

Supporting Information

Synthesis and In Vitro Anti-influenza Virus Evaluation of Novel Sialic Acid (C-5 and C-9)-Pentacyclic Triterpene Derivatives

Xu Han ^{1,†}, Long-Long Si ^{1,†}, Yong-Ying Shi ¹, Zi-Bo Fan ¹, Shou-Xin Wang ^{1,3}, Zhen-Yu Tian ¹, Man Li ¹, Jia-Qi Sun ¹, Ping-Xuan Jiao ¹, Fu-Xiang Ran ¹, Yong-Min Zhang ², De-Min Zhou ¹, Su-Long Xiao ^{1,*}

1. State Key Laboratory of Natural and Biomimetic Drugs, School of Pharmaceutical Sciences, Peking University, Beijing 100191, China; E-Mails: ax_han@126.com (X. H.); silonglong@bjmu.edu.cn (L.-L. S.); sygne24501@sina.com (Y.-Y. S.); fancyfzb@163.com (Z.-B. F.); shouxinwang@126.com (S.-X. W.); fashankc@163.com (Z.-Y.T.), 18811711762@163.com (M.L.), jiaqi.sun@pku.edu.cn (J.-Q.S.); 15022326072@163.com (P.-X.J.); rfx@bjmu.edu.cn (F.-X. R); Deminzhou@bjmu.edu.cn (D.-M. Z)
2. Institut Parisien de Chimie Moléculaire, CNRS UMR 8232, Université Pierre & Marie Curie-Paris 6, 4 Place Jussieu, 75005 Paris, France; yongmin.zhang@upmc.fr (Y.-M. Z)
3. School of Pharmacy, Jining Medical University, Rizhao 276826, China

1. **Table S1.** The cytotoxicity of compounds **26** and **42** against HL-60, HeLa and A549 cell lines. Selected ¹H, ¹³C NMR and HRMS spectra.

NMR or HRMS	Page
¹ H NMR of compound 9	S4
¹³ C NMR of compound 9	S4
HRMS of compound 9	S5
¹ H NMR of compound 18	S5
¹³ C NMR of compound 18	S6
HRMS of compound 18	S6
¹ H NMR of compound 19	S7
¹³ C NMR of compound 19	S7
HRMS of compound 19	S8
¹ H NMR of compound 20	S8
¹³ C NMR of compound 20	S9
HRMS of compound 20	S9
¹ H NMR of compound 21	S10
¹³ C NMR of compound 21	S10

HRMS of compound 21	S11
¹ H NMR of compound 22	S11
¹³ C NMR of compound 22	S12
HRMS of compound 22	S12
¹ H NMR of compound 23	S13
¹³ C NMR of compound 23	S13
HRMS of compound 23	S14
¹ H NMR of compound 24	S14
¹³ C NMR of compound 24	S15
HRMS of compound 24	S15
¹ H NMR of compound 25	S16
¹³ C NMR of compound 25	S16
HRMS of compound 25	S17
¹ H NMR of compound 26	S17
¹³ C NMR of compound 26	S18

HRMS of compound 26	S18
¹ H NMR of compound 28	S19
¹³ C NMR of compound 28	S19
HRMS of compound 28	S20
¹ H NMR of compound 29	S20
¹³ C NMR of compound 29	S21
HRMS of compound 29	S21
¹ H NMR of compound 30	S22
¹³ C NMR of compound 30	S22
HRMS of compound 30	S23
¹ H NMR of compound 34	S23
¹³ C NMR of compound 34	S24
HRMS of compound 34	S24
¹ H NMR of compound 35	S25
¹³ C NMR of compound 35	S25
HRMS of compound 35	S26
¹ H NMR of compound 36	S26
¹³ C NMR of compound 36	S27
HRMS of compound 36	S27
¹ H NMR of compound 37	S28
¹³ C NMR of compound 37	S28
HRMS of compound 37	S29
¹ H NMR of compound 38	S29

¹³ C NMR of compound 38	S30
HRMS of compound 38	S30
¹ H NMR of compound 39	S31
¹³ C NMR of compound 39	S32
HRMS of compound 39	S32
¹ H NMR of compound 40	S33
¹³ C NMR of compound 40	S33
HRMS of compound 40	S34
¹ H NMR of compound 41	S34
¹³ C NMR of compound 41	S35
HRMS of compound 41	S35
¹ H NMR of compound 42	S36
¹³ C NMR of compound 42	S36
HRMS of compound 42	S37
¹ H NMR of compound 44	S37
¹³ C NMR of compound 44	S38
HRMS of compound 44	S38
¹ H NMR of compound 45	S39
¹³ C NMR of compound 45	S39
HRMS of compound 45	S40
¹ H NMR of compound 46	S40
¹³ C NMR of compound 46	S41
HRMS of compound 46	S41

1. **Table S1.** The cytotoxicity of compounds **26** and **42** against HL-60, HeLa and A549 cell lines.

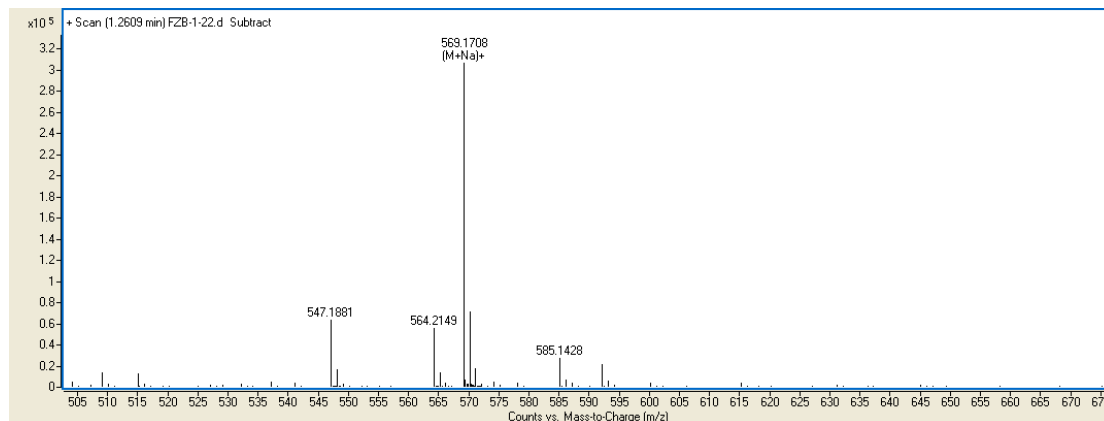
Compounds	Cell lines	0.1 μ M	1 μ M	10 μ M
26	HL-60	3.52	4.01	2.33
	HeLa	-3.34	6.6	9.46
	A549	2.16	5.23	0.21
42	HL-60	-2	13.6	53
	HeLa	1.18	20.13	6.04
	A549	2.33	-0.37	17.7
5-Fu	HL-60	85.22 ^a		
	HeLa	90.32 ^a		
	A549	77.20 ^a		

^a Measured in a dose of 0.5 μ M.

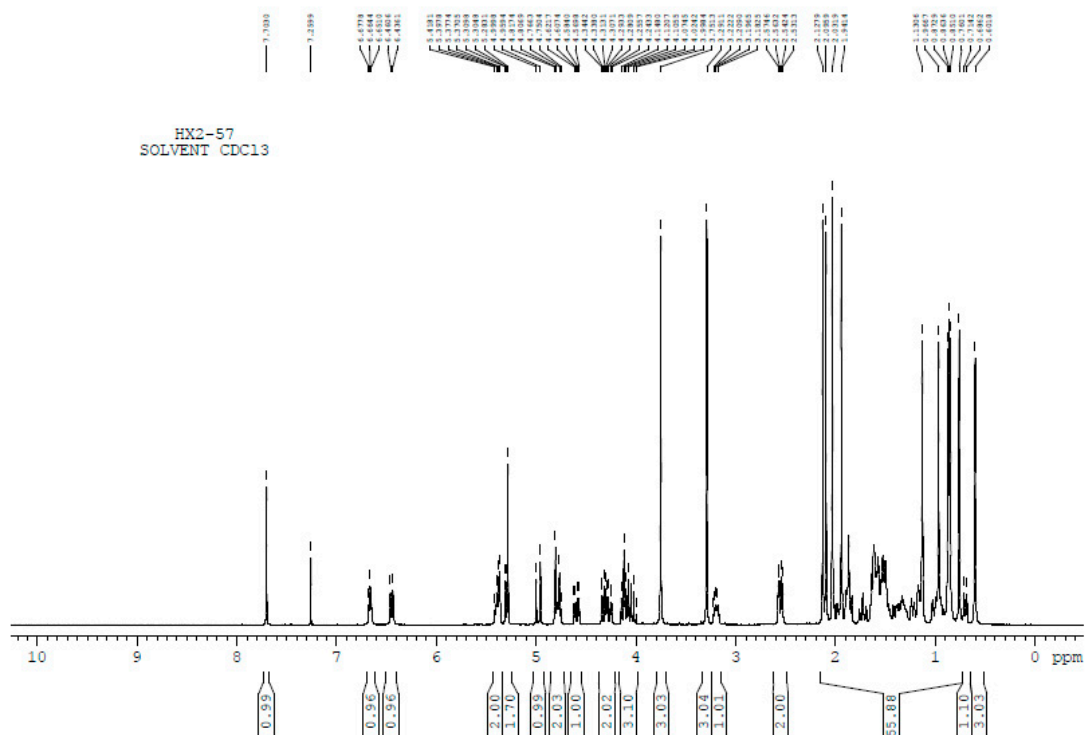
3. HR-ESI-MS spectrum of compound 9

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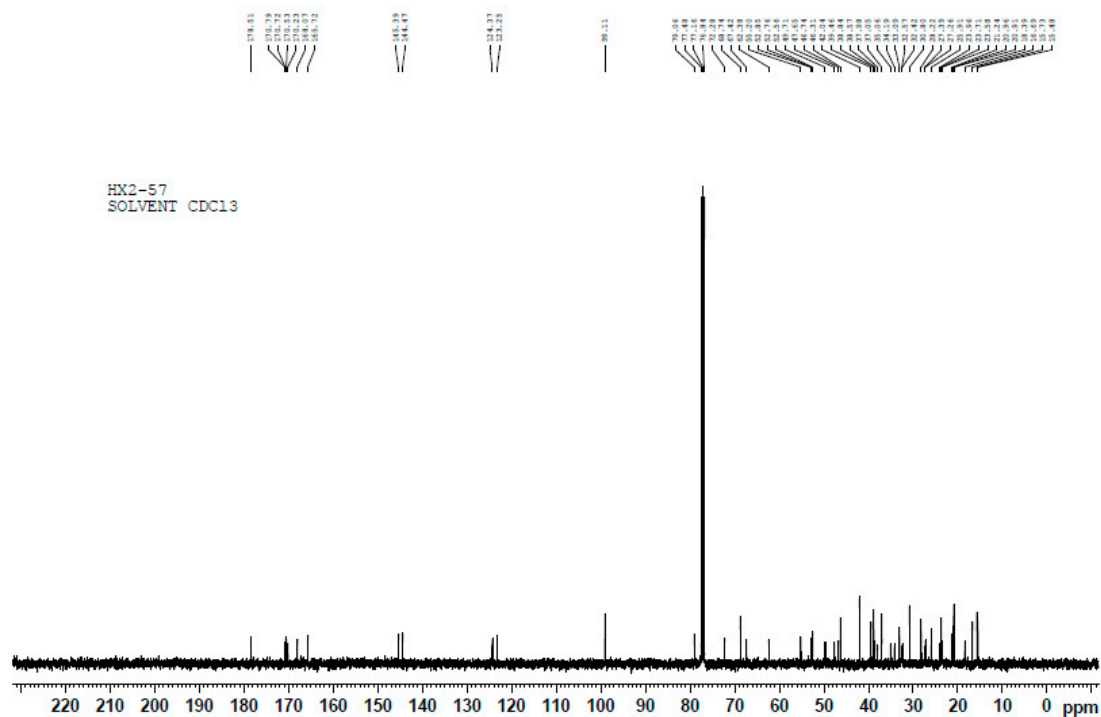
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
FZB1-22	C ₂₁ H ₃₀ N ₄ O ₁₃	C ₂₁ H ₃₀ N ₄ NaO ₁₃	569.1708	569.1702	-1.21



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



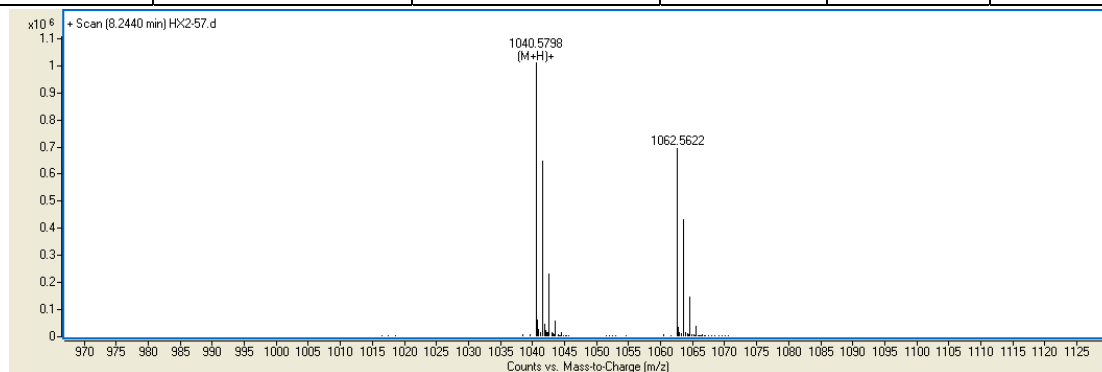
5. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **18**



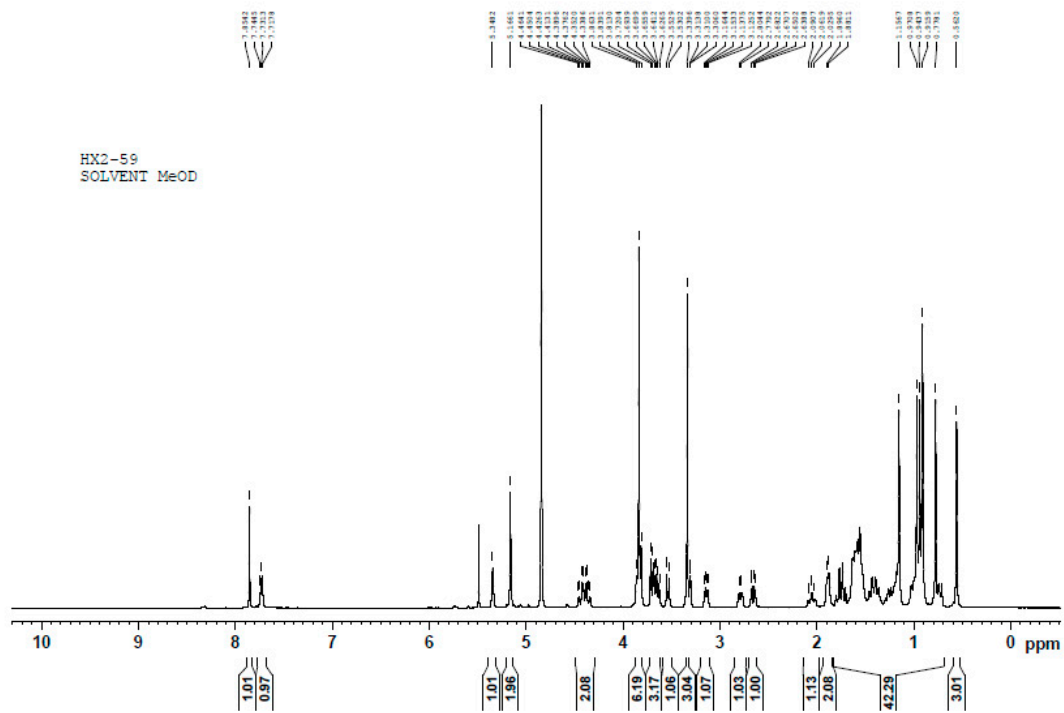
6. HR-ESI-MS spectrum of compound **18**

HIGH RESOLUTION MASS SPECTROMETRY REPORT

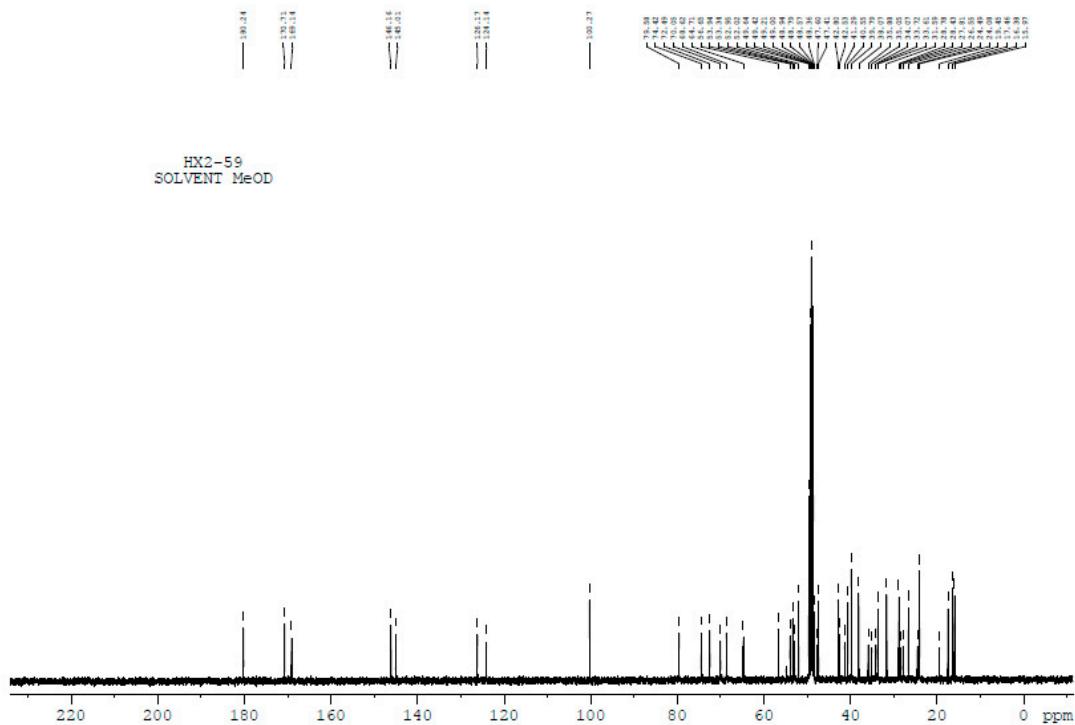
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-57	$\text{C}_{54}\text{H}_{81}\text{N}_5\text{O}_{15}$	$\text{C}_{54}\text{H}_{82}\text{N}_5\text{O}_{15}$	1040.5798	1040.5802	0.37



7. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 19



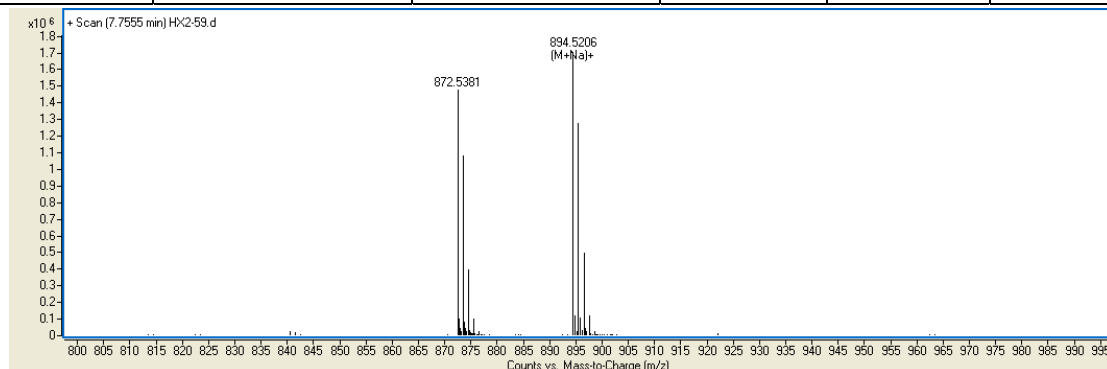
8. ¹³C NMR (100 MHz, CD₃OD) spectrum of compound 19



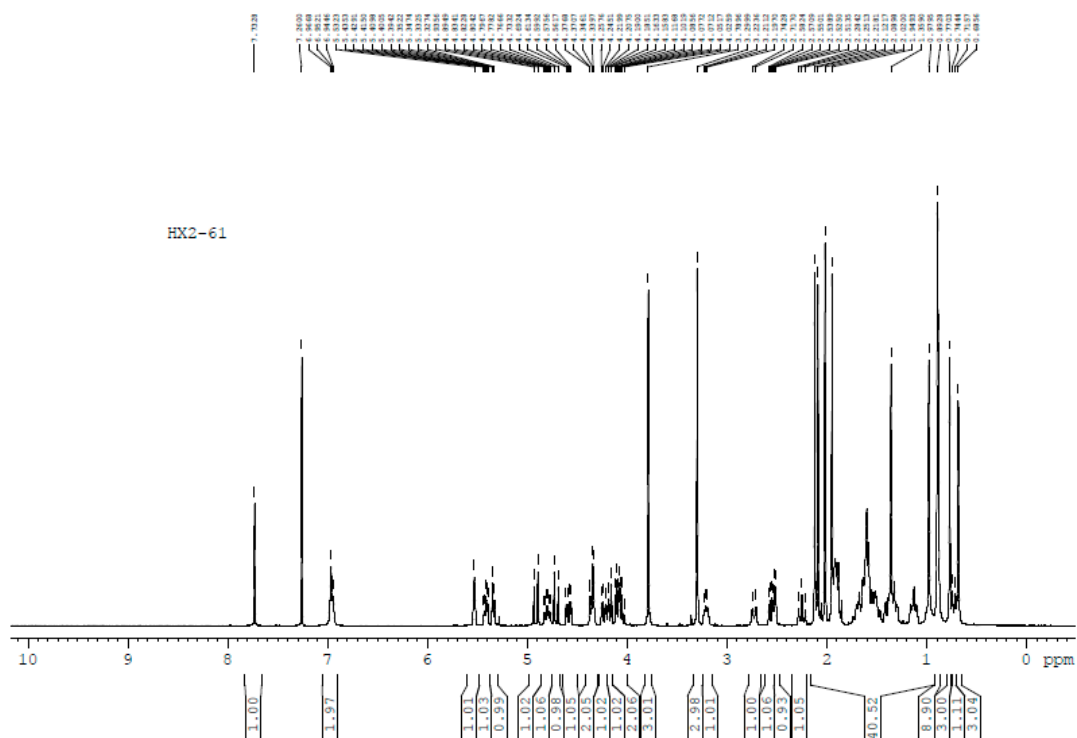
9. HR-ESI-MS spectrum of compound 19

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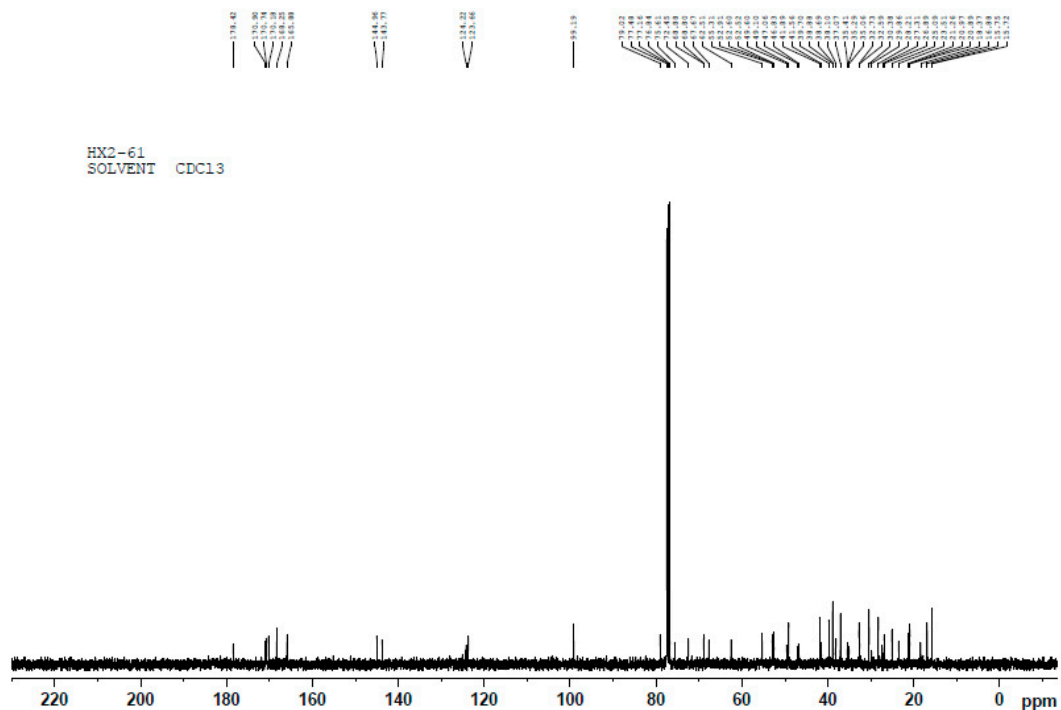
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-59	C ₄₆ H ₇₃ N ₅ O ₁₁	C ₄₆ H ₇₃ N ₅ Na O ₁₁	894.5206	894.5199	-1.23



10. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 20



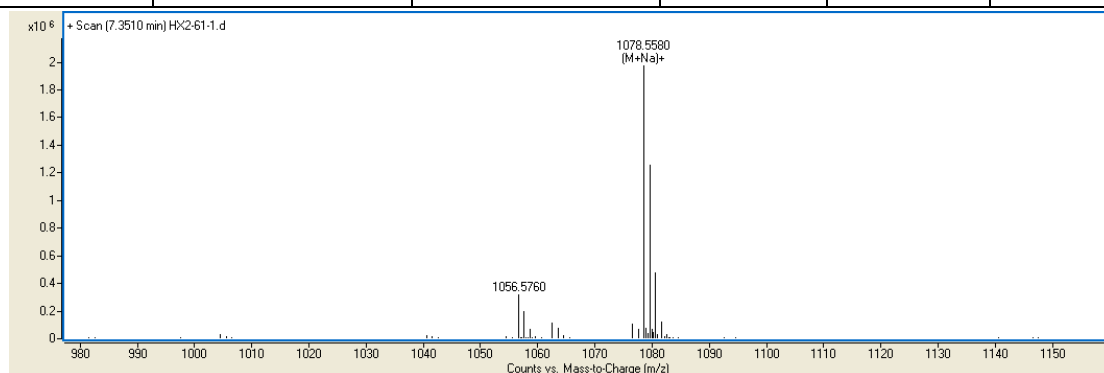
11. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound 20



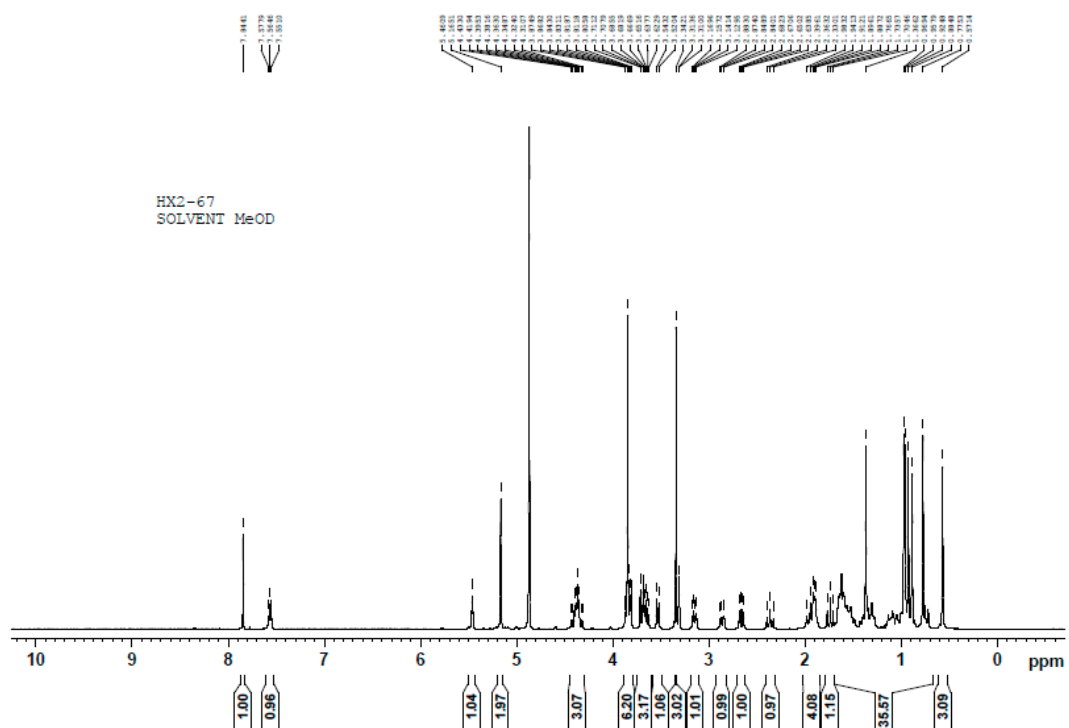
12. HR-ESI-MS spectrum of compound 20

HIGH RESOLUTION MASS SPECTROMETRY REPORT

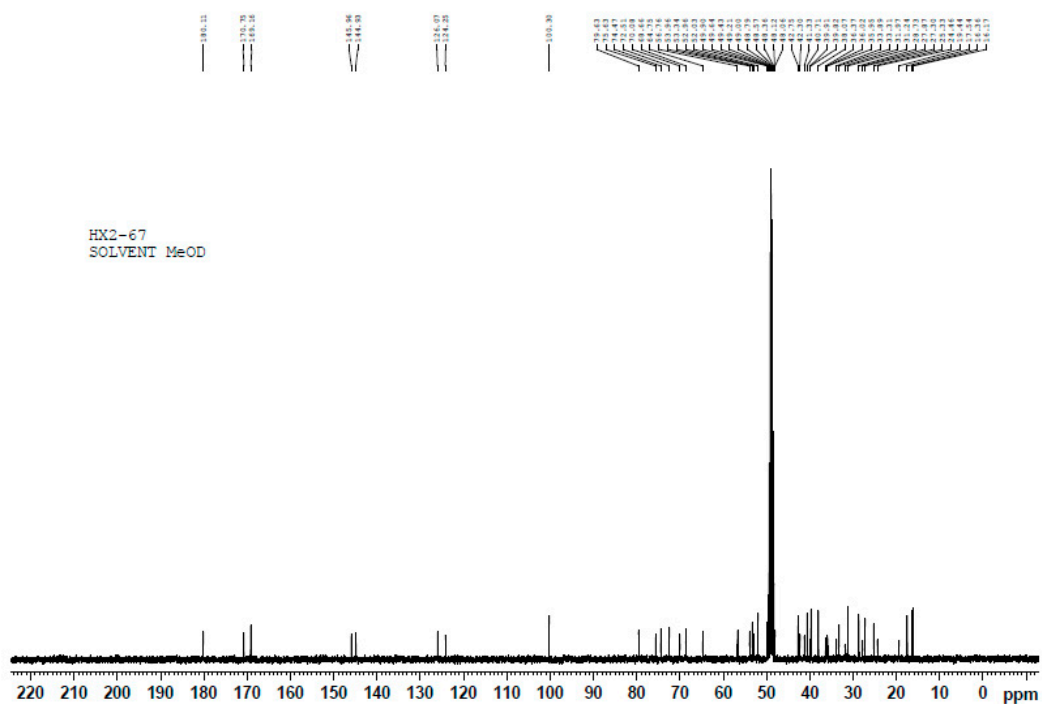
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HX2-61	C ₅₄ H ₈₁ N ₅ O ₁₆	C ₅₄ H ₈₁ N ₅ Na O ₁₆	1078.558	1078.5571	-1.01



13. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 21



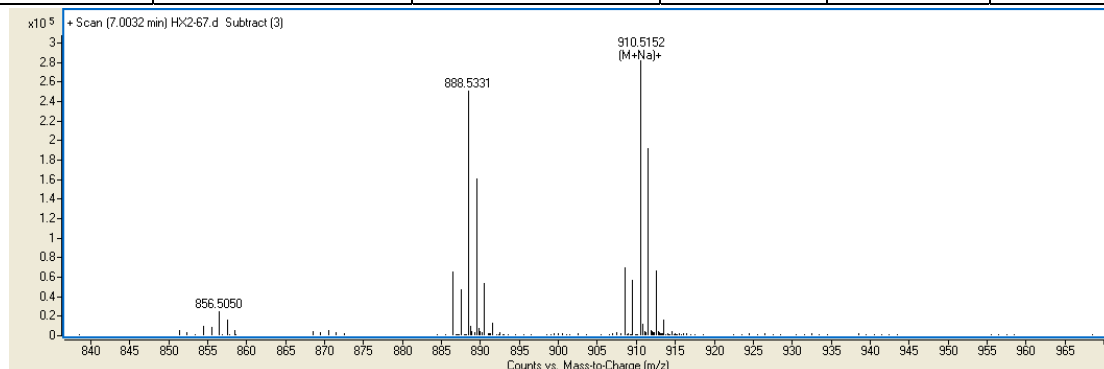
14. ¹³C NMR (100 MHz, CD₃OD) spectrum of compound 21



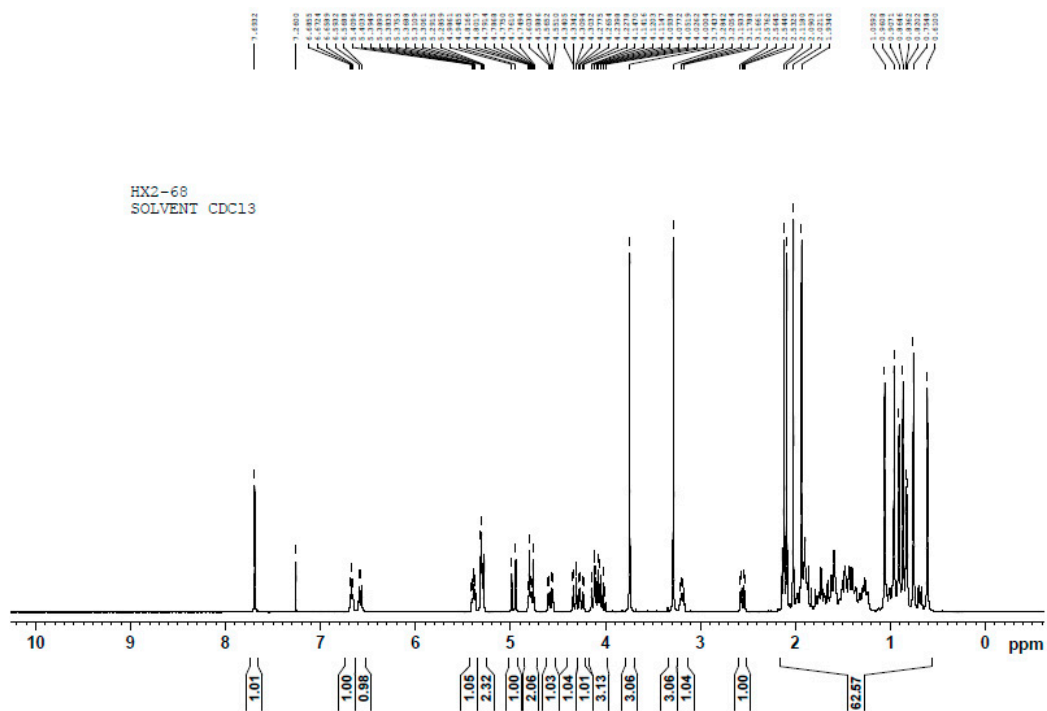
15. HR-ESI-MS spectrum of compound 21

HIGH RESOLUTION MASS SPECTROMETRY REPORT

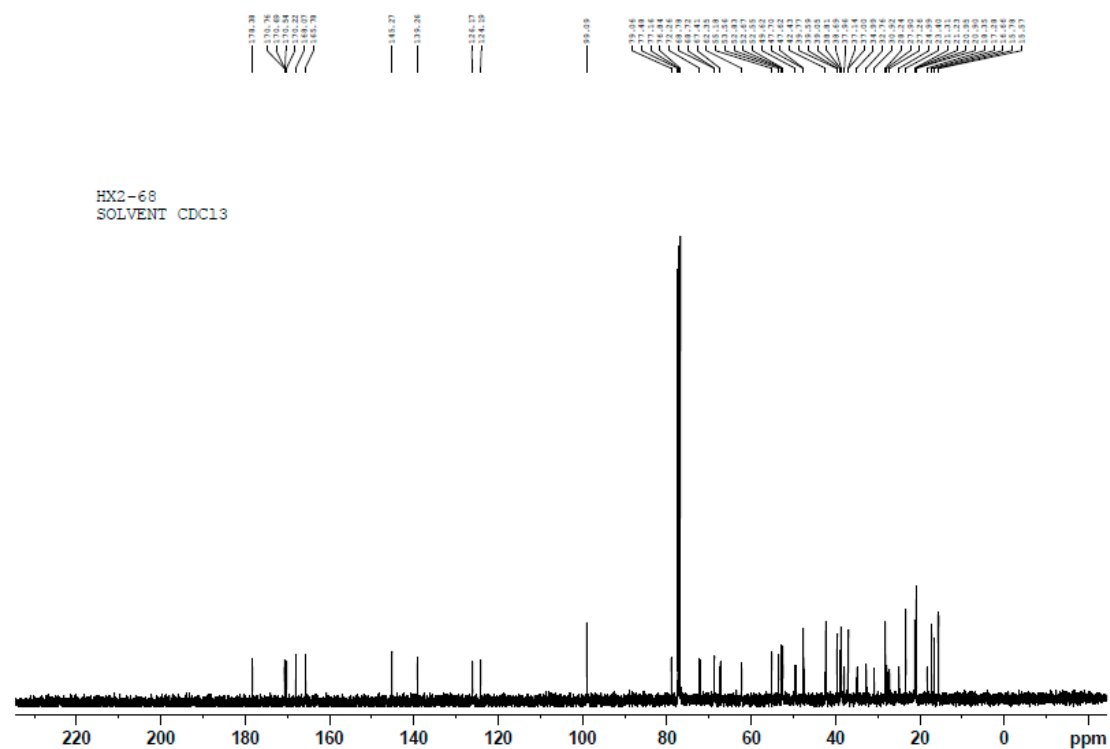
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-67	C ₄₆ H ₇₃ N ₅ O ₁₂	C ₄₆ H ₇₃ N ₅ NaO ₁₂	910.5152	910.5148	-0.77



16. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 22



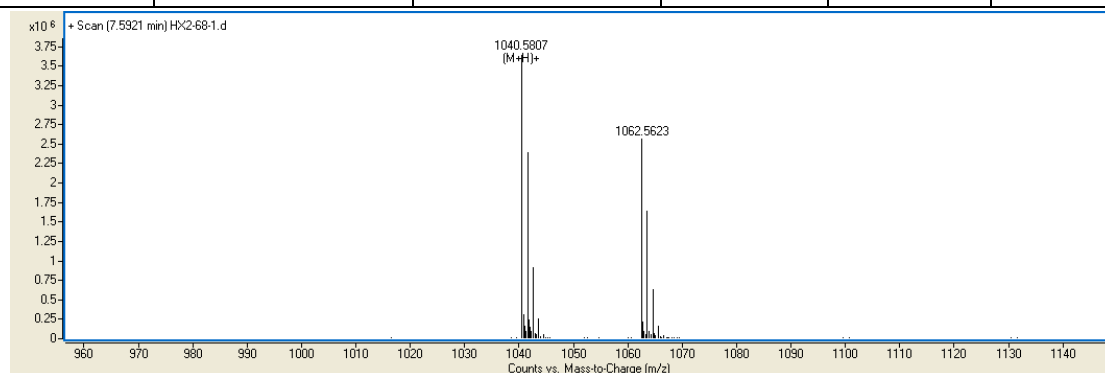
17. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound **22**



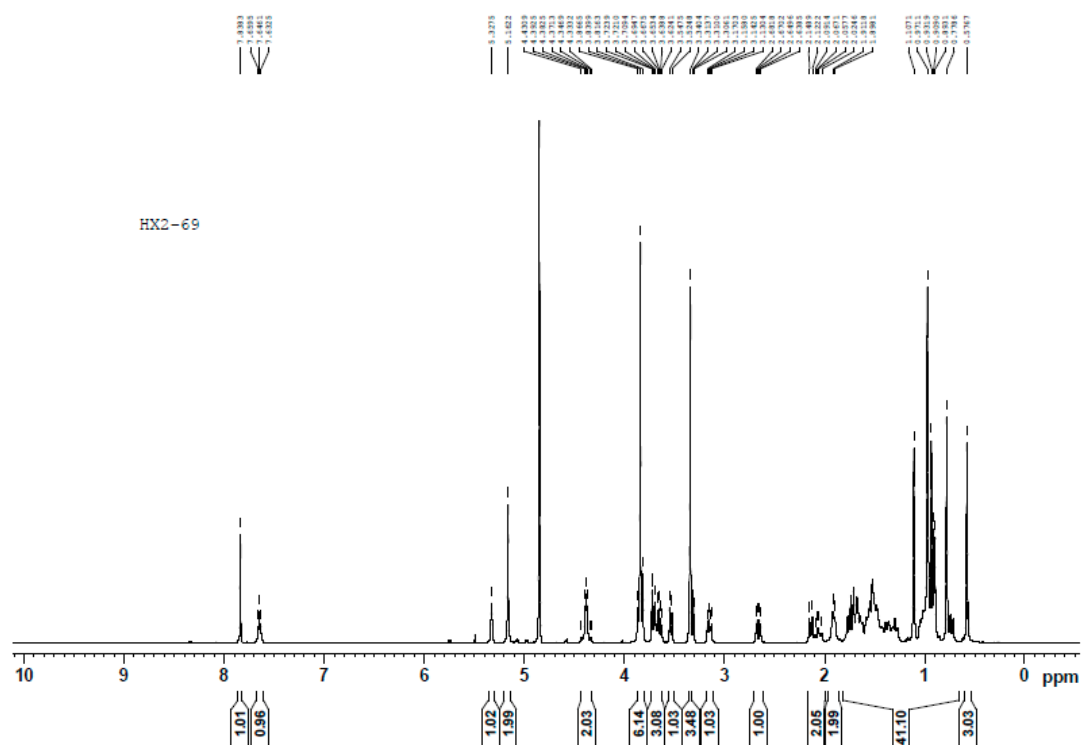
18. HR-ESI-MS spectrum of compound **22**

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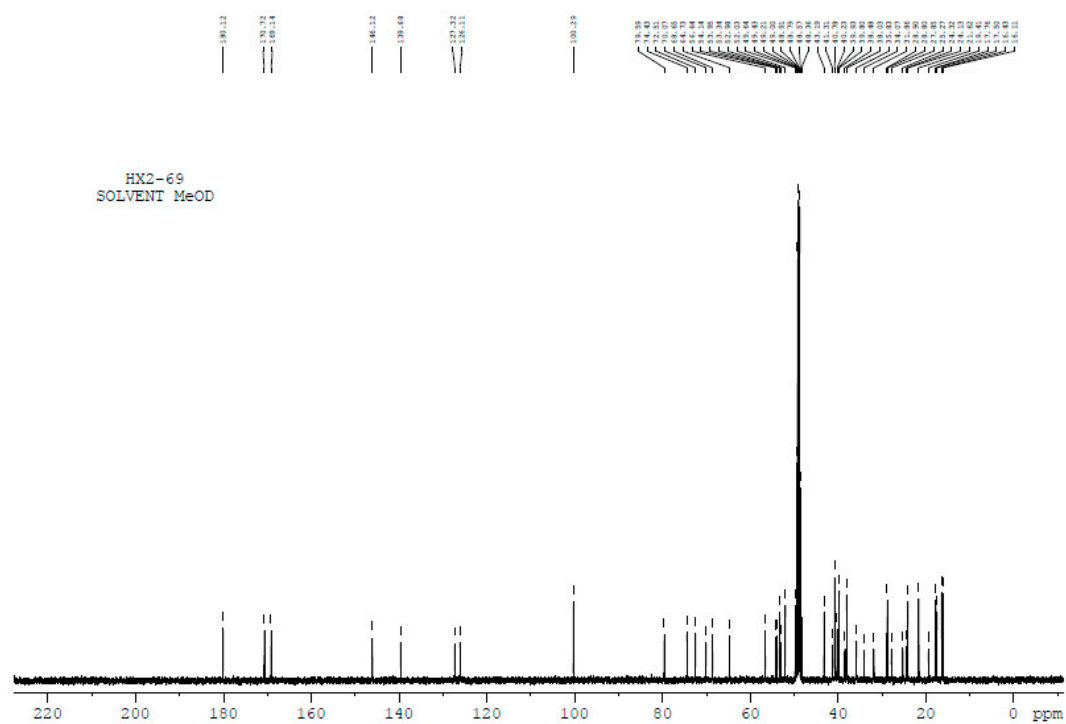
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-68	C ₅₄ H ₈₁ N ₅ O ₁₅	C ₅₄ H ₈₂ N ₅ O ₁₅	1040.5807	1040.58	-0.34



19. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 23



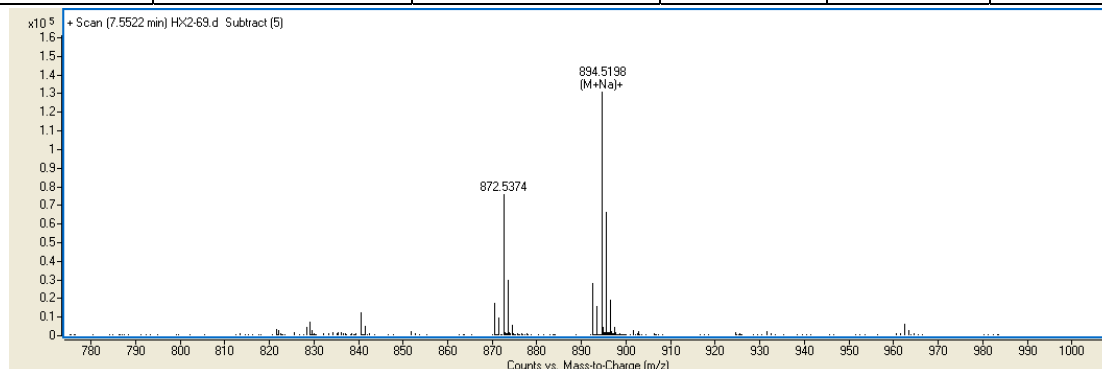
20. ¹³C NMR (100 MHz, CD₃OD) spectrum of compound 23



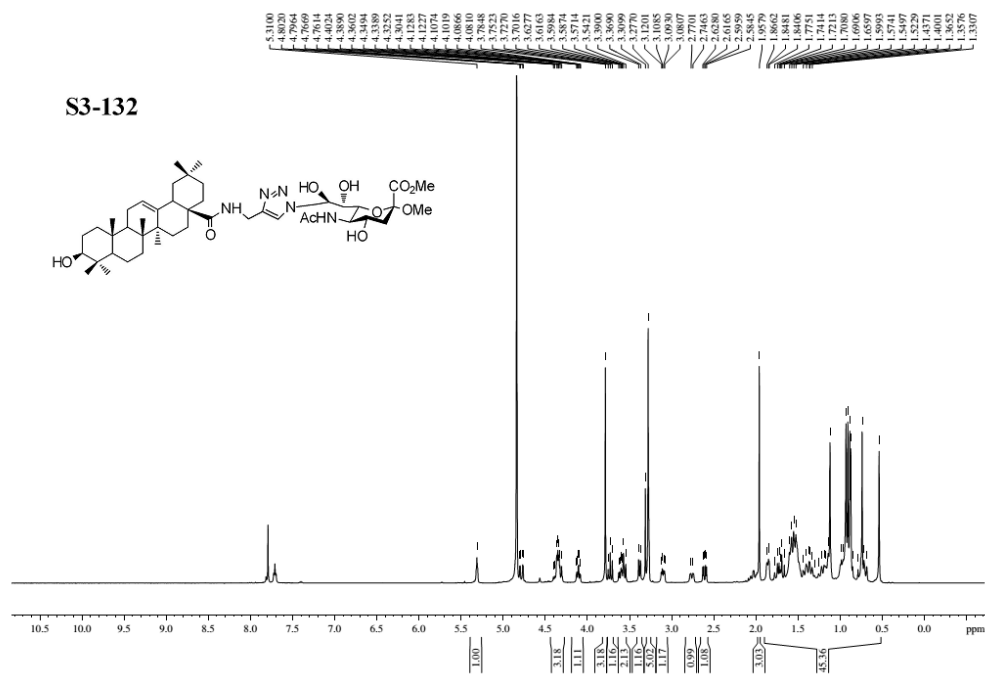
21. HR-ESI-MS spectrum of compound 23

HIGH RESOLUTION MASS SPECTROMETRY REPORT

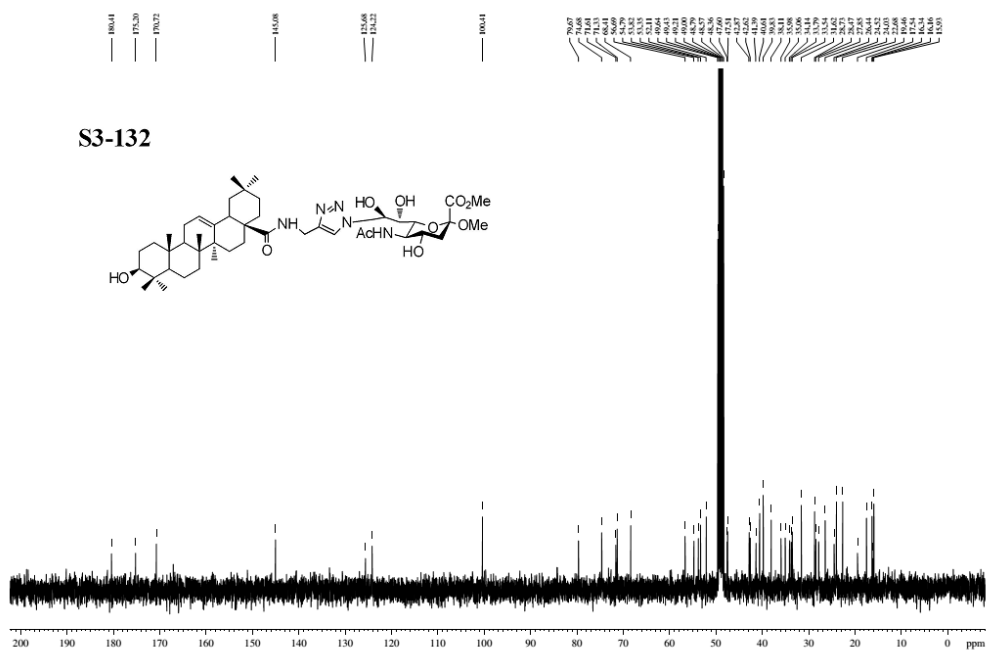
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-69	C ₄₆ H ₇₃ N ₅ O ₁₁	C ₄₆ H ₇₃ N ₅ Na O ₁₁	894.5198	894.5199	0.03



22. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 24



23. ¹³C NMR (100 MHz, CD₃OD) spectrum of compound 24



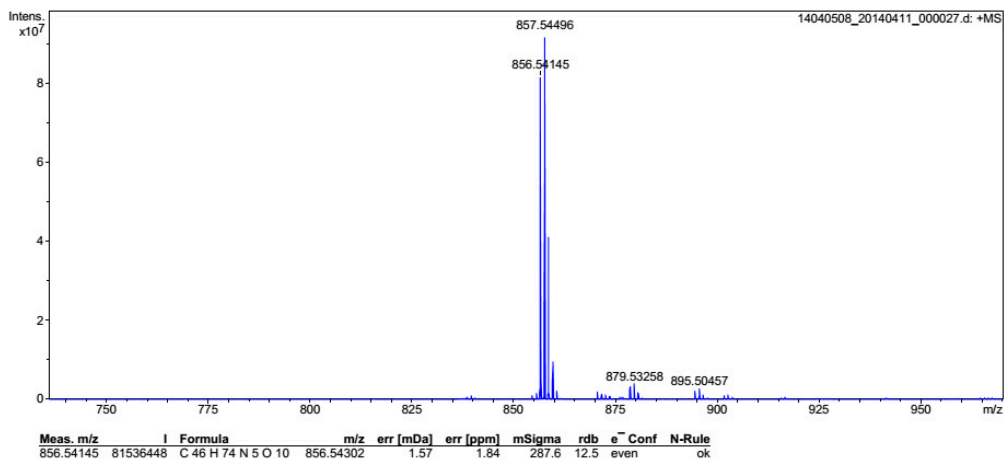
24. HR-ESI-MS spectrum of compound 24

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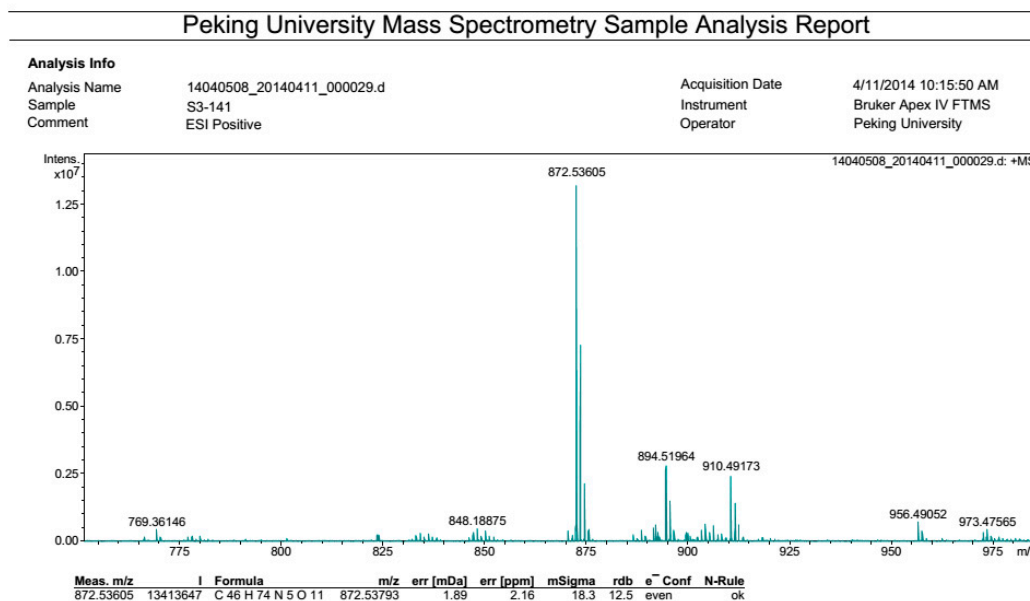
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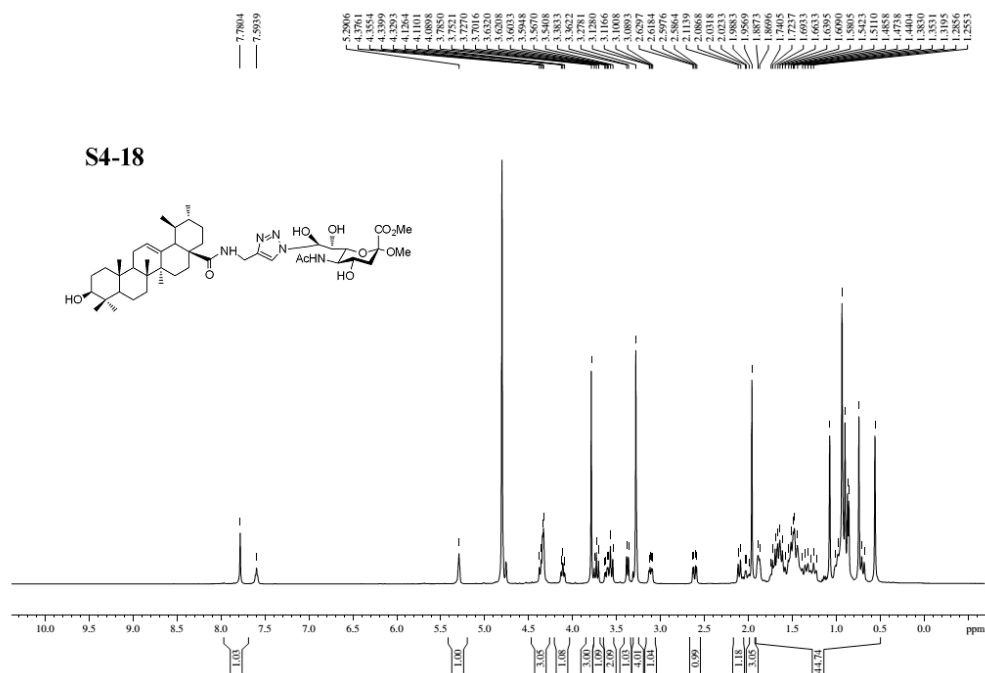
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 Instrument Bruker Apex IV FTMS
 Operator Peking University



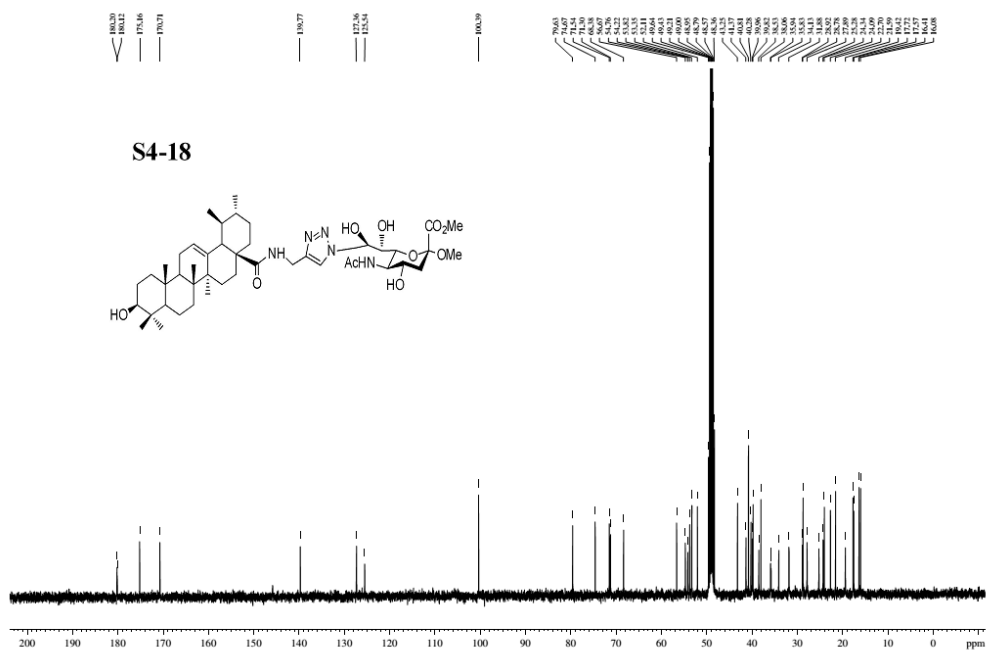
27. HR-ESI-MS spectrum of compound 25



28. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 26



29. ¹³C NMR (100 MHz, CD₃OD) spectrum of compound 26

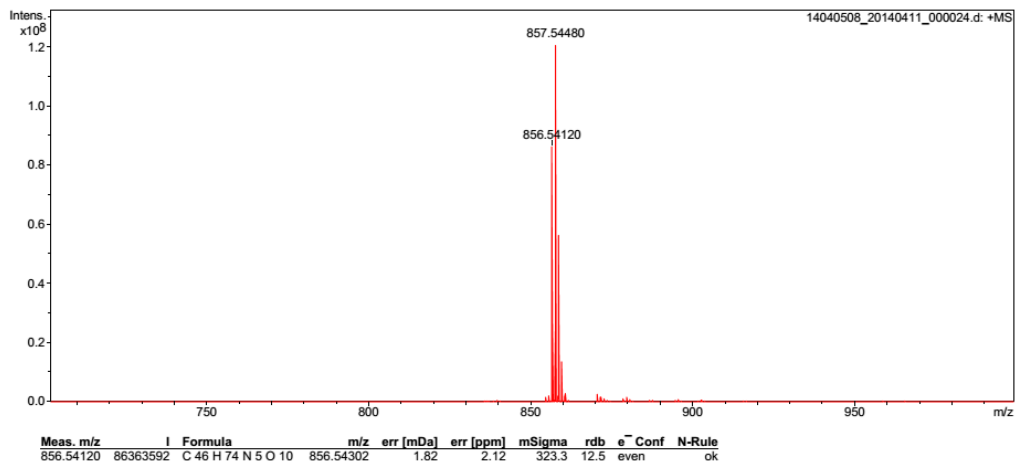


30. HR-ESI-MS spectrum of compound 26

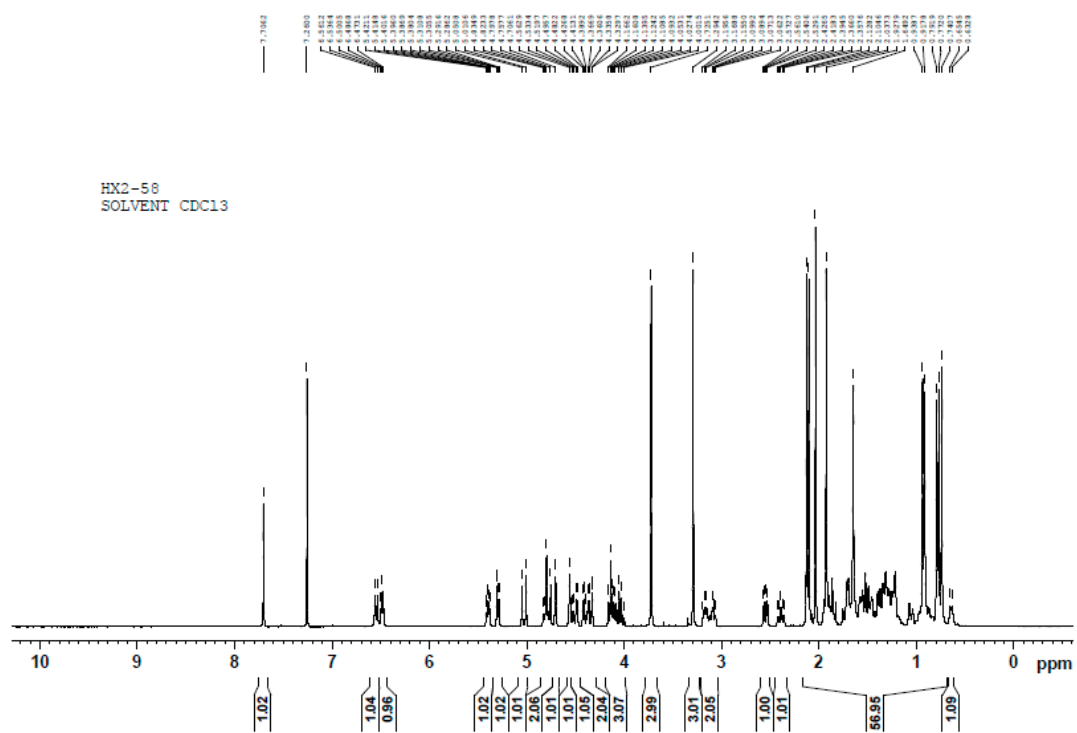
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

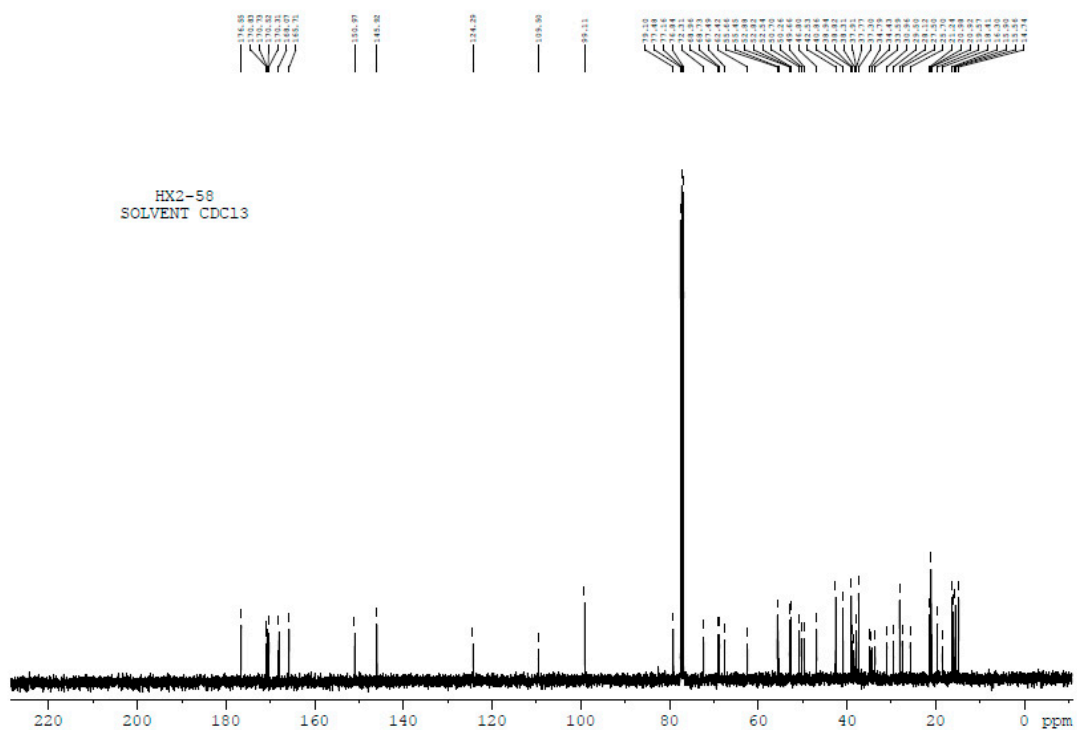
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Comment	ESI Positive	Operator	Peking University



31. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 28



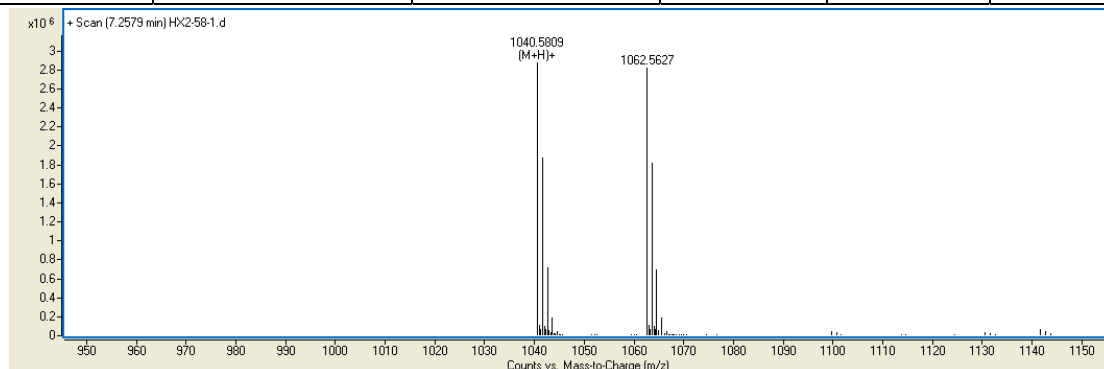
32. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound 28



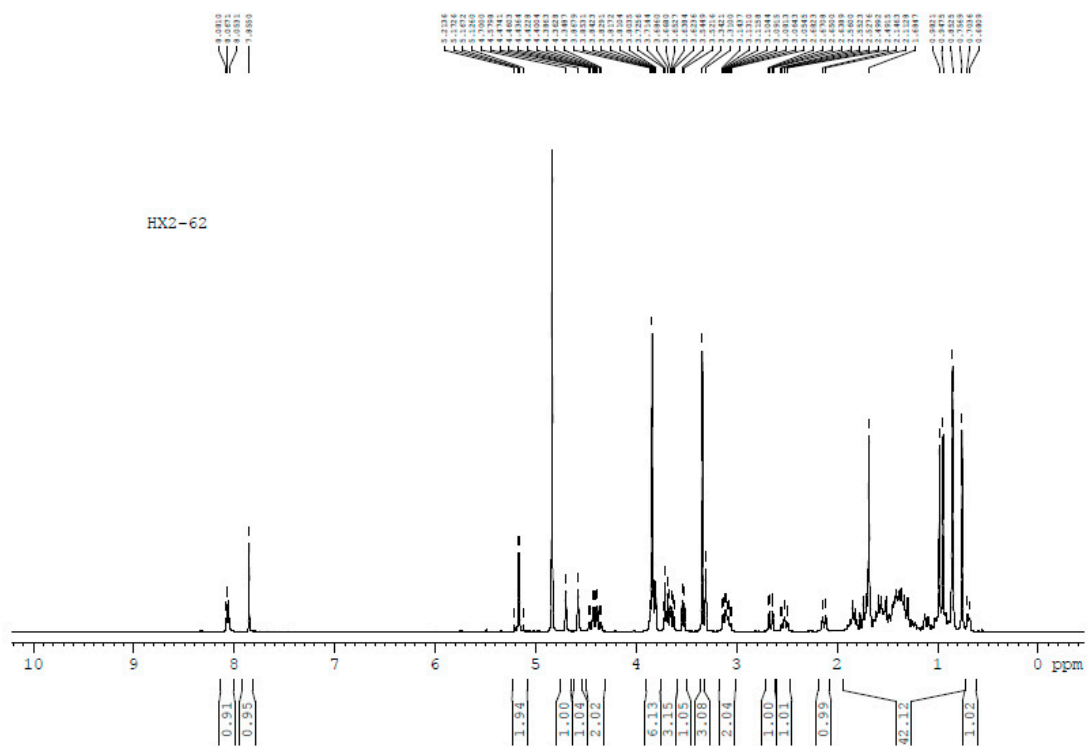
33. HR-ESI-MS spectrum of compound 28

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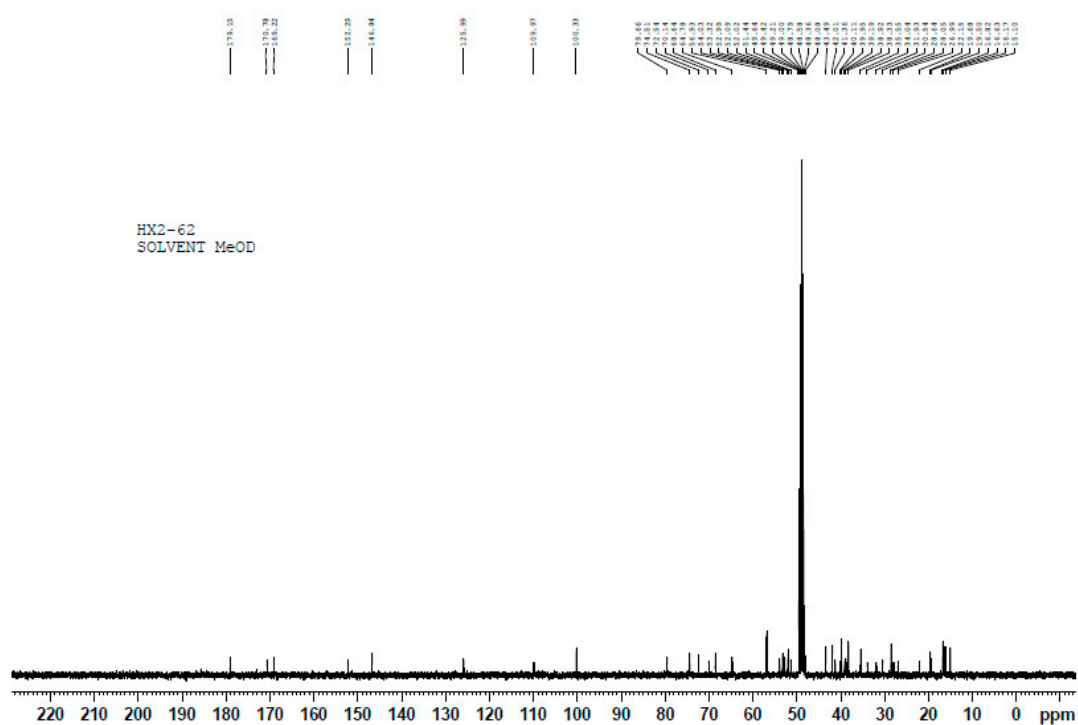
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-58	C ₅₄ H ₈₁ N ₅ O ₁₅	C ₅₄ H ₈₂ N ₅ O ₁₅	1040.5809	1040.5802	-0.59



34. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 29



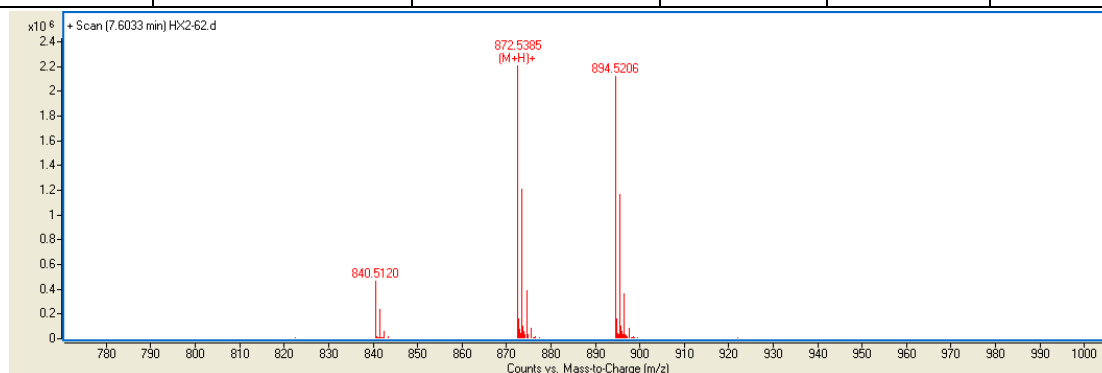
35. ¹³C NMR (100 MHz, CD₃OD) spectrum of compound **29**



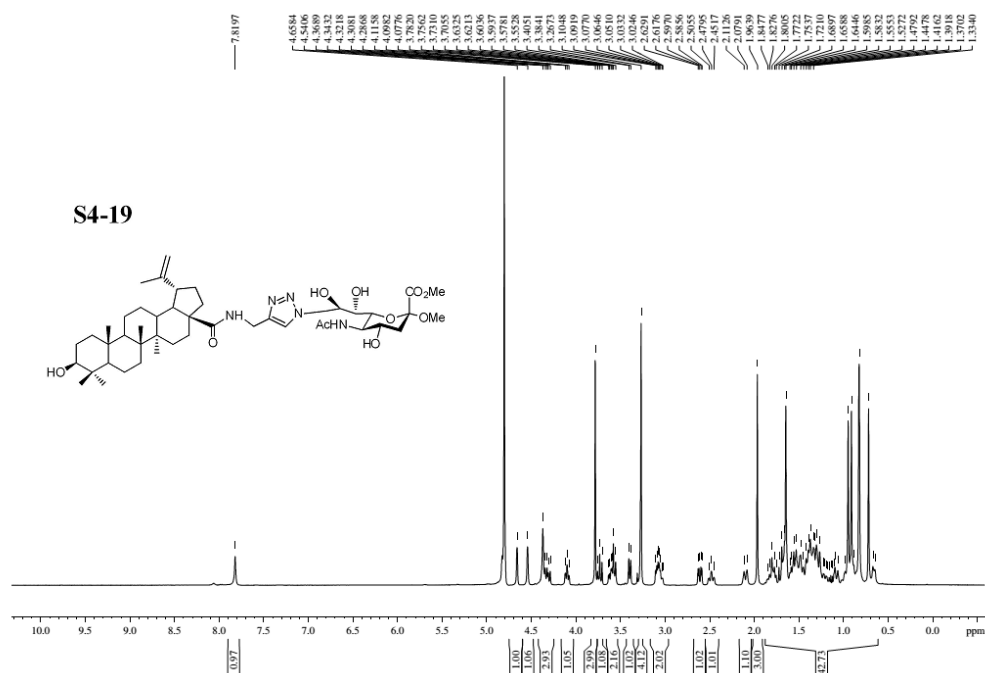
36. HR-ESI-MS spectrum of compound **29**

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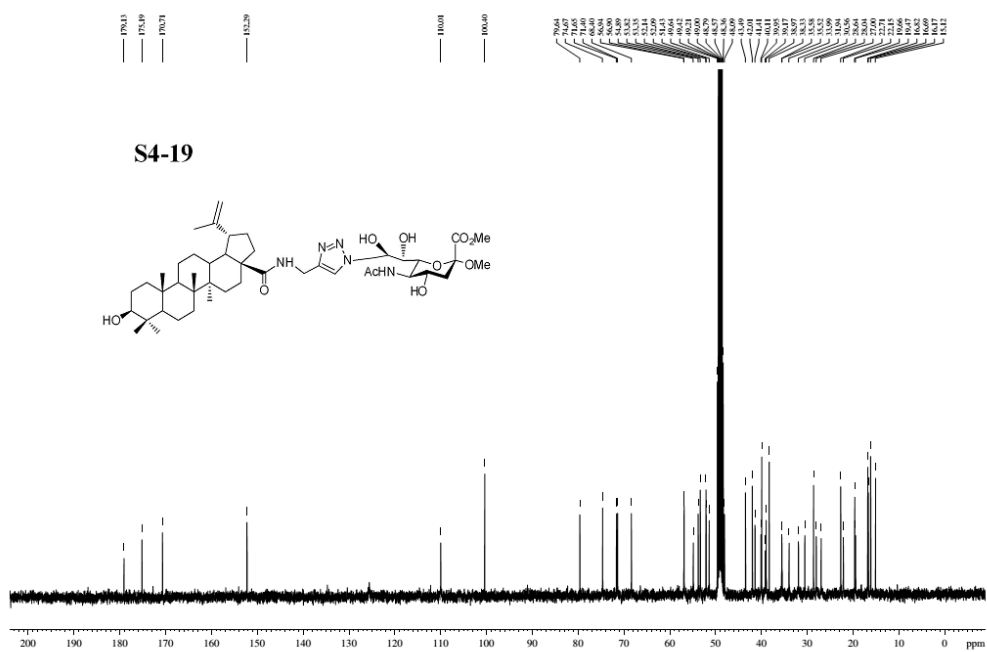
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-62	C ₄₆ H ₇₃ N ₅ O ₁₁	C ₄₆ H ₇₄ N ₅ O ₁₁	872.5385	872.5379	-0.73



37. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 30



38. ¹³C NMR (100 MHz, CD₃OD) spectrum of compound 30



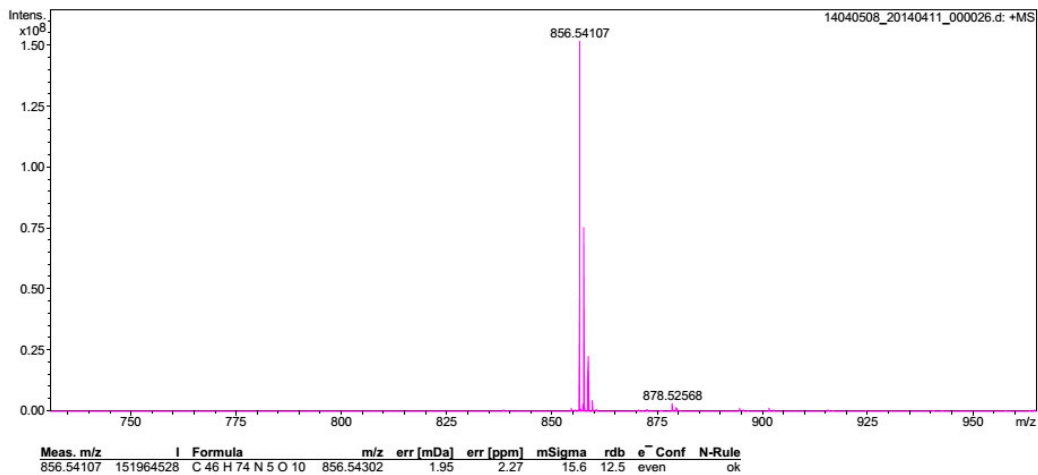
39. HR-ESI-MS spectrum of compound 30

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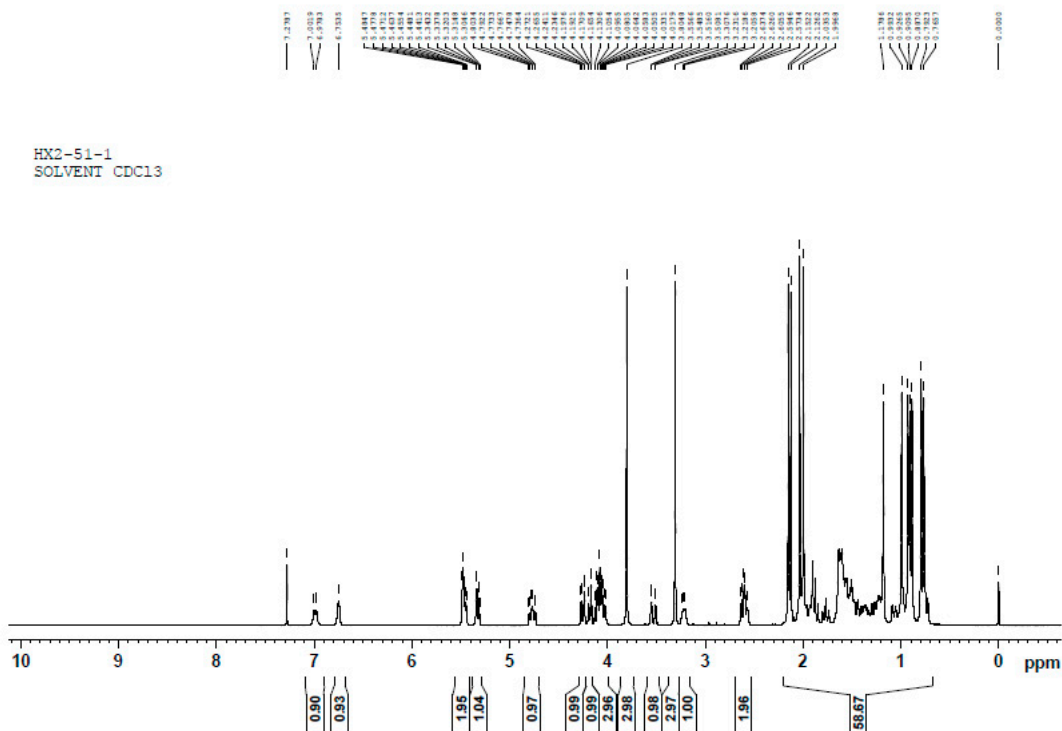
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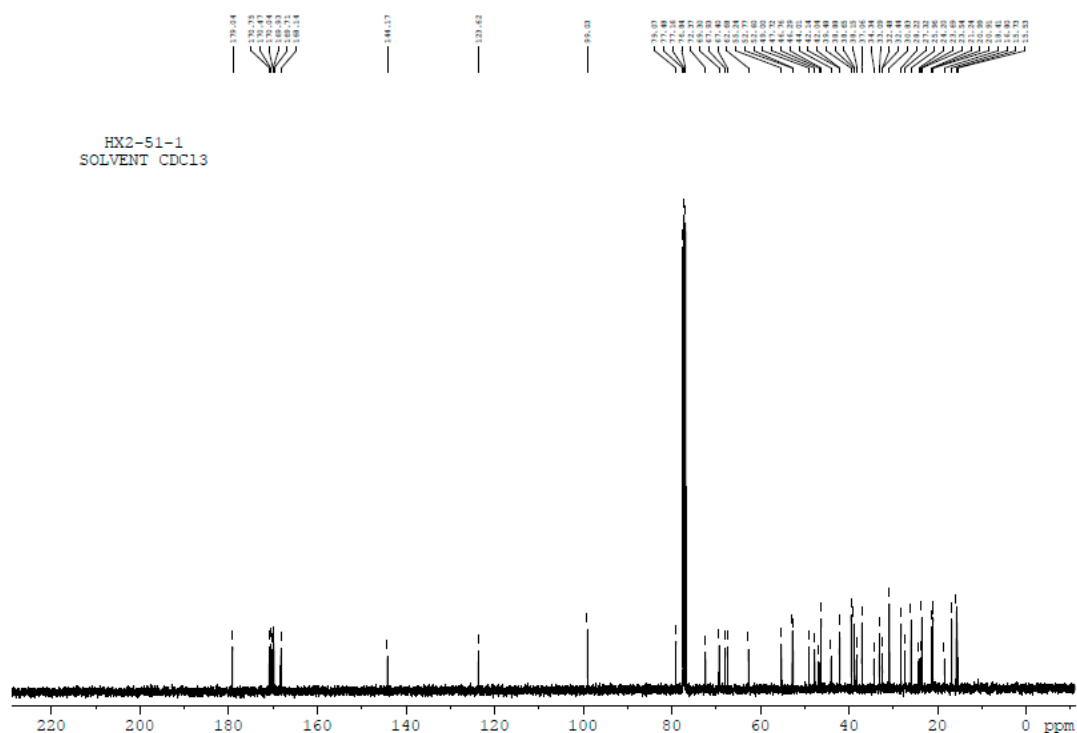
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 Instrument Bruker Apex IV FTMS
 Operator Peking University



40. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 34



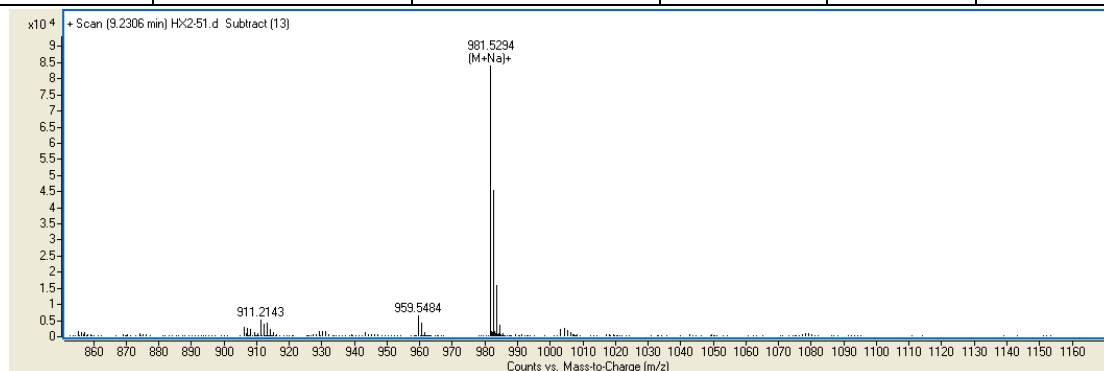
41. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound 34



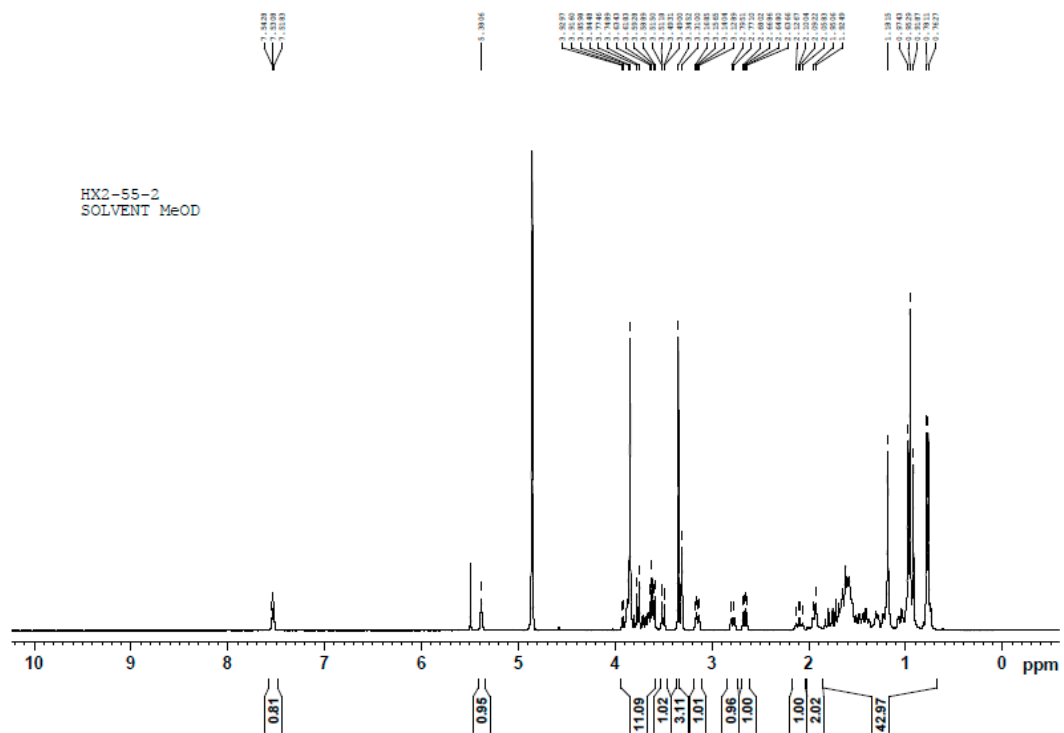
42. HR-ESI-MS spectrum of compound 34

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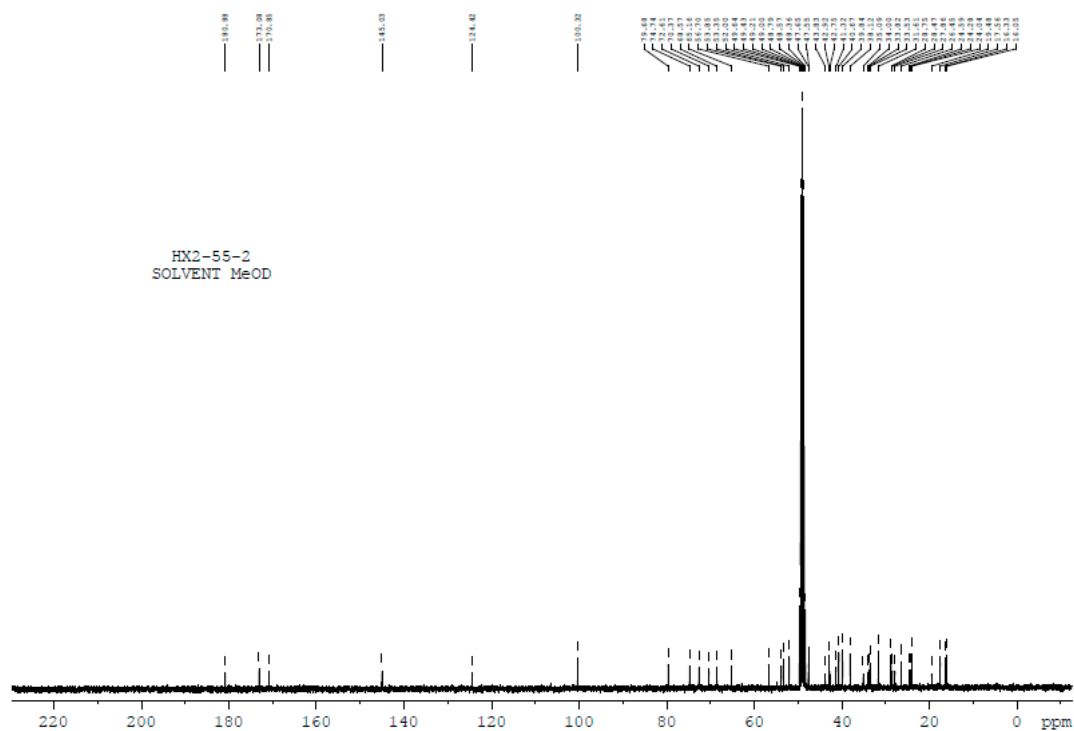
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-51	C ₅₁ H ₇₈ N ₂ O ₁₅	C ₅₁ H ₇₈ N ₂ NaO ₁₅	981.5294	981.5294	0



43. ^1H NMR (400 MHz, CD_3OD) spectrum of compound 35



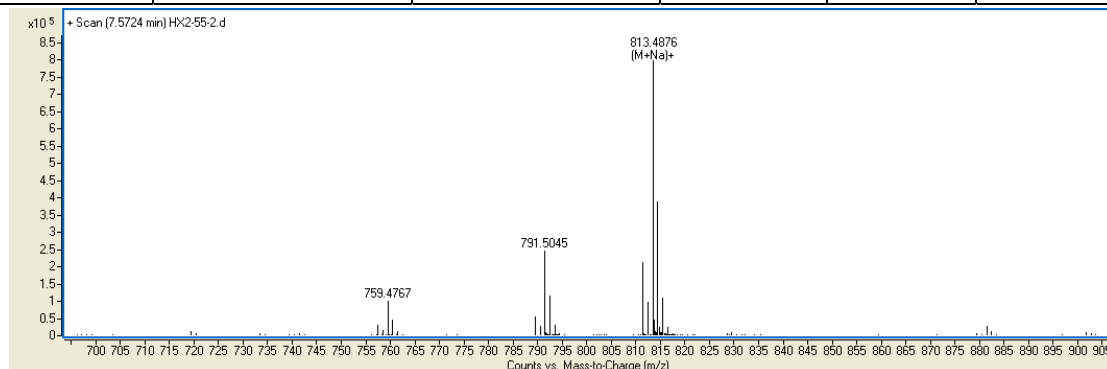
44. ^{13}C NMR (100 MHz, CD_3OD) spectrum of compound 35



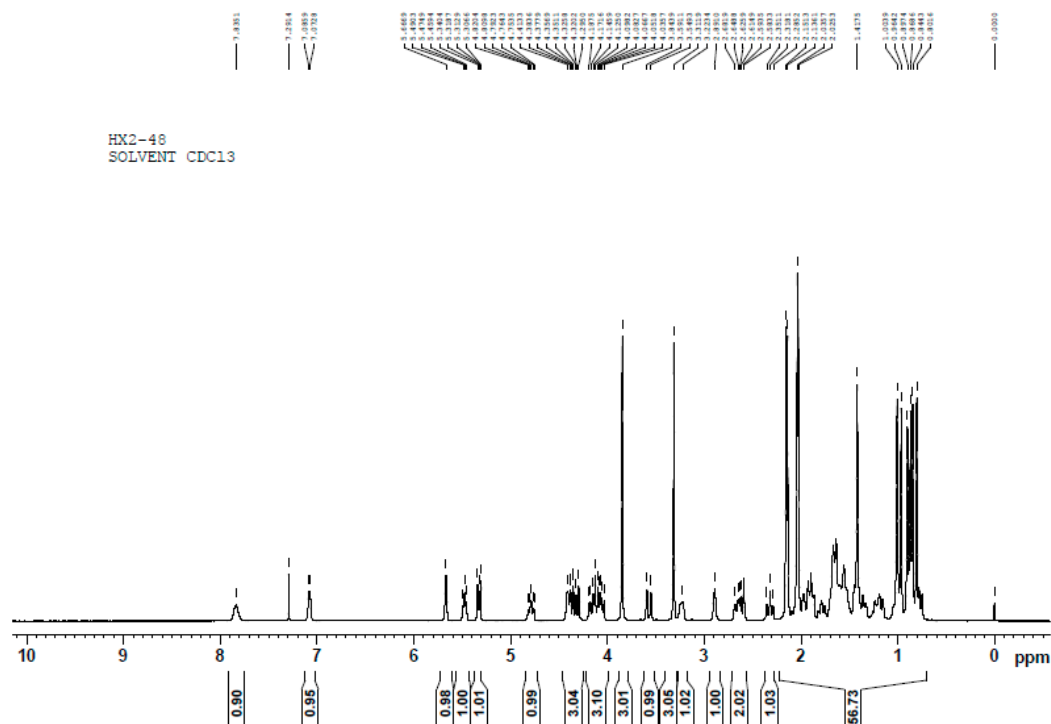
45. HR-ESI-MS spectrum of compound 35

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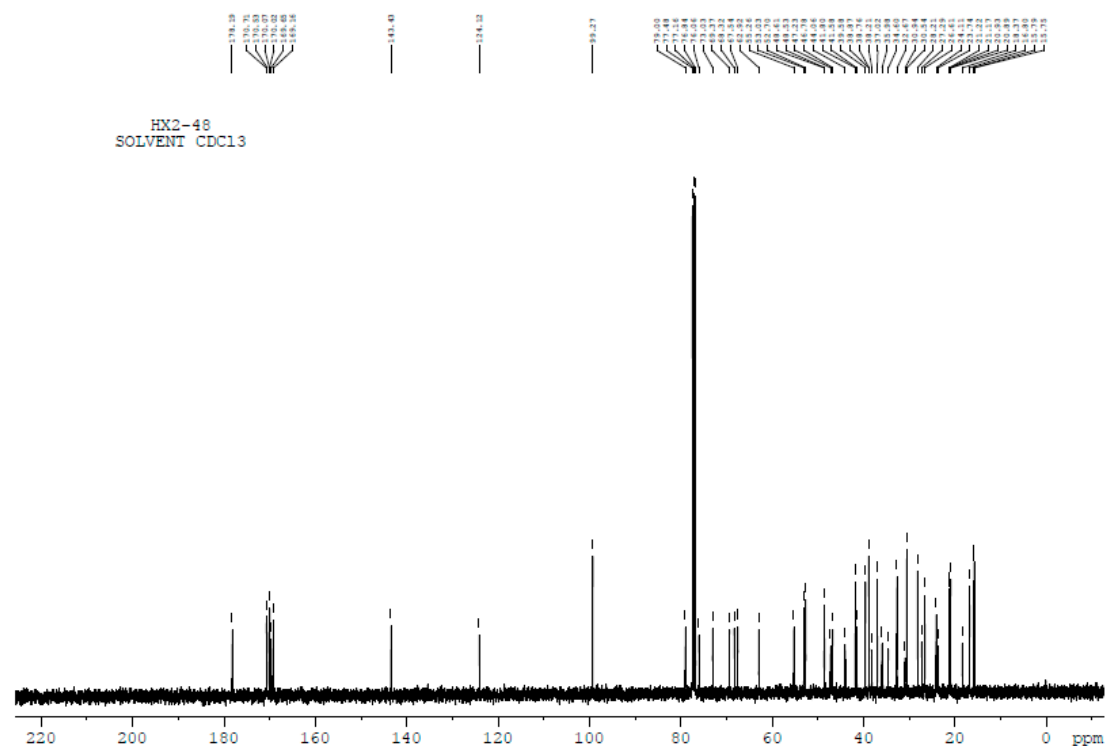
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-55-2	C43 H70 N2 O11	C43 H70 N2 Na O11	813.4876	813.4872	-0.39



46. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 36



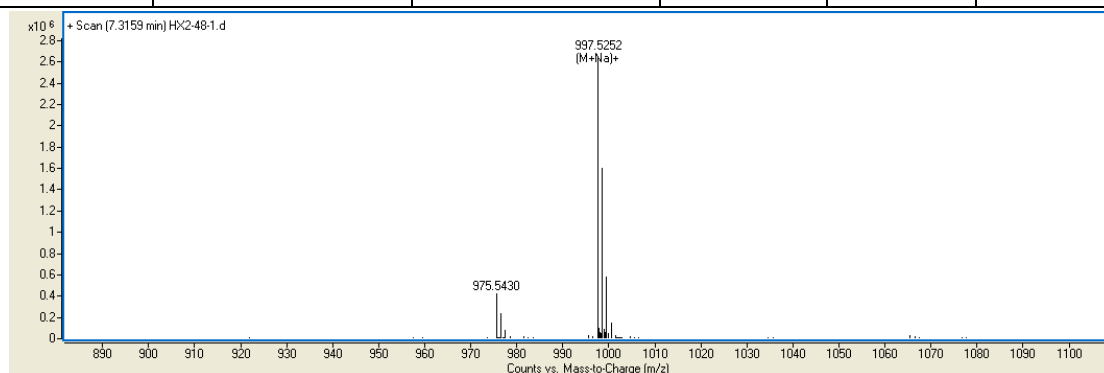
47. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound 36



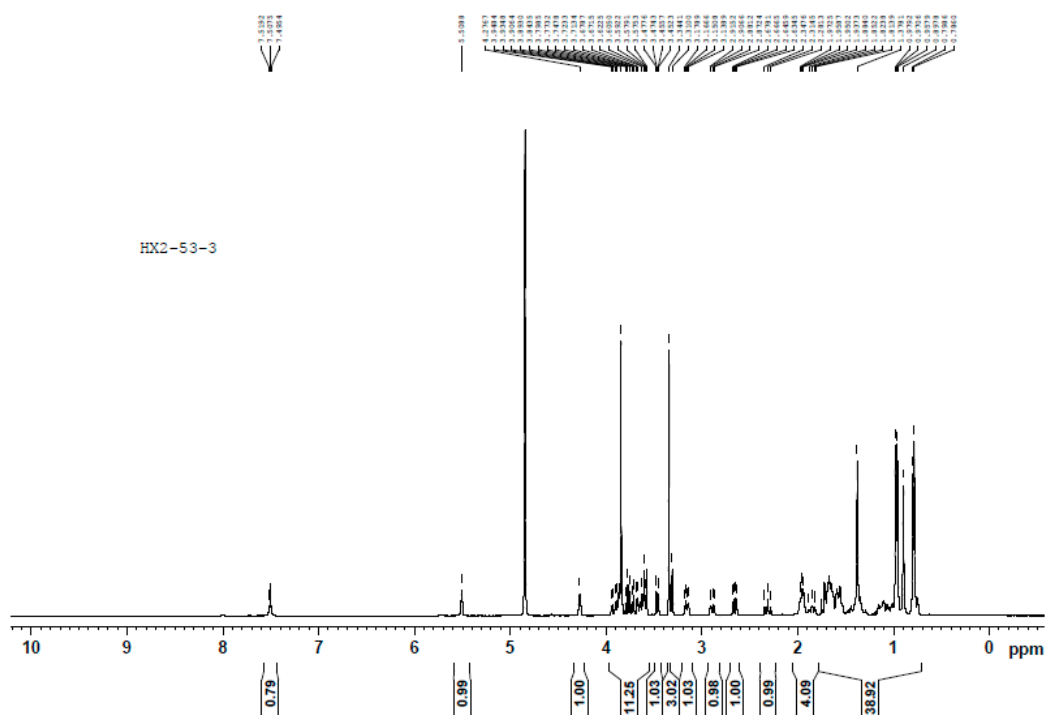
48. HR-ESI-MS spectrum of compound 36

HIGH RESOLUTION MASS SPECTROMETRY REPORT

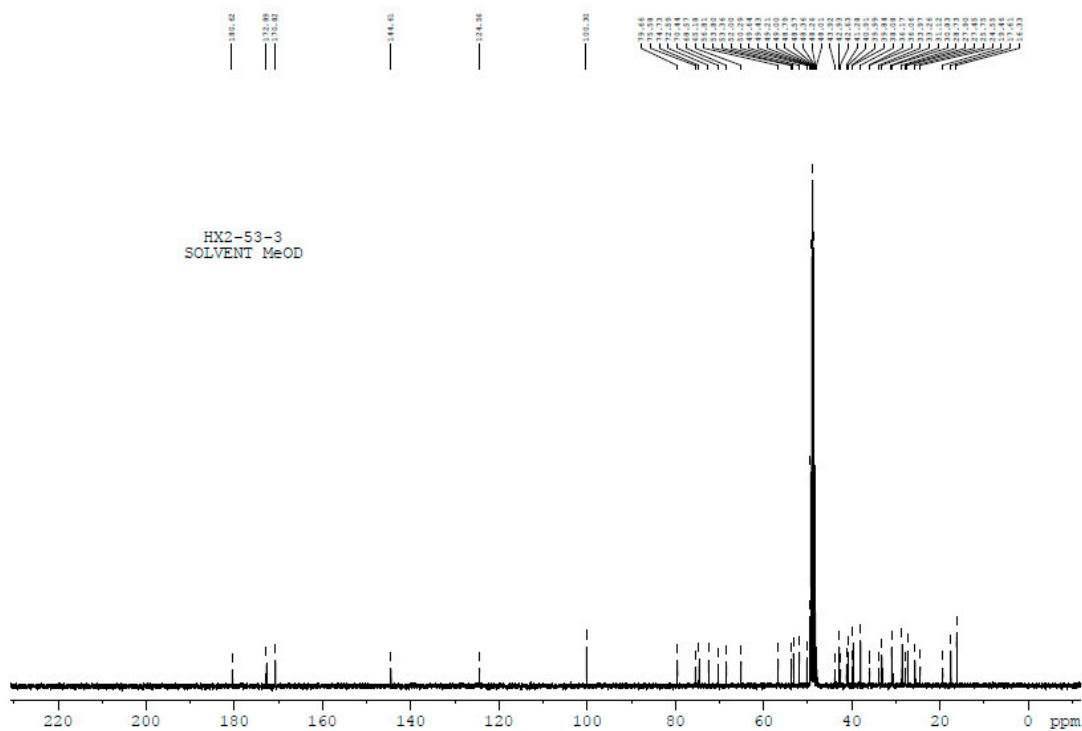
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-48	C ₅₁ H ₇₈ N ₂ O ₁₆	C ₅₁ H ₇₈ N ₂ Na O ₁₆	997.5252	997.5244	-0.83



49. ^1H NMR (400 MHz, CD_3OD) spectrum of compound **37**



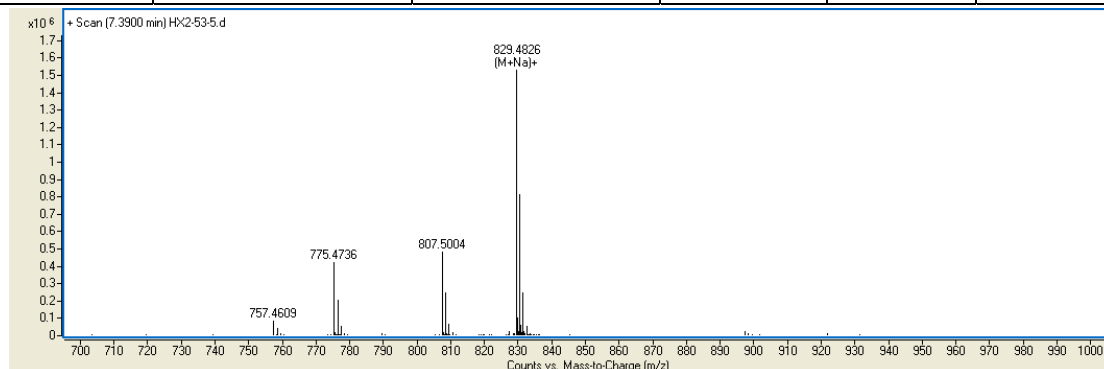
50. ^{13}C NMR (100 MHz, CD_3OD) spectrum of compound **37**



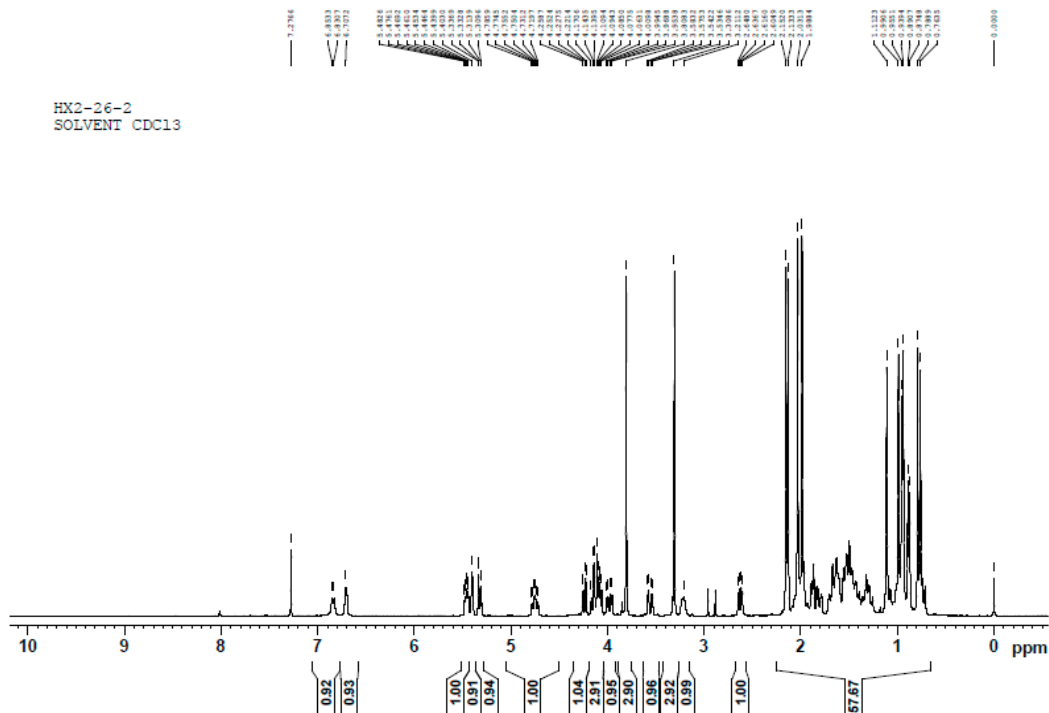
51. HR-ESI-MS spectrum of compound 37

HIGH RESOLUTION MASS SPECTROMETRY REPORT

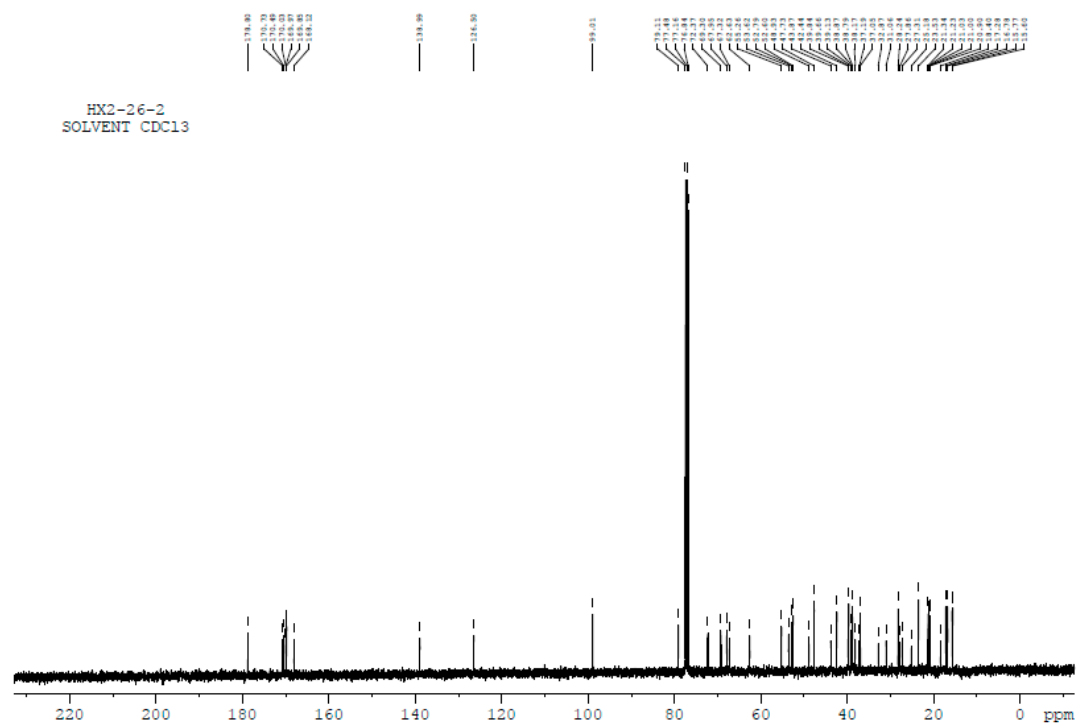
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-53-5	C43 H70 N2 O12	C43 H70 N2 Na O12	829.4826	829.4821	-0.84



52. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 38



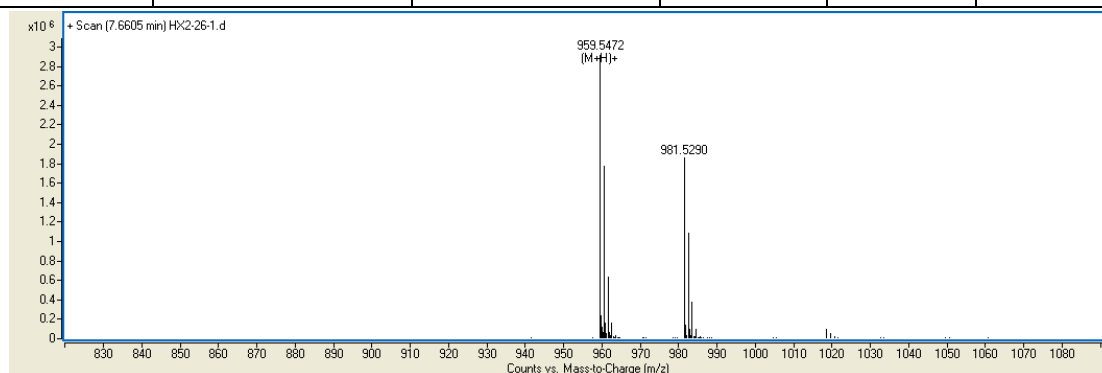
53. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound 38



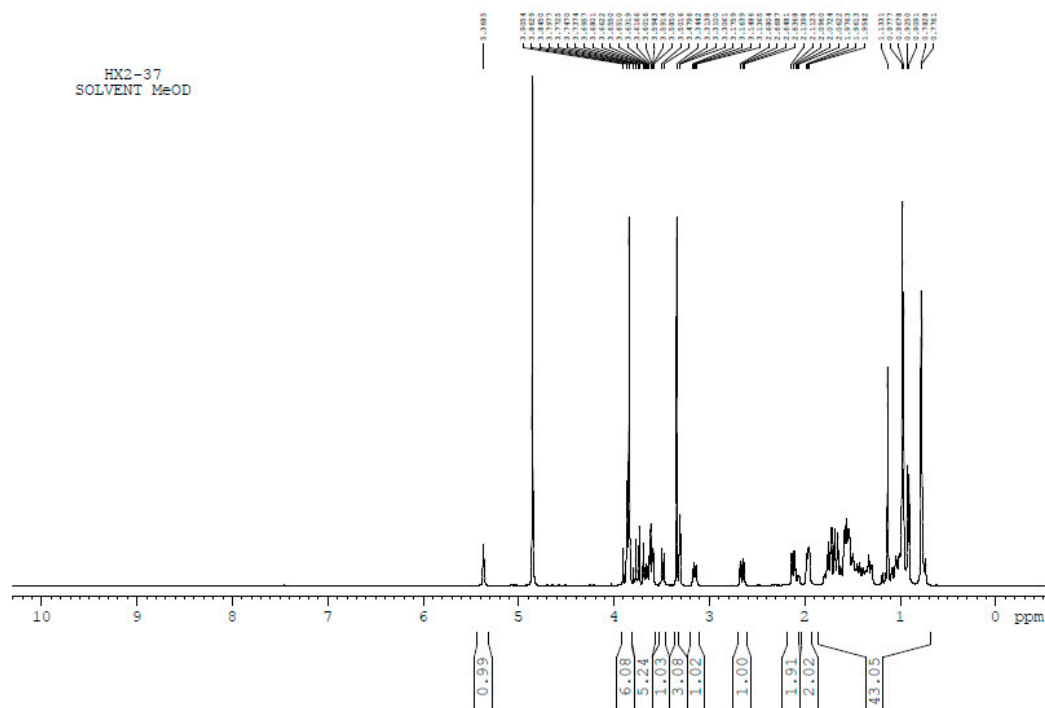
54. HR-ESI-MS spectrum of compound 38

HIGH RESOLUTION MASS SPECTROMETRY REPORT

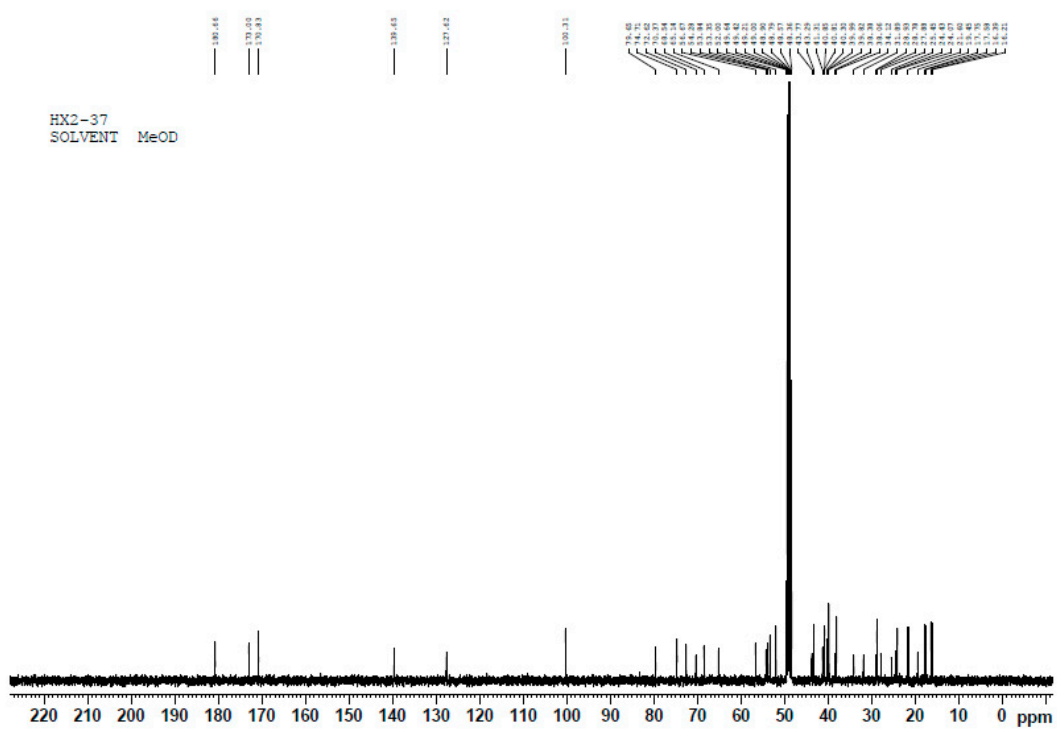
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-26	C ₅₁ H ₇₈ N ₂ O ₁₅	C ₅₁ H ₇₉ N ₂ O ₁₅	959.5472	959.5475	0.34



55. ^1H NMR (400 MHz, CD_3OD) spectrum of compound 39



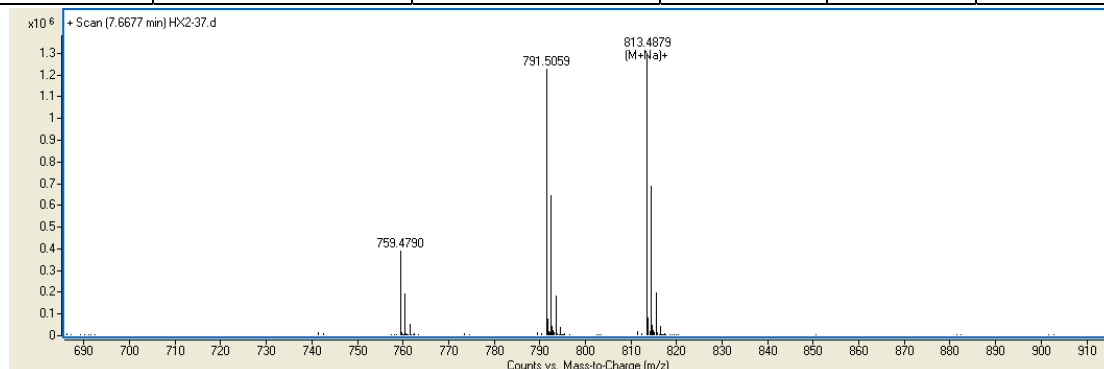
56. ^{13}C NMR (100 MHz, CD_3OD) spectrum of compound 39



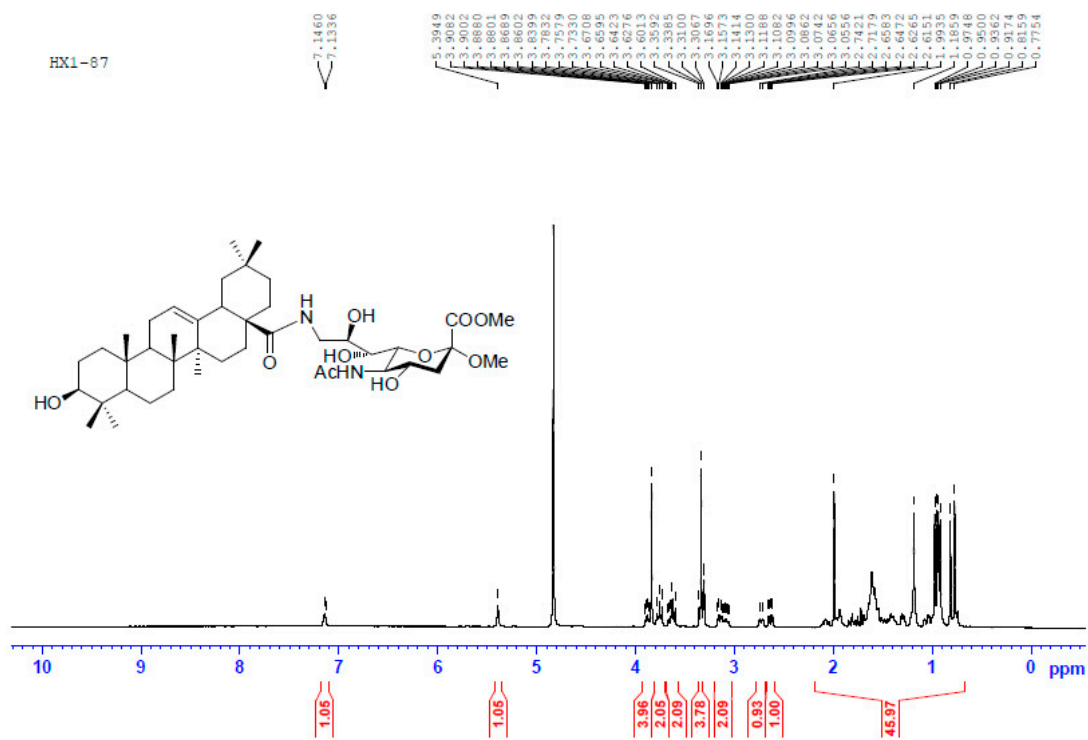
57. HR-ESI-MS spectrum of compound 39

HIGH RESOLUTION MASS SPECTROMETRY REPORT

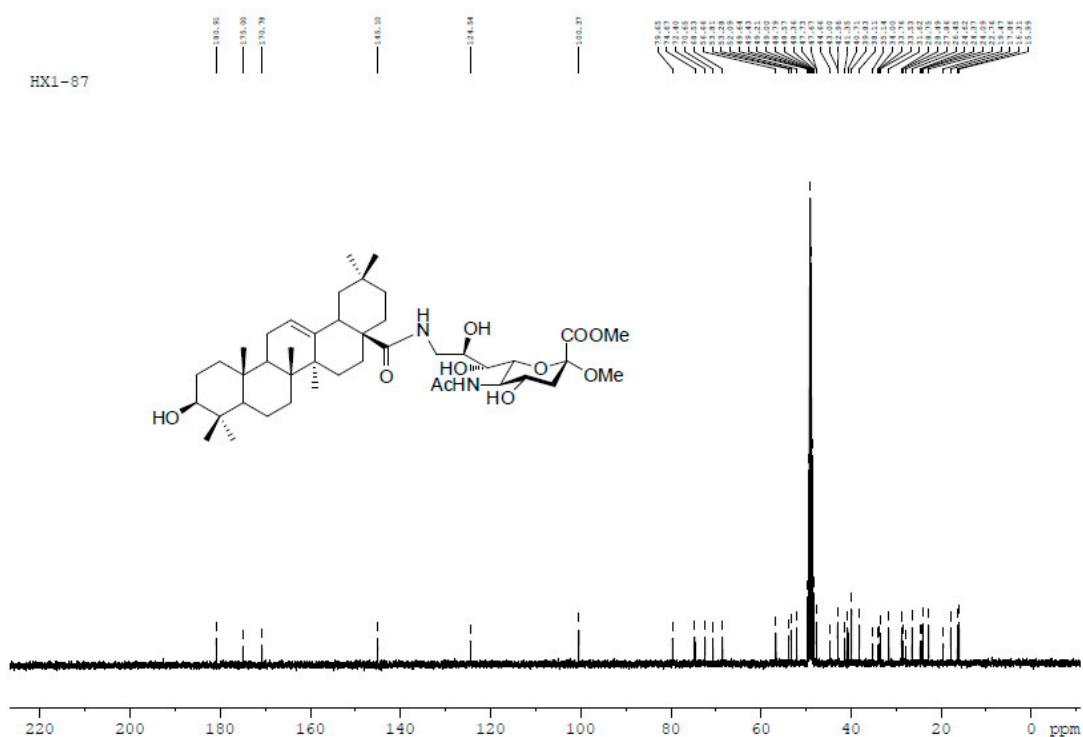
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-37	C ₄₃ H ₇₀ N ₂ O ₁₁	C ₄₃ H ₇₀ N ₂ Na O ₁₁	813.4879	813.4872	-1.05



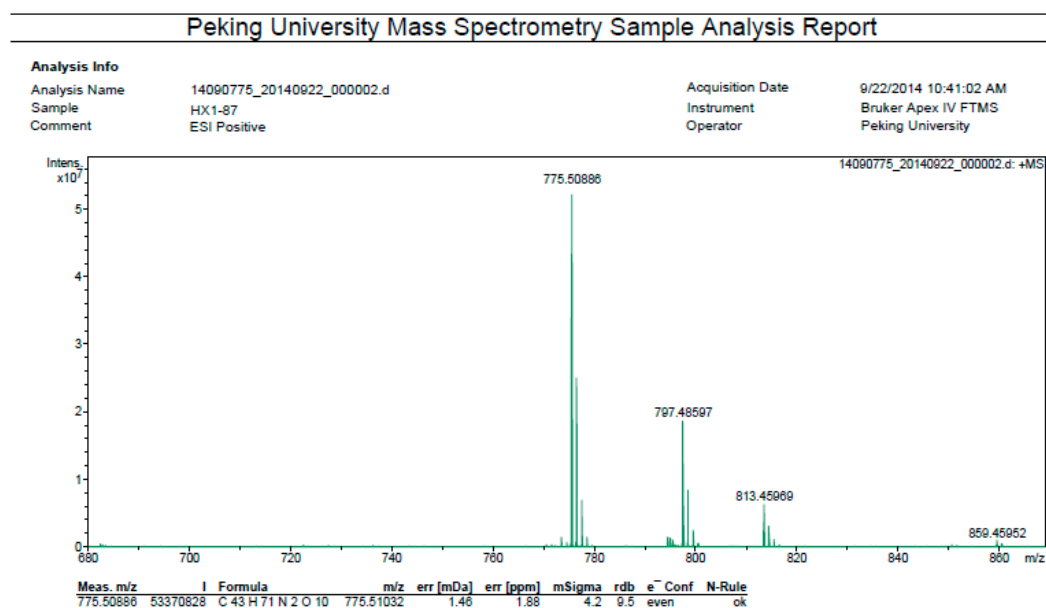
58. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 40



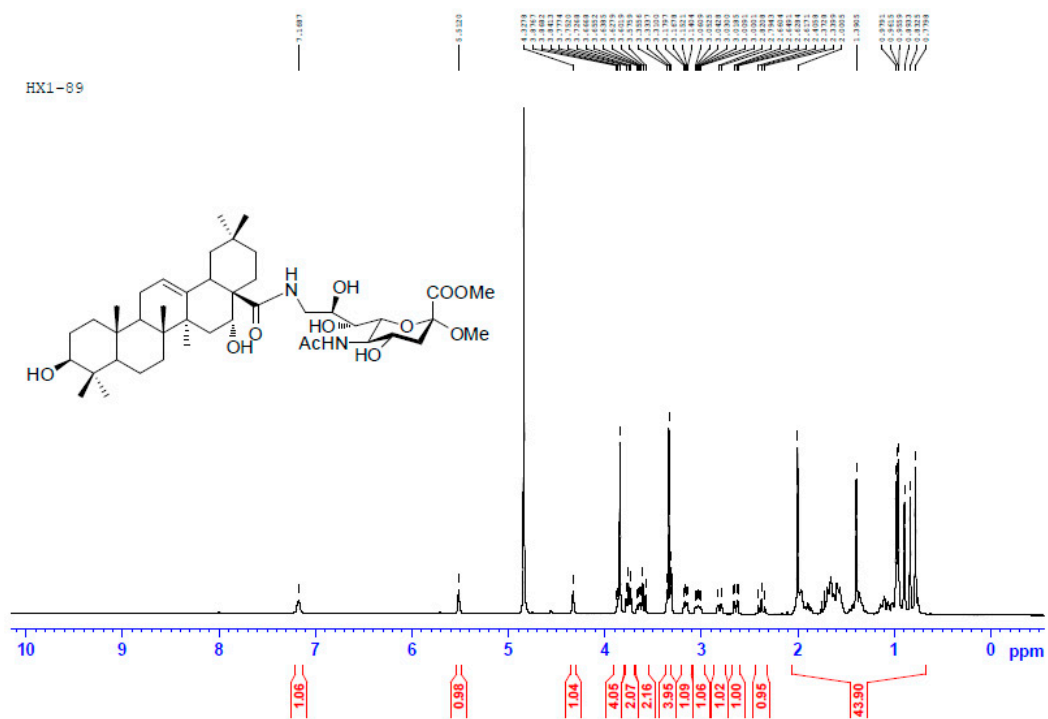
59. ^{13}C NMR (100 MHz, CD_3OD) spectrum of compound 40



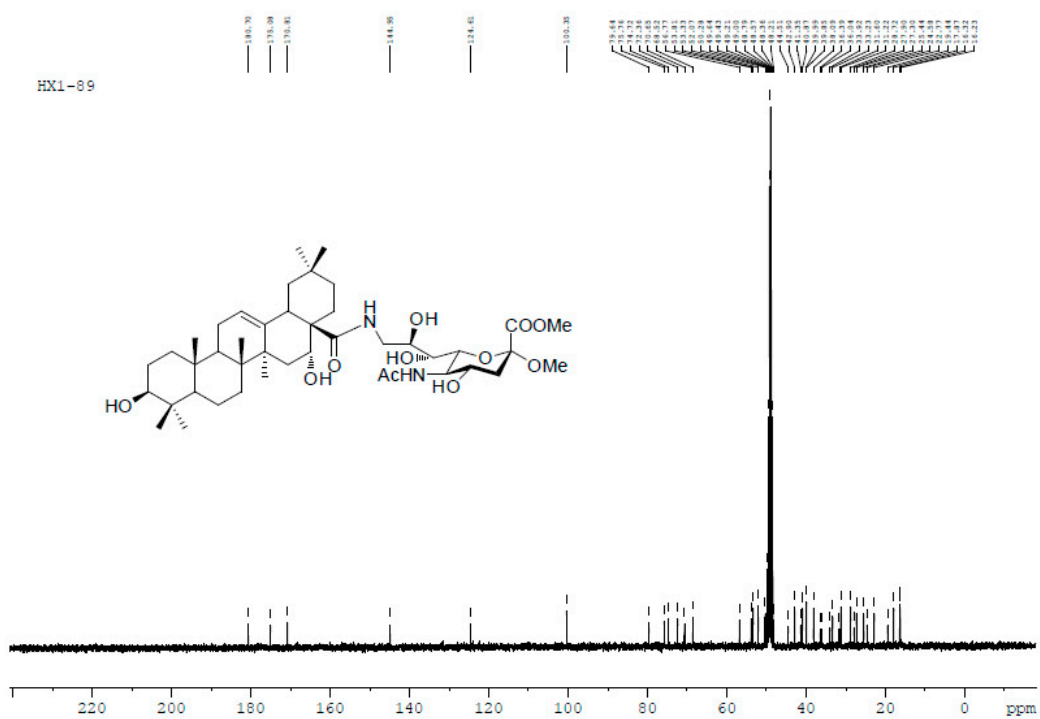
60. HR-ESI-MS spectrum of compound 40



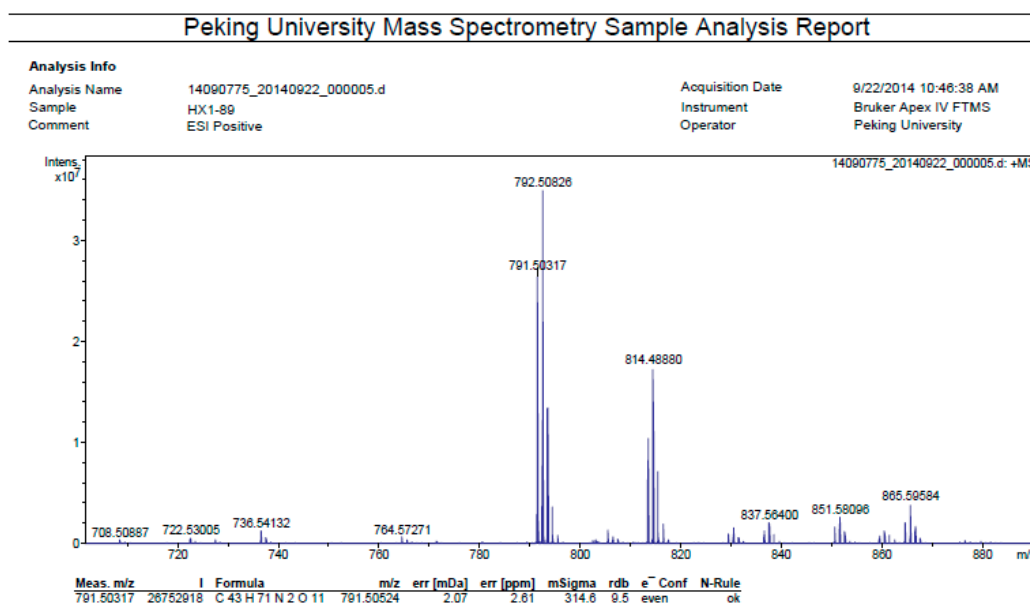
61. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 41



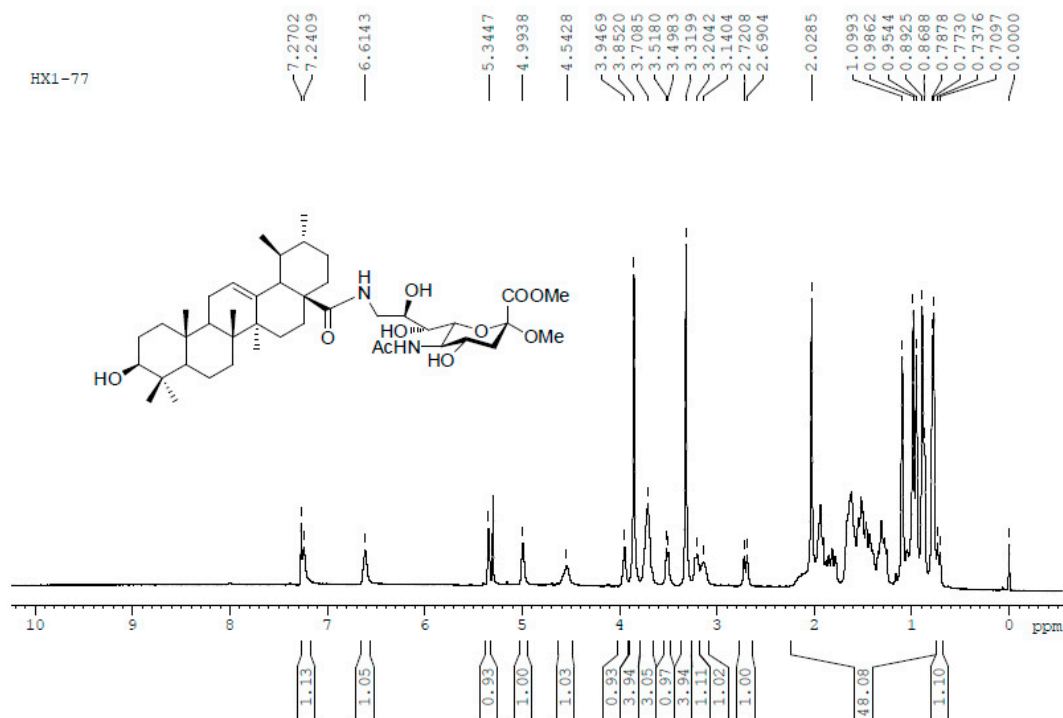
62. ¹³C NMR (100 MHz, CD₃OD) spectrum of compound 41



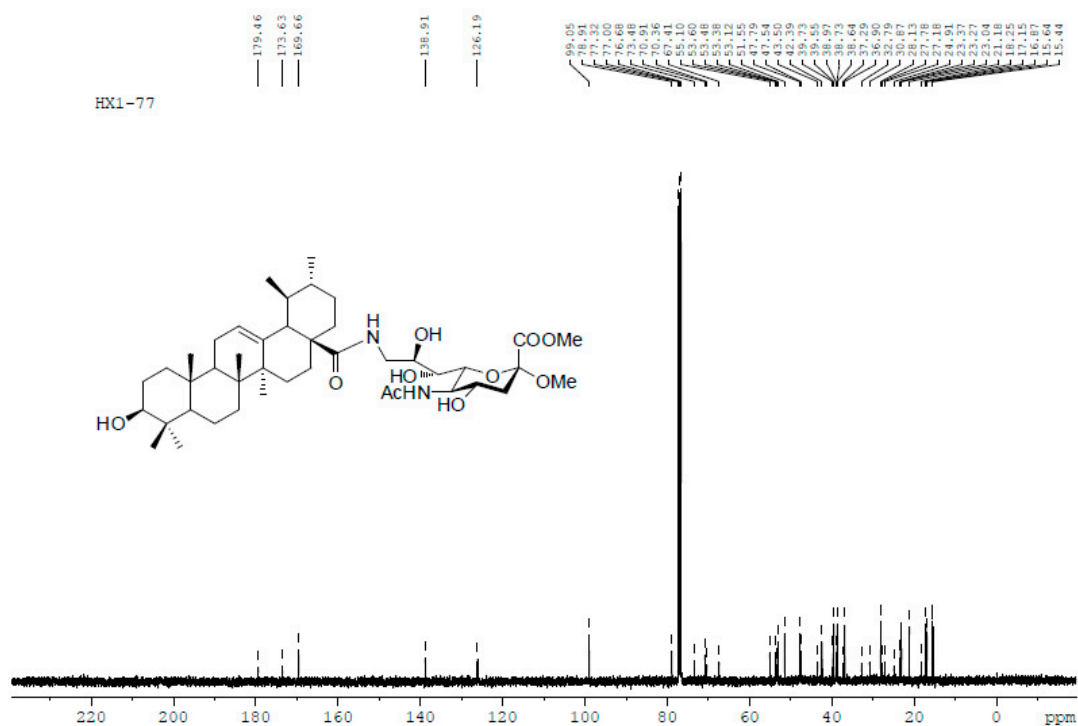
63. HR-ESI-MS spectrum of compound 41



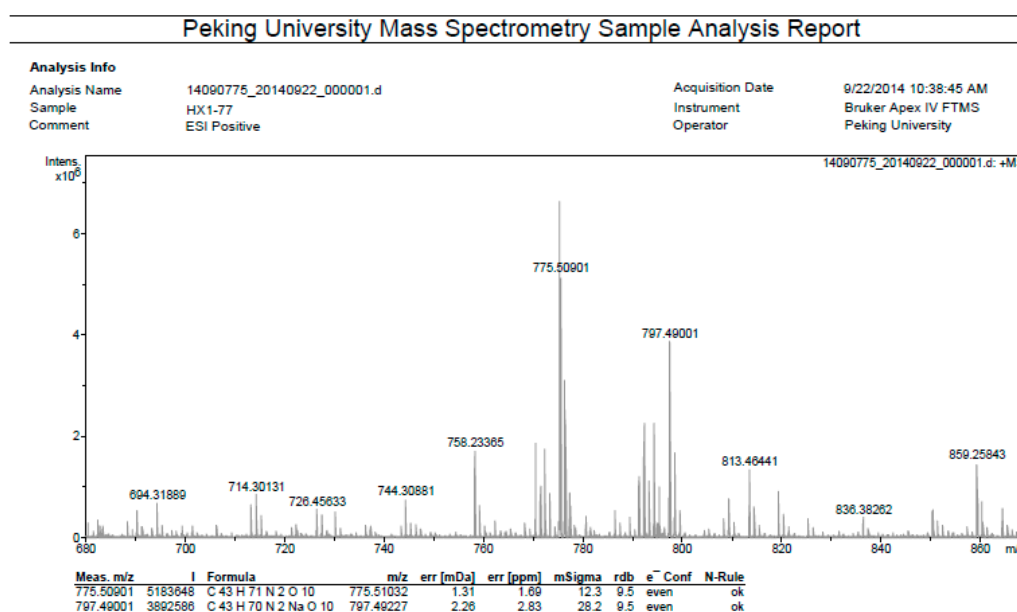
64. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 42



65. ¹³C NMR (100 MHz, CD₃OD) spectrum of compound 42



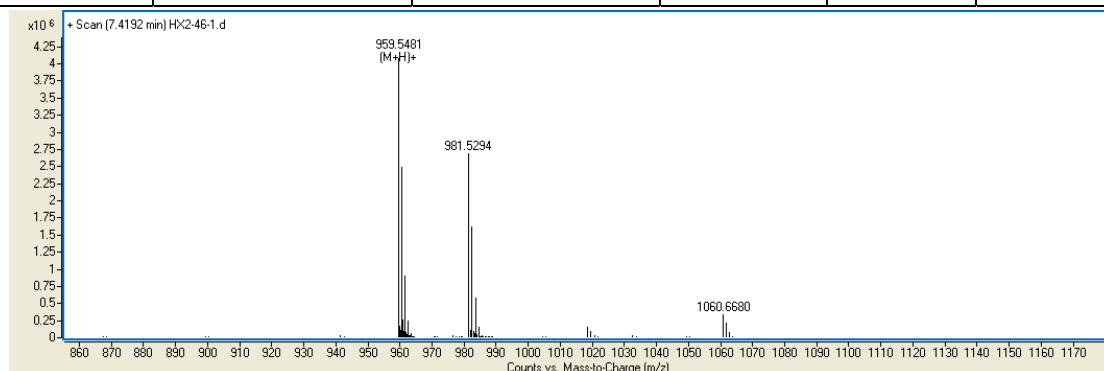
66. HR-ESI-MS spectrum of compound 42



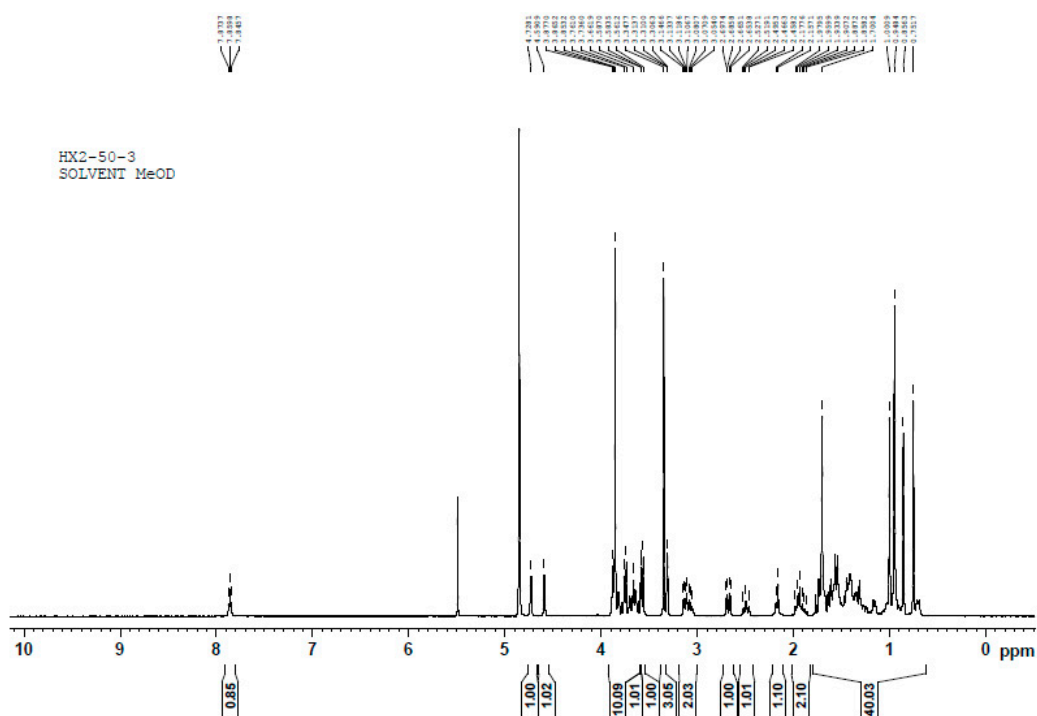
69. HR-ESI-MS spectrum of compound 44

HIGH RESOLUTION MASS SPECTROMETRY REPORT

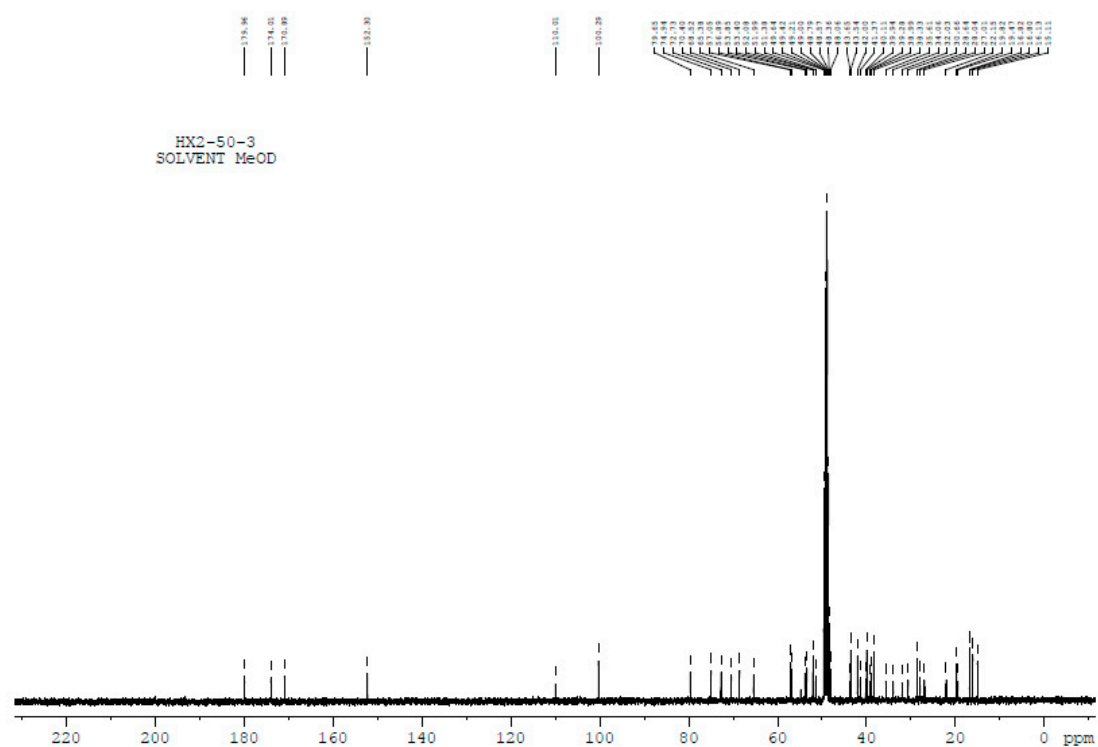
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-46	C51 H78 N2 O15	C51 H79 N2 O15	959.5481	959.5475	-0.45



70. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 45



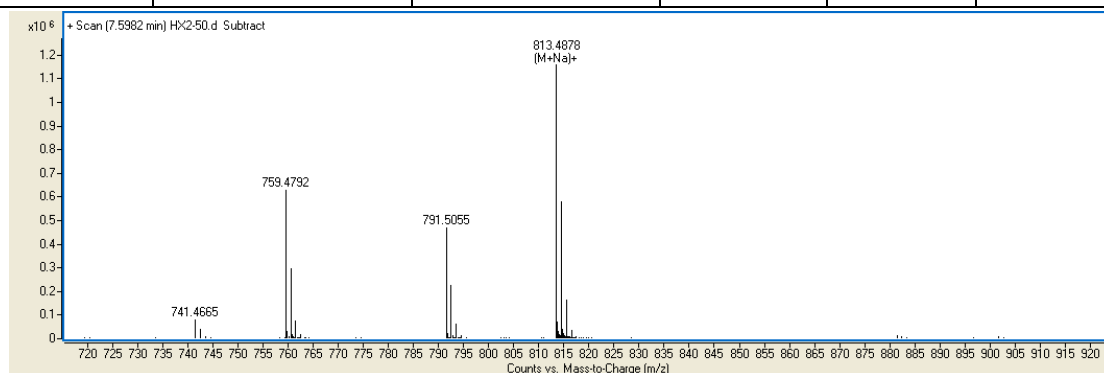
71. ¹³C NMR (100 MHz, CD₃OD) spectrum of compound 45



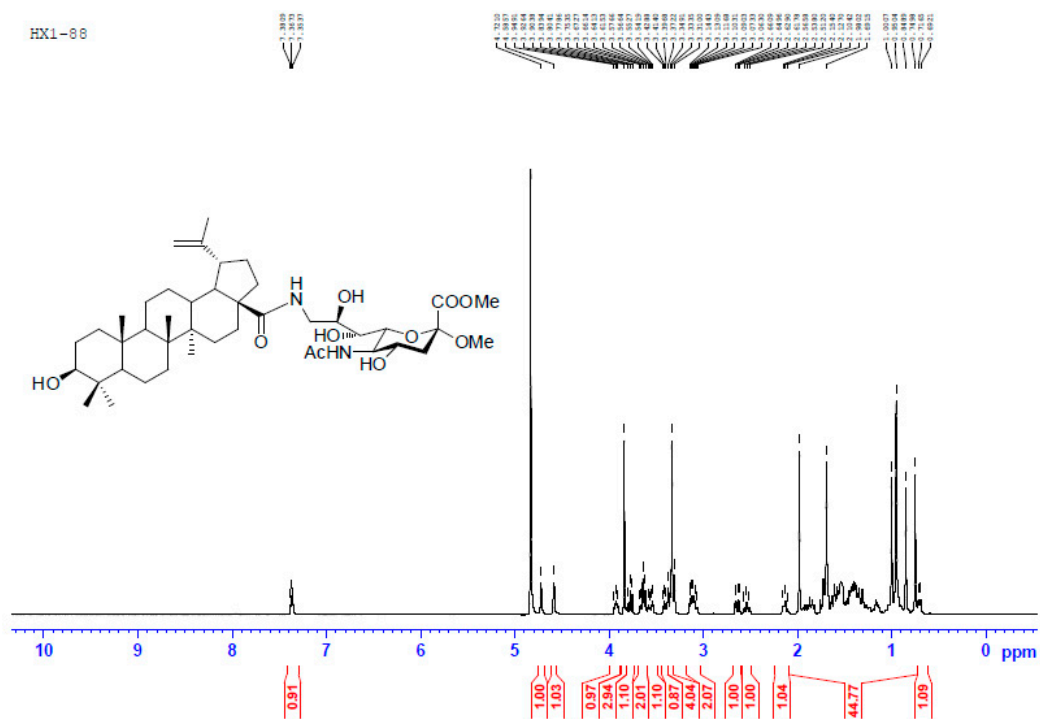
72. HR-ESI-MS spectrum of compound 45

HIGH RESOLUTION MASS SPECTROMETRY REPORT

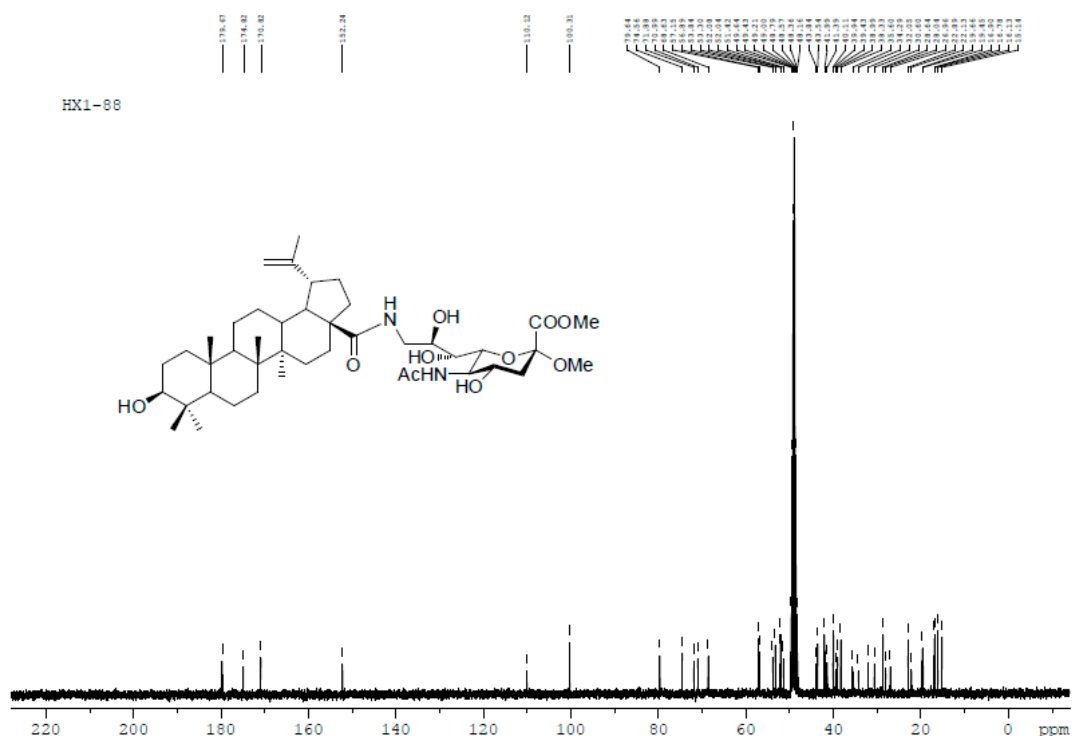
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
HX2-50	C ₄₃ H ₇₀ N ₂ O ₁₁	C ₄₃ H ₇₀ N ₂ Na O ₁₁	813.4878	813.4872	-0.82



73. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 46



74. ¹³C NMR (100 MHz, CD₃OD) spectrum of compound 46



75. HR-ESI-MS spectrum of compound 46

Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name 14090775_20140922_000003.d
 Sample HX1-88
 Comment ESI Positive

Acquisition Date 9/22/2014 10:42:48 AM
 Instrument Bruker Apex IV FTMS
 Operator Peking University

