

Electronic Supplementary Information

Synthesis and immunological evaluation of MUC1 glycopeptide conjugates bearing *N*-acetyl modified STn derivatives as antitumor vaccines

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Table of Contents

IgG titers of immunological evaluation.....	S3
¹ H and ¹³ C NMR spectra of compound 3	S4
¹ H and ¹³ C NMR spectra of compound 4	S5
¹ H and ¹³ C NMR spectra of compound 5	S6
¹ H and ¹³ C NMR spectra of compound 6	S7
¹ H and ¹³ C NMR spectra of compound 9	S8
¹ H and ¹³ C NMR spectra of compound 14	S9
¹ H and ¹³ C NMR spectra of compound 15	S10
¹ H and ¹³ C NMR spectra of compound 16	S11
¹ H and ¹³ C NMR spectra of compound 18	S12
¹ H and ¹³ C NMR spectra of compound 19	S13
¹ H and ¹³ C NMR spectra of compound 20	S14
¹ H and ¹³ C NMR spectra of compound 22	S15
¹ H and ¹³ C NMR spectra of compound 23	S16
¹ H and ¹³ C NMR spectra of compound 24	S17
Analytical HPLC and MALDI-TOF mass spectrum of glycopeptide 25	S18
Analytical HPLC and MALDI-TOF mass spectrum of glycopeptide 26	S19
Analytical HPLC and MALDI-TOF mass spectrum of glycopeptide 27	S20
Analytical HPLC and MALDI-TOF mass spectrum of glycopeptide 28	S21
Analytical HPLC and MALDI-TOF mass spectrum of glycopeptide 29	S22

Analytical HPLC and MALDI-TOF mass spectrum of glycopeptide 30	S23
Analytical HPLC and MALDI-TOF mass spectrum of glycopeptide 31	S24
Analytical HPLC and MALDI-TOF mass spectrum of glycopeptide 32	S25
Analytical HPLC and MALDI-TOF mass spectrum of glycopeptide 33	S26
Analytical HPLC and MALDI-TOF mass spectrum of glycopeptide 34	S27
Analytical HPLC and MALDI-TOF mass spectrum of glycopeptide 35	S28
Analytical HPLC and MALDI-TOF mass spectrum of glycopeptide 36	S29

Table S1. IgG titers against STn-MUC1-BSA of individual mouse serum 14 days after the 4th vaccination

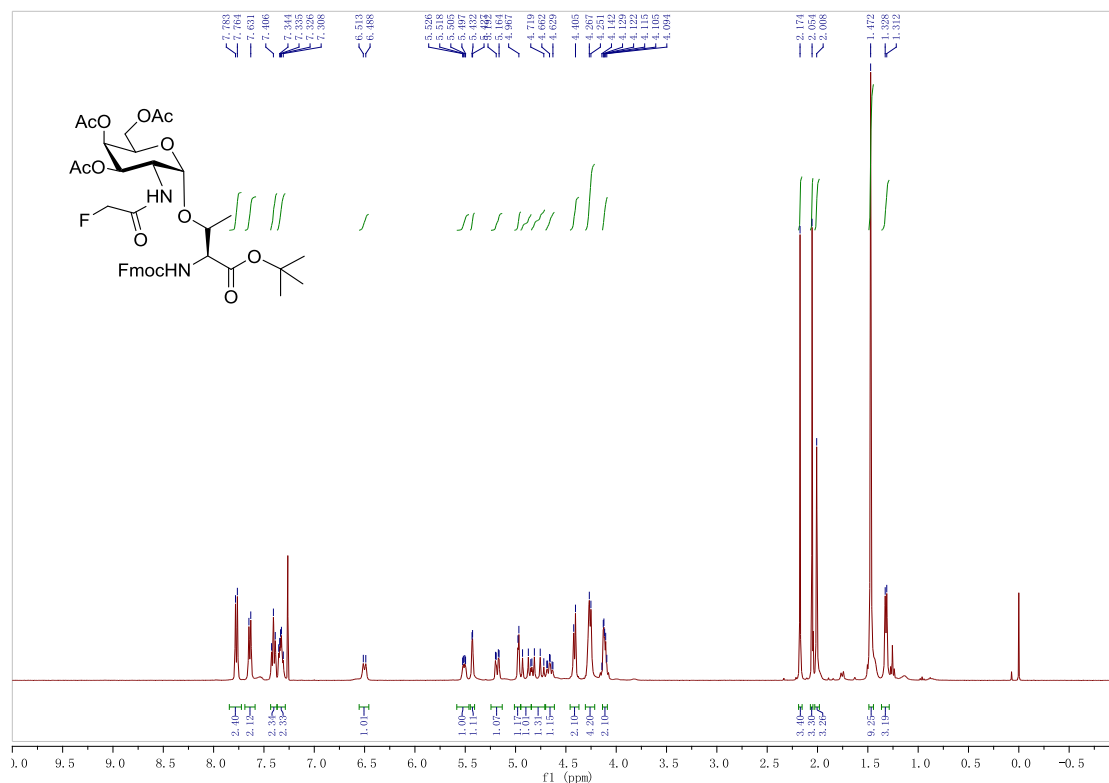
	V1	V2	V3	V4
Mouse 1	716726	2065005	1215059	491241
Mouse 2	584300	714066	1081360	884544
Mouse 3	195219	3621392	447224	91857
Mouse 4	403722	1127029	478388	1674453
Mouse 5	1314481	2424080	5820127	1085042
Mouse 6	5003014	343585	171749	606525
Median	650513	1596017	779874	745534

Table S2. Pooled sera IgG titers against STn-MUC1-BSA and against corresponding modified-STn-MUC1-BSA after the 4th vaccination.

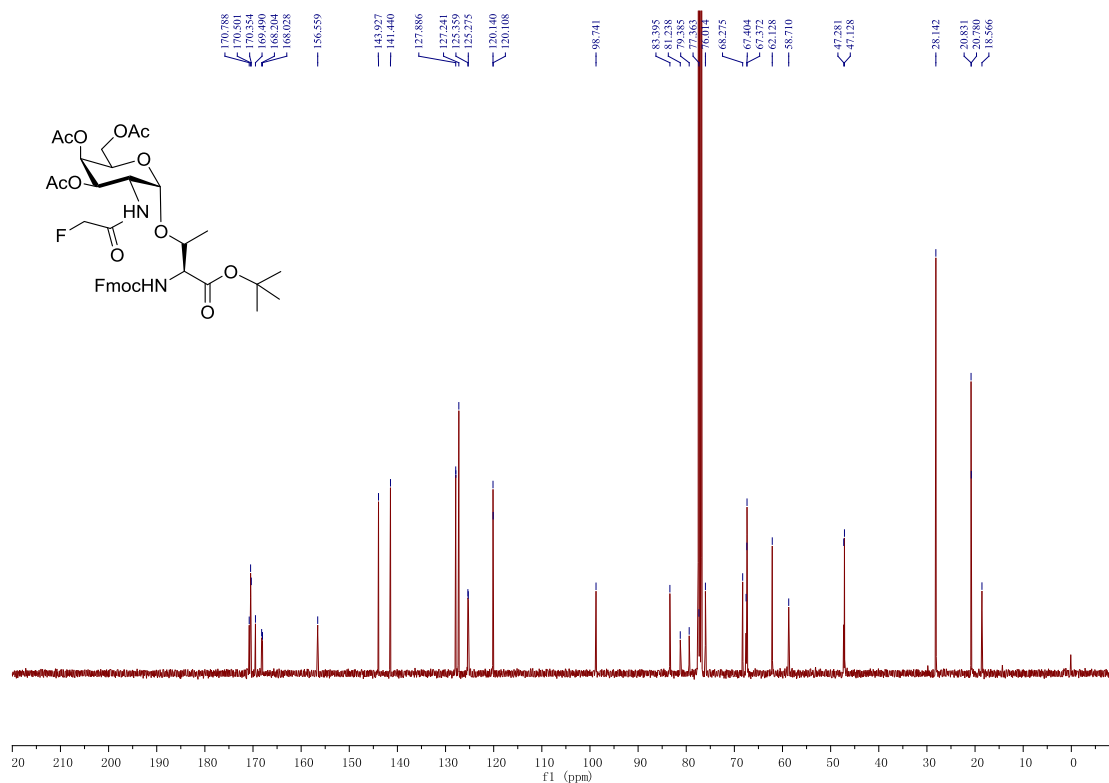
	against STn-MUC1-BSA	against corresponding Modified-STn-MUC1-BSA
V1	1273825	1273825
V2	1575932	1696947
V3	1235774	1551093
V4	1002516	1364358

Table S3. IgG2a titers against STn-MUC1-BSA of individual mouse serum 14 days after the 4th vaccination

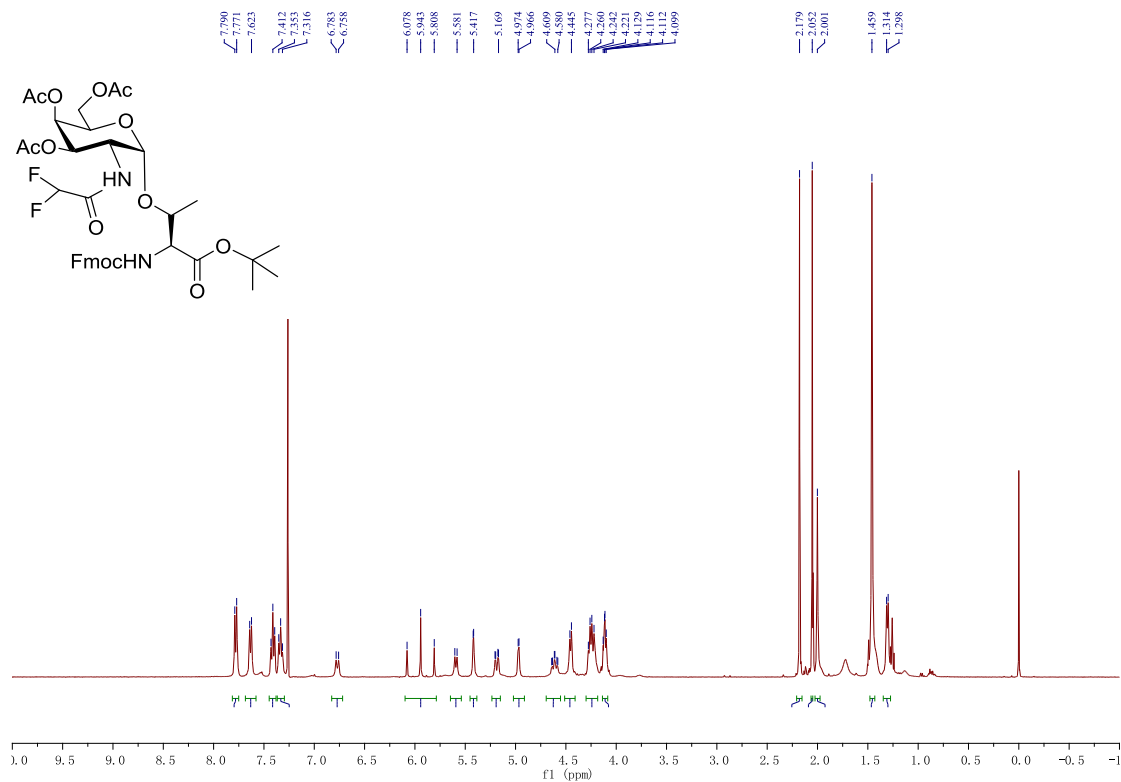
	V1	V2	V3	V4
Mouse 1	7827	3178	3783	7806
Mouse 2	2138	3790	1593	21386
Mouse 3	1913	236244	2352	784
Mouse 4	4837	49602	2113	25324
Mouse 5	6373	21613	29224	738
Mouse 6	6406	311359	1788	2081
Median	5605	35607	2232	4944



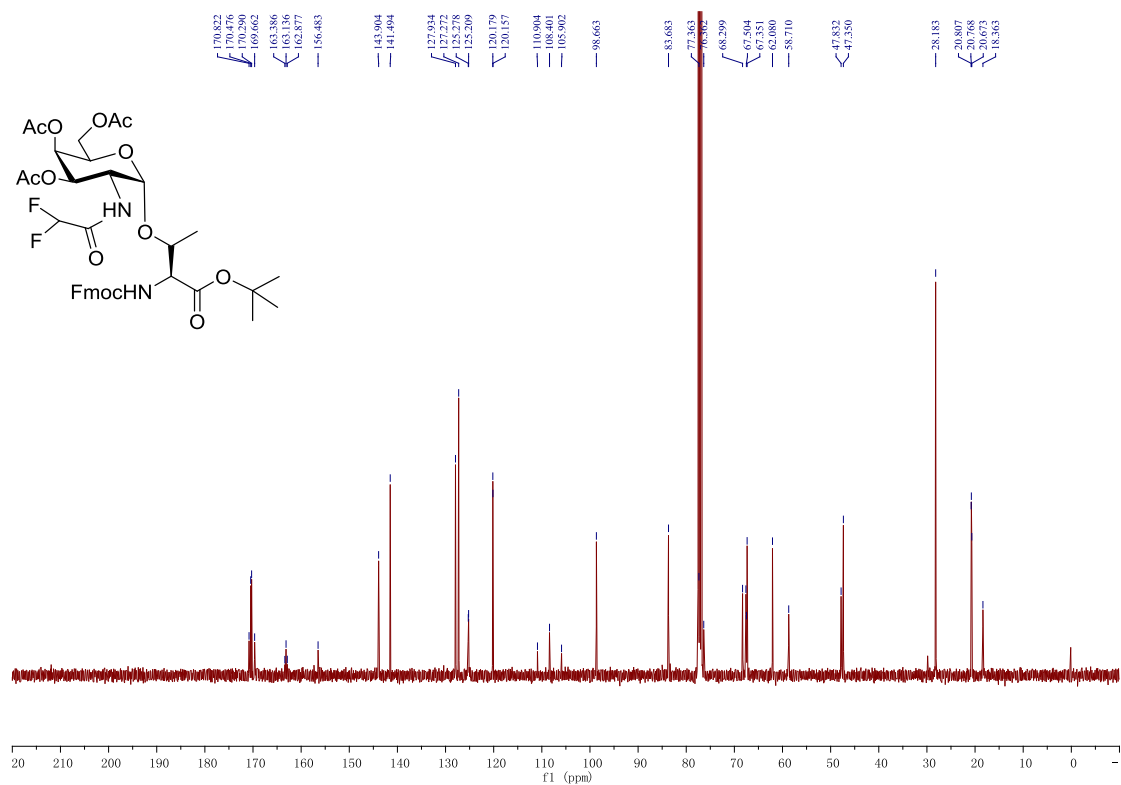
¹H NMR spectrum of compound 3 (400 MHz, CDCl₃)



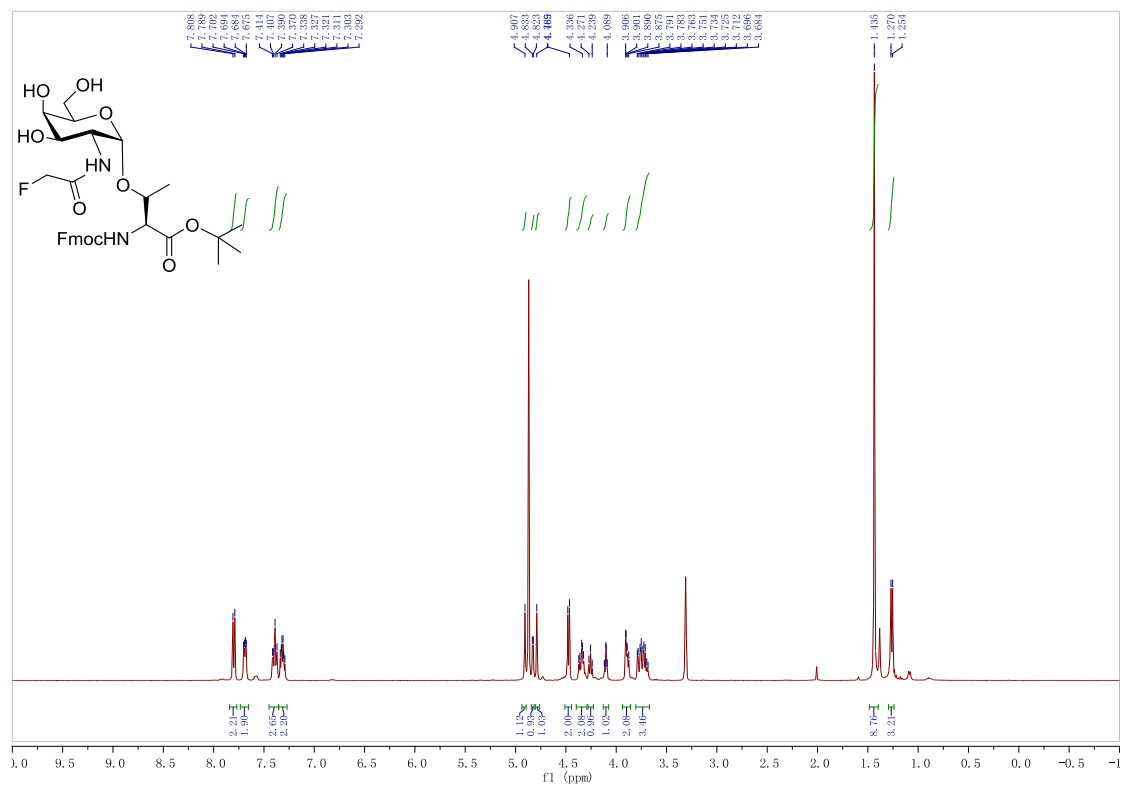
¹³C NMR spectrum of compound 3 (100 MHz, CDCl₃)



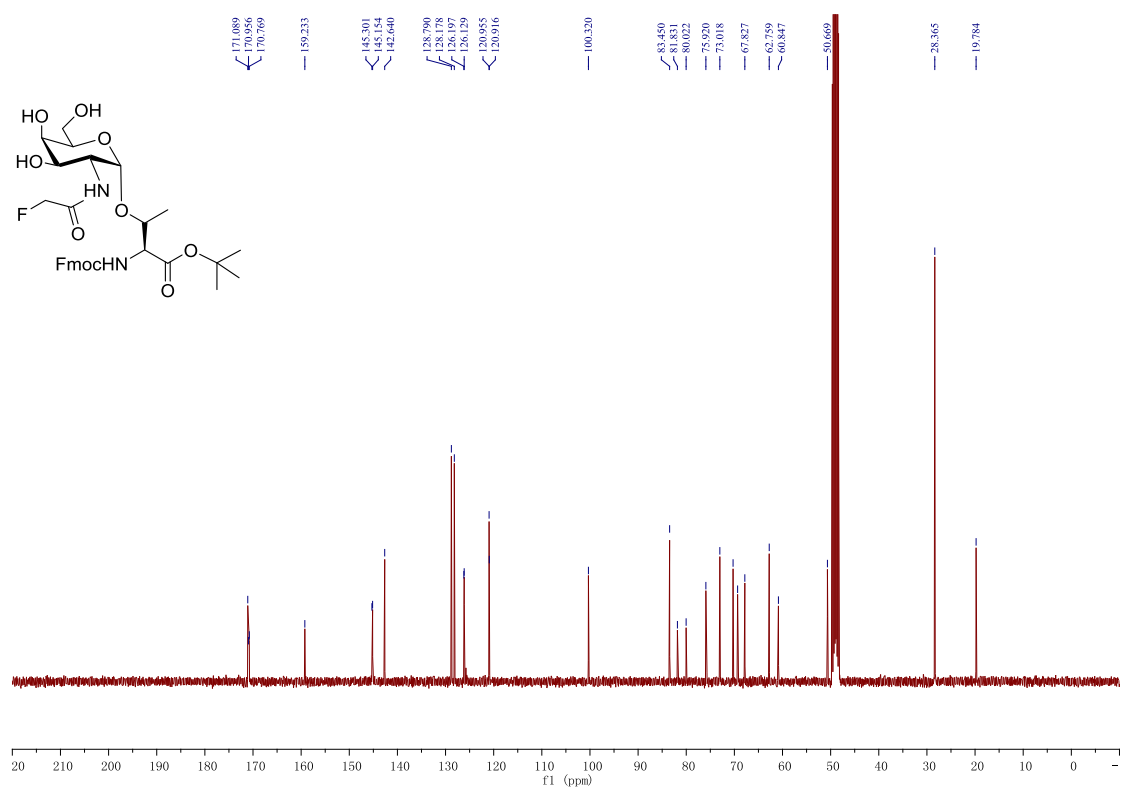
¹H NMR spectrum of compound 4 (400 MHz, CDCl₃)



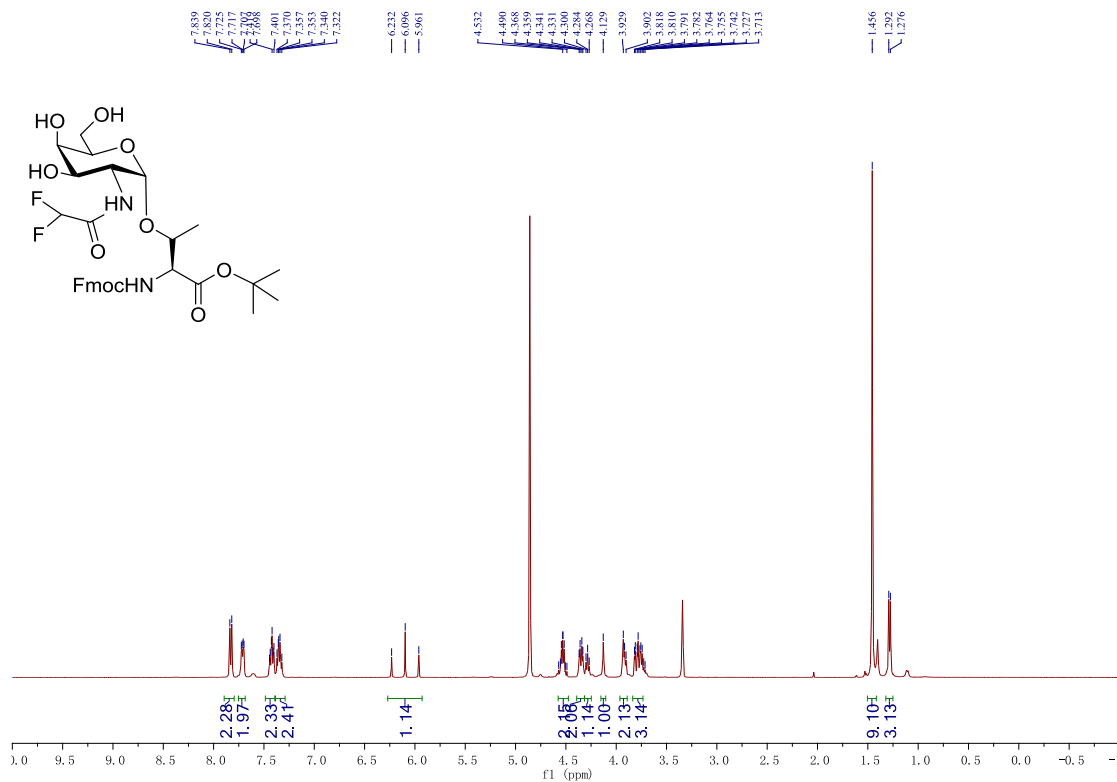
¹³C NMR spectrum of compound 4 (100 MHz, CDCl₃)



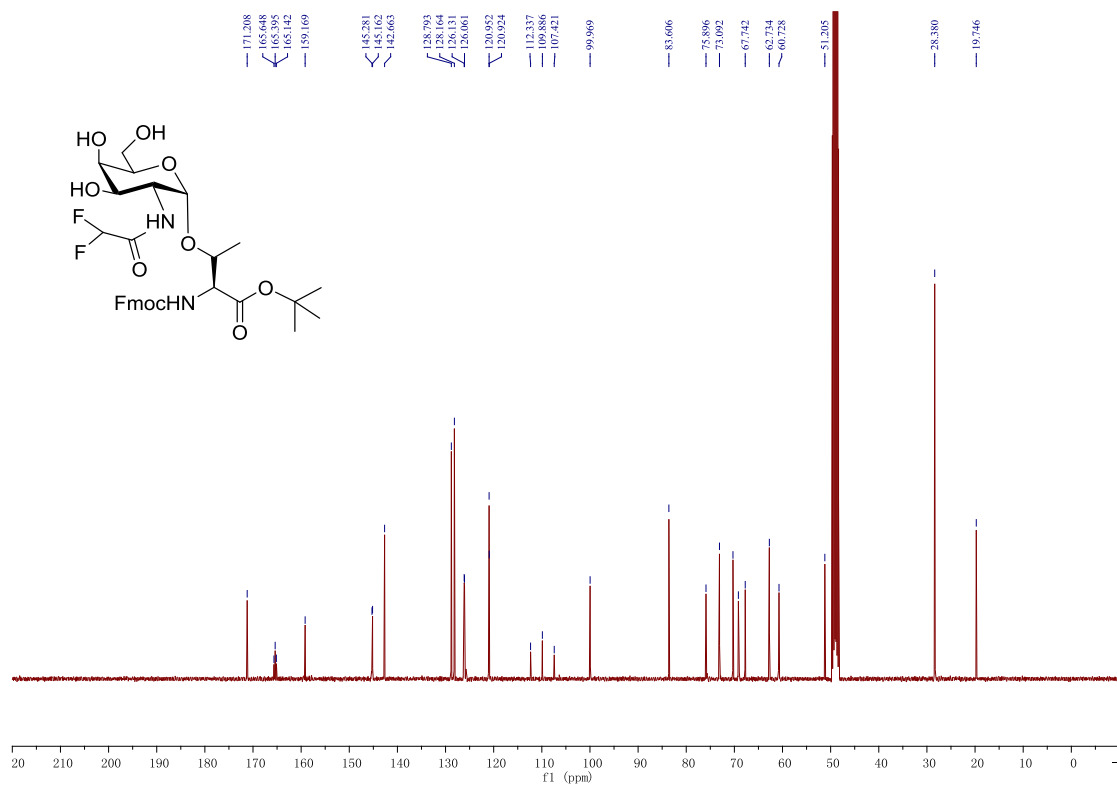
¹H NMR spectrum of compound 5 (400 MHz, CD₃OD)



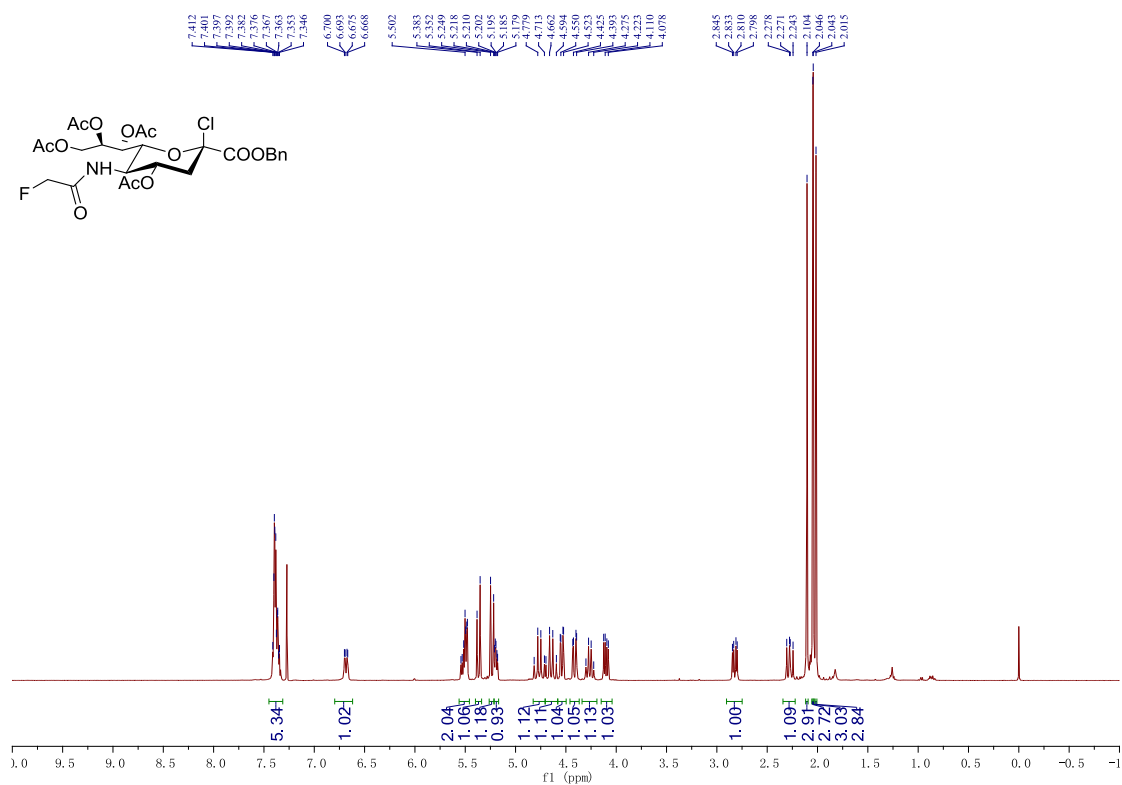
¹³C NMR spectrum of compound 5 (100 MHz, CD₃OD)



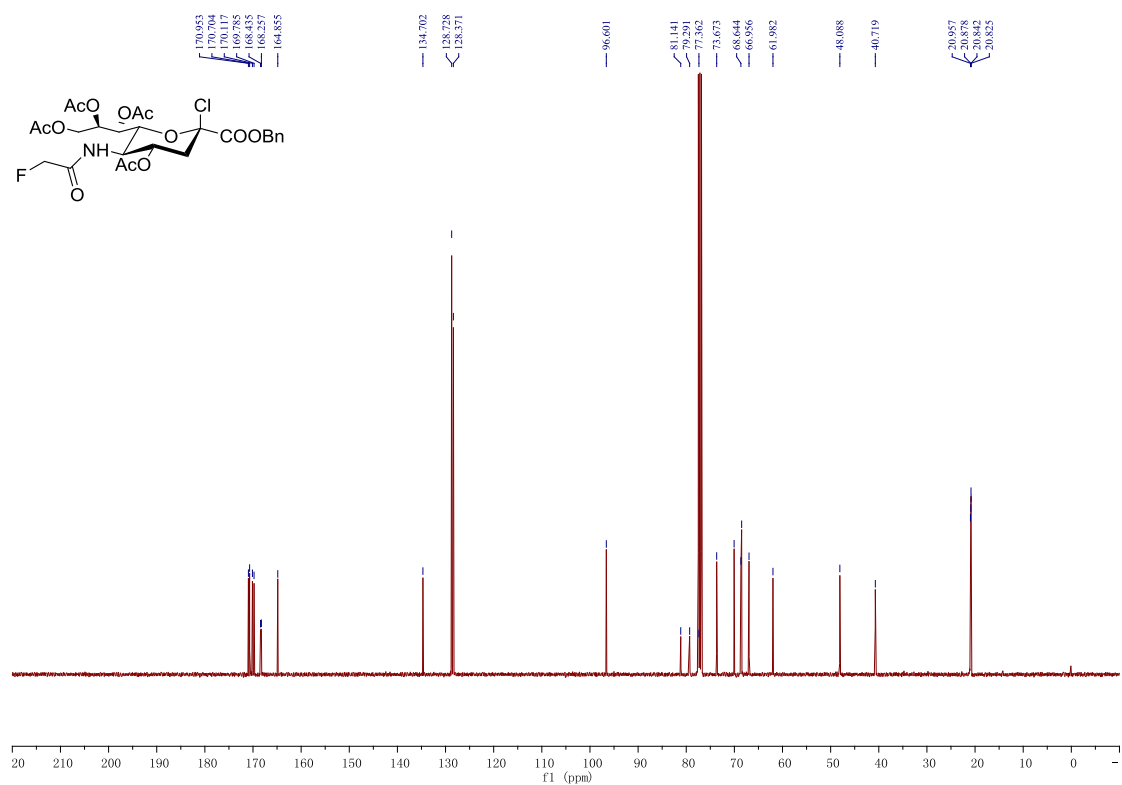
¹H NMR spectrum of compound 6 (400 MHz, CD₃OD)



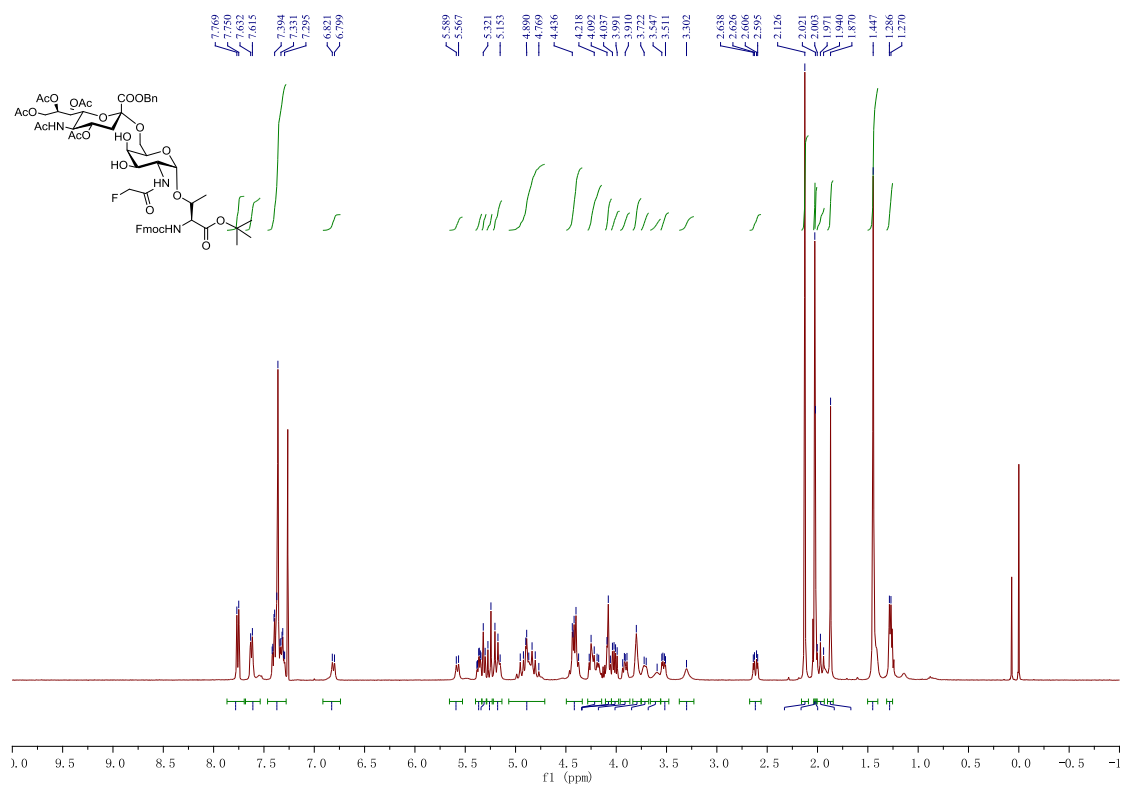
¹³C NMR spectrum of compound 6 (100 MHz, CD₃OD)



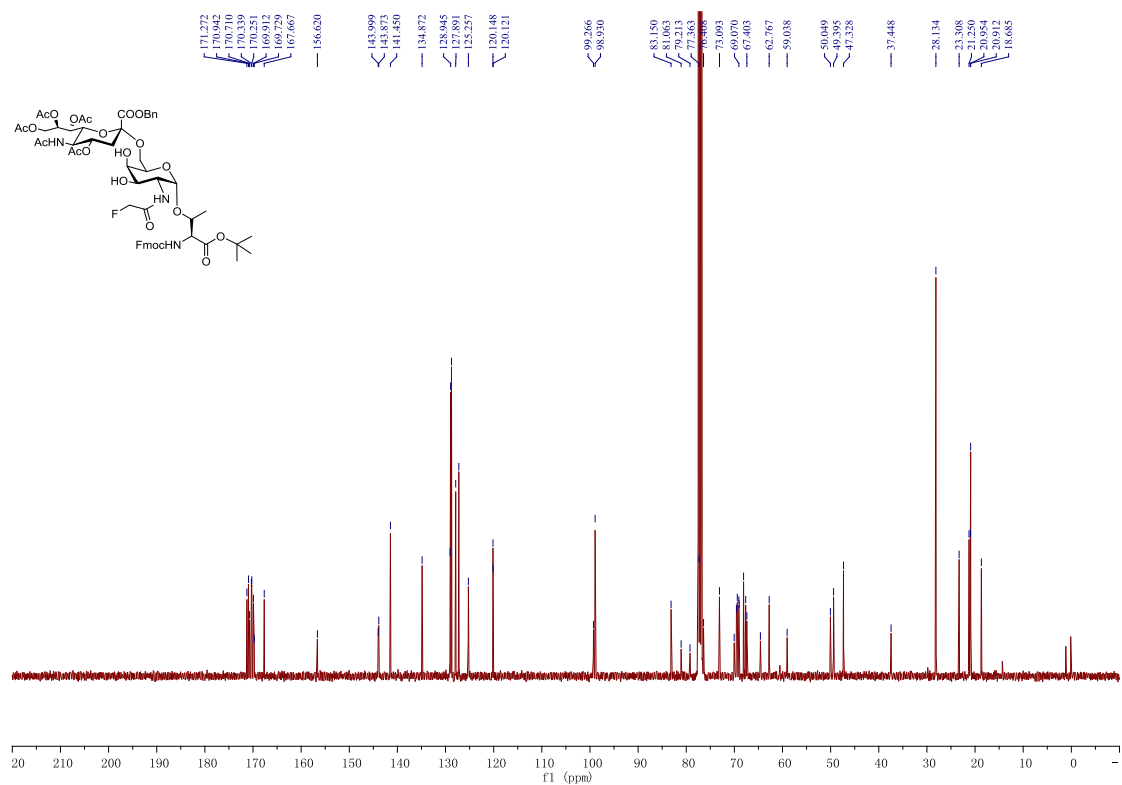
¹H NMR spectrum of compound 9 (400 MHz, CDCl₃)



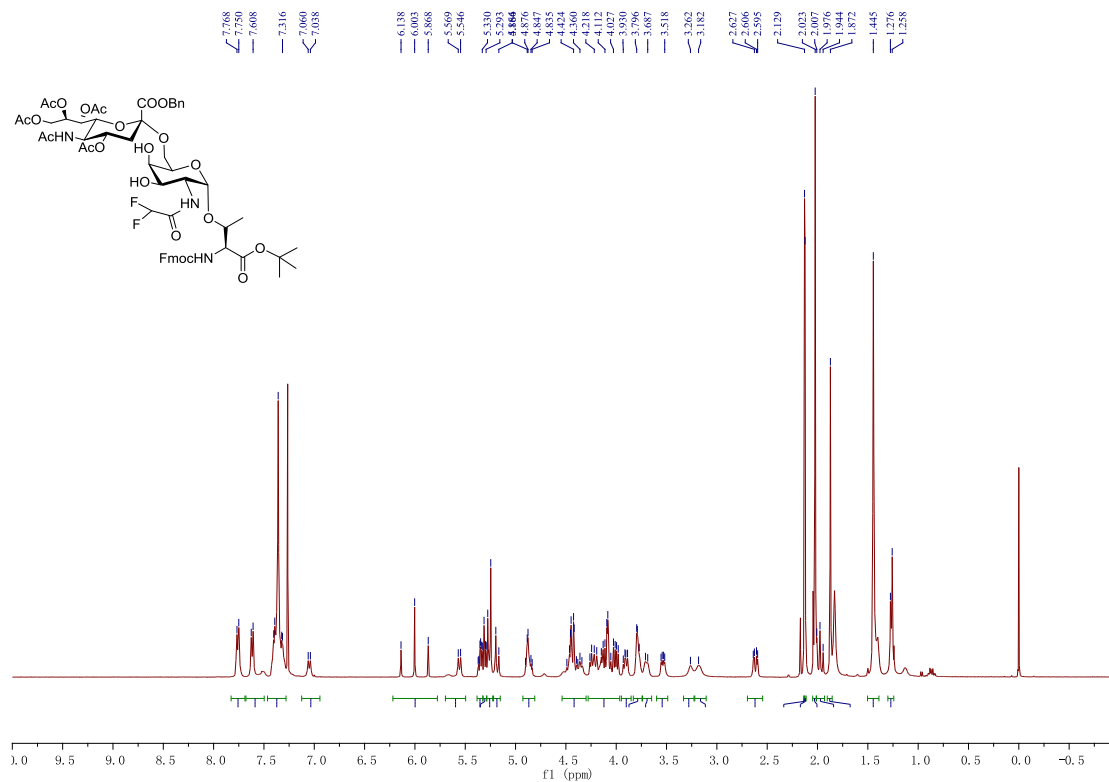
¹³C NMR spectrum of compound 9 (100 MHz, CDCl₃)



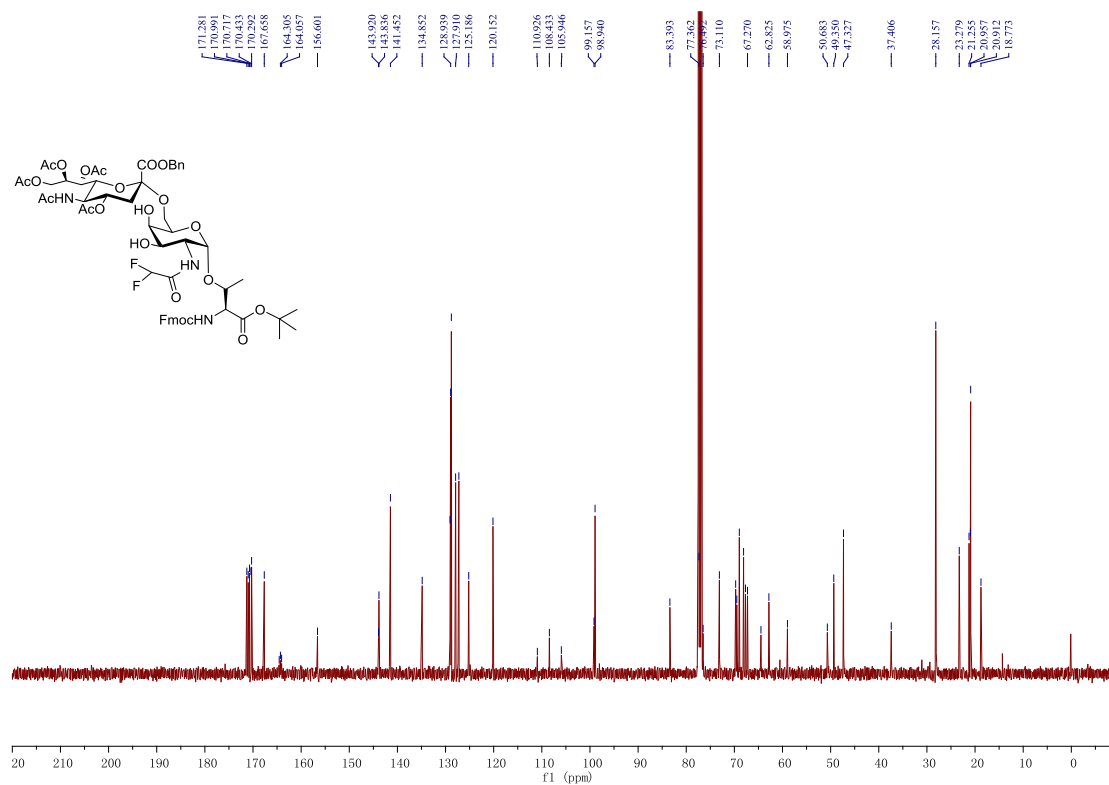
¹H NMR spectrum of compound 14 (400 MHz, CDCl₃)



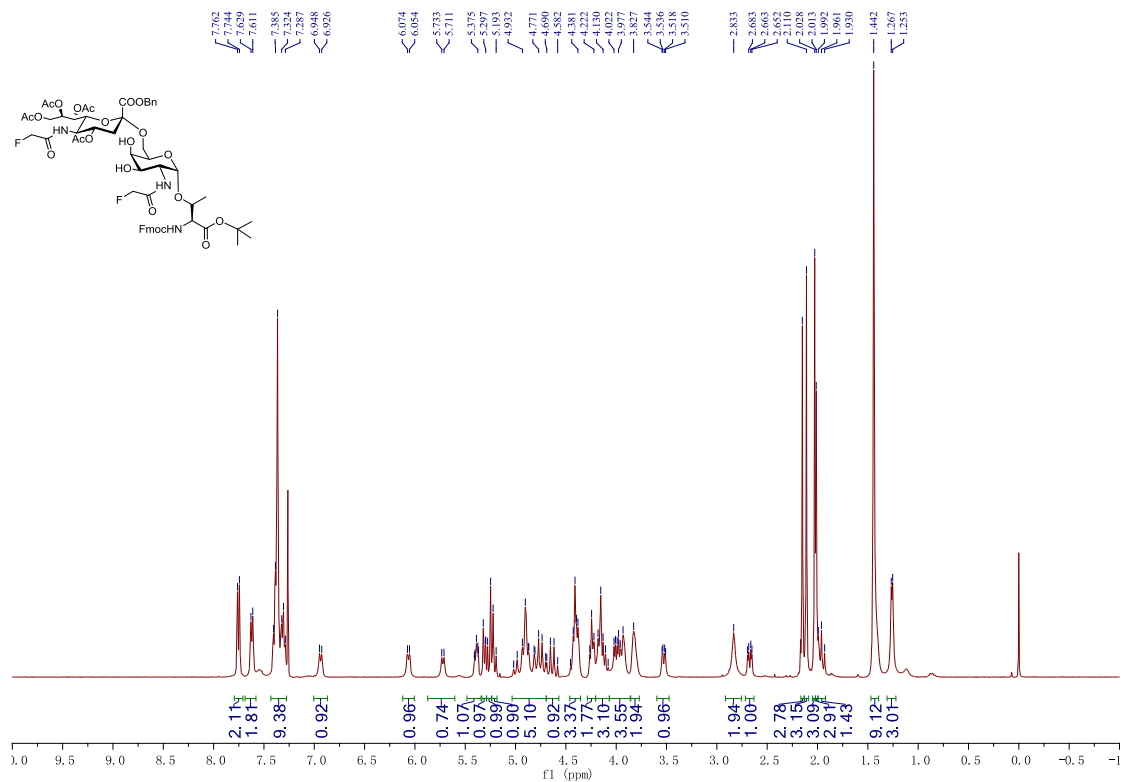
¹³C NMR spectrum of compound 14 (100 MHz, CDCl₃)



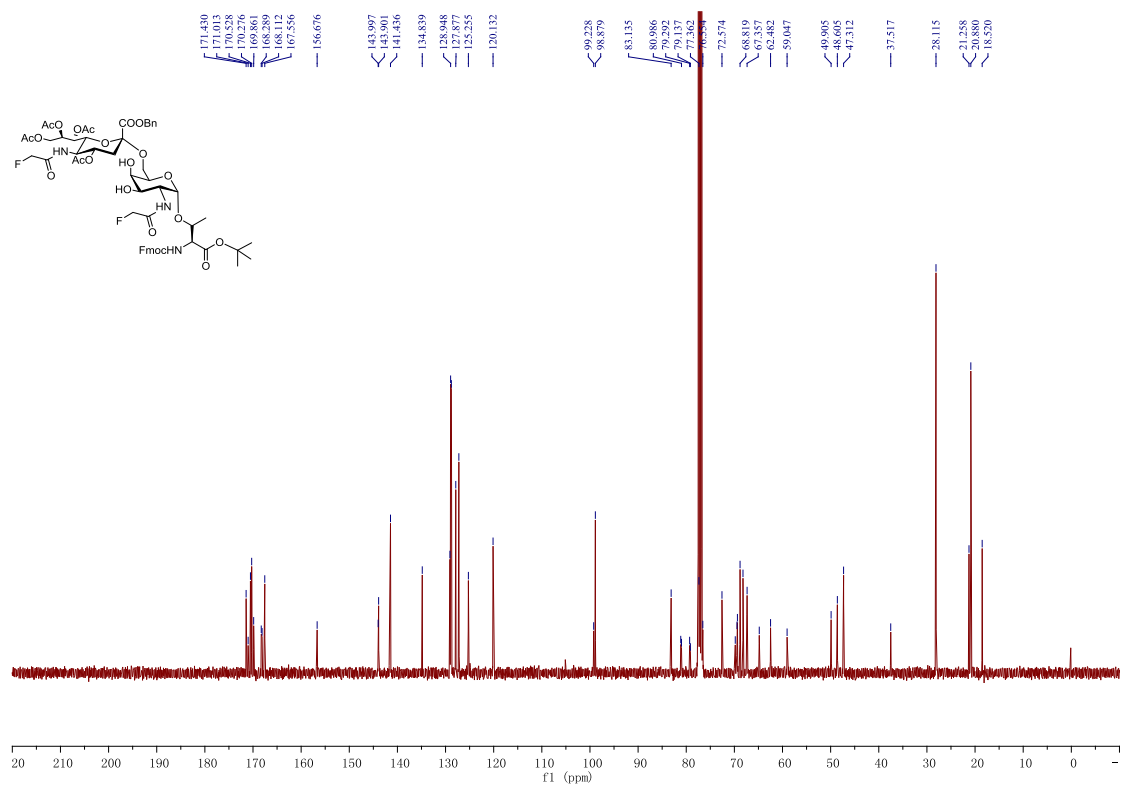
¹H NMR spectrum of compound **15** (400 MHz, CDCl₃)



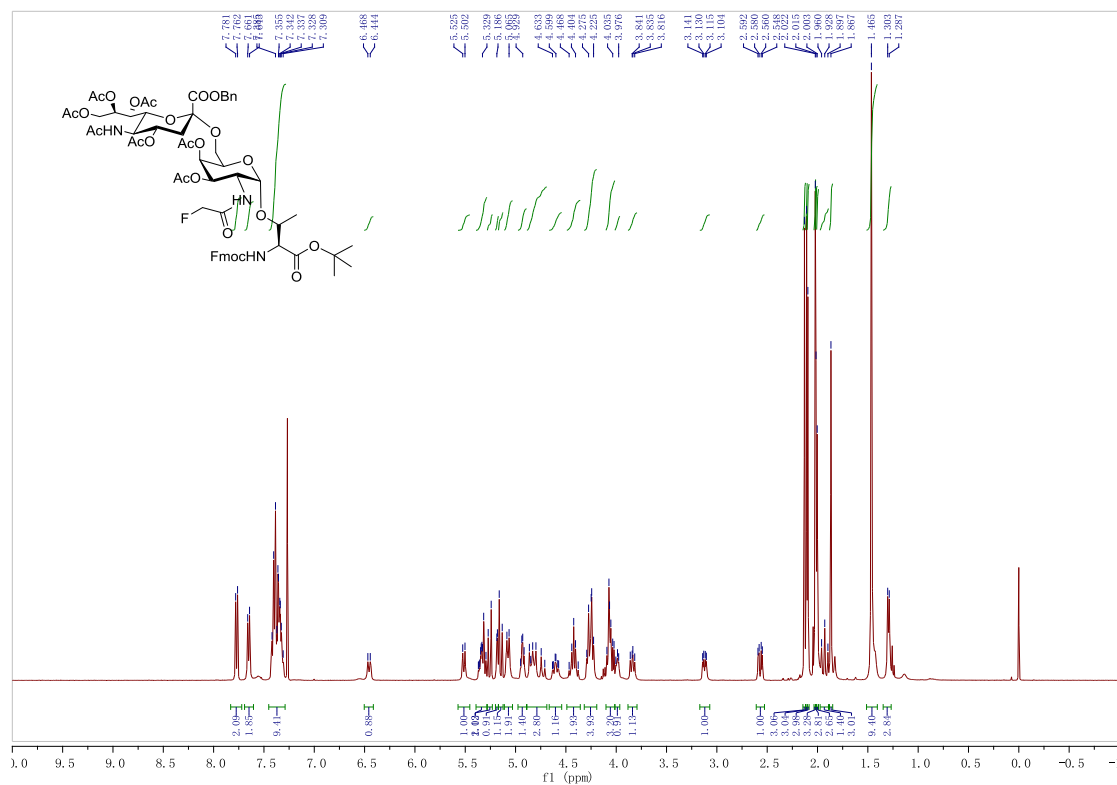
¹³C NMR spectrum of compound **15** (100 MHz, CDCl₃)



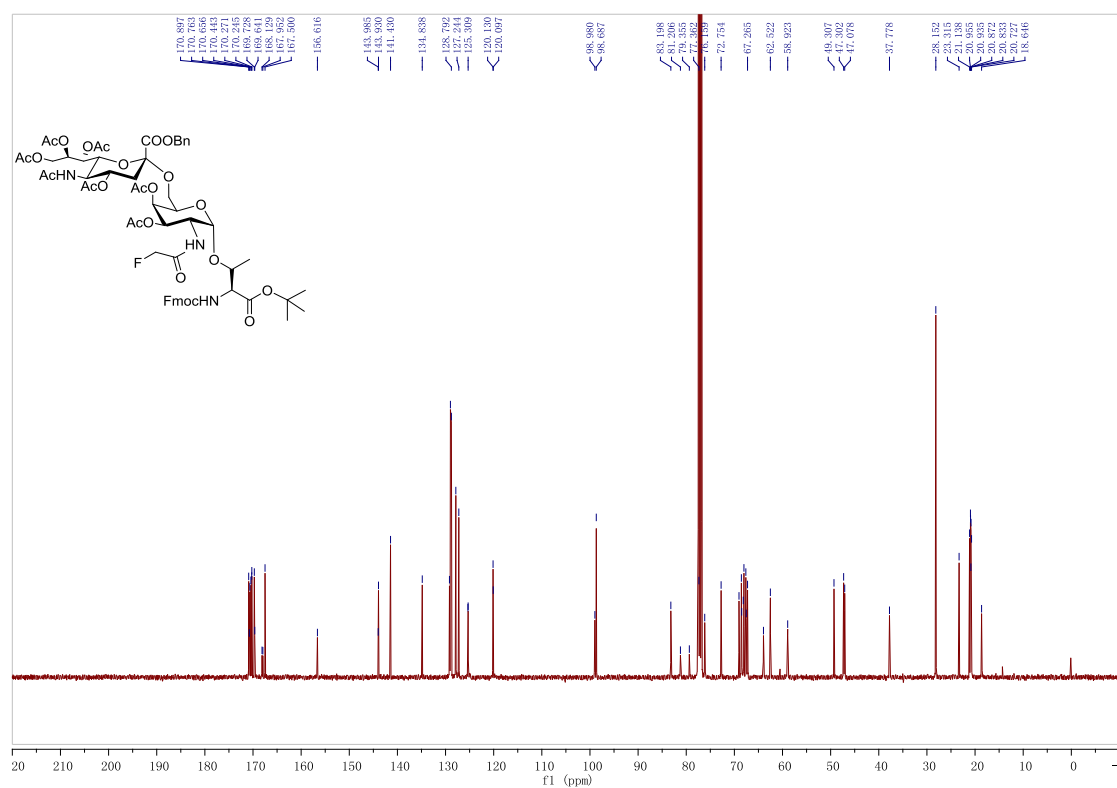
¹H NMR spectrum of compound 16 (400 MHz, CDCl₃)



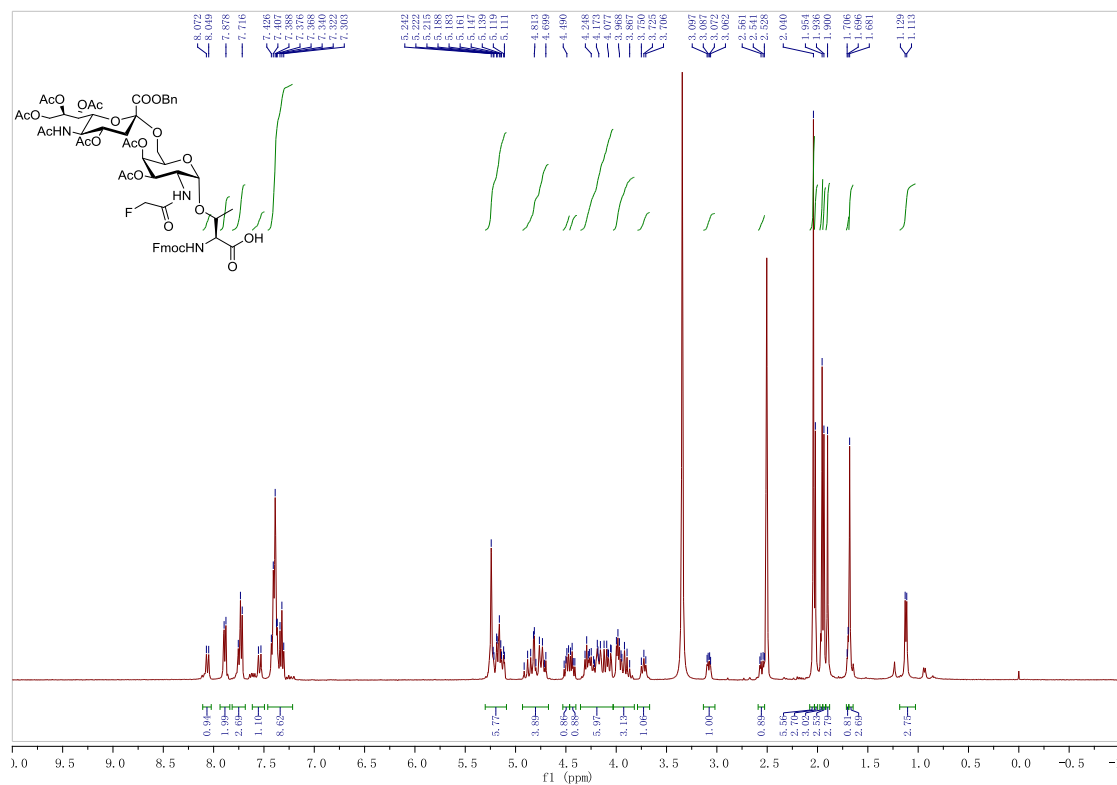
¹³C NMR spectrum of compound 16 (100 MHz, CDCl₃)



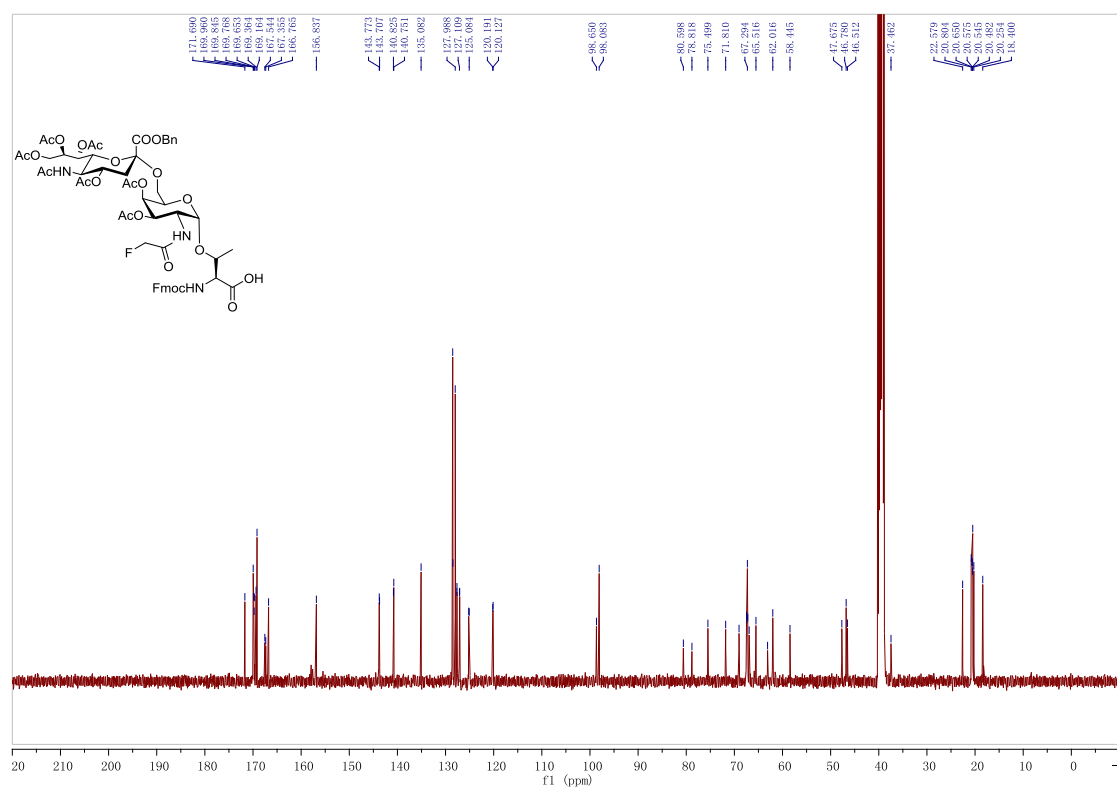
¹H NMR spectrum of compound 18 (400 MHz, CDCl₃)



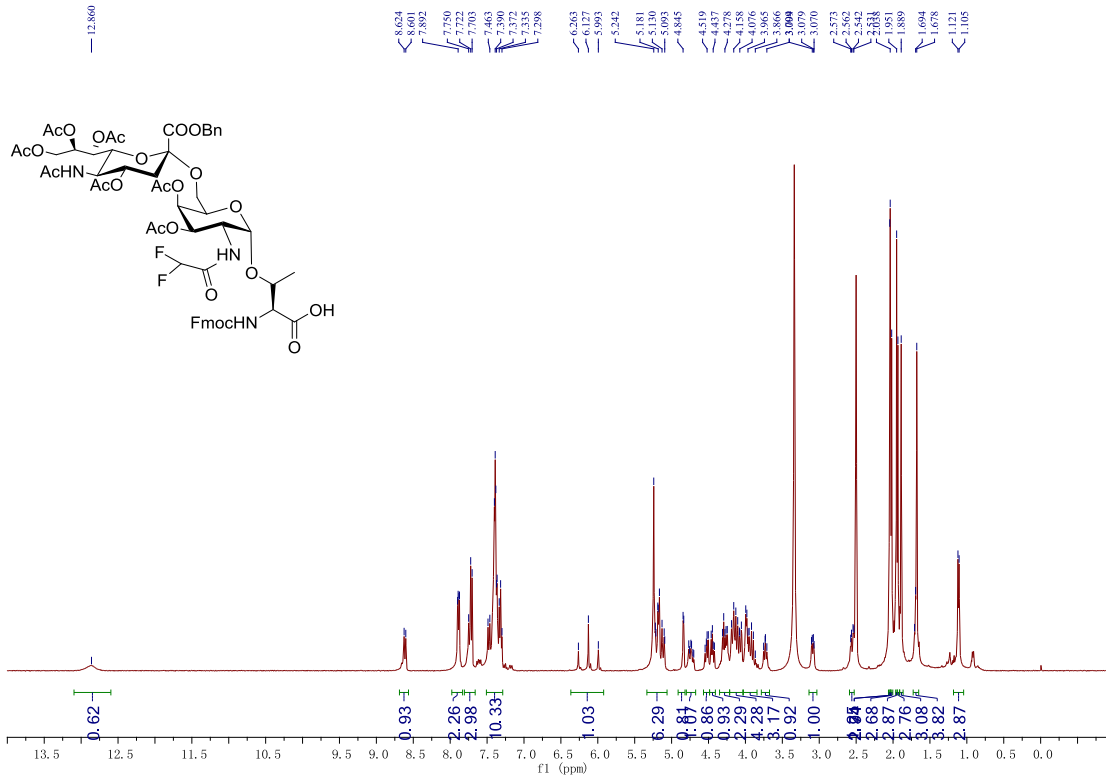
¹³C NMR spectrum of compound 18 (100 MHz, CDCl₃)



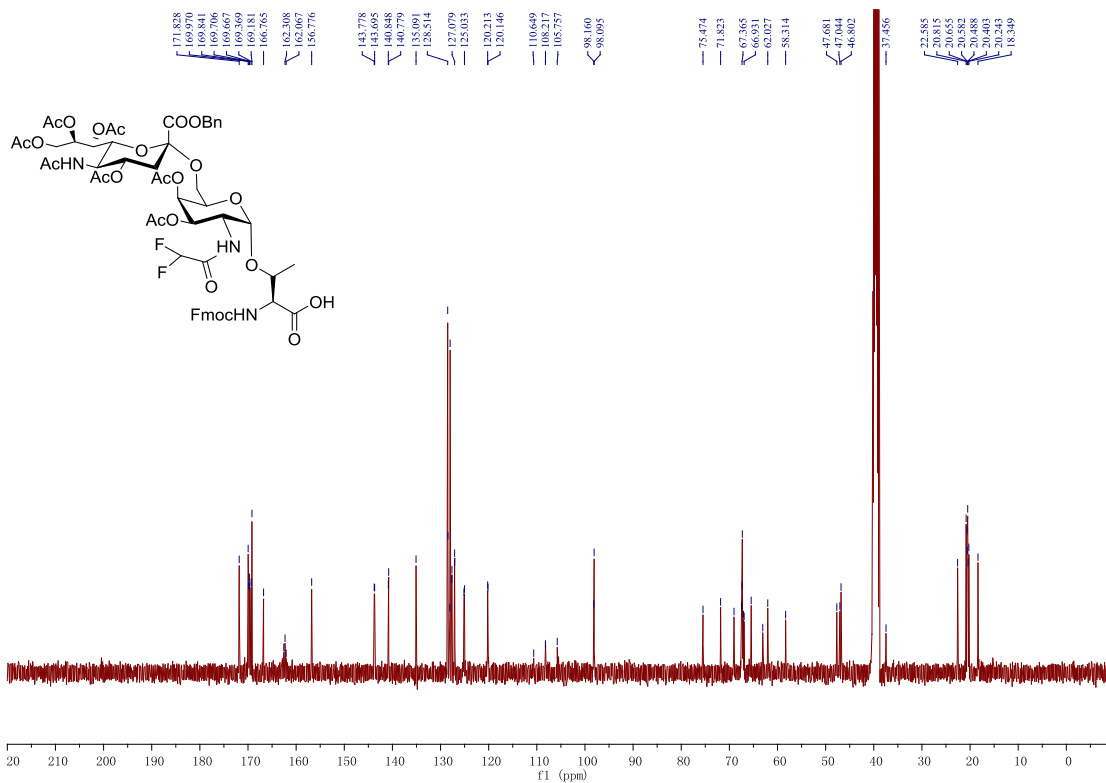
¹H NMR spectrum of compound 22 (400 MHz, DMSO-d₆)



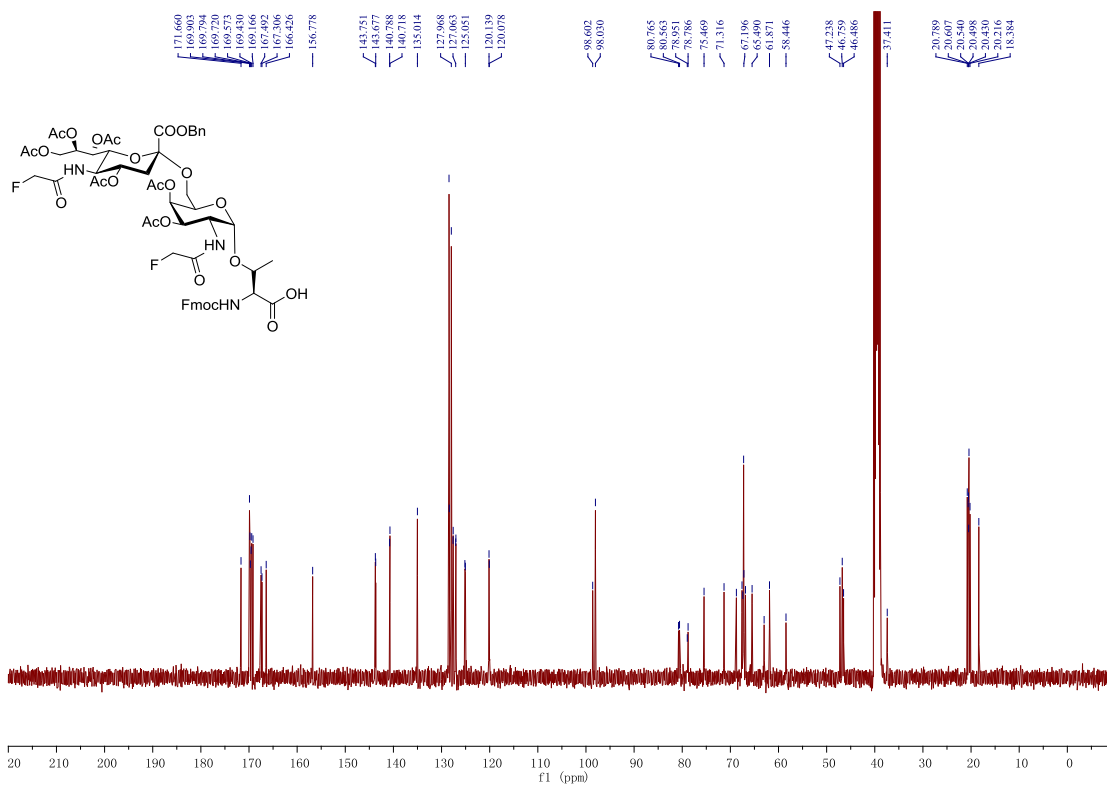
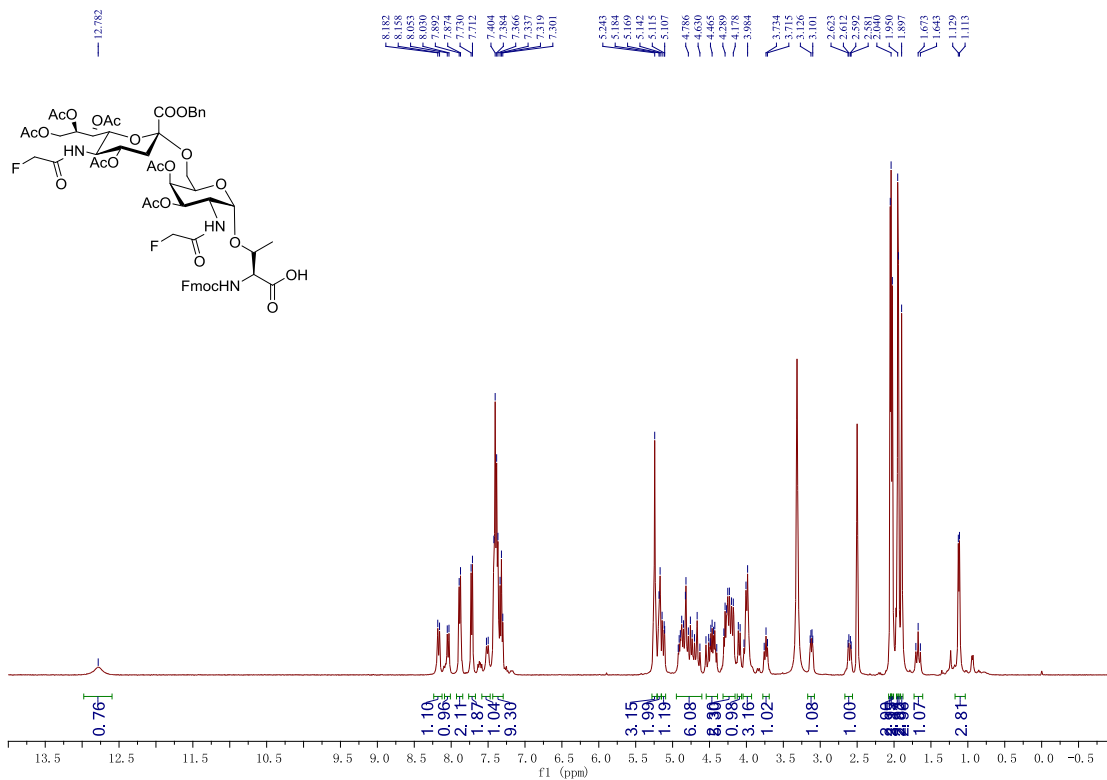
¹³C NMR spectrum of compound 22 (100 MHz, DMSO-d₆)

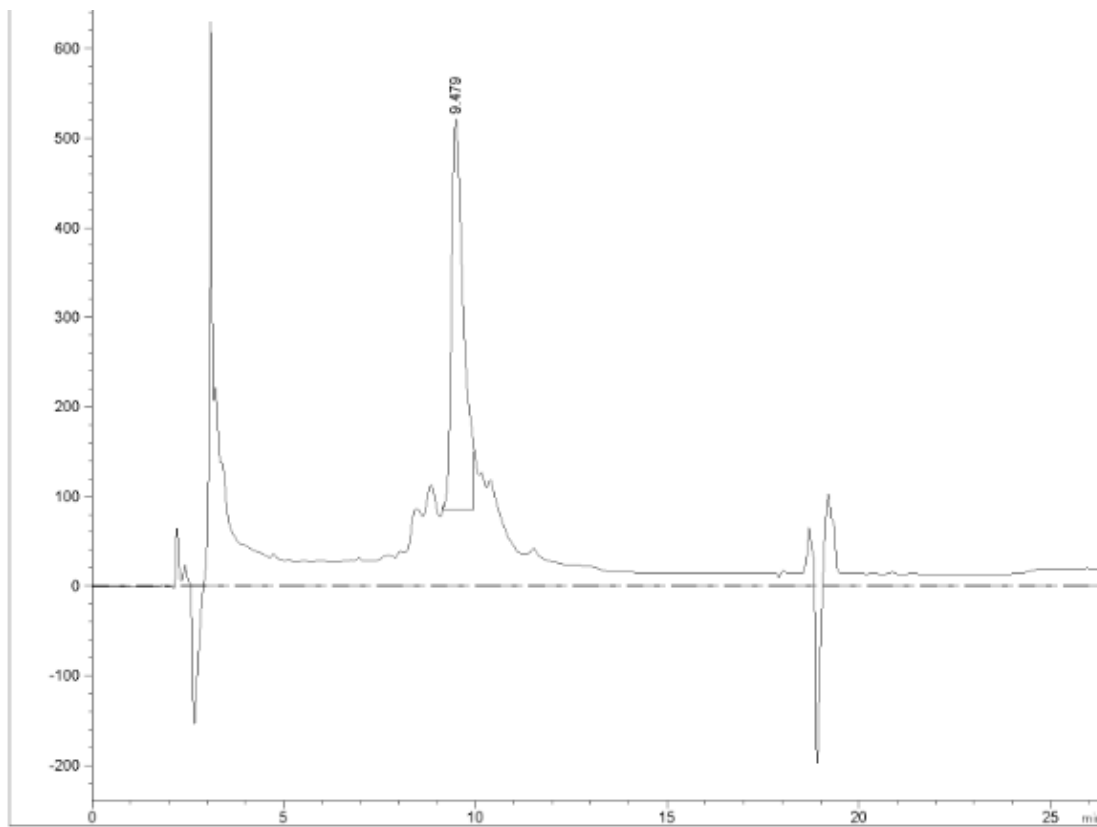


¹H NMR spectrum of compound 23 (400 MHz, DMSO-d₆)

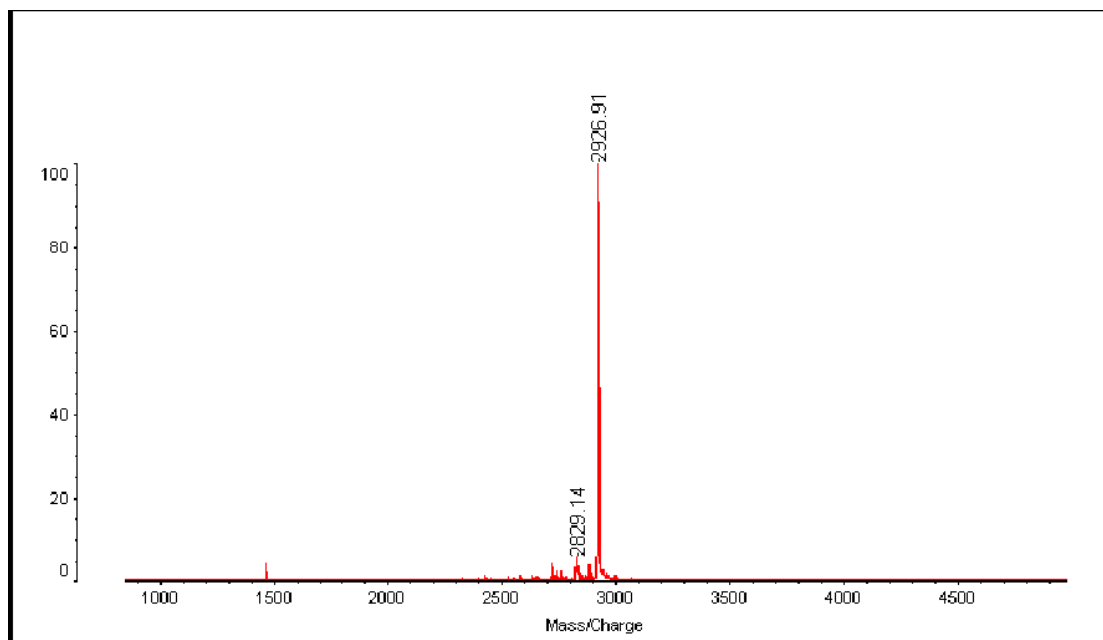


¹³C NMR spectrum of compound 23 (100 MHz, DMSO-d₆)

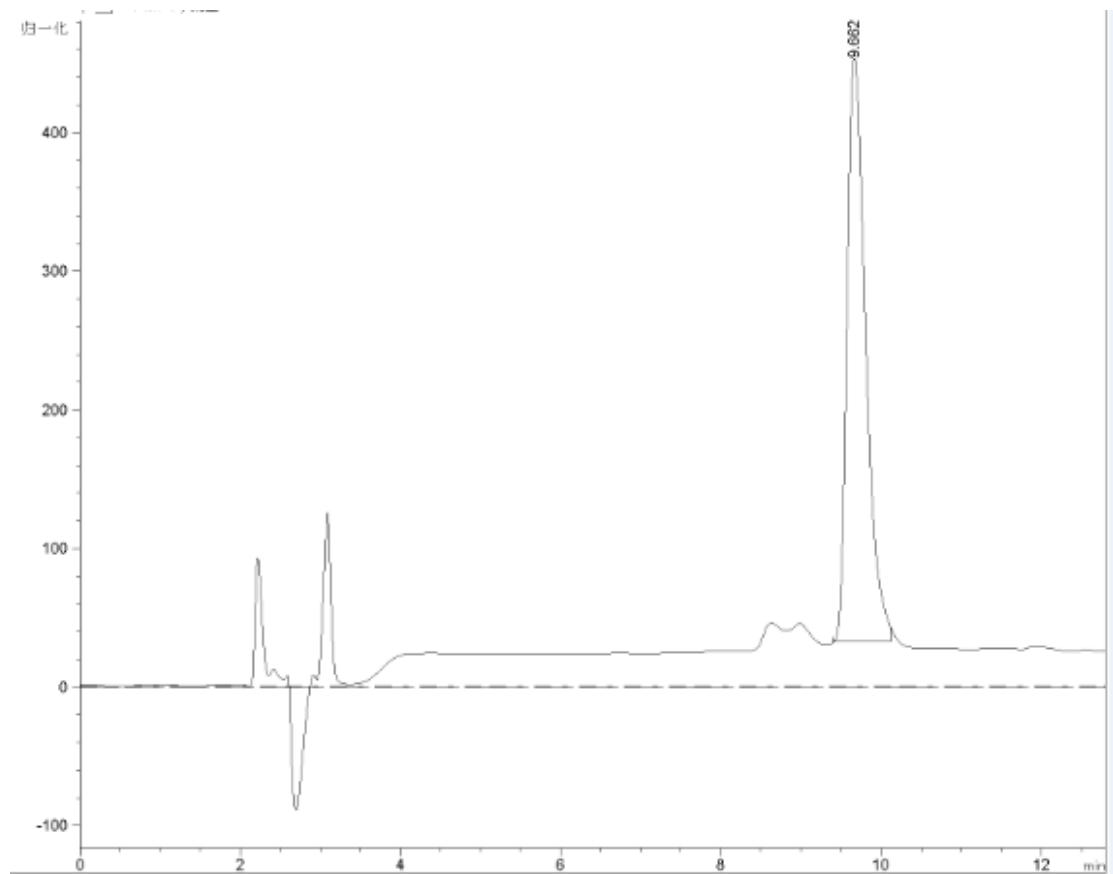




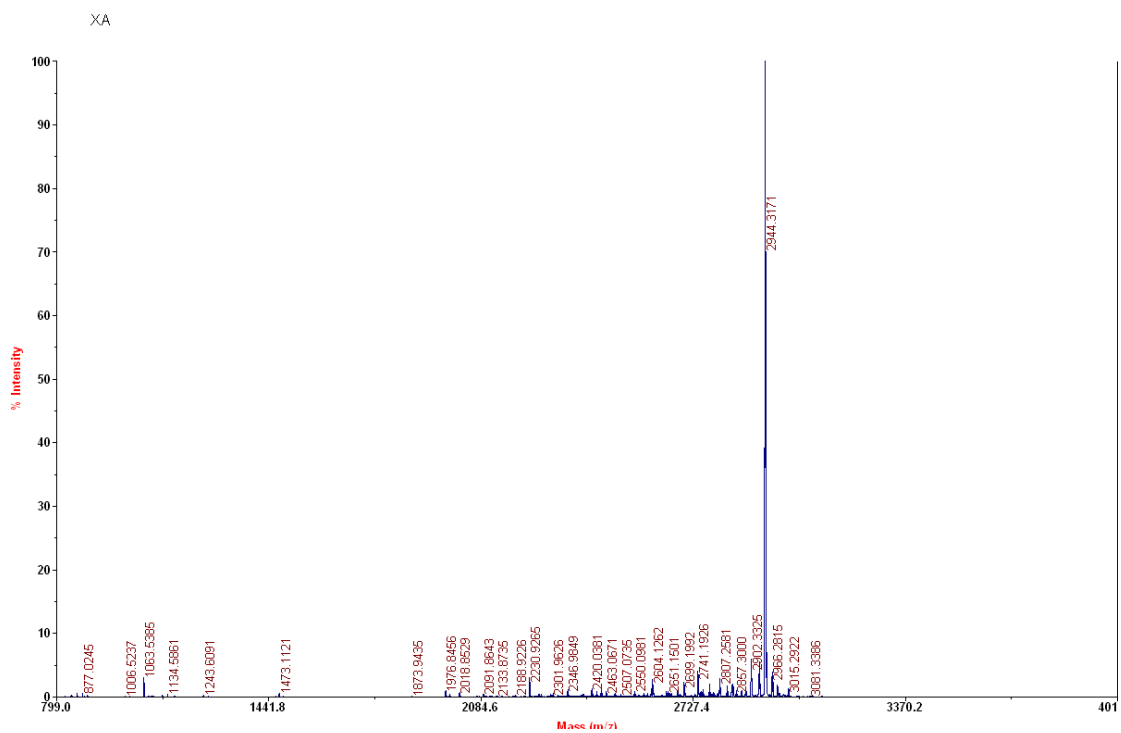
Analytical HPLC of glycopeptide **25**



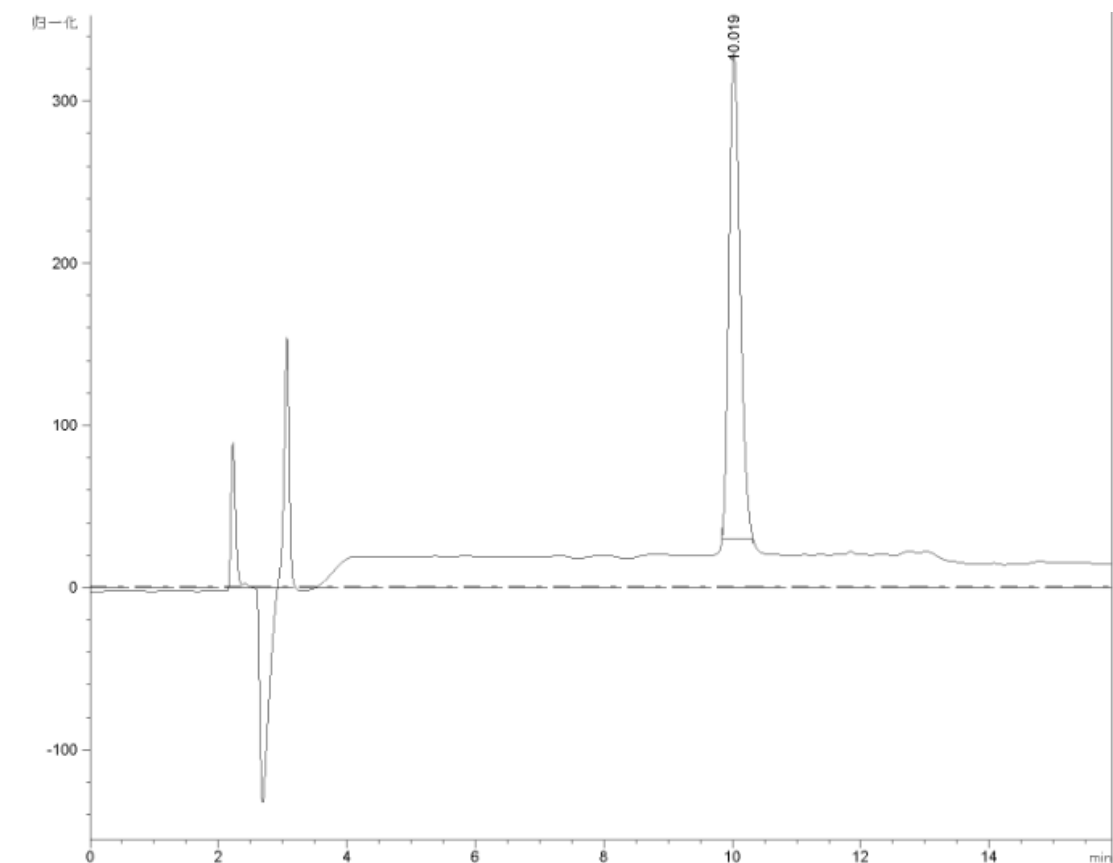
MALDI-TOF mass spectrum of glycopeptide **25**



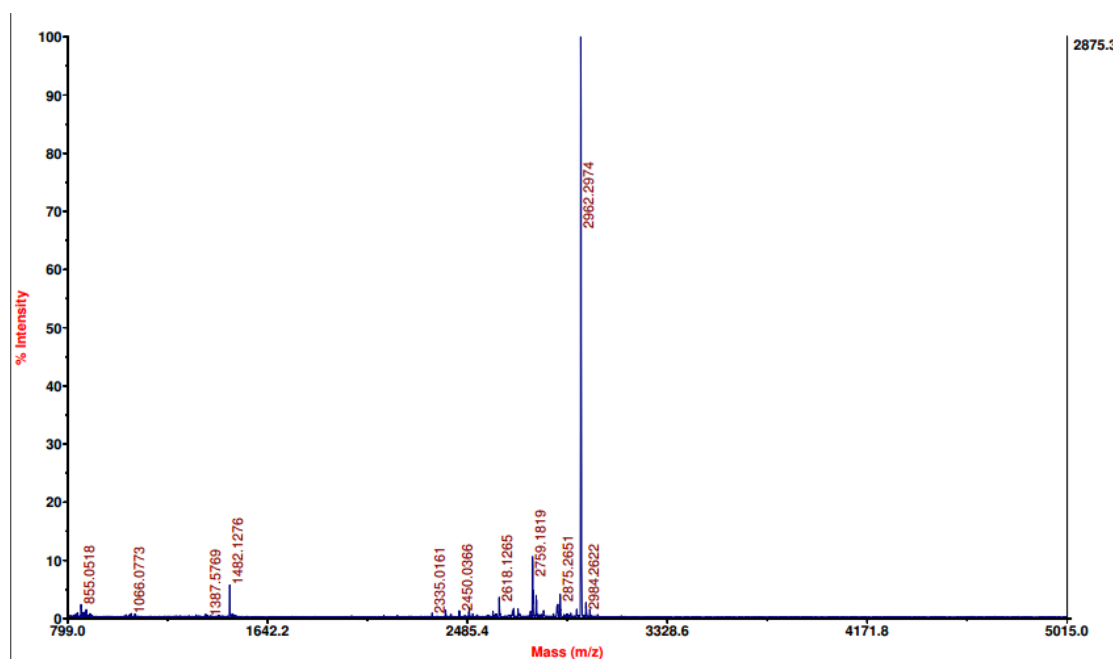
Analytical HPLC of glycopeptide **26**



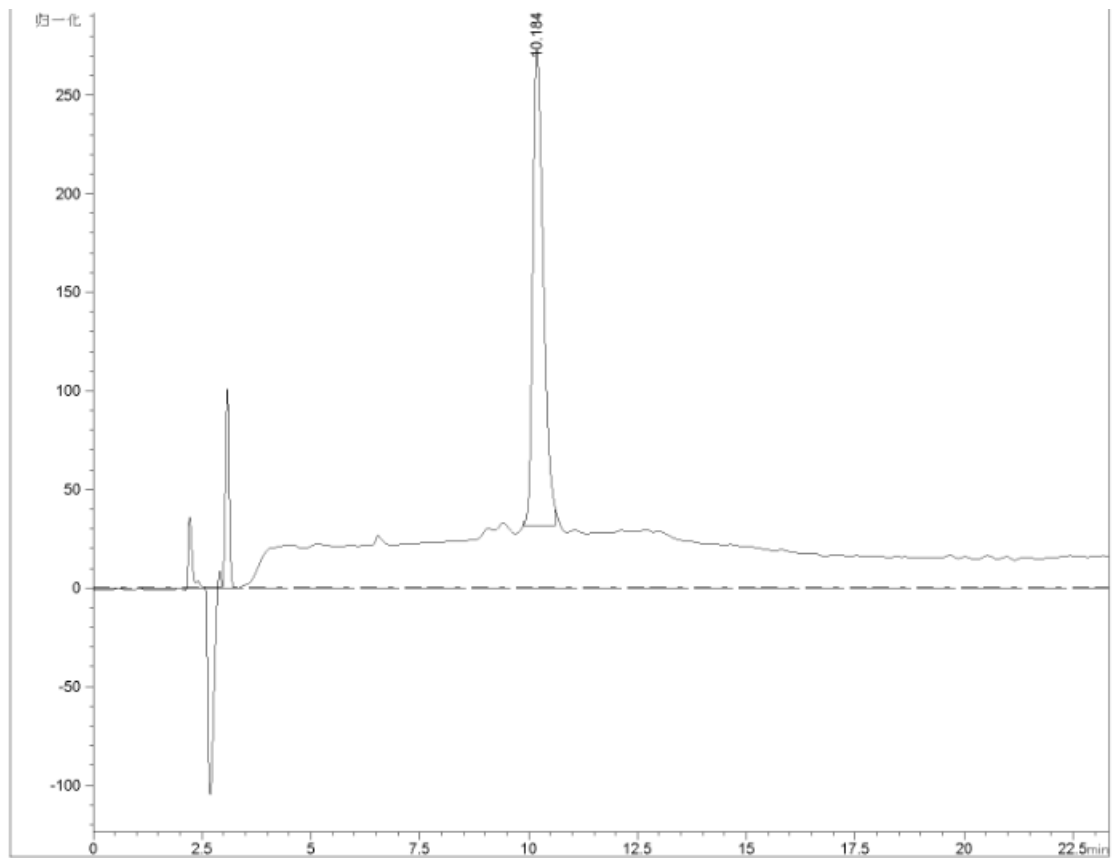
MALDI-TOF mass spectrum of glycopeptide **26**



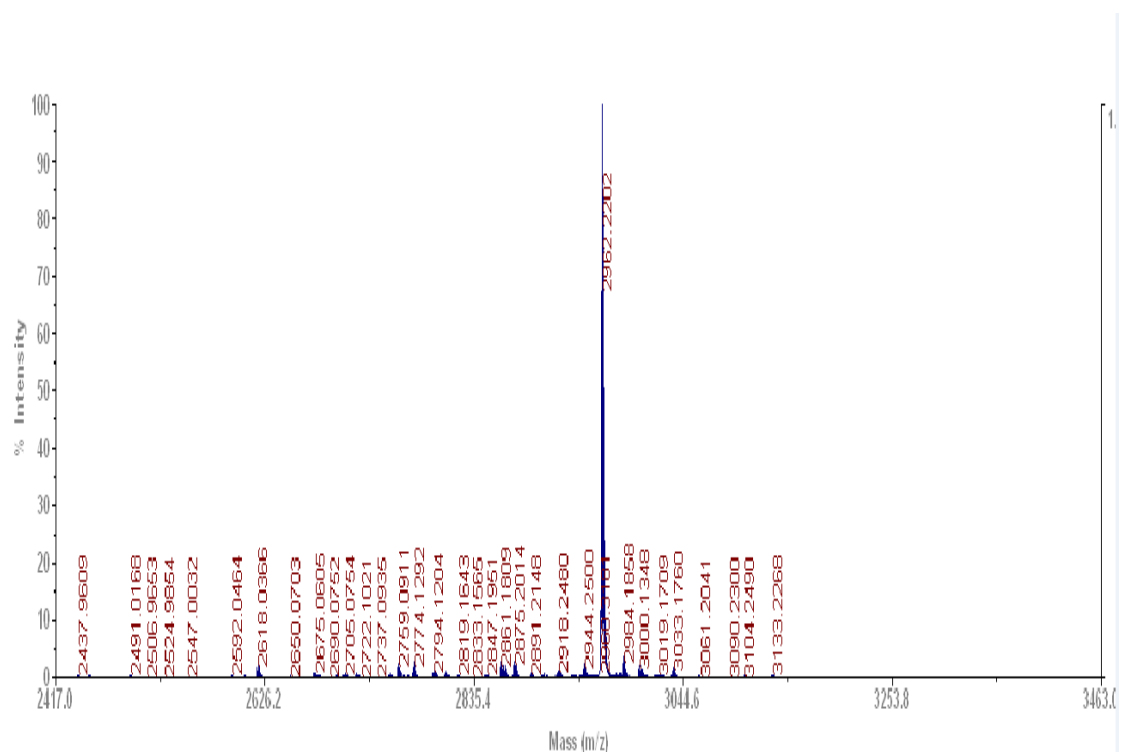
Analytical HPLC of glycopeptide **27**



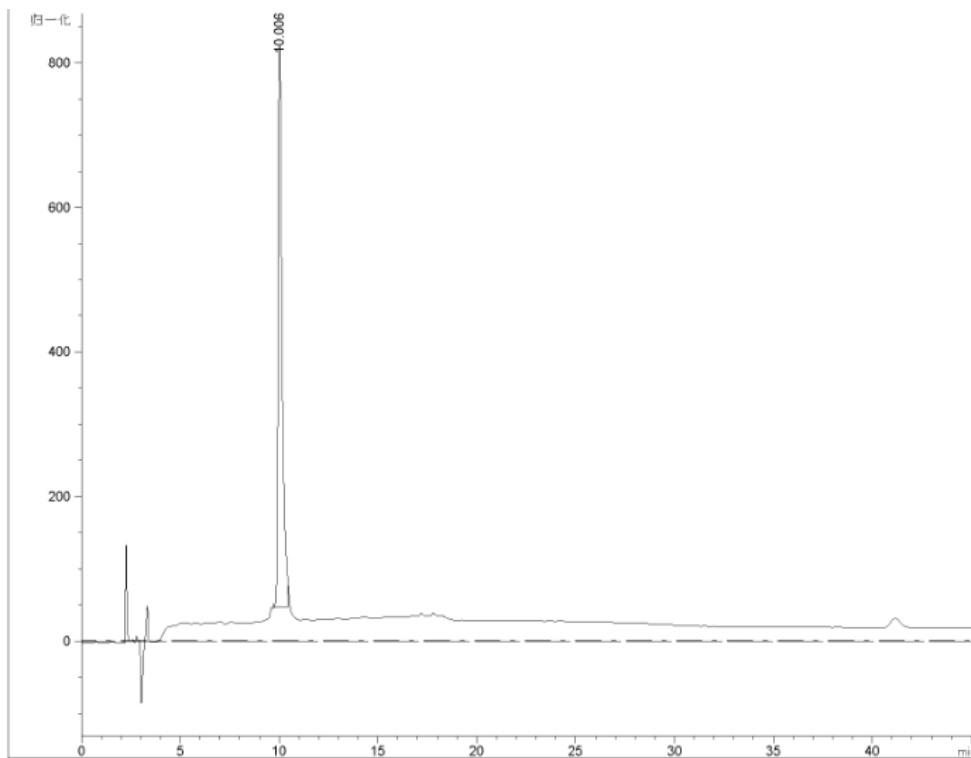
MALDI-TOF mass spectrum of glycopeptide **27**



Analytical HPLC of glycopeptide **28**



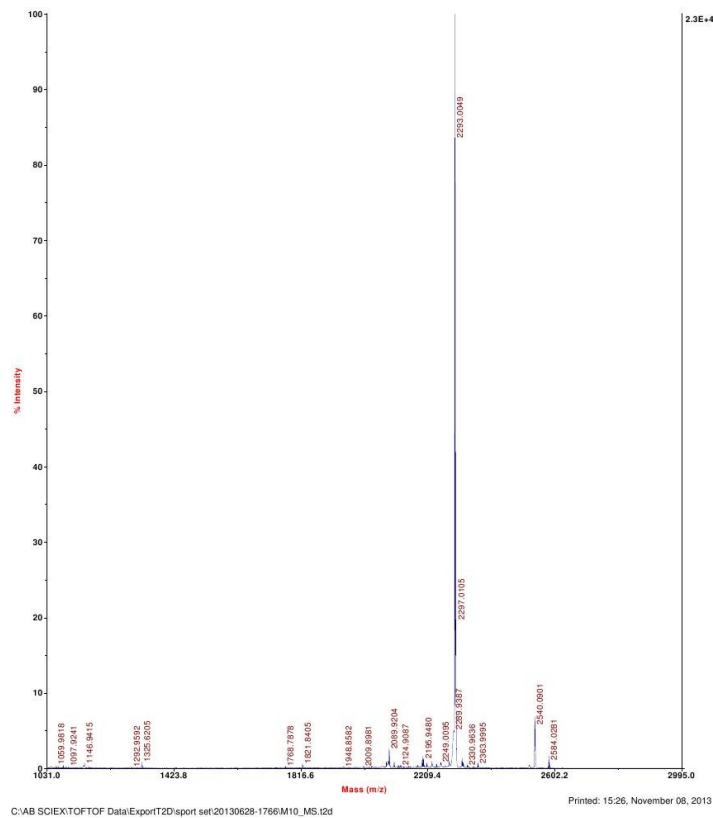
MALDI-TOF mass spectrum of glycopeptide **28**



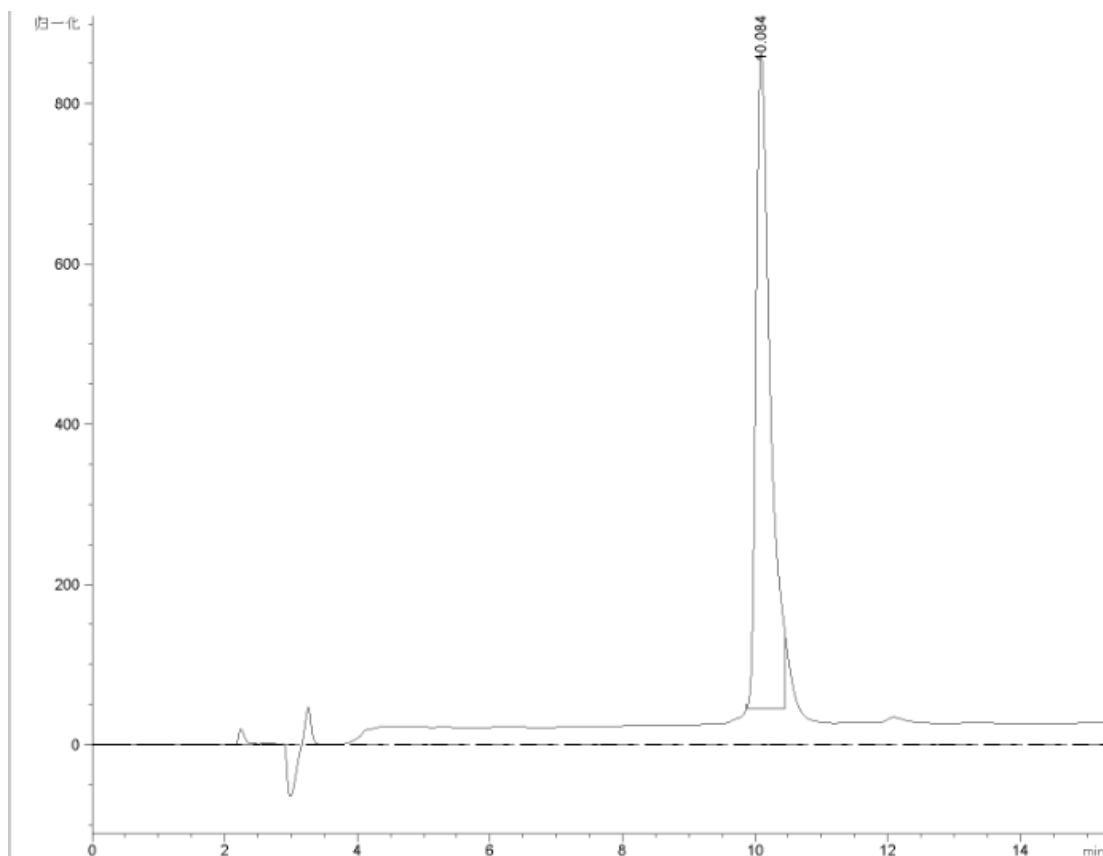
Analytical HPLC of glycopeptide **29**

AB Sciex TOF/TOF™ Series Explorer™ 72115

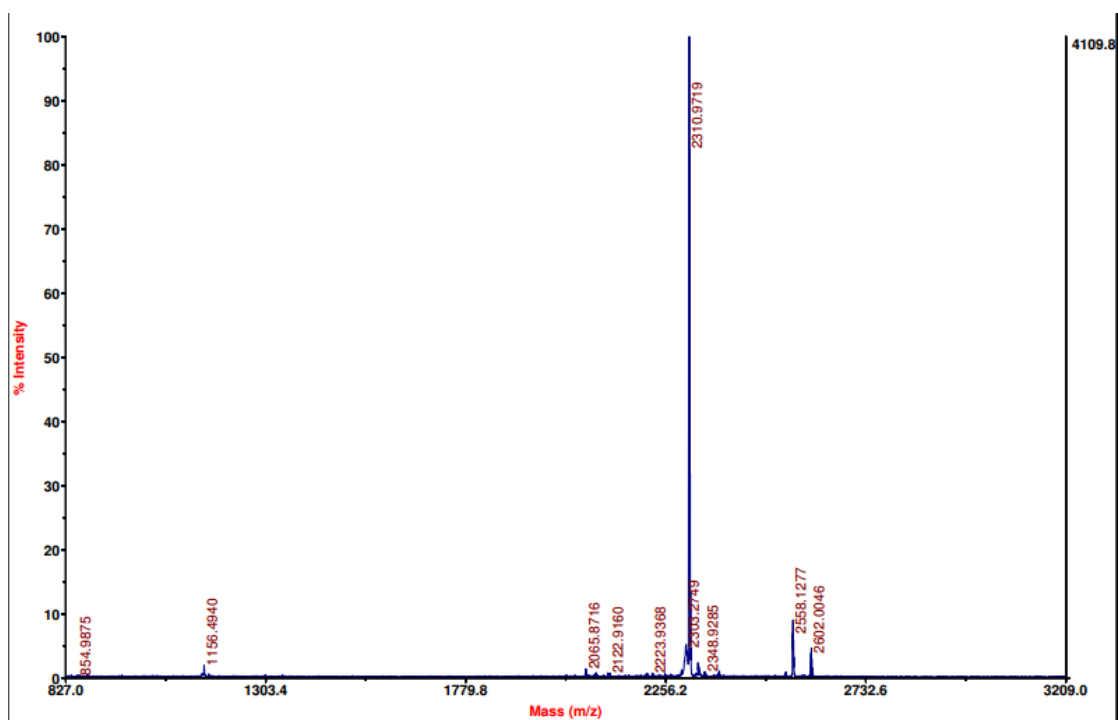
TOF/TOF™ Reflector Spec #1 MC[BP = 2294.0, 23263]



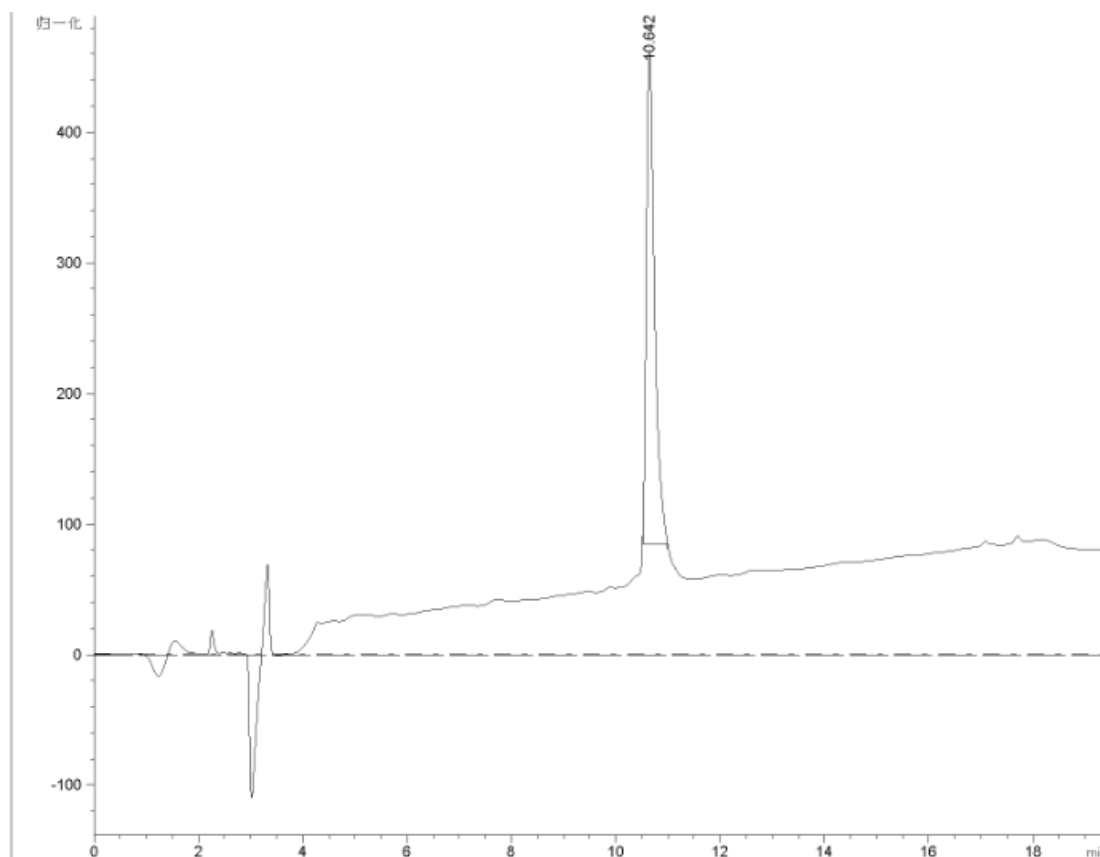
MALDI-TOF mass spectrum of glycopeptide **29**



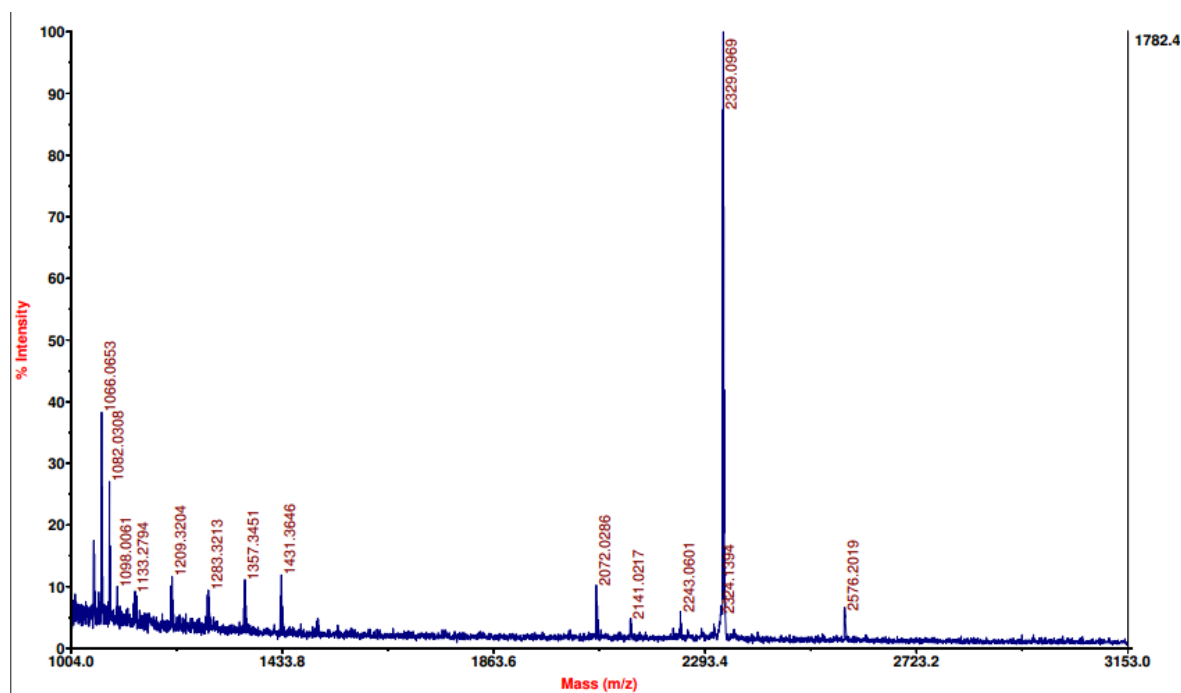
Analytical HPLC of glycopeptide **30**



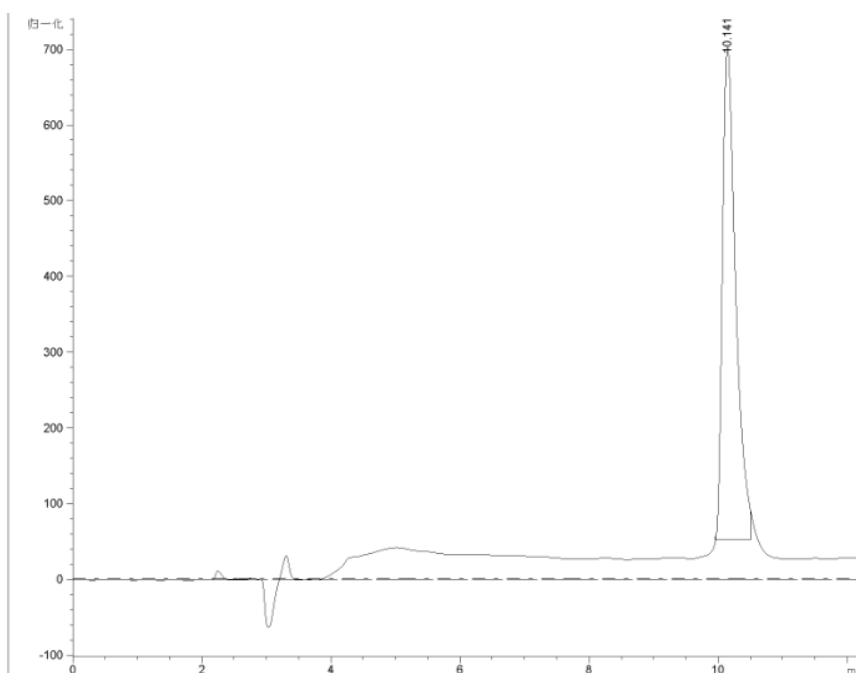
MALDI-TOF mass spectrum of glycopeptide **30**



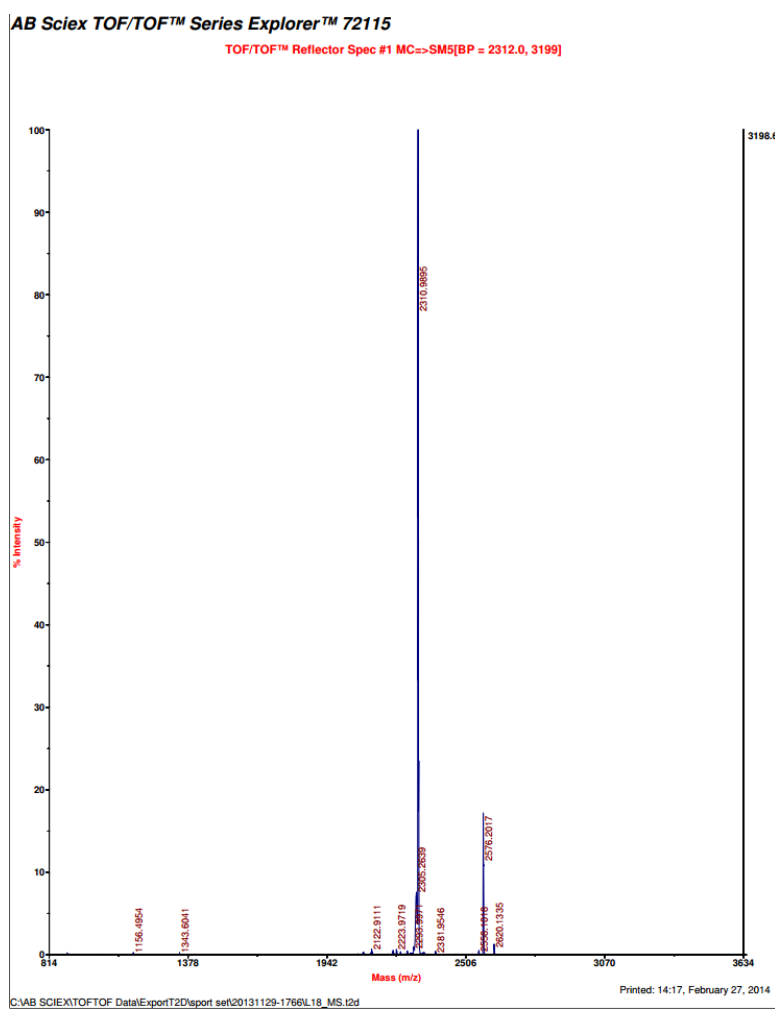
Analytical HPLC of glycopeptide 31



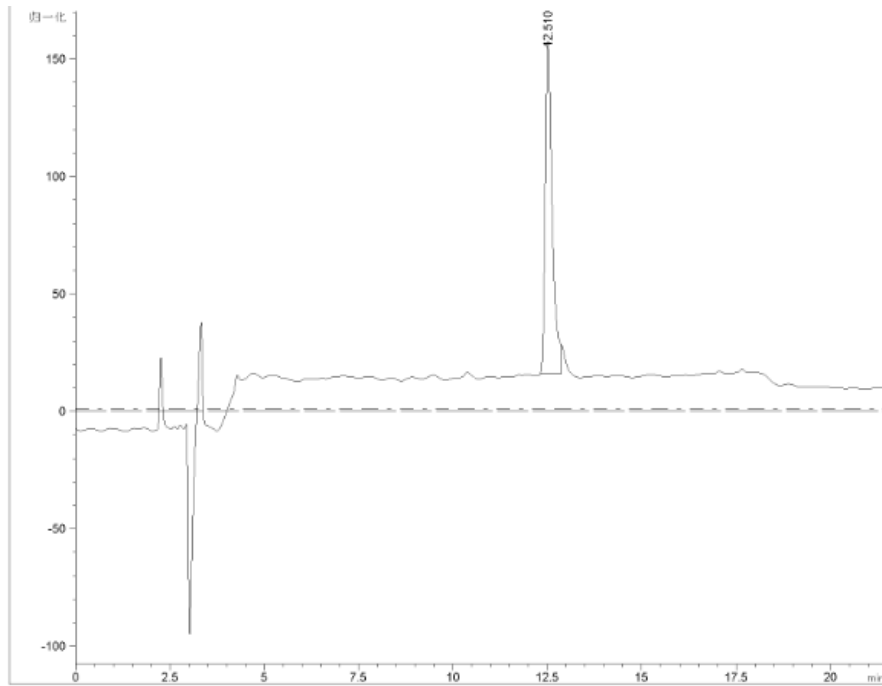
MALDI-TOF mass spectrum of glycopeptide 31



Analytical HPLC of glycopeptide **32**



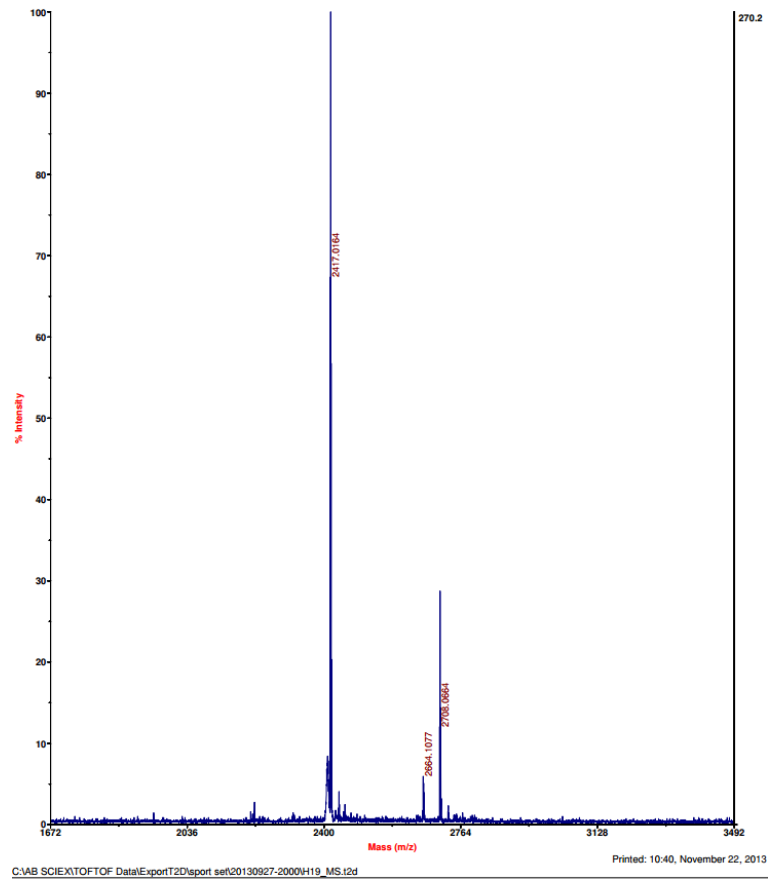
MALDI-TOF mass spectrum of glycopeptide **32**



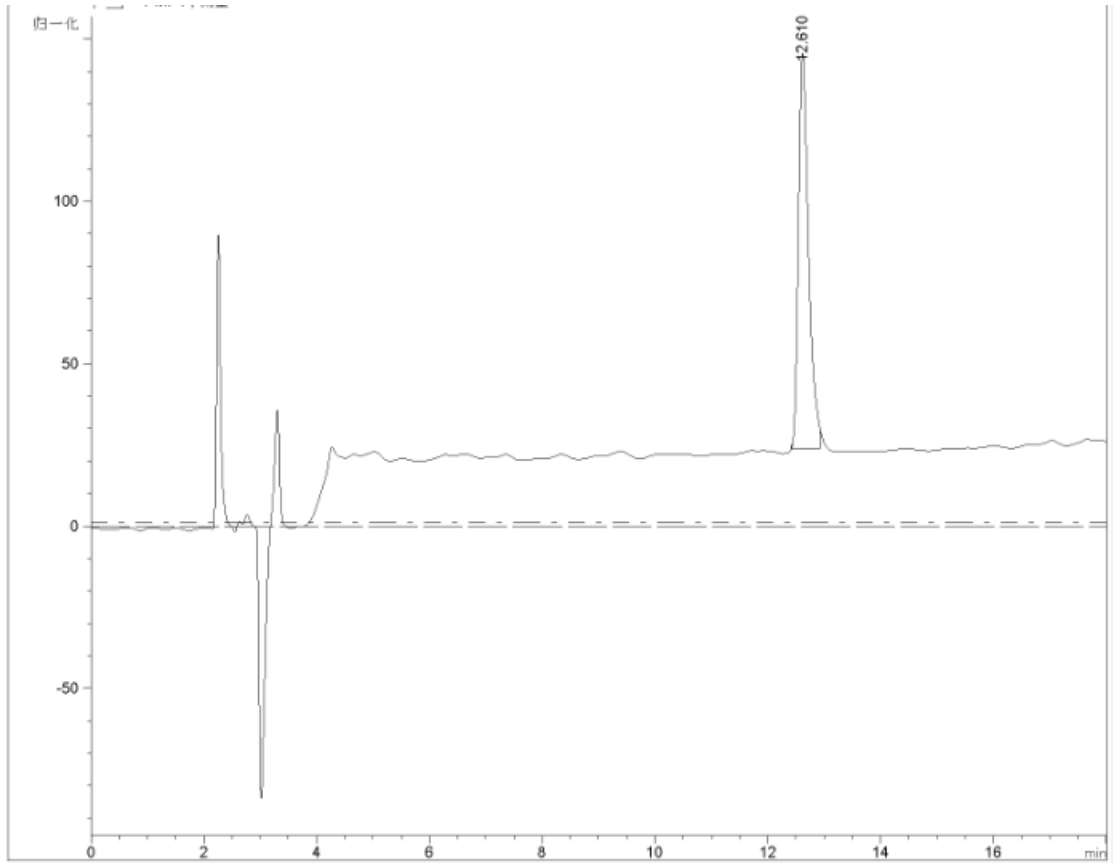
Analytical HPLC of glycopeptide **33**

AB Sciex TOF/TOF™ Series Explorer™ 72115

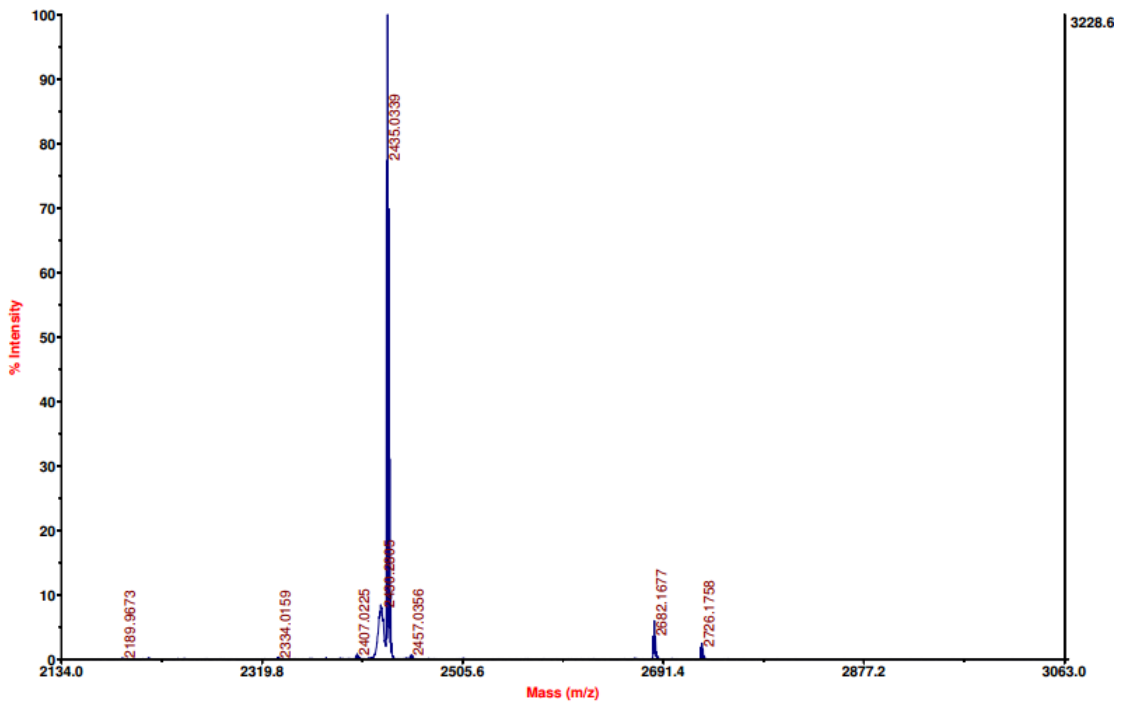
TOF/TOF™ Reflector Spec #1 MC[BP = 2418.0, 270]



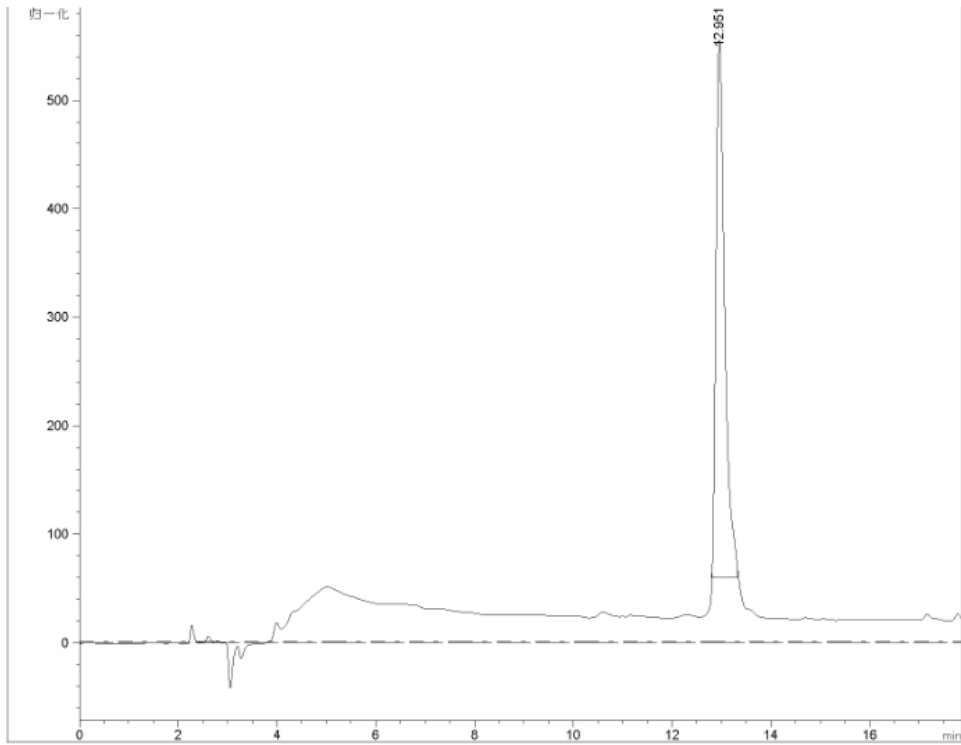
MALDI-TOF mass spectrum of glycopeptide **33**



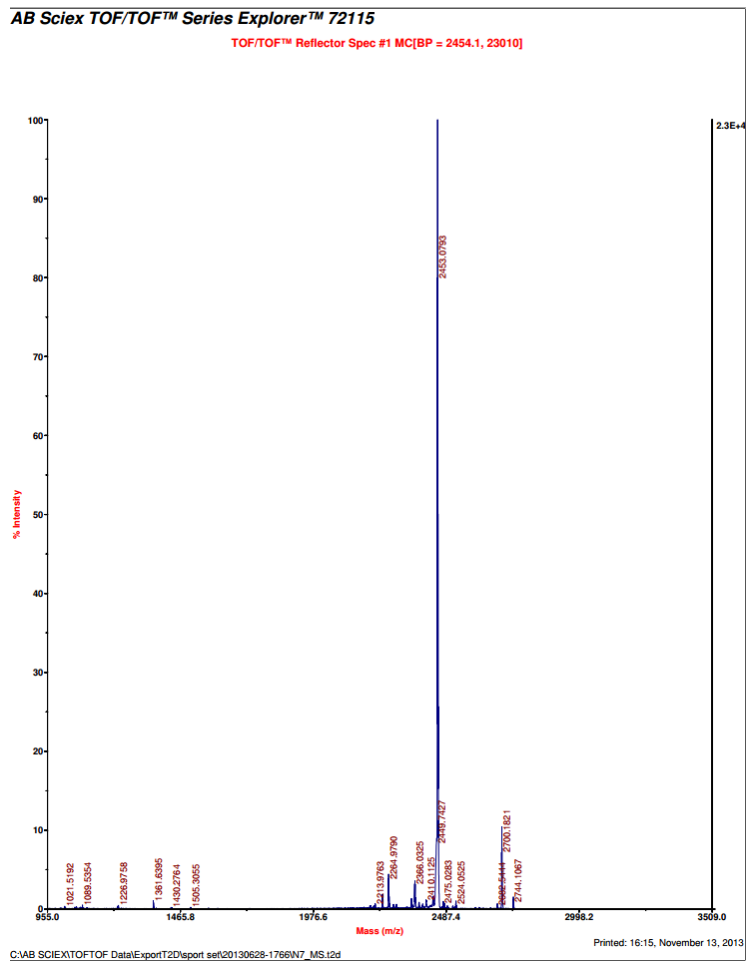
Analytical HPLC of glycopeptide **34**



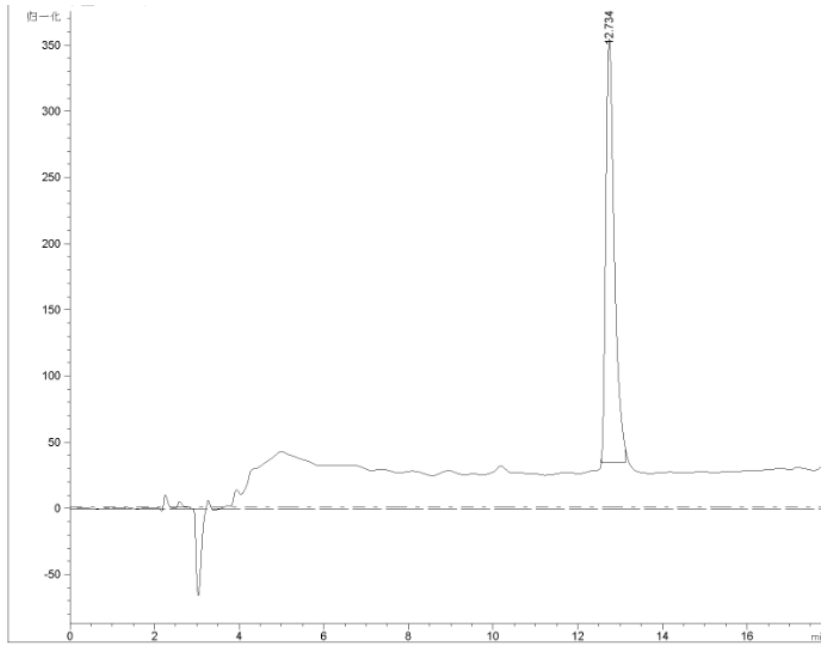
MALDI-TOF mass spectrum of glycopeptide **34**



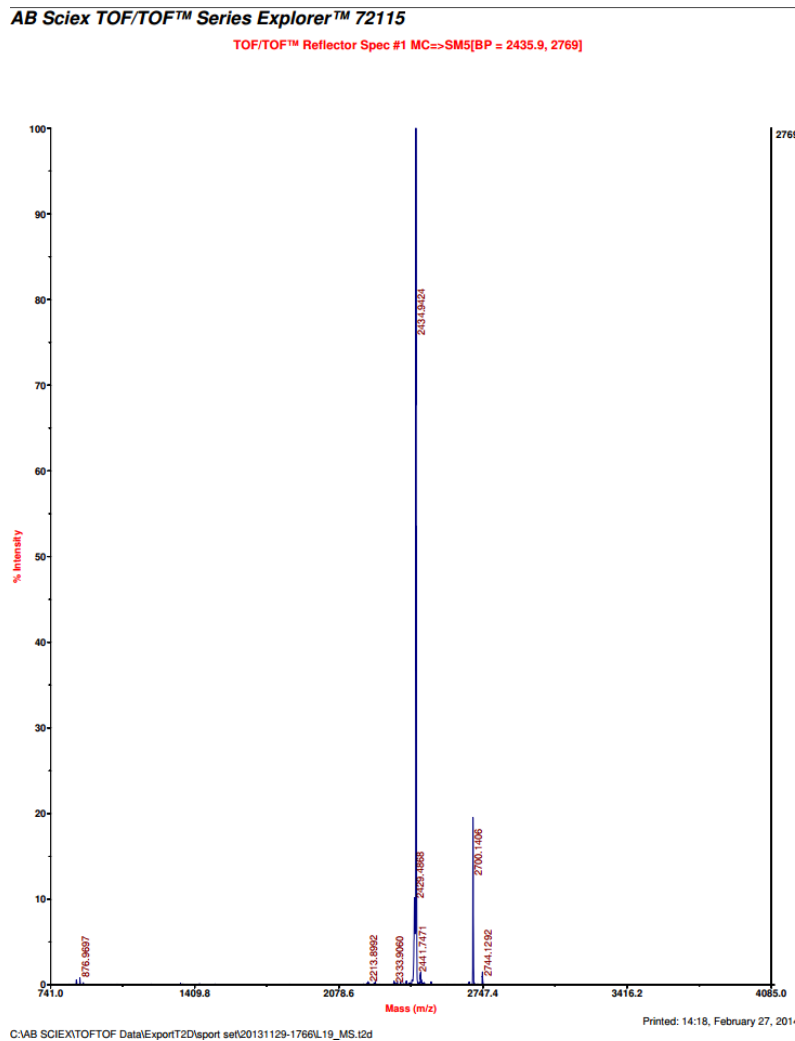
Analytical HPLC of glycopeptide 35



MALDI-TOF mass spectrum of glycopeptide 35



Analytical HPLC of glycopeptide **36**



MALDI-TOF mass spectrum of glycopeptide **36**