

Two novel oxetane containing lignans and a new megastigmane from *Paronychia*

arabica and *in silico* analysis as prospective SARS-CoV-2 Inhibitors

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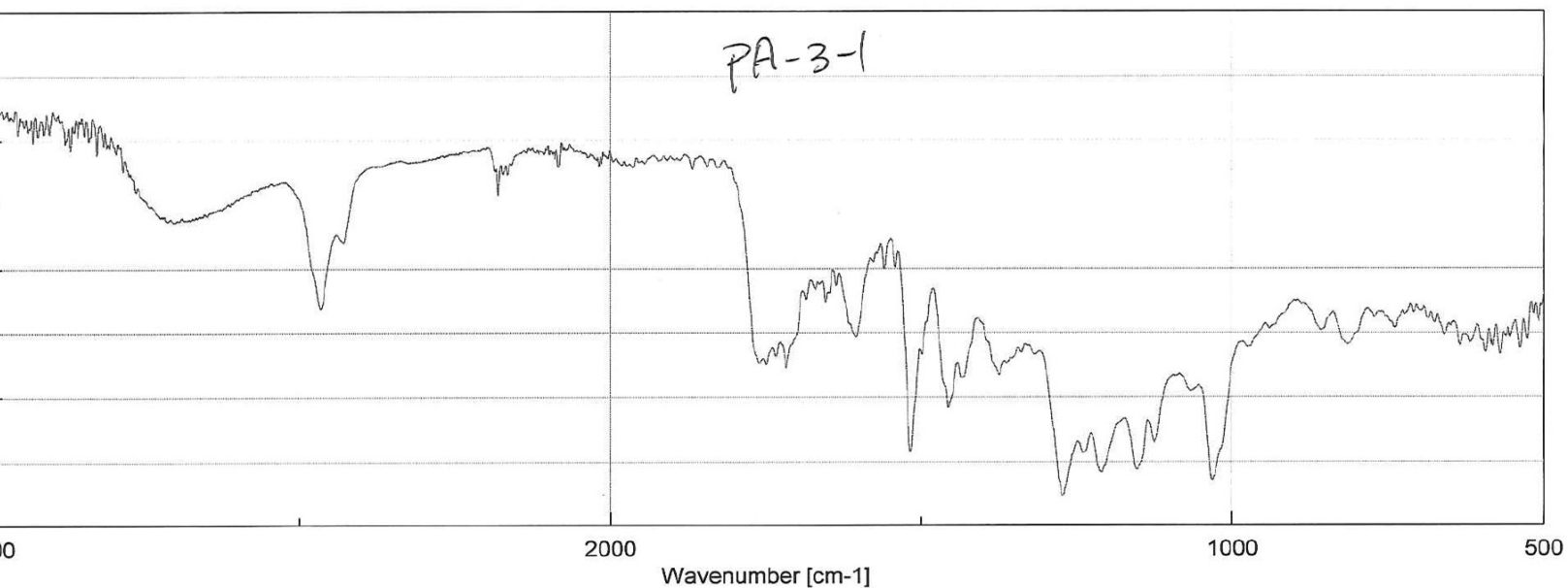
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^e Molecular Genetics and Genome Mapping Laboratory, Genome Mapping Department, Agricultural Genetic Engineering Research Institute (AGERI), Agriculture Research Center (ARC), Giza, 12619, Egypt

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Supporting data	Page
S1: FT-IR of 11	3
S2: TOF-ESI-MS of 1	4
S3: ¹ H NMR of compound 1 (500 Hz, MeOD).....	6
S4: ¹³ C NMR of compound 1 (125 Hz, MeOD)	7
S5: DEPT NMR of compound 1	8
S6: HSQC of compound 1	9
S7: HMBC NMR of compound 1	10
S8: ¹ H ¹ H COSY NMR of compound 1	11
S9: NOESY of compound 1	12
S10: FT-IR of 2	12
S11: CIMS of 2	13

S11: HRCIMS of 2	14
S12: ¹ H NMR of compound 2 (500 Hz, MeOD).....	15
S14: ¹³ H NMR of compound 2 (125 Hz, MeOD)	16
S15: DEPT NMR of compound 2	17
S16: HSQC of compound 2	18
S17: HMBC NMR of compound 2	19
S18: ¹ H ¹ H COSY NMR of compound 2	20
S19: NOESY of compound 2	21
S20: FT-IR of 3	22
S21: FAB-ESIMS of 3	23
S22 HRFAB-ESIMS of 3	24
S23: ¹ H NMR of compound 3 (500 Hz, MeOD).....	25
S24: ¹³ H NMR of compound 3 (125 Hz, MeOD)	26
S25: DEPT NMR of compound 3	27
S26: HSQC of compound 3	28
S27: HMBC NMR of compound 3	29
S28: ¹ H ¹ H COSY NMR of compound 3	30
S29: NOESY of compound 3	31



[測定情報]

機種名 FT/IR-4200typeA
シリアル番号 C094361018

Memory-3

付属品名 ATR PRO470-H
付属品シリアルNo. A012061293
入射角 45 度

測定日時 2019/03/27 11:32

光源 標準光源
検出器 TGS
積算回数 64
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (16)
アパーチャー Auto (7.1 mm)

徳島文理大学

2019/03/27 11:33

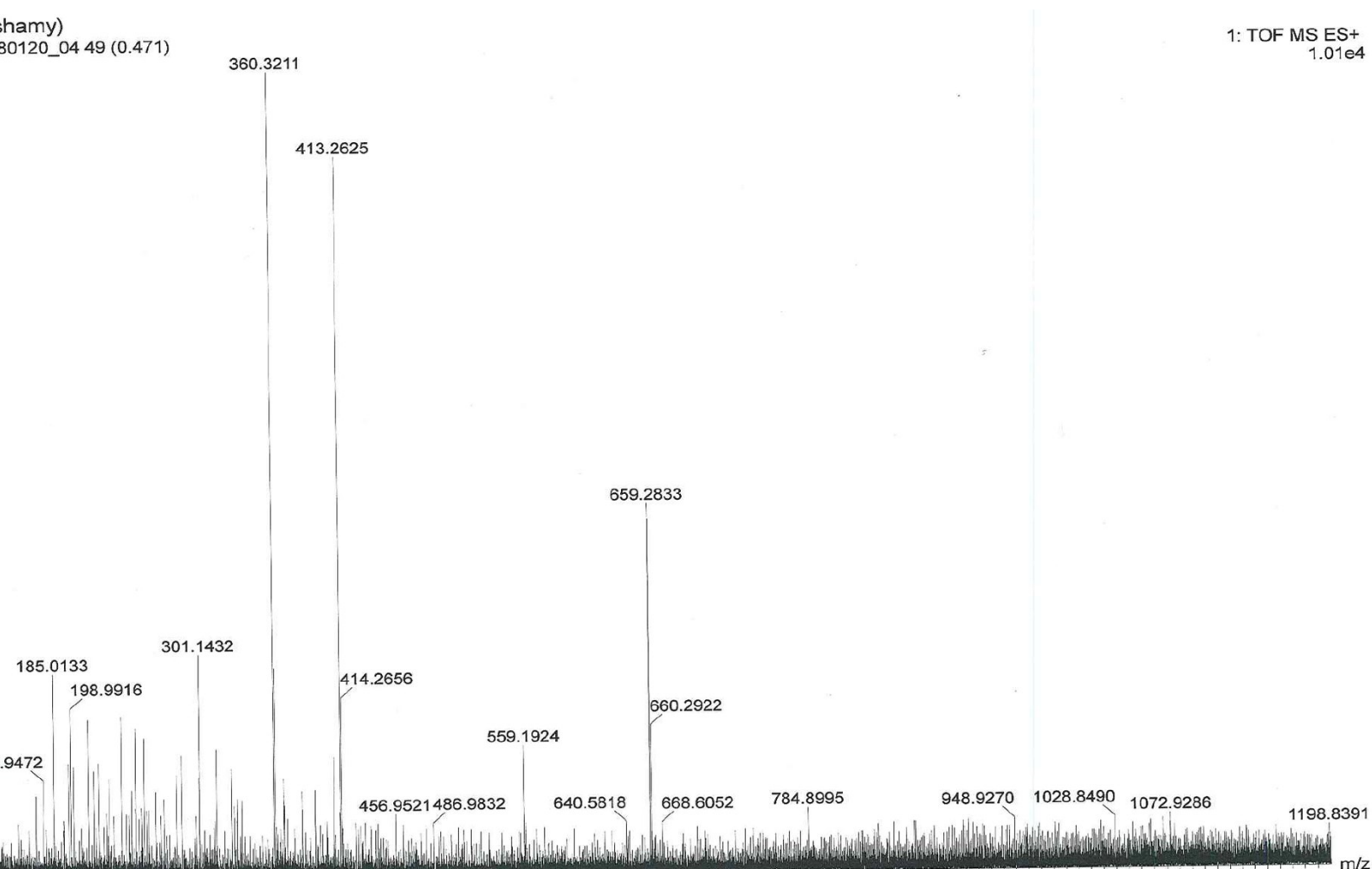
等間隔データ
Wavenumber [cm-1]

%T
499.473 cm-1
4000.6 cm-1
0.964233 cm-1

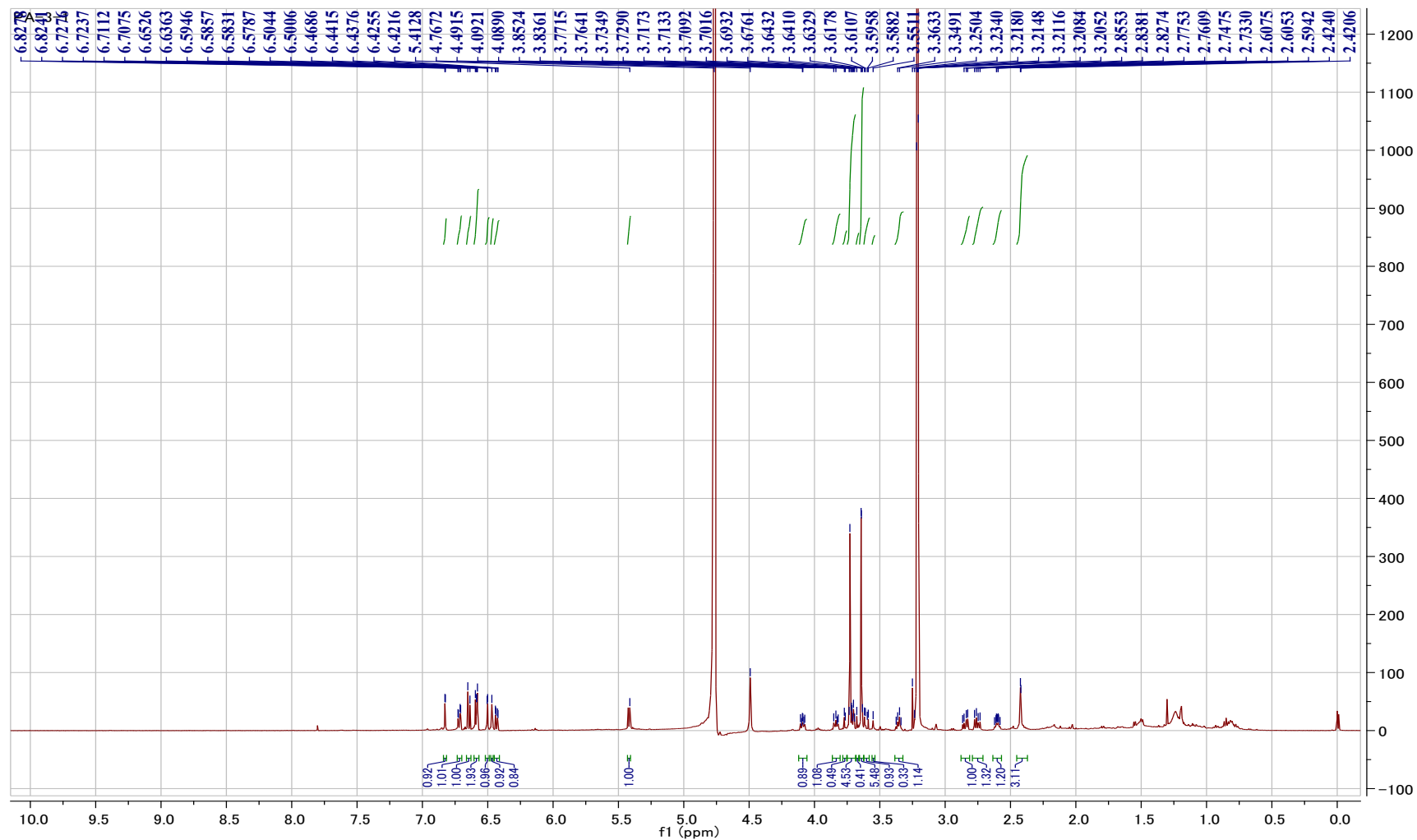
S1: FT-IR of 1

shamy)
80120_04 49 (0.471)

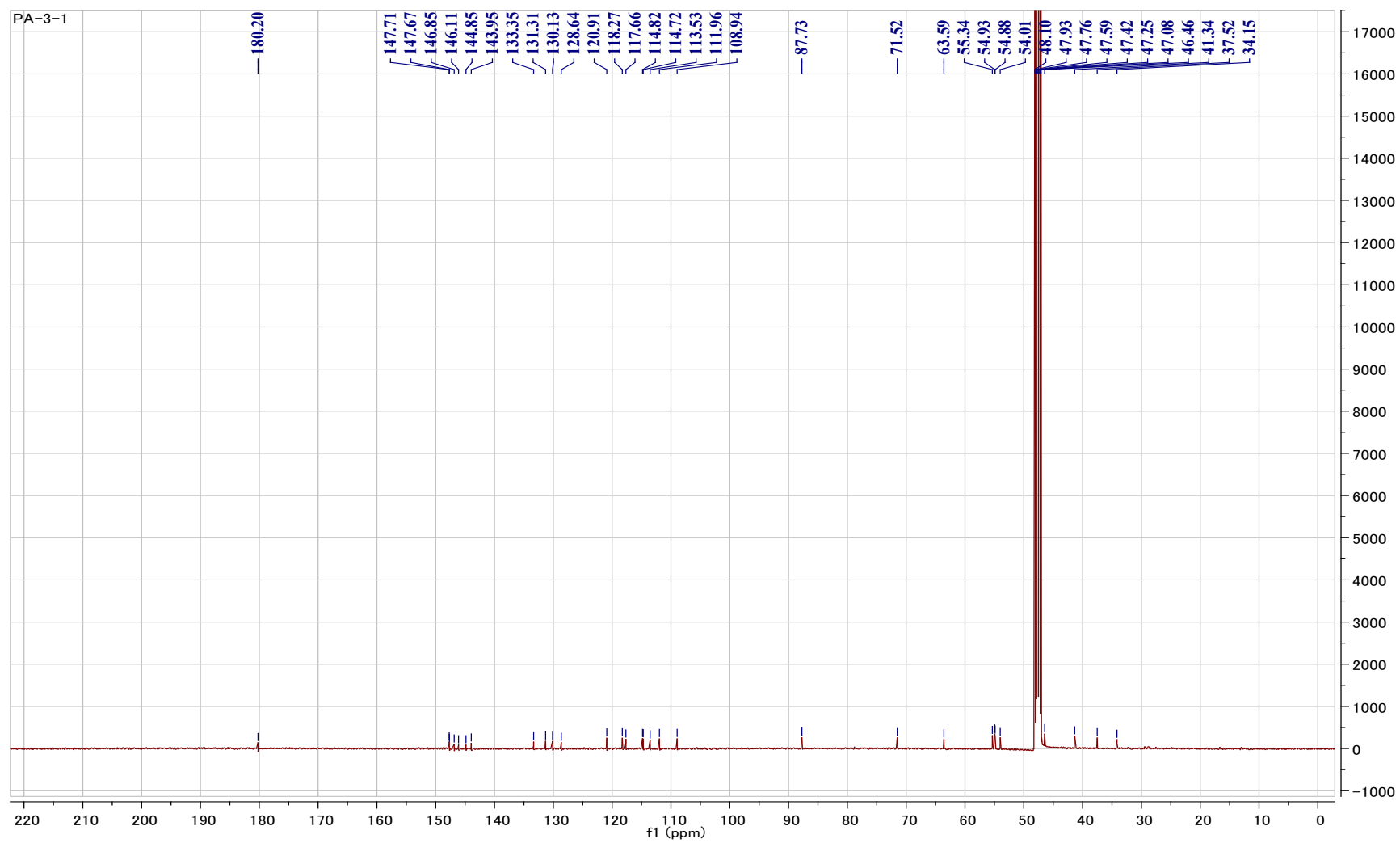
1: TOF MS ES+
1.01e4



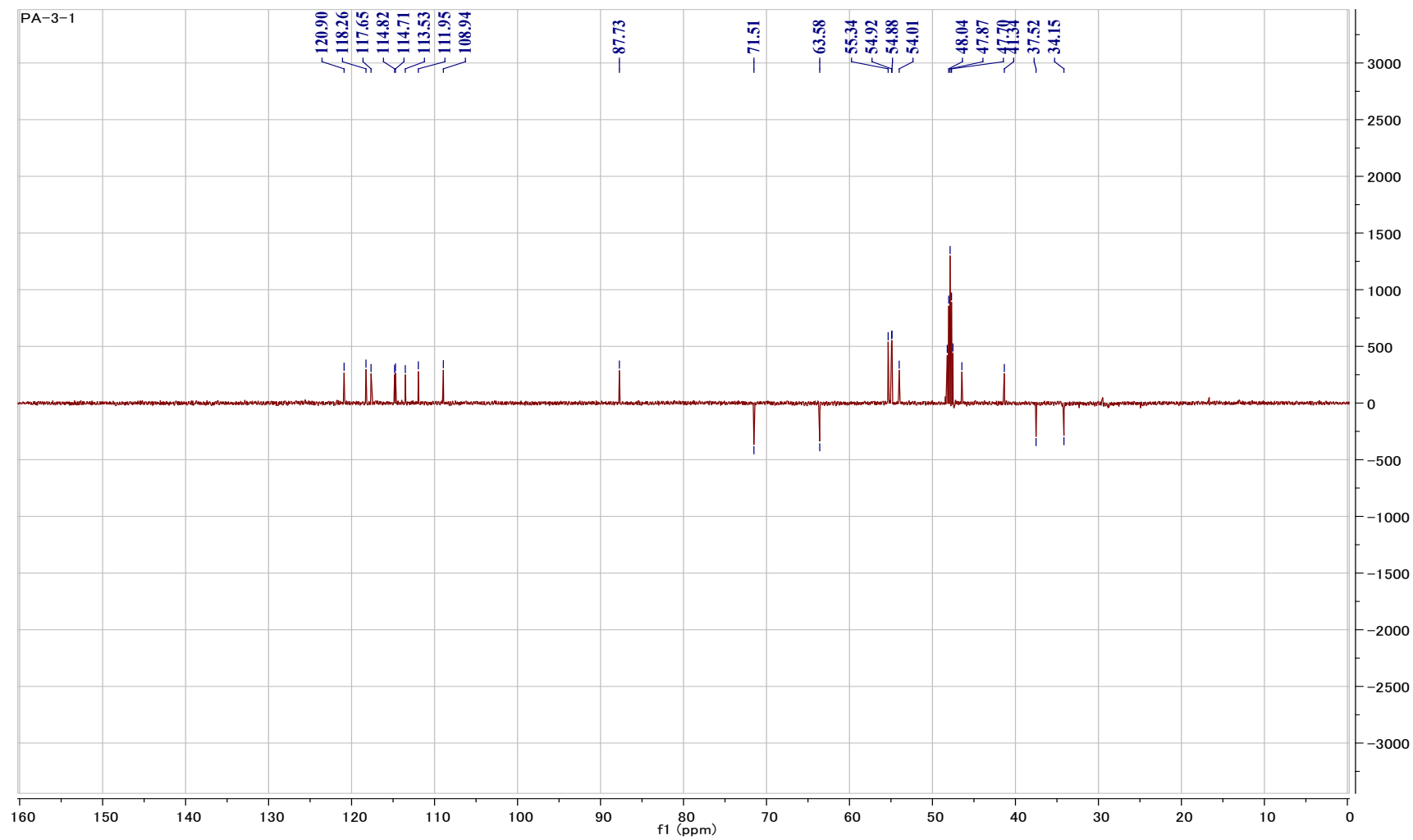
S2: TOF-ESI-MS of 1



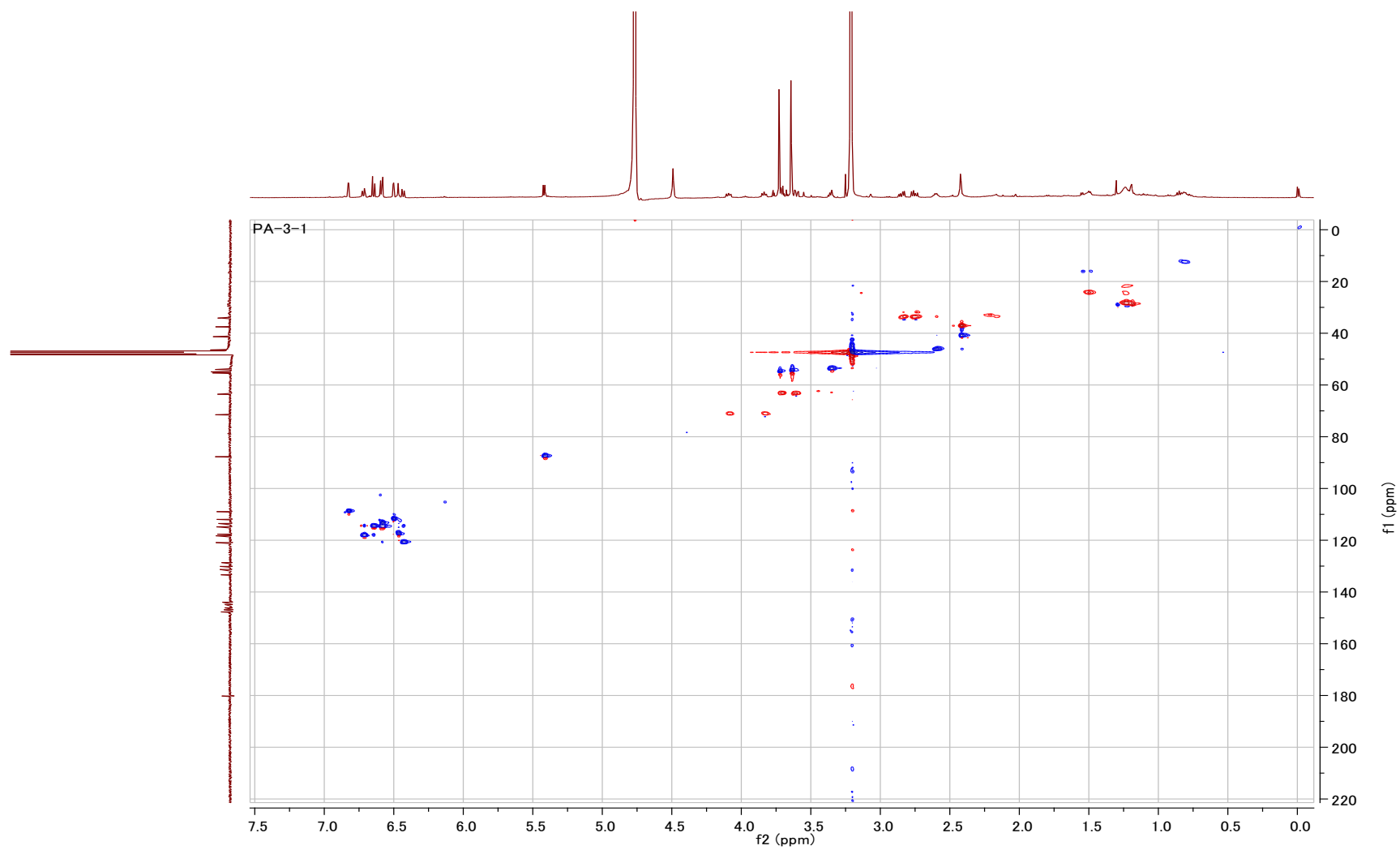
S3: ^1H NMR of **1** (500 Hz, MeOD)



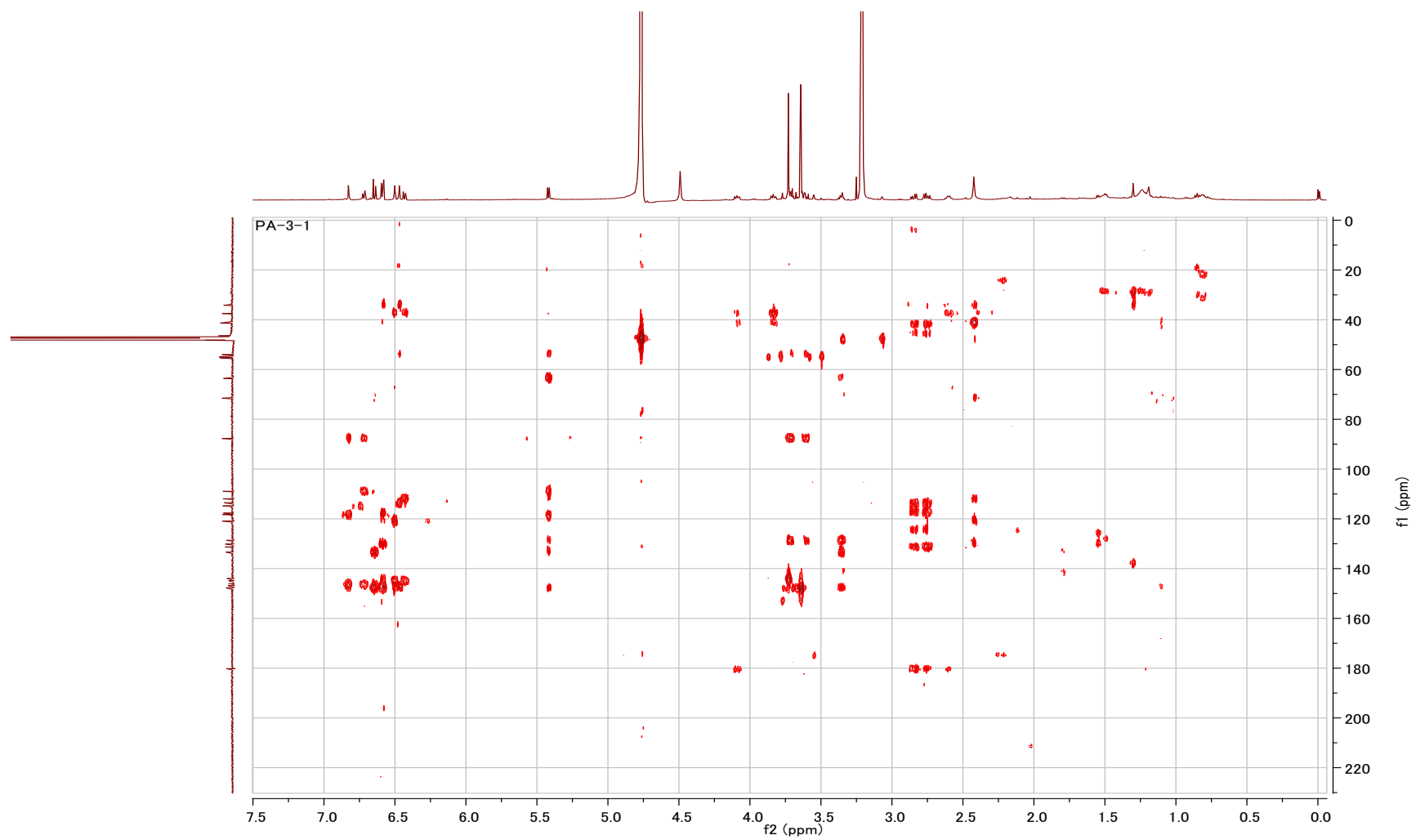
S4: ^{13}C NMR of **1** (125 Hz, MeOD)



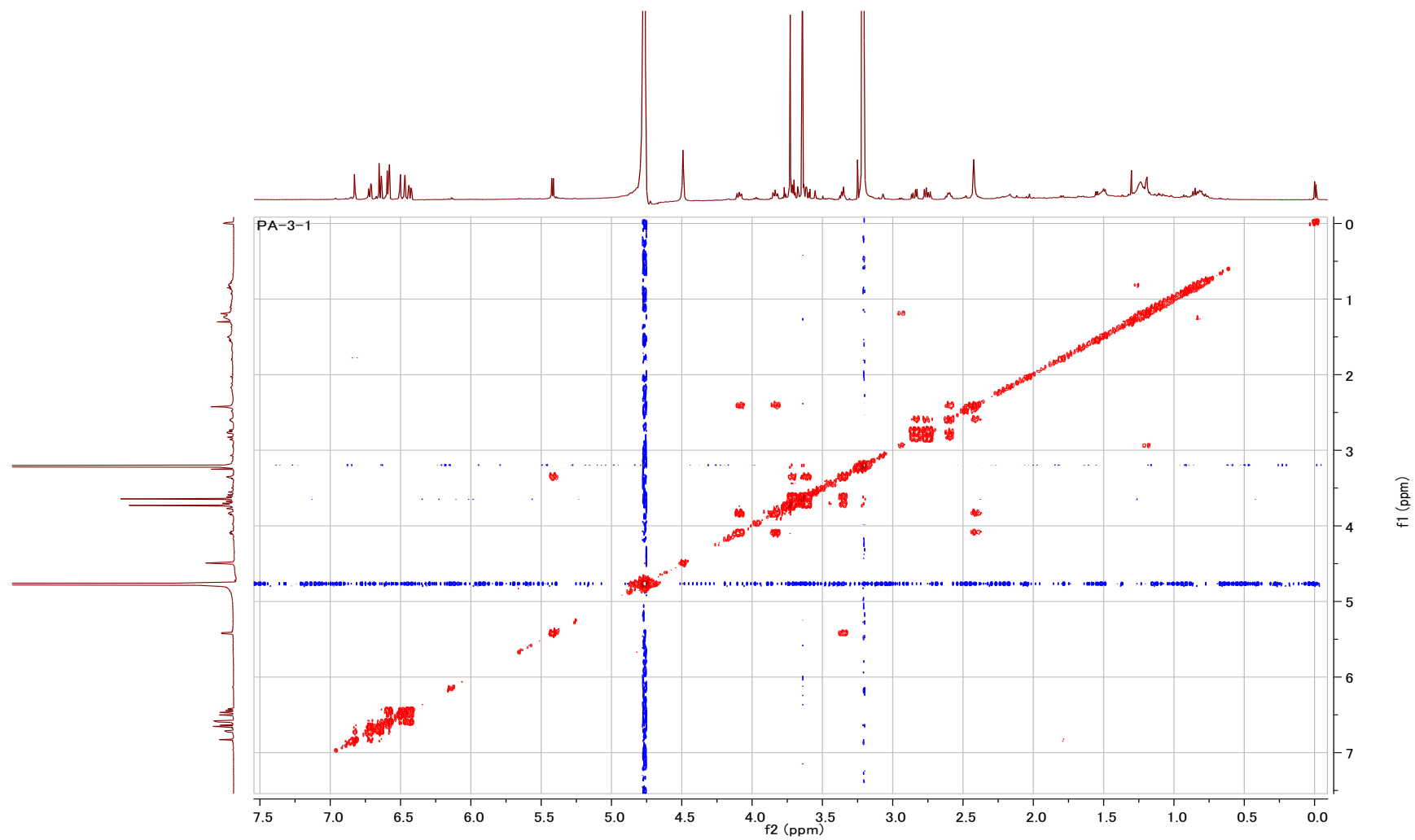
S5: DEPT-135 of 1



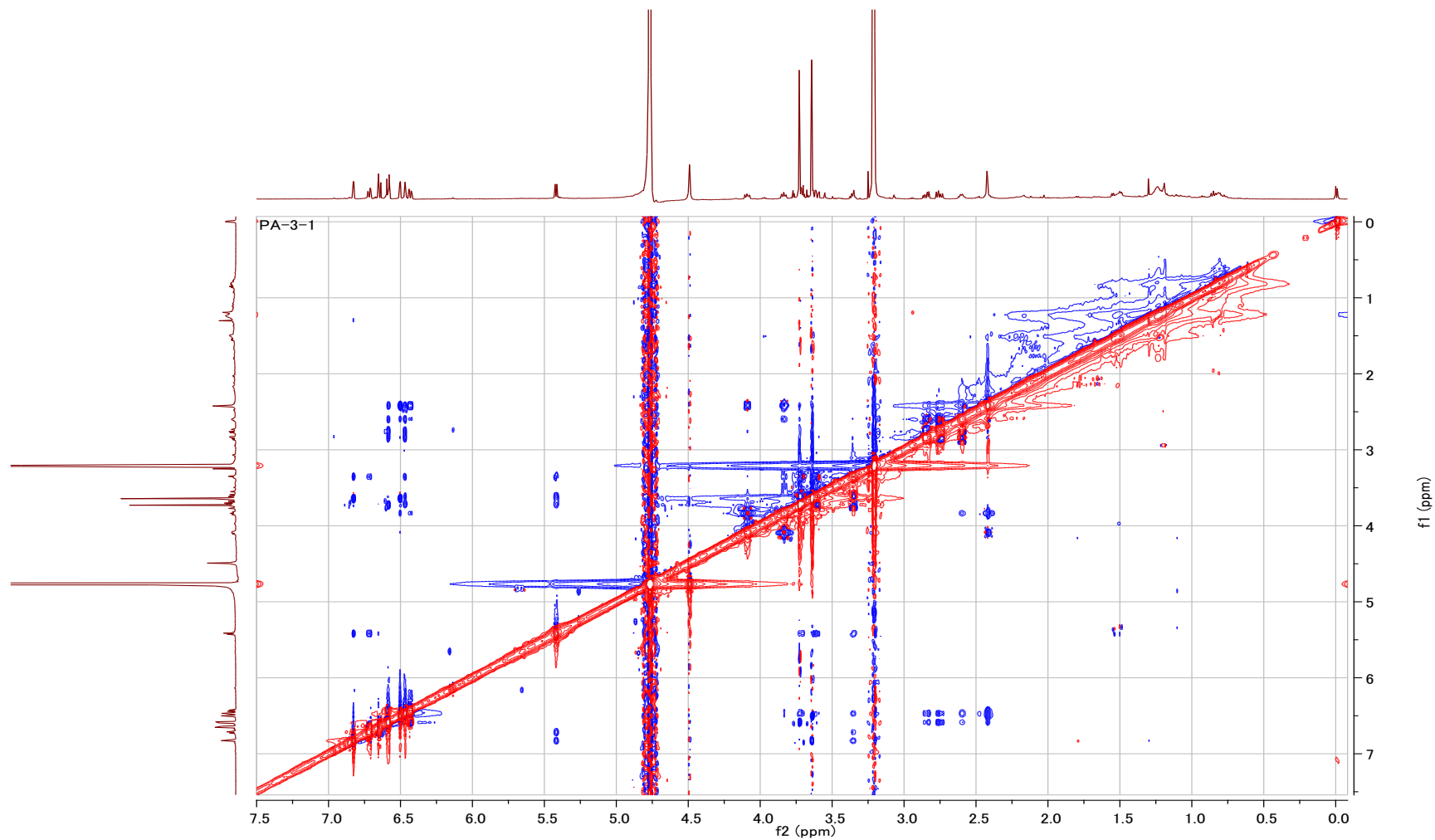
S6: HSQC of 1



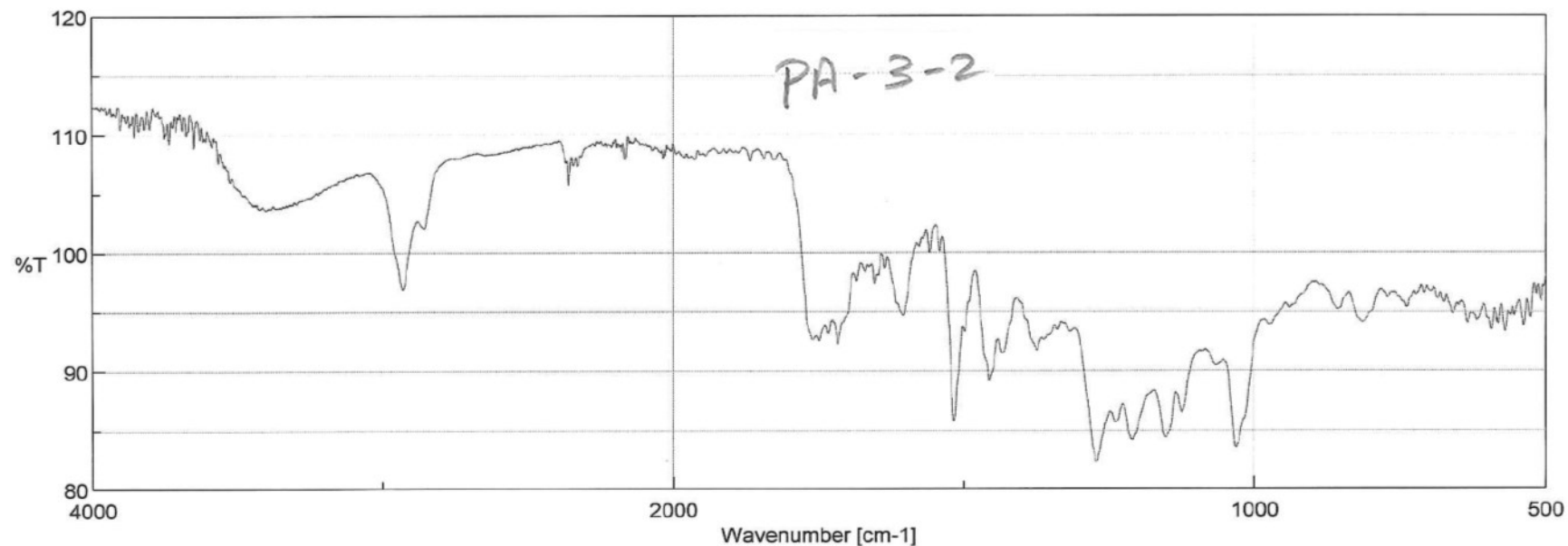
S7: HMBC of **1**



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



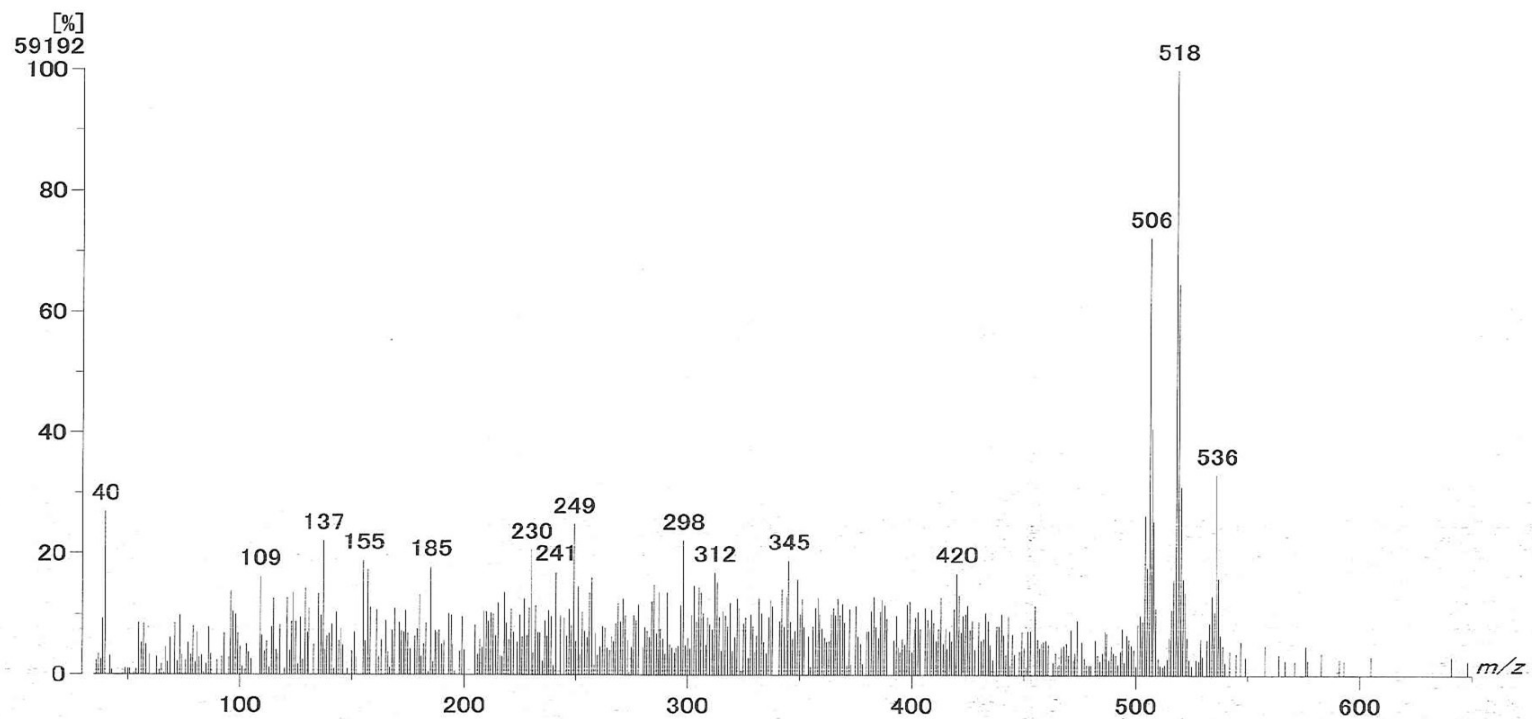
S9: NOESY of 1



[コメント情報]		[測定情報]		Memory-3
試料名		機種名	FT/IR-4200typeA	
コメント		シリアル番号	C094361018	
測定者		付属品名	ATR PRO470-H	
所属		付属品シリアルNo.	A012061293	
会社	徳島文理大学	入射角	45 度	
[データ情報]		測定日時	2019/03/27 11:32	
作成日時	2019/03/27 11:33	光源	標準光源	
データタイプ	等間隔データ	検出器	TGS	
		積算回数	64	
横軸	Wavenumber [cm-1]	分解	4 cm-1	
縦軸	%T	ゼロフィリング	On	
スタート	499.473 cm-1	アポダイゼーション	Cosine	
エンド	4000.6 cm-1	ゲイン	Auto (16)	
データ間隔	0.964233 cm-1	アパーチャー	Auto (7.1 mm)	
データ数	3632	スキャンスピード	Auto (2 mm/sec)	
		フィルタ	Auto (30000 Hz)	

S10: FTIR of 2

um]
na-CI.18-Mar-2019.005 Date : 18-Mar-2019 17:26
-2(CH4)
on
Ion Mode : CI+
e : Normal Ion [MF-Linear]
Scan# : (97,99)-k(16)[k=1.0]
Int. : 5.64 (59192)
nge : 35 to 650 Cut Level : 0.00 %



S11: CIMS of 2

Data : Umeyama-CIHR.18-Mar-2019.004

Date : 18-Mar-2019 18:04

Instrument : MStation

Sample : PA-3-2

Note : MStation

Inlet : Direct Ion Mode : CI+

RT : 2.65 min Scan# : 70

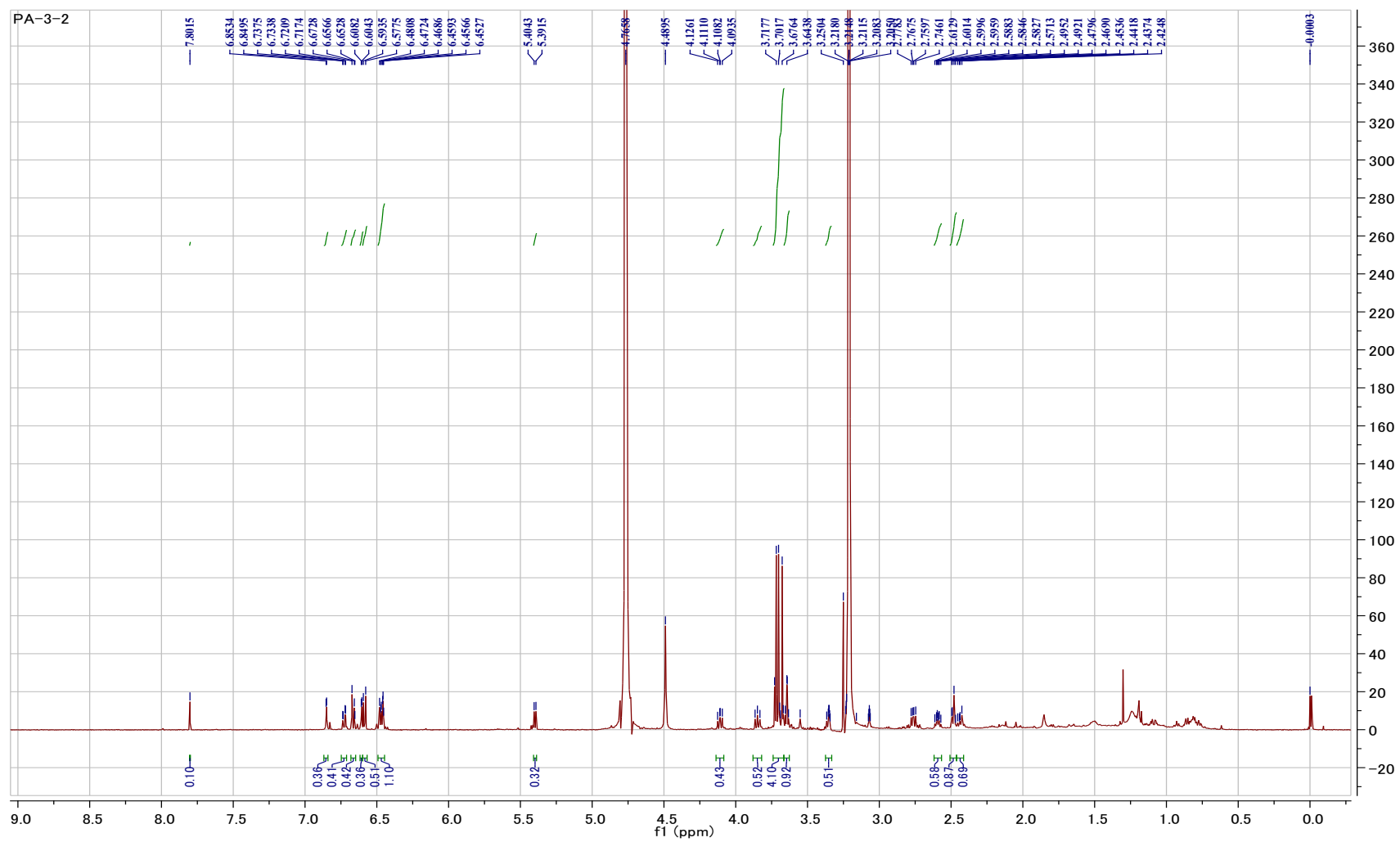
Elements : C 150/0, H 250/0, O 50/0

Mass Tolerance : 5mmu

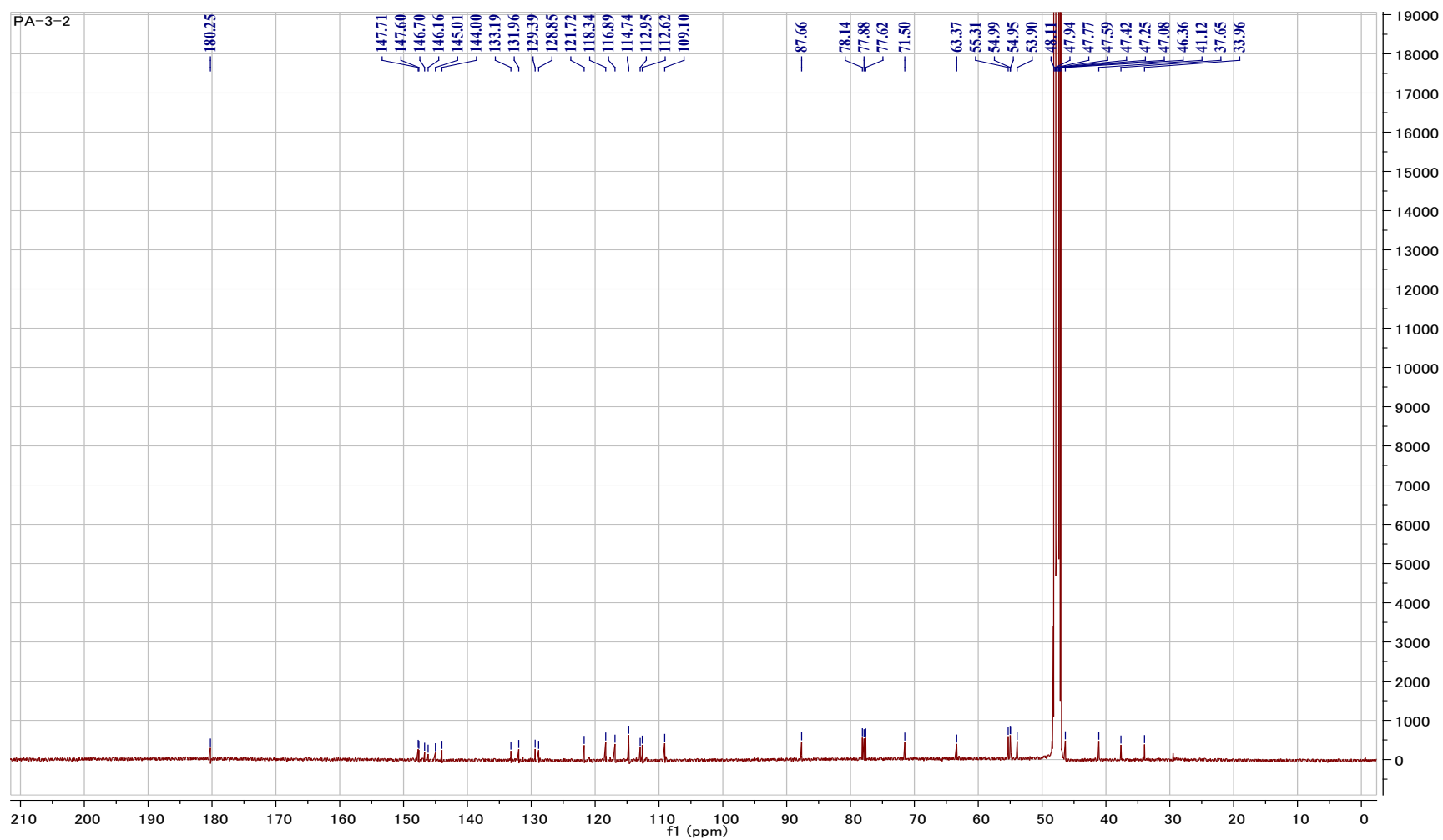
Unsaturation (U.S.) : 0.0 - 20.0

	Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
1	536.2030	3.05	-3.0 / -1.6	15.0 C30 H32 O9

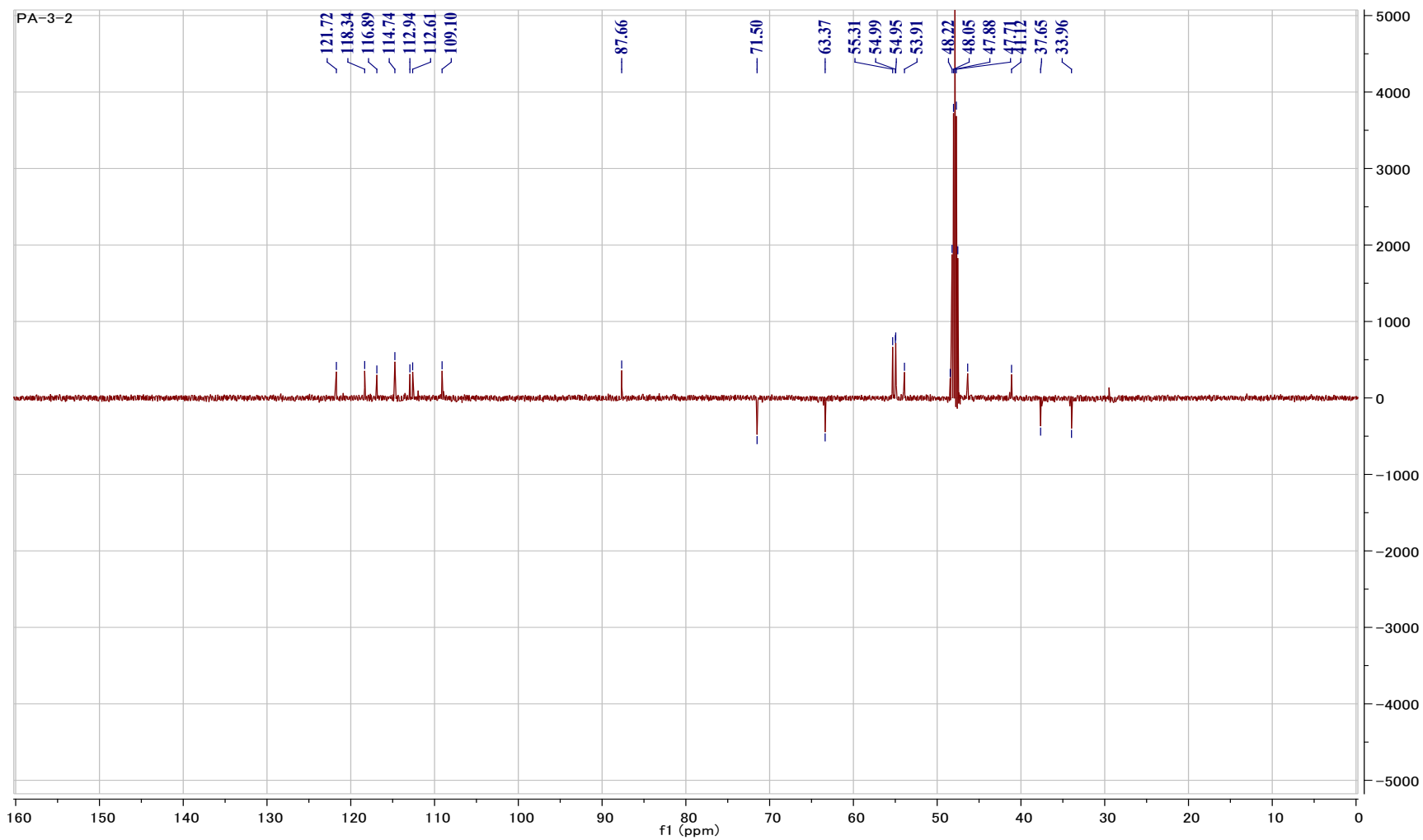
S12: HRCIMS of 2



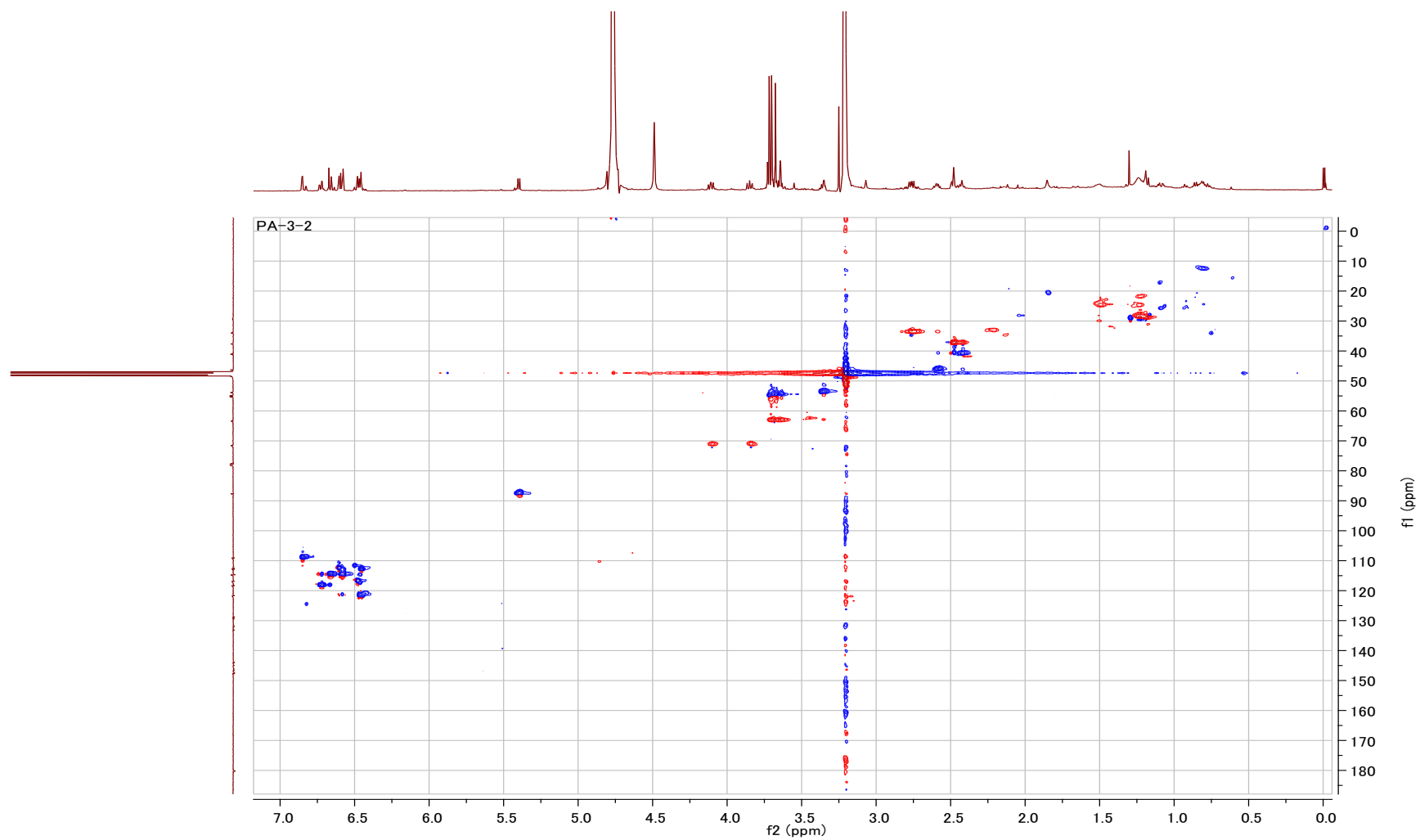
S13: ^1H NMR of **2** (500 Hz, MeOD)



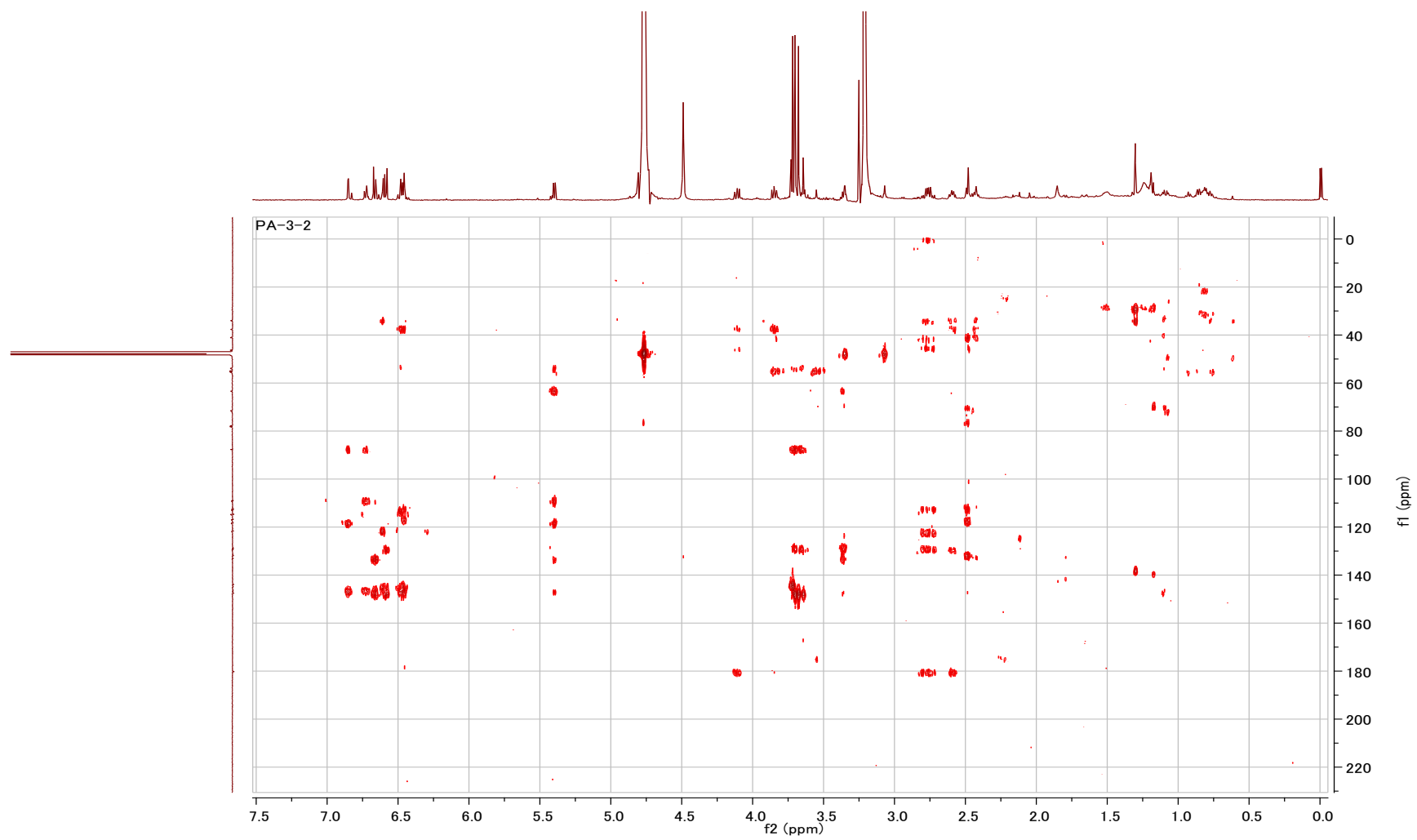
S14: ^{13}C NMR of **2** (125 Hz, MeOD)



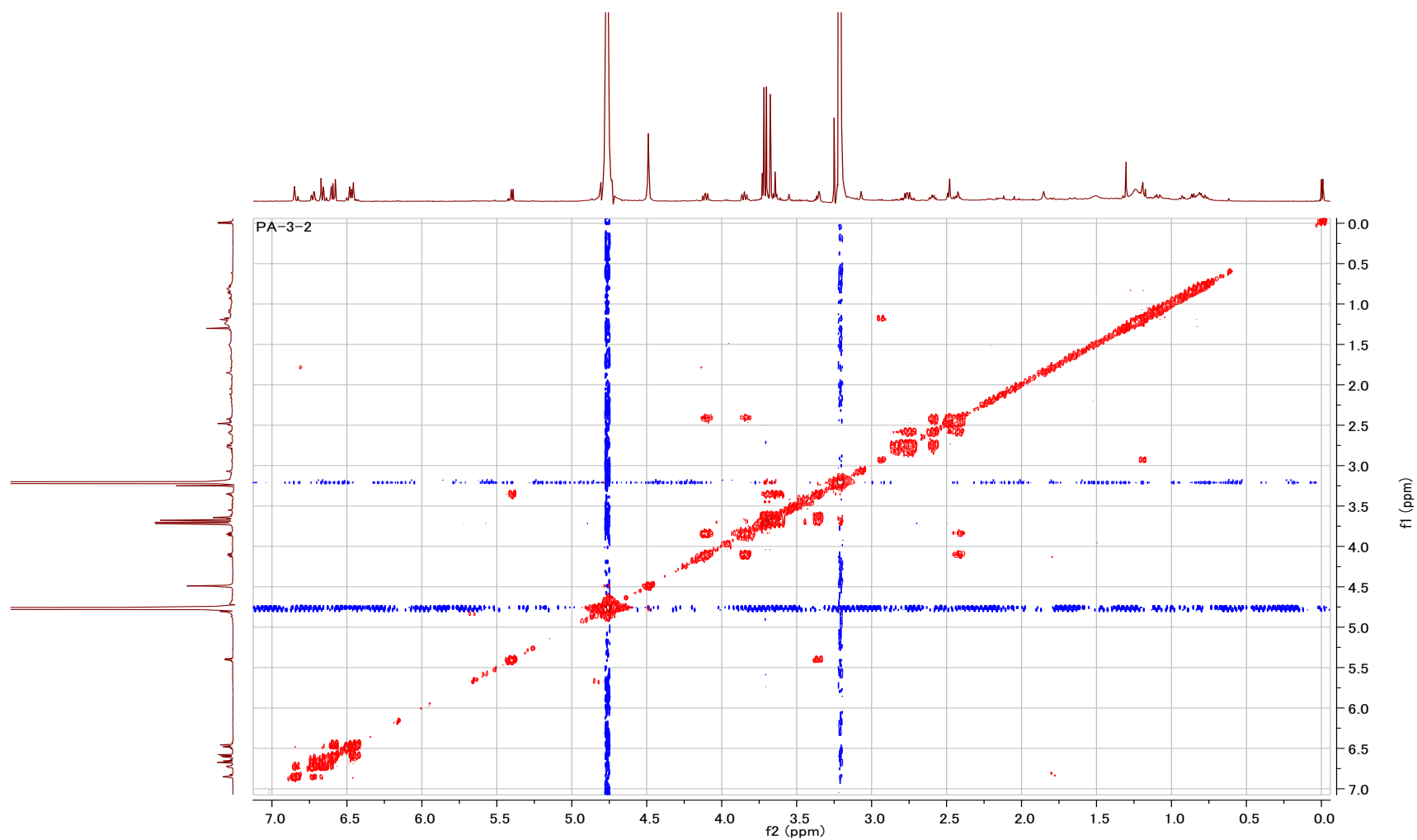
S15: DEPT-135 of **2**



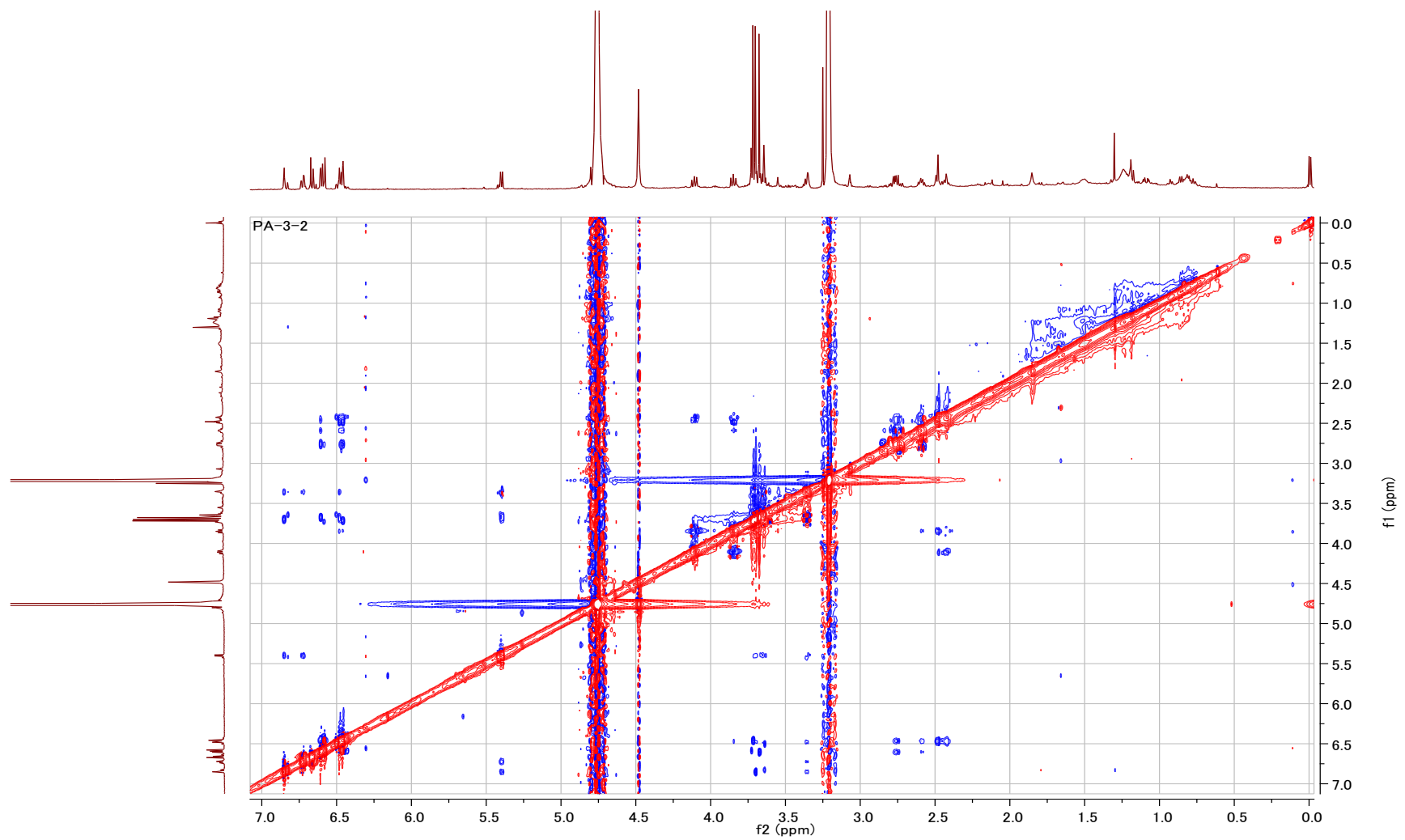
S16: HSQC of **2**



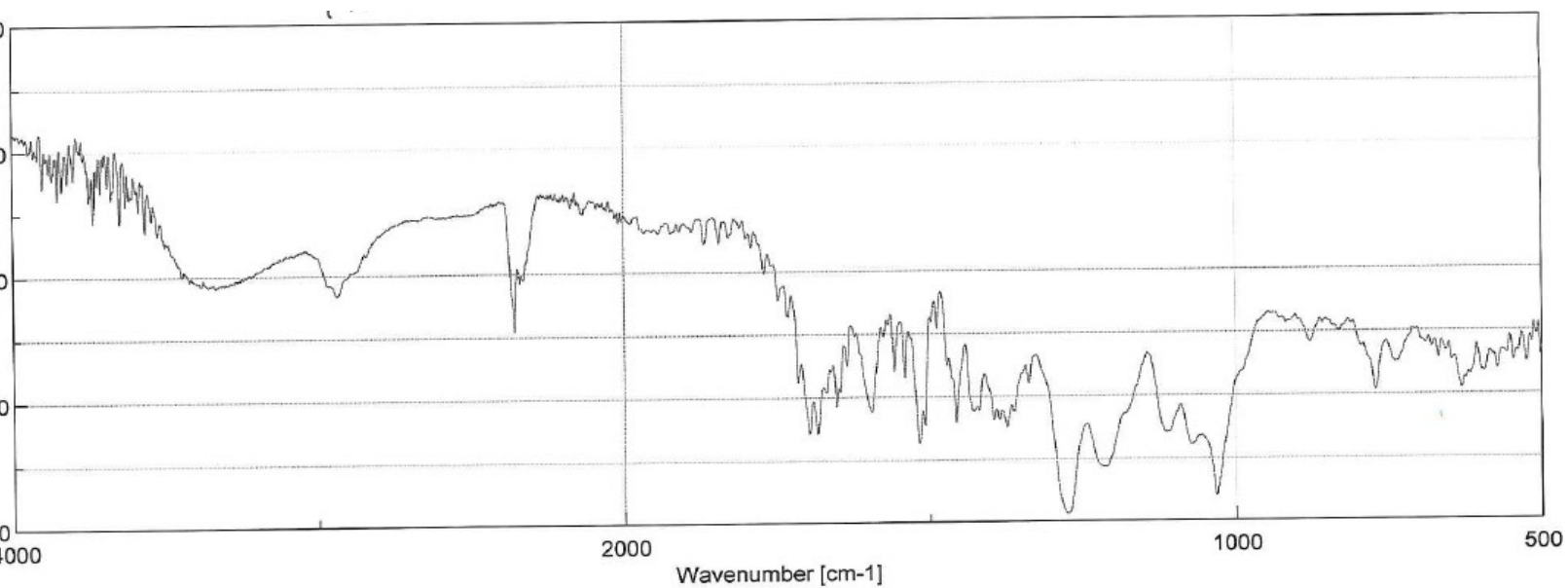
S17: HMBC of 2



S18: ^1H - ^1H COSY of 2



S19: NOESY of **2**



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2019/03/27 11:53
等間隔データ
Wavenumber [cm-1]
%T
499.473 cm-1
4000.6 cm-1
0.964233 cm-1

[測定情報]

機種名 FT/IR-4200typeA
シリアル番号 C094361018

付属品名 ATR PRO470-H
付属品シリアルNo. A012061293
入射角 45 度

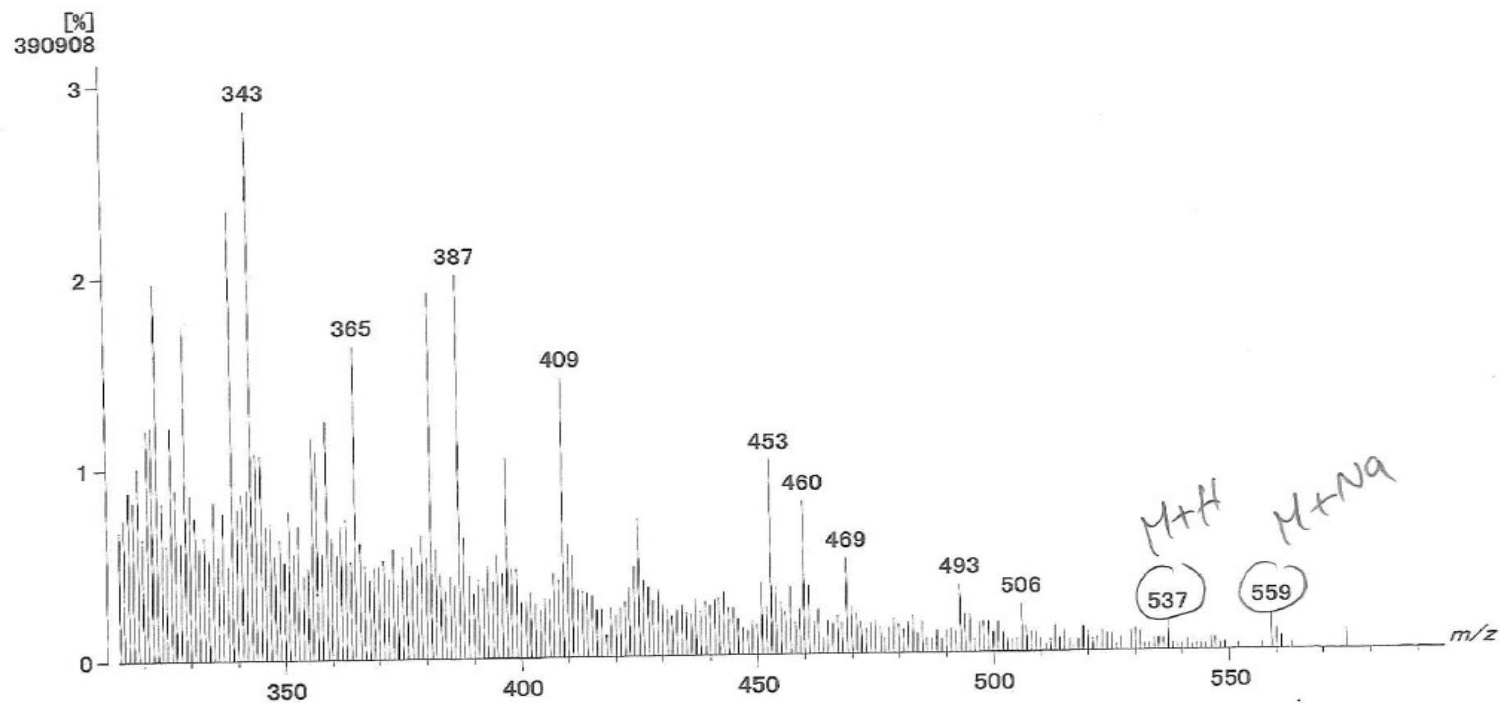
測定日時 2019/03/27 11:53

光源 標準光源
検出器 TGS
積算回数 64
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (16)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)

Memory-1

S20: FT-IR of 3

rum]
ma-FAB.12-Dec-2017.001 Date : 12-Dec-2017 10:35
-1-83-4/m-NBA
ion
Ion Mode : FAB+
pe : Normal Ion [MF-Linear]
Scan# : (2,6)
Int. : 1194.87 (12529100)
range : 315 to 596 Cut Level : 0.00 %

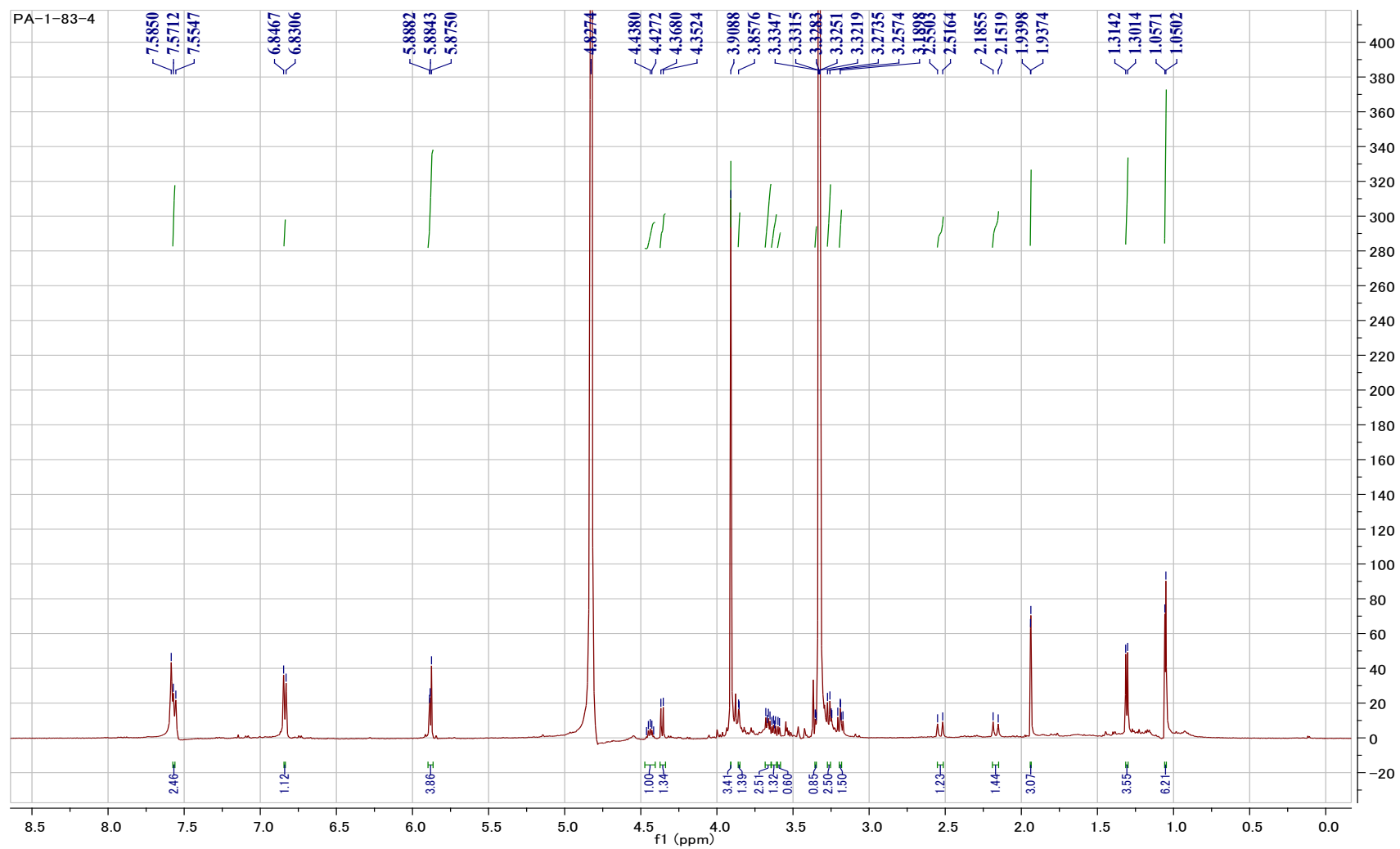


S21: FAB-ESIMS of 3

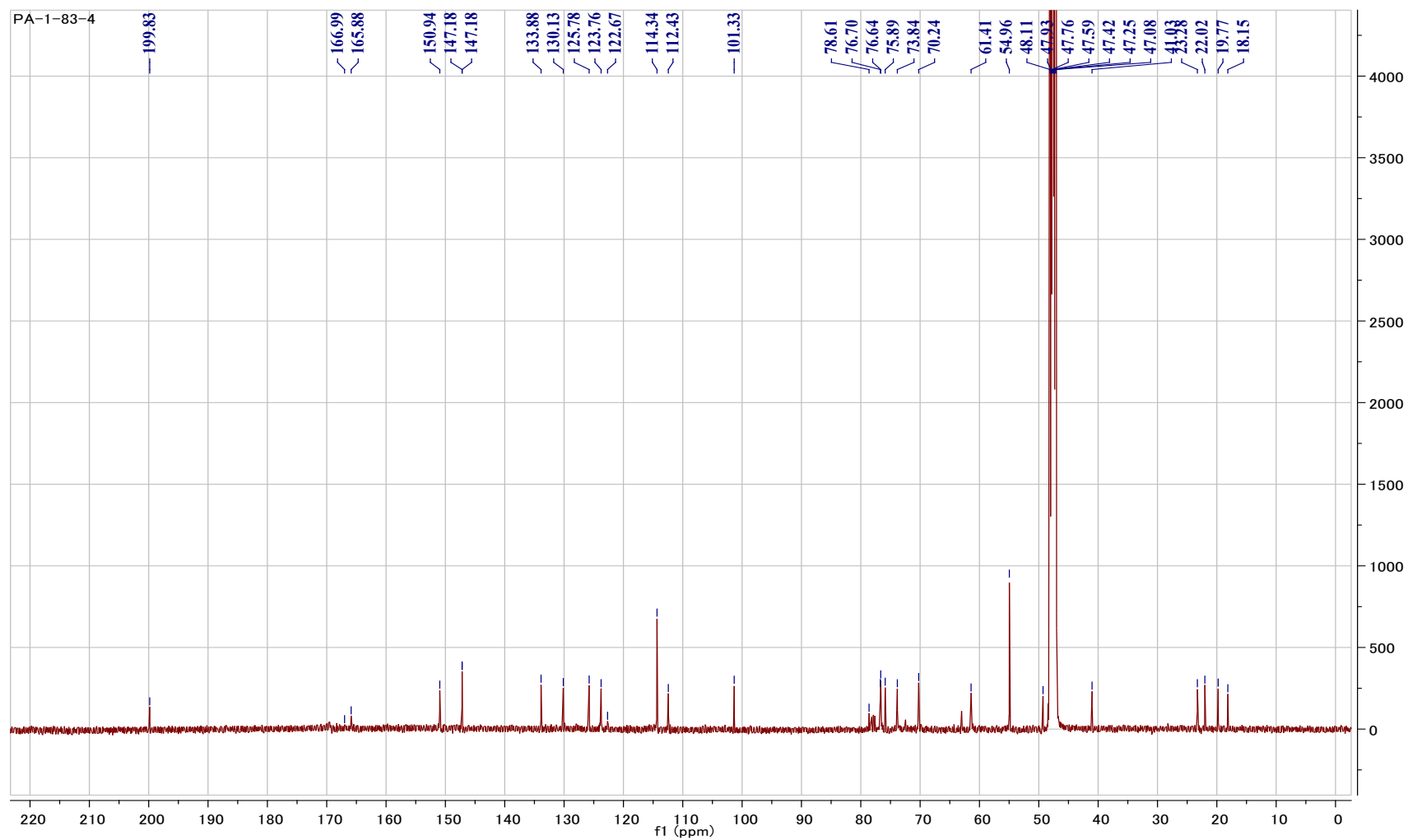
Data : Umeyama-FABHR.26-Mar-2019.002 Date : 26-Mar-2019 08:46
Instrument : MS700D
Sample : PA-1-83-4
Note : MStation
Inlet : Direct Ion Mode : FAB+
RT : 11.83 min Scan# : 44
Elements : C 150/0, H 250/0, O 50/0, Na 1/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : 0.0 - 15.0

	Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
1	559.2157	7.12	-4.0 / -2.2	12.5	C29 H35 O11
2			+0.3 / +0.2	9.5	C27 H36 O11 Na

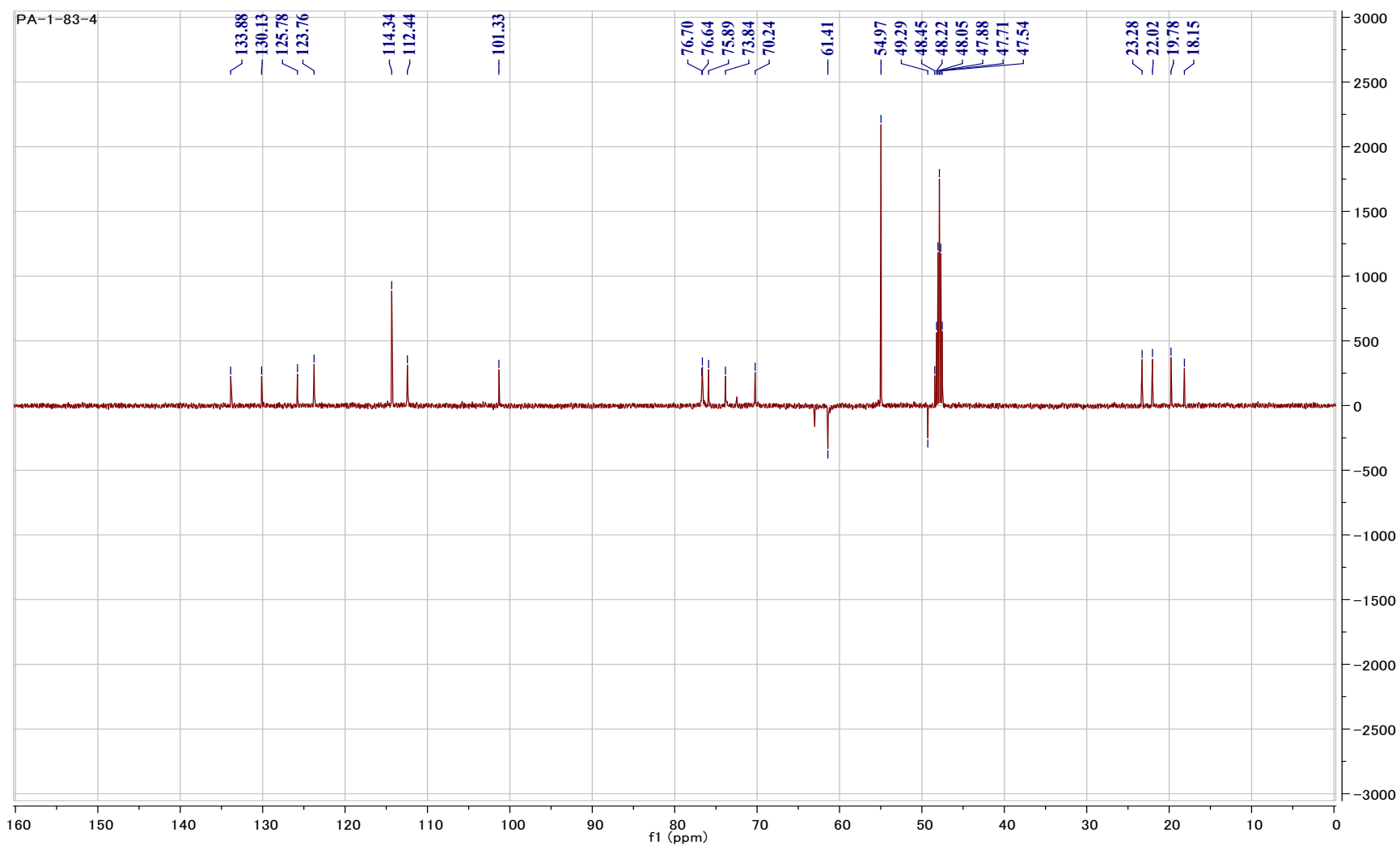
S22: HRFAB-ESIMS of 3



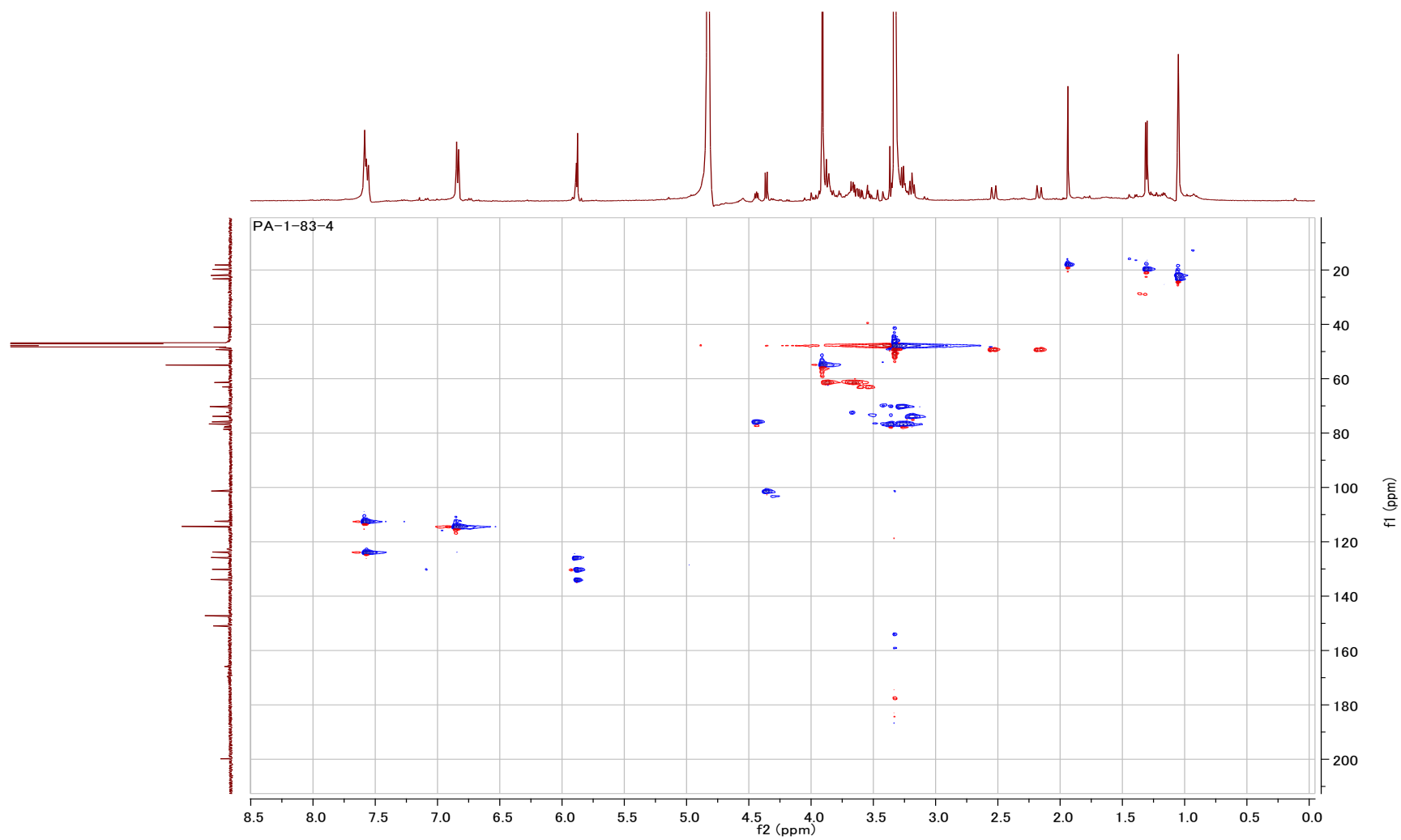
S23: ^1H NMR of **3** (500 Hz, MeOD)



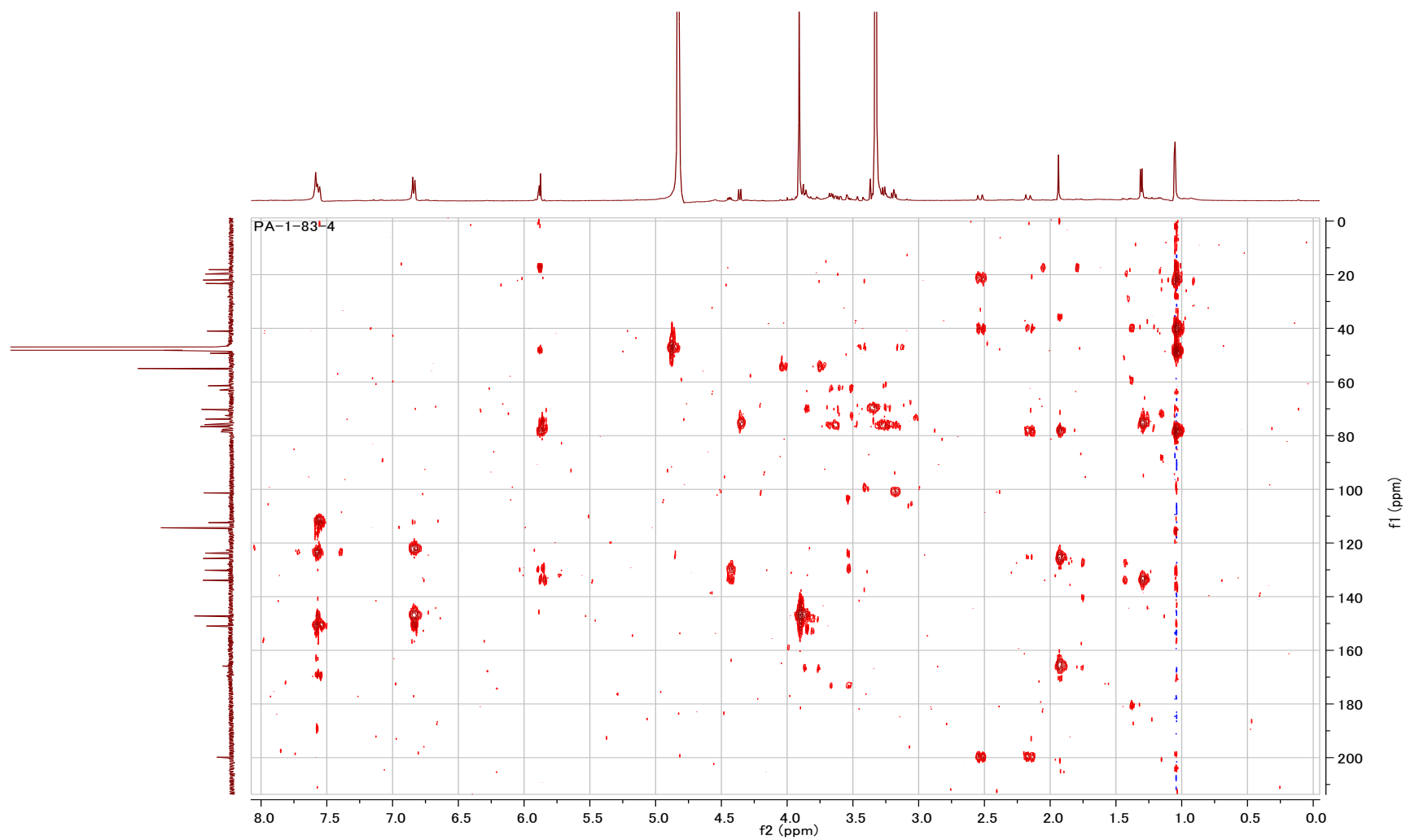
S24: ^{13}C NMR of **3** (125 Hz, MeOD)



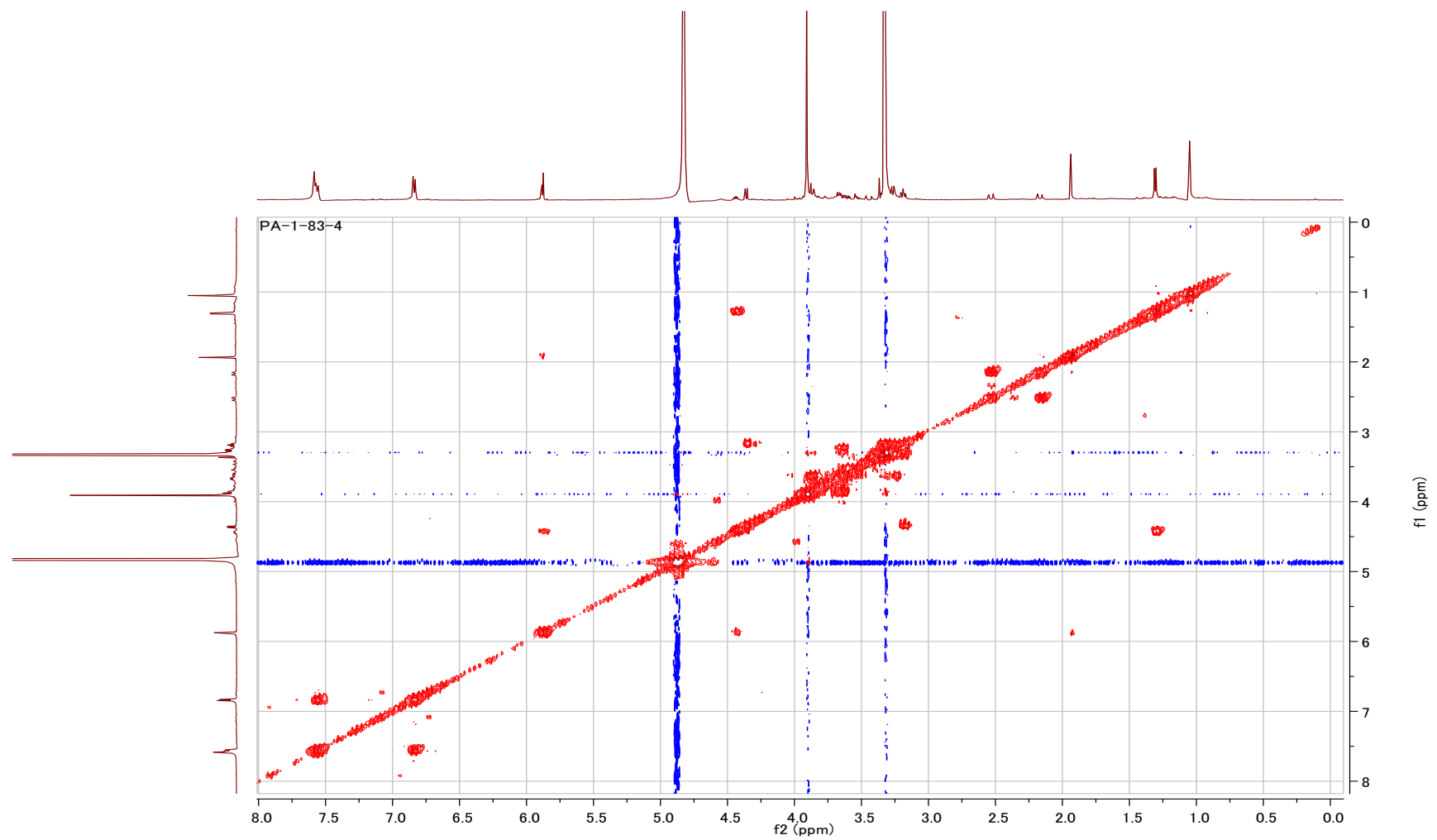
S25: DEPT-135 of **3**



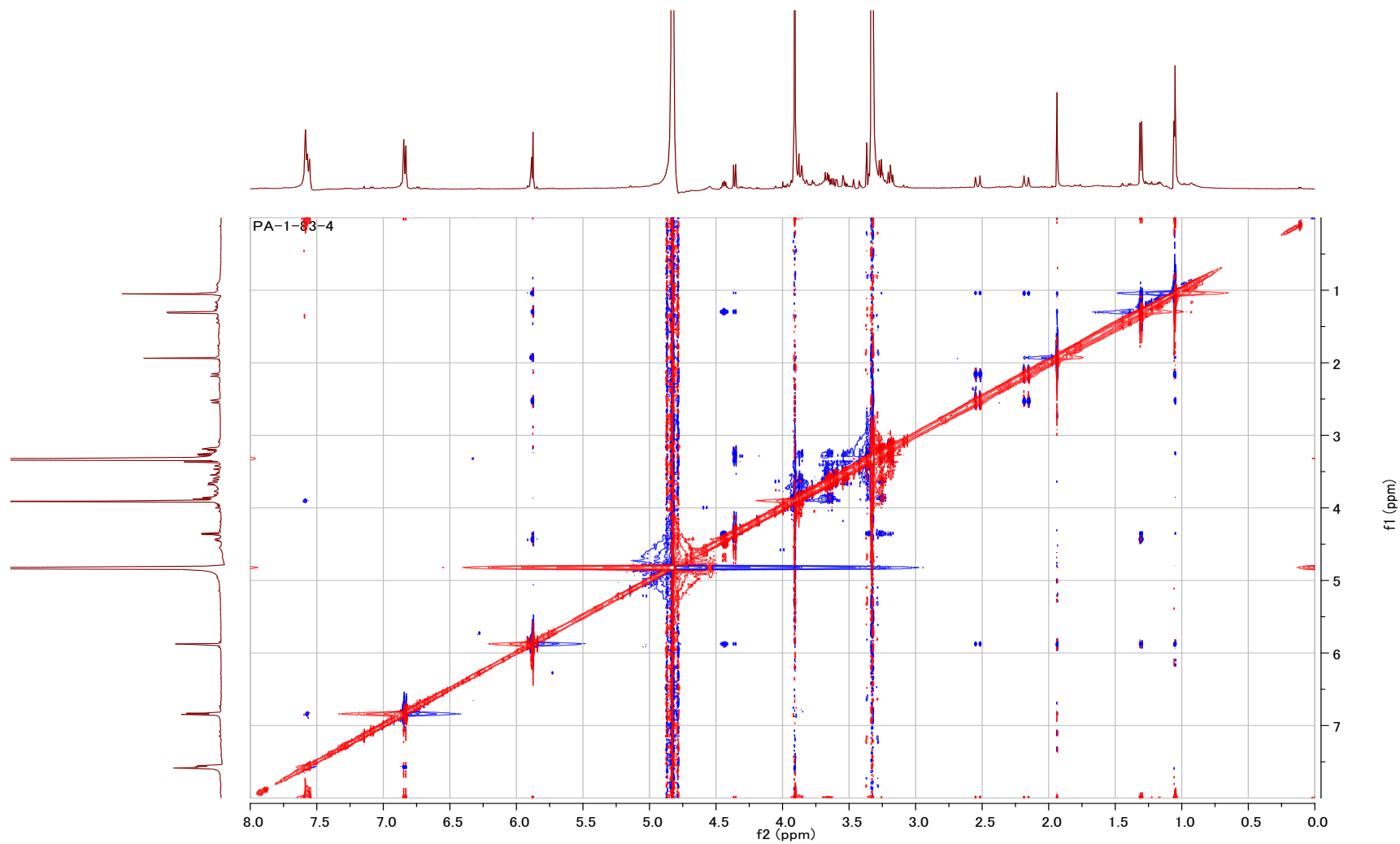
S26: HSQC of 3



S27: HMBC of **3**



S28: ^1H - ^1H COSY of **3**



S29: NOESY of 3