

Supplementary Material

Solution-Phase Total Synthesis of Teixobactin

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Content

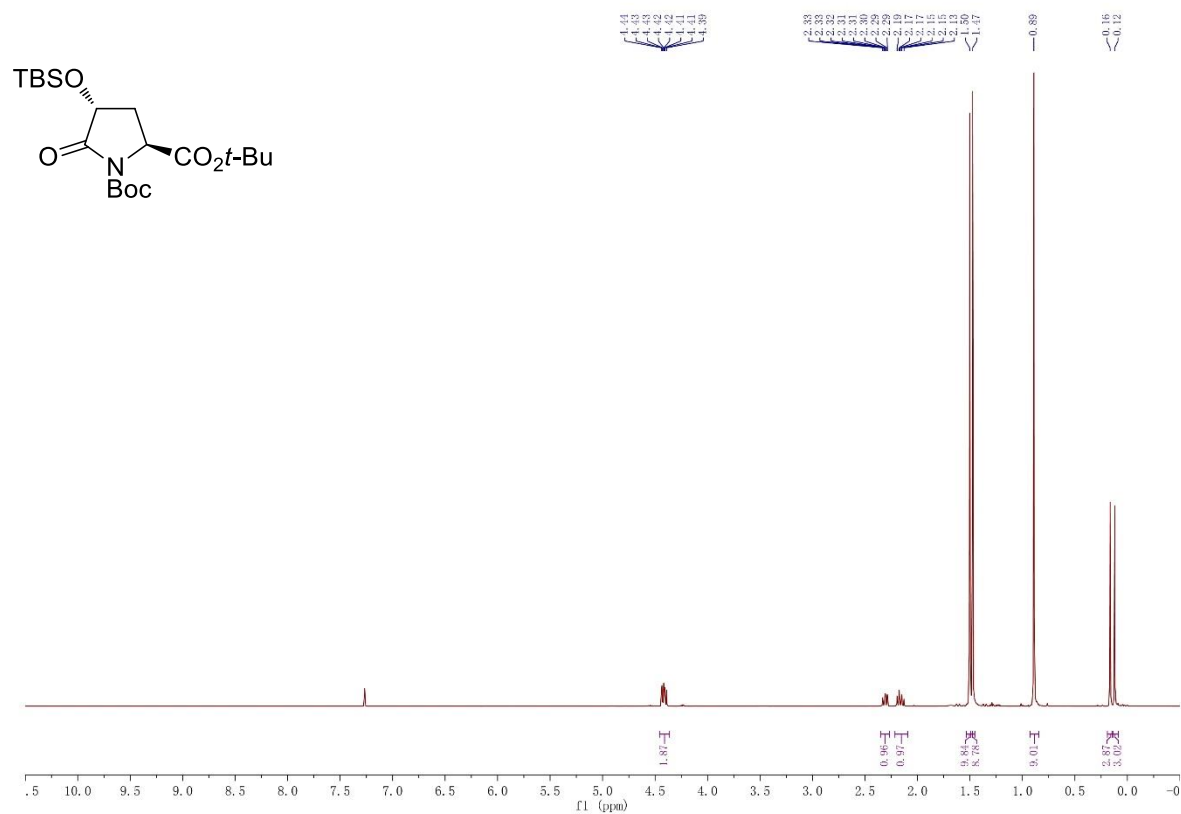
Spectra for new compounds	S2-S22
MIC determination	S23-S24
HPLC analysis of teixobactin	S25

TBS ether of 8, ¹H NMR (500 MHz, CDCl₃)

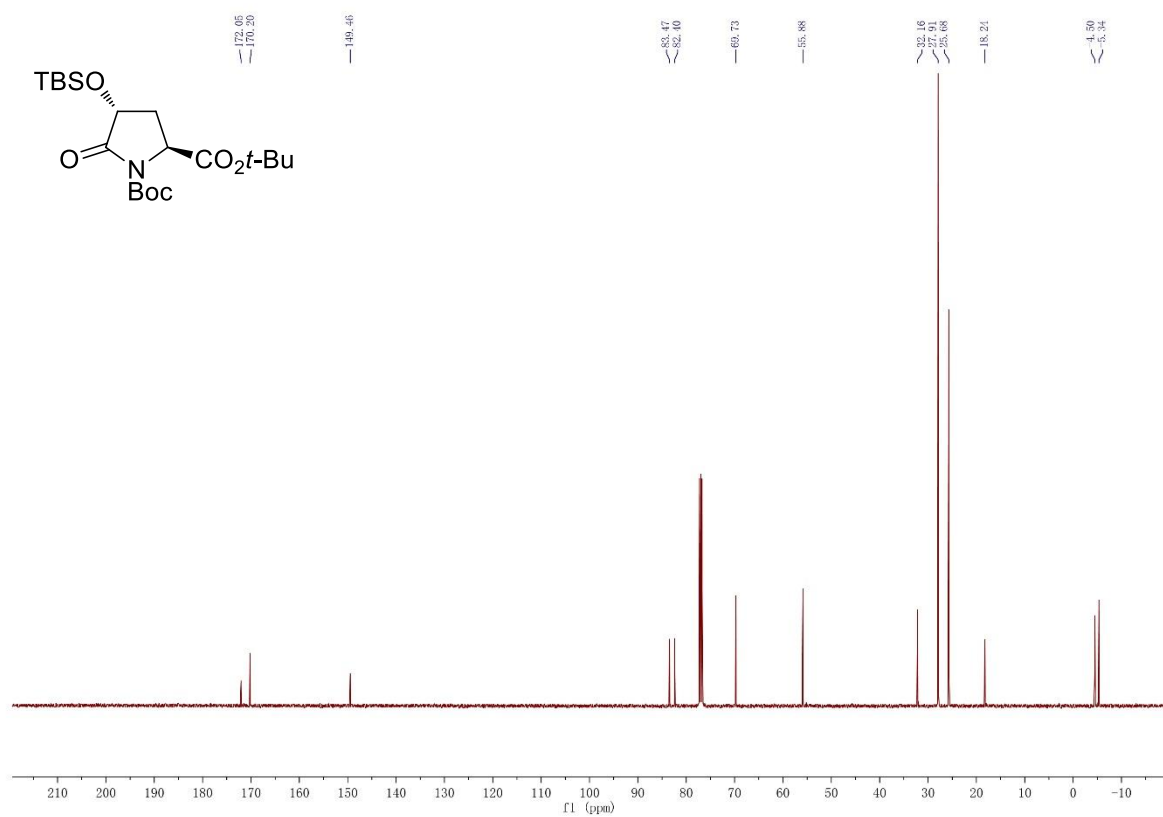


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Pyroglutamate 9, ^1H NMR (500 MHz, CDCl_3)

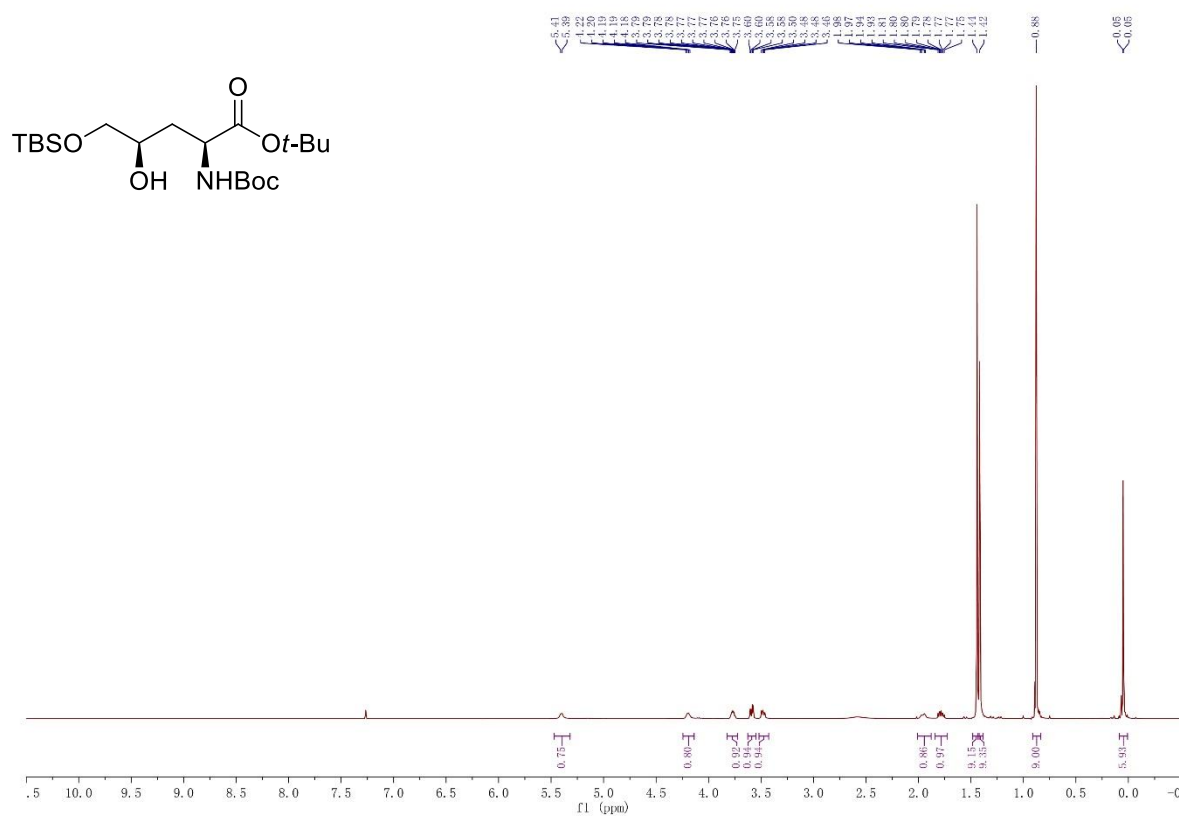


Pyroglutamate 9, ^{13}C NMR (125 MHz, CDCl_3)

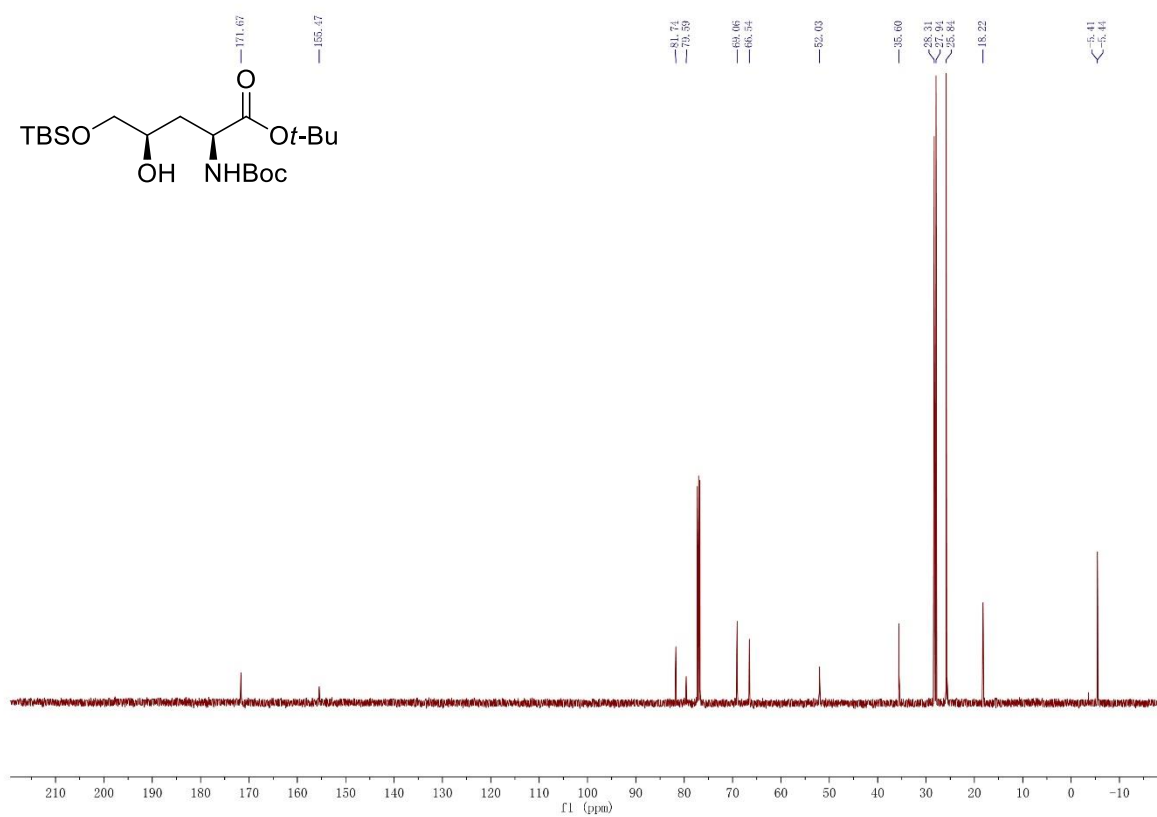


Supplementary Material

Alcohol 10, ^1H NMR (500 MHz, CDCl_3)



Alcohol 10, ^{13}C NMR (125 MHz, CDCl_3)



Ketone 11, ¹H NMR (500 MHz, CDCl₃)

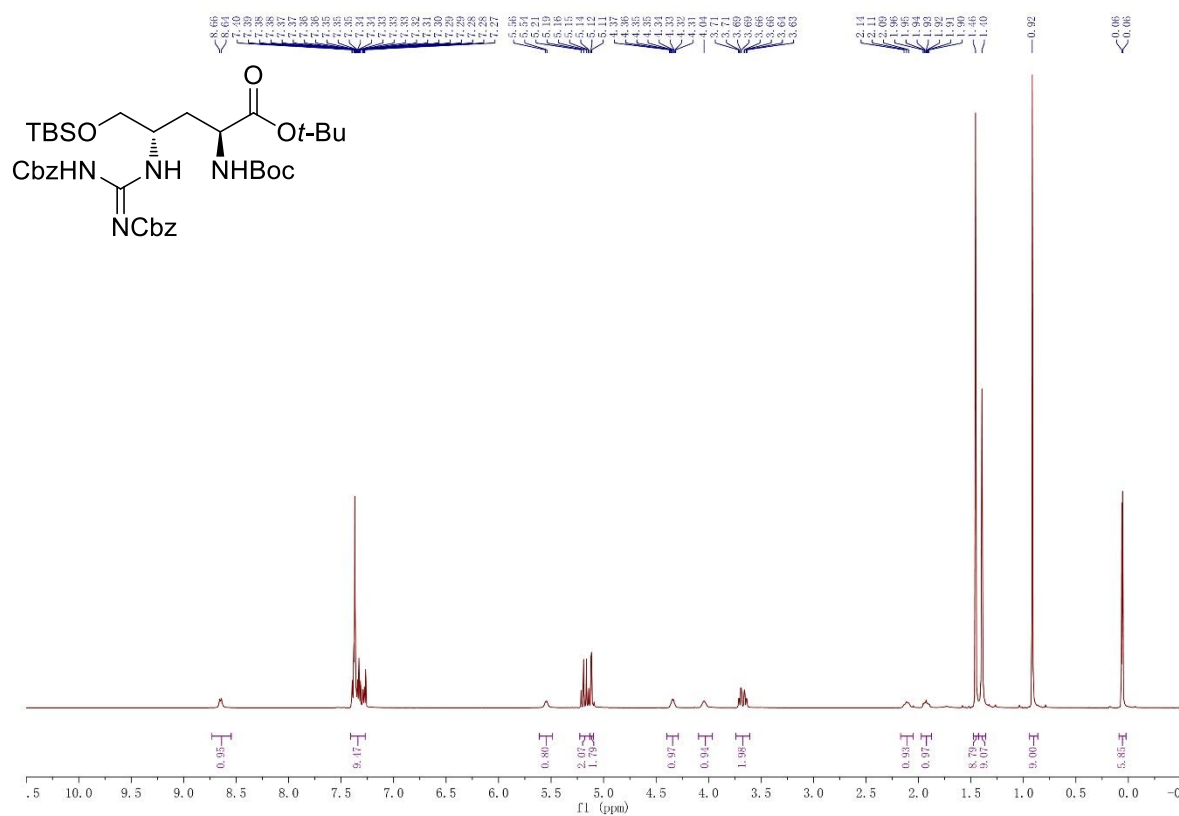


Amine 12, ^1H NMR (500 MHz, CDCl_3)

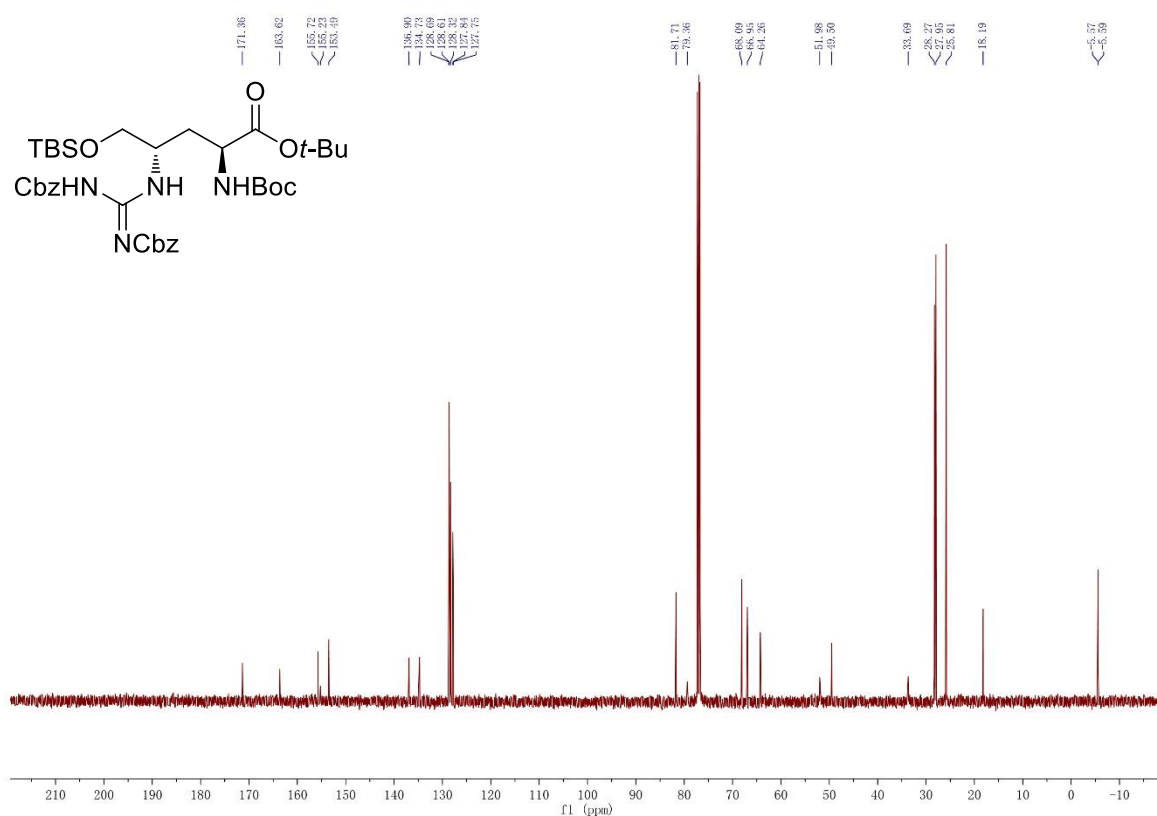


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Guanidinyl compound 14, ^1H NMR (500 MHz, CDCl_3)

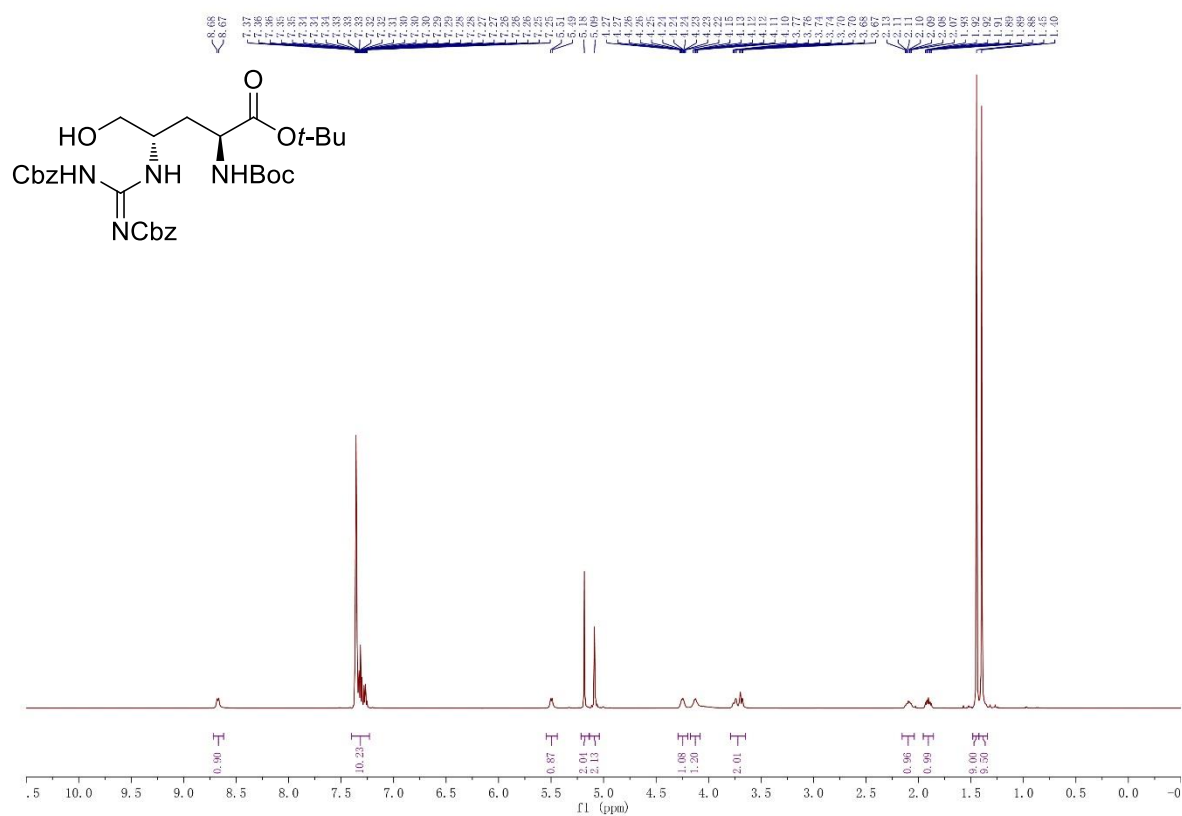


Guanidinyl compound 14, ^{13}C NMR (125 MHz, CDCl_3)

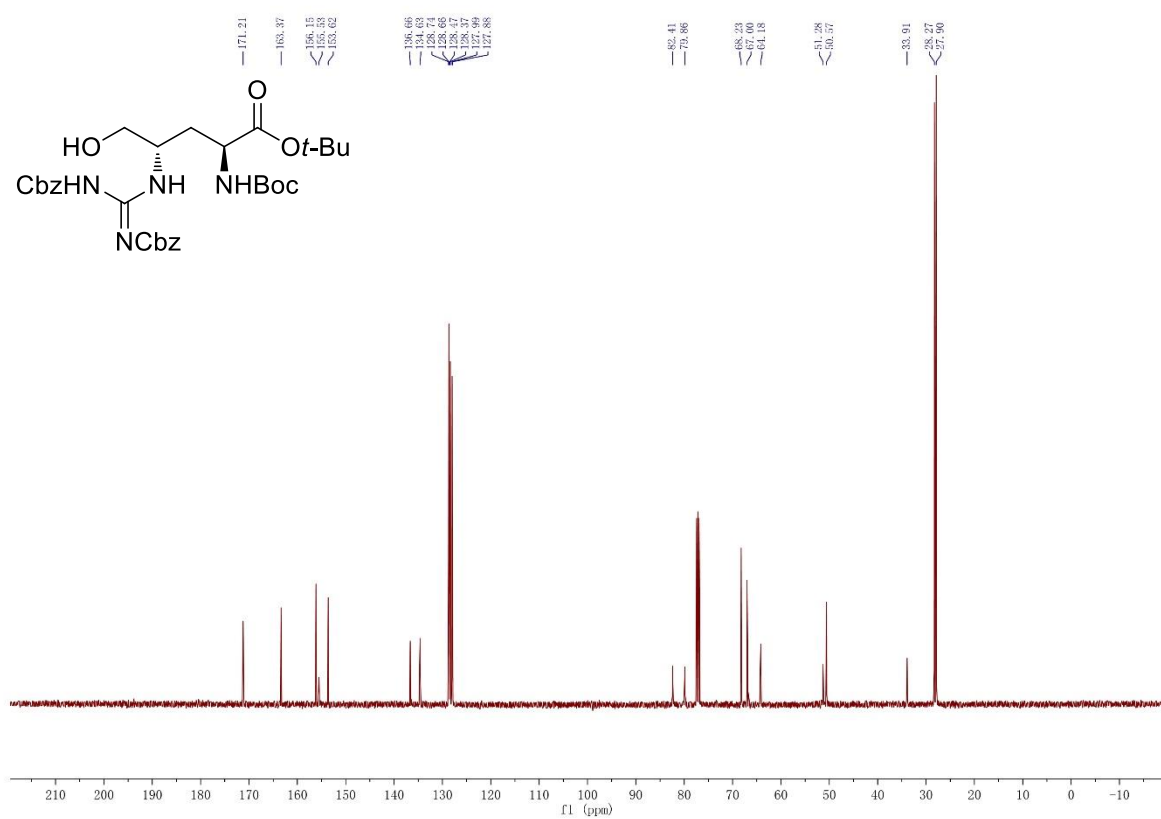


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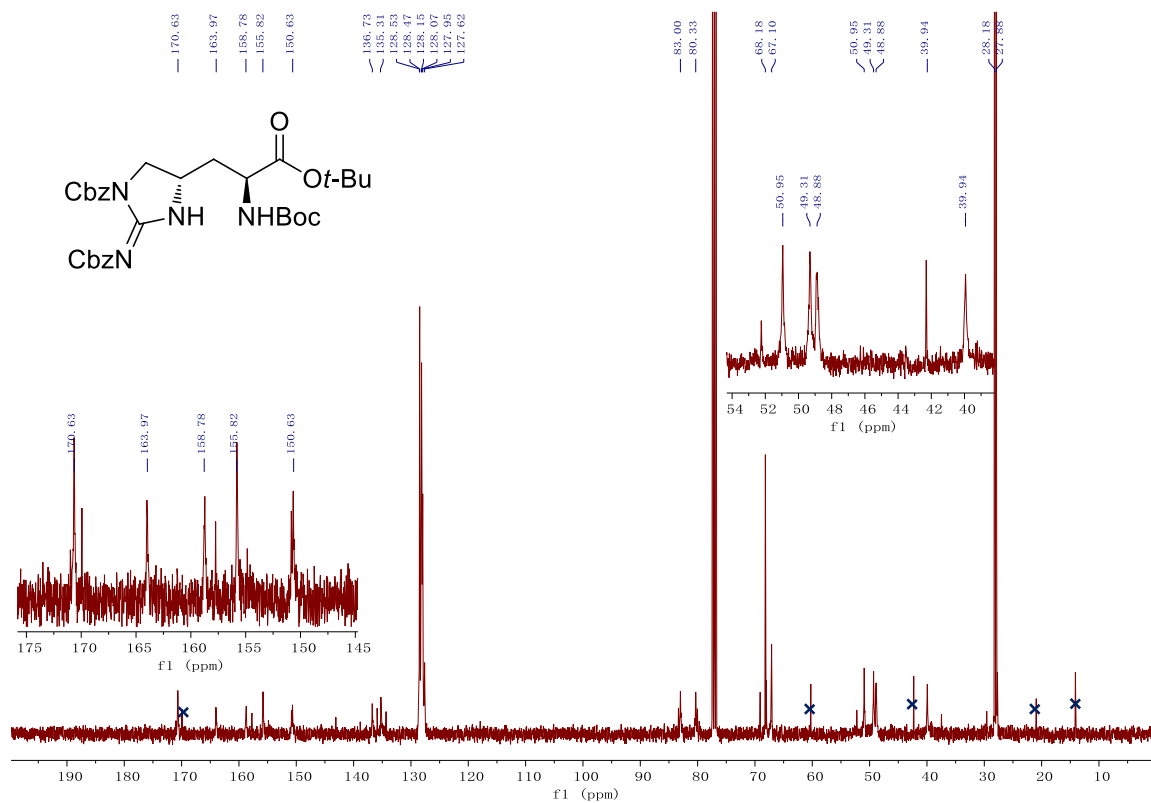
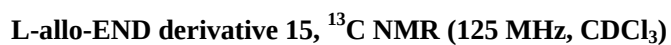
Primary alcohol, ^1H NMR (500 MHz, CDCl_3)



Primary alcohol, ^{13}C NMR (125 MHz, CDCl_3)

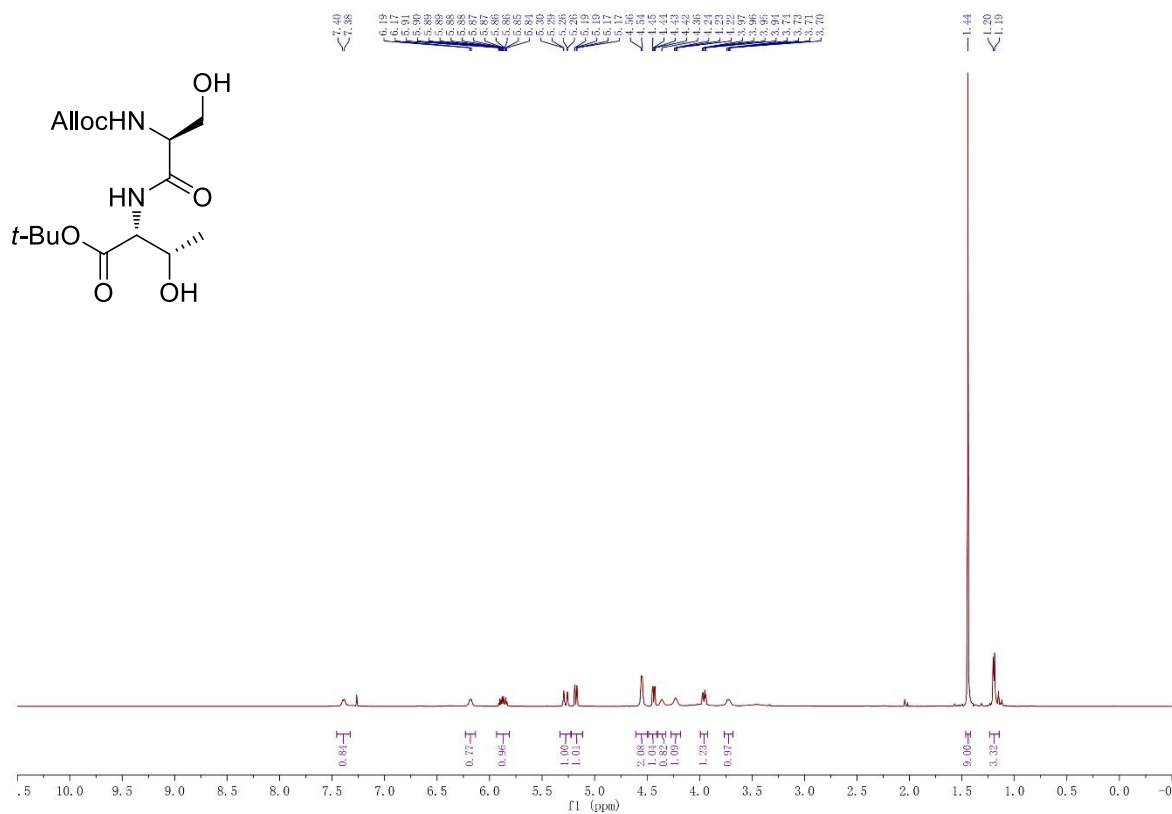


L-*allo*-END derivative 15, ¹H NMR (500 MHz, CDCl₃)

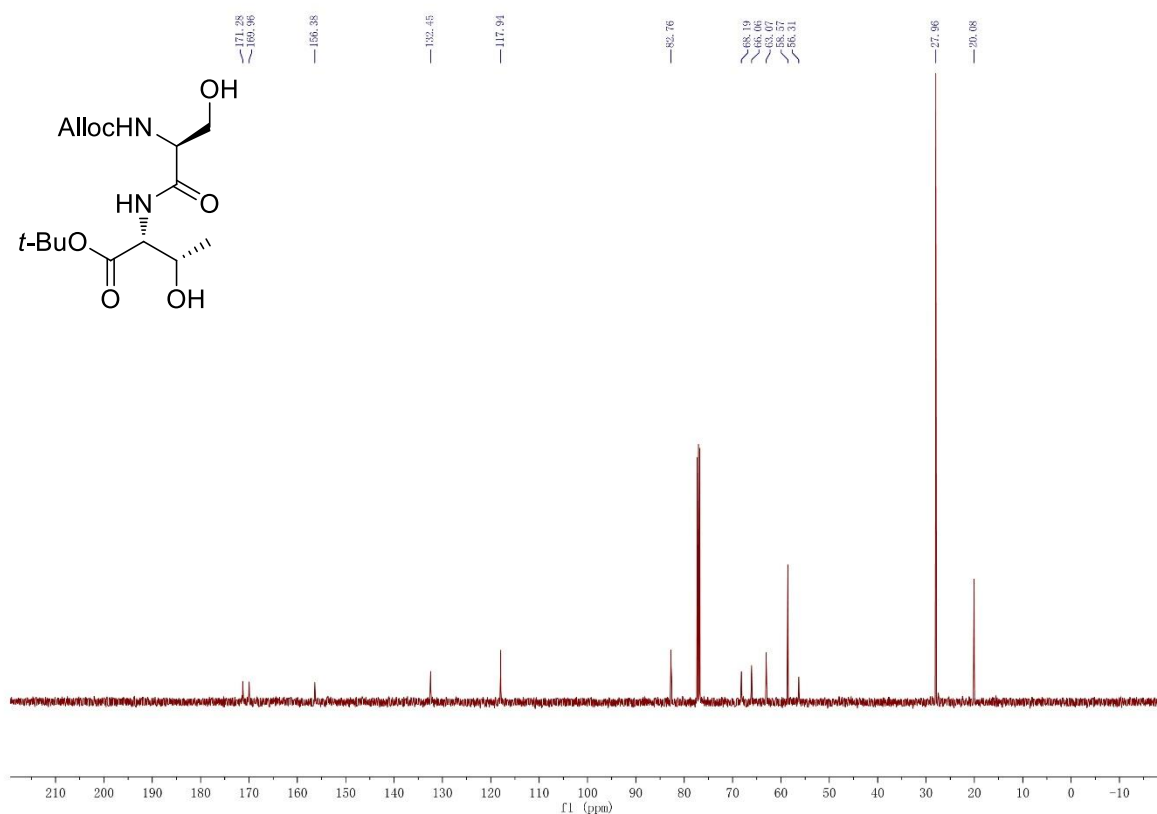


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Alloc-Ser-Thr-OBu^t, ¹H NMR (500 MHz, CDCl₃)

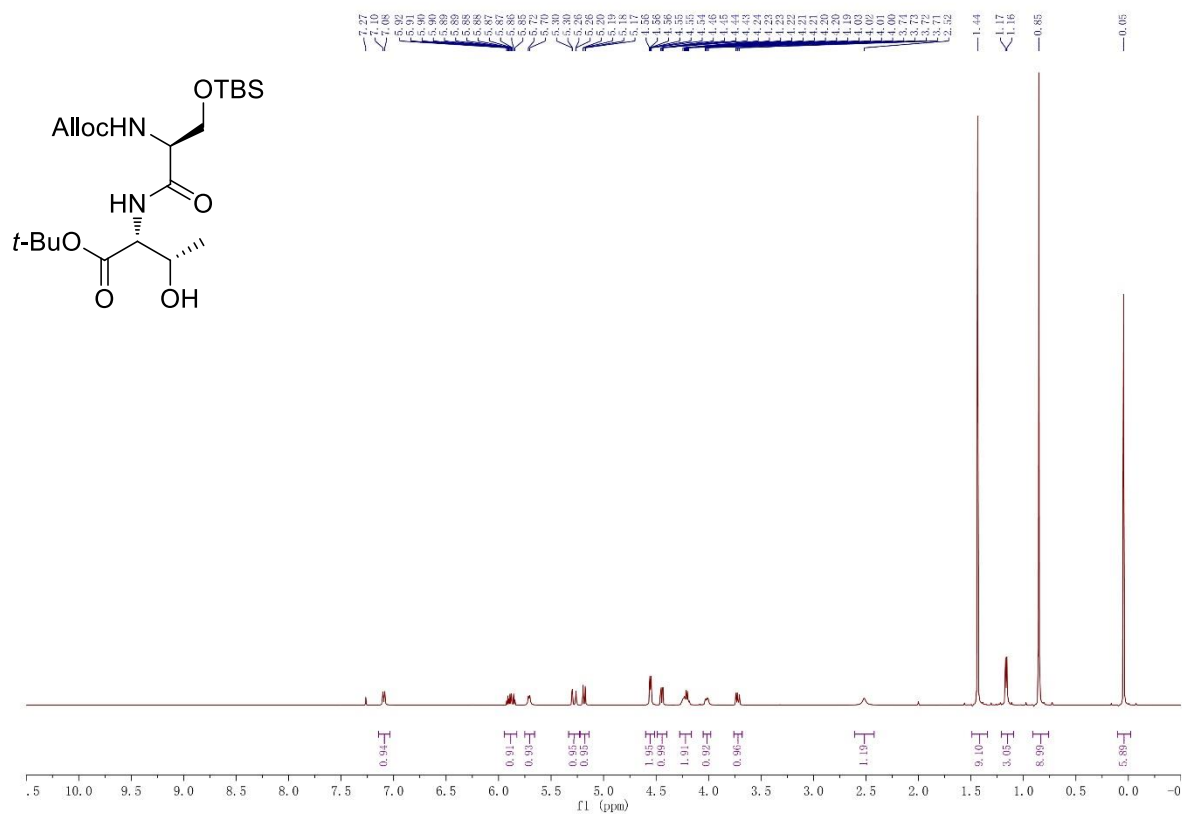


Alloc-Ser-Thr-OBu^t, ¹³C NMR (125 MHz, CDCl₃)

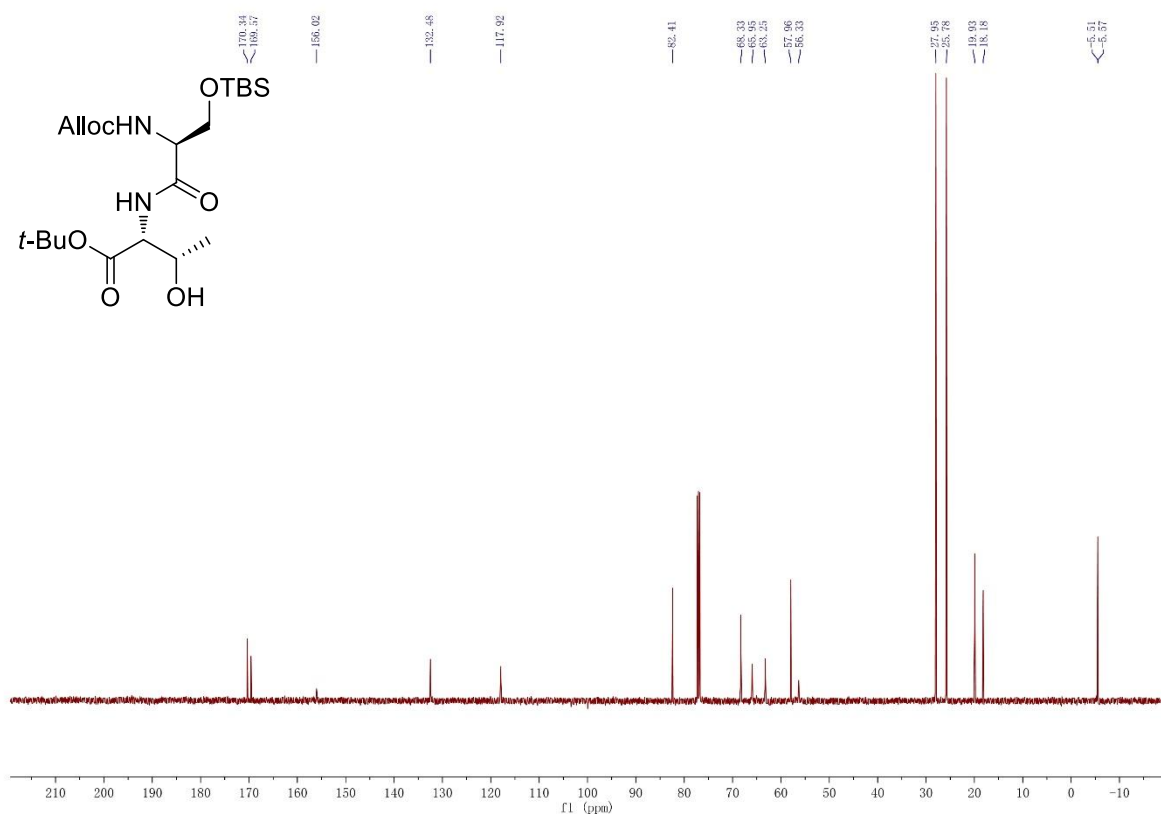


Supplementary Material

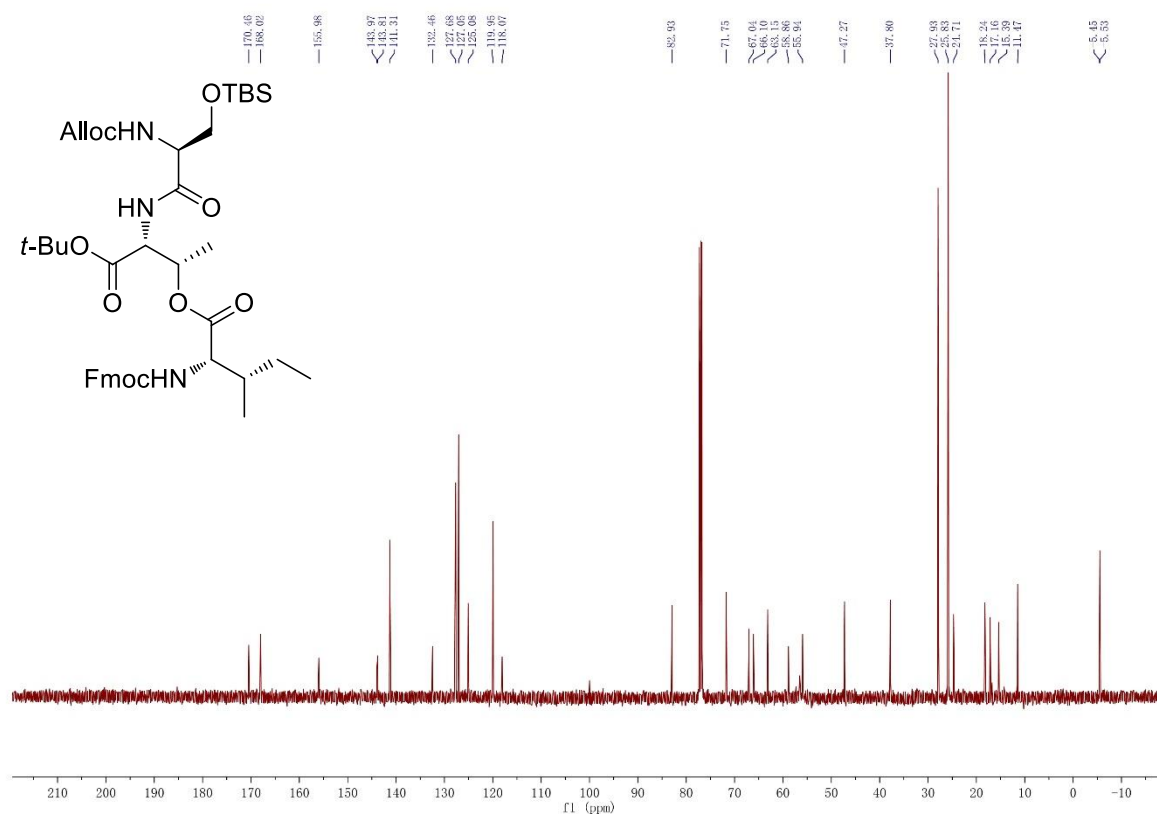
Dipeptide 24, ^1H NMR (500 MHz, CDCl_3)



Dipeptide 24, ^{13}C NMR (125 MHz, CDCl_3)



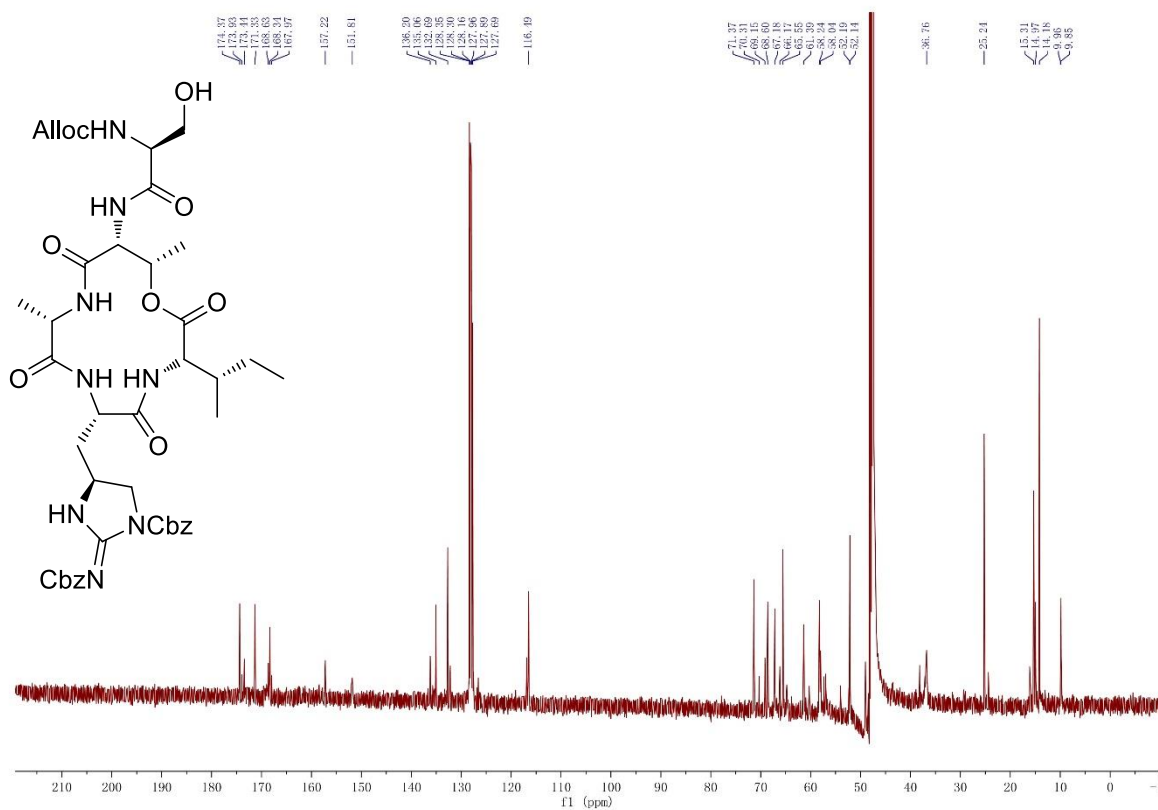
Tripeptide 6a, ¹H NMR (500 MHz, CDCl₃)



Pentapeptide 25, ^1H NMR (500 MHz, CDCl_3)

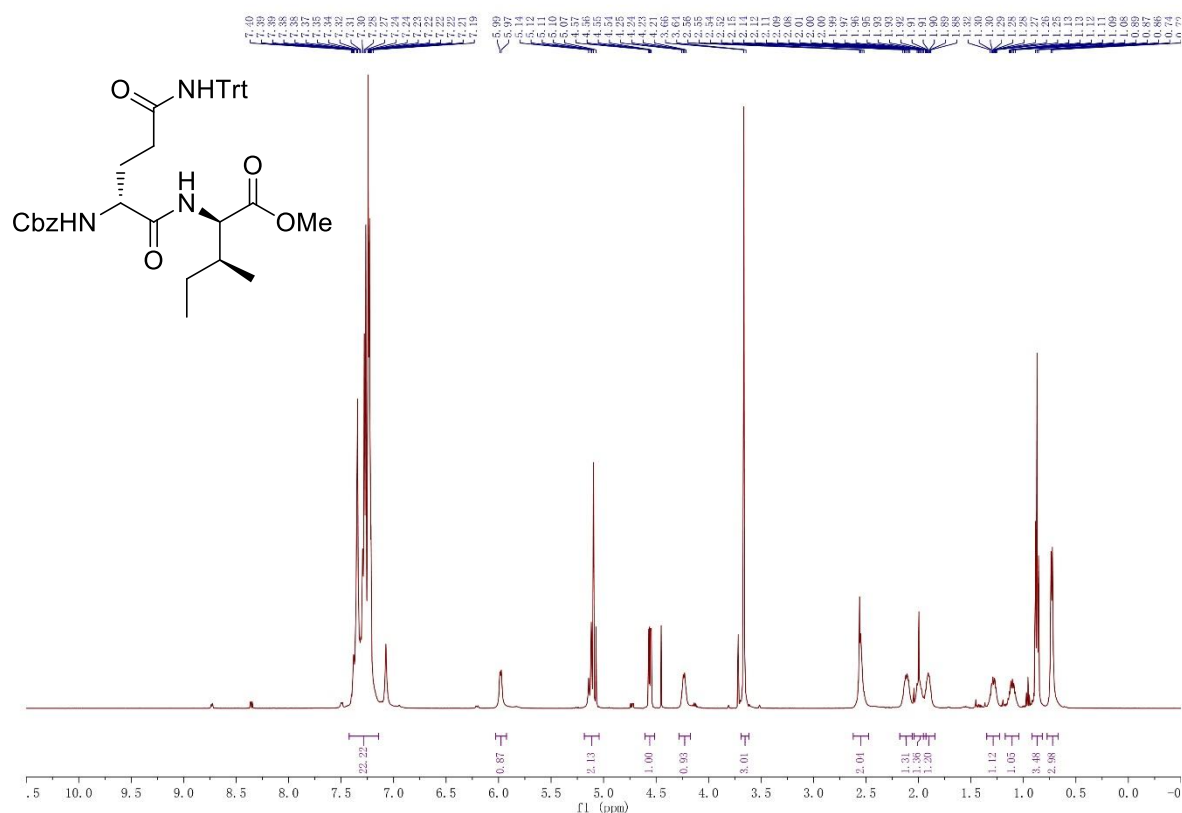


Compound 3a, ¹H NMR (500 MHz, CD₃OD)

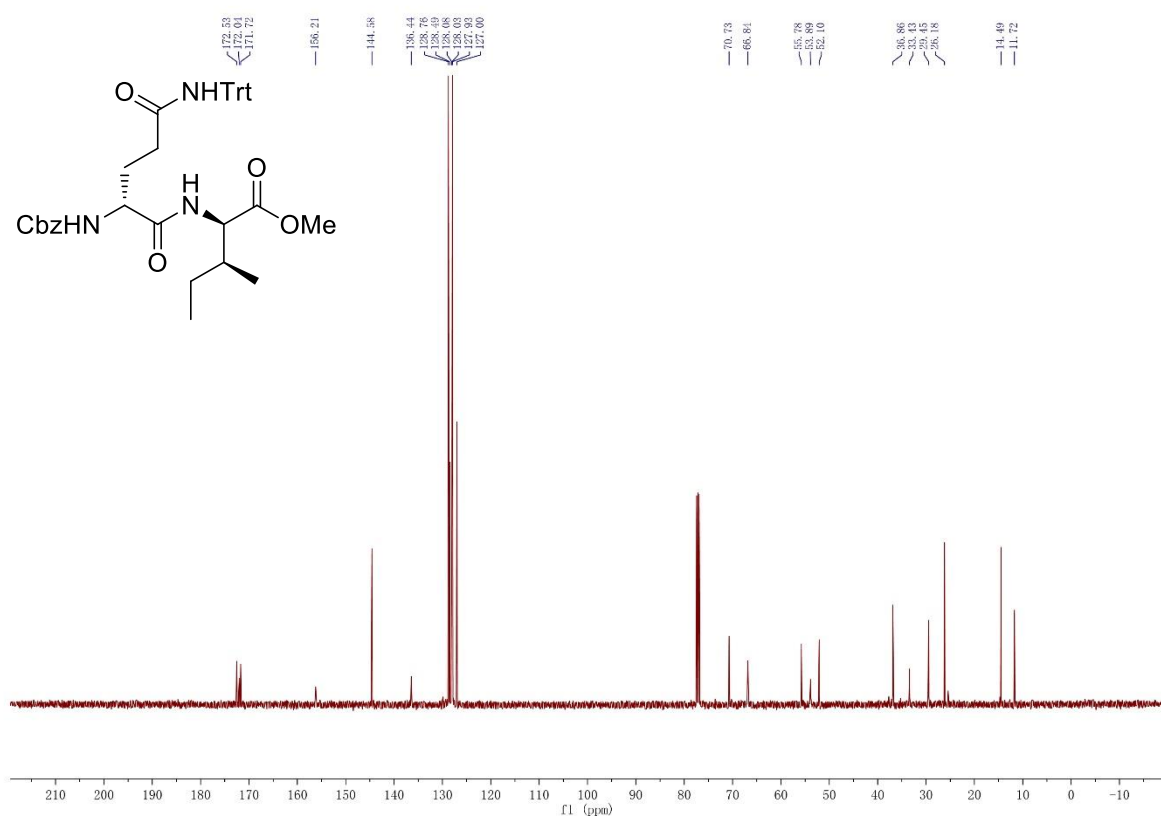


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Cbz-Gln(Tr)-allo-Ile-OMe, ^1H NMR (500 MHz, CDCl_3)



Cbz-Gln(Tr)-allo-Ile-OMe, ^{13}C NMR (125 MHz, CDCl_3)

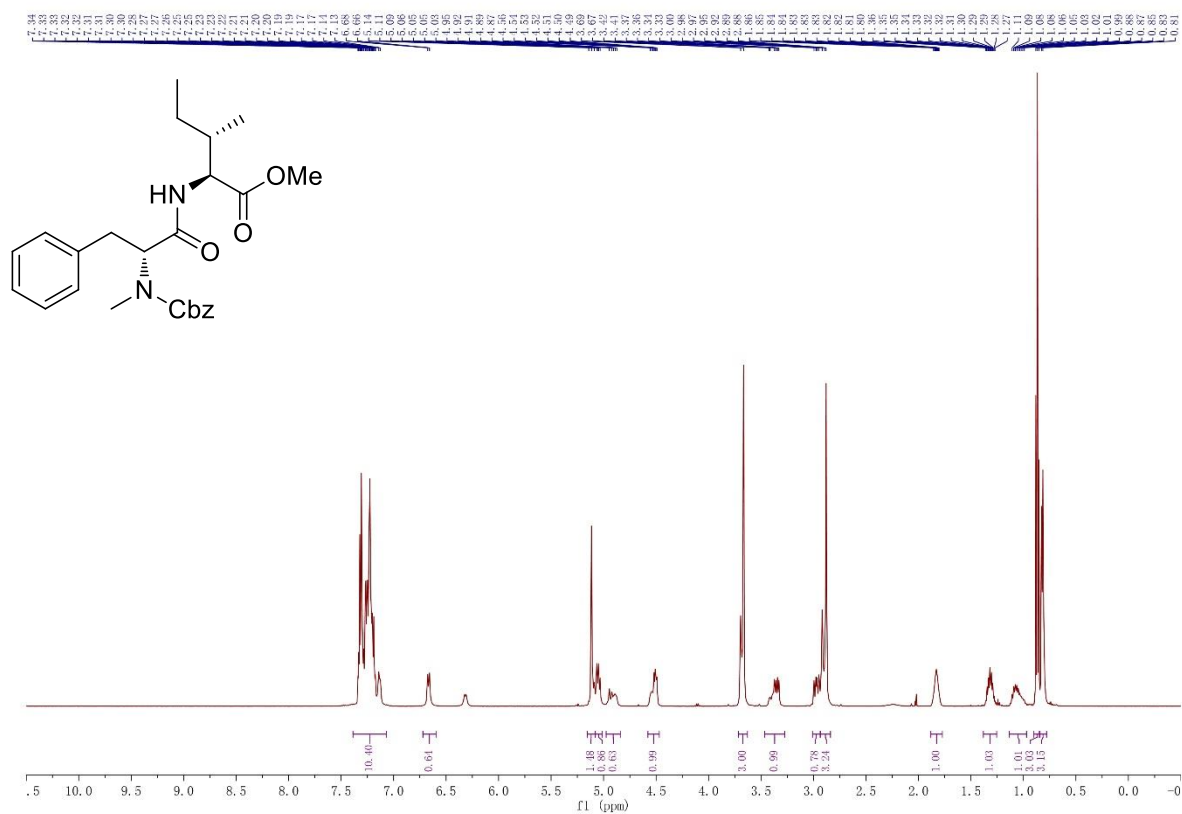


Tripeptide 4, ¹H NMR (500 MHz, CDCl₃)

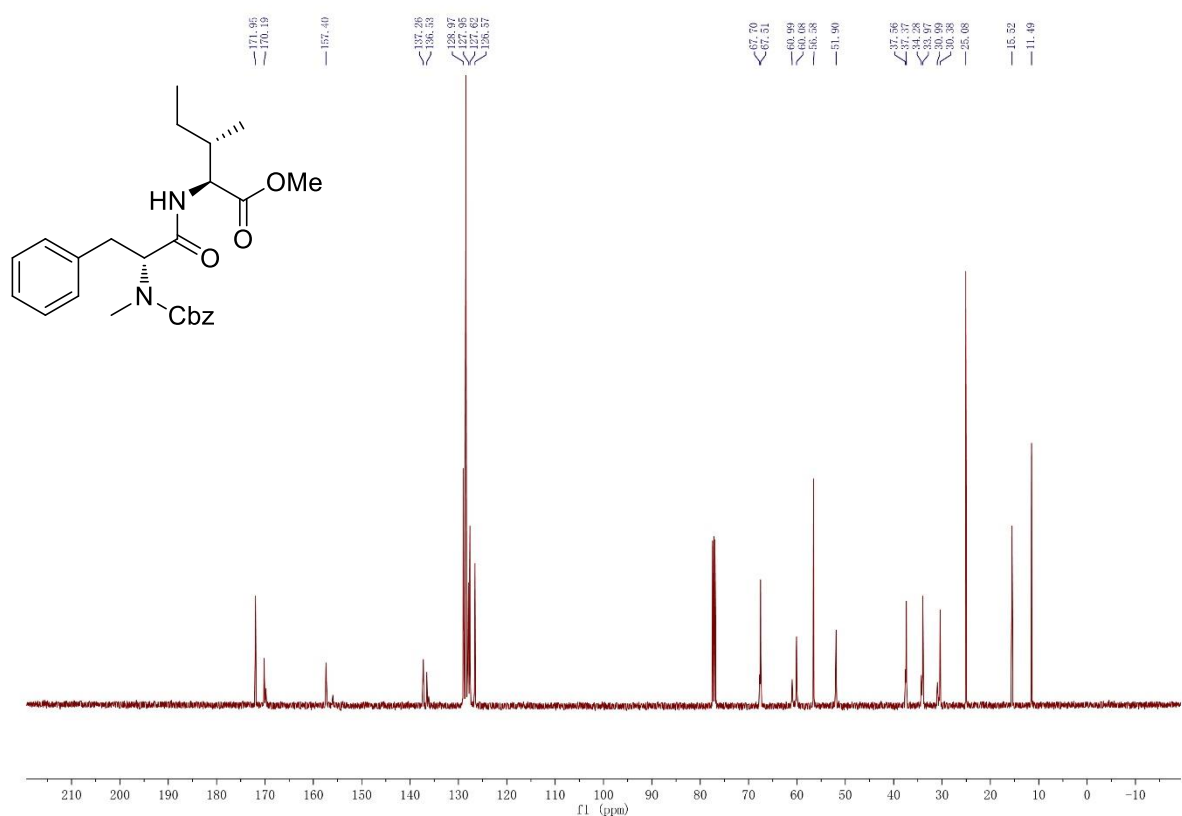


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Cbz-NMe-Phe-Ile-OMe, ^1H NMR (500 MHz, CDCl_3)

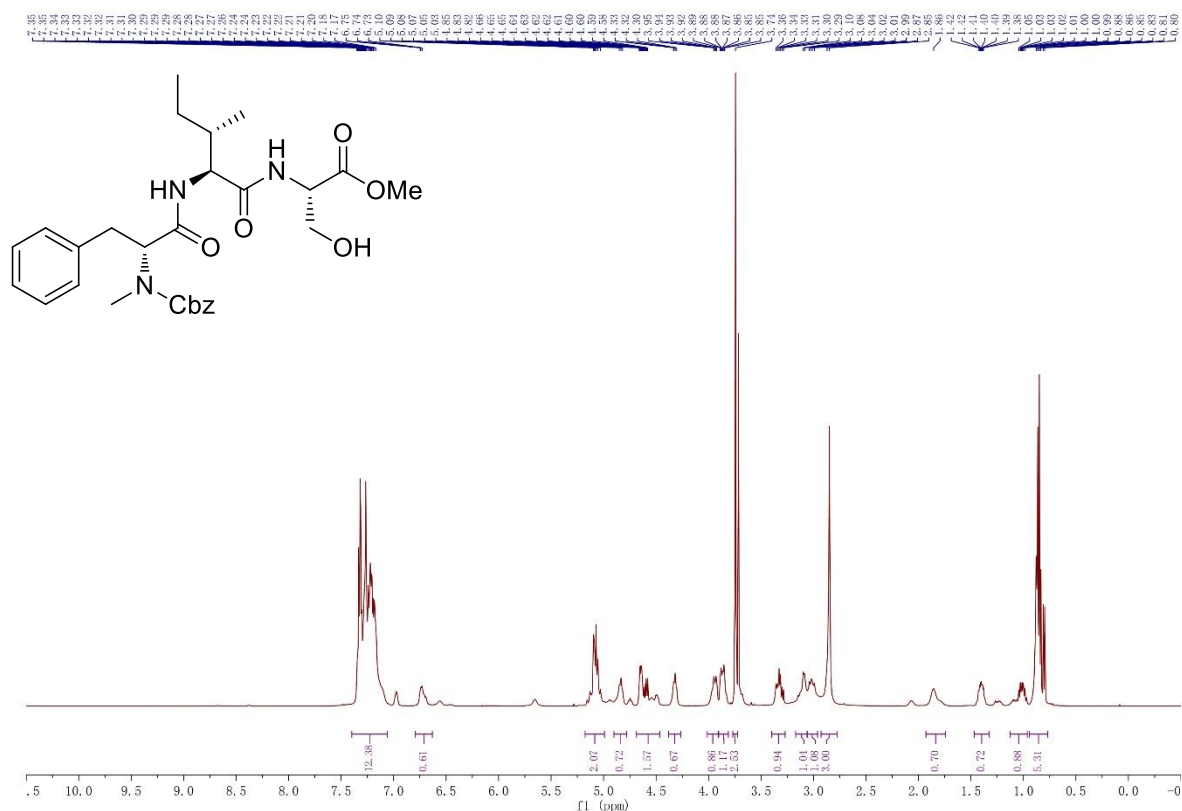


Cbz-NMe-Phe-Ile-OMe, ^{13}C NMR (125 MHz, CDCl_3)

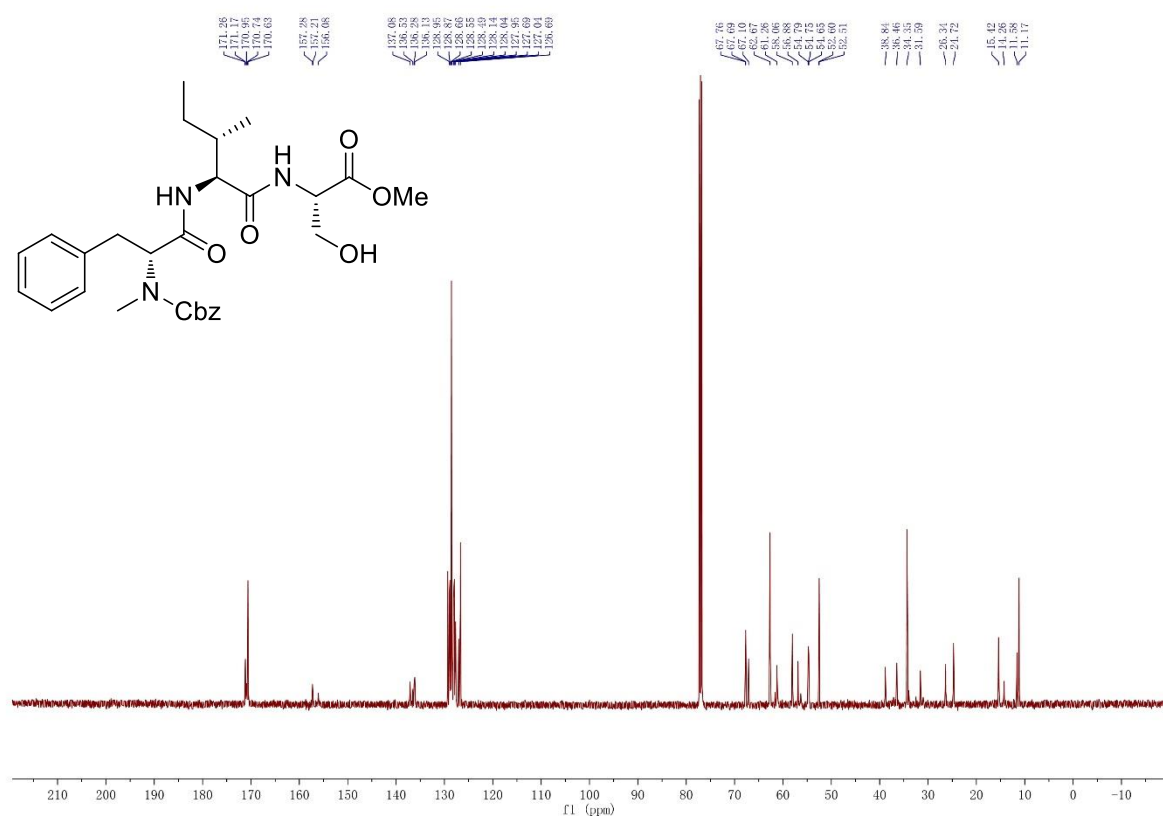


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Tripeptide 30, ^1H NMR (500 MHz, CDCl_3)

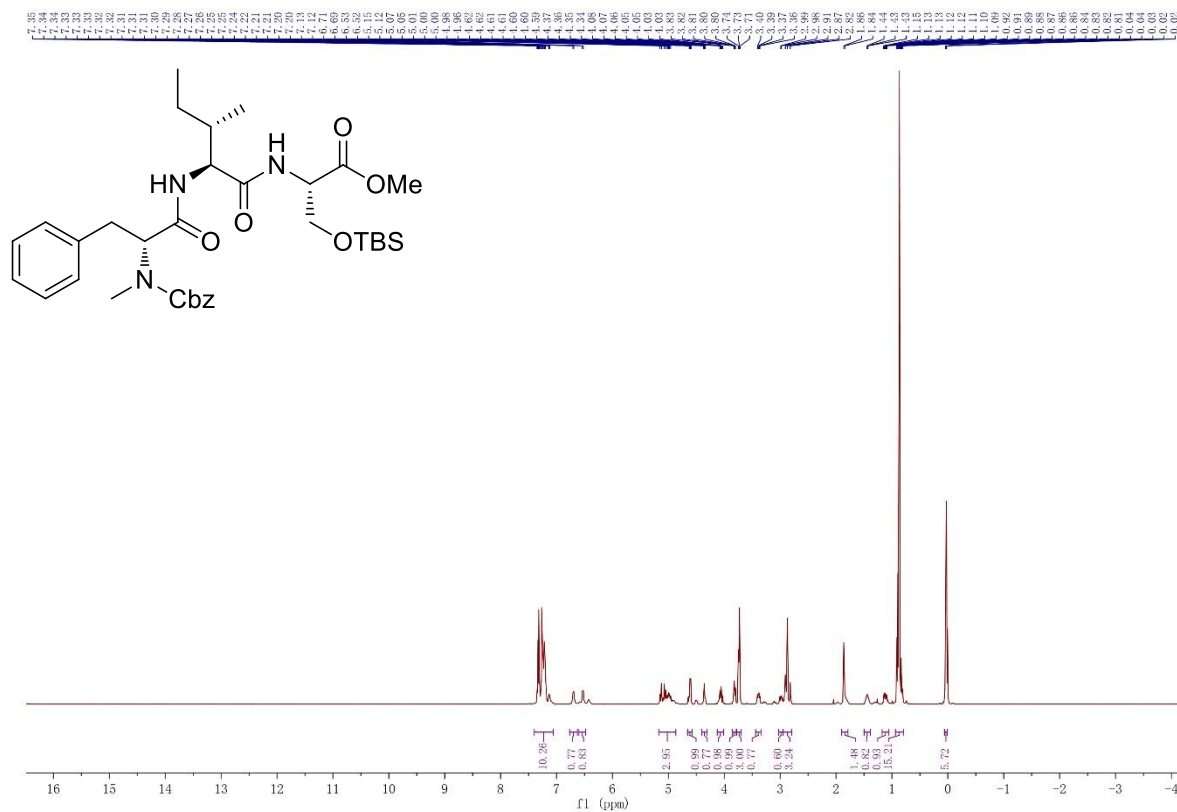


Tripeptide 30, ^{13}C NMR (125 MHz, CDCl_3)

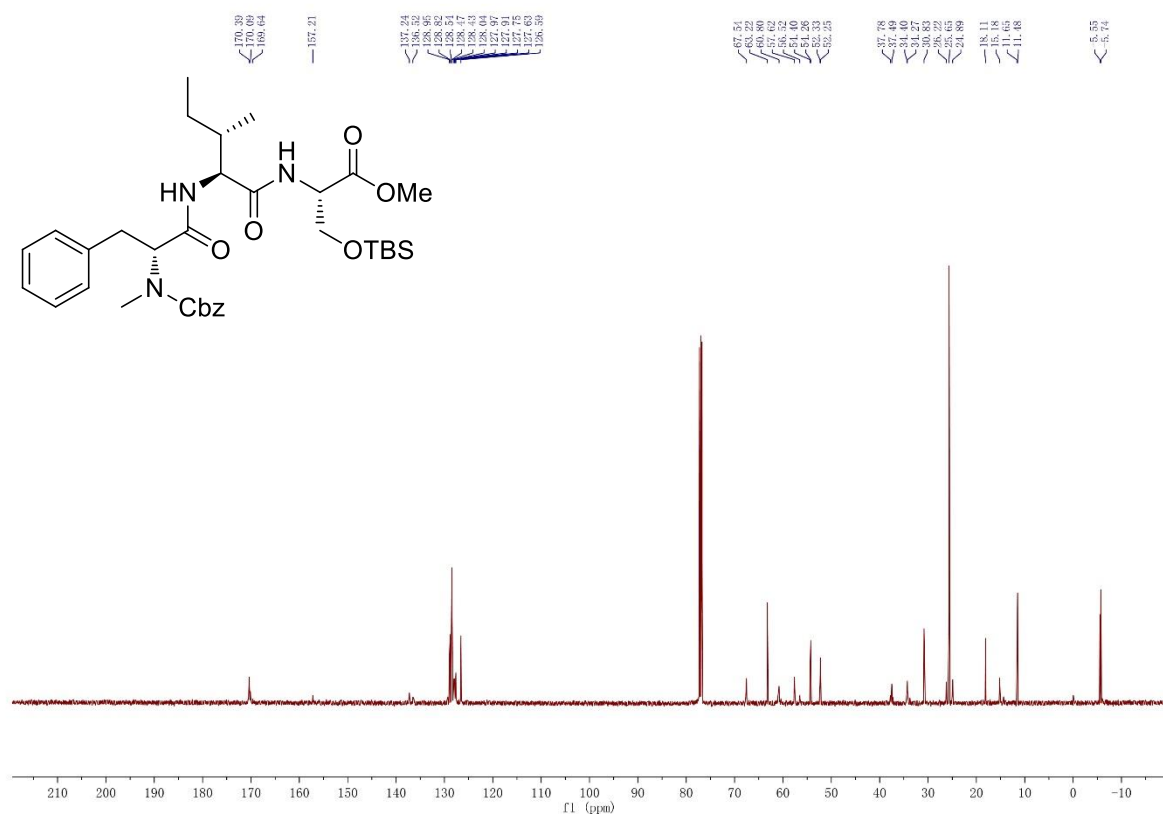


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Tripeptide 5, ^1H NMR (500 MHz, CDCl_3)

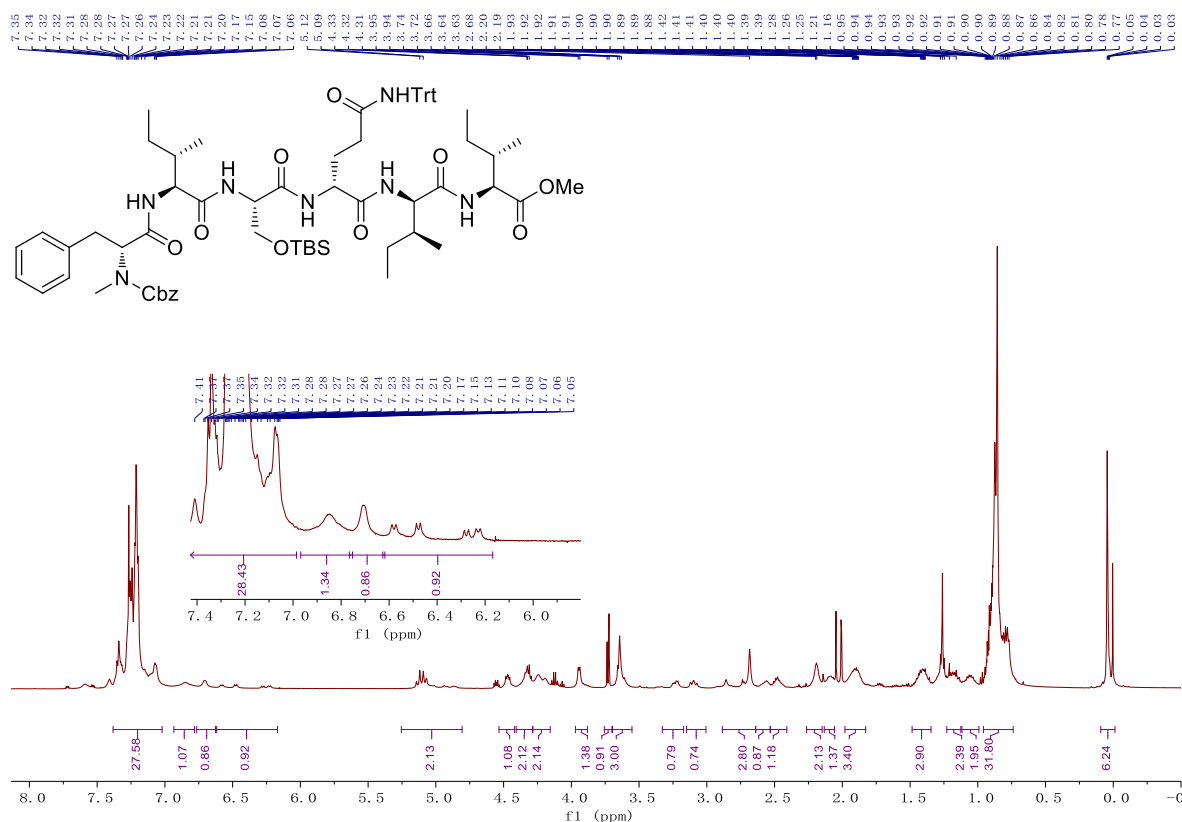


Tripeptide 5, ^{13}C NMR (125 MHz, CDCl_3)

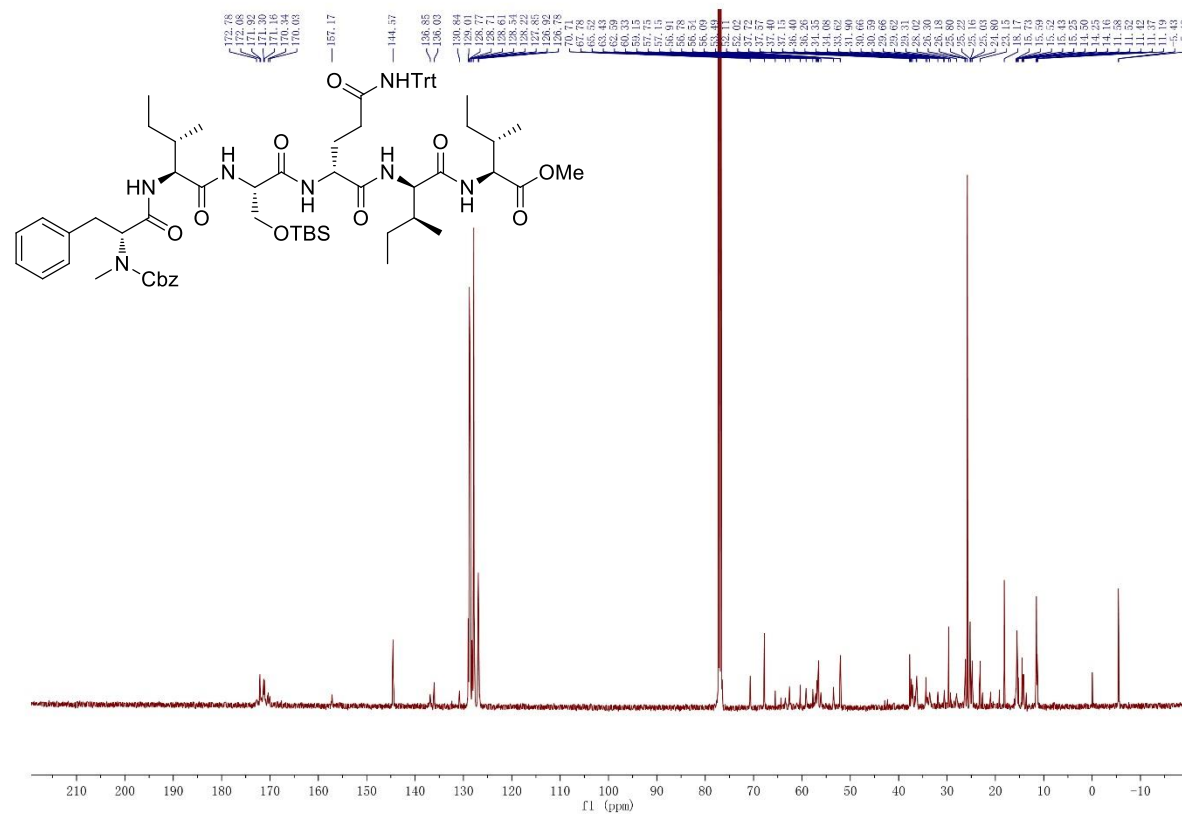


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Side-chain hexapeptide 2, ^1H NMR (500 MHz, CDCl_3)

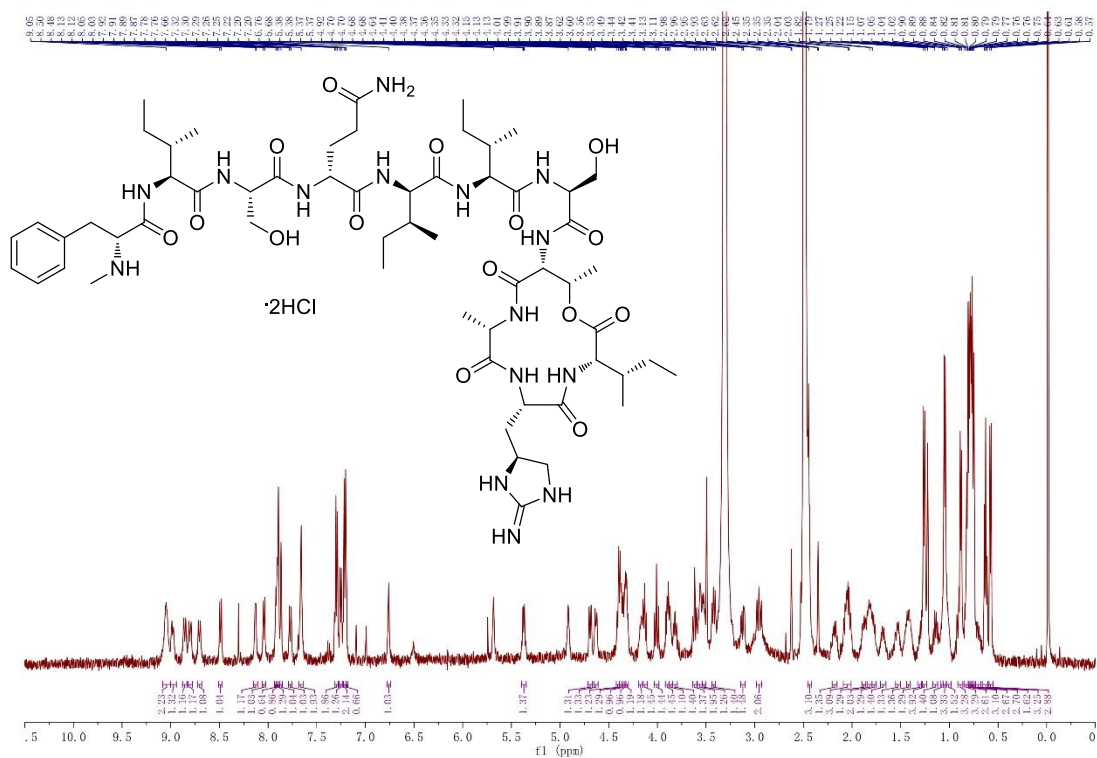


Side-chain hexapeptide 2, ^{13}C NMR (125 MHz, CDCl_3)

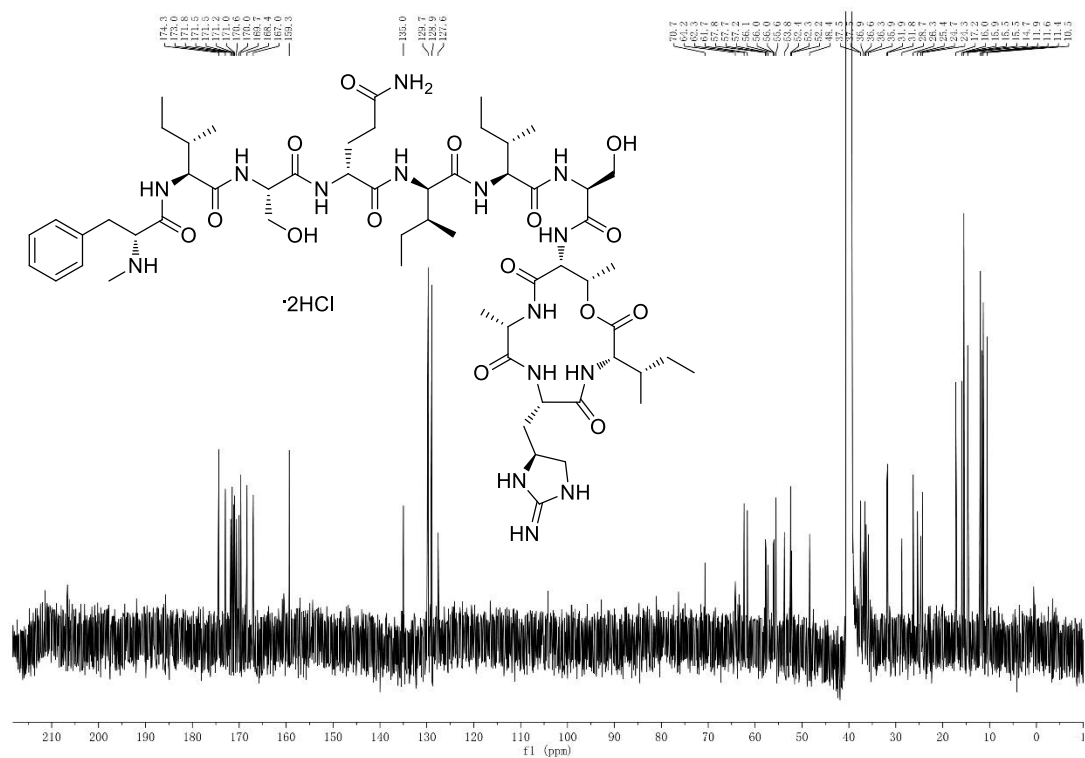


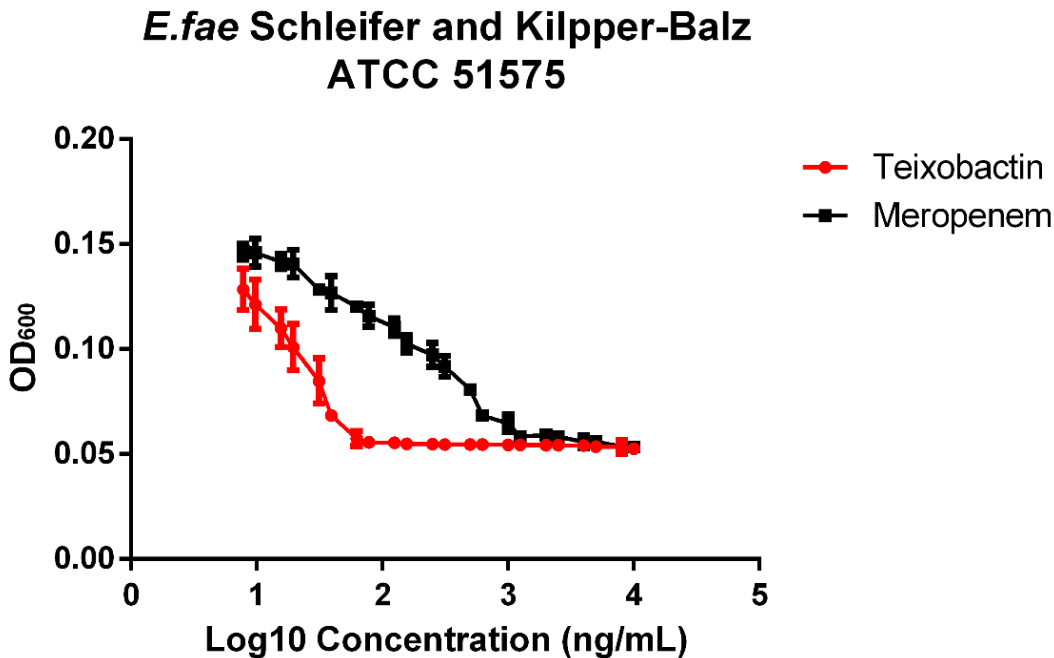
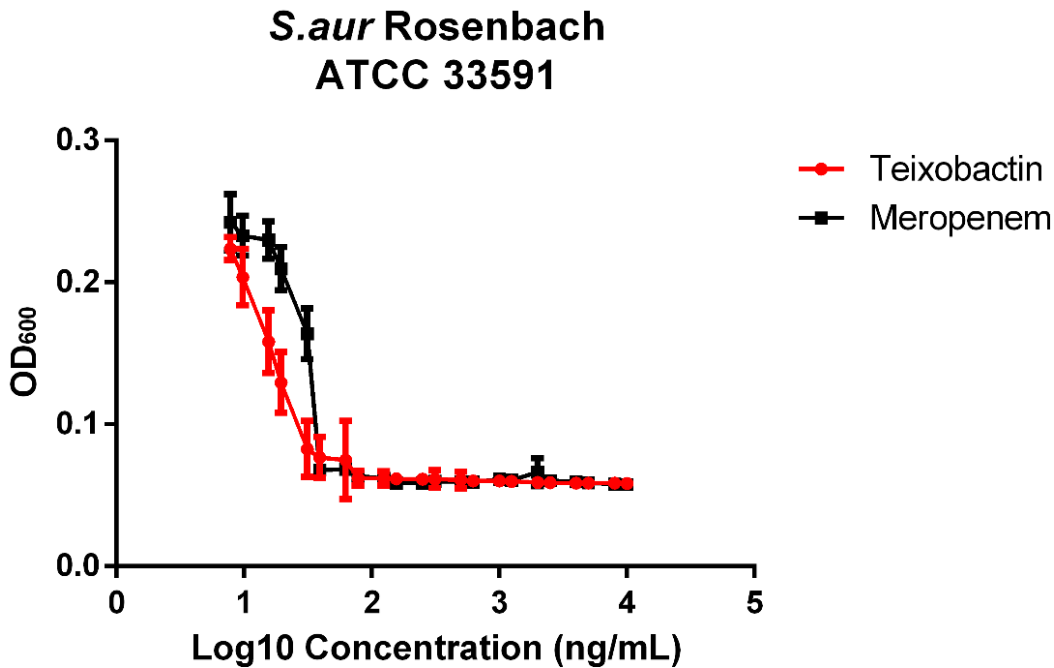
Supplementary Material

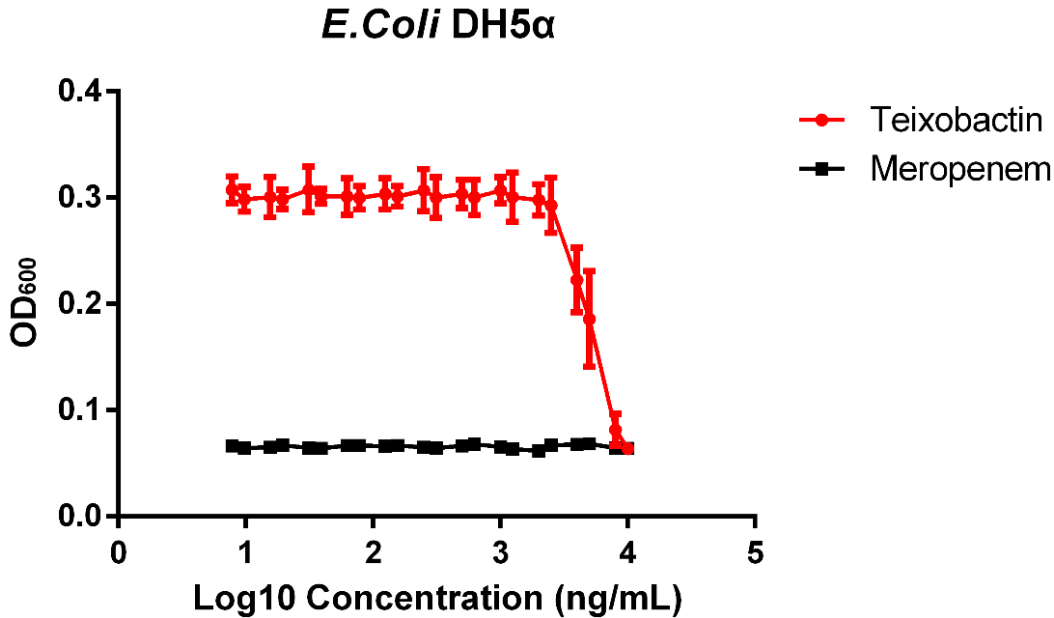
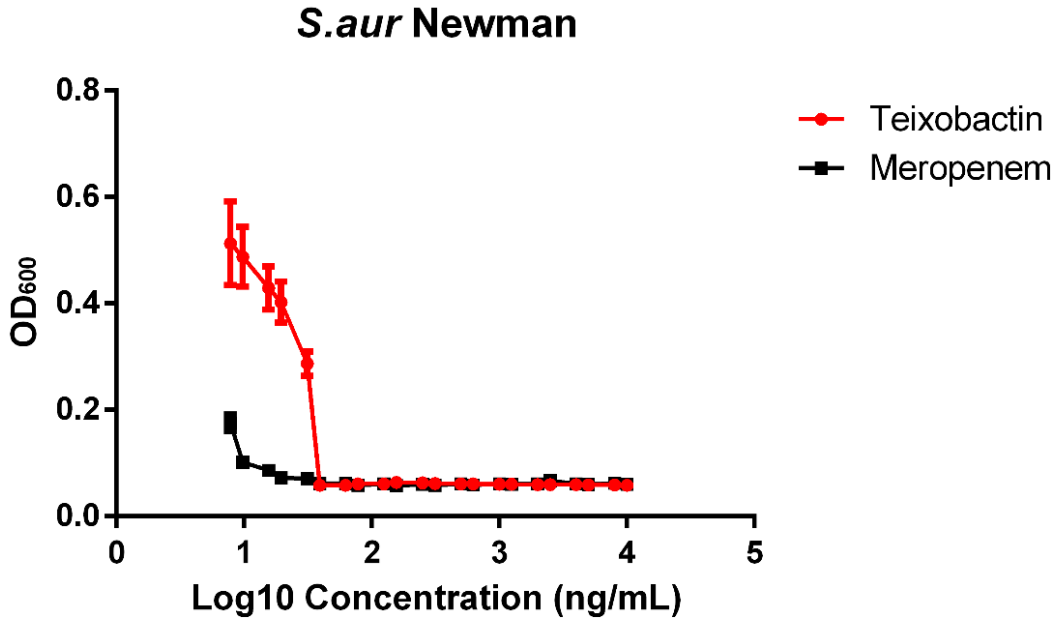
Teixobactin 1, ^1H NMR (500 MHz, $\text{DMSO-}d_6$)



Teixobactin 1, ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$)







HPLC Report of Teixobactin

Sample Name: Tei-pur004
Volume Injected: 100(μL)
Method: Default
Date: 2018-05-21 16:39:45

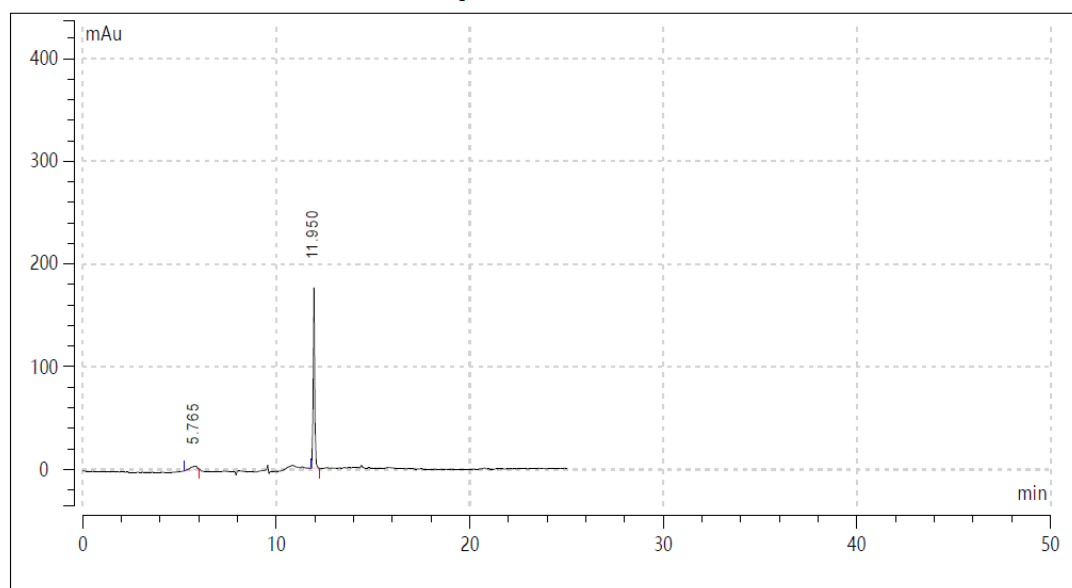
Sample ID: NEWID259
Chanel: Tei-pur004-(UV-ch1-254)
Operator: SG Chen
Print Time:

The analysis was carried out on SAIPU (Separation (Beijing) Technology Co Ltd., Beijing, China) with a MWD UV detector (254 nm).

Column: YMC-Pack ODS-A column (250 mm × 4.6 mm, i.d., S-5 μm, 12 nm, AA12S05-2546WT Ser.No. 109FA70186, YMC Co. Ltd., Japan).

Mobile phase: MeCN : Water-0.1% TFA: 0-20 min, from 95 : 5 (v/v) to 5 : 95 (v/v), then 20-25 min, 0 : 100 (v/v). Flow rate: 1.0 mL/min.

Tei-pur004-(UV-ch1-254)



峰列表

No	名称	保留时间 (min)	峰面积 (mAu*s)	峰宽 (min)	半峰宽 (min)	峰高 (mAu)	面积百分比 (%)	峰类型
1	N. A.	5.765	78.74077	0.337	0.363	3.472	7.559	BB
2	N. A.	11.950	962.97078	0.136	0.080	182.060	92.441	BB
3	总计							

峰列表: Peak list

名称: Name 保留时间: Retention Time 峰面积: Area of Peak
峰宽: Width 半峰宽: Full Width at Half Maxiam 峰高: Height of Peak
面积百分比: Percentage of Area 峰类型: Type of Peak
