

SUPPORTING INFORMATION

Synthesis and Conformational Analysis of Hydantoin-Based Universal Peptidomimetics

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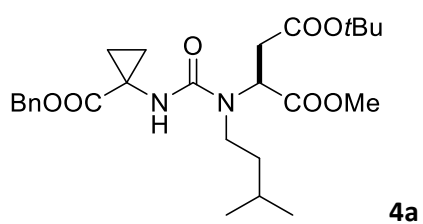
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[‡] Consiglio Nazionale delle Ricerche, Istituto di Scienze e Tecnologie Chimiche “G. Natta” (SCITEC), via Mario Bianco 9, 20131 Milan, Italy

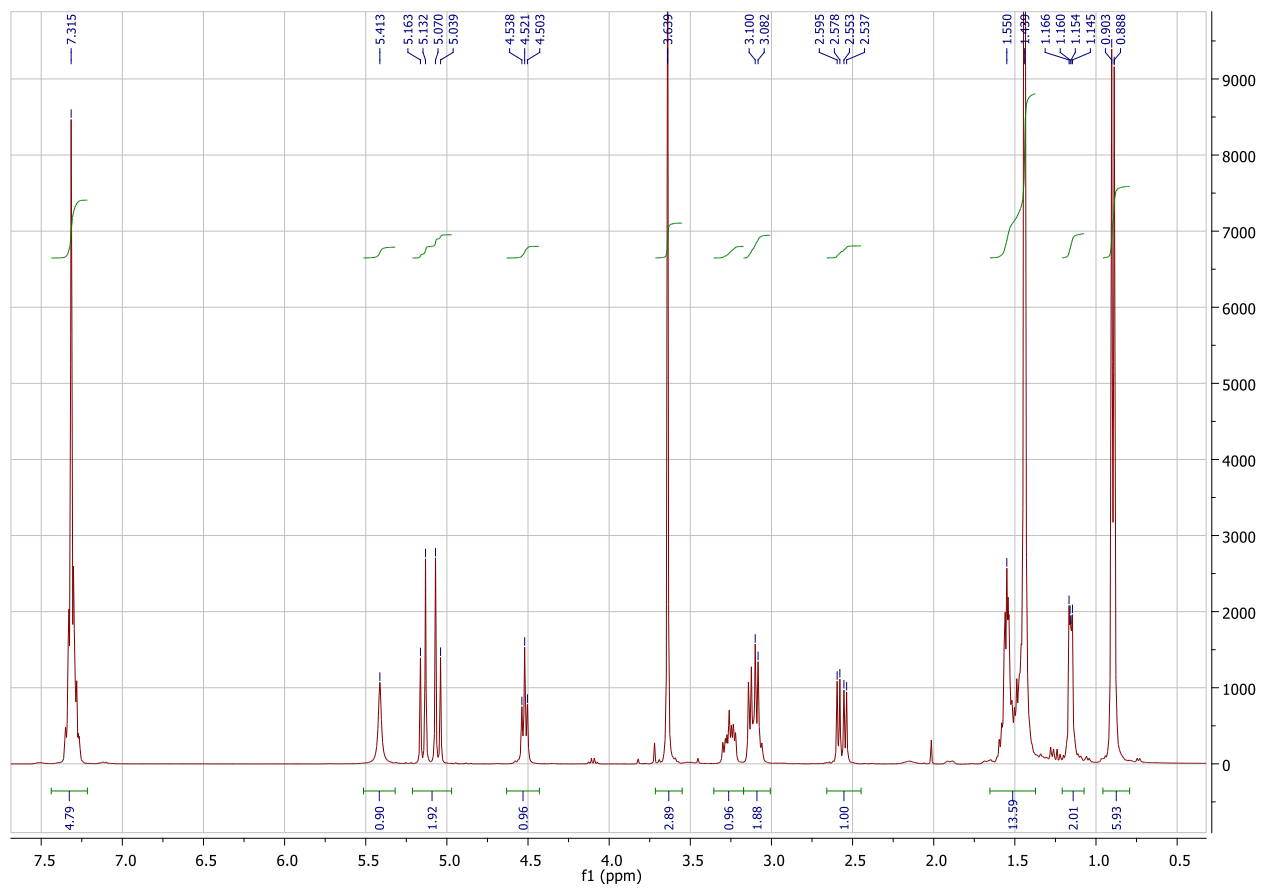
alessandro.volonterio@polimi.it; alessandro.sacchetti@polimi.it

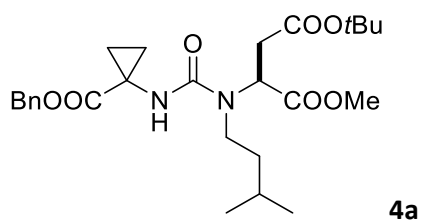
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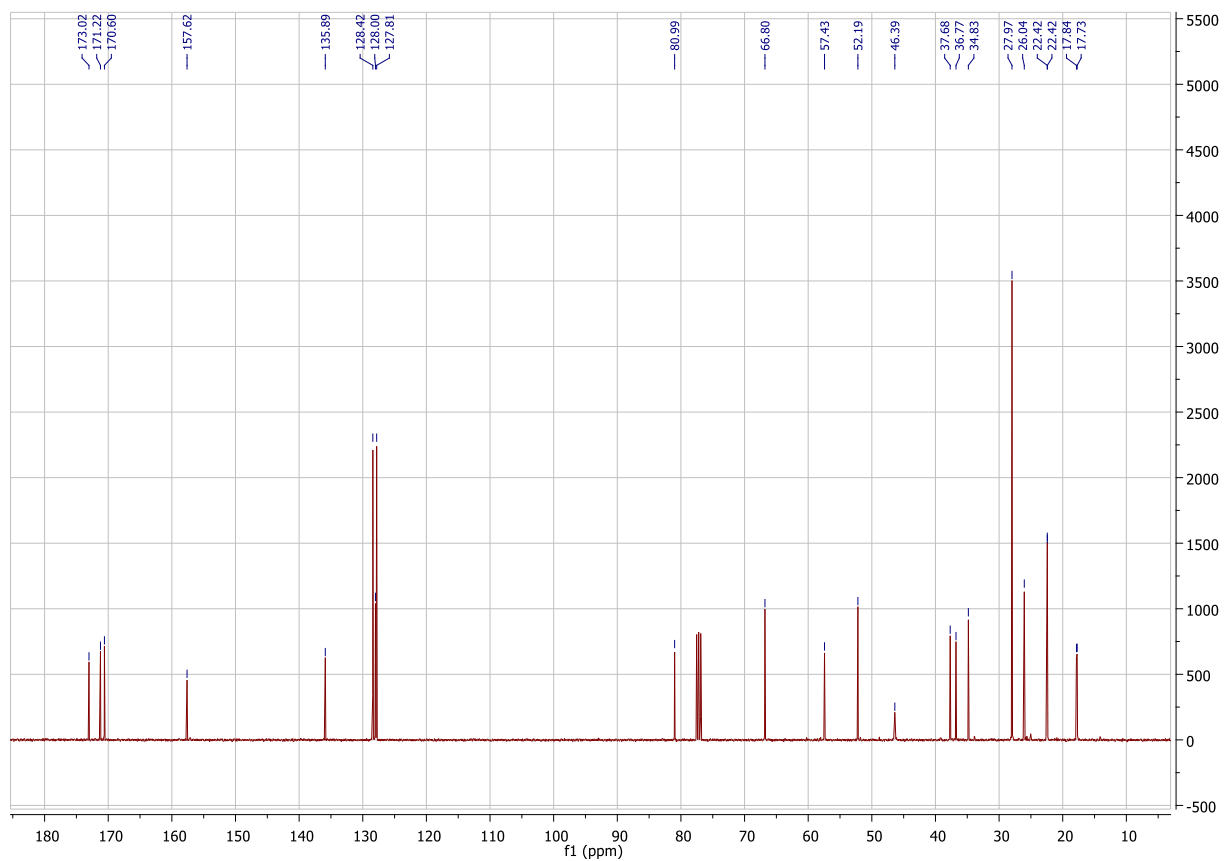


¹H-NMR (400 MHz, CDCl₃)



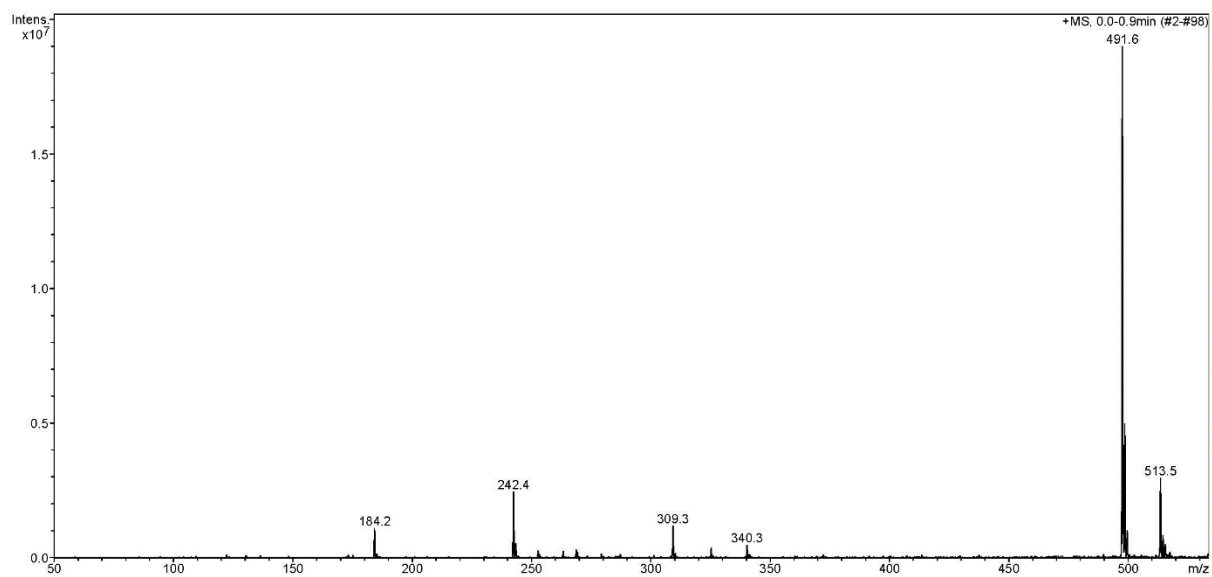


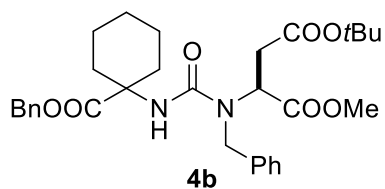
$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)



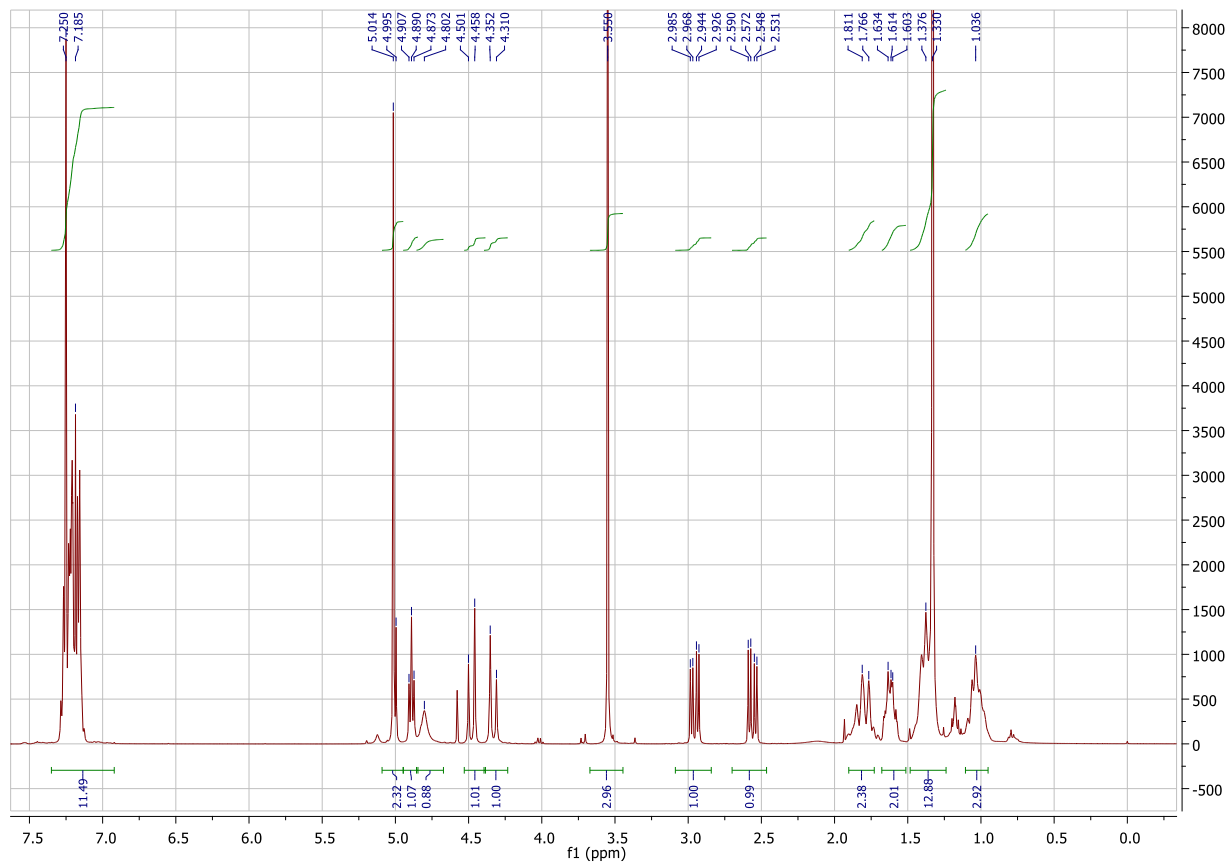
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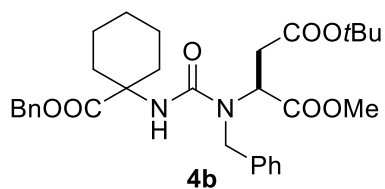
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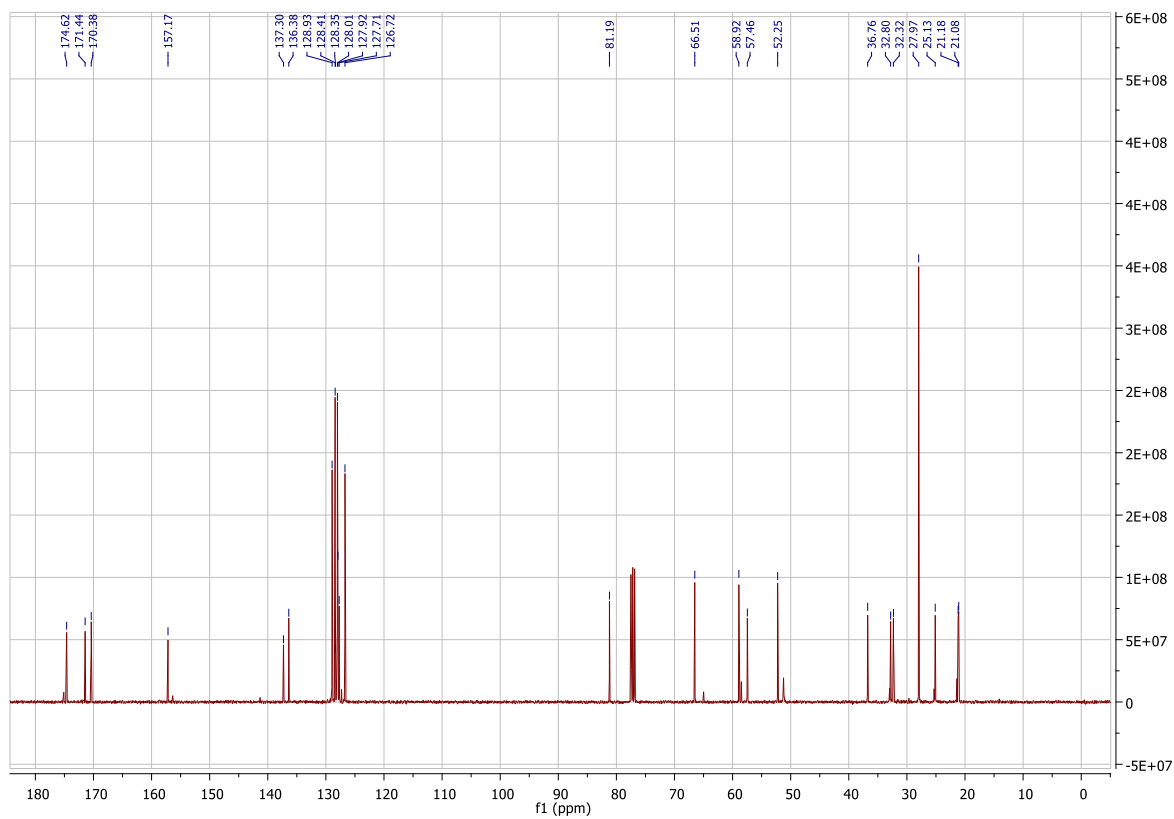


$^1\text{H-NMR}$ (400 MHz, CDCl_3)





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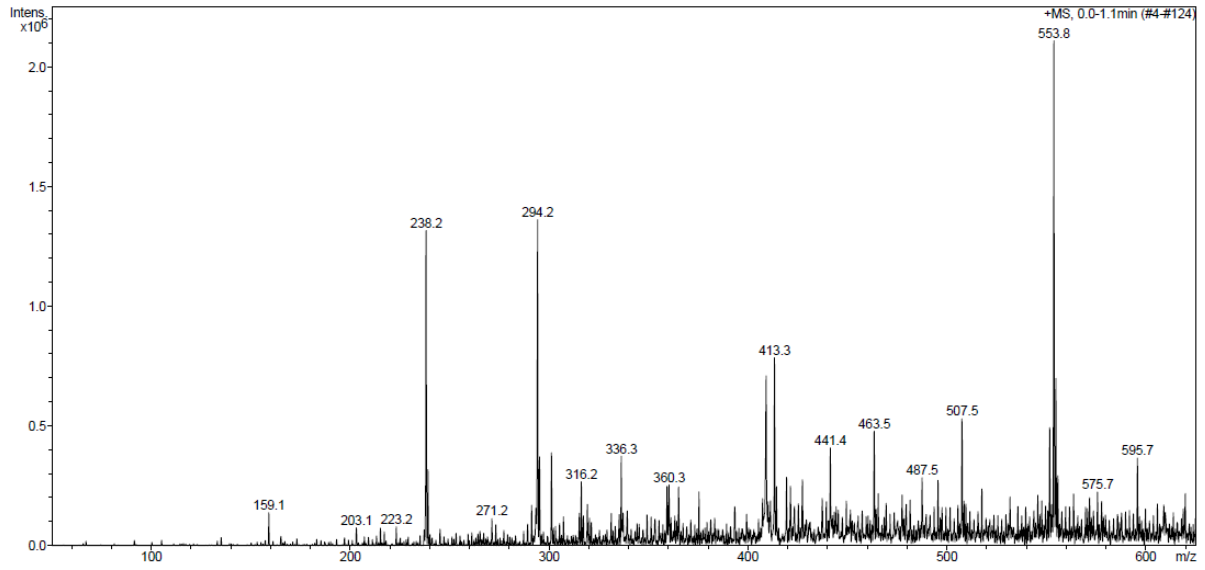


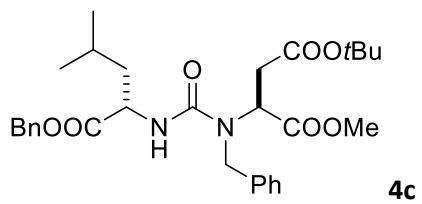
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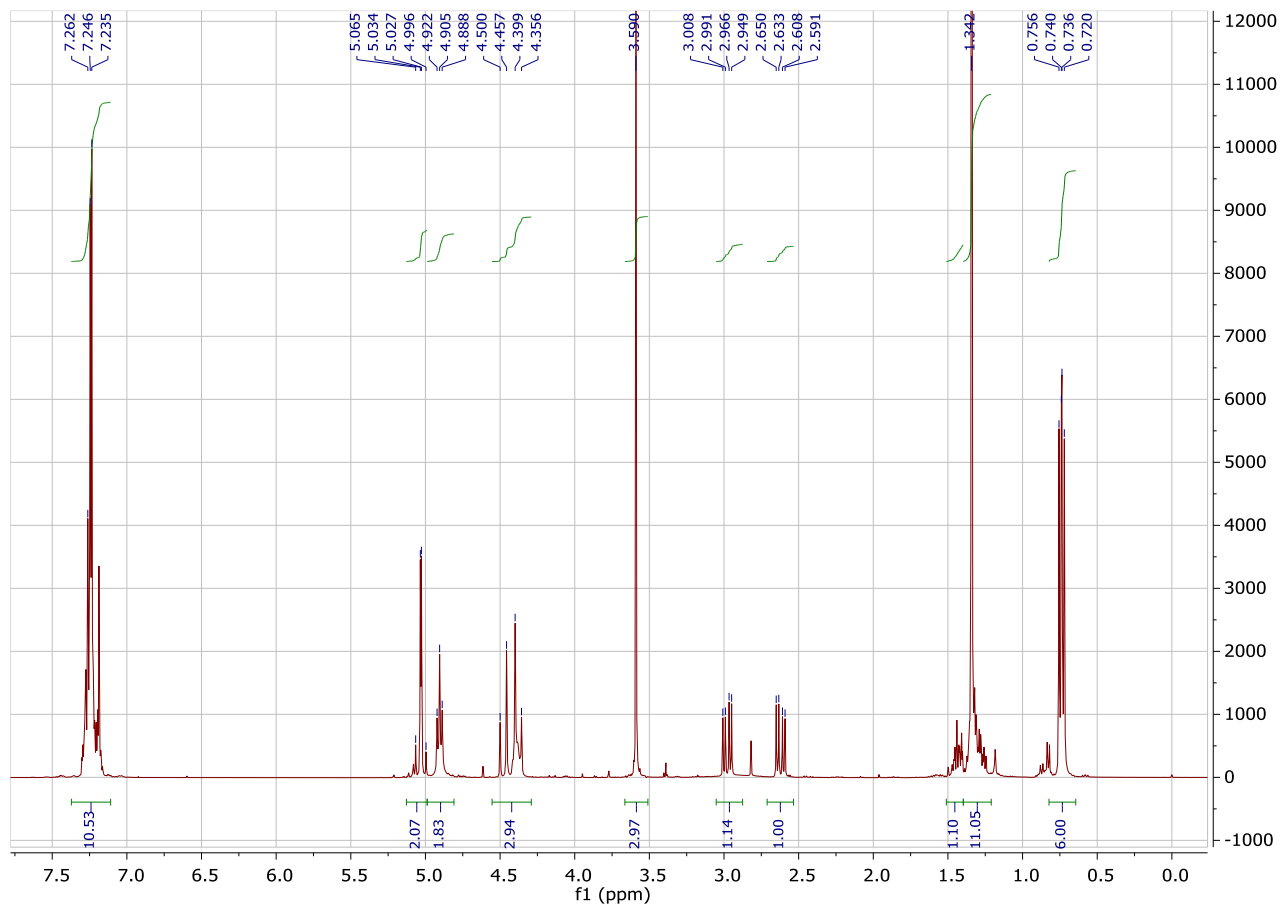
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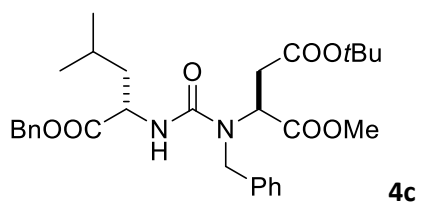
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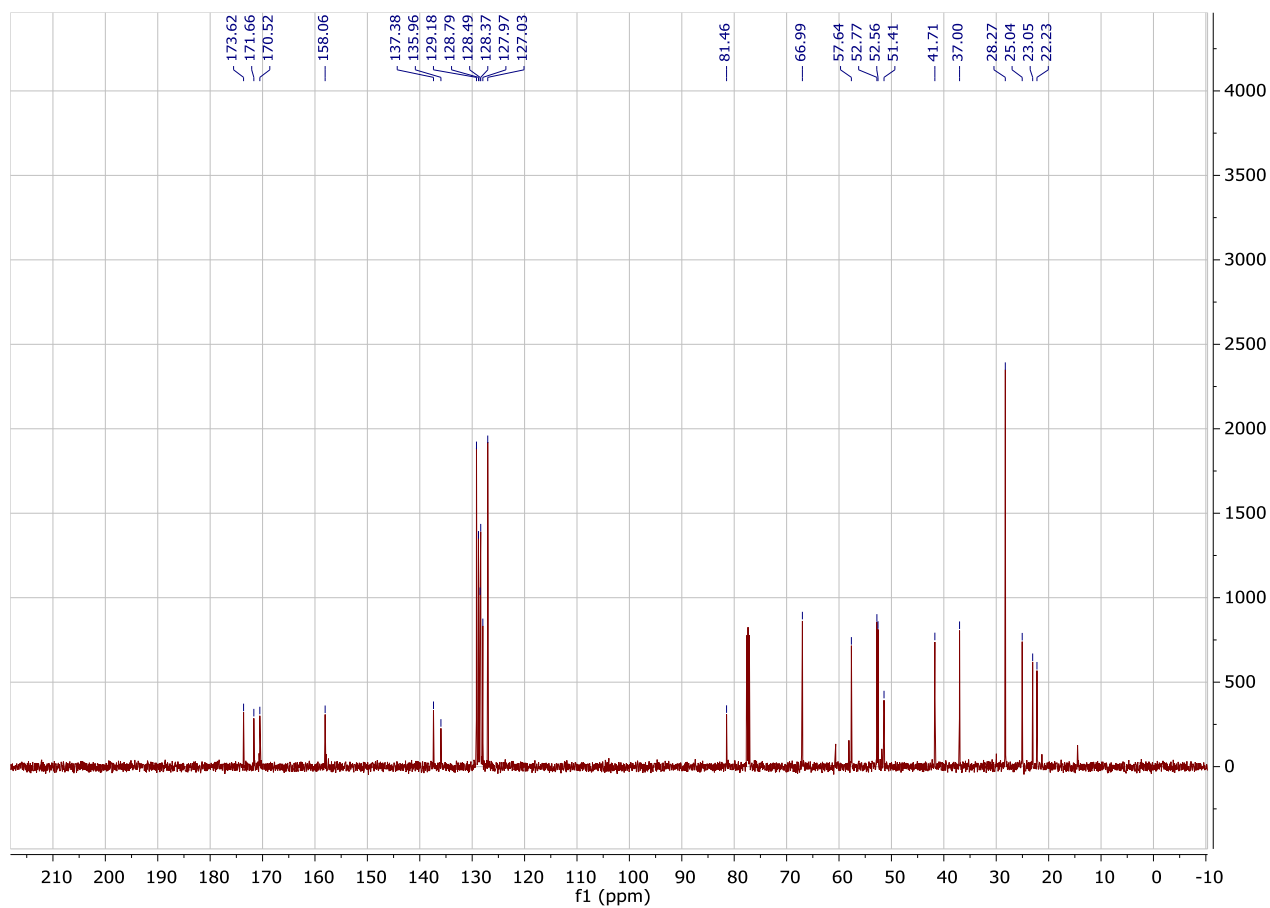


$^1\text{H-NMR}$ (400 MHz, CDCl_3)



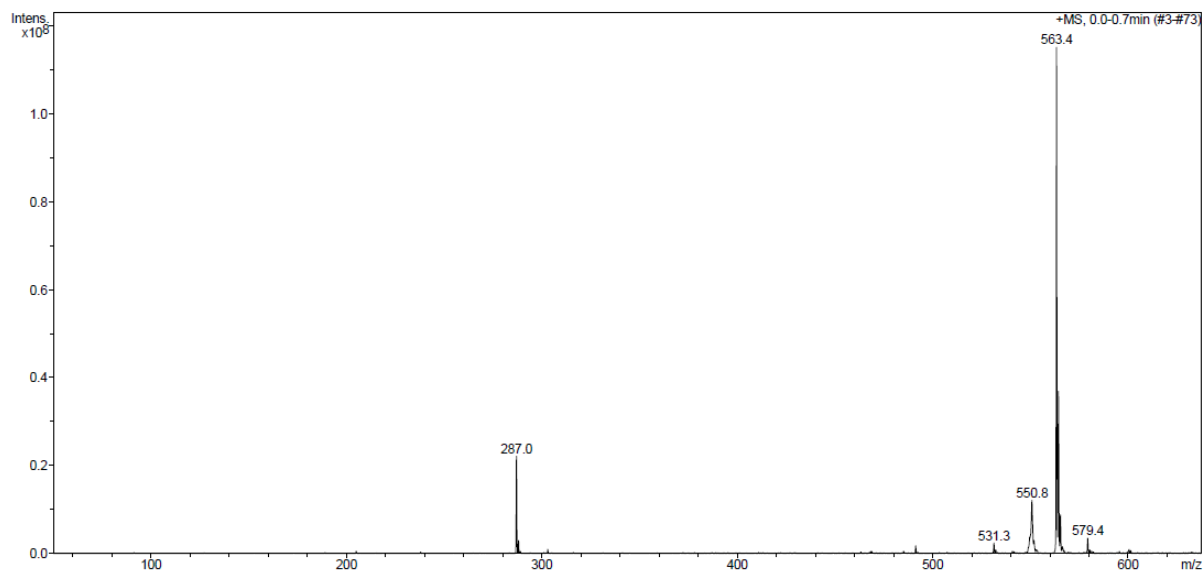


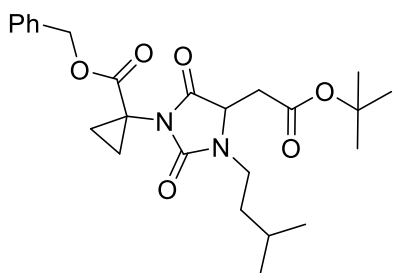
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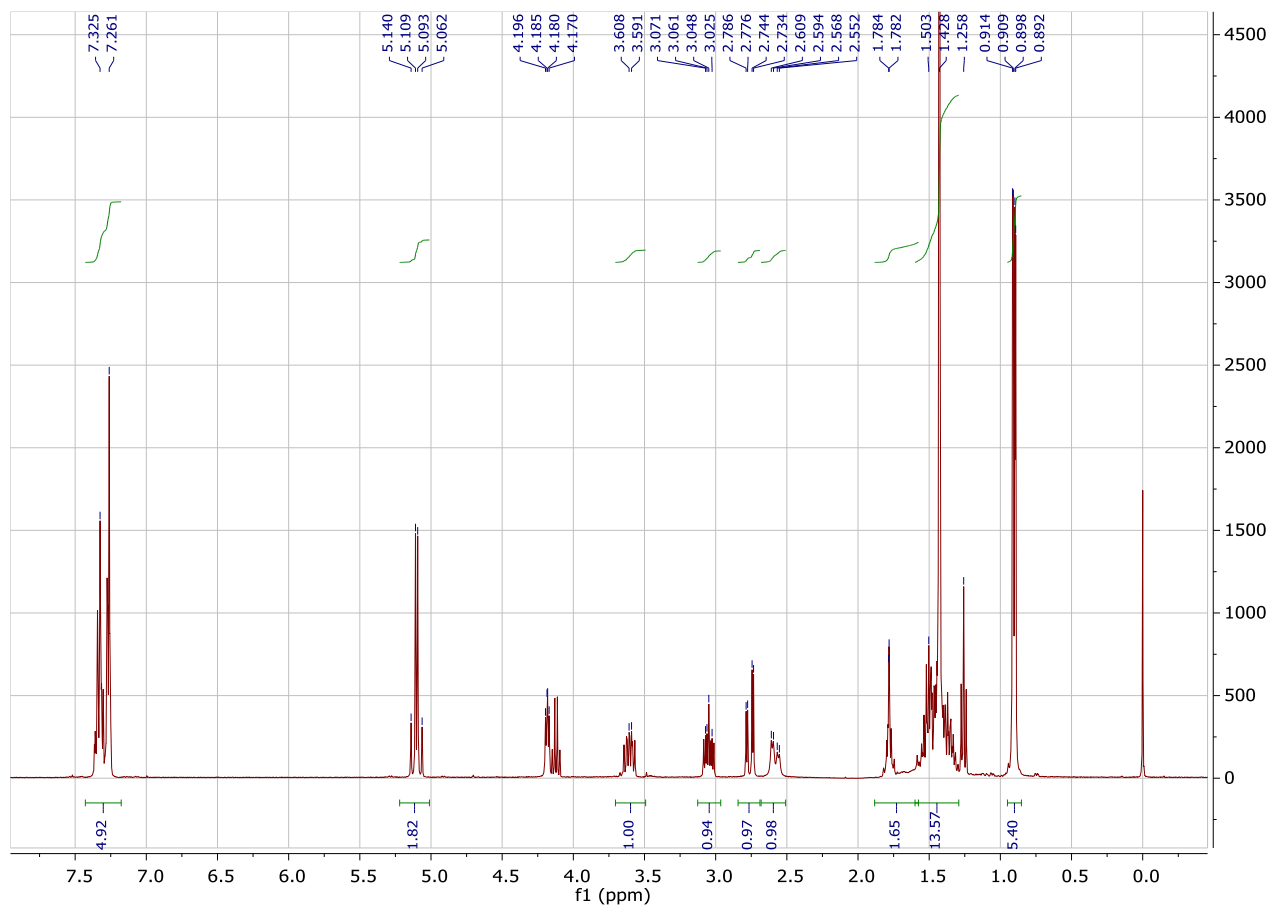
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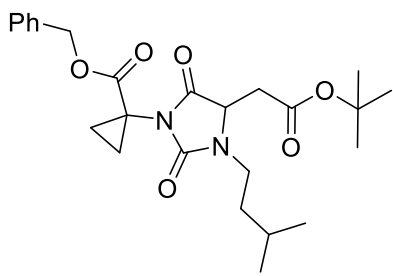




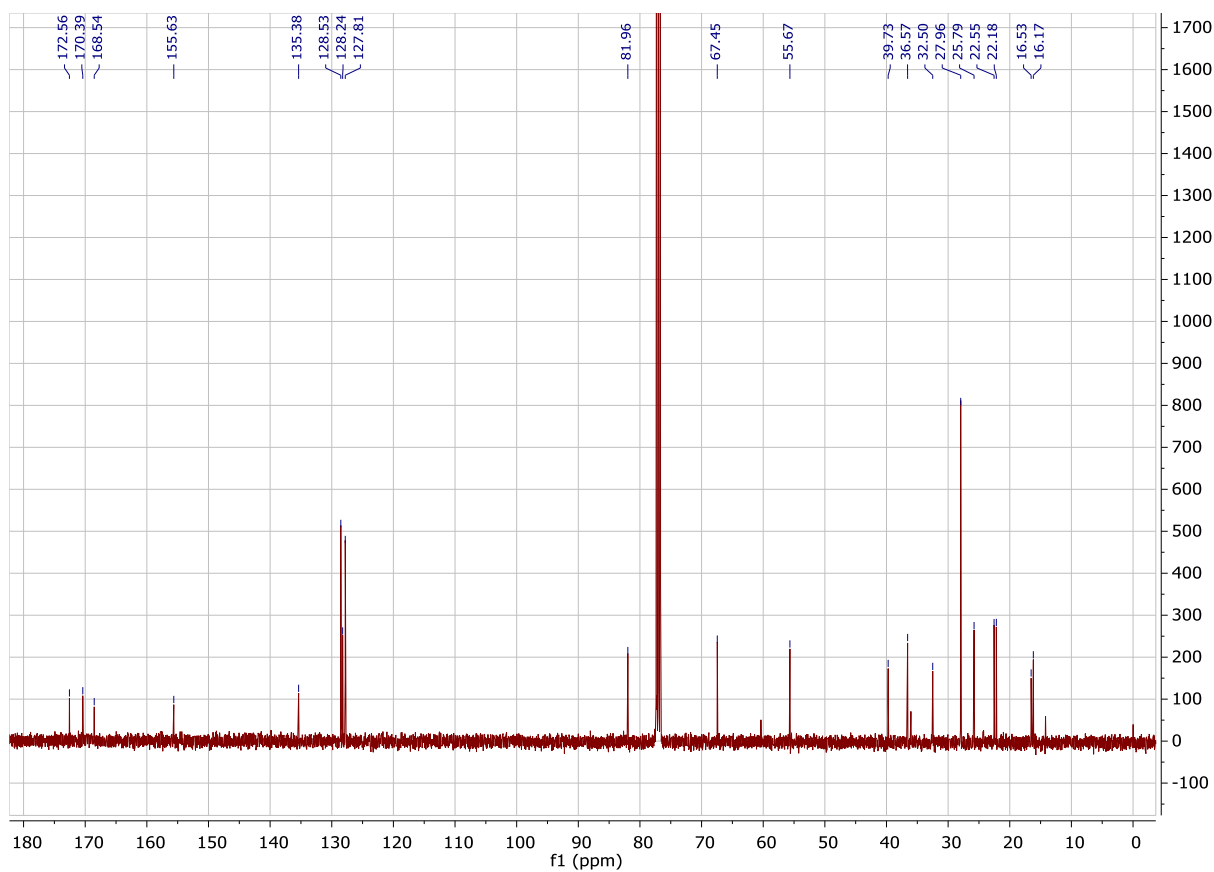
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$^1\text{H-NMR}$ (400 MHz, CDCl_3)





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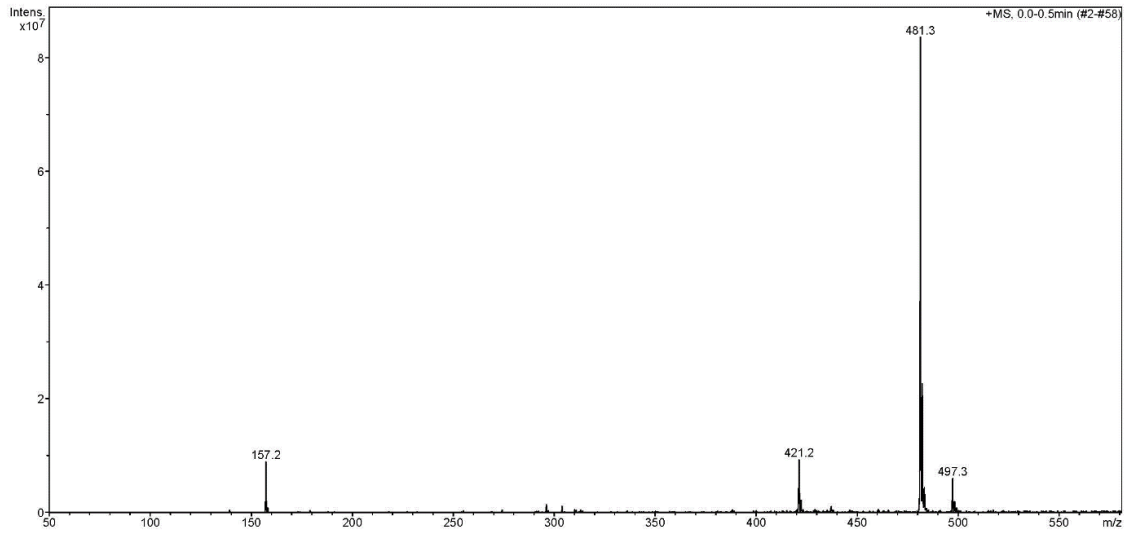


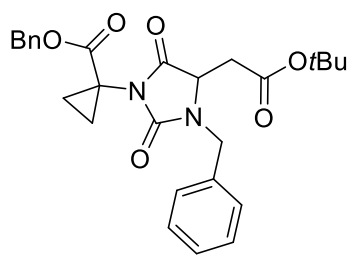
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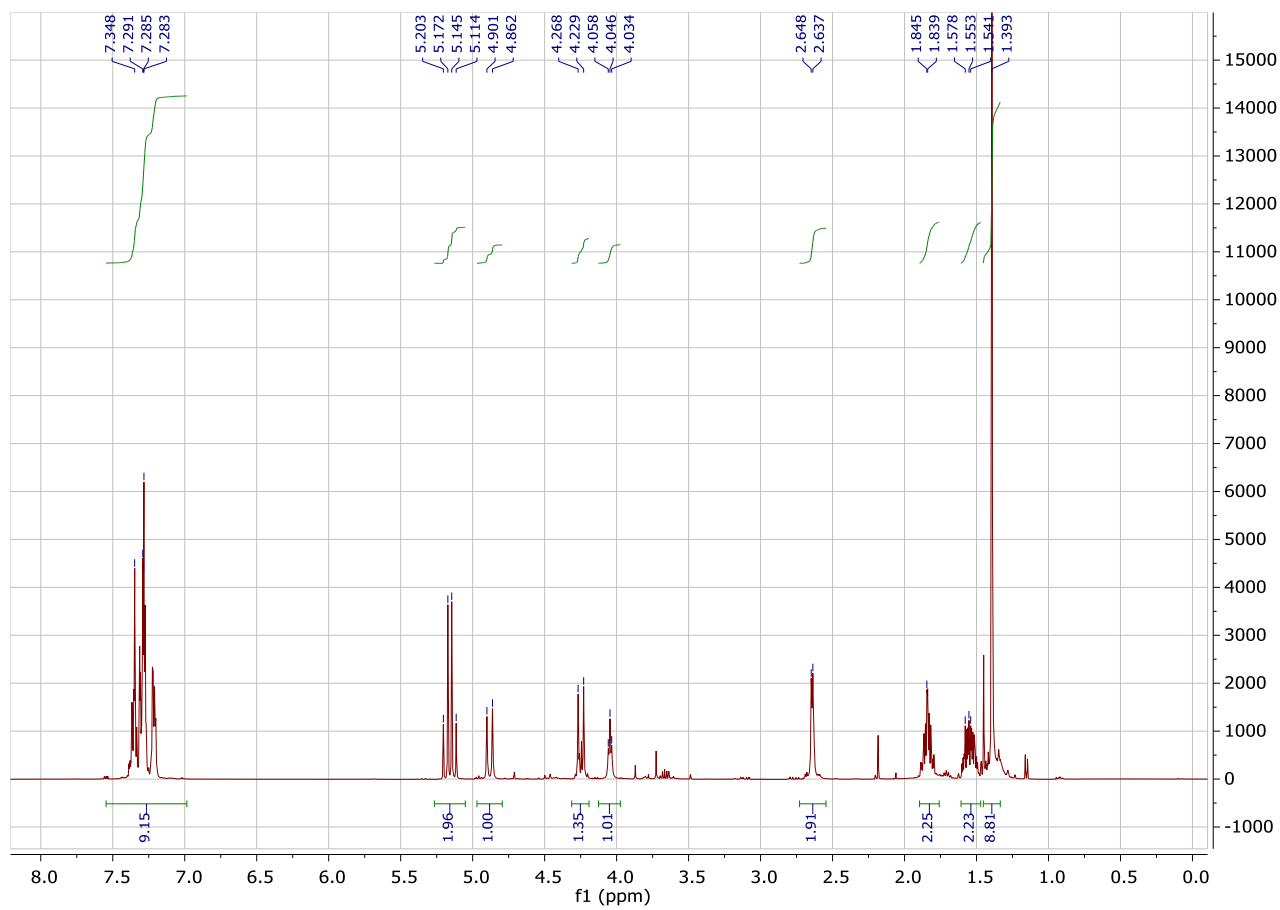
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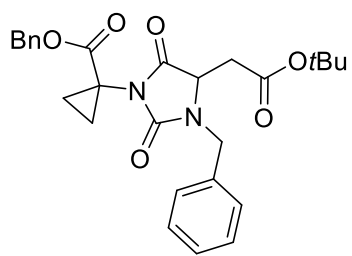




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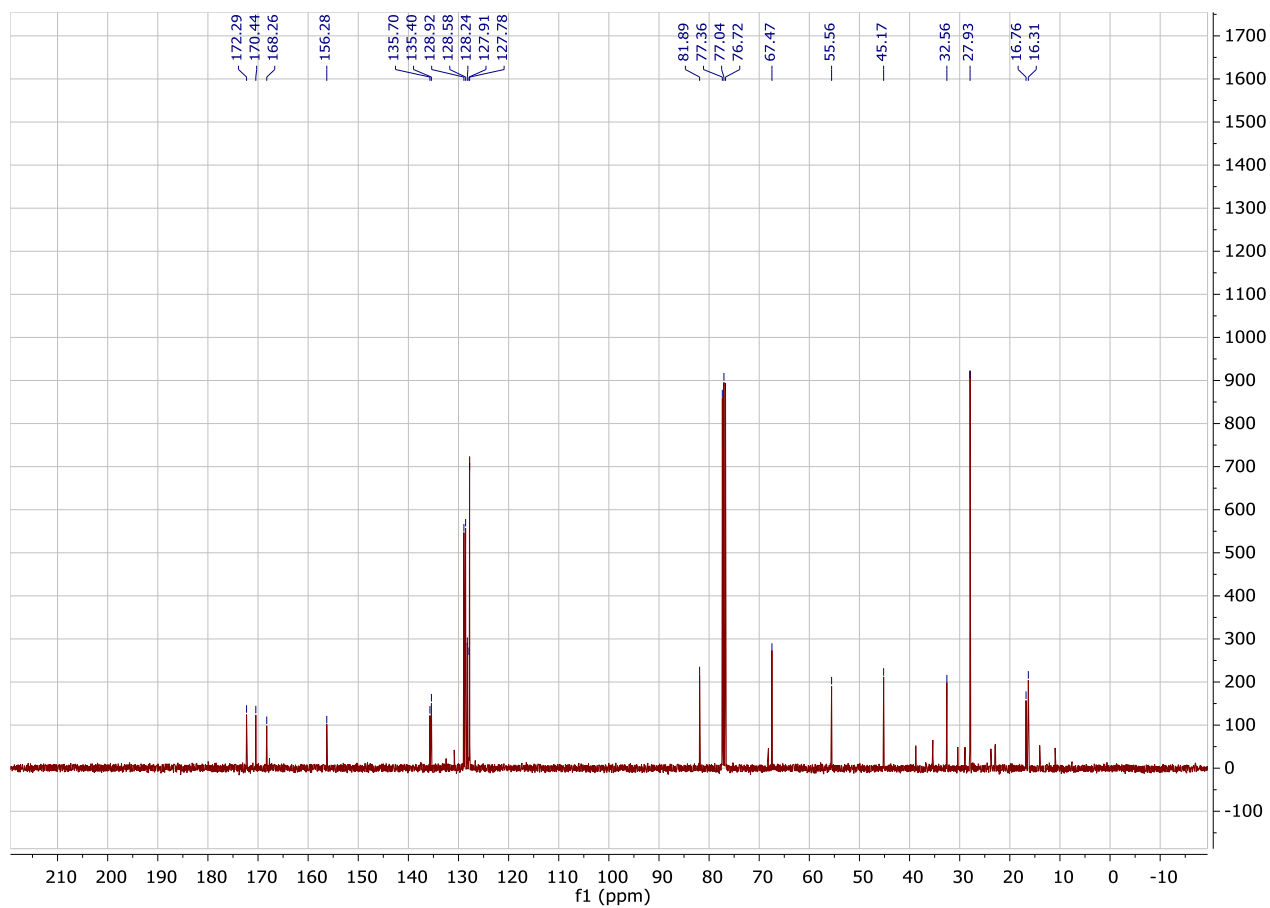
$^1\text{H-NMR}$ (400 MHz, CDCl_3)





5b

$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)



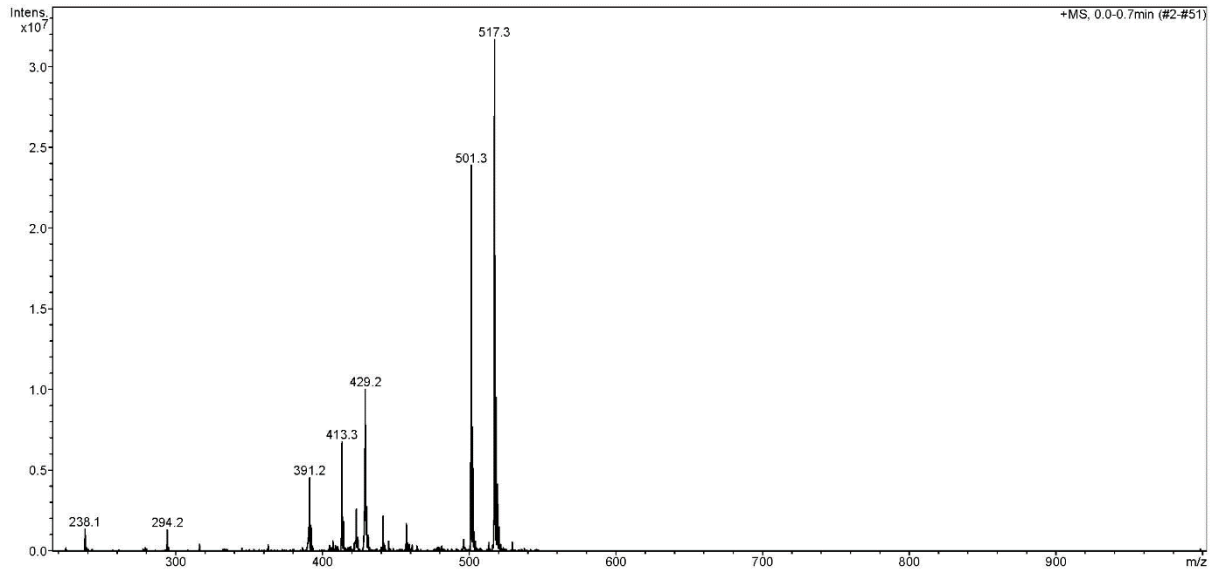
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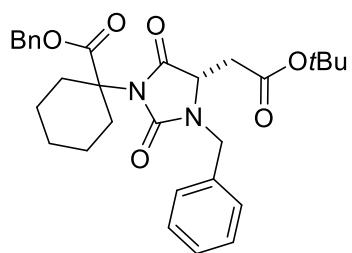
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Operator
Instrument

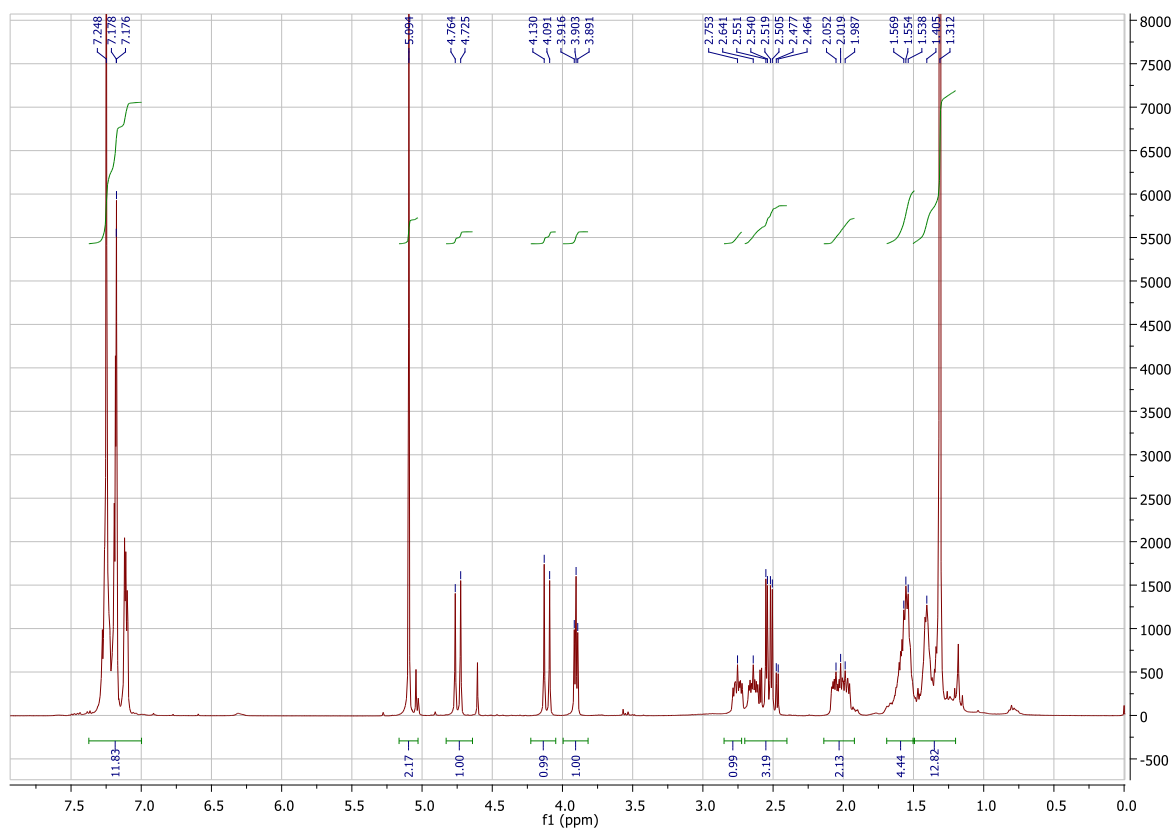
Walter Panzeri
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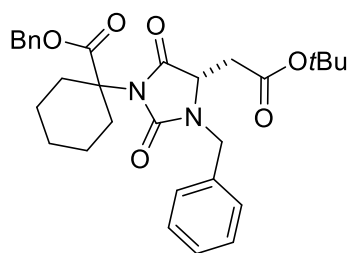




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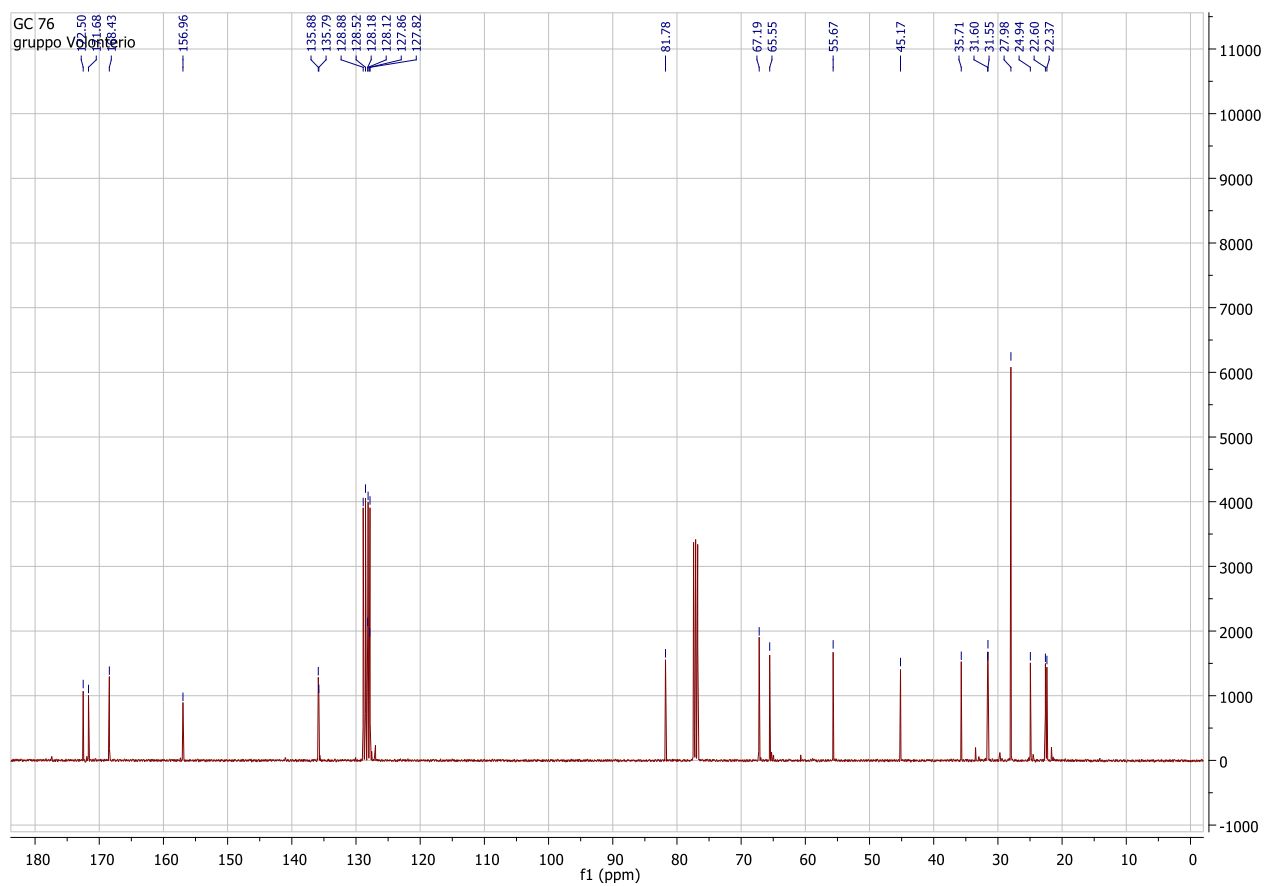
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$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)

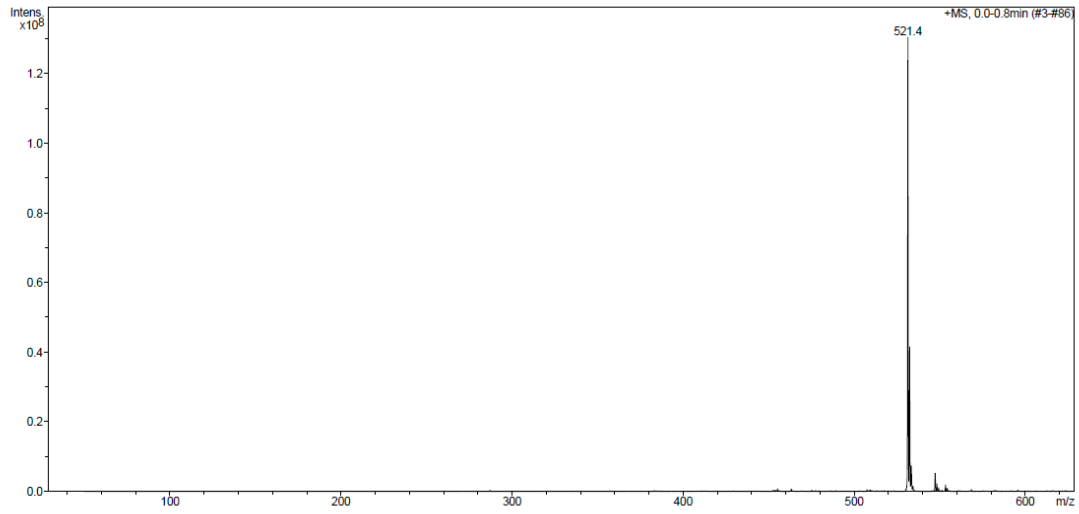


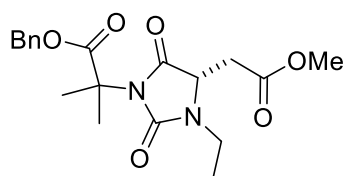
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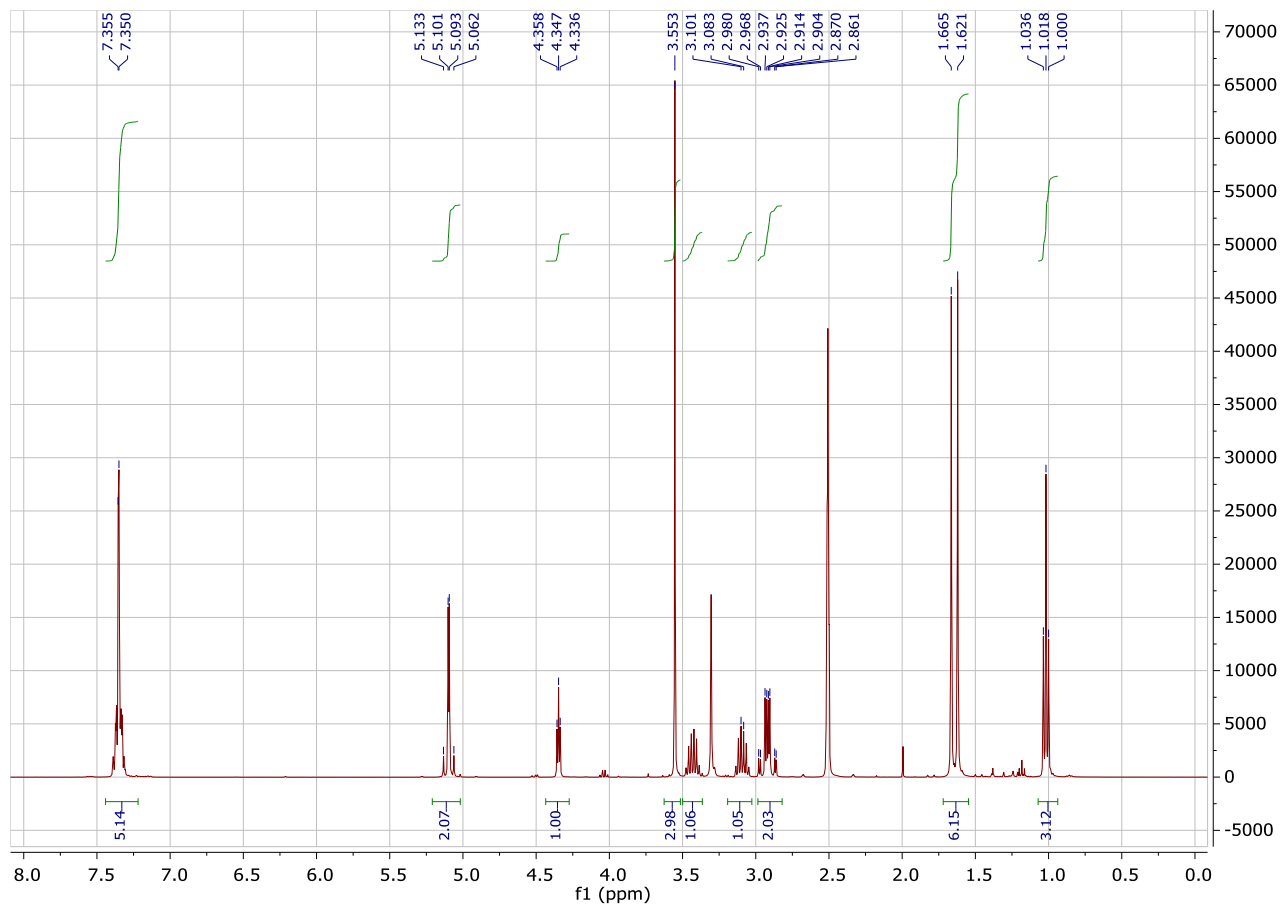
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Instrument esquire3000plus

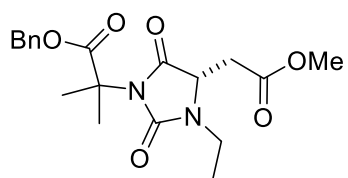




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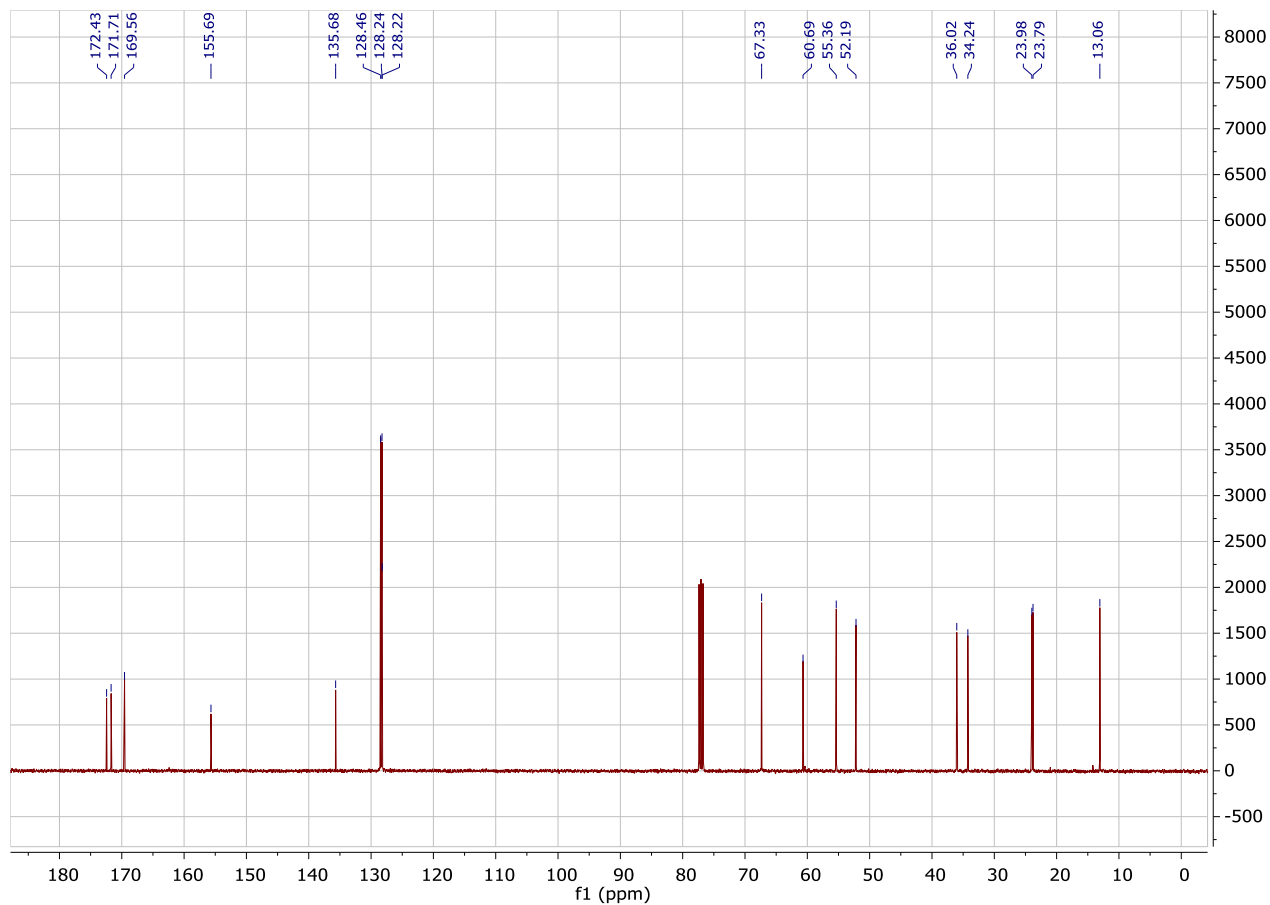
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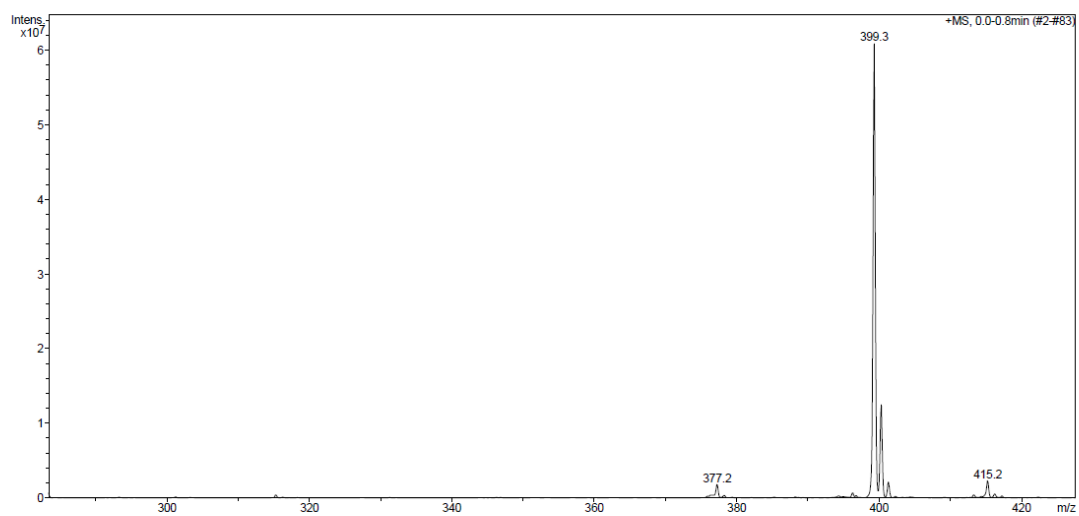
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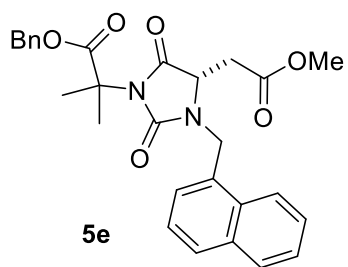
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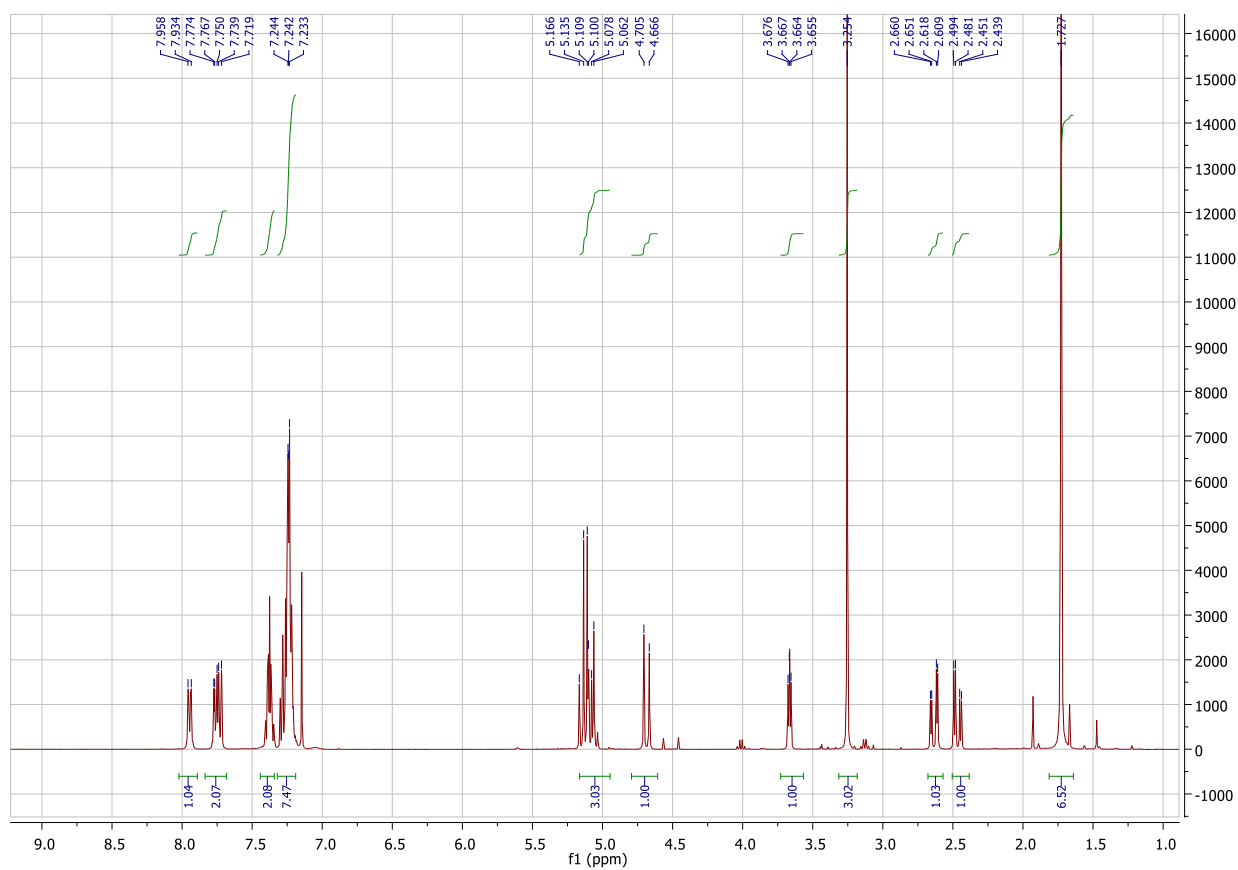
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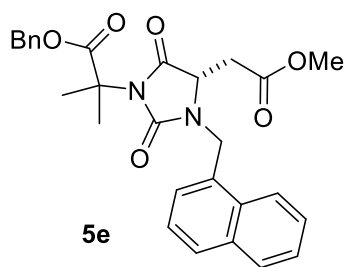
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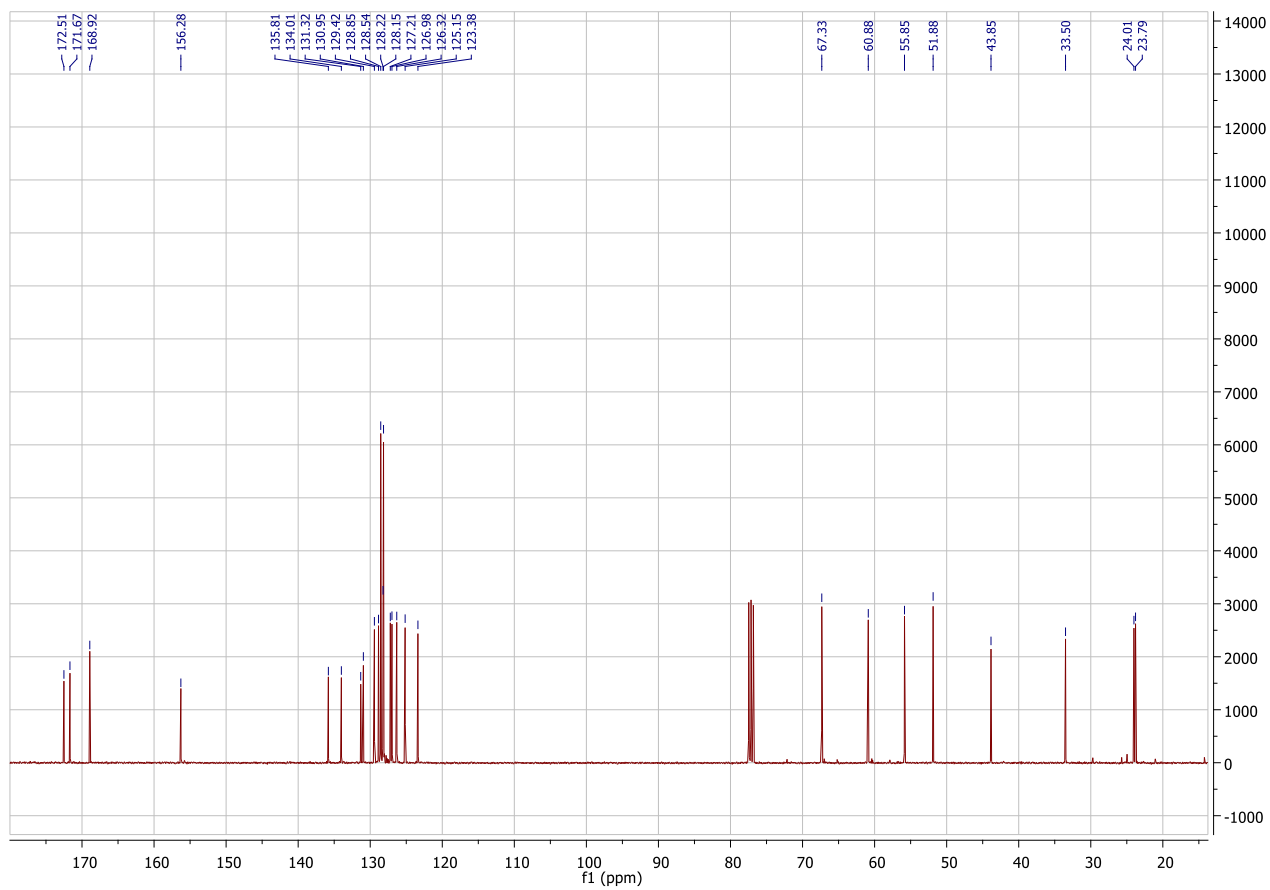


¹H-NMR (400 MHz, CDCl₃)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)

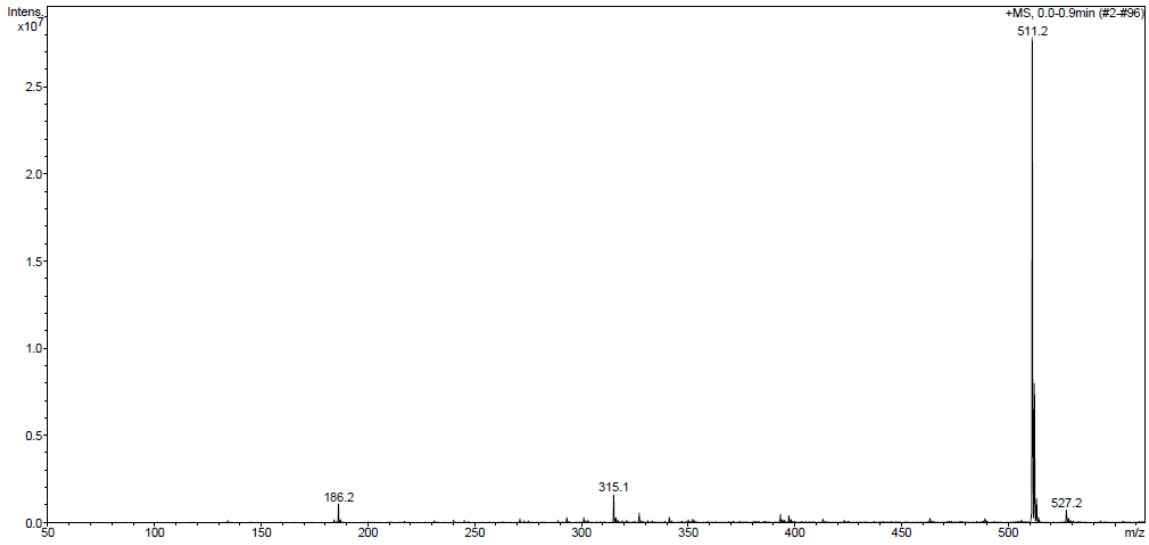


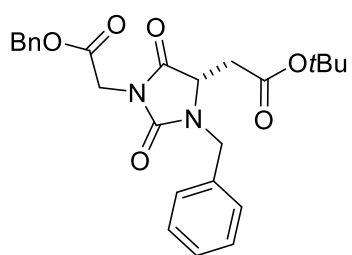
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

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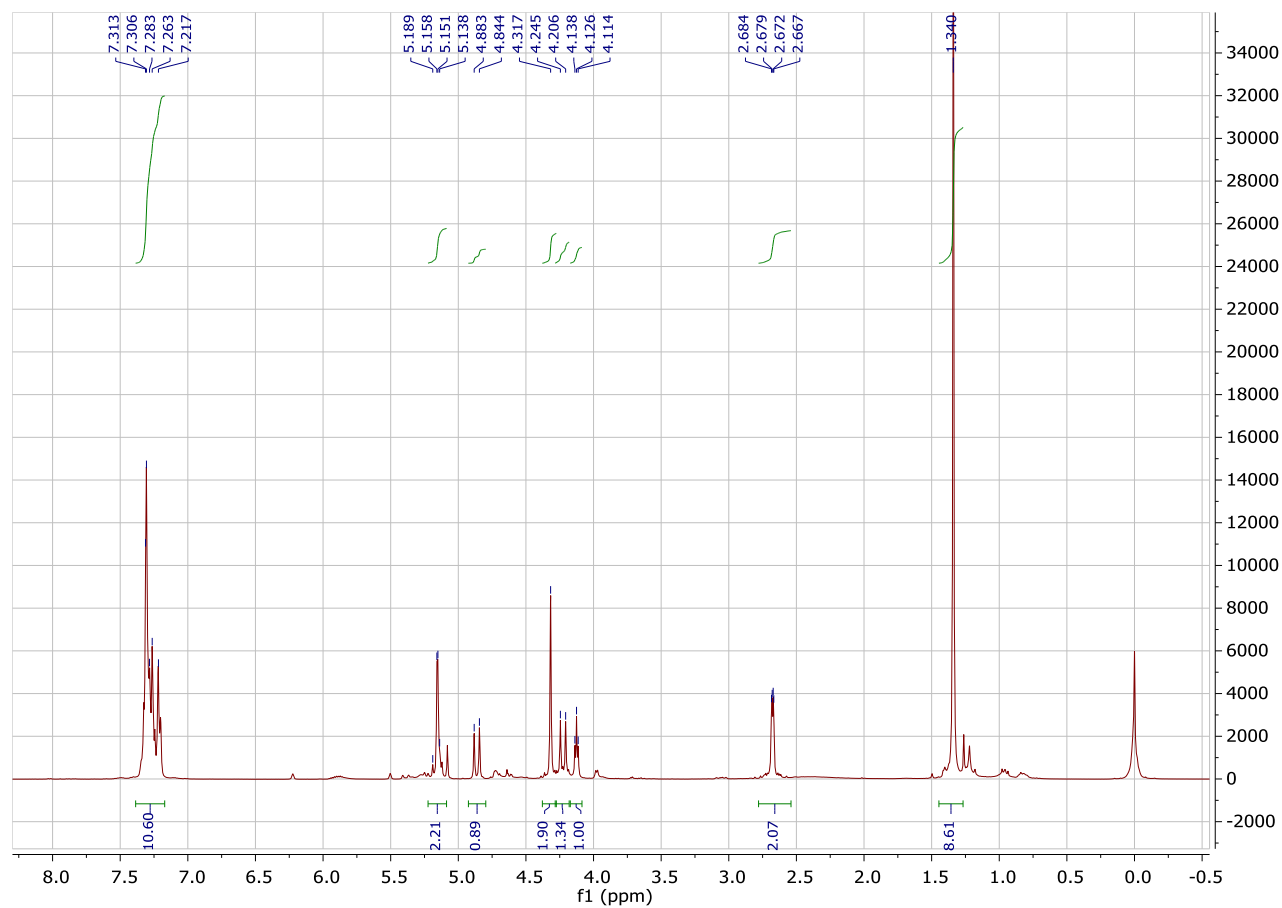
Operator Walter Panzeri
Instrument esquire3000plus

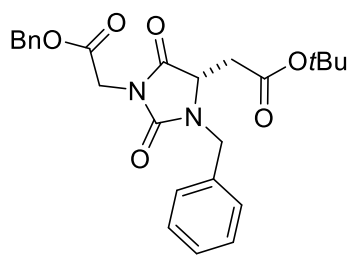




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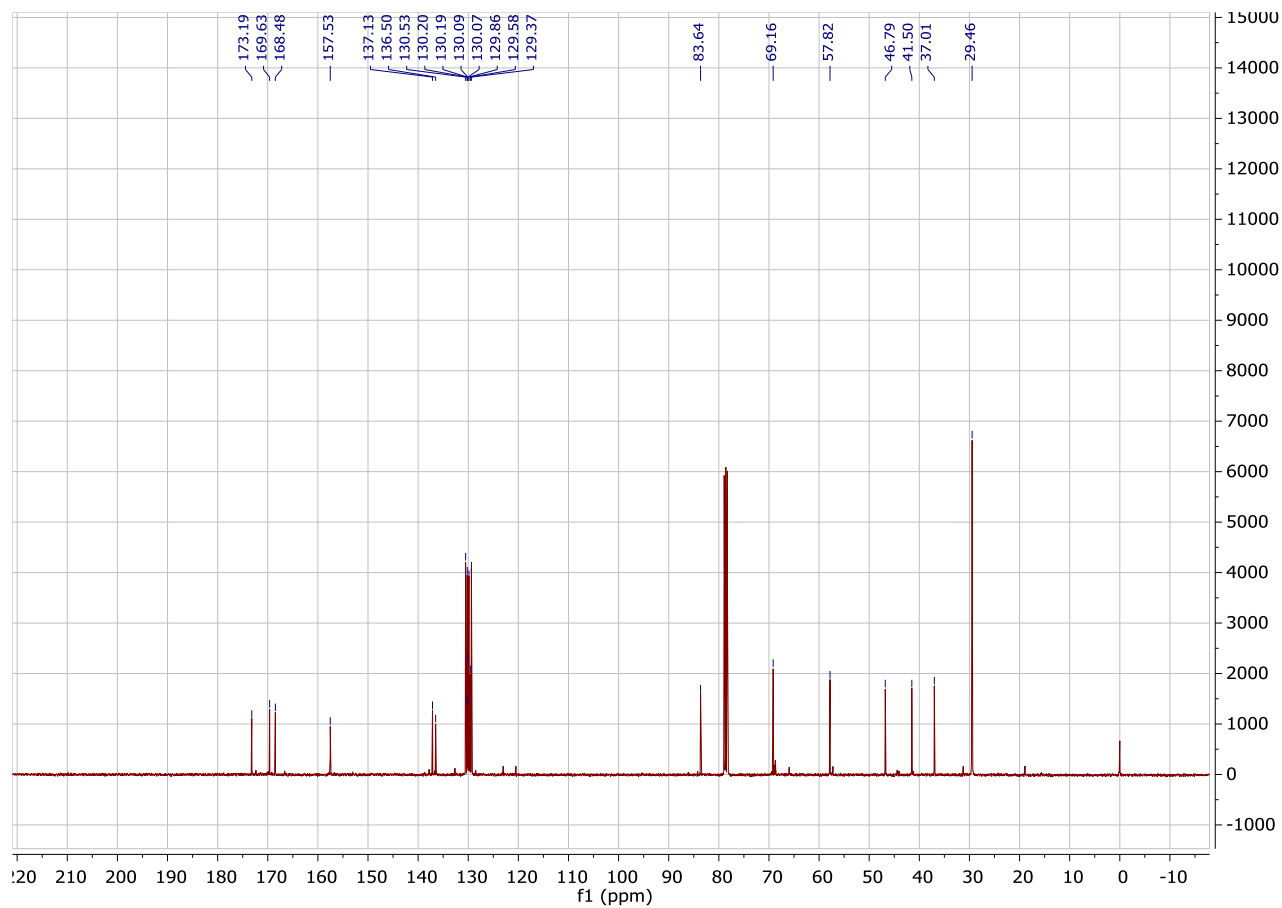
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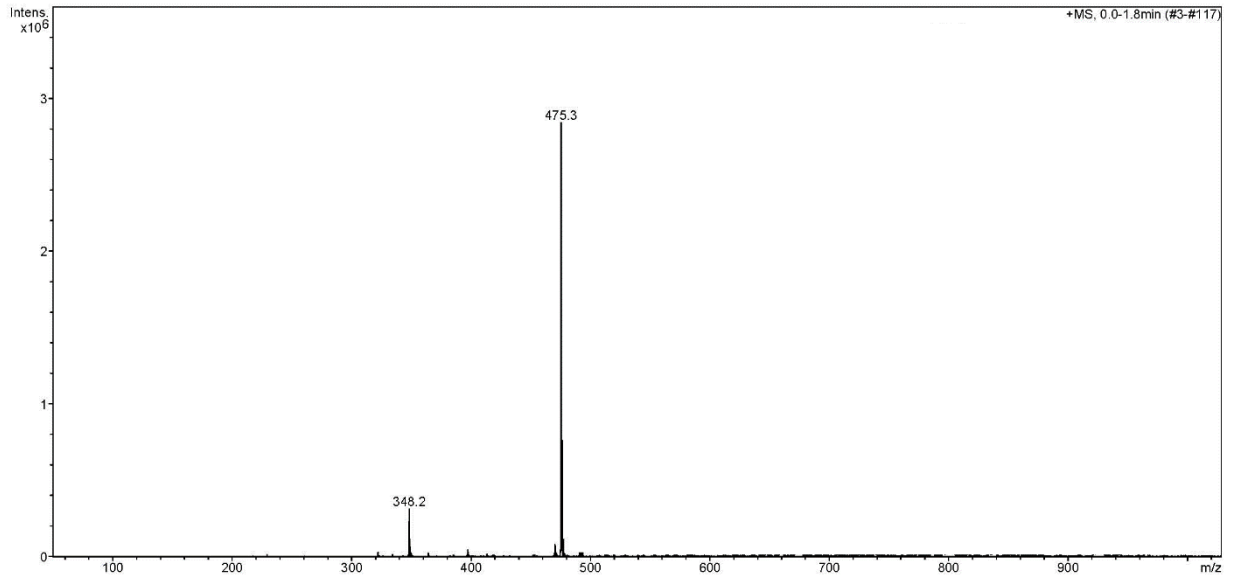
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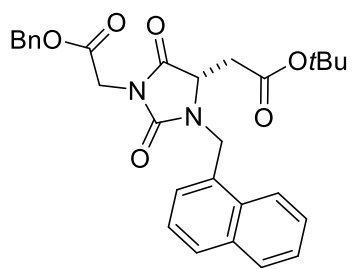
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-L.G.S. - Laboratorio Grandi Strumenti - Display Report

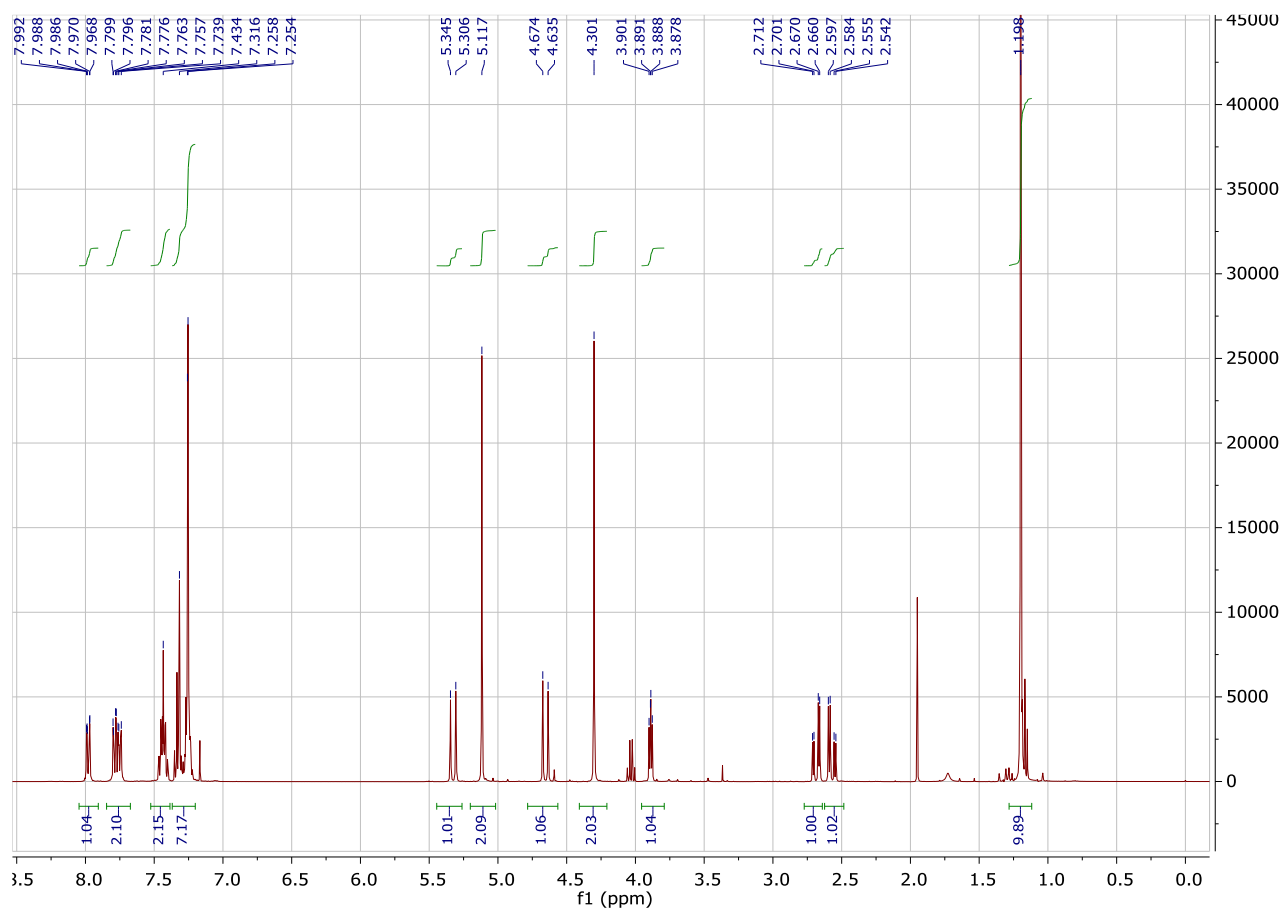
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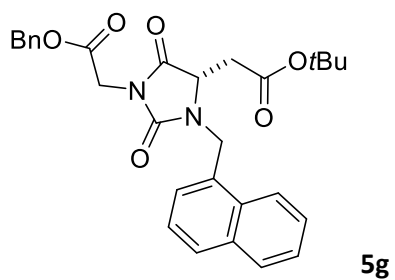




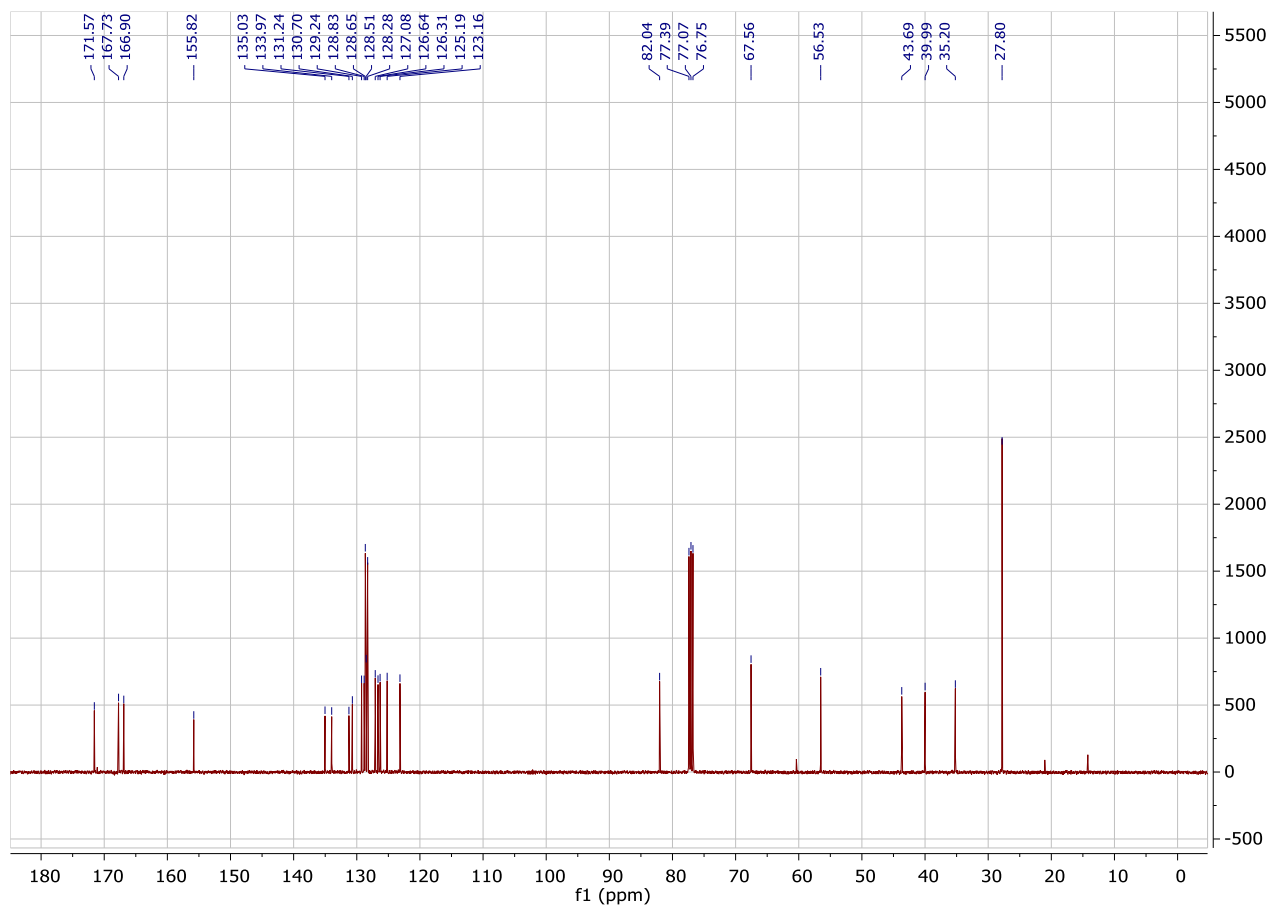
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$^1\text{H-NMR}$ (400 MHz, CDCl_3)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)



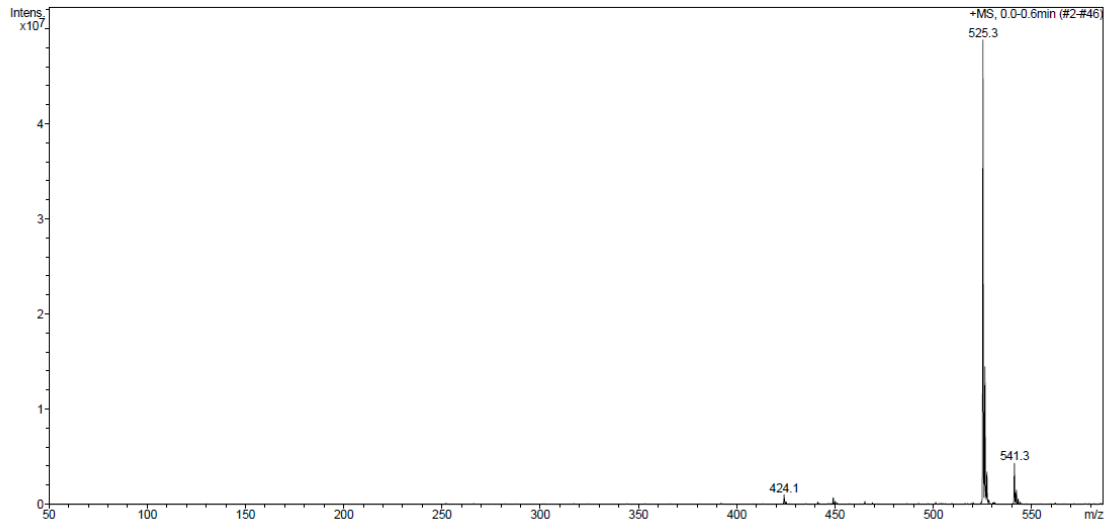
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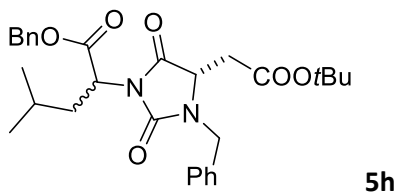
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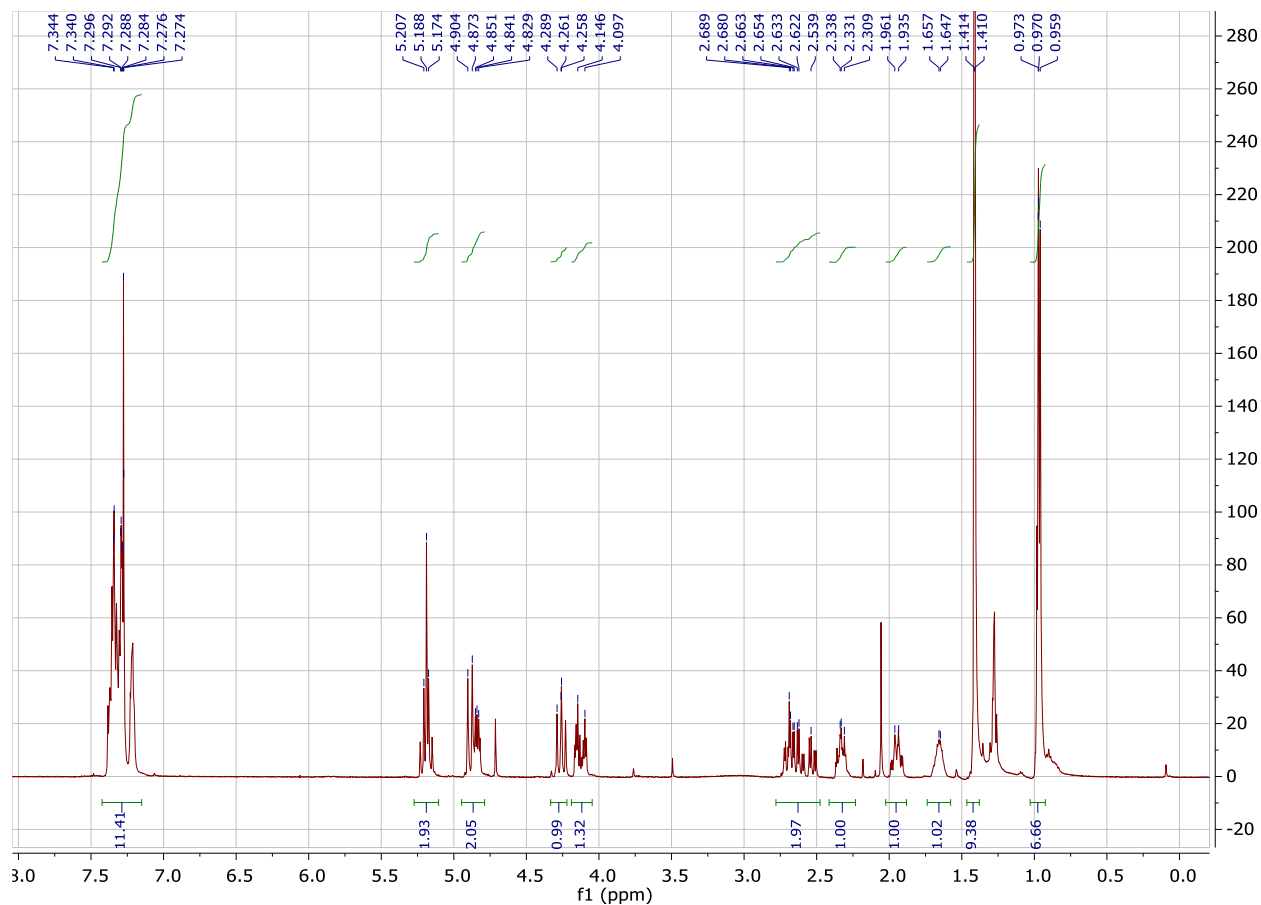
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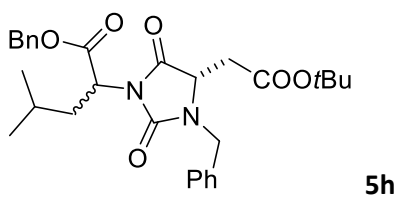
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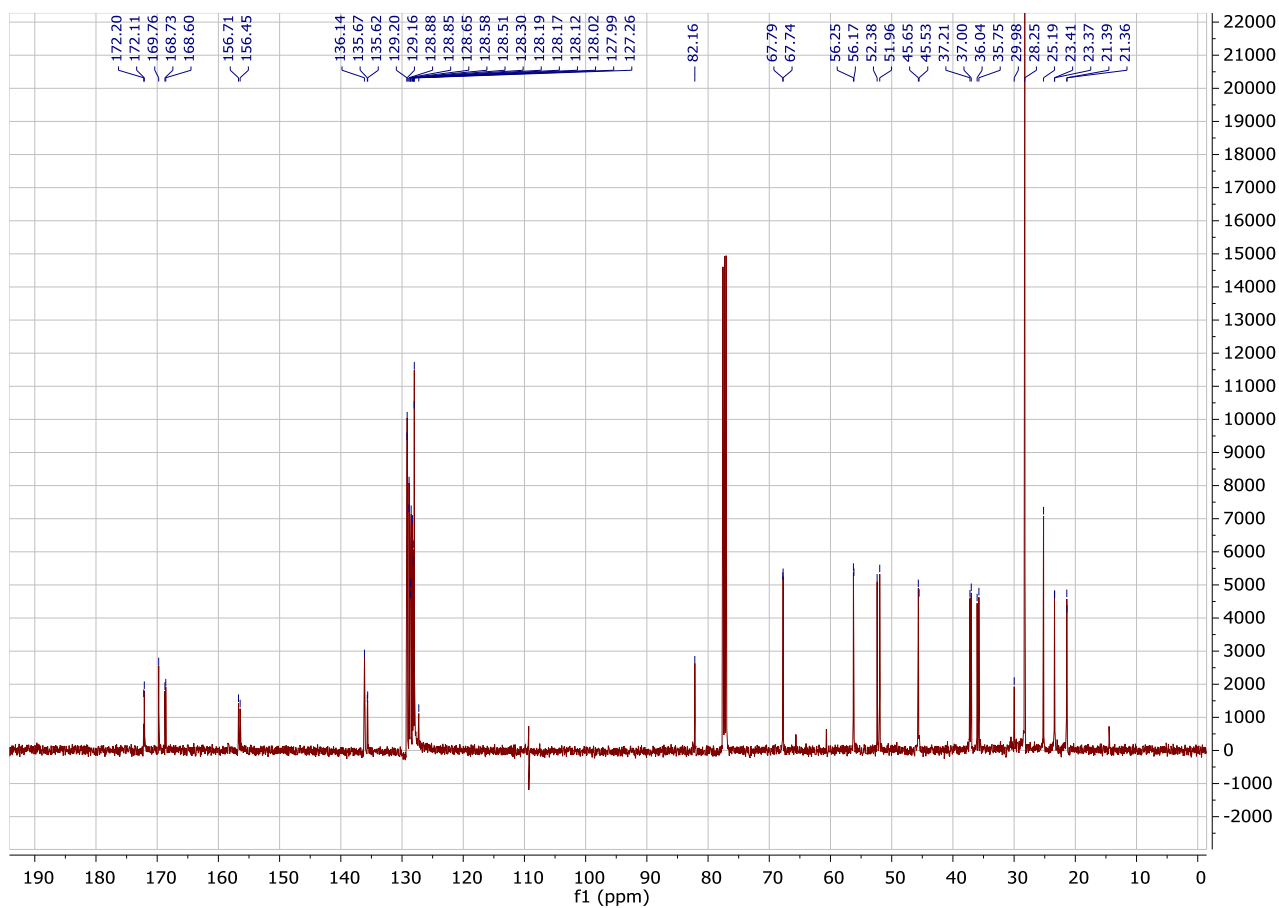


$^1\text{H-NMR}$ (400 MHz, CDCl_3)





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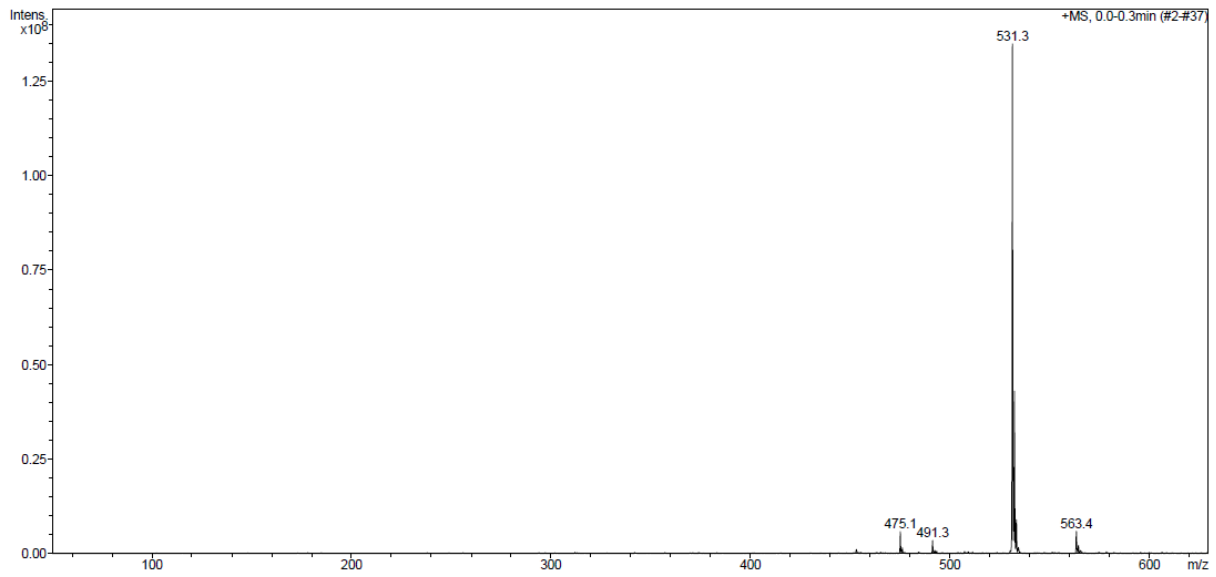
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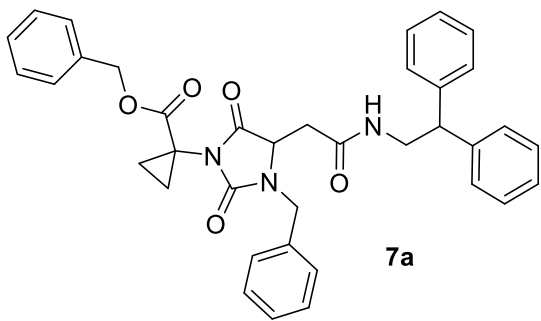
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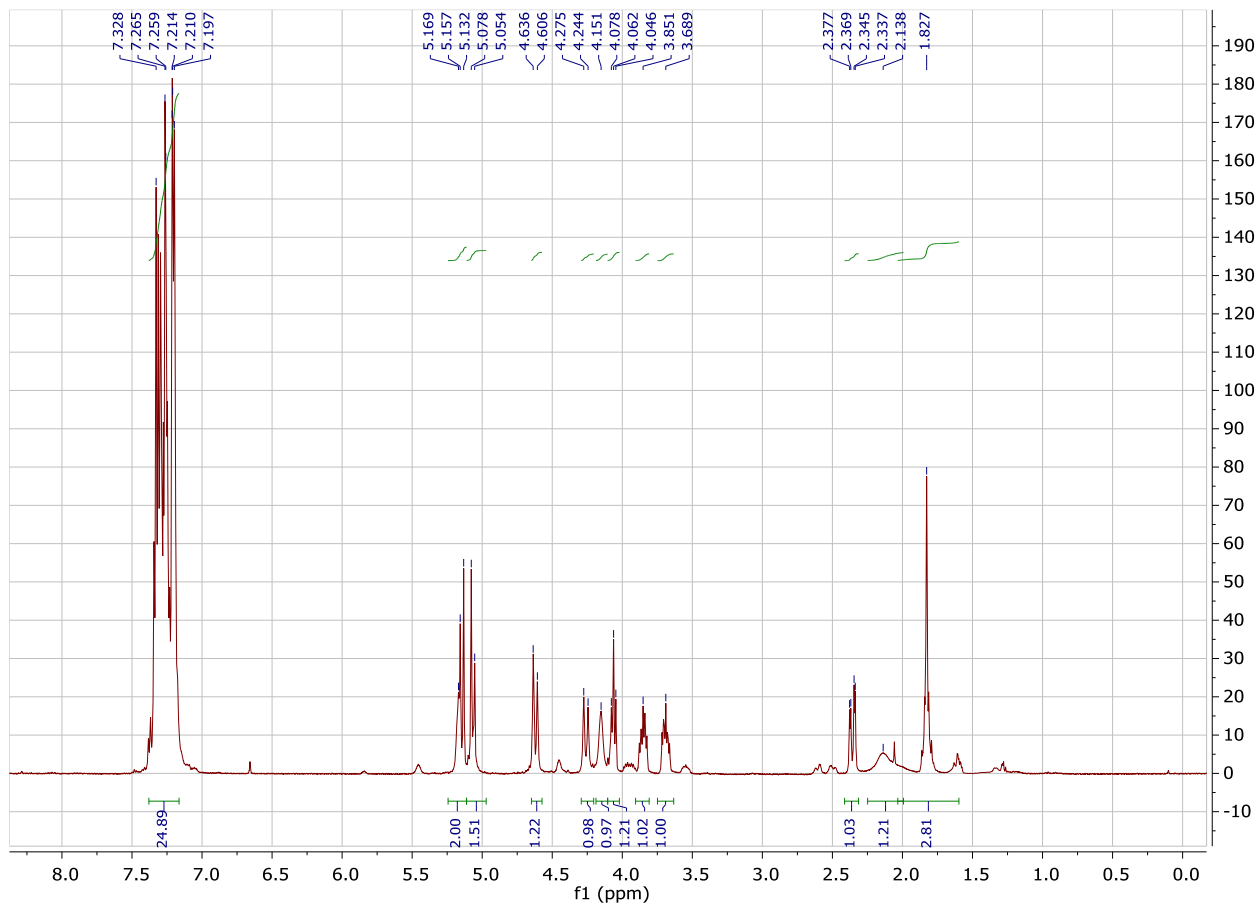
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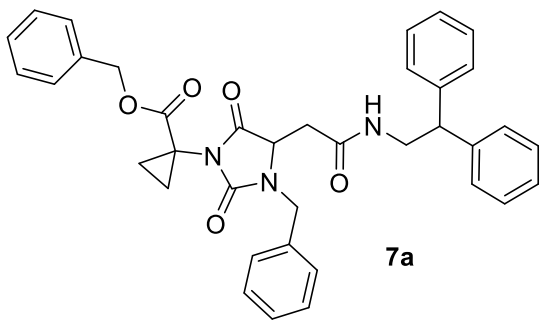
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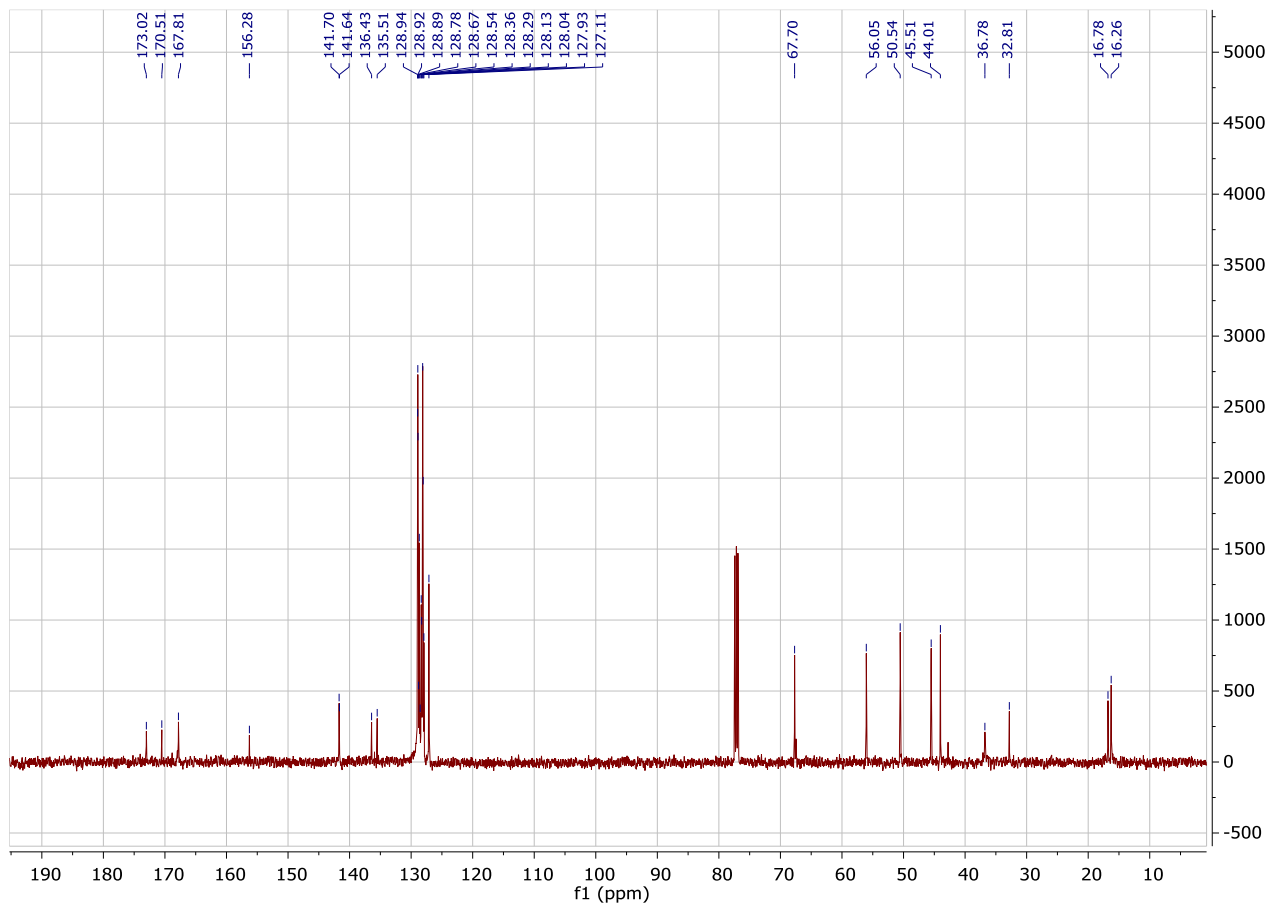


$^1\text{H-NMR}$ (400 MHz, CDCl_3)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)

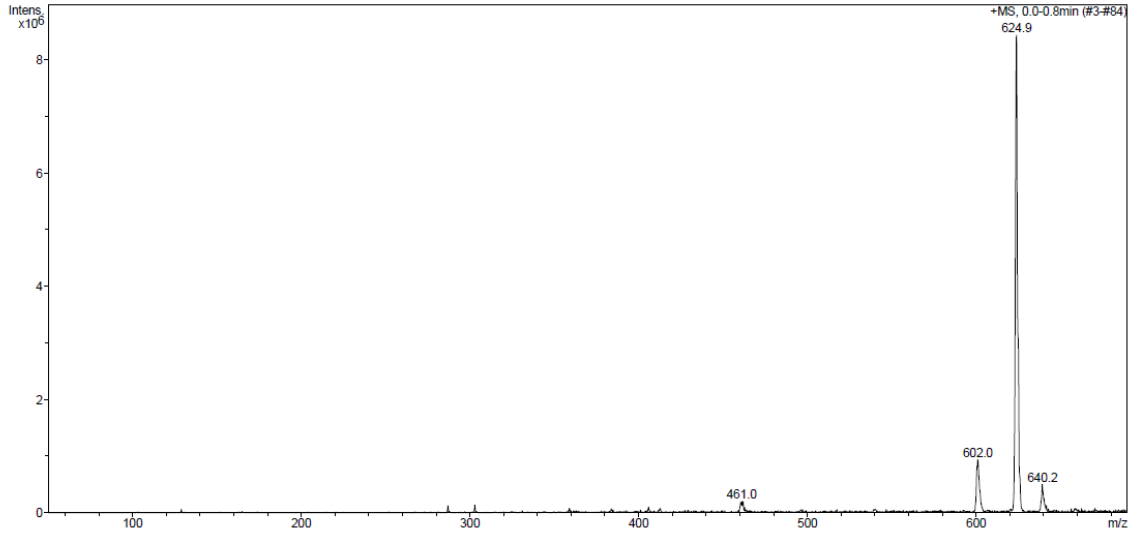


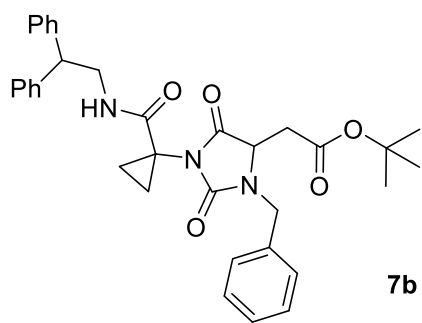
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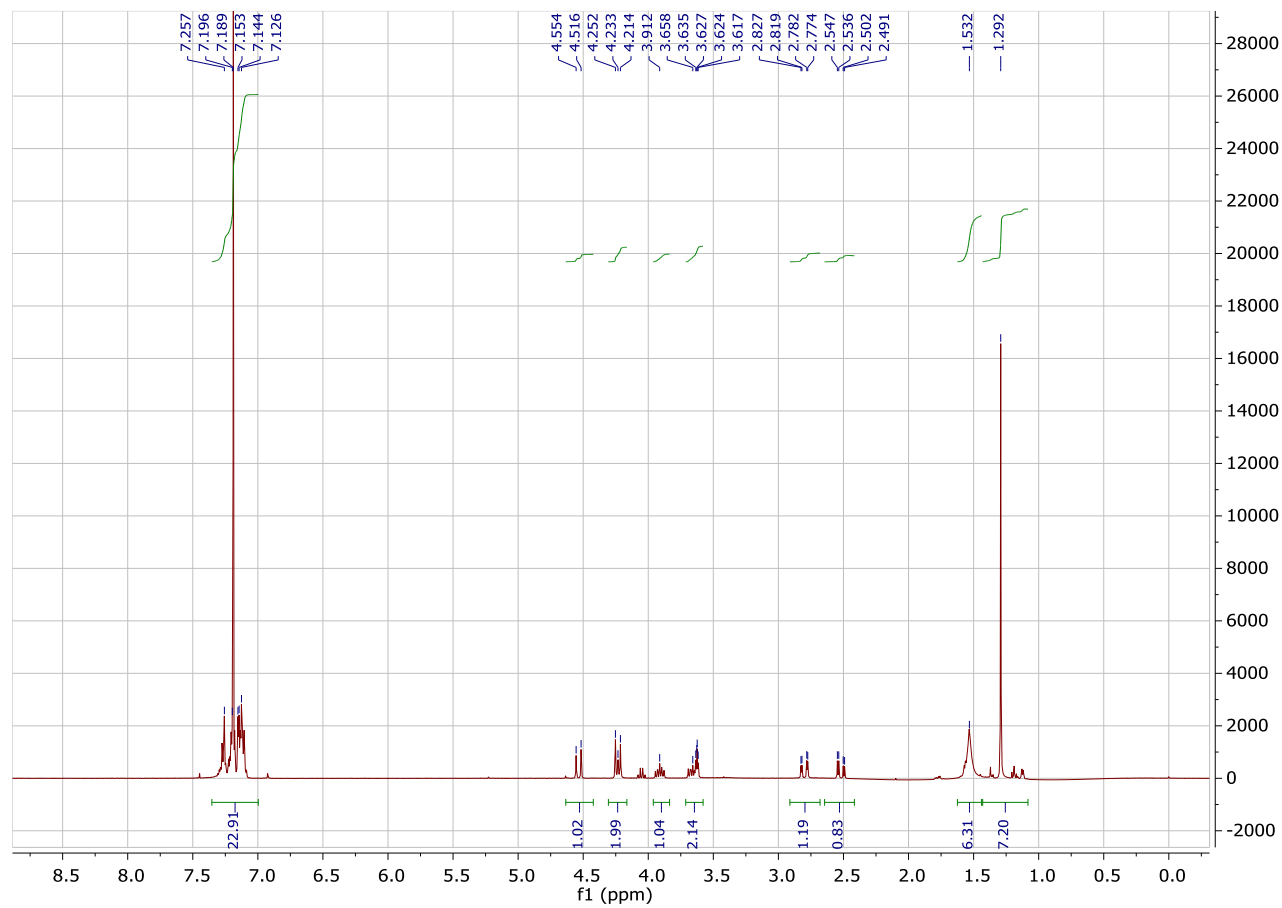
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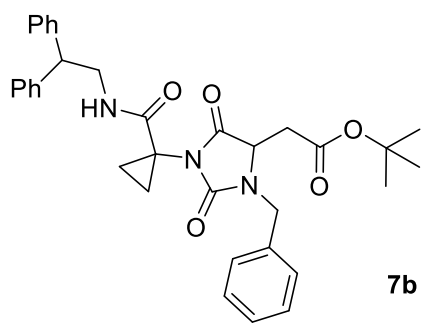
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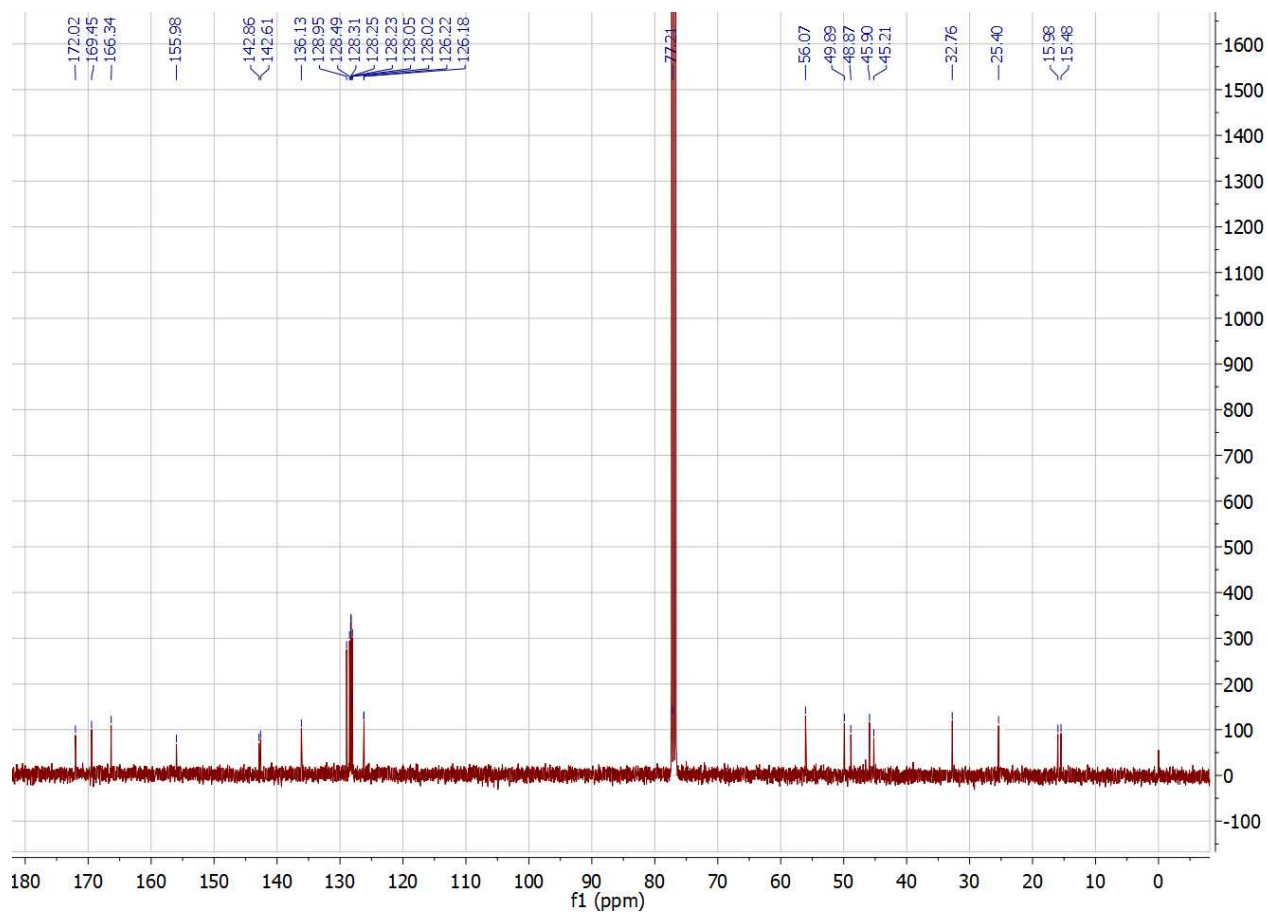


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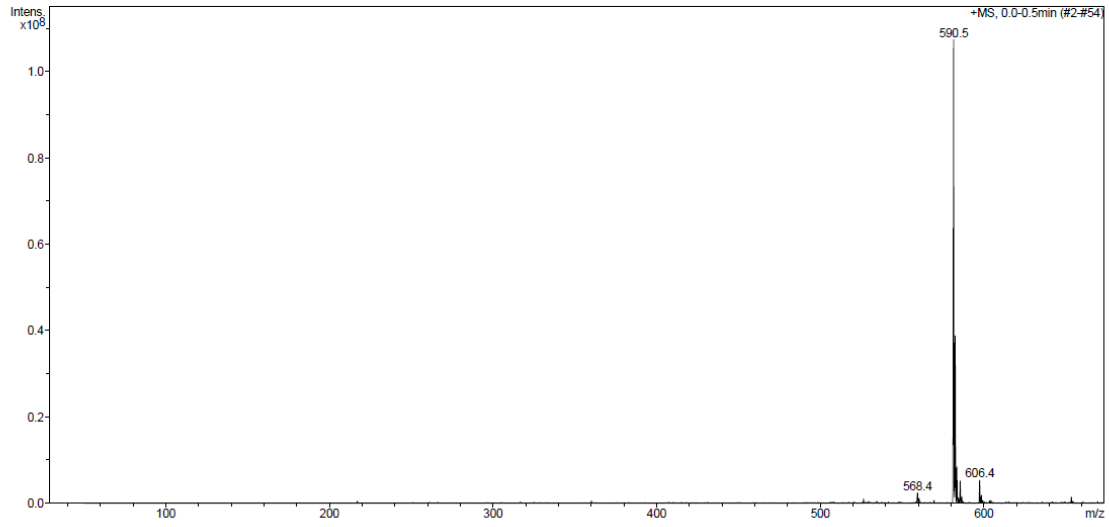


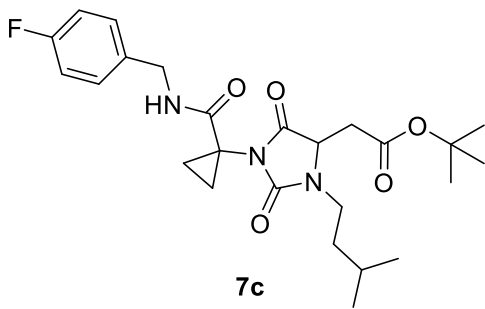
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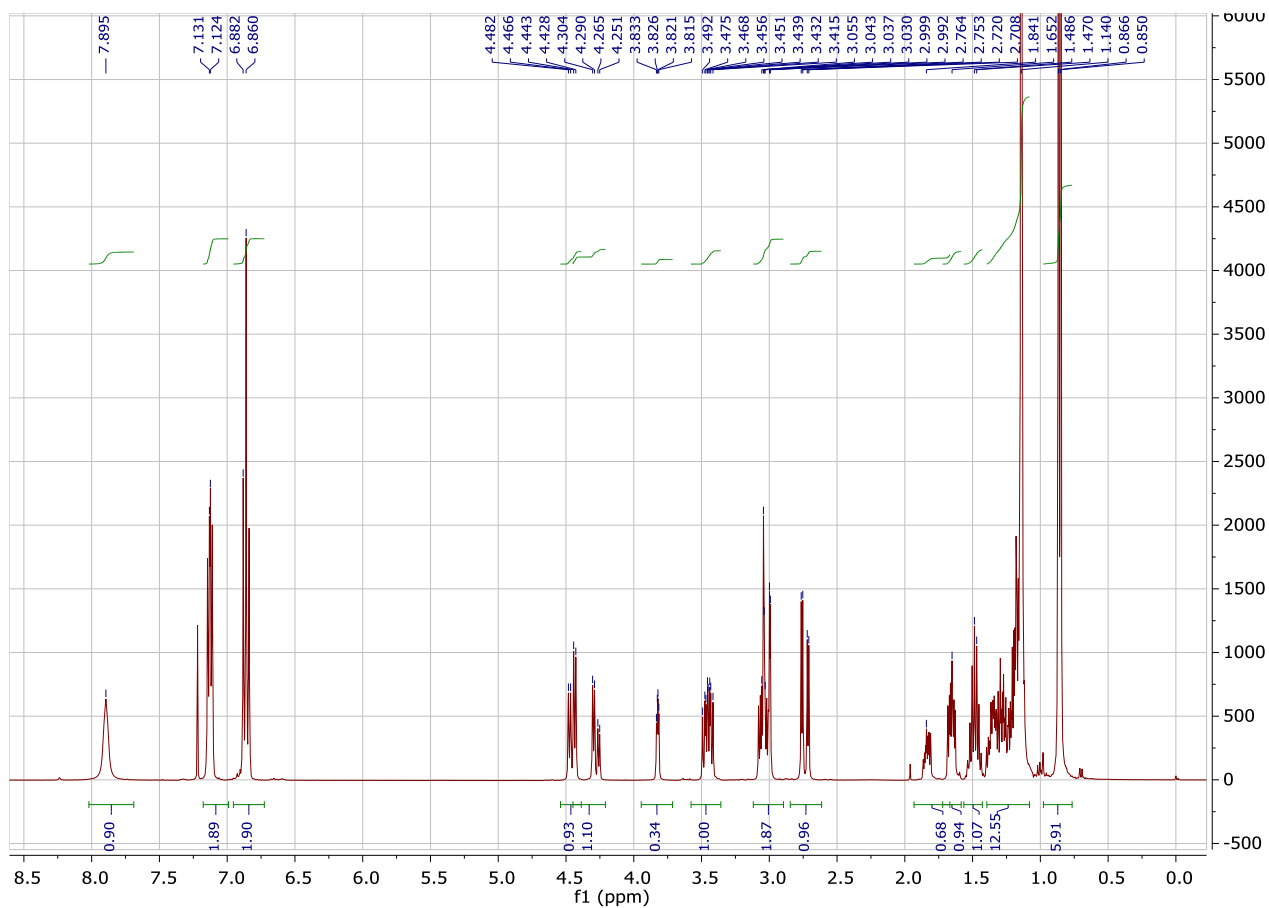
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

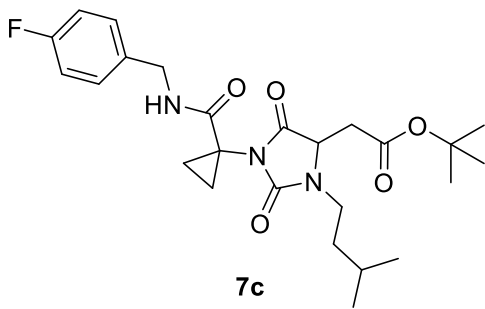
Analysis Name	av gc132.d	Acquisition Date	07/01/19 14:41:30	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg	Instrument	esquire3000plus
Comment	1mg/ml dil 1:100 MeOH Richiedente: Cristina		Im.MS		



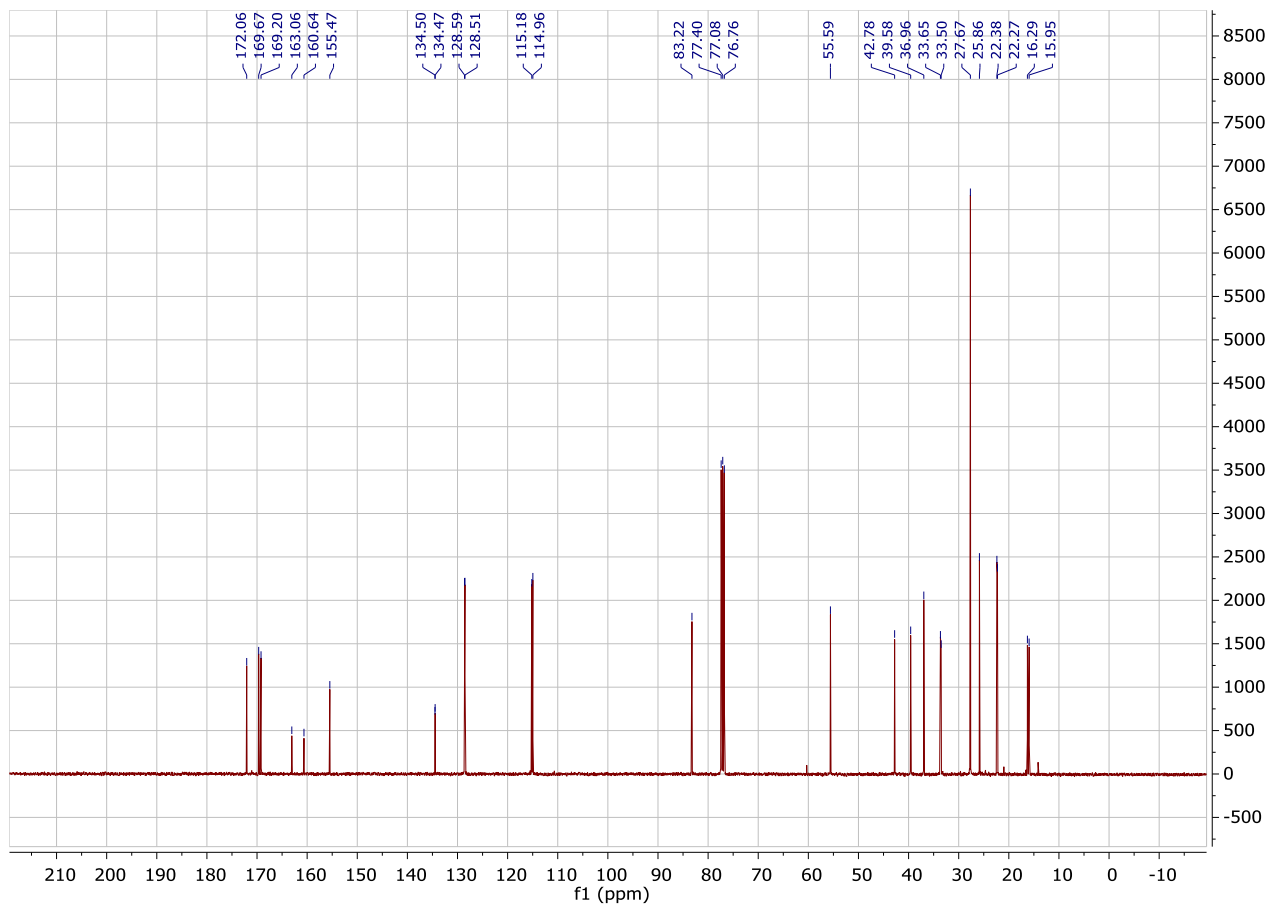


$^1\text{H-NMR}$ (400 MHz, CDCl_3)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)

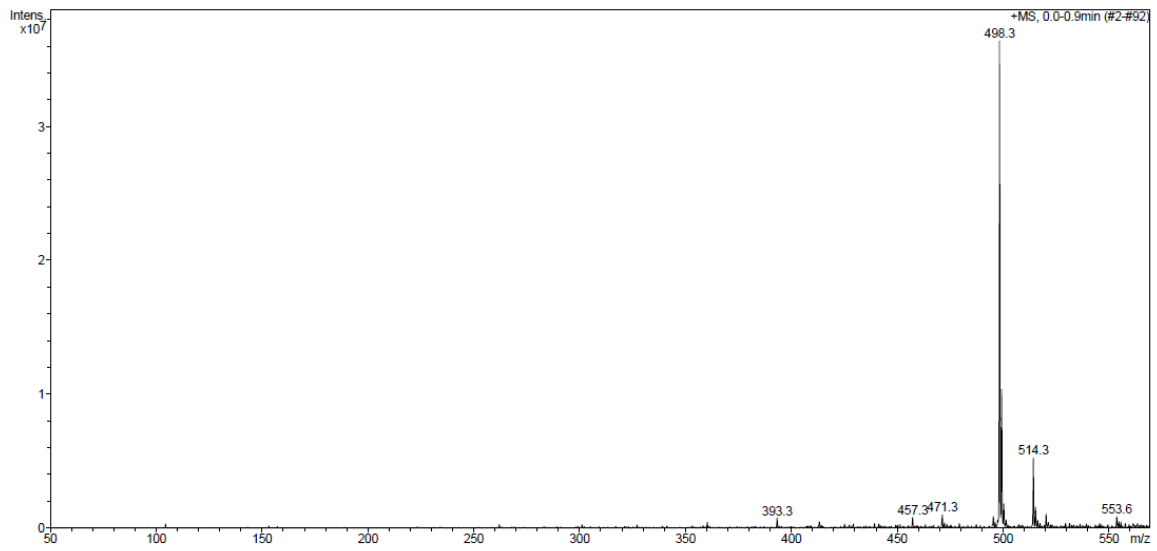


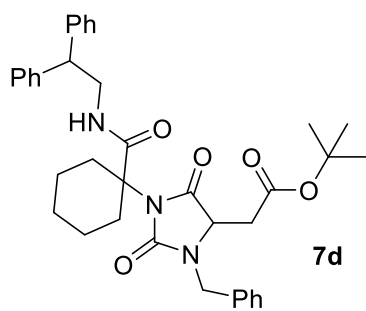
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name av gc120.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Cristina

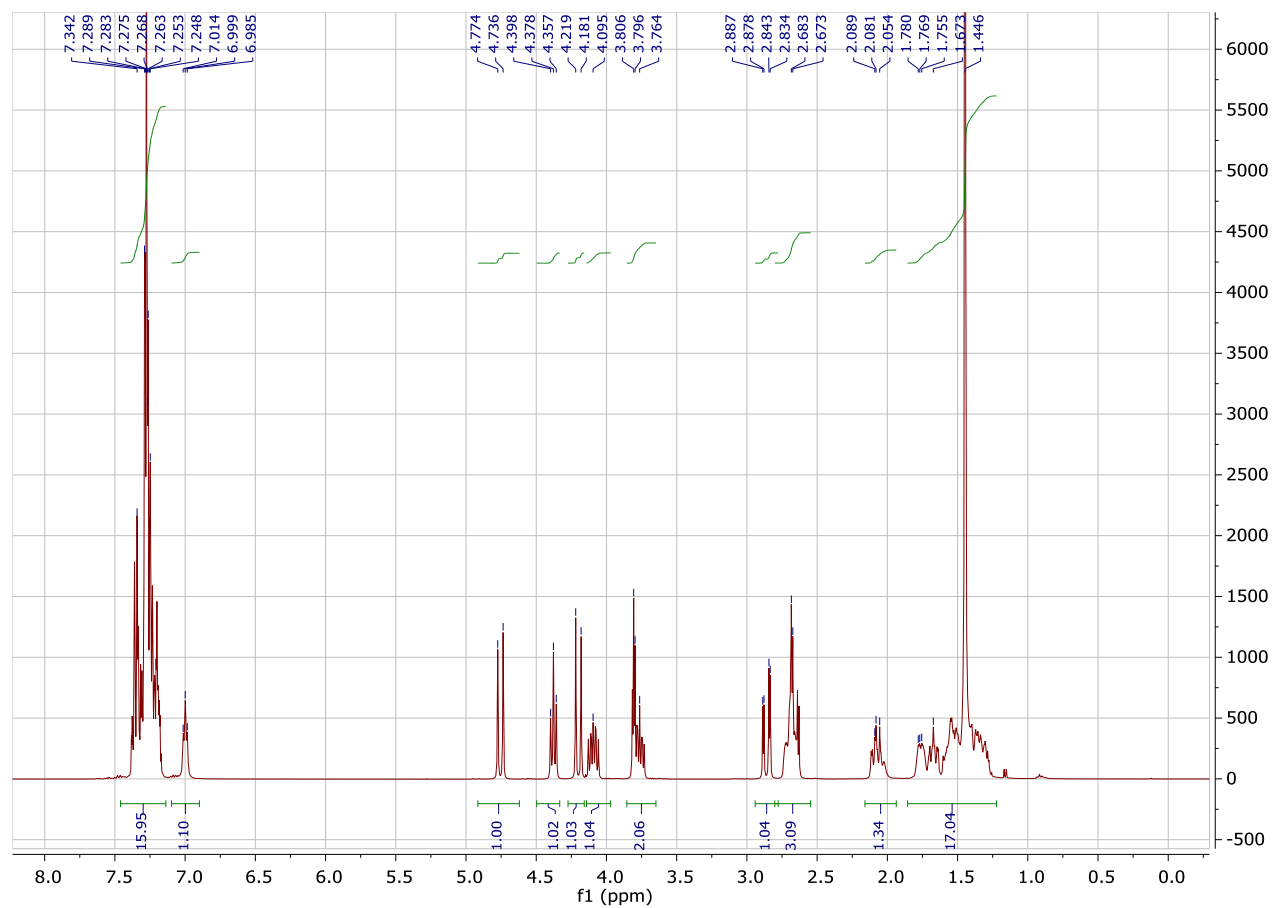
Acquisition Date 04/05/19 13:14:49
Method Copy of _01tmix_posneg
In.MS

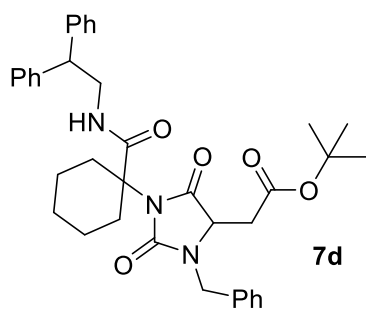
Operator Walter Panzeri
Instrument esquire3000plus



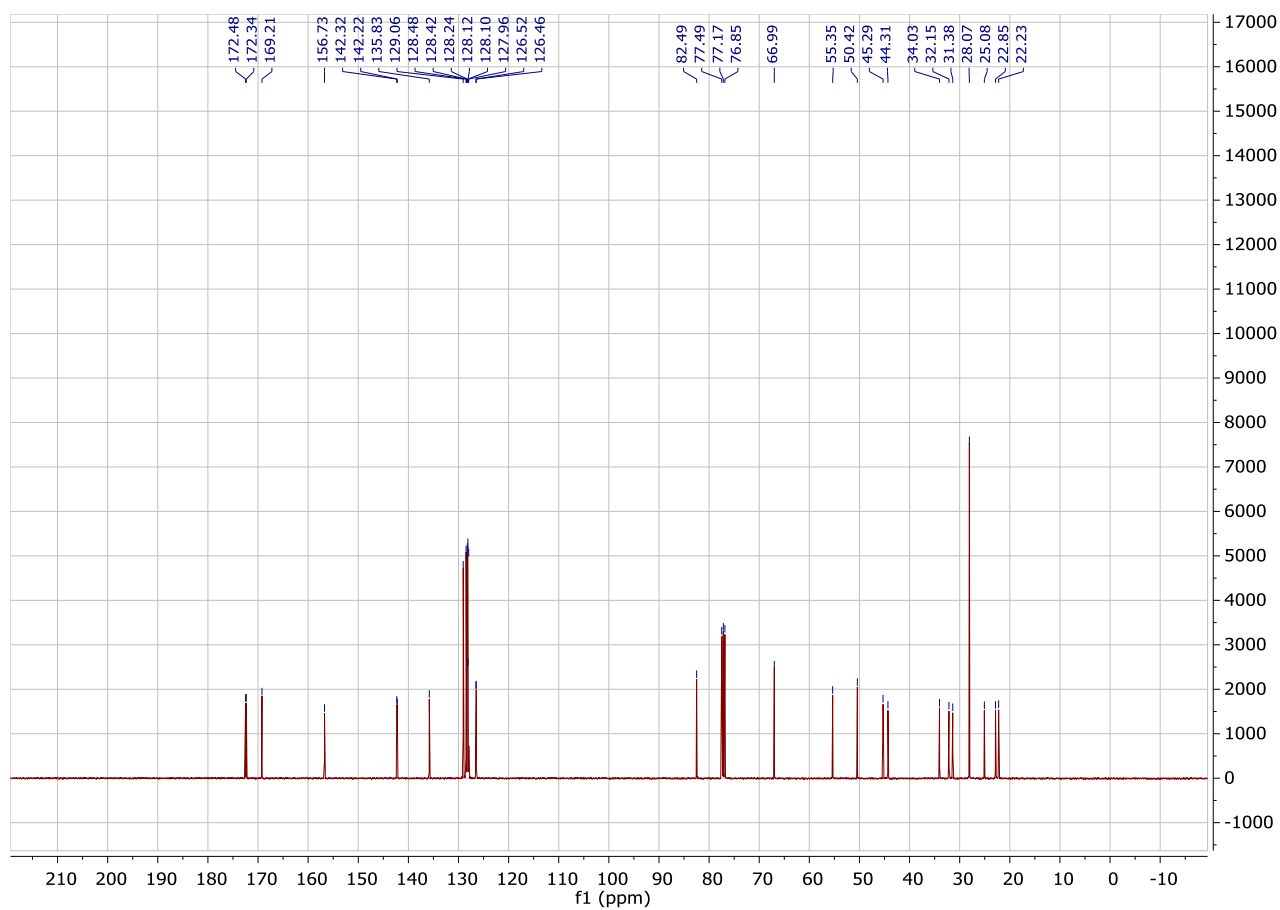


$^1\text{H-NMR}$ (400 MHz, CDCl_3)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)



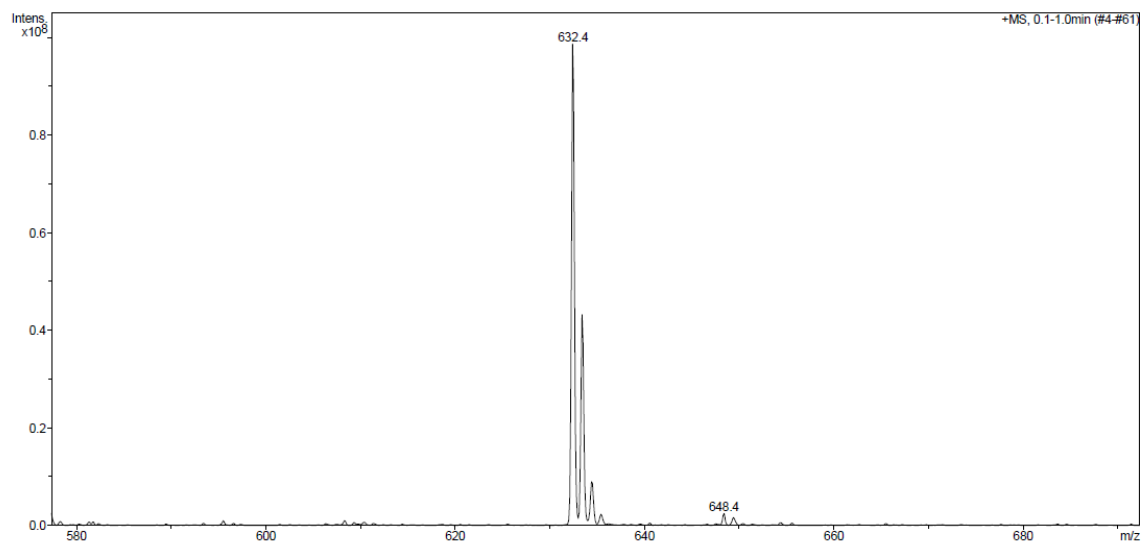
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

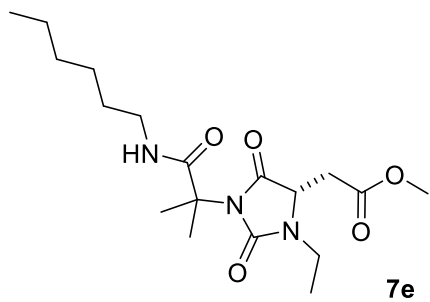
Analysis Name av gc78.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Cristina

Acquisition Date 07/25/18 15:35:31
Method Copy of _01tmix_posneg
Im.MS

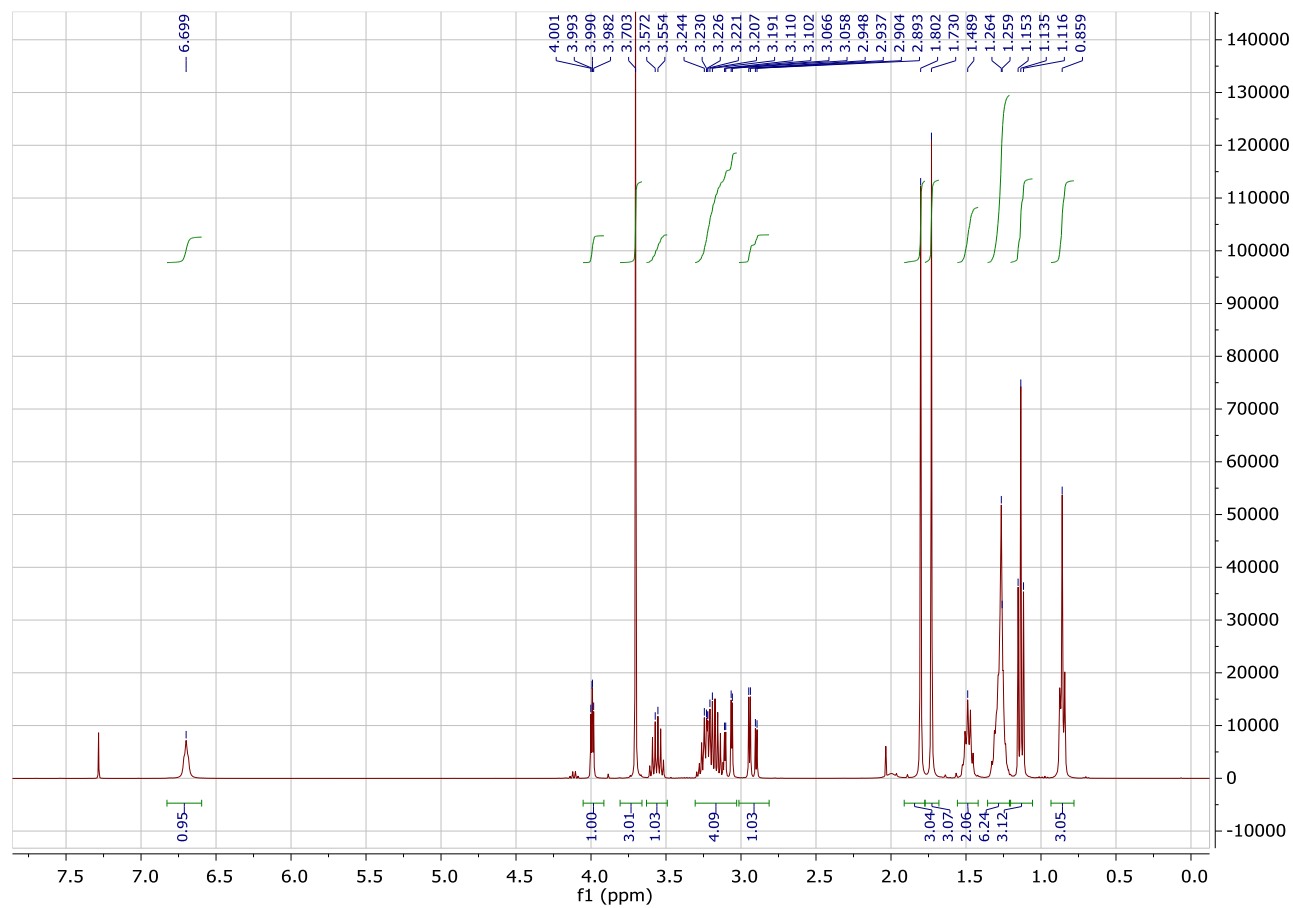
Operator
Instrument

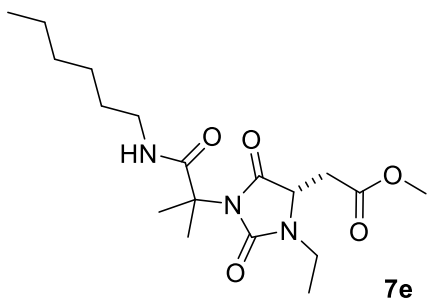
Walter Panzeri
esquire3000plus



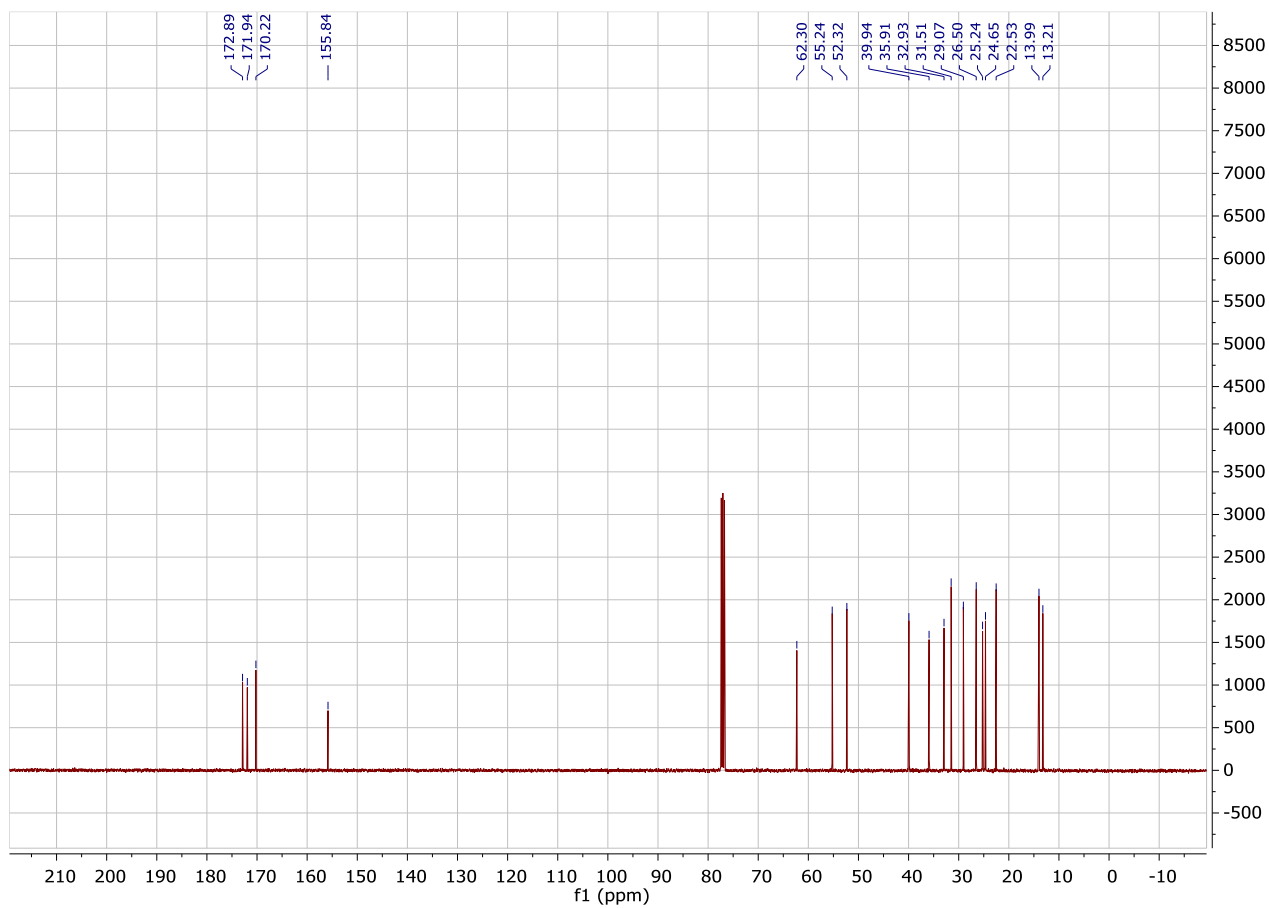


$^1\text{H-NMR}$ (400 MHz, CDCl_3)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)

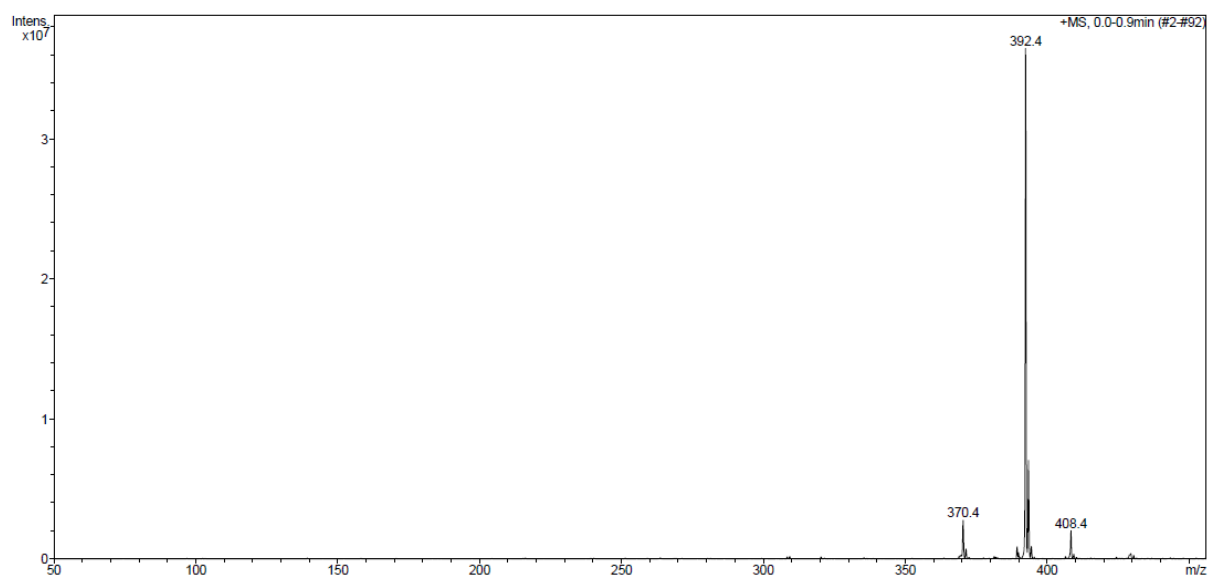


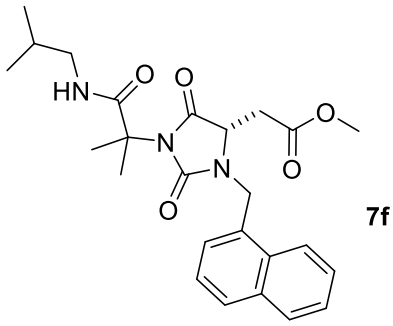
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name av gc20_c.d
Sample Name
Comment 1 mg/ml H2O
Richiedente: Cristina

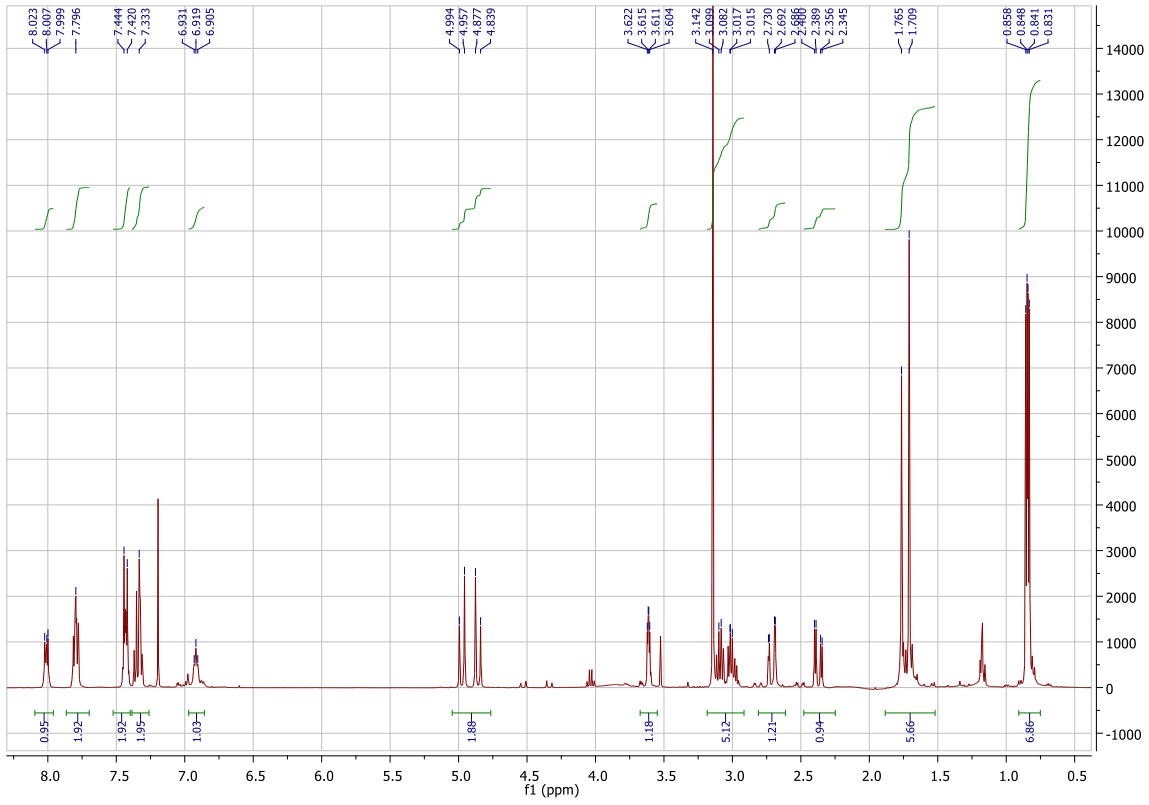
Acquisition Date 01/26/18 14:43:10
Method Copy of _01tmix_posneg
Im.MS

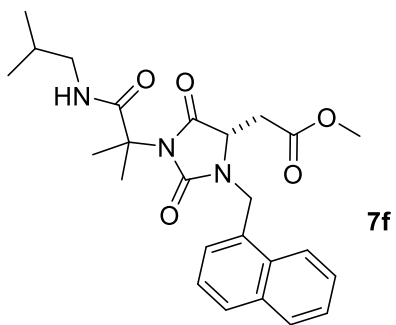
Operator Walter Panzeri
Instrument esquire3000plus



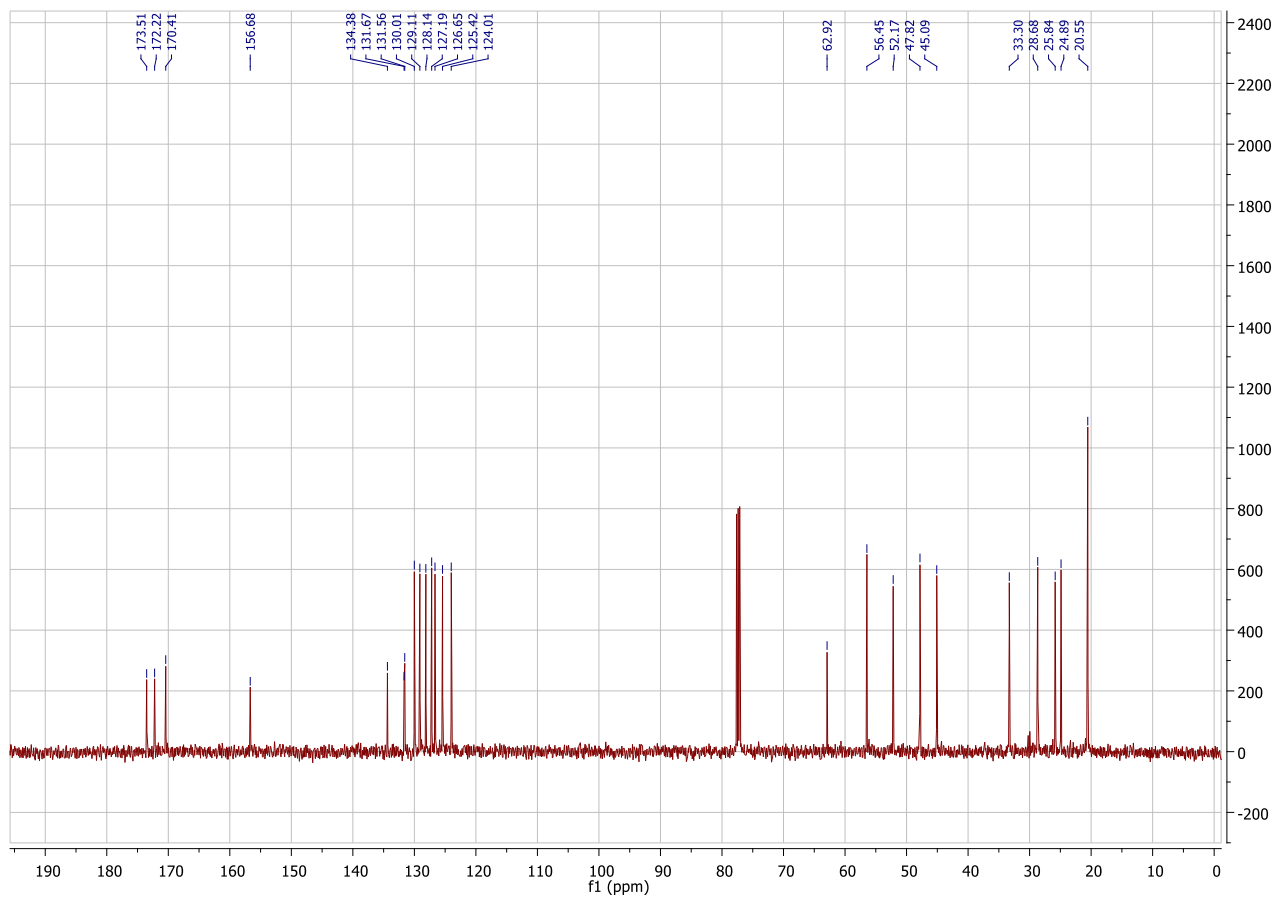


$^1\text{H-NMR}$ (400 MHz, CDCl_3)



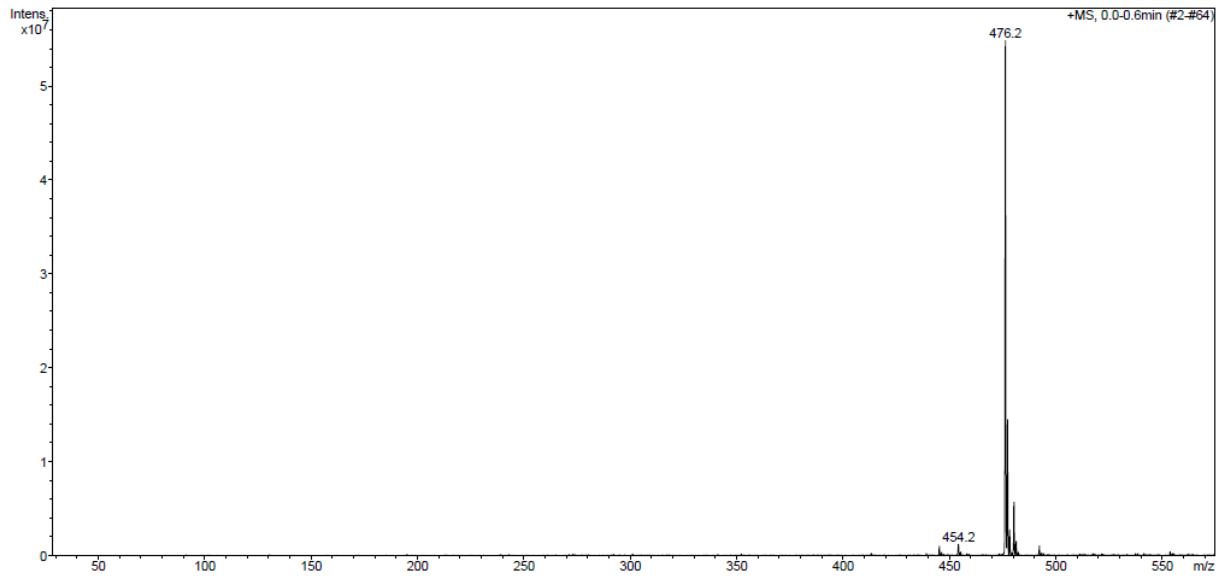


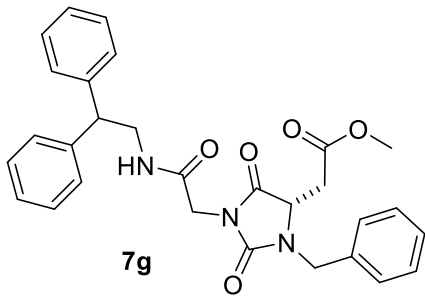
$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)



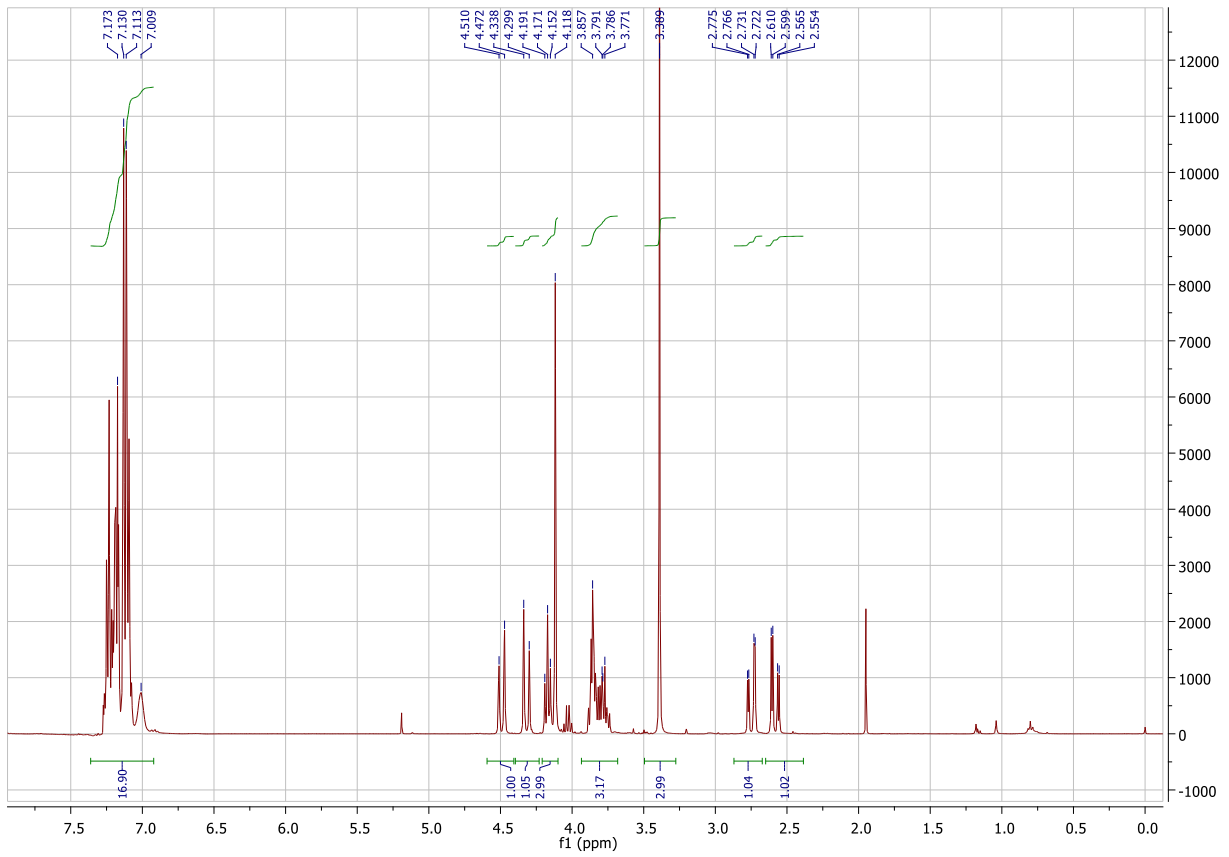
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

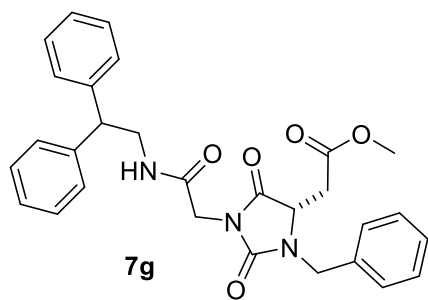
Analysis Name	av gc50.d	Acquisition Date	05/22/18 12:26:44	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Cristina		Im.MS		



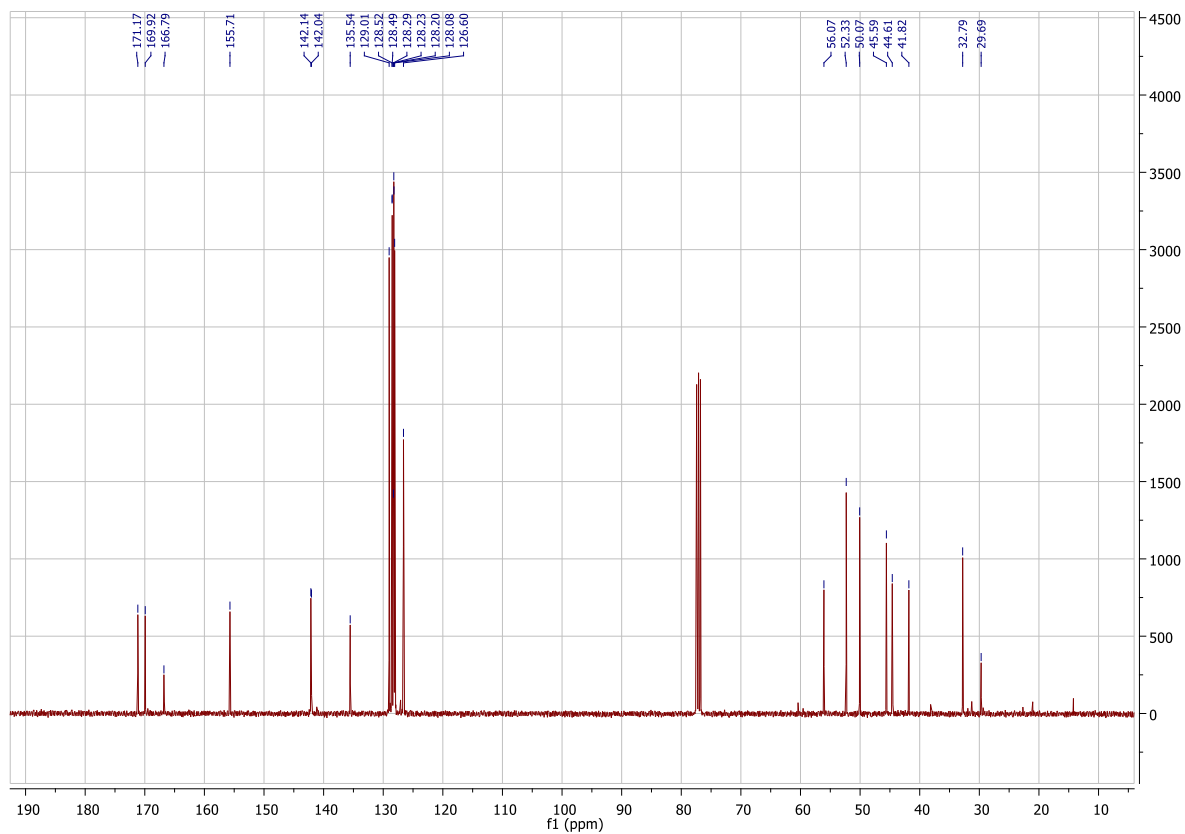


$^1\text{H-NMR}$ (400 MHz, CDCl_3)



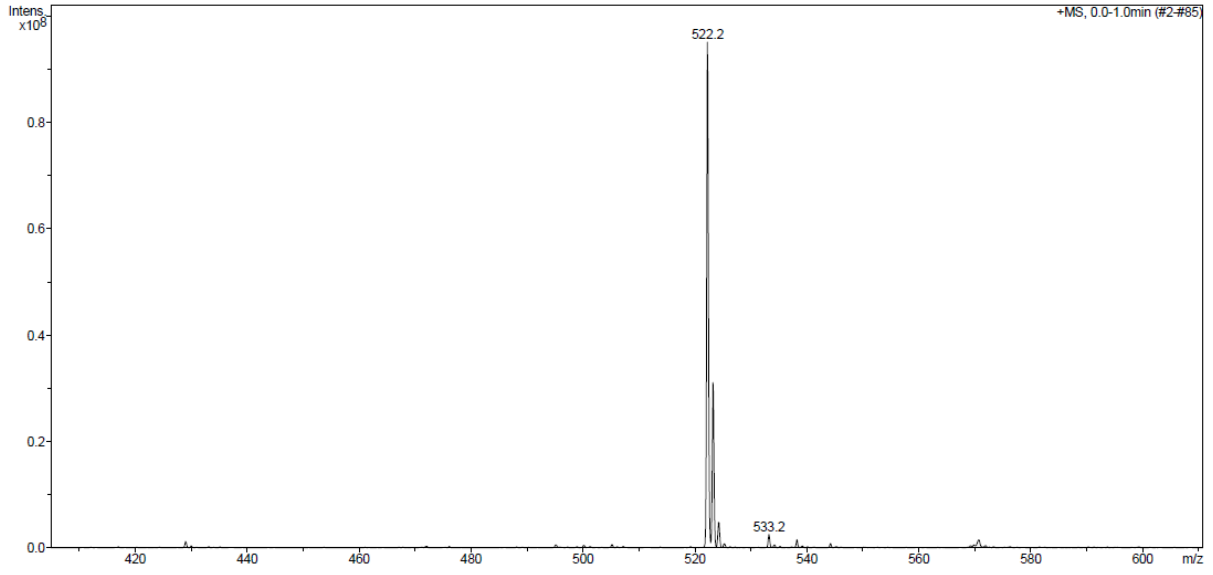


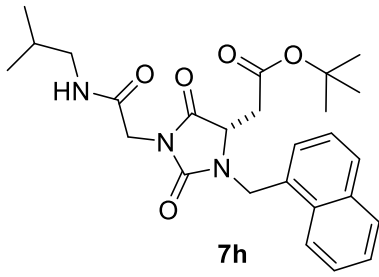
$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)



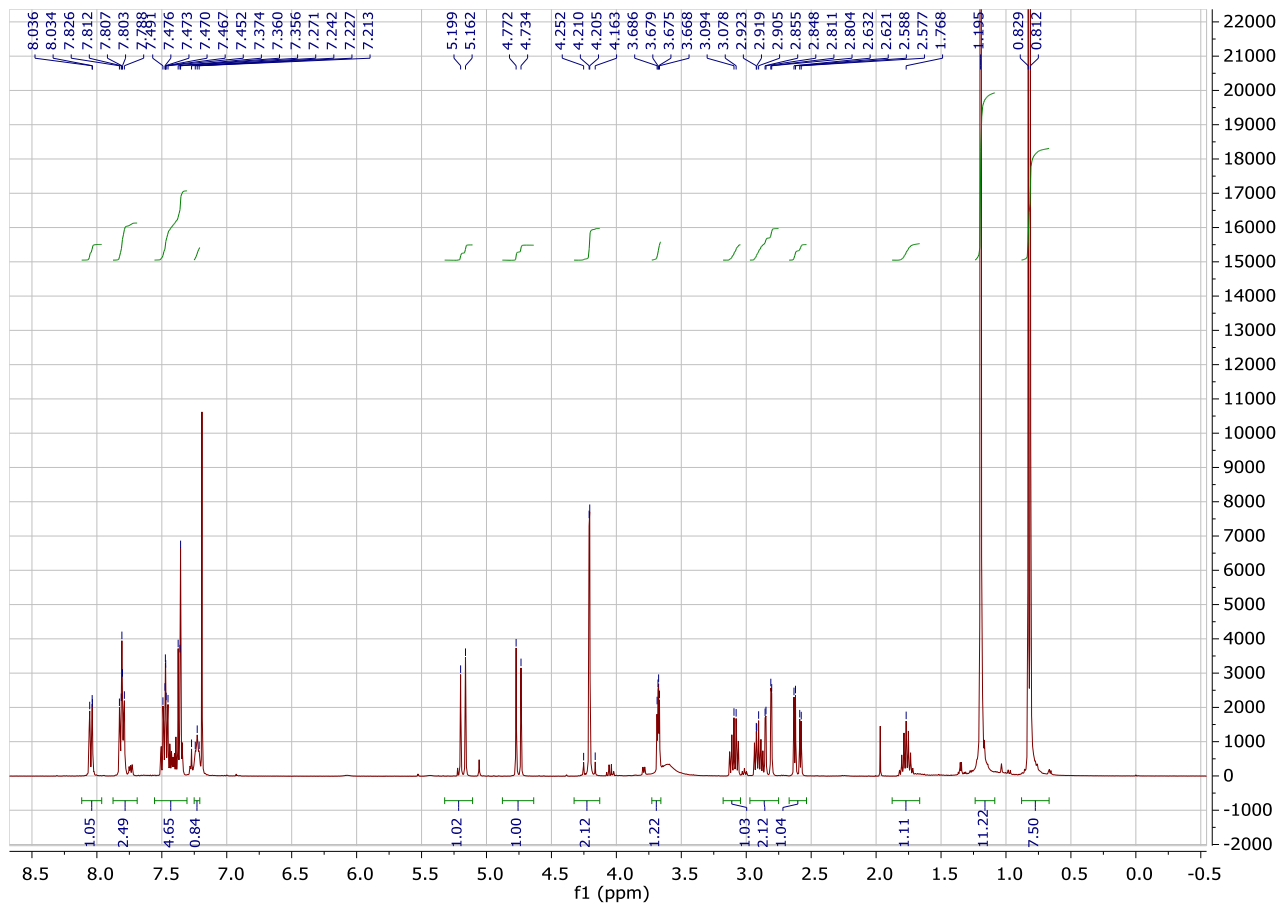
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

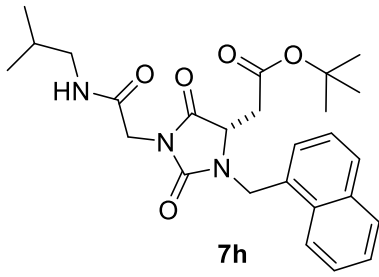
Analysis Name	av gc38.d	Acquisition Date	04/16/18 09:30:16	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg Im.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Cristina				



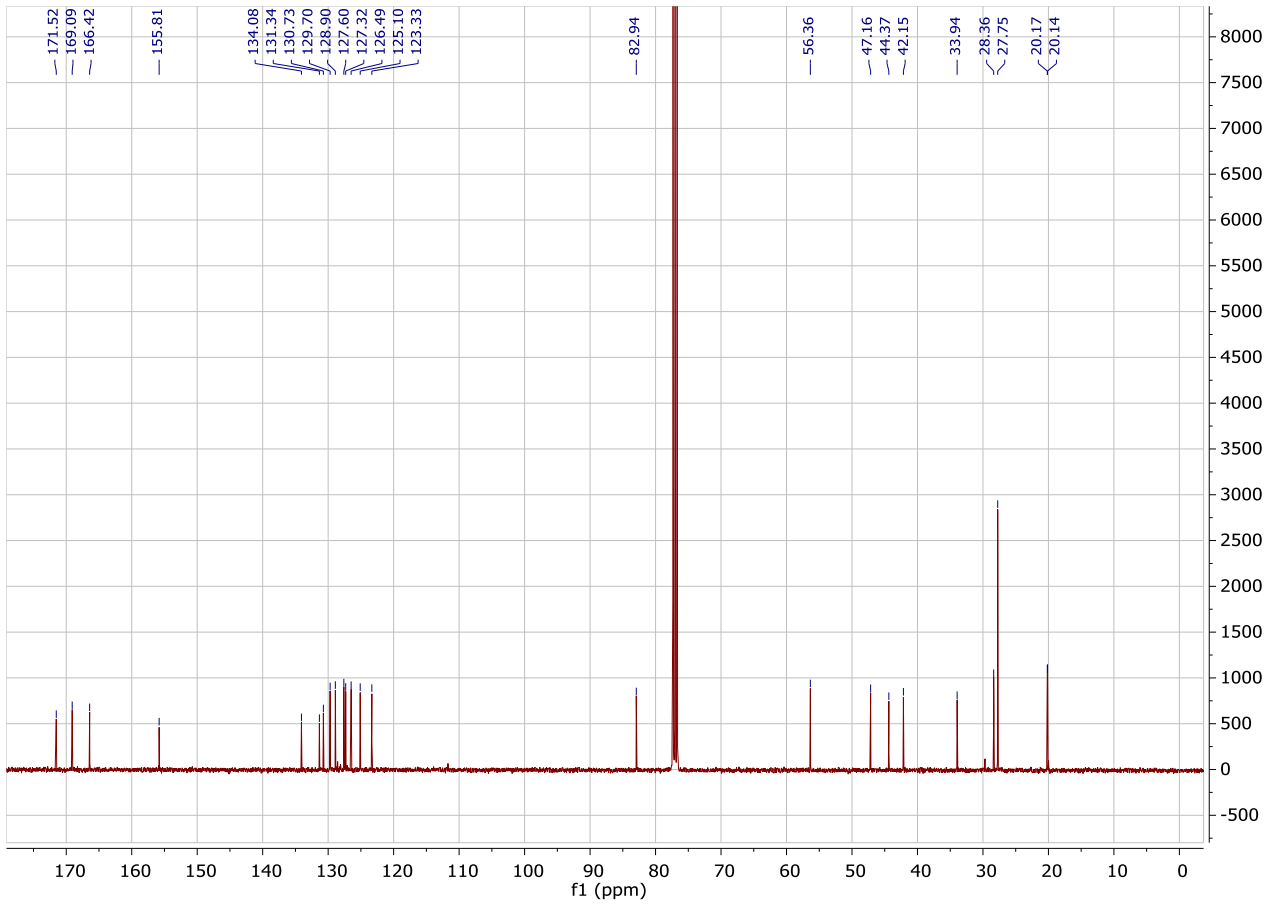


$^1\text{H-NMR}$ (400 MHz, CDCl_3)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)

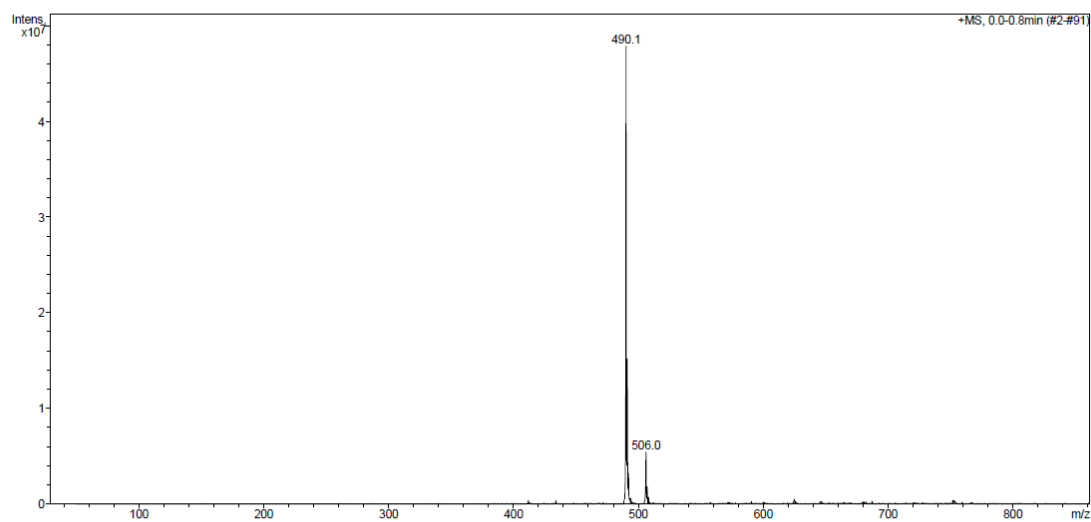


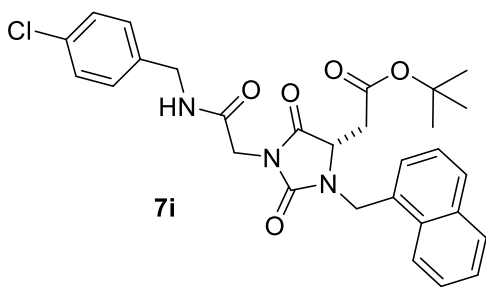
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name av ac069.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Caramiello

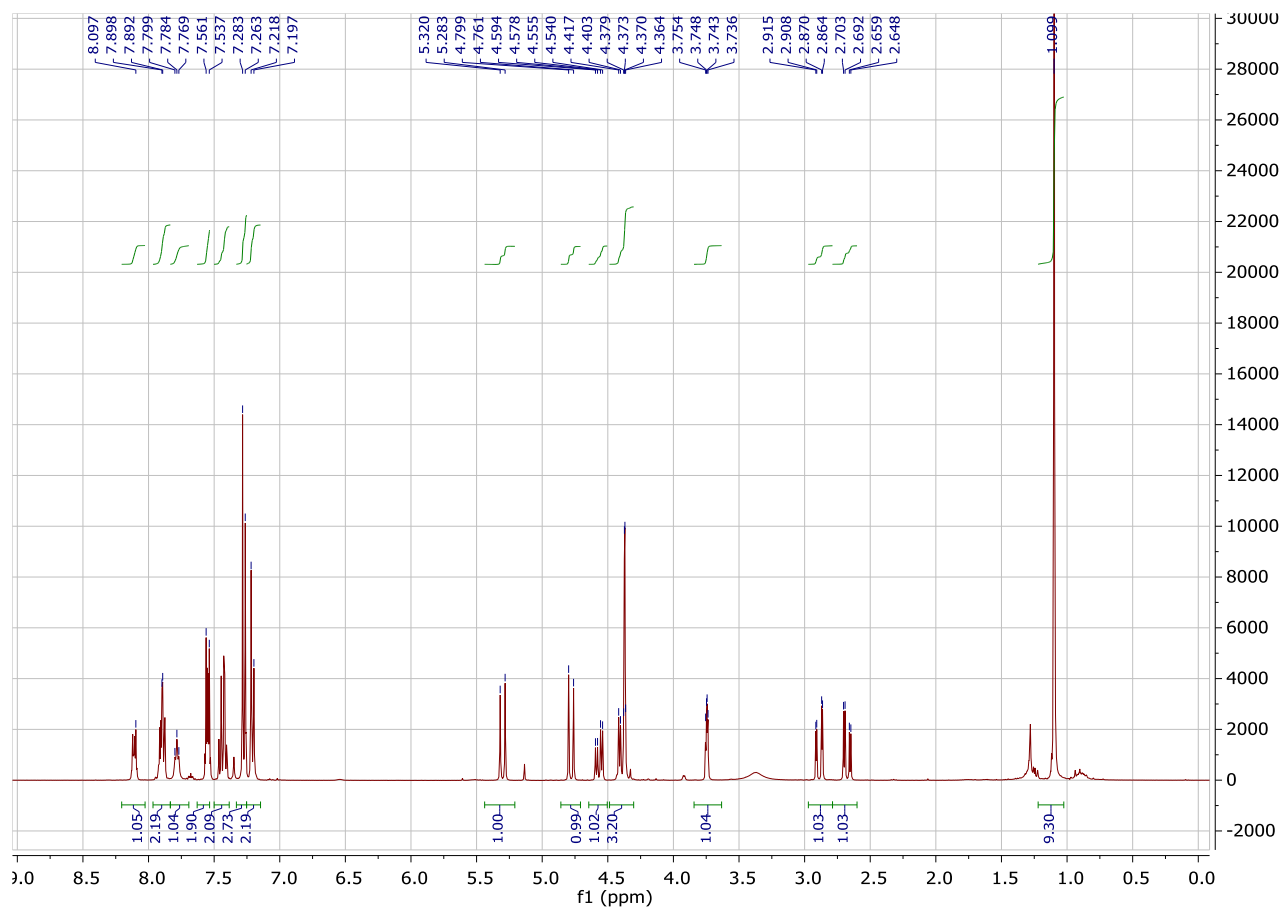
Acquisition Date 08/31/20 13:39:32
Method Copy of SPW_TBLM.MS

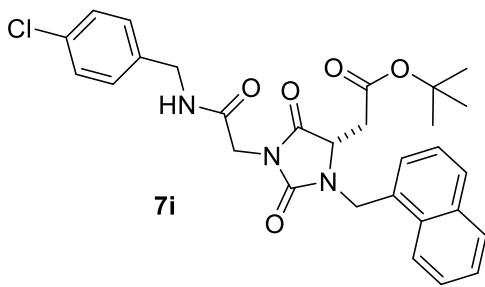
Operator Walter Panzeri
Instrument esquire3000plus



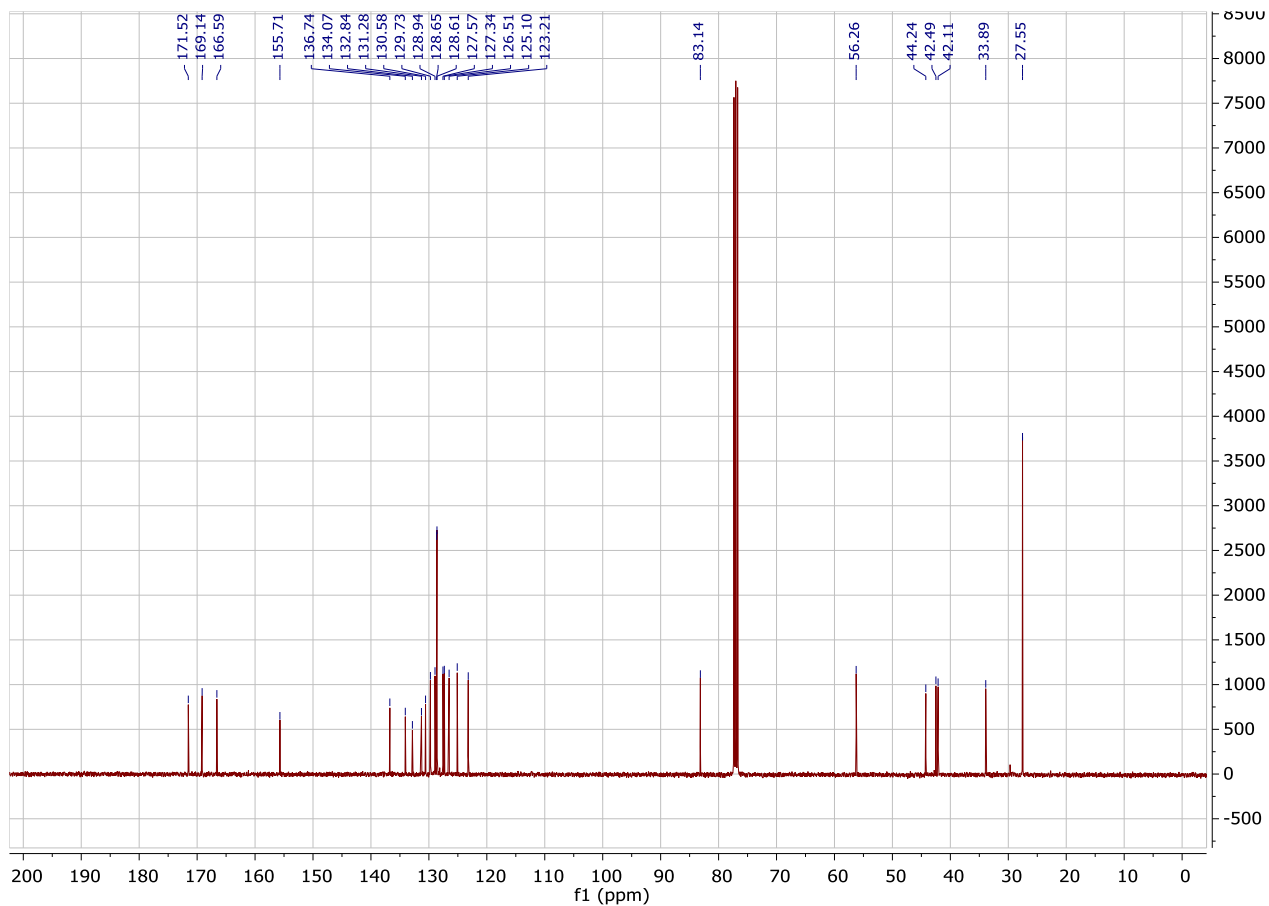


$^1\text{H-NMR}$ (400 MHz, CDCl_3)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)

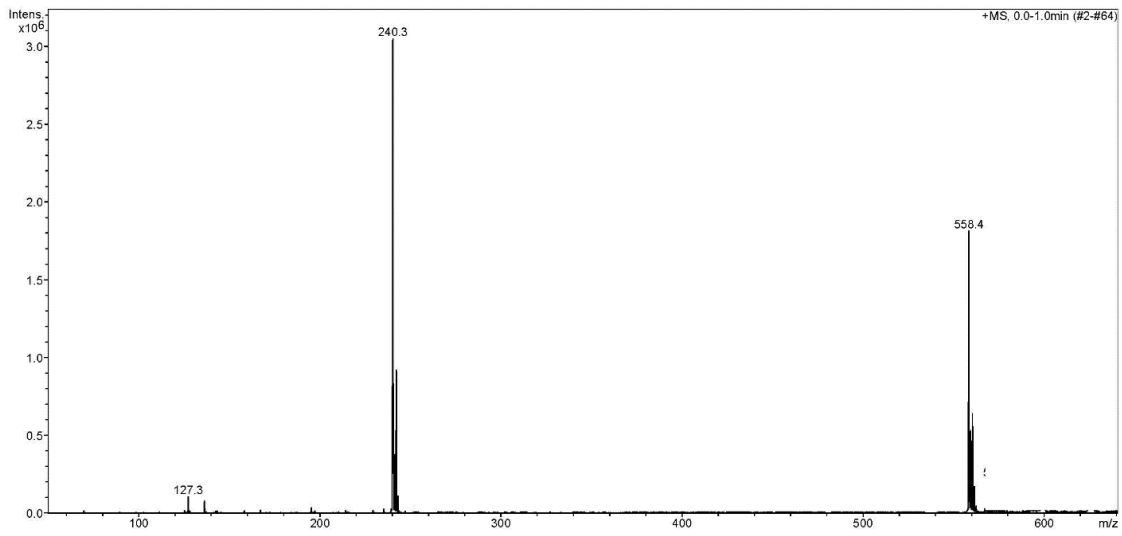


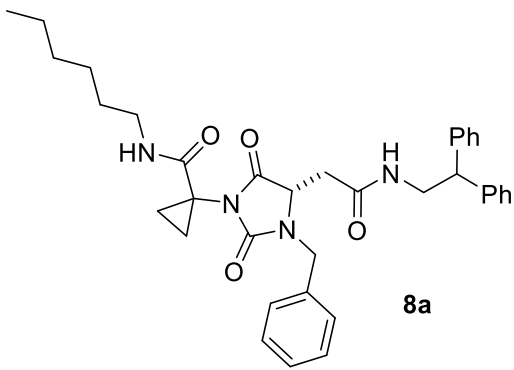
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name av ac194.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Mapanesi Alessia

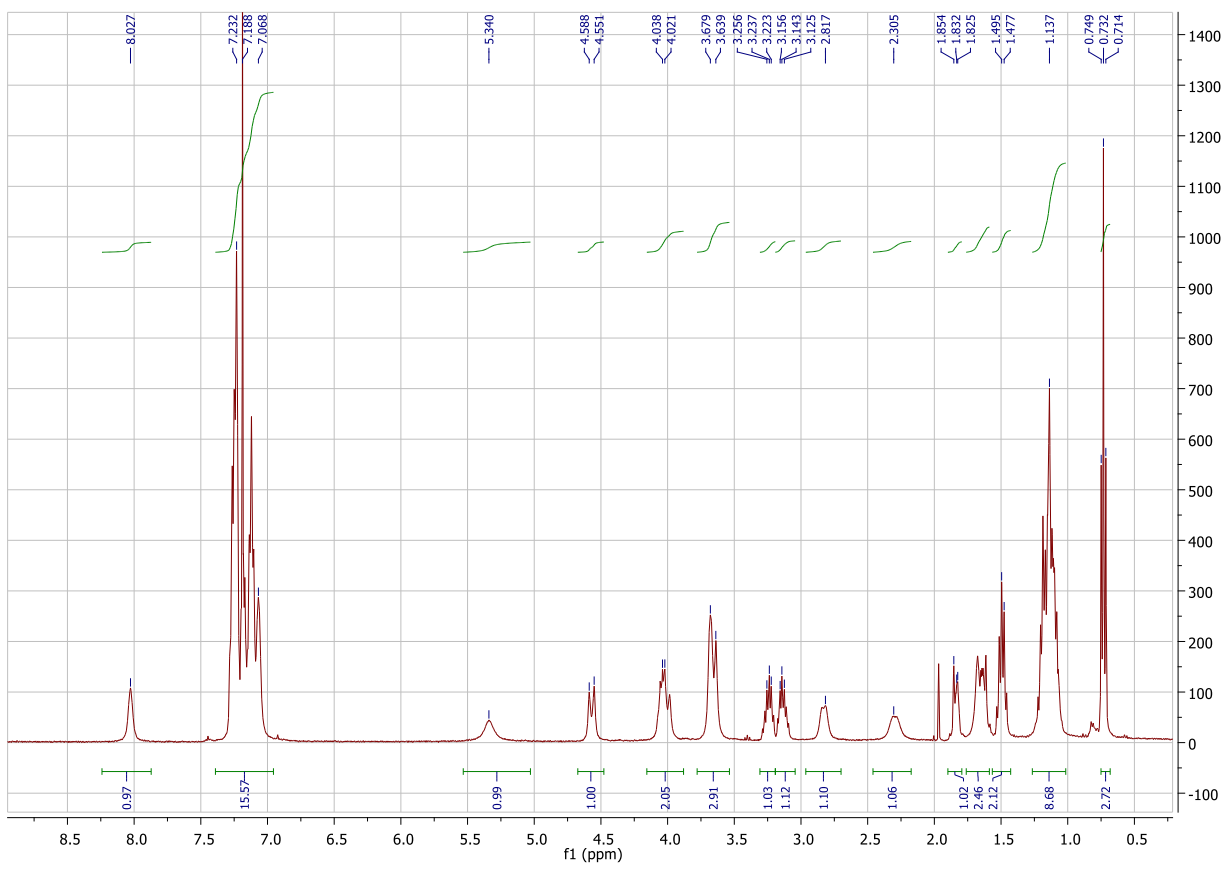
Acquisition Date 03/18/22 11:28:34
Method Copy of \$opt0622.MS

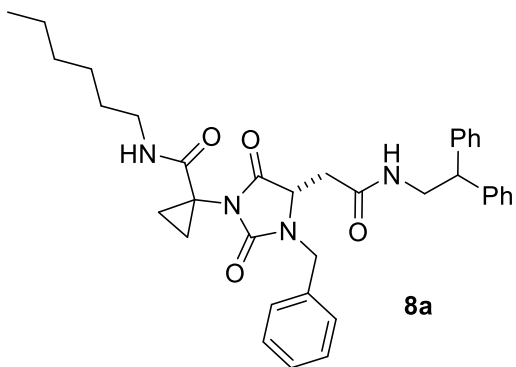
Operator Walter Panzeri
Instrument esquire3000plus



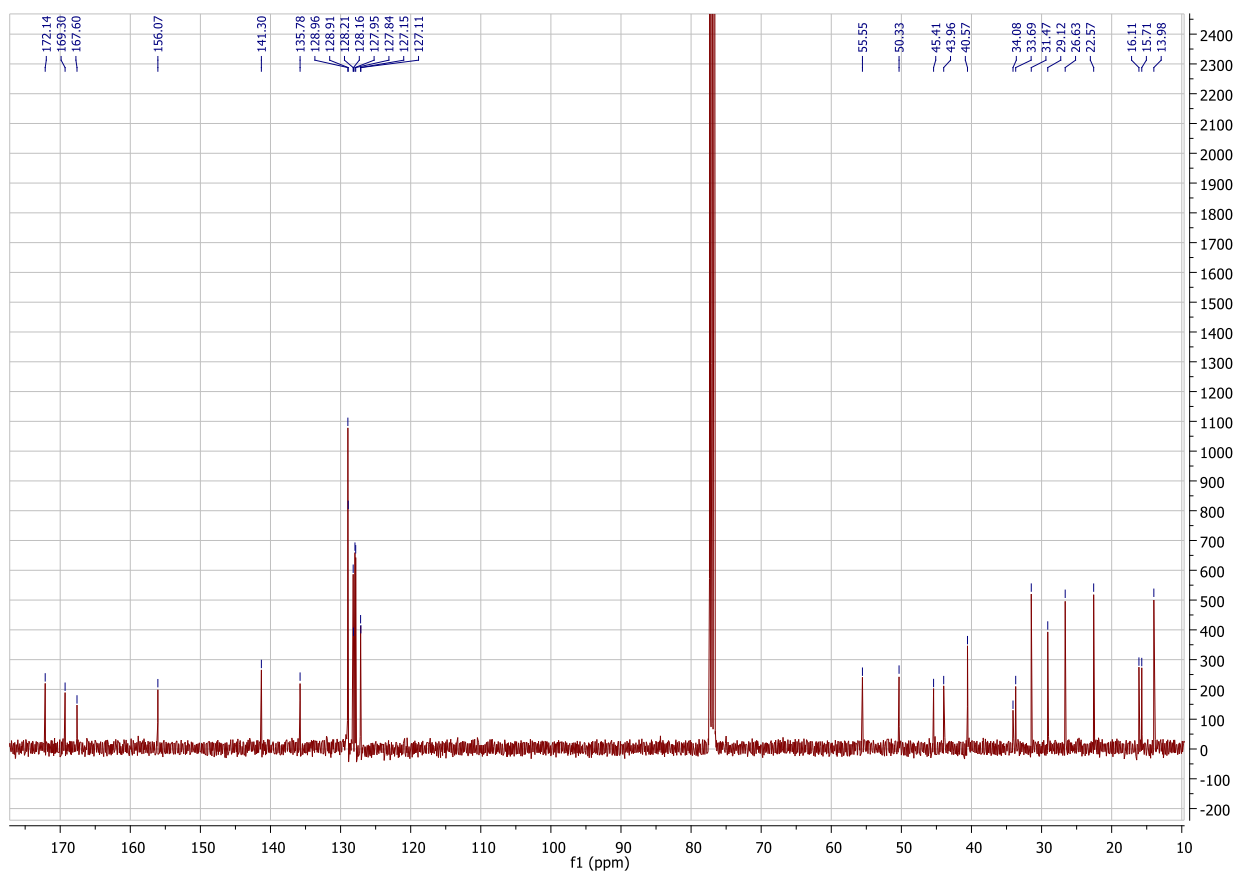


$^1\text{H-NMR}$ (400 MHz, CDCl_3)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)

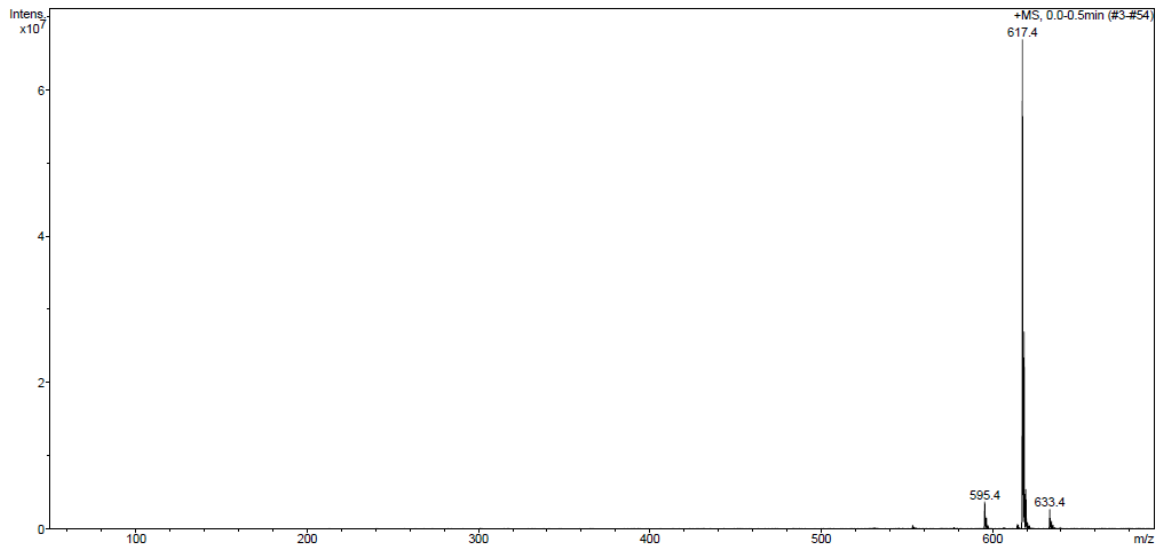


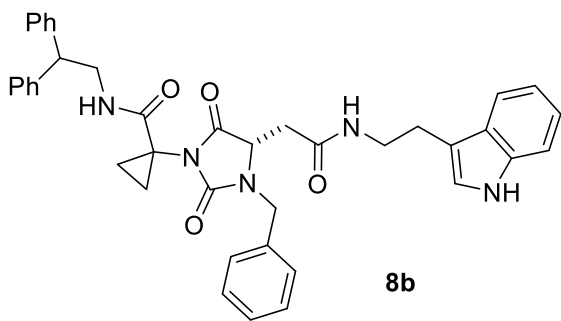
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name av fm2856.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Frigeno

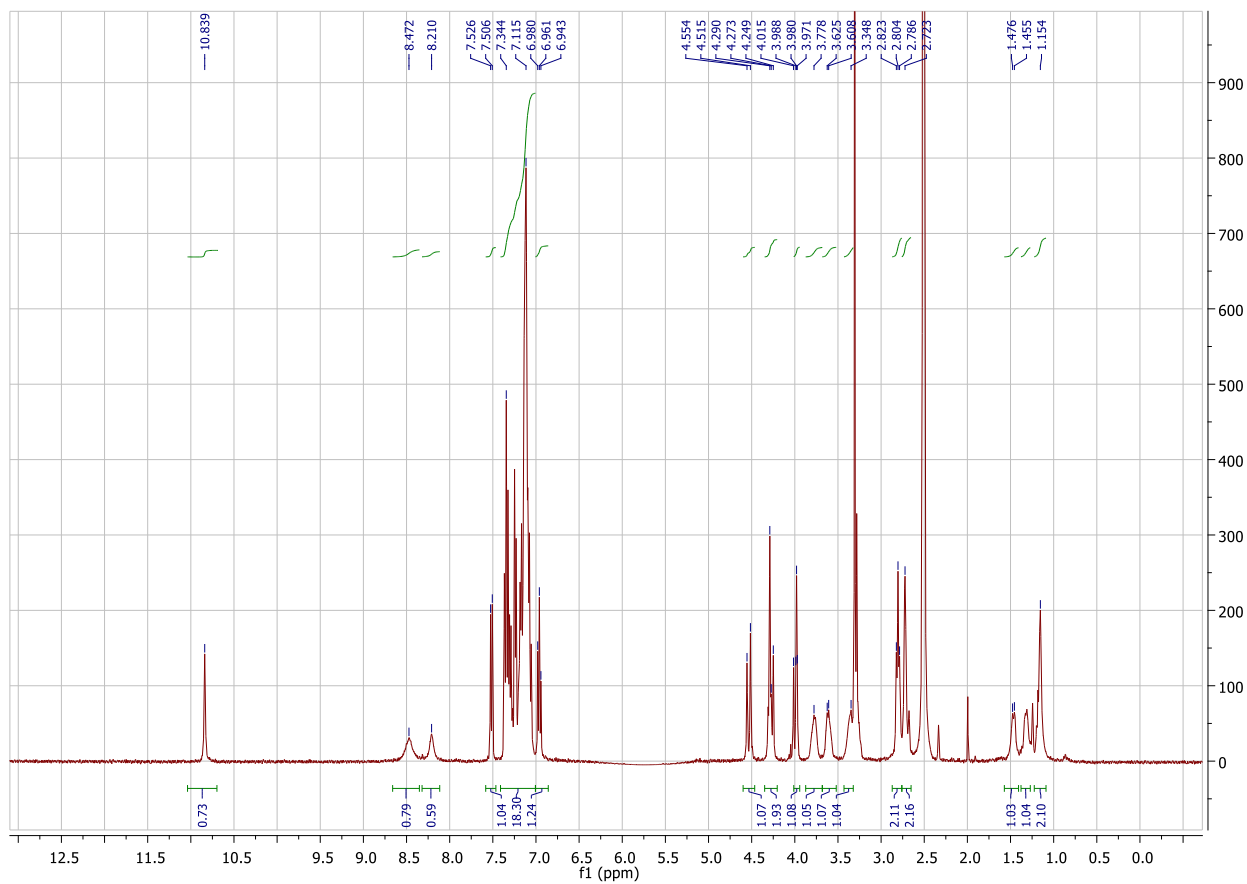
Acquisition Date 07/13/17 13:23:26
Method Copy of _01tmix_posneg
Im.MS

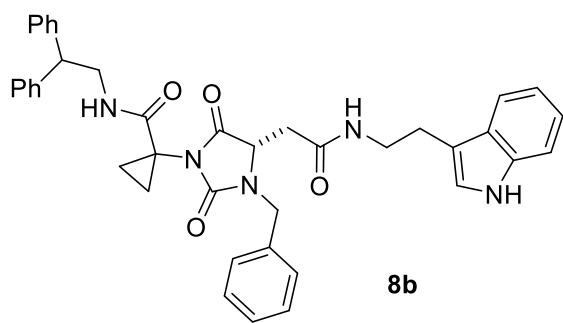
Operator Walter Panzeri
Instrument esquire3000plus



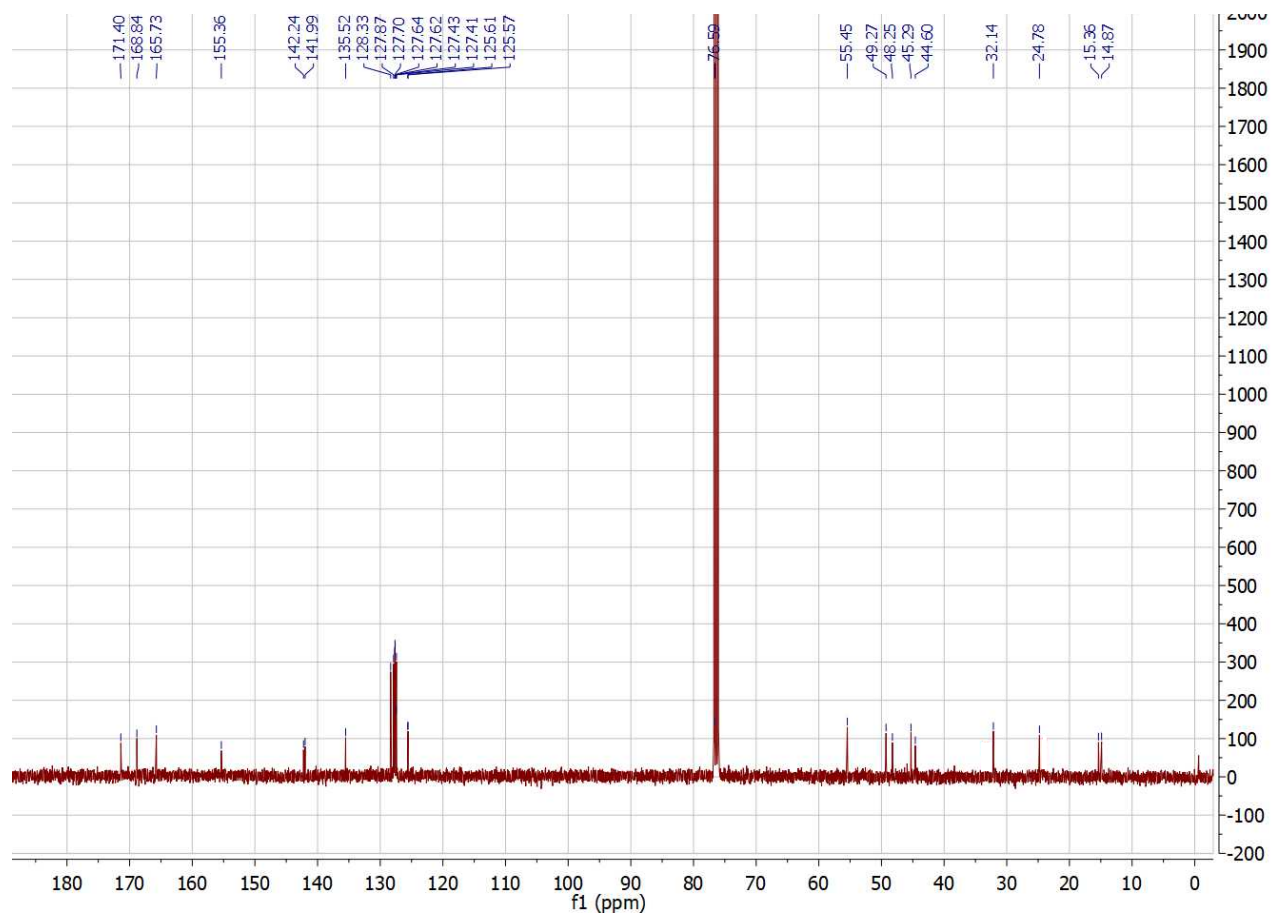


$^1\text{H-NMR}$ (101 MHz, $\text{dms}\text{-d}_6$)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)

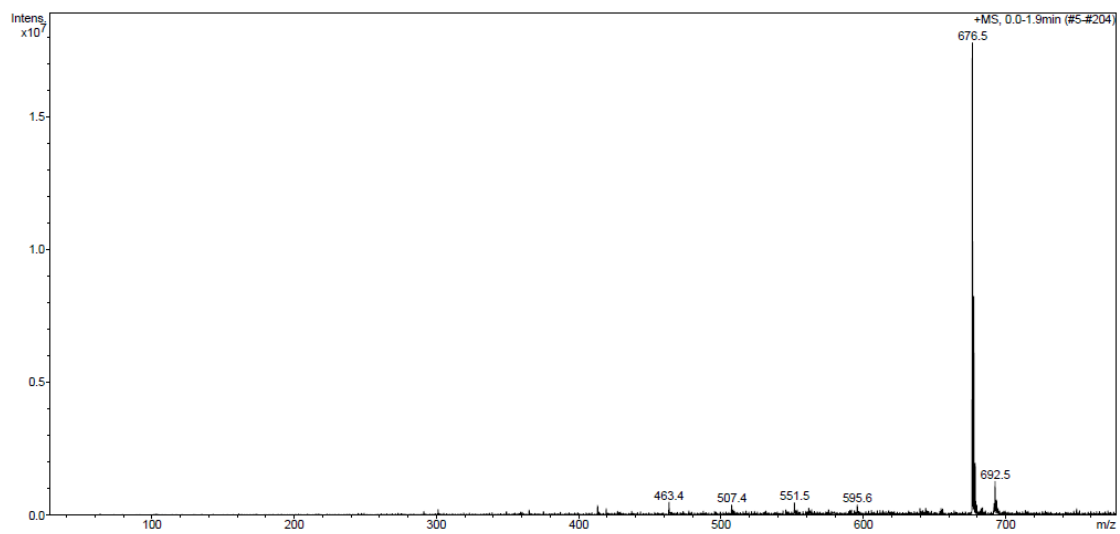


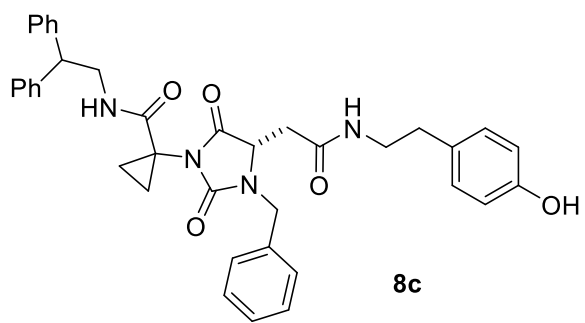
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name av gc111.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Cristina

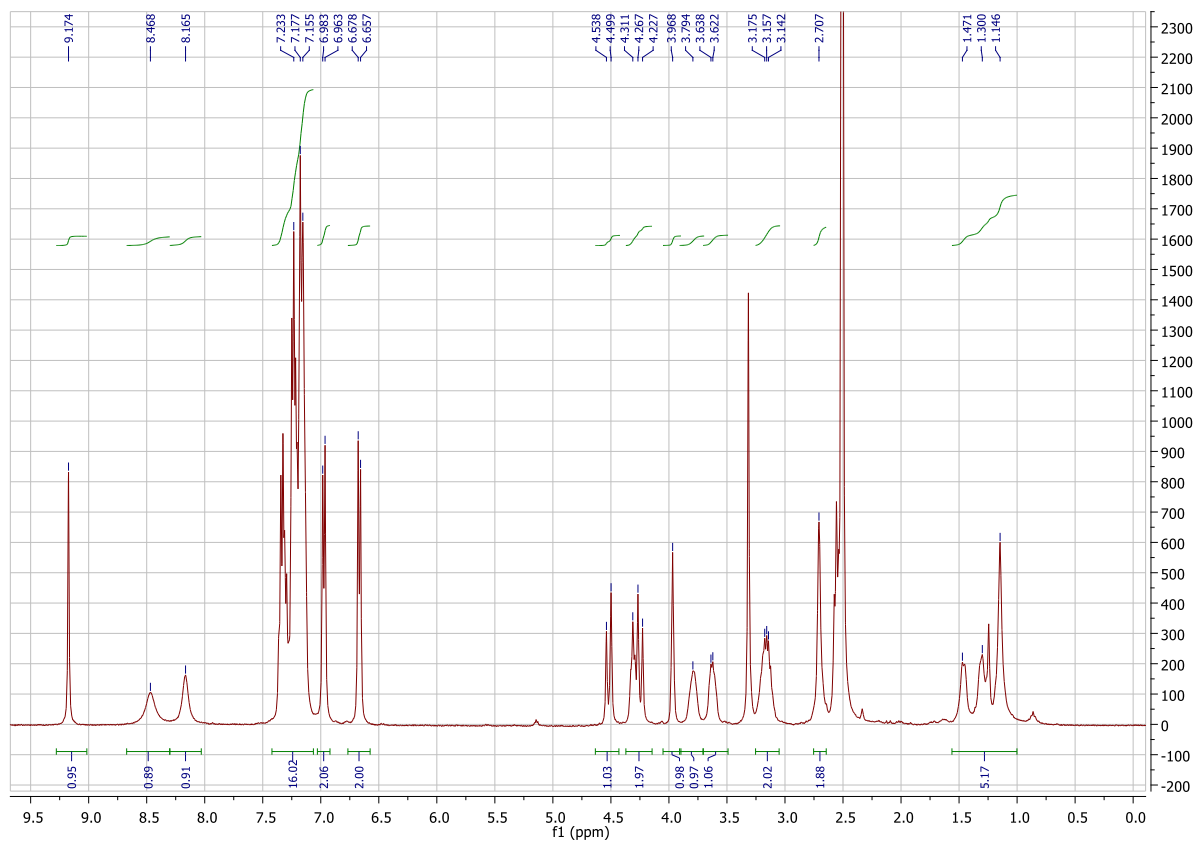
Acquisition Date 02/08/19 14:15:22
Method Copy of _01tmix_posneg
Im.MS

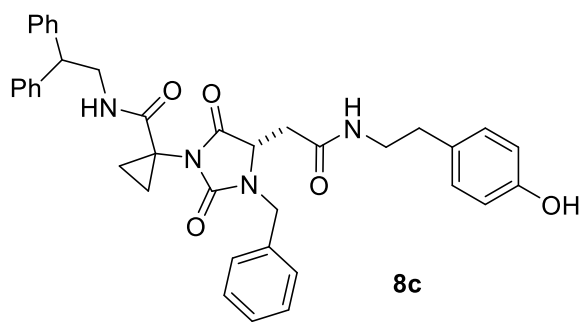
Operator Walter Panzeri
Instrument esquire3000plus



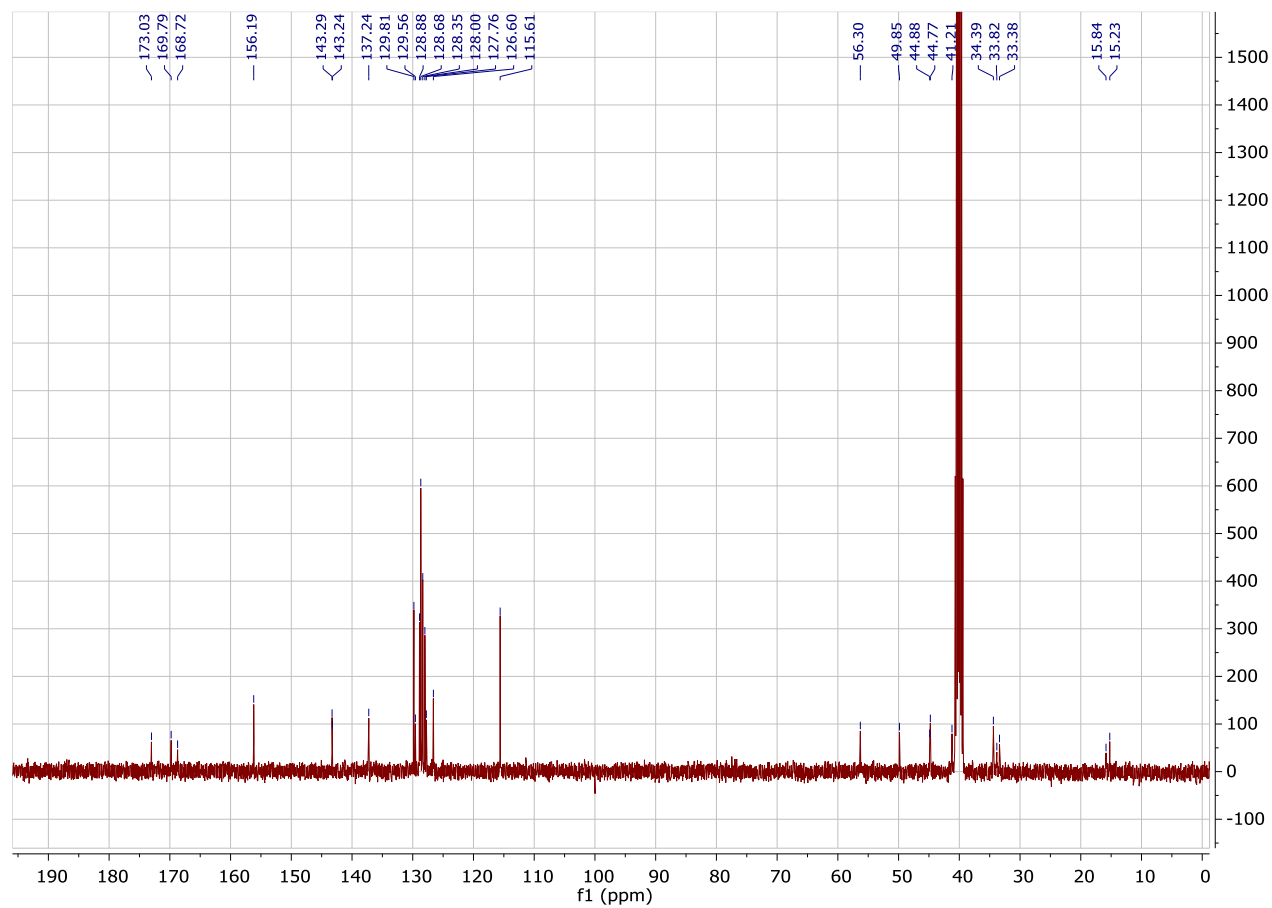


$^1\text{H-NMR}$ (400 MHz, $\text{dms}\text{-d}_6$)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, $\text{dms}\text{-d}_6$)



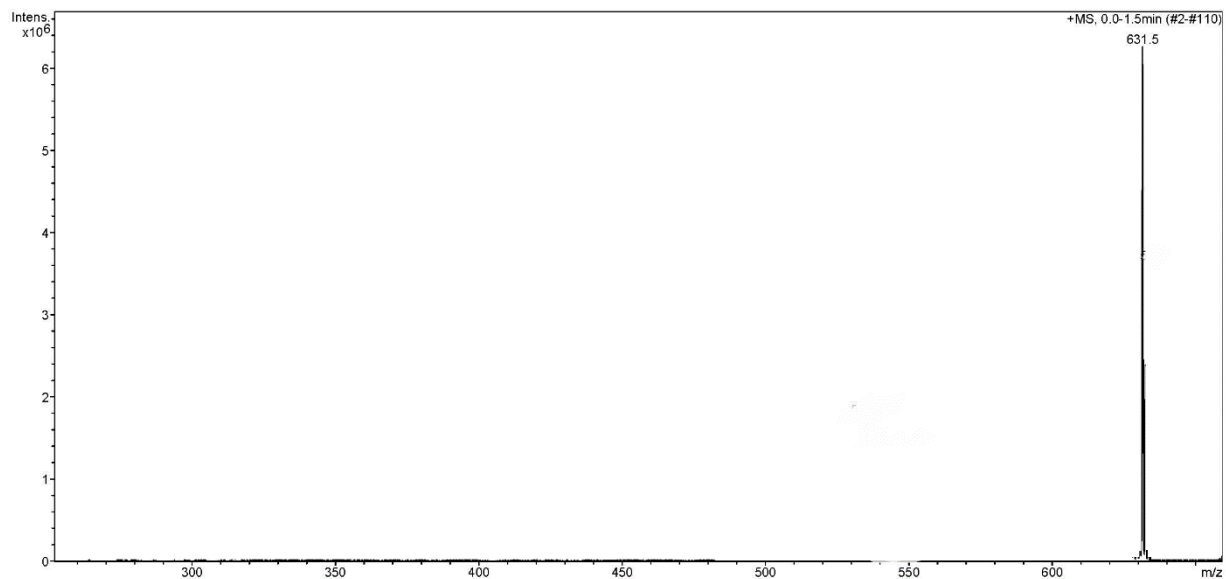
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

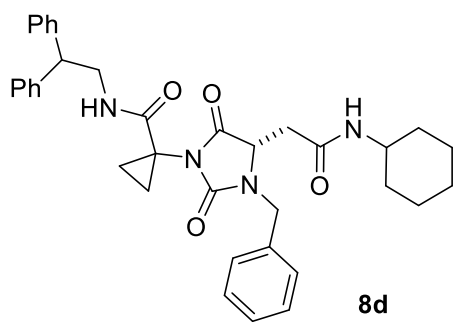
Analysis Name av ac 172.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
 Richiedente: Caramiello

Acquisition Date 11/10/21 10:44:30
Method Copy of \$opt0622.MS

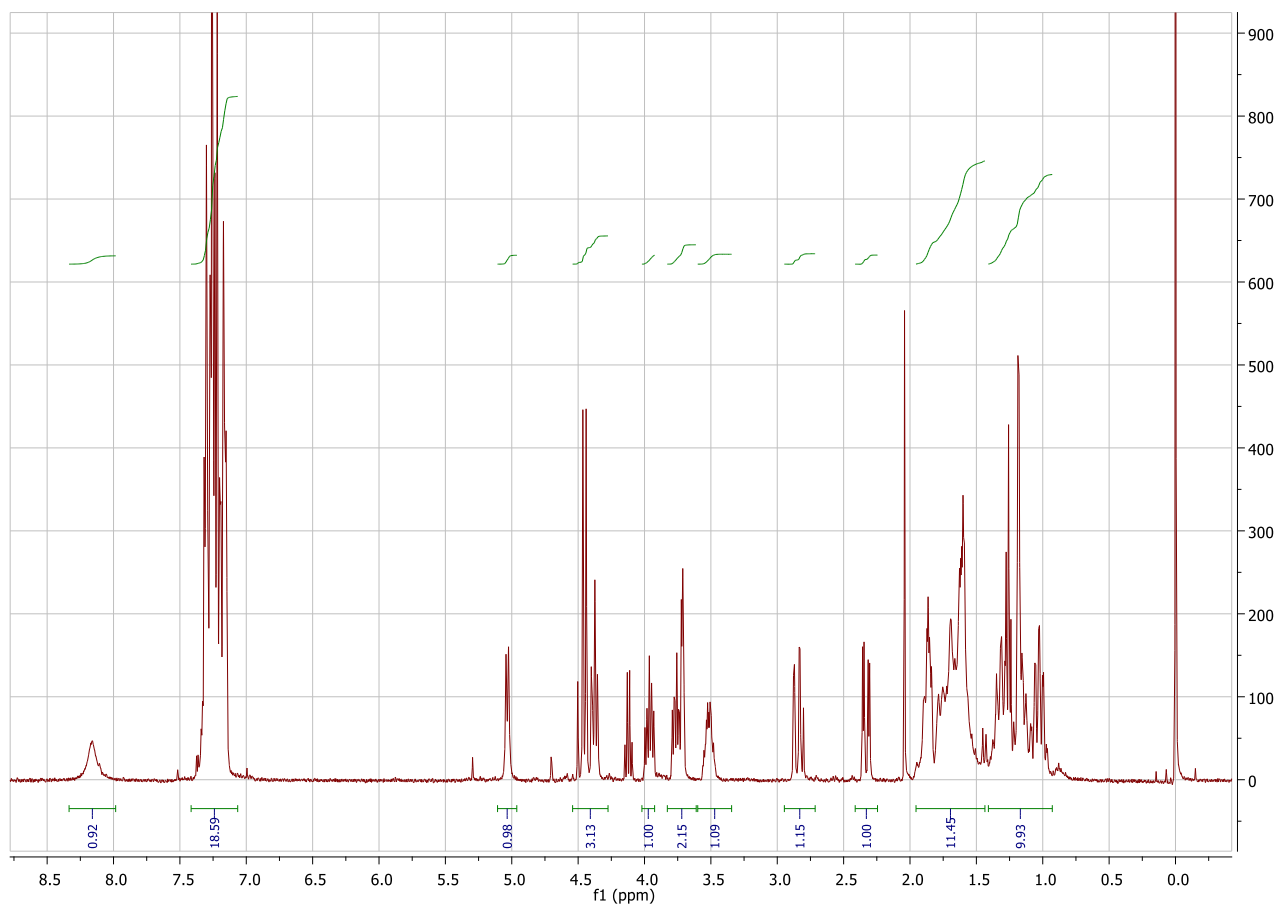
Operator
Instrument

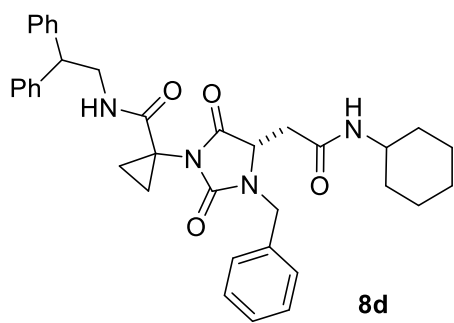
Walter Panzeri
esquire3000plus



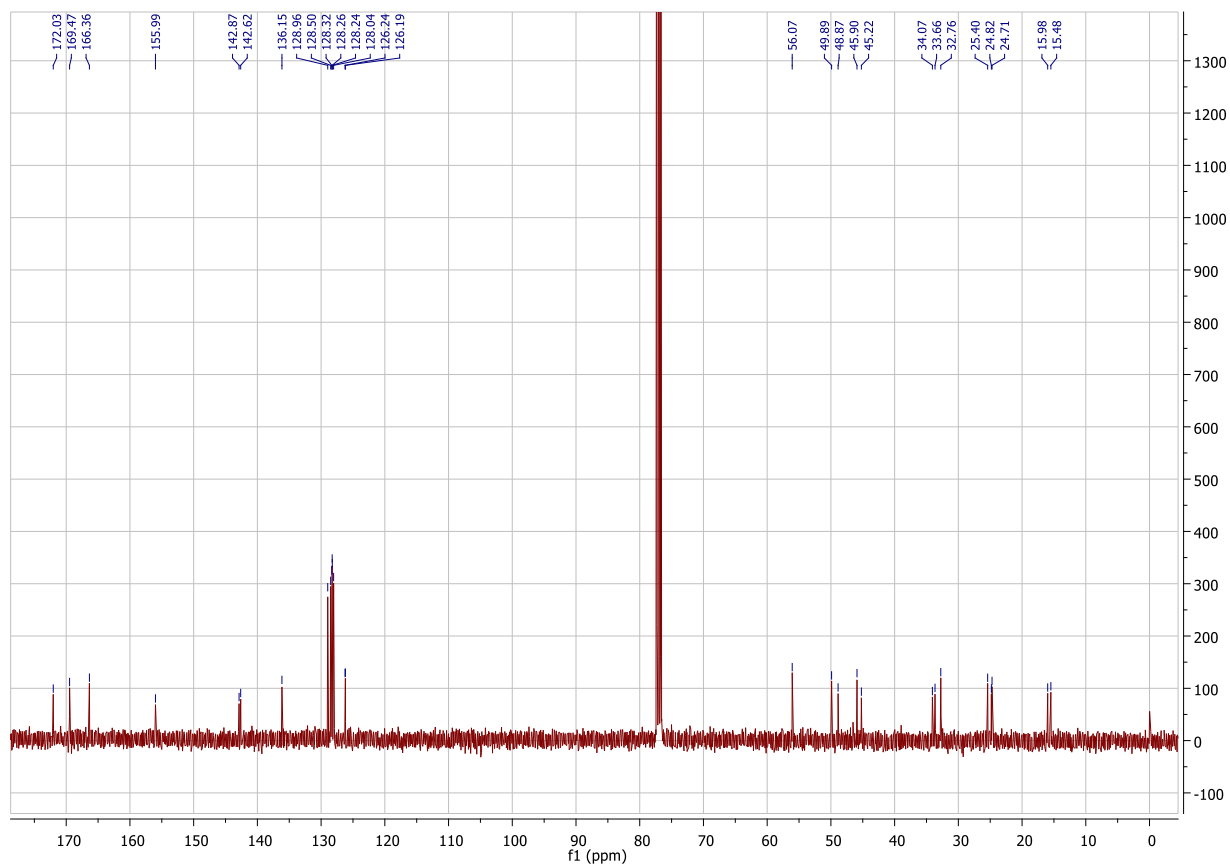


¹H-NMR (400 MHz, CDCl₃)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)

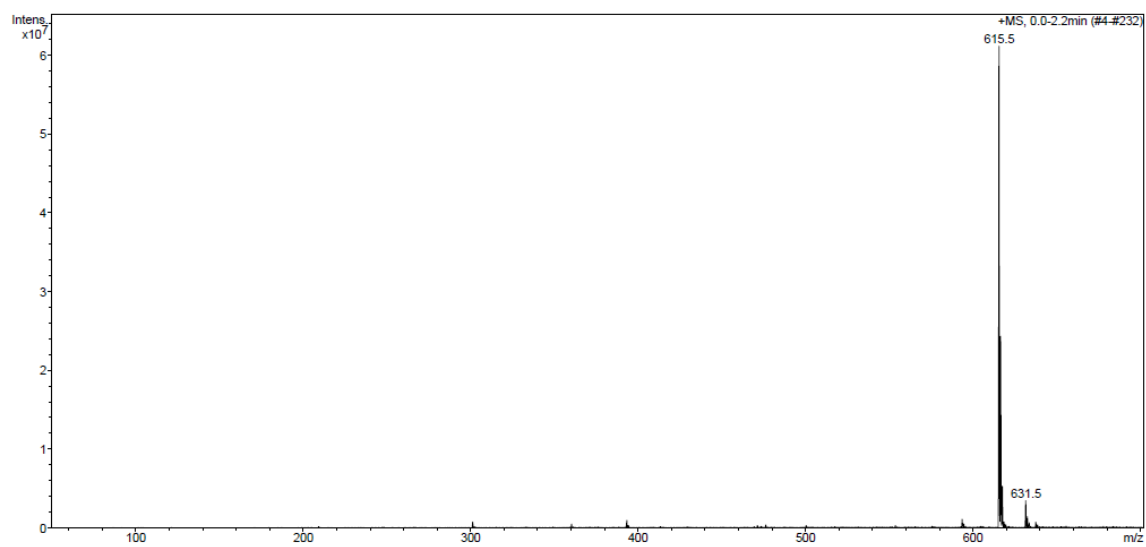


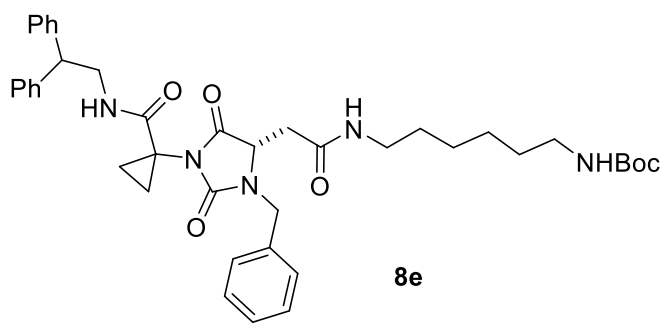
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name av fv2063.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Viani

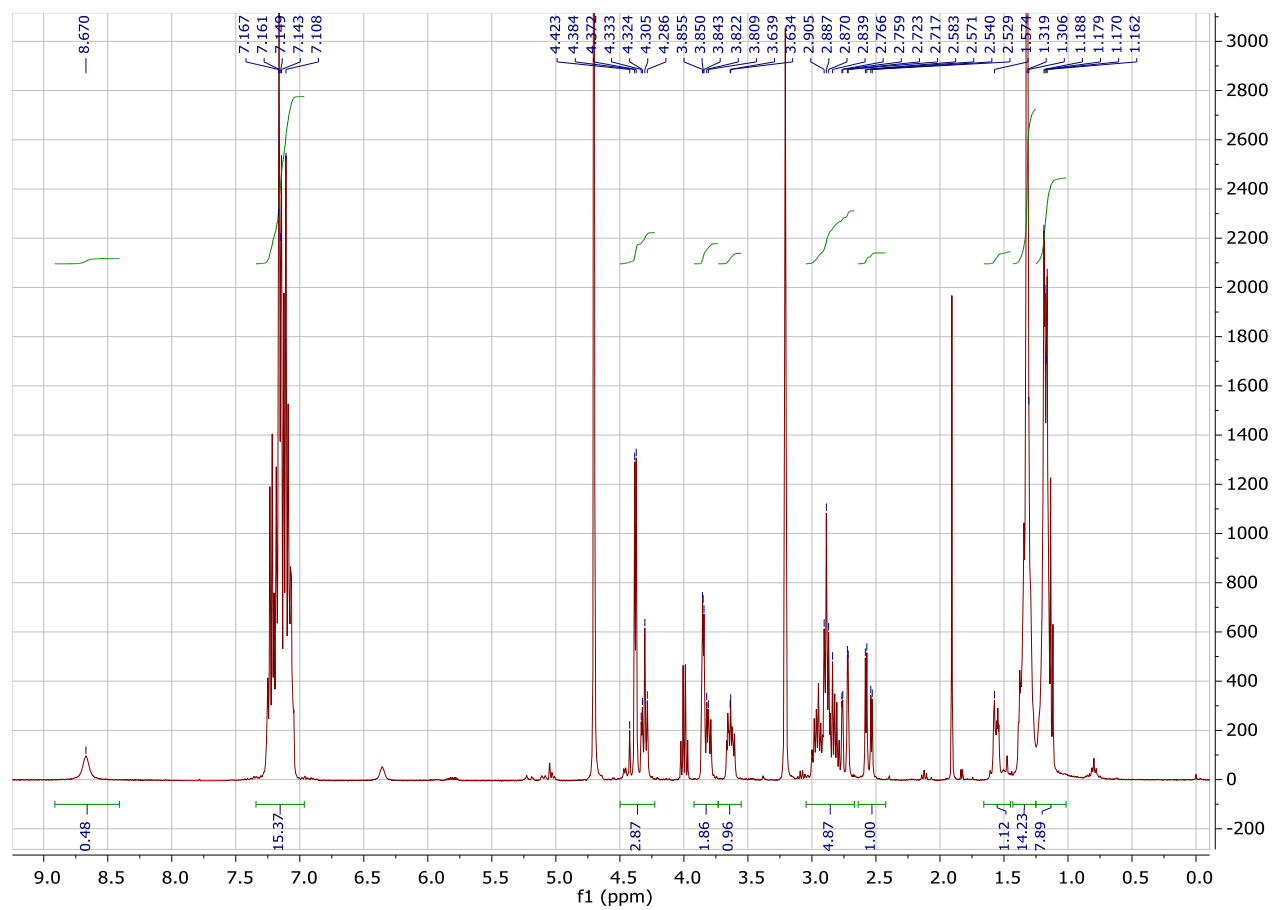
Acquisition Date 02/04/19 14:42:37
Method Copy of _01tmix_posneg
Int.MS

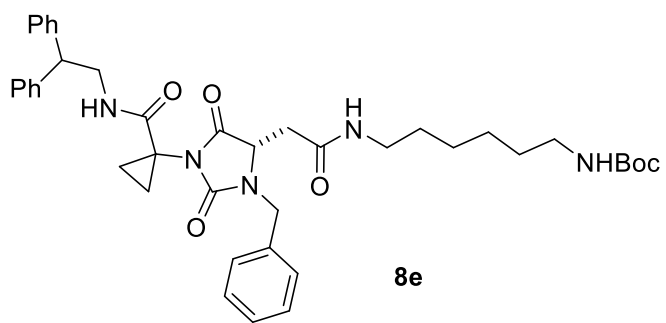
Operator Walter Panzeri
Instrument esquire3000plus



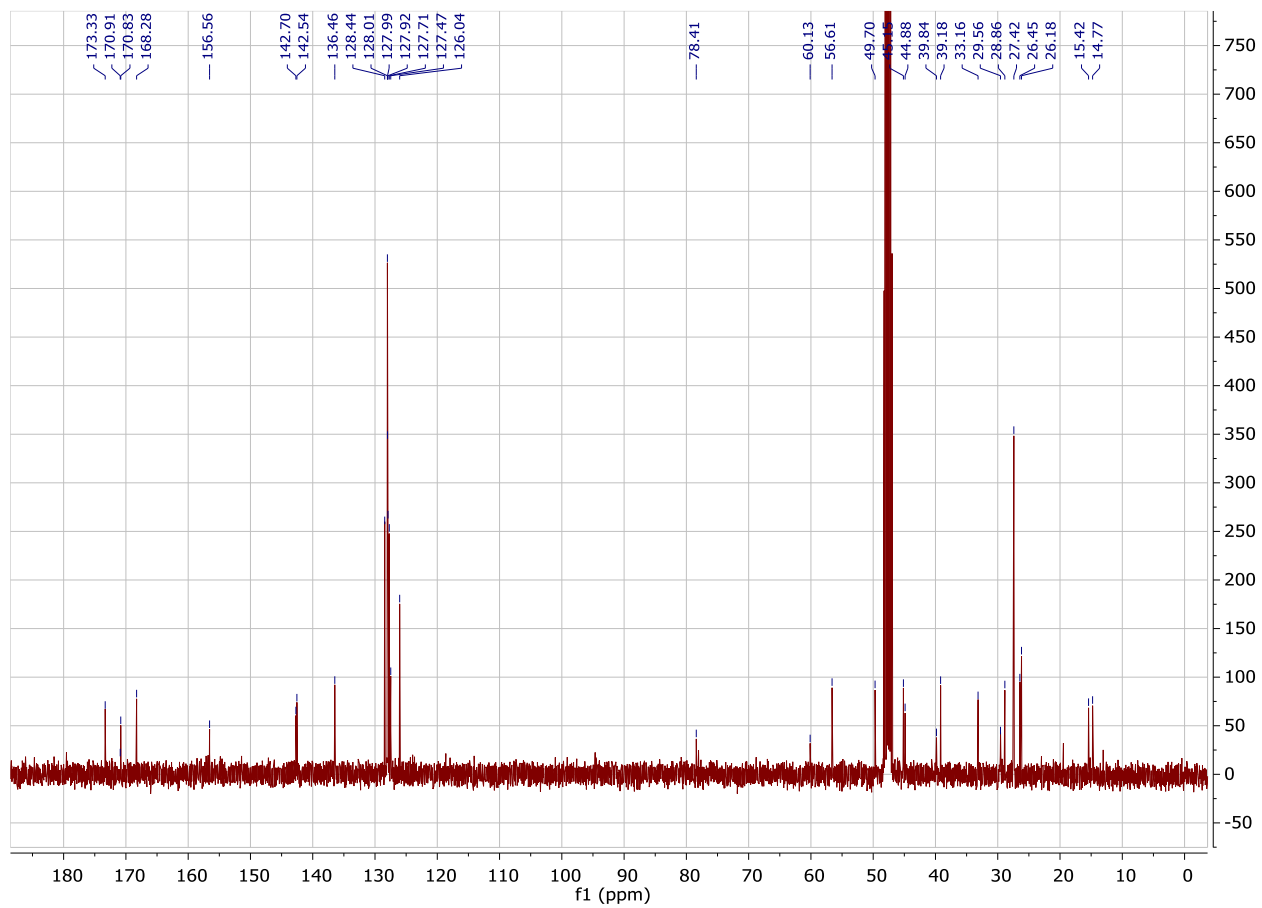


¹H-NMR (400 MHz, CD₃OD)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CD_3OD)

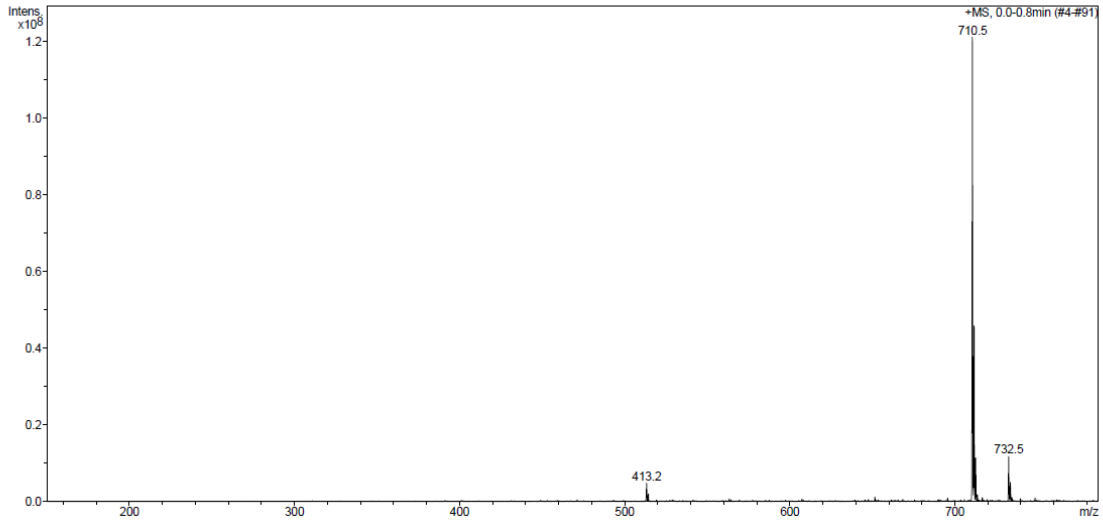


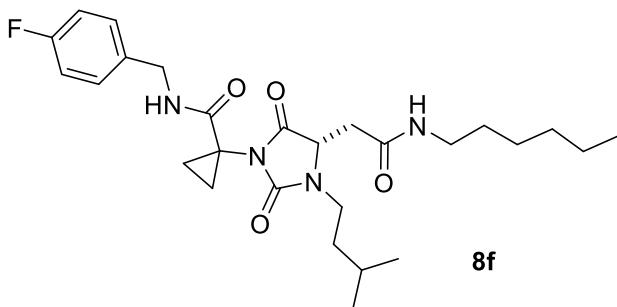
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name av gc113.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Cristina

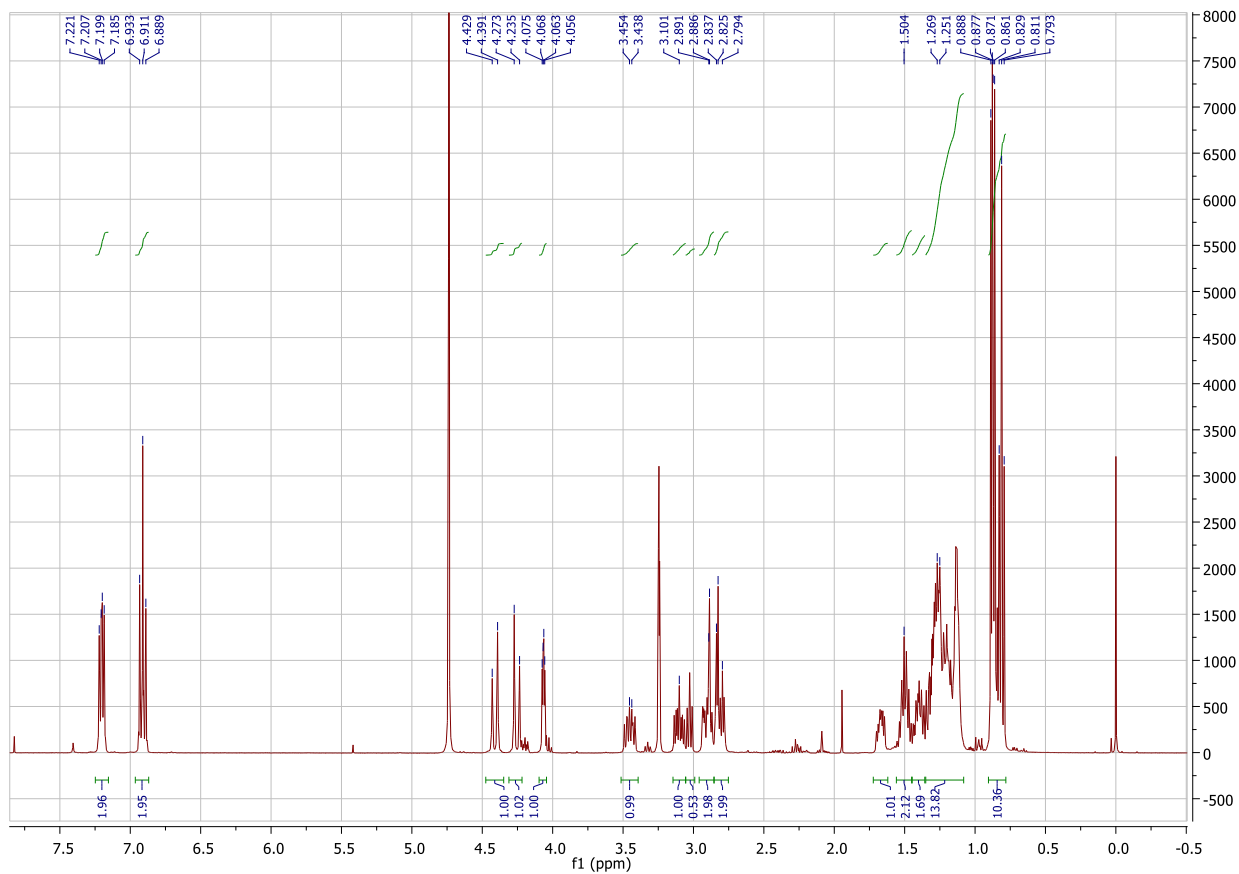
Acquisition Date 03/06/19 14:49:10
Method Copy of _01tmix_posneg
Im.MS

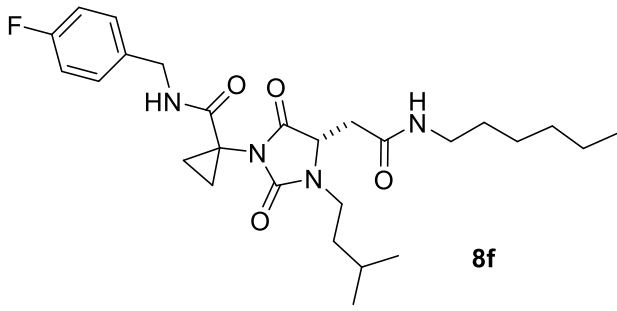
Operator Walter Panzeri
Instrument esquire3000plus



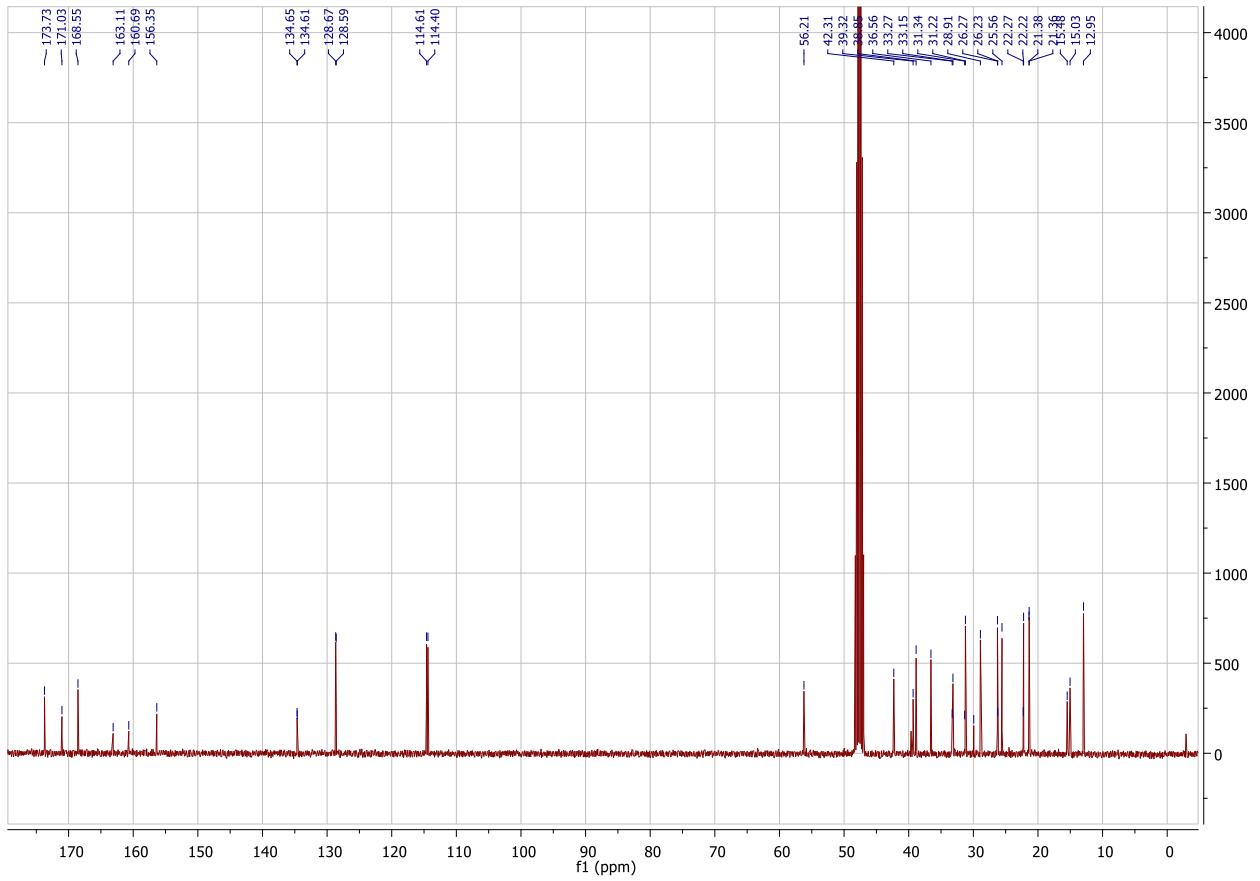


$^1\text{H-NMR}$ (400 MHz, CD_3OD)



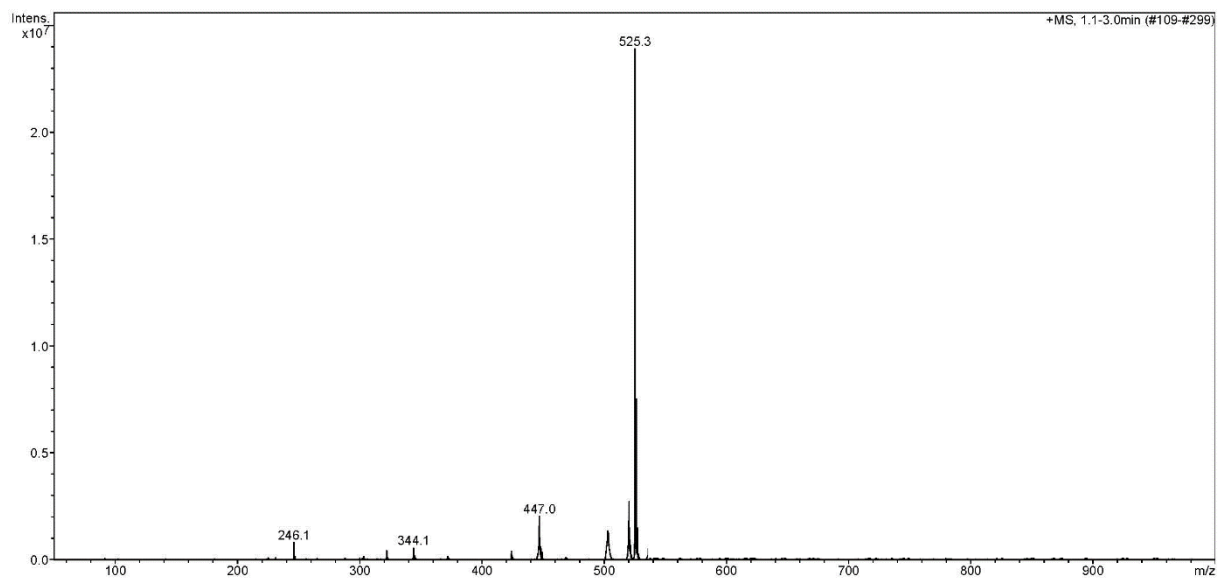


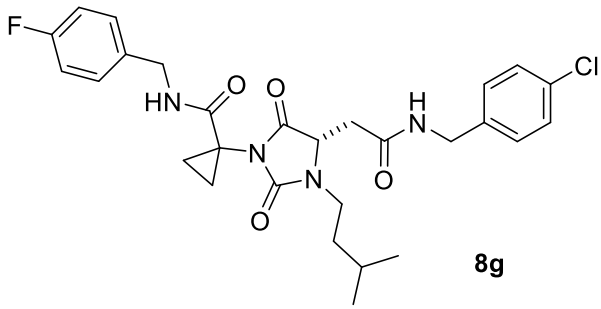
$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CD_3OD)



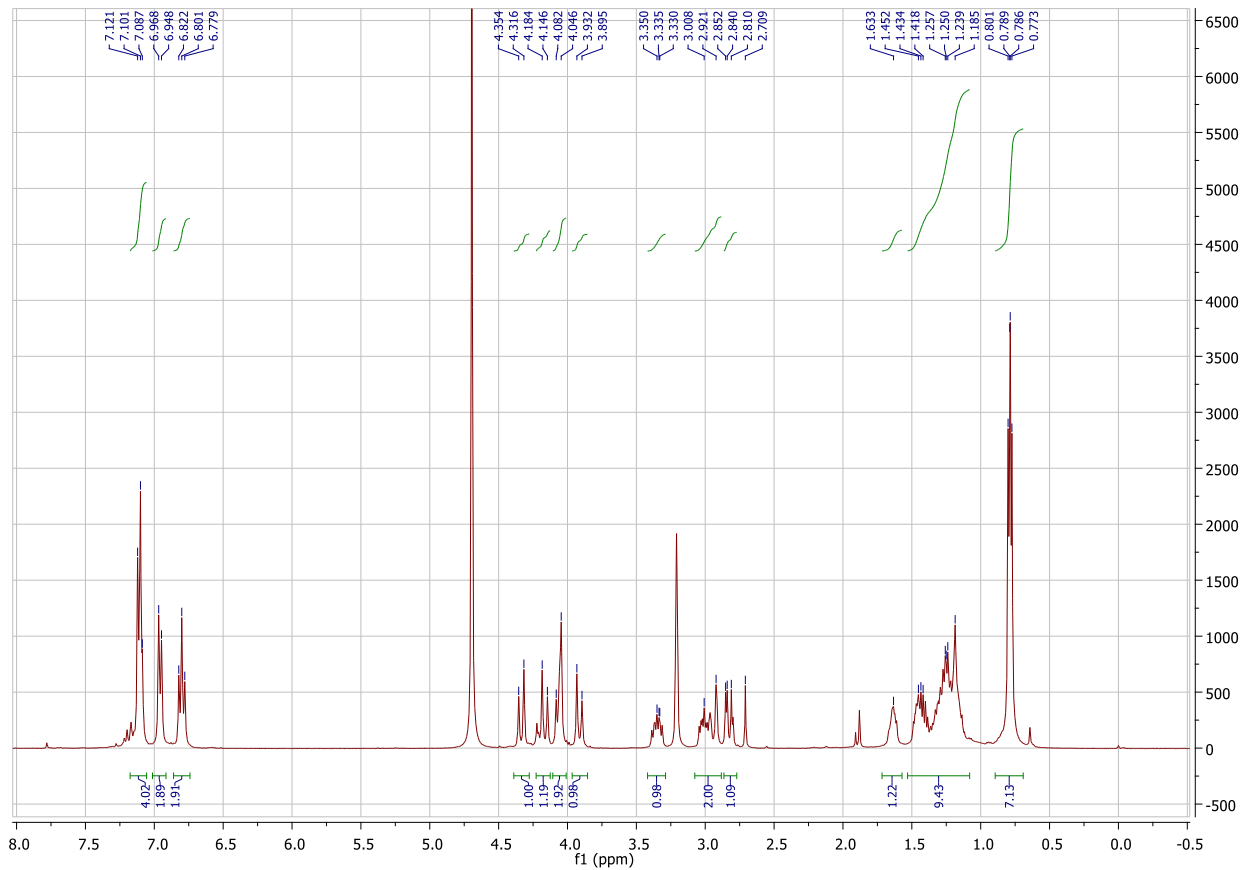
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

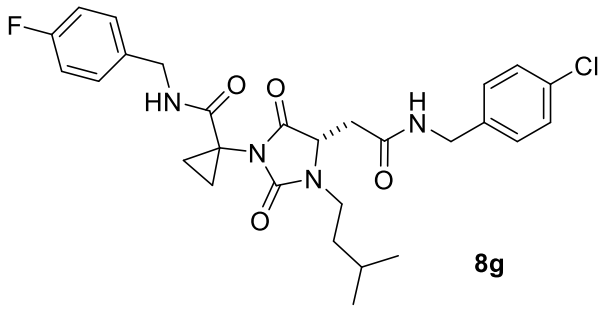
Analysis Name: av ac132c.d
Sample Name: 1 mg/ml dil 1:100 MeOH
Comment: Richiedente: Caramiello
Acquisition Date: 04/13/21 15:57:54
Method: Copy of \$PW_TBLM.MS
Operator: Walter Panzeri
Instrument: esquire3000plus



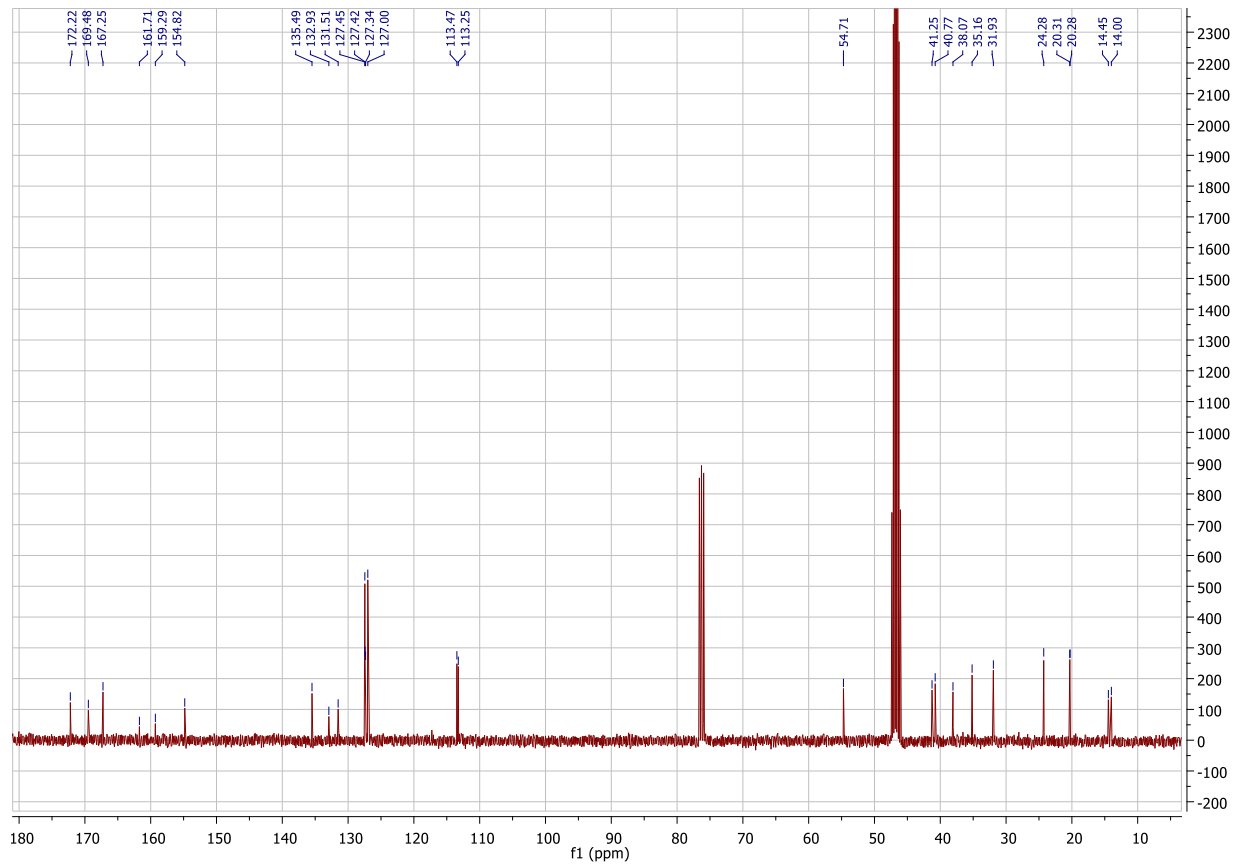


$^1\text{H-NMR}$ (101 MHz, CD_3OD)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CD_3OD)



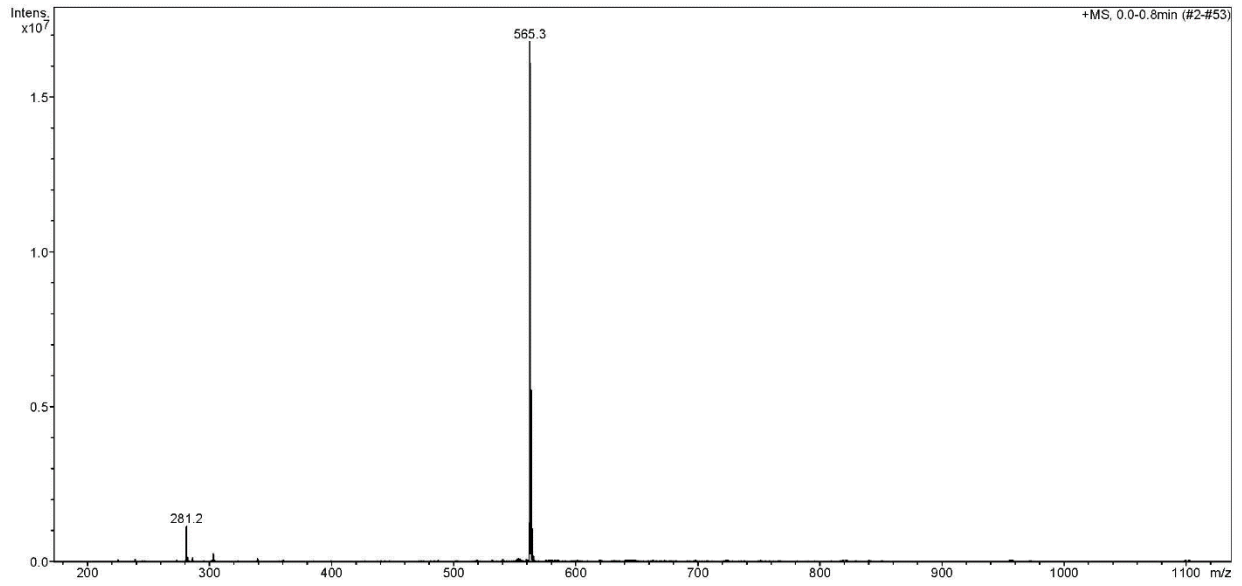
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

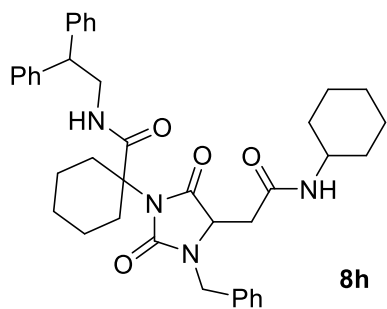
Analysis Name av.ms2057.d
Sample Name
Comment 1 mg/mL dil 1:100 MeOH
Richiedente: Sani

Acquisition Date 07/08/22 09:17:41
Method Copy of Sopt0622.MS

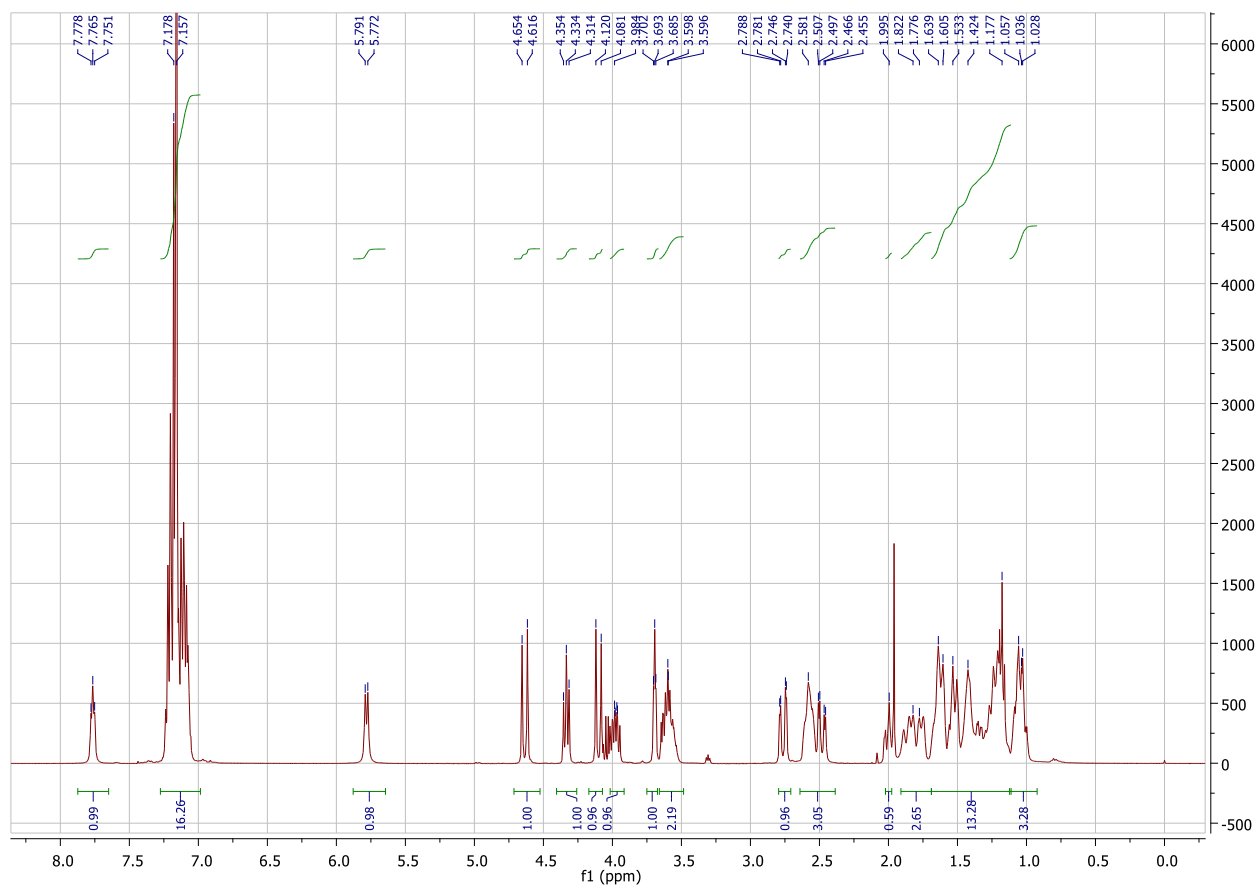
Operator
Instrument

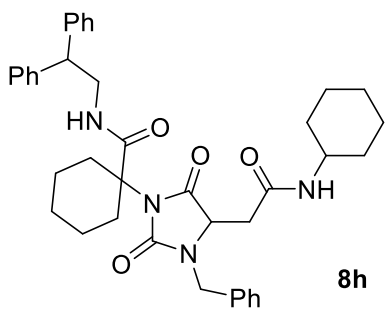
Walter Panzeri
esquire3000plus



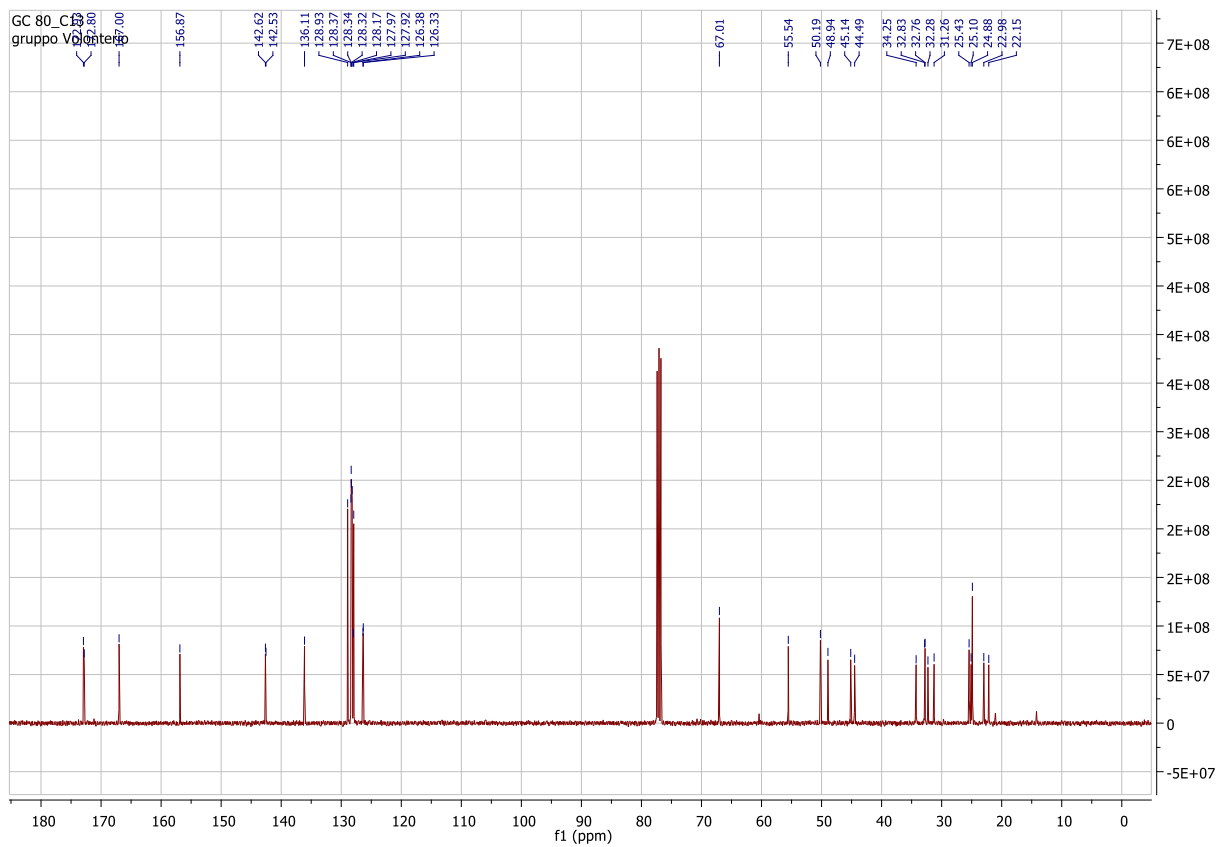


$^1\text{H-NMR}$ (400 MHz, CDCl_3)



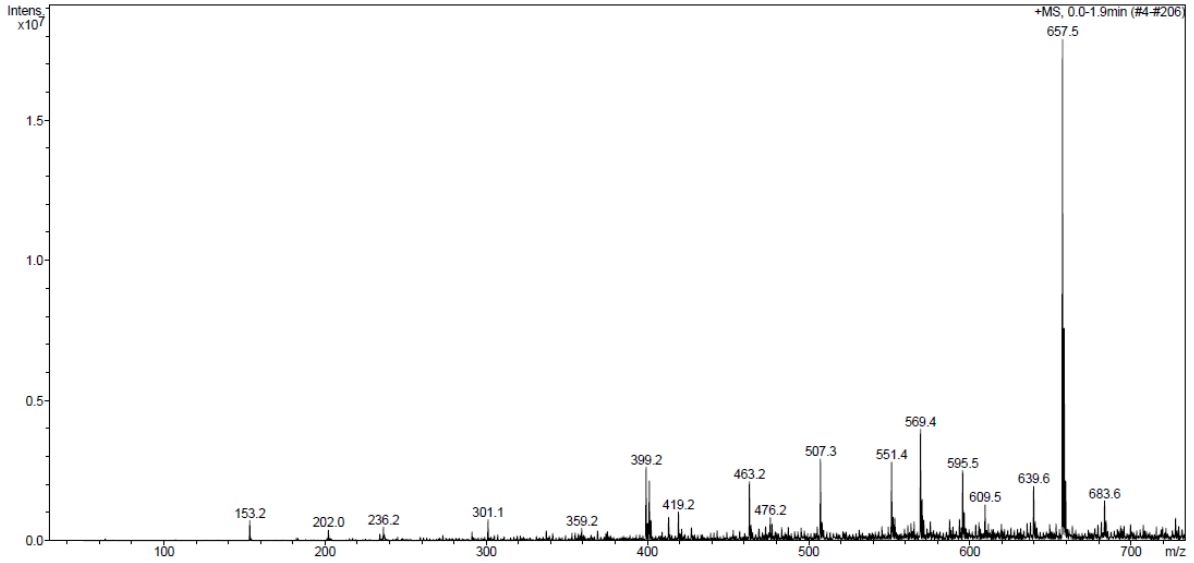


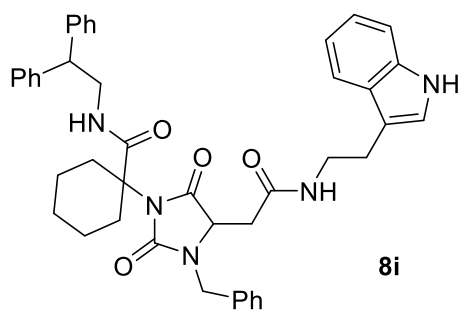
$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)



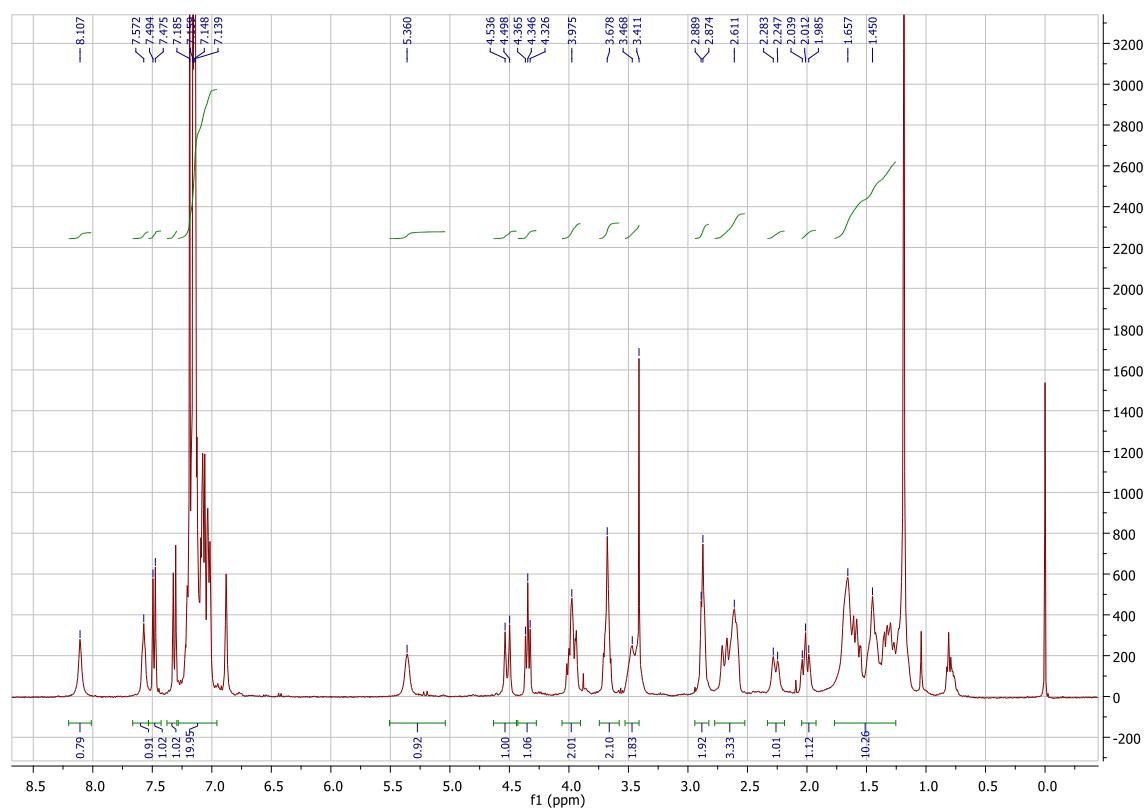
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

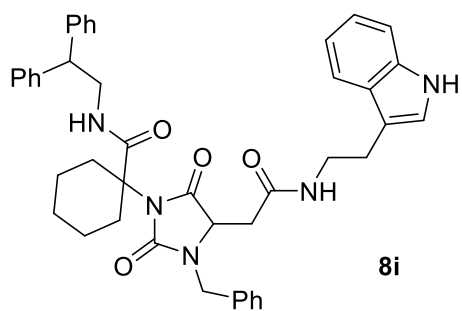
Analysis Name av gc80.d Acquisition Date 09/14/18 10:53:50 Operator Walter Panzeri
Sample Name Method Copy of _01tmix_posneg Instrument esquire3000plus
Comment 1 mg/ml dil 1:100 MeOH Im.MS
Richiedente: Cristina



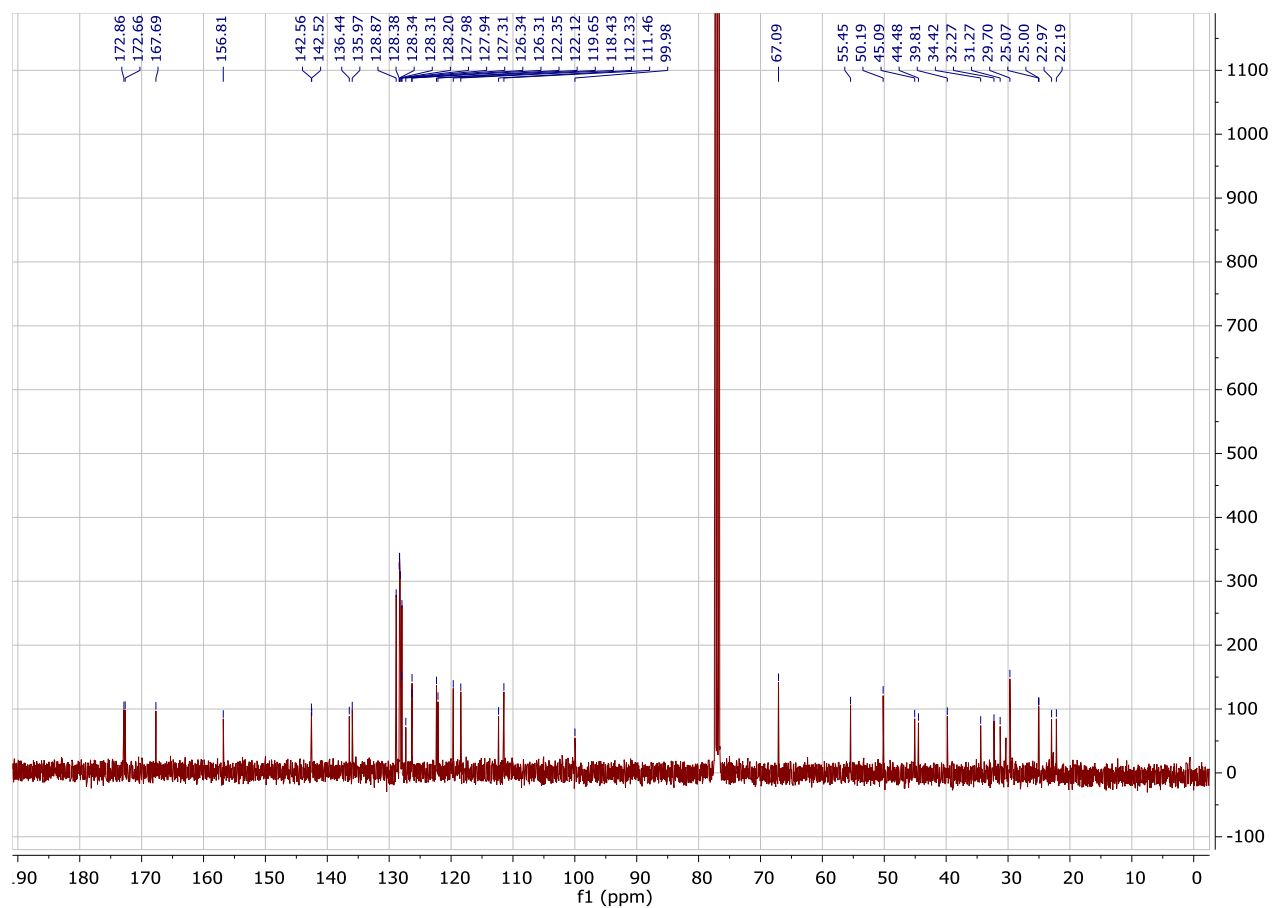


$^1\text{H-NMR}$ (400 MHz, CDCl_3)



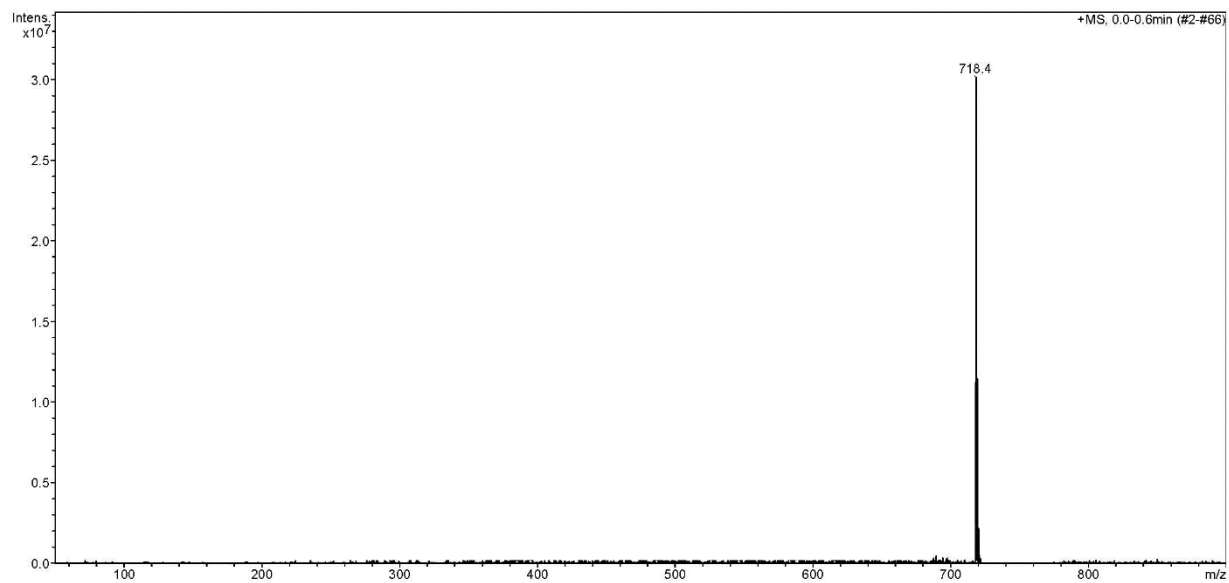


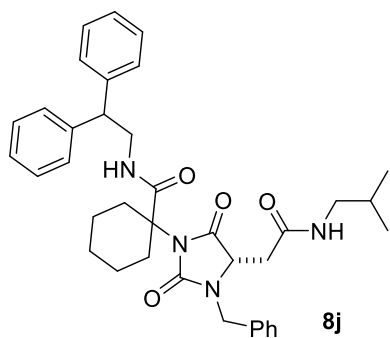
$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)



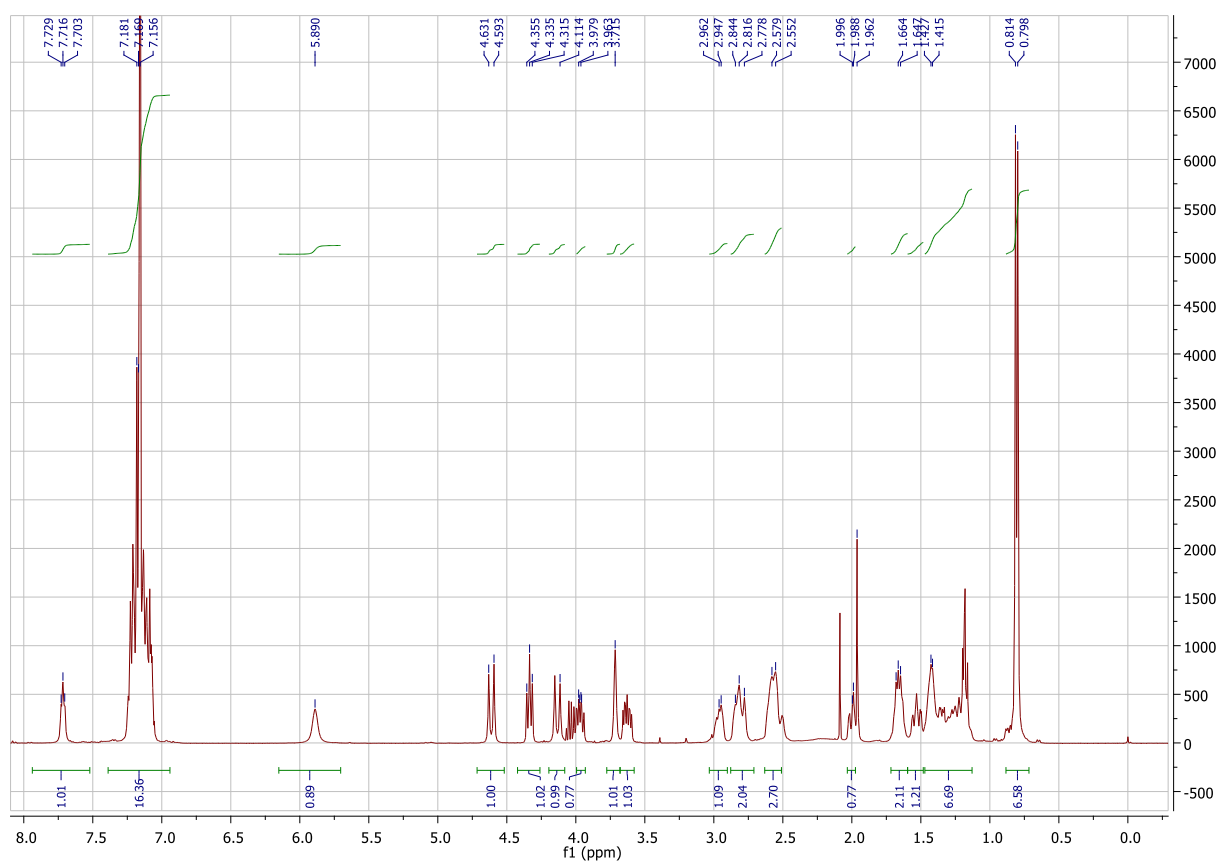
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

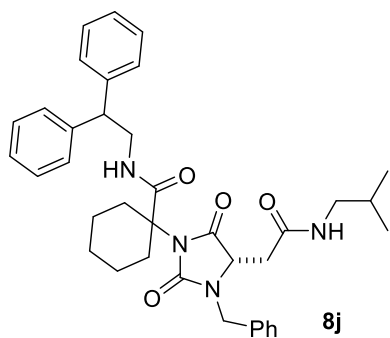
Analysis Name	av md20g_f.d	Acquisition Date	04/24/19 14:19:55	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 CH3CN Richiedente: Viani		Im.MS		



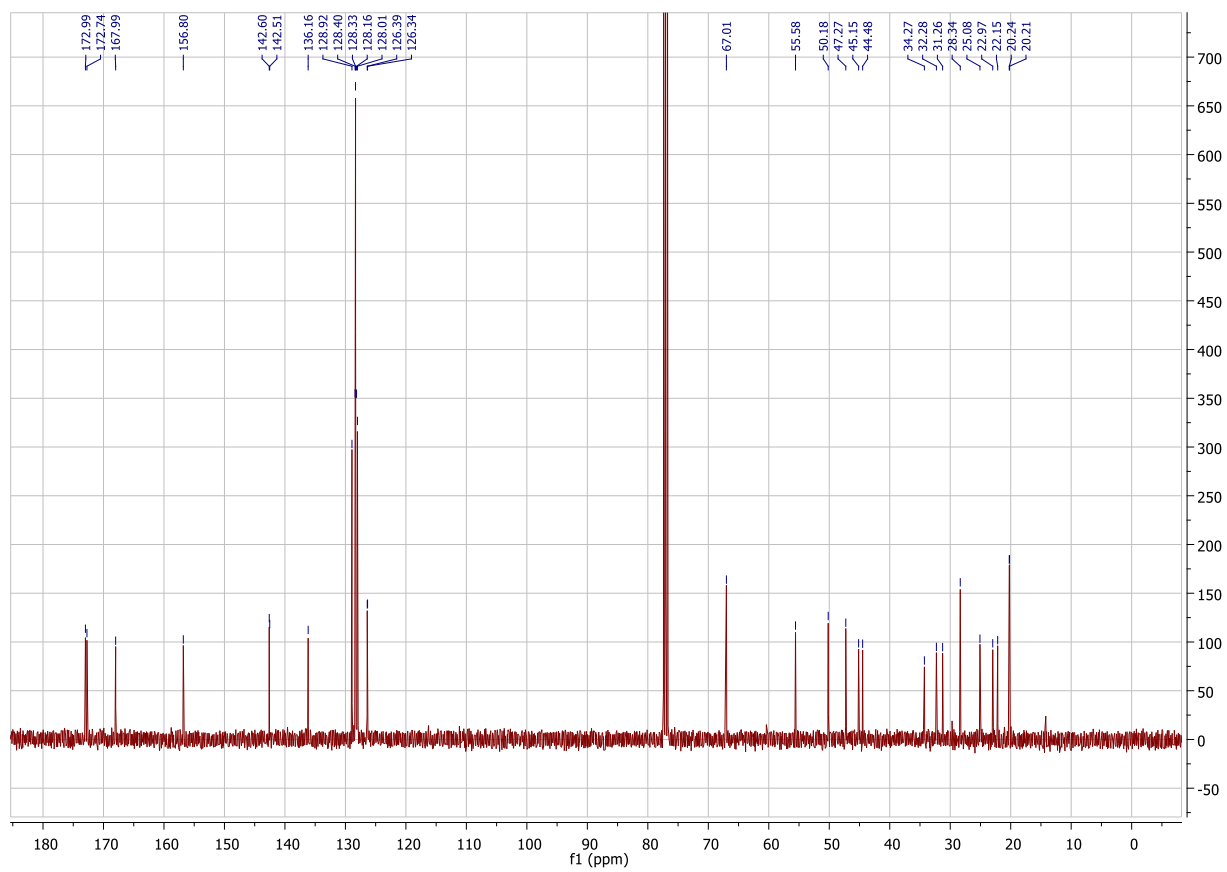


$^1\text{H-NMR}$ (400 MHz, CDCl_3)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)

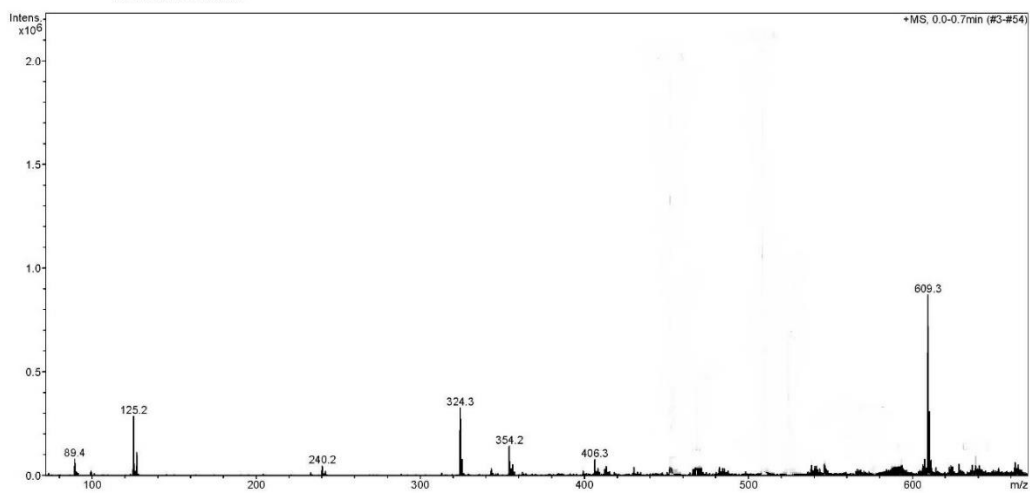


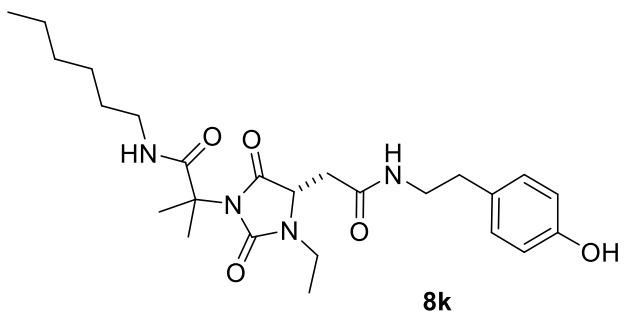
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name av ac176a.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Caramiello

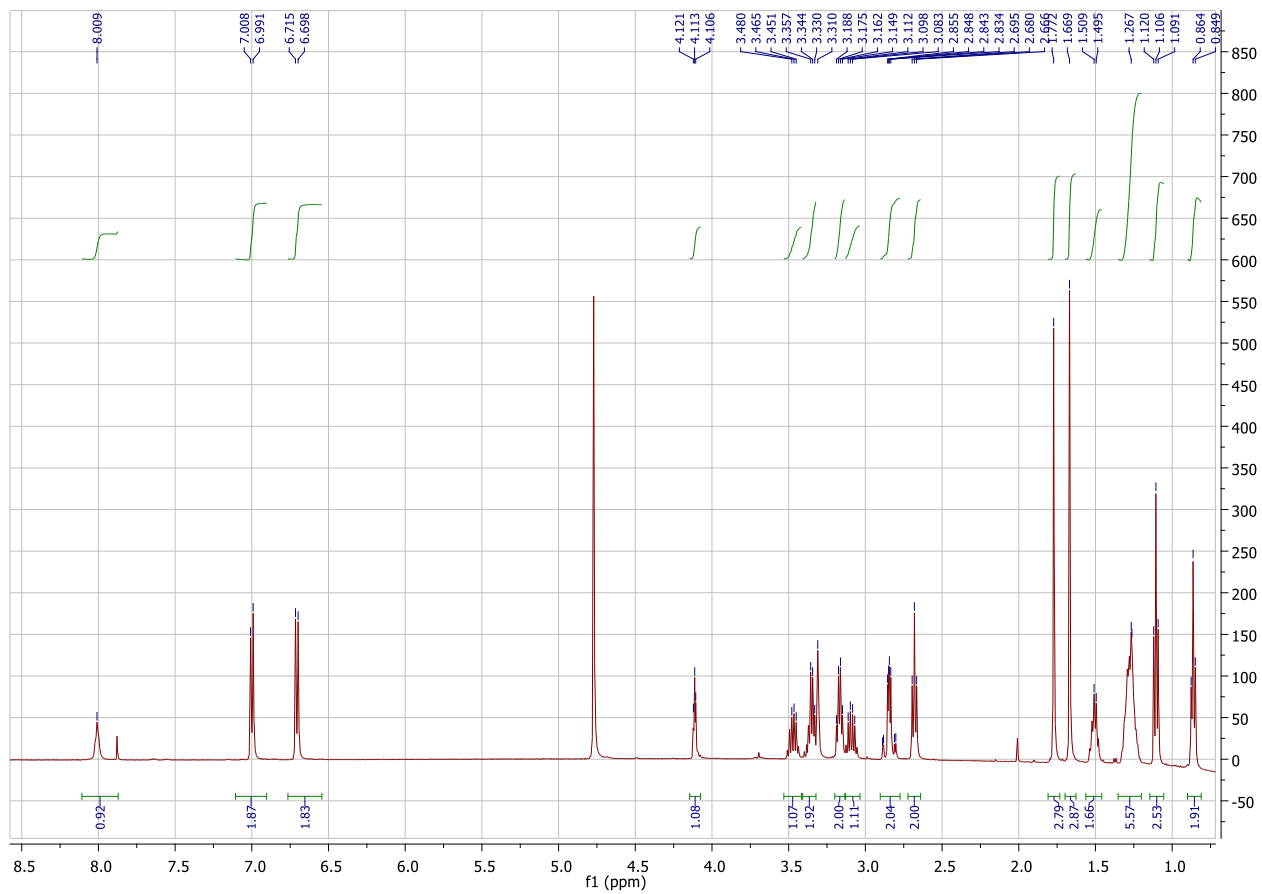
Acquisition Date 02/02/22 14:07:38
Method Copy of \$opt0922.MS

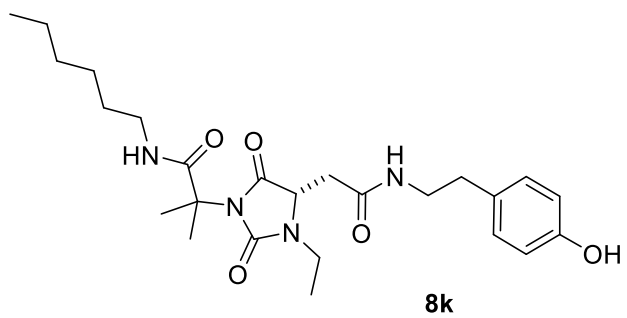
Operator Walter Panzeri
Instrument esquire3000plus



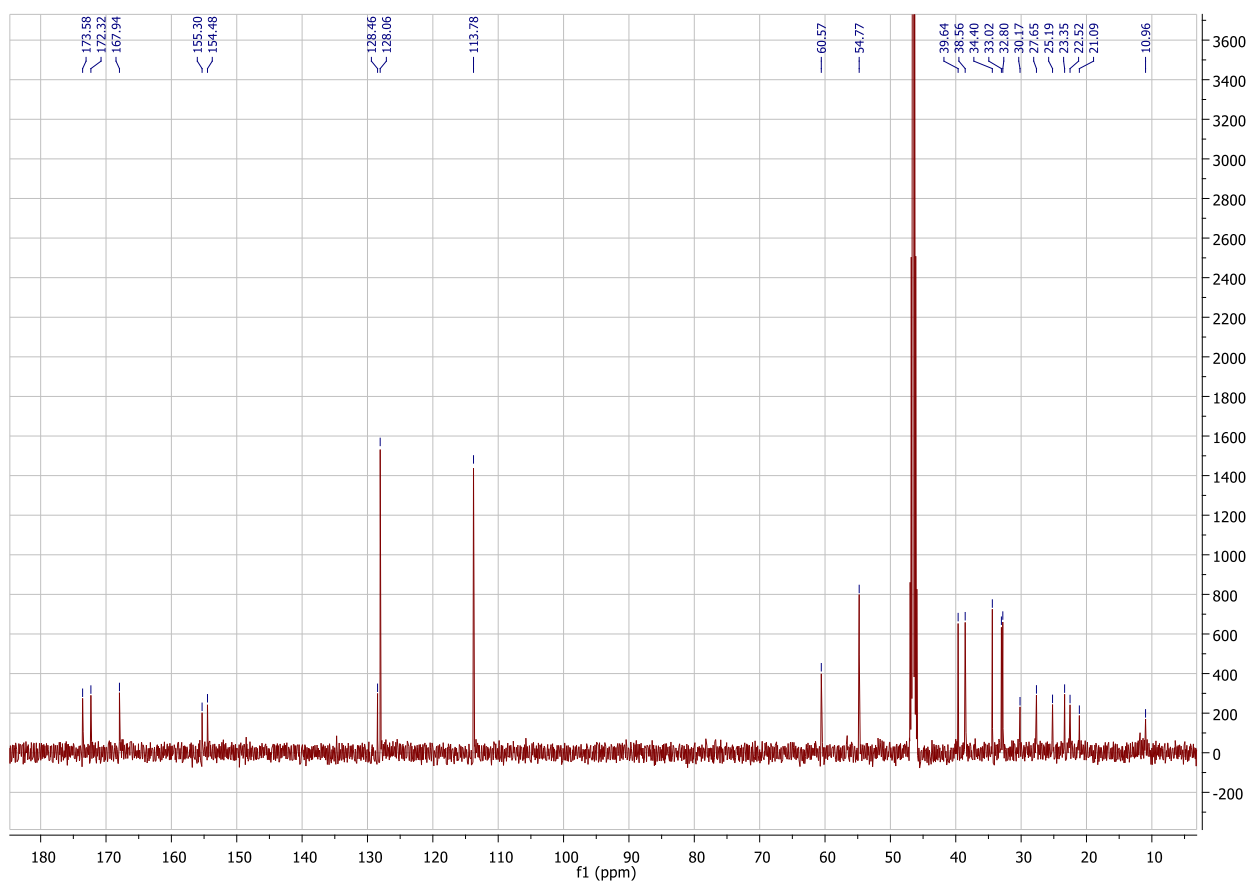


$^1\text{H-NMR}$ (400 MHz, CD_3OD)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CD_3OD)

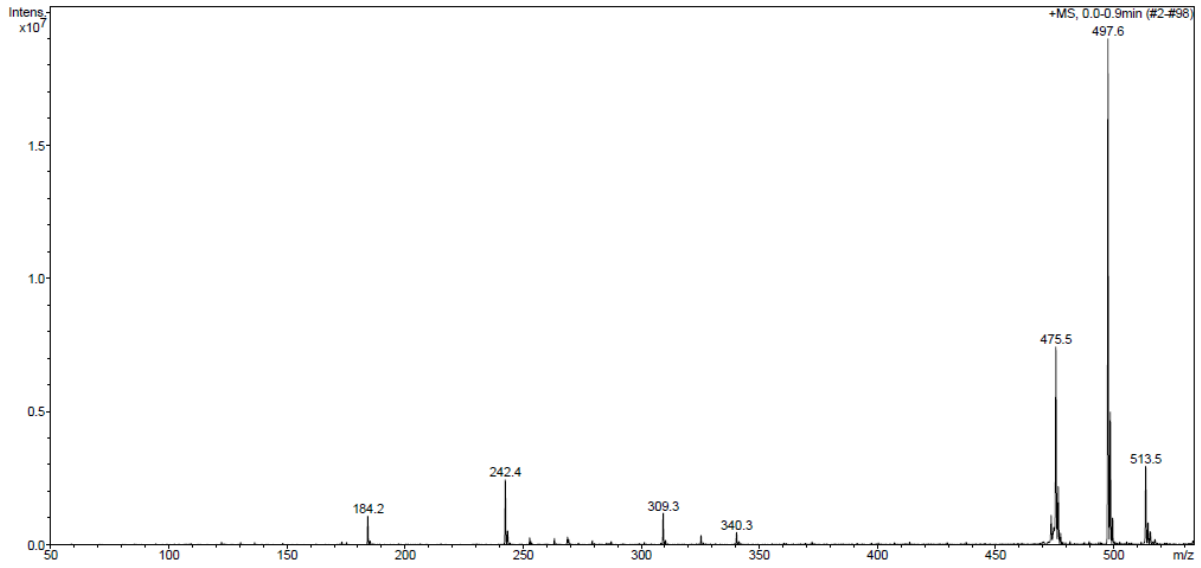


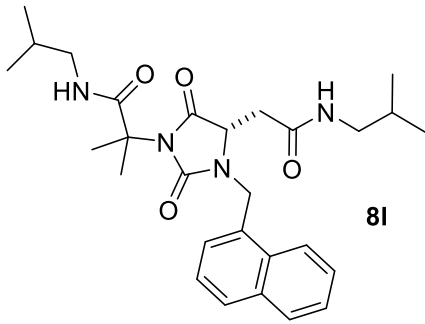
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name av_gc22b.d
Sample Name
Comment 1 mg/ml dil 1:100 CH3CN
Richiedente: Cristina

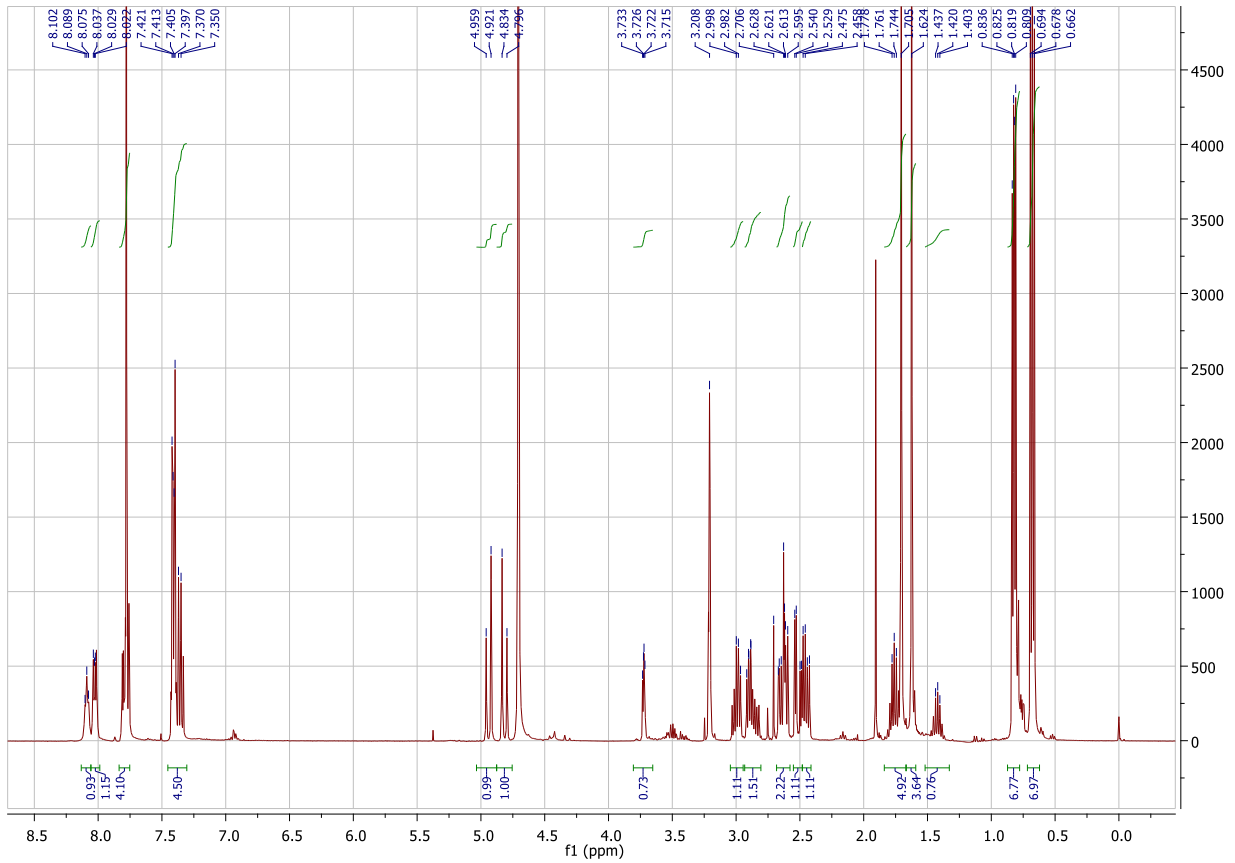
Acquisition Date 02/08/18 14:19:50
Method Copy of _01tmix_posneg
In.MS

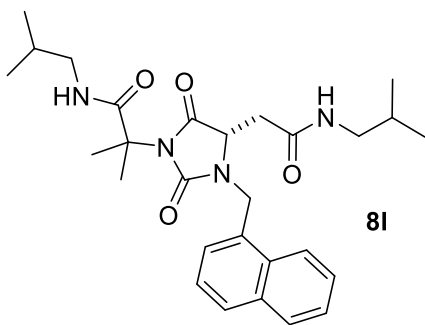
Operator Walter Panzeri
Instrument esquire3000plus



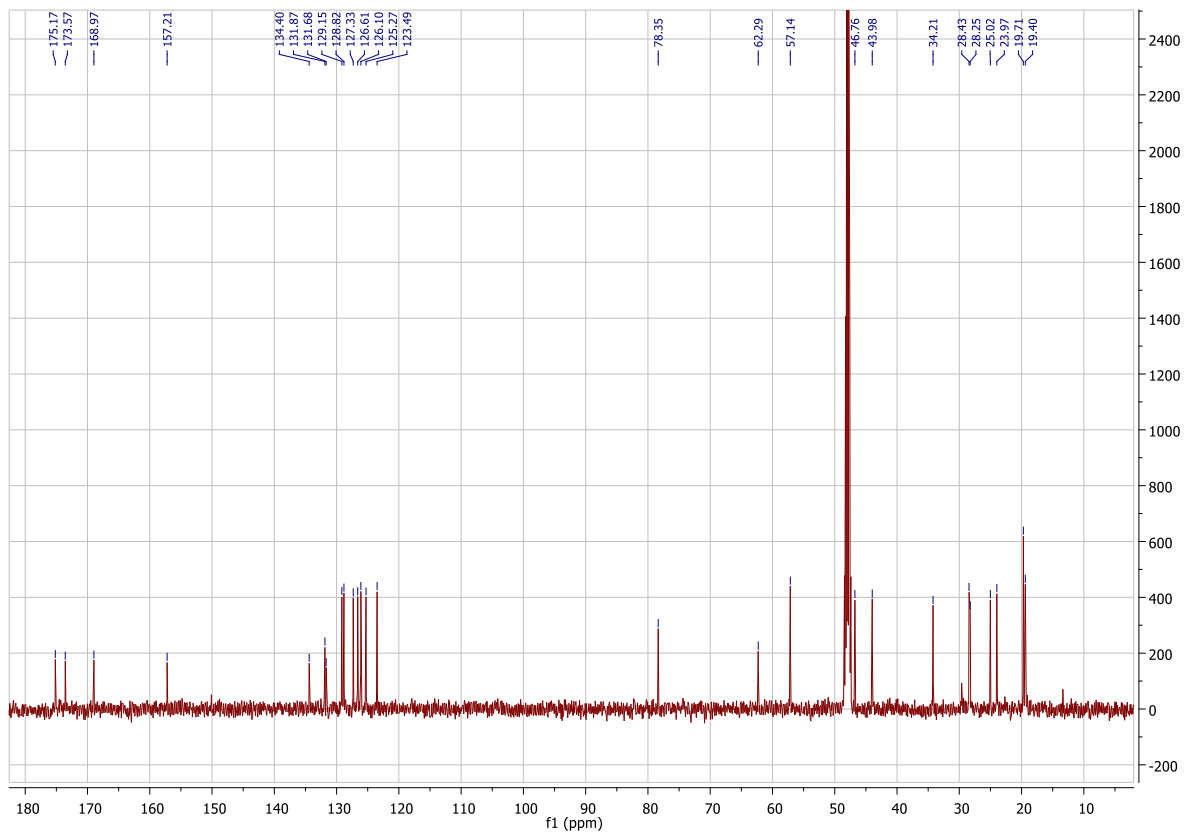


¹H-NMR (400 MHz, CD₃OD)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CD_3OD)



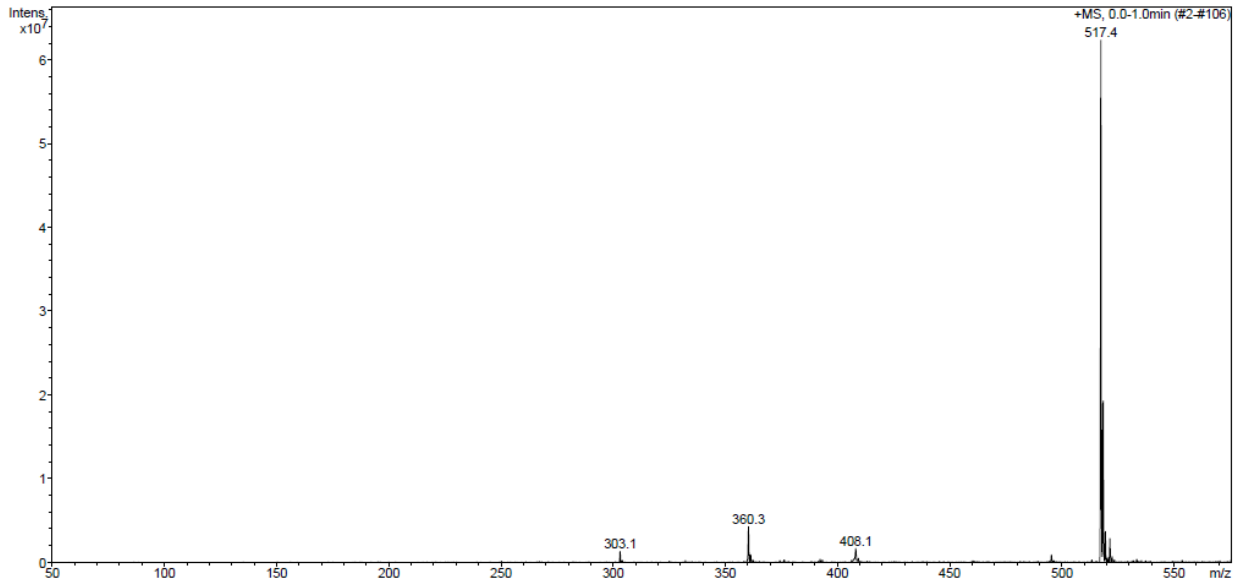
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

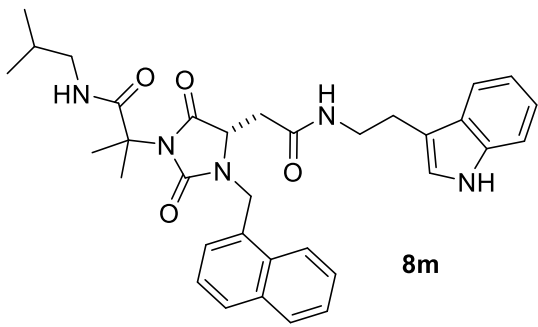
Analysis Name av gc62.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Cristina

Acquisition Date 06/13/18 10:46:23
Method Copy of _01tmix_posneg
Im.MS

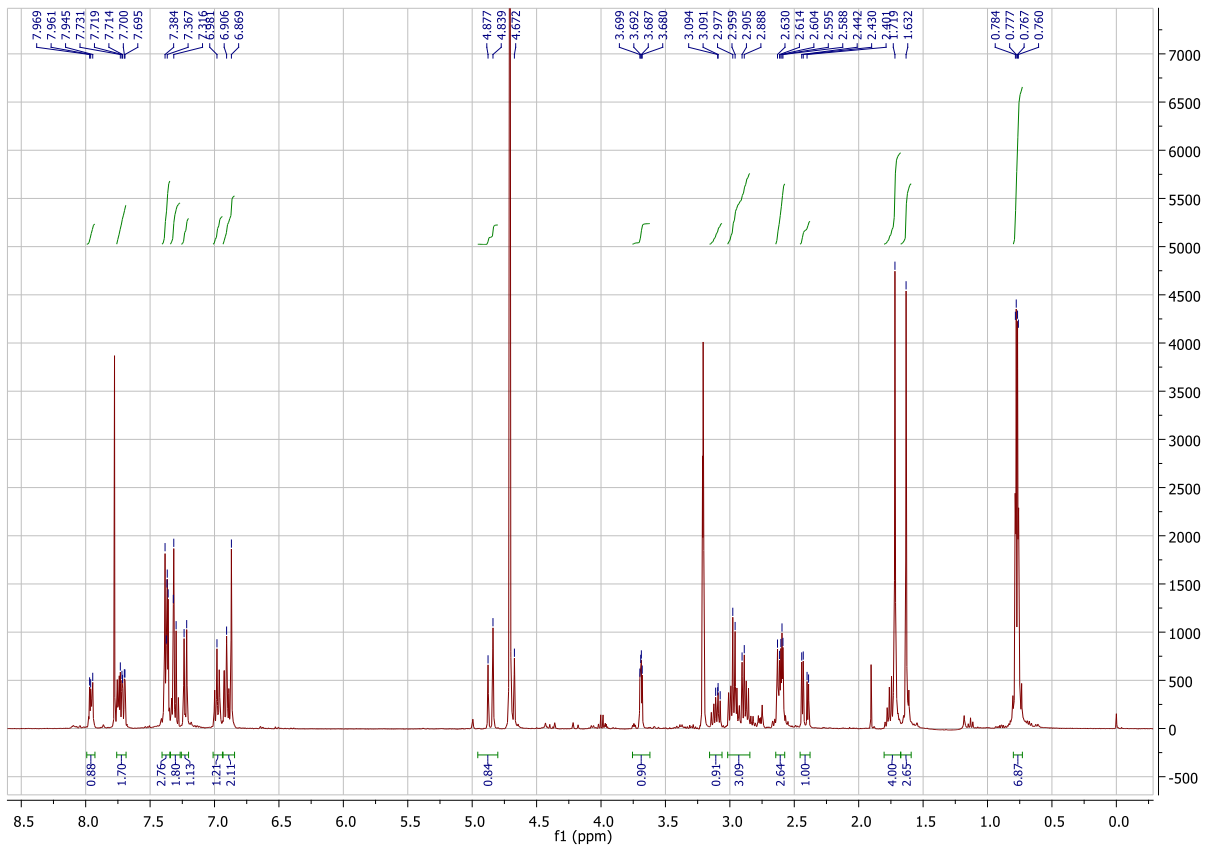
Operator
Instrument

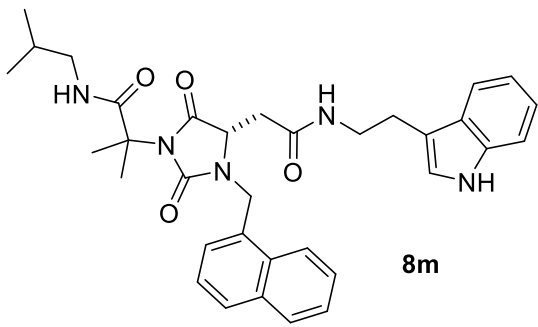
Walter Panzeri
esquire3000plus



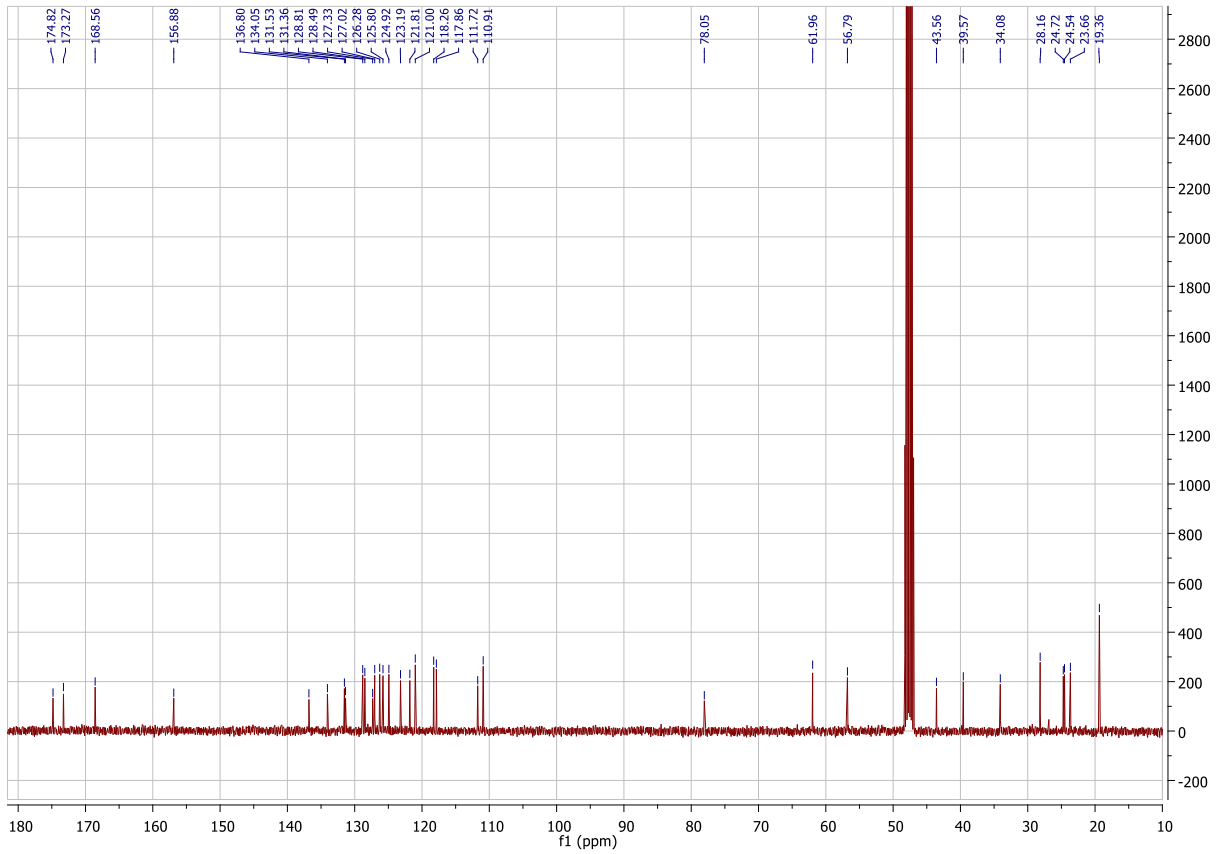


$^1\text{H-NMR}$ (400 MHz, CD_3OD)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CD_3OD)

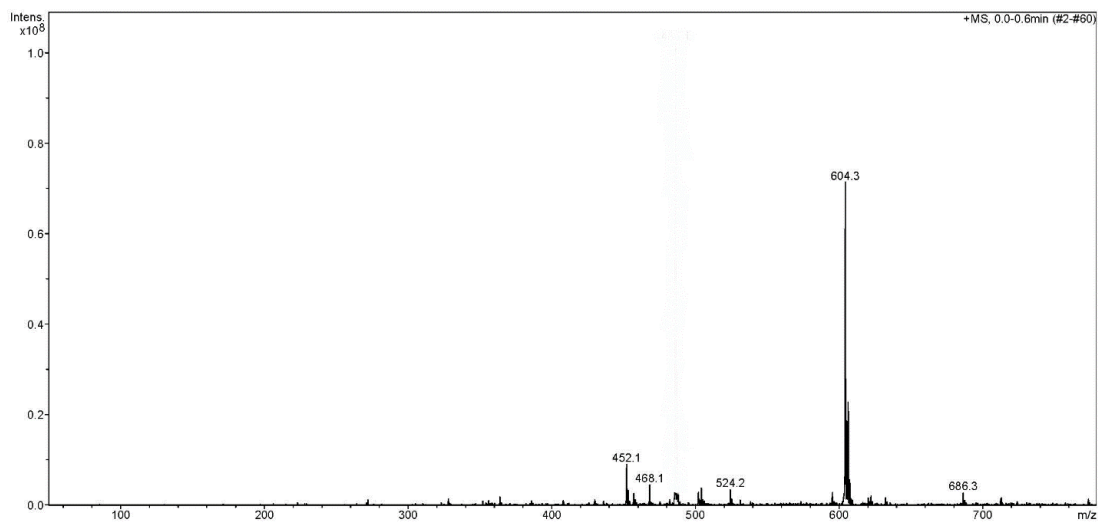


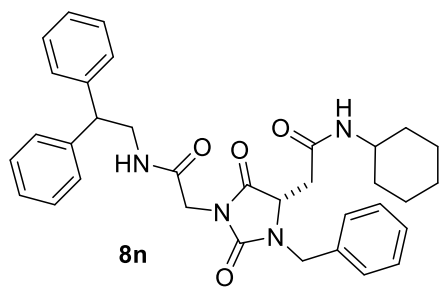
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name k.ms1671.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Sani

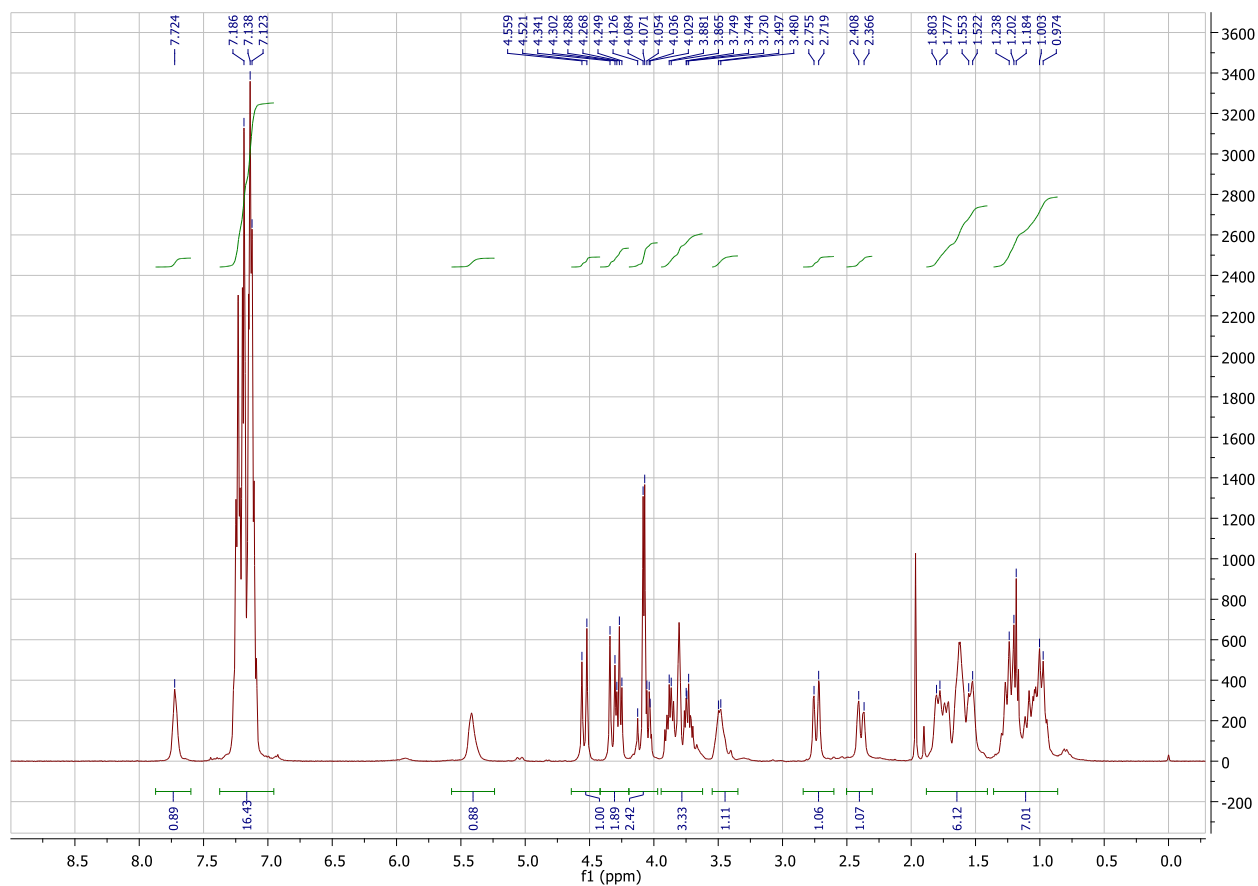
Acquisition Date 03/28/18 11:55:09
Method Copy_of_01tmix_posneg
Im.MS

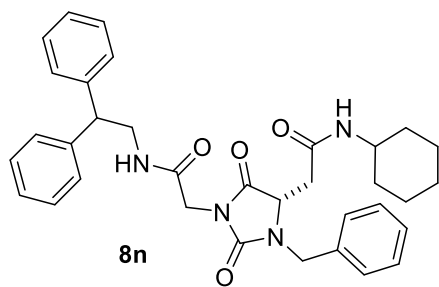
Operator Walter Panzeri
Instrument esquire3000plus



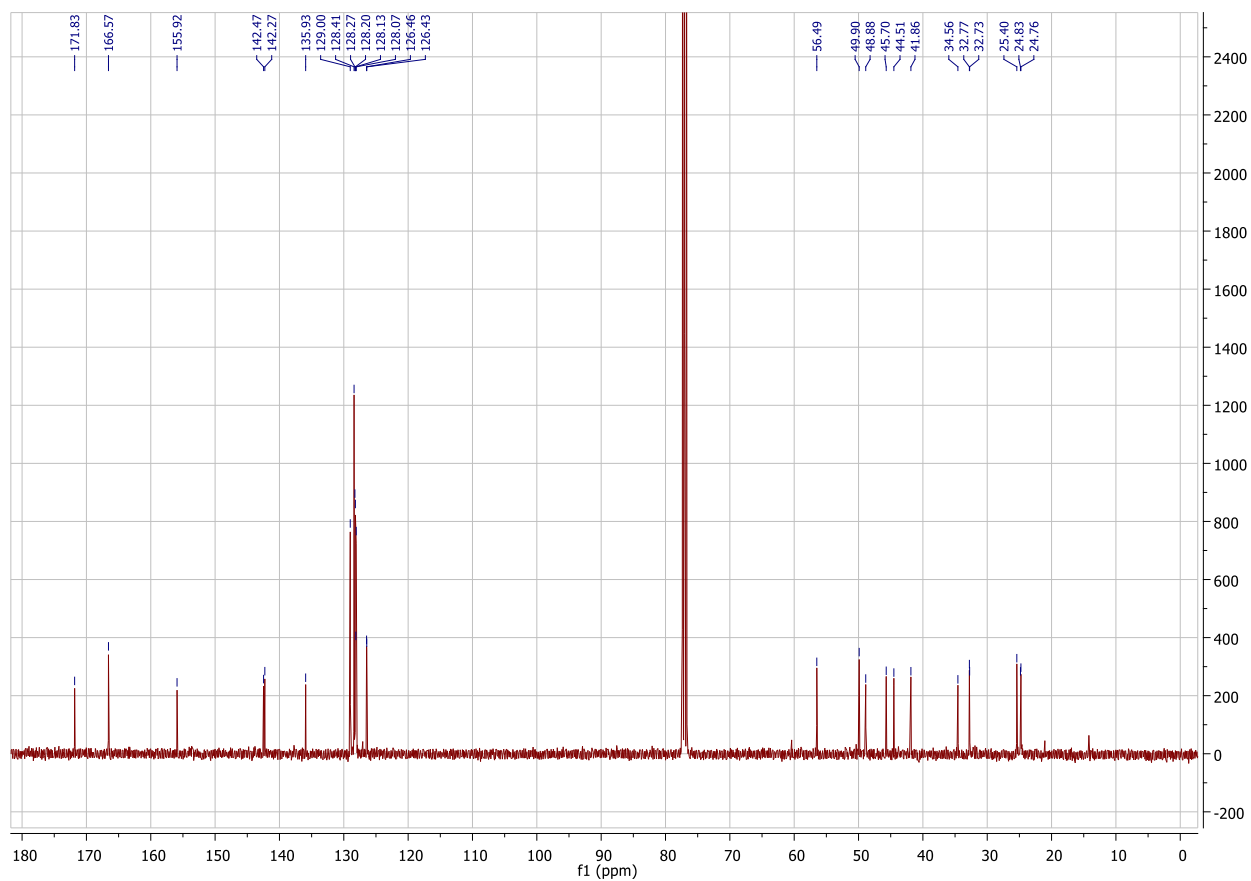


$^1\text{H-NMR}$ (400 MHz, CDCl_3)



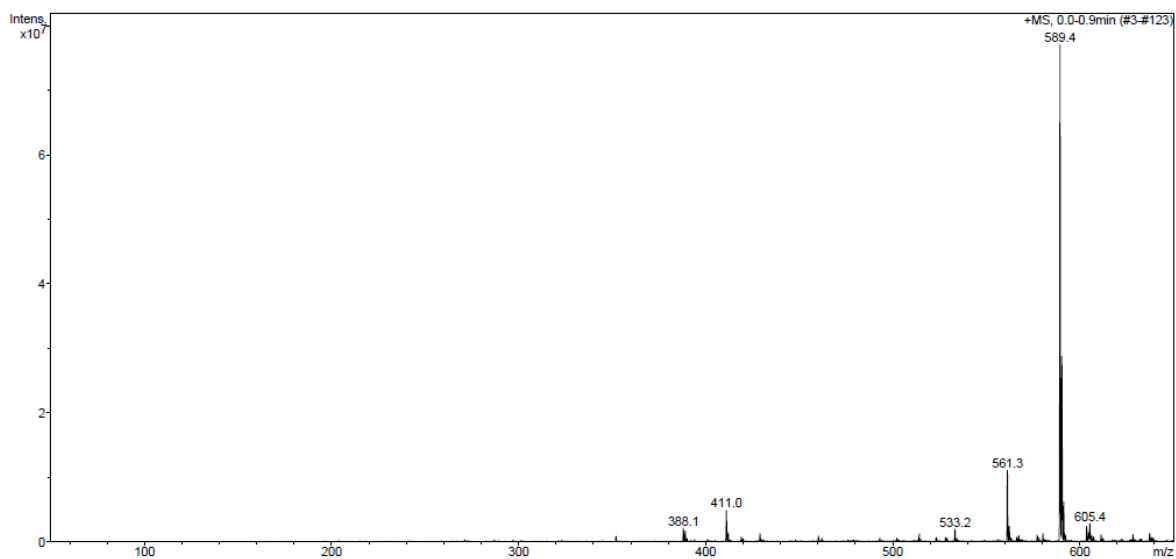


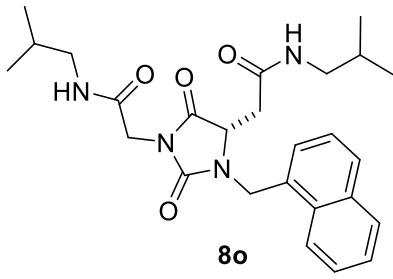
$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)



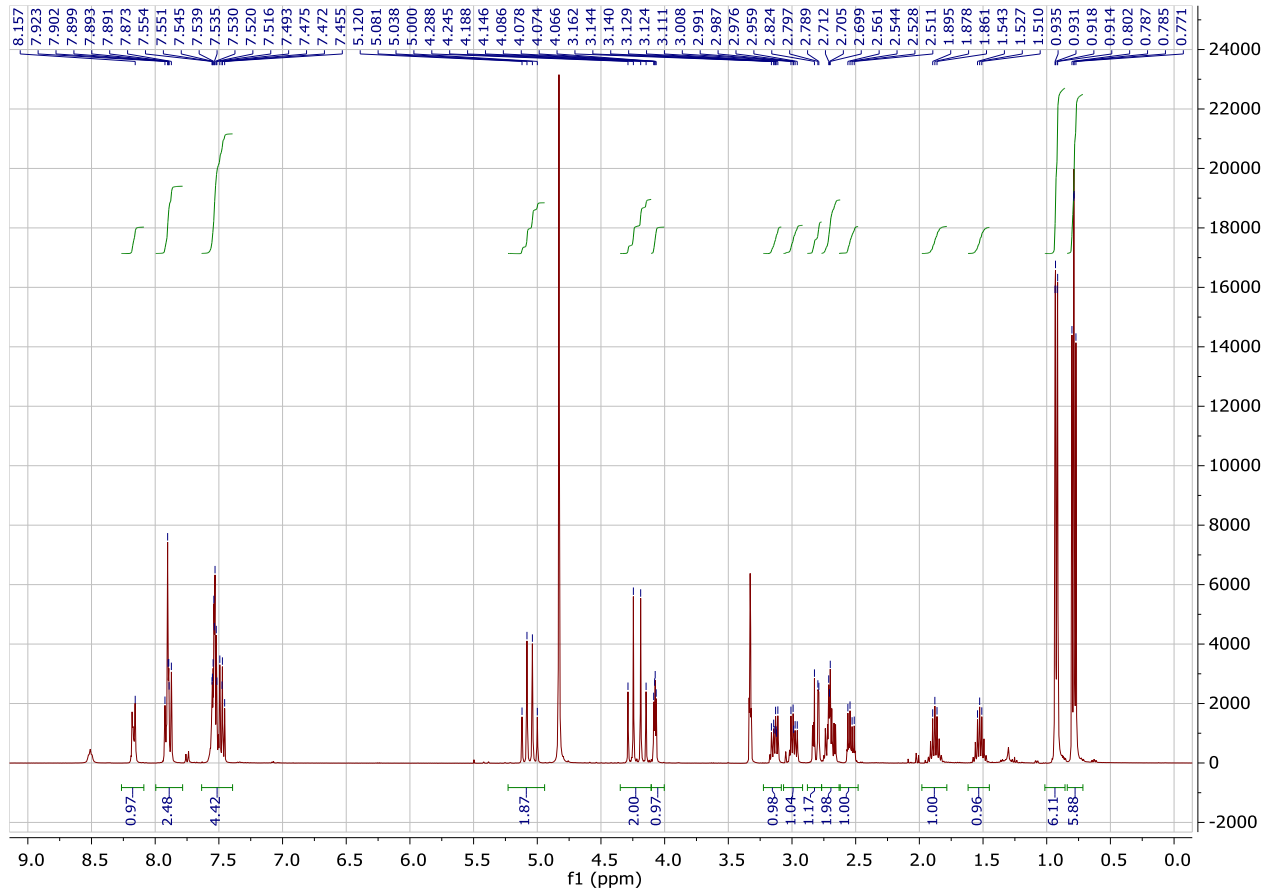
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

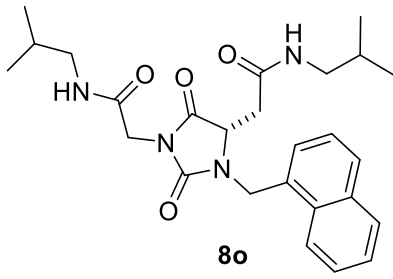
Analysis Name	av gc40.d	Acquisition Date	04/19/18 09:25:10	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg Im.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Cristina				



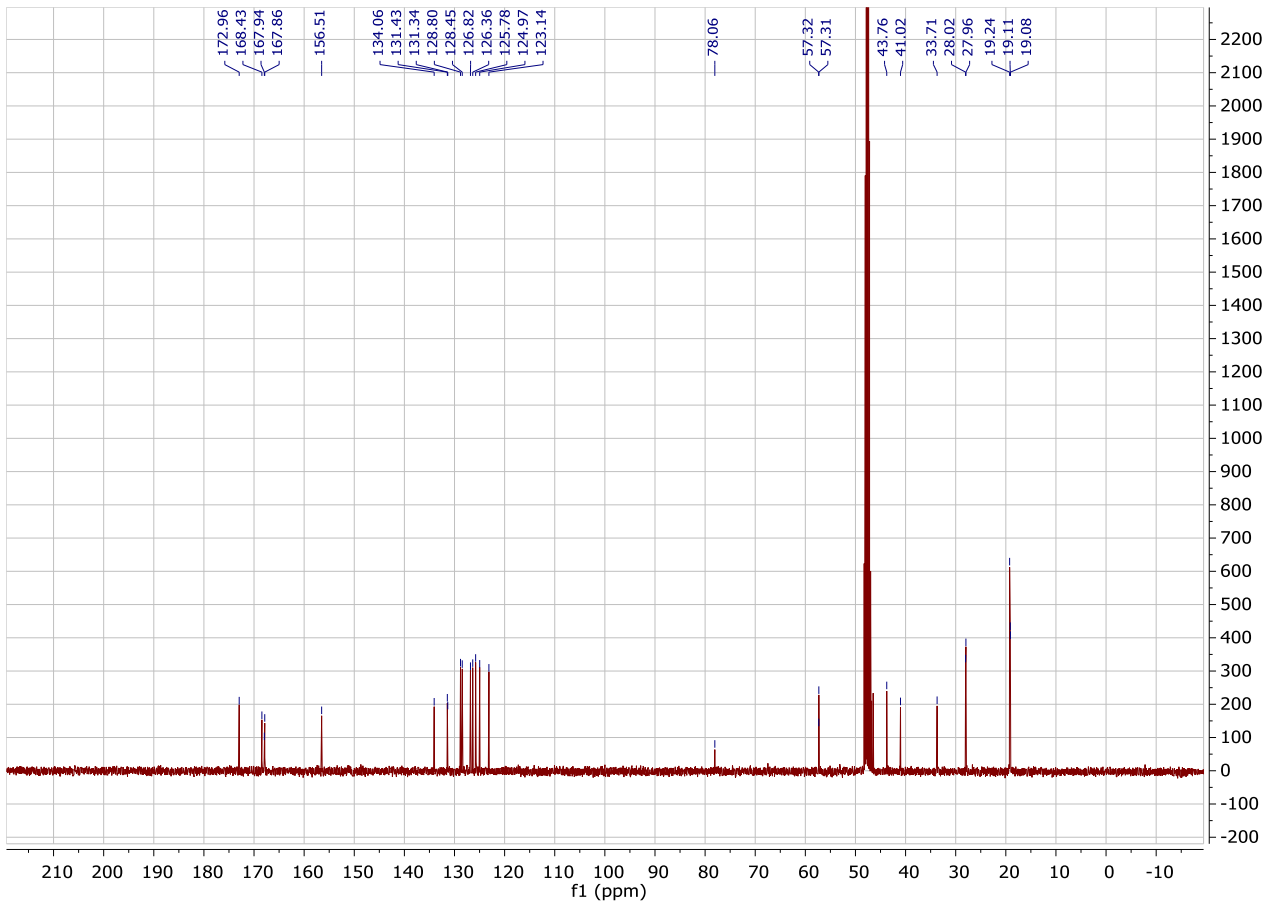


¹H-NMR (101 MHz, CD₃OD)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CD_3OD)

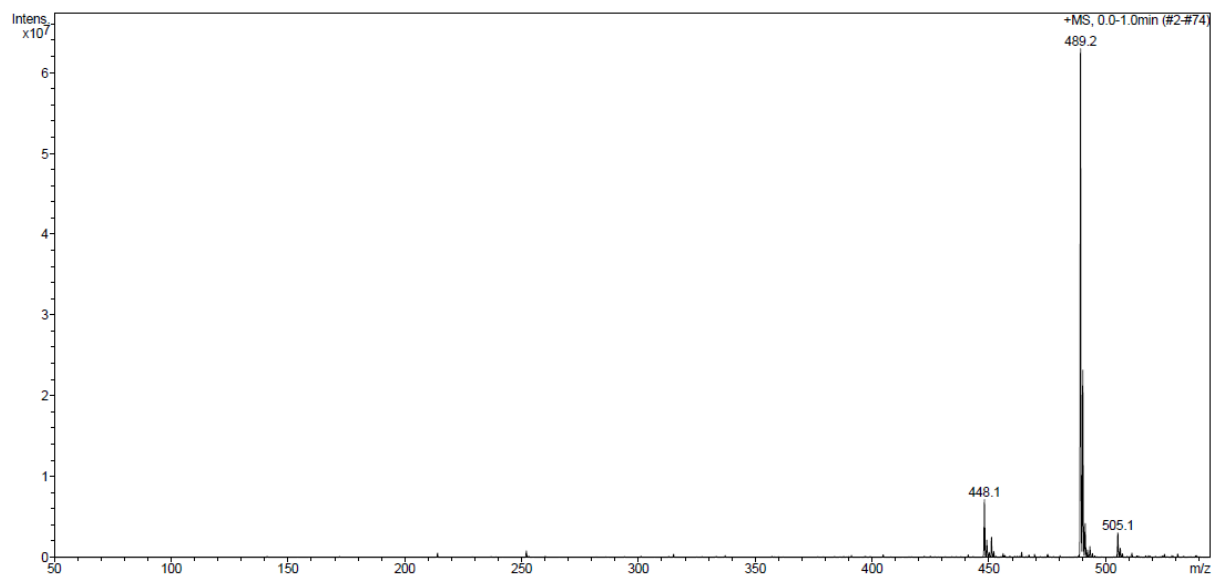


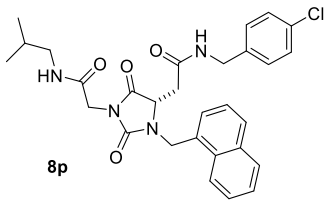
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name av ac065.d
Sample Name
Comment 1mg/ml dil 1:100 MeOH
Richiedente: Caramiello

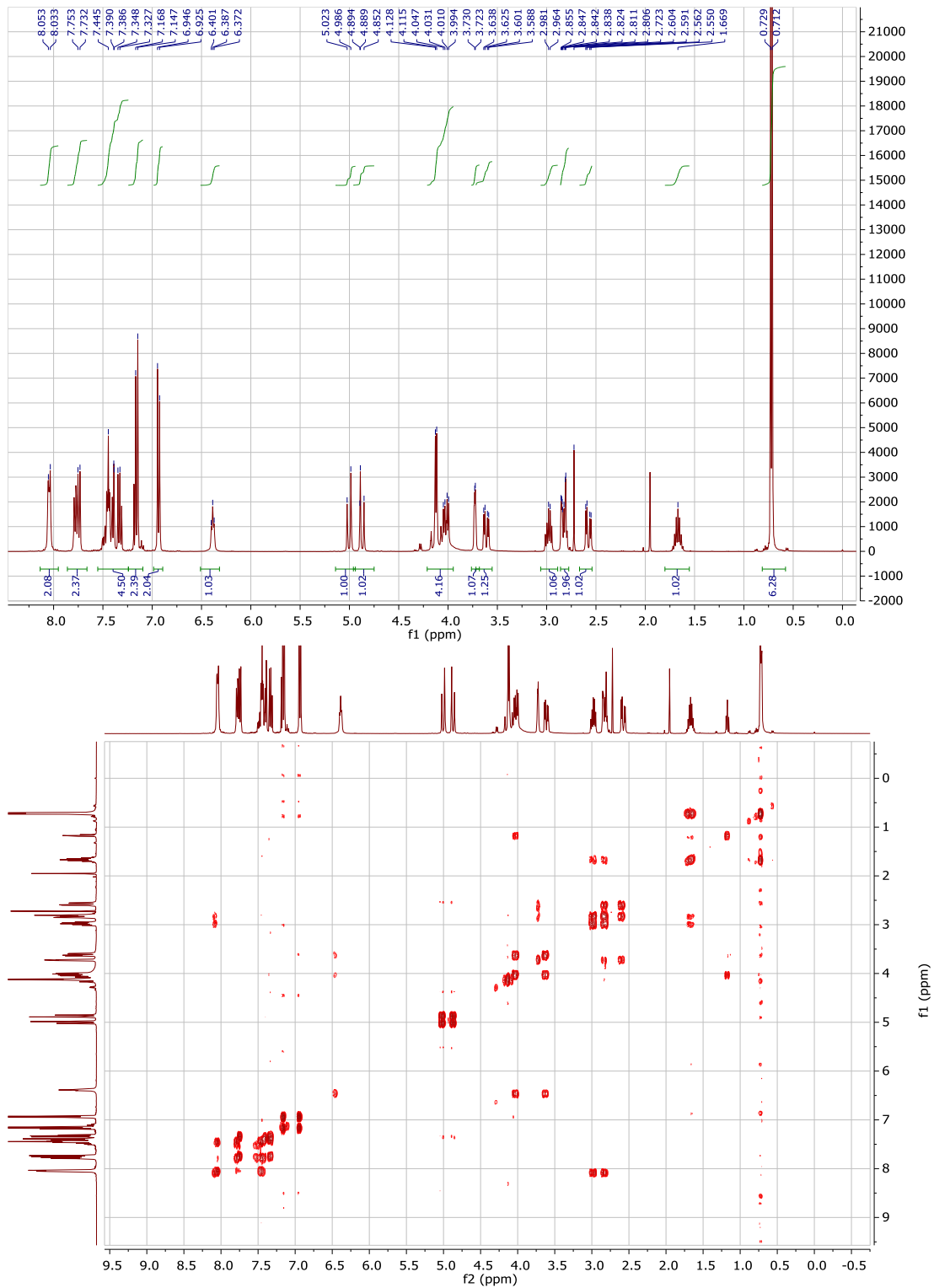
Acquisition Date 07/20/20 14:27:00
Method Copy of _01tmix_posneg
In.MS

Operator Walter Panzeri
Instrument esquire3000plus

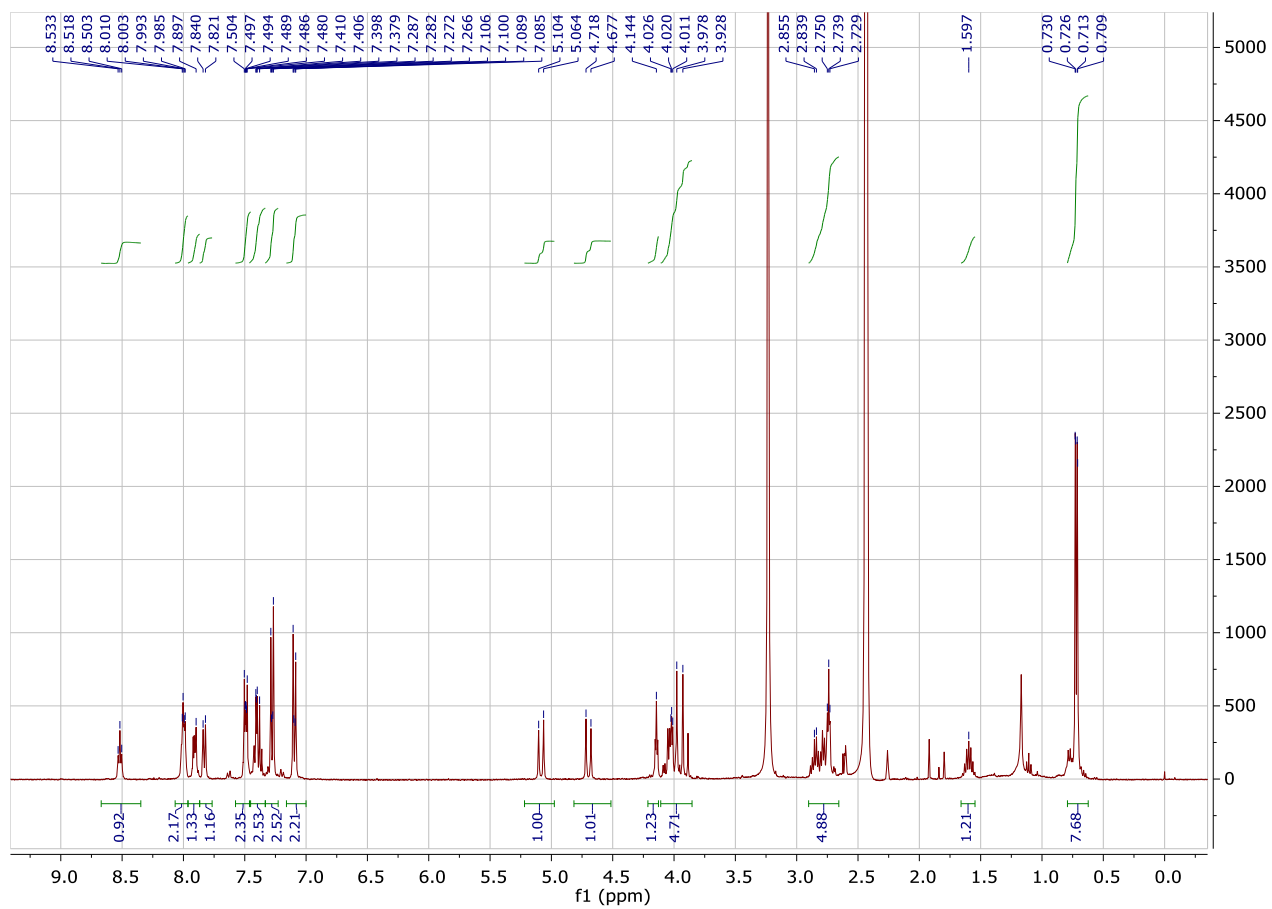


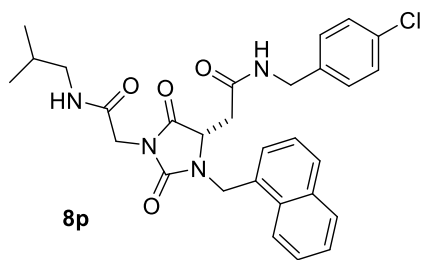


^1H NMR and COSY in CDCl_3 (400 MHz)

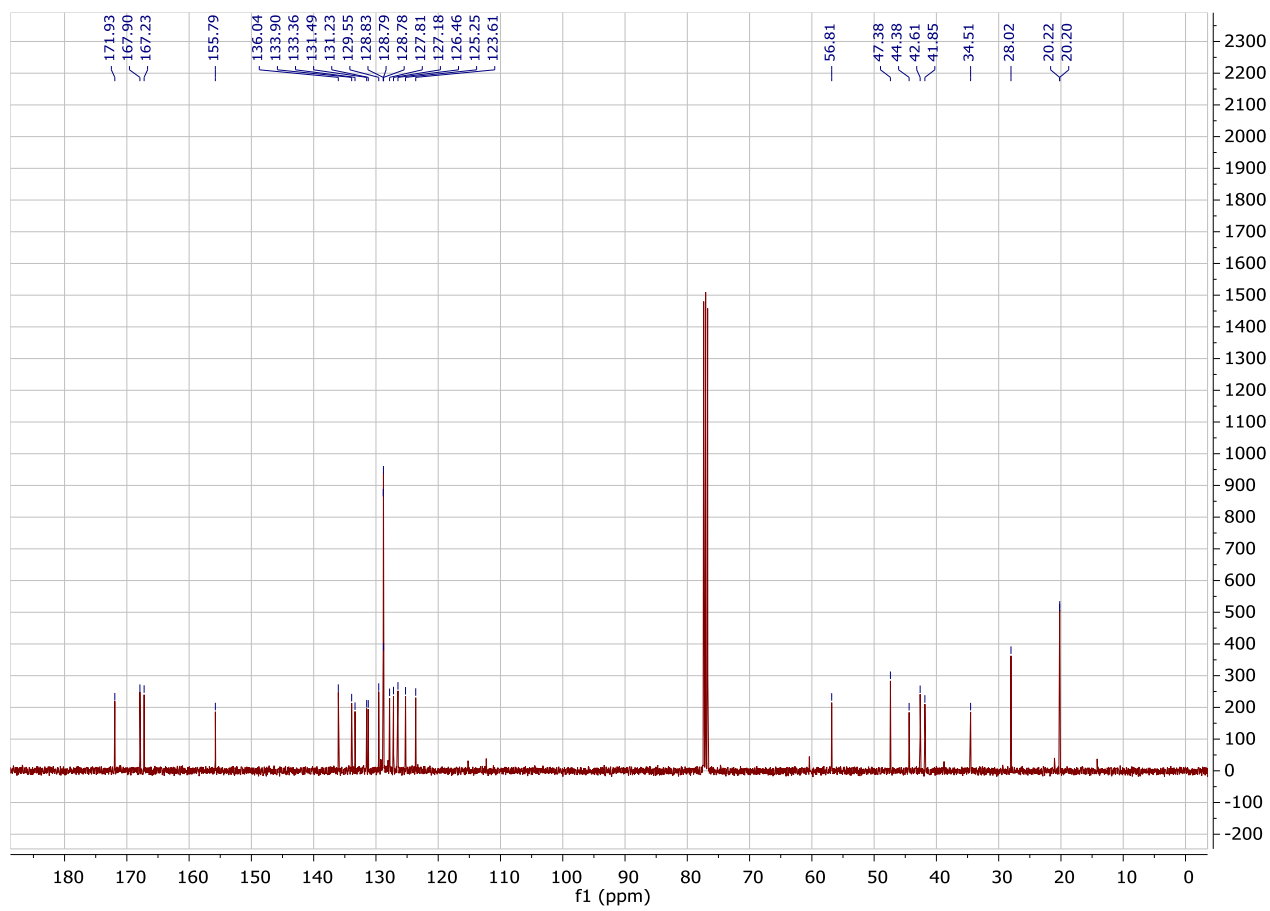


¹H NMR (400 MHz, dms0-d₆)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)

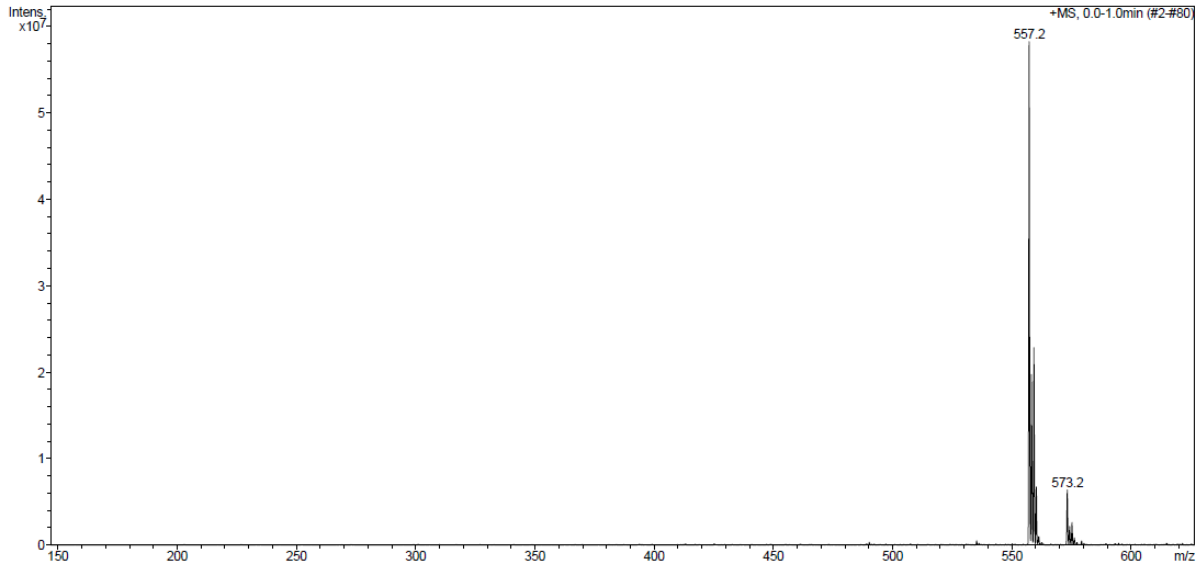


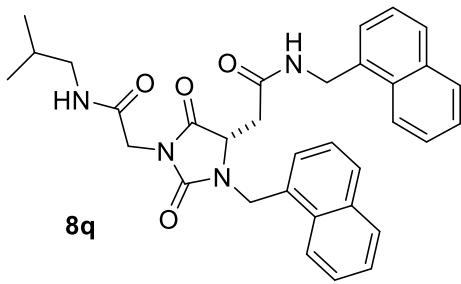
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name av ac073.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Caramiello

Acquisition Date 09/08/20 10:52:09
Method Copy of \$PW_TBLM.MS

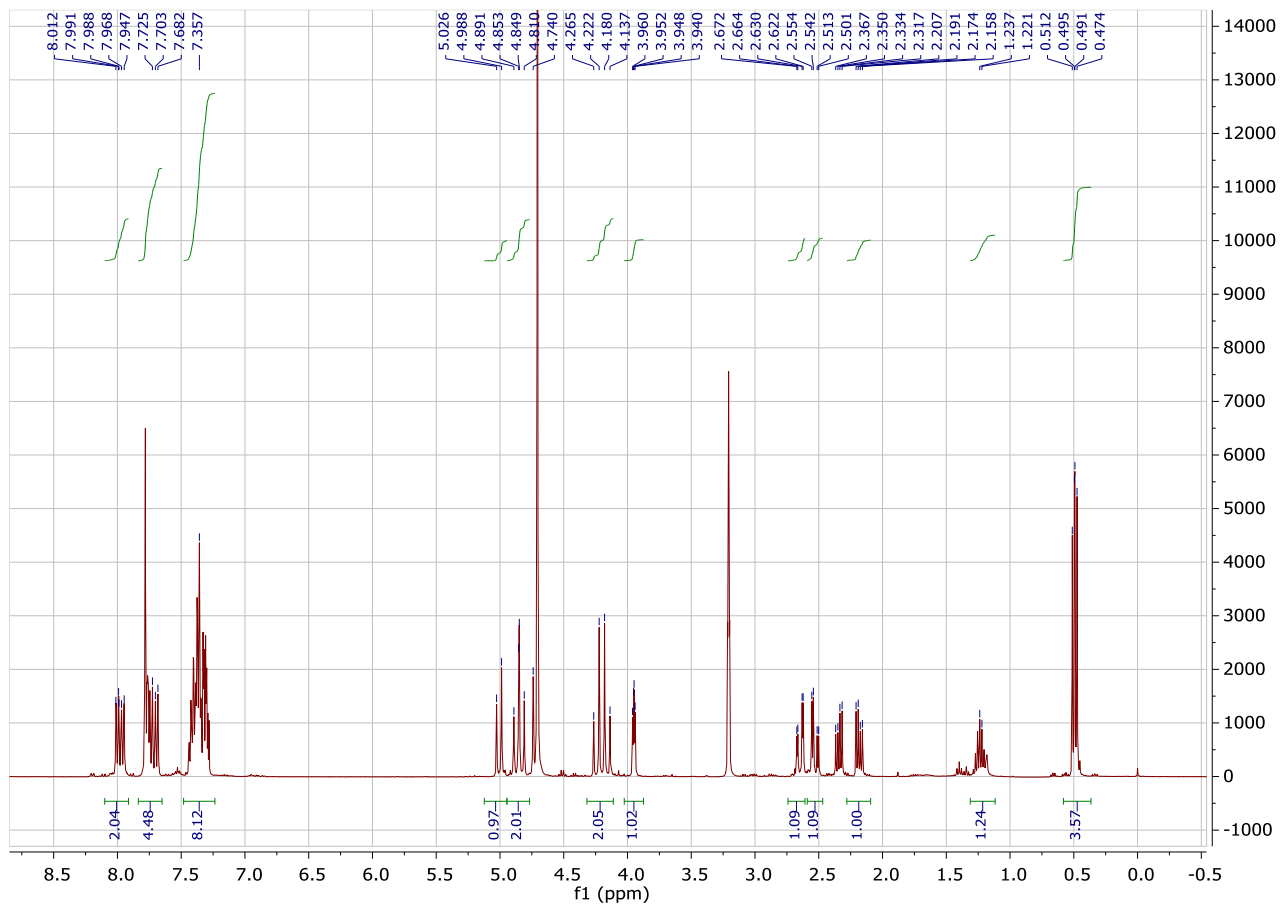
Operator Walter Panzeri
Instrument esquire3000plus

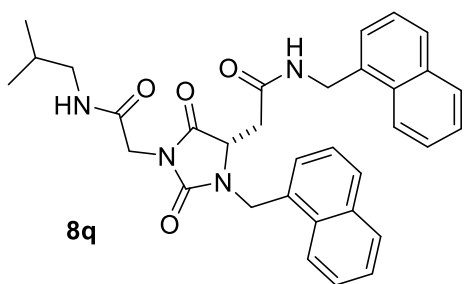




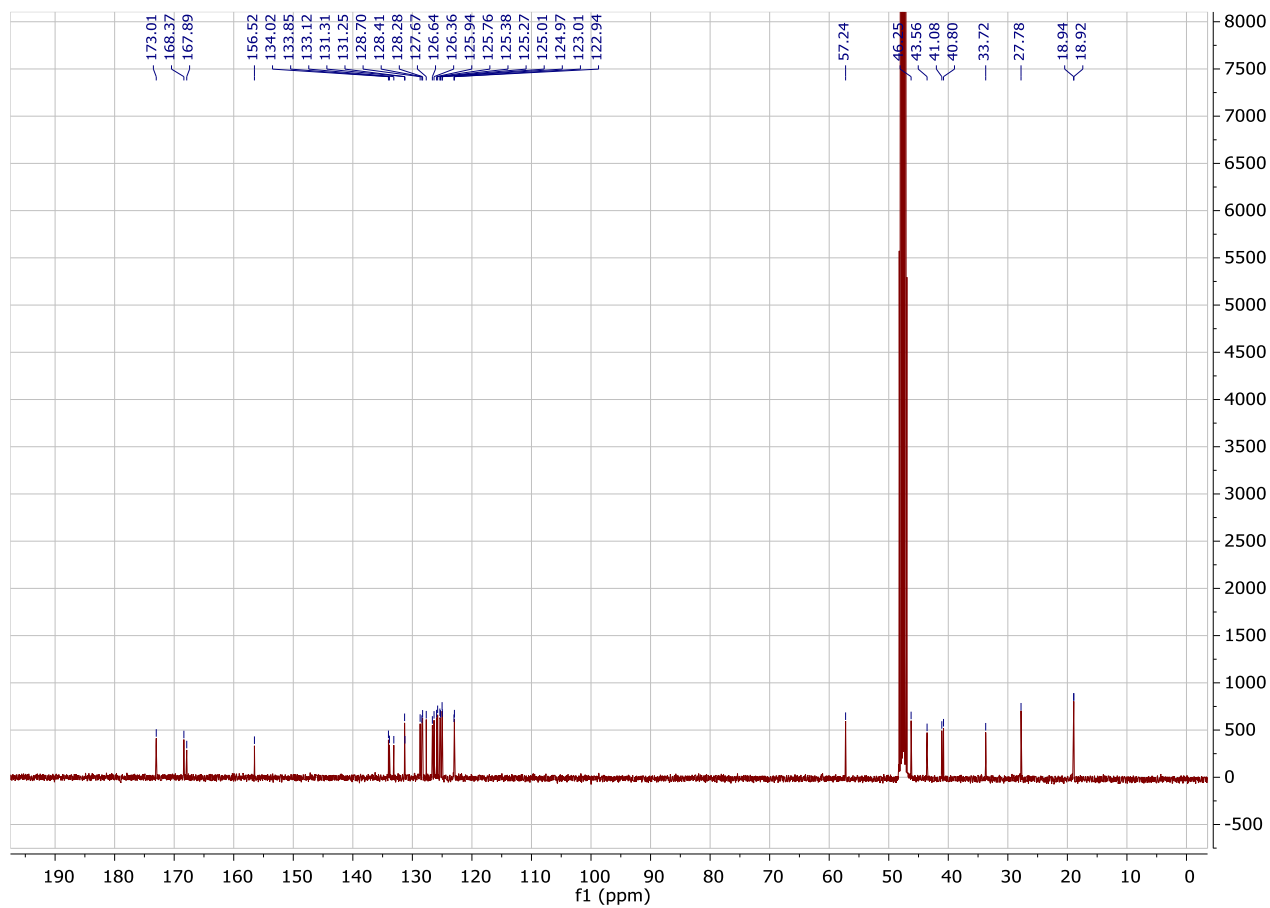
8q

$^1\text{H-NMR}$ (400 MHz, CD_3OD)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CD_3OD)



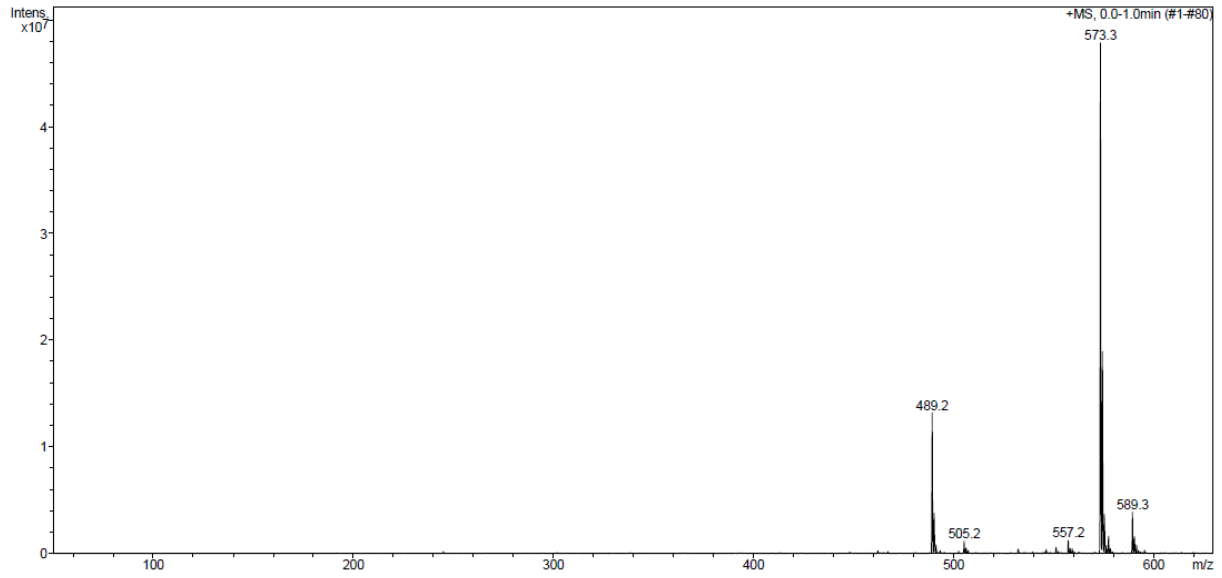
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

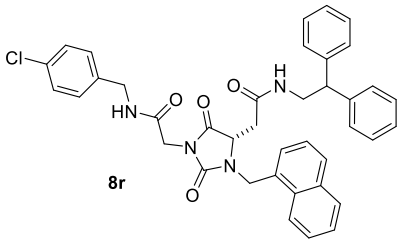
Analysis Name av ac074.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Caramiello

Acquisition Date 09/08/20 10:45:32
Method Copy of \$PW_TB.LM.MS

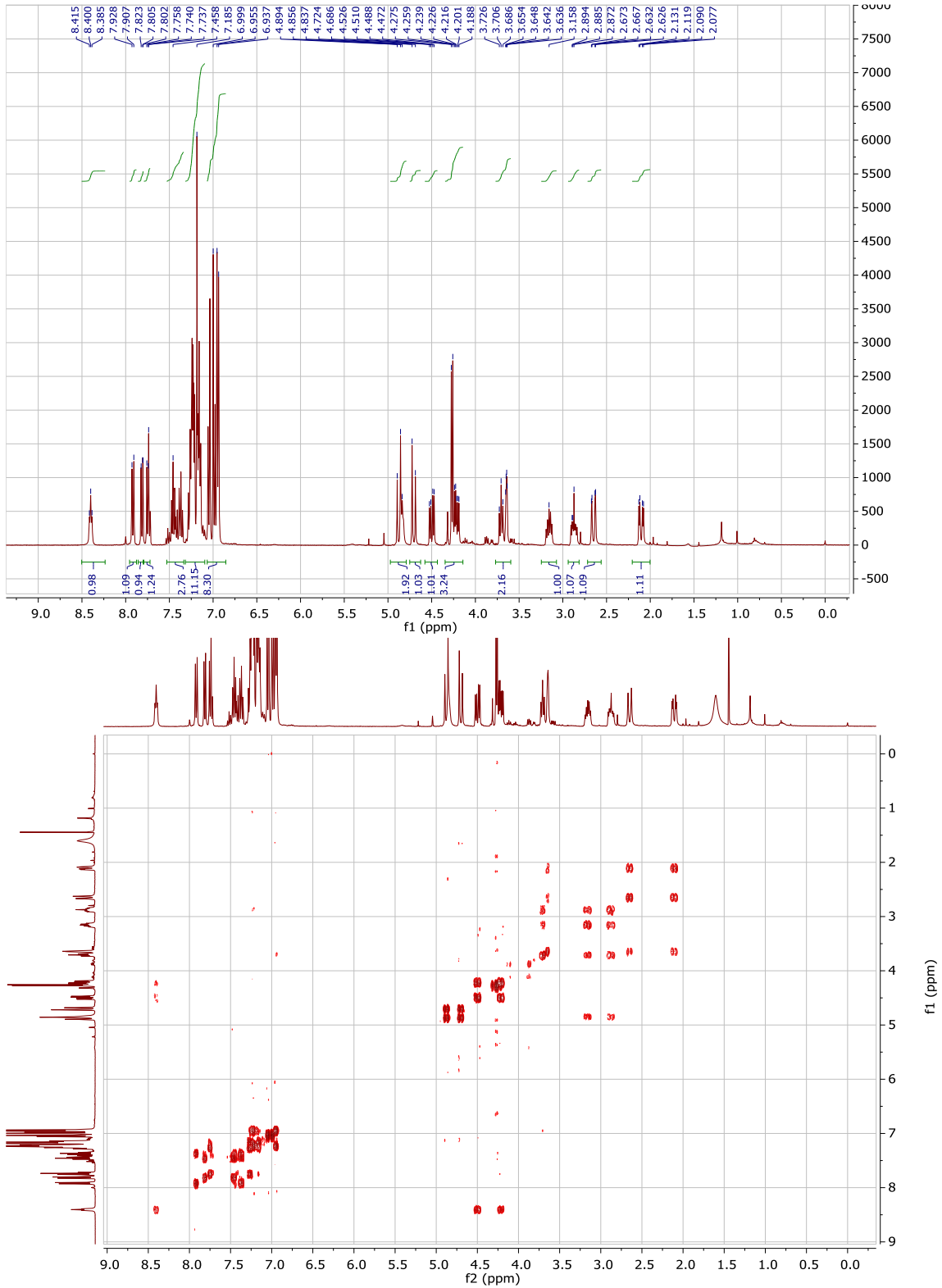
Operator
Instrument

Walter Panzeri
esquire3000plus

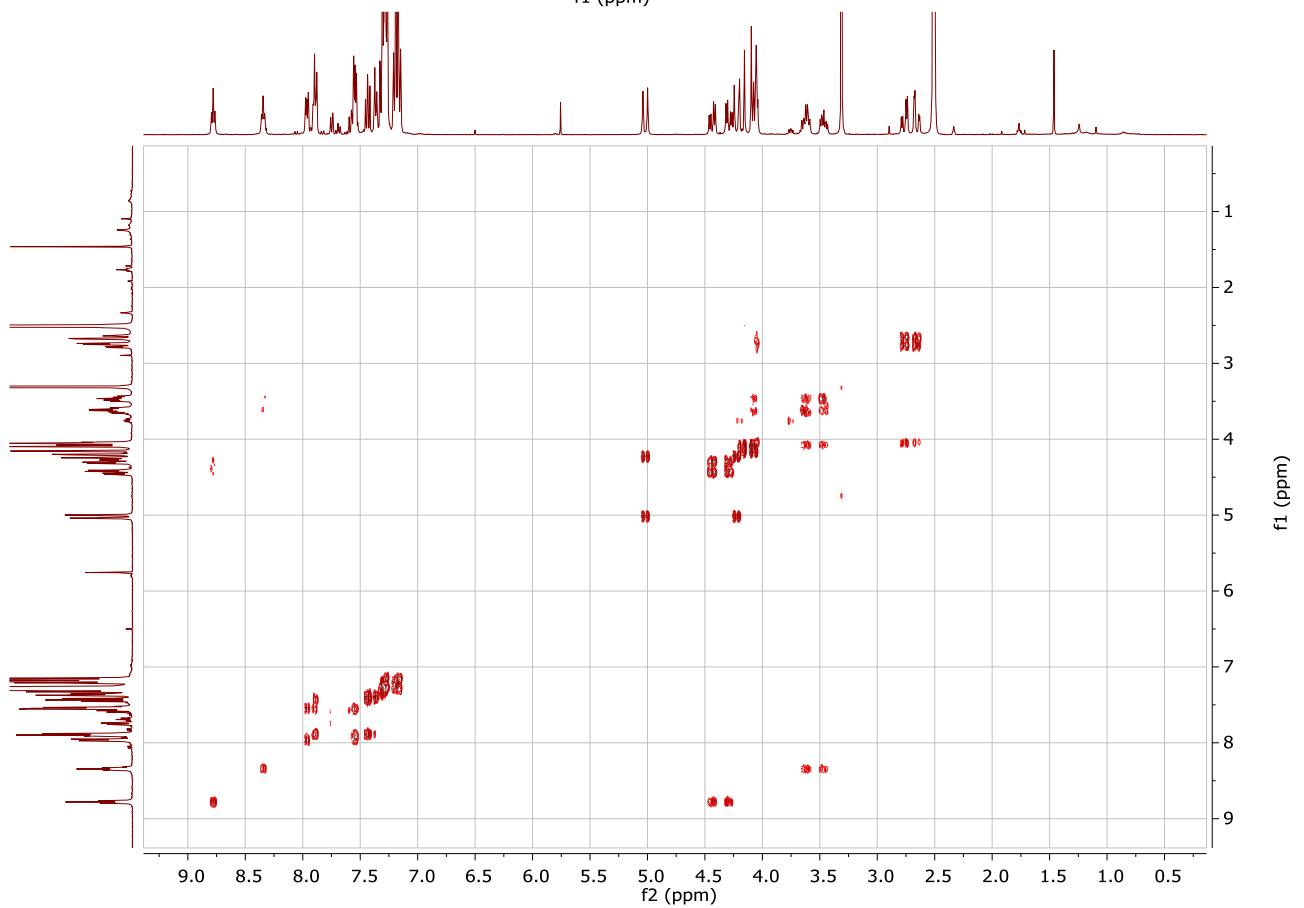
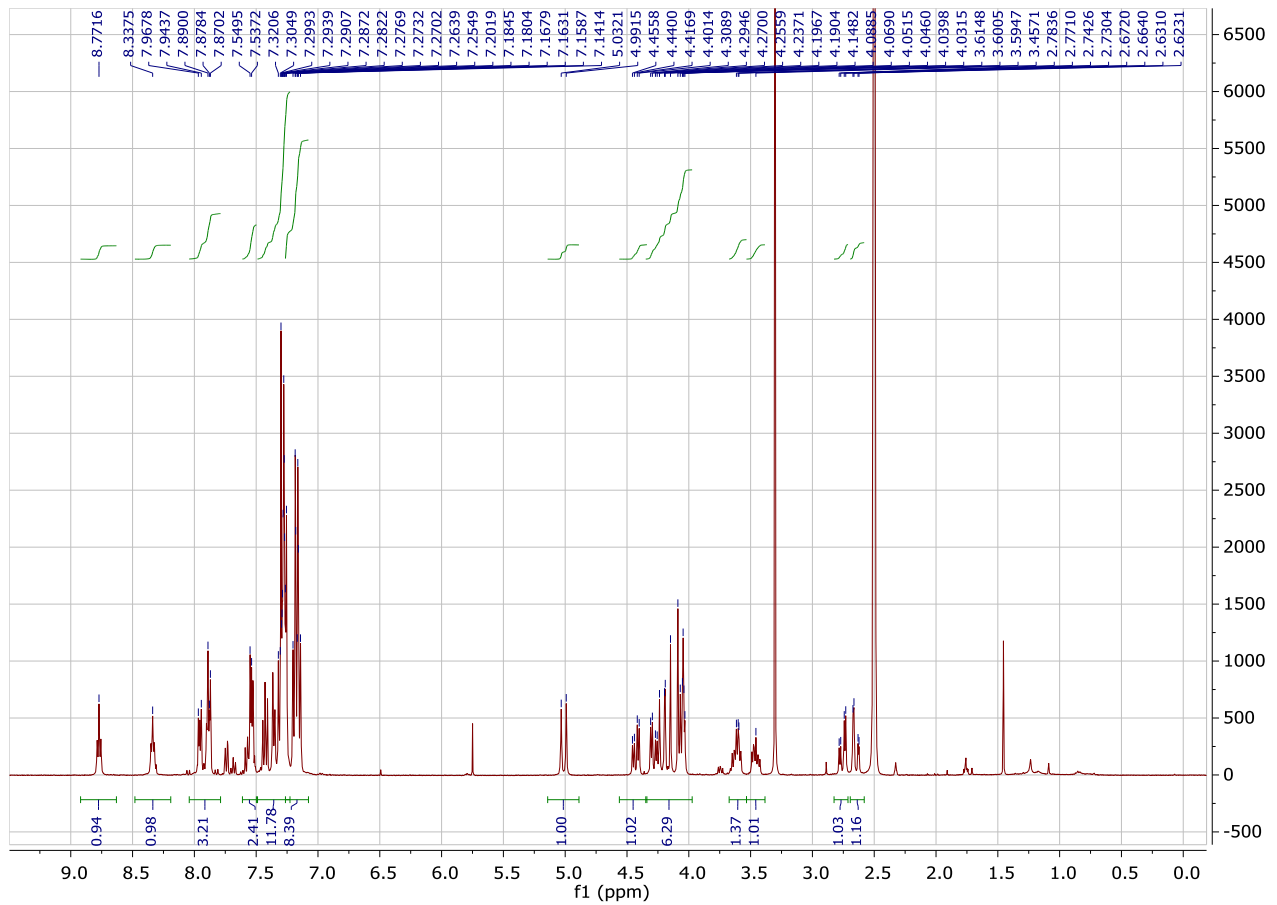


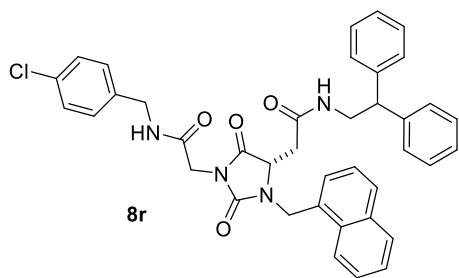


¹H NMR and COSY in CDCl₃ (400 MHz)

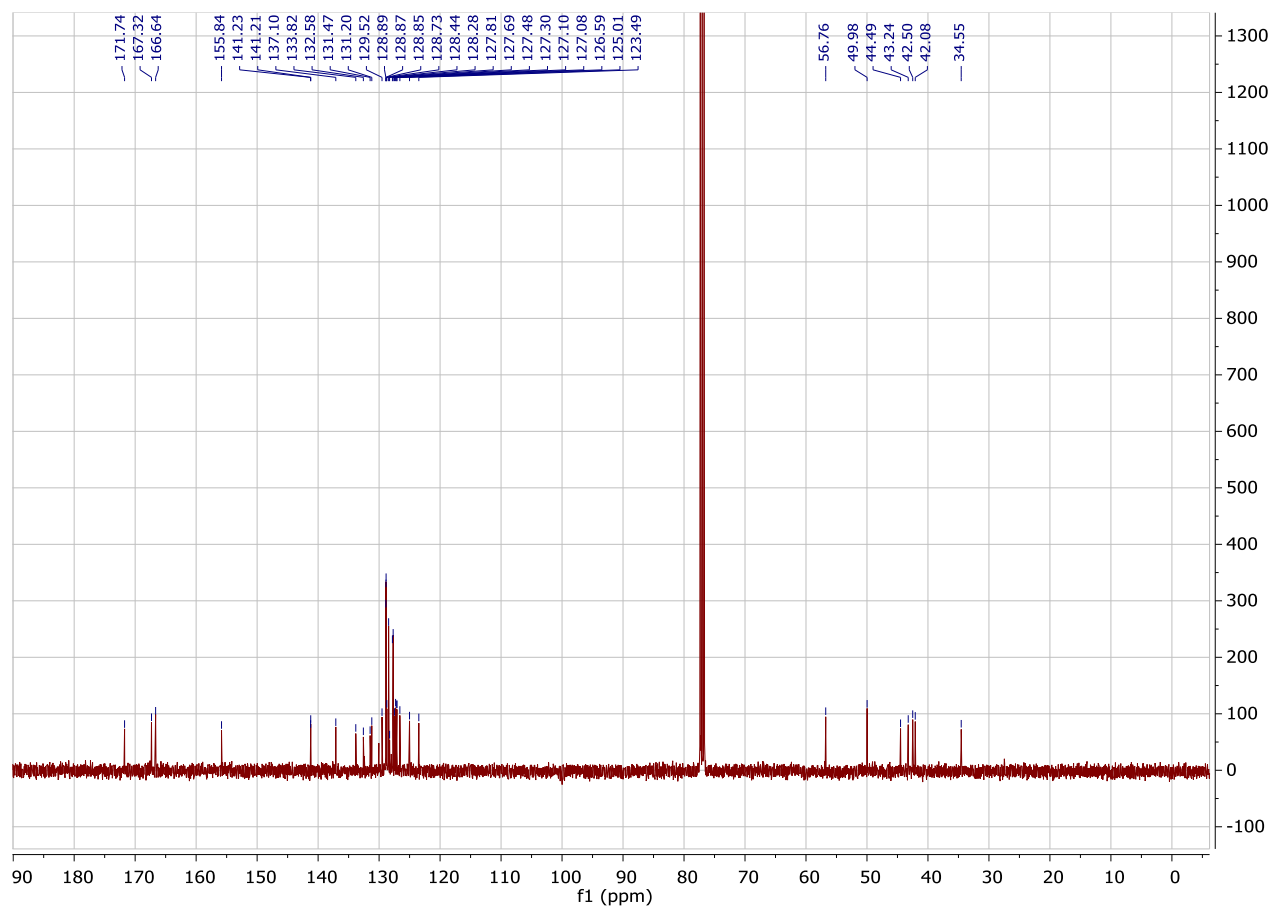


¹H NMR and COSY in dms_o-d₆ (400 MHz)





$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)



-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name av ac192.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Caramiello

Acquisition Date 03/09/22 10:19:08
Method Copy of \$opt0622.MS

Operator
Instrument

Walter Panzeri
esquire3000plus

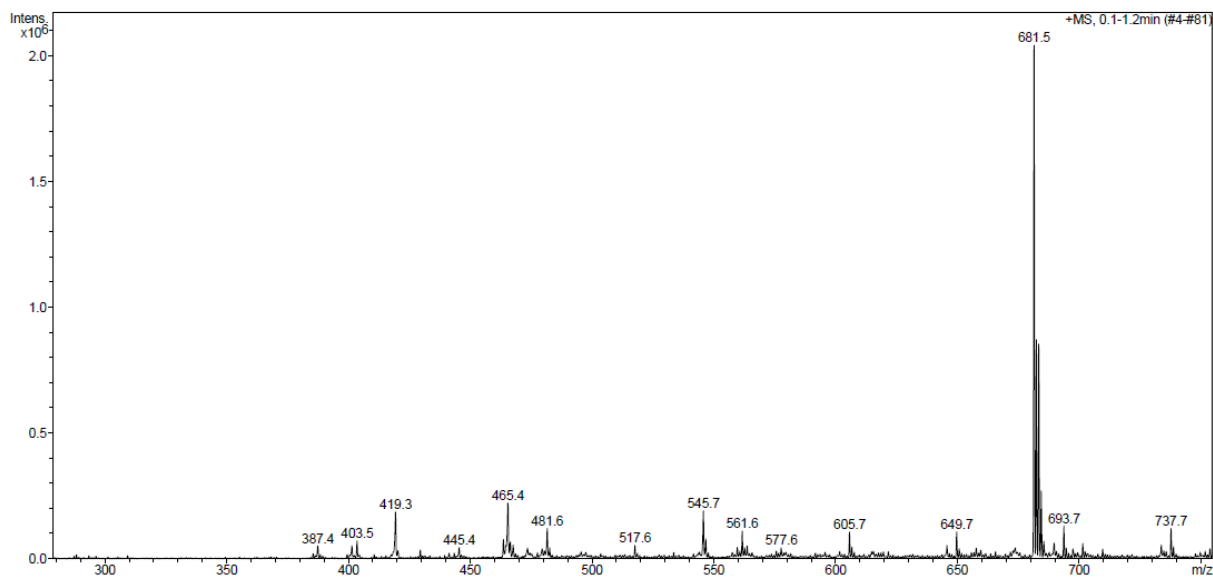


Figure S1. Results from Monte Carlo/MM conformational analysis. For each compounds the percentage of conformers meeting the geometrical requirements for β -turn, α -helix and 3_{10} -helix are reported.

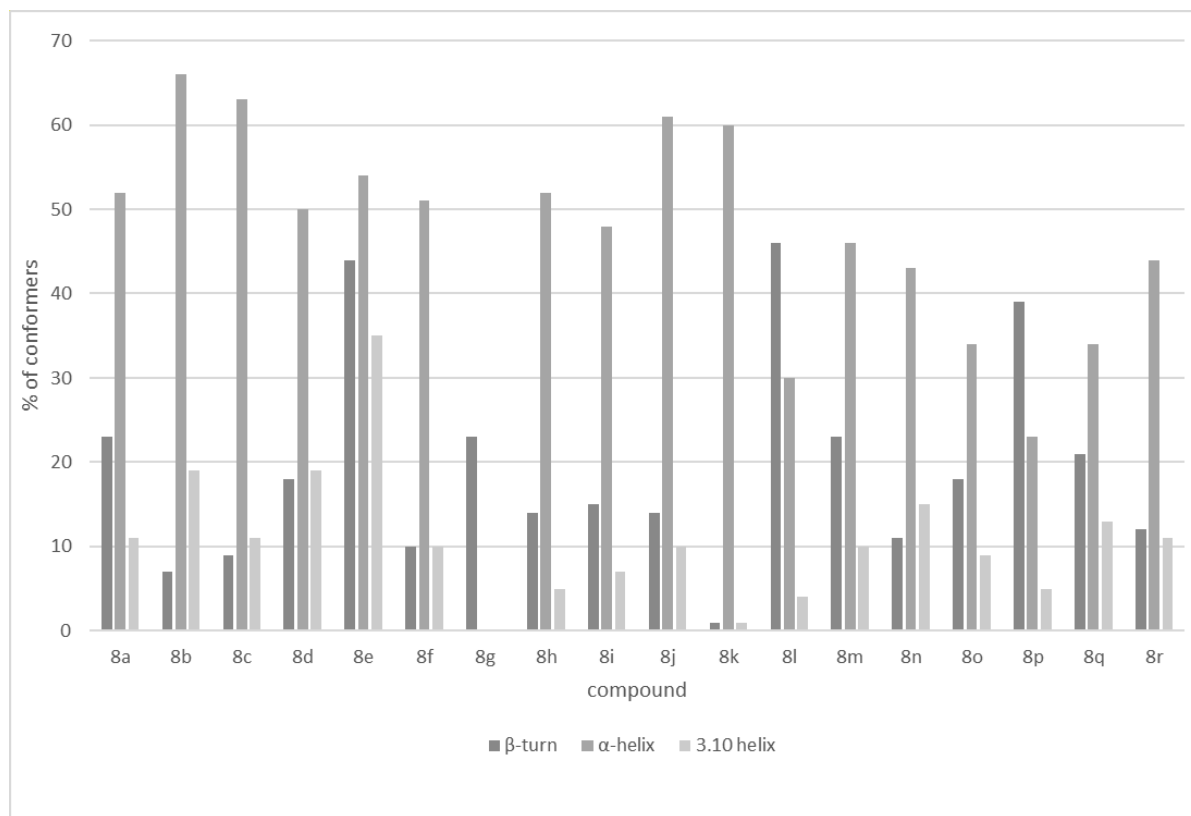


Figure S2. VT ^1H NMR spectra of **8o** (400 MHz)

From the bottom to the top: a) ^1H NMR in CDCl_3 at 302 K, b) ^1H NMR in CDCl_3 at 306 K, c) ^1H NMR in CDCl_3 at 310 K, d) ^1H NMR in CDCl_3 at 314 K, e) ^1H NMR in CDCl_3 at 318 K.

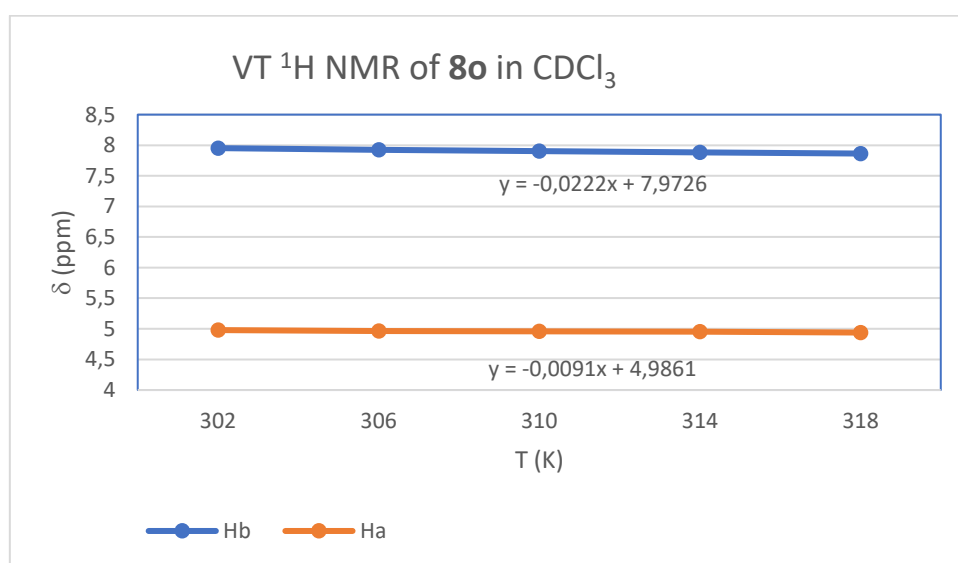
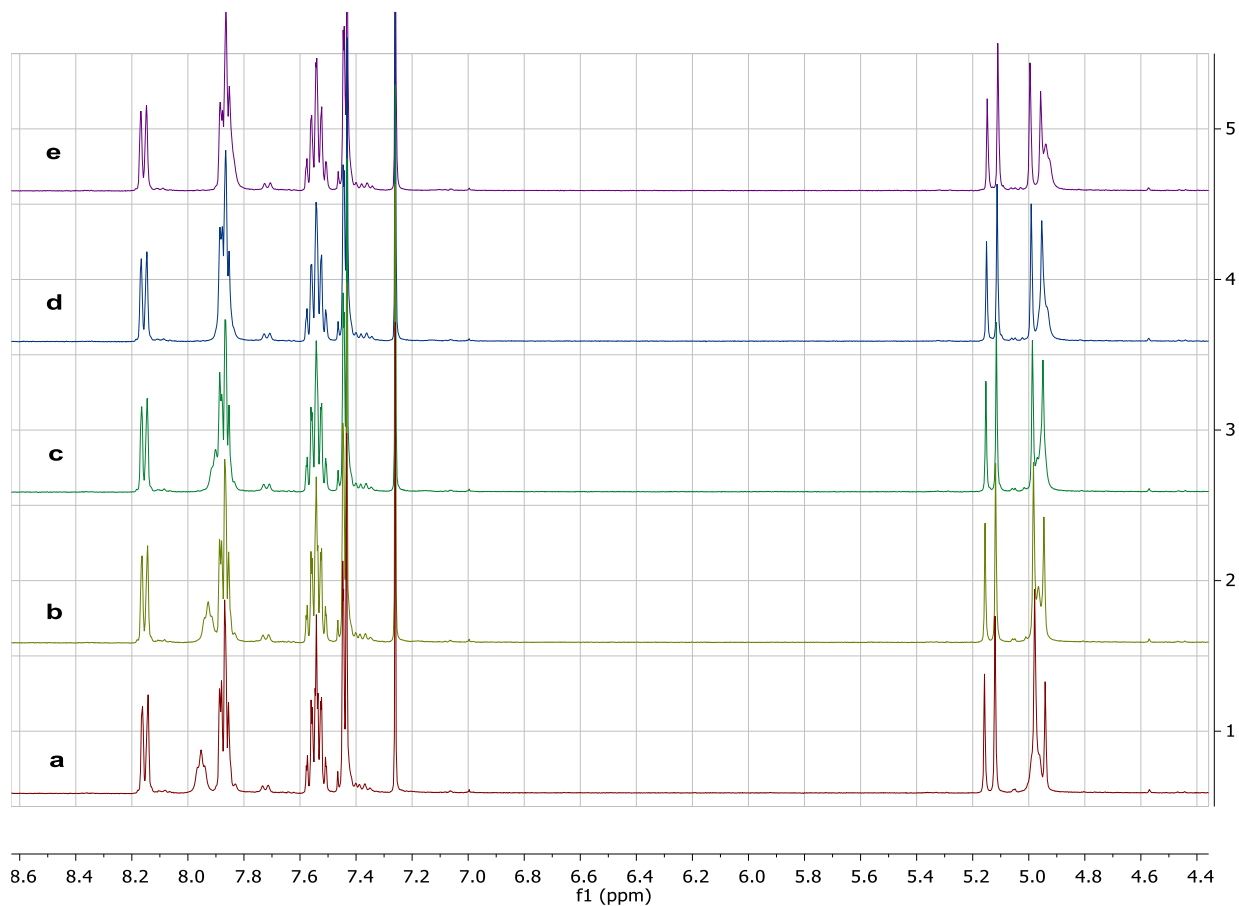


Figure S3. VT ^1H NMR spectra of **8p** (400 MHz)

From the bottom to the top: a) ^1H NMR in CDCl_3 at 302 K, b) ^1H NMR in CDCl_3 at 306 K, c) ^1H NMR in CDCl_3 at 310 K, d) ^1H NMR in CDCl_3 at 314 K, e) ^1H NMR in CDCl_3 at 318 K.

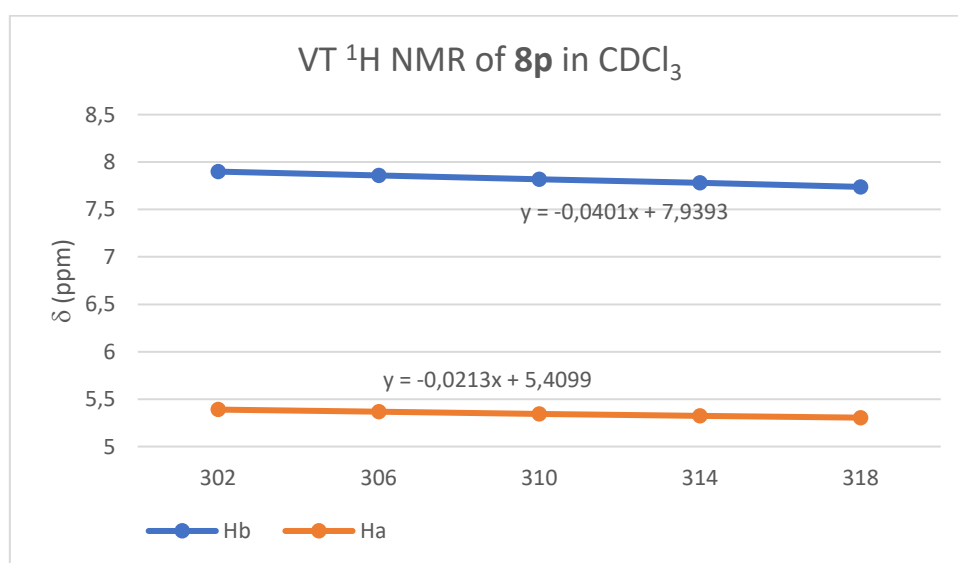
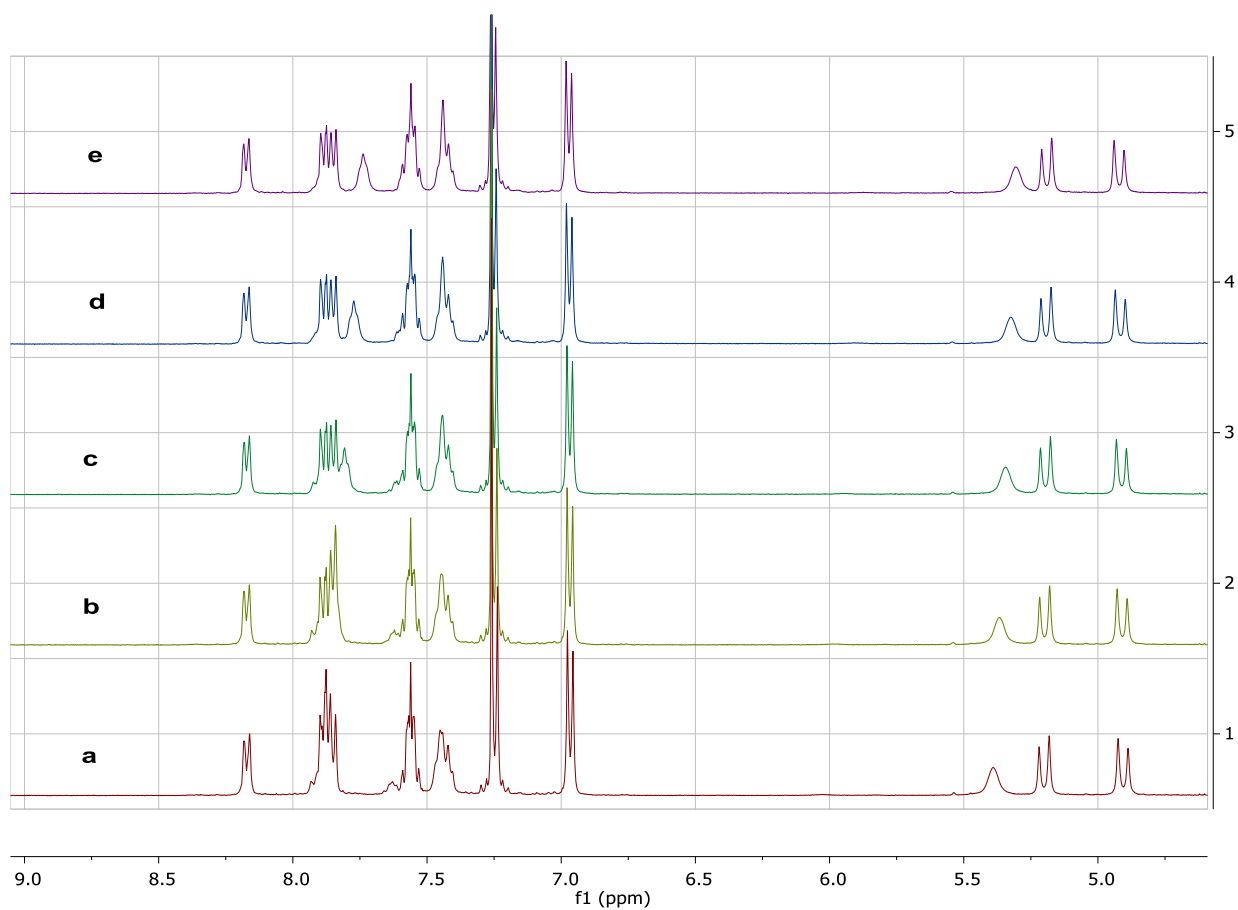


Figure S4. VT ^1H NMR spectra of **8r** in CDCl_3 (400 MHz)

From the bottom to the top: a) ^1H NMR in CDCl_3 at 302 K, b) ^1H NMR in CDCl_3 at 306 K, c) ^1H NMR in CDCl_3 at 310 K, d) ^1H NMR in CDCl_3 at 314 K, e) ^1H NMR in CDCl_3 at 318 K.

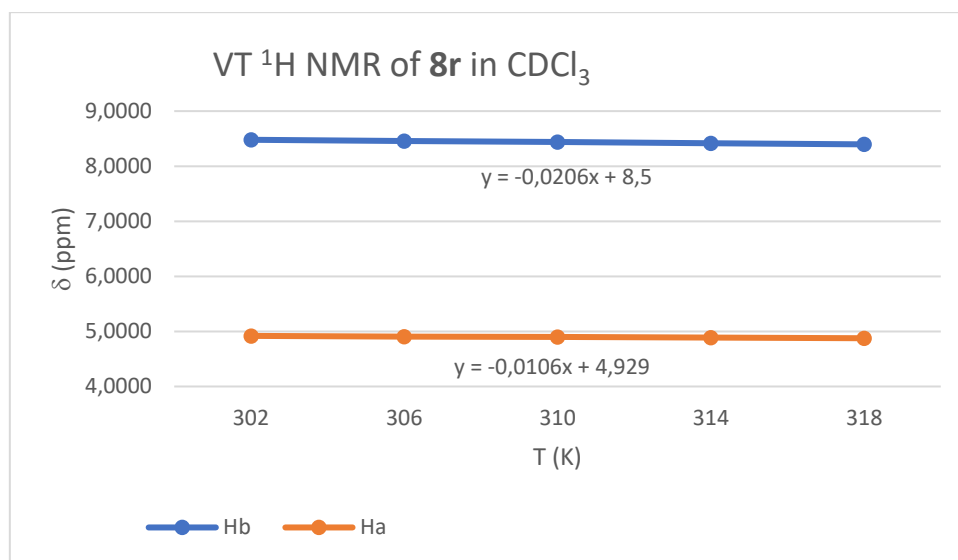
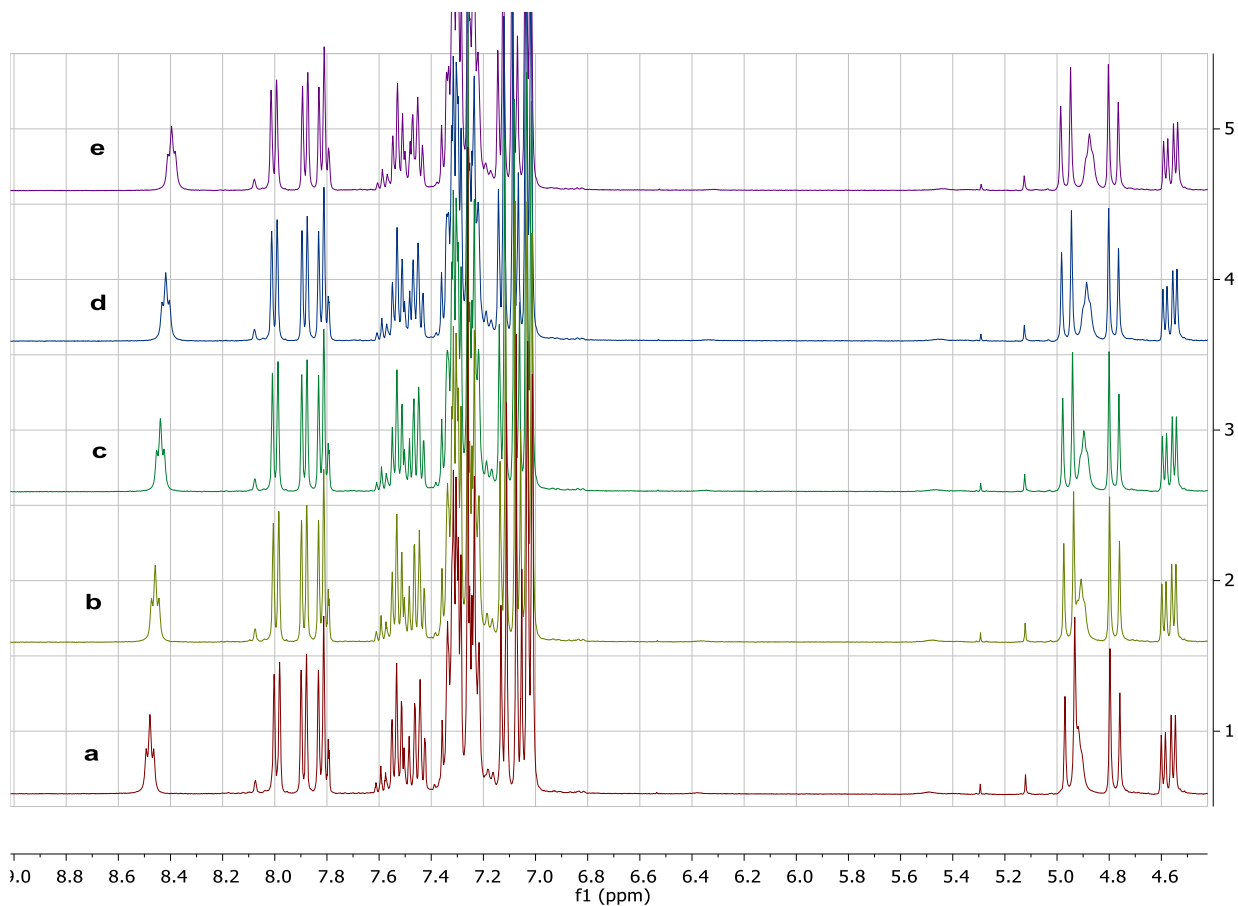


Figure S5. VT ^1H NMR spectra of **8p** in $\text{dms}\text{-d}_6$ (400 MHz)

From the bottom to the top: a) ^1H NMR in $\text{dms}\text{-d}_6$ at 302 K, b) ^1H NMR in $\text{dms}\text{-d}_6$ at 306 K, c) ^1H NMR in $\text{dms}\text{-d}_6$ at 310 K, d) ^1H NMR in $\text{dms}\text{-d}_6$ at 314 K, e) ^1H NMR in $\text{dms}\text{-d}_6$ at 318 K.

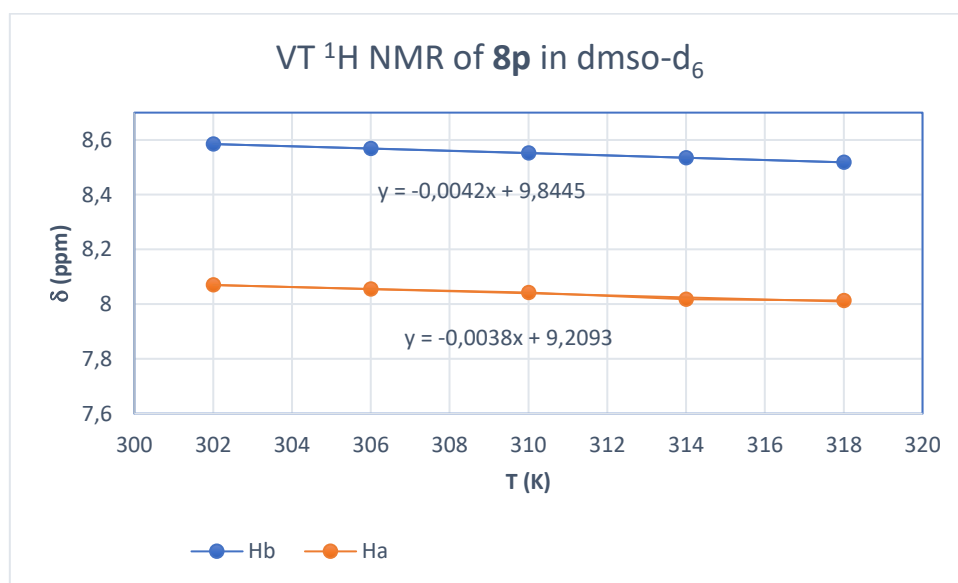
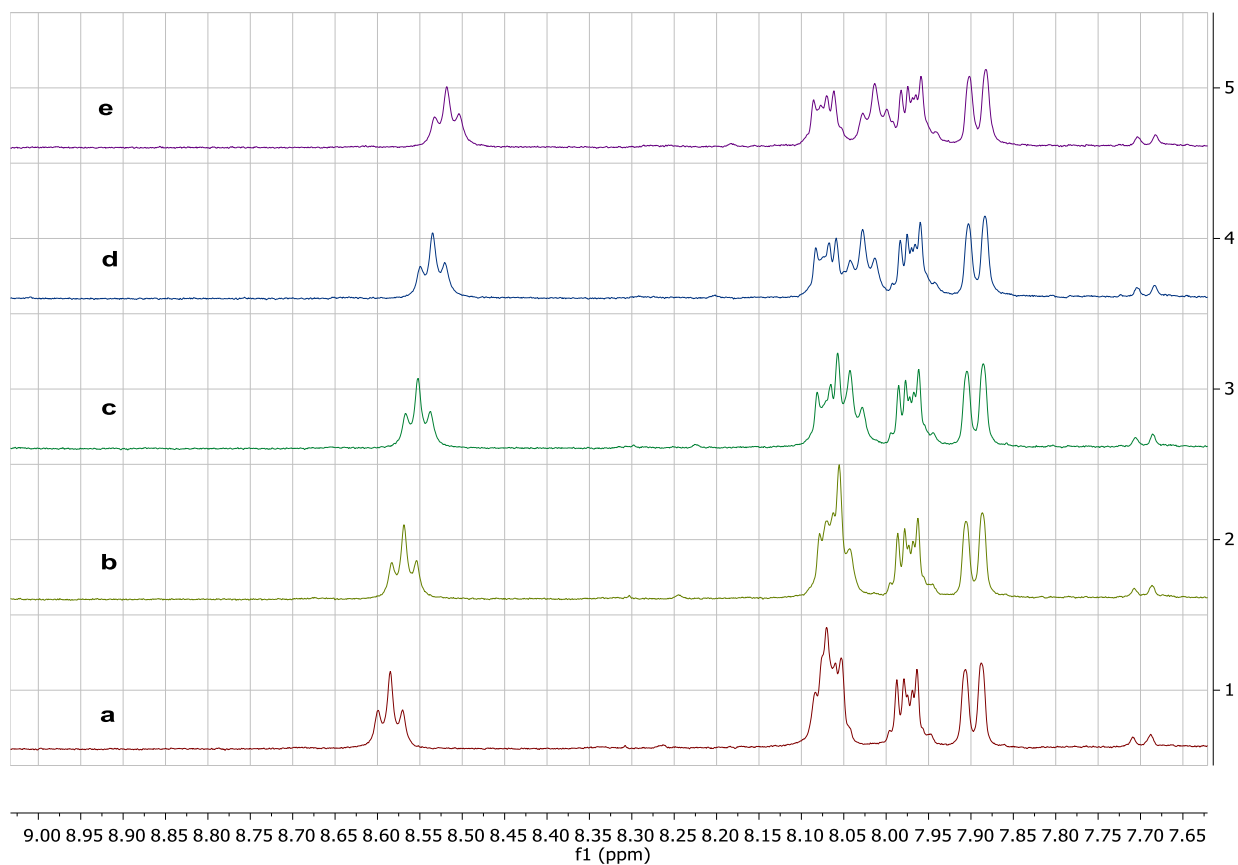


Figure S6. VT ^1H NMR spectra of **8r** in $\text{dms}\text{-d}_6$ (400 MHz)

From the bottom to the top: a) ^1H NMR in $\text{dms}\text{-d}_6$ at 302 K, b) ^1H NMR in $\text{dms}\text{-d}_6$ at 304 K, c) ^1H NMR in $\text{dms}\text{-d}_6$ at 306 K, d) ^1H NMR in $\text{dms}\text{-d}_6$ at 310 K, e) ^1H NMR in $\text{dms}\text{-d}_6$ at 314 K, f) ^1H NMR in $\text{dms}\text{-d}_6$ at 318 K.

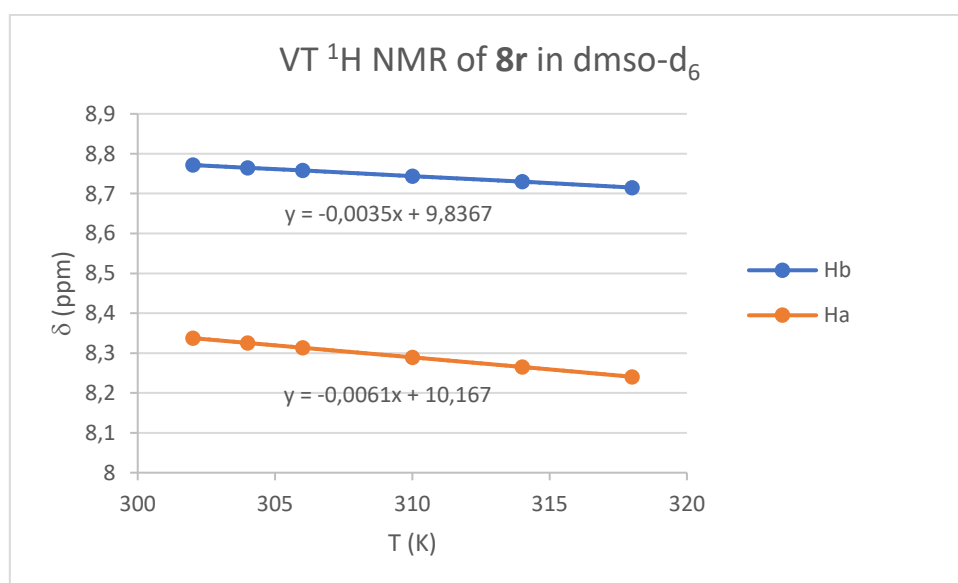
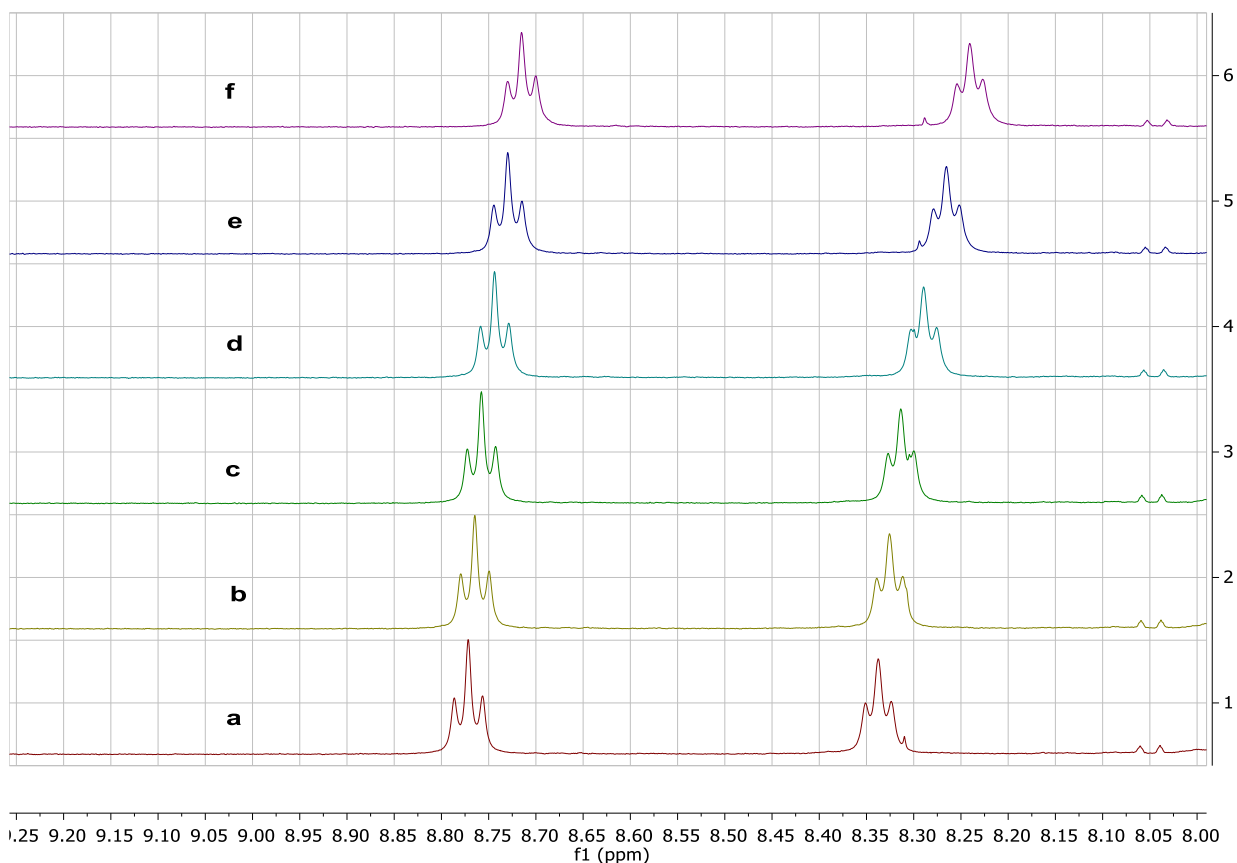


Figure S7. DMSO titration ^1H NMR spectra of **8p** (500 MHz)

From the bottom to the top: a) ^1H NMR in CDCl_3 , b) ^1H NMR in CDCl_3 + 5 μL of DMSO, c) ^1H NMR in CDCl_3 + 10 μL of DMSO, d) ^1H NMR in CDCl_3 + 15 μL of DMSO, e) ^1H NMR in CDCl_3 + 20 μL of DMSO, f) ^1H NMR in CDCl_3 + 25 μL of DMSO; g) ^1H NMR in CDCl_3 + 30 μL of DMSO; h) ^1H NMR in CDCl_3 + 35 μL of DMSO, i) ^1H NMR in CDCl_3 + 40 μL of DMSO.

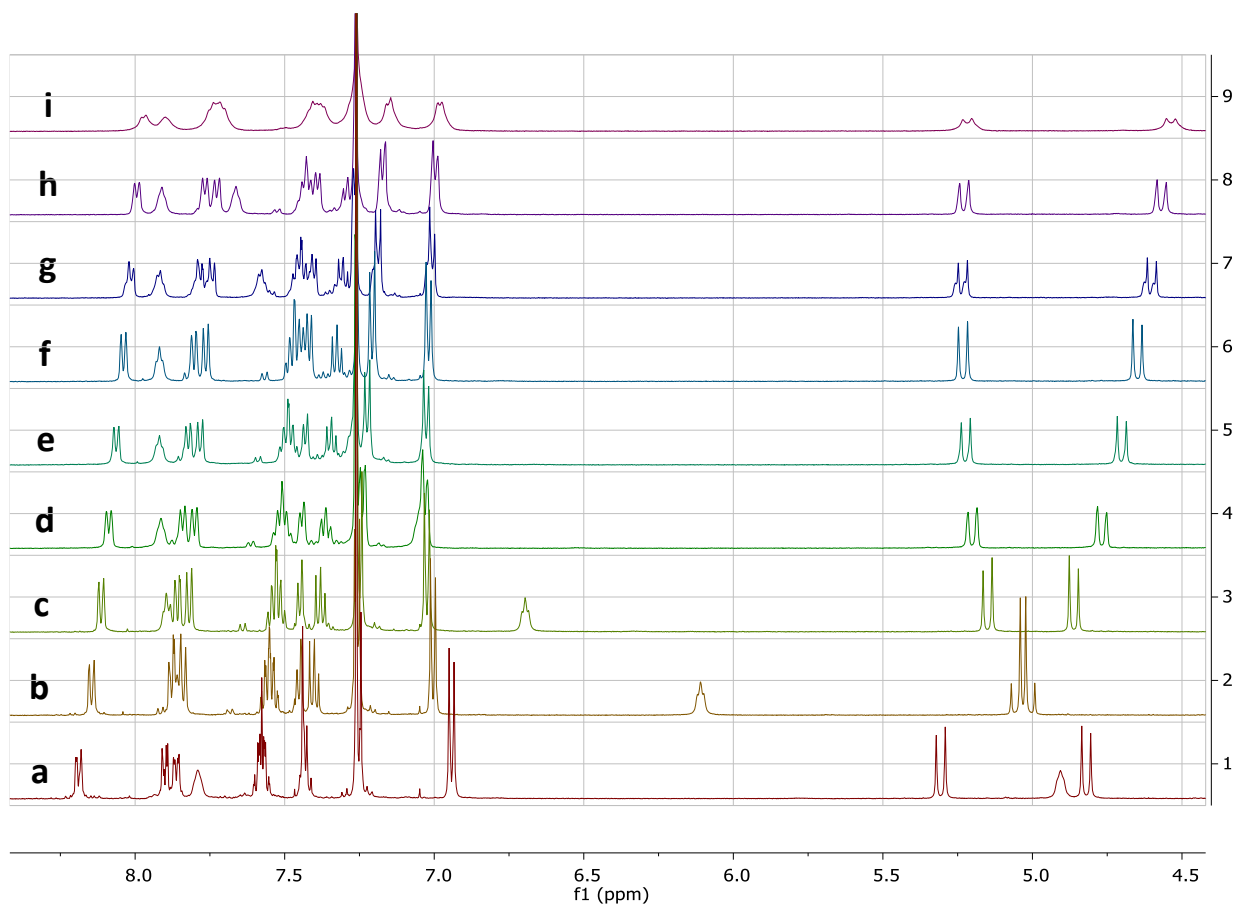


Figure S8. DMSO titration ^1H NMR spectra of **8r** (500 MHz)

From the bottom to the top: a) ^1H NMR in CDCl_3 , b) ^1H NMR in CDCl_3 + 5 μL of DMSO, c) ^1H NMR in CDCl_3 + 10 μL of DMSO, d) ^1H NMR in CDCl_3 + 15 μL of DMSO, e) ^1H NMR in CDCl_3 + 20 μL of DMSO, f) ^1H NMR in CDCl_3 + 25 μL of DMSO; g) ^1H NMR in CDCl_3 + 30 μL of DMSO; h) ^1H NMR in CDCl_3 + 35 μL of DMSO, i) ^1H NMR in CDCl_3 + 40 μL of DMSO, j) ^1H NMR in CDCl_3 + 45 μL of DMSO, k) ^1H NMR in CDCl_3 + 50 μL of DMSO

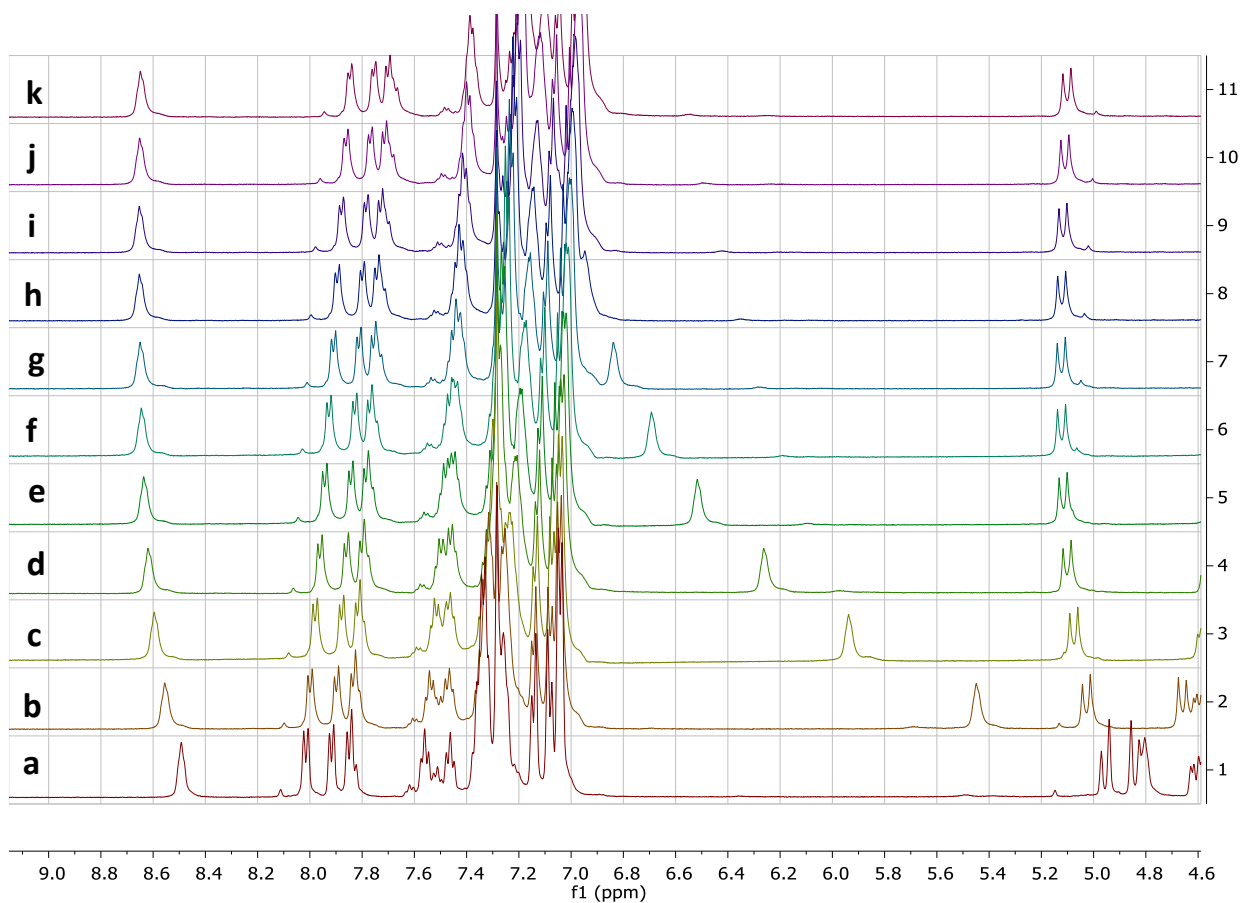


Table S1. Selected H-bond distances and angles.

Bond	D...A (Å)	D-H...A (Å)	D-H...A (°)	Equivalent positions
N3-H3N...O4	2.727(9)	1.965(6)	147.2(5)	x,y,z
N4-H4N...O3	2.843(9)	2.001(6)	166.1(5)	x,y-1,z
C38-H38...O1	3.651(12)	2.738(6)	167.5(6)	x,y,z
C31-H31...O3	3.751(11)	2.947(6)	145.5(6)	x,y-1,z
C32-H32...O1	3.784(13)	2.894(6)	160.5(7)	x,y-1,z
C25-H25...Cl1	3.775(20)	2.895(5)	158(1)	1-x,y,1-z