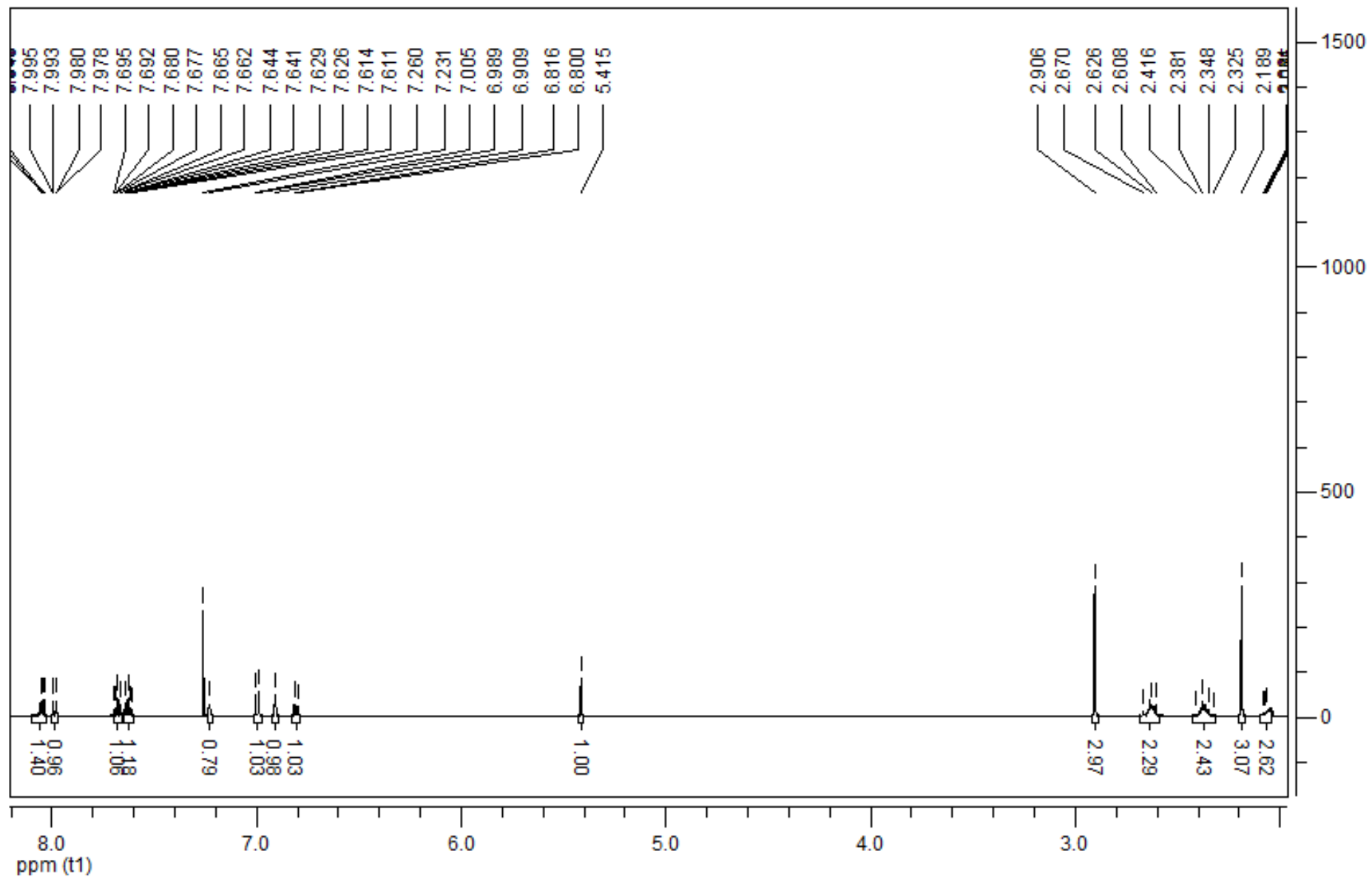
Exact Mass: 434,0392

**5h**

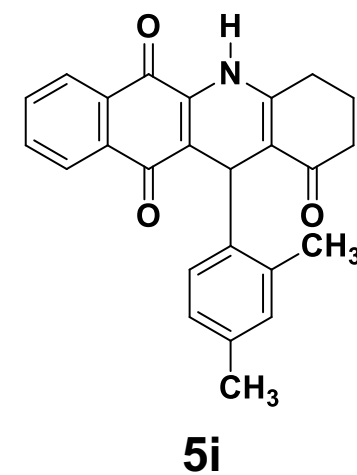
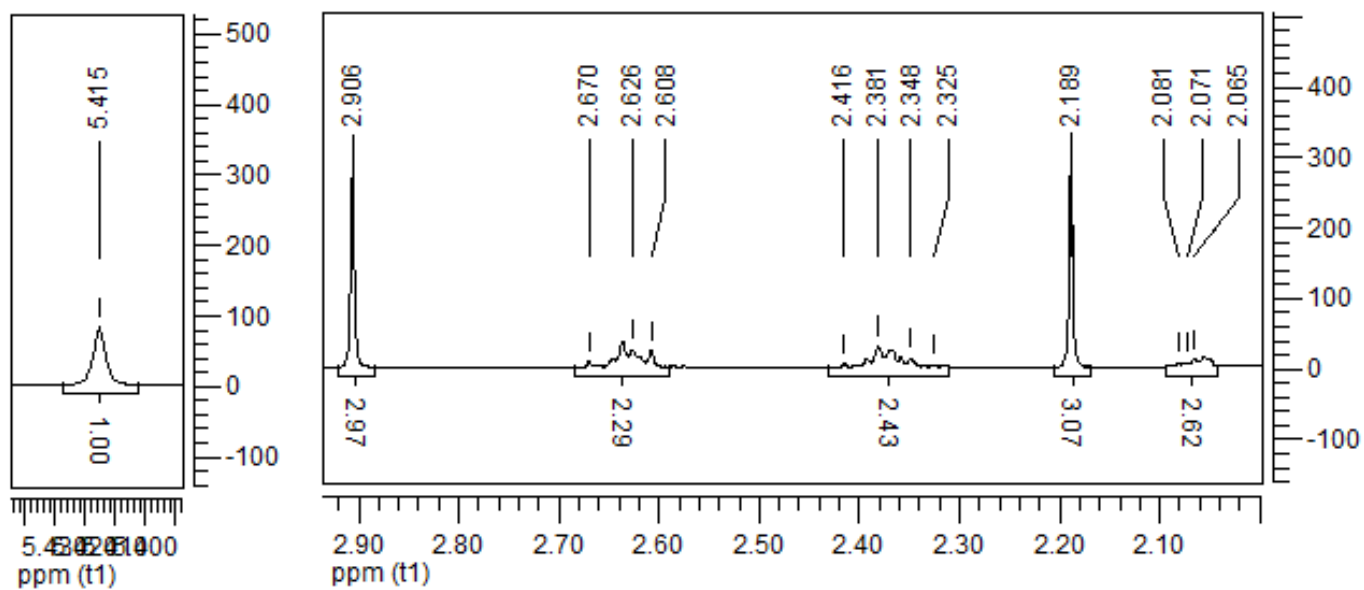
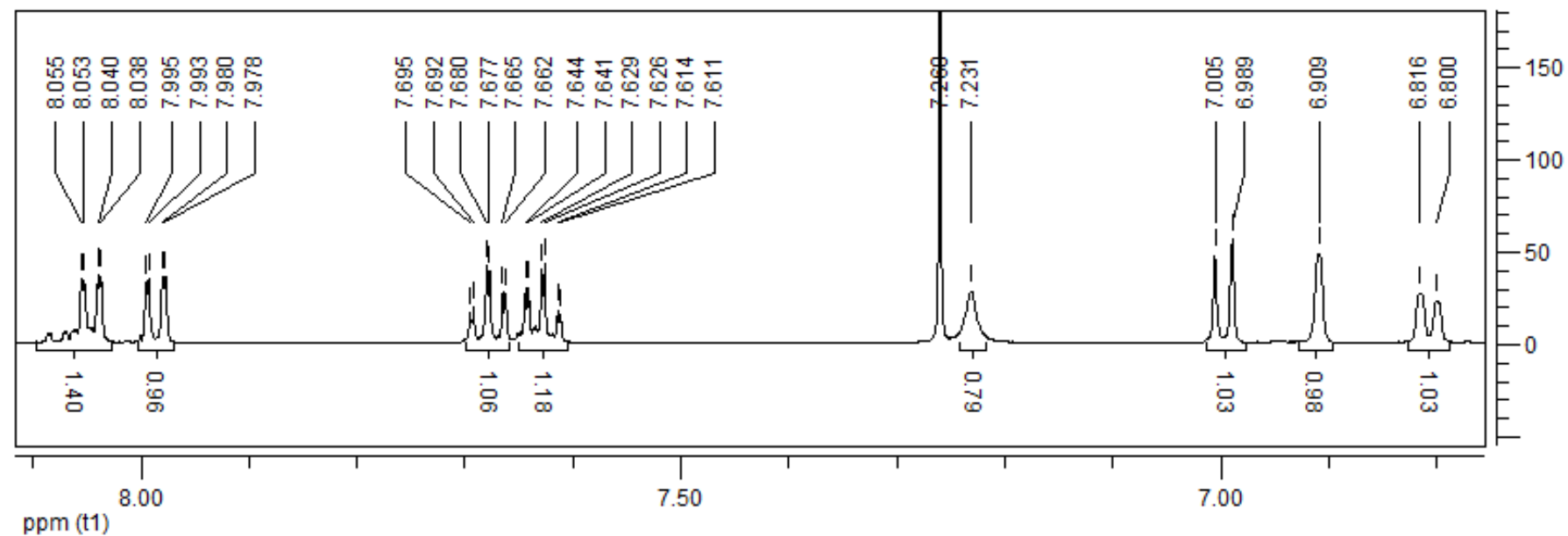
HRMS of compound **5h**



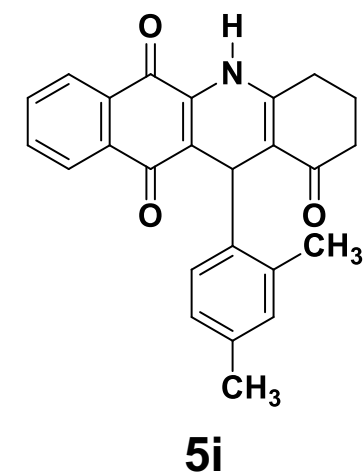
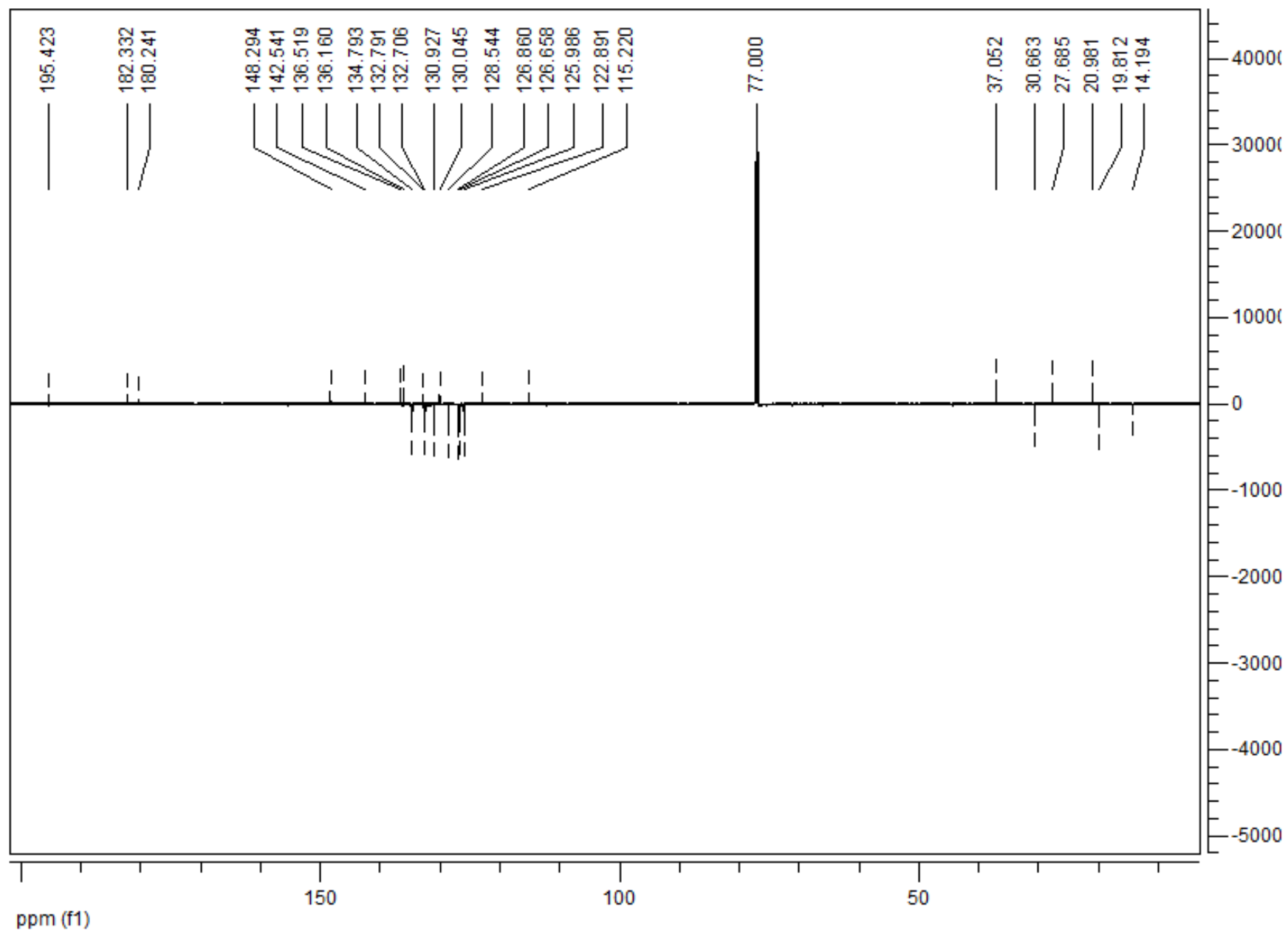
IR spectrum of compound **5i**



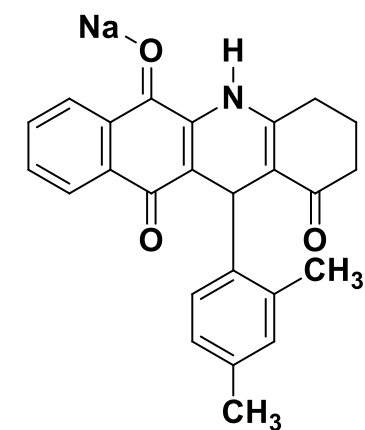
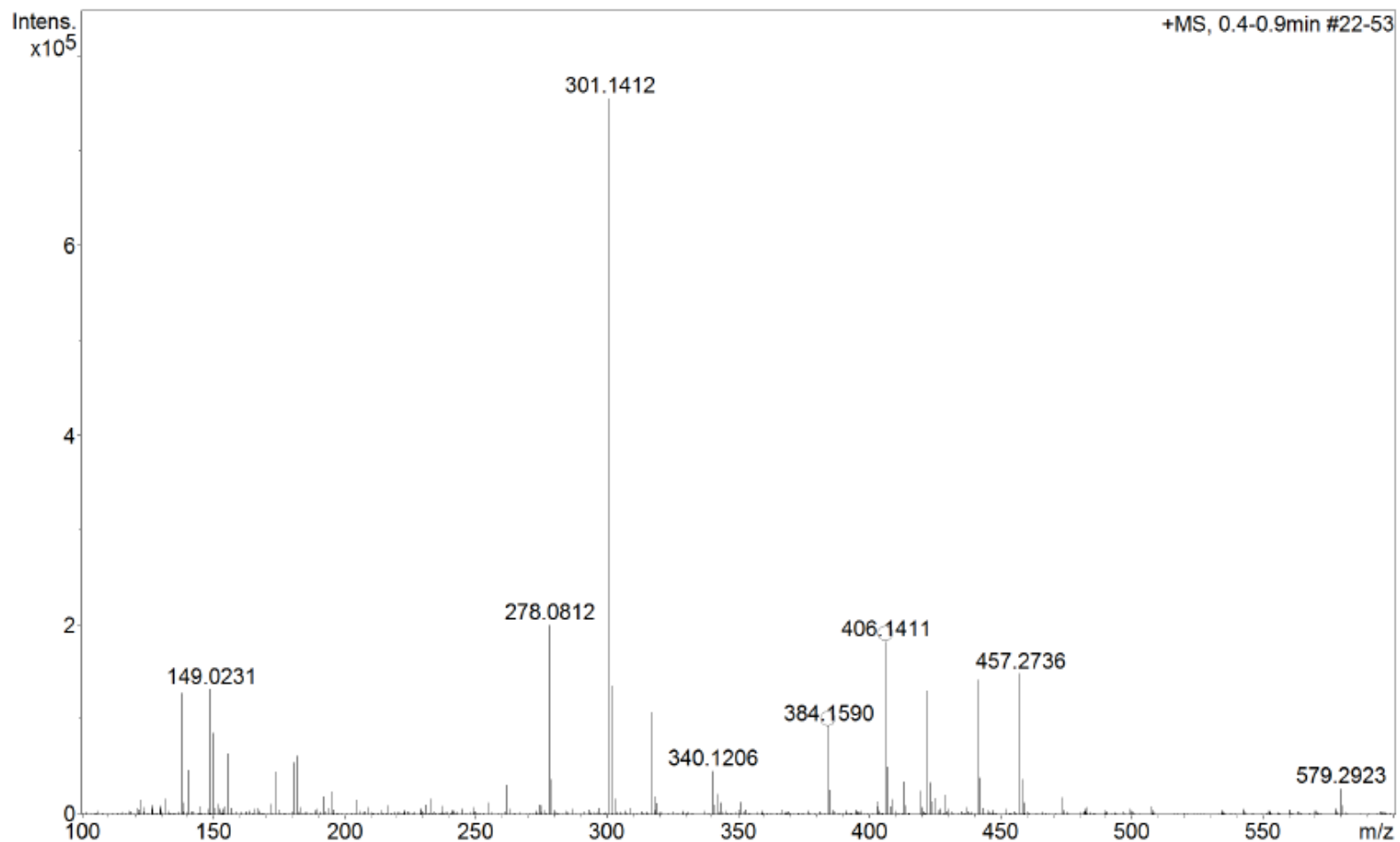
<sup>1</sup>H NMR spectrum of compound **5i** (500.00 MHz, CDCl<sub>3</sub>)



<sup>1</sup>H NMR spectrum of compound **5i** (500.00 MHz, CDCl<sub>3</sub>)



+MS, 0.4-0.9min #22-53

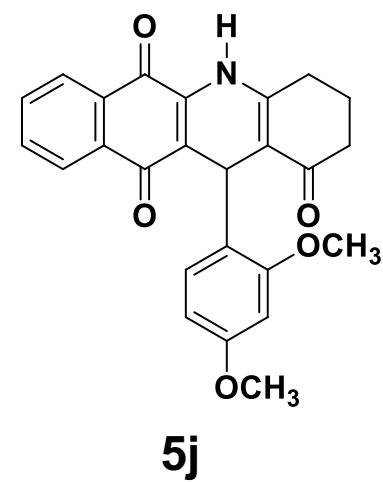
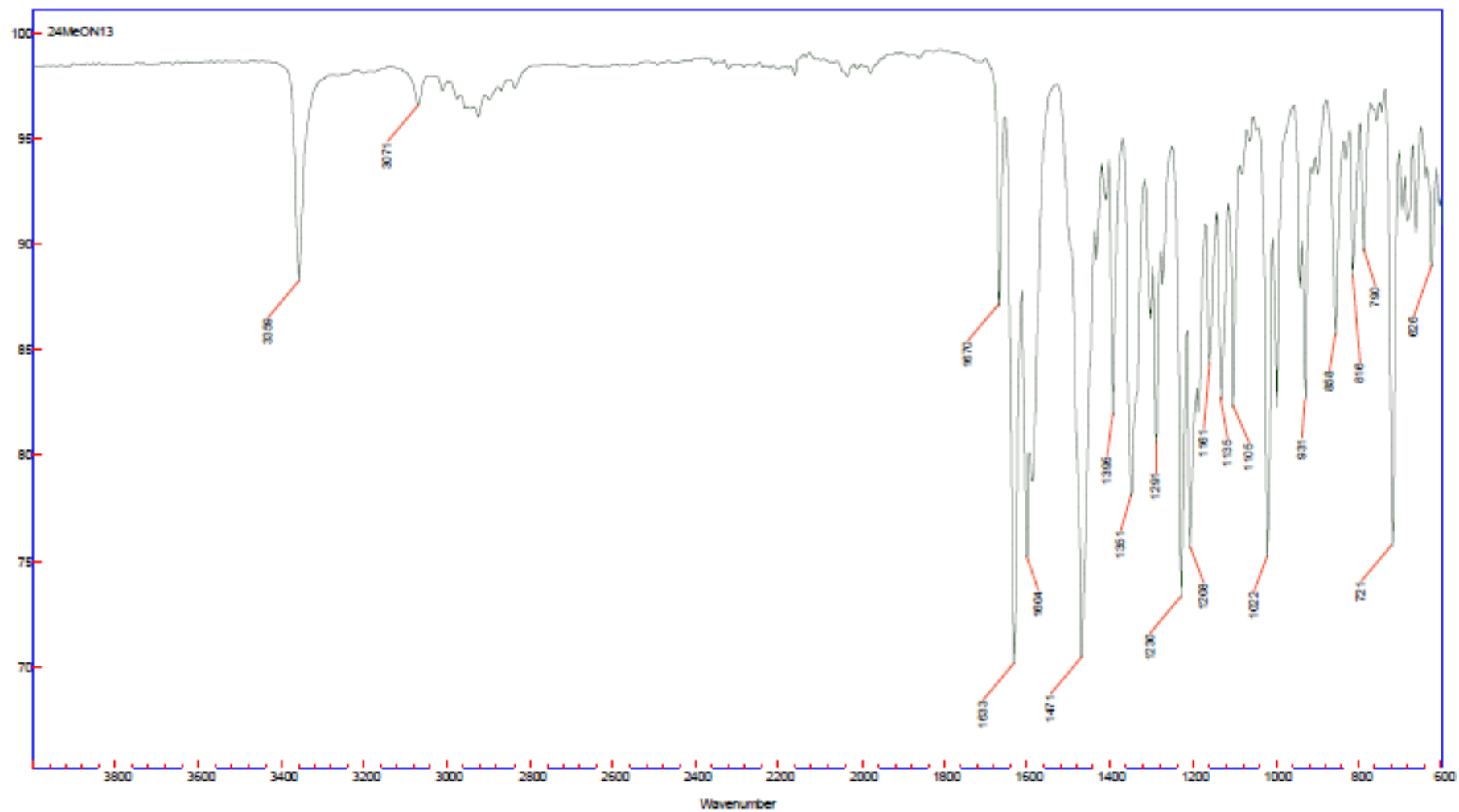


Exact Mass: 406,1419

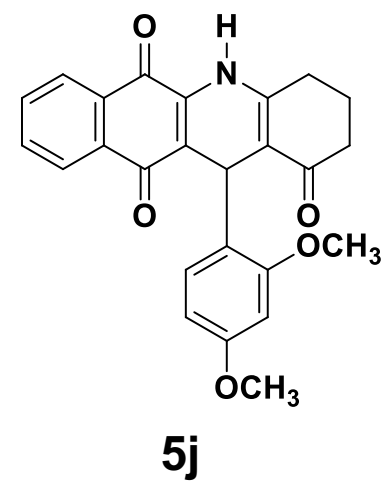
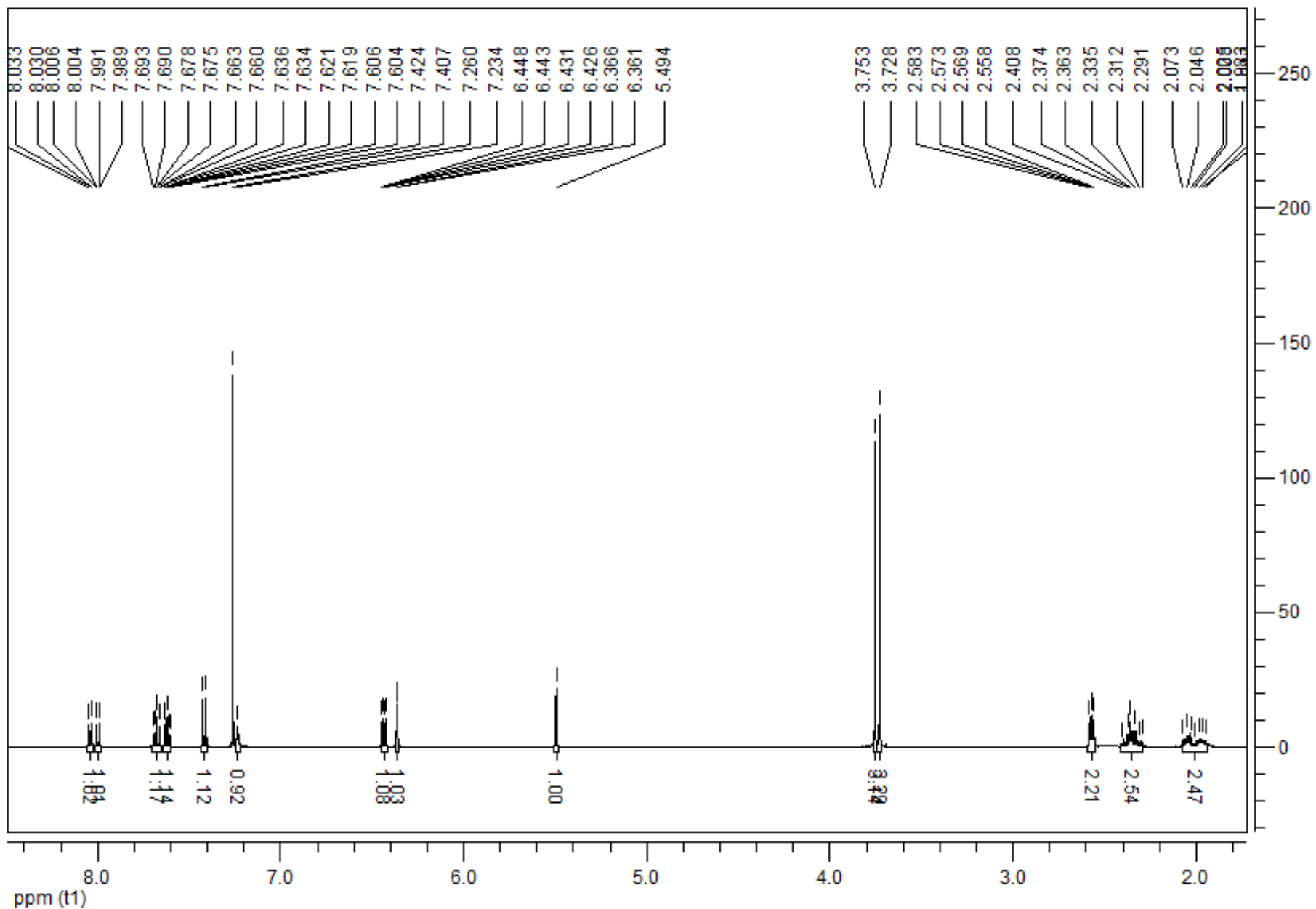
**5i**

Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
384.159038	1	C <sub>25</sub> H <sub>22</sub> NO <sub>3</sub>	384.159420	1.0	2.0	15.5	ok	even		3.1	4.5	n.a.	n.a.	n.a.	n.a.	n.a.			
	2	C <sub>21</sub> H <sub>18</sub> N <sub>7</sub> O	384.156735	-6.0	-5.8	16.5	ok	even		11.4	19.5	n.a.	n.a.	n.a.	n.a.	n.a.			
	3	C <sub>20</sub> H <sub>22</sub> N <sub>3</sub> O <sub>5</sub>	384.155397	-9.5	-9.0	11.5	ok	even		23.8	37.8	n.a.	n.a.	n.a.	n.a.	n.a.			
406.141135	1	C <sub>25</sub> H <sub>21</sub> NNaO <sub>3</sub>	406.141364	0.6	1.3	15.5	ok	even		4.7	7.2	n.a.	n.a.	n.a.	n.a.	n.a.			
	2	C <sub>21</sub> H <sub>17</sub> N <sub>7</sub> NaO	406.138679	-6.0	-6.1	16.5	ok	even		9.7	16.8	n.a.	n.a.	n.a.	n.a.	n.a.			
	3	C <sub>20</sub> H <sub>21</sub> N <sub>3</sub> NaO <sub>5</sub>	406.137341	-9.3	-9.0	11.5	ok	even		22.2	35.1	n.a.	n.a.	n.a.	n.a.	n.a.			

HRMS of compound **5i**

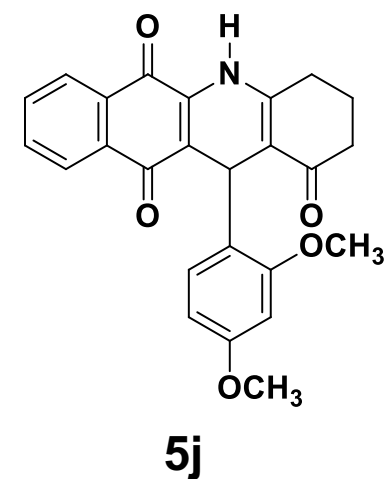
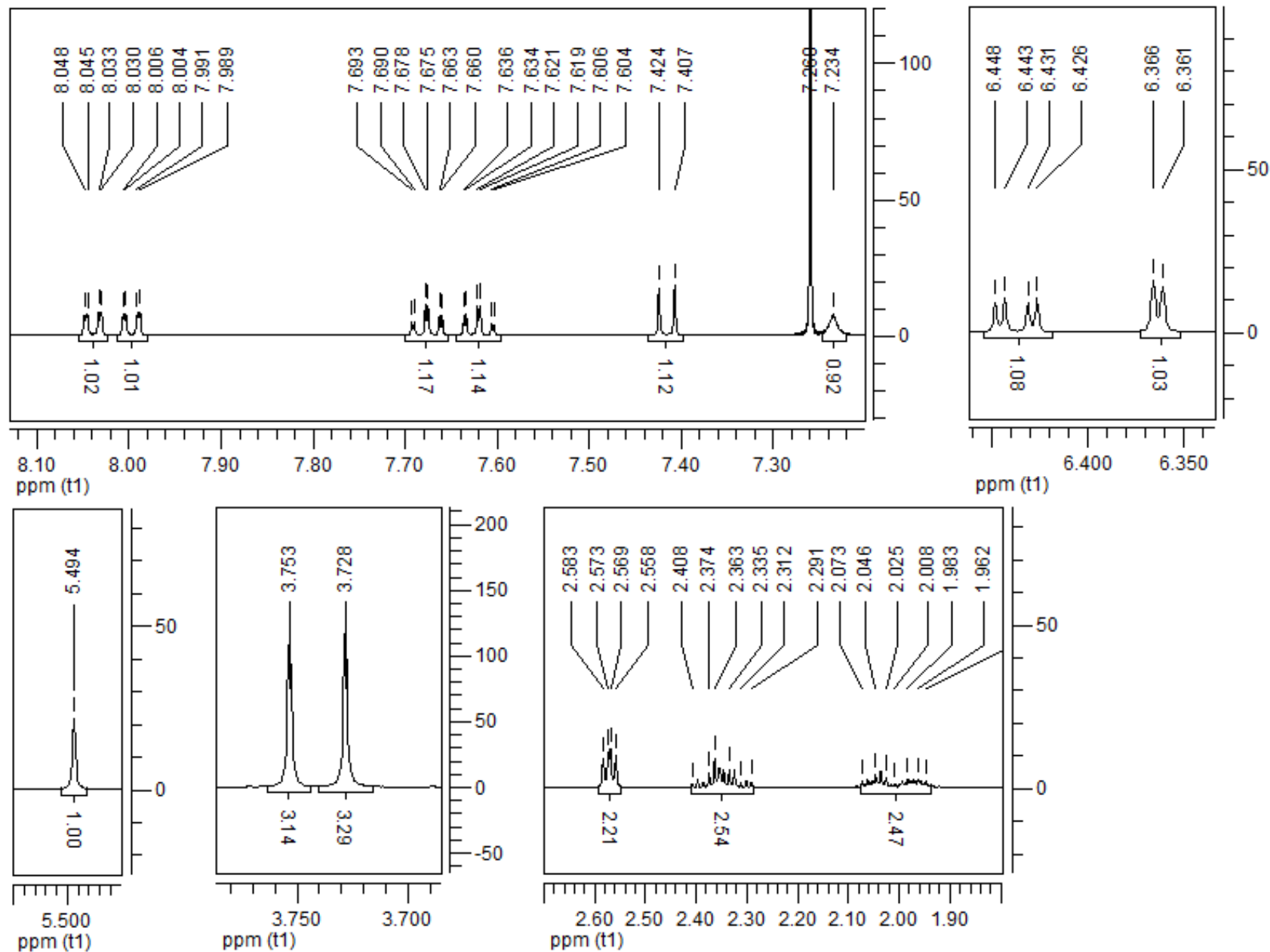


IR spectrum of compound **5j**

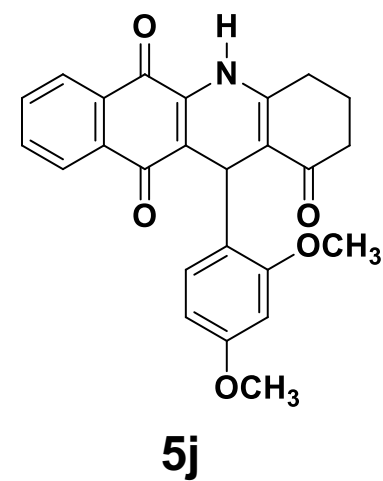
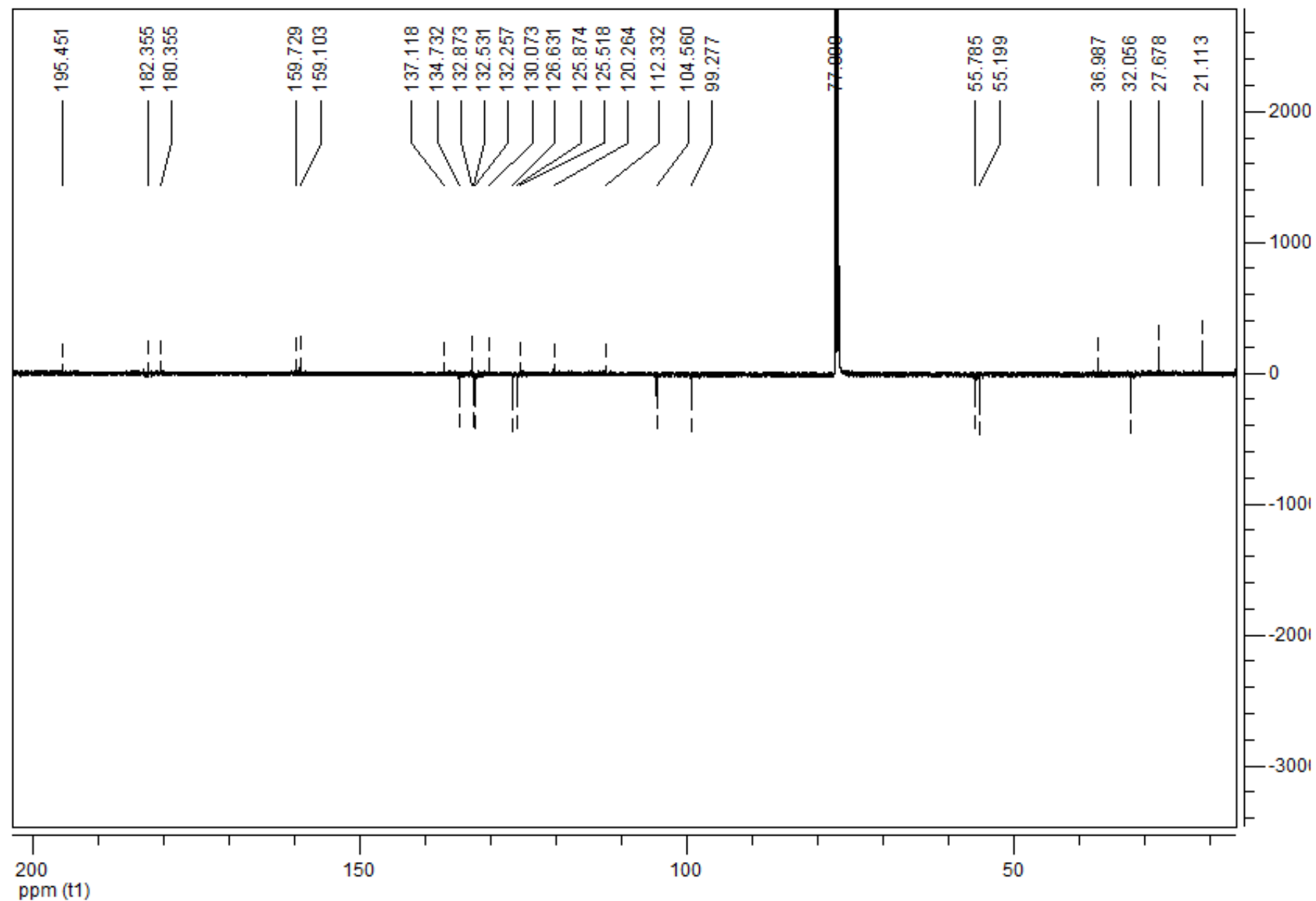


<sup>1</sup>H NMR spectrum of compound **5j** (500.00 MHz, CDCl<sub>3</sub>)



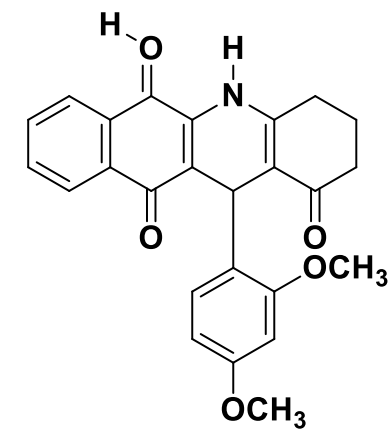
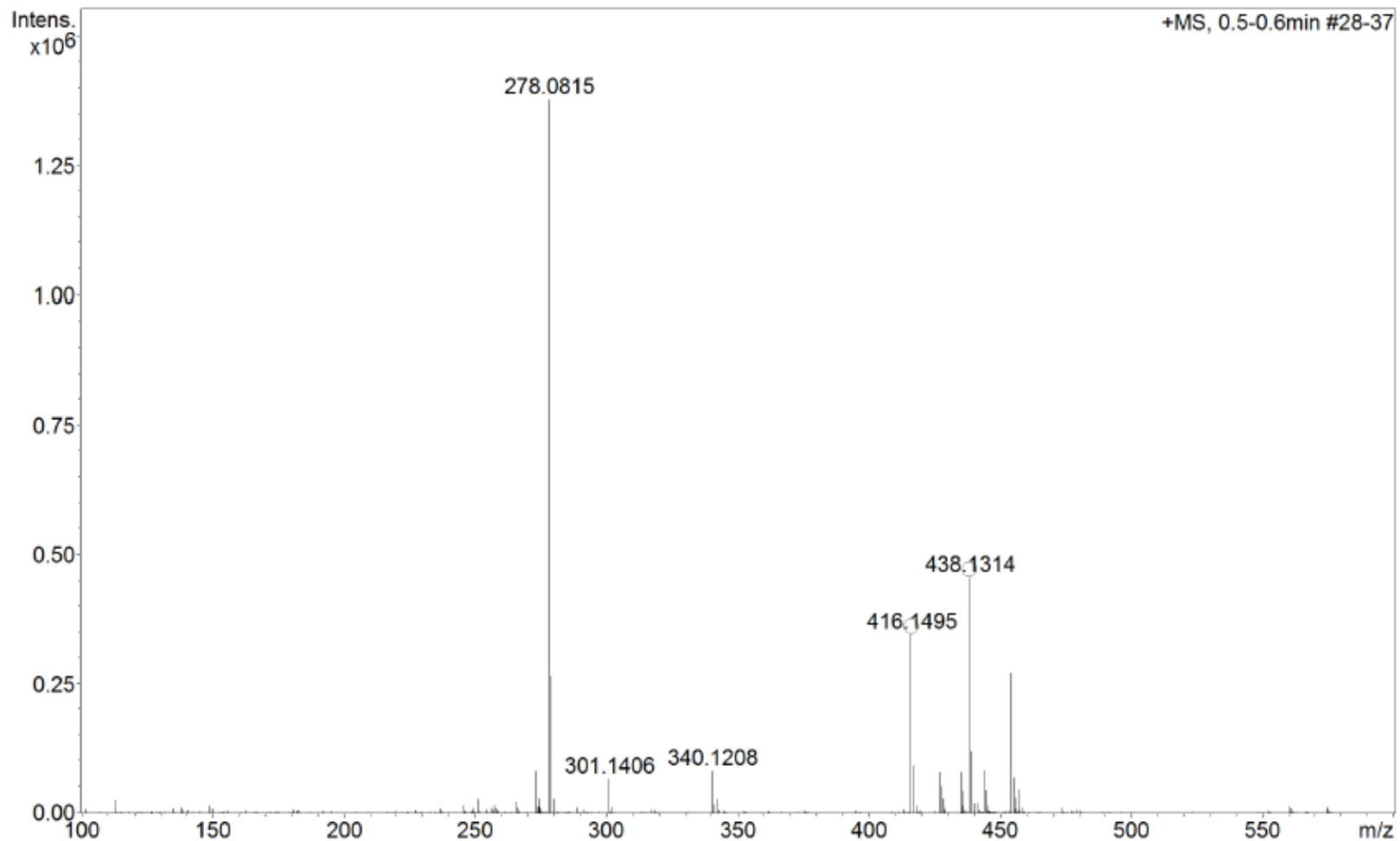


$^1\text{H}$  NMR spectrum of compound **5j** (500.00 MHz,  $\text{CDCl}_3$ )



<sup>13</sup>C NMR spectrum of compound **5j** (75.0 MHz, CDCl<sub>3</sub>)

+MS, 0.5-0.6min #28-37

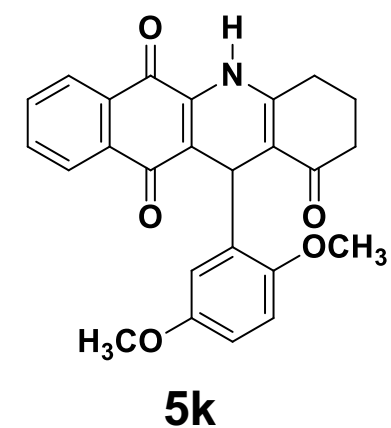
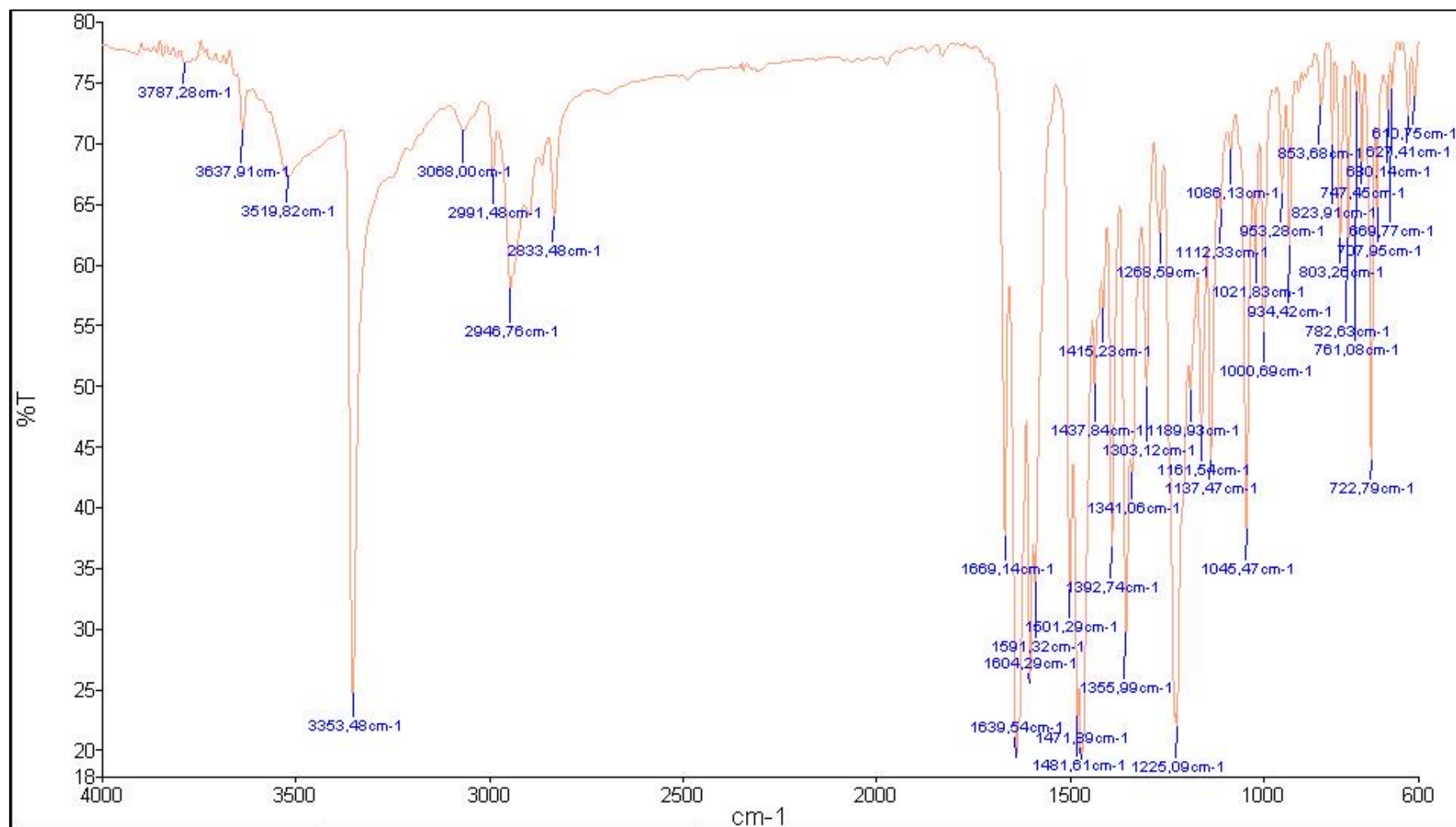


Exact Mass: 416,1498

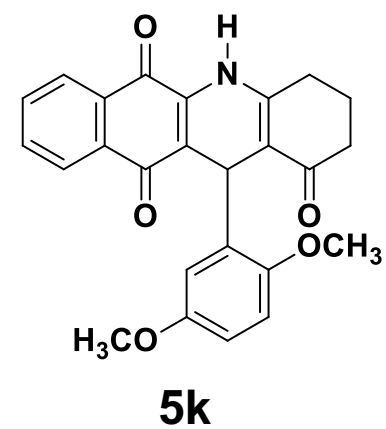
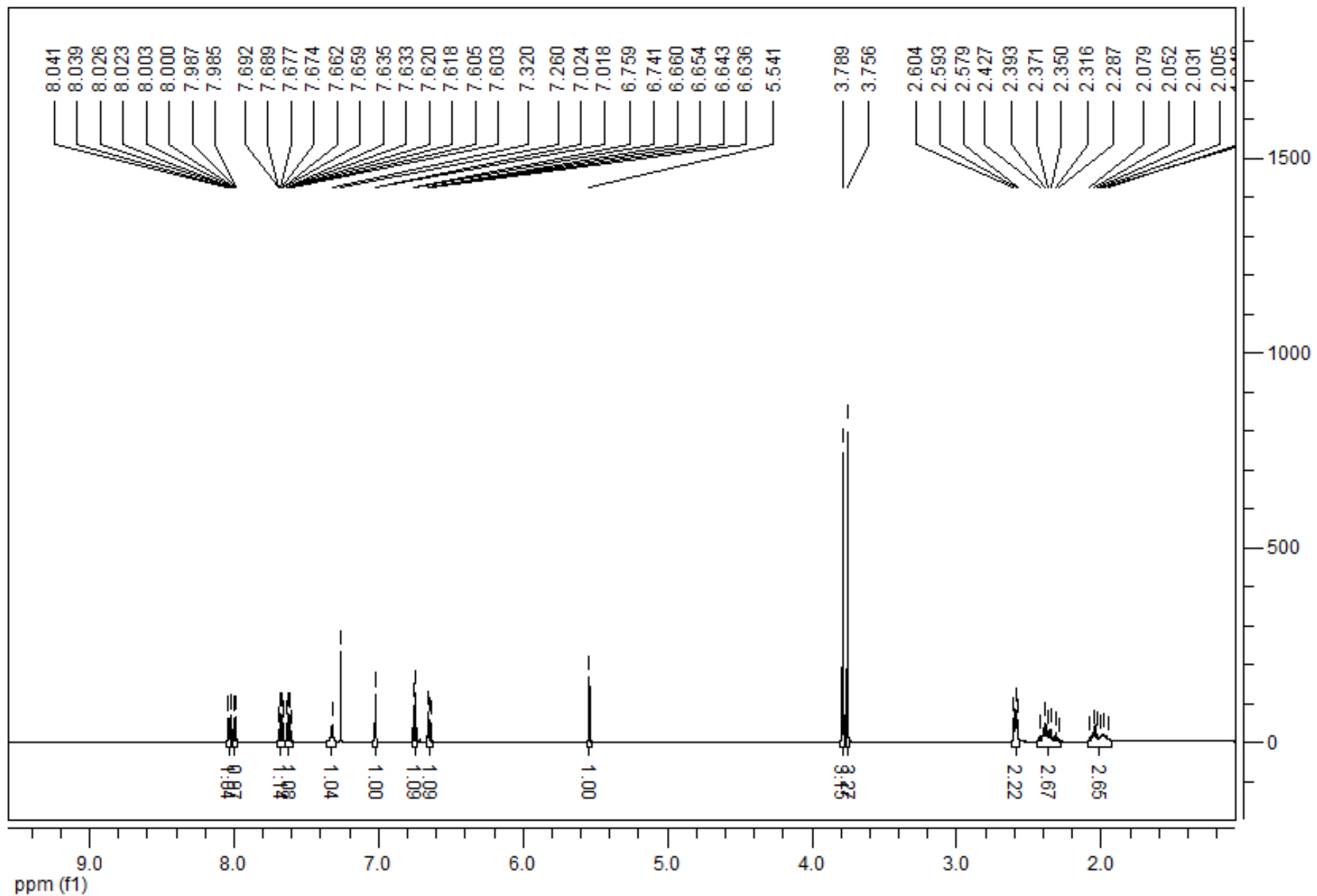
**5j**

Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
416.149467	1	C <sub>25</sub> H <sub>22</sub> NO <sub>5</sub>	416.149249	-0.5	0.1	15.5	ok	even		8.4	13.8		n.a.		n.a.		n.a.		n.a.
	2	C <sub>26</sub> H <sub>18</sub> N <sub>5</sub> O	416.150587	2.7	3.1	20.5	ok	even		21.3	31.5		n.a.		n.a.		n.a.		n.a.
438.131436	1	C <sub>25</sub> H <sub>21</sub> NNaO <sub>5</sub>	438.131193	-0.6	0.3	15.5	ok	even		11.7	19.3		n.a.		n.a.		n.a.		n.a.
	2	C <sub>26</sub> H <sub>17</sub> N <sub>5</sub> NaO	438.132531	2.5	3.1	20.5	ok	even		24.4	36.9		n.a.		n.a.		n.a.		n.a.

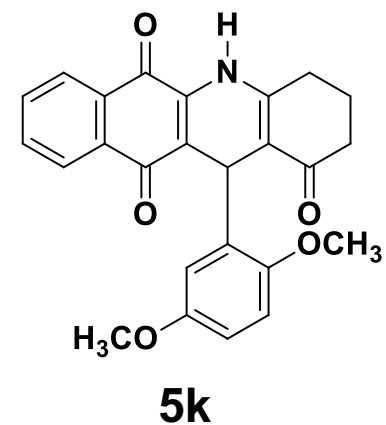
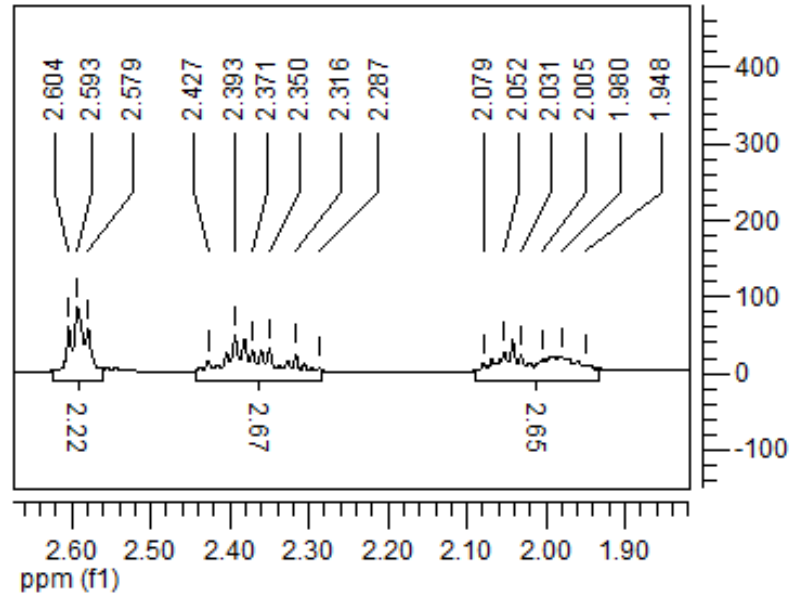
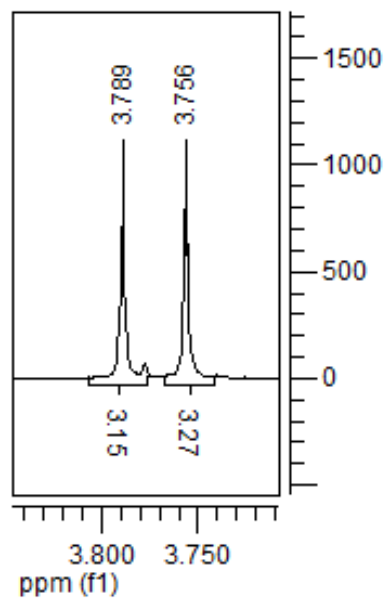
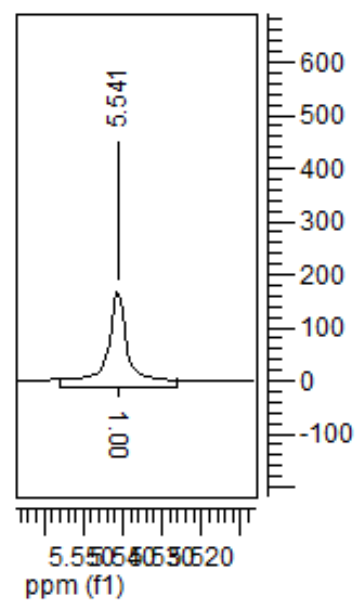
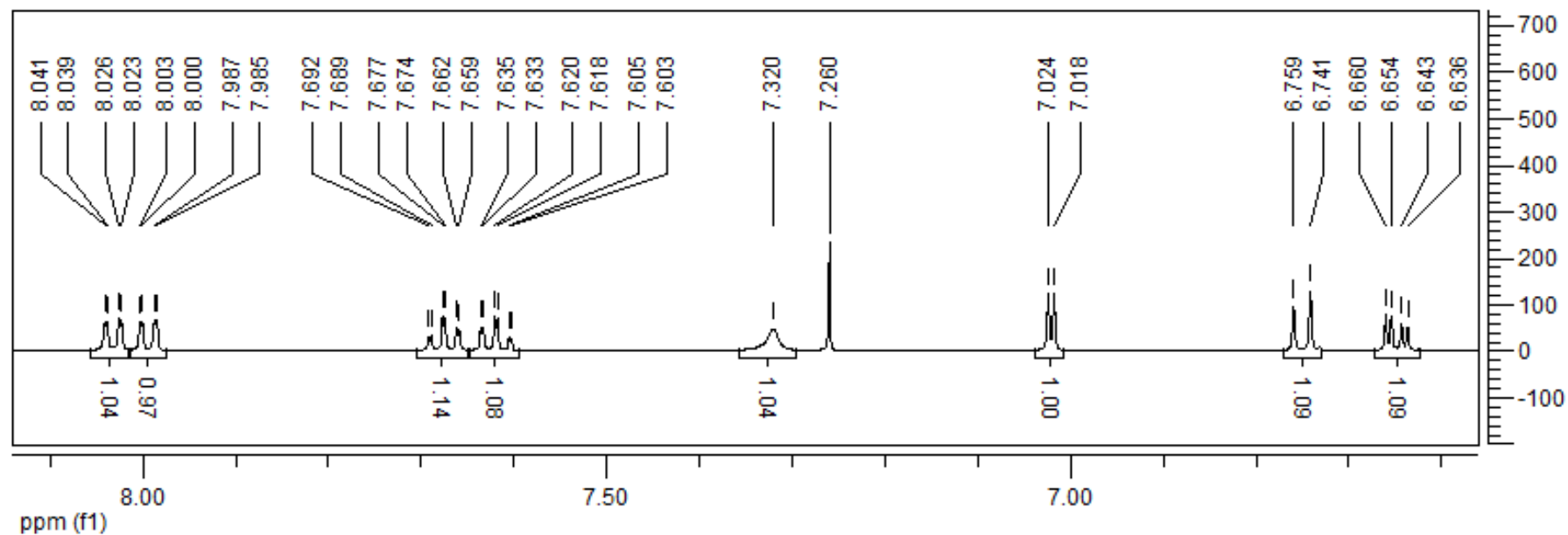
HRMS of compound **5j**



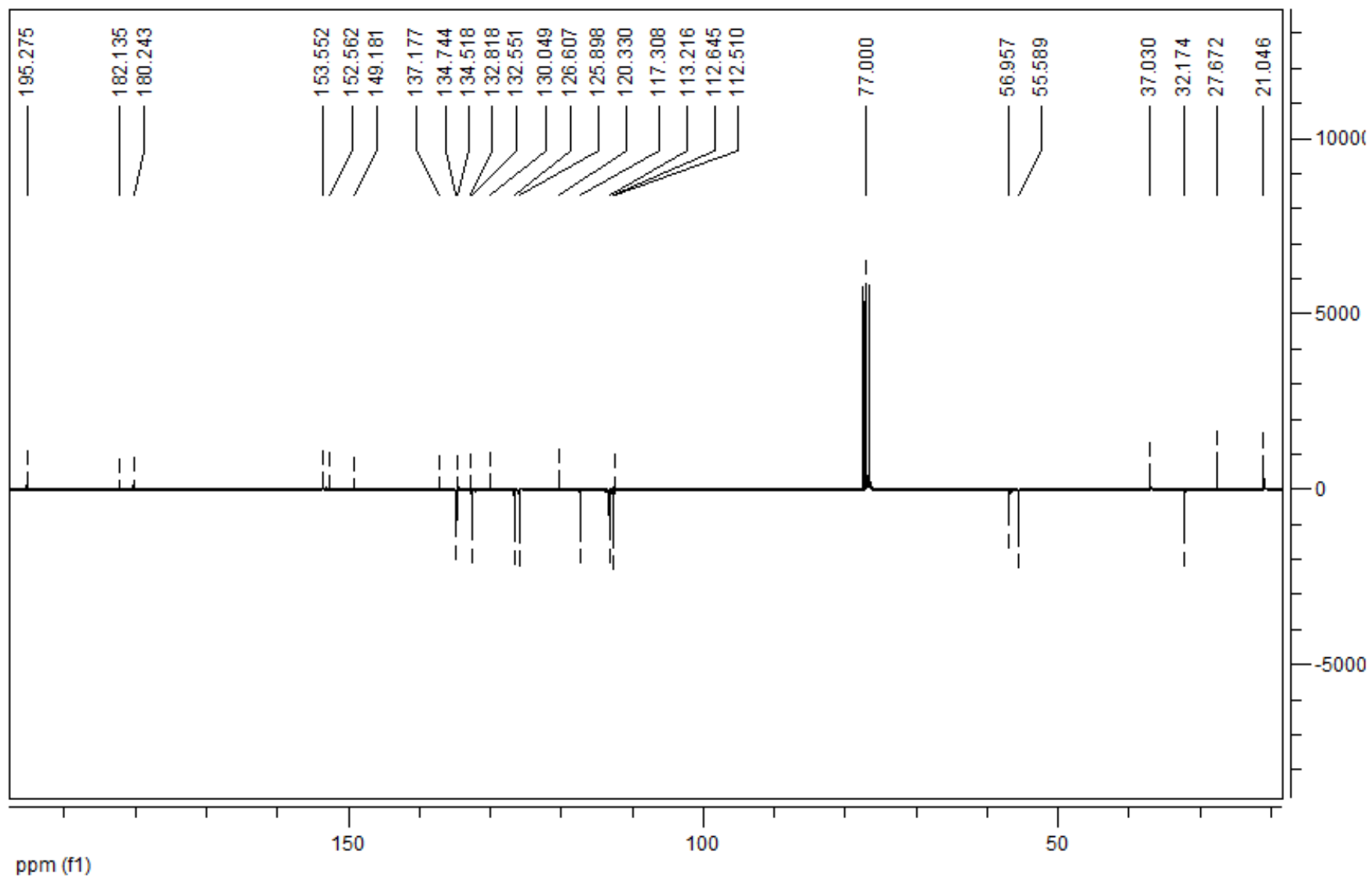
IR spectrum of compound **5k**



<sup>1</sup>H NMR spectrum of compound **5k** (500.00 MHz, CDCl<sub>3</sub>)

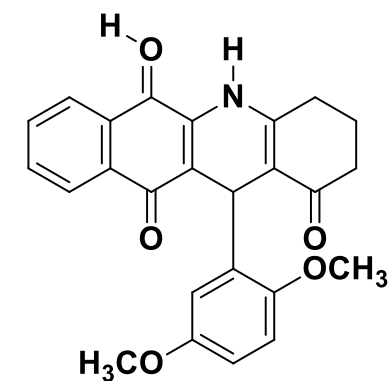
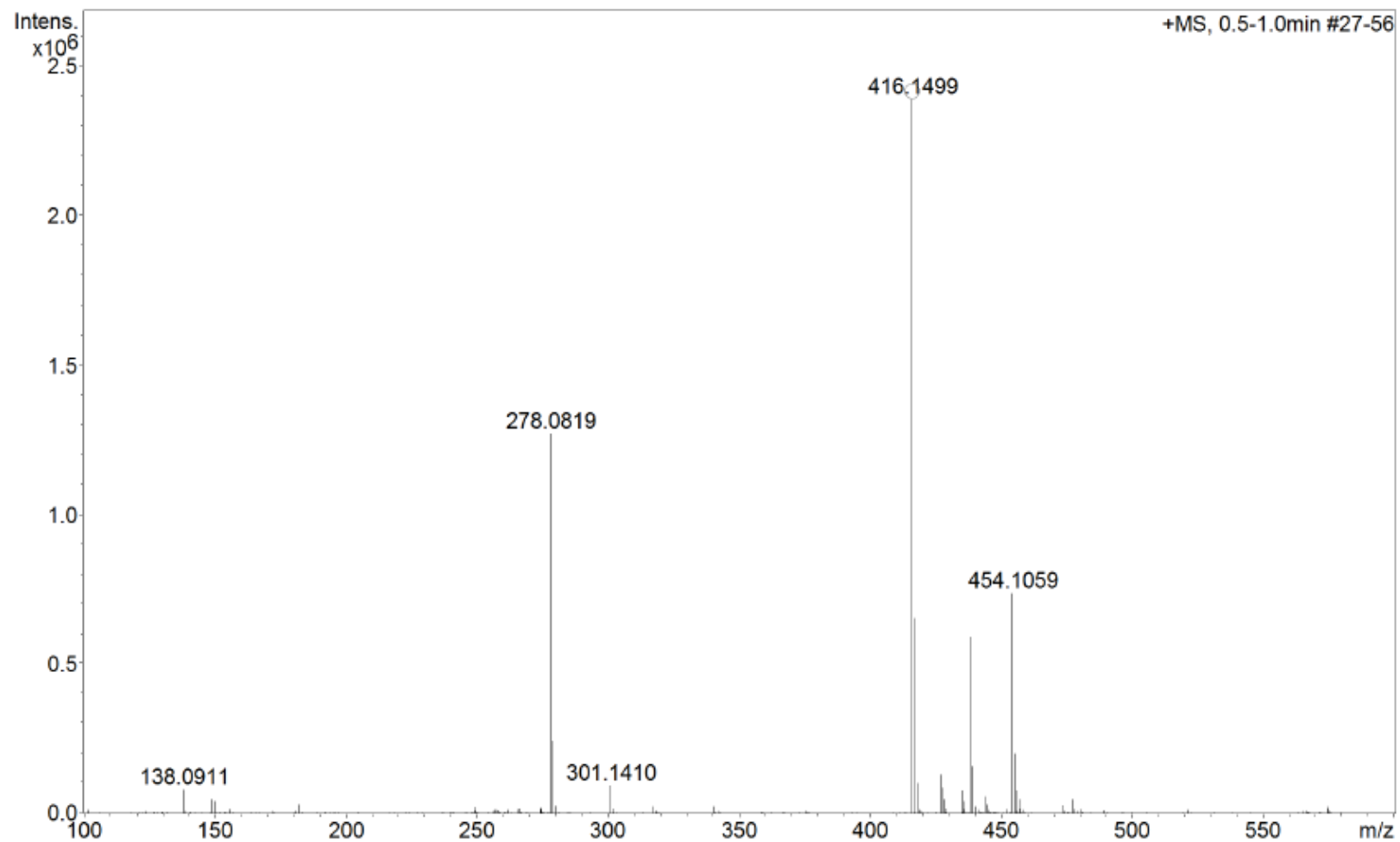


$^1\text{H}$  NMR spectrum of compound **5k** (500.00 MHz,  $\text{CDCl}_3$ )



$^{13}\text{C}$  NMR spectrum of compound **5k** (125.0 MHz,  $\text{CDCl}_3$ )

+MS, 0.5-1.0min #27-56



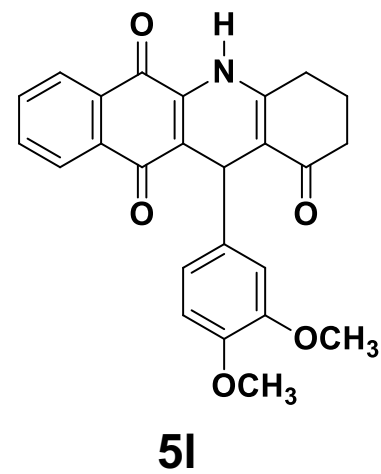
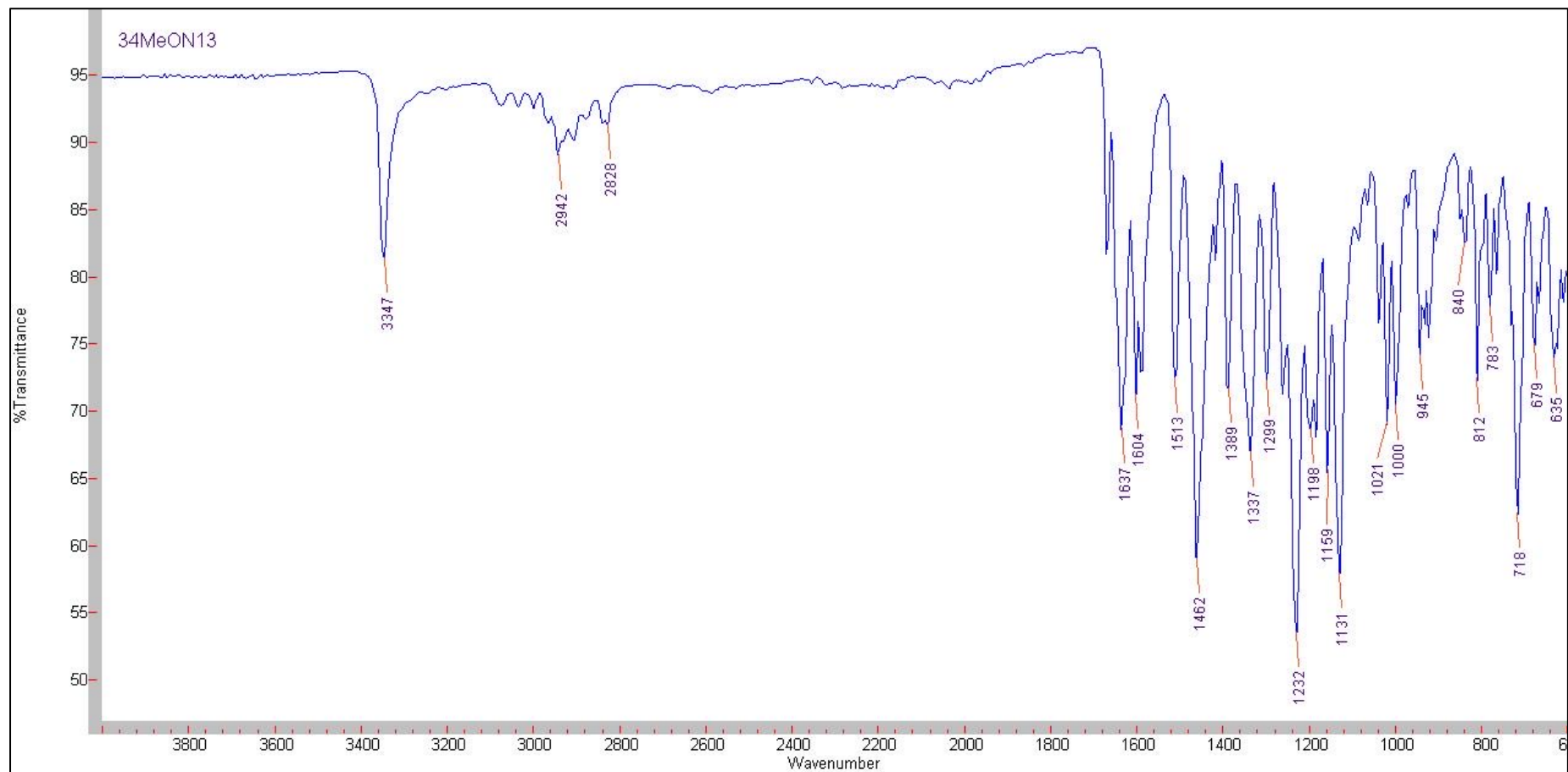
Exact Mass: 416,1498

**5k**

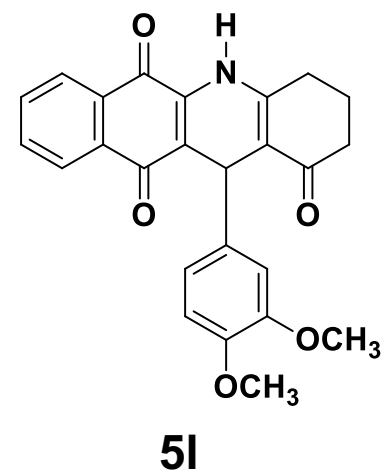
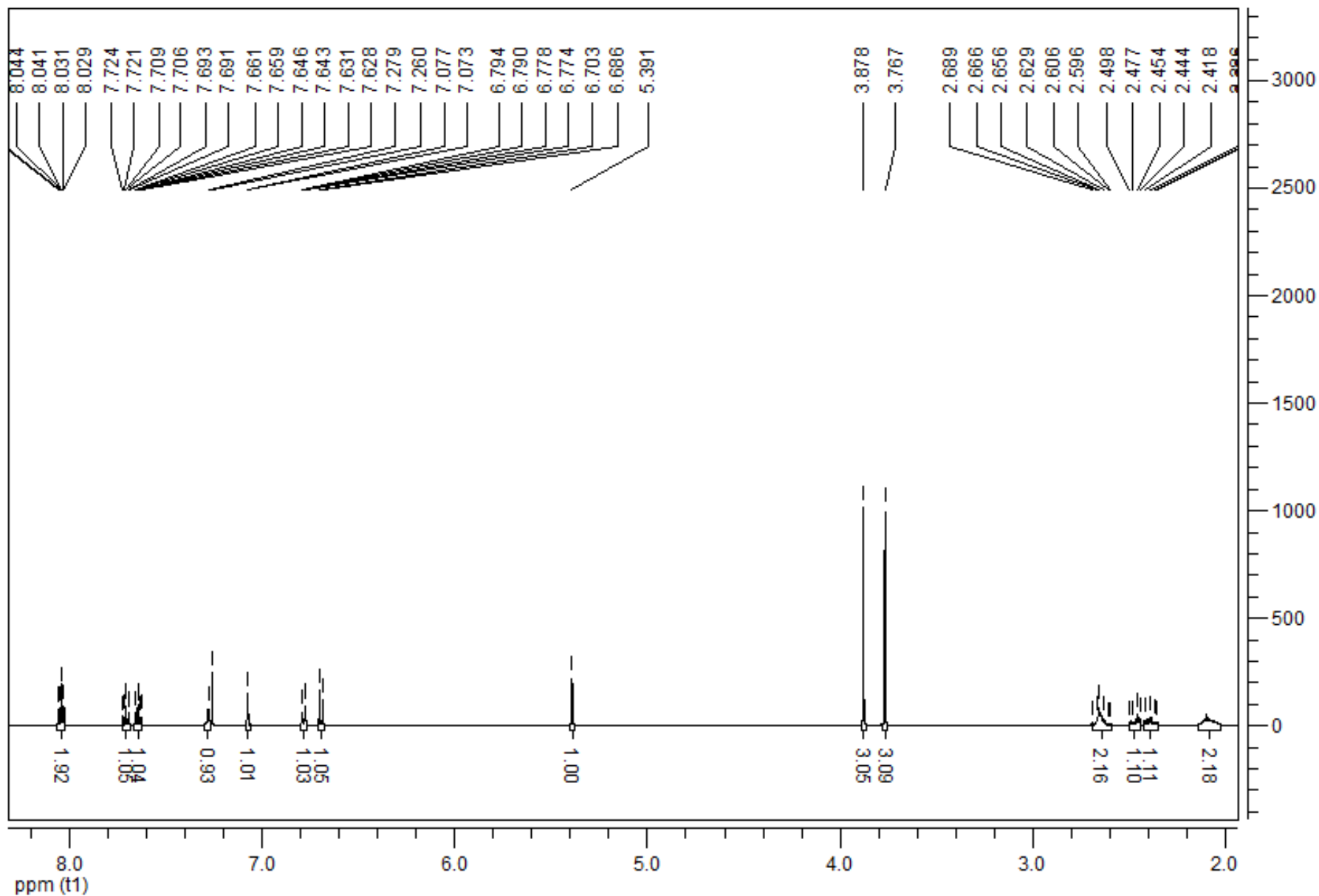
Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std	Mean m/z	Std I	VarNorm	Std m/z	Diff	Std	Comb	Dev
416.1499	1	C25H22NO5	416.149249	-1.6	-1.8	15.5	ok	even		4.0	7.1		n.a.		n.a.		n.a.		n.a.	
	2	C21H18N7O3	416.146564	-8.0	-9.0	16.5	ok	even		10.9	17.2		n.a.		n.a.		n.a.		n.a.	
	3	C26H18N5O	416.150587	1.6	1.1	20.5	ok	even		16.1	23.8		n.a.		n.a.		n.a.		n.a.	

HRMS of compound **5k**

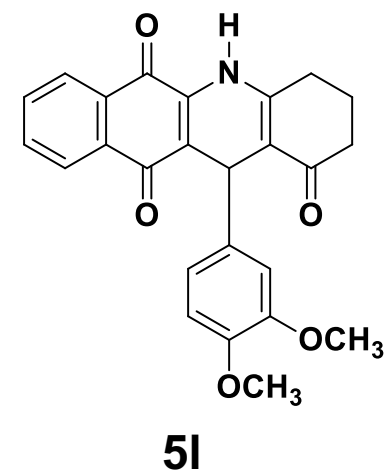
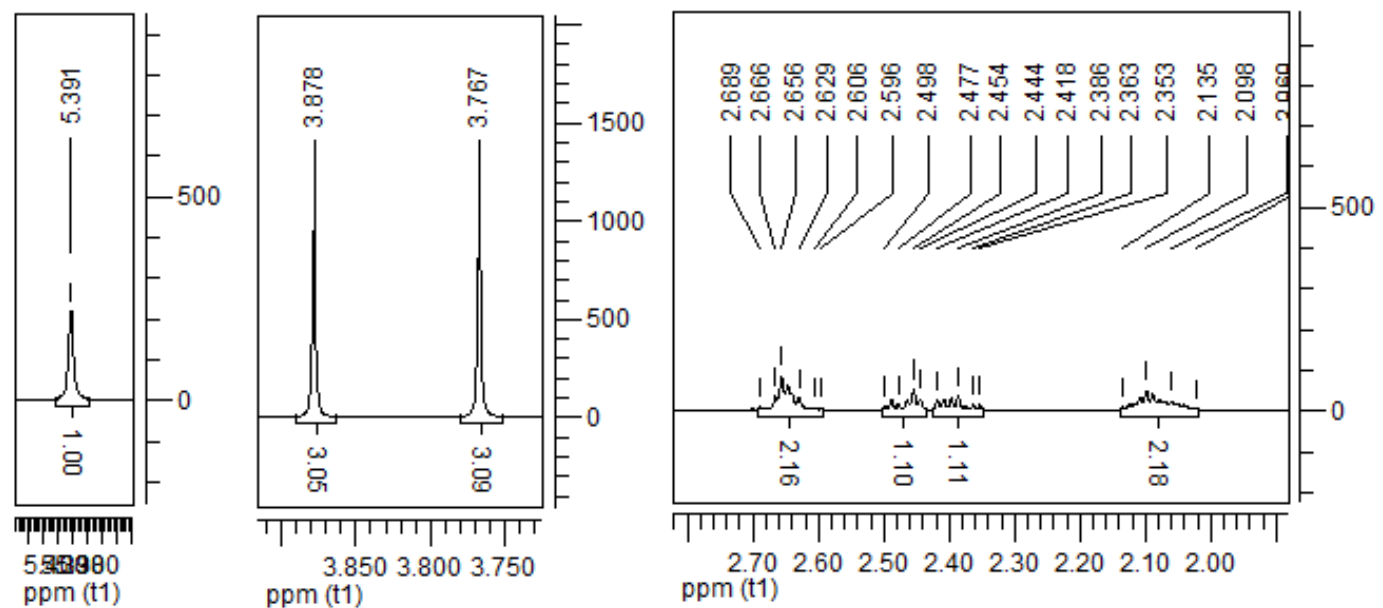
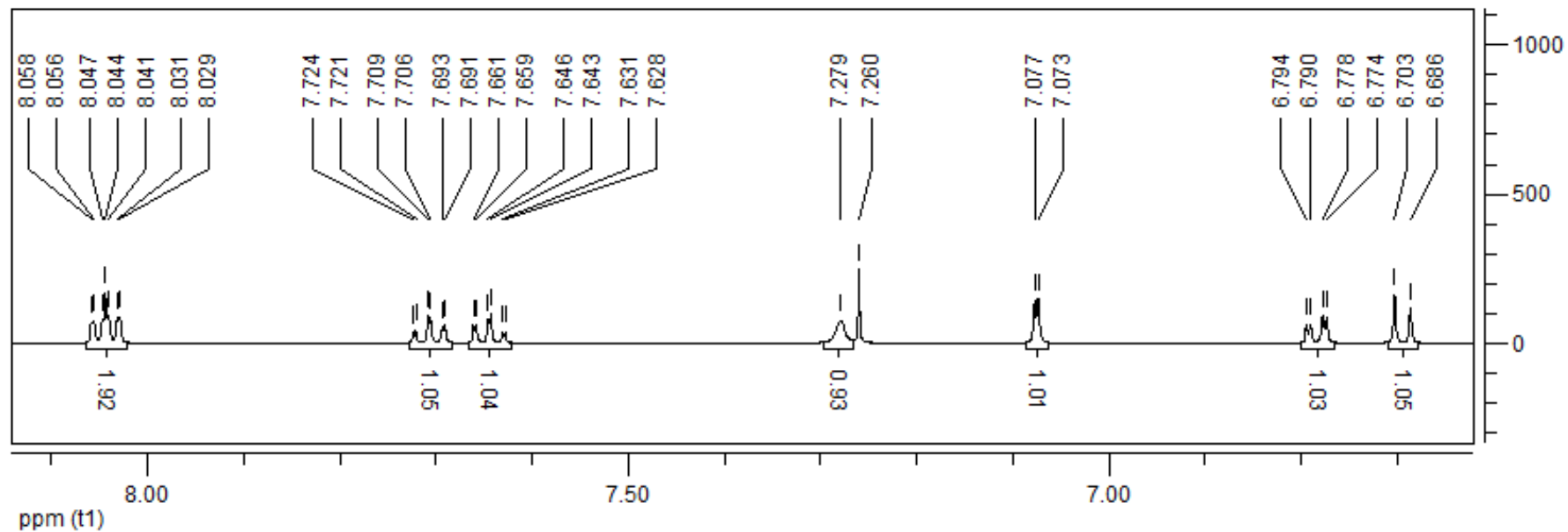




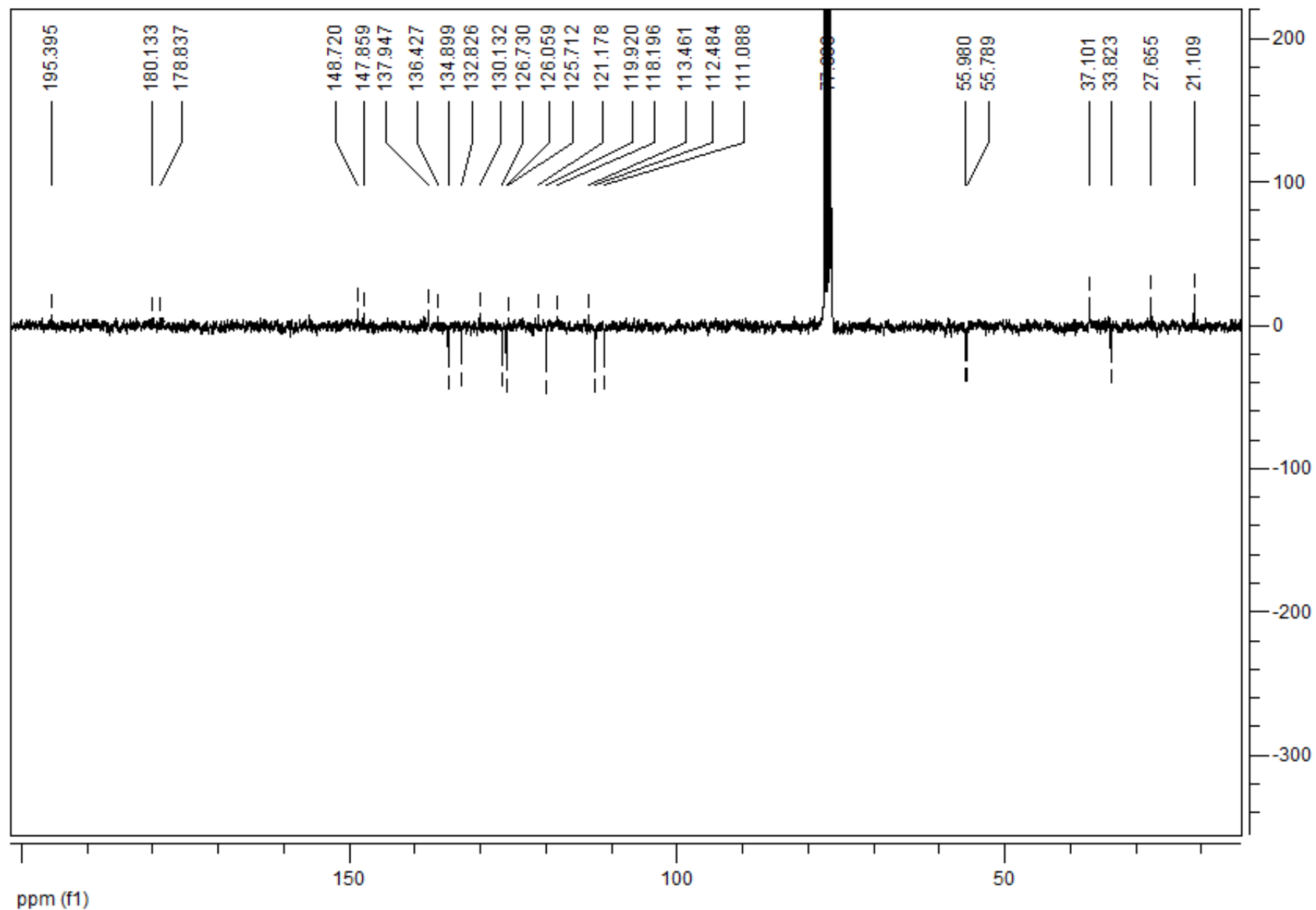
IR spectrum of compound **51**



<sup>1</sup>H NMR spectrum of compound **5I** (500.00 MHz, CDCl<sub>3</sub>)

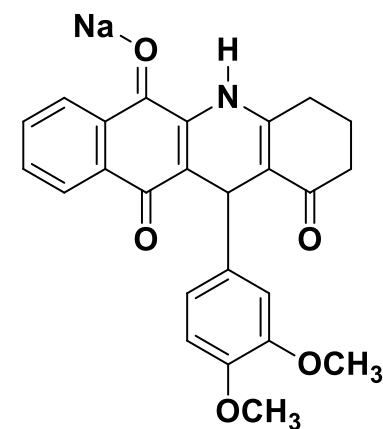
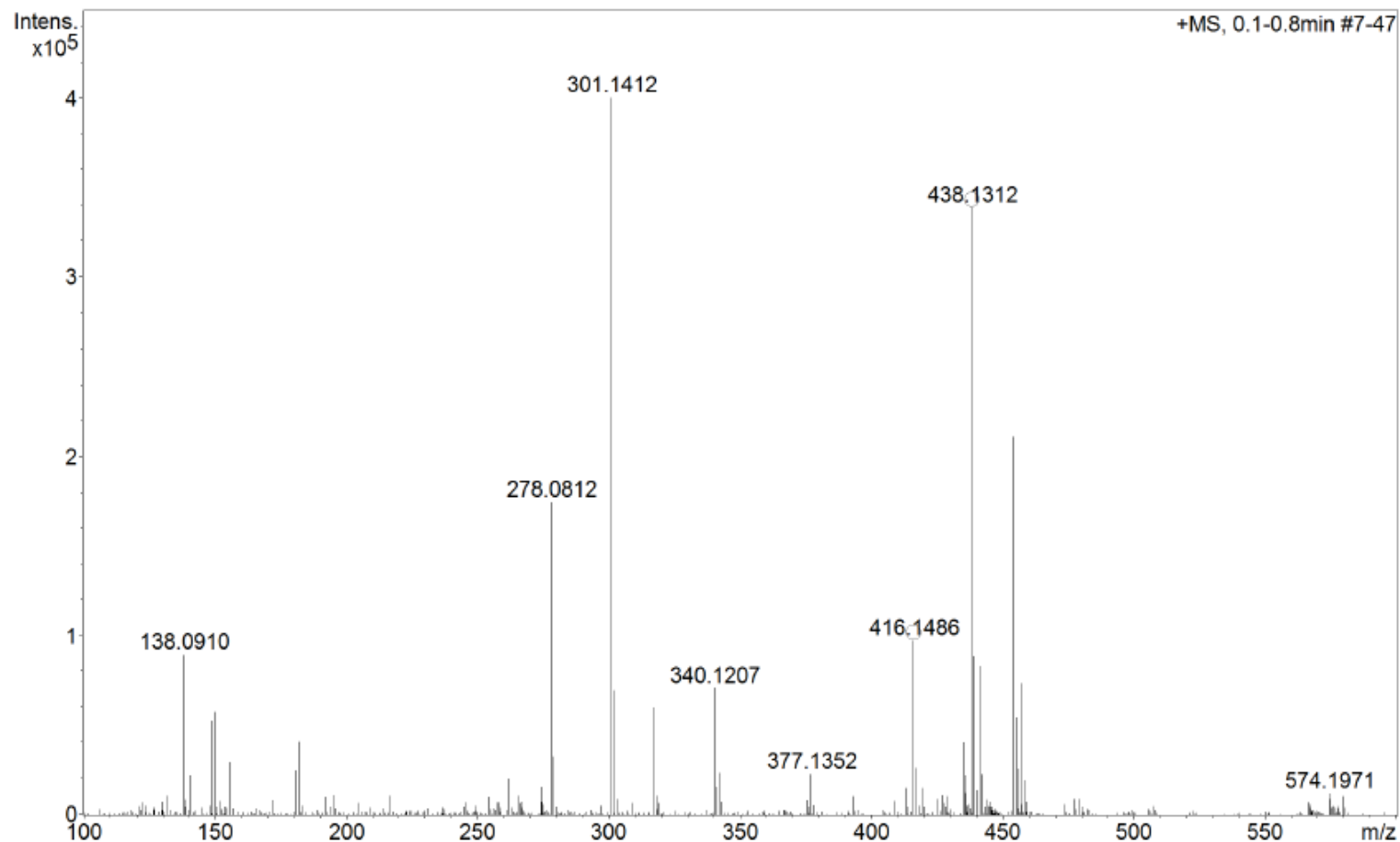


<sup>1</sup>H NMR spectrum of compound **5l** (500.00 MHz, CDCl<sub>3</sub>)



$^{13}\text{C}$  NMR spectrum of compound **5I** (75.0 MHz,  $\text{CDCl}_3$ )

+MS, 0.1-0.8min #7-47

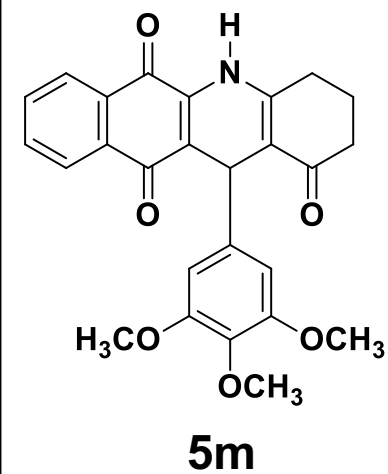
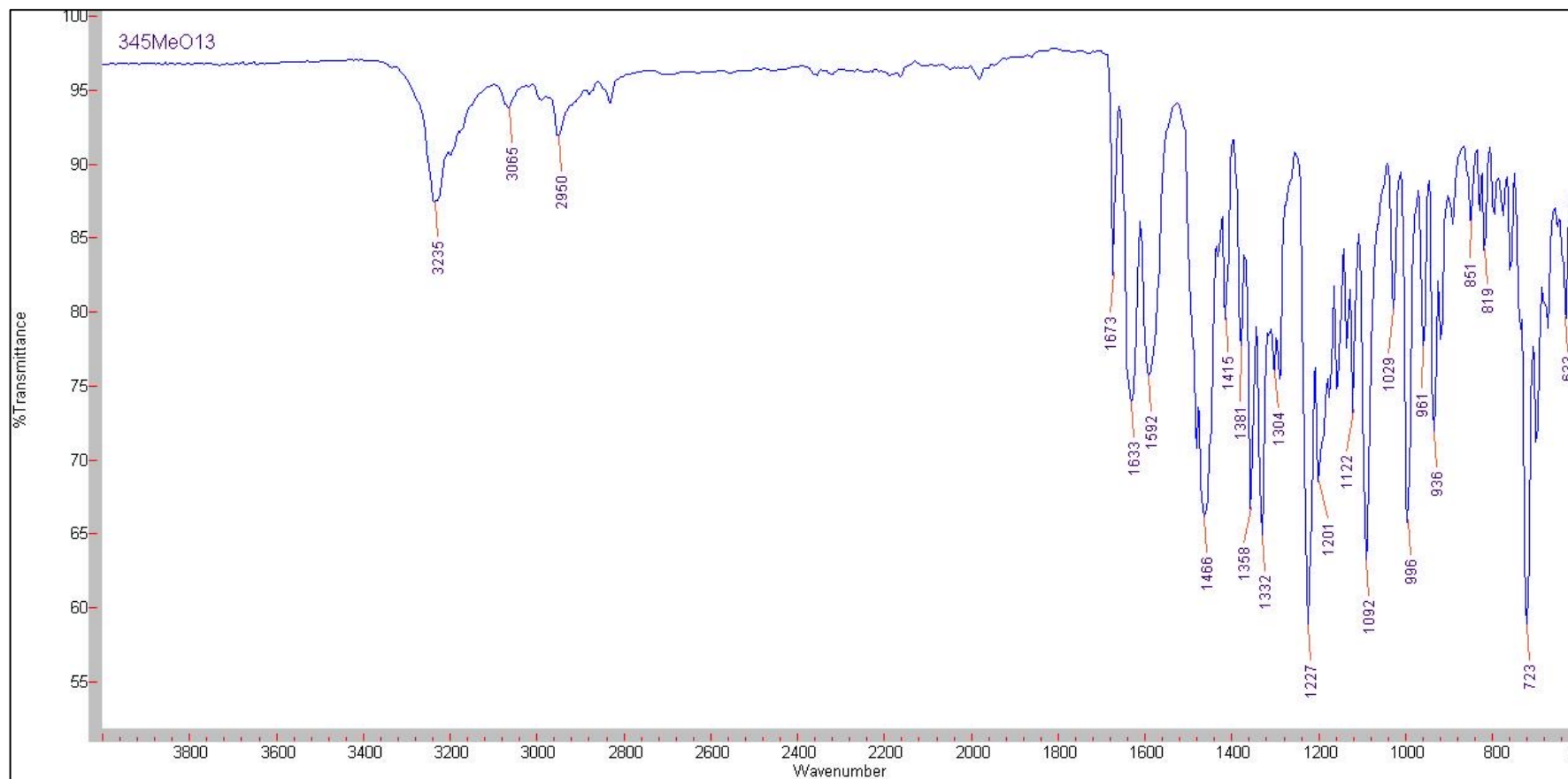


Exact Mass: 438,1317

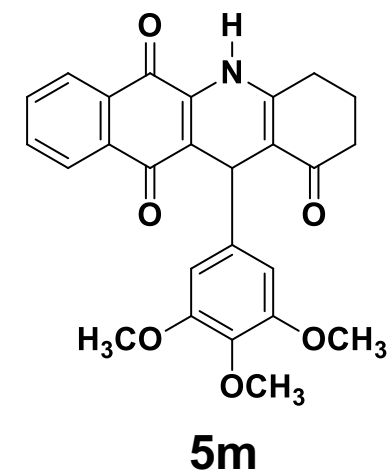
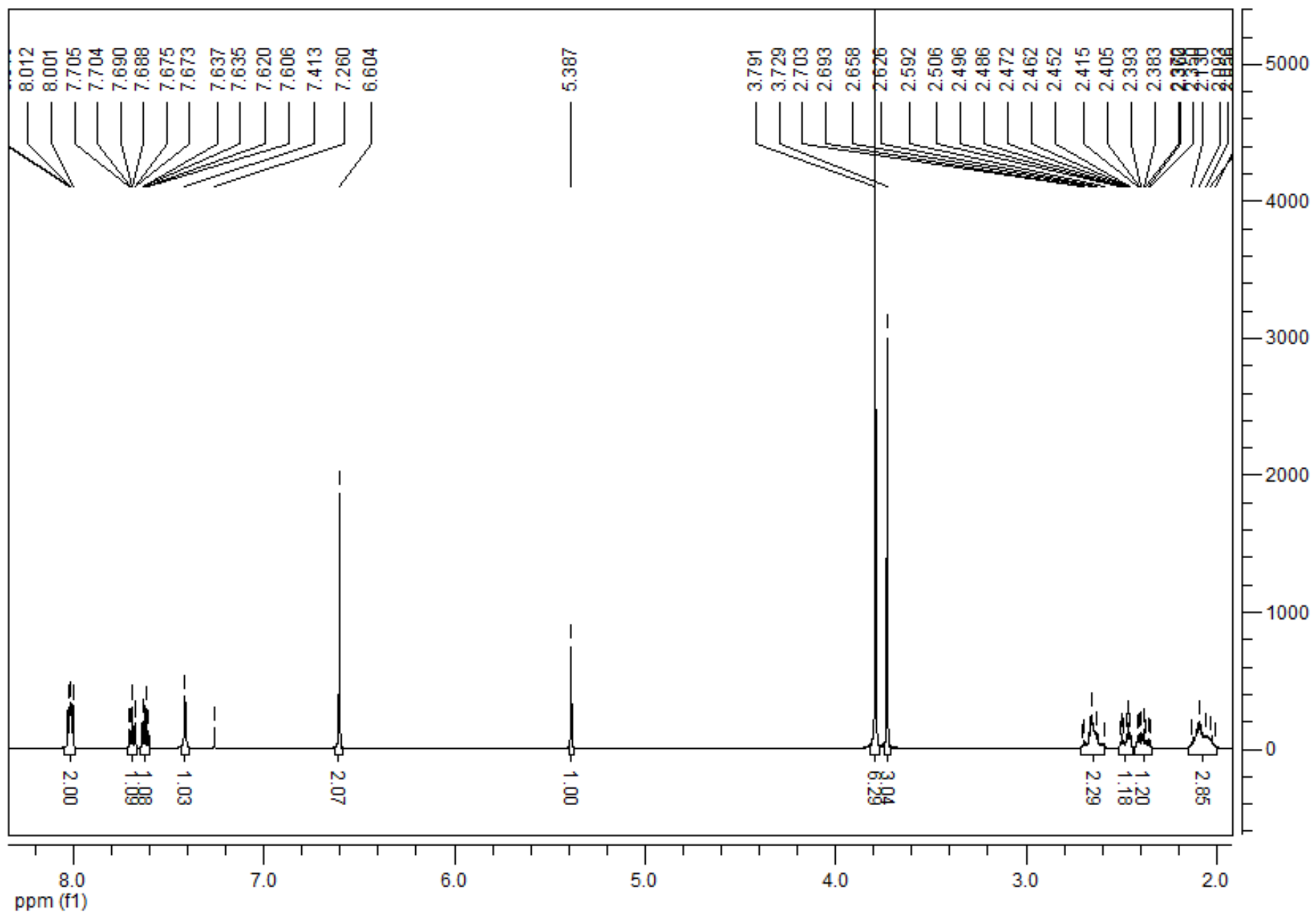
**51**

Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std Mean	m/z	Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
416.1486	36	1 C <sub>25</sub> H <sub>22</sub> NO <sub>5</sub>	416.149249	1.5	1.2	15.5	ok	even		8.6	11.5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
	2	C <sub>21</sub> H <sub>18</sub> N <sub>7</sub> O <sub>3</sub>	416.146564	-5.0	-6.0	16.5	ok	even		9.2	16.4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
	3	C <sub>20</sub> H <sub>22</sub> N <sub>3</sub> O <sub>7</sub>	416.145226	-8.2	-8.9	11.5	ok	even		19.3	32.1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
	4	C <sub>26</sub> H <sub>18</sub> N <sub>5</sub> O	416.150587	4.7	4.1	20.5	ok	even		22.1	30.0	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
438.1312	37	1 C <sub>25</sub> H <sub>21</sub> NNaO <sub>5</sub>	438.131193	-0.1	0.6	15.5	ok	even		10.3	16.9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
	2	C <sub>26</sub> H <sub>17</sub> N <sub>5</sub> NaO	438.132531	3.0	3.3	20.5	ok	even		23.2	34.6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	

HRMS of compound **51**



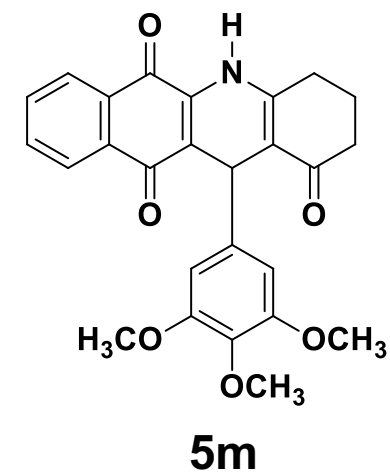
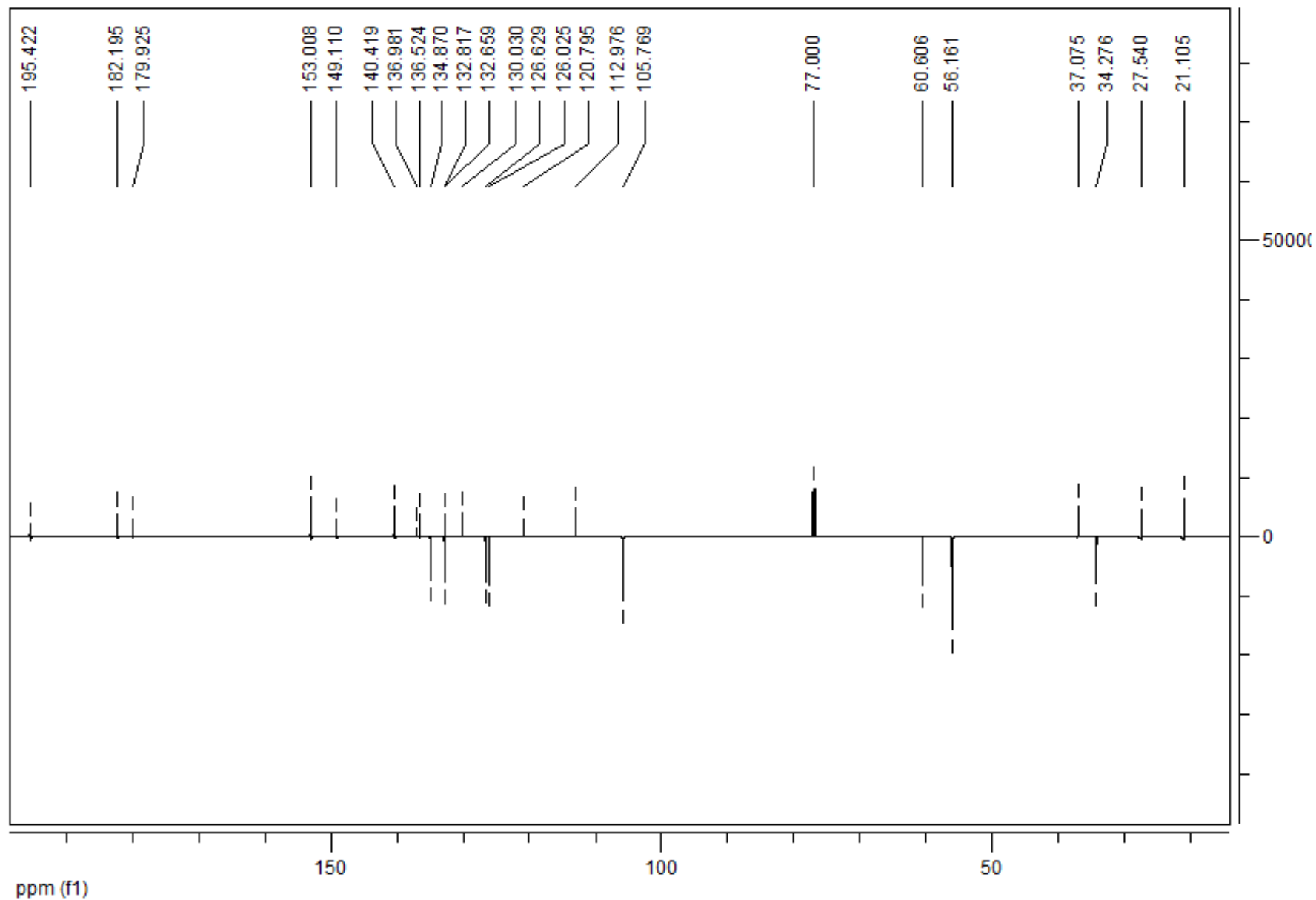
IR spectrum of compound **5m**



<sup>1</sup>H NMR spectrum of compound **5m** (500.00 MHz, CDCl<sub>3</sub>)

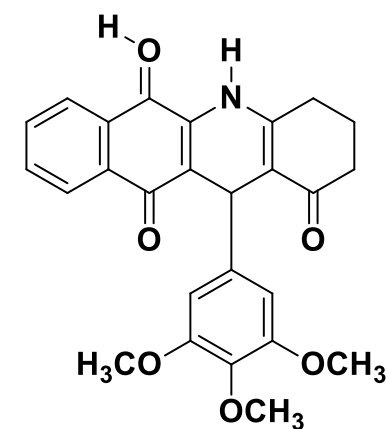
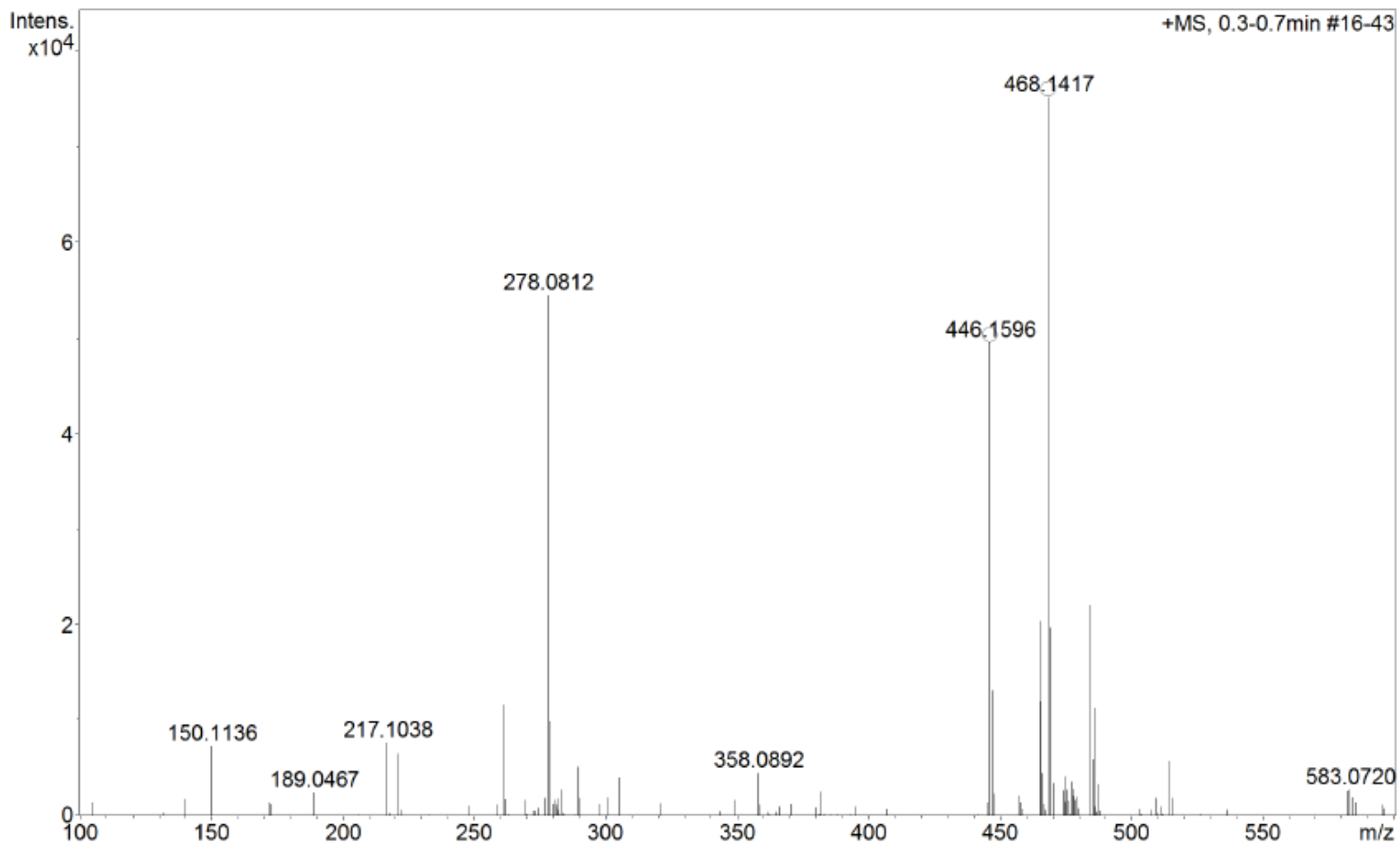






<sup>13</sup>C NMR spectrum of compound **5m** (75.0 MHz, CDCl<sub>3</sub>)

+MS, 0.3-0.7min #16-43



Exact Mass: 446,1604

**5m**

Meas. m/z #	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup>	Conf	mSigma	Std I	Std	Mean m/z	Std I	VarNorm	Std	m/z	Diff	Std	Comb	Dev
446.159604	1 C <sub>26</sub> H <sub>24</sub> NO <sub>6</sub>	446.159814	0.5	1108.5	15.5	ok	even		14.0	27.5		n.a.		n.a.		n.a.		n.a.		n.a.
	2 C <sub>23</sub> H <sub>16</sub> N <sub>11</sub>	446.158466	-2.6	-2.7	21.5	ok	even		15.6	21.4		n.a.		n.a.		n.a.		n.a.		n.a.
	3 C <sub>27</sub> H <sub>20</sub> N <sub>5</sub> O <sub>2</sub>	446.161151	3.5	4.1	20.5	ok	even		28.7	42.0		n.a.		n.a.		n.a.		n.a.		n.a.
468.141660	1 C <sub>26</sub> H <sub>23</sub> NNaO <sub>6</sub>	468.141758	0.2	1056.4	15.5	ok	even		14.9	29.0		n.a.		n.a.		n.a.		n.a.		n.a.
	2 C <sub>23</sub> H <sub>15</sub> N <sub>11</sub> Na	468.140410	-2.7	-2.6	21.5	ok	even		16.8	23.1		n.a.		n.a.		n.a.		n.a.		n.a.
	3 C <sub>27</sub> H <sub>19</sub> N <sub>5</sub> NaO <sub>2</sub>	468.143096	3.1	3.8	20.5	ok	even		29.8	43.6		n.a.		n.a.		n.a.		n.a.		n.a.

HRMS of compound **5m**