

## Supplementary Material

### Synthesis and characterization of peptidomimetics containing oxazolidin-2-one and oxazolidine scaffolds

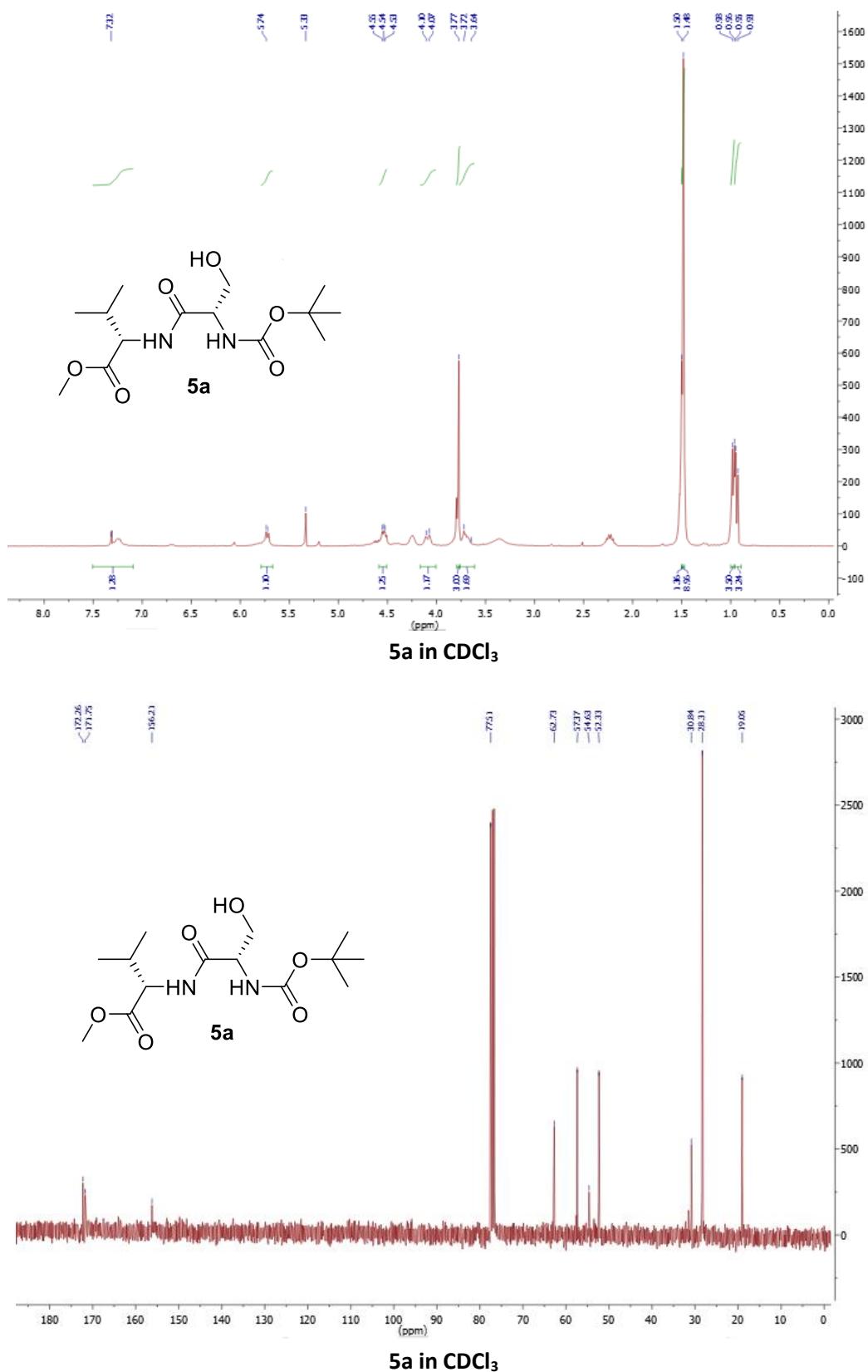
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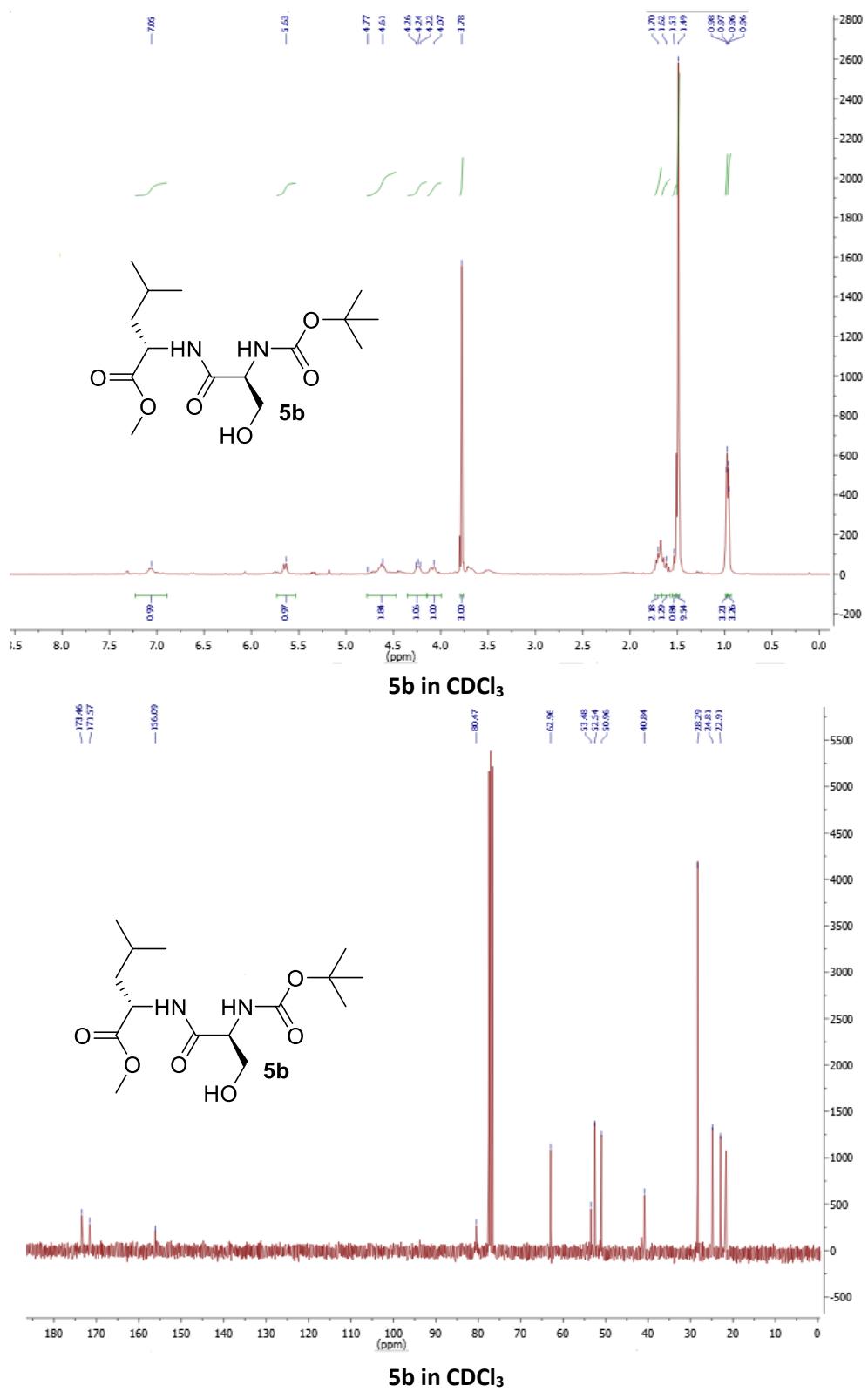
<sup>b</sup>Université de Paris, CiTCoM, CNRS, 4 avenue de l'observatoire F-75006 Paris, France  
Email: [w\\_medjahed@yahoo.fr](mailto:w_medjahed@yahoo.fr)

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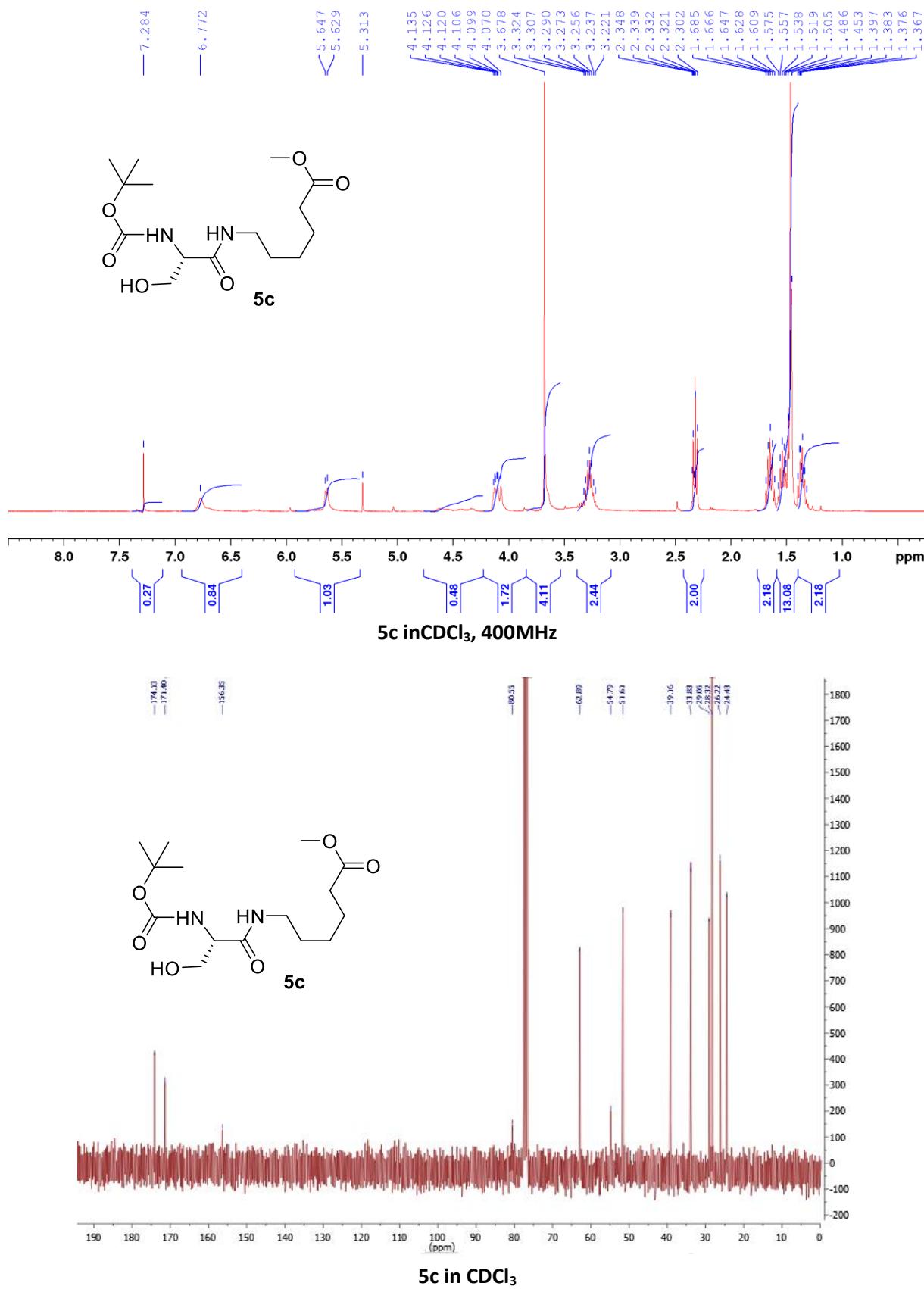
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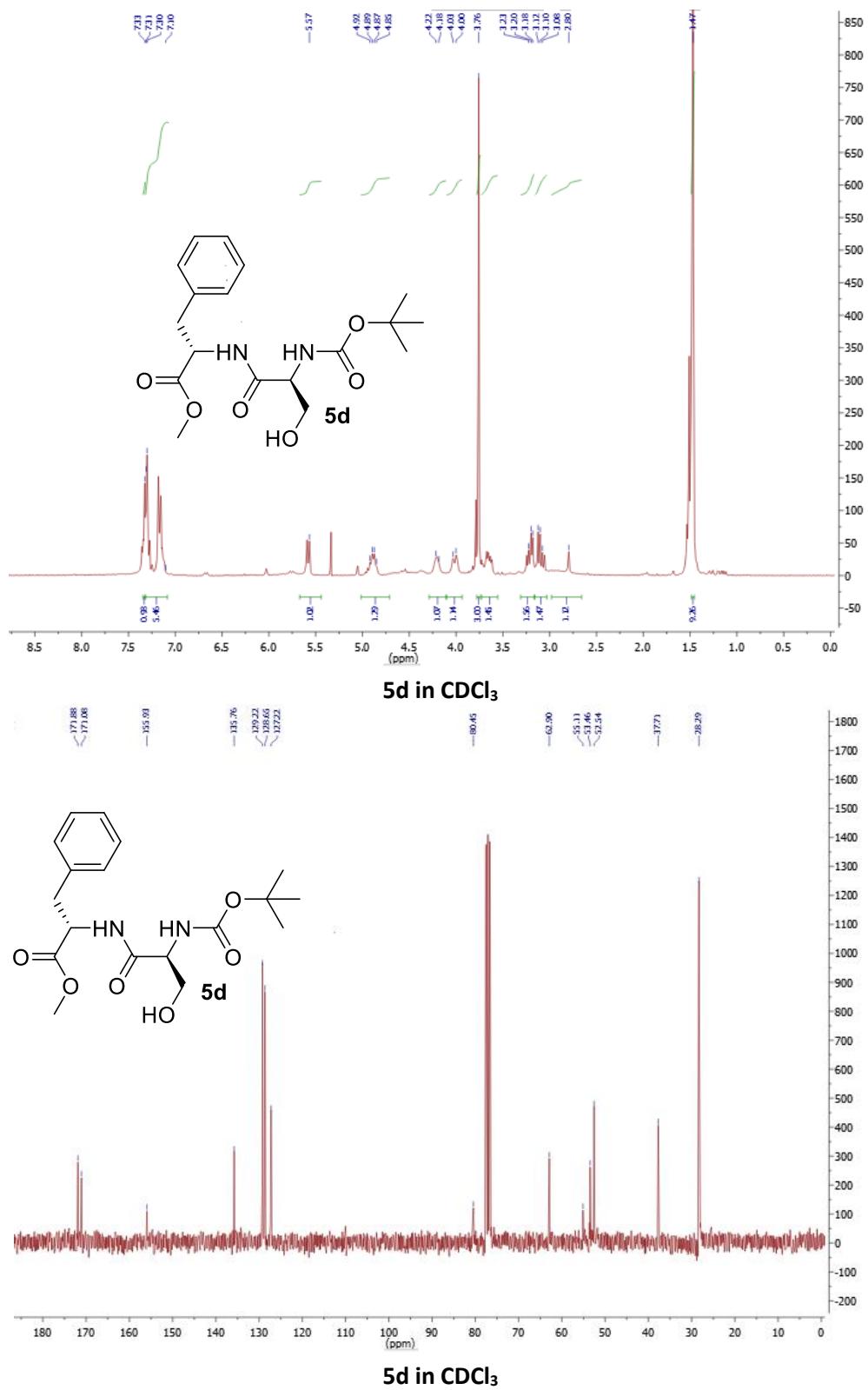
**Figure 1**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound 5a.



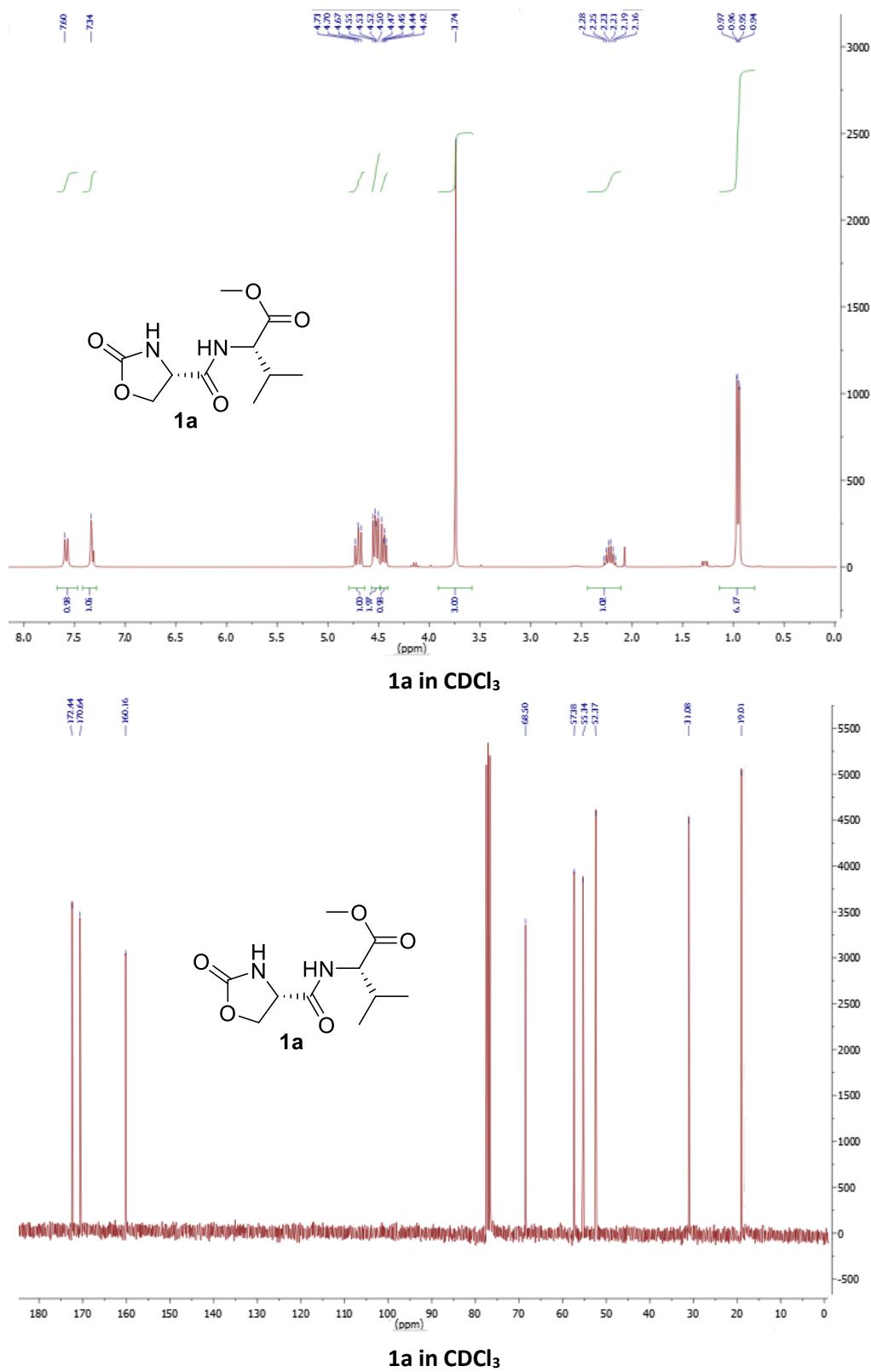
**Figure 2**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound **5b**.



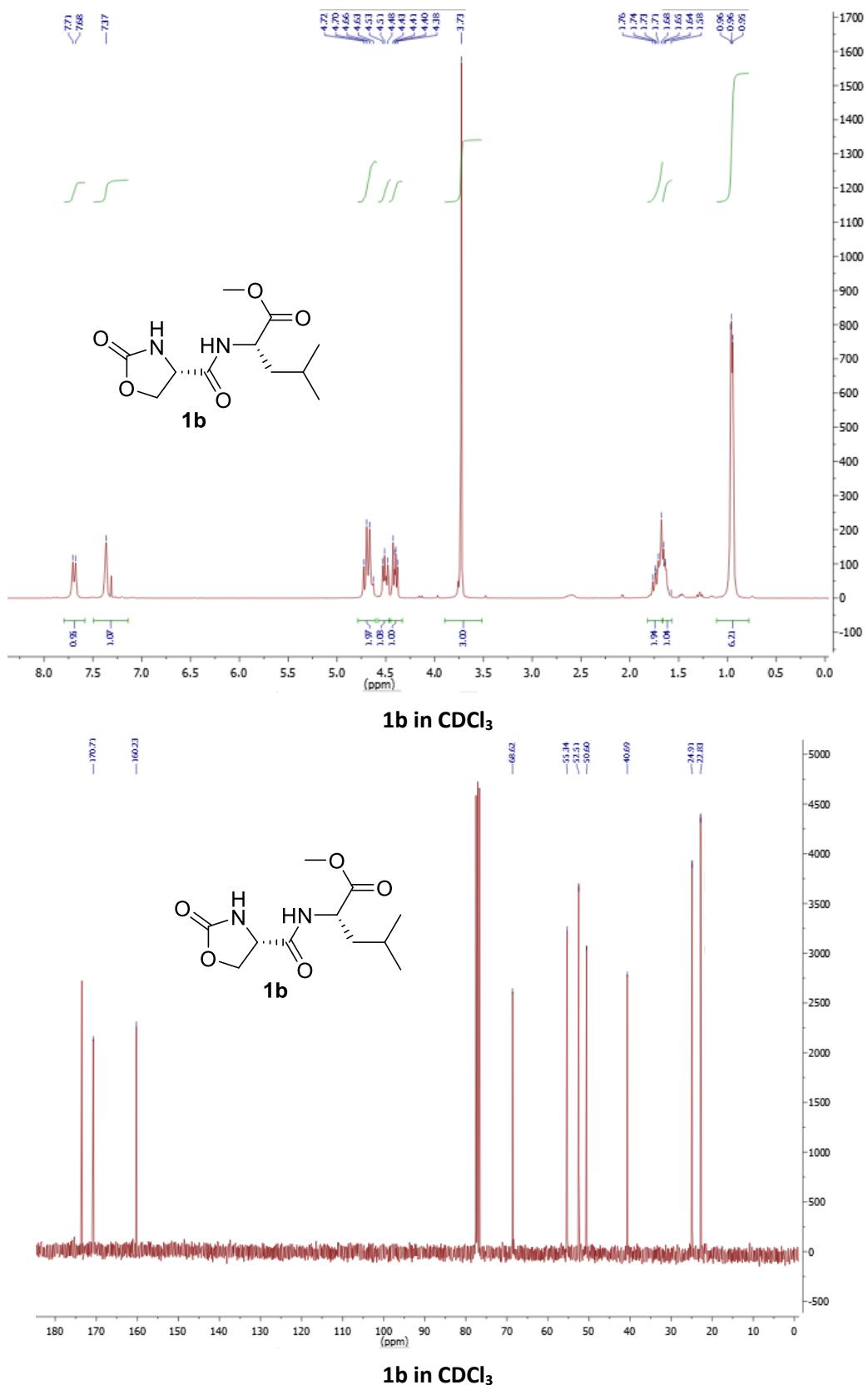
**Figure 3** <sup>1</sup>H and <sup>13</sup>C NMR of compound **5c**.



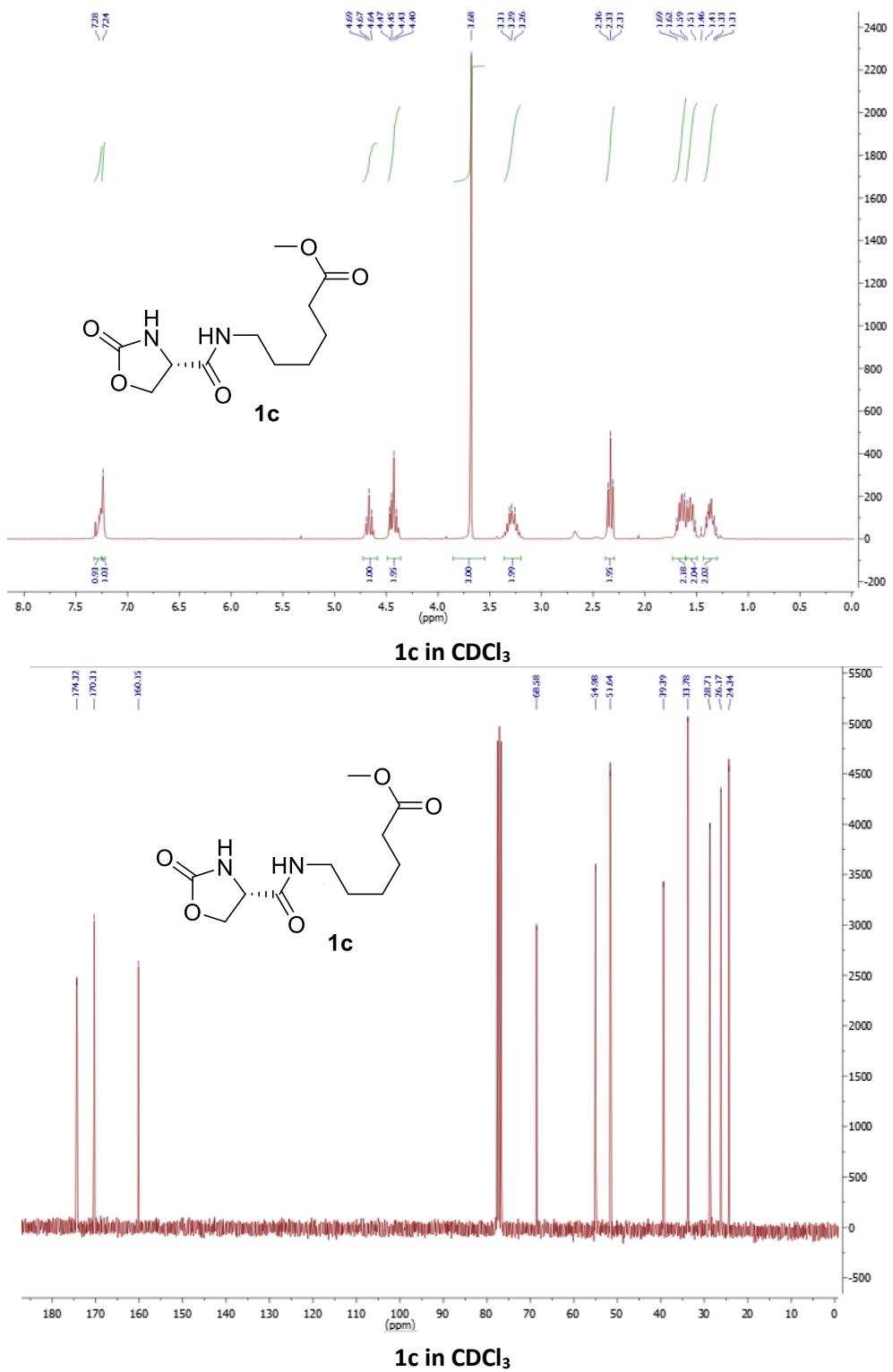
**Figure 4**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound 5d.



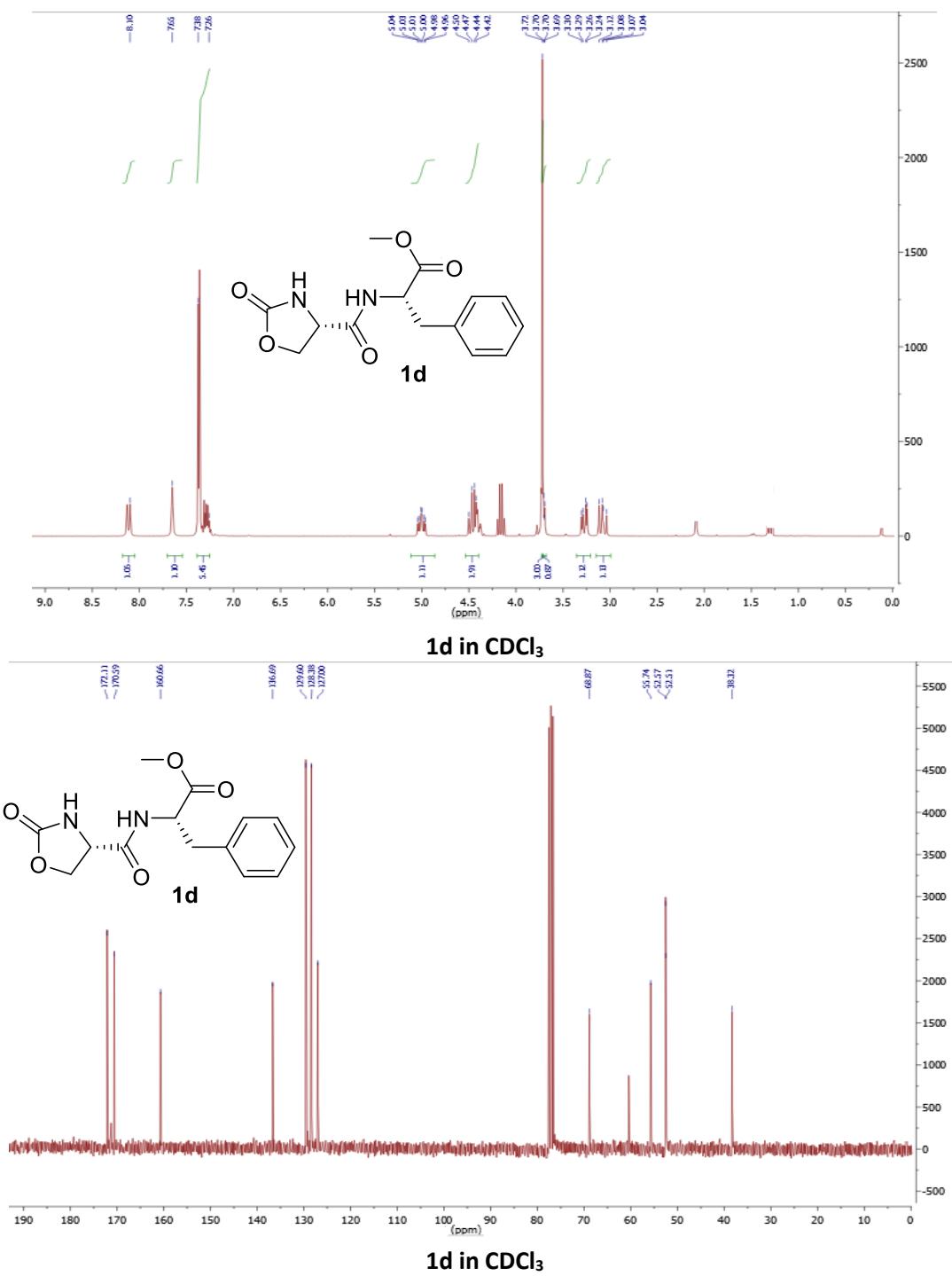
**Figure 5**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound 1a.



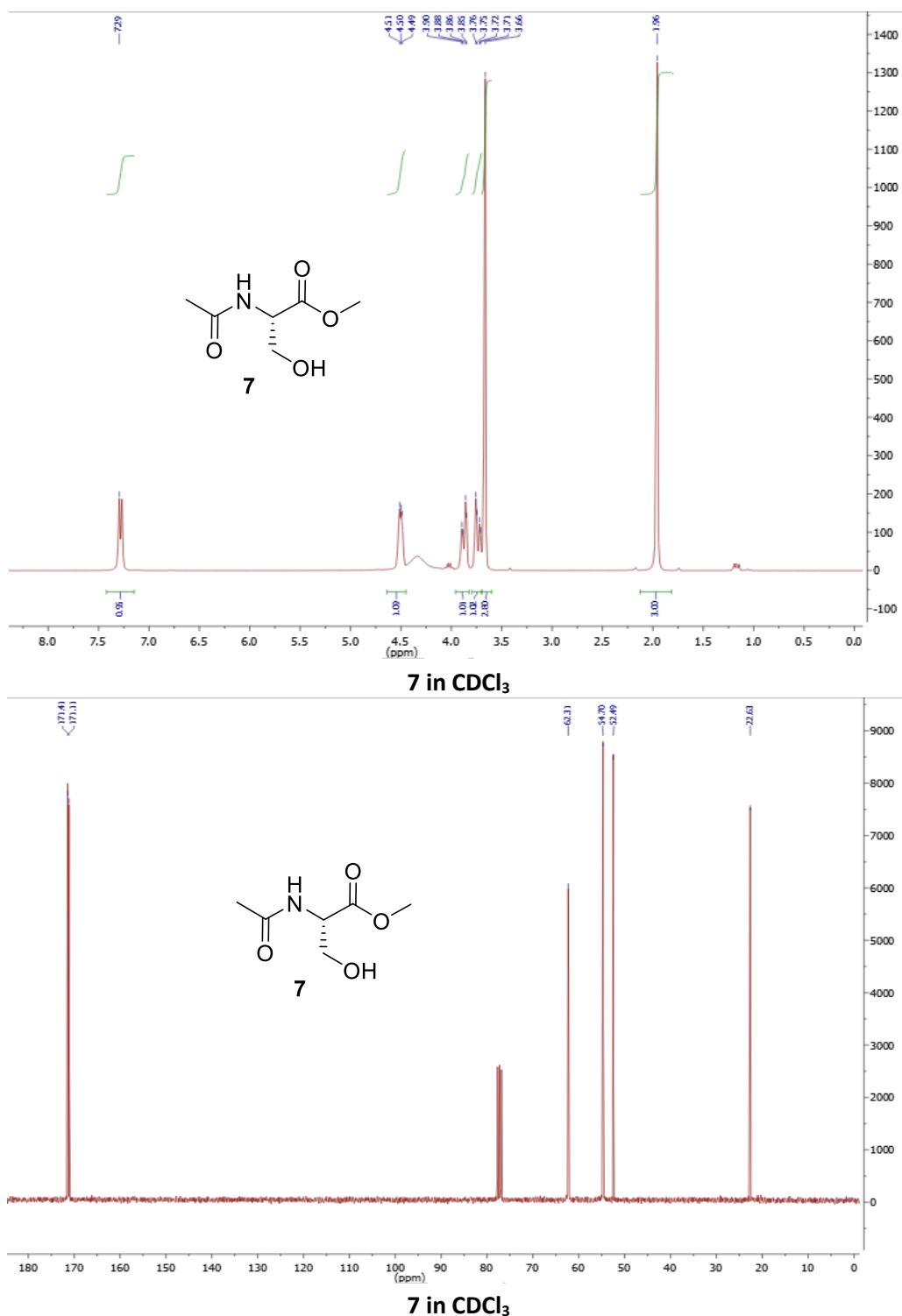
**Figure 6**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound **1b**.



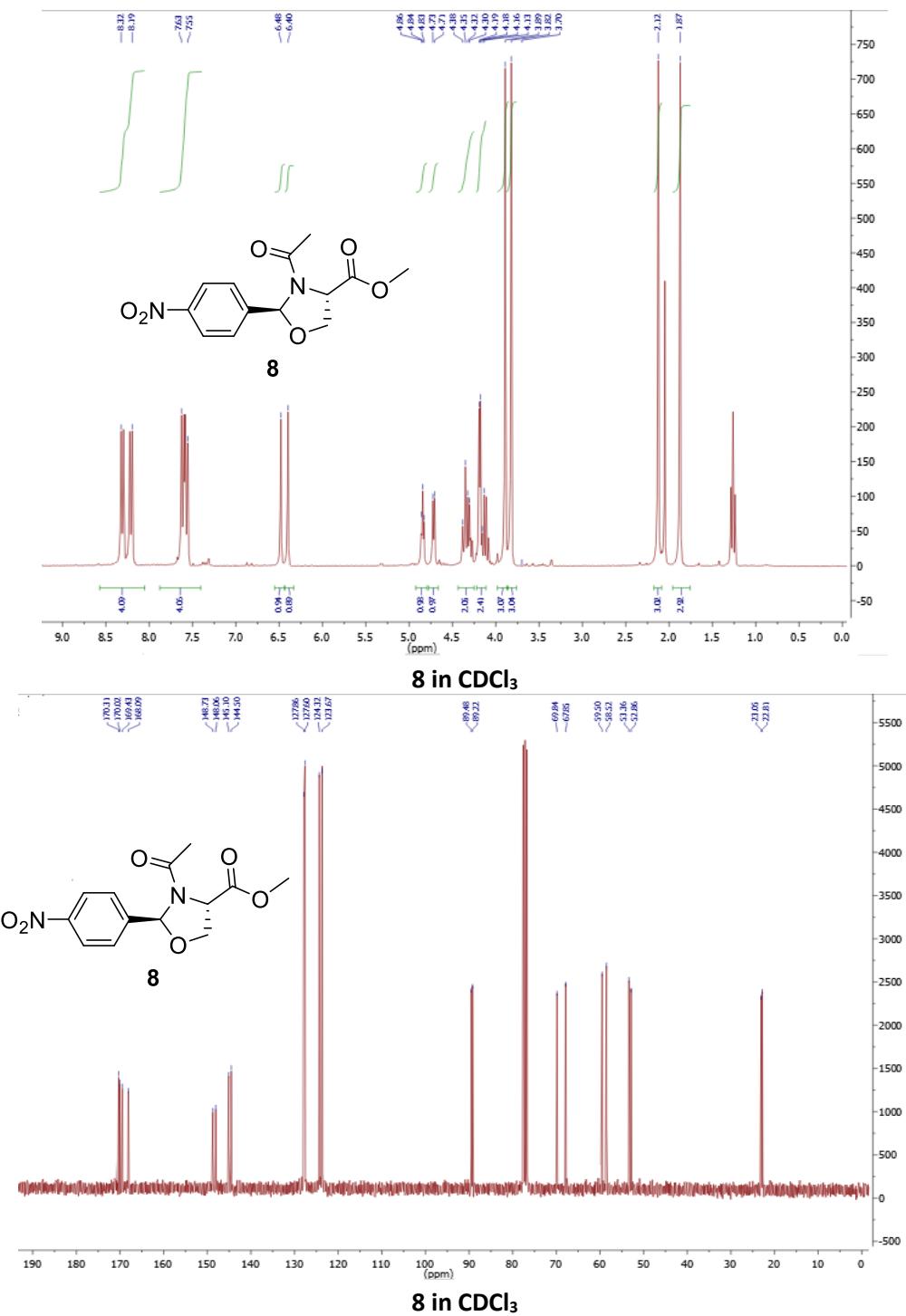
**Figure 7**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound **1c**.



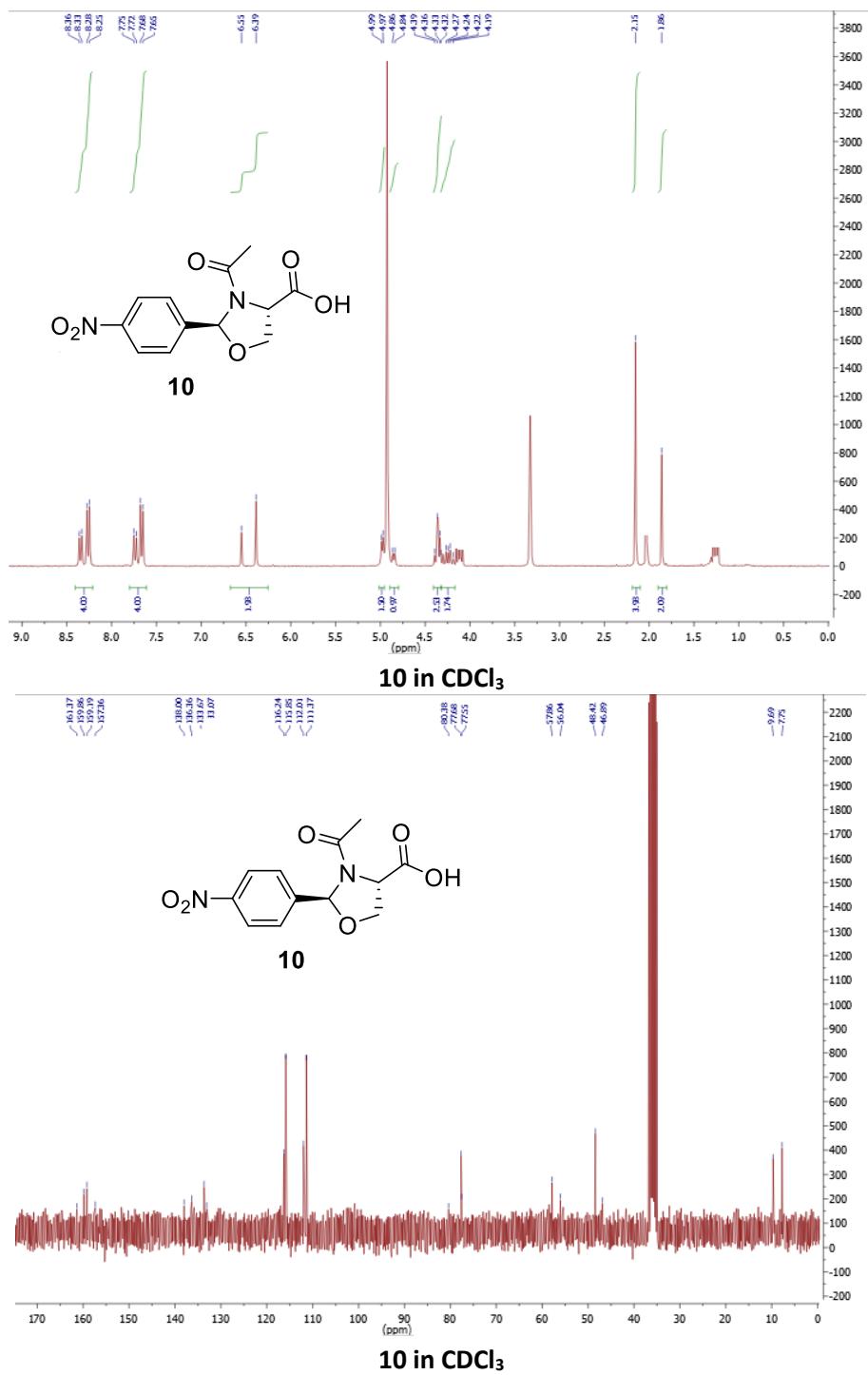
**Figure 8**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound **1d**.



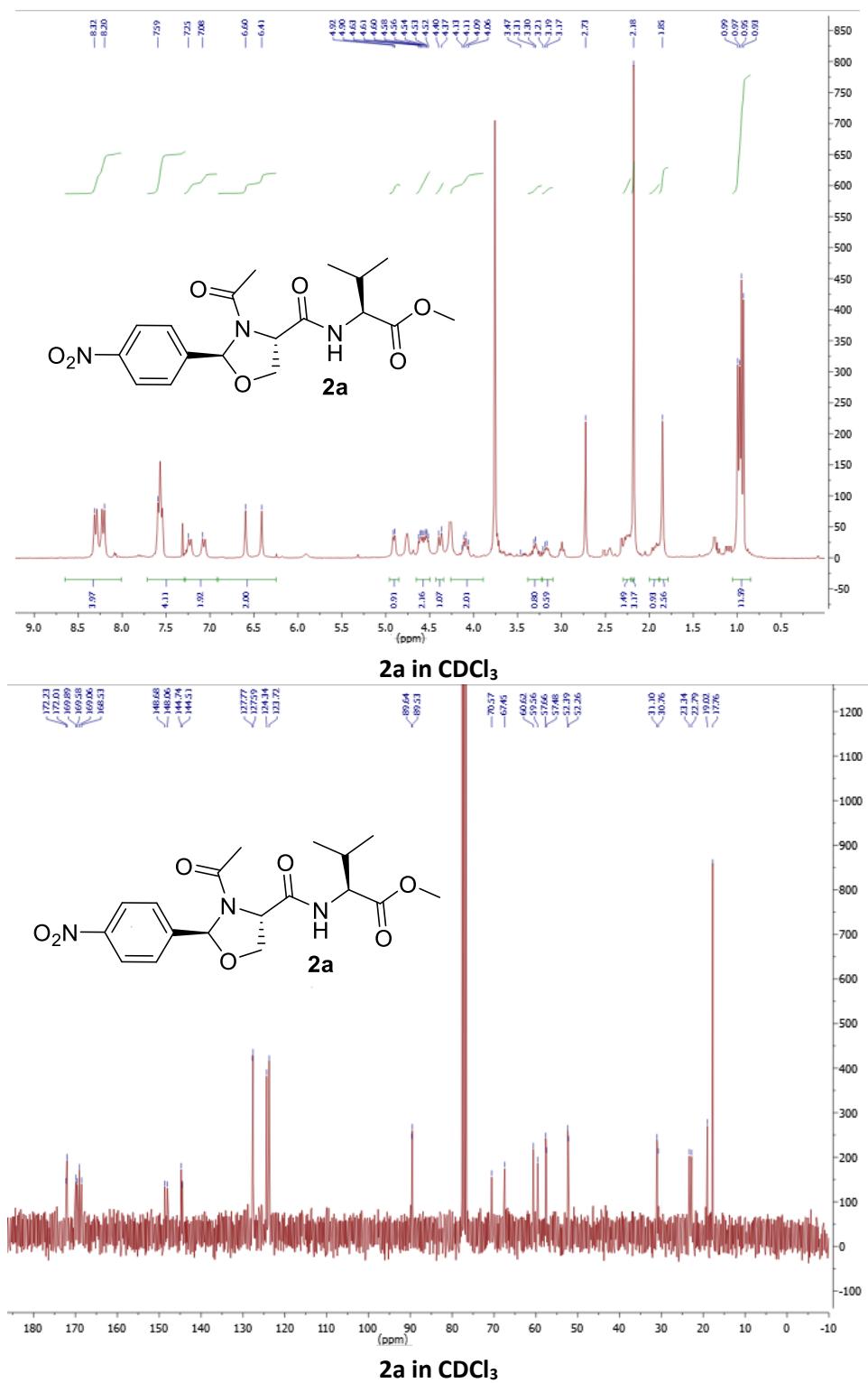
**Figure 9**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound 7.



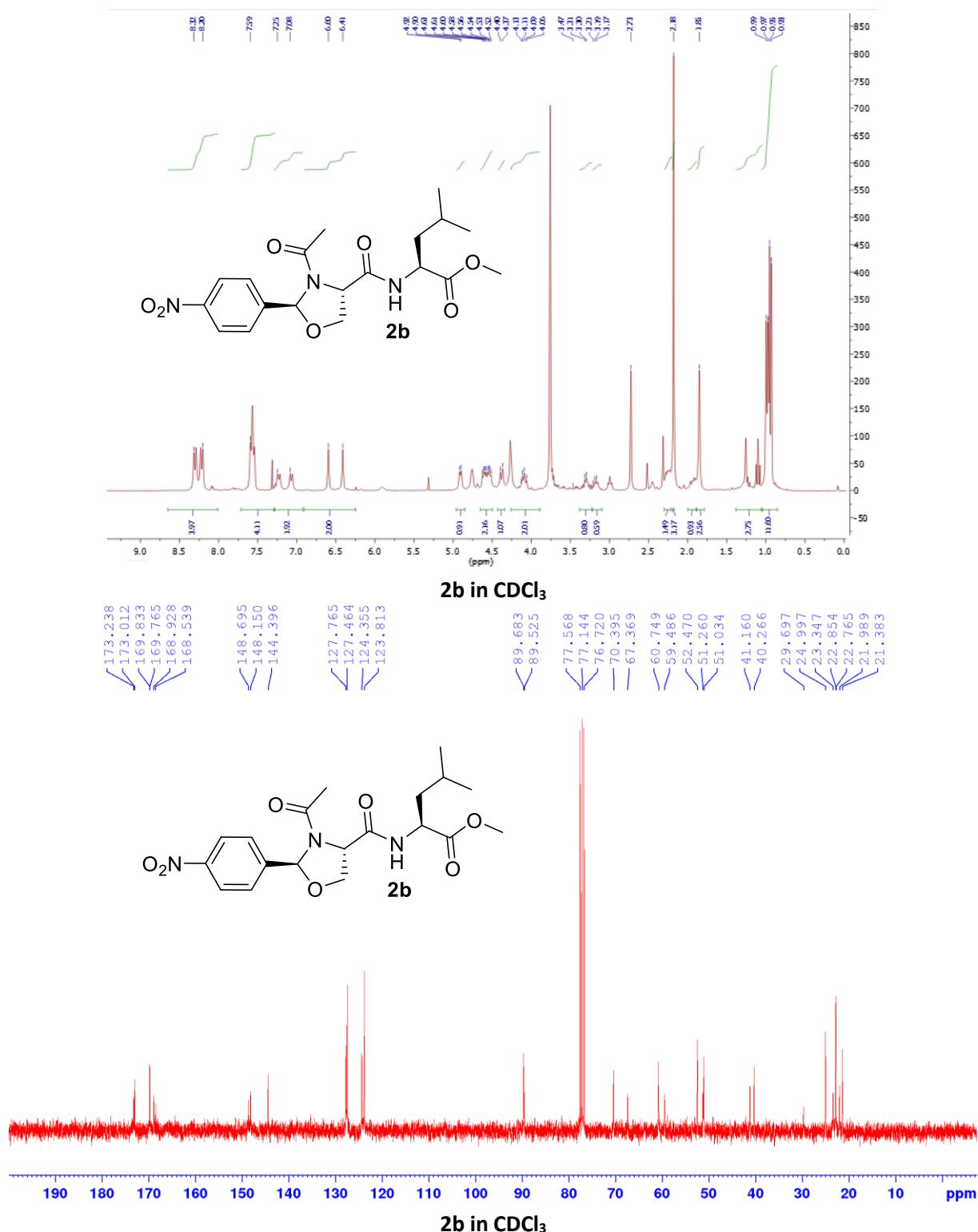
**Figure 10**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound **8**.



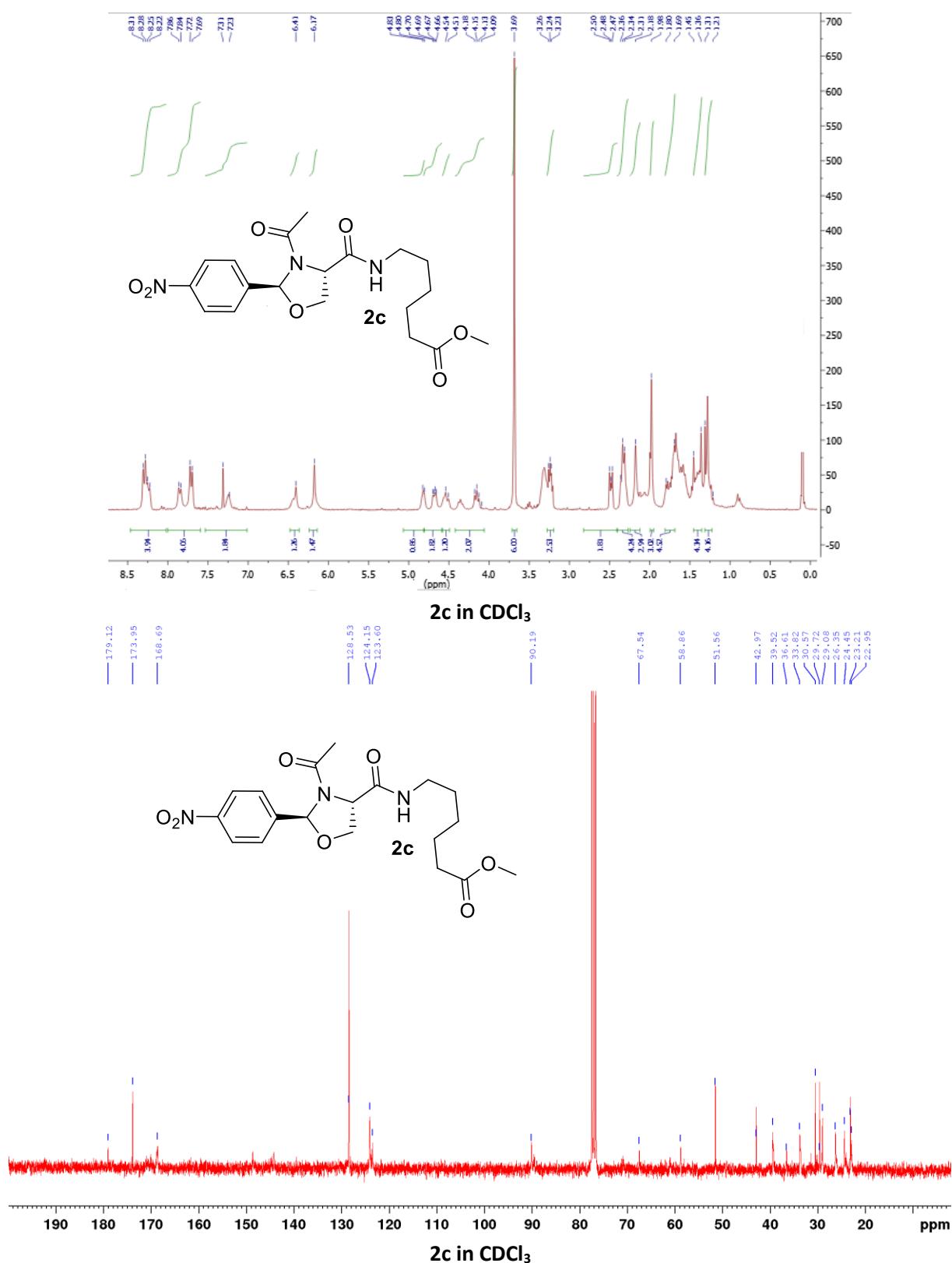
**Figure 11**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound 10.



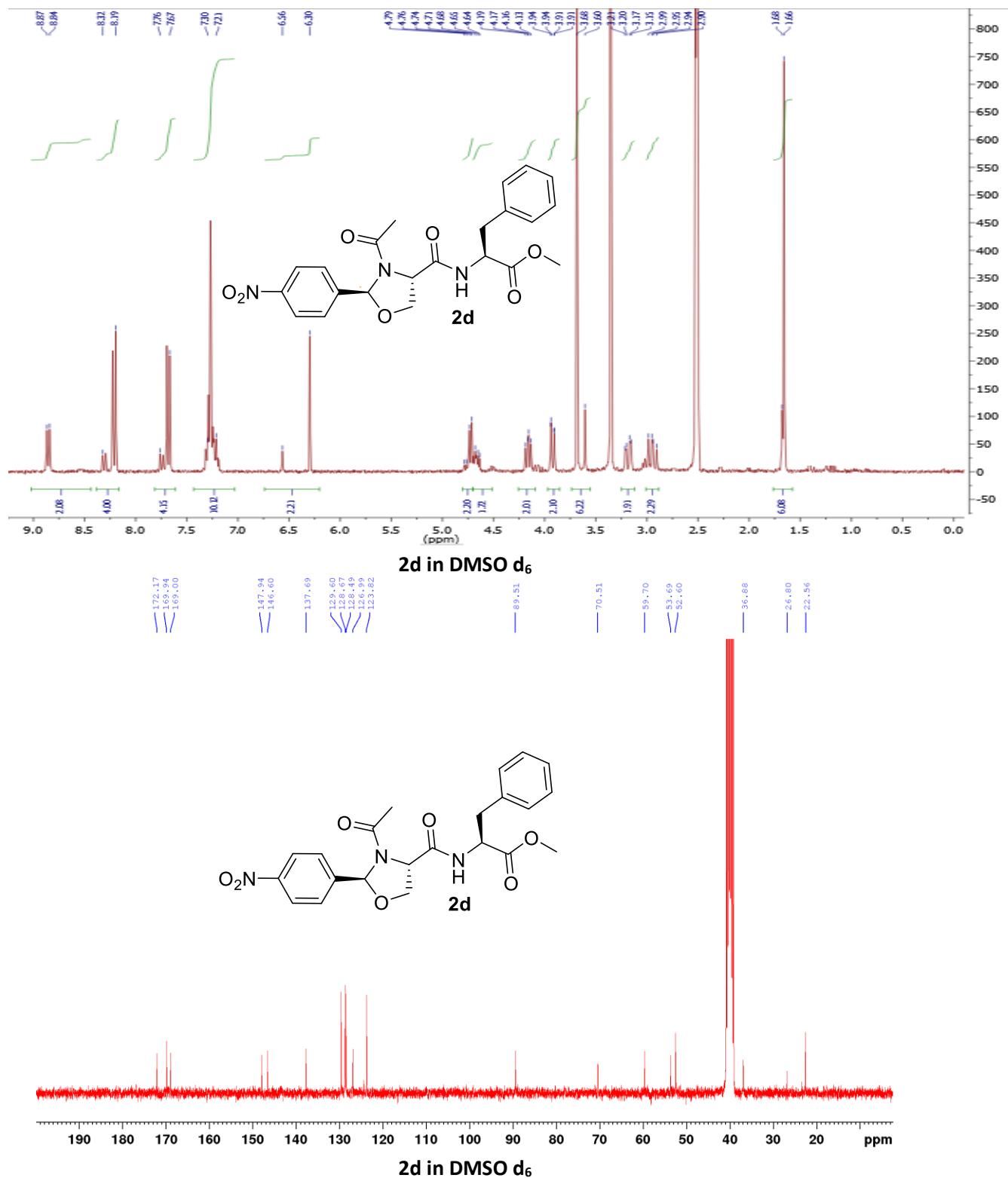
**Figure 12**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound 2a.



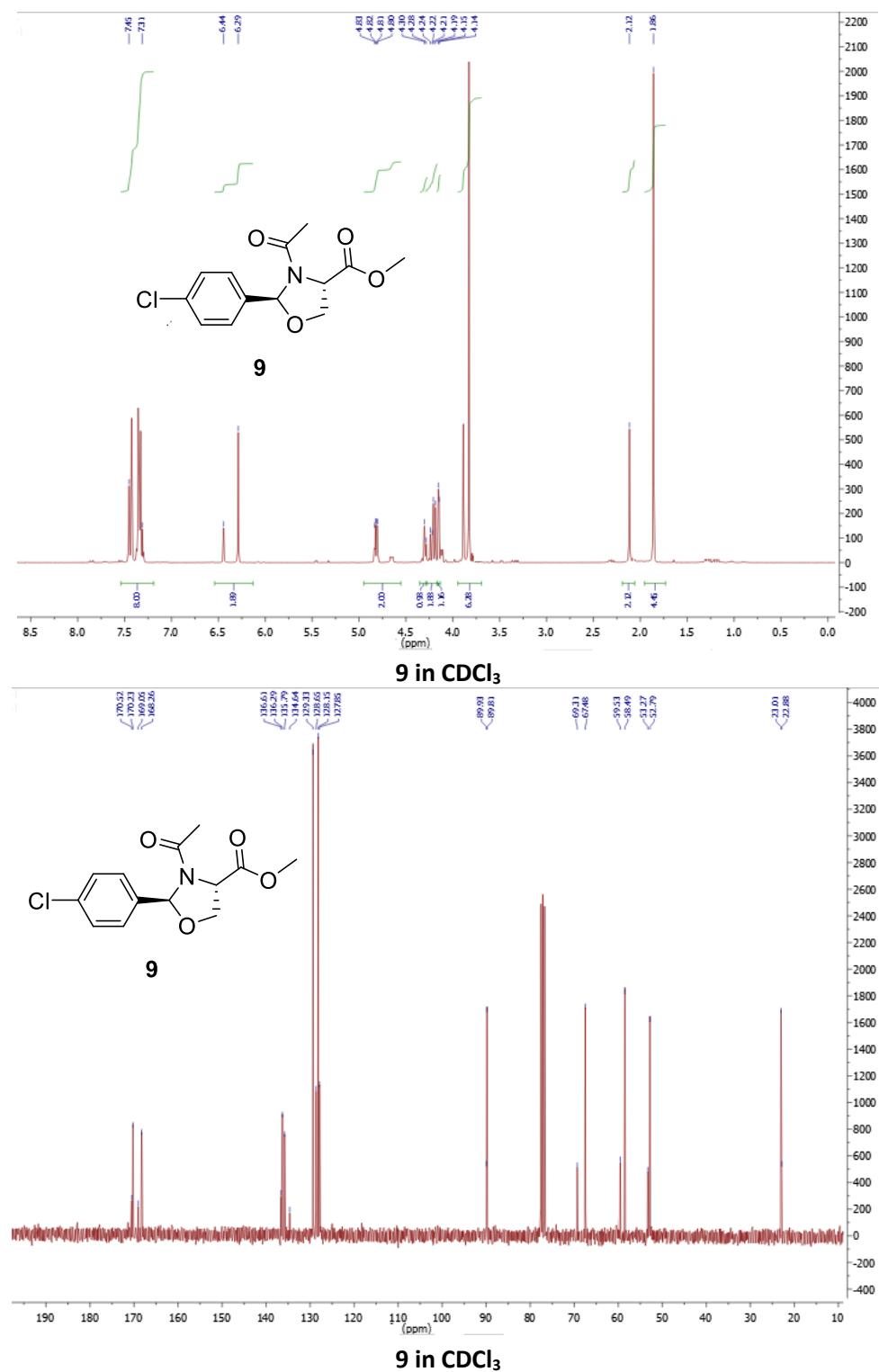
**Figure 13**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound **2b**.



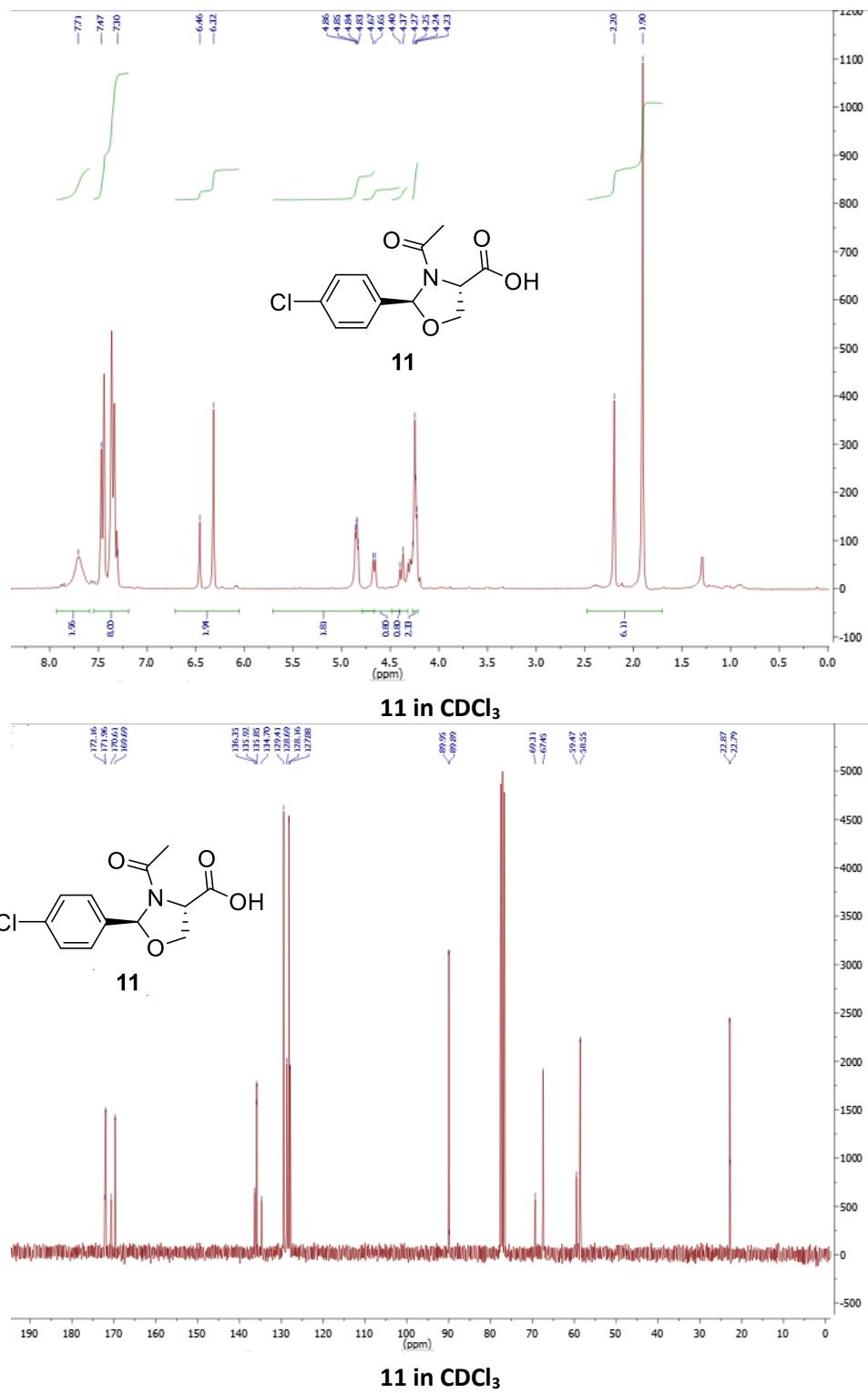
**Figure 14**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound **2c**.



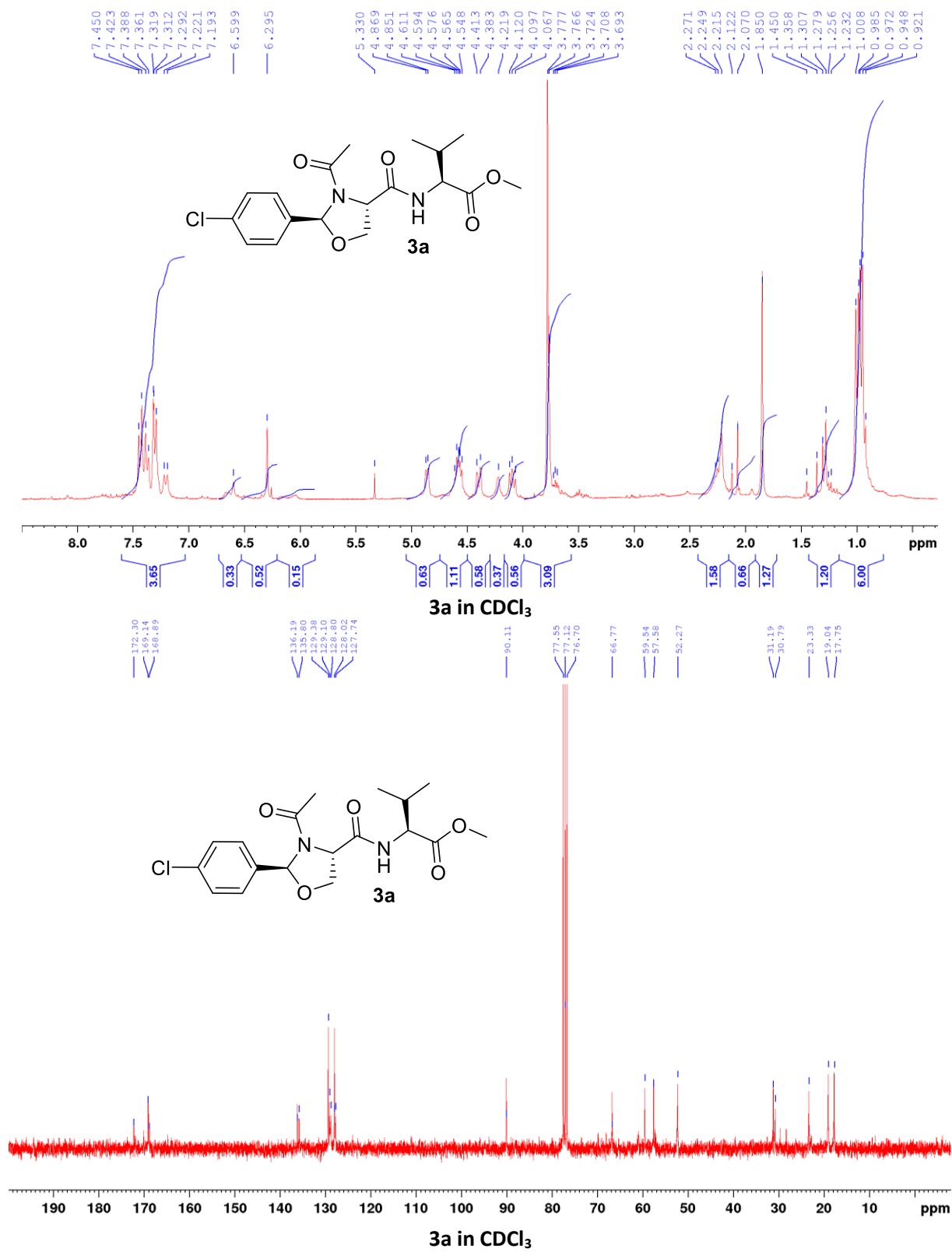
**Figure 15**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound **2d**.



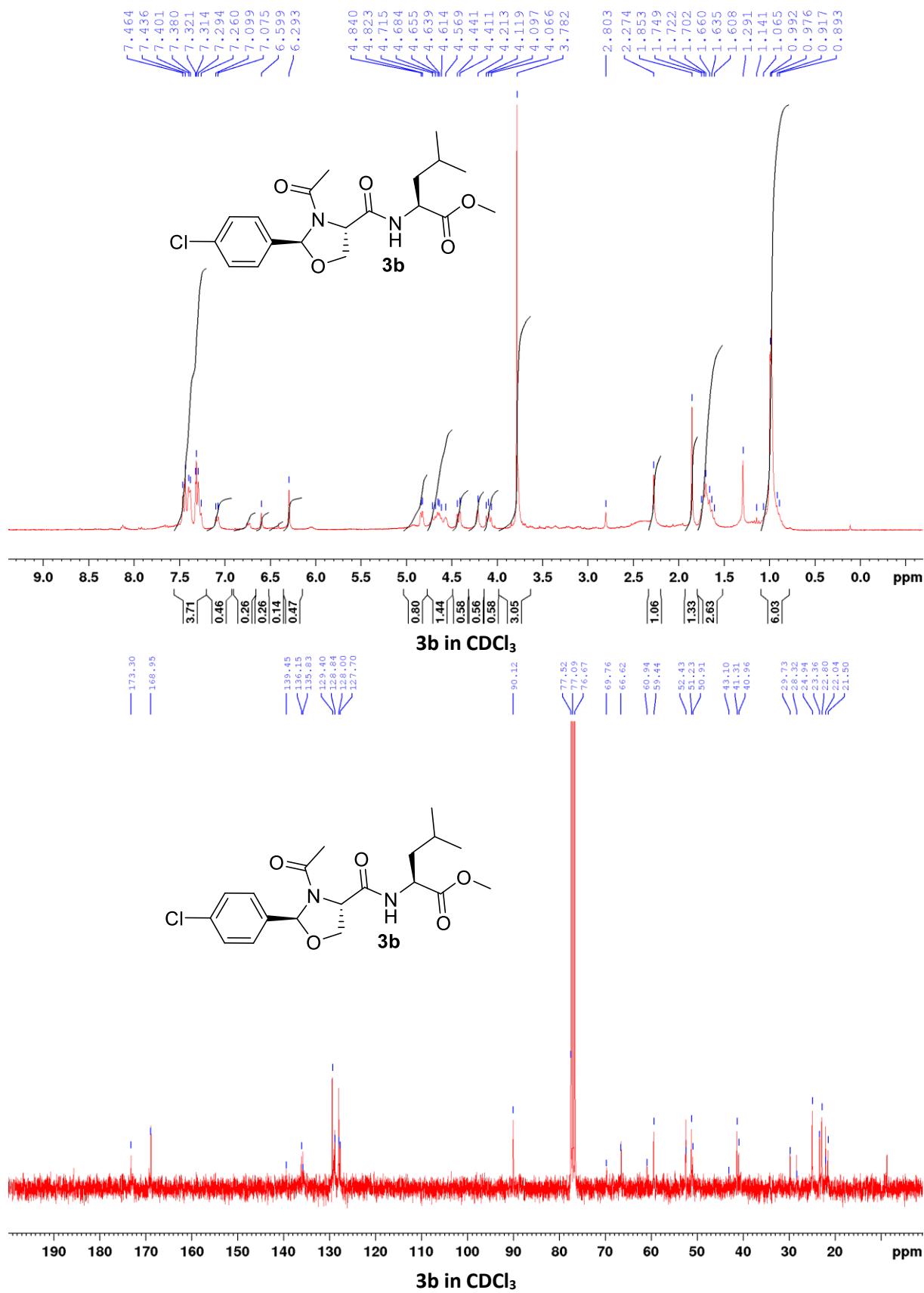
**Figure 16**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound 9.



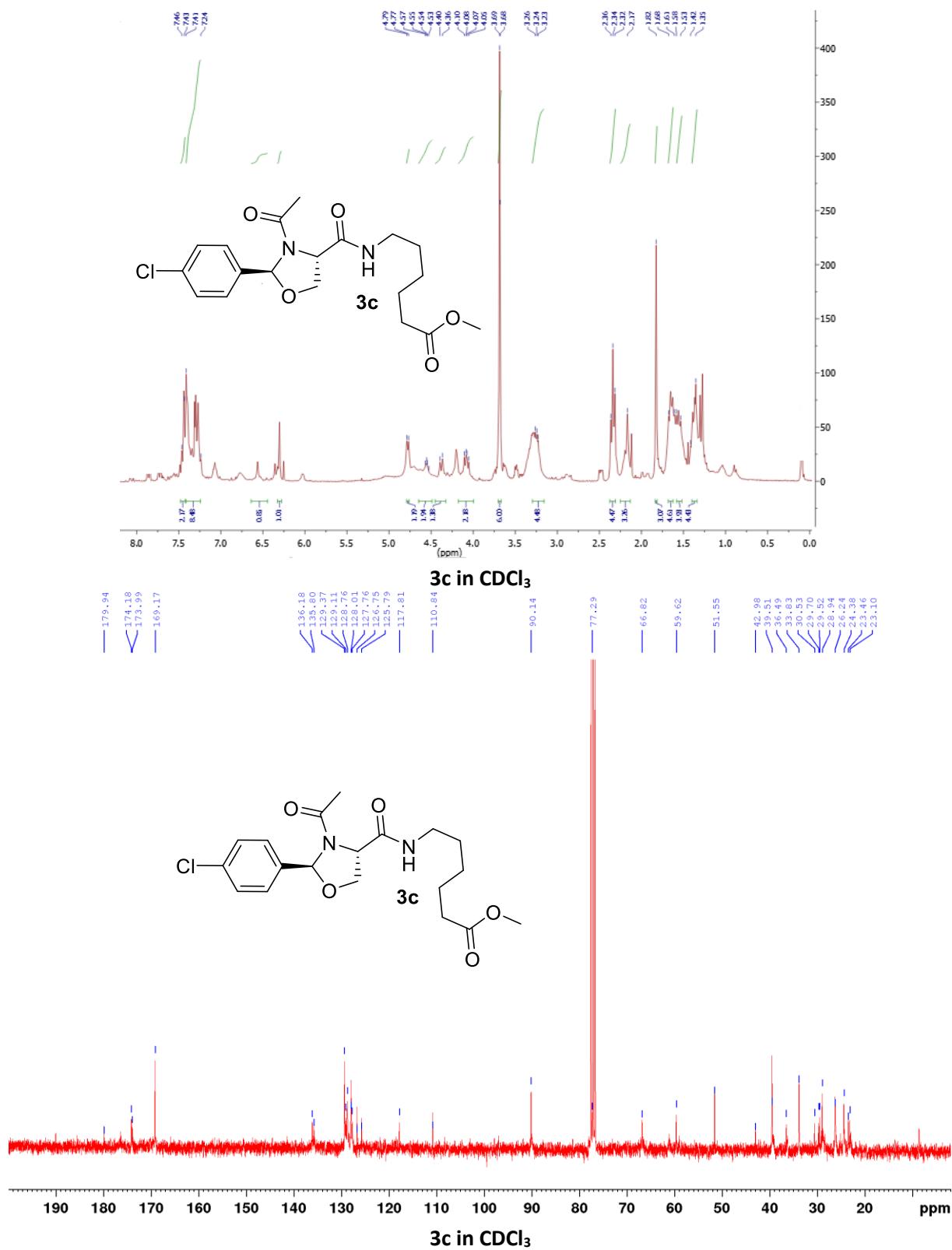
**Figure 17**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound **11**.



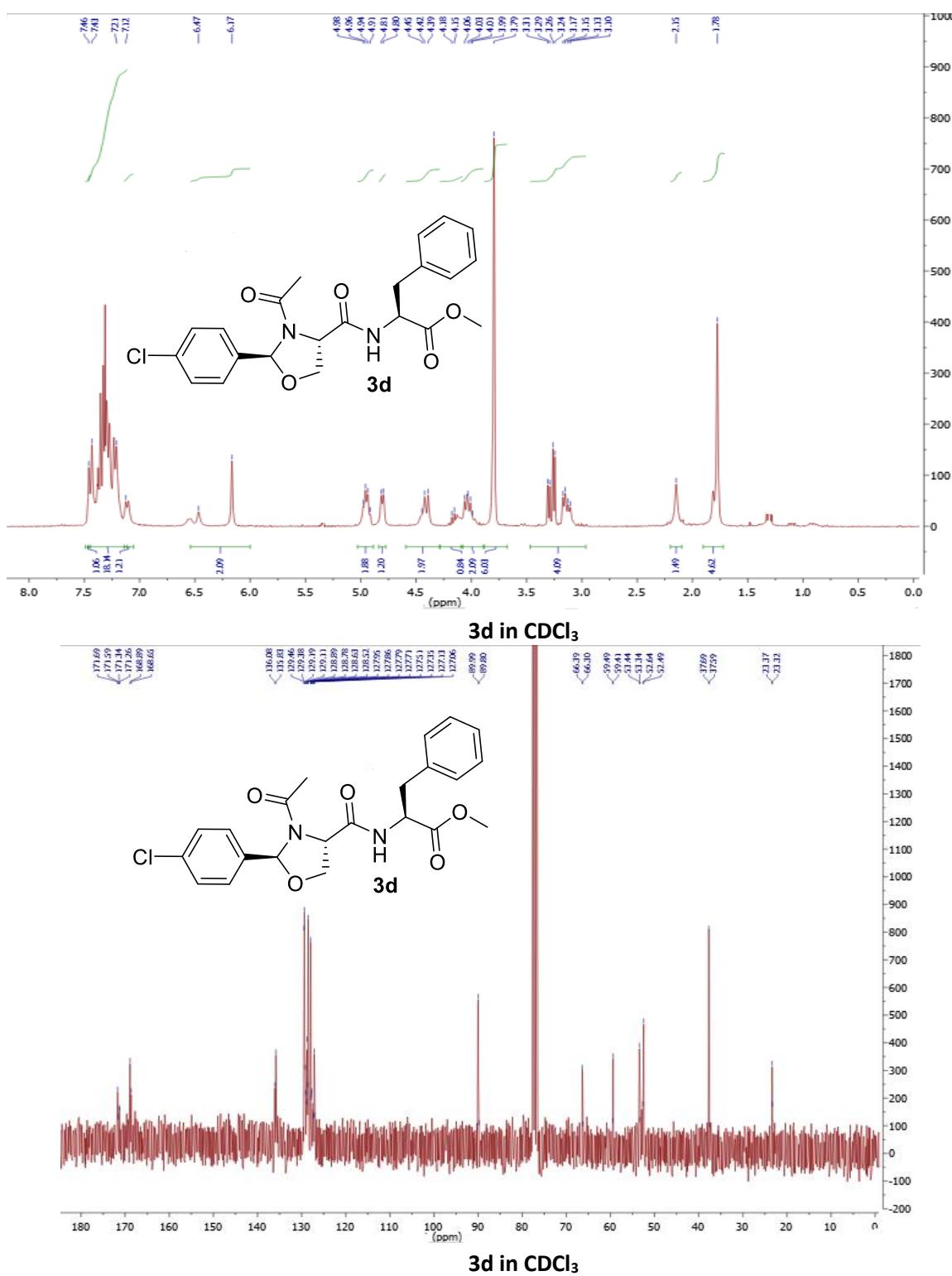
**Figure 18**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound 3a.

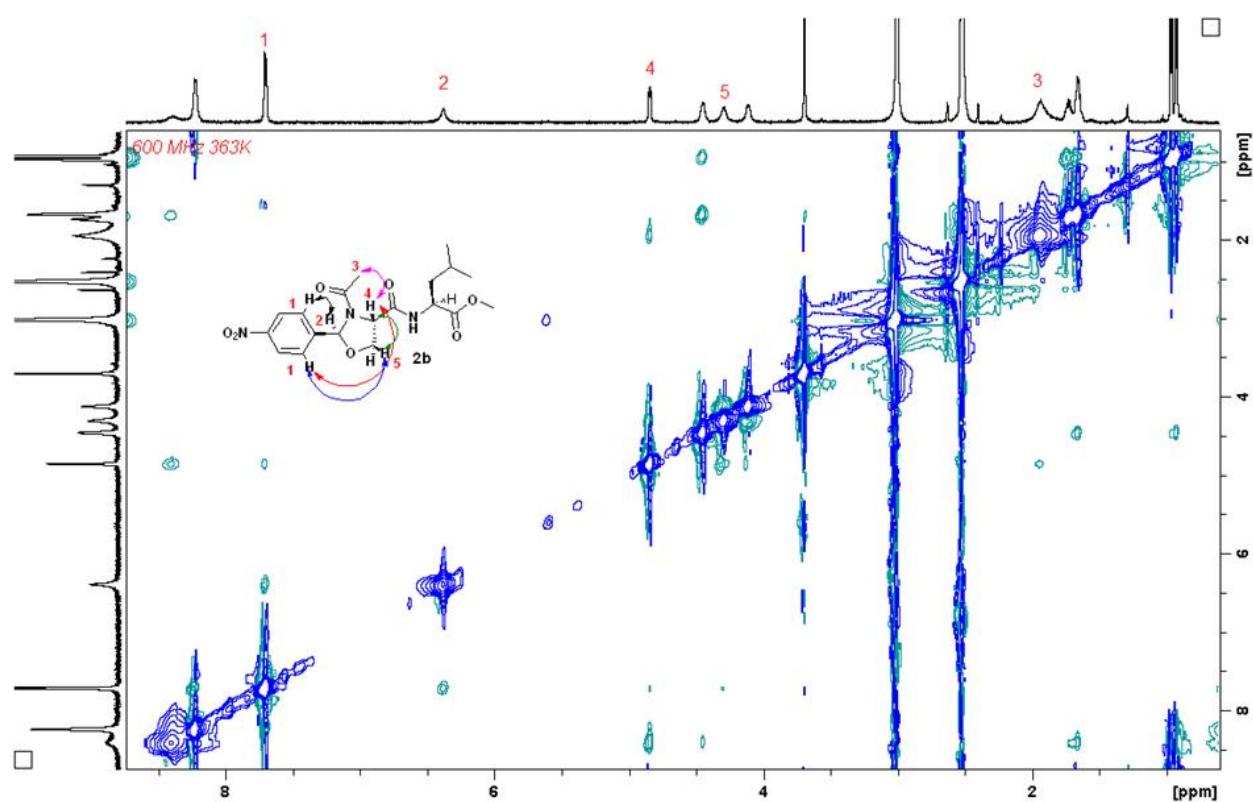


**Figure 19**  $^1\text{H}$  and  $^{13}\text{C}$  NMR of compound **3b**.

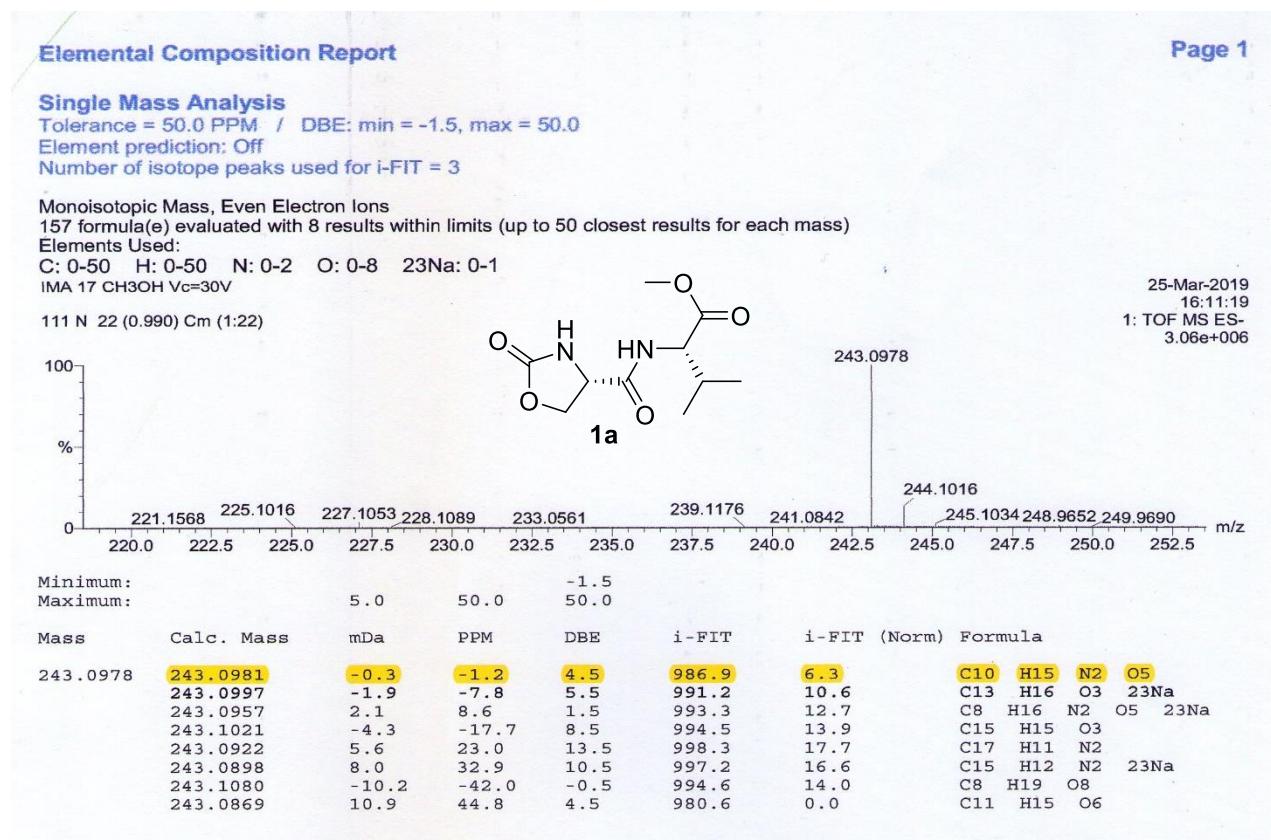
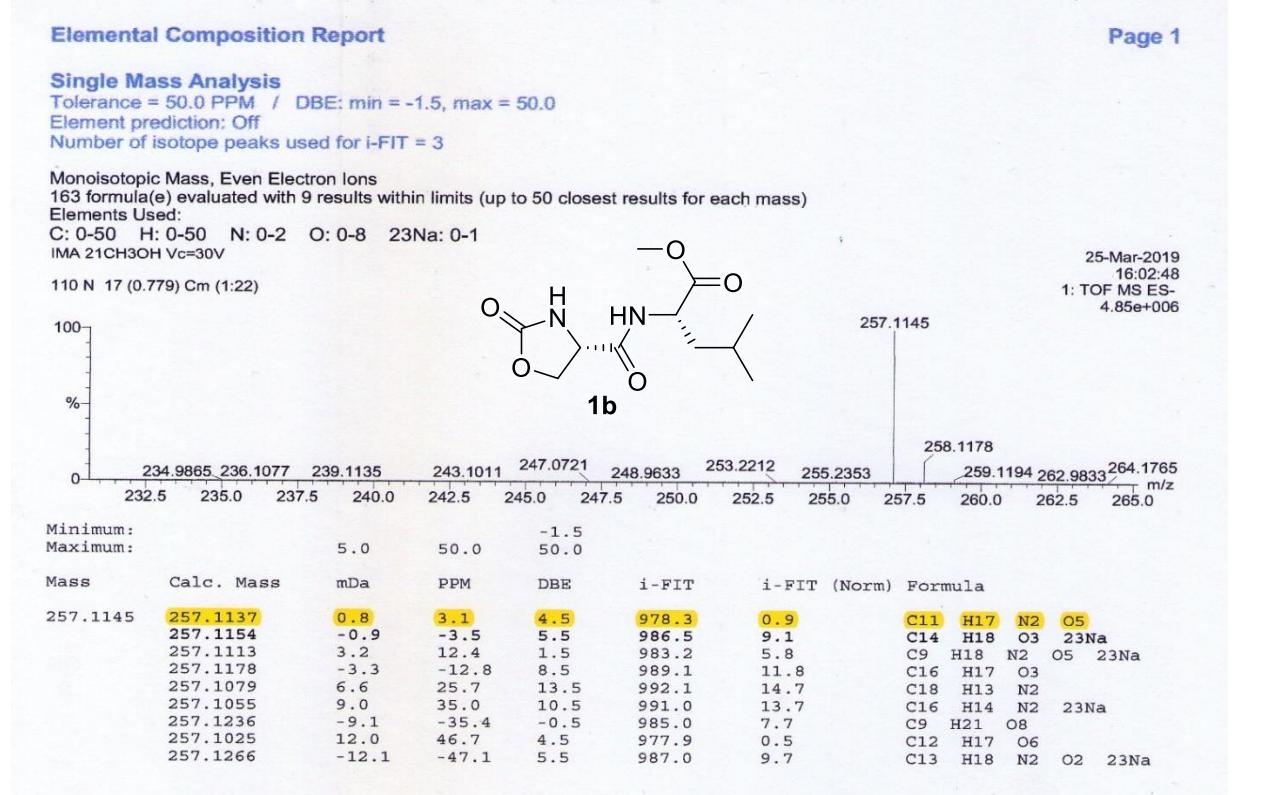


**Figure 20** <sup>1</sup>H and <sup>13</sup>C NMR of compound **3c**.





**Figure 22** nOe of compound **2b**.

**Figure 23 HRMS of compound 1a (IMA 17)****Figure 24 HRMS of compound 1b (IMA 21)**

## Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

163 formula(e) evaluated with 9 results within limits (up to 50 closest results for each mass)

Elements Used:

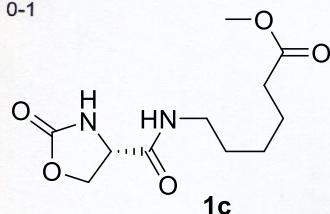
C: 0-50 H: 0-50 N: 0-2 O: 0-8 23Na: 0-1

IMA 24 CH<sub>3</sub>OH Vc=30V

109 N 15 (0.671) Cm (1:15)

100 %

0 234.9877 239.1187 242.9495 243.9496 247.5 250.0 252.5 255.2375 257.5 260.0 262.5 m/z



257.1144

258.1180

 25-Mar-2019  
 15:53:09  
 1: TOF MS ES-  
 3.30e+006

 Minimum:  
 Maximum: 5.0 50.0 -1.5 50.0

Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

257.1144	257.1137	0.7	2.7	4.5	884.2	3.5	C11 H17 N2 O5
	257.1154	-1.0	-3.9	5.5	891.0	10.3	C14 H18 O3 23Na
	257.1113	3.1	12.1	1.5	889.6	8.9	C9 H18 N2 O5 23Na
	257.1178	-3.4	-13.2	8.5	893.8	13.1	C16 H17 O3
	257.1079	6.5	25.3	13.5	897.0	16.4	C18 H13 N2
	257.1055	8.9	34.6	10.5	896.0	15.3	C16 H14 N2 23Na
	257.1236	-9.2	-35.8	-0.5	890.8	10.1	C9 H21 O8
	257.1025	11.9	46.3	4.5	880.7	0.0	C12 H17 O6
	257.1266	-12.2	-47.4	5.5	892.0	11.3	C13 H18 N2 O2 23Na

Figure 25 HRMS of compound 1c (IMA 24)

## Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

203 formula(e) evaluated with 14 results within limits (up to 50 closest results for each mass)

Elements Used:

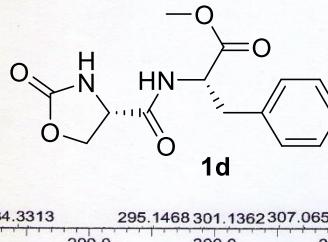
C: 0-50 H: 0-50 N: 0-2 O: 0-8 23Na: 0-1

IMA 27 CH<sub>3</sub>OH Vc=30V

108 P 41 (1.811) Cm (35:41)

100 %

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315.0956

316.0983 327.0841

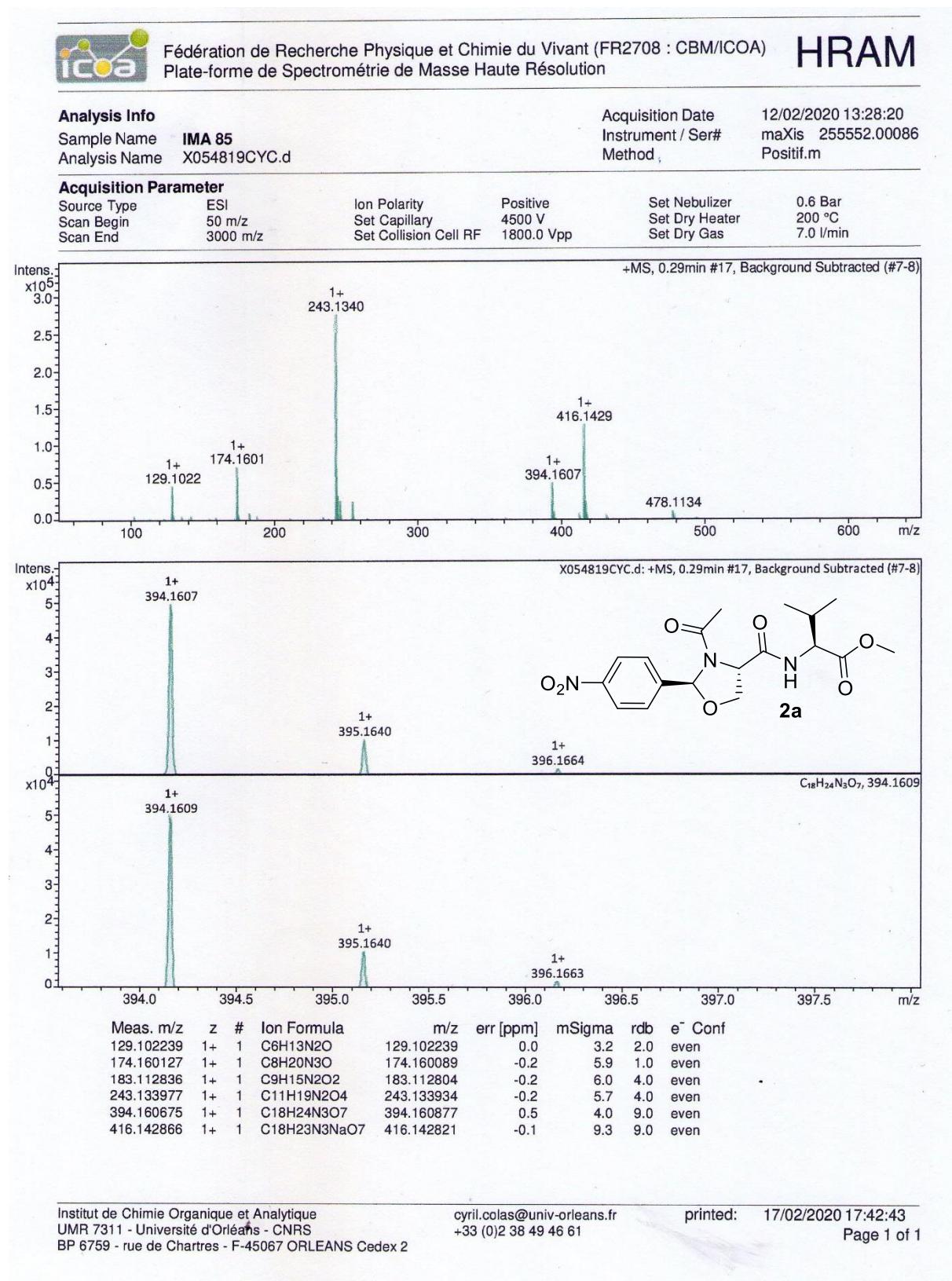
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 Minimum:  
 Maximum: 5.0 50.0 -1.5 50.0

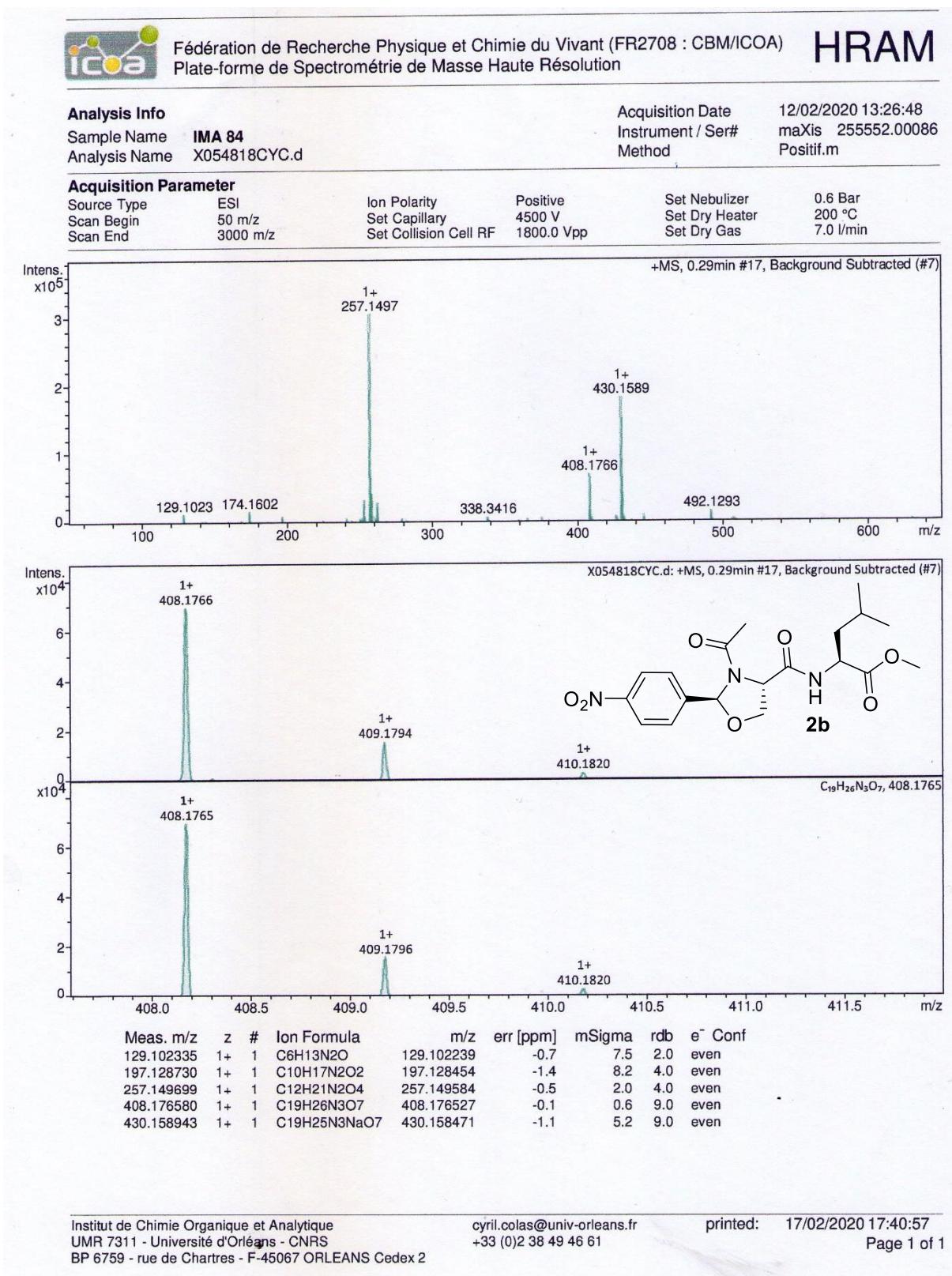
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

315.0956	315.0957	-0.1	-0.3	7.5	668.4	1.6	C14 H16 N2 O5 23Na
	315.0981	-2.5	-7.9	10.5	667.9	1.1	C16 H15 N2 O5
	315.0922	3.4	10.8	19.5	675.7	8.9	C23 H11 N2
	315.0997	-4.1	-13.0	11.5	672.7	5.9	C19 H16 O3 23Na
	315.0898	5.8	18.4	16.5	674.9	8.1	C21 H12 N2 23Na
	315.1021	-6.5	-20.6	14.5	674.8	8.0	C21 H15 O3
	315.0869	8.7	27.6	10.5	670.2	3.4	C17 H15 O6
	315.1056	-10.0	-31.7	2.5	674.4	7.6	C12 H20 O8 23Na
	315.0845	11.1	35.2	7.5	667.7	0.9	C15 H16 O6 23Na
	315.1080	-12.4	-39.4	5.5	670.6	3.8	C14 H19 O8
	315.0828	12.8	40.6	6.5	673.5	6.7	C12 H15 N2 O8
	315.0810	14.6	46.3	19.5	678.2	11.4	C24 H11 O
	315.0804	15.2	48.2	3.5	676.5	9.7	C10 H16 N2 O8 23Na
	315.1109	-15.3	-48.6	11.5	673.9	7.1	C18 H16 N2 O2 23Na

Figure 26 HRMS of compound 1d (IMA 27)



**Figure 27** HRMS of compound **2a** (IMA 85)



**Figure 28** HRMS of compound **2b** (IMA 84)



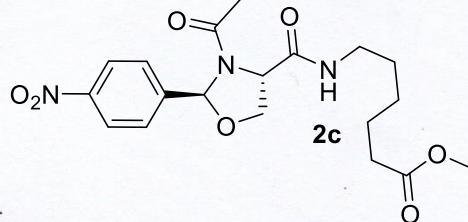
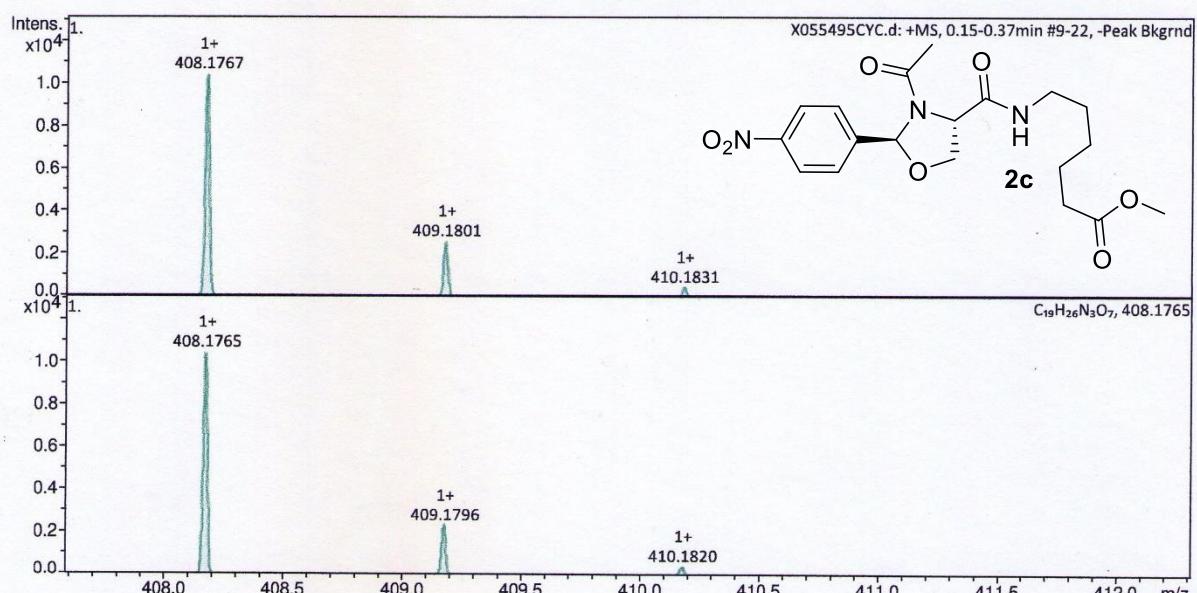
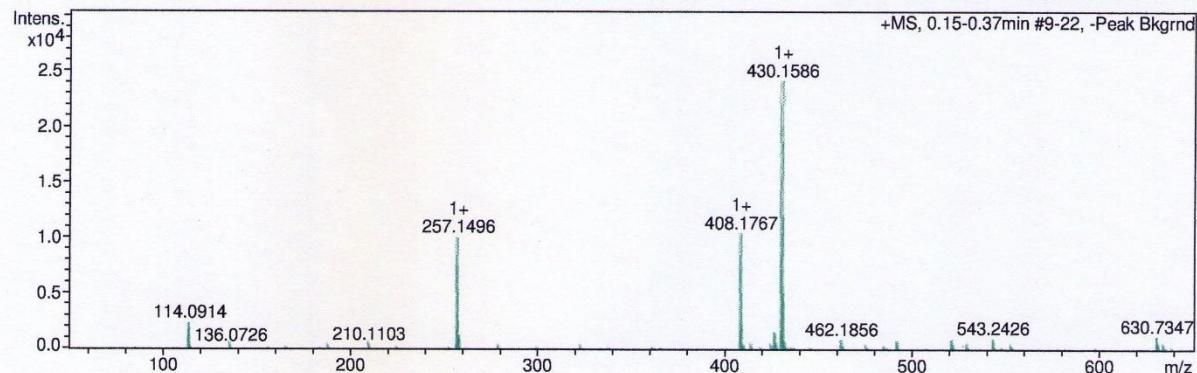
**Analysis Info**

Sample Name **IMA 92**  
Analysis Name X055495CYC.d

Acquisition Date 11/03/2020 19:09:56  
Instrument / Ser# maXis 255552.00086  
Method Positif.m

**Acquisition Parameter**

Source Type ESI	Ion Polarity Positive	Set Nebulizer 0.6 Bar
Scan Begin 50 m/z	Set Capillary 4500 V	Set Dry Heater 200 °C
Scan End 3000 m/z	Set Collision Cell RF 1800.0 Vpp	Set Dry Gas 7.0 l/min



Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf
114.091351	1+	1	C <sub>6</sub> H <sub>12</sub> NO	114.091340	-0.1	n.a.	2.0	even
257.149626	1+	1	C <sub>12</sub> H <sub>21</sub> N <sub>2</sub> O <sub>4</sub>	257.149584	-0.2	4.5	4.0	even
408.176650	1+	1	C <sub>19</sub> H <sub>26</sub> N <sub>3</sub> O <sub>7</sub>	408.176527	-0.3	15.2	9.0	even
430.158599	1+	1	C <sub>19</sub> H <sub>25</sub> N <sub>3</sub> NaO <sub>7</sub>	430.158471	-0.3	12.4	9.0	even

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**Figure 29 HRMS of compound 2c (IMA 92)**



Fédération de Recherche Physique et Chimie du Vivant (FR2708 : CBM/ICOA)  
Plate-forme de Spectrométrie de Masse Haute Résolution

HRAM

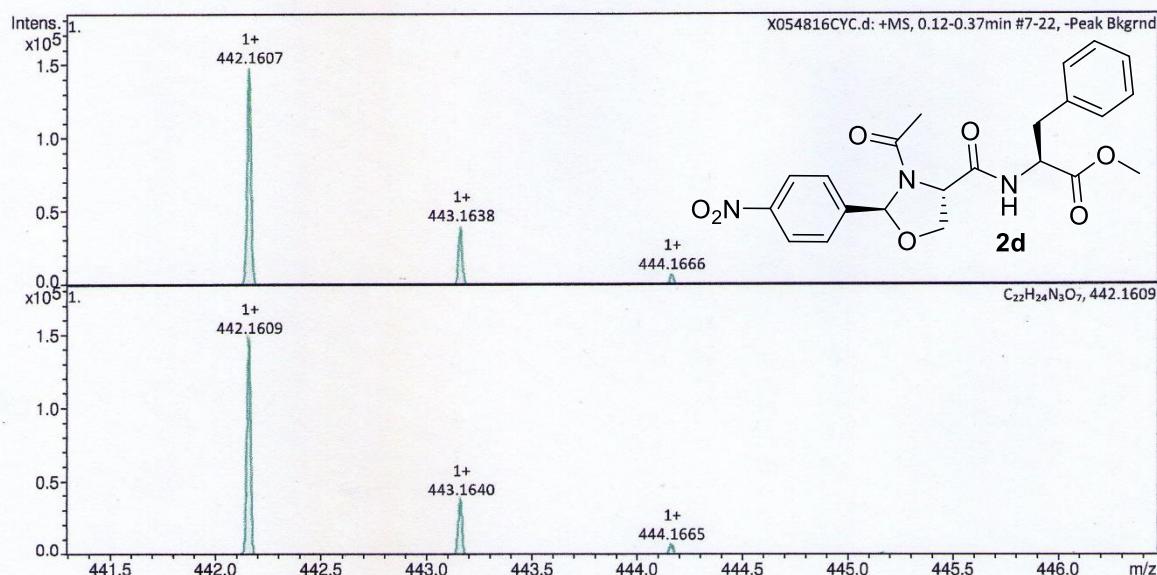
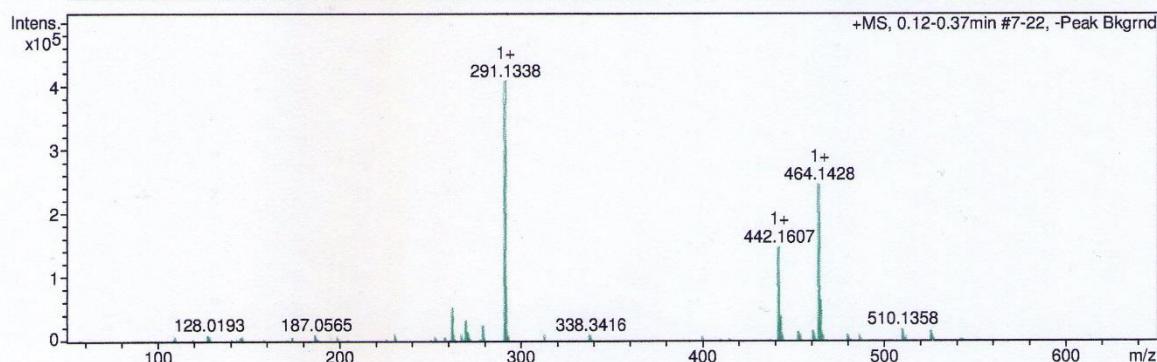
**Analysis Info**

Sample Name **IMA 67**  
Analysis Name X054816CYC.d

Acquisition Date 12/02/2020 13:23:46  
Instrument / Ser# maXis 255552.00086  
Method Positif.m

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan End	3000 m/z	Set Collision Cell RF	1800.0 Vpp	Set Dry Gas	7.0 l/min



Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf
291.133758	1+	1	C <sub>15</sub> H <sub>19</sub> N <sub>2</sub> O <sub>4</sub>	291.133934	0.6	11.2	8.0	even
442.160672	1+	1	C <sub>22</sub> H <sub>24</sub> N <sub>3</sub> O <sub>7</sub>	442.160877	0.5	7.6	13.0	even
464.142763	1+	1	C <sub>22</sub> H <sub>23</sub> N <sub>3</sub> NaO <sub>7</sub>	464.142821	0.1	6.5	13.0	even

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**Figure 30 HRMS of compound 2d (IMA 67)**



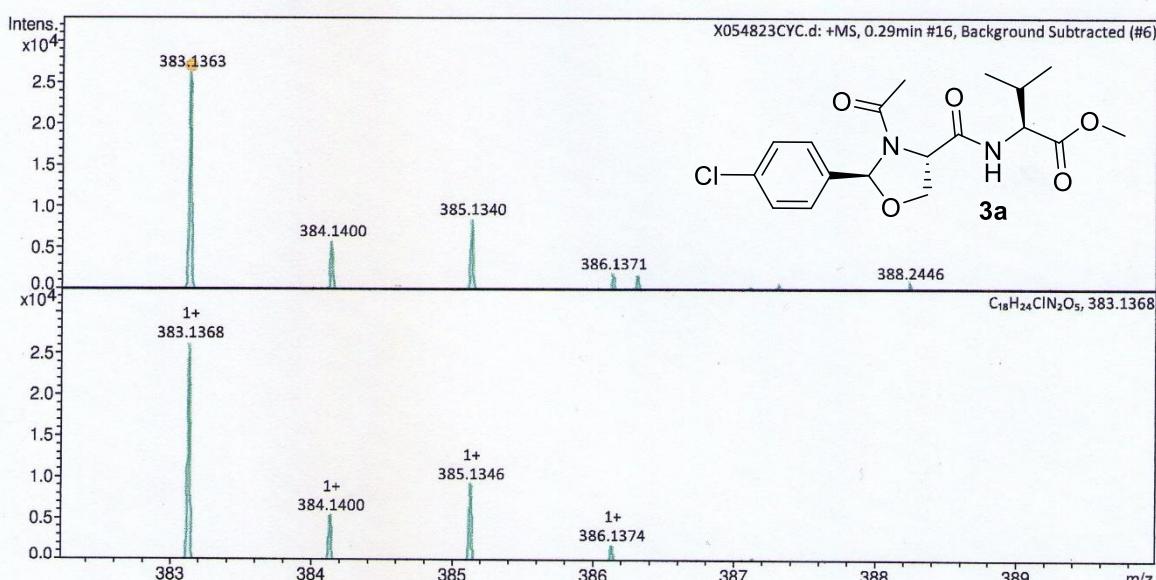
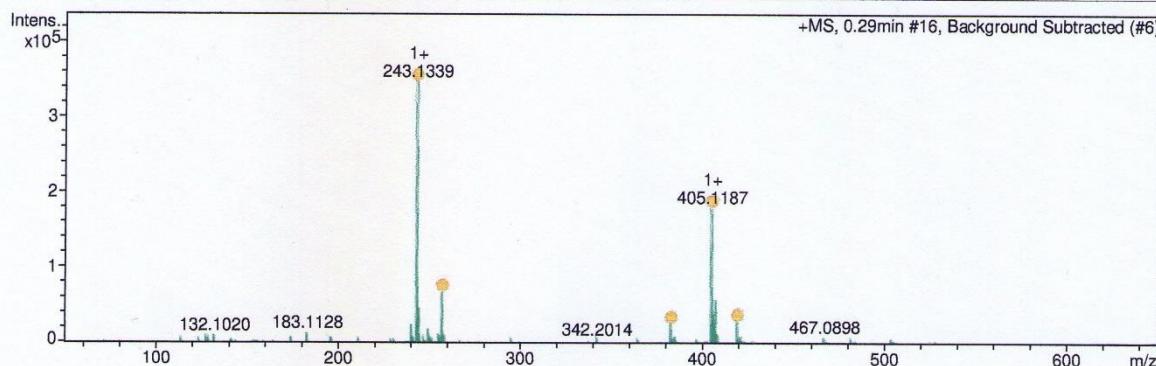
**Analysis Info**

Sample Name **IMA 95**  
Analysis Name X054823CYC.d

Acquisition Date 12/02/2020 13:38:05  
Instrument / Ser# maXis 255552.00086  
Method Positif.m

**Acquisition Parameter**

Source Type ESI	Ion Polarity Positive	Set Nebulizer 0.6 Bar
Scan Begin 50 m/z	Set Capillary 4500 V	Set Dry Heater 200 °C
Scan End 3000 m/z	Set Collision Cell RF 1800.0 Vpp	Set Dry Gas 7.0 l/min



Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf
243.133936	1+	1	C11H19N2O4	243.133934	-0.0	2.4	4.0	even
257.149485	1+	1	C12H21N2O4	257.149584	0.4	17.0	4.0	even
383.136254	1+	1	C18H24ClN2O5	383.136826	1.5	14.6	8.0	even
405.118697	1+	1	C18H23ClN2NaO5	405.118770	0.2	13.7	8.0	even
419.134152	1+	1	C19H25ClN2NaO5	419.134420	0.6	18.1	8.0	even

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**Figure 31 HRMS of compound 3a (IMA 95)**

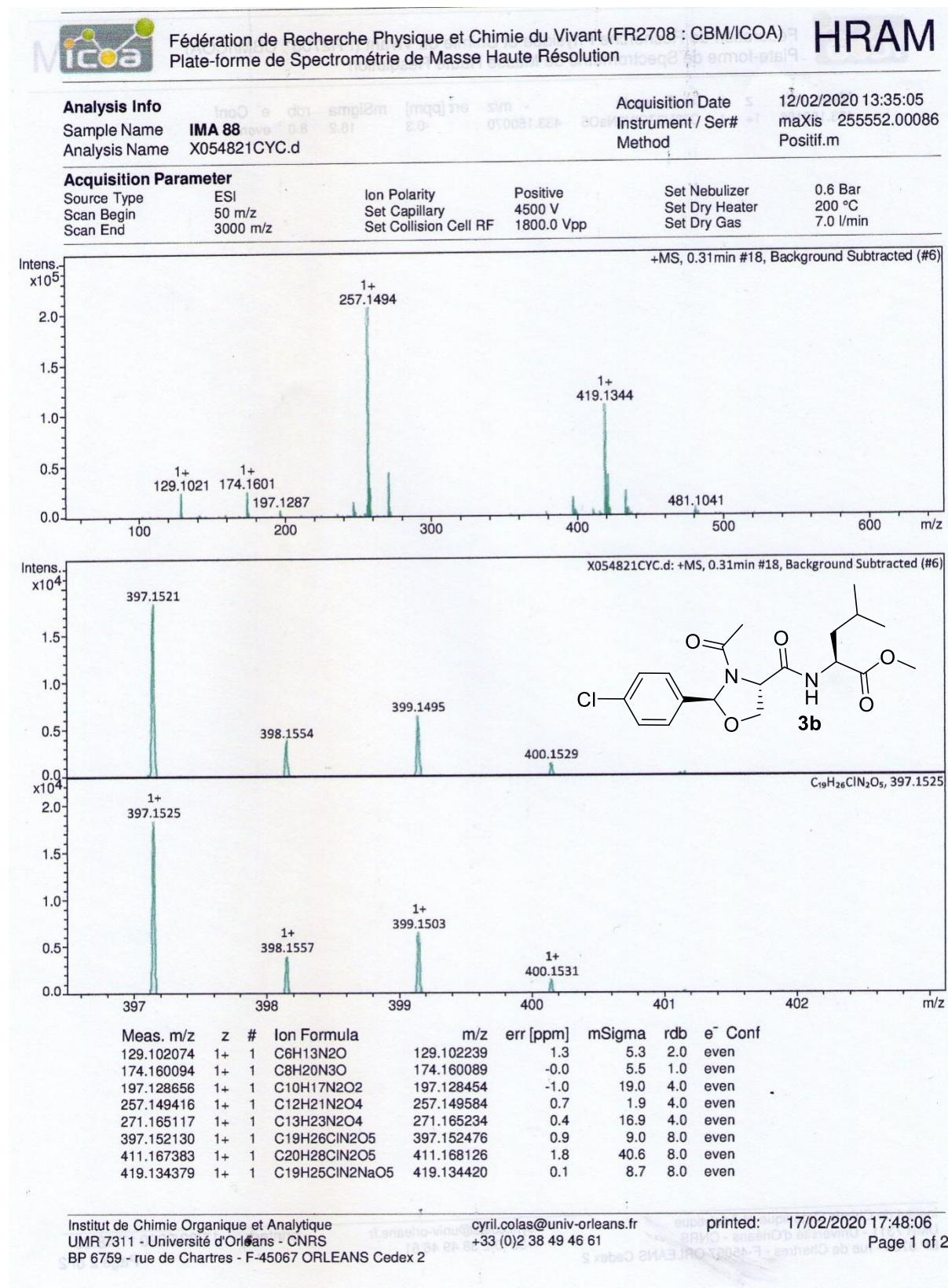
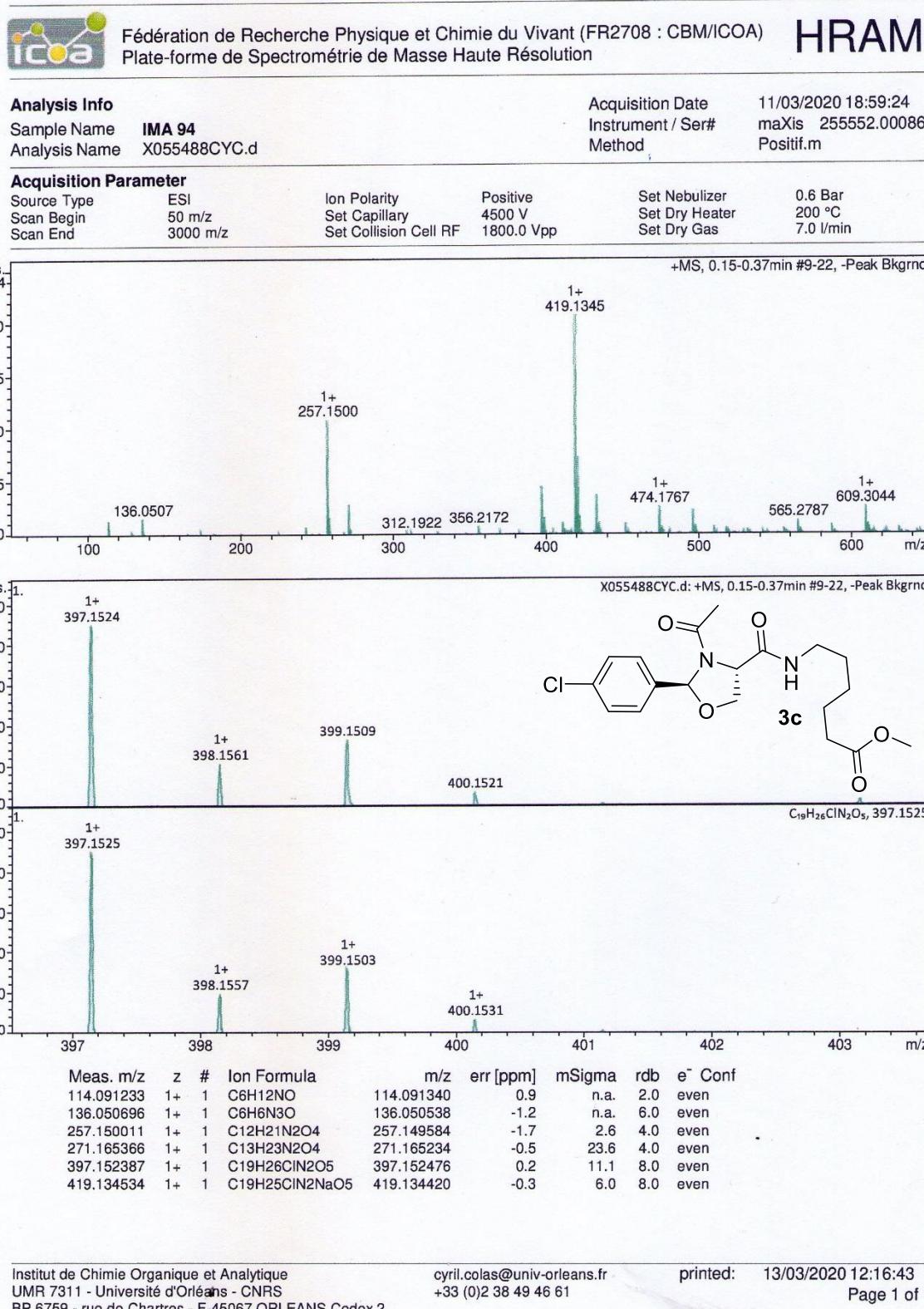


Figure 32 HRMS of compound 3b (IMA 88)



**Figure 33** HRMS of compound **3c** (IMA 94)

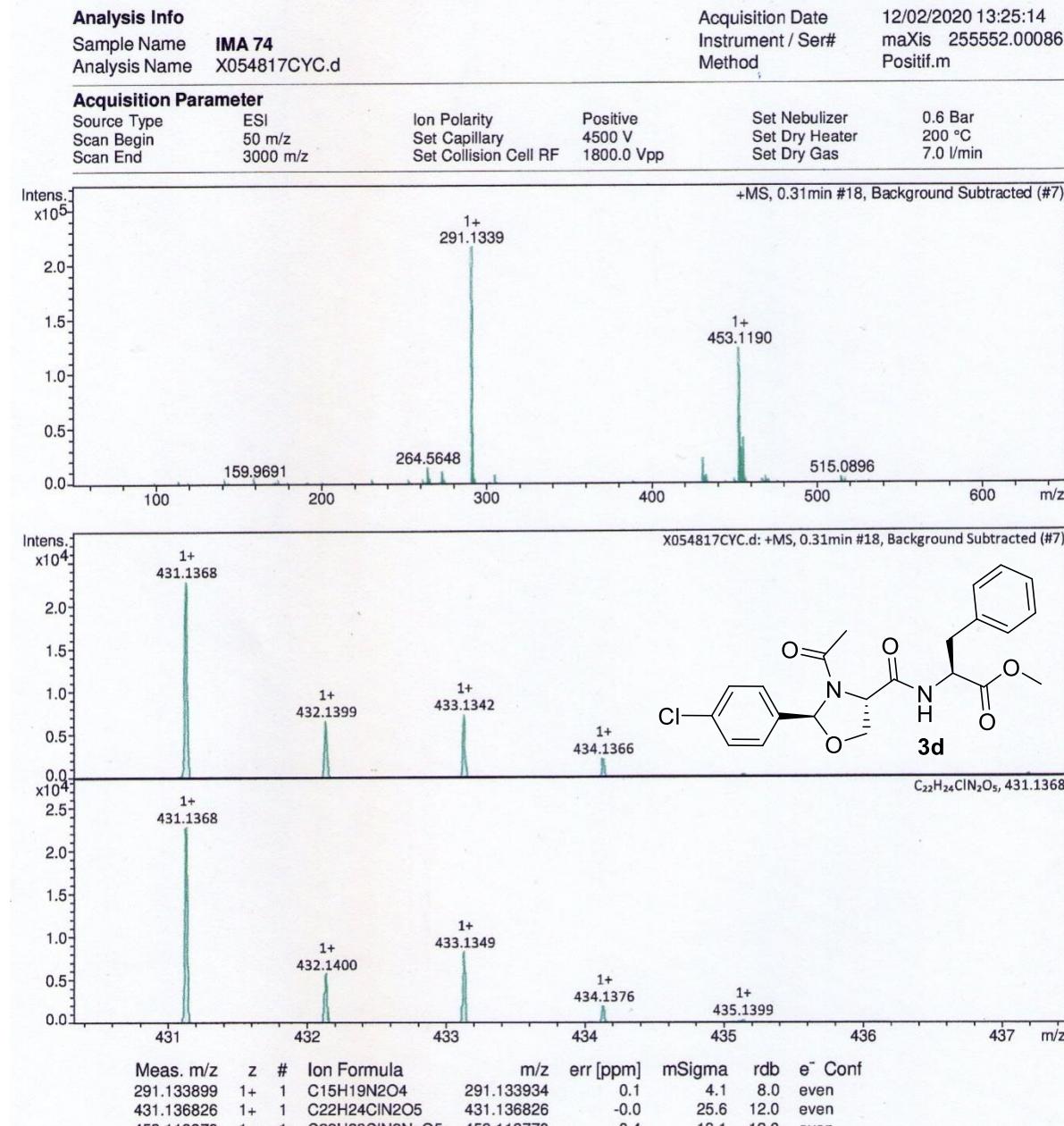


Figure 34 HRMS of compound 3d (IMA 74)