

Supplementary Information II (Figures)

Figure Captions

Figure S1. ¹H-NMR (1-a), ¹³C-NMR (1-b) and HR-ESI-MS (1-c) spectra of compound 2

Figure S2. ¹H-NMR (2-a), ¹³C-NMR (2-b) and HR-ESI-MS (2-c) spectra of compound 3

Figure S3. ¹H-NMR (3-a), ¹³C-NMR (3-b) and HR-ESI-MS (3-c) spectra of compound 4

Figure S4. ¹H-NMR (4-a), ¹³C-NMR (4-b) and HR-ESI-MS (4-c) spectra of compound 5

Figure S5. ¹H-NMR (5-a), ¹³C-NMR (5-b) and HR-ESI-MS (5-c) spectra of compound 6

Figure S6. ¹H-NMR (6-a), ¹³C-NMR (6-b) and HR-ESI-MS (6-c) spectra of compound 7

Figure S7. ¹H-NMR (7-a), ¹³C-NMR (7-b) and HR-ESI-MS (7-c) spectra of compound 8

Figure S8. ¹H-NMR (8-a), ¹³C-NMR (8-b) and HR-ESI-MS (8-c) spectra of compound 9

Figure S9. ¹H-NMR (9-a), ¹³C-NMR (9-b) and HR-ESI-MS (9-c) spectra of compound 10

Figure S10. ¹H-NMR (10-a), ¹³C-NMR (10-b) and HR-ESI-MS (10-c) spectra of compound 11

Figure S11. ¹H-NMR (11-a), ¹³C-NMR (11-b) and HR-ESI-MS (11-c) spectra of compound 12

Figure S12. ¹H-NMR (12-a), ¹³C-NMR (12-b) and HR-ESI-MS (12-c) spectra of compound 13

Figure S13. ¹H-NMR (13-a), ¹³C-NMR (13-b) and HR-ESI-MS (13-c) spectra of compound 14

Figure S14. ¹H-NMR (14-a), ¹³C-NMR (14-b) and HR-ESI-MS (14-c) spectra of compound 15

Figure S15. ¹H-NMR (15-a), ¹³C-NMR (15-b) and HR-ESI-MS (15-c) spectra of compound 16

Figure S16. ¹H-NMR (16-a), ¹³C-NMR (16-b) and HR-ESI-MS (16-c) spectra of compound 17

Figure S17. ¹H-NMR (17-a), ¹³C-NMR (17-b) and HR-ESI-MS (17-c) spectra of compound 18

Figure S18. ¹H-NMR (18-a), ¹³C-NMR (18-b) and HR-ESI-MS (18-c) spectra of compound 19

Figure S19. Purity test of compound 2 by HPLC ($\lambda=210$ nm)

Figure S20. Purity test of compound 3 by HPLC ($\lambda=210$ nm)

Figure S21. Purity test of compound 4 by HPLC ($\lambda=210$ nm)

Figure S22. Purity test of compound 5 by HPLC ($\lambda=210$ nm)

Figure S23. Purity test of compound 6 by HPLC ($\lambda=210$ nm)

Figure S24. Purity test of compound 7 by HPLC ($\lambda=210$ nm)

Figure S25. Purity test of compound 8 by HPLC ($\lambda=210$ nm)

Figure S26. Purity test of compound 9 by HPLC ($\lambda=210$ nm)

Figure S27. Purity test of compound 10 by HPLC ($\lambda=210$ nm)

Figure S28. Purity test of compound 11 by HPLC ($\lambda=210$ nm)

Figure S29. Purity test of compound 12 by HPLC ($\lambda=210$ nm)

Figure S30. Purity test of compound 13 by HPLC ($\lambda=210$ nm)

Figure S31. Purity test of compound 14 by HPLC ($\lambda=210$ nm)

Figure S32. Purity test of compound 15 by HPLC ($\lambda=210$ nm)

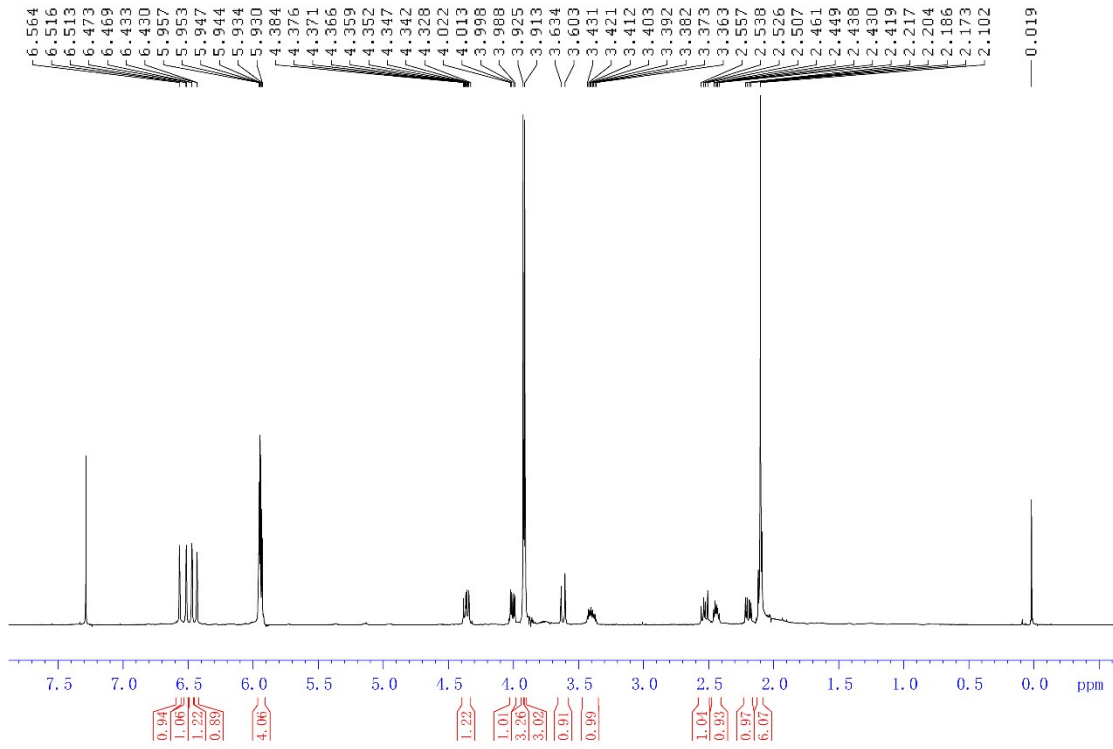
Figure S33. Purity test of compound 16 by HPLC ($\lambda=210$ nm)

Figure S34. Purity test of compound 17 by HPLC ($\lambda=210$ nm)

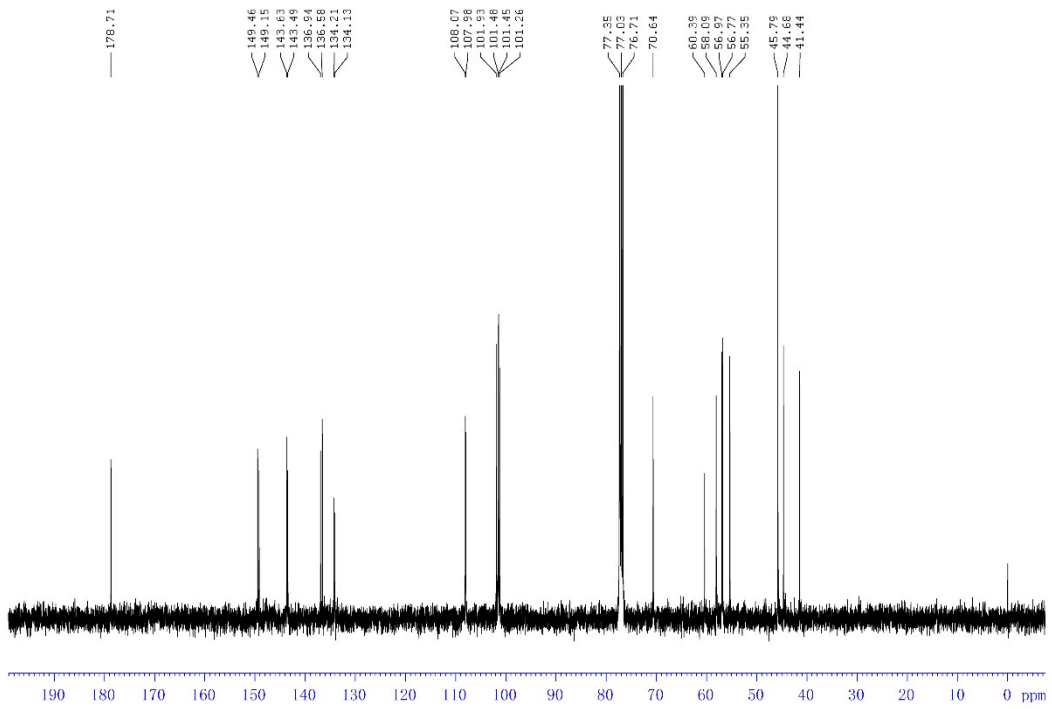
Figure S35. Purity test of compound 18 by HPLC ($\lambda=210$ nm)

Figure S36. Purity test of compound 19 by HPLC ($\lambda=210$ nm)

1-a



1-b



1-c

Spectrum from DataSET11.wiff (sample 1) - pepAME-1, Experiment 1, +TOF MS (100 - 1000)

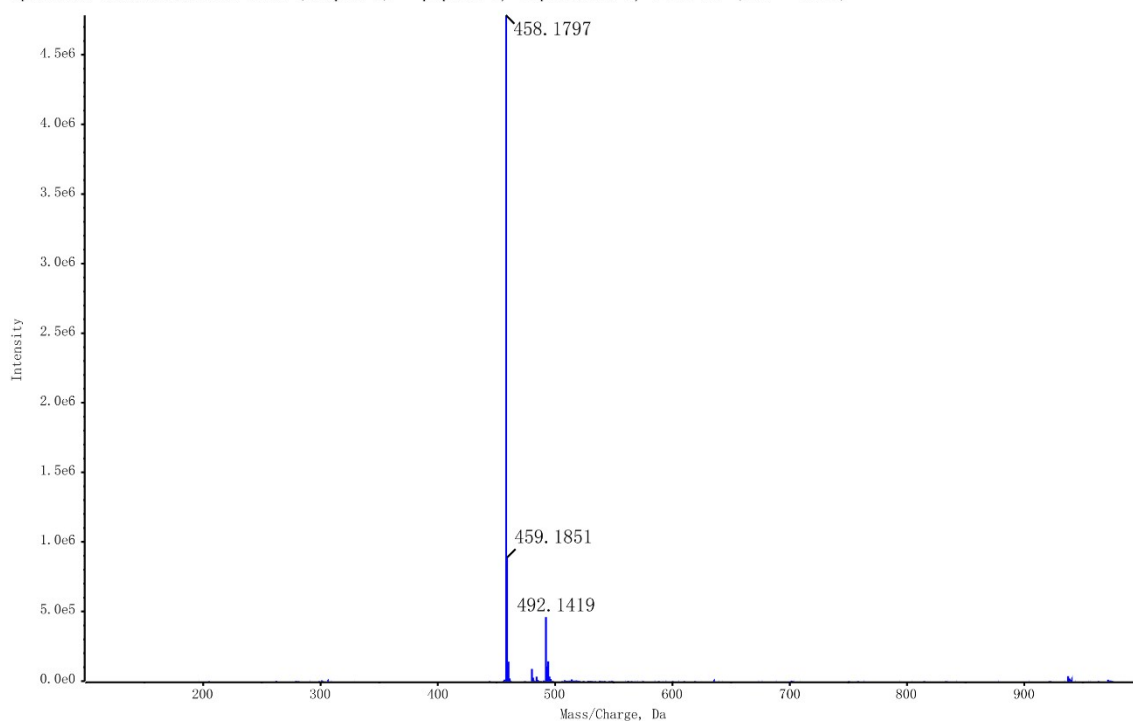
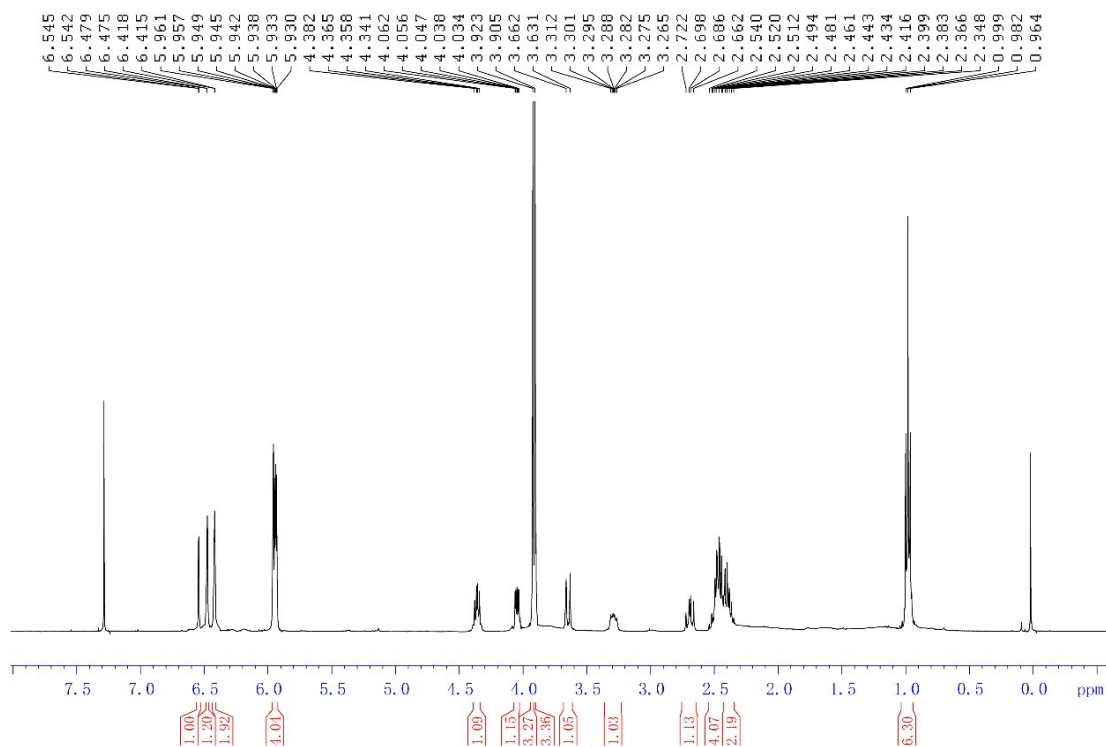
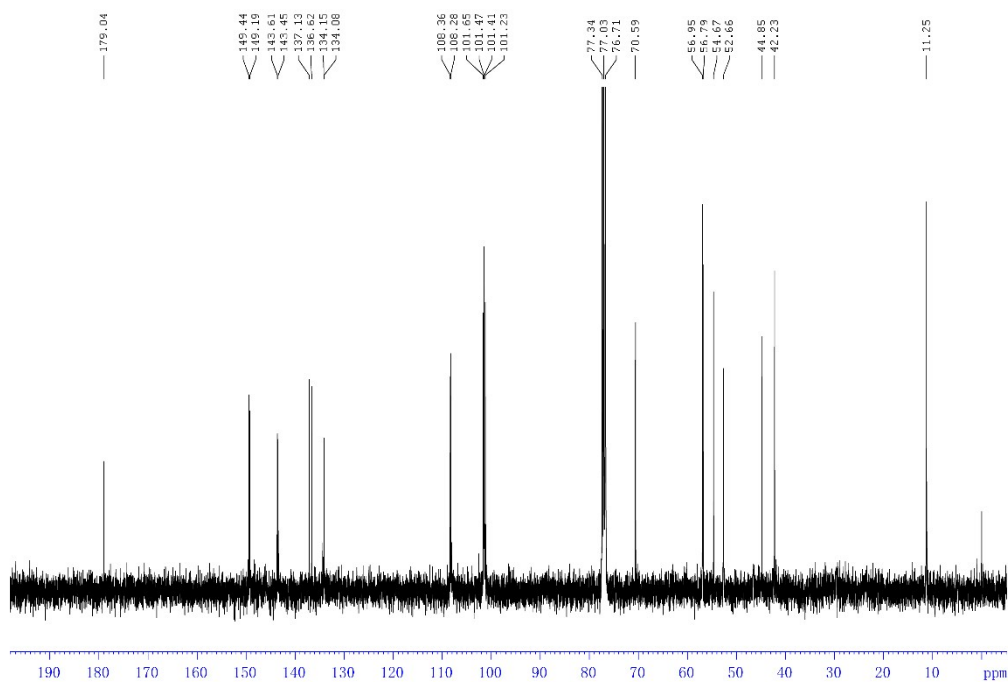


Figure S1. $^1\text{H-NMR}$ (1-a), $^{13}\text{C-NMR}$ (1-b) and HR-ESI-MS (1-c) spectra of compound 2

2-a



2-b



2-c

Spectrum from DataSET12.wiff (sample 2) - pepAME-2, Experiment1, +TOF MS (100 - 1000)

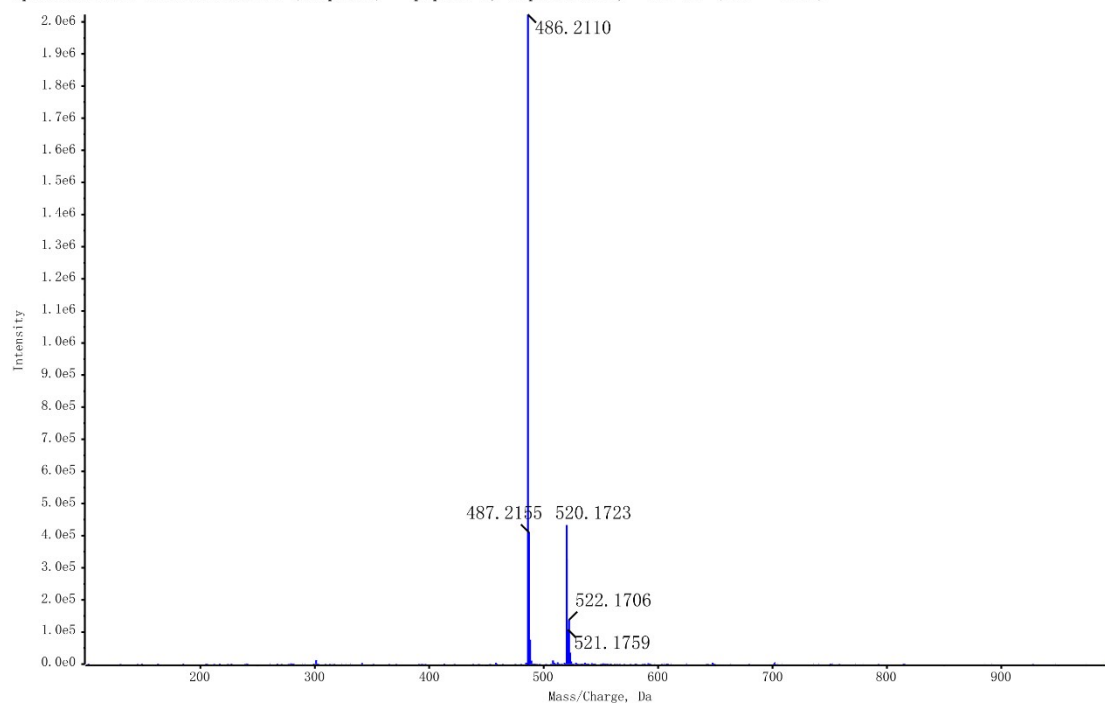
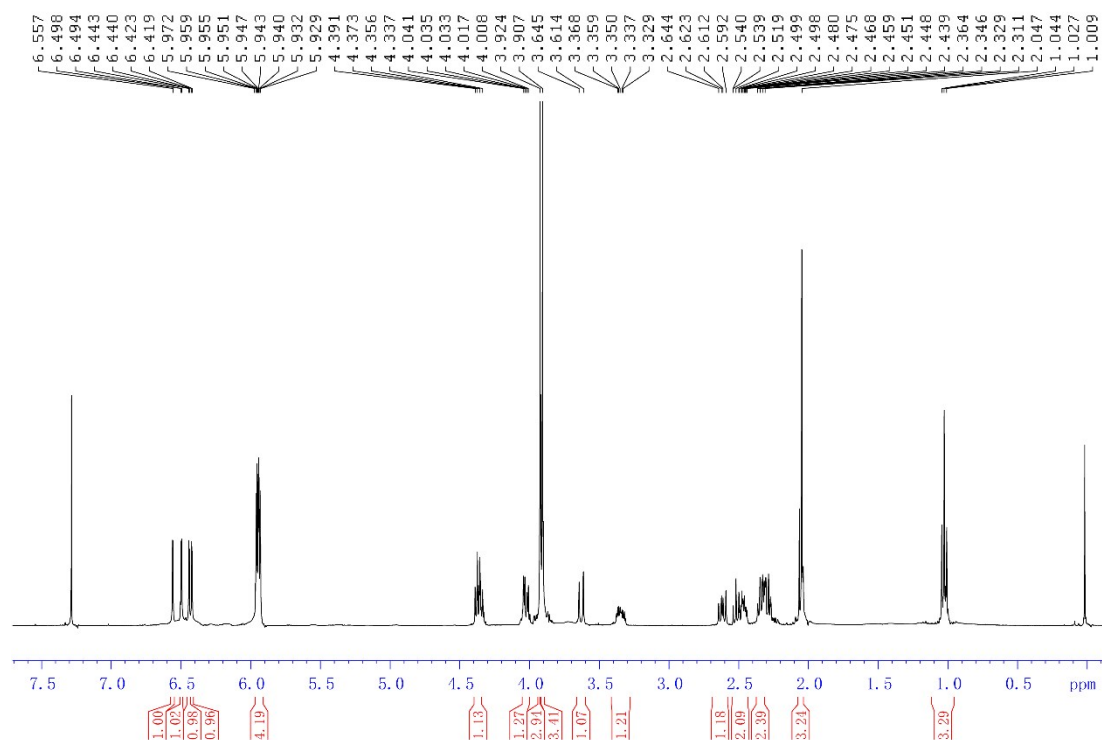
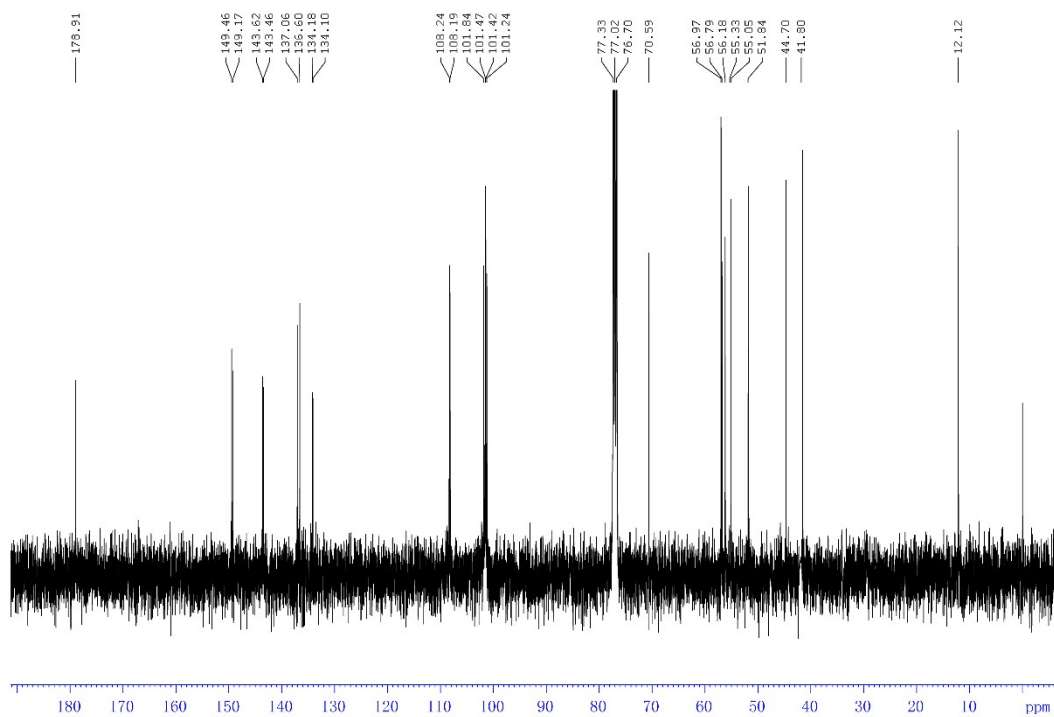


Figure S2. ¹H-NMR (2-a), ¹³C-NMR (2-b) and HR-ESI-MS (2-c) spectra of compound 3

3-a



3-b



3-c

Spectrum from DataSET110.wiff (sample 3) - pepAME-3, Experiment 1, +TOF MS (100 - 1000)

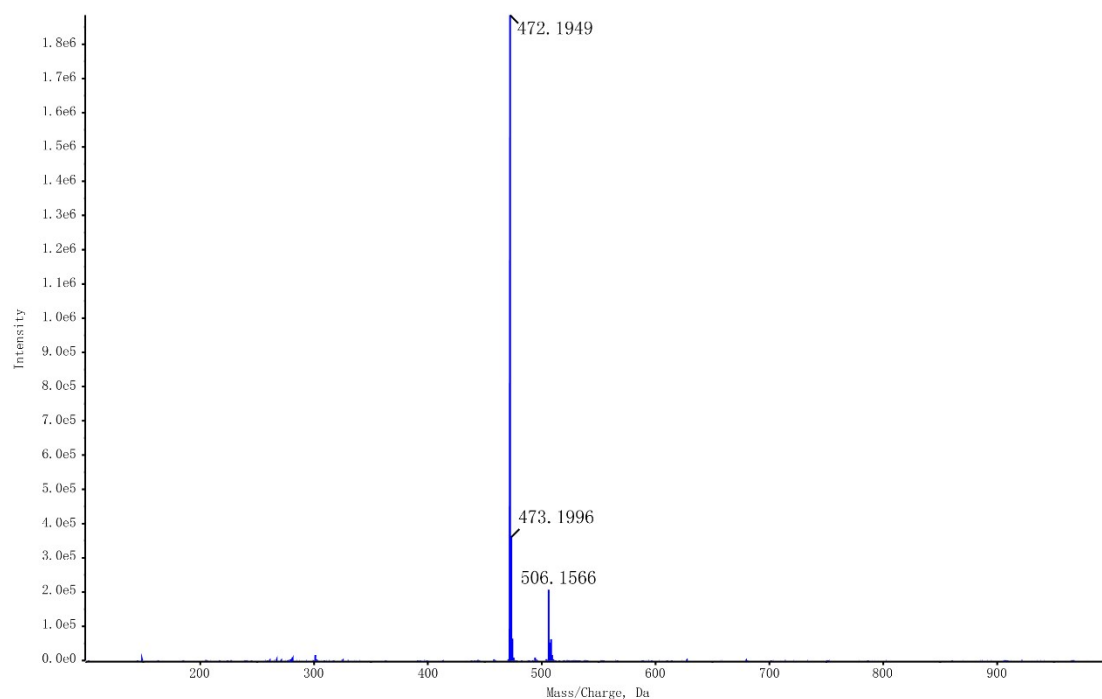
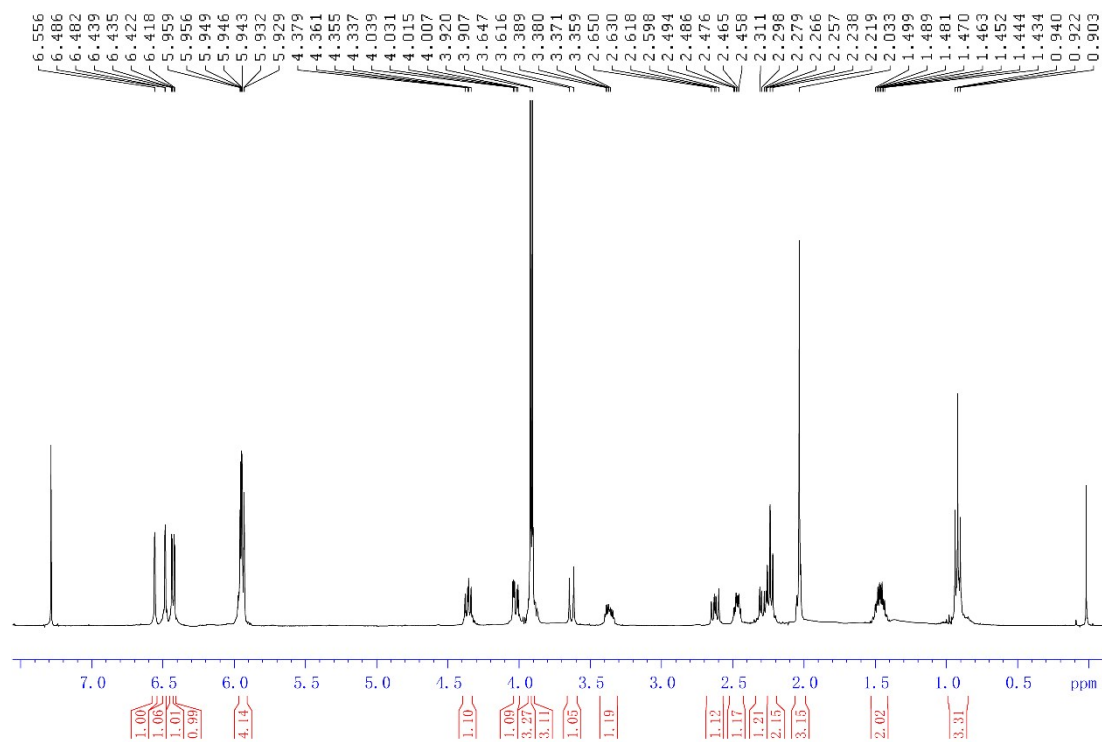
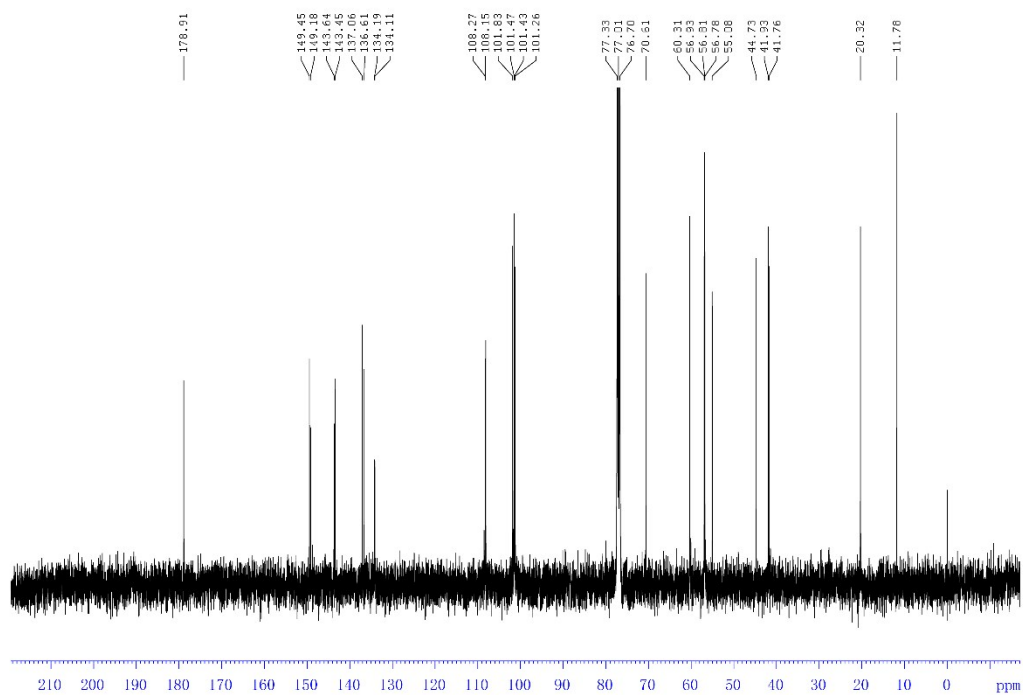


Figure S3. $^1\text{H-NMR}$ (3-a), $^{13}\text{C-NMR}$ (3-b) and HR-ESI-MS (3-c) spectra of compound 4

4-a



4-b



4-c

Spectrum from DataSET113.wiff (sample 4) - pepAME-4, Experiment 1, +TOF MS (100 - 1000)

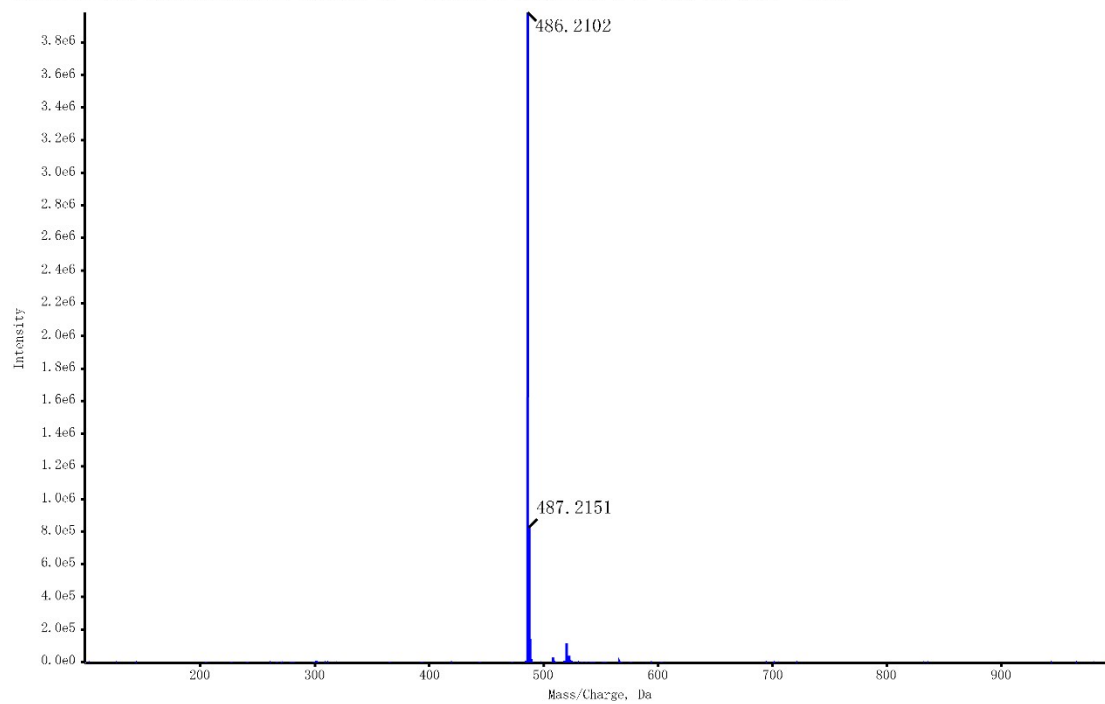
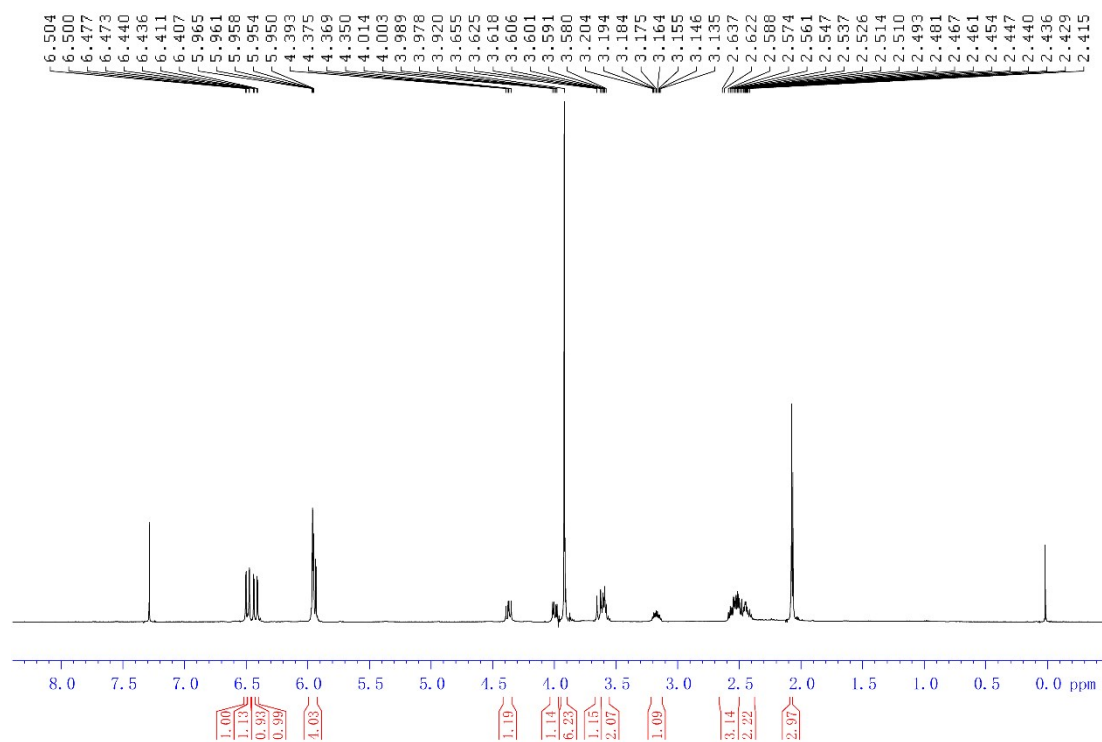
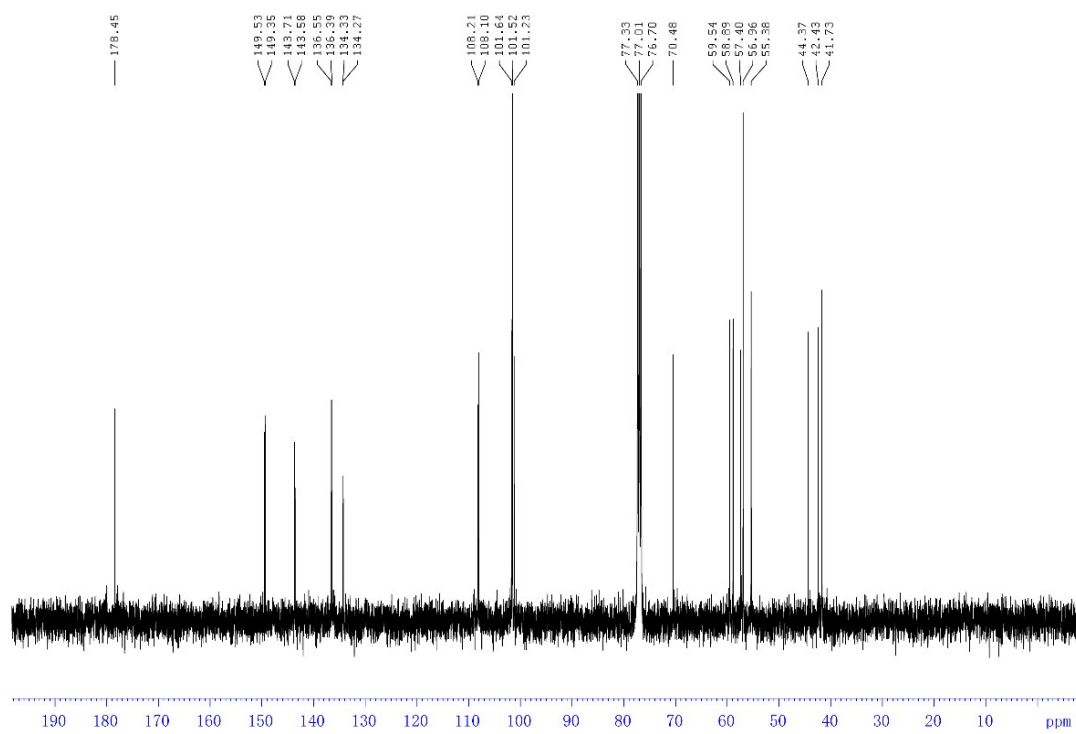


Figure S4. ¹H-NMR (4-a), ¹³C-NMR (4-b) and HR-ESI-MS (4-c) spectra of compound 5

5-a



5-b



5-c

Spectrum from DataSET17.wiff (sample 5) - pepAME-5, Experiment1, +TOF MS (100 - 1000)

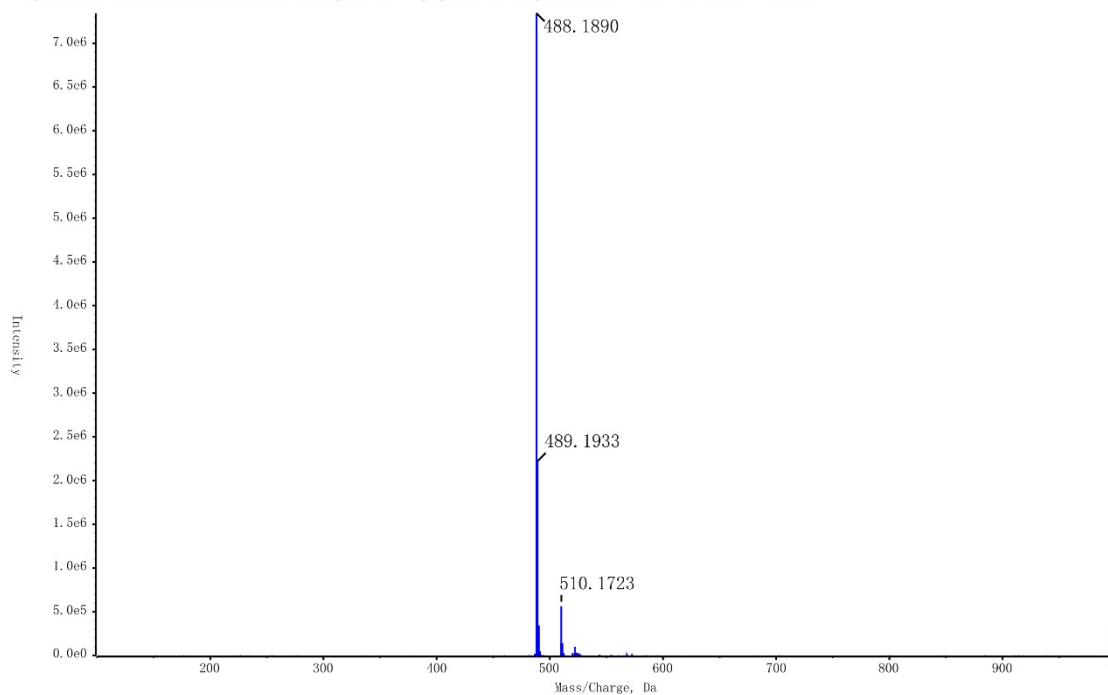
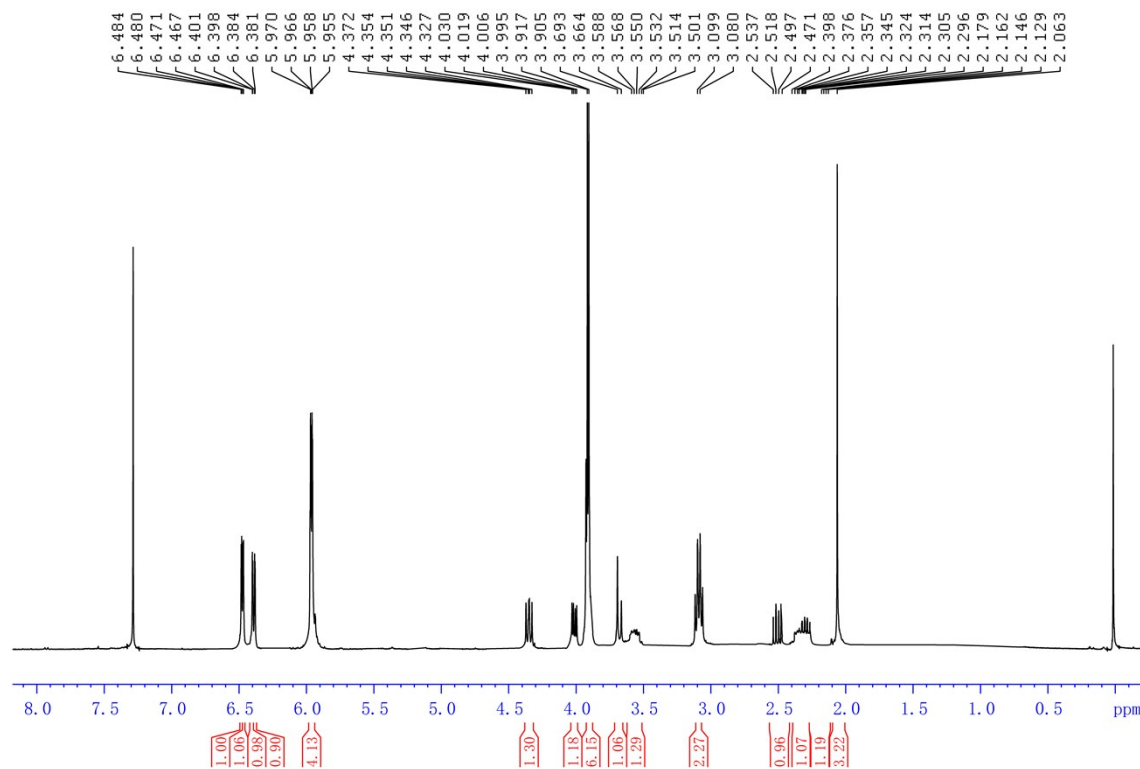
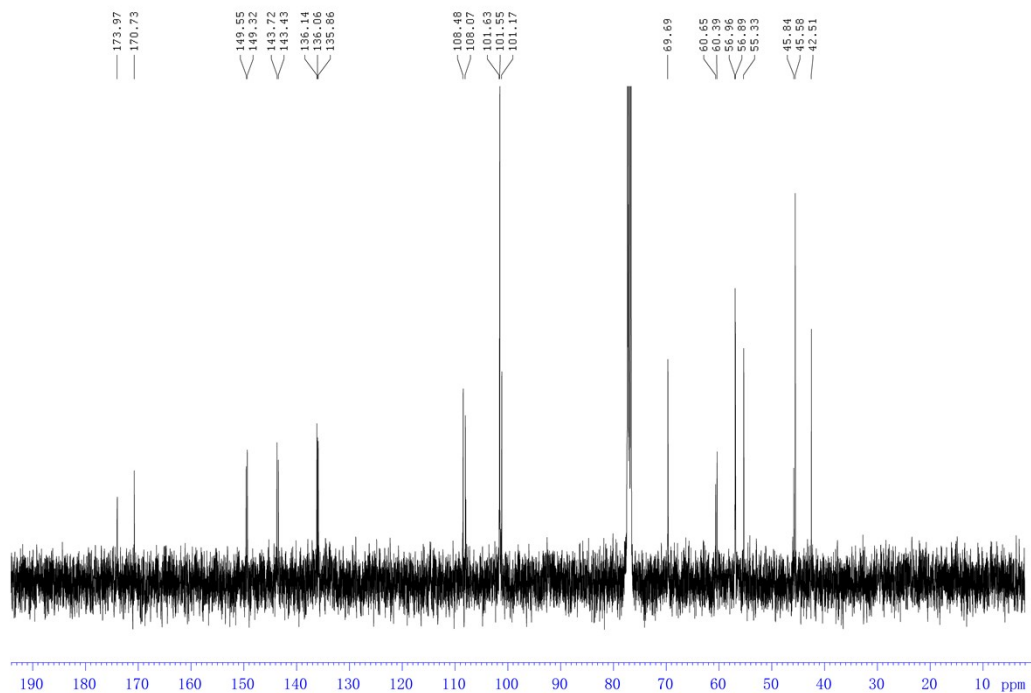


Figure S5. ¹H-NMR (5-a), ¹³C-NMR (5-b) and HR-ESI-MS (5-c) spectra of compound 6

6-a



6-b



6-c

Spectrum from DataSET120.wiff (sample 6) - Sample006, Experiment 1, +TOF MS (50 - 1500)

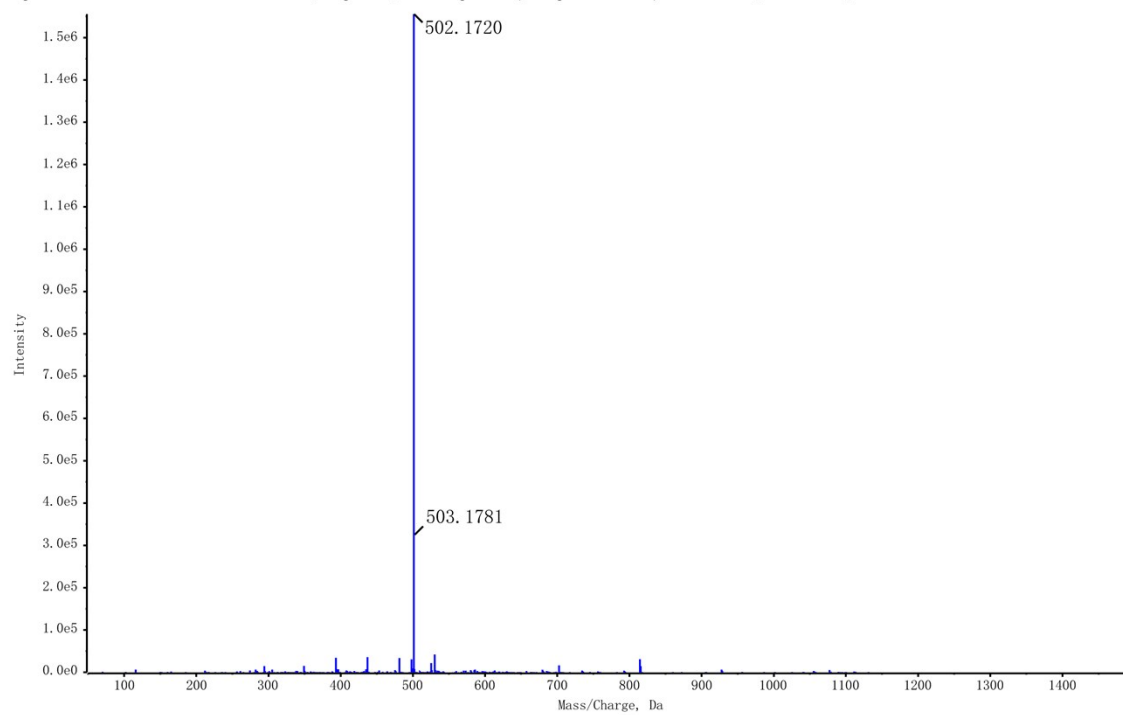
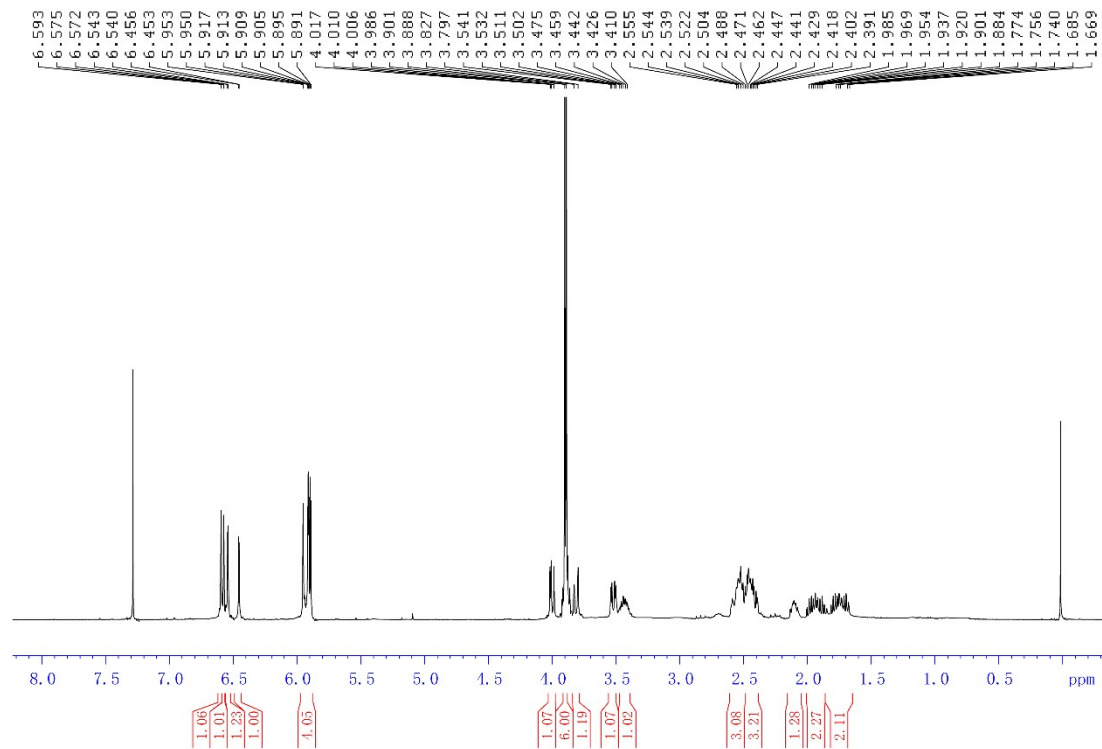
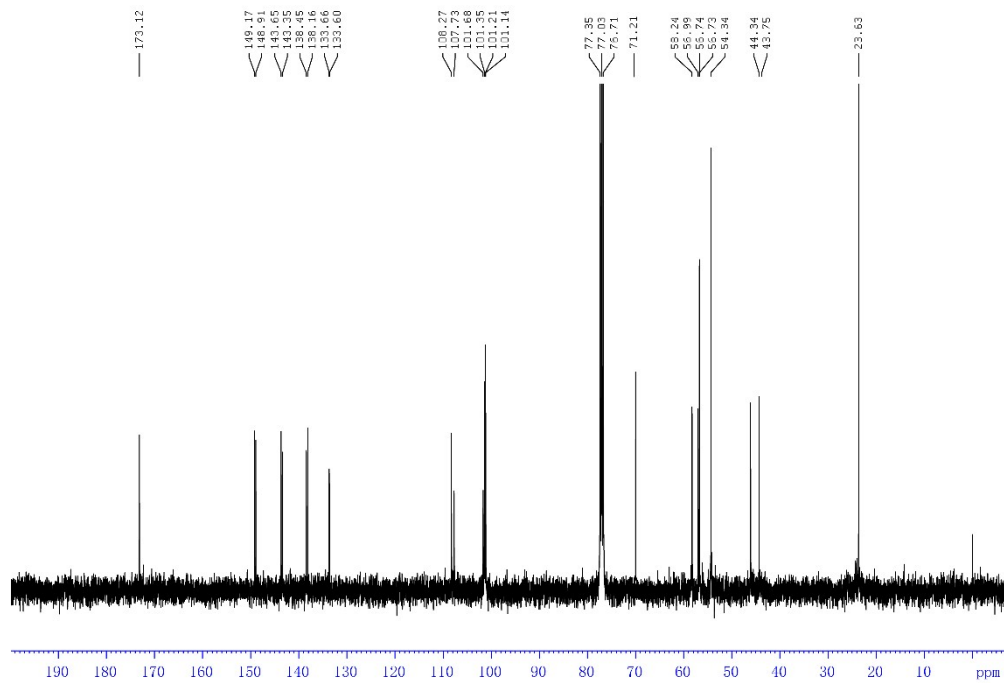


Figure S6. ¹H-NMR (6-a), ¹³C-NMR (6-b) and HR-ESI-MS (6-c) spectra of compound 7

7-a



7-b



7-c

Spectrum from DataSET11.wiff (sample 7) - pepAME-7, Experiment1, +TOF MS (100 - 1000)

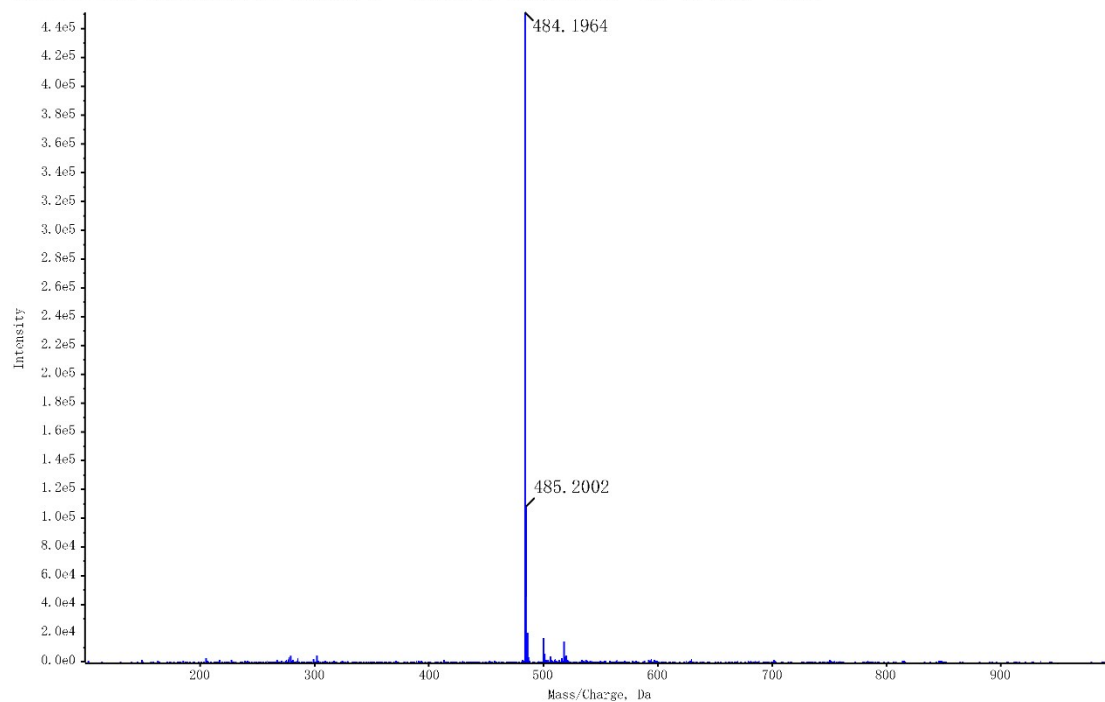
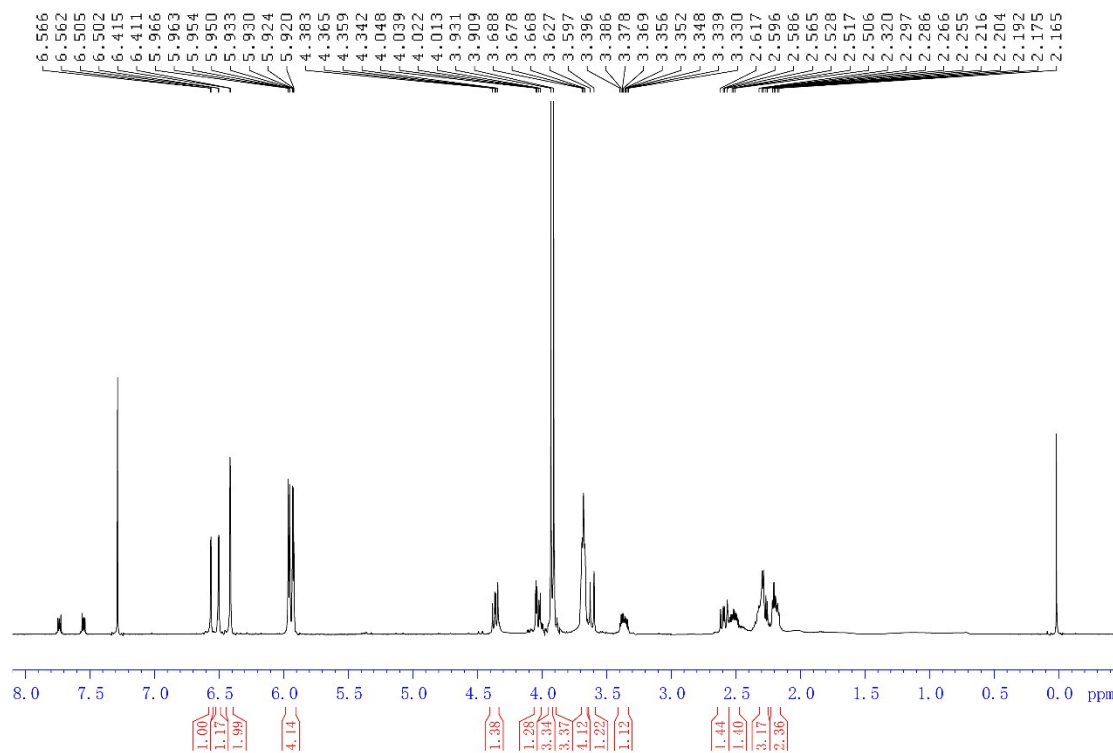
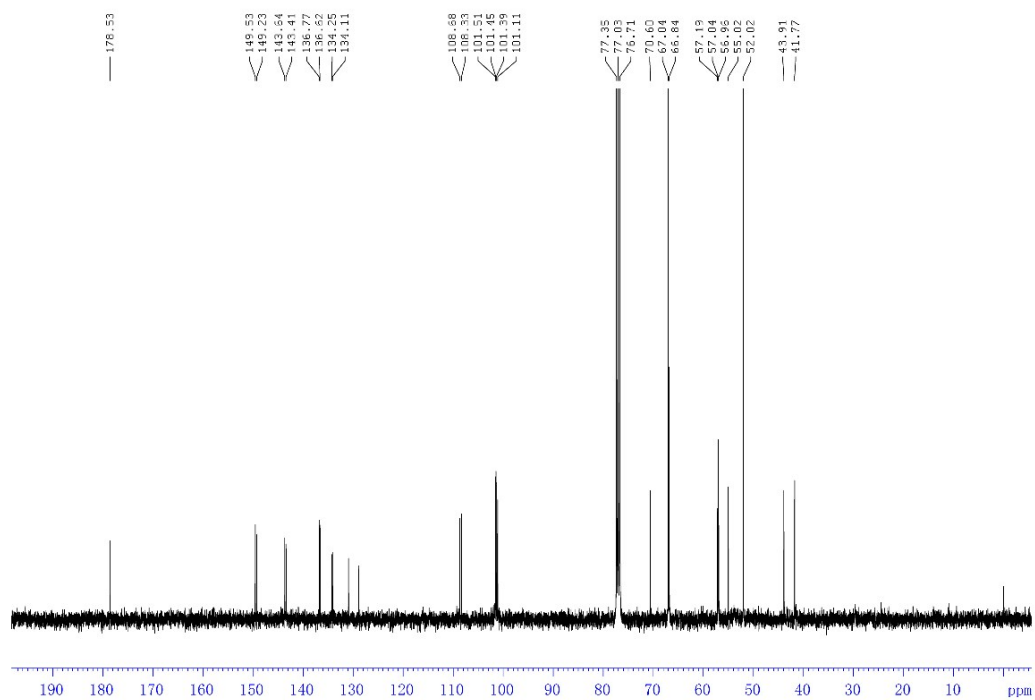


Figure S7. $^1\text{H-NMR}$ (7-a), $^{13}\text{C-NMR}$ (7-b) and HR-ESI-MS (7-c) spectra of compound 8

8-a



8-b



8-c

Spectrum from DataSET13.wiff (sample 8) - pepAME-8, Experiment1, +TOF MS (100 - 1000)

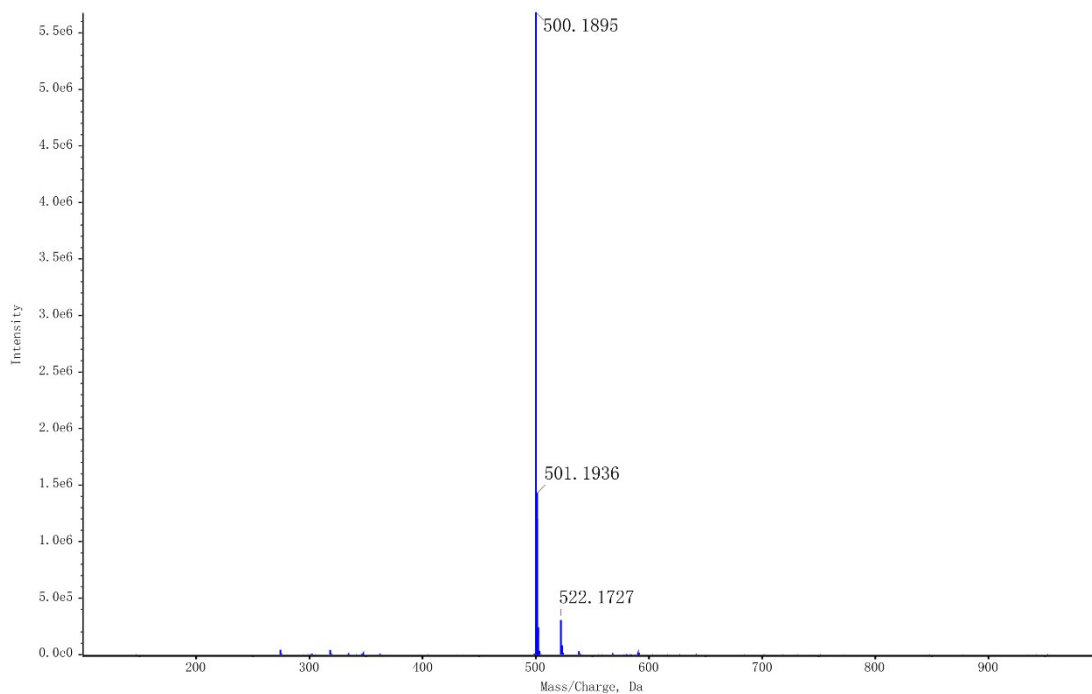
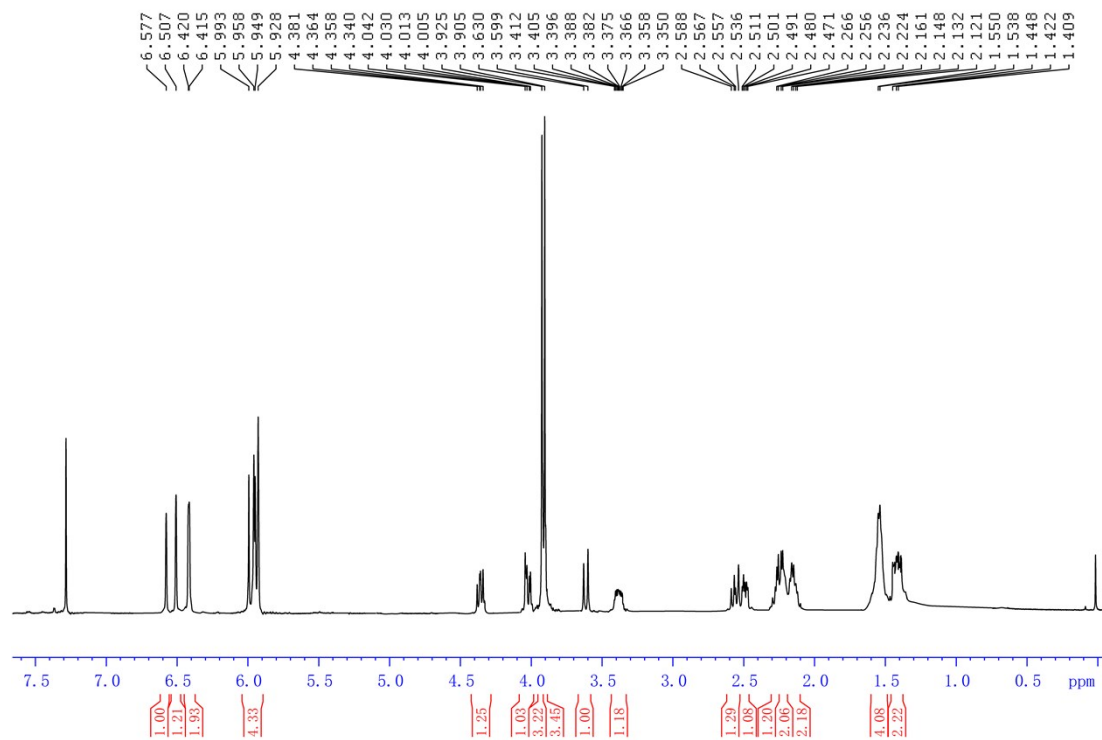
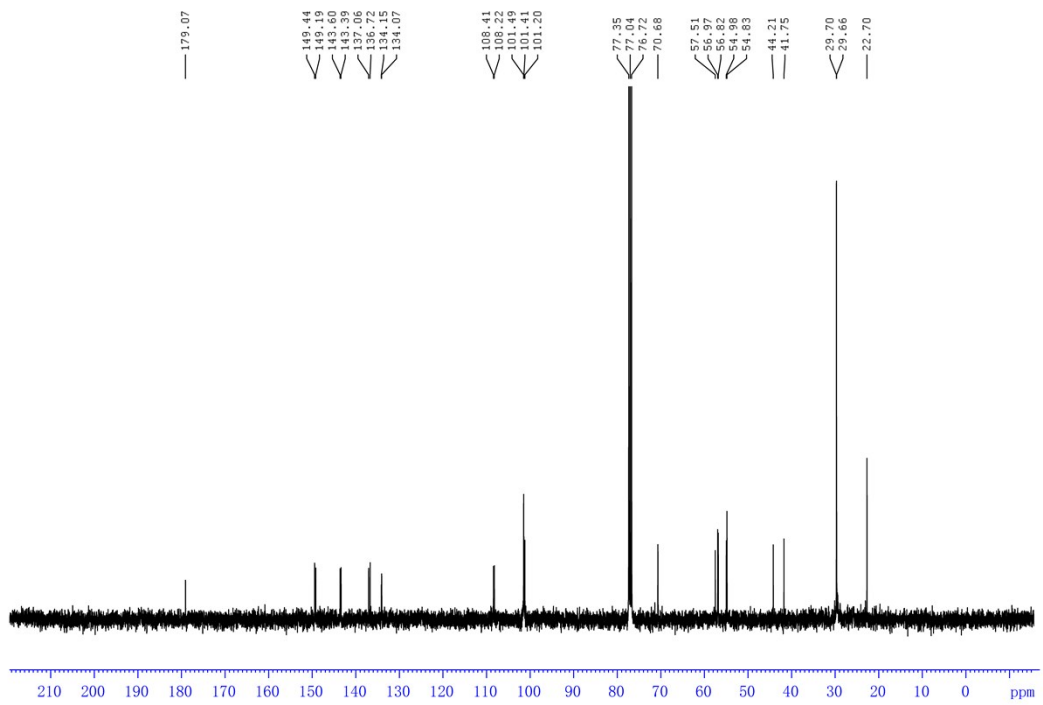


Figure S8. ¹H-NMR (8-a), ¹³C-NMR (8-b) and HR-ESI-MS (8-c) spectra of compound 9

9-a



9-b



9-c

Spectrum from DataSET119.wiff (sample 9) - Sample009, Experiment 1, +TOF MS (50 - 1500)

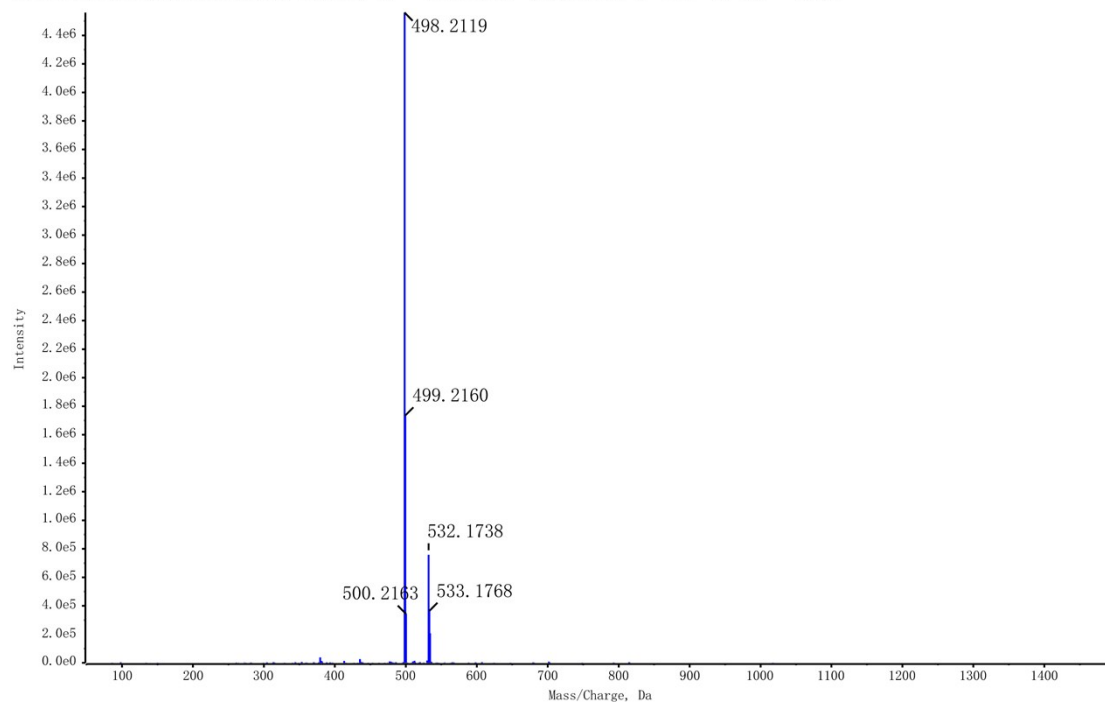
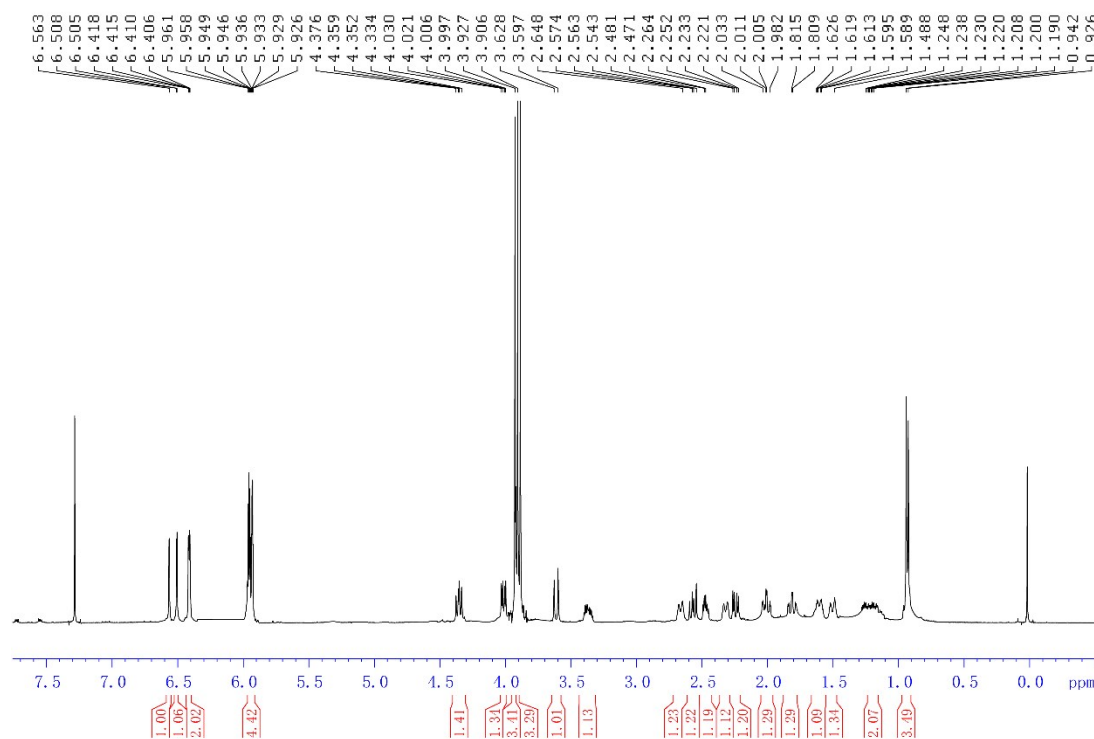
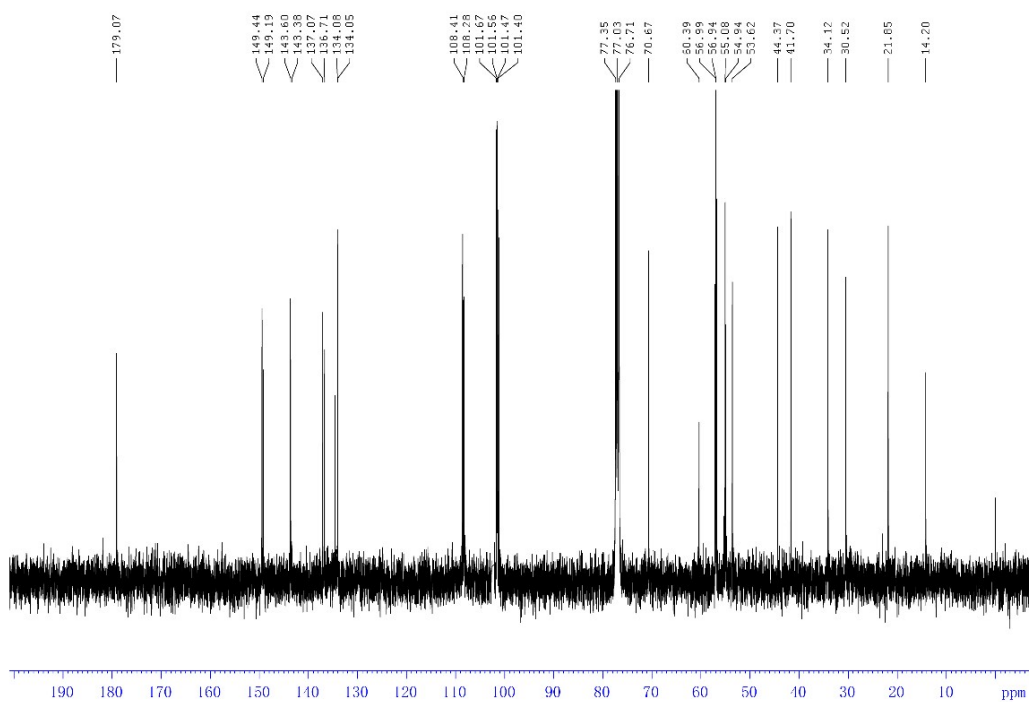


Figure S9. $^1\text{H-NMR}$ (9-a), $^{13}\text{C-NMR}$ (9-b) and HR-ESI-MS (9-c) spectra of compound 10

10-a



10-b



10-c

Spectrum from DataSET14.wiff (sample 10) - pepAME-10, Experiment 1, +TOF MS (100 - 1000)

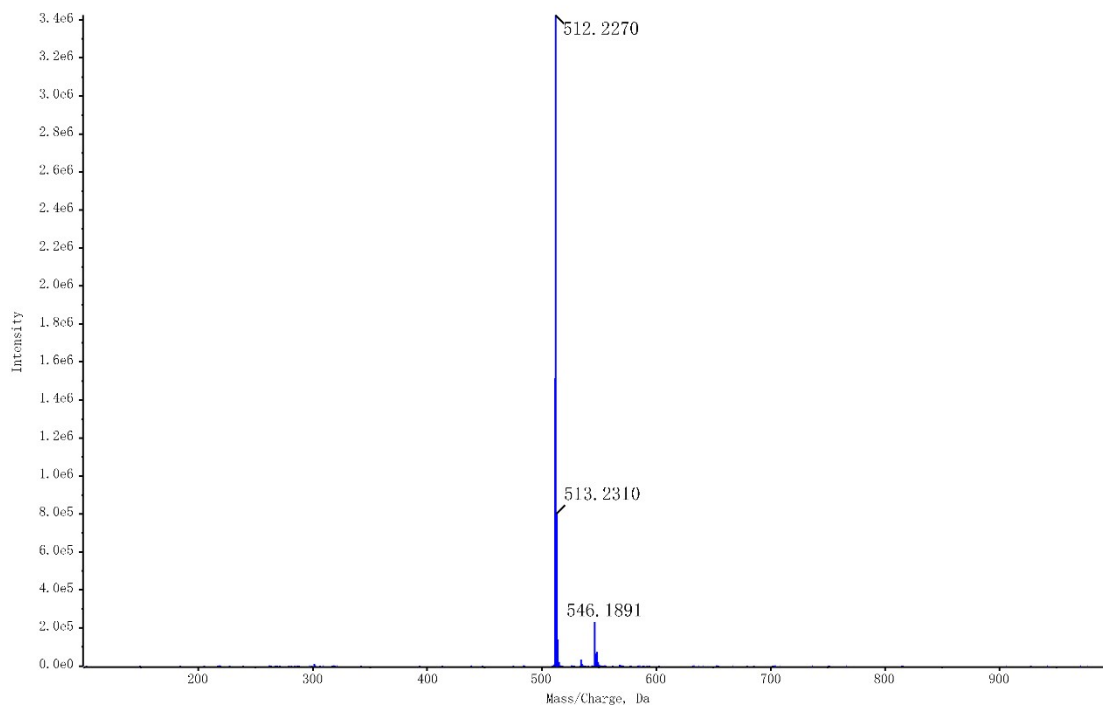
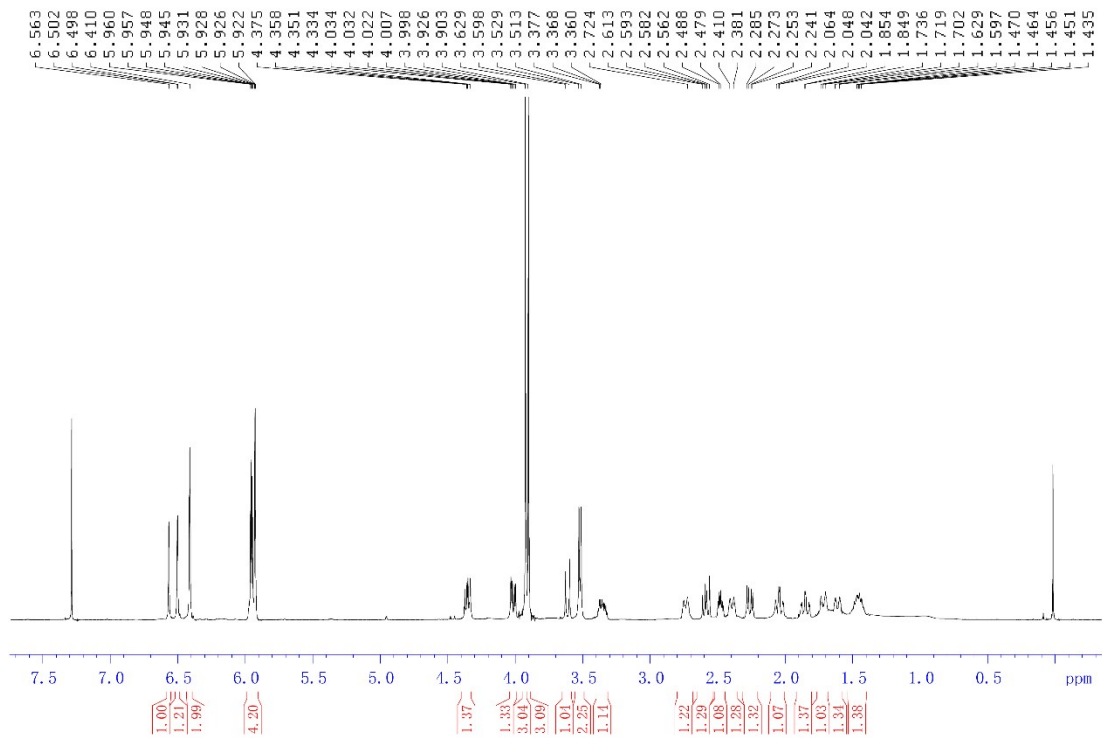
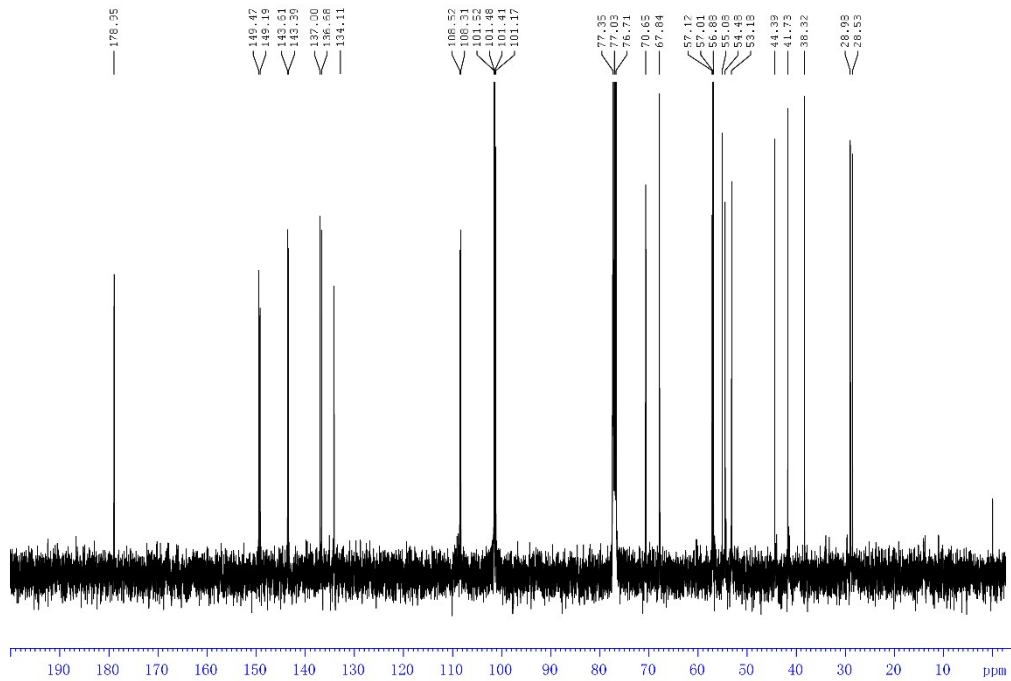


Figure S10. $^1\text{H-NMR}$ (10-a), $^{13}\text{C-NMR}$ (10-b) and HR-ESI-MS (10-c) spectra of compound 11

11-a



11-b



11-c

Spectrum from DataSET15.wiff (sample 11) - pepAME-11, Experiment1, +TOF MS (100 - 1000)

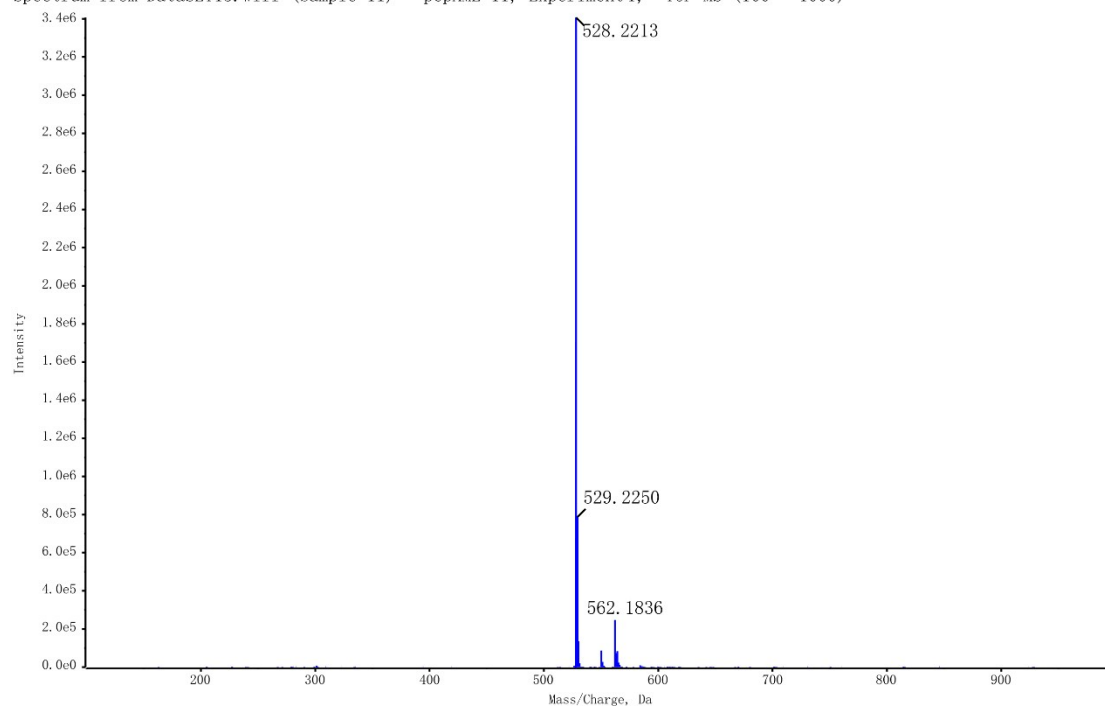
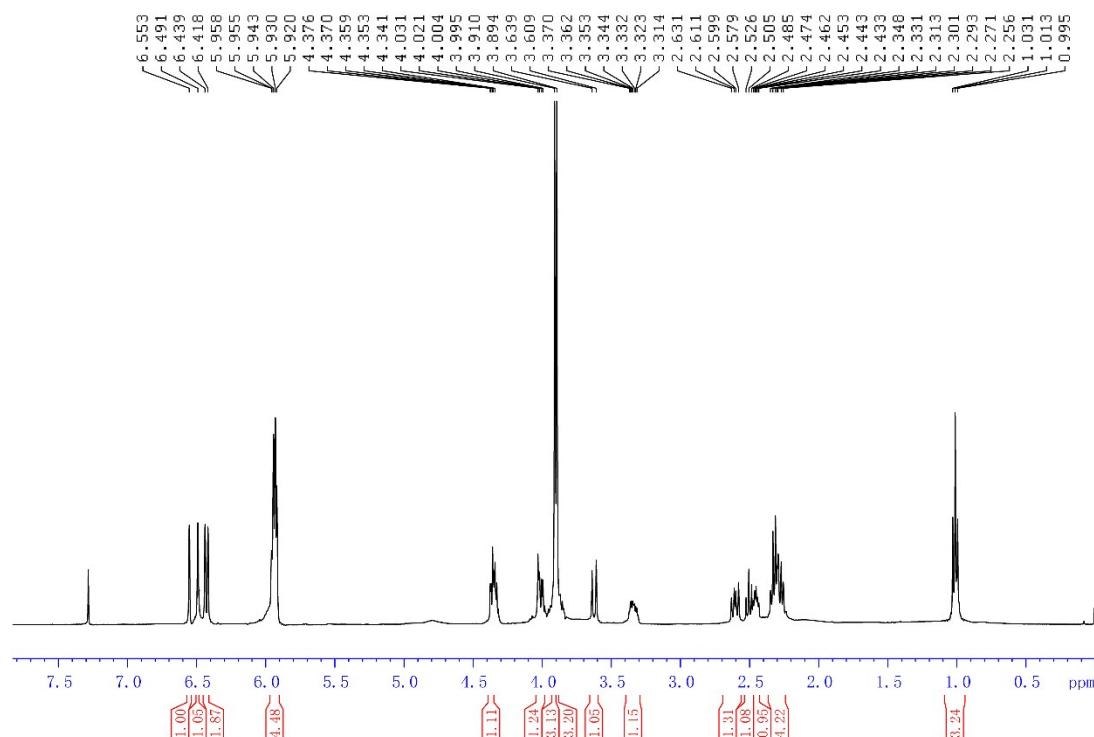
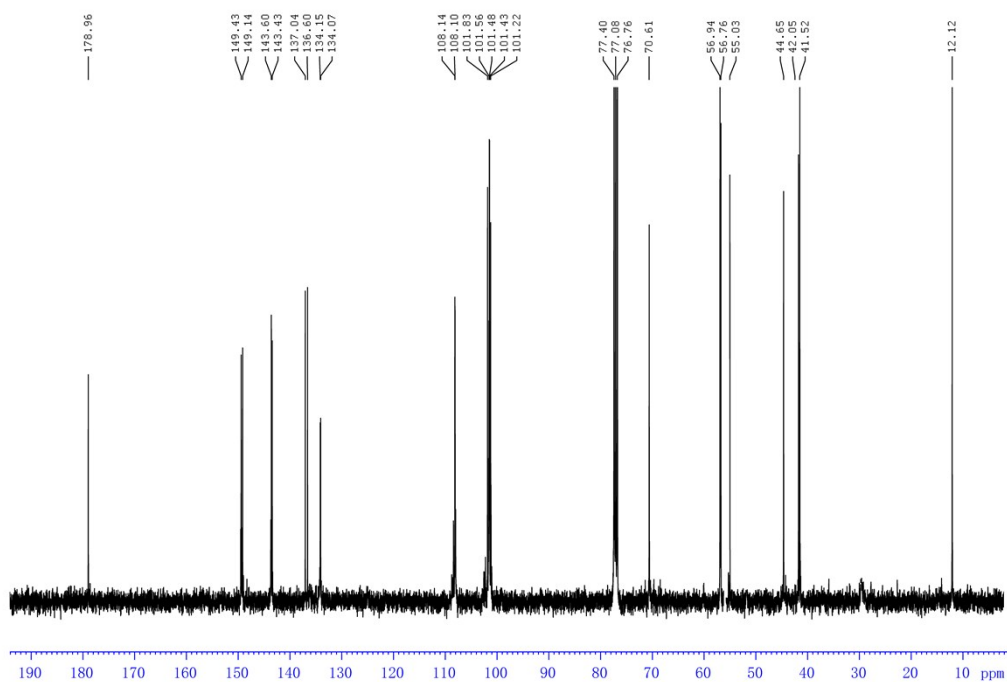


Figure S11. $^1\text{H-NMR}$ (11-a), $^{13}\text{C-NMR}$ (11-b) and HR-ESI-MS (11-c) spectra of compound 12

12-a



12-b



12-c

Spectrum from DataSET110.wiff (sample 12) - pepAME-12, Experiment 1, +TOF MS (100 - 1000)

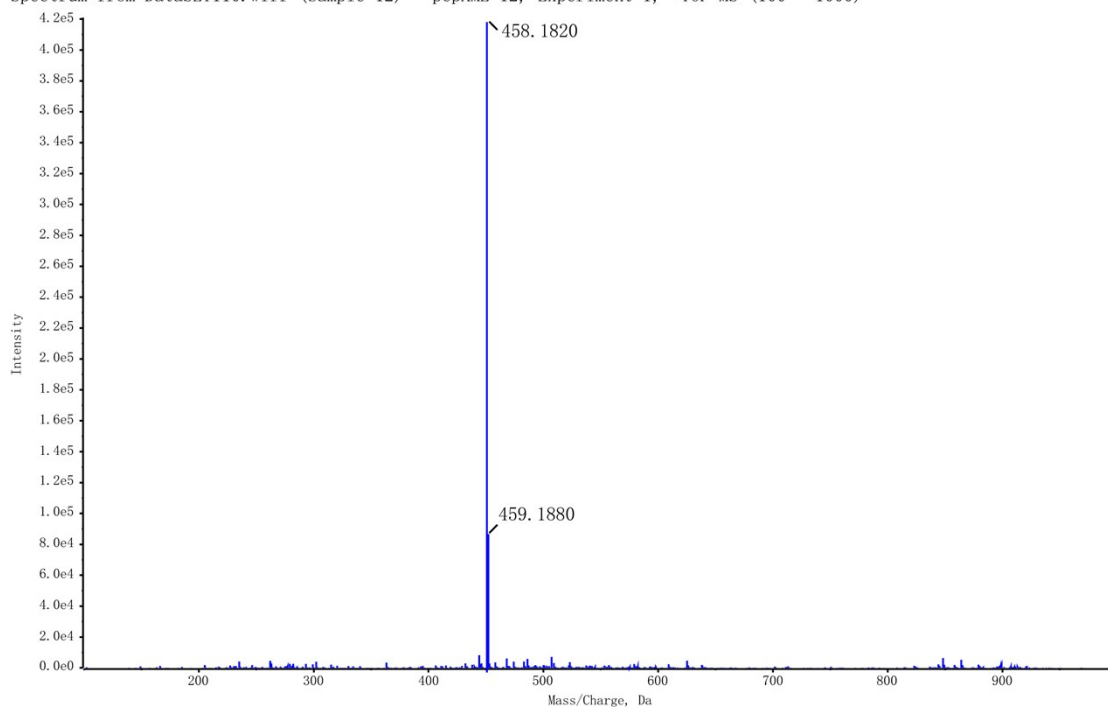
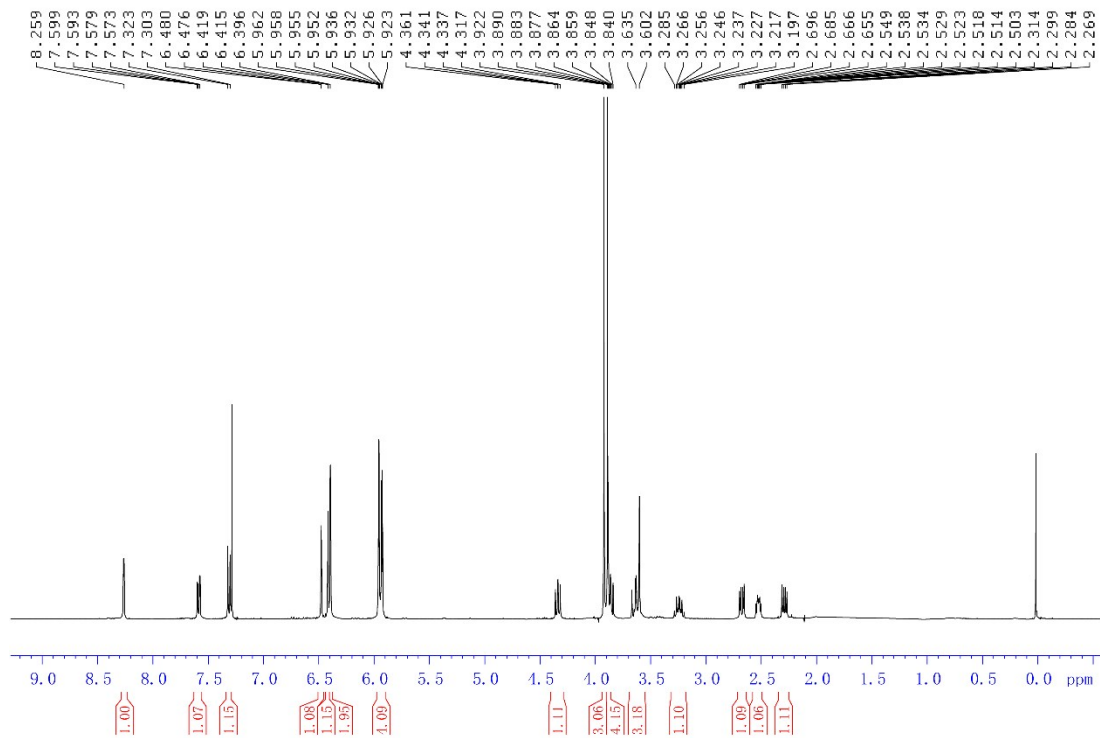
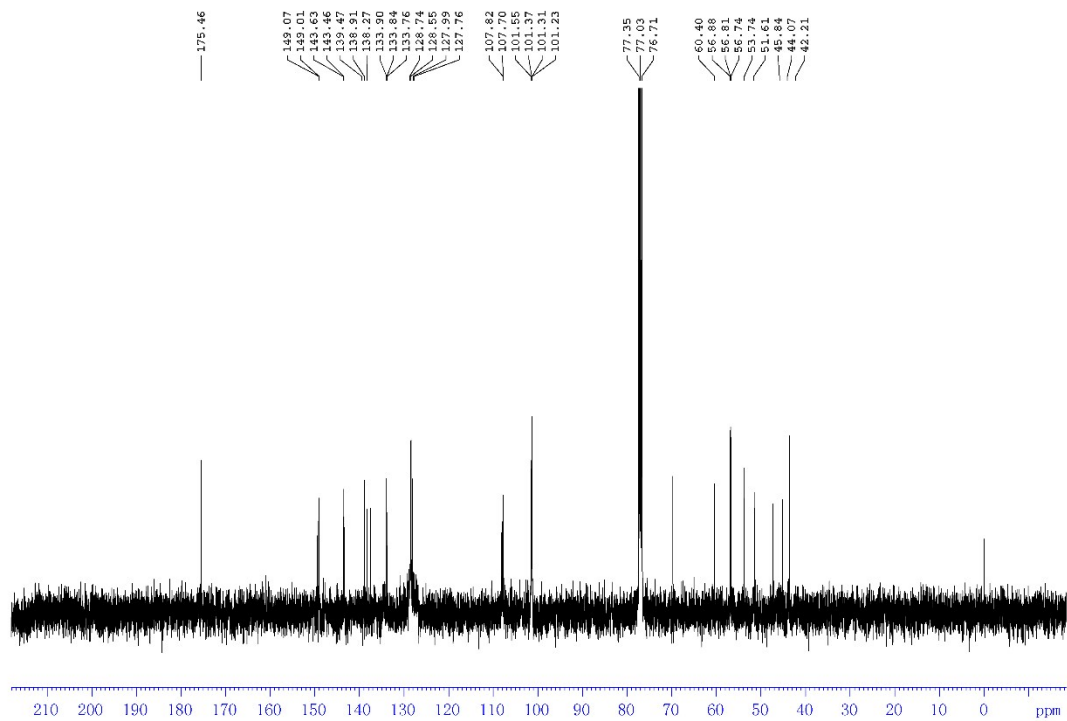


Figure S12. $^1\text{H-NMR}$ (12-a), $^{13}\text{C-NMR}$ (12-b) and HR-ESI-MS (12-c) spectra of compound 13

13-a



13-b



13-c

Spectrum from DataSET111.wiff (sample 13) - pepAME-13, Experiment 1, +TOF MS (100 - 1000)

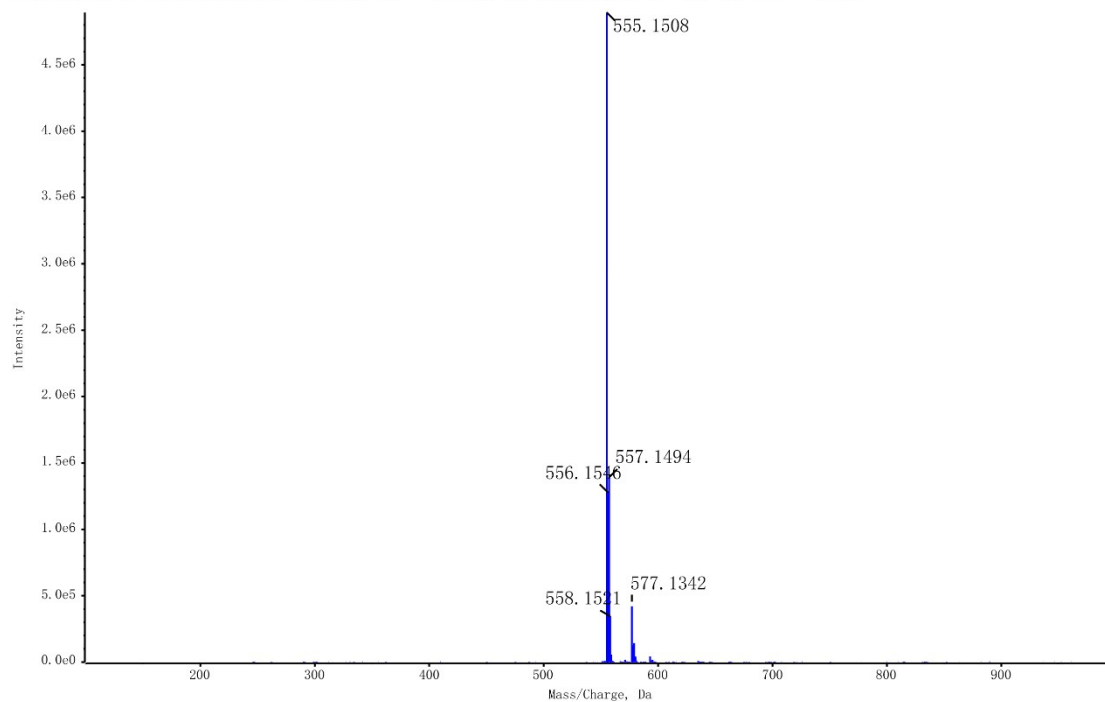
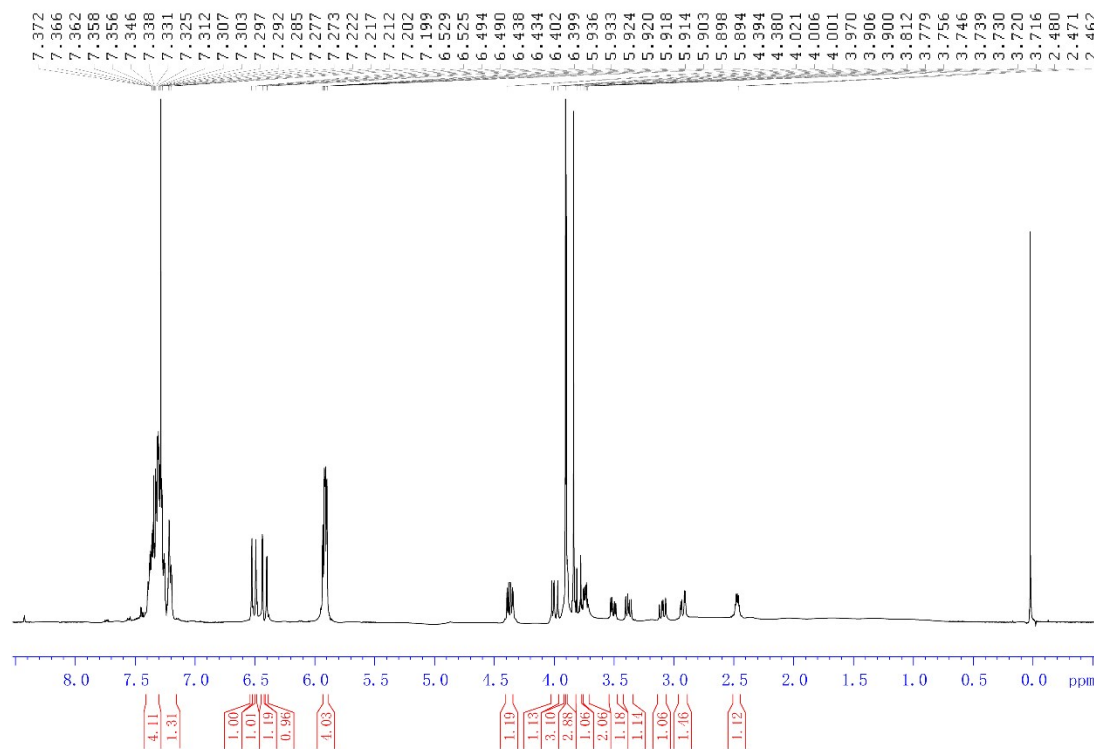
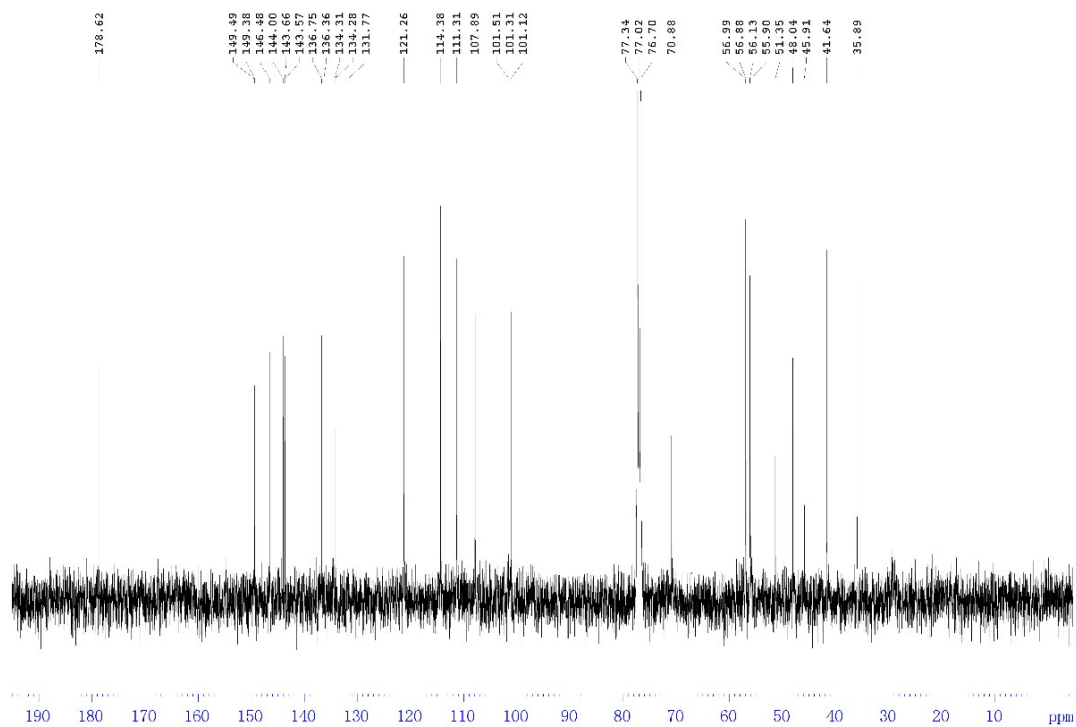


Figure S13. $^1\text{H-NMR}$ (13-a), $^{13}\text{C-NMR}$ (13-b) and HR-ESI-MS (13-c) spectra of compound 14

14-a



14-b



14-c

Spectrum from DataSET16.wiff (sample 14) - pepAME-14, Experiment 1, +TOF MS (100 - 1000)

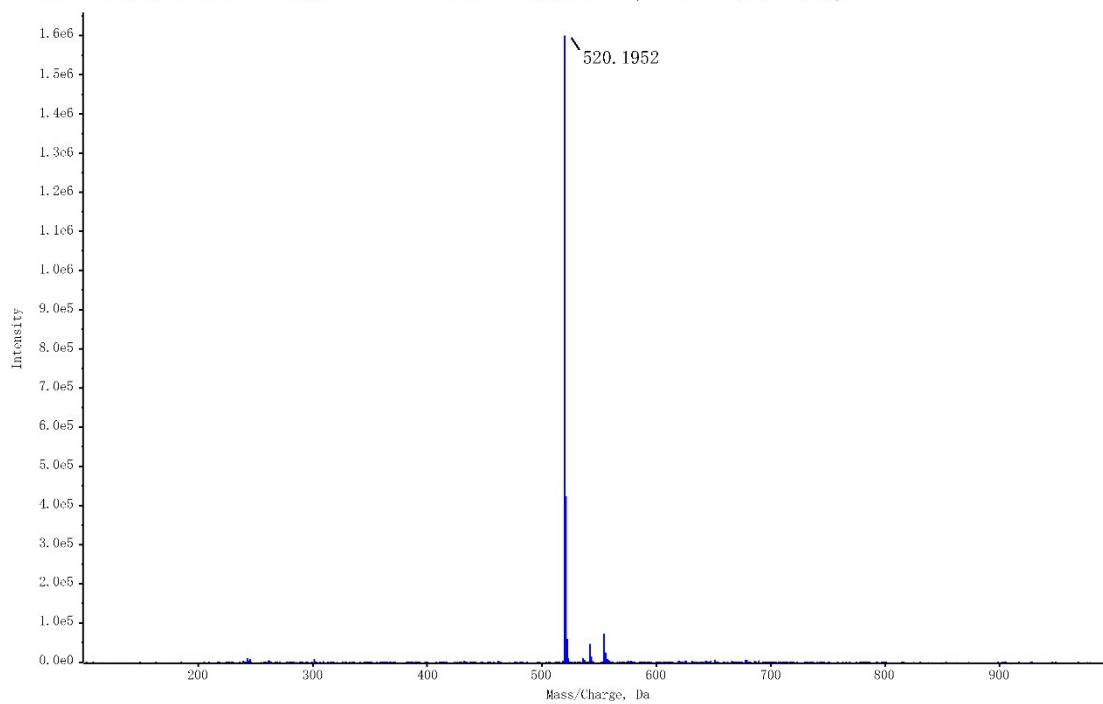
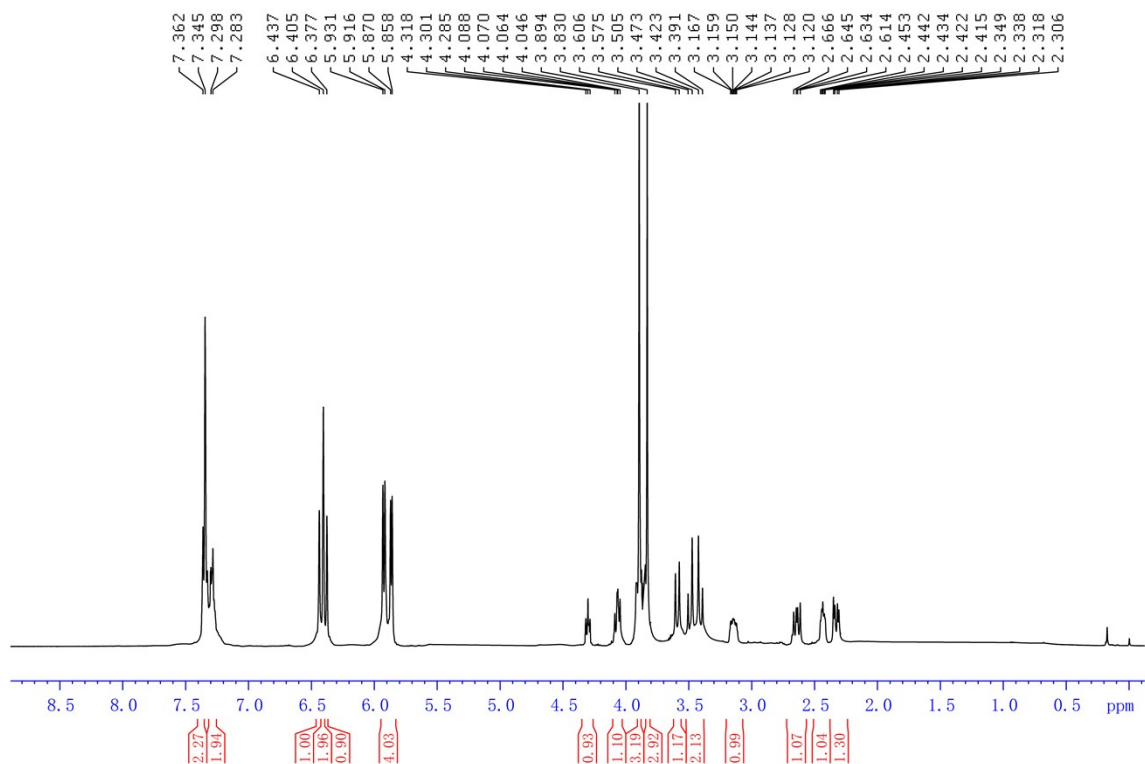
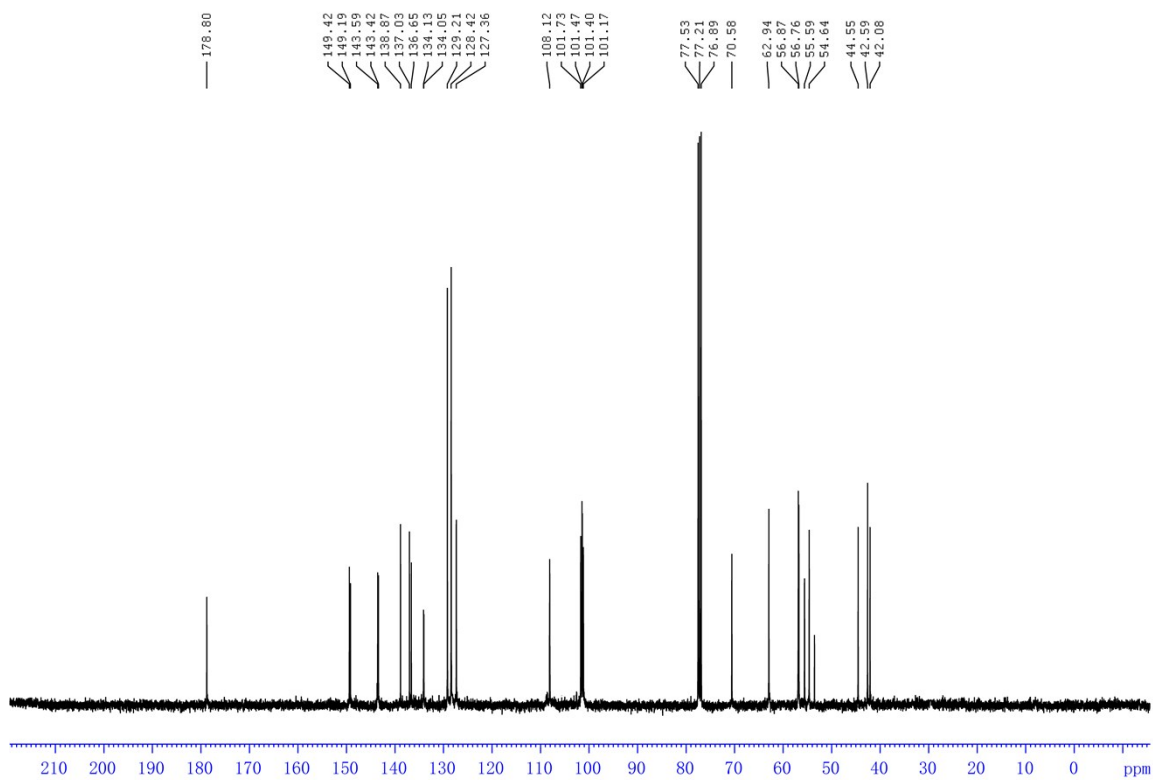


Figure S14. ^1H -NMR (14-a), ^{13}C -NMR (14-b) and HR-ESI-MS (14-c) spectra of compound 15

15-a



15-b



15-c

Spectrum from DataSET121.wiff (sample 1) - Sample003, Experiment 1, +TOF MS (50 - 1500)

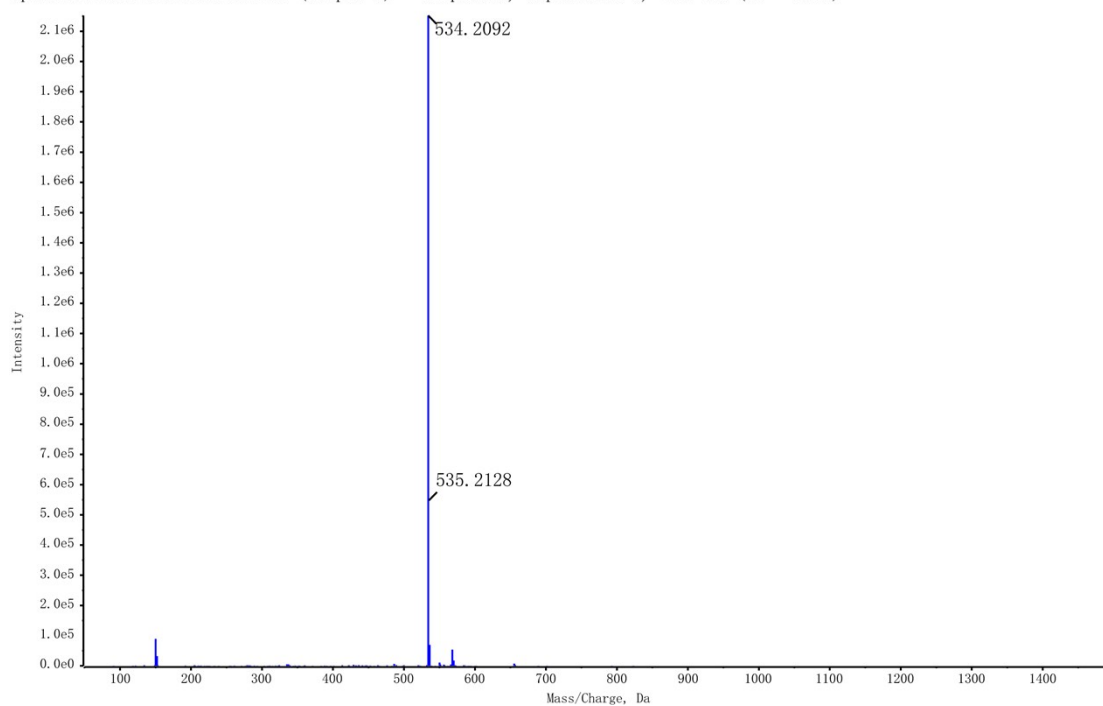
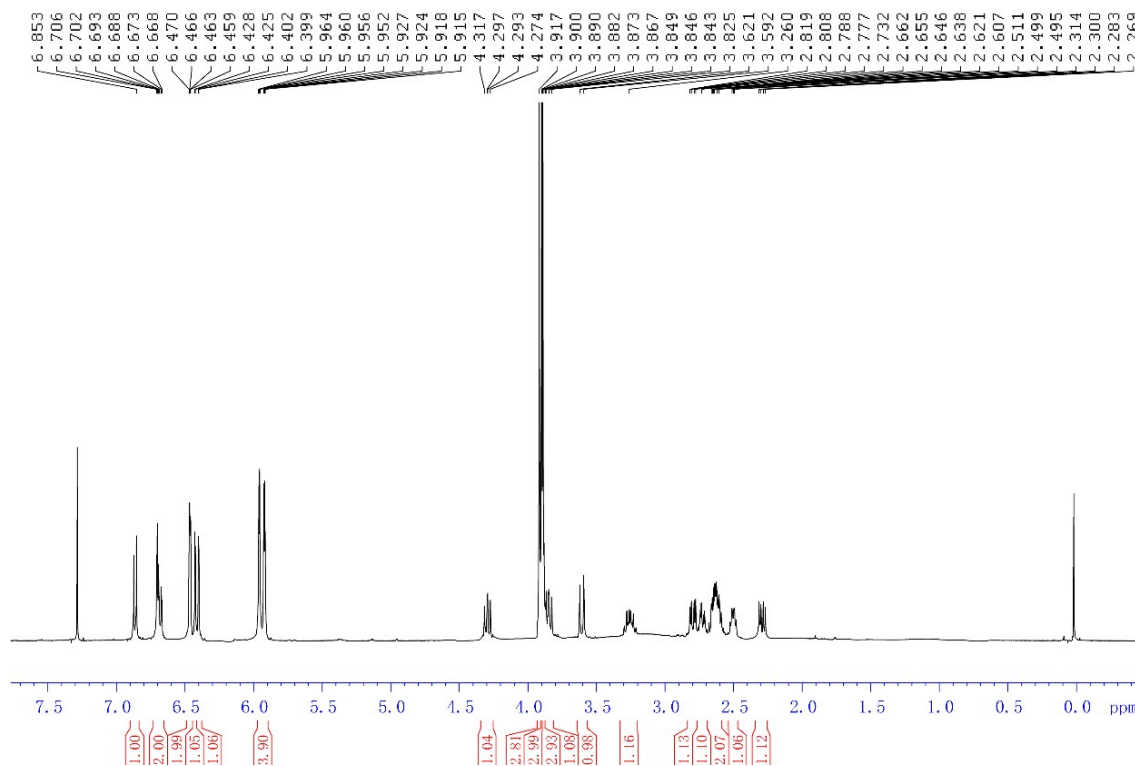
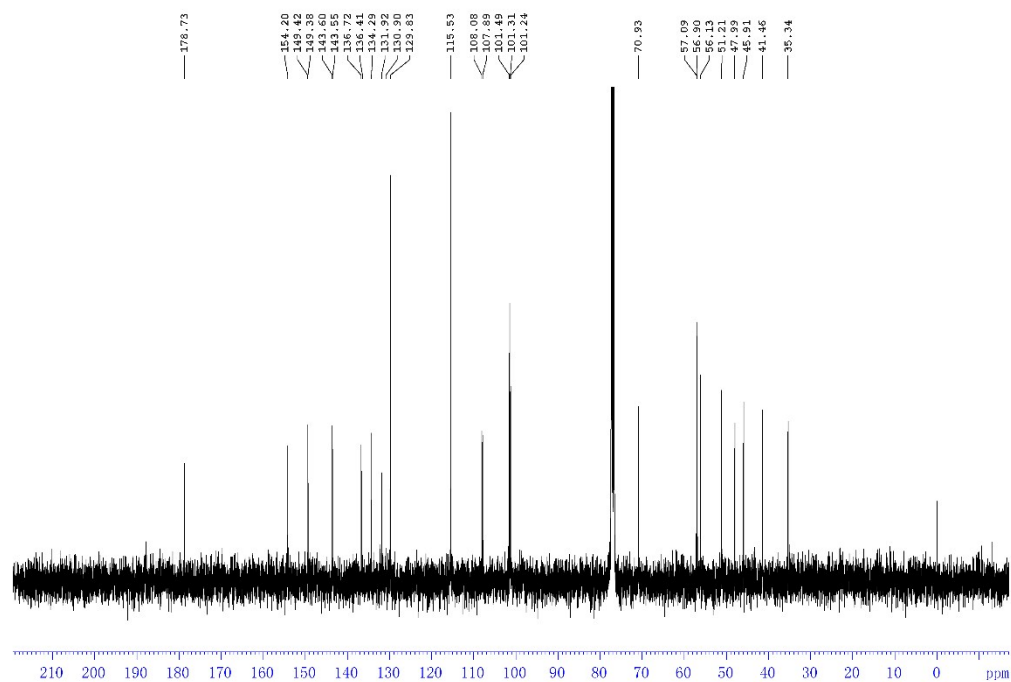


Figure S15. $^1\text{H-NMR}$ (15-a), $^{13}\text{C-NMR}$ (15-b) and HR-ESI-MS (15-c) spectra of compound 16

16-a



16-b



16-c

Spectrum from DataSET19.wiff (sample 16) - pepAME-16, Experiment 1, +TOF MS (100 - 1000)

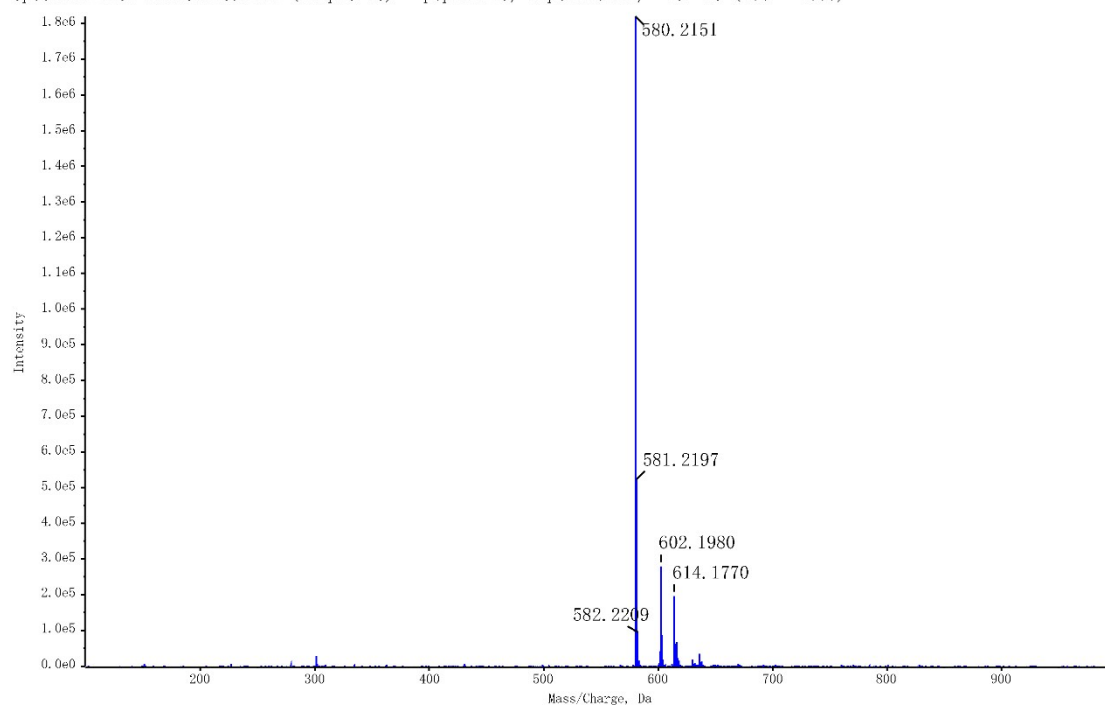
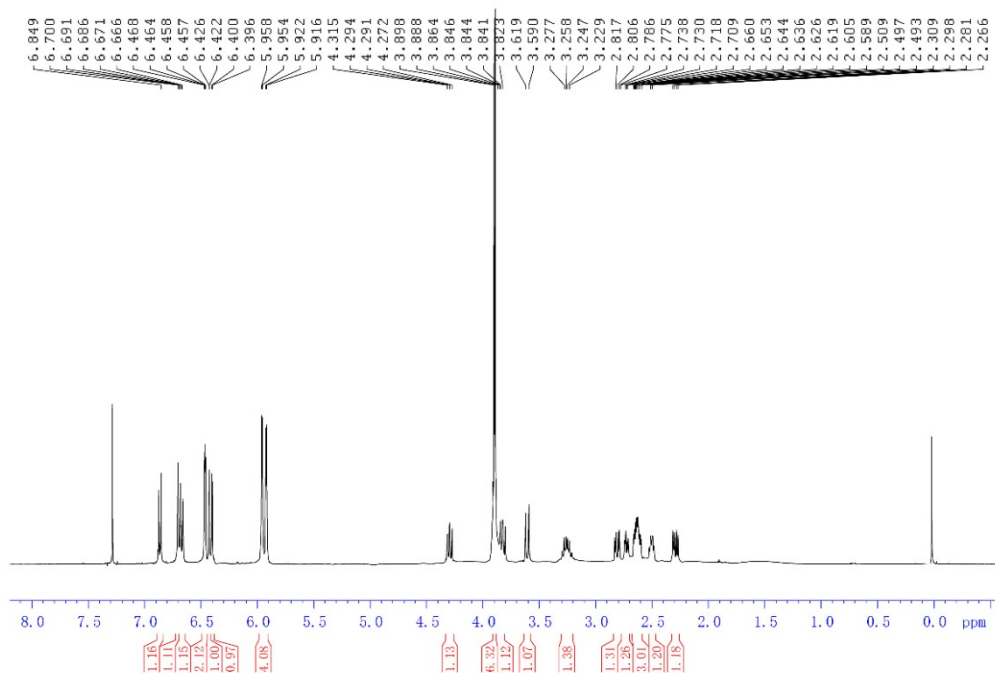
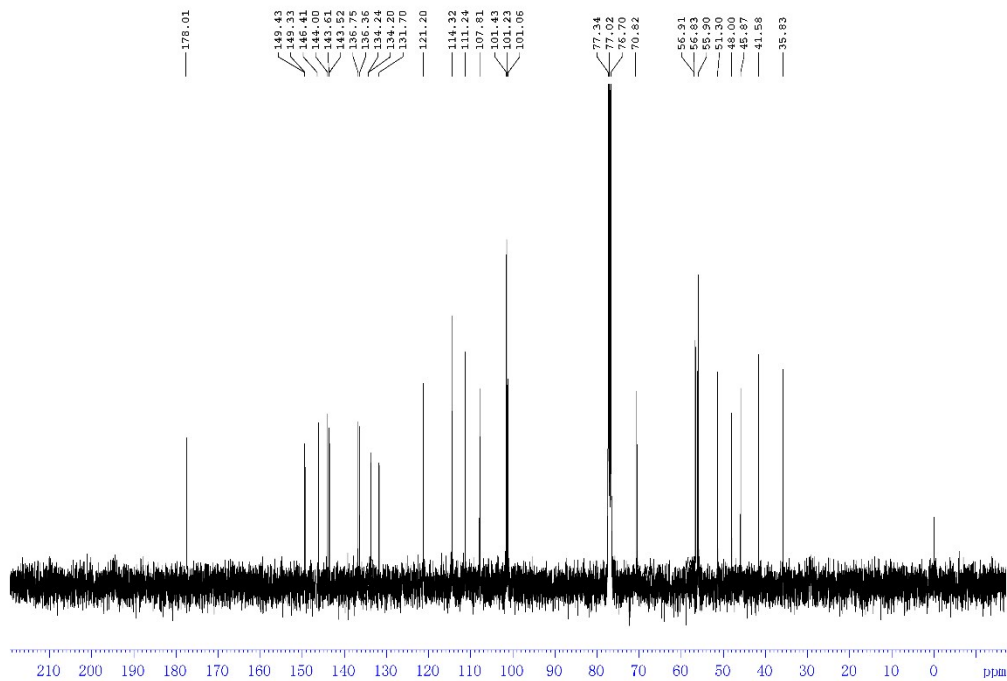


Figure S16. ¹H-NMR (16-a), ¹³C-NMR (16-b) and HR-ESI-MS (16-c) spectra of compound 17

17-a



17-b



17-c

Spectrum from DataSET114.wiff (sample 17) - pepAME-17, Experiment 1, +TOF MS (100 - 1000)

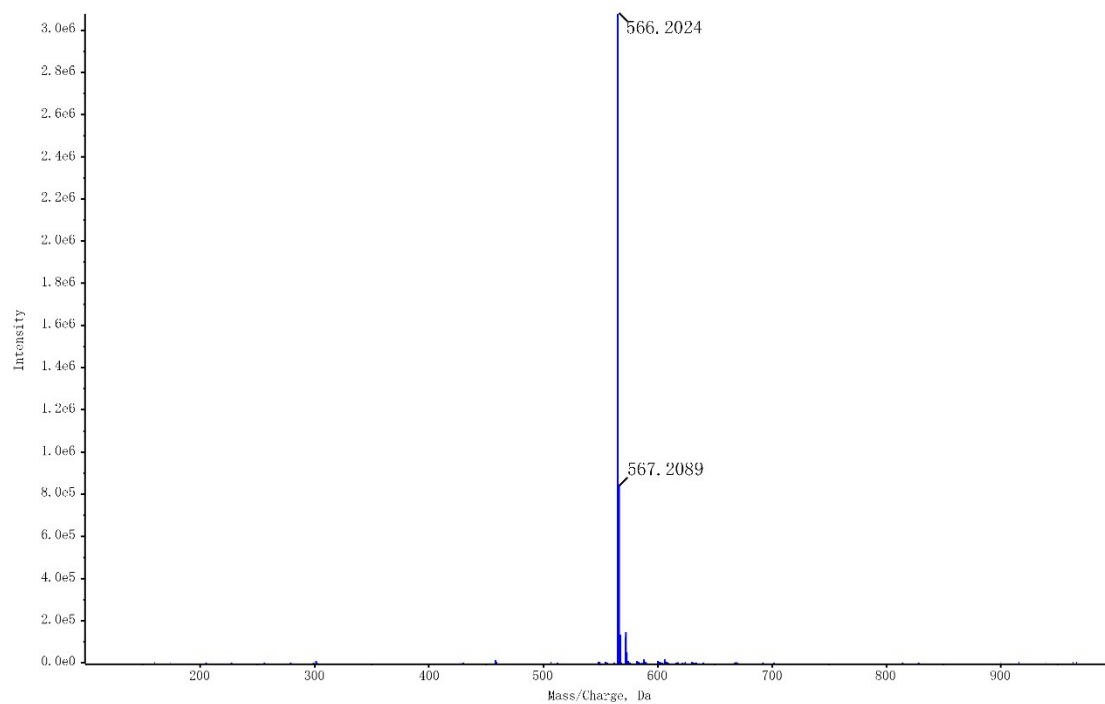
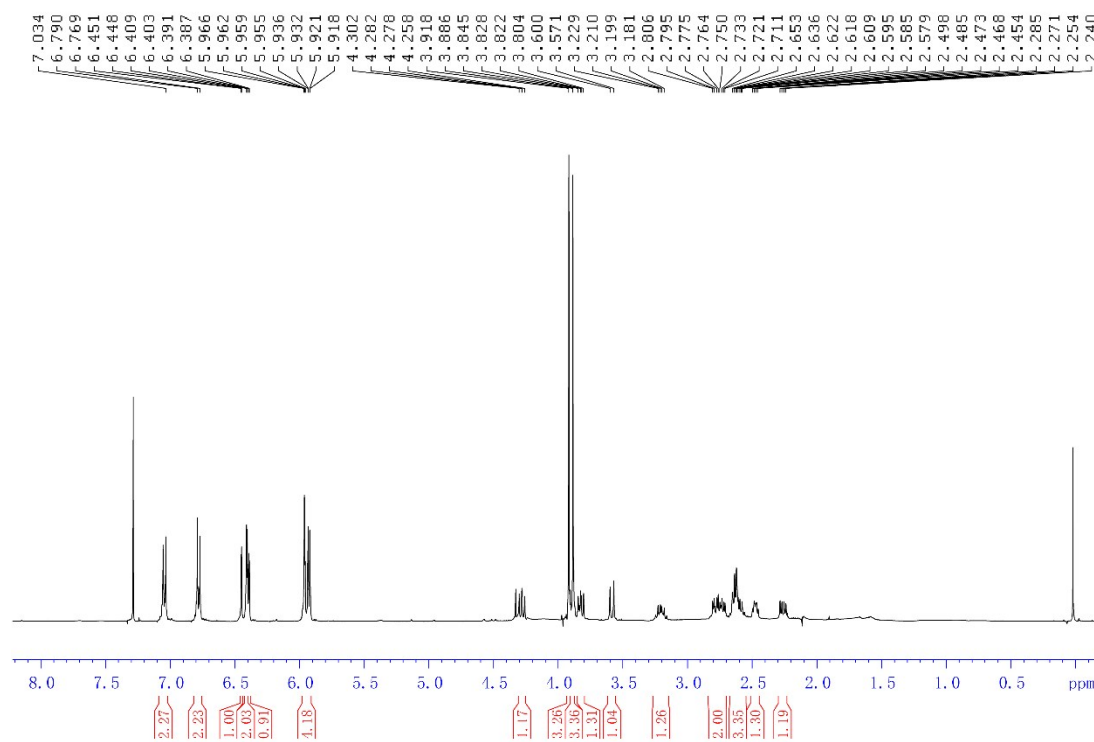
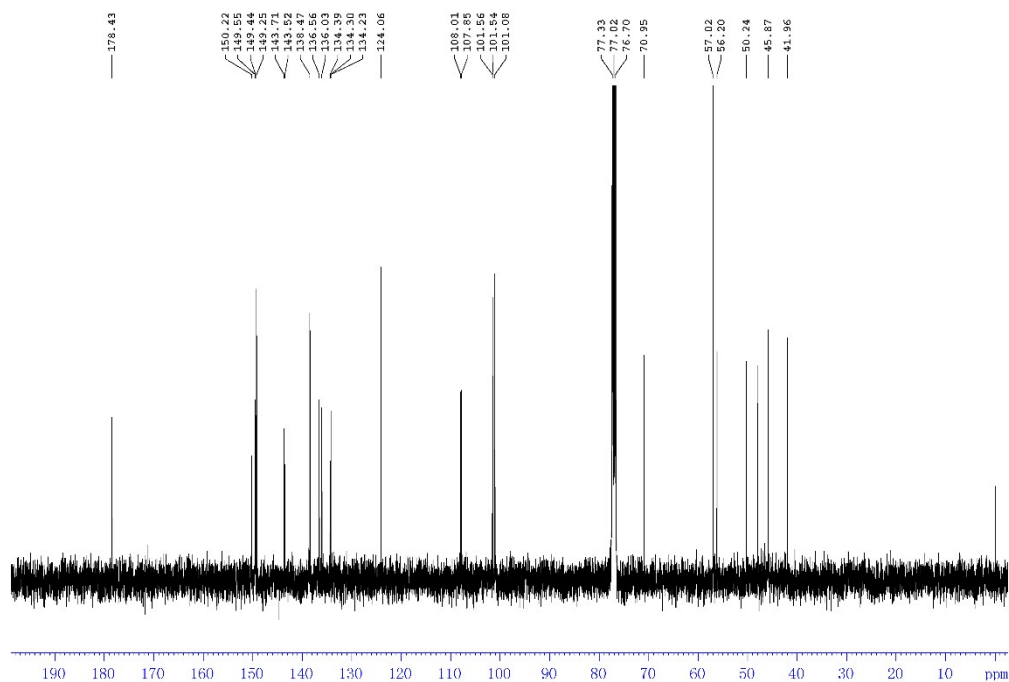


Figure S17. $^1\text{H-NMR}$ (17-a), $^{13}\text{C-NMR}$ (17-b) and HR-ESI-MS (17-c) spectra of compound 18

18-a



18-b



18-c

Spectrum from DataSET114.wiff (sample 18) - pepAME-18, Experiment 1, +TOF MS (100 - 1000)

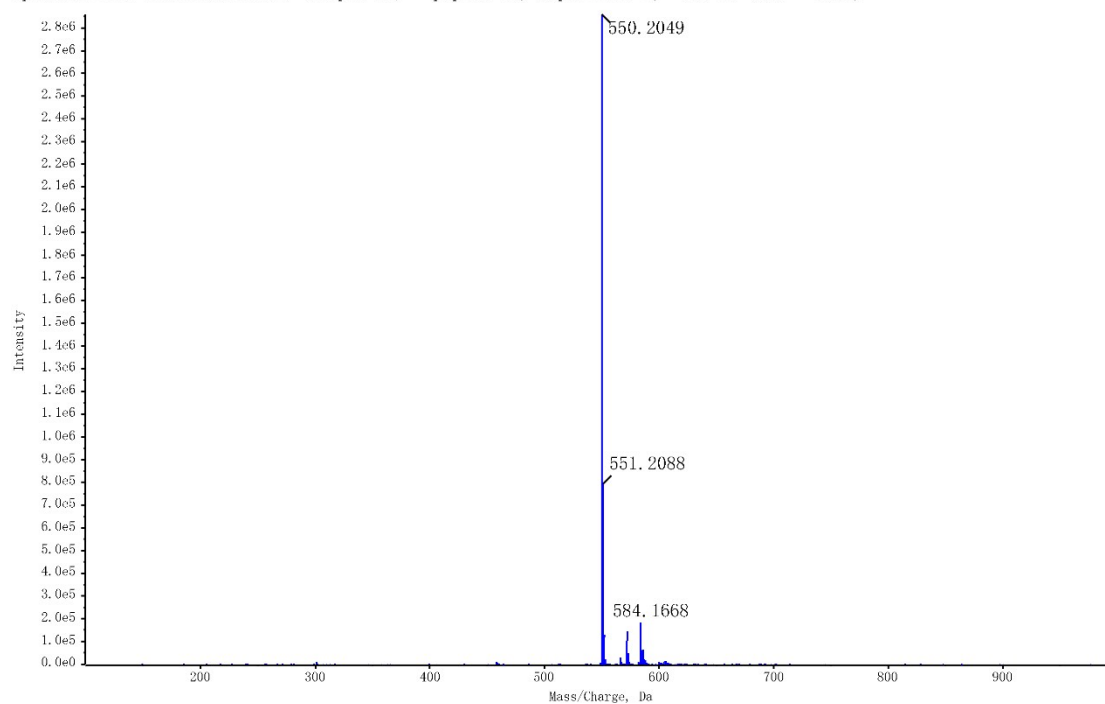


Figure S18. ^1H -NMR (18-a), ^{13}C -NMR (18-b) and HR-ESI-MS (18-c) spectra of compound 19

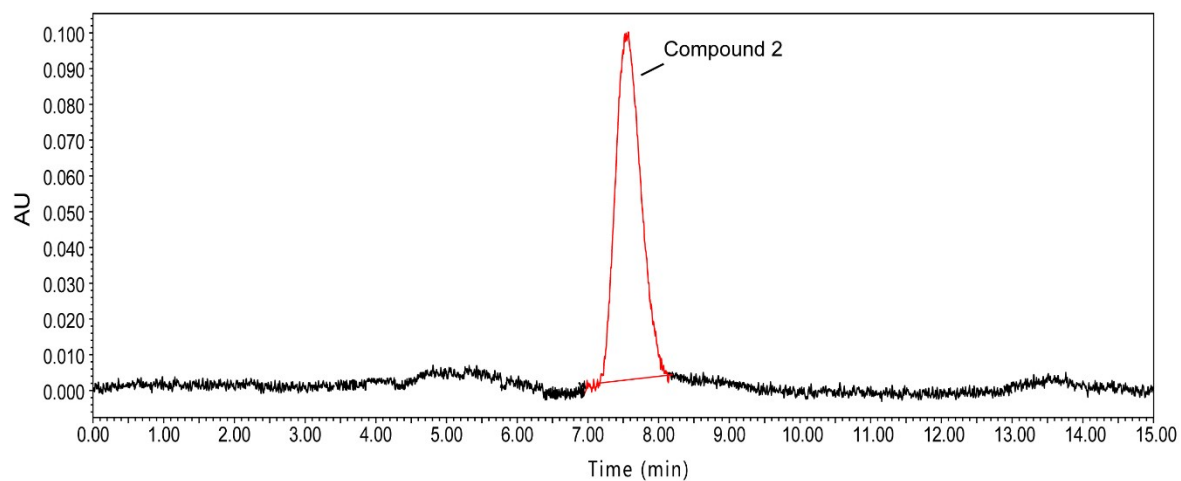


Figure S19. Purity test of compound 2 by HPLC ($\lambda=210$ nm)

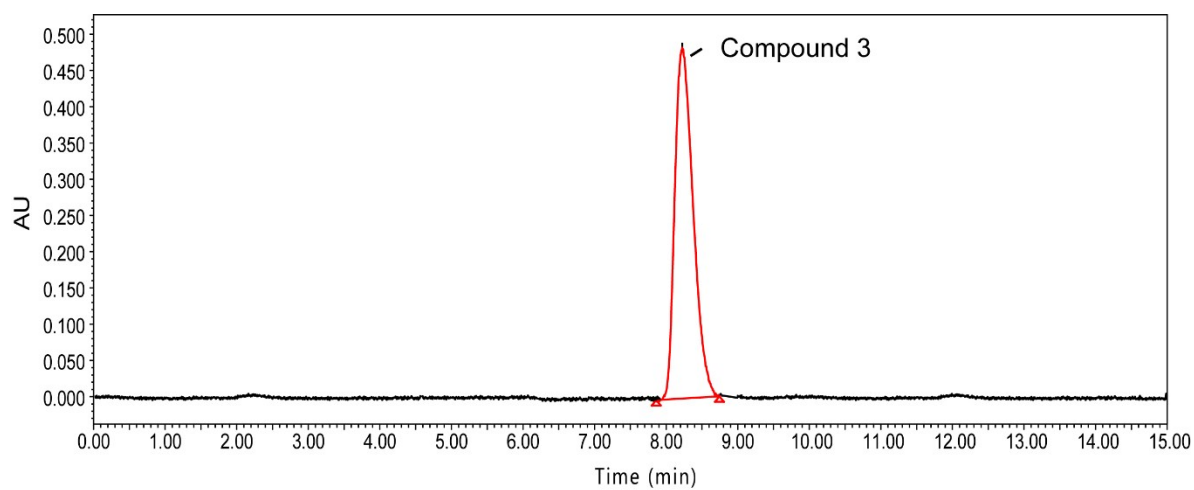


Figure S20. Purity test of compound 3 by HPLC ($\lambda=210$ nm)

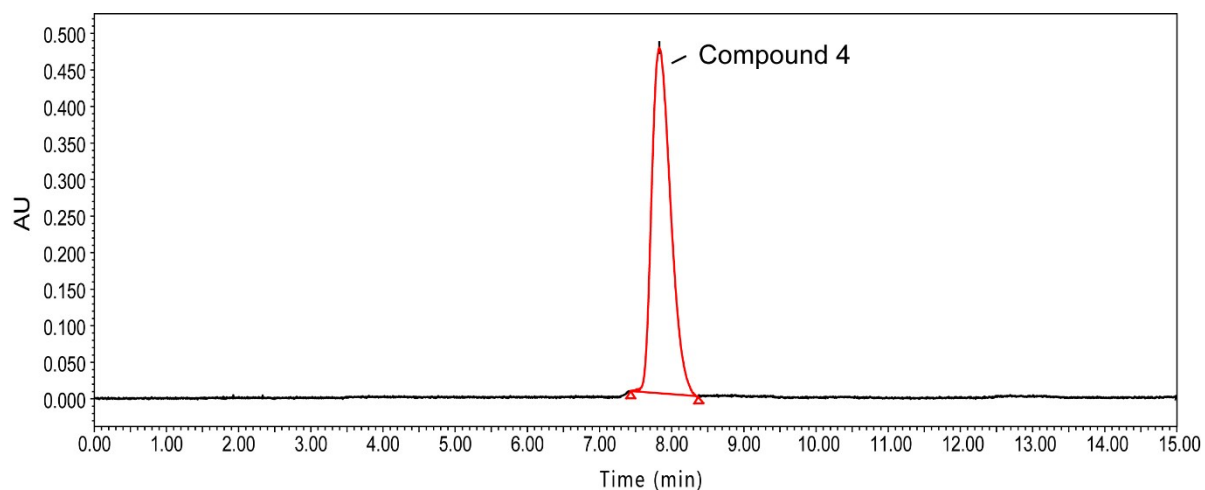


Figure S21. Purity test of compound 4 by HPLC ($\lambda=210$ nm)

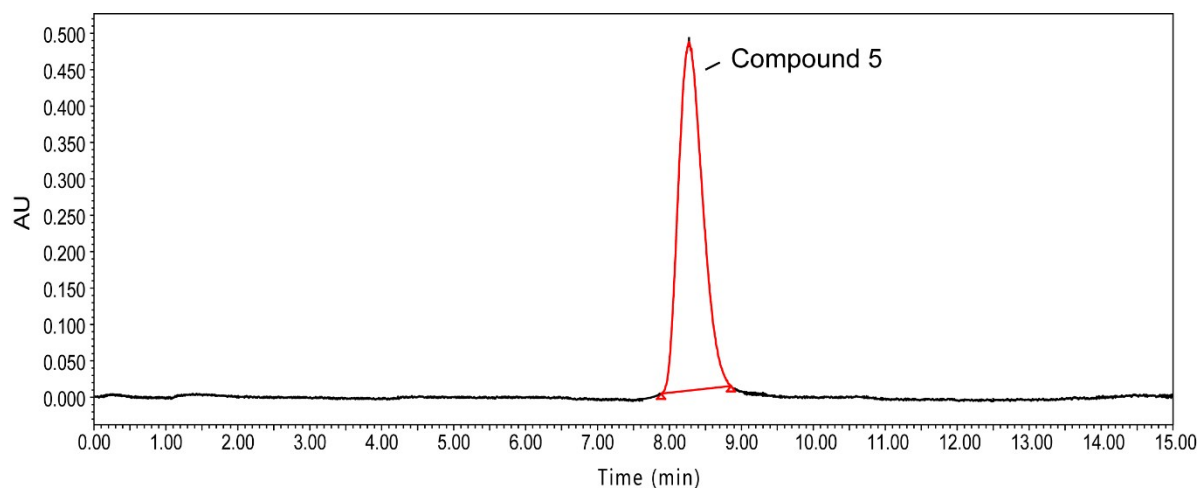


Figure S22. Purity test of compound 5 by HPLC ($\lambda=210$ nm)

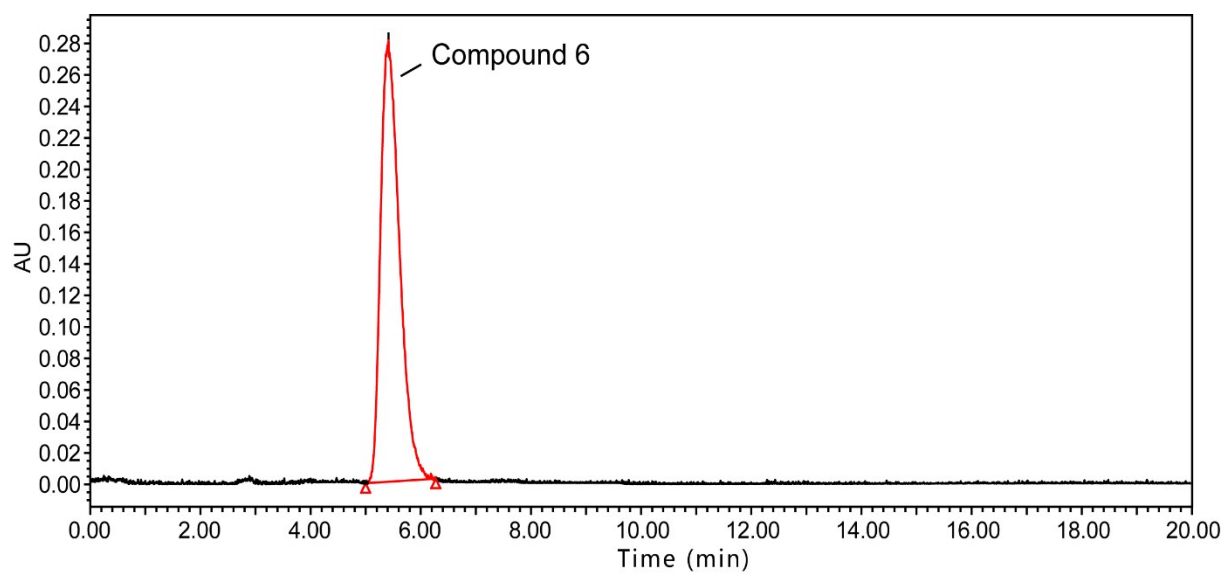


Figure S23. Purity test of compound 6 by HPLC ($\lambda=210$ nm)

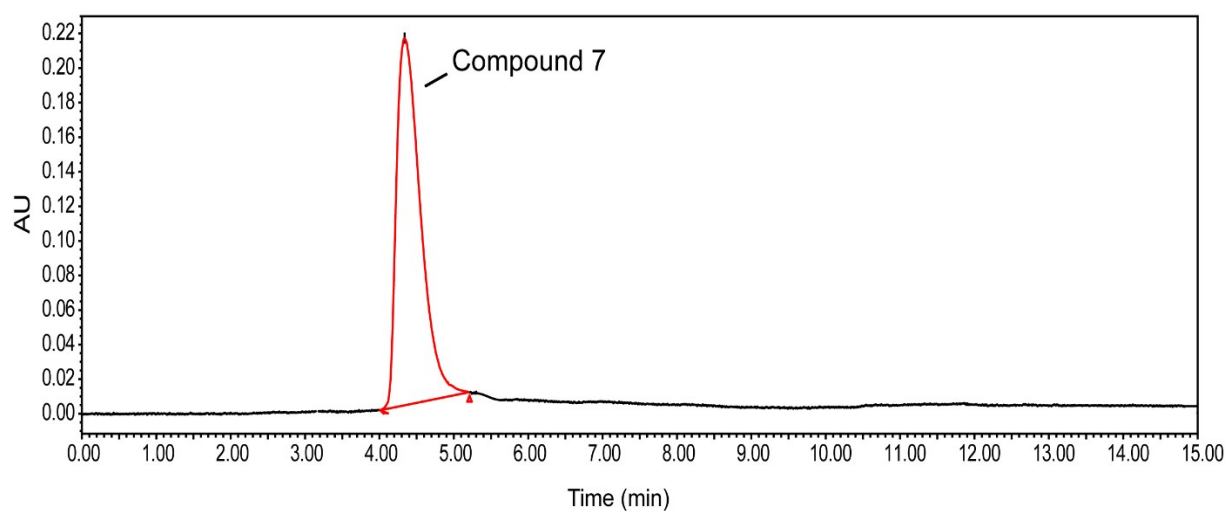


Figure S24. Purity test of compound 7 by HPLC ($\lambda=210$ nm)

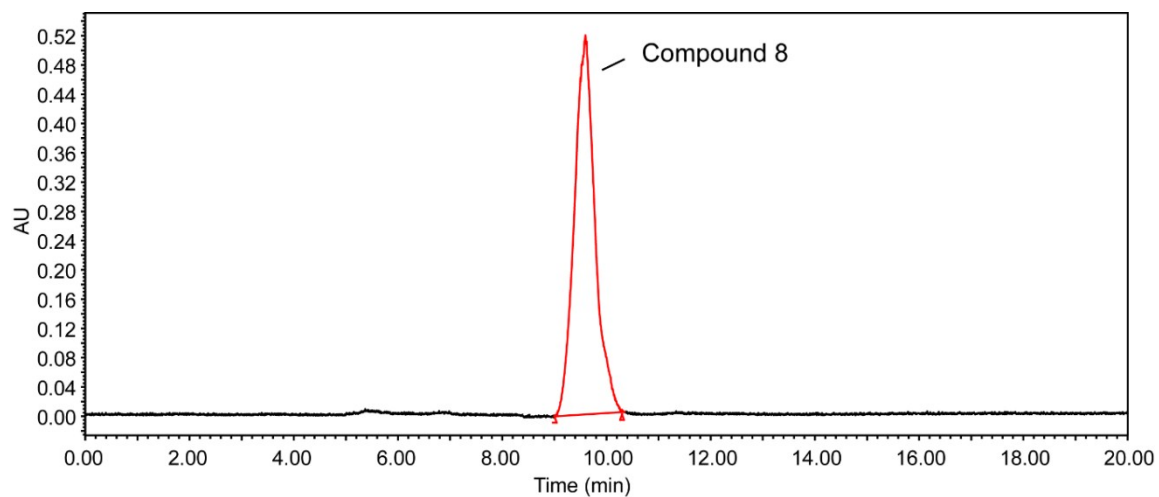


Figure S25. Purity test of compound 8 by HPLC ($\lambda=210$ nm)

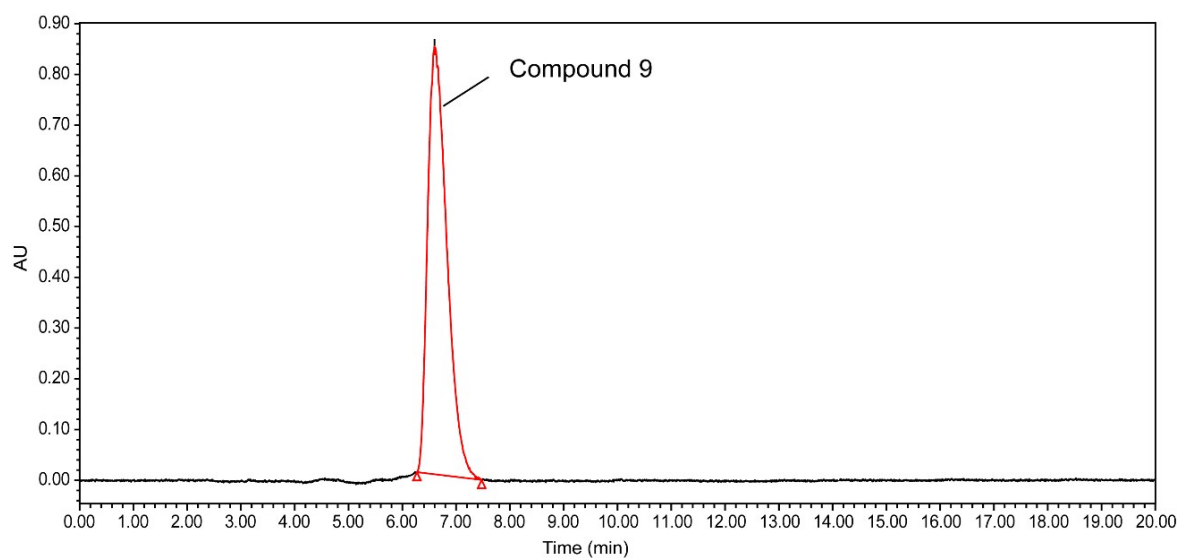


Figure S26. Purity test of compound 9 by HPLC ($\lambda=210$ nm)

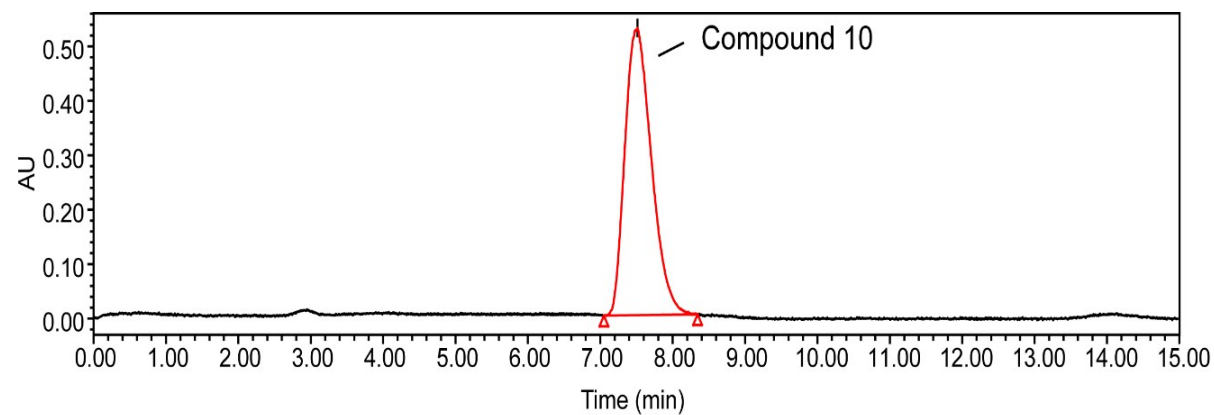


Figure S27. Purity test of compound 10 by HPLC ($\lambda=210$ nm)

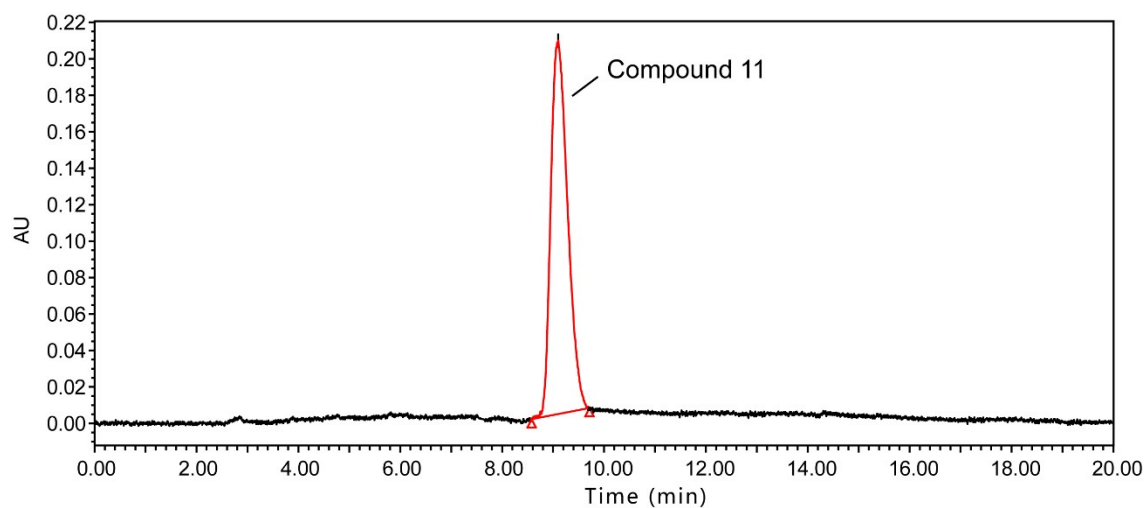


Figure S28. Purity test of compound 11 by HPLC ($\lambda=210$ nm)

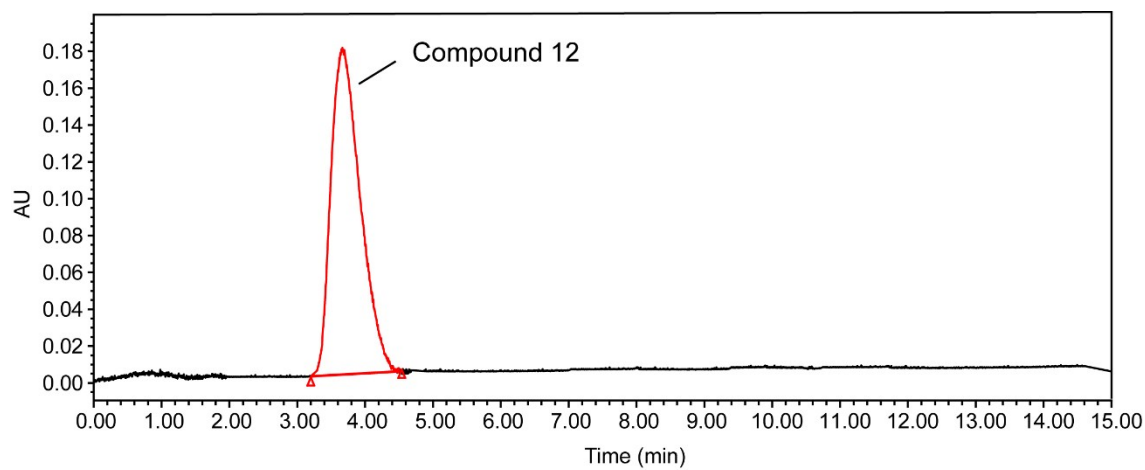


Figure S29. Purity test of compound 12 by HPLC ($\lambda=210$ nm)

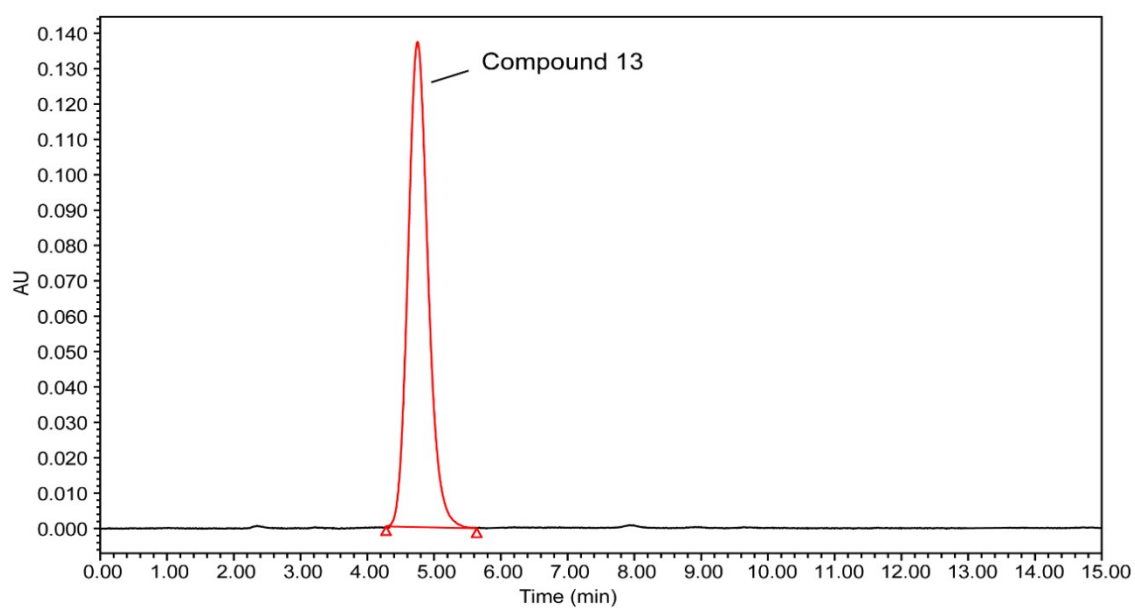


Figure S30. Purity test of compound 13 by HPLC ($\lambda=210$ nm)

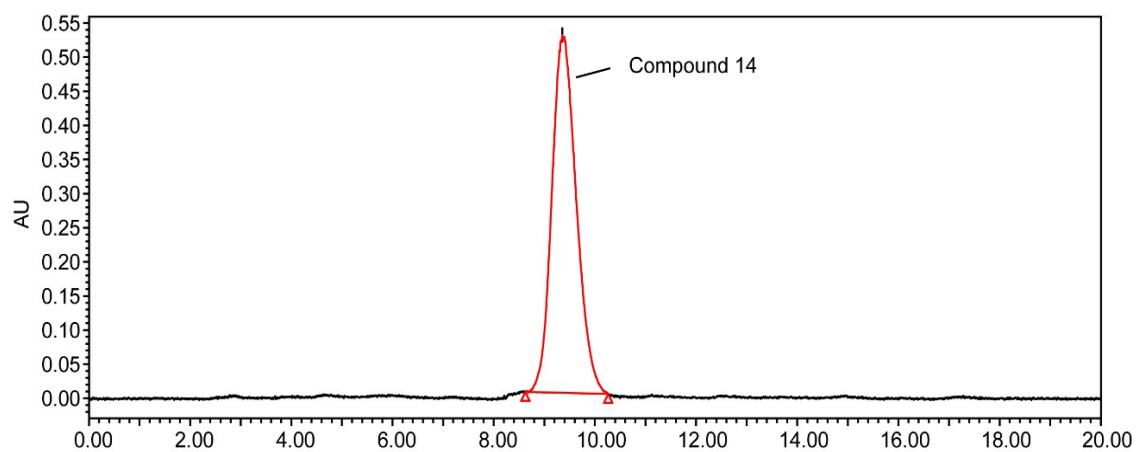


Figure S31. Purity test of compound 14 by HPLC ($\lambda=210$ nm)

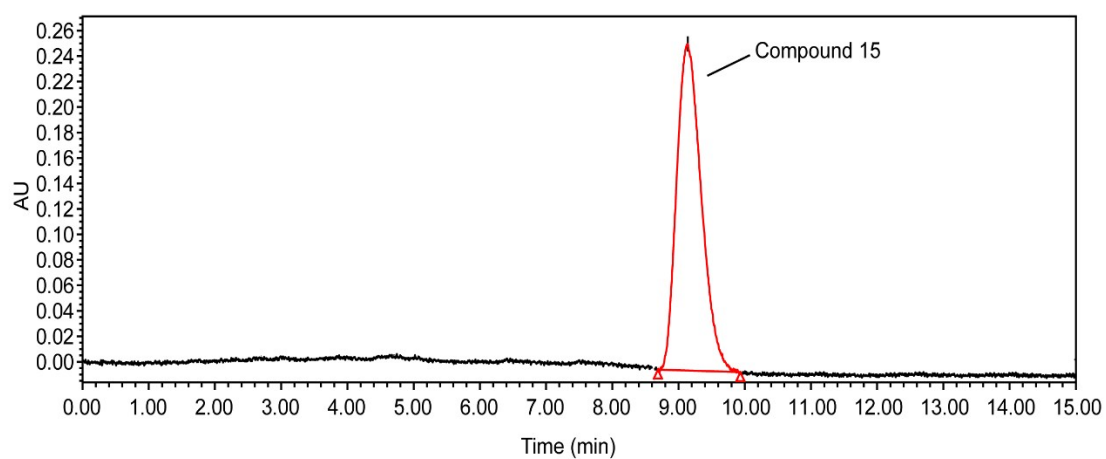


Figure S32. Purity test of compound 15 by HPLC ($\lambda=210$ nm)

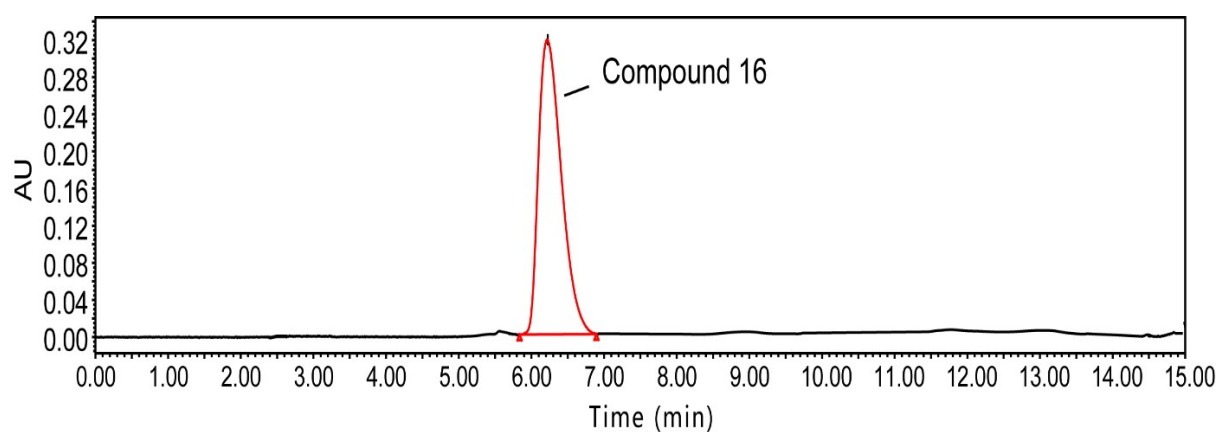


Figure S33. Purity test of compound 16 by HPLC ($\lambda=210$ nm)

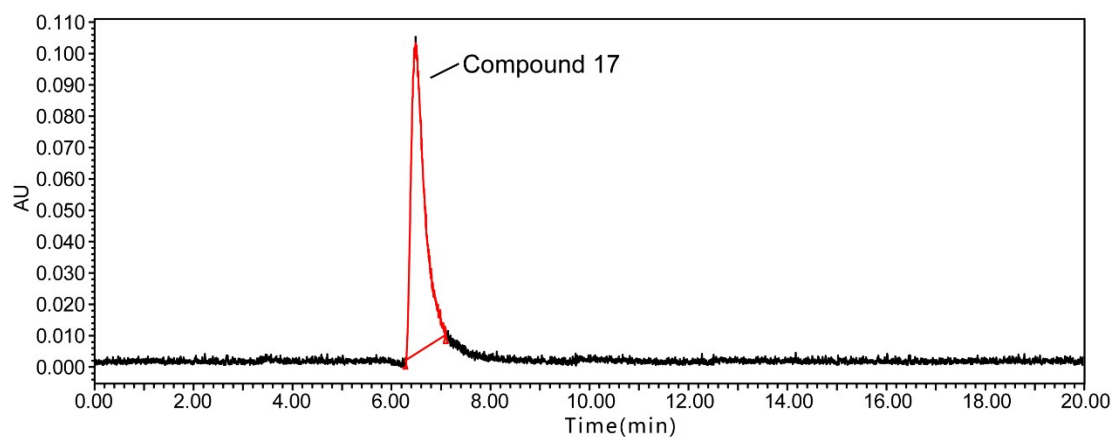


Figure S34. Purity test of compound 17 by HPLC ($\lambda=210$ nm)

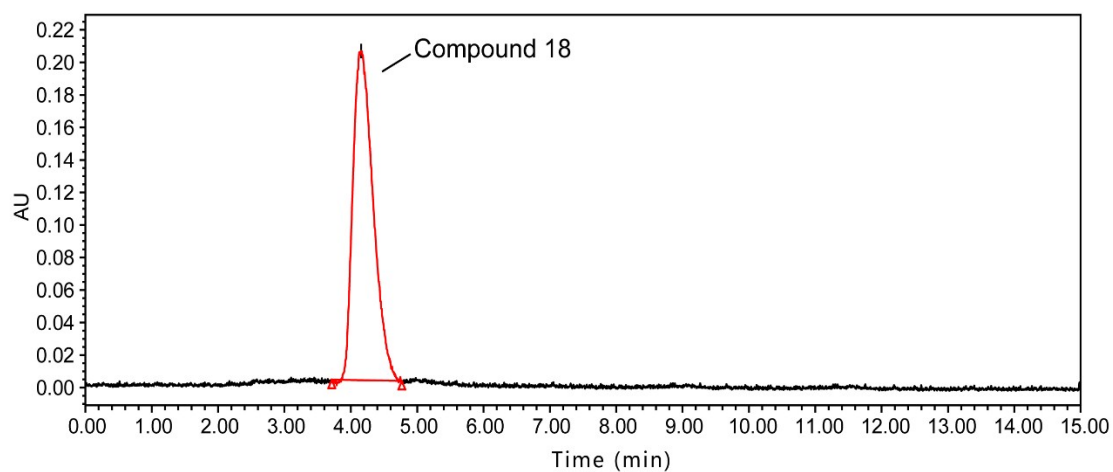


Figure S35. Purity test of compound 18 by HPLC ($\lambda=210$ nm)

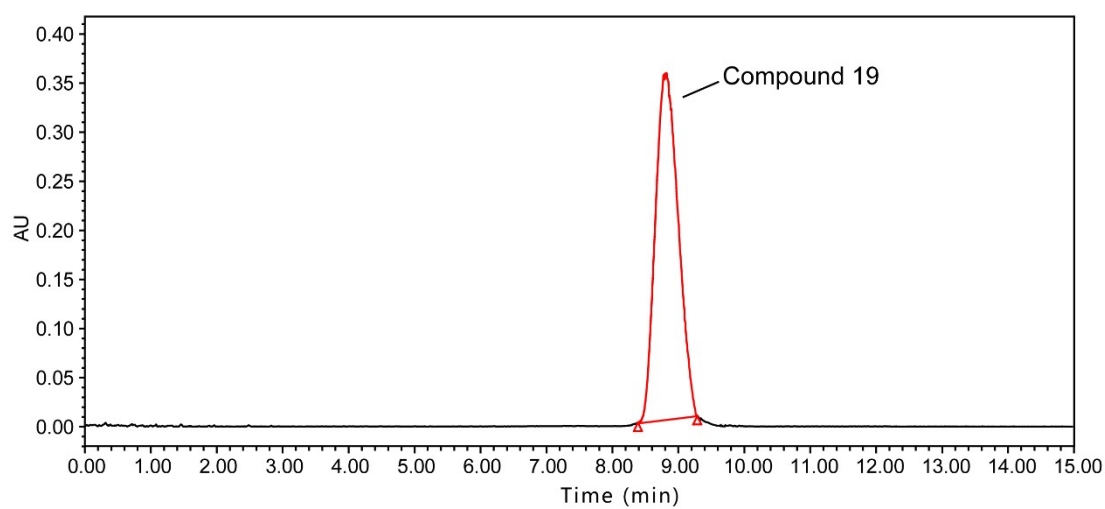


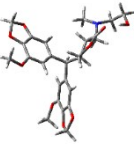
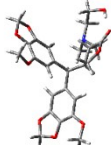
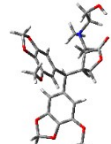
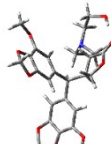
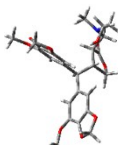
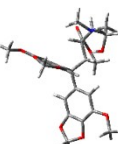
Figure S36. Purity test of compound 19 by HPLC ($\lambda=210$ nm)

Supplementary Information I (Tables)

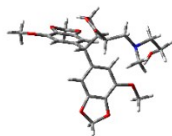
Table S1. Energies of the dominative conformers of **6** at MMFF94 force field.

Configuration	Conformer	Energy (kcal/mol)	Population (%)
a	1	110.44	67.51
	2	111.18	19.18
	3	111.77	7.16
	4	112.40	2.47
b	1	98.01	82.94
	2	99.53	6.35
	3	99.67	5.07

Table S2. Energies of the conformers of **6** at B3LYP/6-311G** in methanol.

Configuration	Conformation	Structure	E (Hartree)	E (kcal/mol)	Population (%)
a	1		-1702.250555	-1068178.34	96.57
	2		-1702.246519	-1068175.81	1.34
	3		-1702.243212	-1068173.73	0.04
	4		-1702.246924	-1068176.06	2.05
b	1		-1702.254118	-1068180.58	5.54
	2		-1702.254164	-1068180.61	5.82

3



-1702.256079 -1068181.81 44.32

Table S3. the parameters of σ and UV-shift for each configuration of **6**

Configuration	UV-shift value (nm)	σ - shift value (eV)
a	0.36	10
b	0.36	-1