

Ahmpatinin ⁱBu, a new HIV-1 protease inhibitor, from a *Streptomyces* sp. CPCC 202950

Ming-Hua Chen,^{†ac} Shan-Shan Chang,^{†ab} Biao Dong,^a Li-Yan Yu,^a Ye-Xiang Wu,^a
Ren-Zhong Wang,^a Wei Jiang,^a Zeng-Ping Gao,^{*b} Shu-Yi Si^{*a}

^{a.} *Institute of Medicinal Biotechnology, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing 100050, China. E-mail: sisymb@hotmail.com (S. Si)*

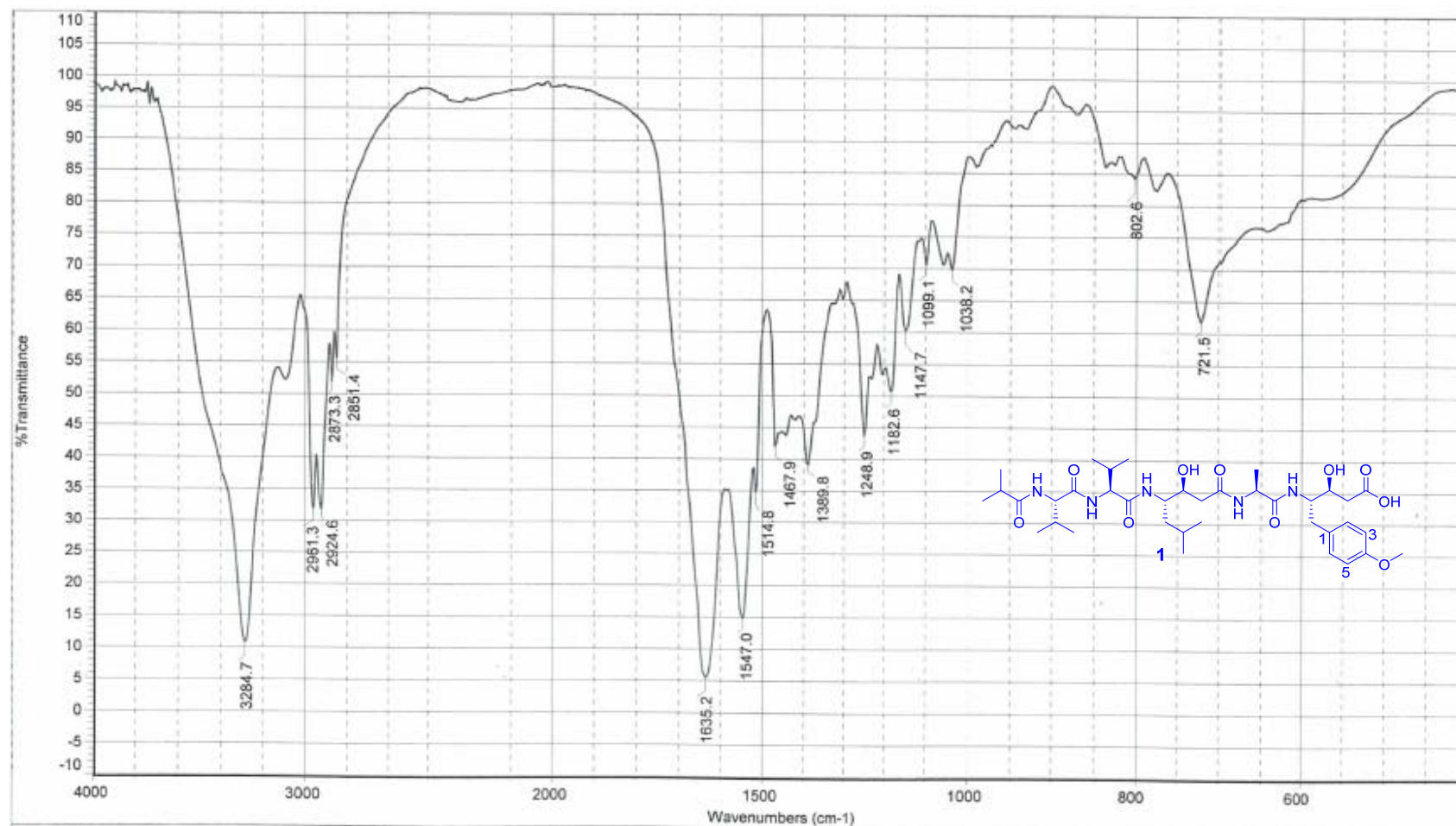
^{b.} *School of Chinese Materia Medica, Beijing University of Chinese Medicine, Beijing 100102, China. E-mail: gaozp@bucm.edu.cn (Z. Gao)*

^{c.} *Key Laboratory for Uighur Medicine, Institute of Materia Medica of Xinjiang, Urumqi 830004, China.*

Supporting Information

List of Content

No.	Content	Page
1	Figure S1. The IR Spectrum of Compound 1	S3
2	Figure S2. The (+)-HRESIMS Spectroscopic Data of Compound 1	S4
3	Figure S3. The ^1H NMR Spectrum of Compound 1 in $\text{DMSO}-d_6$	S5
4	Figure S4. The ^{13}C NMR Spectrum of Compound 1 in $\text{DMSO}-d_6$	S6
5	Figure S5. The DEPT Spectrum of Compound 1 in $\text{DMSO}-d_6$	S7
6	Figure S6. The ^1H - ^1H COSY Spectrum of Compound 1 in $\text{DMSO}-d_6$	S8
7	Figure S7. The HSQC Spectrum of Compound 1 in $\text{DMSO}-d_6$	S9
8	Figure S8. The HMBC Spectrum of Compound 1 in $\text{DMSO}-d_6$	S10
9	Figure S9. The NOESY Spectrum of Compound 1 in $\text{DMSO}-d_6$	S11
10	Figure S10. The IR Spectrum of Compound 2	S12
11	Figure S11. The (-)-HRESIMS Spectroscopic Data of Compound 2	S13
12	Figure S12. The ^1H NMR Spectrum of Compound 2 in $\text{DMSO}-d_6$	S14
13	Figure S13. The ^{13}C NMR Spectrum of Compound 2 in $\text{DMSO}-d_6$	S15
14	Figure S14. The DEPT Spectrum of Compound 2 in $\text{DMSO}-d_6$	S16
15	Figure S15. The ^1H - ^1H COSY Spectrum of Compound 2 in $\text{DMSO}-d_6$	S17
16	Figure S16. The HSQC Spectrum of Compound 2 in $\text{DMSO}-d_6$	S18
17	Figure S17. The HMBC Spectrum of Compound 2 in $\text{DMSO}-d_6$	S19
18	Figure S18. The NOESY Spectrum of Compound 2 in $\text{DMSO}-d_6$	S20
19	Figure S19. The IR Spectrum of Compound 3	S21
20	Figure S20. The (+)-HRESIMS Spectroscopic Data of Compound 3	S22
21	Figure S21. The ^1H NMR Spectrum of Compound 3 in $\text{DMSO}-d_6$	S23
22	Figure S22. The ^{13}C NMR Spectrum of Compound 3 in $\text{DMSO}-d_6$	S24
23	Figure S23. The DEPT Spectrum of Compound 3 in $\text{DMSO}-d_6$	S25
24	Figure S24. The ^1H - ^1H COSY Spectrum of Compound 3 in $\text{DMSO}-d_6$	S26
25	Figure S25. The HSQC Spectrum of Compound 3 in $\text{DMSO}-d_6$	S27
26	Figure S26. The HMBC Spectrum of Compound 3 in $\text{DMSO}-d_6$	S28
27	Figure S27. Marfey's Analysis of Acid Hydrolysate of Compound 1	S29
28	Figure S28. Chiral-phase HPLC Analysis of Acid Hydrolysate of Compound 1	S30



日期: 星期一 7月 11 15:16:47 2016 (GMT+08:00) Sample Name: CSS - 26

(显微镜透射法FT- IR Microscope Transmission)

扫描次数: 100

傅里叶变换显微镜红外(FT-IR Microscope): Centaurus

分辨率: 8.000

美国热电公司(Thermo)傅里叶变换红外光谱仪:Nicolet 5700

Figure S1. The IR Spectrum of Compound 1

20160407 CSS-26
 Bruker AVIIIHD 600 20160407
 PROTON DMSO D:\ DATA2016 3

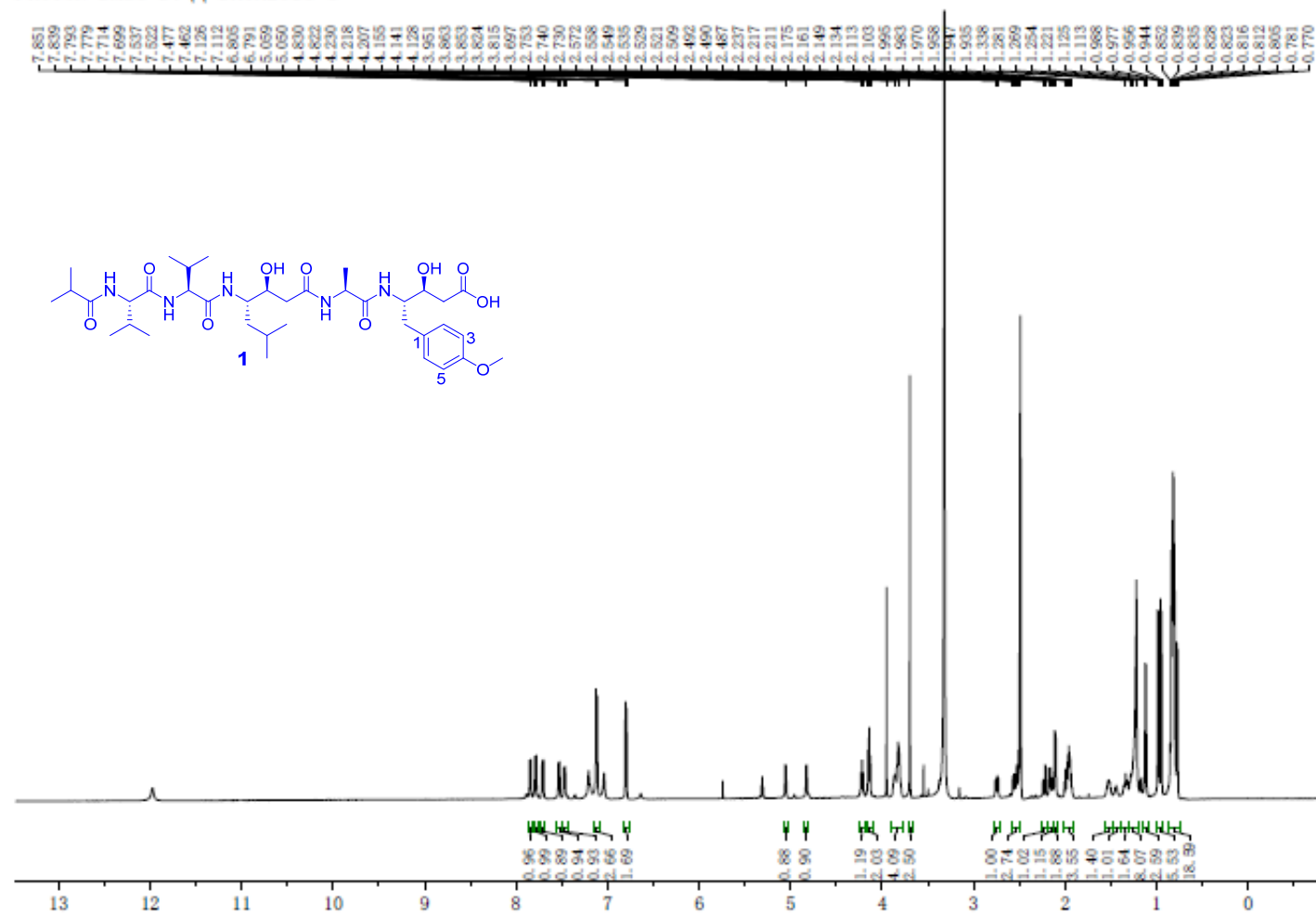


Figure S3. The ¹H NMR Spectrum of Compound **1** in DMSO-*d*₆

20160408 CSS-26
 Bruker AVIIIHD 600 20160408
 C13 DMSO D:\ DATA2016 29

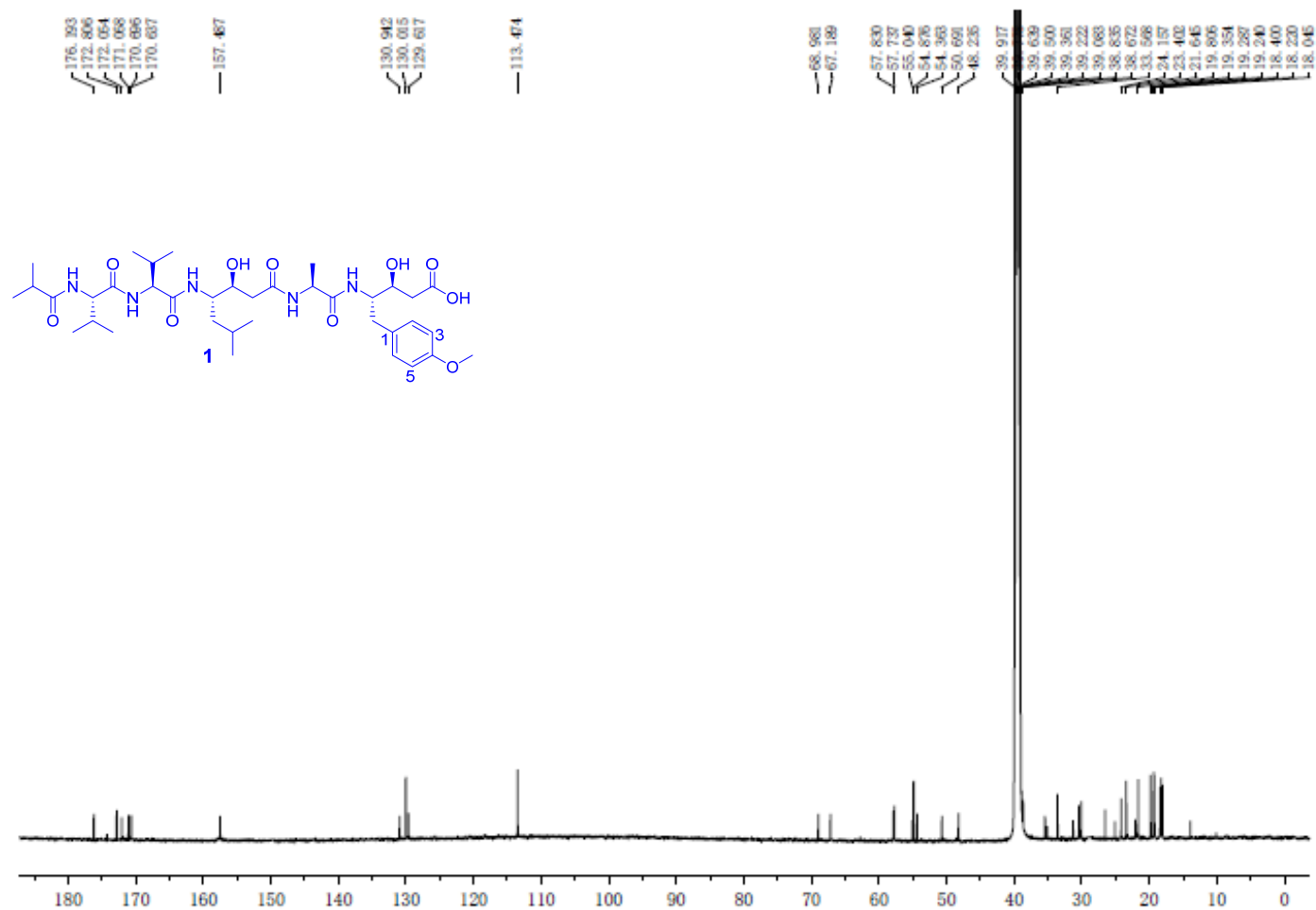
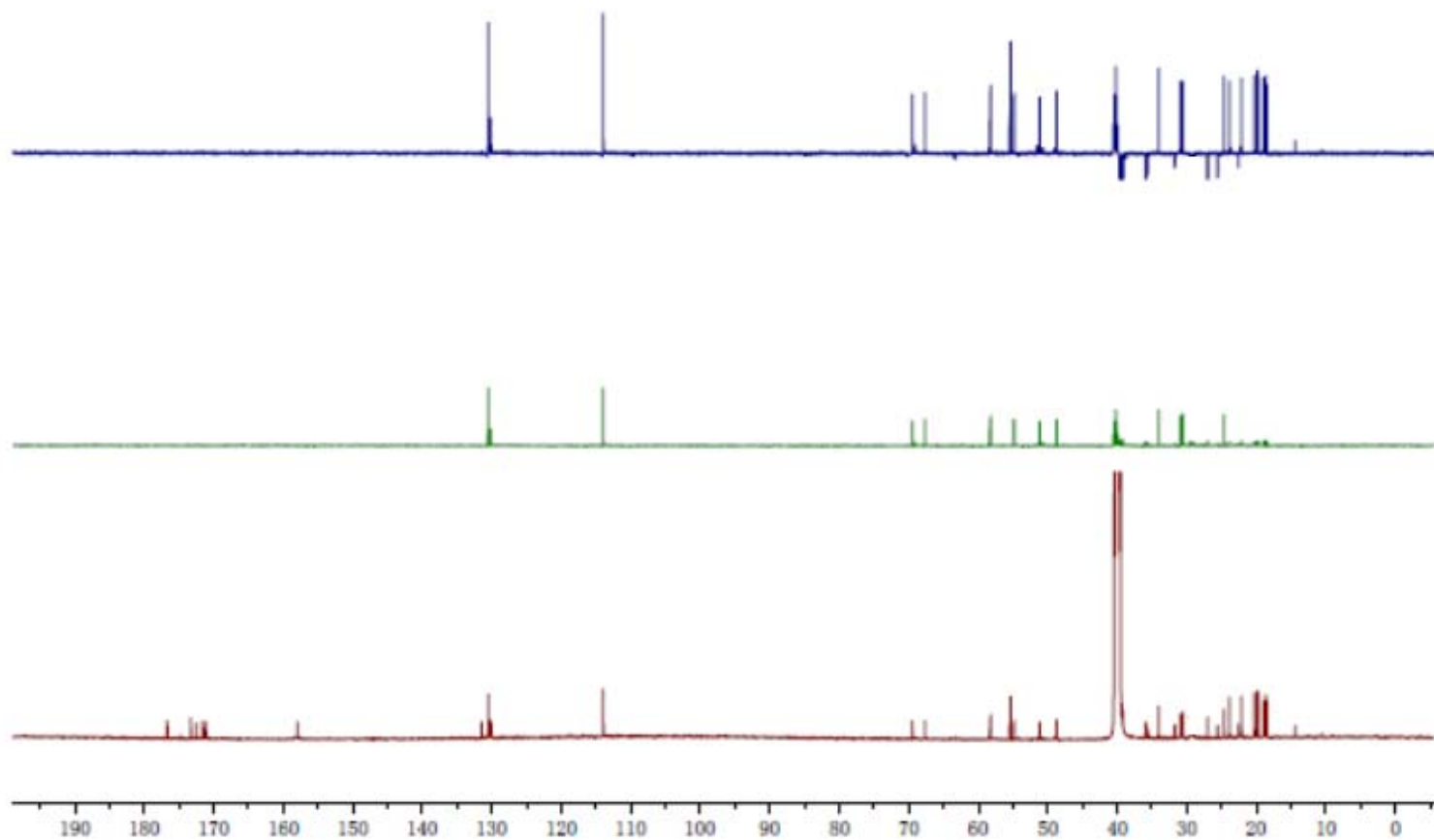


Figure S4. The ^{13}C NMR Spectrum of Compound 1 in $\text{DMSO}-d_6$

1



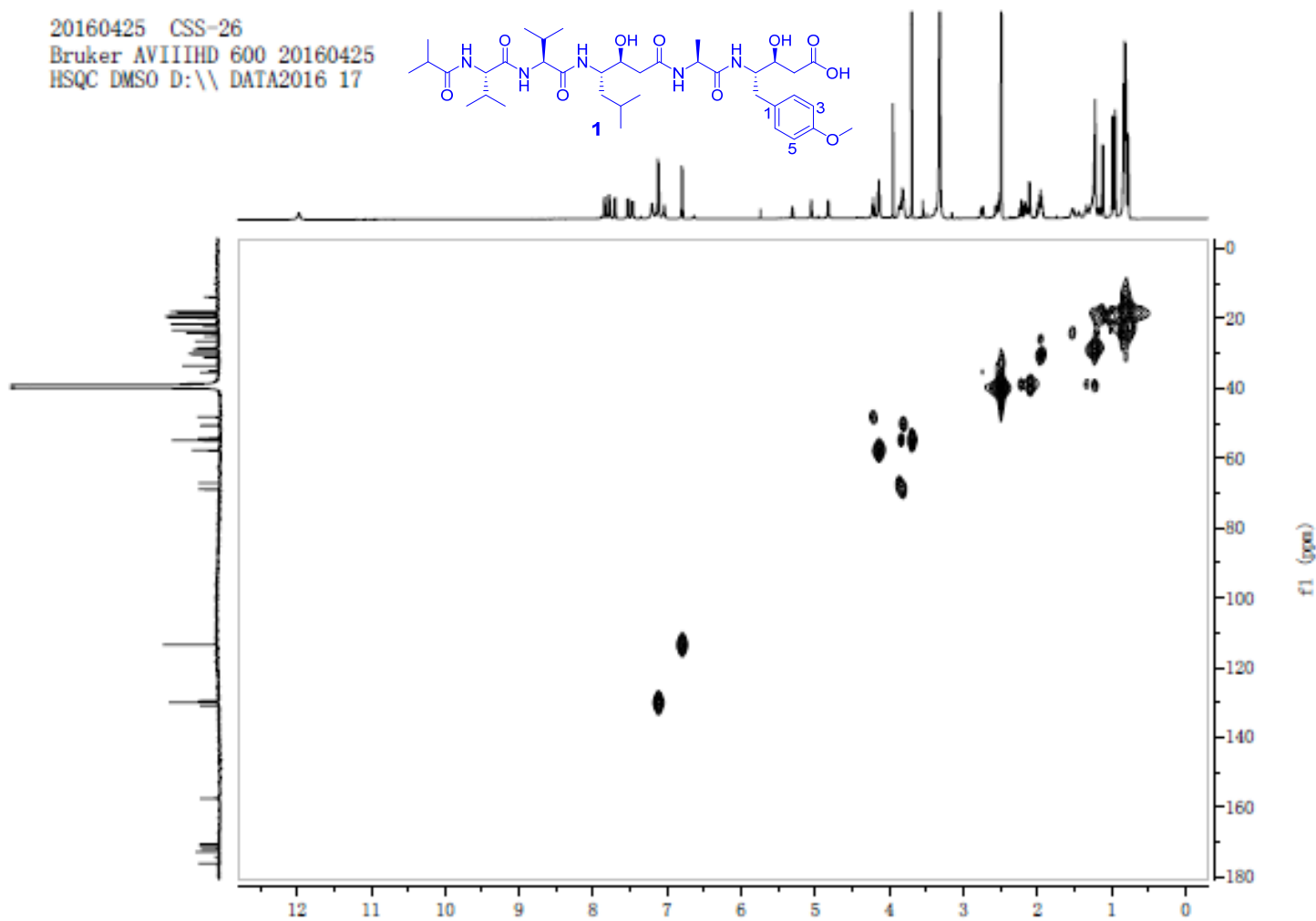
S7

20160425 CSS-26
Bruker AVIIIHD 600 20160425
COSY_MQF DMSO D:\ DATA2016 17

Chemical structure of compound 1 is shown in the bottom right corner of the plot area:

CC(C)C(O)C(=O)NC(C)C(=O)NC(C)C(=O)NC(C)C(=O)O

Figure S6. The ^1H - ^1H COSY Spectrum of Compound **1** in $\text{DMSO}-d_6$

[illegible]

S9

20160628 CSS-26
Bruker AVIIIHD 600 20160628
HMBC DMSO D:\ DATA2016 54

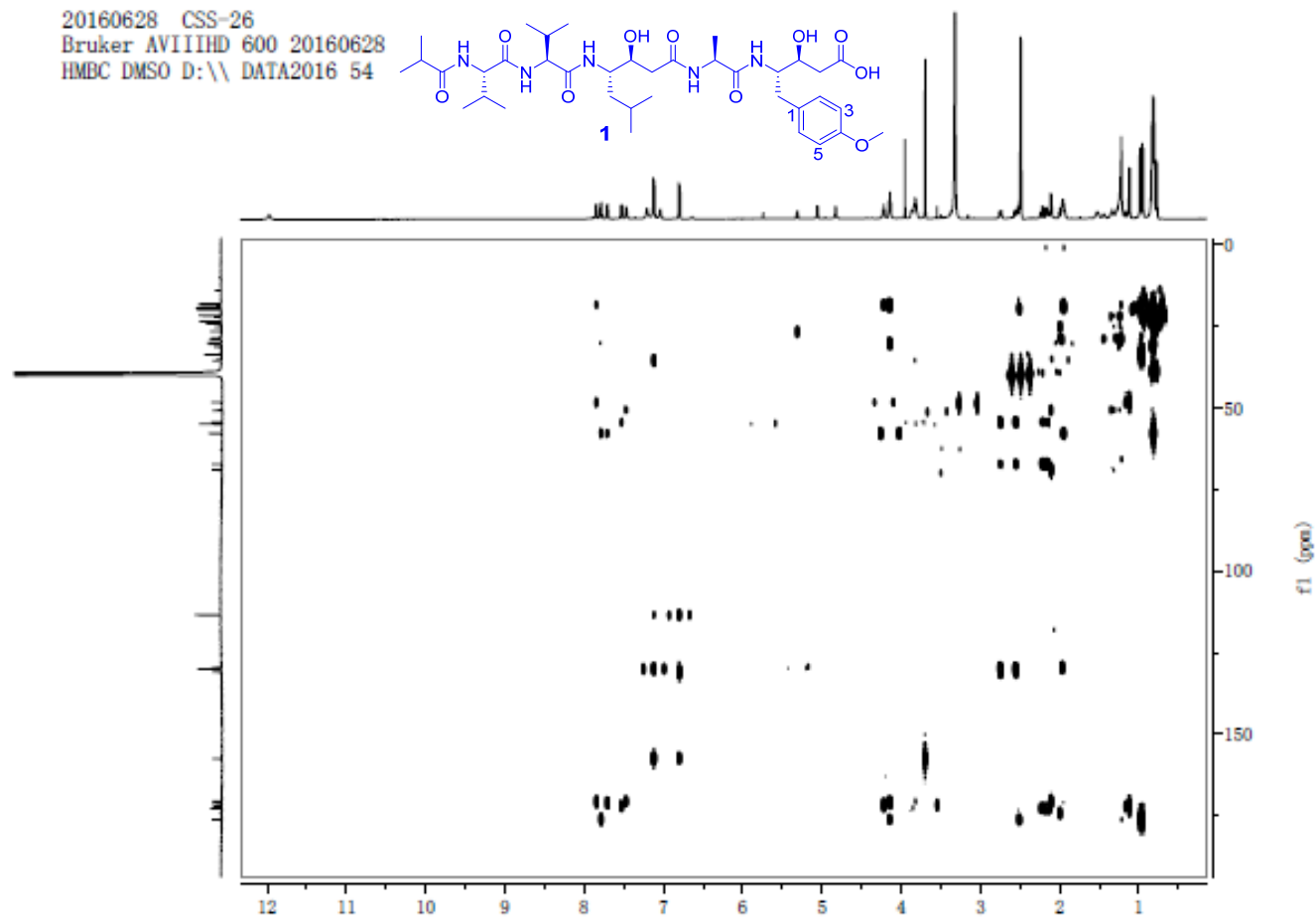
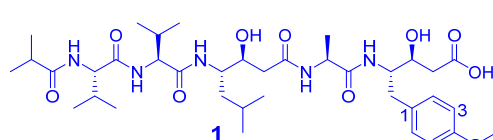


Figure S8. The HMBC Spectrum of Compound **1** in DMSO- d_6

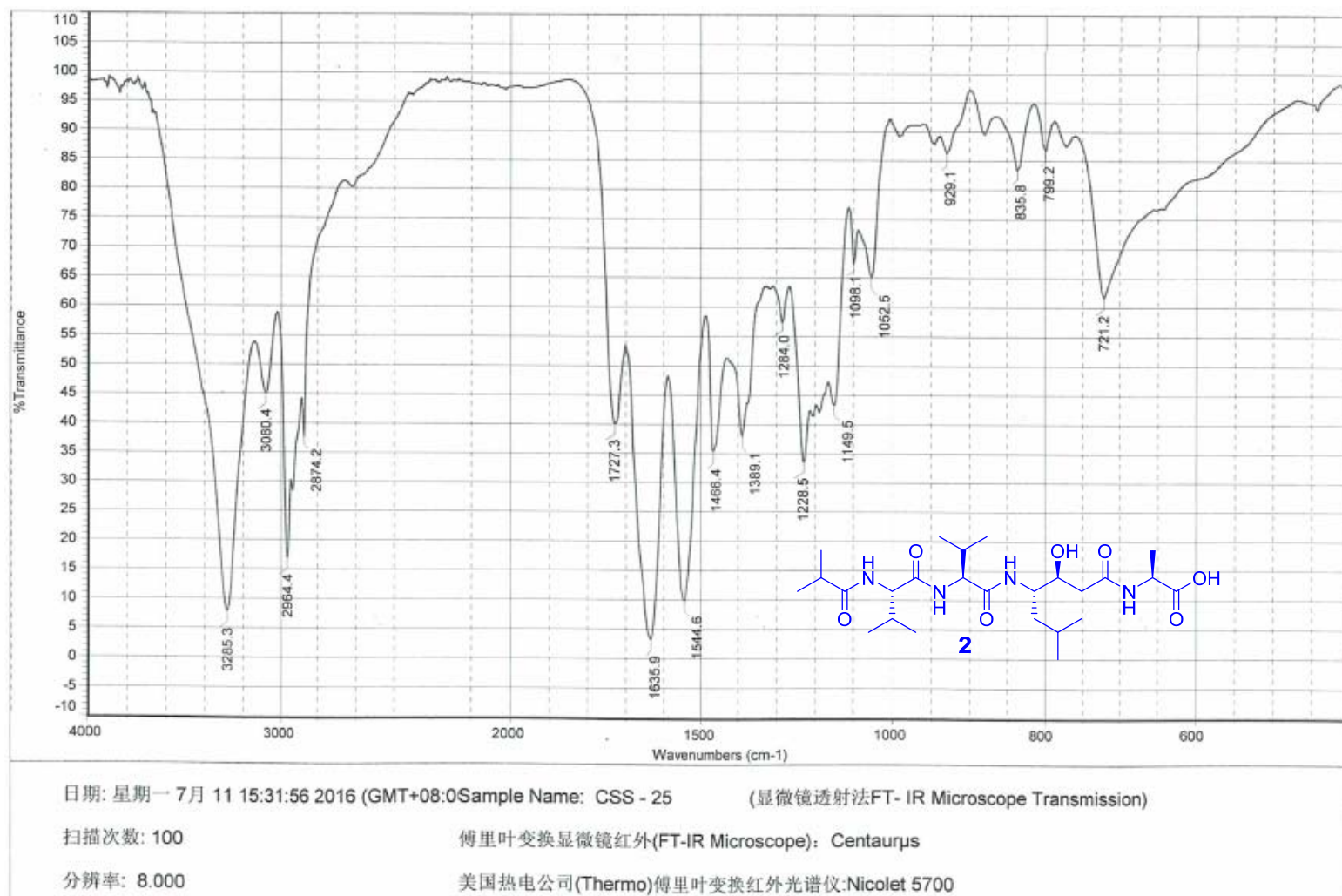


Figure S10. The IR Spectrum of Compound 2

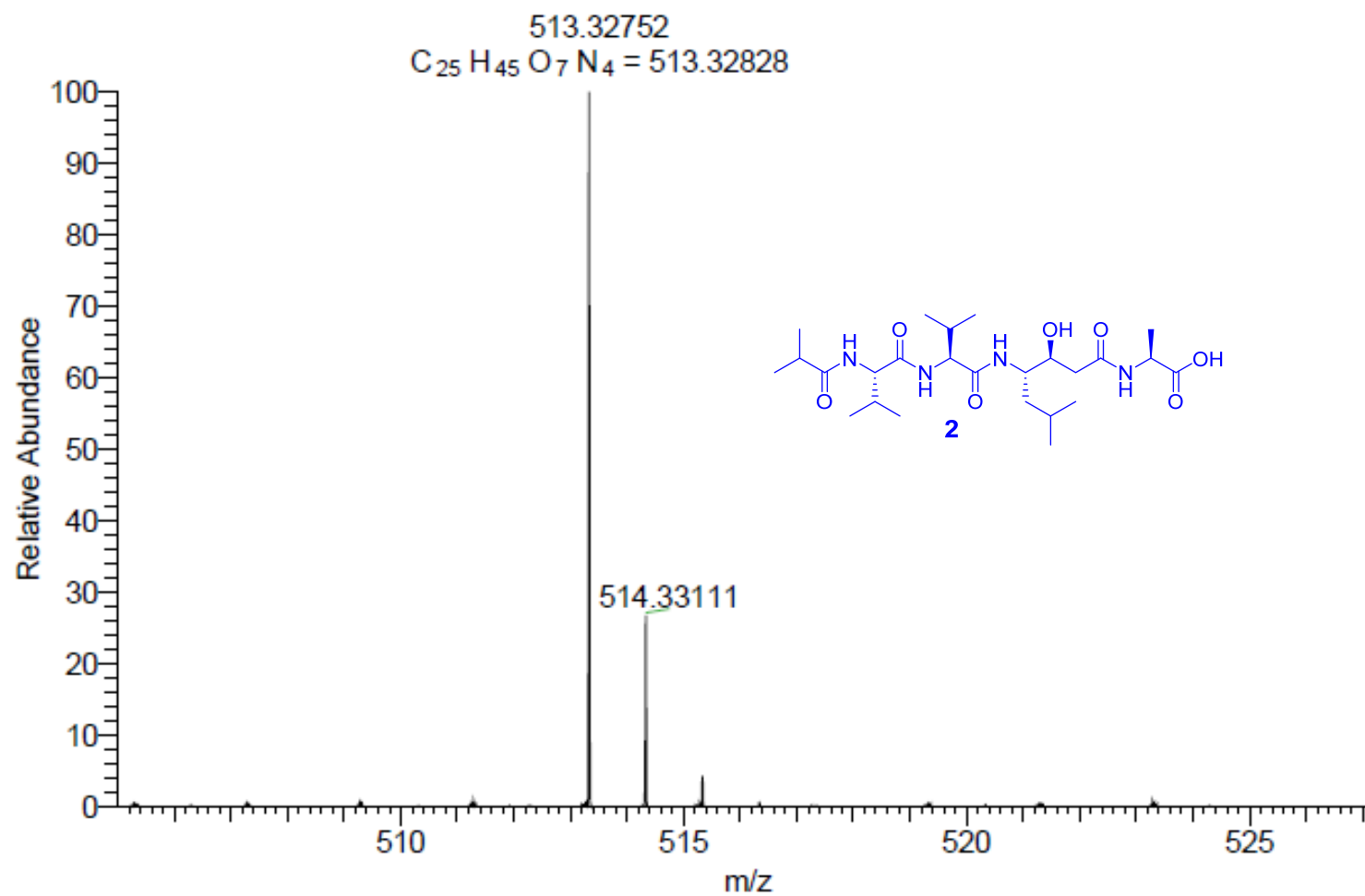


Figure S11. The (-)-HRESIMS Spectroscopic of Compound **2**

20160113 CSS-25
 Bruker AVIIIHD 600 20160113
 PROTON DMSO D:\ DATA2016 20

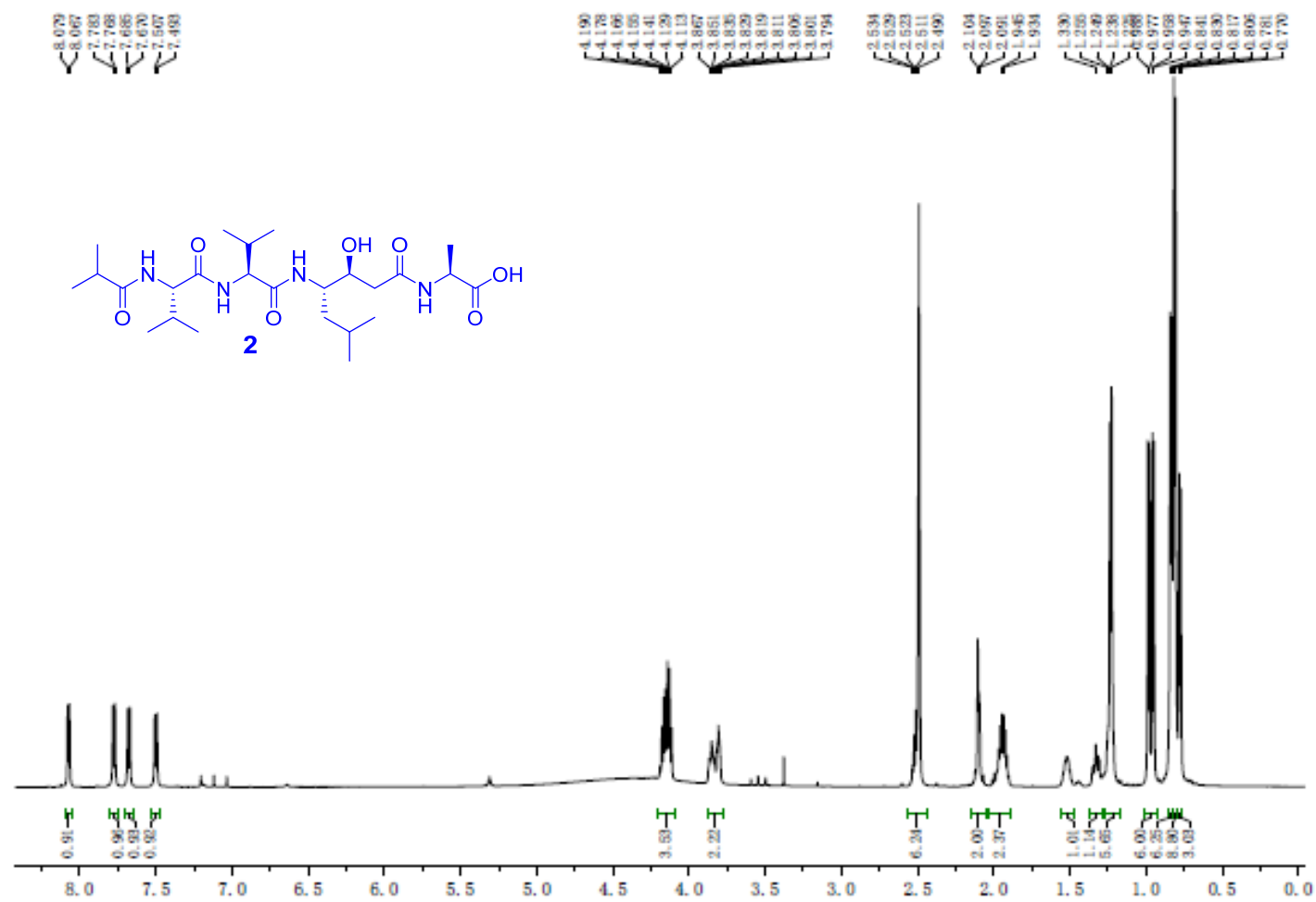


Figure S12. The ¹H NMR Spectrum of Compound **2** in DMSO-*d*₆

20160116 CSS-25
 Bruker AVIIIHD 600 20160116
 C13 DMSO D:\ DATA2016 48

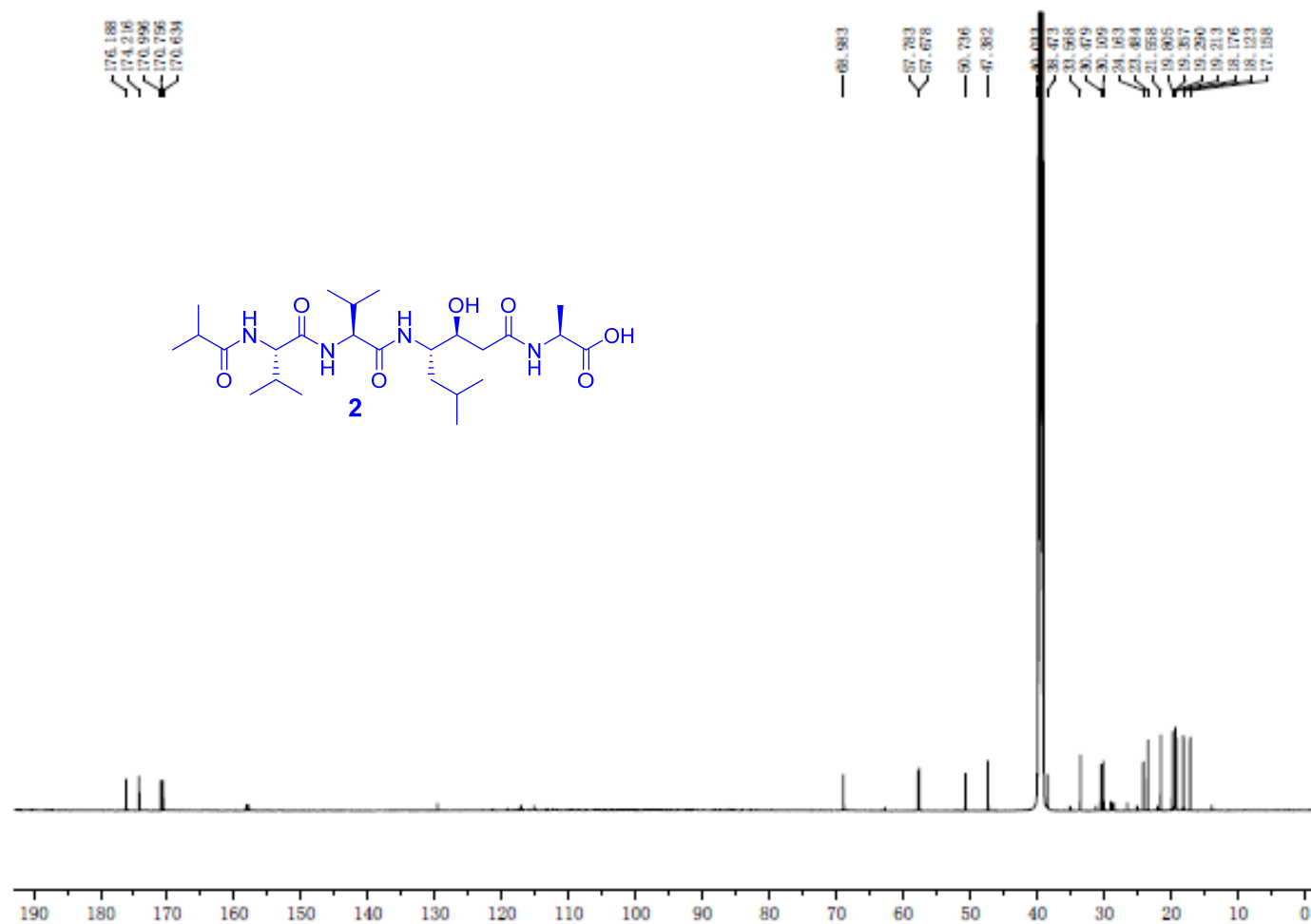


Figure S13. The ¹³C NMR Spectrum of Compound **2** in DMSO-*d*₆

20160116 CSS-25
Bruker AVIIIHD 600 20160116
DEPT90/135 DMSO D:\ DATA2016 48

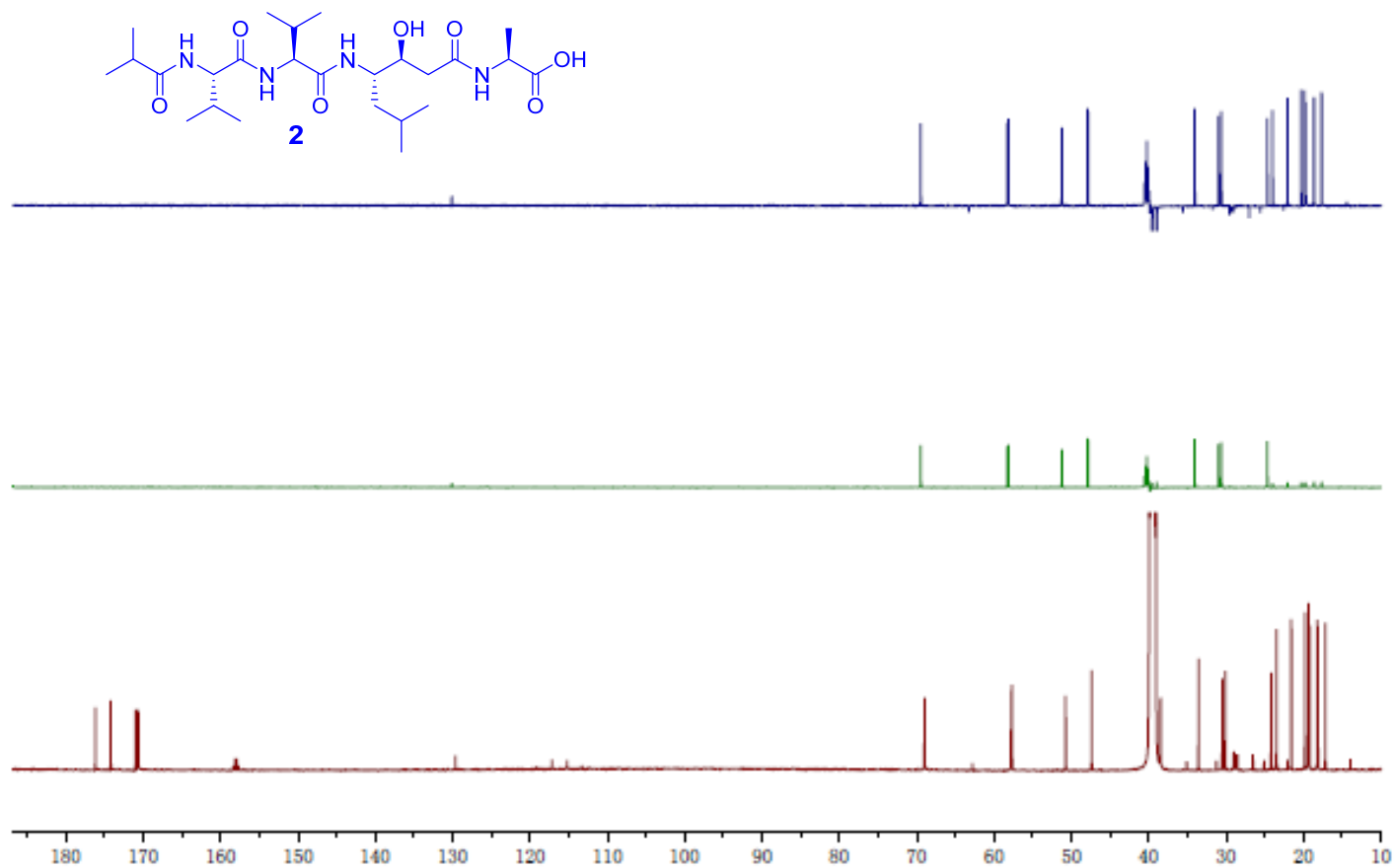


Figure S14. The DEPT Spectrum of Compound **2** in DMSO- d_6

20160122 CSS-25
Bruker AVIIIHD 600 20160122
COSY_MQF DMSO D:\ DATA2016 32

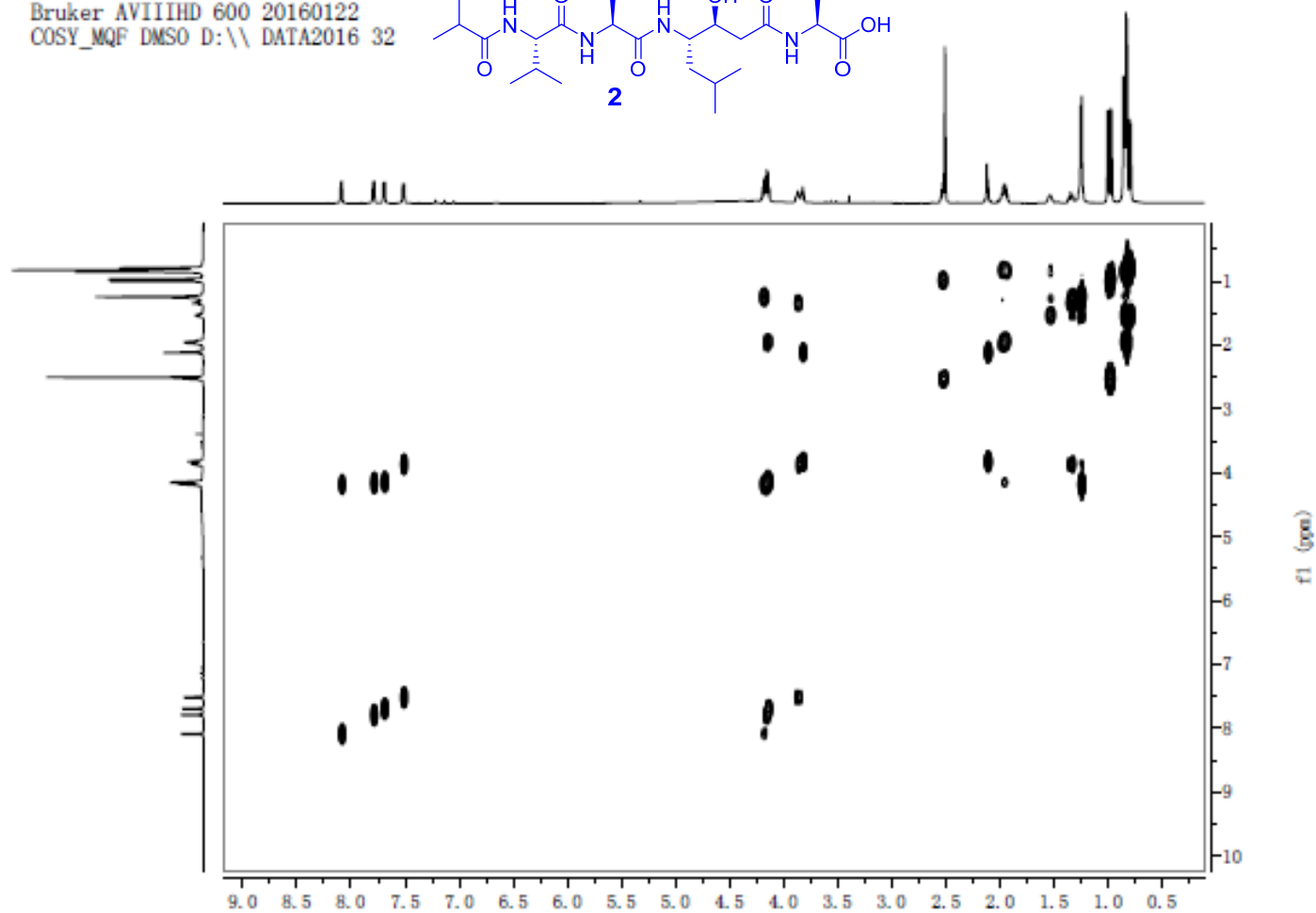
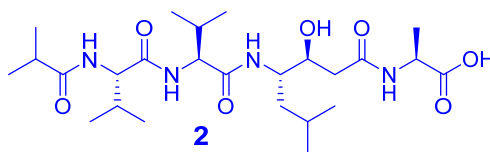


Figure S15. The ^1H - ^1H COSY Spectrum of Compound **2** in $\text{DMSO}-d_6$

20160122 CSS-25
Bruker AVIIIHD 600 20160122
HSQC DMSO D:\ DATA2016 32

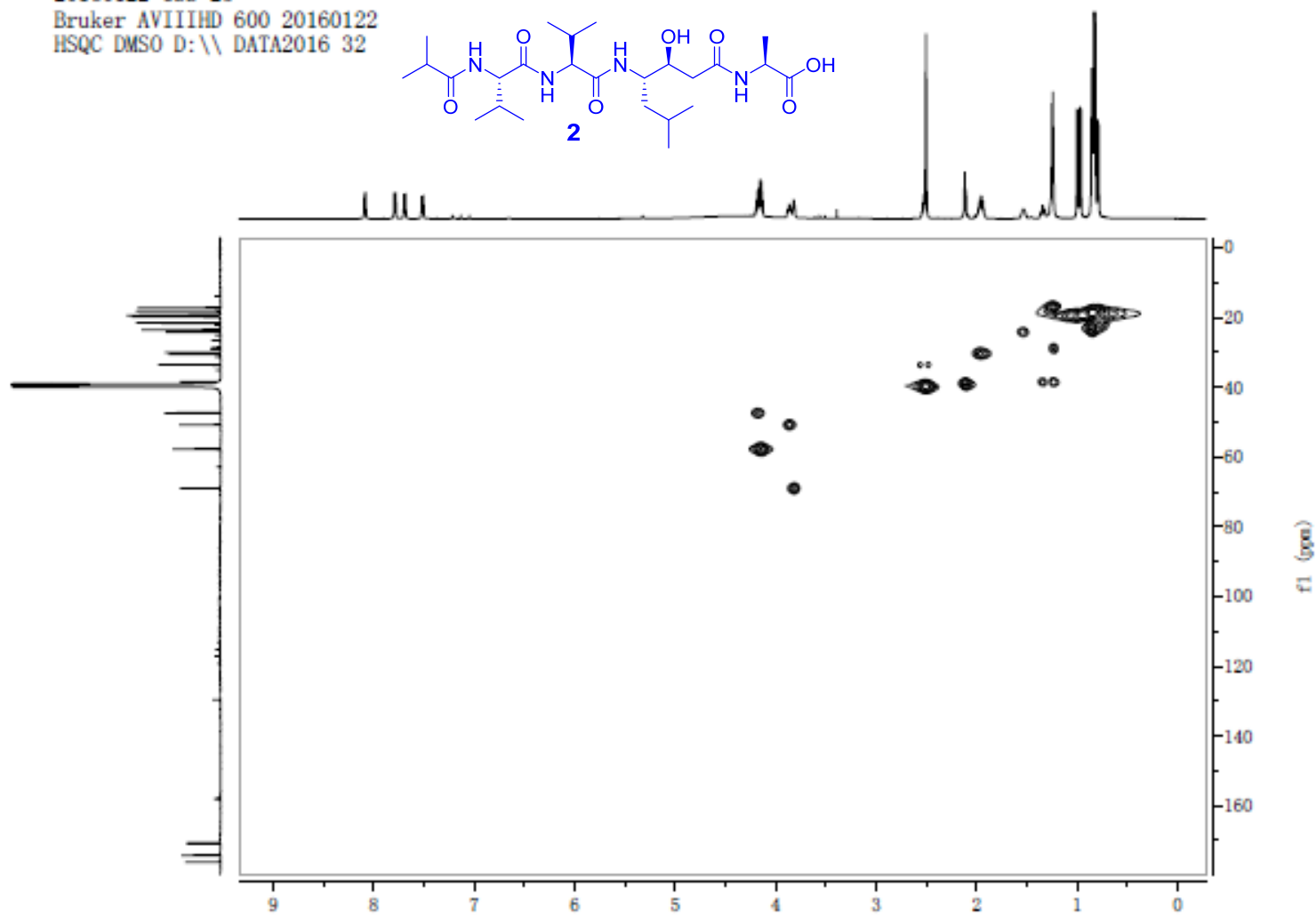
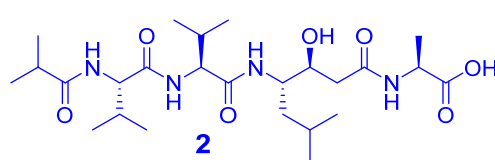


Figure S17. The HSQC Spectrum of Compound **2** in DMSO-*d*₆

20160122 CSS-25
Bruker AVIIIHD 600 20160122
HMBC DMSO D:\ DATA2016 32

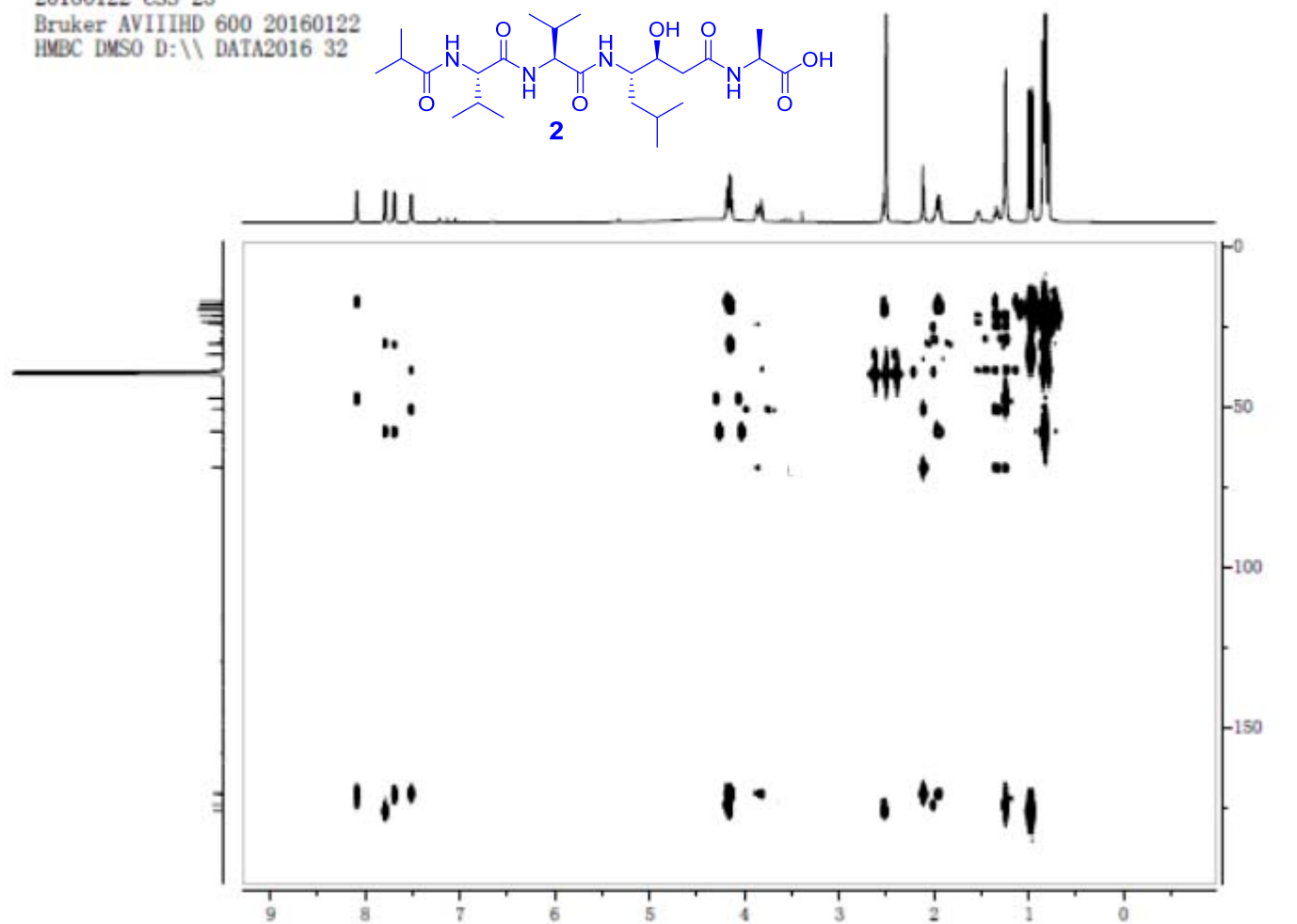


Figure S17. The HMBC Spectrum of Compound 2 in DMSO- d_6

Bruker AVIIIHD 600 20160122
NOESY_2D DMSO D:\ DATA2016 32



Current Data Parameters
NAME 20160122 CSS-25
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160125
Time 2.00
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG noesygppbpb
TD 2048
SOLVENT DMSO
NS 16
DS 16
SWH 8417.509 Hz
FIDRES 4.110112 Hz
AQ 0.1216512 sec
RG 144
DW 59.400 usec
DE 20.00 usec
TE 298.0 K
DO 0.00004476 sec
D1 1.20000005 sec
D8 0.60000002 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00011880 sec

===== CHANNEL f1 =====
SFO1 600.2539016 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
P17 2500.00 usec
PLW1 12.93200016 W
PLW0 2.52999997 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPE1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 160
SFO1 600.2539 MHz
FIDRES 52.609428 Hz
SW 14.023 ppm
PRMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.2500000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.2500000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

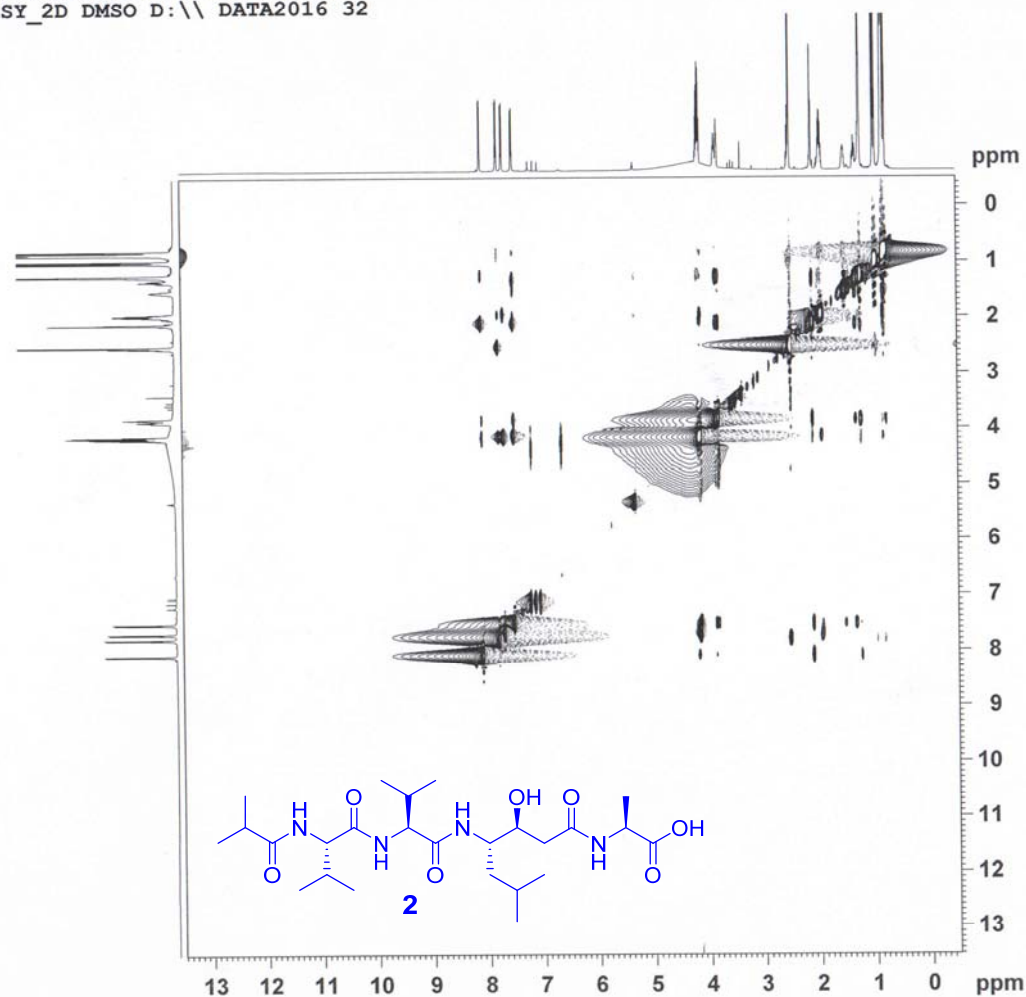


Figure S18. The NOESY Spectrum of Compound 1 in DMSO- d_6

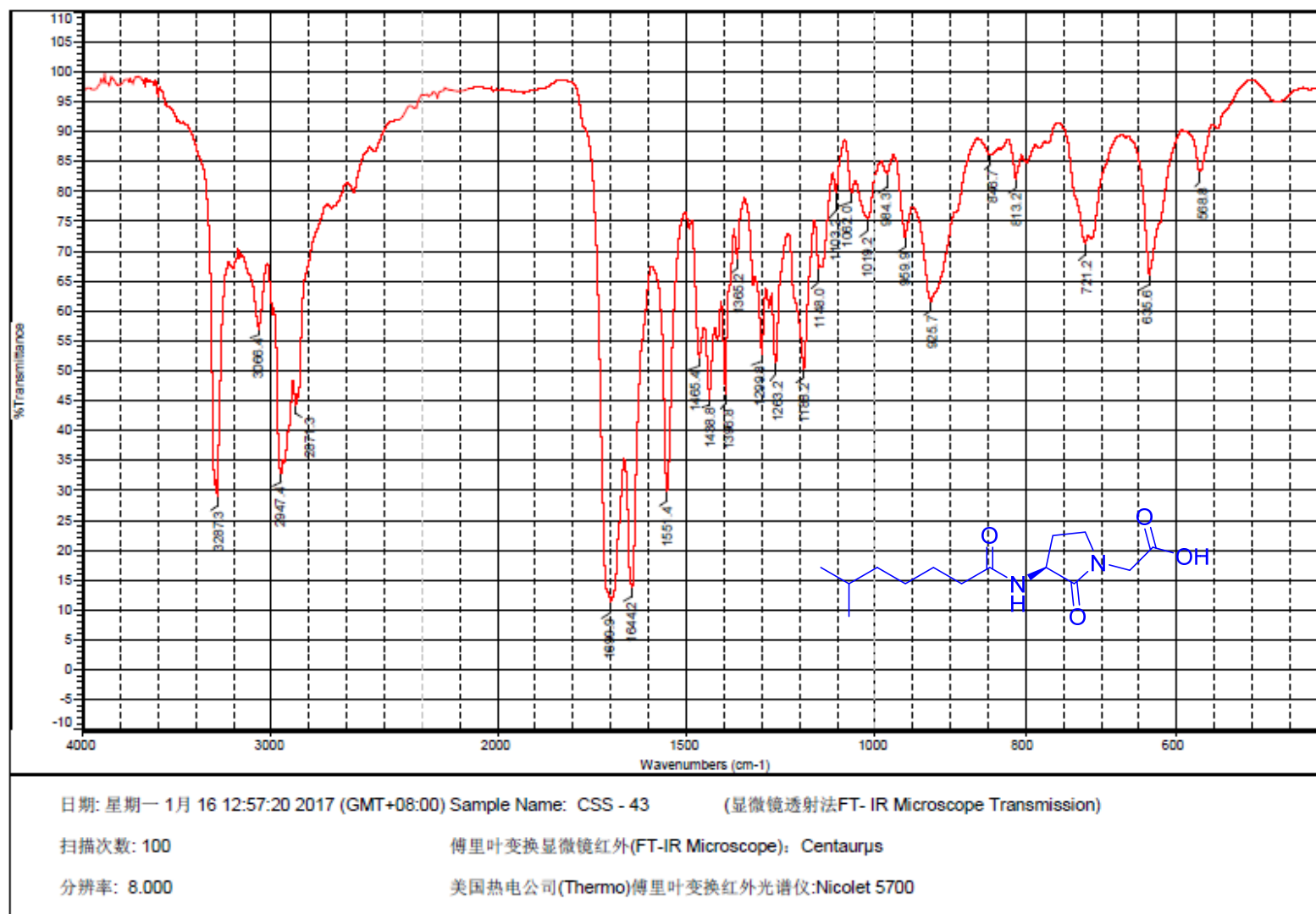


Figure S19. The IR Spectrum of Compound 3

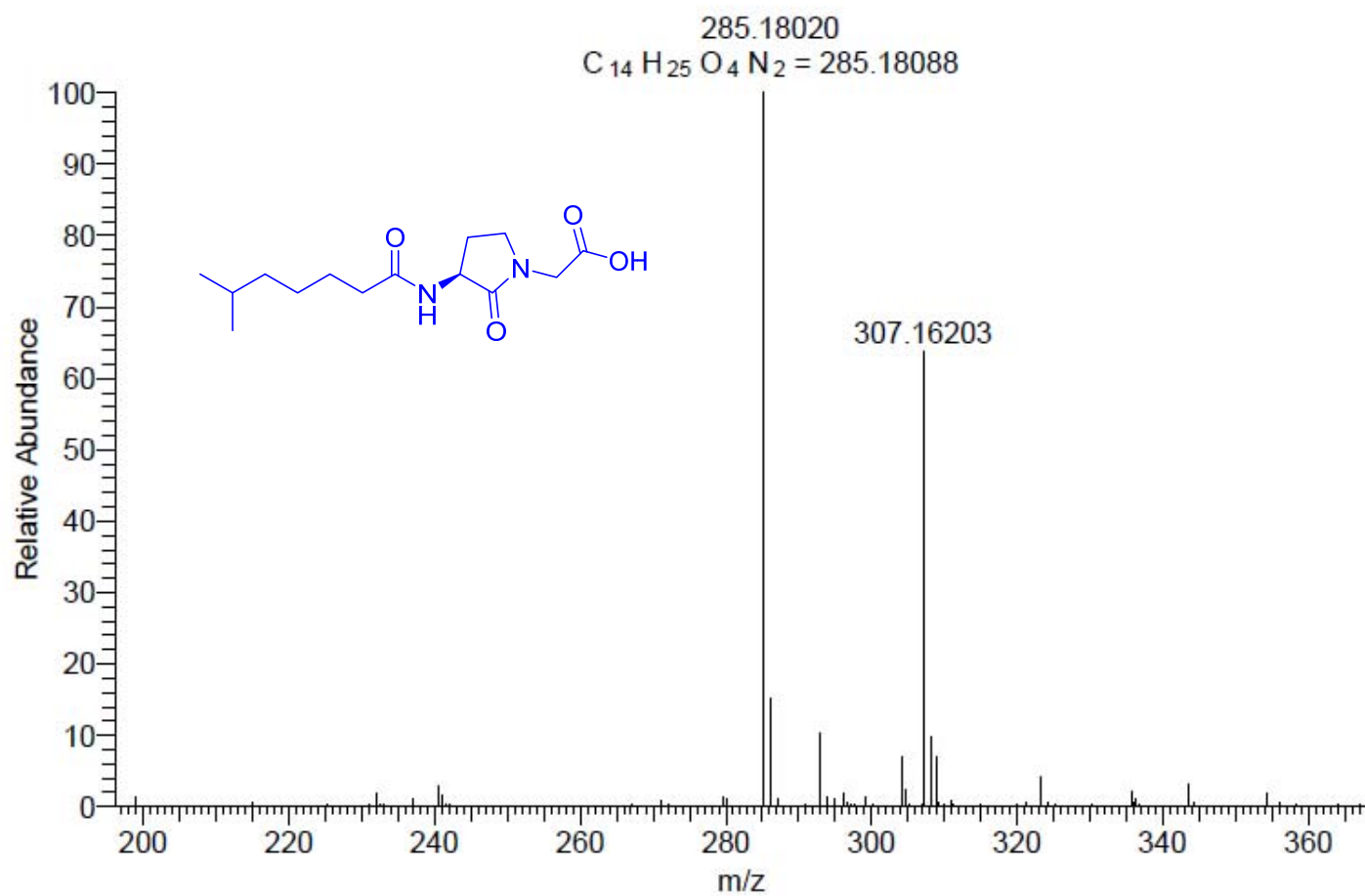


Figure S20. The (+)-HRESIMS Spectroscopic Data of Compound **3**

20160829 css-43
 Bruker AVIIIHD 600 20160829
 PROTON DMSO D:\ DATA2016 9

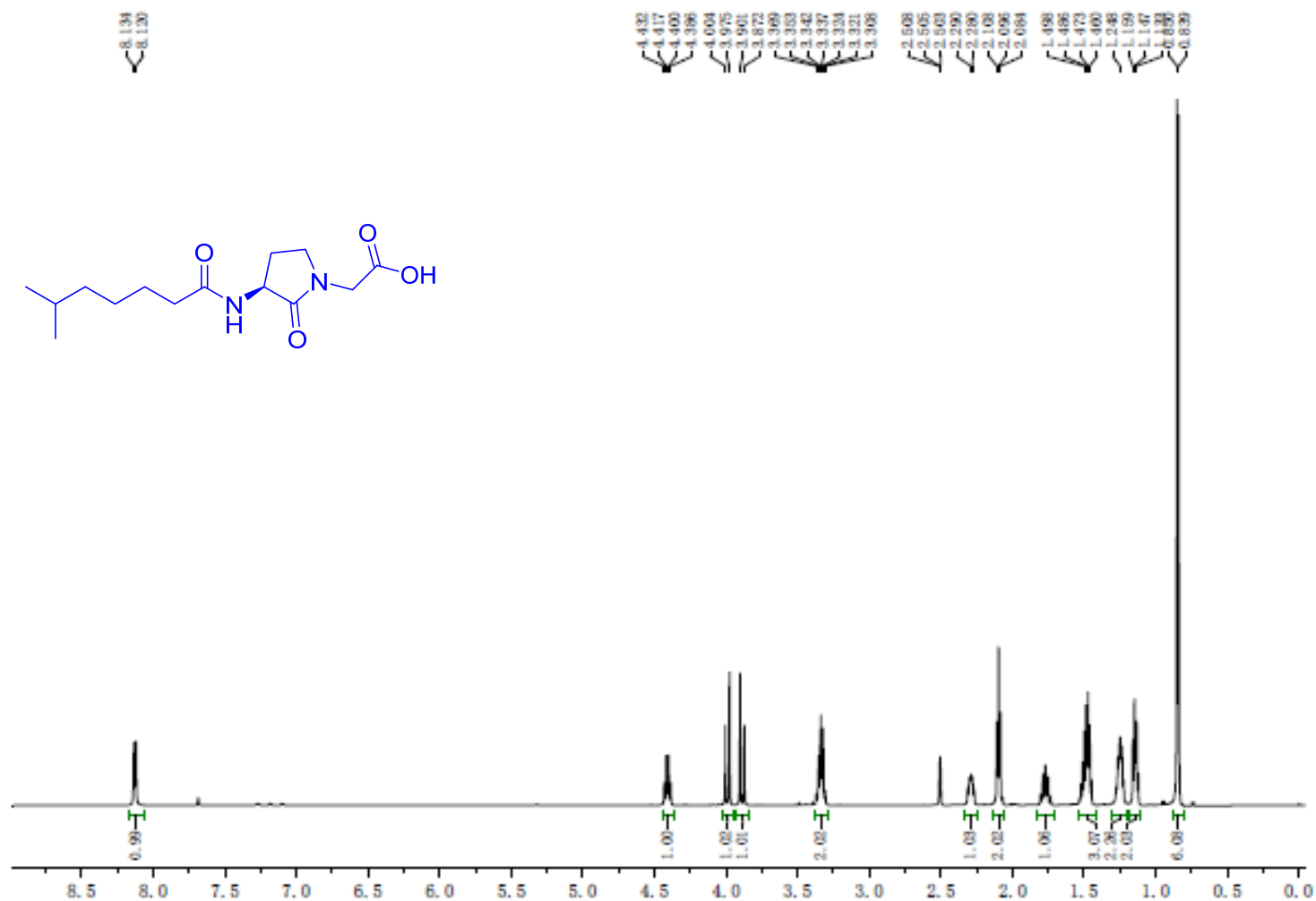


Figure S21. The ¹H NMR Spectrum of Compound **3** in DMSO-*d*₆

20160831 CSS-43
Bruker AVIIIHD 600 20160831
C13 CD3OD D:\ DATA2016 53

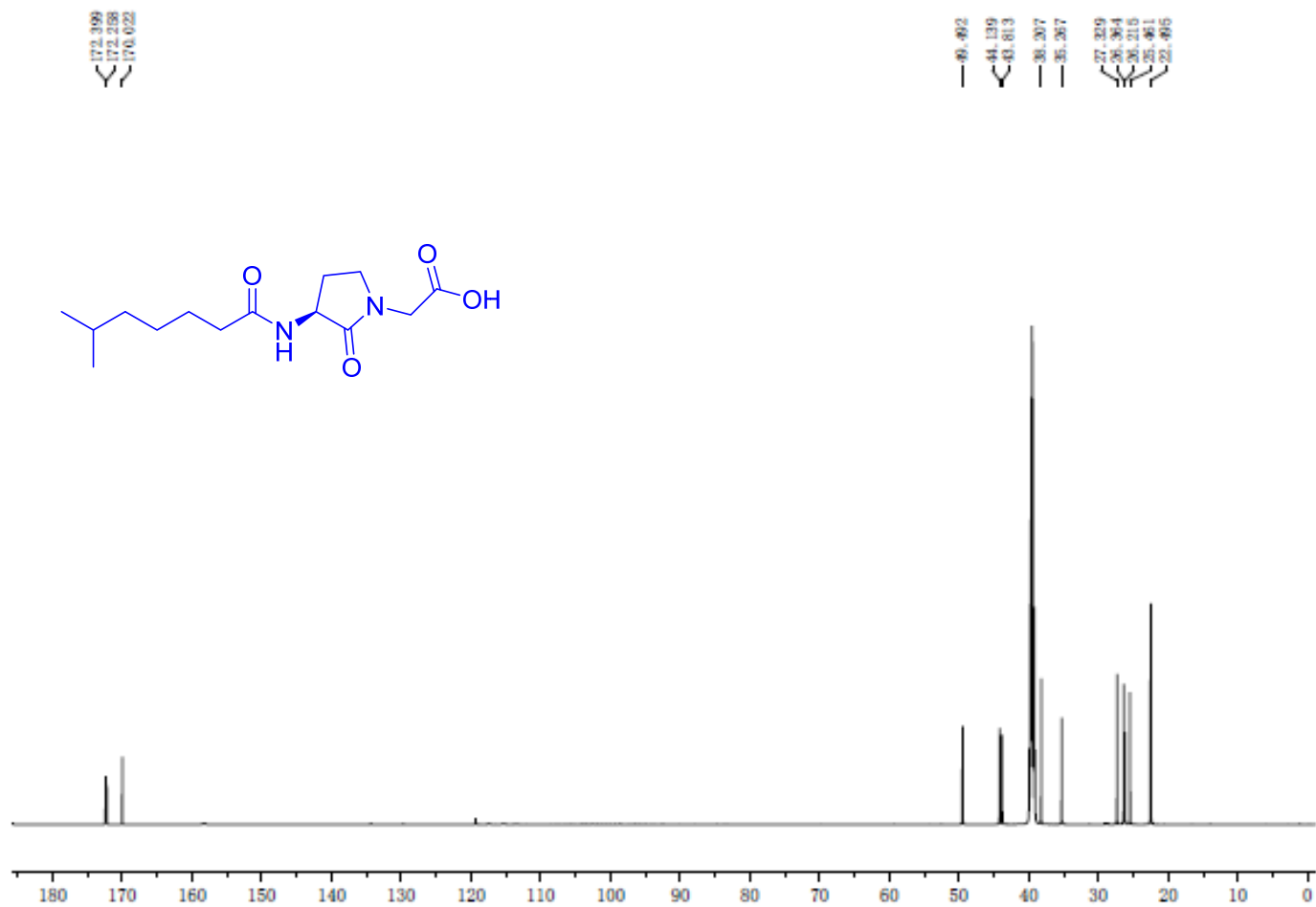


Figure S22. The ¹³C NMR Spectrum of Compound **3** in DMSO-*d*₆

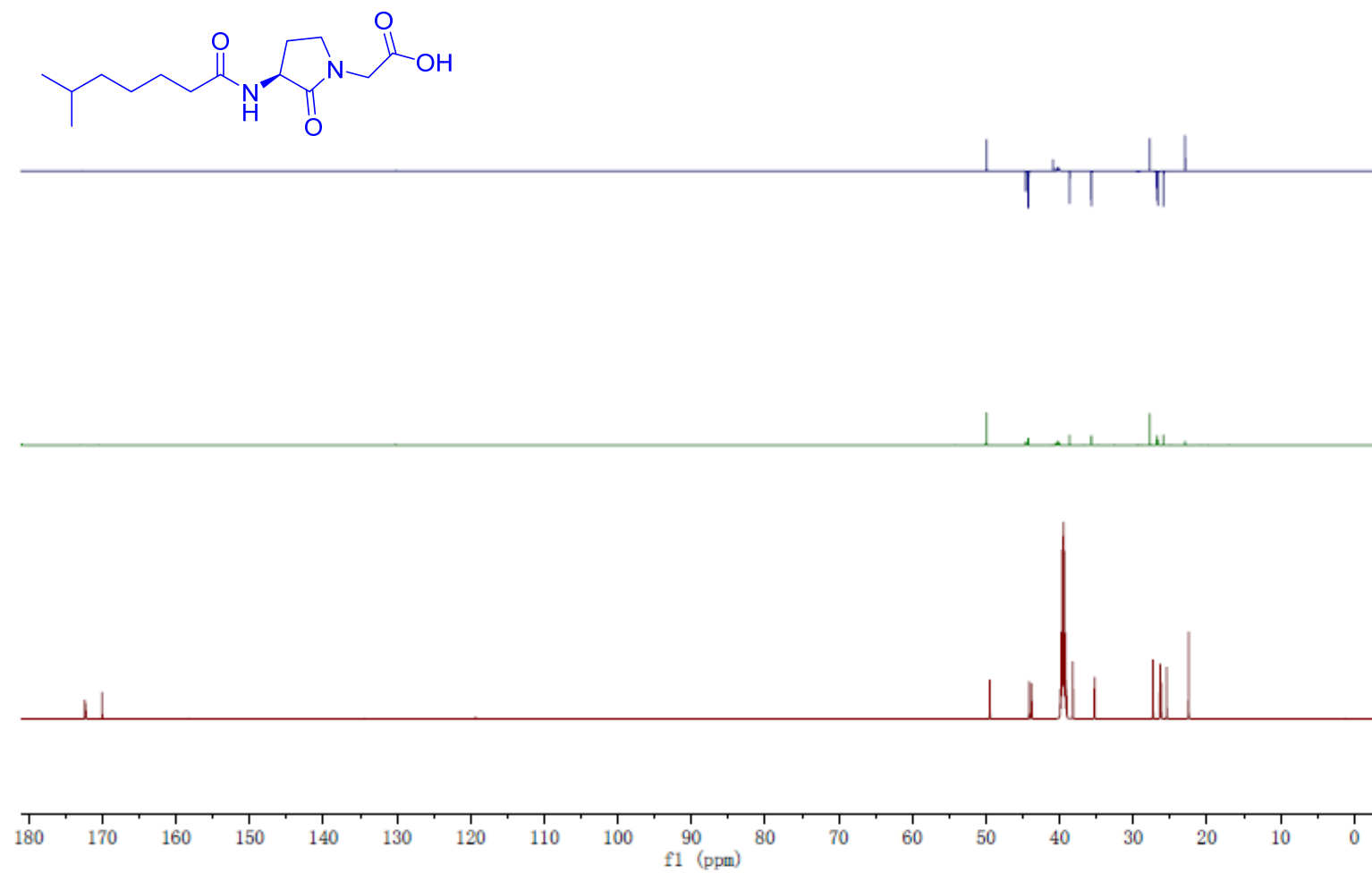


Figure S23. The DEPT Spectrum of Compound **3** in DMSO- d_6

20160914 CSS-43
Bruker AVIIIHD 600 20160914
COSY_MQF DMSO D:\ DATA2016 12

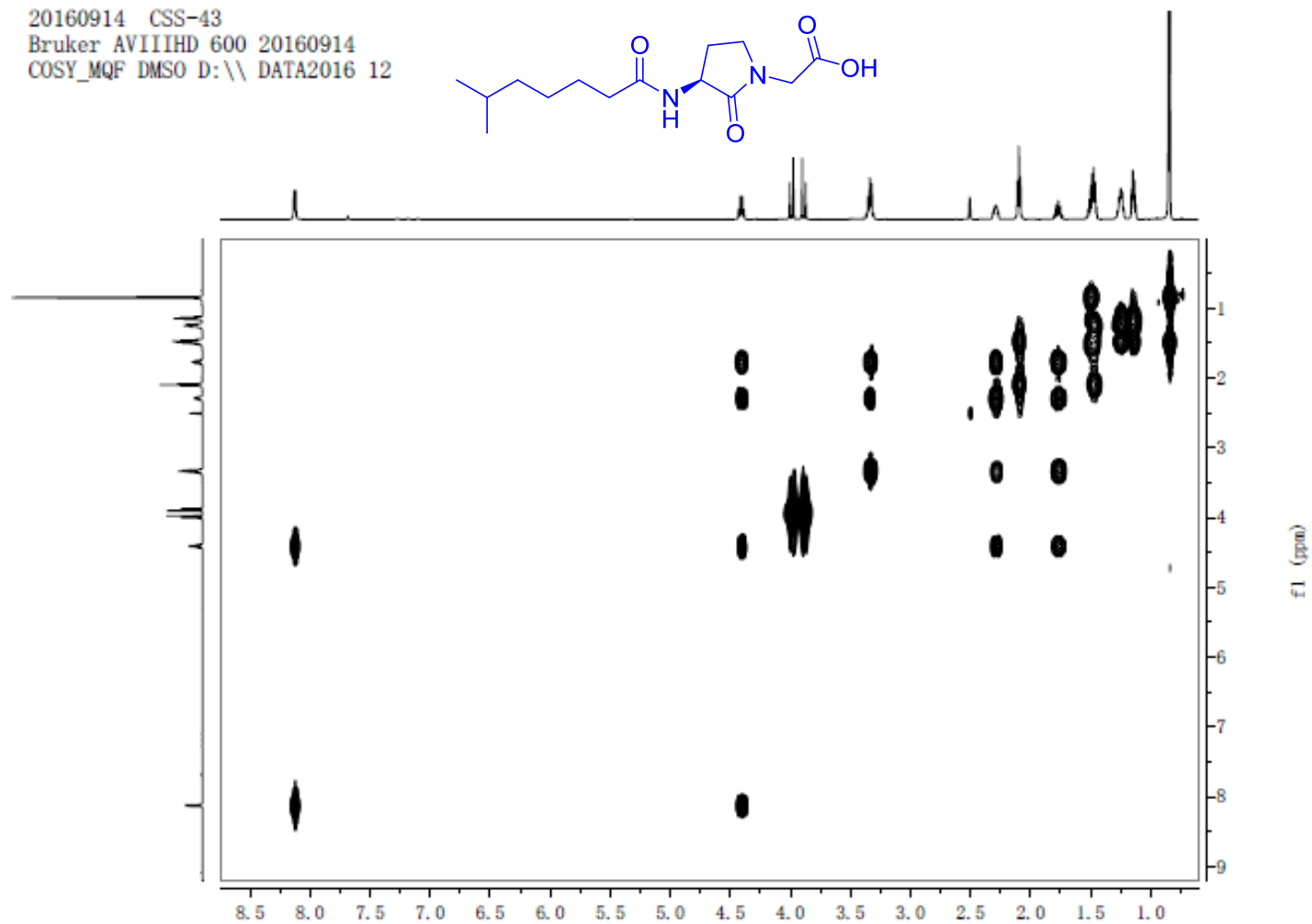


Figure S24. The ^1H - ^1H COSY Spectrum of Compound **3** in $\text{DMSO}-d_6$

20160914 CSS-43
Bruker AVIIIHD 600 20160914
HSQC DMSO D:\ DATA2016 12

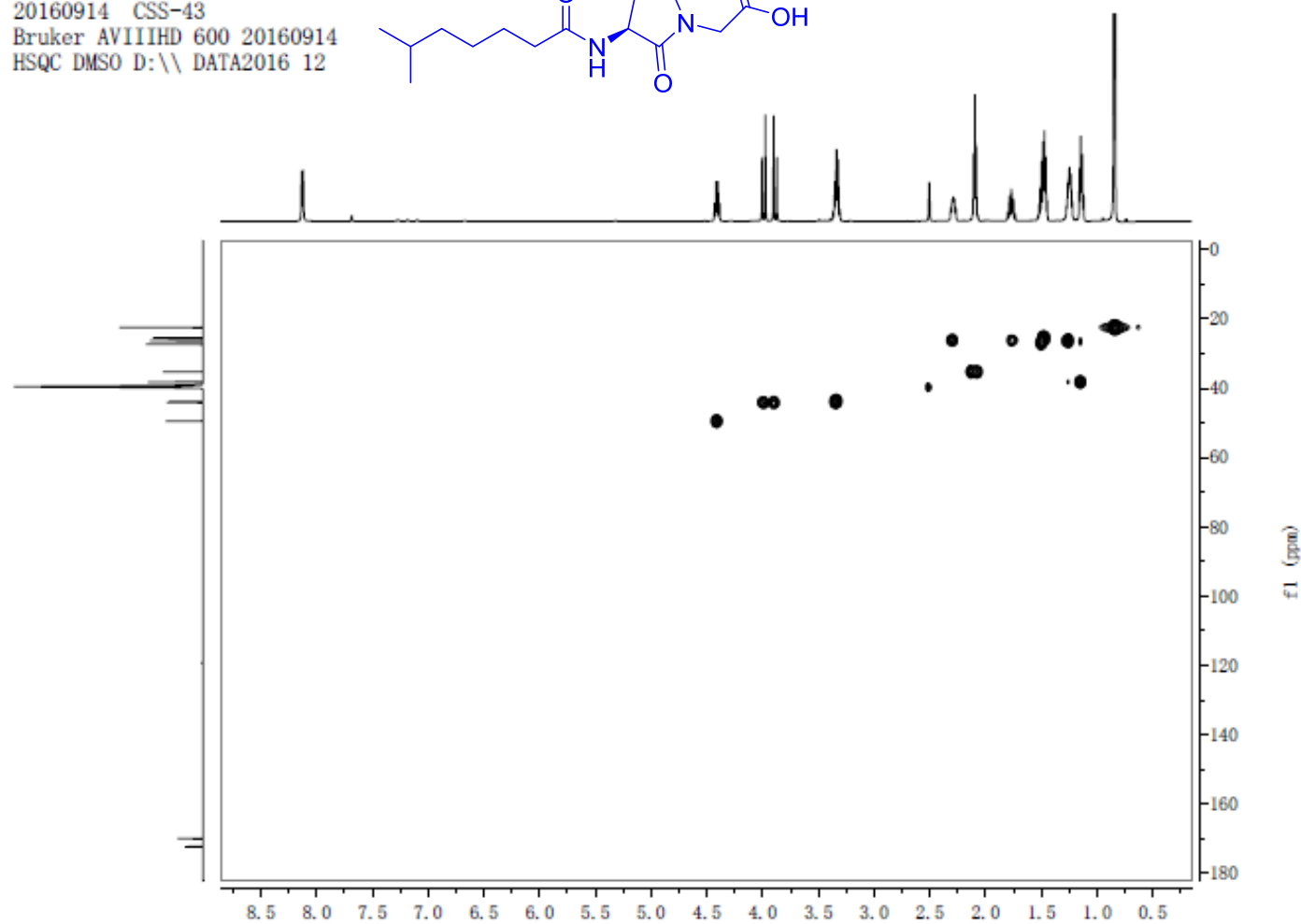
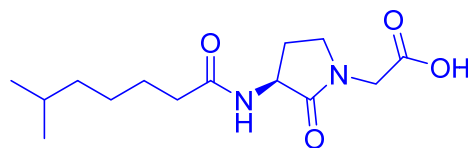


Figure S25. The HSQC Spectrum of Compound **3** in $\text{DMSO}-d_6$

20160914 CSS-43
Bruker AVIIIHD 600 20160914
HMBC DMSO D:\ DATA2016 12

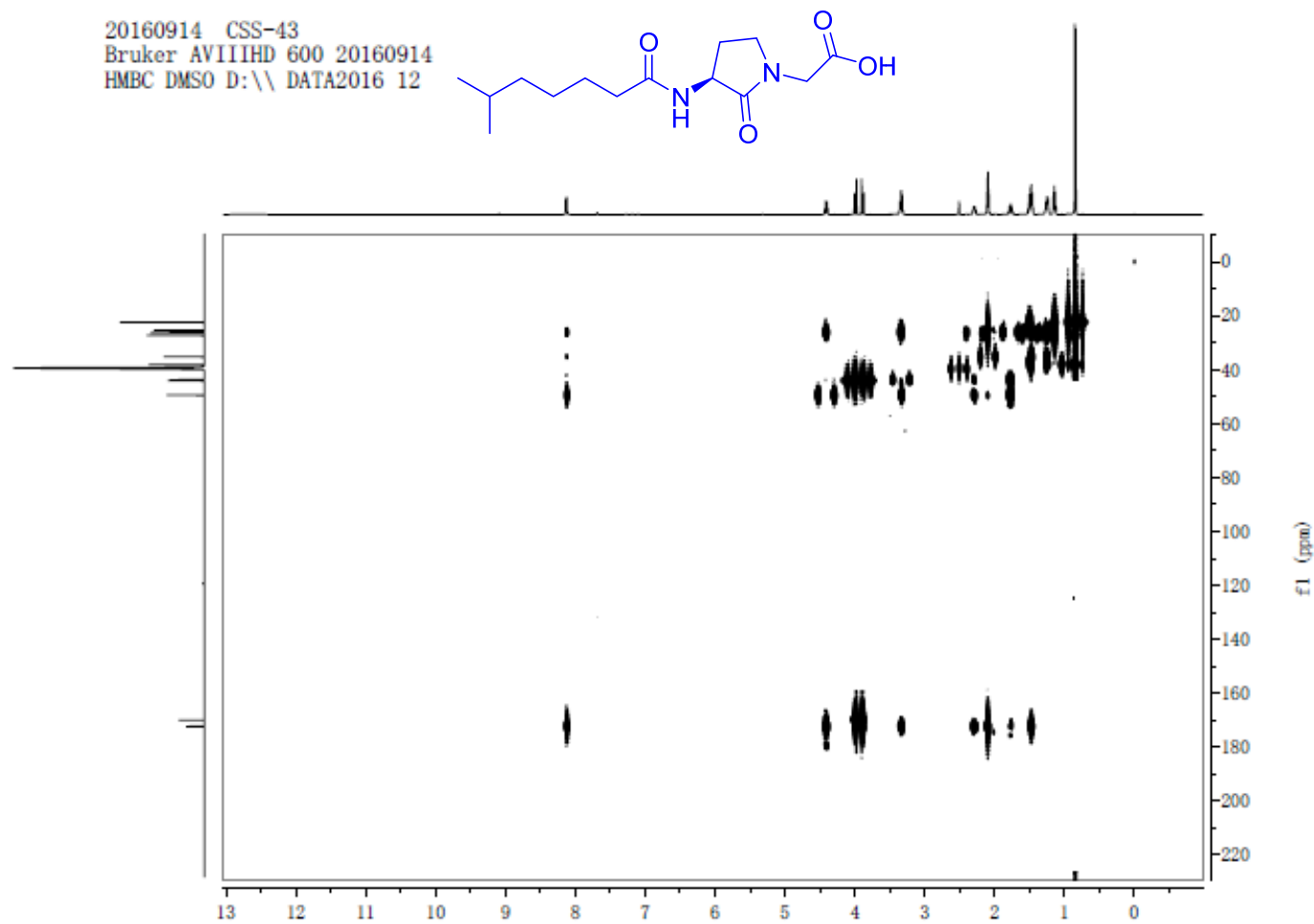


Figure S26. The HMBC Spectrum of Compound **3** in DMSO- d_6

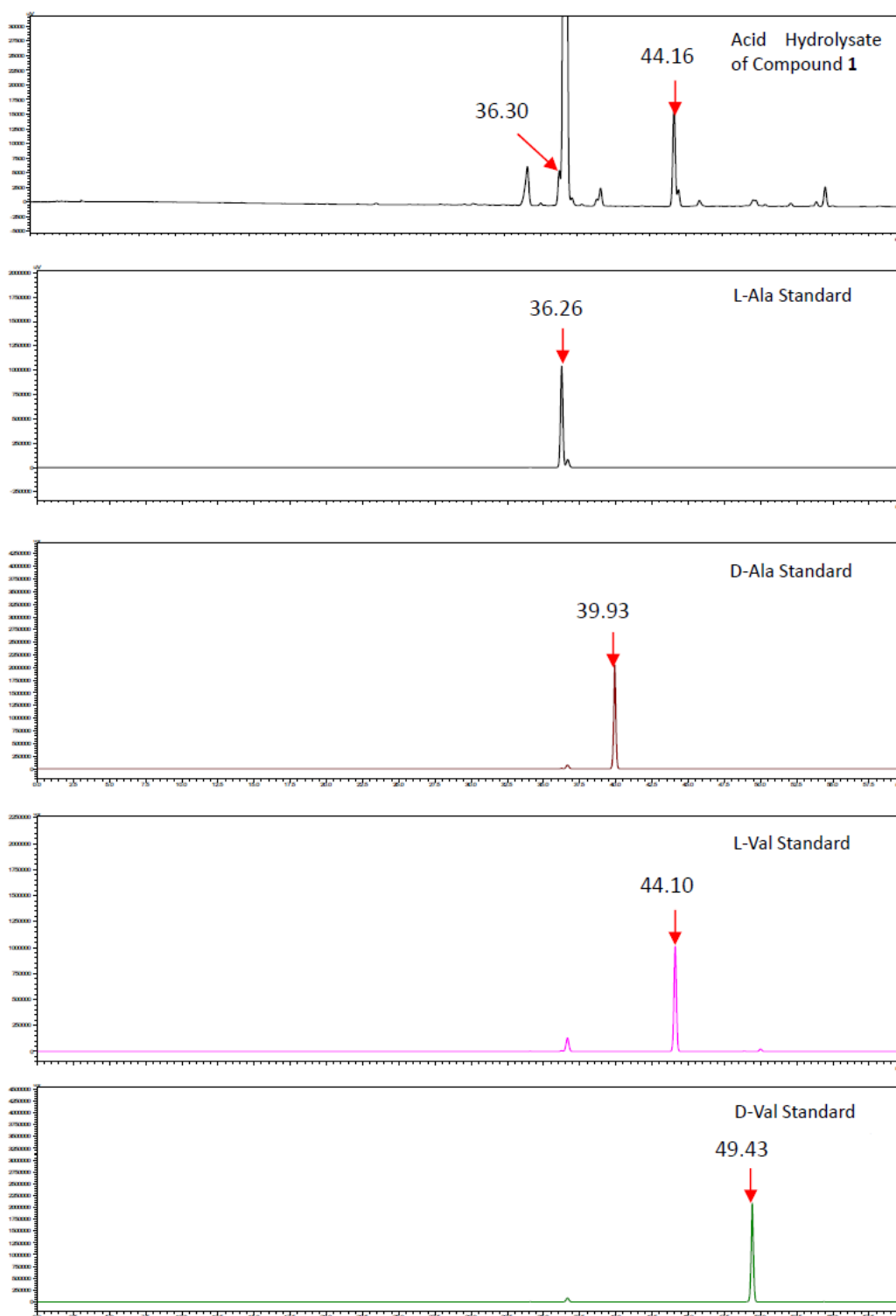


Figure S27. Marfey's Analysis of Acid Hydrolysate of Compound 1 (t_R min)

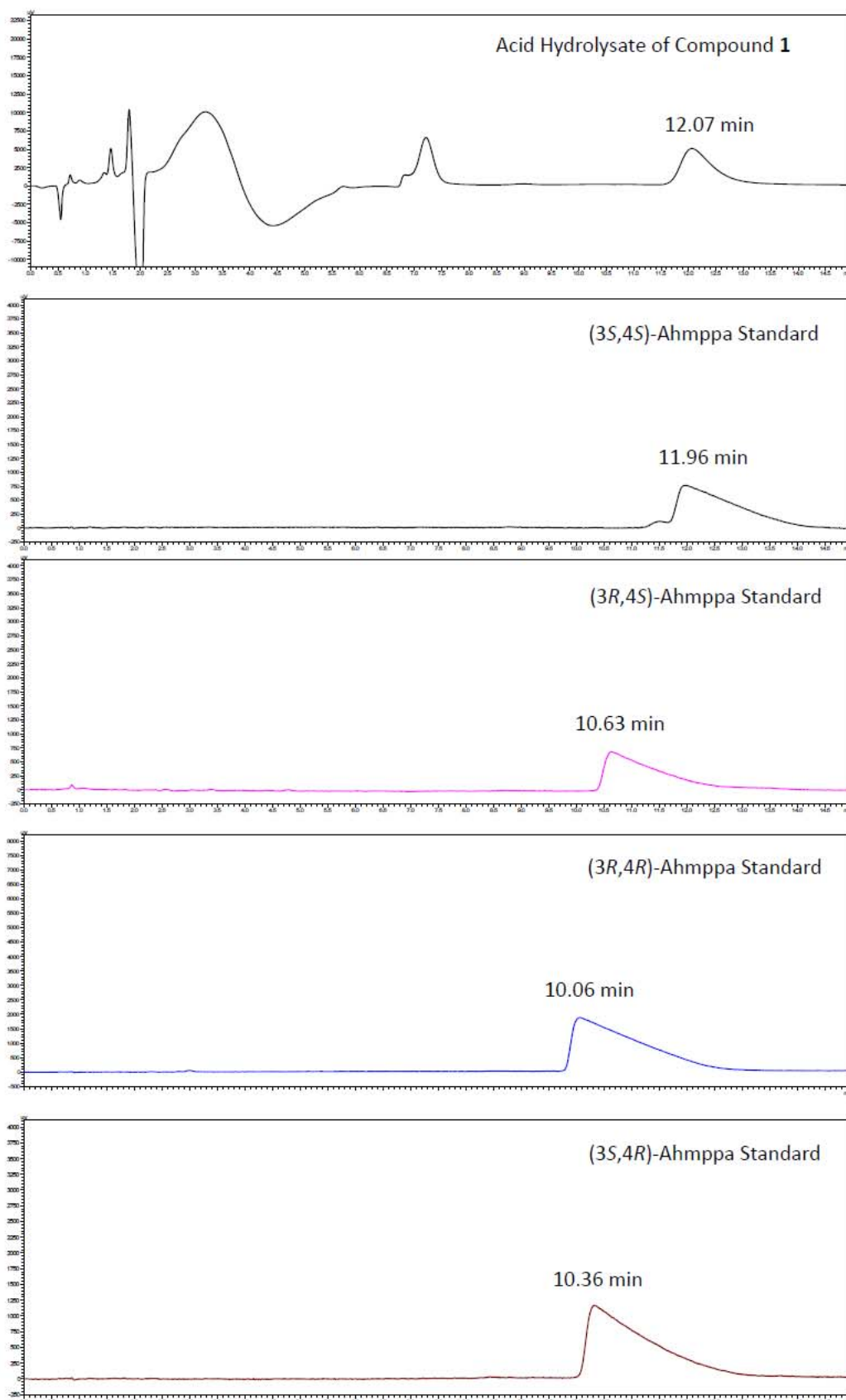


Figure S28. Chiral-phase HPLC Analysis of Acid Hydrolysate of Compound **1** (t_R min)