Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Aziridine Derived Electrophilic Handle for Asparatic Ligation

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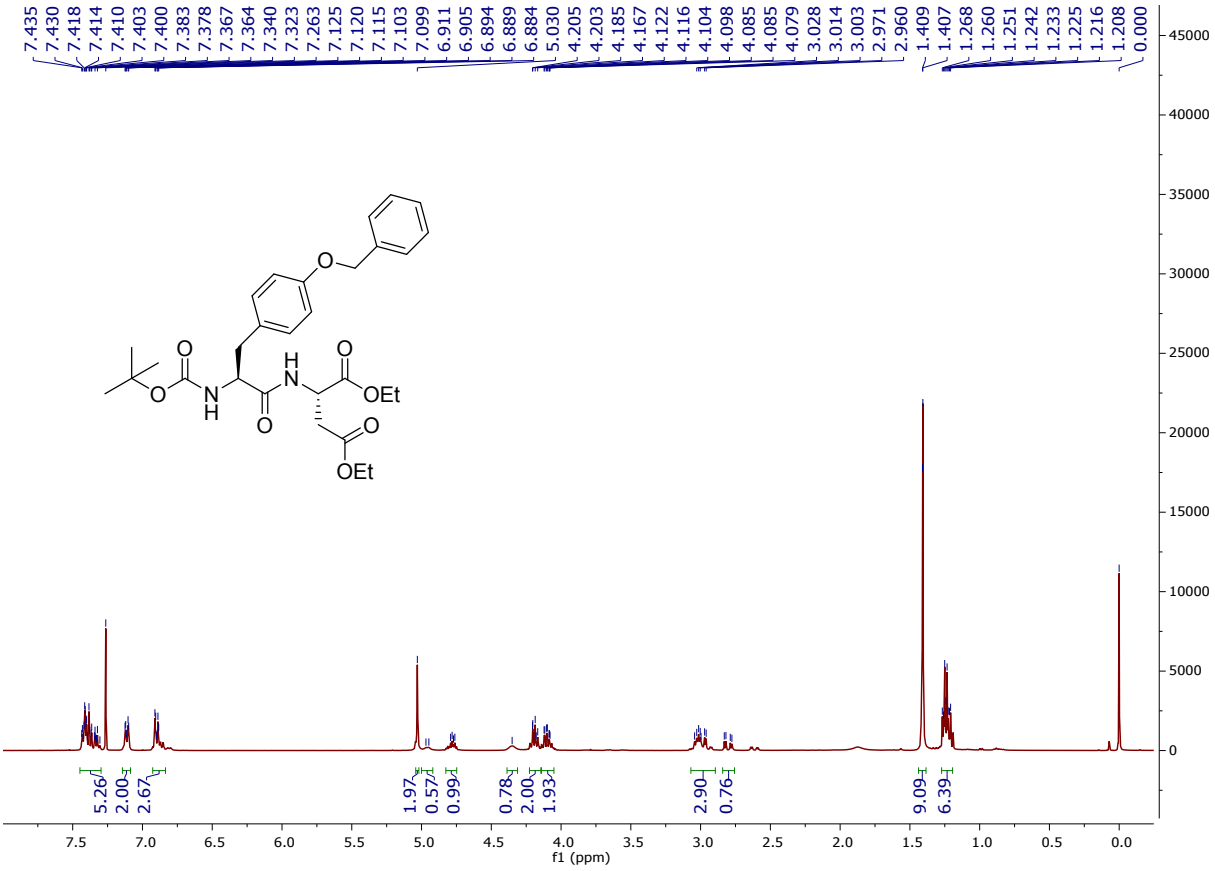
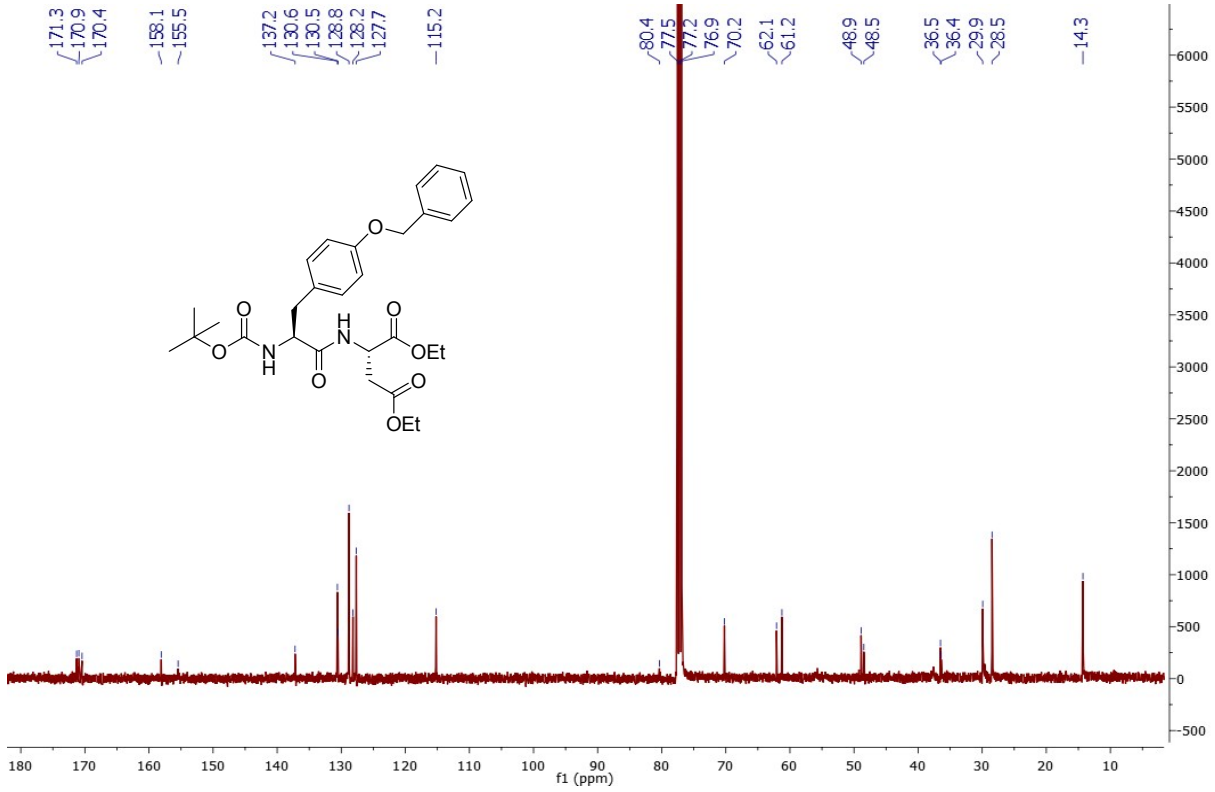
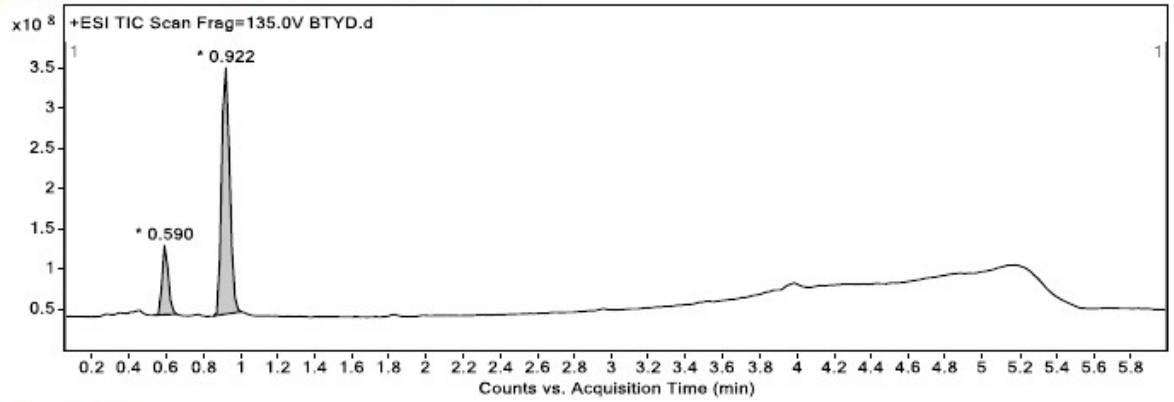




[1] H NMR (400 MHz, $CDCl_3$) and [13]C NMR (100 MHz, $CDCl_3$) of compound **5c**

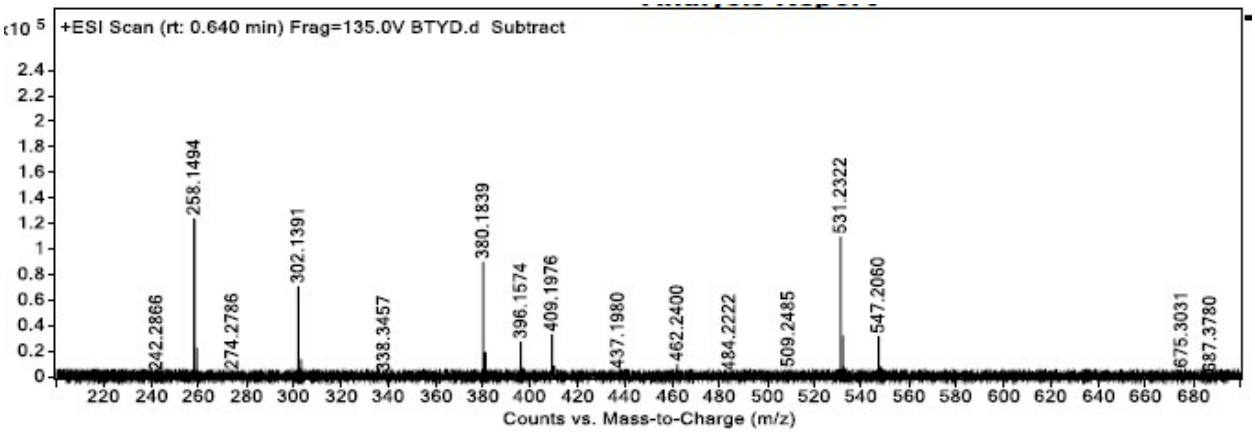
User Chromatograms

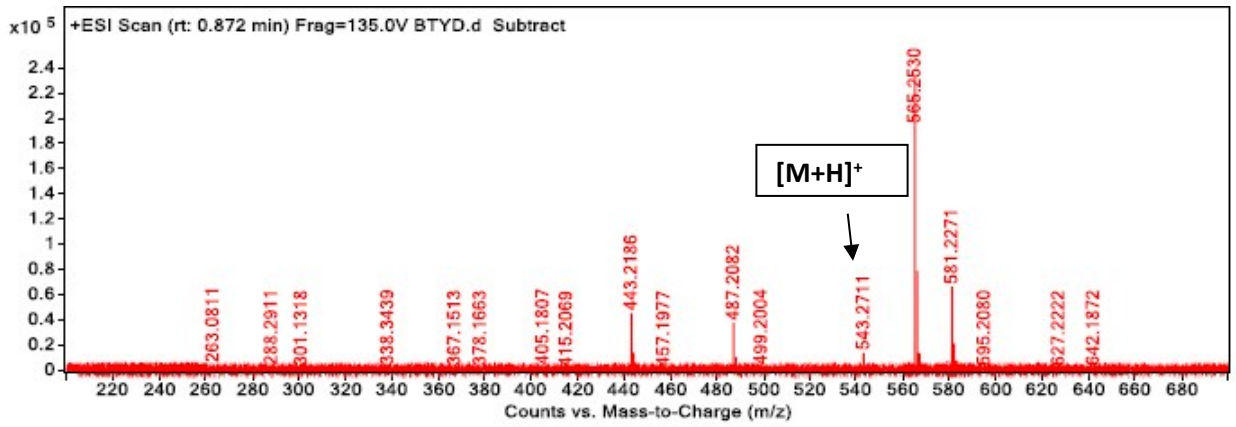
Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI



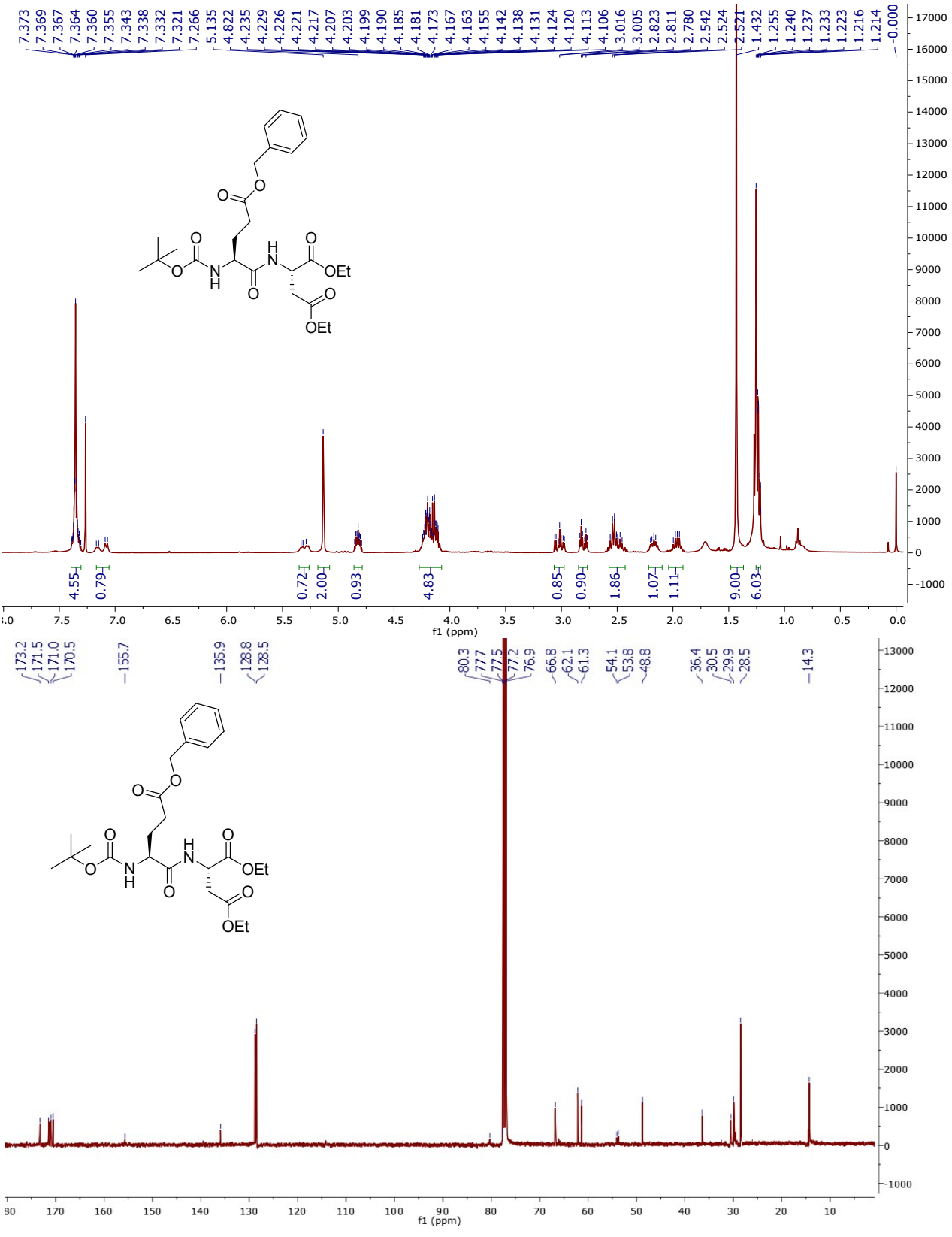
Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.541	0.59	0.657	86748755	200408185	21.34
2	0.855	0.922	1.004	307146976	939319964	100

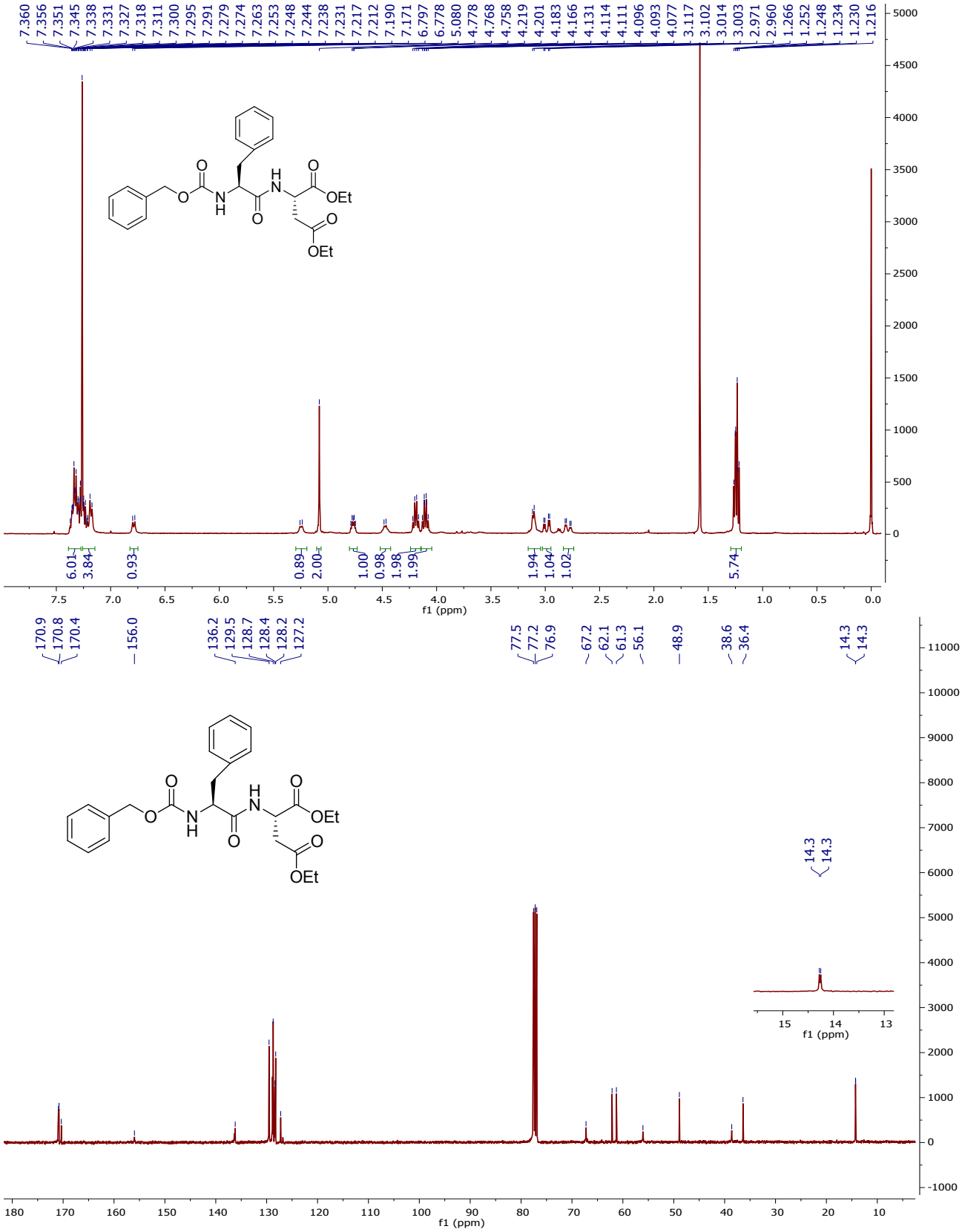




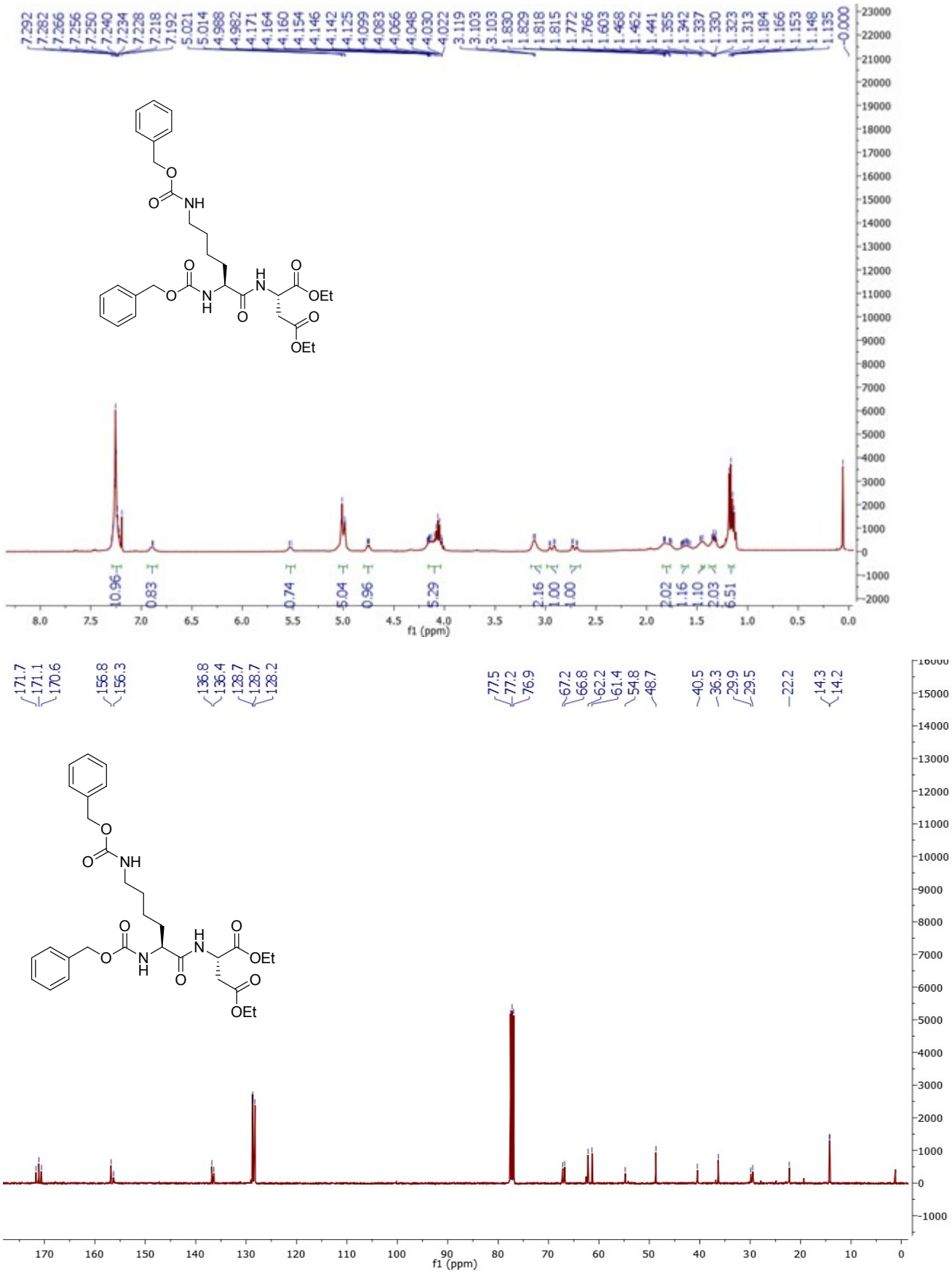
LC-HRMS of compound 5c



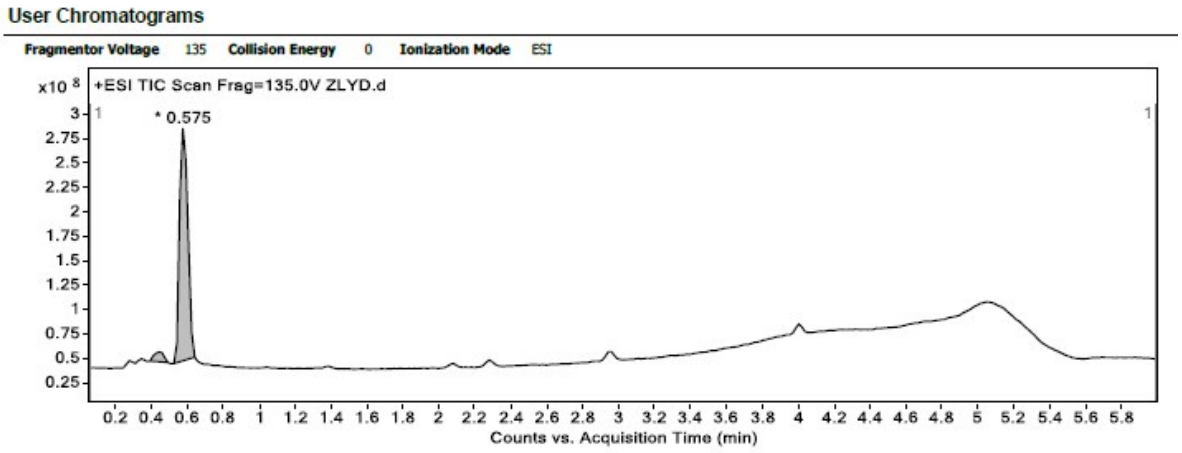
^{1} H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **5d**



^{1} H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **5e**



^{1} H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **5f**



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
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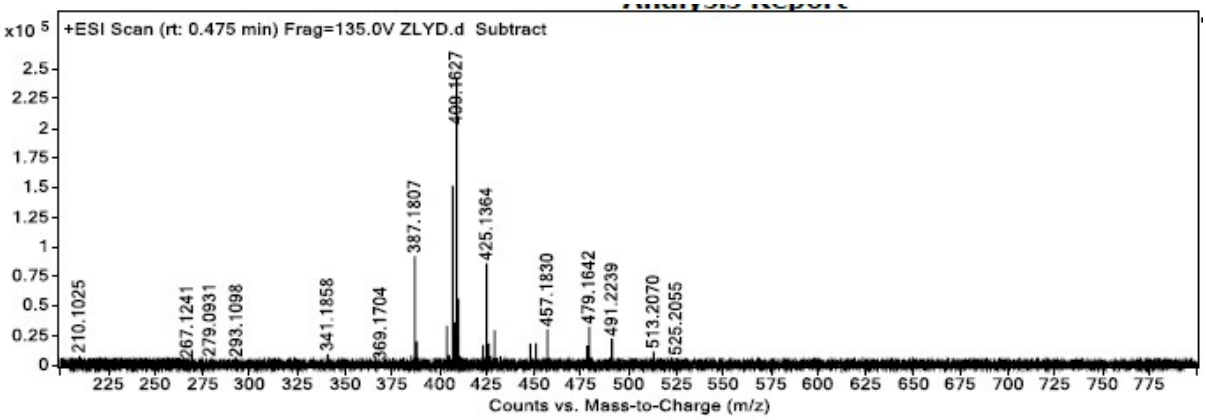
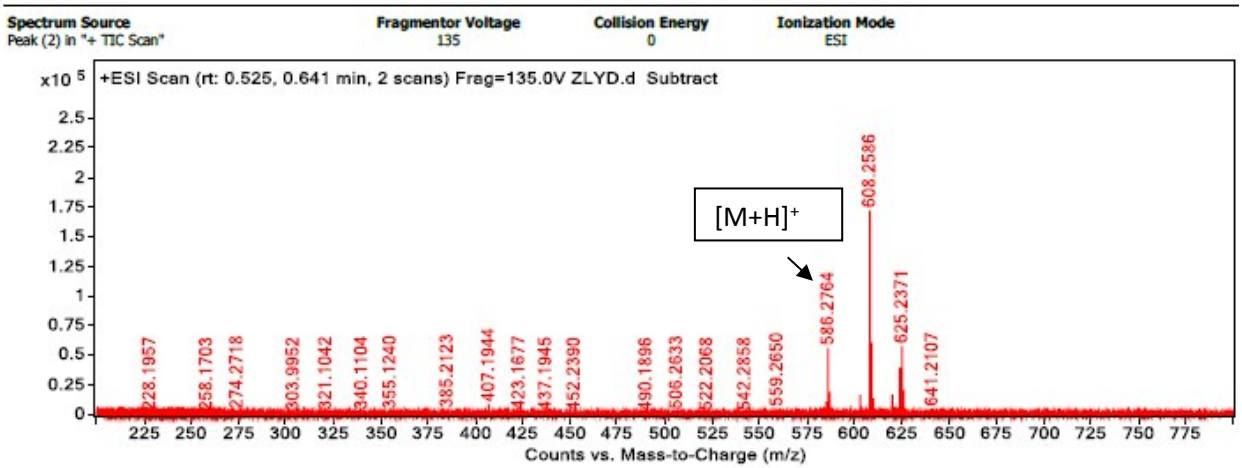
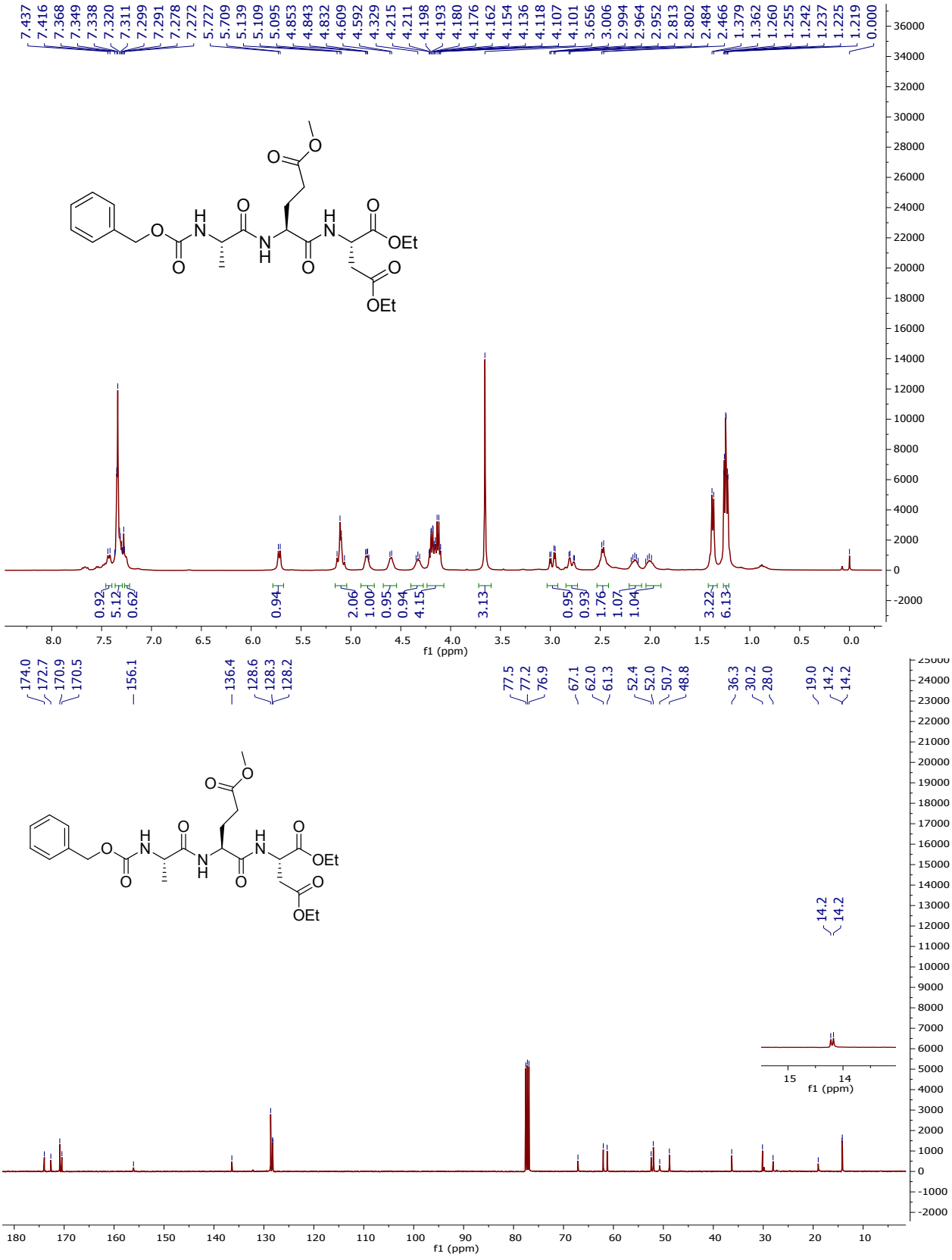
2	0.525	0.575	0.641	237358035	763546149	100

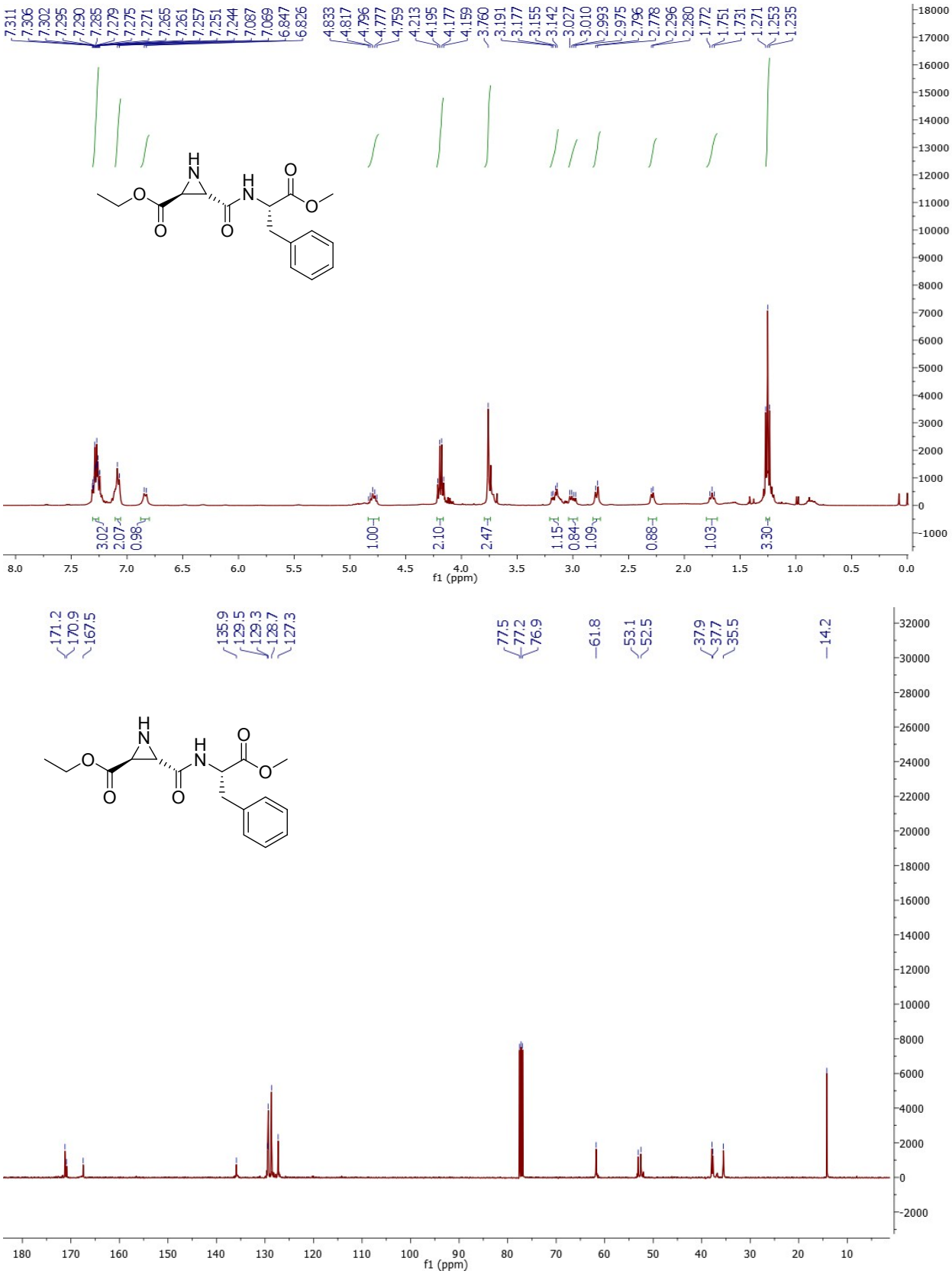




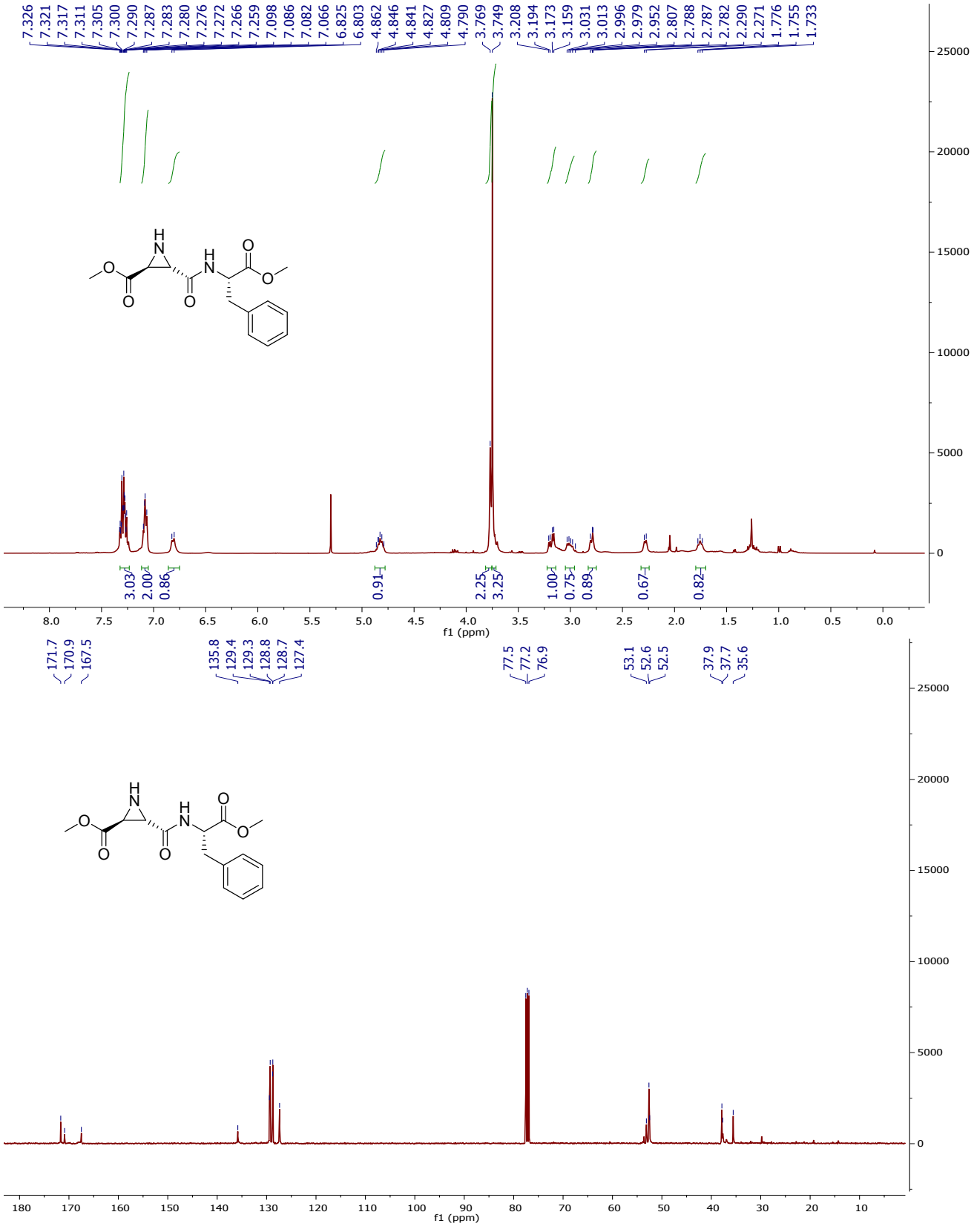
LC-HRMS of compound **5f**



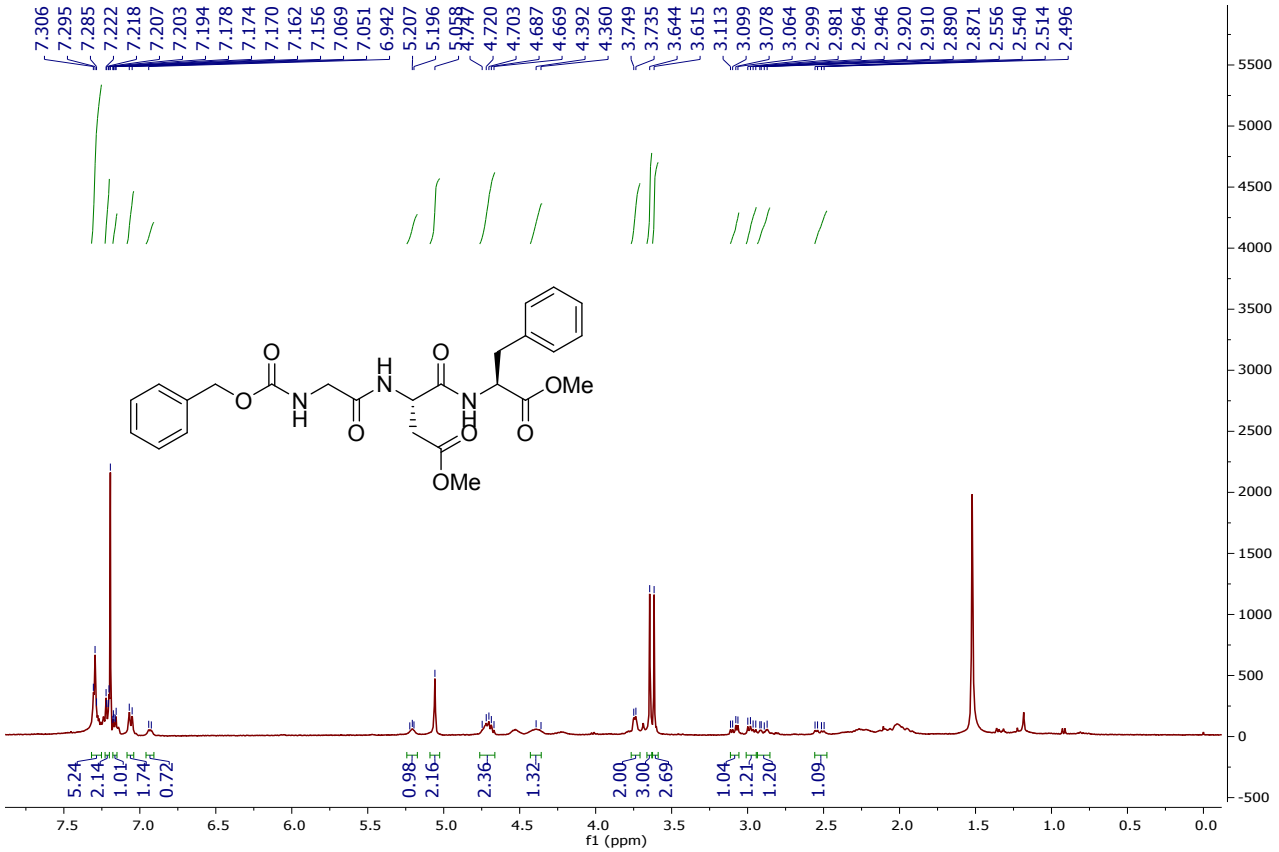
^{1} H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **5g**

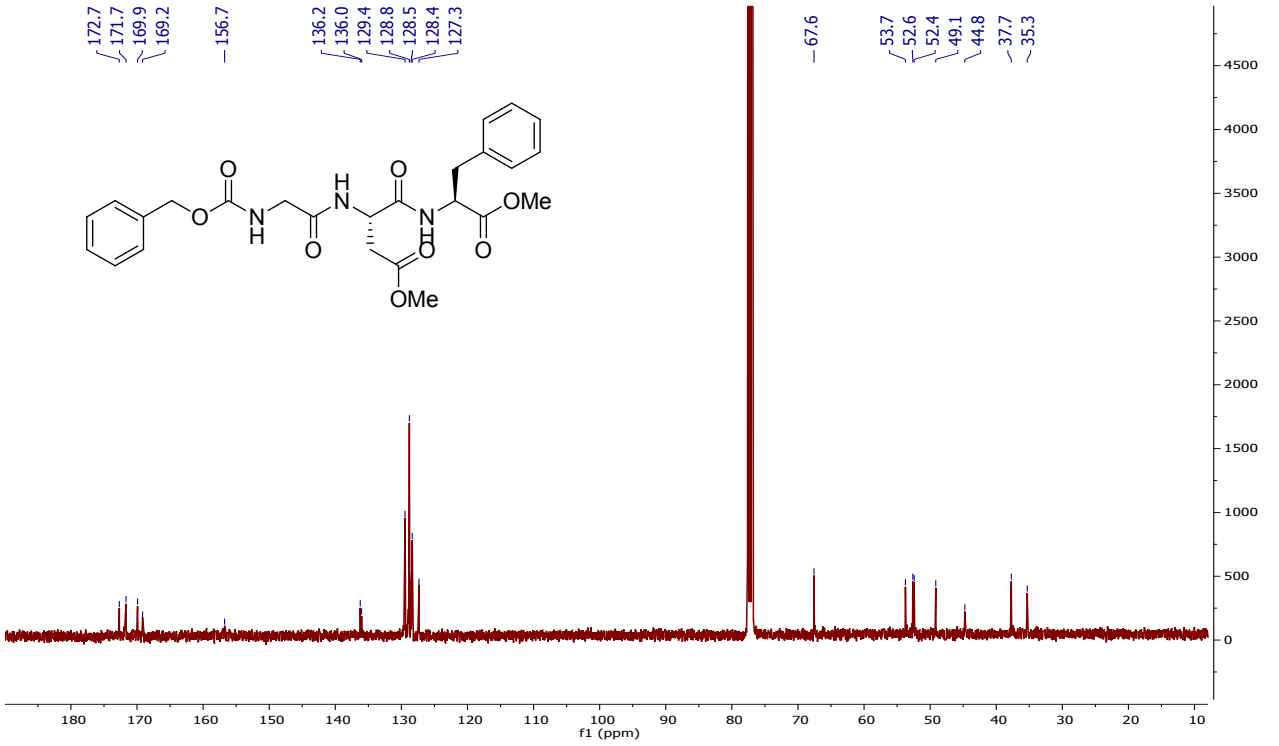


^{1} H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **6a**

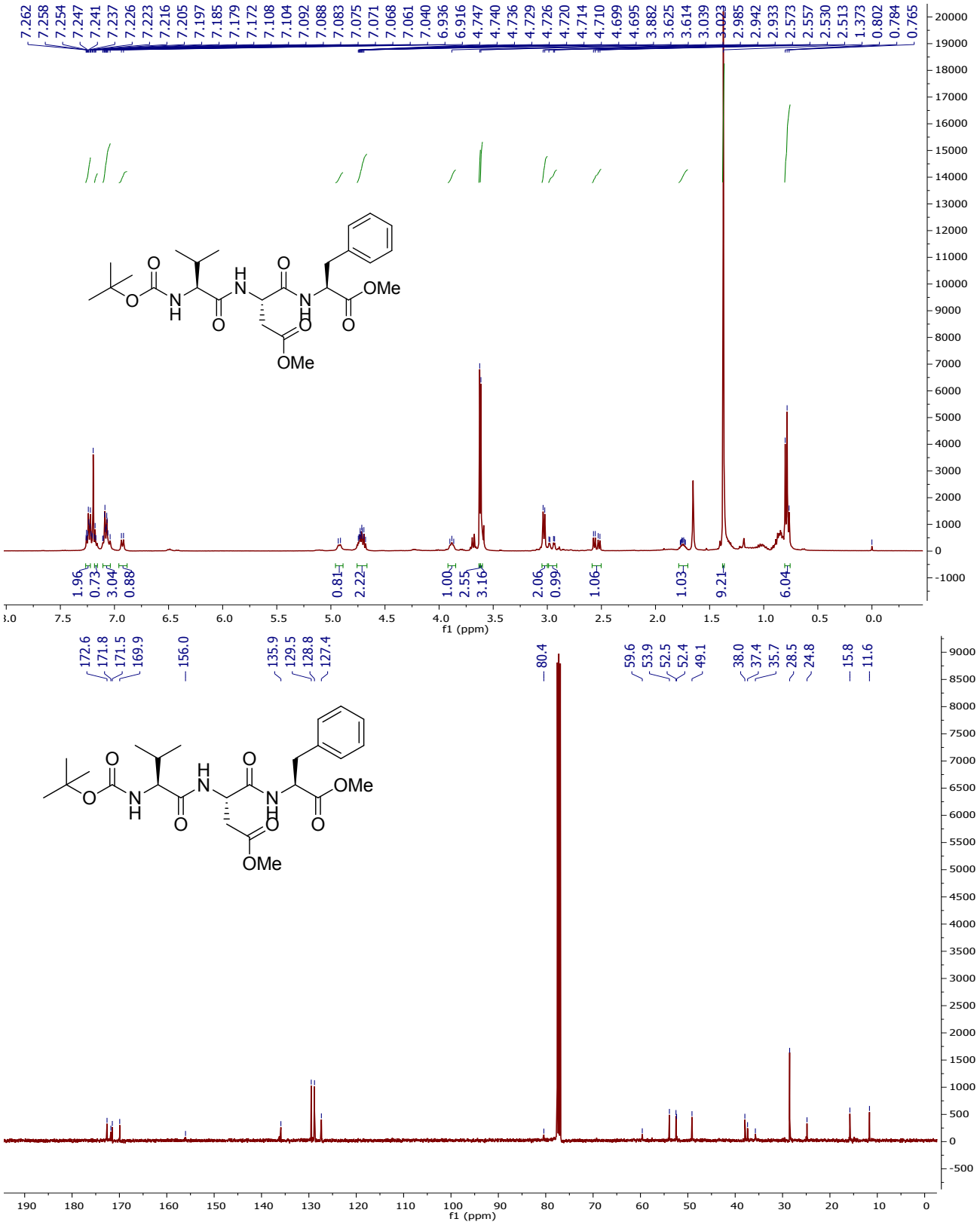


^{1} H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **6b**

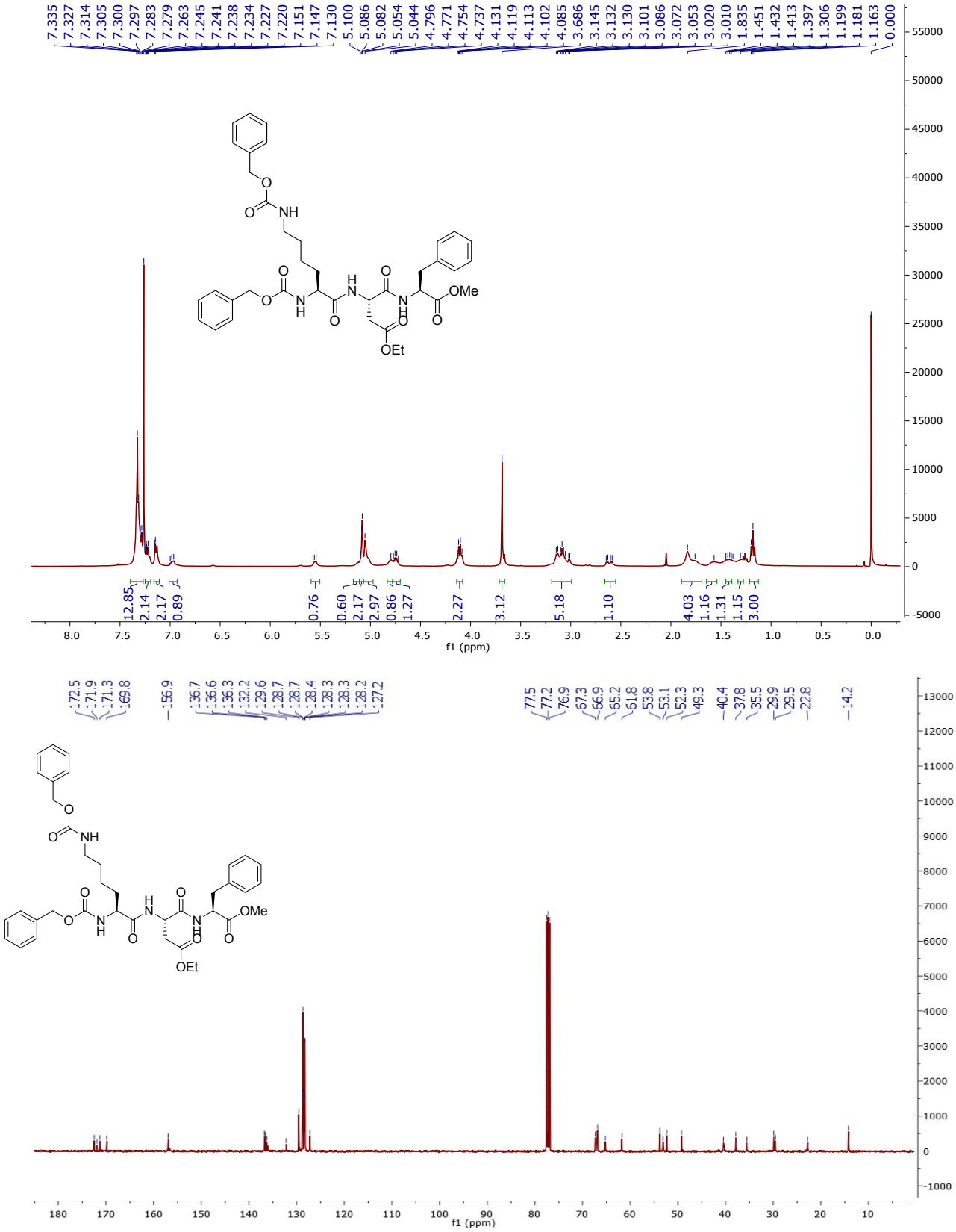




^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **7a**



^{1} H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **7b**



^{1} H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **7c**

Data Filename	LDP.d	Sample Name	LDP
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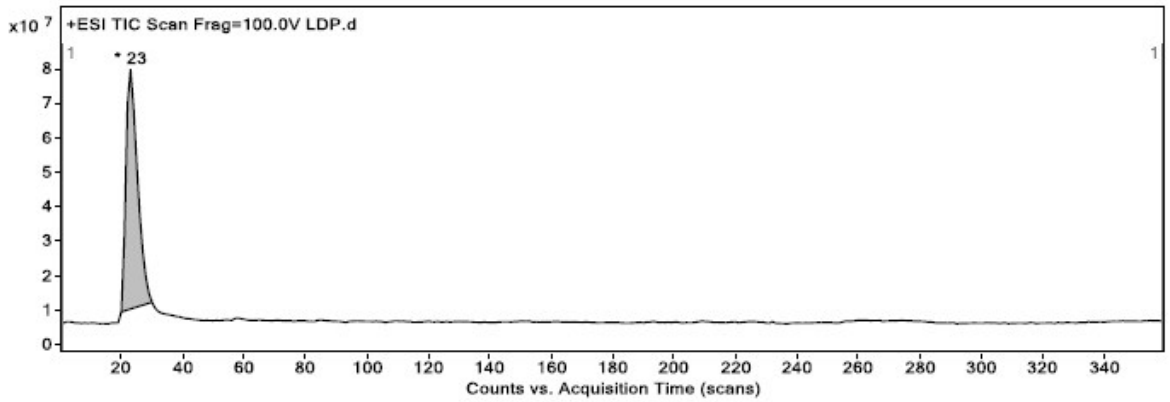
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

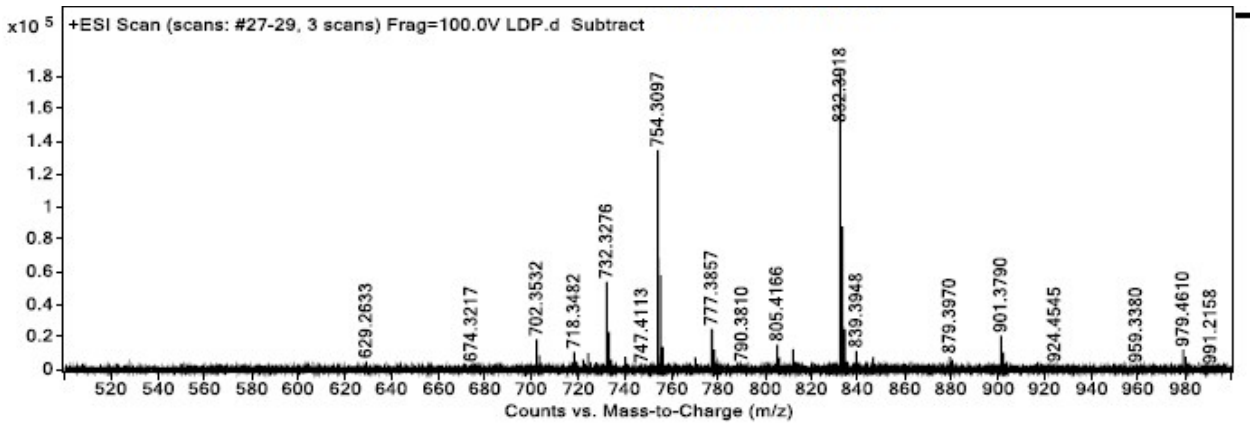
User Chromatograms

Fragmentor Voltage 100 **Collision Energy** 0 **Ionization Mode** ESI

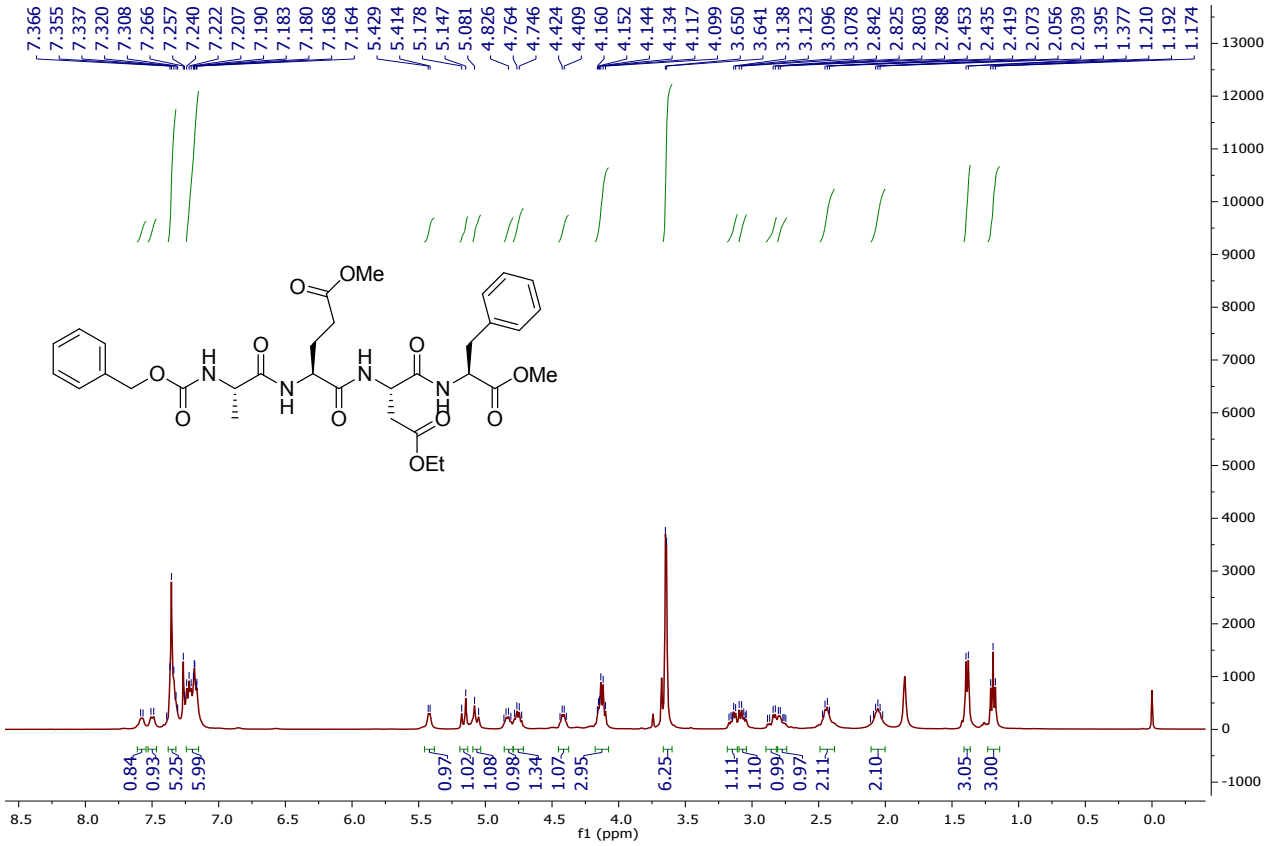


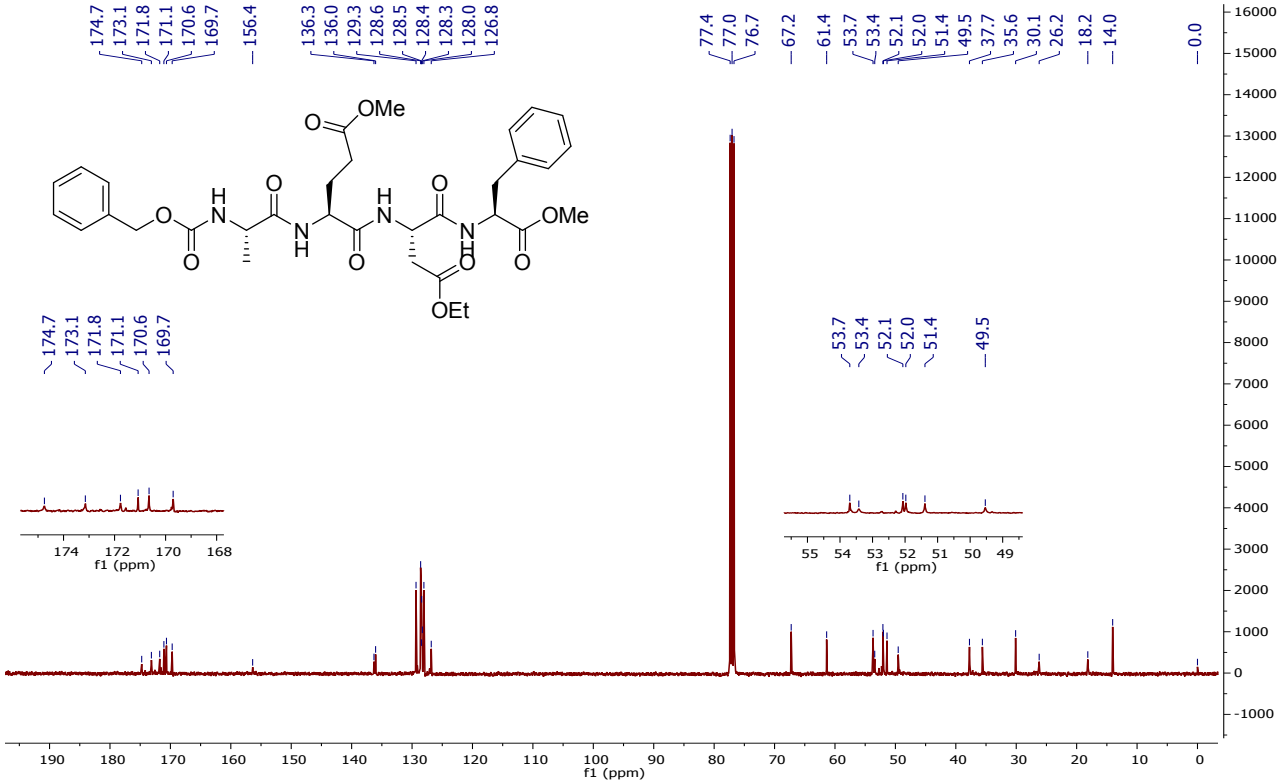
Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	20	23	30	69480800	303545459	100

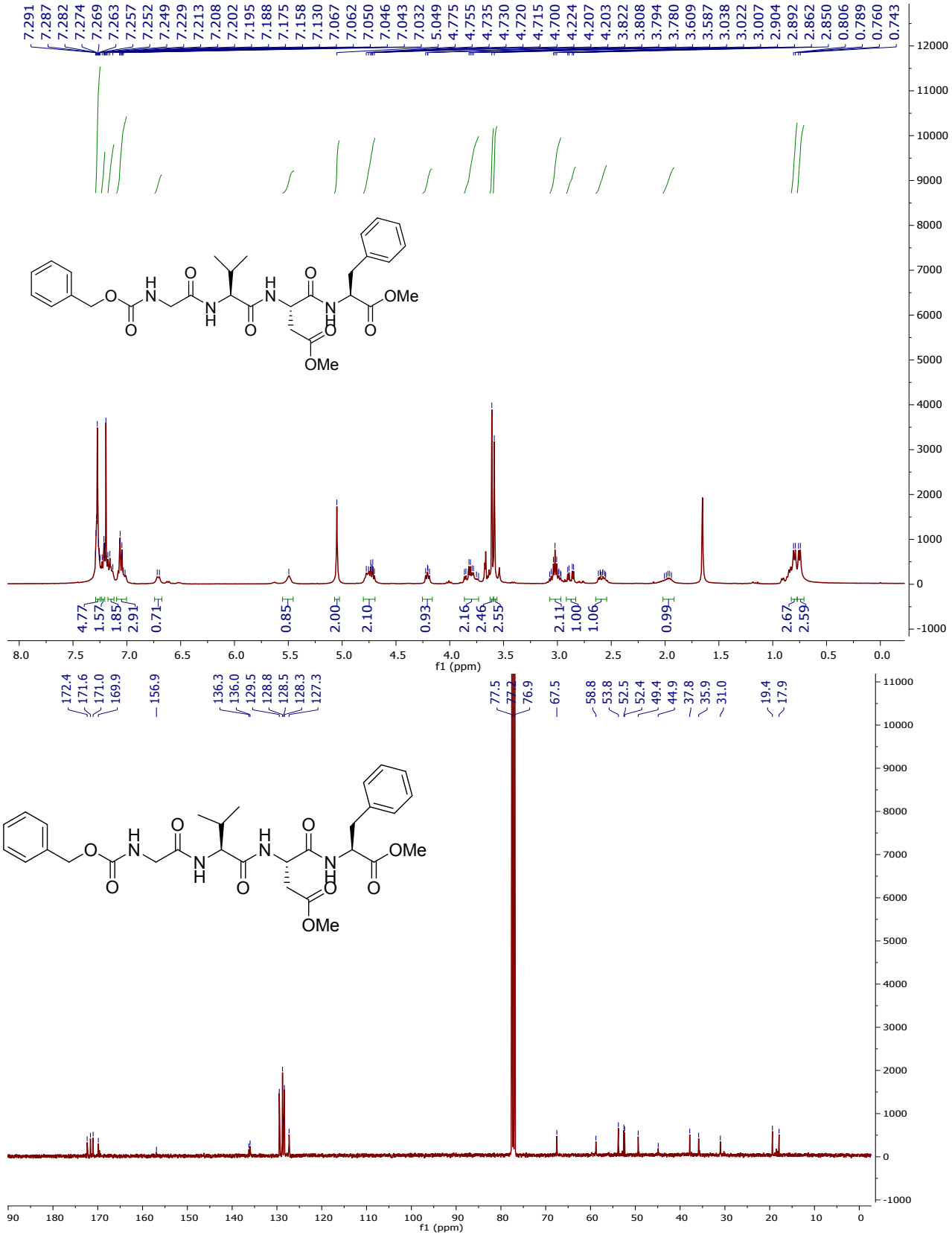


HPLC- of compound **7c**

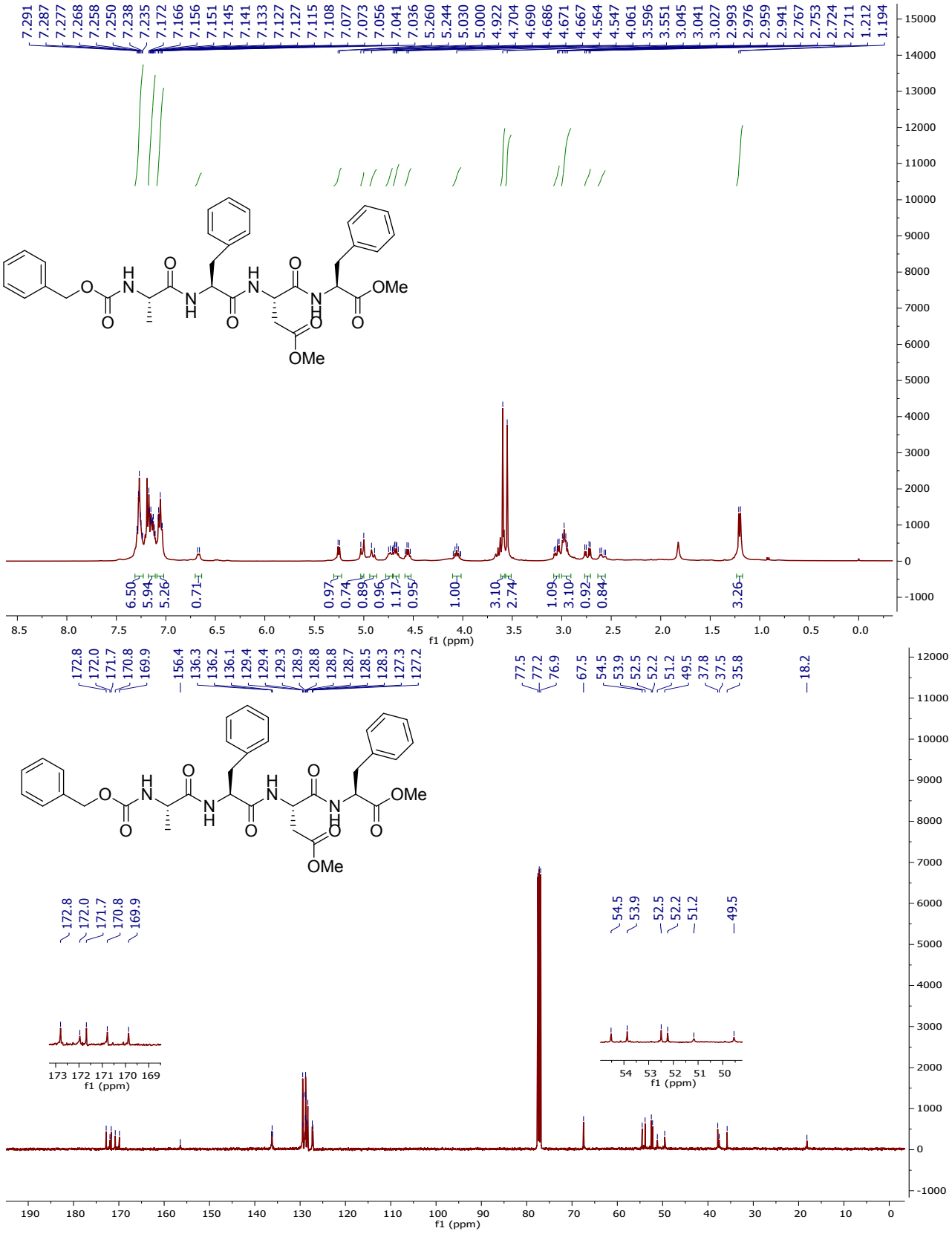




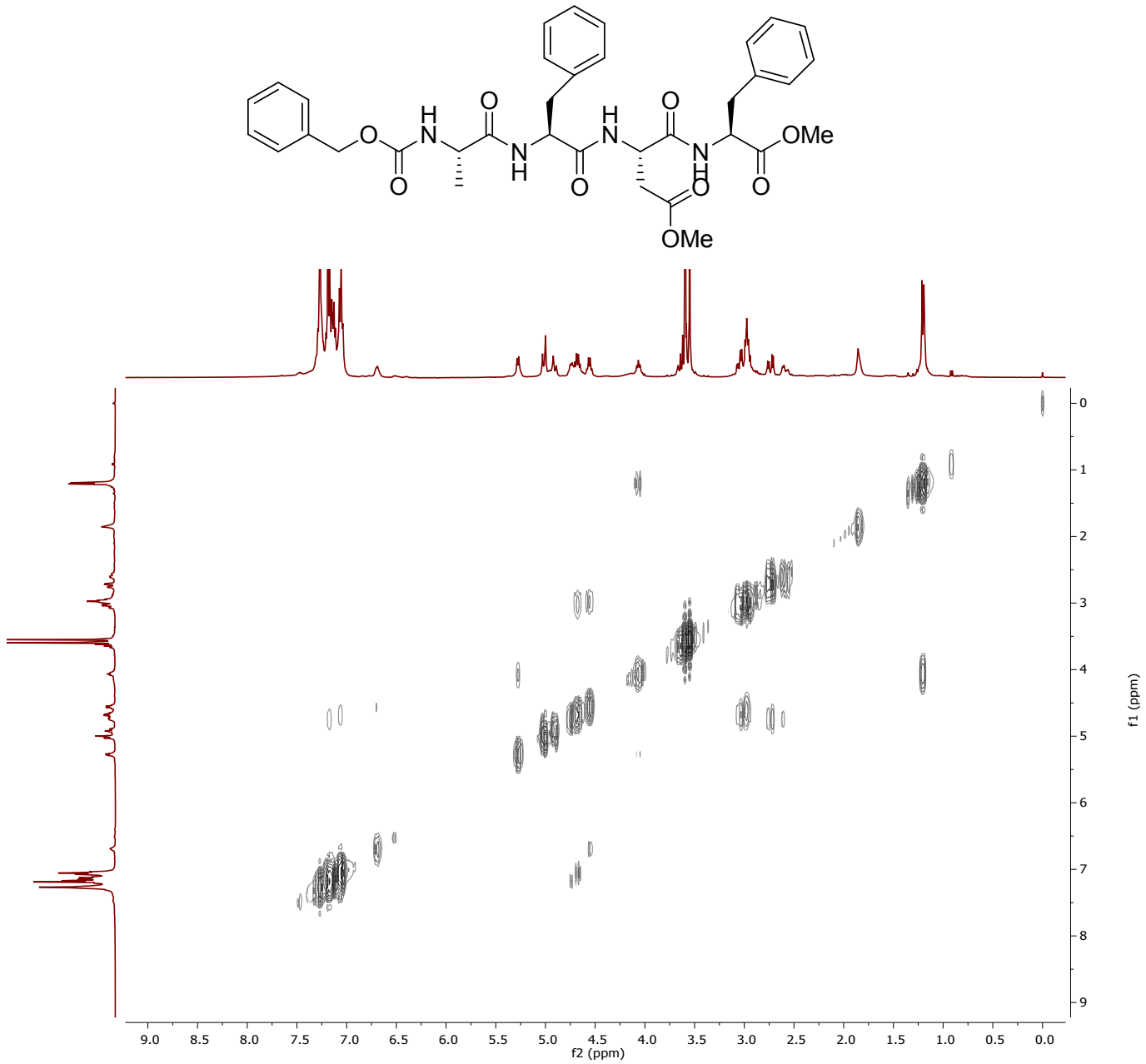
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **7d**



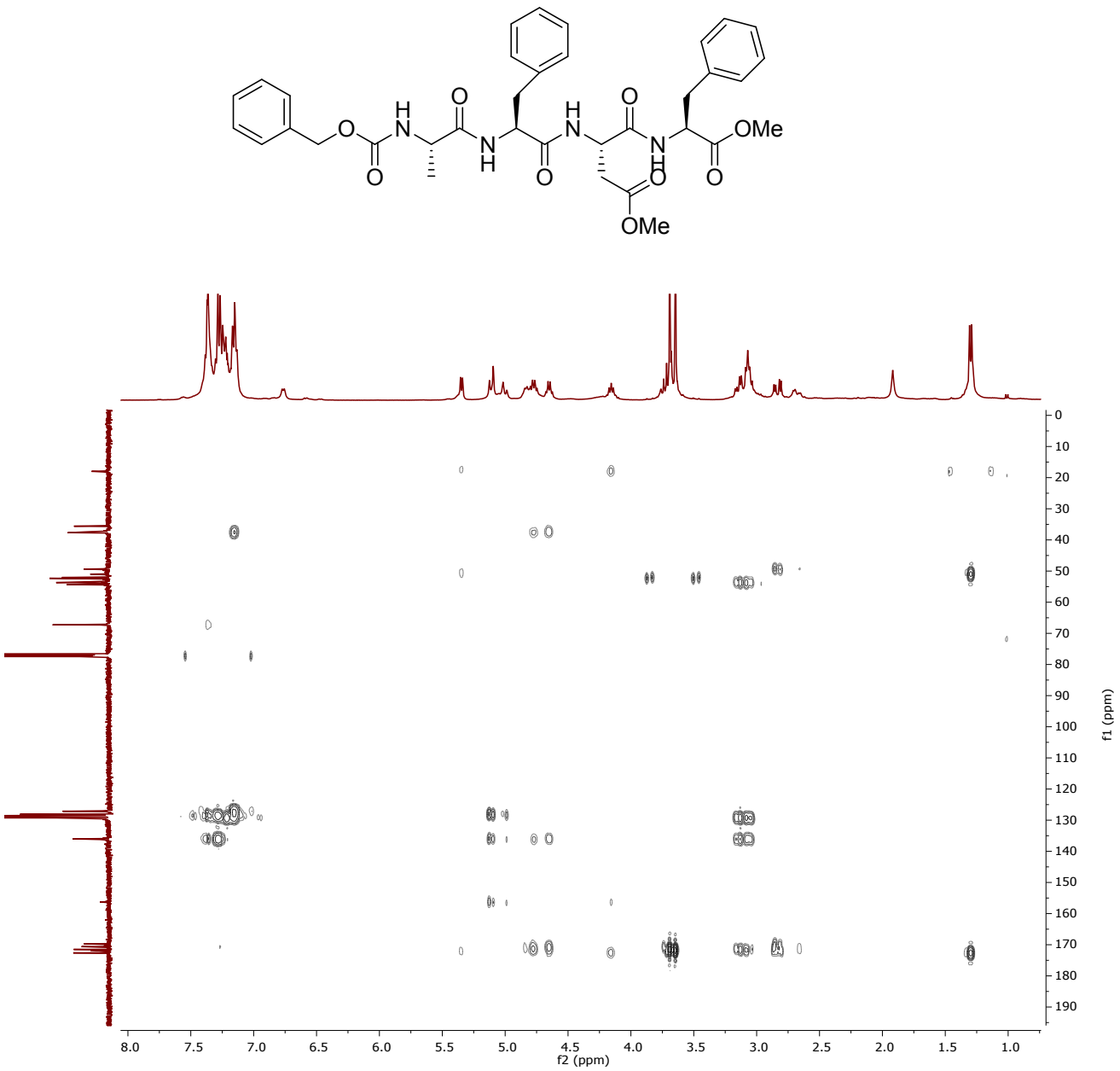
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **7e**



^{1} H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **7f**

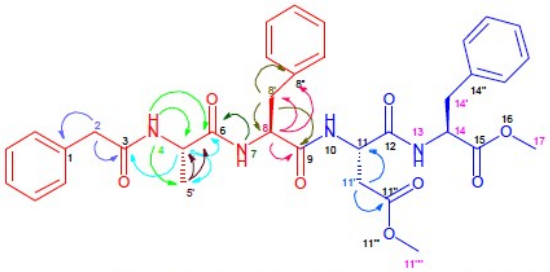


COSY NMR of compound **7f**

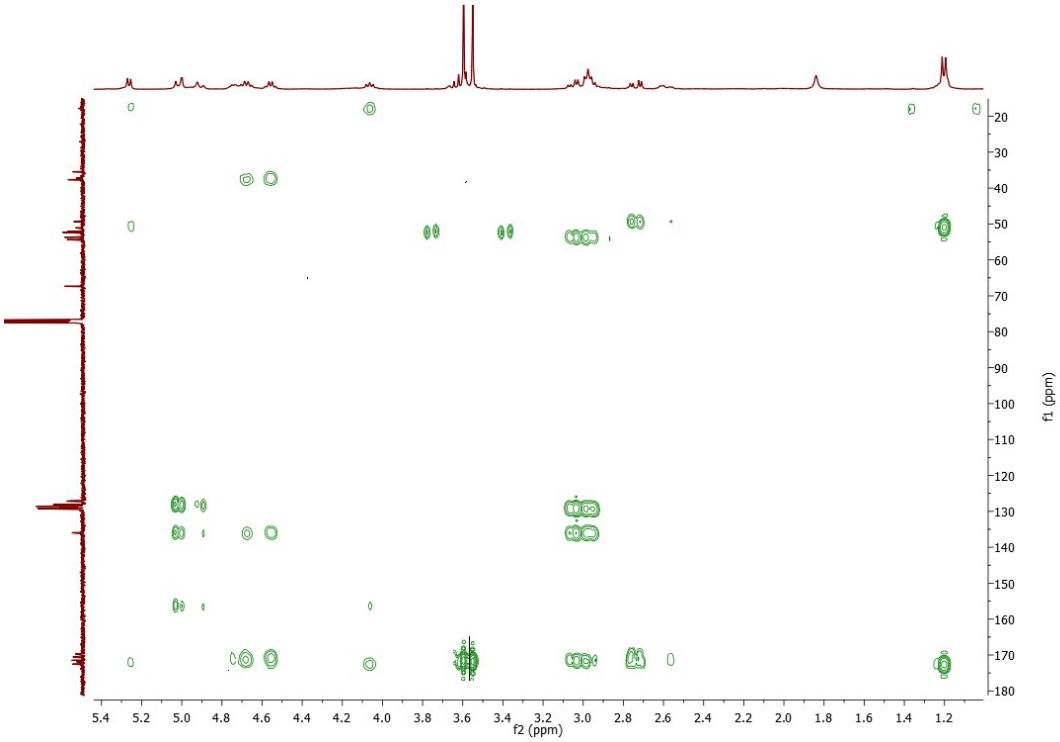


HSQC NMR of compound **7f**

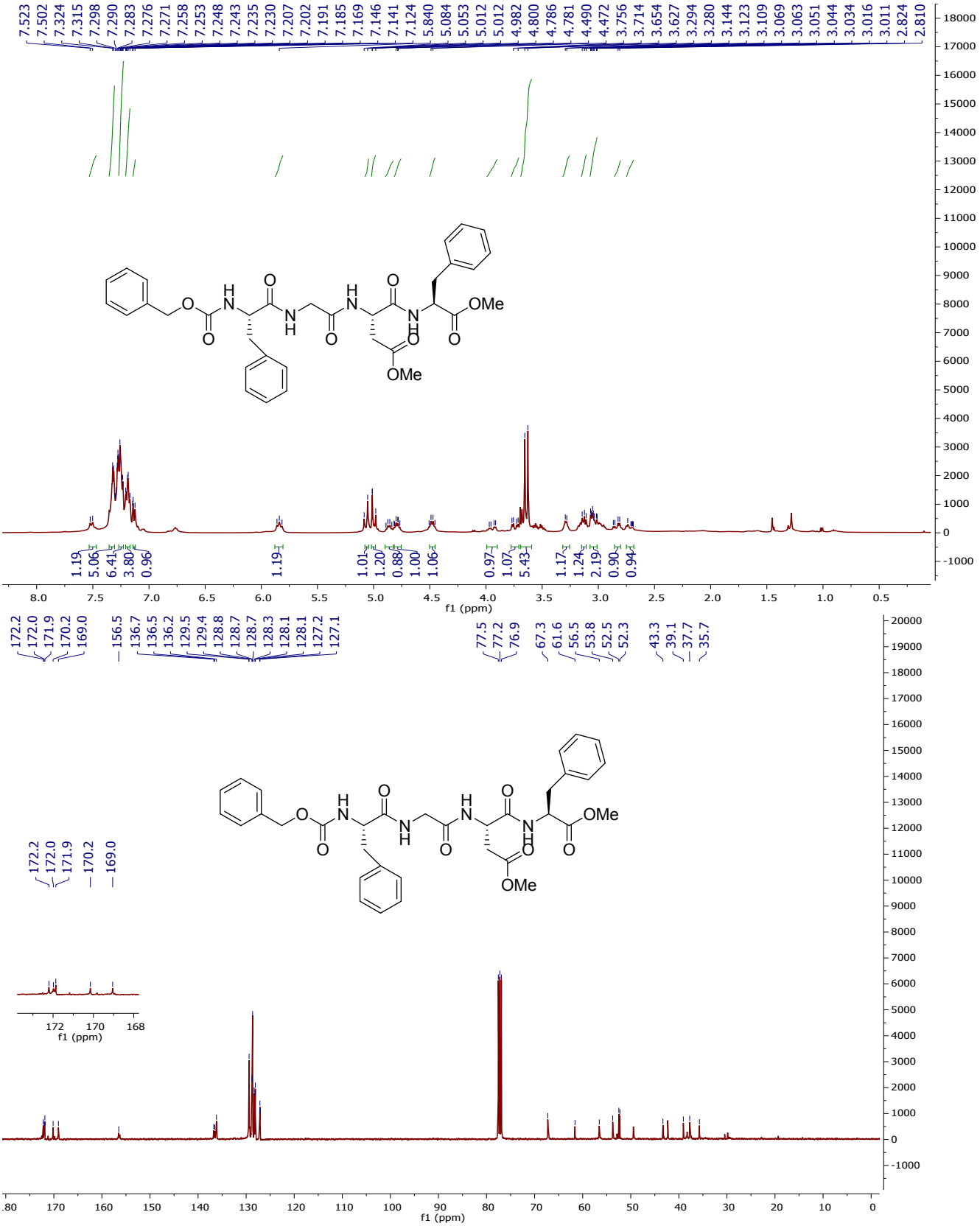
Atom No.	^{1}H NMR	^{13}C NMR	HMBC
1	-	136.2	-
2	4.91, 5.02	67.5	C-1, C-3
3	-	156.4	-
4	5.28	-	C-5', C-6, C-5
5	4.06	51.2	C-5', C-3, C-6
5'	1.21	18.2	C-5, C-6
6	-	172.8	-
7	6.69	-	C-6
8	4.55	53.9	C-8', C-8", C-9
8'	2.98	37.5	C-8, C-8", C-9, correlations with C-8" (b-g)
8"	-	136.9	-
8"-(b-f)	Overlapped signals between 7.00-7.29		Multiple correlations
9	-	169.9	-
10	7.17	-	C-9
11	4.74	49.4	C-11', C_12
11'	2.58, 2.73	35.8	C-11, C-11"
11"	-	- 171.5	
11"'	-	-	
11""	3.59	52.2	C-11"
12	-	170.8	-
13	7.06	-	C-14', C-12
14	4.67	54.5	C-15, C-14', C-14"
14'	3.02	37.8	C-14, C-14", C-15
14"	-	135.9	-
14" (b-f)	Overlapped signals between 7.00-7.29		Multiple correlations
15	-	171.8	-
16	-	-	
17	3.55	52.5	C-15



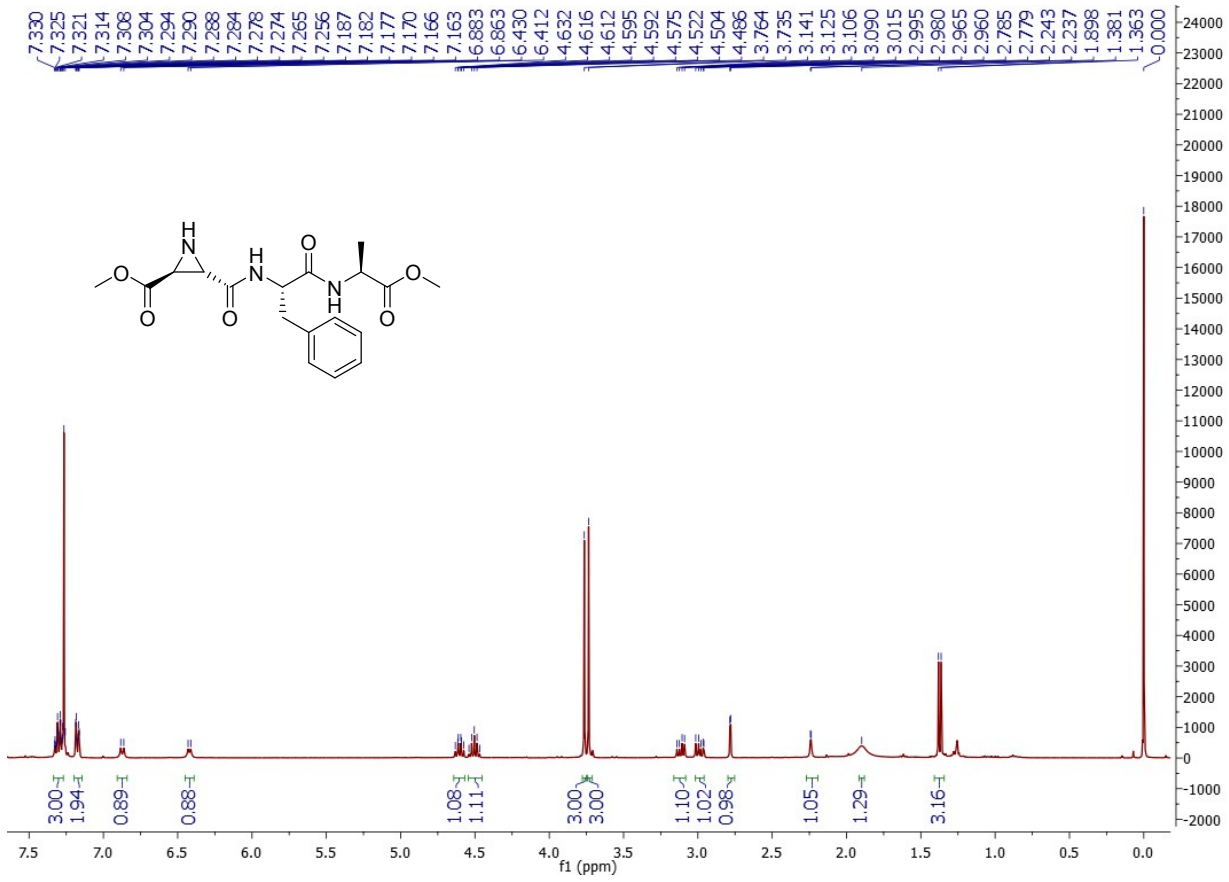
Isomer 1: α–tetrapeptide: Cbz-L-Ala-L-Phe-L-Asp(OMe)-L-Phe-OMe

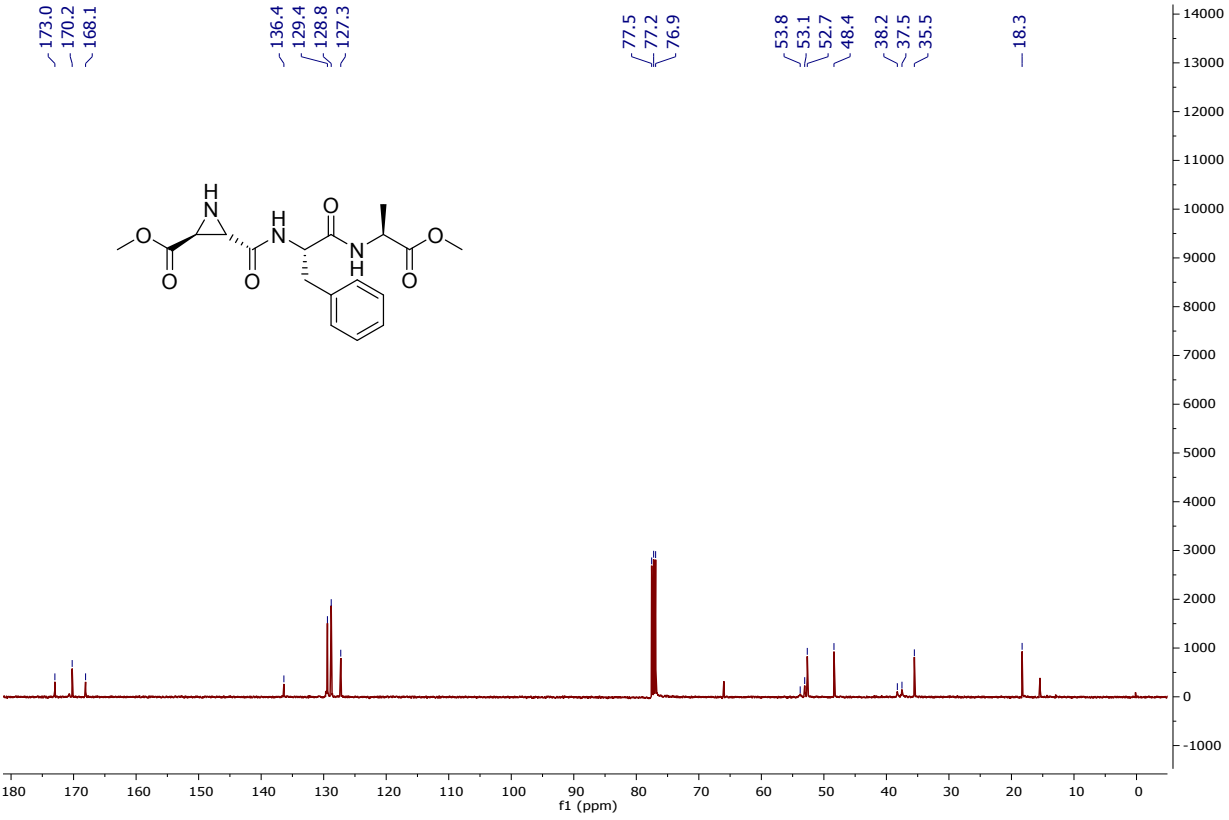


HMBC NMR of compound **7f**

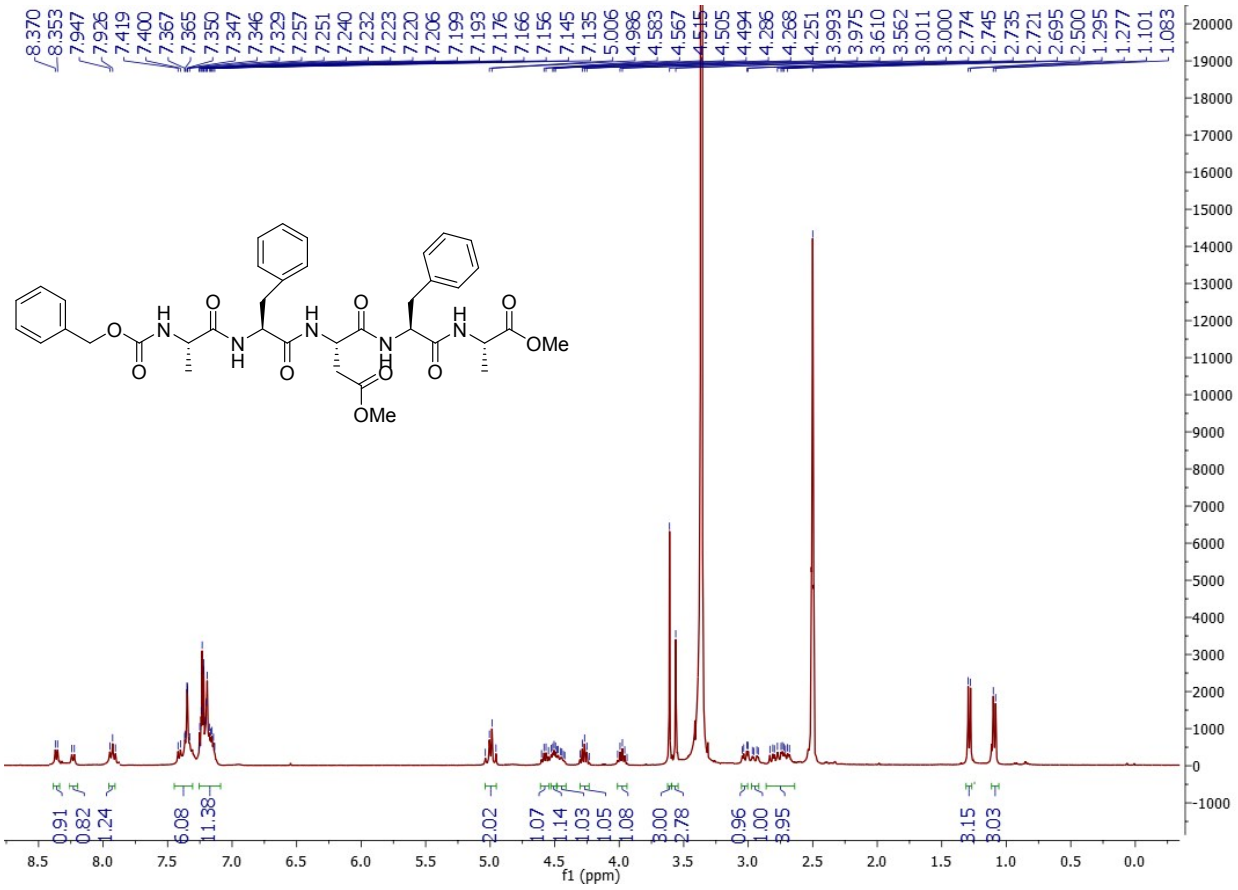


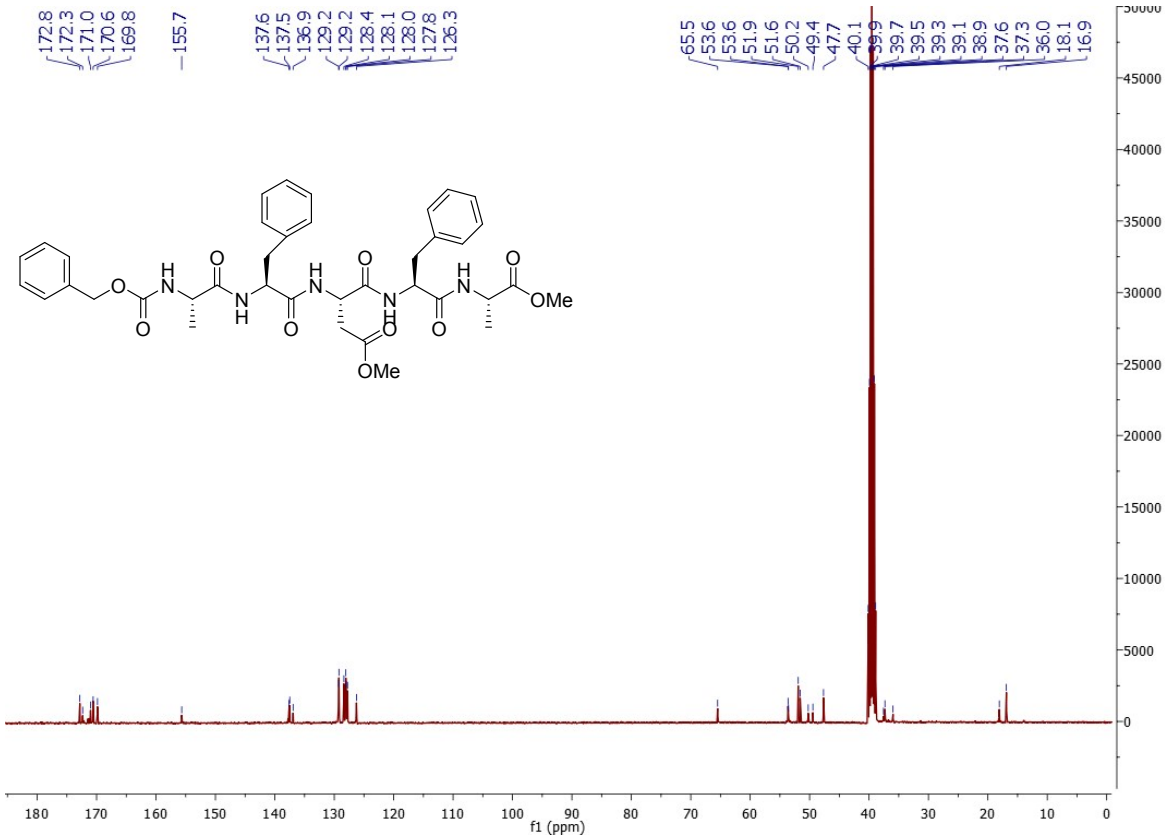
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **7g**





^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **6c**





^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) of compound **8**