

Supplementary material

Paralemnolins X and Y, New Antimicrobial Sesquiterpenoids from the Soft Coral *Paralemnalia thyrsoide*

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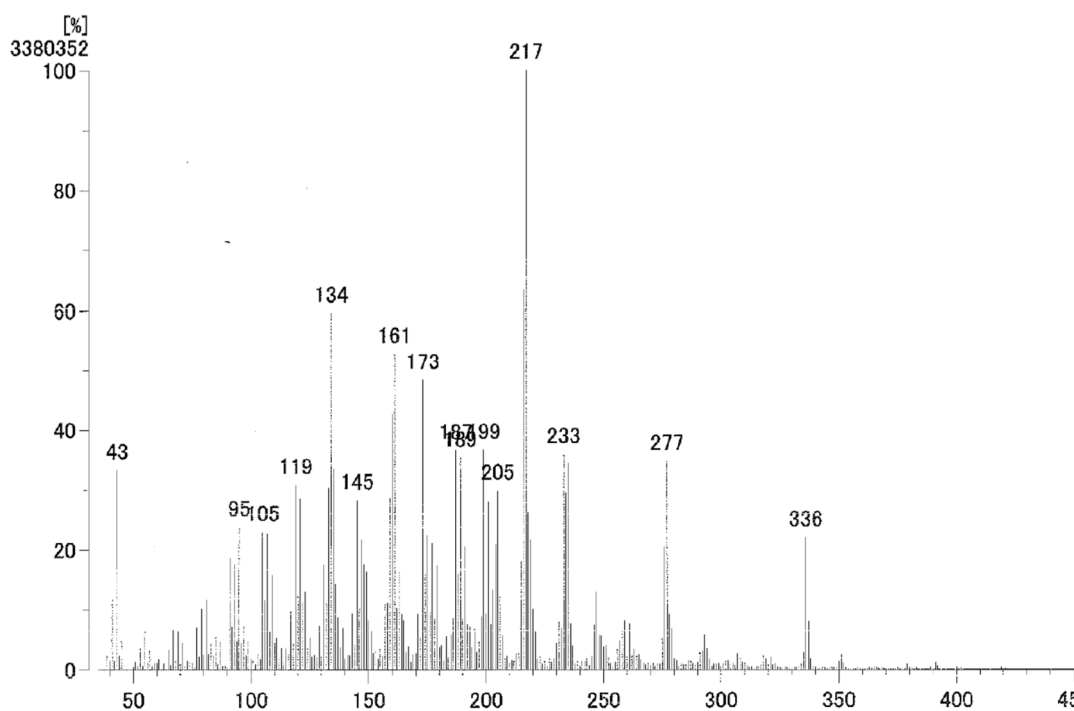
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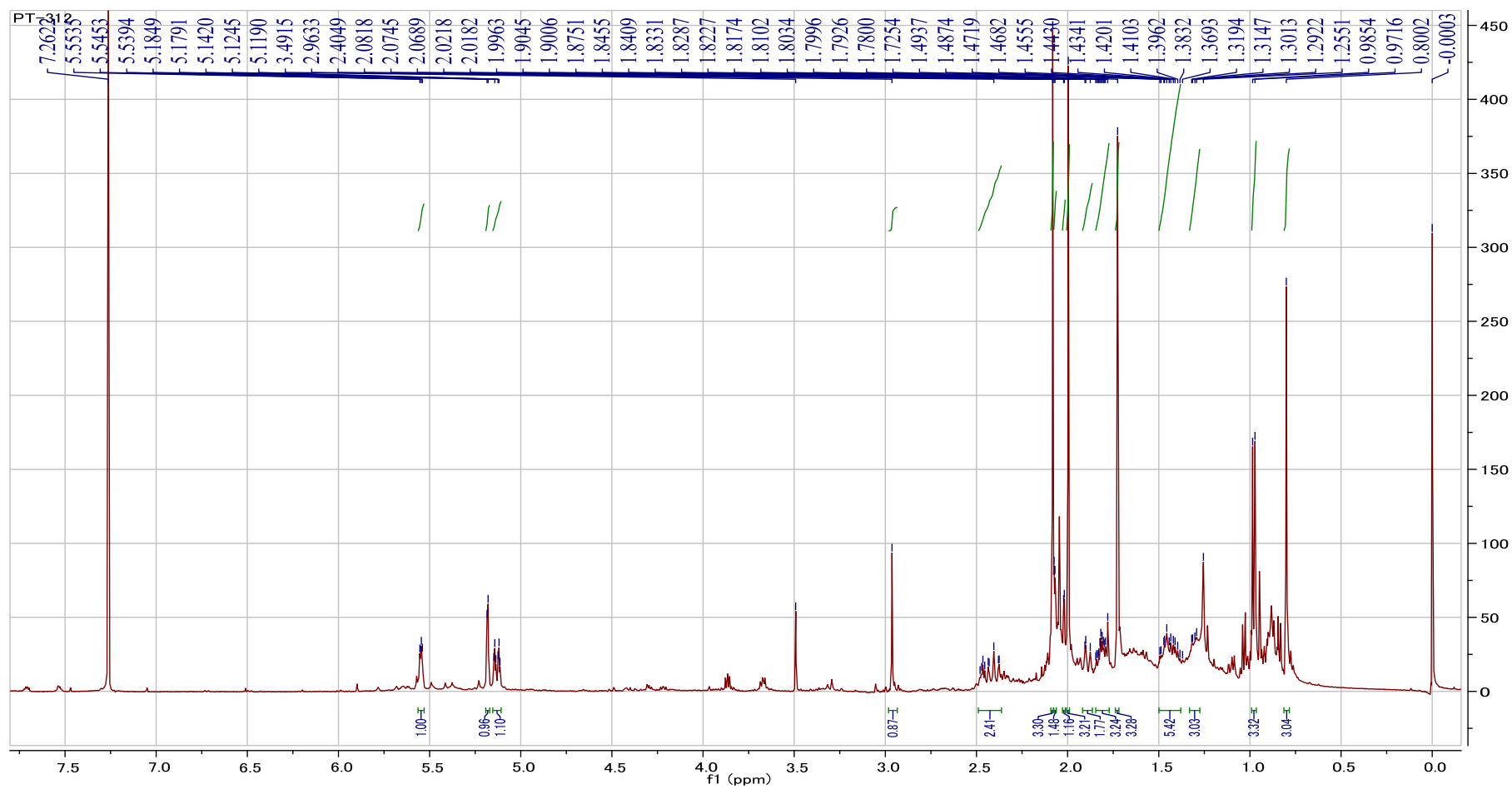


S1: LRCIMS of 1

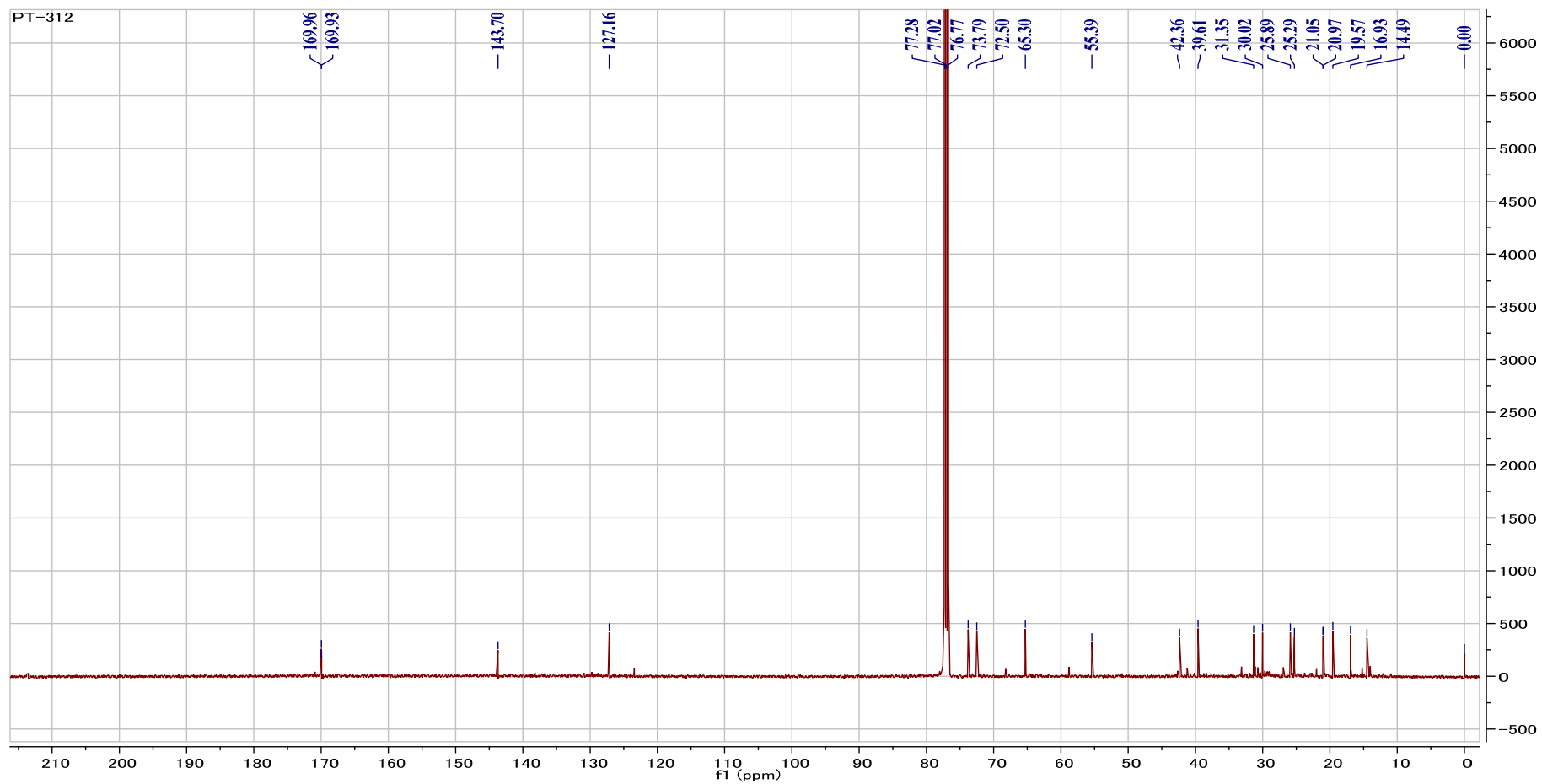
Data : Umeyama-CIHR.06-Aug-2019.001 Date : 06-Aug-2019 15:54
 Instrument : MStation
 Sample : PT-312
 Note : MStation
 Inlet : Direct Ion Mode : CI+
 RT : 0.56 min Scan# : 15
 Elements : C 150/0, H 250/0, O 50/0
 Mass Tolerance : 5mmu
 Unsaturation (U.S.) : 0.0 - 15.0

	Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
1	336.1940	100.00	+1.0 / +0.3	6.0	C19 H28 O5

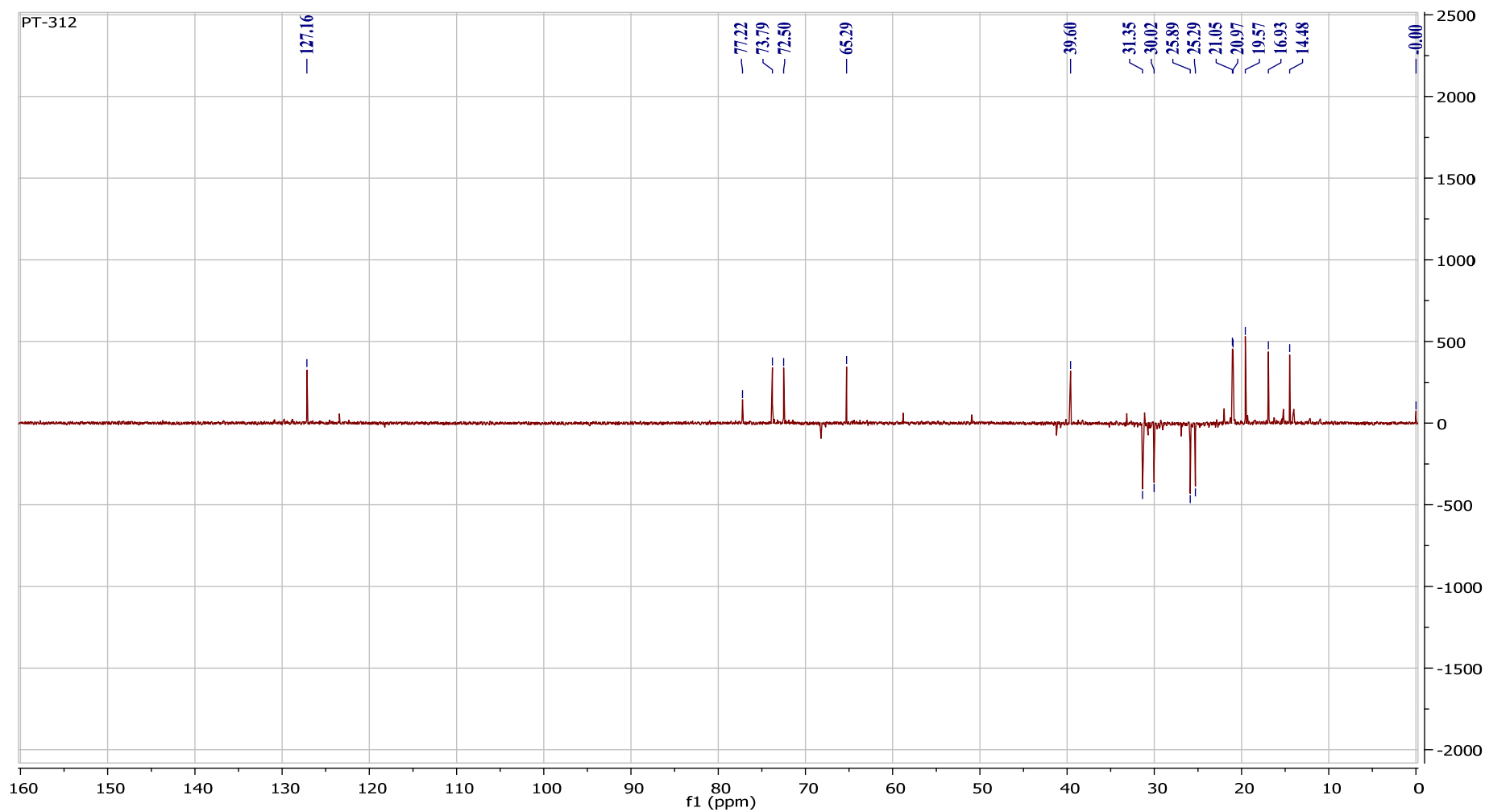
S2: HRCIMS of 1



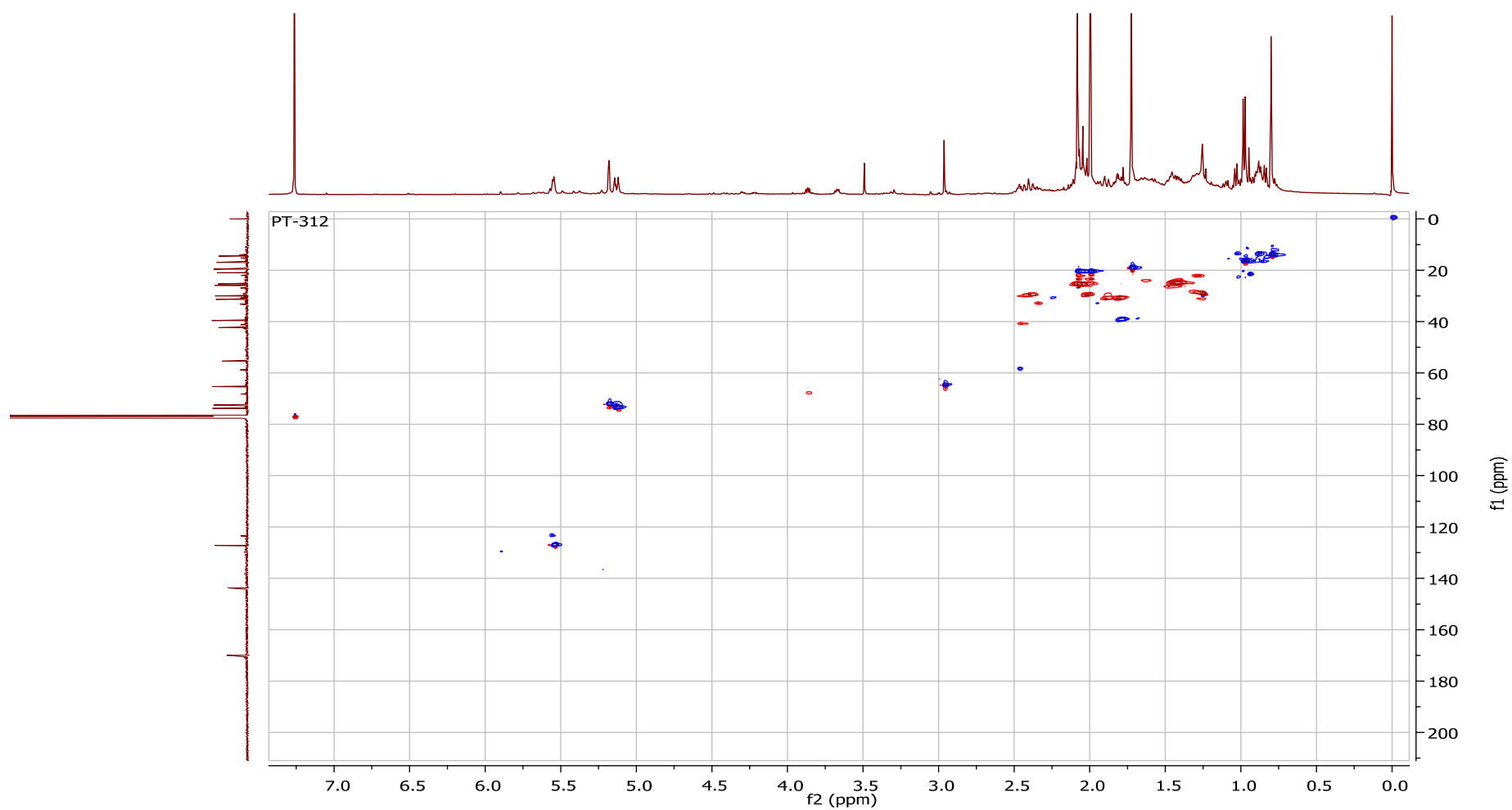
S3: ^1H NMR of **1**



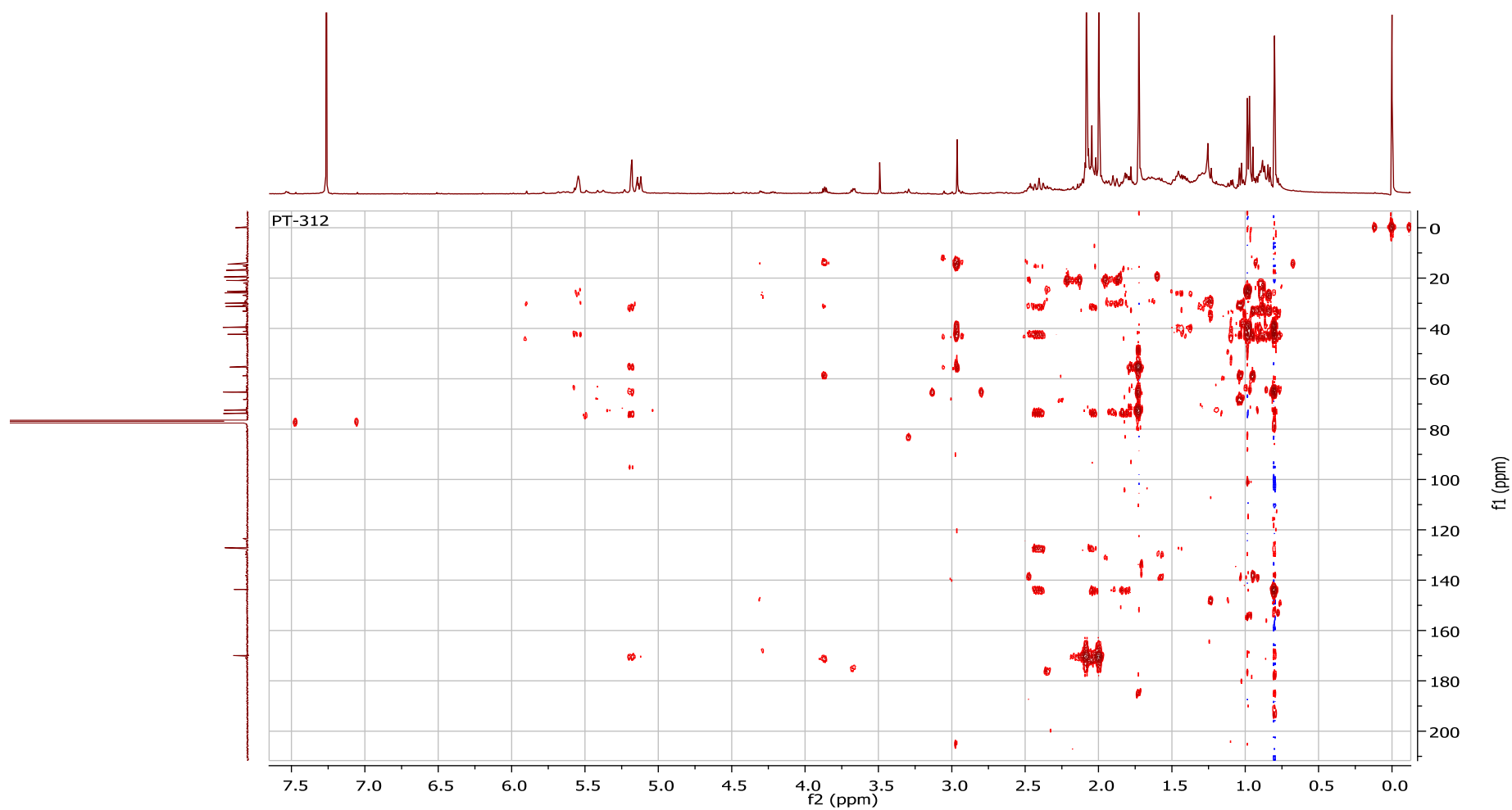
S4: ^{13}C NMR of **1**



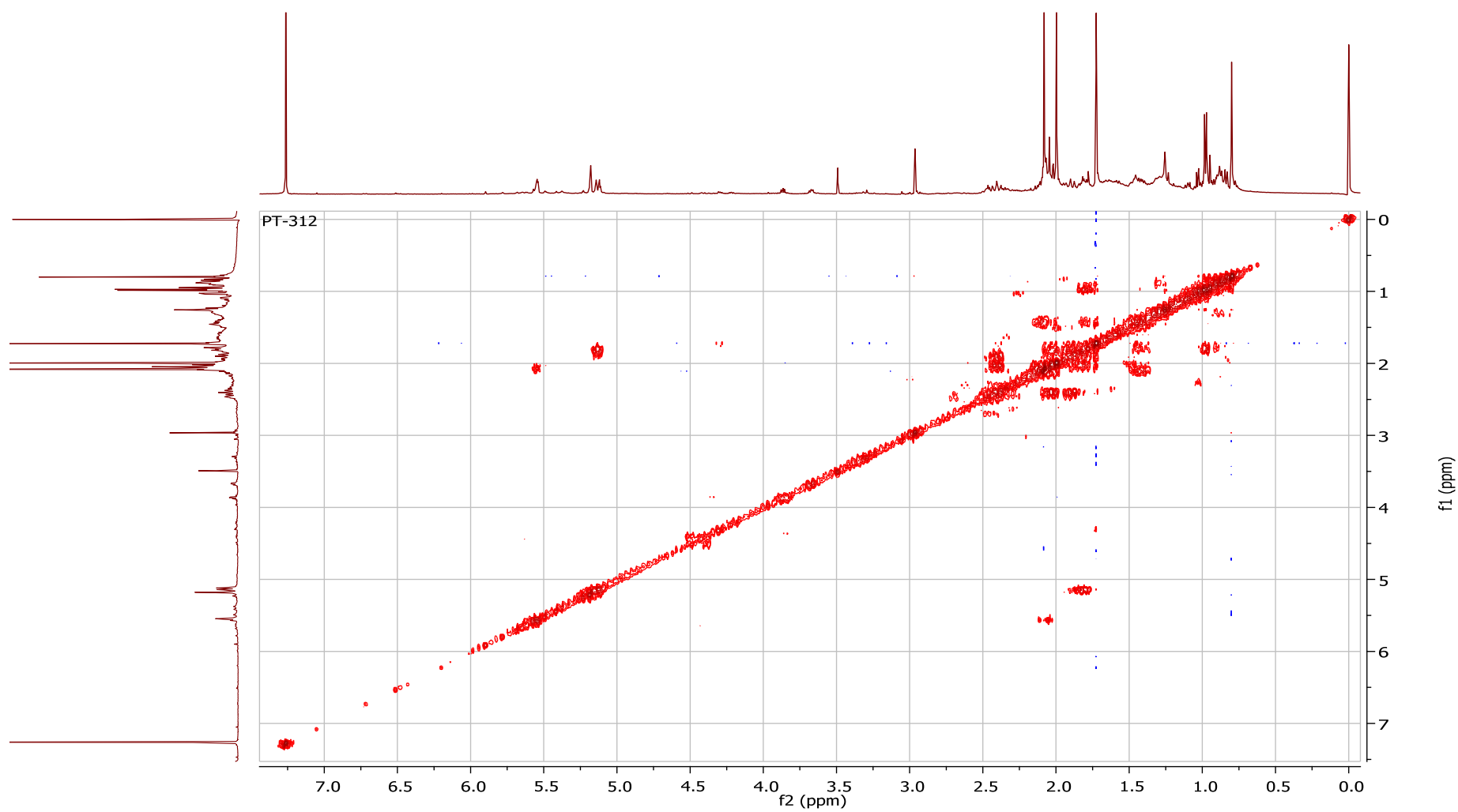
S5: DEPT-135 of 1



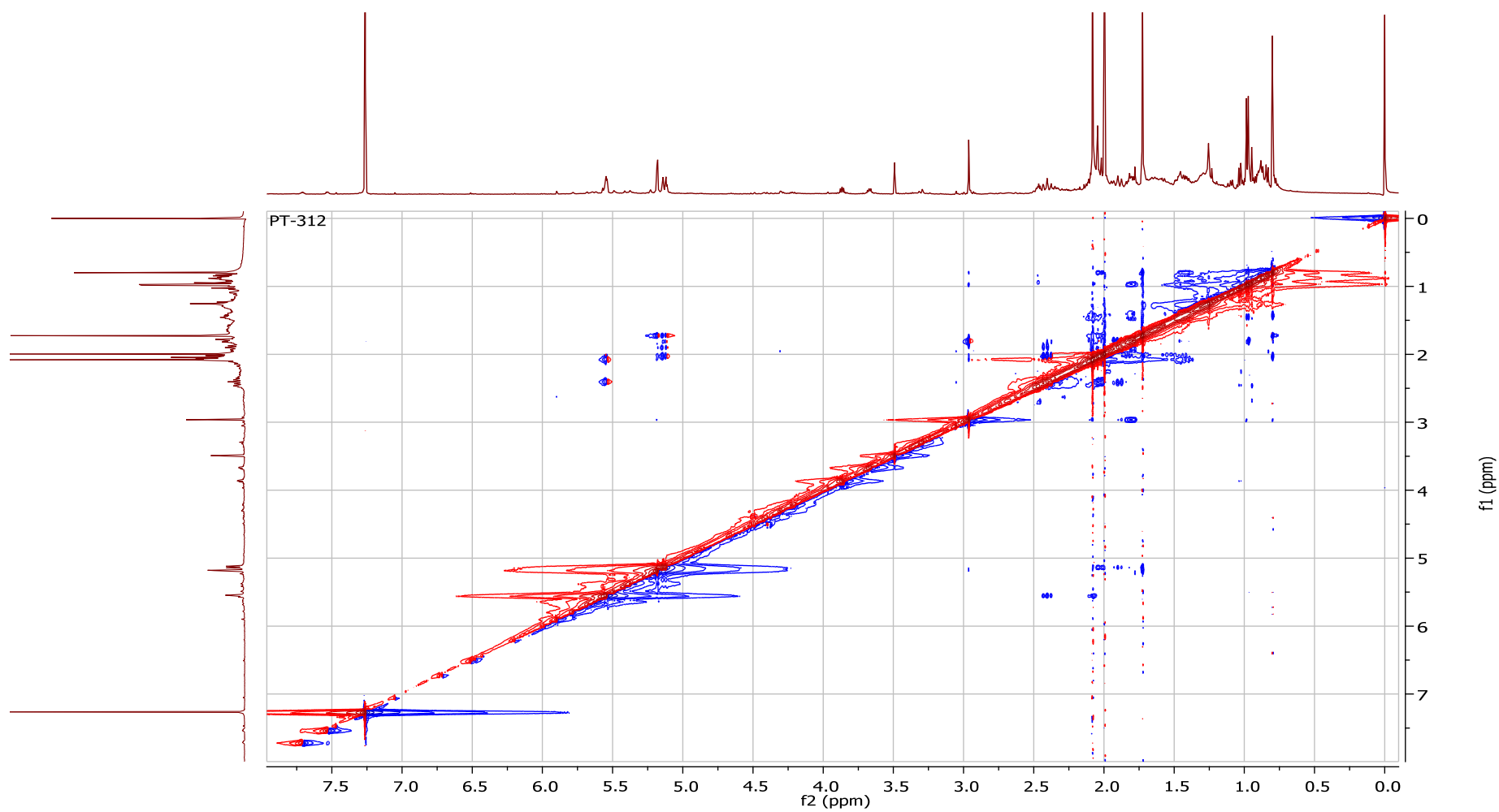
S6: HSQC of **1**



S7: HMBC of **1**

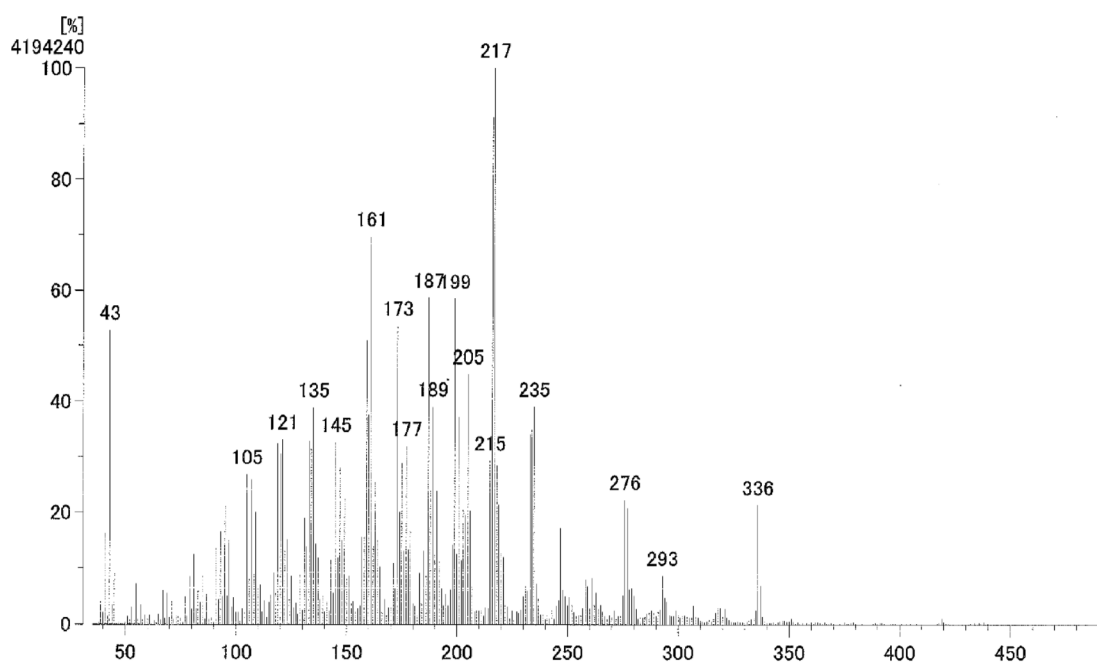


S8: ^1H ^1H COSY of **1**



S9: NOESY of **1**

LRCIMS

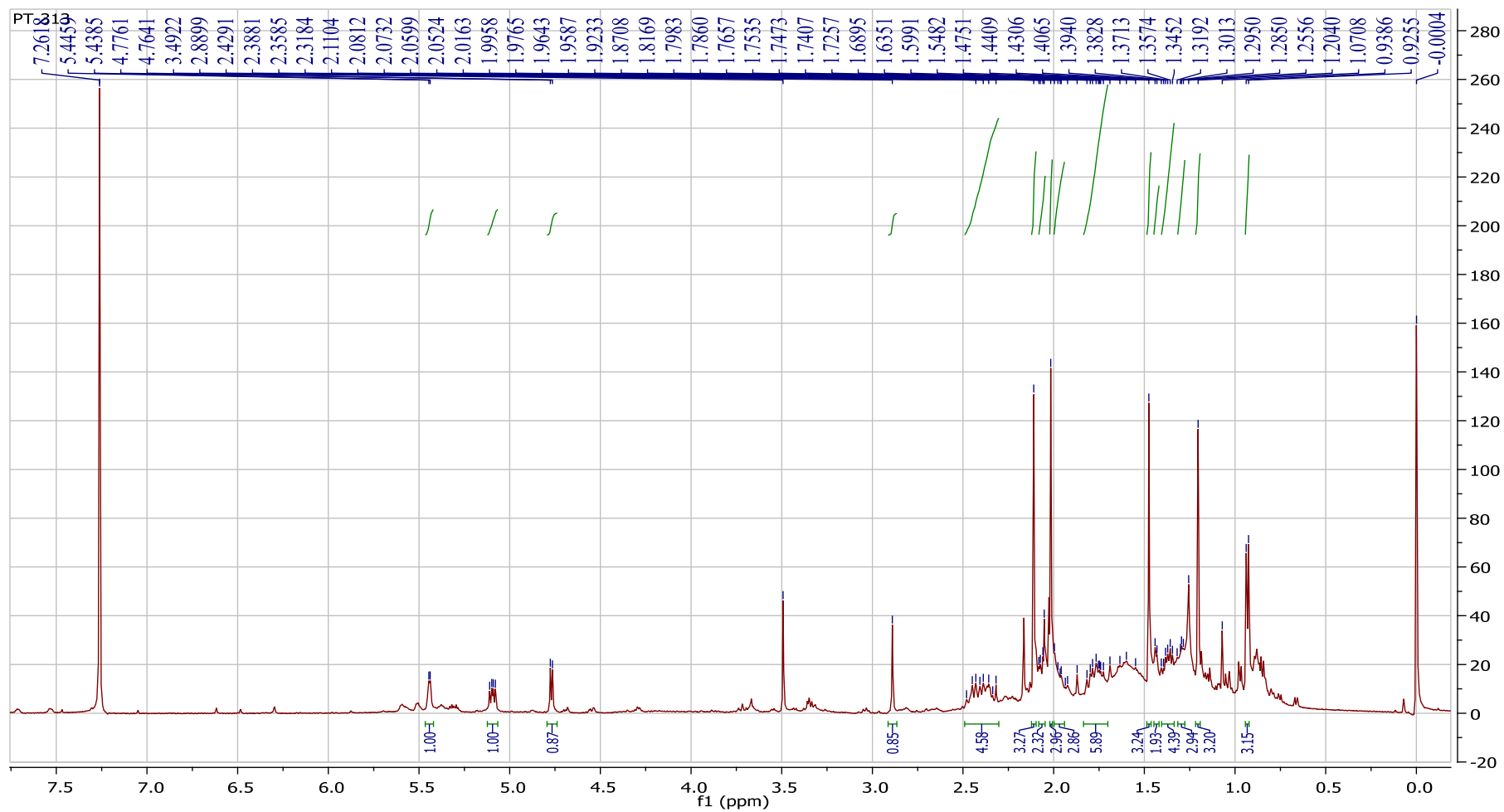


S10: LRCIMS of 2

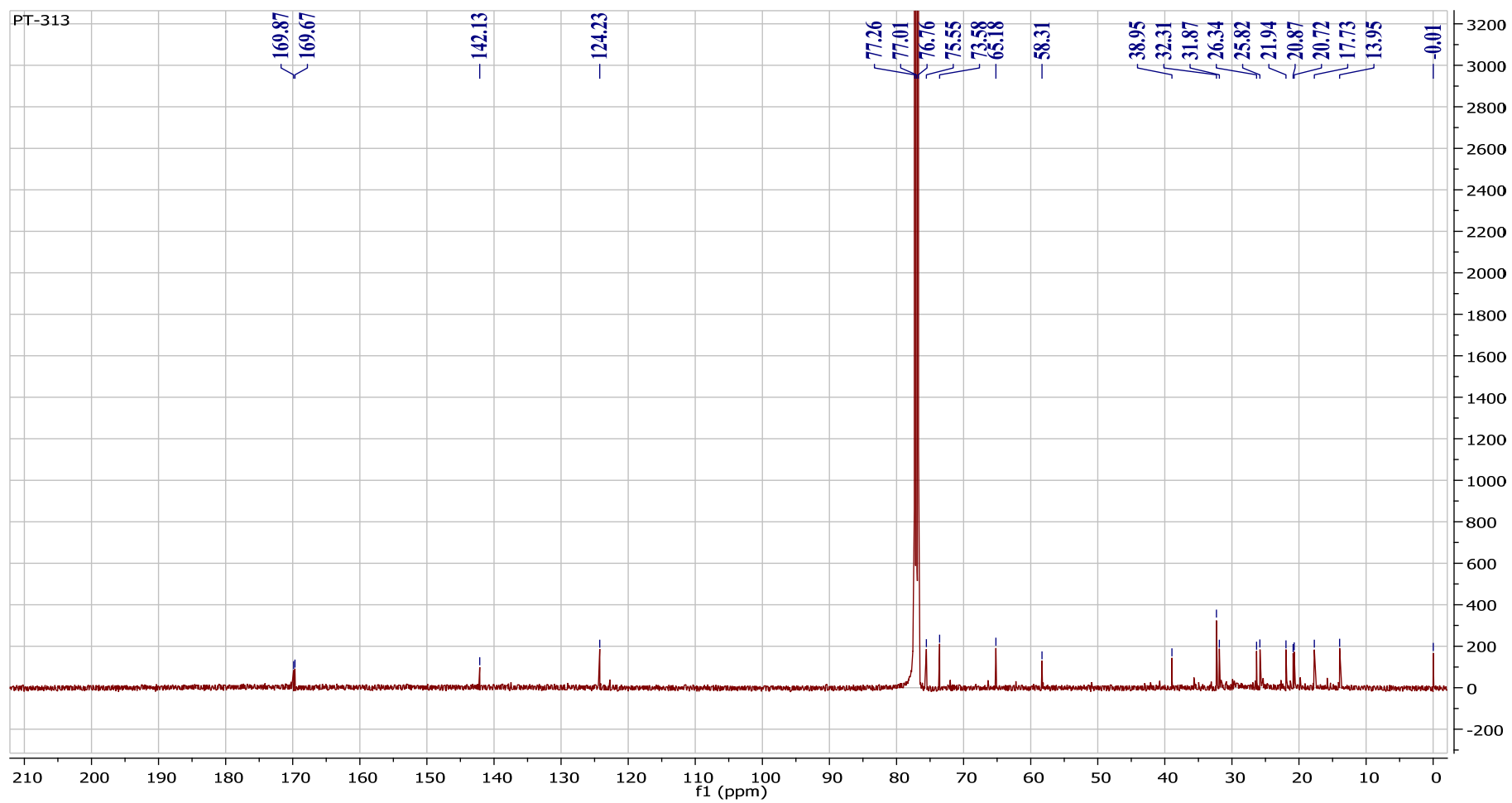
Data : Umeyama-CIHR.10-Aug-2019.001 Date : 10-Aug-2019 09:51
 Instrument : MStation
 Sample : PT-313
 Note : MStation
 Inlet : Direct Ion Mode : CI+
 RT : 0.40 min Scan# : 11
 Elements : C 150/0, H 250/0, O 50/0
 Mass Tolerance : 5mmu
 Unsaturation (U.S.) : 0.0 - 15.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
1	336.1934	21.76	-0.8 / -0.3	6.0 C19 H28 O5

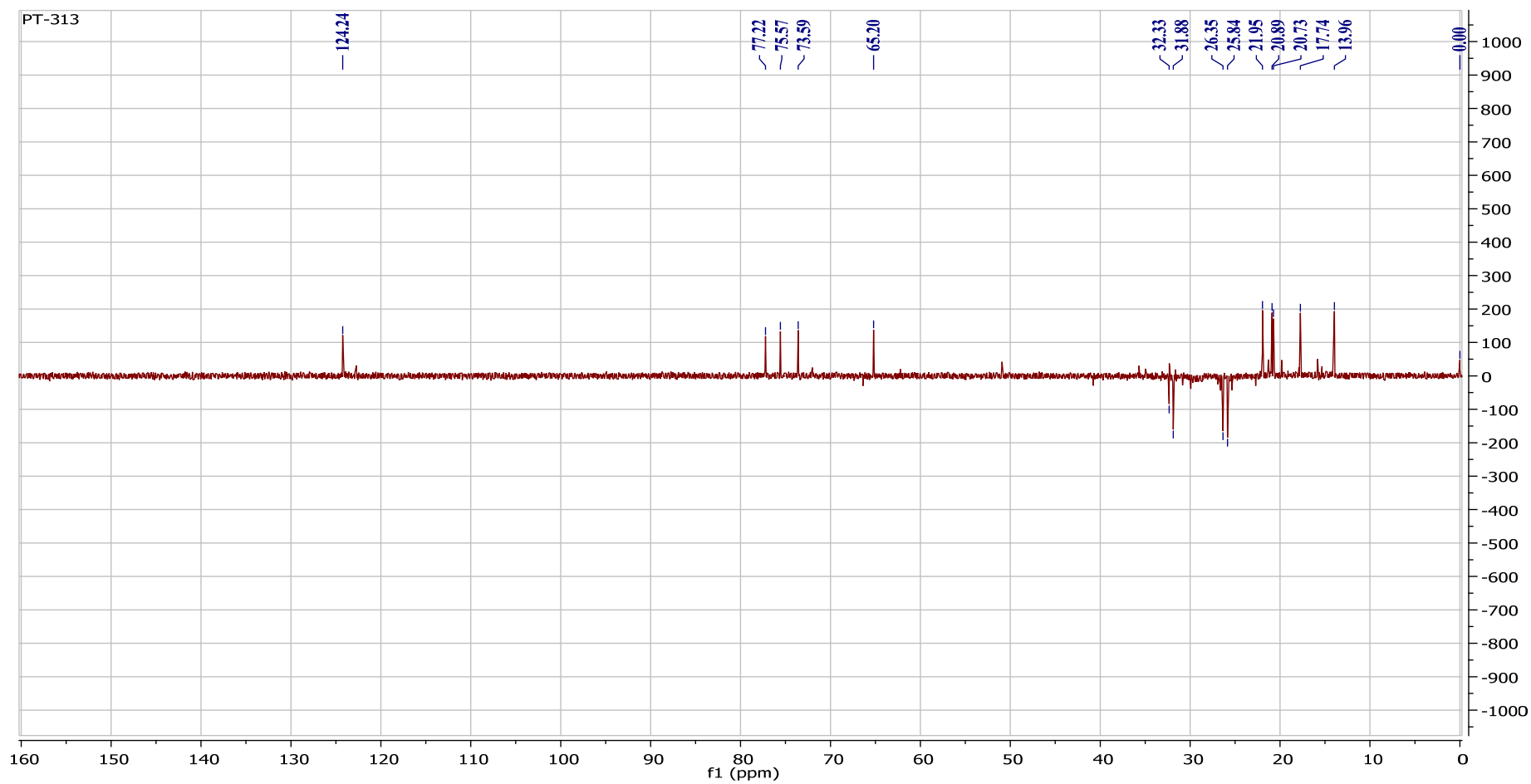
S11: HRCIMS of 2



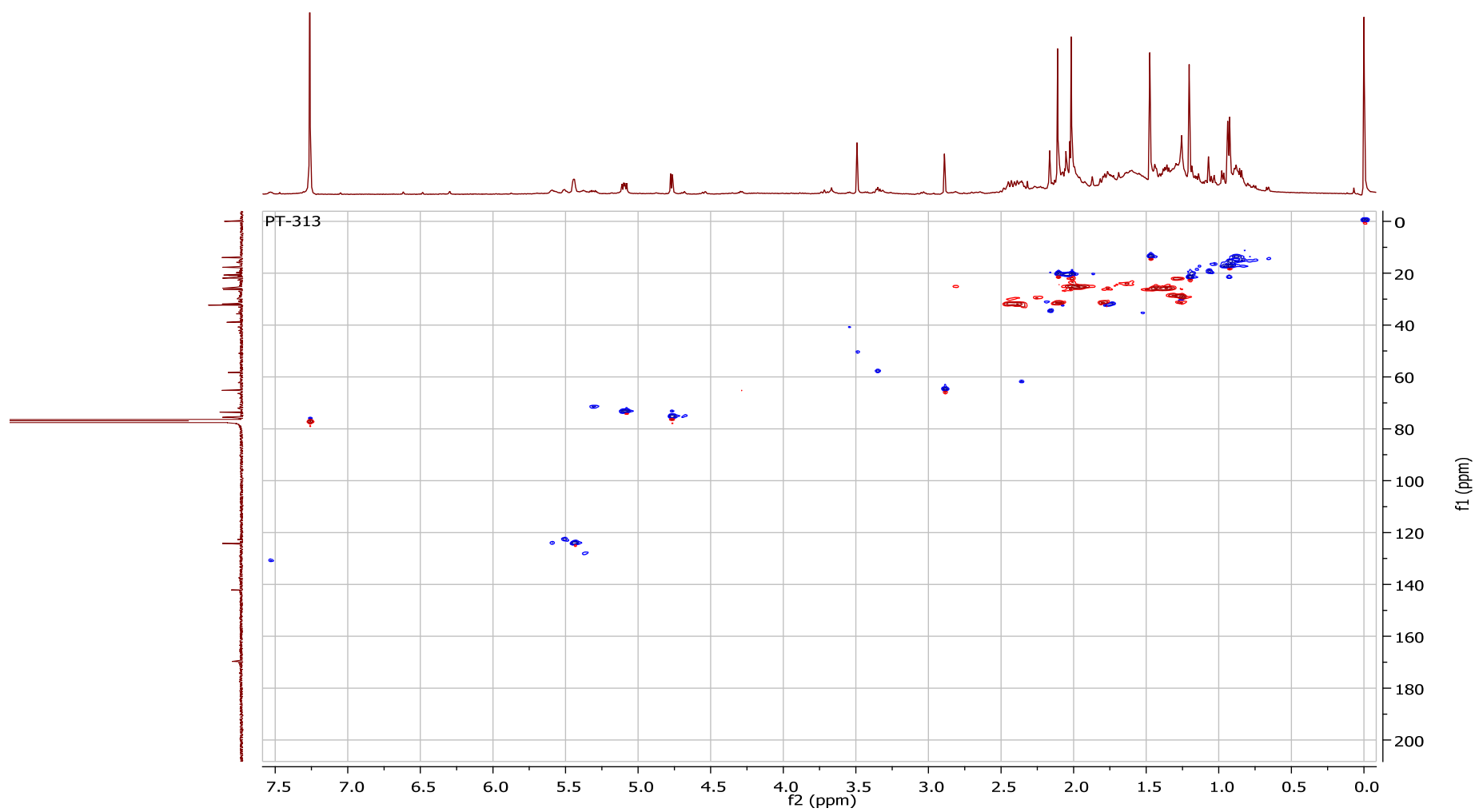
S12: ^1H NMR of **2**



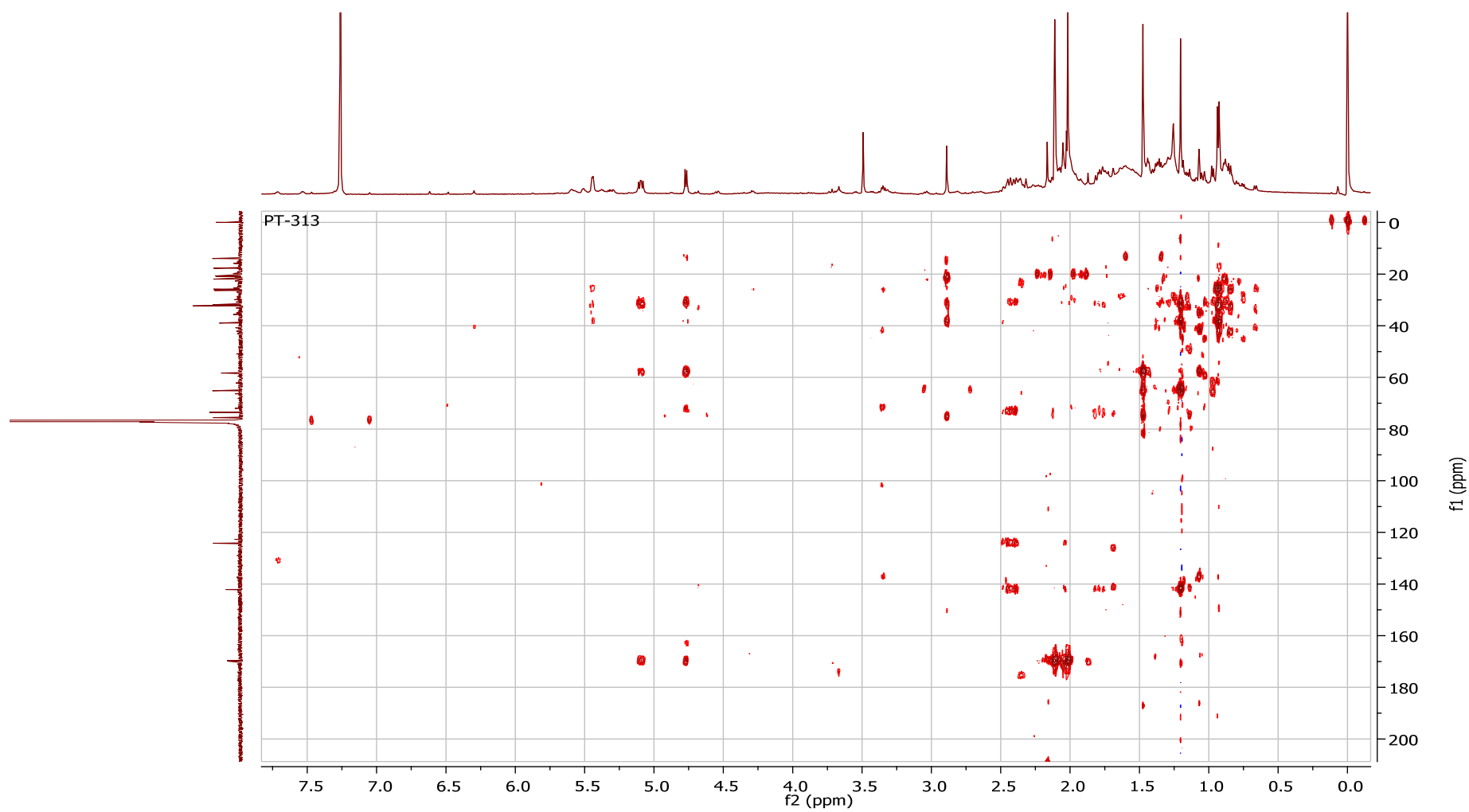
S13: ^{13}C NMR of **2**



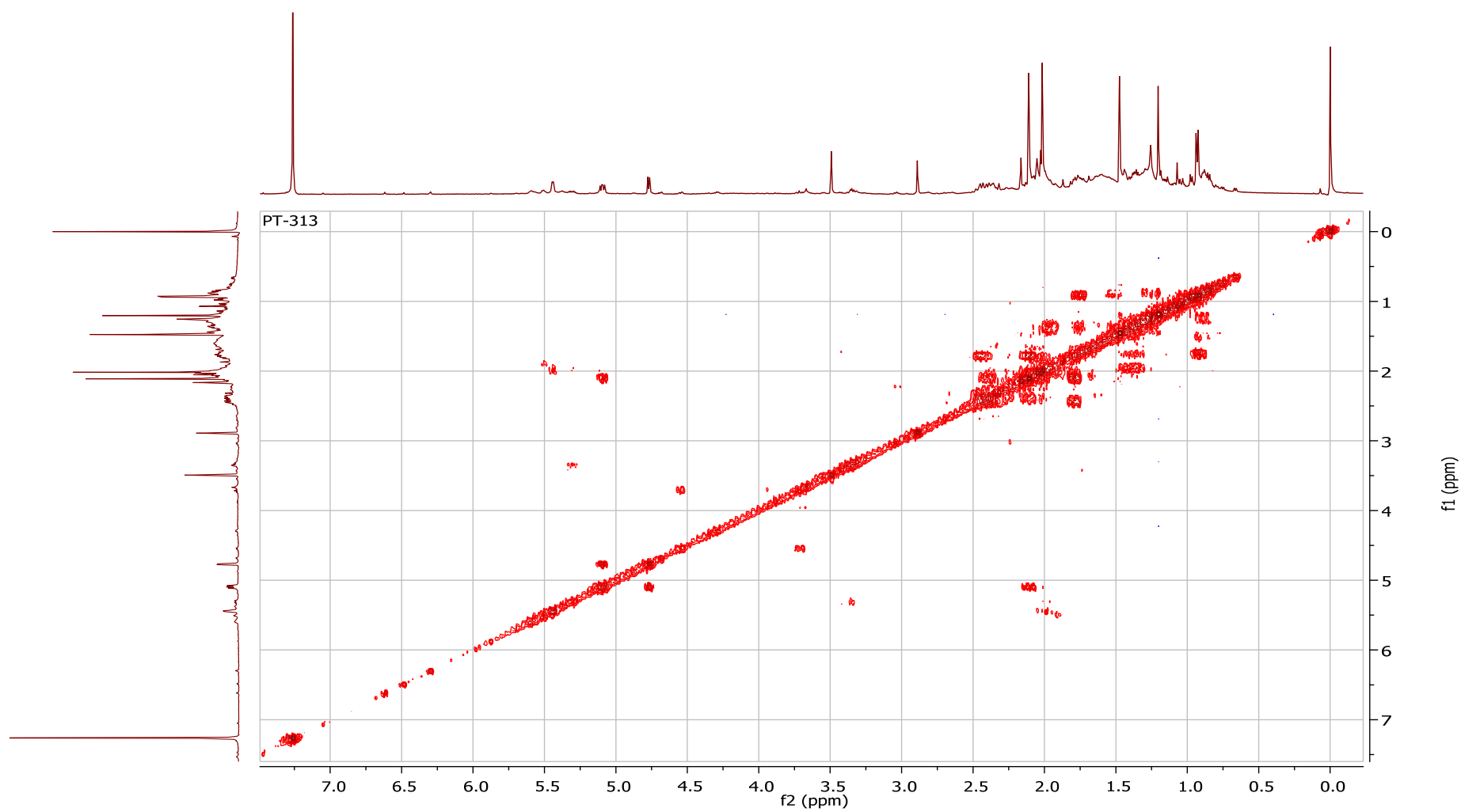
S14: DEPT-135 of 2



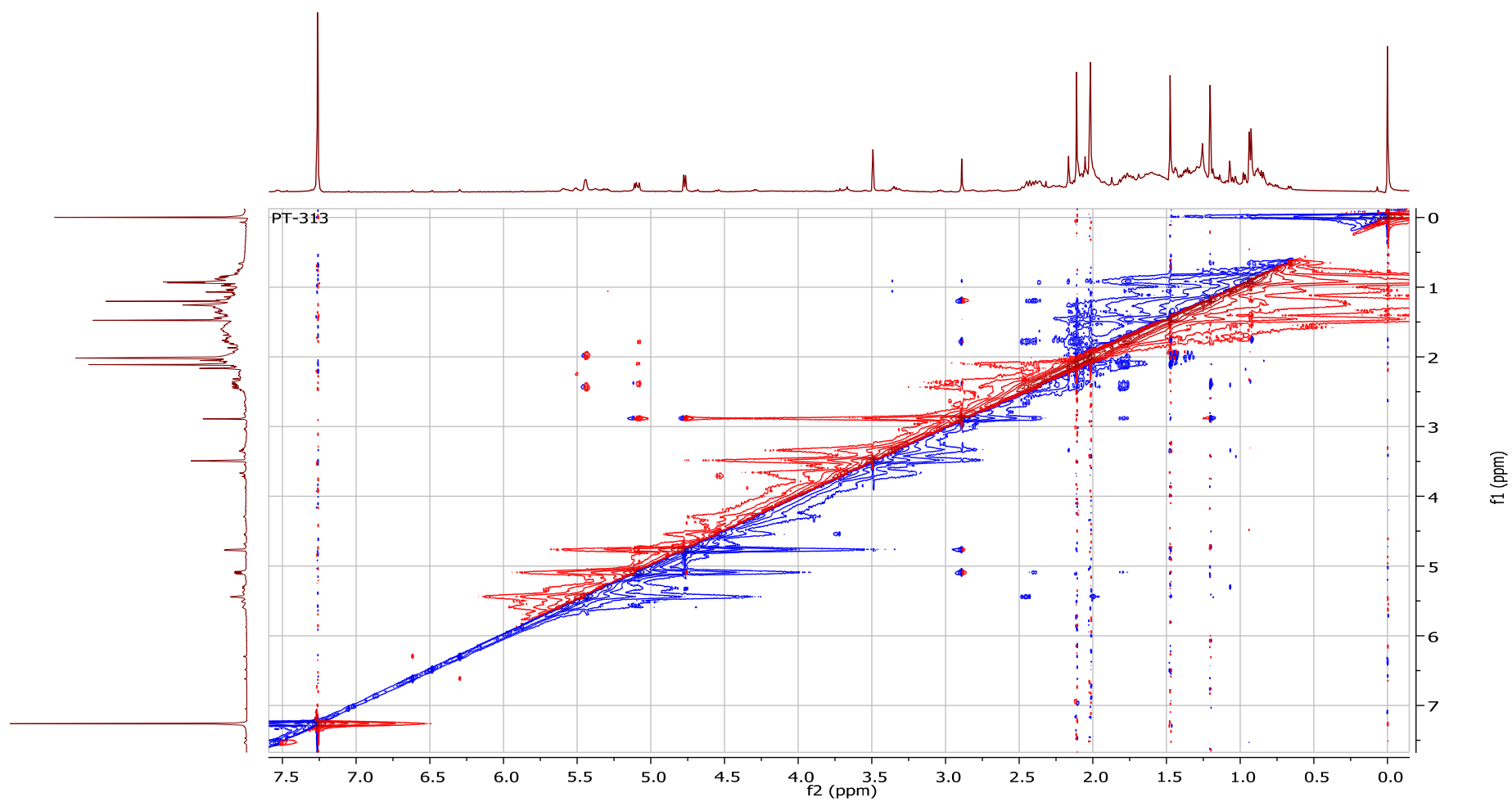
S15: HSQC of **2**



S16: HMBC of **2**

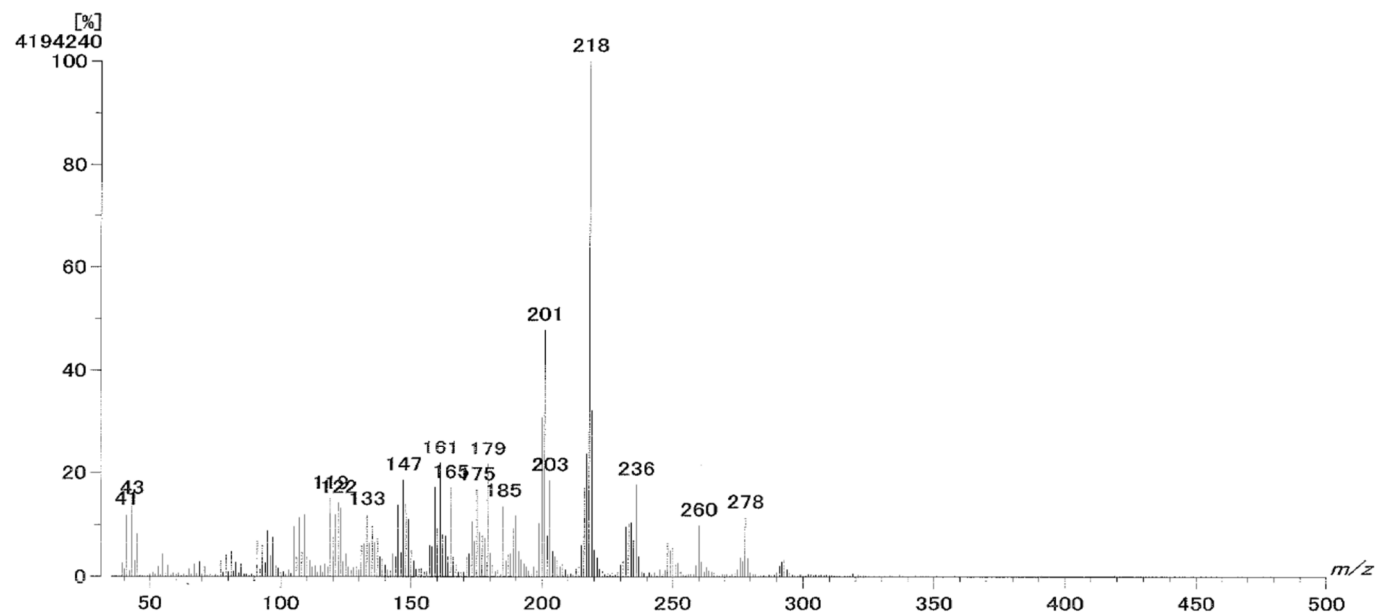


S17: ^1H ^1H COSY of **2**

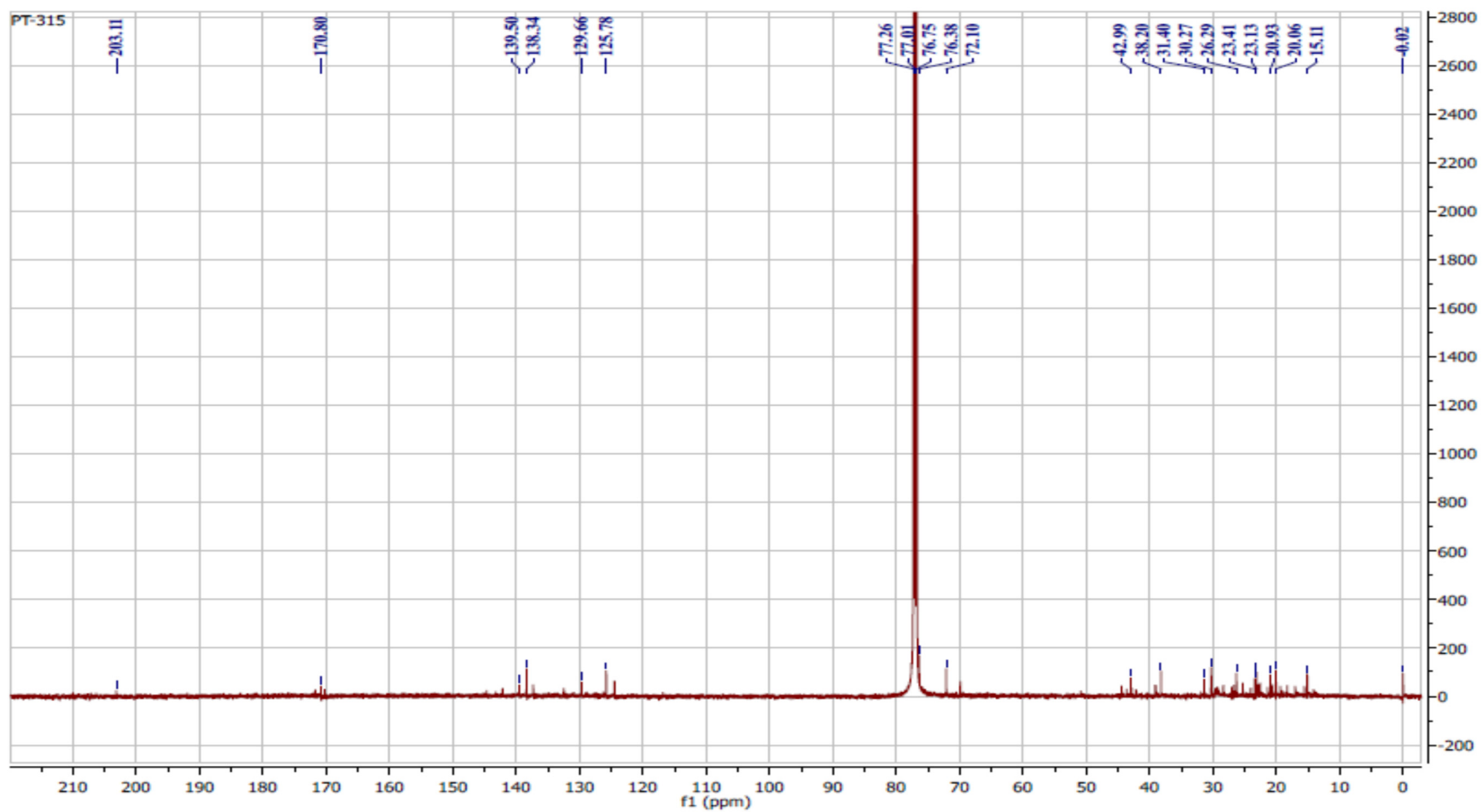


S18: NOESY of **2**

[Mass Spectrum]
Data : Umeyama-Cl.17-Aug-2019.003 Date : 17-Aug-2019 10:37
Sample : PT-315(CH4)
Note : MStation
Inlet : Direct Ion Mode : CI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.63 min Scan# : 24
BP : m/z 218 Int. : 399.99 (4194240)
Output m/z range : 35 to 500 Cut Level : 0.00 %



S19: LRCIMS of 3



S21: ^{13}C -NMR of **3**

[Mass Spectrum]

Data : Umeyama-Cl.29-Jul-2019.002 Date : 29-Jul-2019 08:27

Sample : PT-316(CH4)

Note : MStation

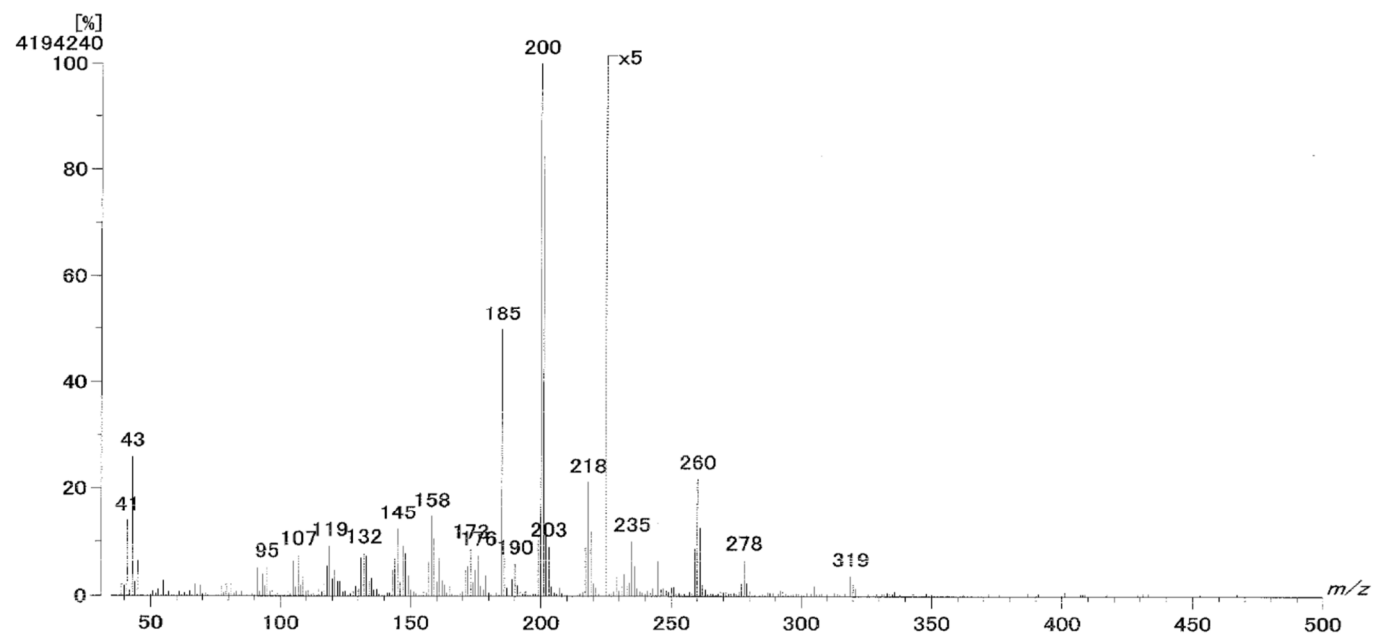
Inlet : Direct Ion Mode : CI+

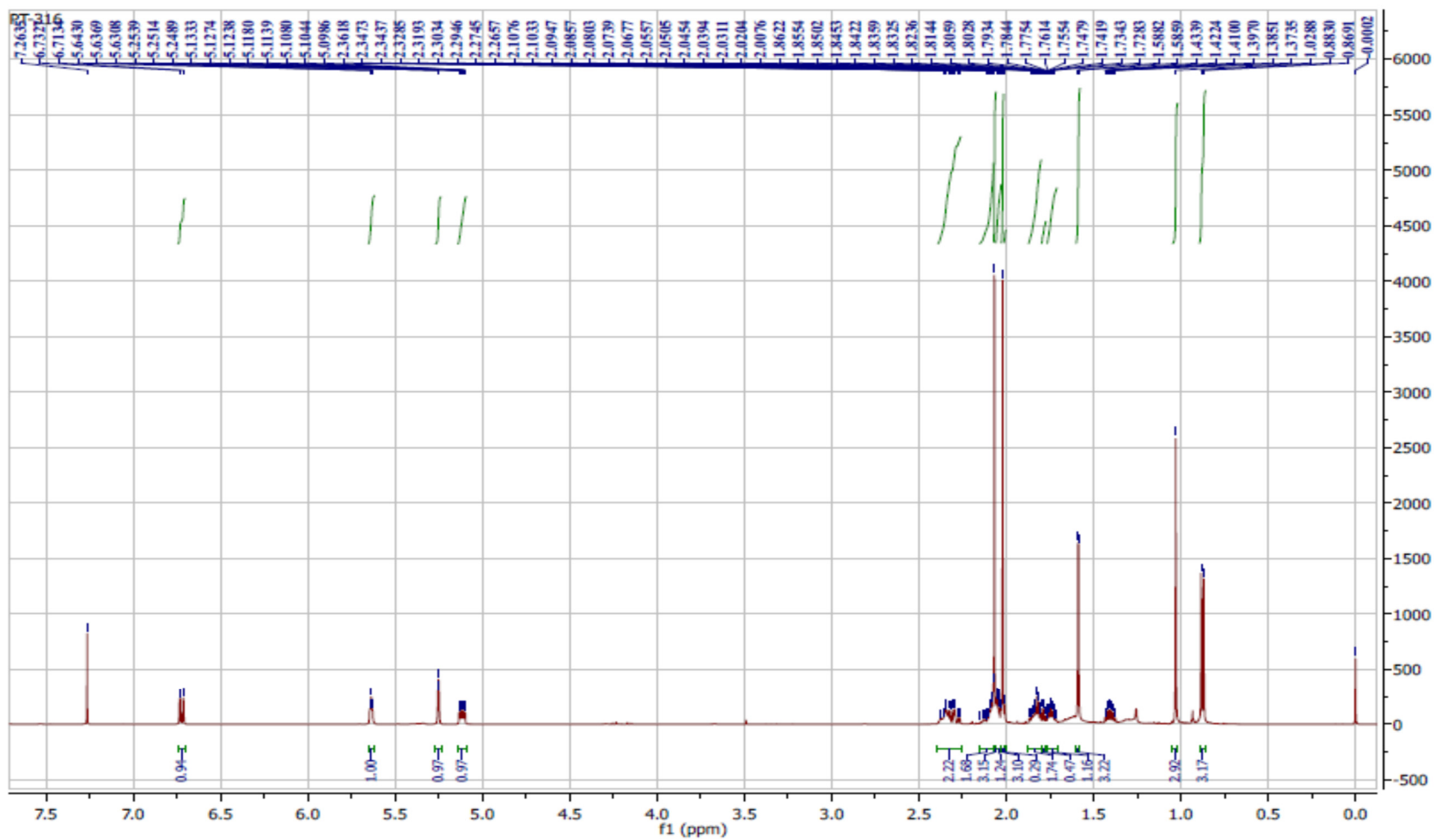
Spectrum Type : Normal Ion [MF-Linear]

RT : 0.55 min Scan# : 21

BP : m/z 200 Int. : 399.99 (4194240)

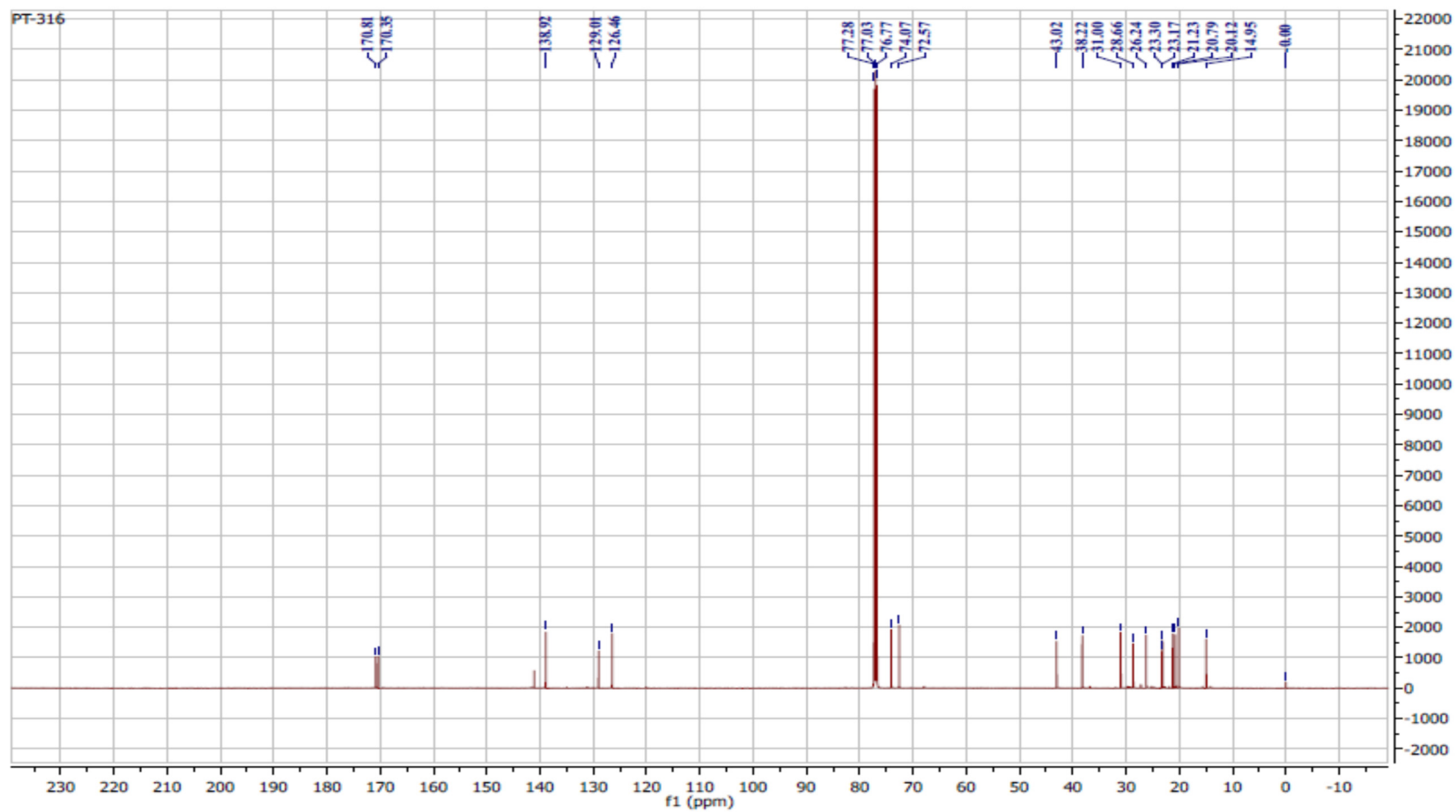
Output m/z range : 35 to 500 Cut Level : 0.00 %





^1H -

S23: NMR of 4



S24: ^{13}C -NMR of 4

[Mass Spectrum]

Data : Umeyama-EI.22-Jul-2019.001 Date : 22-Jul-2019 09:59

Sample : PT-311

Note : MStation

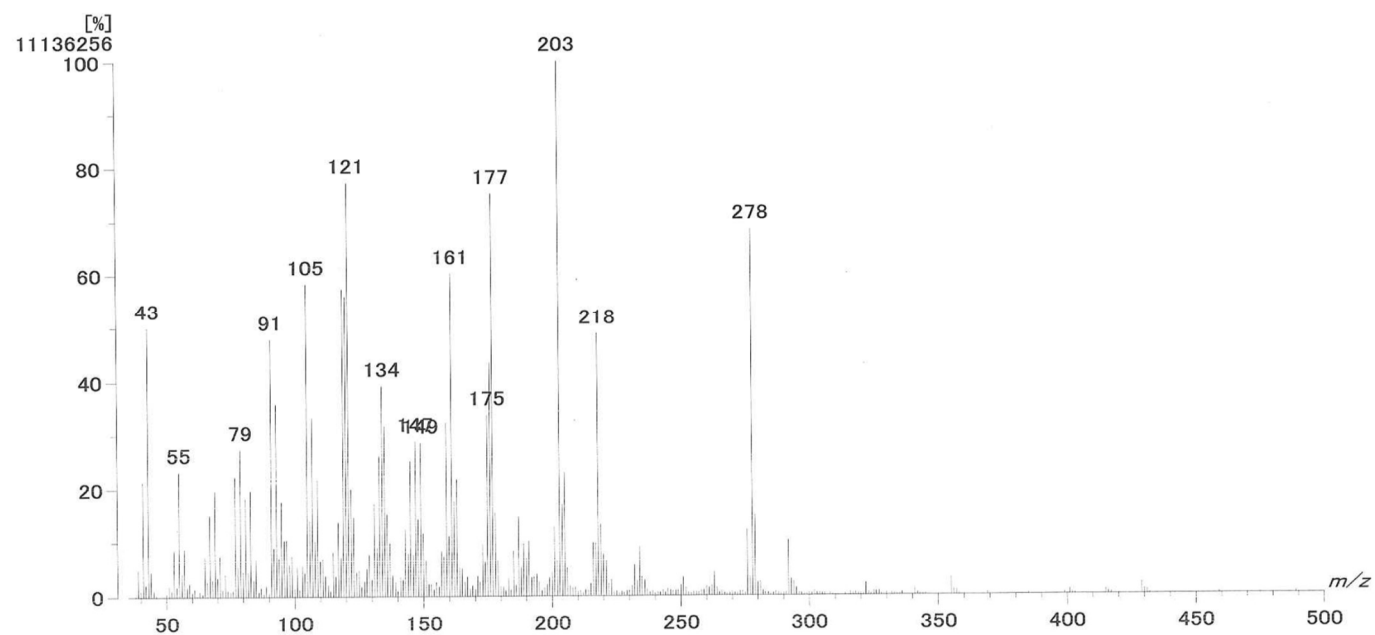
Inlet : Direct Ion Mode : EI+

Spectrum Type : Normal Ion [MF-Linear]

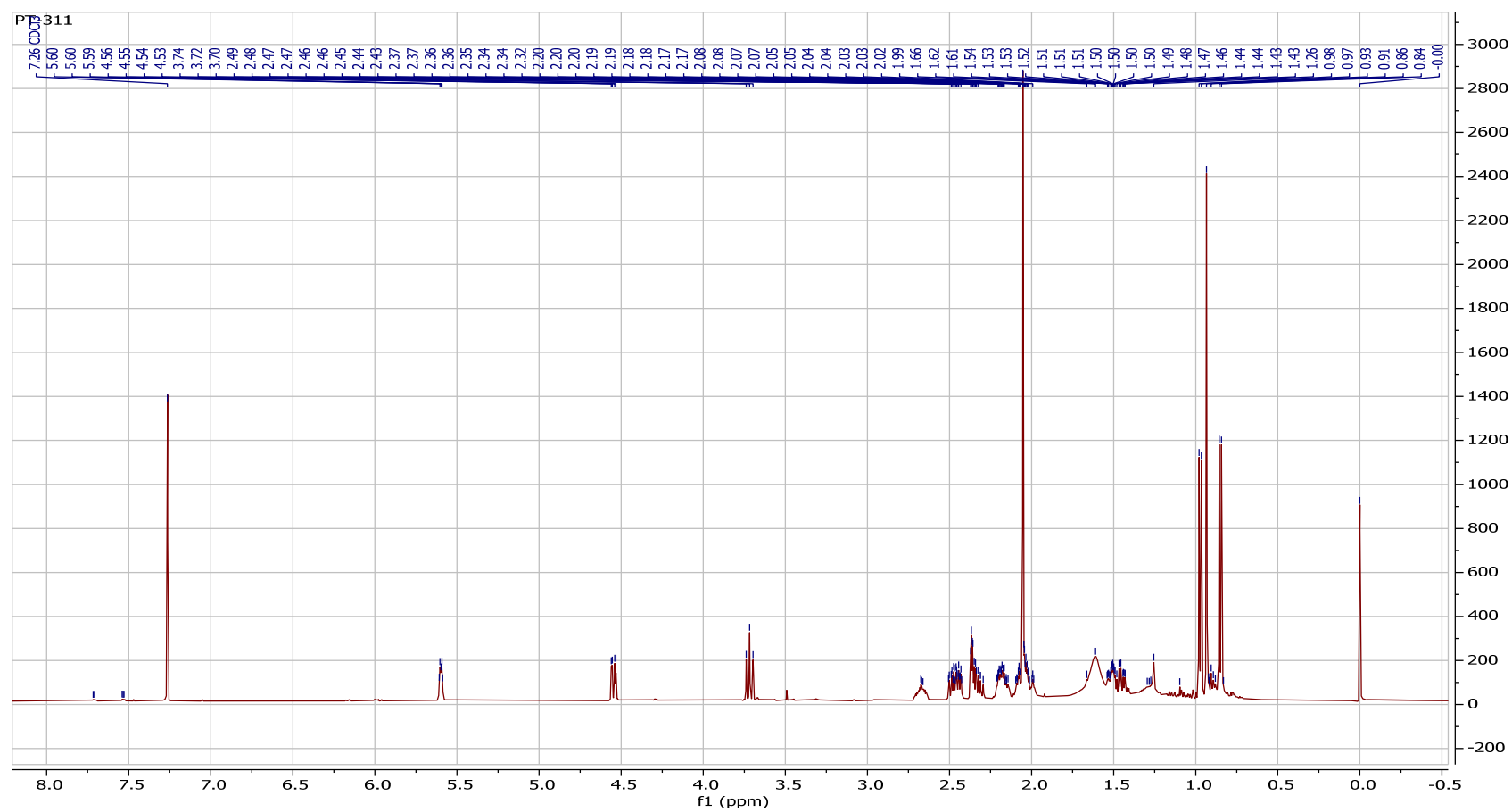
RT : 0.60 min Scan# : 19

BP : m/z 203 Int. : 1062.04 (11136256)

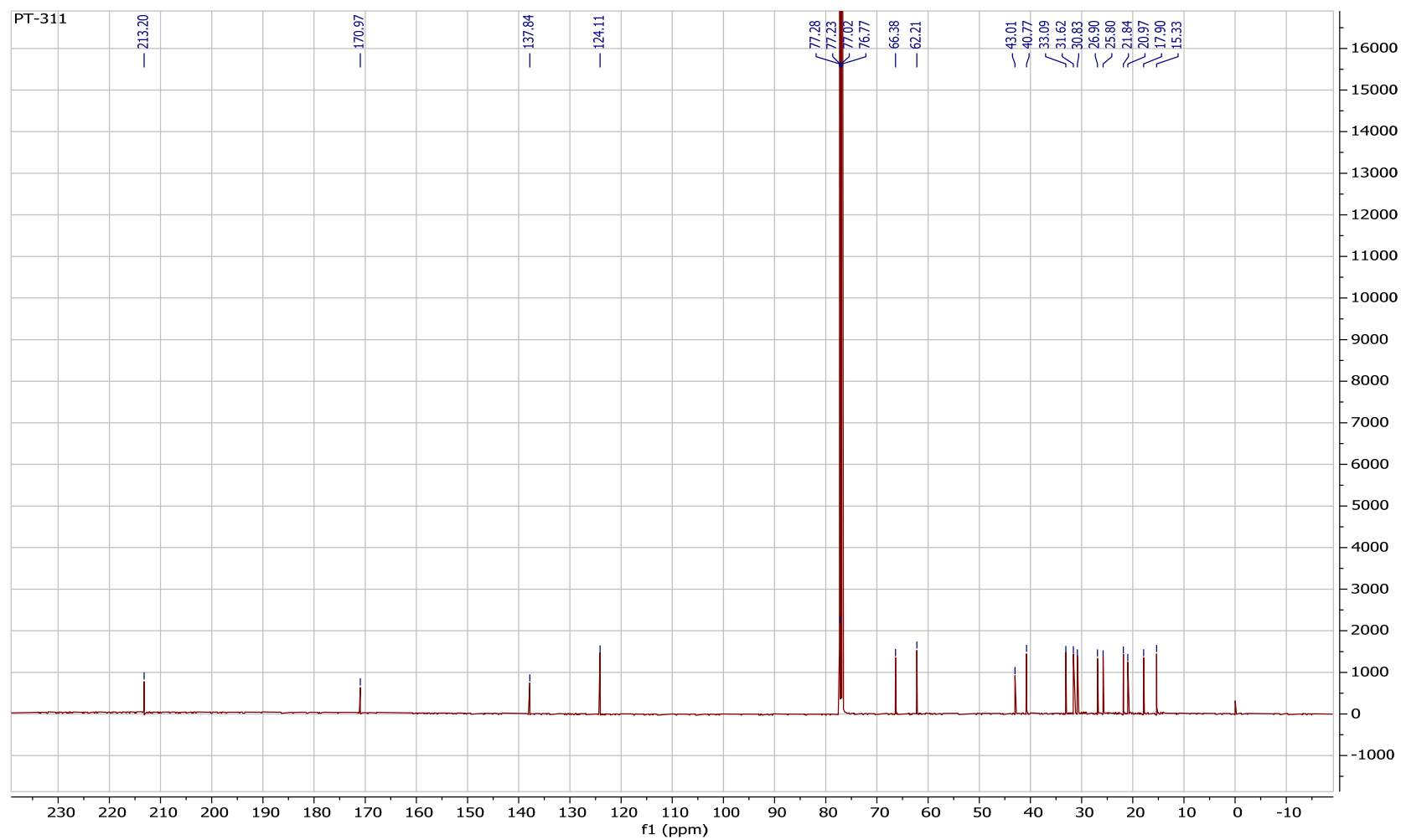
Output m/z range : 35 to 500 Cut Level : 0.00 %



S25: LRCIMS of 5

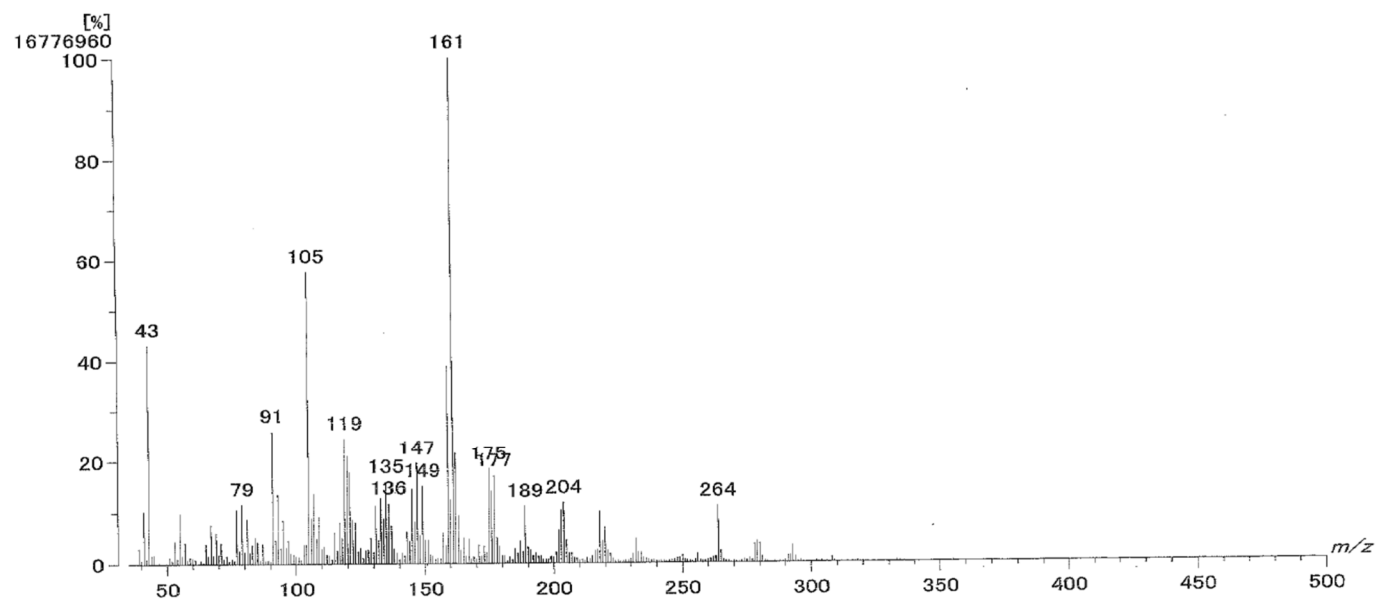


S26: ^1H -NMR of **5**

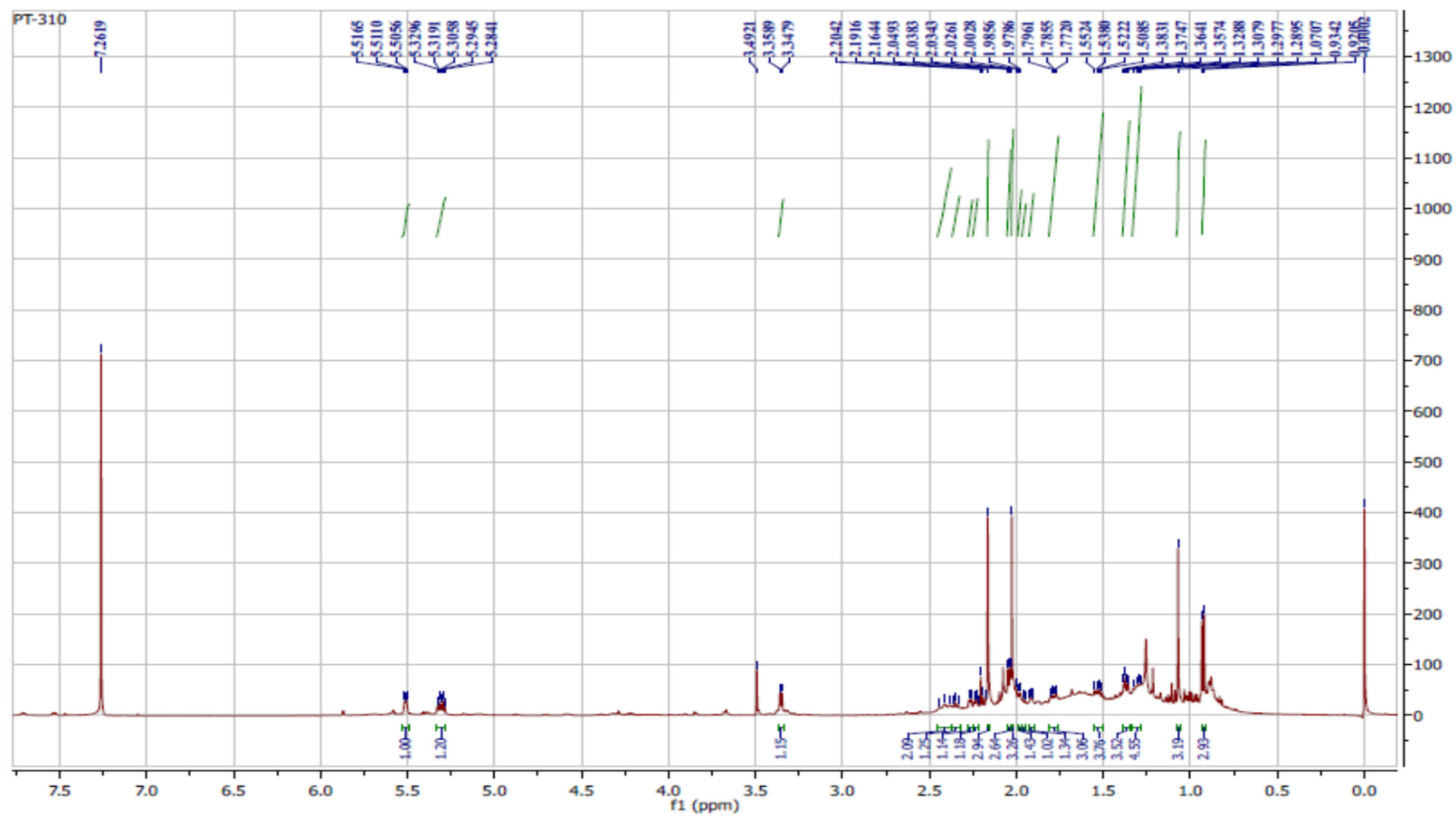


S27: ^{13}C -NMR of **5**

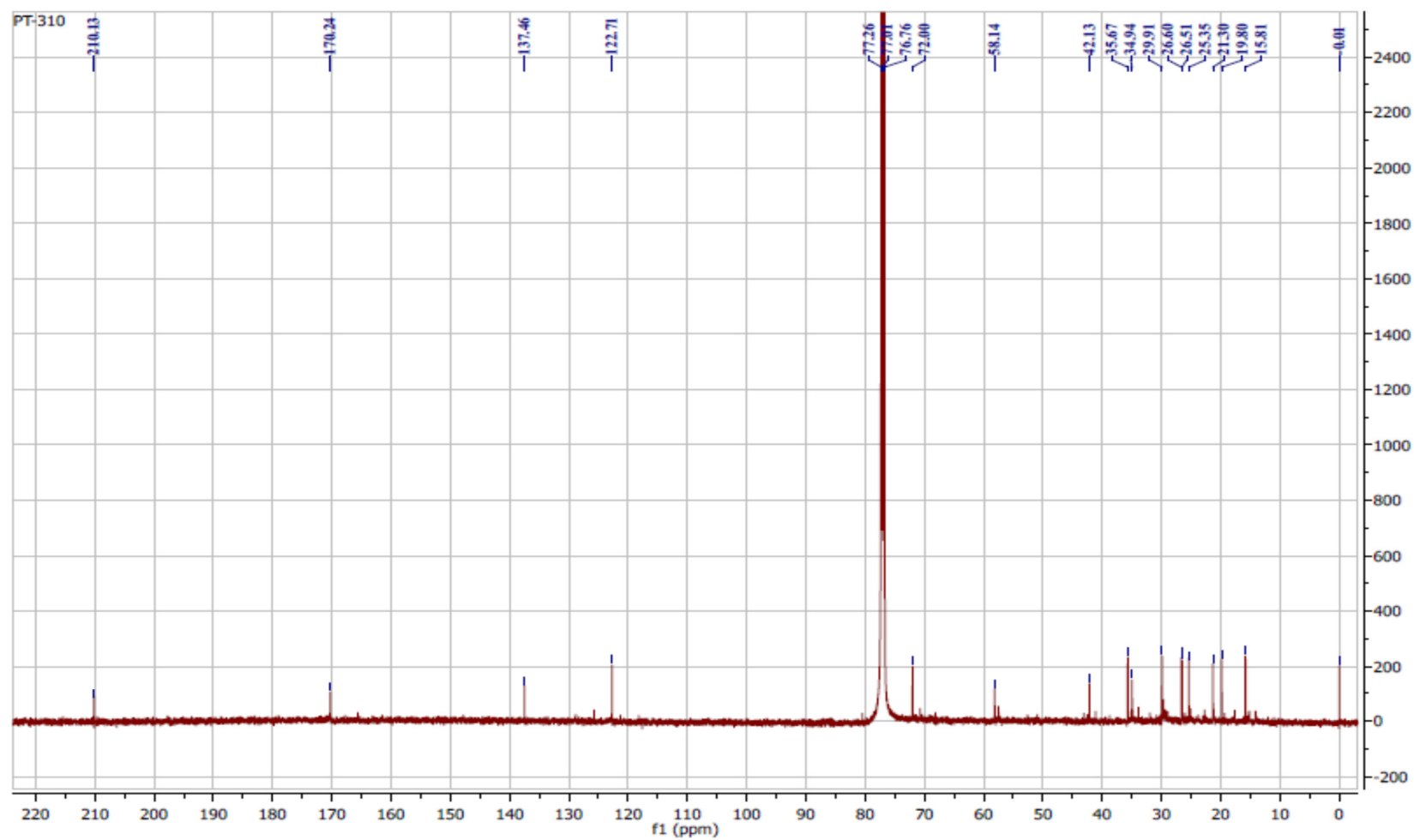
[Mass Spectrum]
Data : Umeyama-El01-Aug-2019.001 Date : 01-Aug-2019 07:58
Sample : PT-310
Note : MStation
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.50 min Scan# : 16
BP : m/z 161 Int. : 1599.98 (16776960)
Output m/z range : 35 to 500 Cut Level : 0.00 %



S28: LRCIMS EI-MS of 6

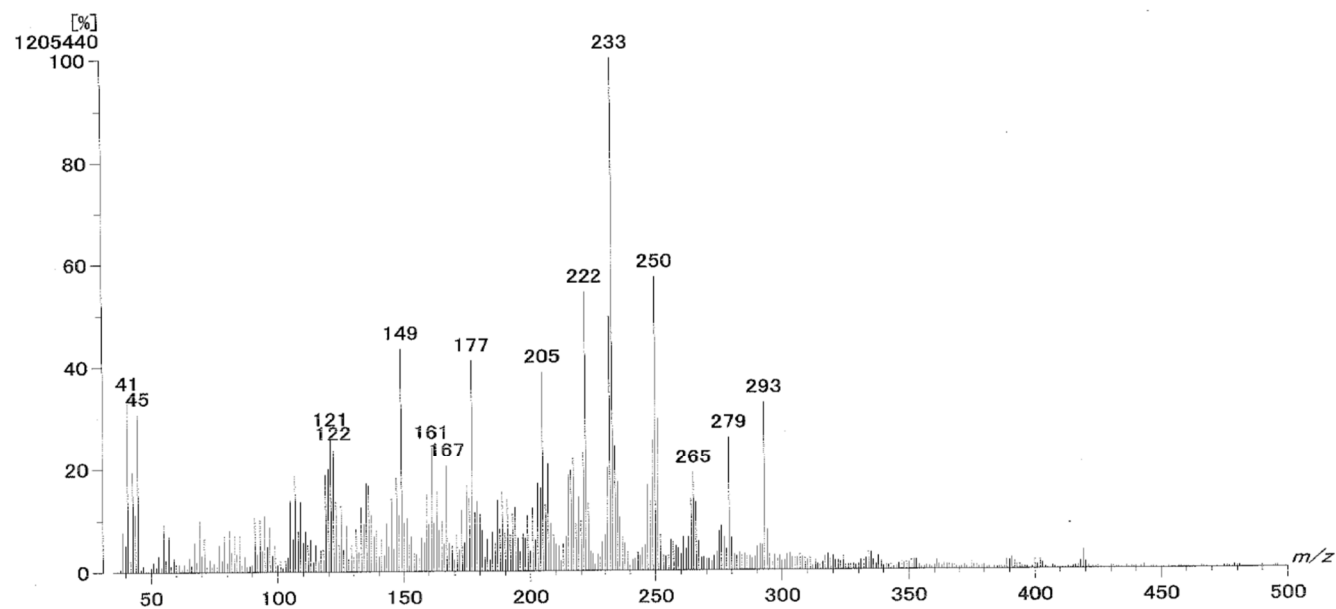


S29: ^1H -NMR of **6**

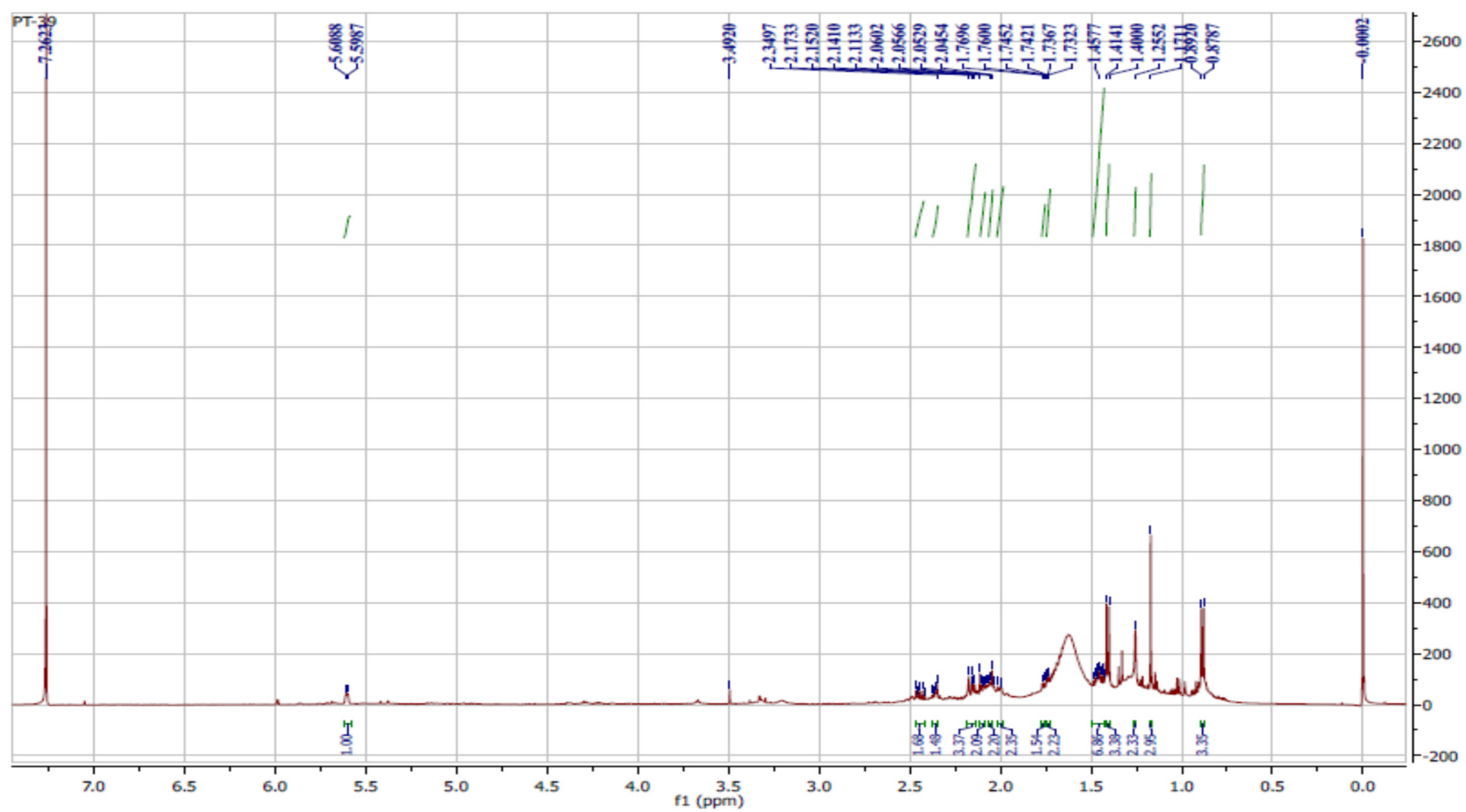


S30: ^{13}C -NMR of **6**

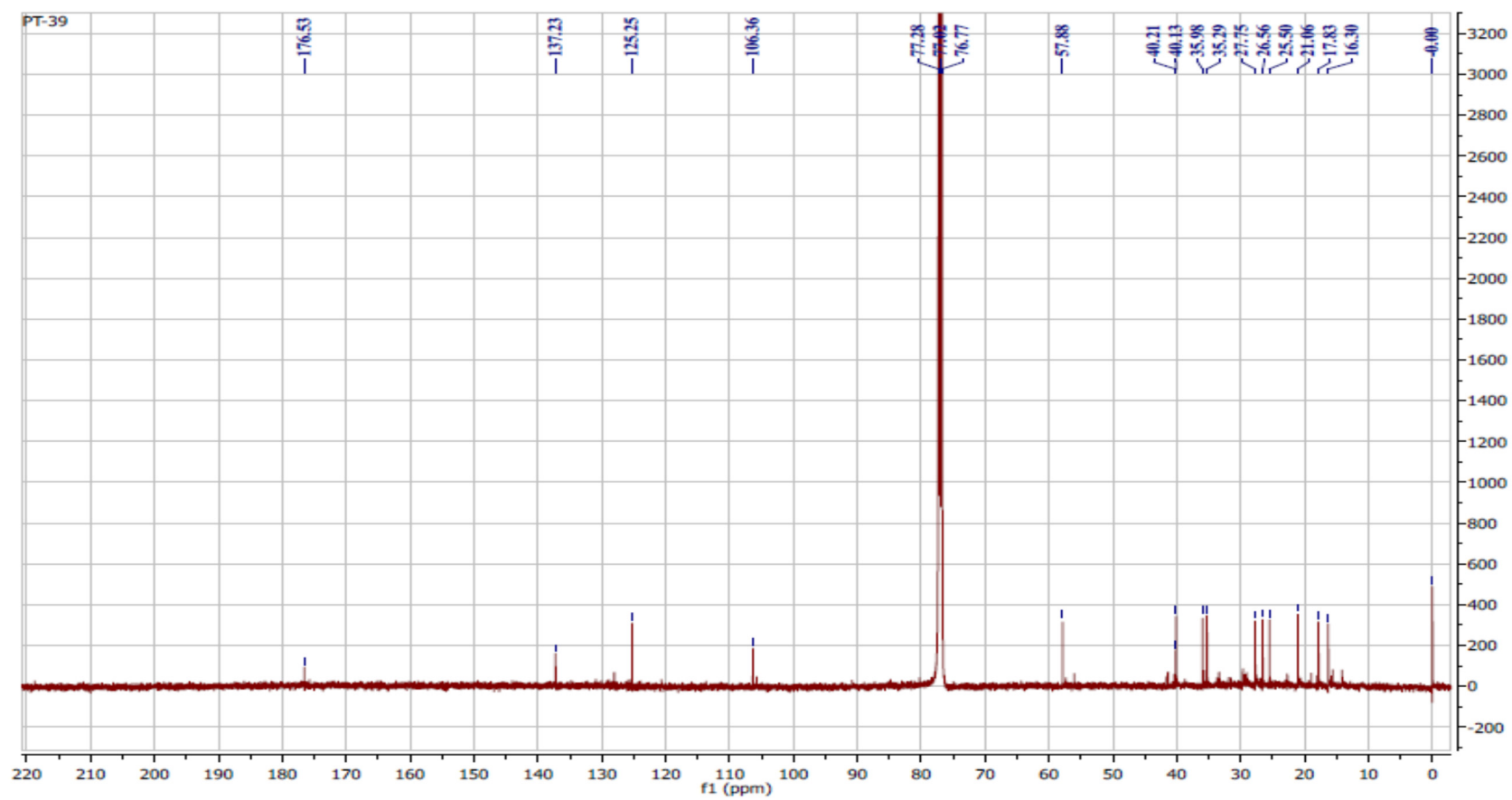
[Mass Spectrum]
Data : Umeyama-C117-Aug-2019.004 Date : 17-Aug-2019 10:44
Sample : PT-39(CH4)
Note : MStation
Inlet : Direct Ion Mode : CI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.79 min Scan# : 30
BP : m/z 233 Int. : 114.96 (1205440)
Output m/z range : 35 to 500 Cut Level : 0.00 %



S31: LRCIMS EI-MS of 7



S32: ^1H -NMR of **7**



S33: ^{13}C -NMR of **7**

[Mass Spectrum]

Data : Umeyama-EL17-Jul-2019.004 Date : 17-Jul-2019 15:21

Sample : PT-42

Note : MStation

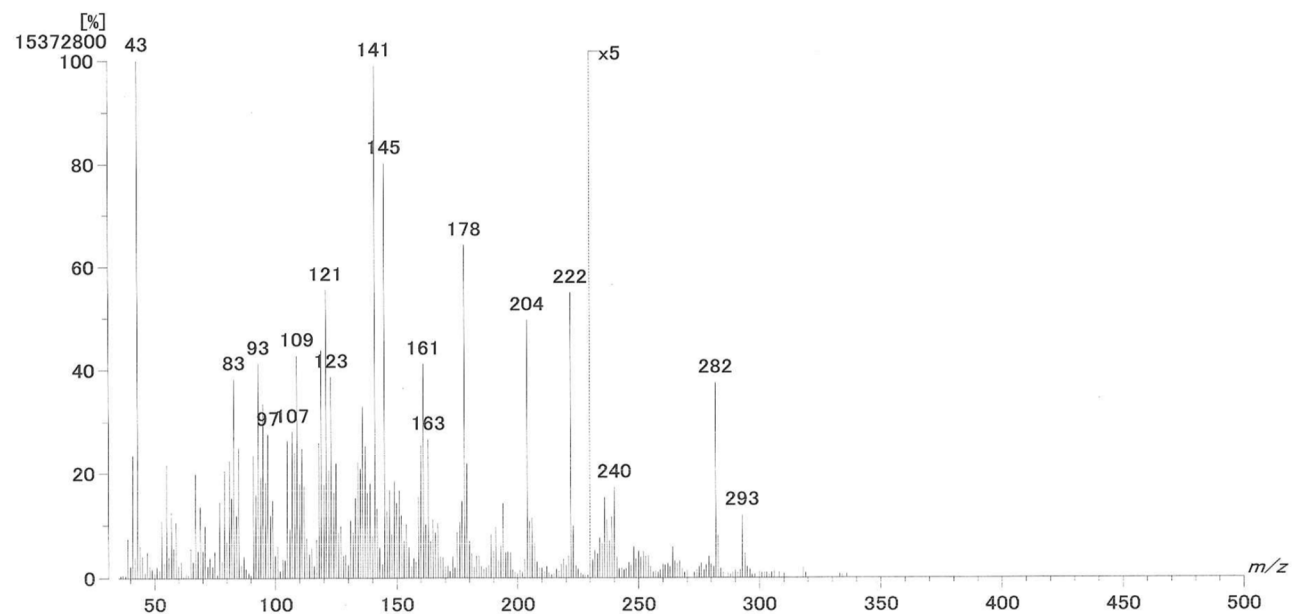
Inlet : Direct Ion Mode : EI+

Spectrum Type : Normal Ion [MF-Linear]

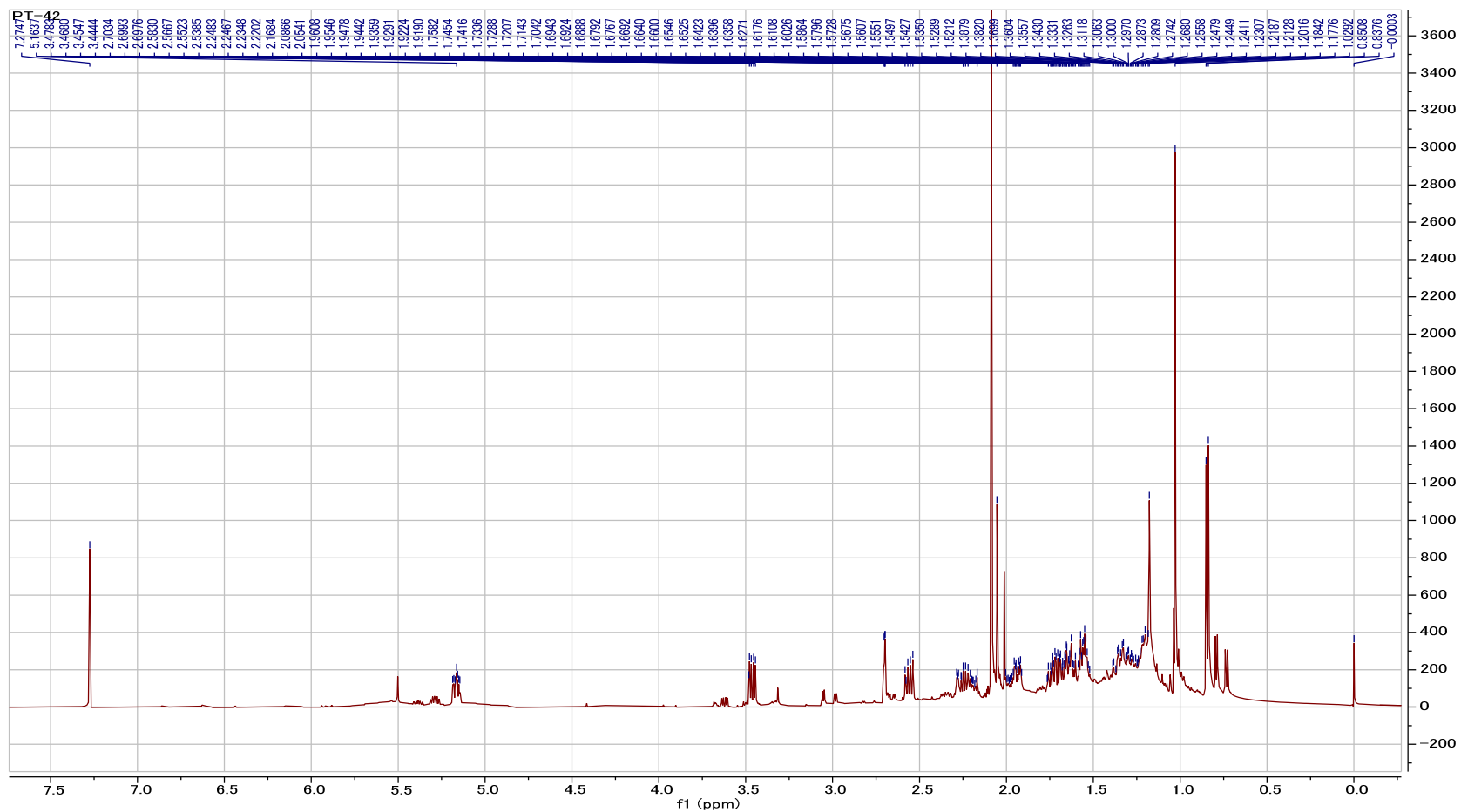
RT : 0.50 min Scan# : 16

BP : m/z 43 Int. : 1466.07 (15372800)

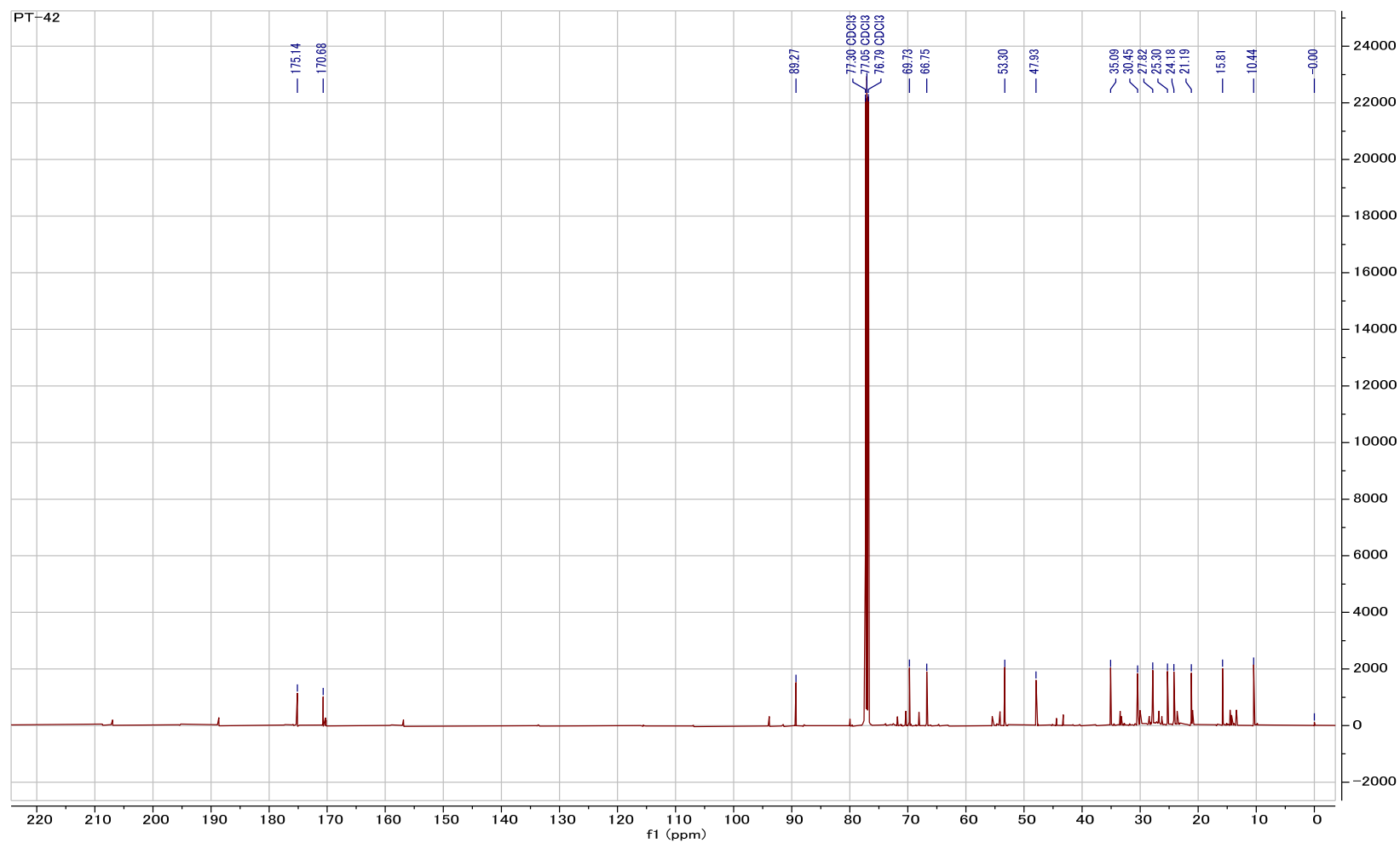
Output m/z range : 35 to 500 Cut Level : 0.00 %



S34:LRCIMS EI-MS of **8**

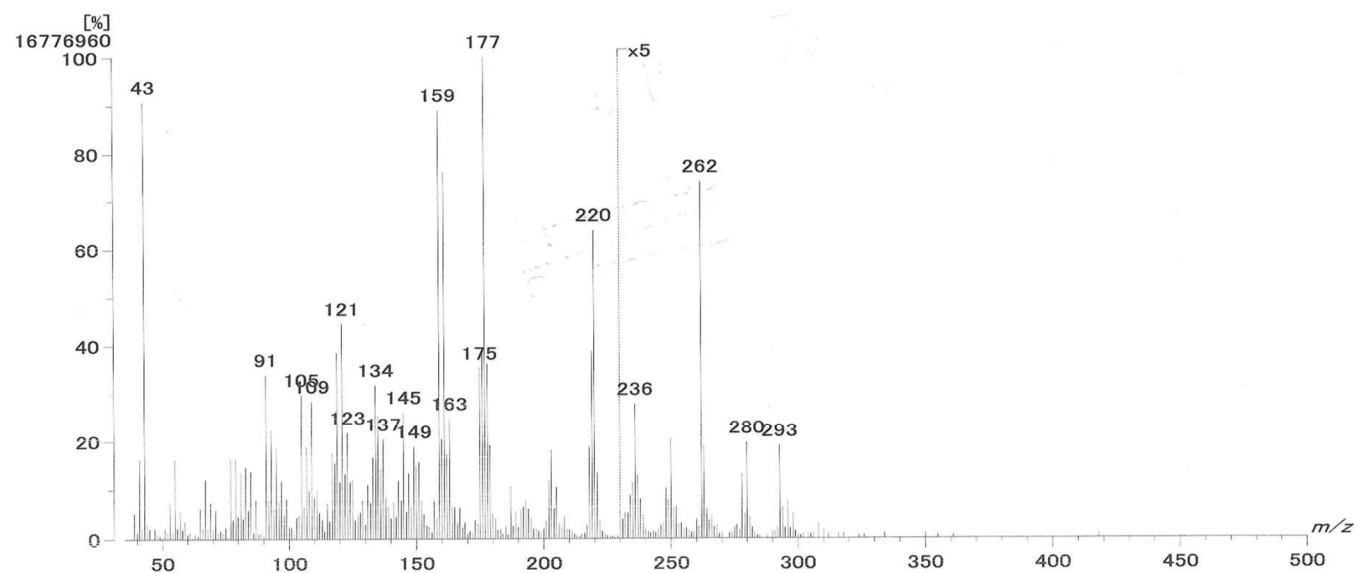


S35: ^1H -NMR of **8**

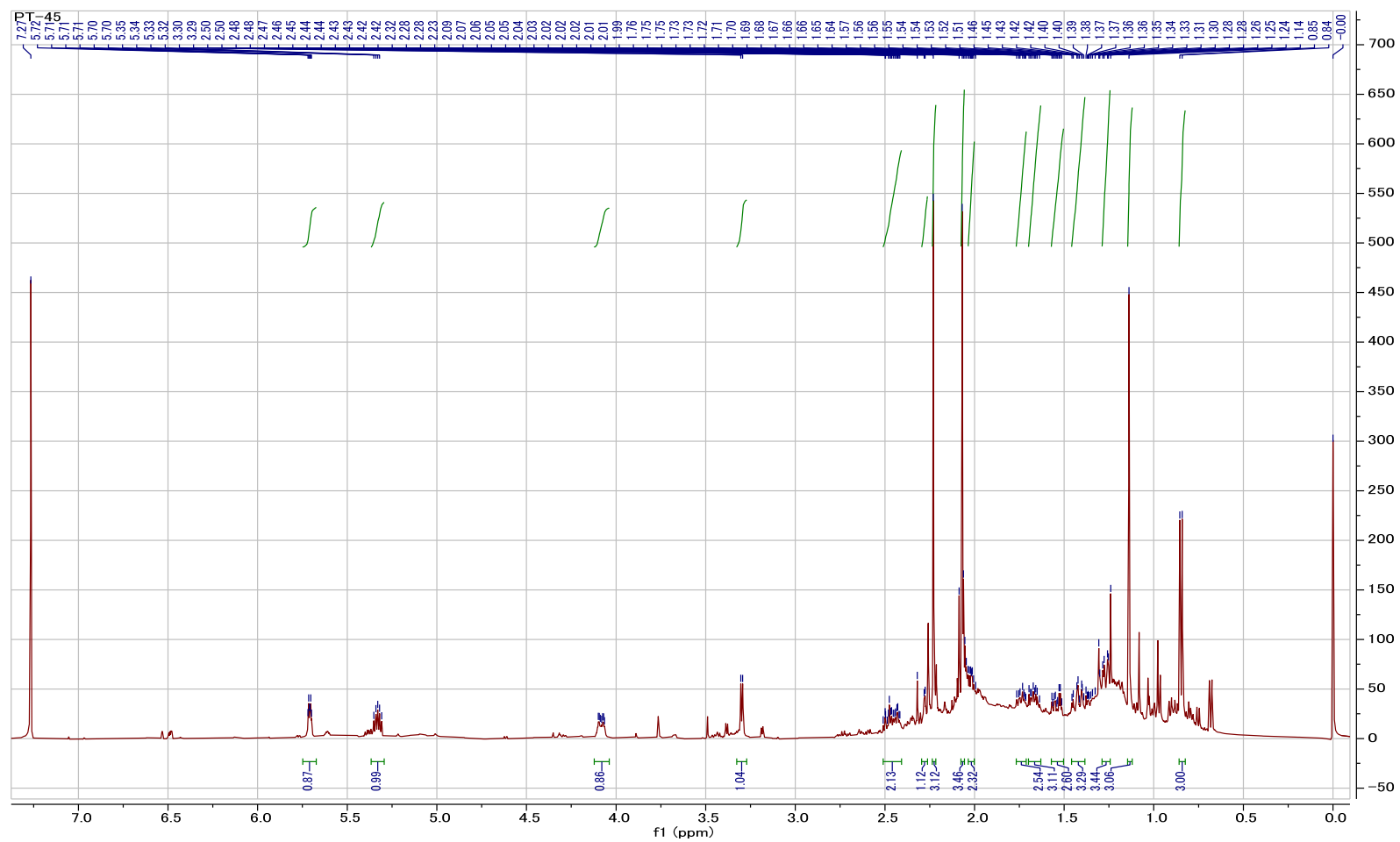


S36: ^{13}C -NMR of **8**

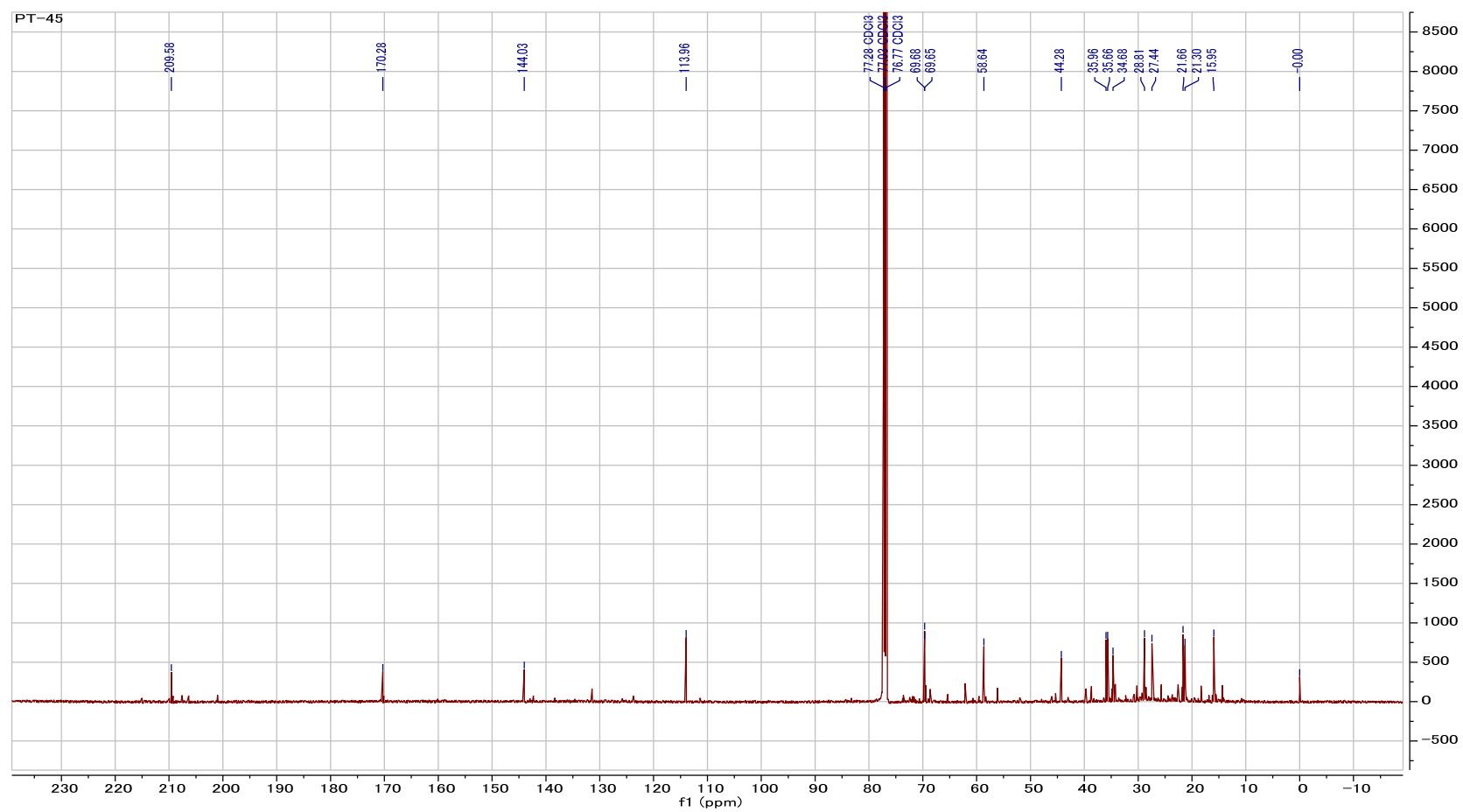
[Mass Spectrum]
Data : Umeyama-EI.17-Jul-2019.005 Date : 17-Jul-2019 15:27
Sample : PT-45
Note : MStation
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.47 min Scan# : 15
BP : m/z 177 Int. : 1599.98 (16776960)
Output m/z range : 35 to 500 Cut Level : 0.00 %



S37: LRCIMS EI-MS of 9



S38: ¹H-NMR of **9**



S39: ^{13}C -NMR of **9**

[Mass Spectrum]

Data : Umeyama-El.09-Jul-2019.002 Date : 09-Jul-2019 13:45

Sample : PT-44

Note : MStation

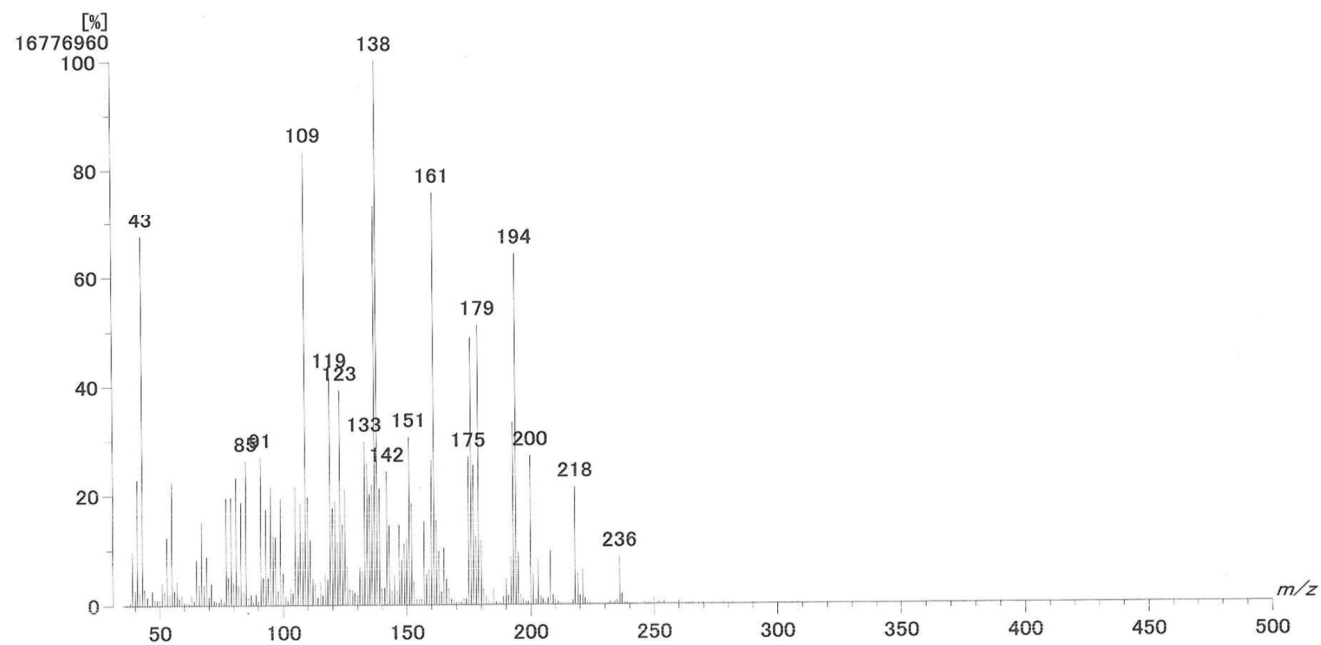
Inlet : Direct Ion Mode : EI+

Spectrum Type : Normal Ion [MF-Linear]

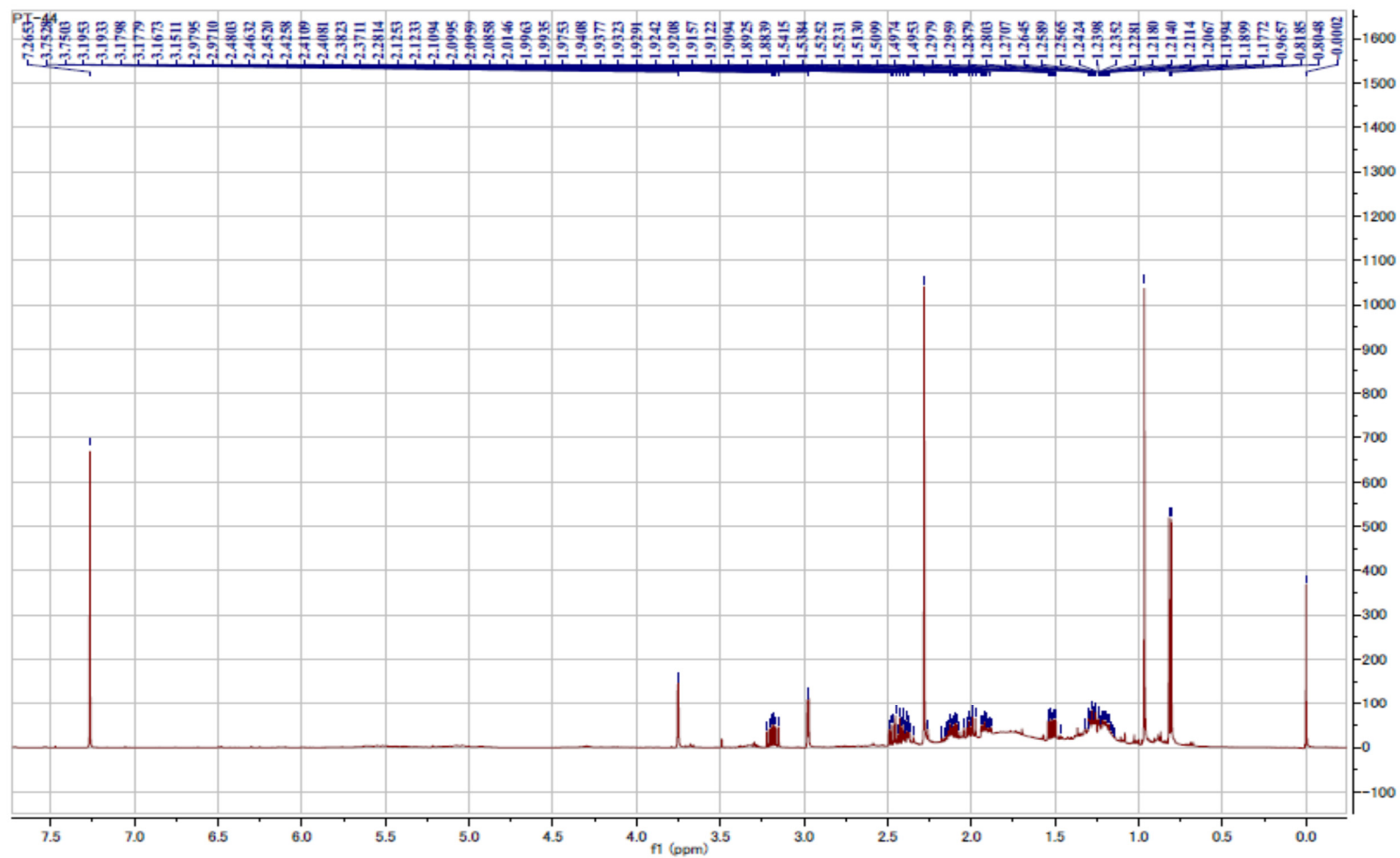
RT : 0.37 min Scan# : 12

BP : m/z 138 Int. : 1599.98 (16776960)

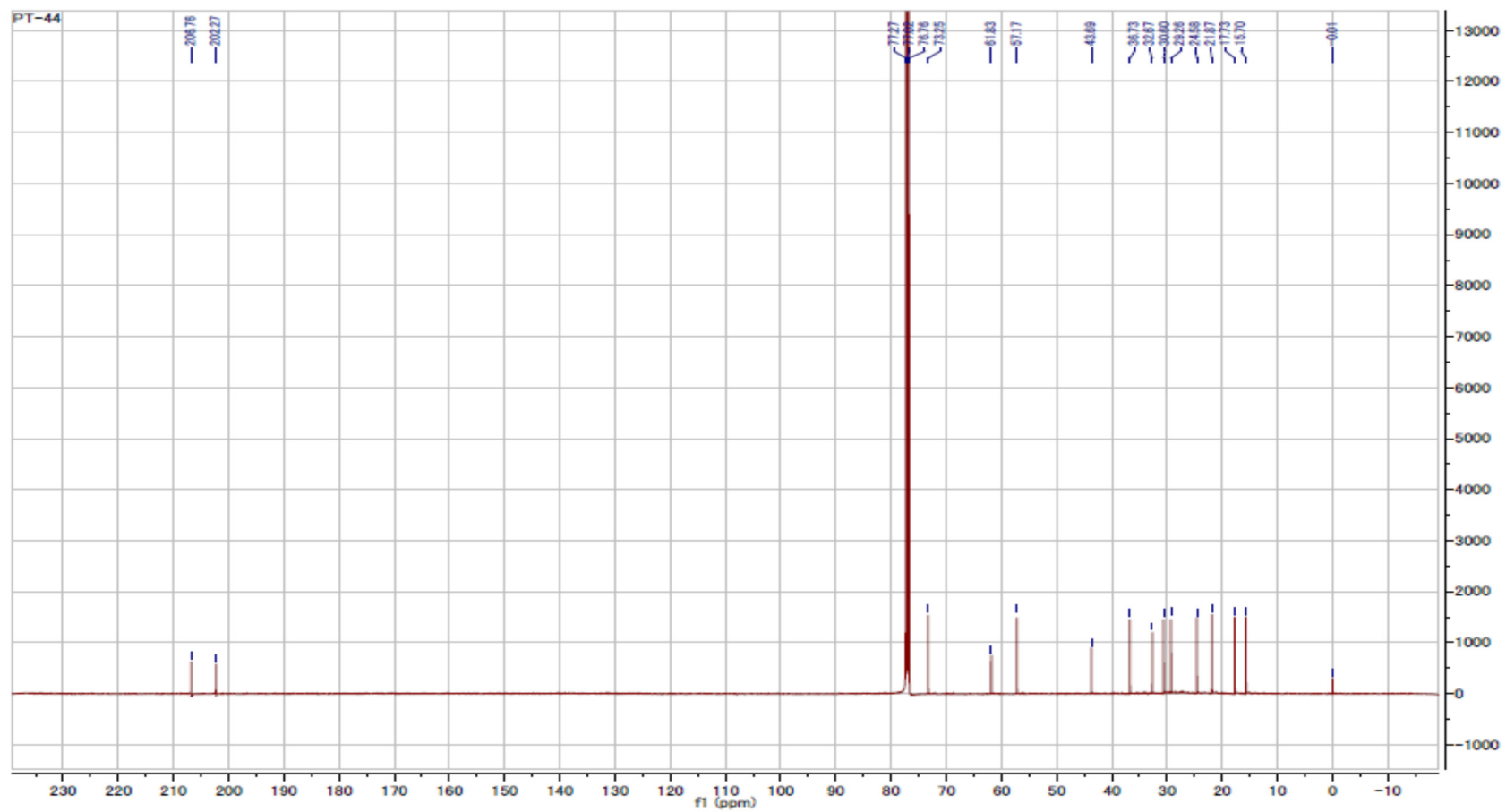
Output m/z range : 35 to 500 Cut Level : 0.00 %



S40: LRCIMS EI-MS of **10**



S41: ^1H -NMR of **10**



S42: ^{13}C -NMR of **10**

[Mass Spectrum]

Data : Umeyama-El24-Jul-2019.001 Date : 24-Jul-2019 16:28

Sample : PT-34

Note : MStation

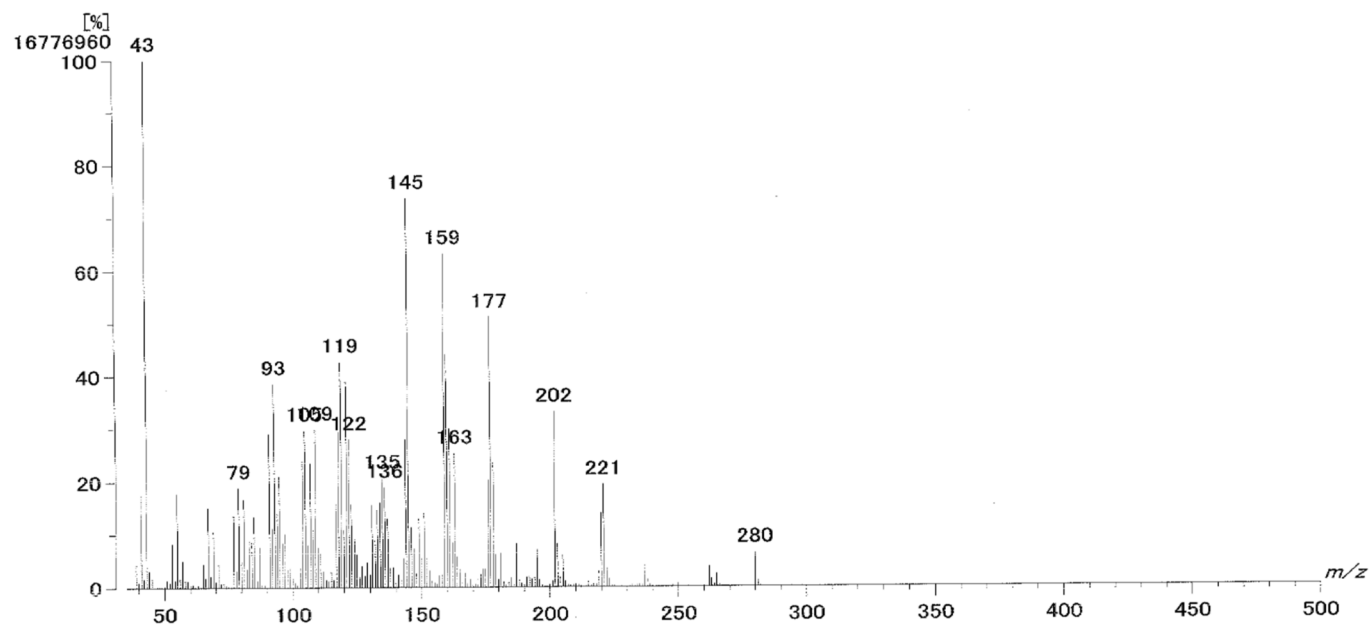
Inlet : Direct Ion Mode : EI+

Spectrum Type : Normal Ion [MF-Linear]

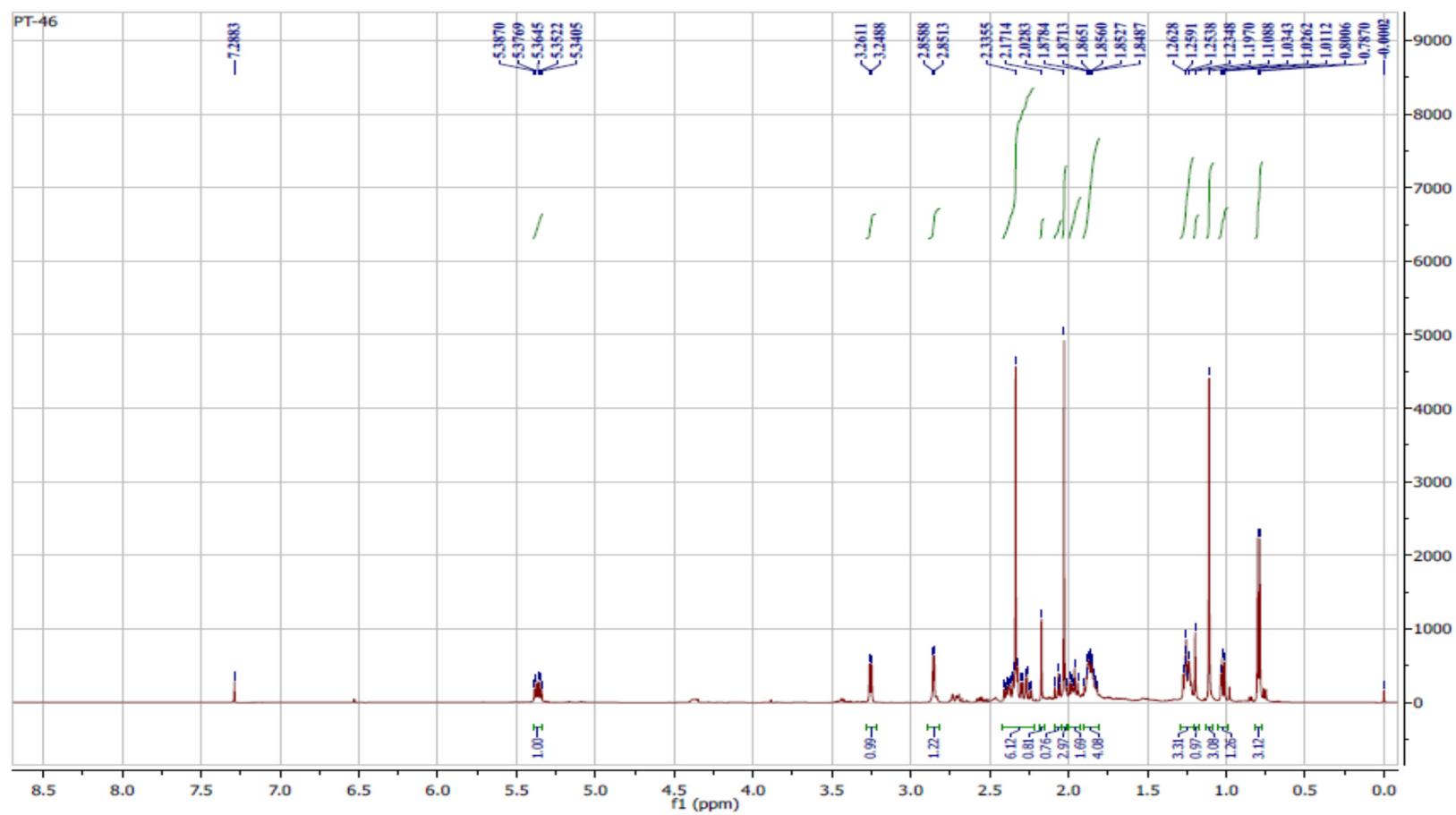
RT : 0.57 min Scan# : 18

BP : m/z 43 Int. : 1599.98 (16776960)

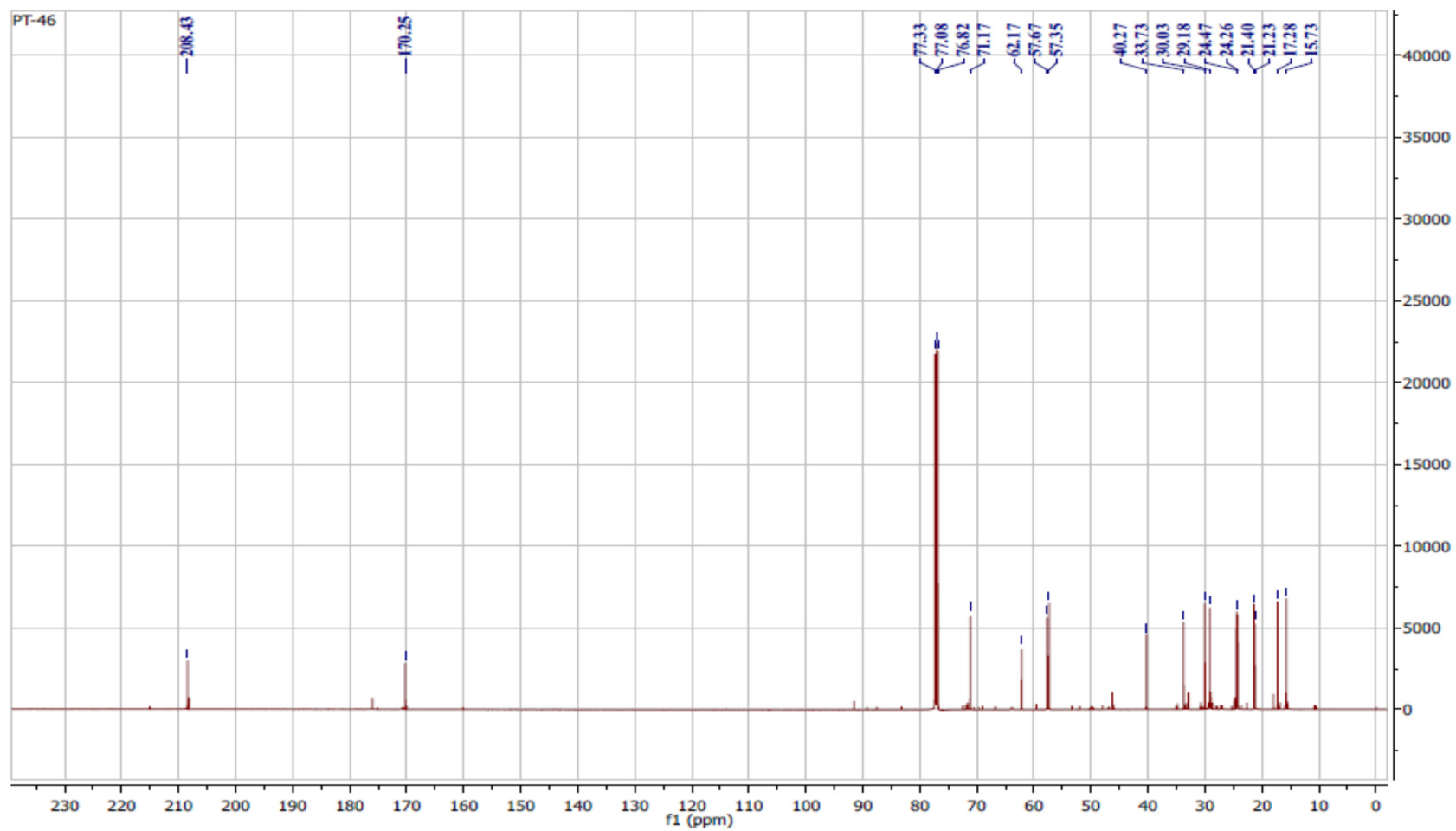
Output m/z range : 35 to 500 Cut Level : 0.00 %



S43: LRCIMS EI-MS of 11

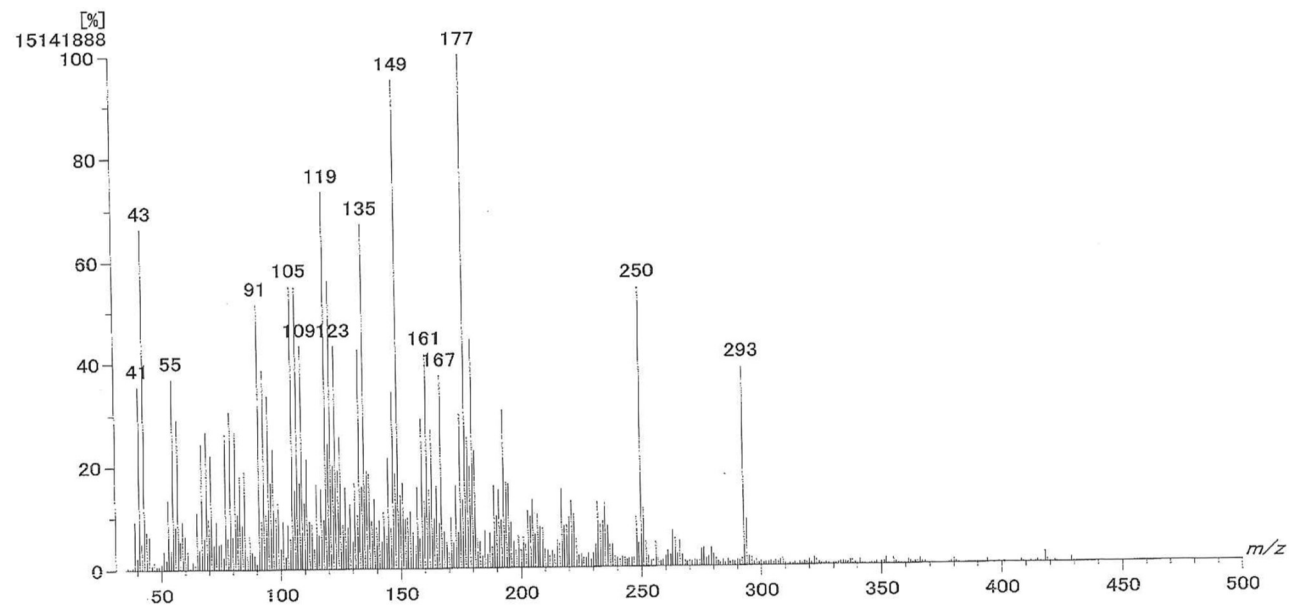


S44: ^1H -NMR of **11**

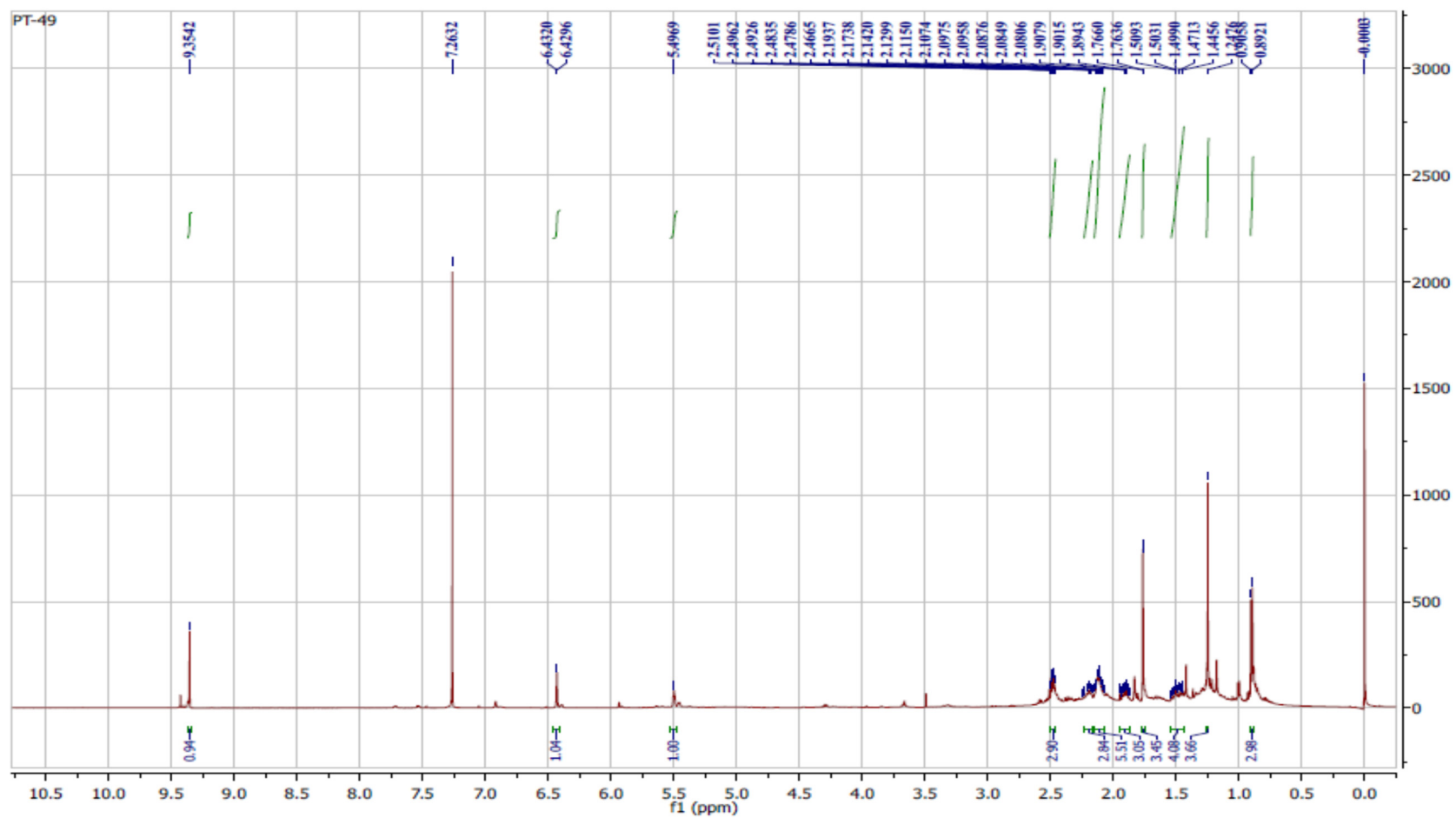


S45: ^{13}C -NMR of **11**

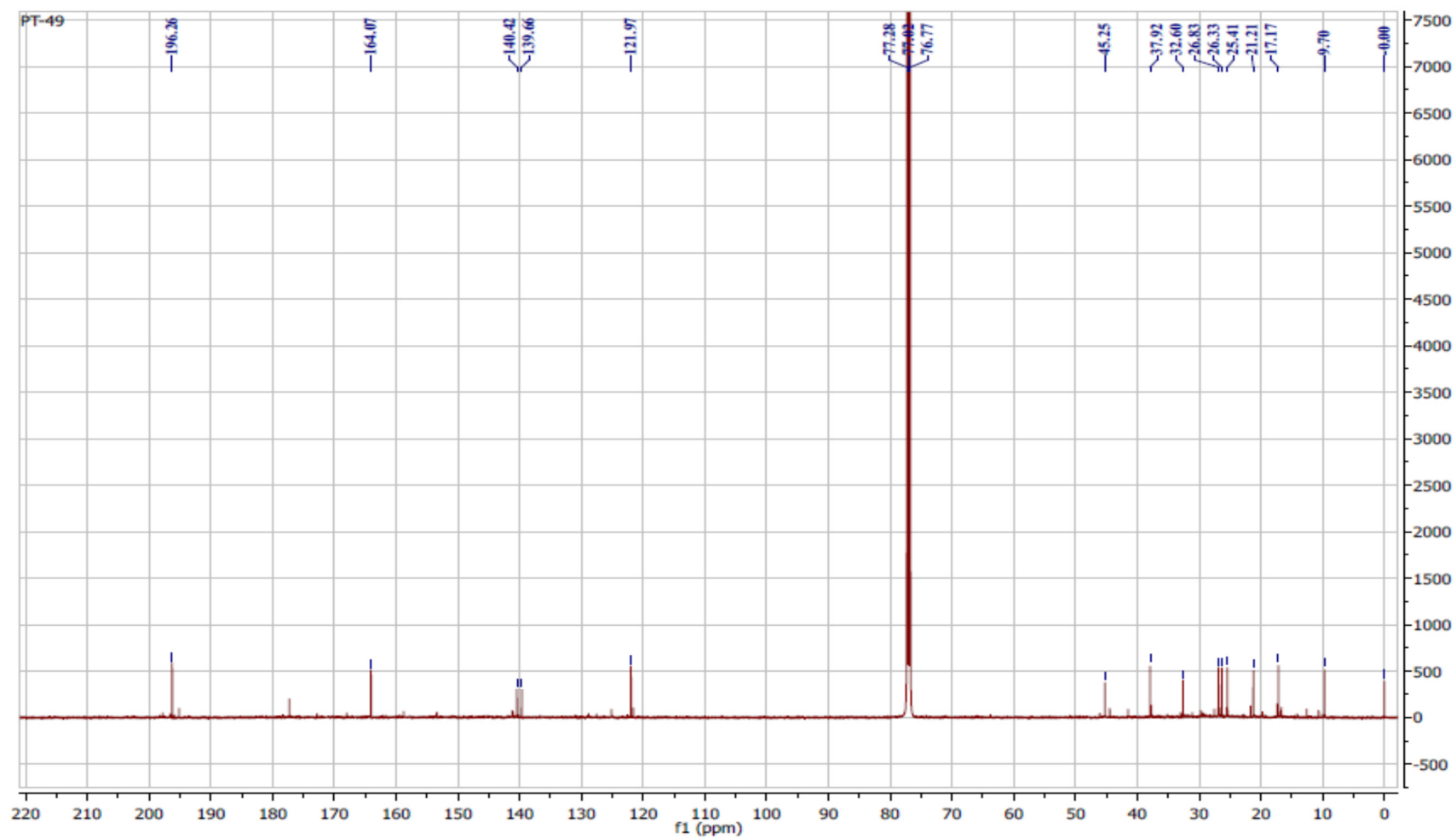
[Mass Spectrum]
Data : Umeyama-EI.17-Jul-2019.001 Date : 17-Jul-2019 10:25
Sample : PT-49
Note : MStation
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.67 min Scan# : 21
BP : m/z 177 Int. : 1444.04 (15141888)
Output m/z range : 35 to 500 Cut Level : 0.00 %



S46: LRCIMS EI-MS of 12



S47: ^1H -NMR of **12**



S48: ^{13}C -NMR of **12**