
Discovery of Novel pleuromutilin derivatives as potent antibacterial agents for the treatment of MRSA infection

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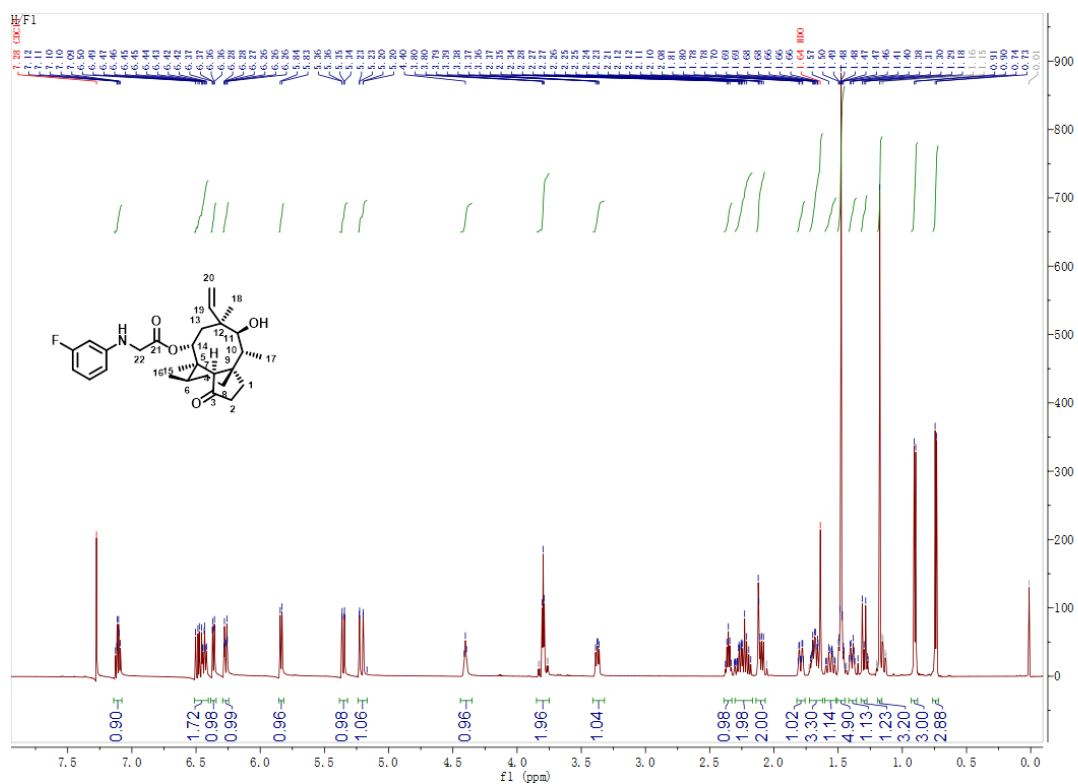


Figure SI 1-1. ¹H-NMR spectrum (CDCl₃, 400MHz) of compound **8**.

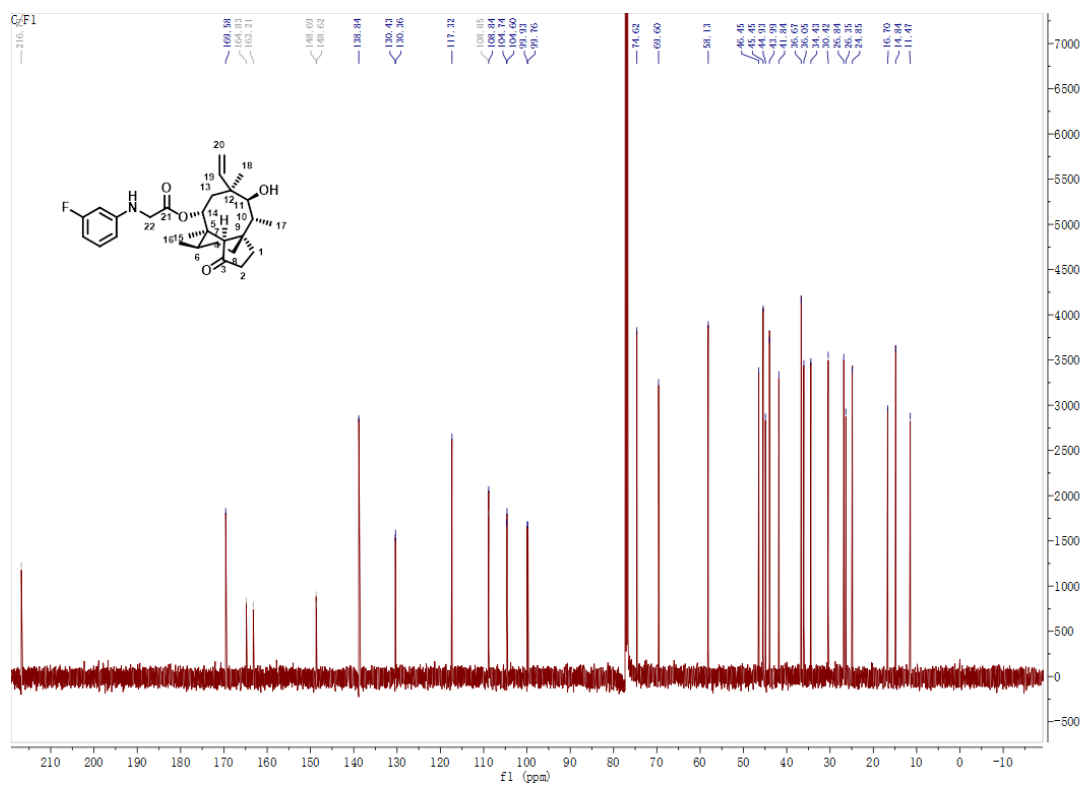


Figure SI 1-2. ¹³C-NMR spectrum (CDCl₃, 101MHz) of compound **8**.

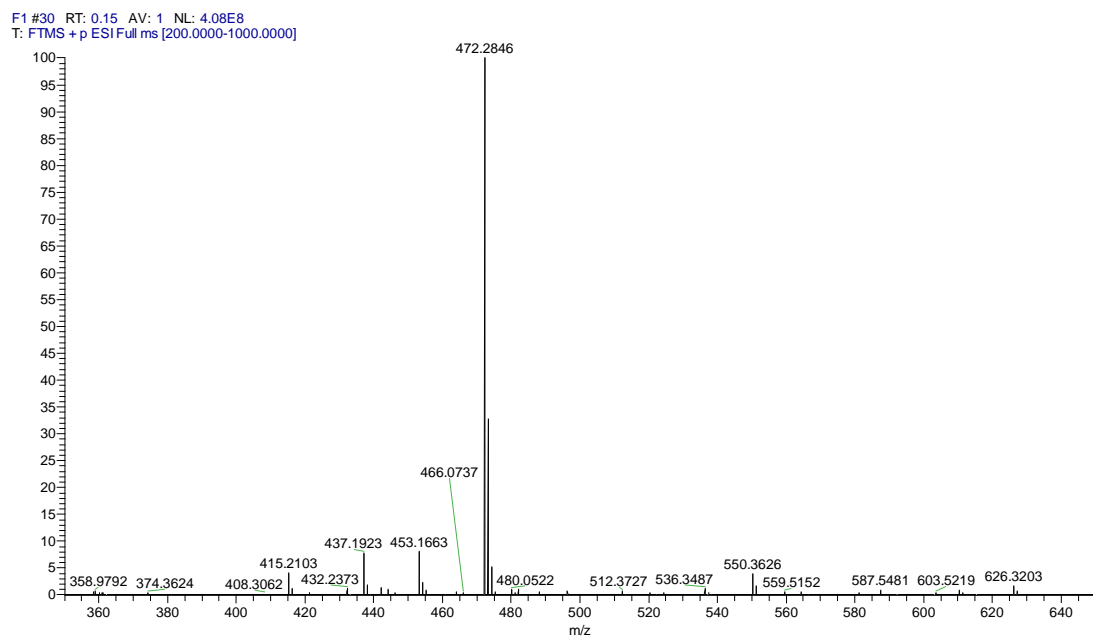


Figure SI 1-3. HR Mass spectrum (ESI) of compound 8.

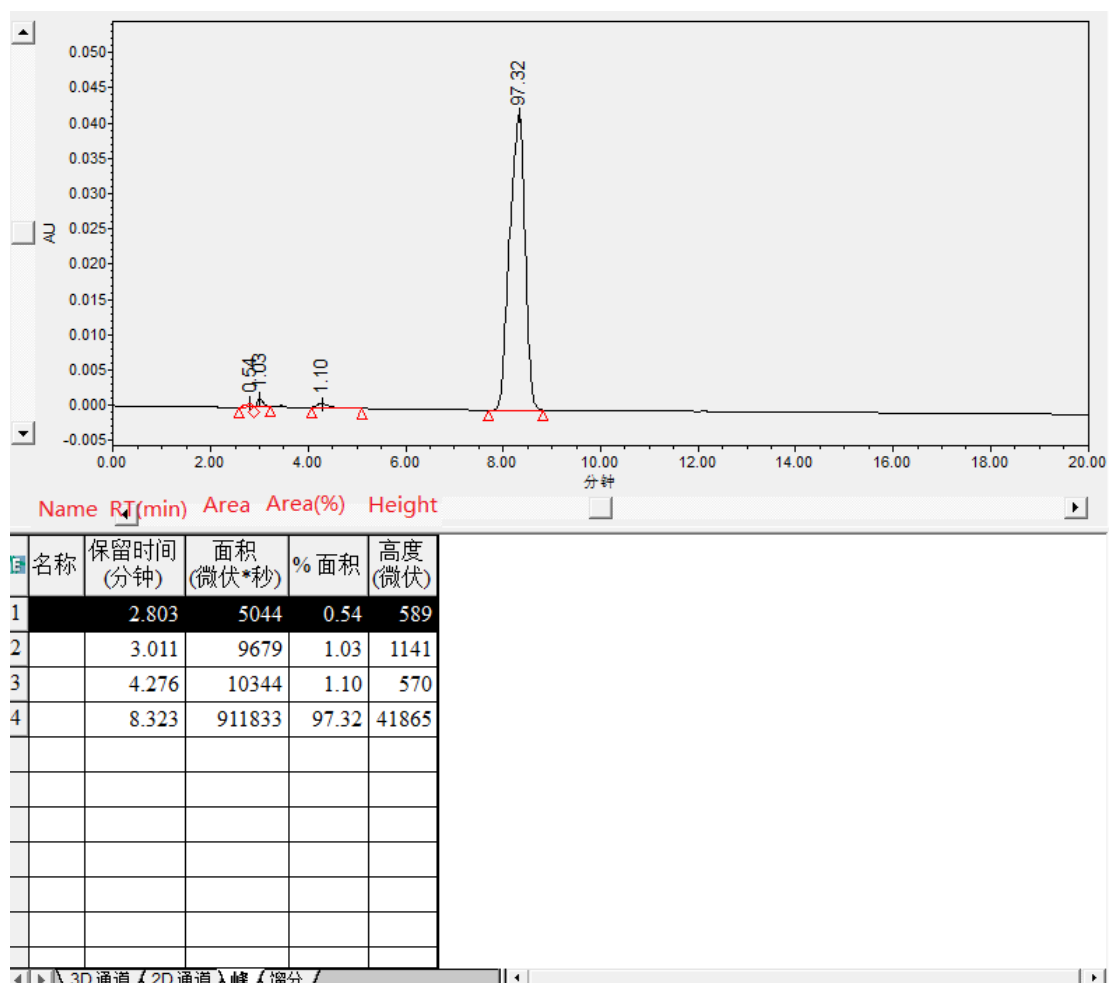


Figure SI 1-4. HPLC of compound 8.

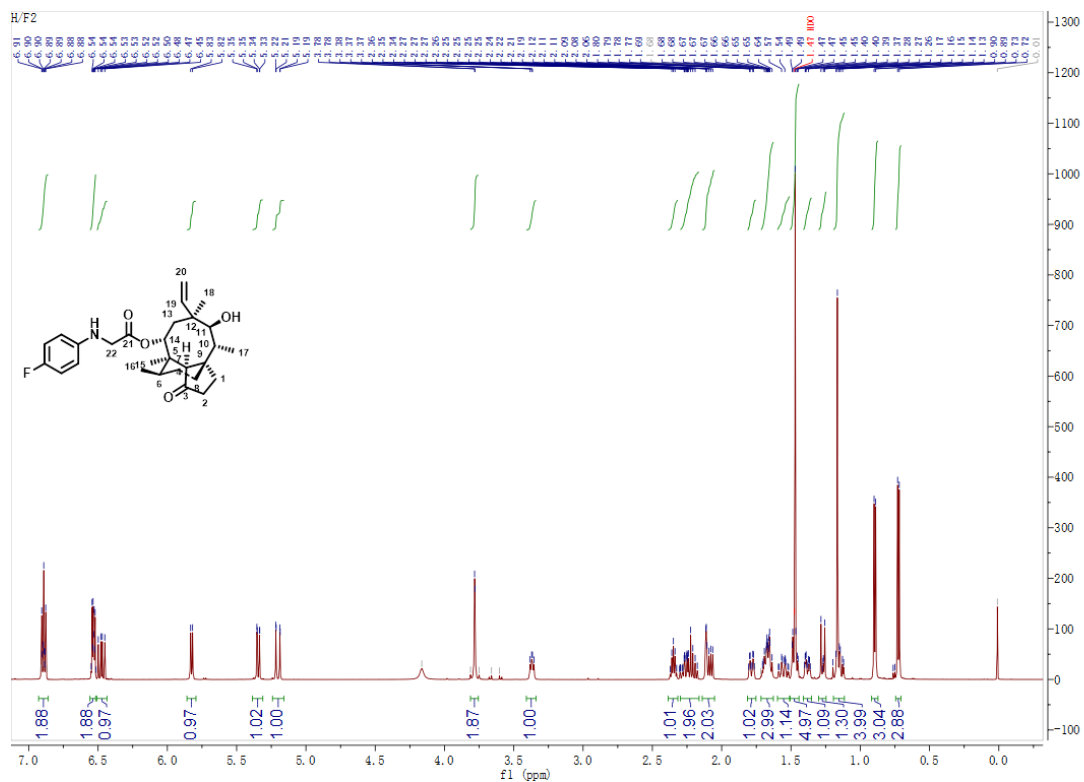


Figure SI 2-1. ^1H -NMR spectrum (CDCl_3 , 400MHz) of compound **9**.

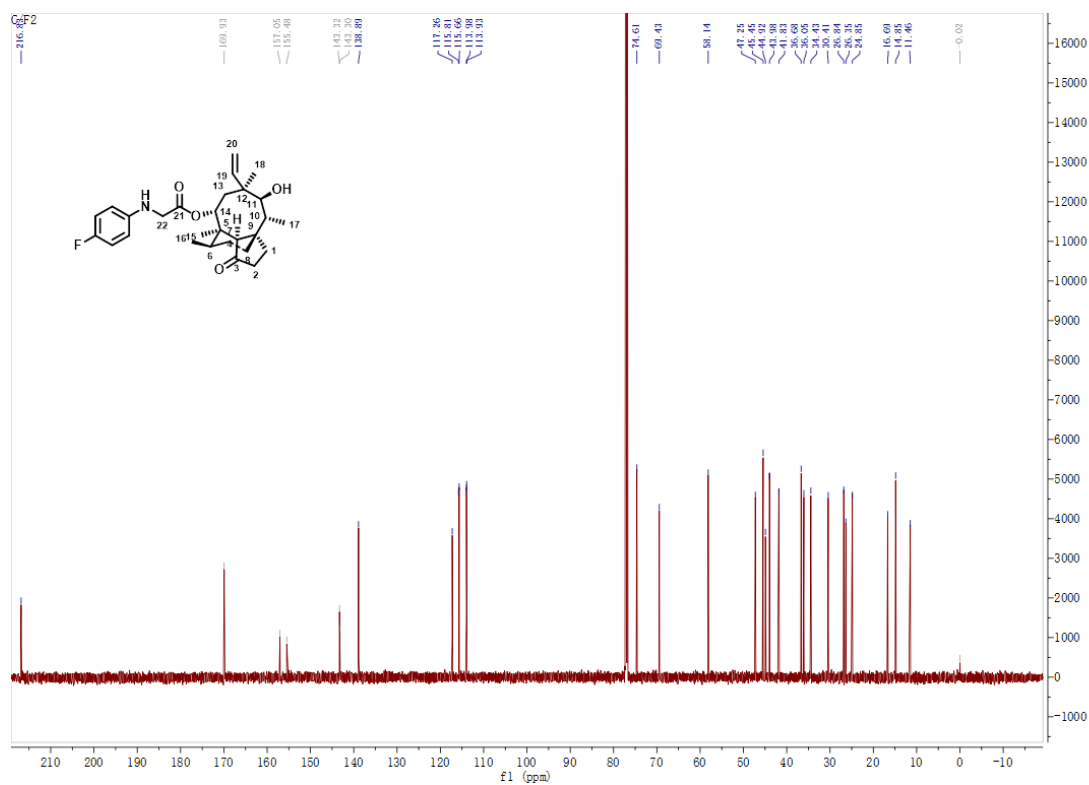


Figure SI 2-2. ^{13}C -NMR spectrum (CDCl_3 , 101MHz) of compound **9**.

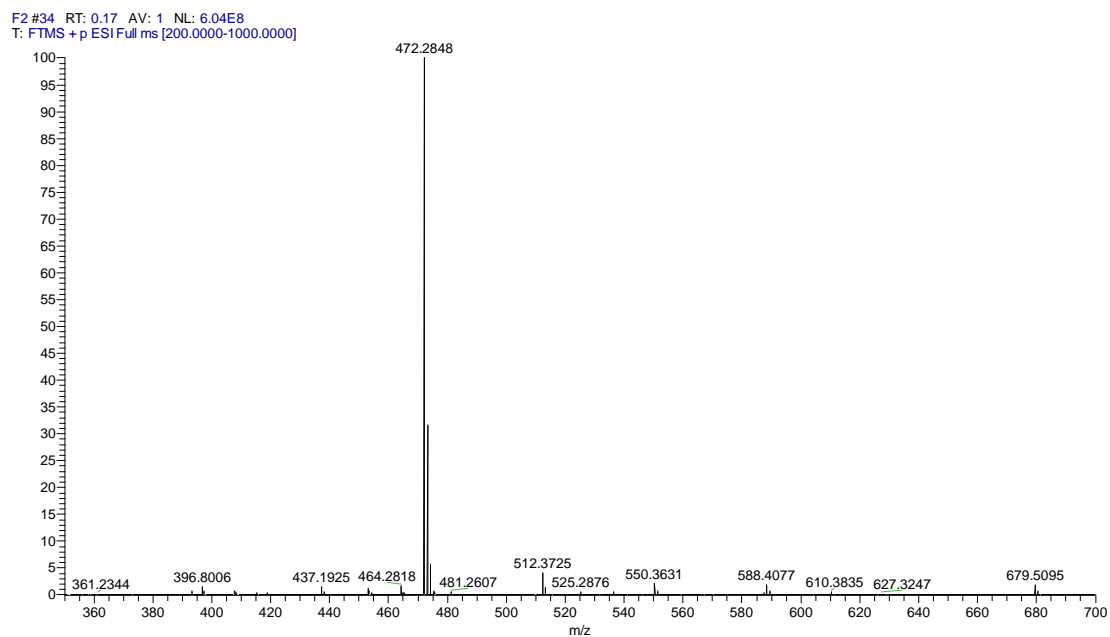


Figure SI 2-3. HR Mass spectrum (ESI) of compound 9.

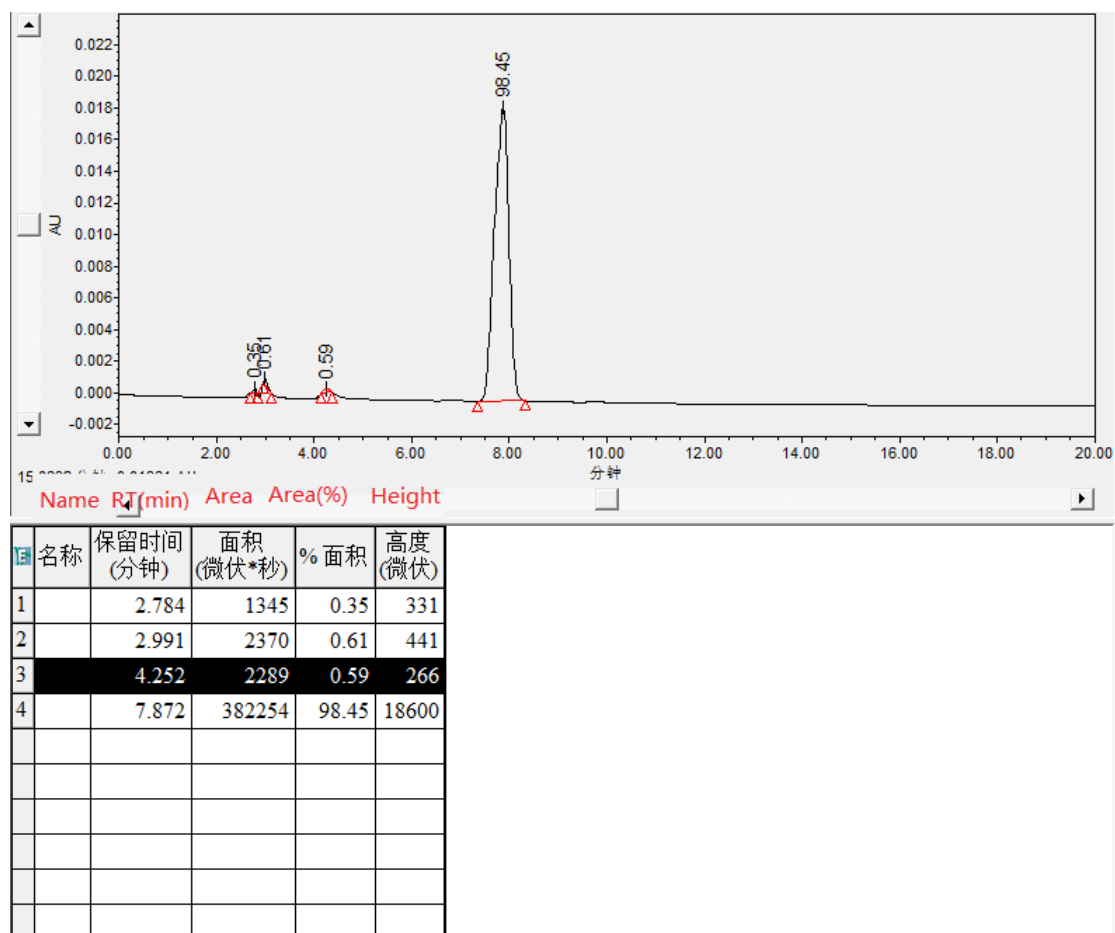


Figure SI 2-4. HPLC of compound 9.

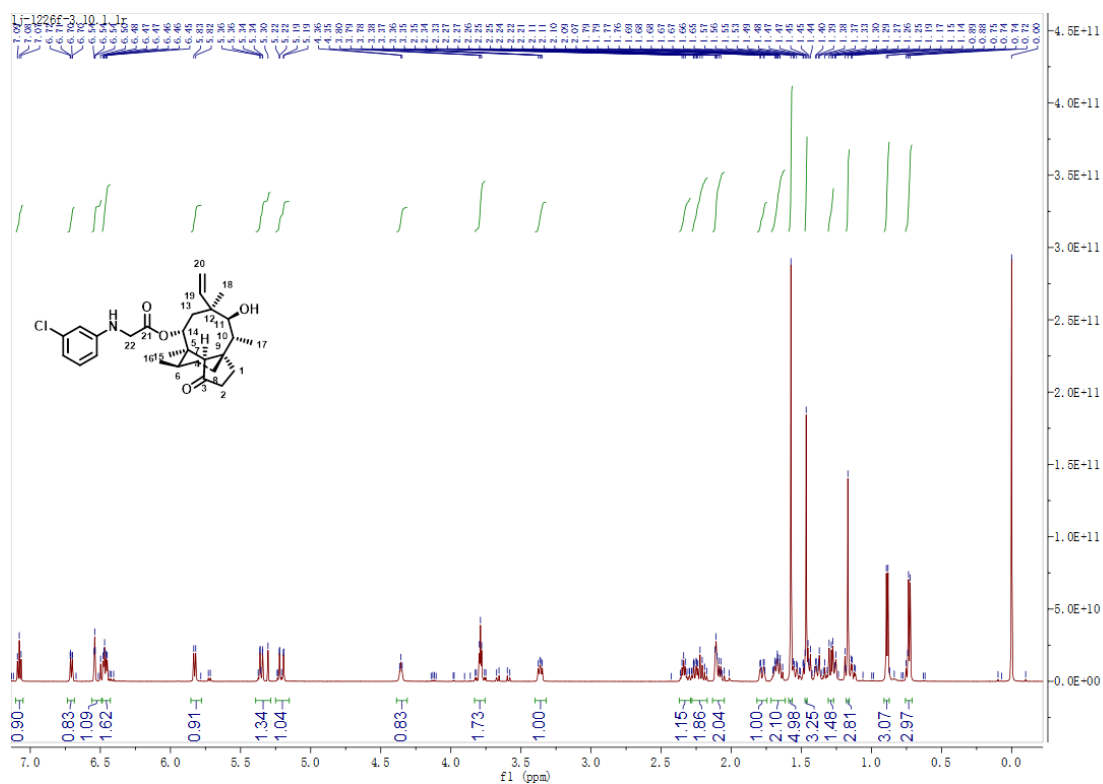


Figure SI 3-1. ^1H -NMR spectrum (CDCl₃, 400MHz) of compound 10.

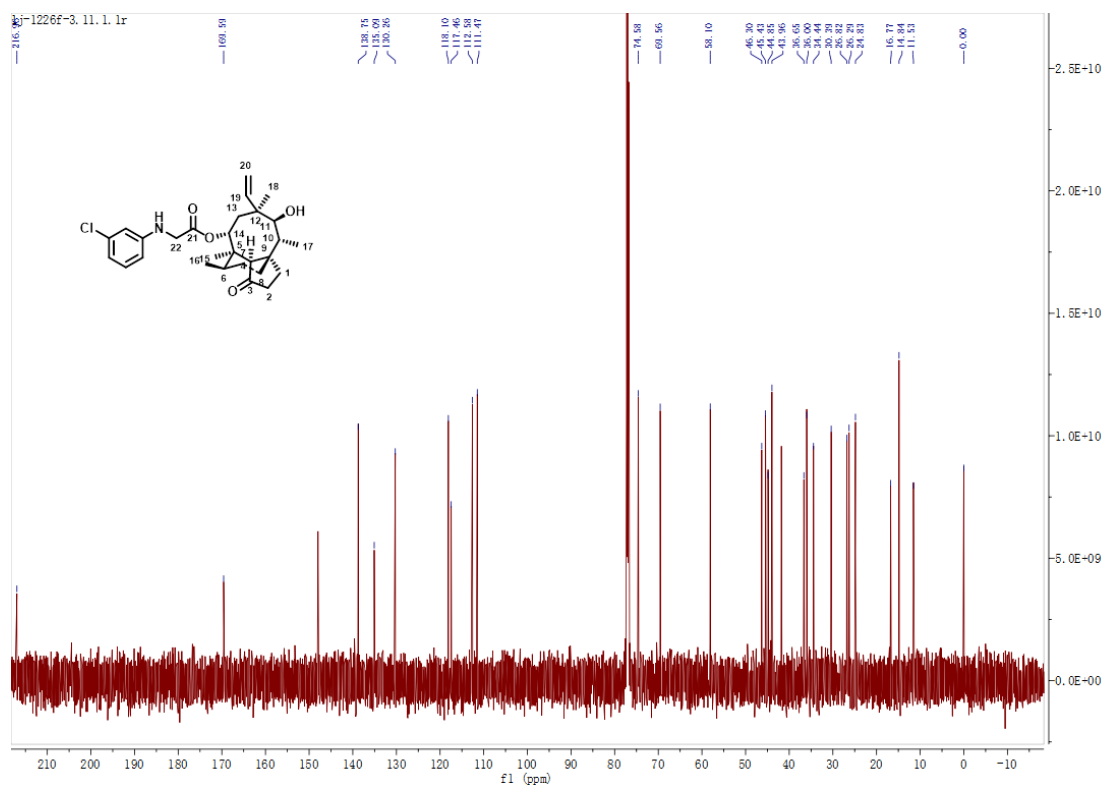


Figure SI 3-2. ^{13}C -NMR spectrum (CDCl₃, 101MHz) of compound 10.

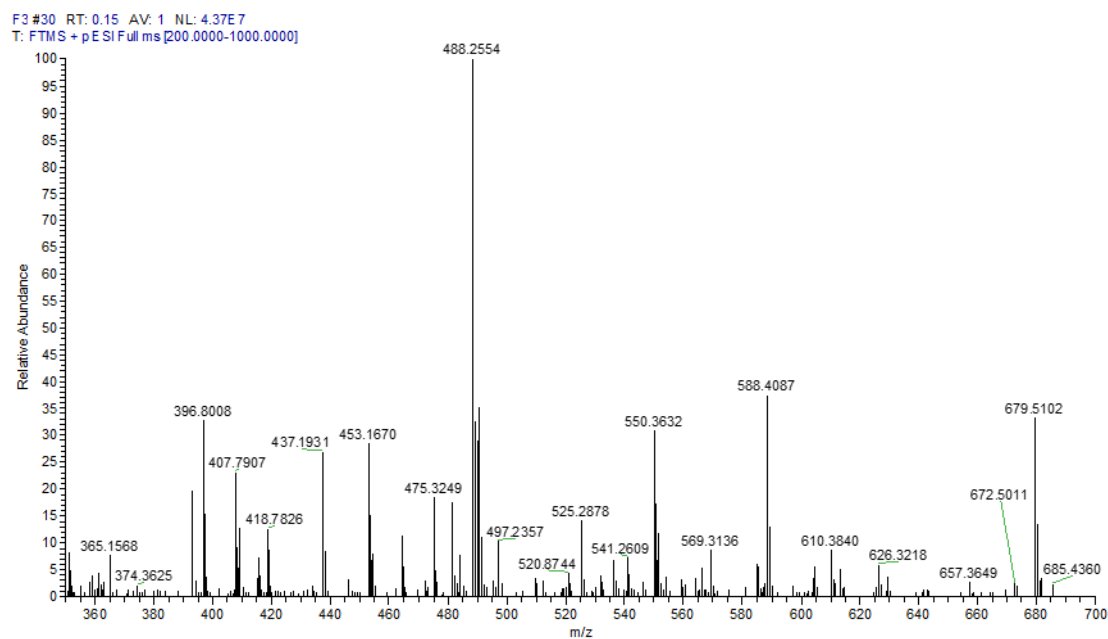


Figure SI 3-3. HR Mass spectrum (ESI) of compound 10.

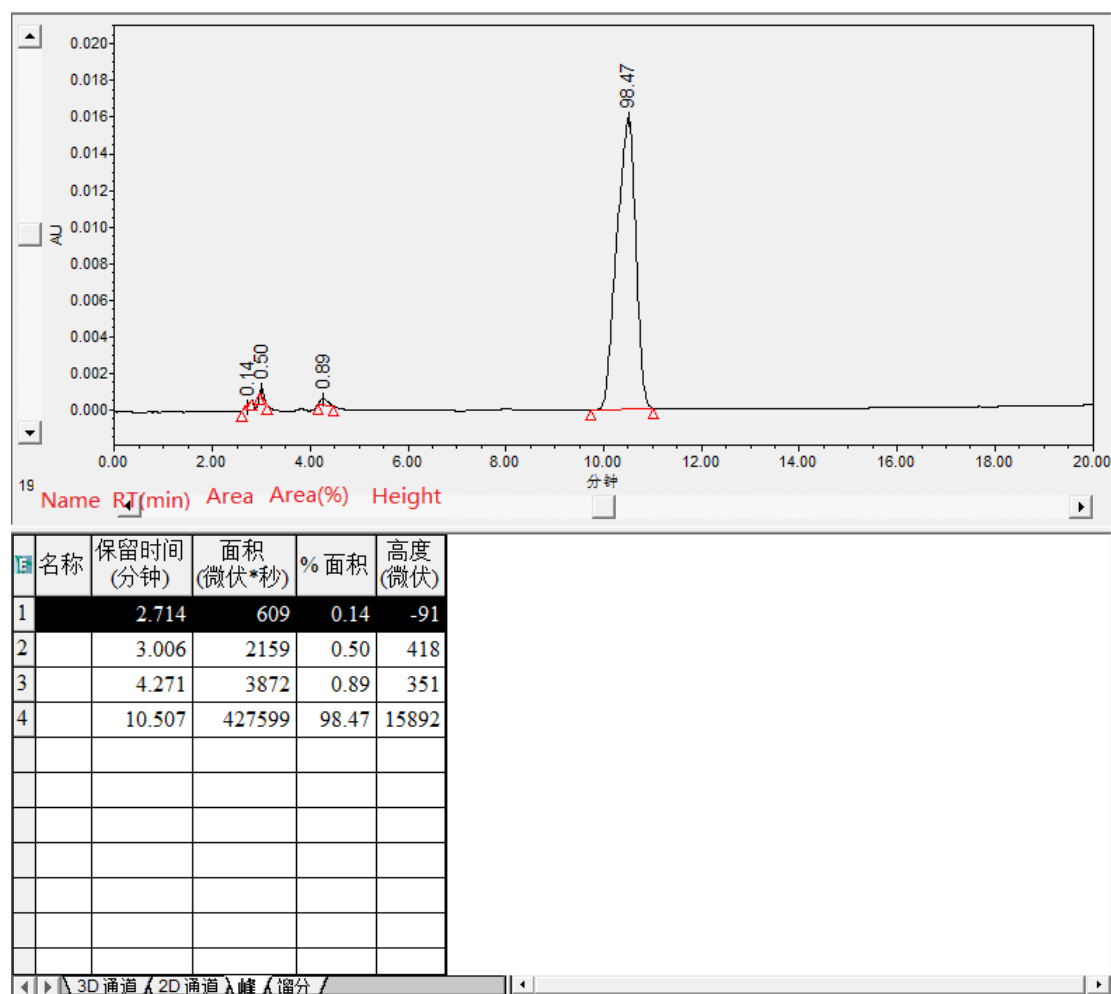


Figure SI 3-4. HPLC of compound 10.

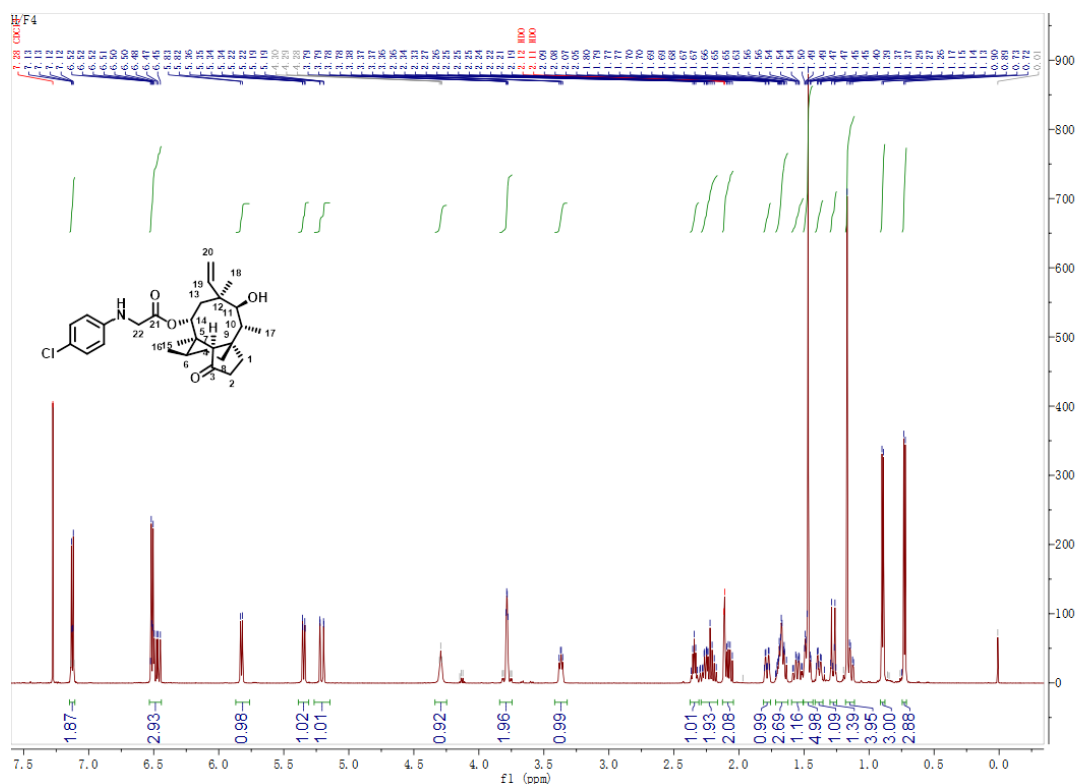


Figure SI 4-1. ¹H-NMR spectrum (CDCl₃, 400MHz) of compound 11.

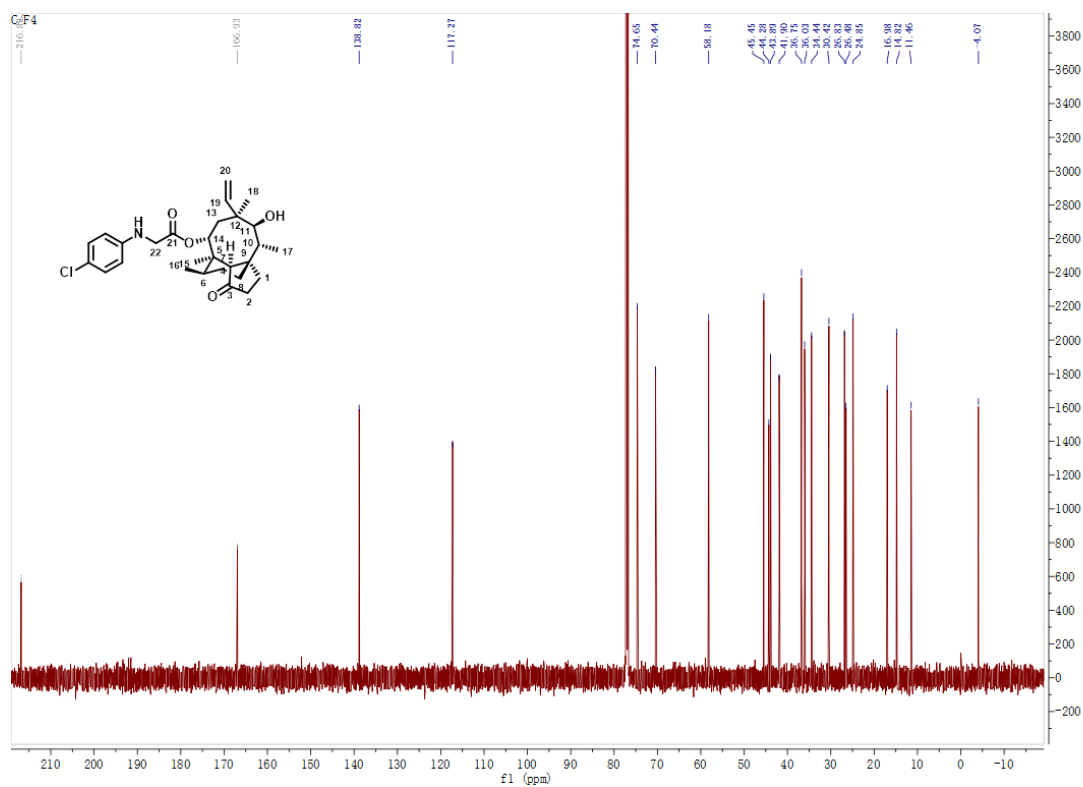


Figure SI 4-2. ¹³C-NMR spectrum (CDCl₃, 101MHz) of compound 11.

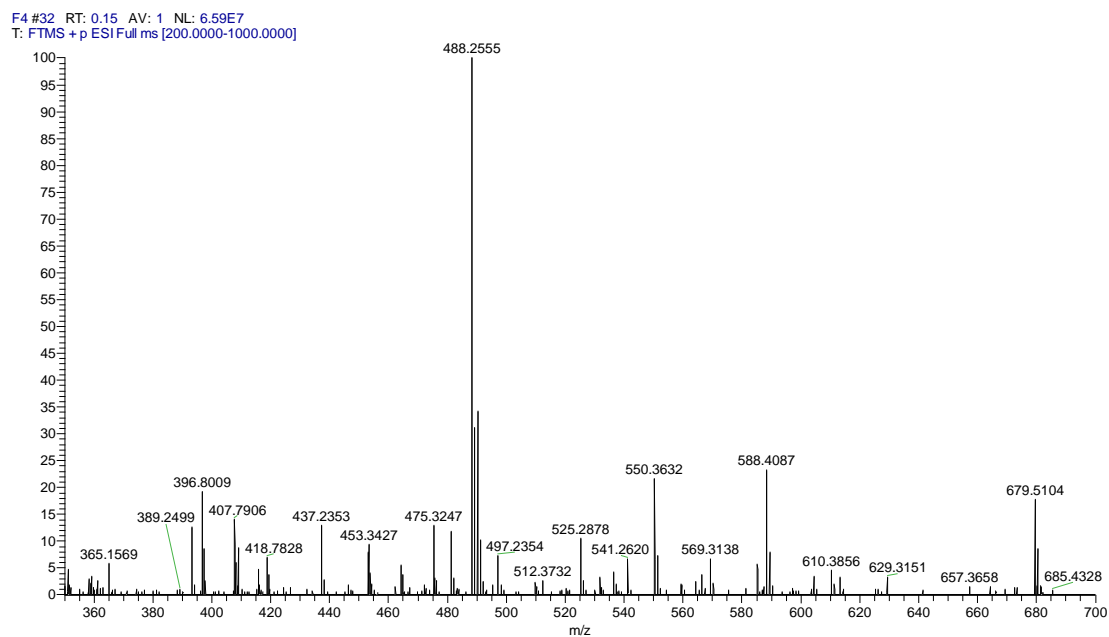


Figure SI 4-3. HR Mass spectrum (ESI) of compound 11.

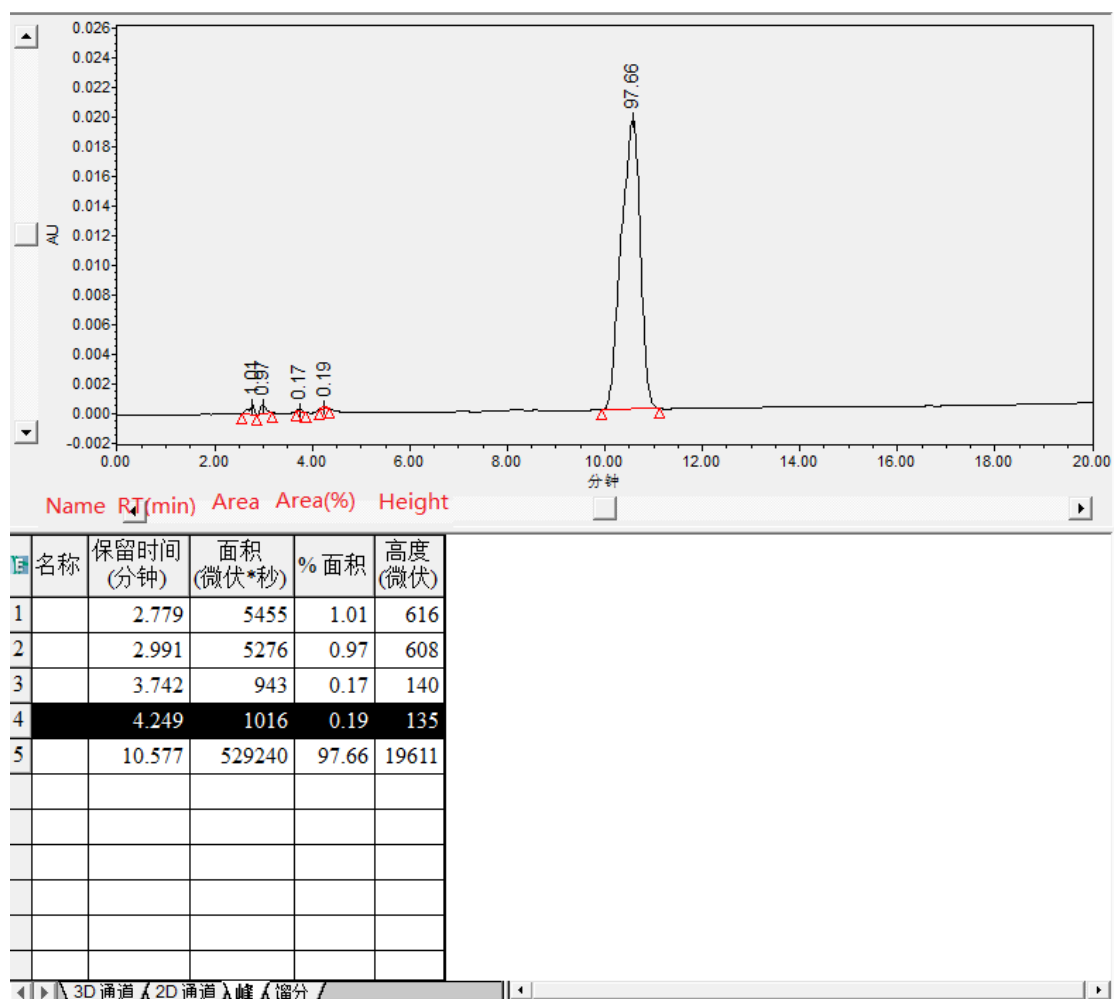


Figure SI 4-4. HPLC of compound 11.

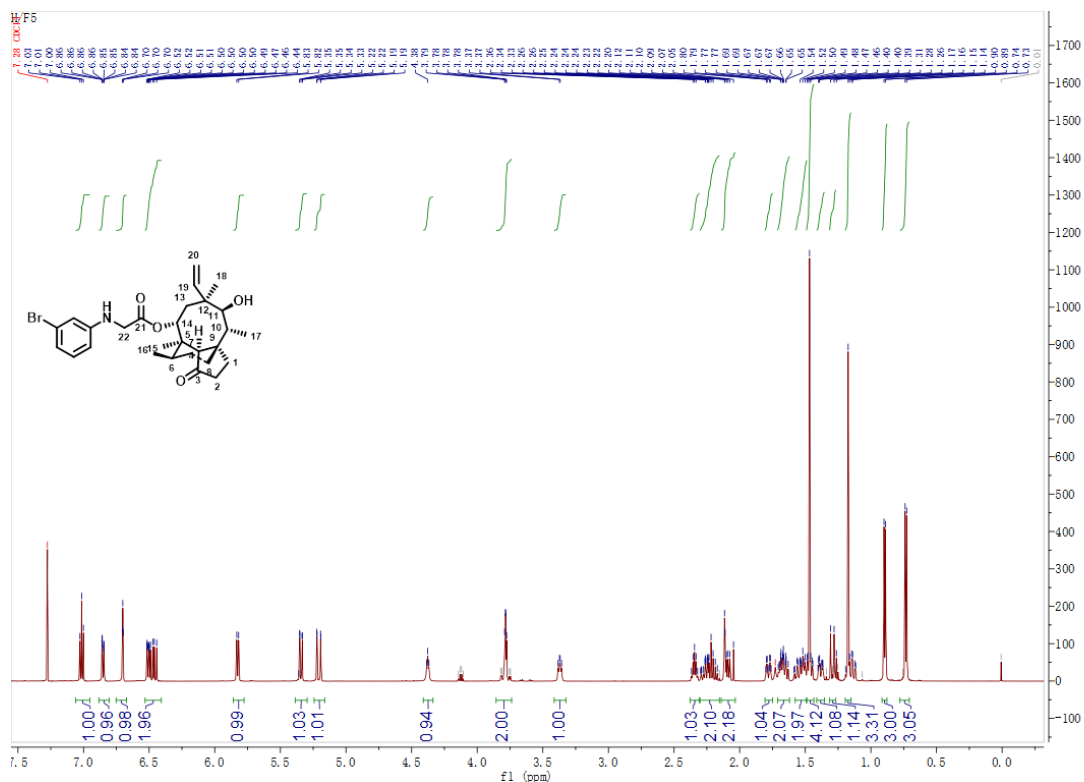


Figure SI 5-1. ¹H-NMR spectrum (CDCl₃, 400MHz) of compound 12.

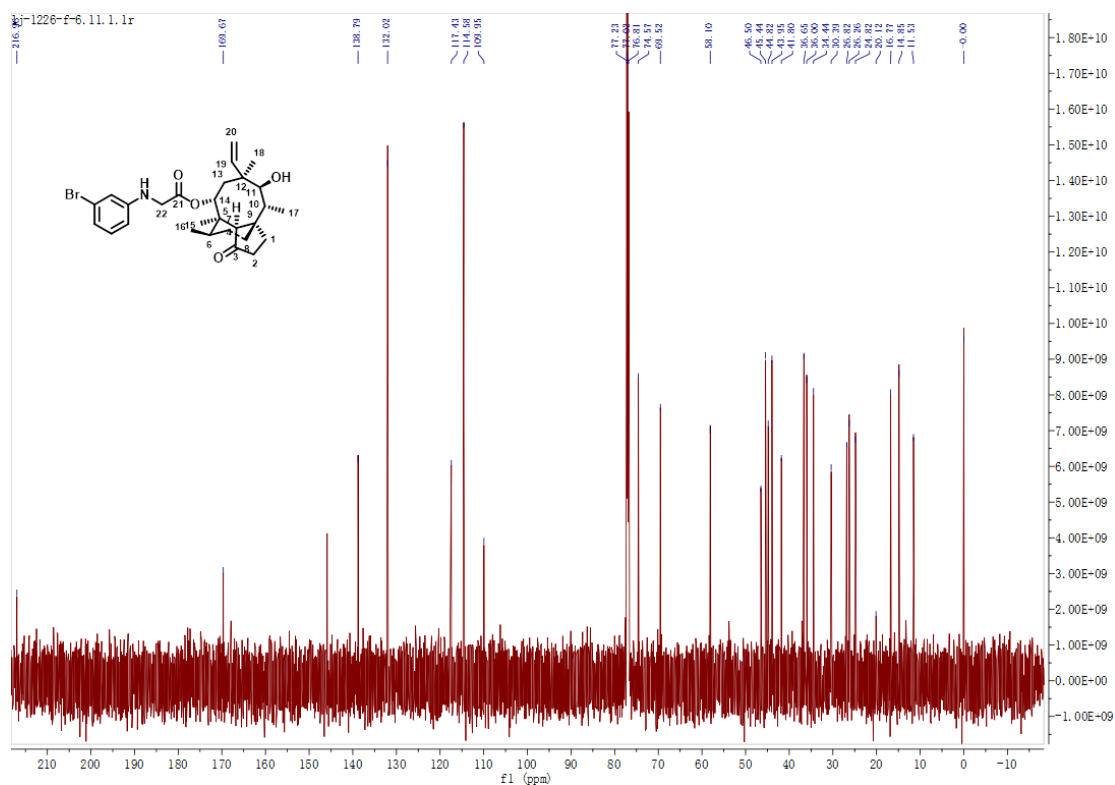


Figure SI 5-2. ¹³C-NMR spectrum (CDCl₃, 101MHz) of compound 12.

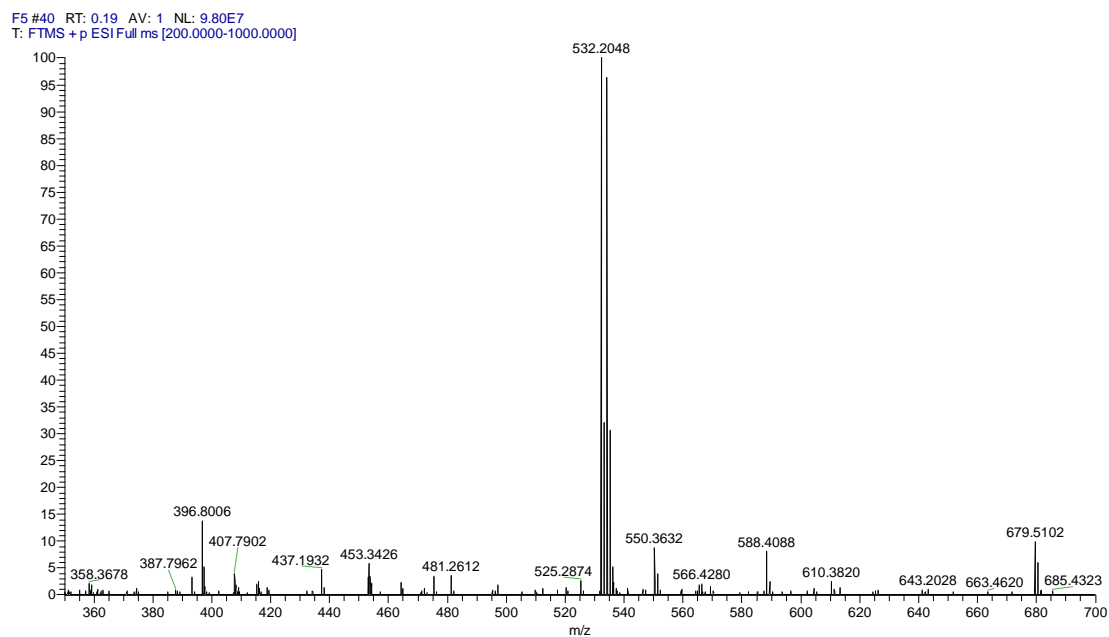


Figure SI 5-3. HR Mass spectrum (ESI) of compound 12.

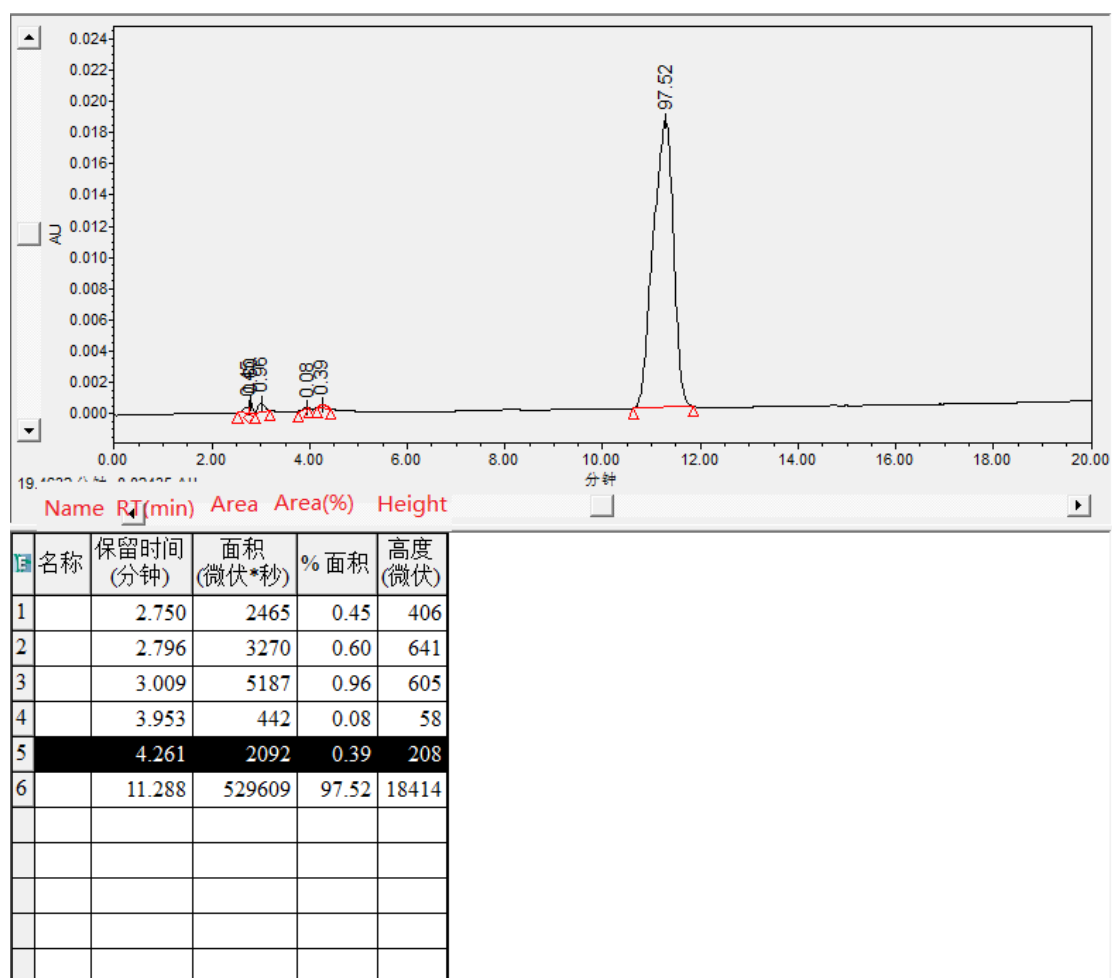


Figure SI 5-4. HPLC of compound 12.

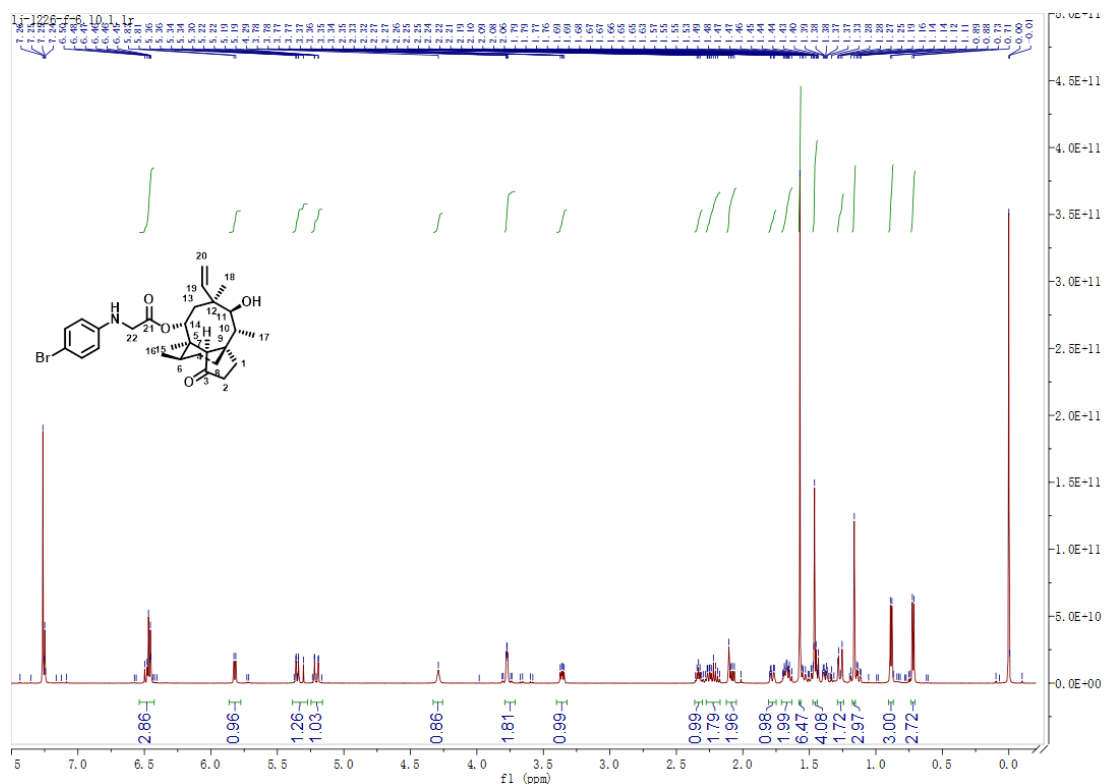


Figure SI 6-1. ^1H -NMR spectrum (CDCl₃, 400MHz) of compound 13.

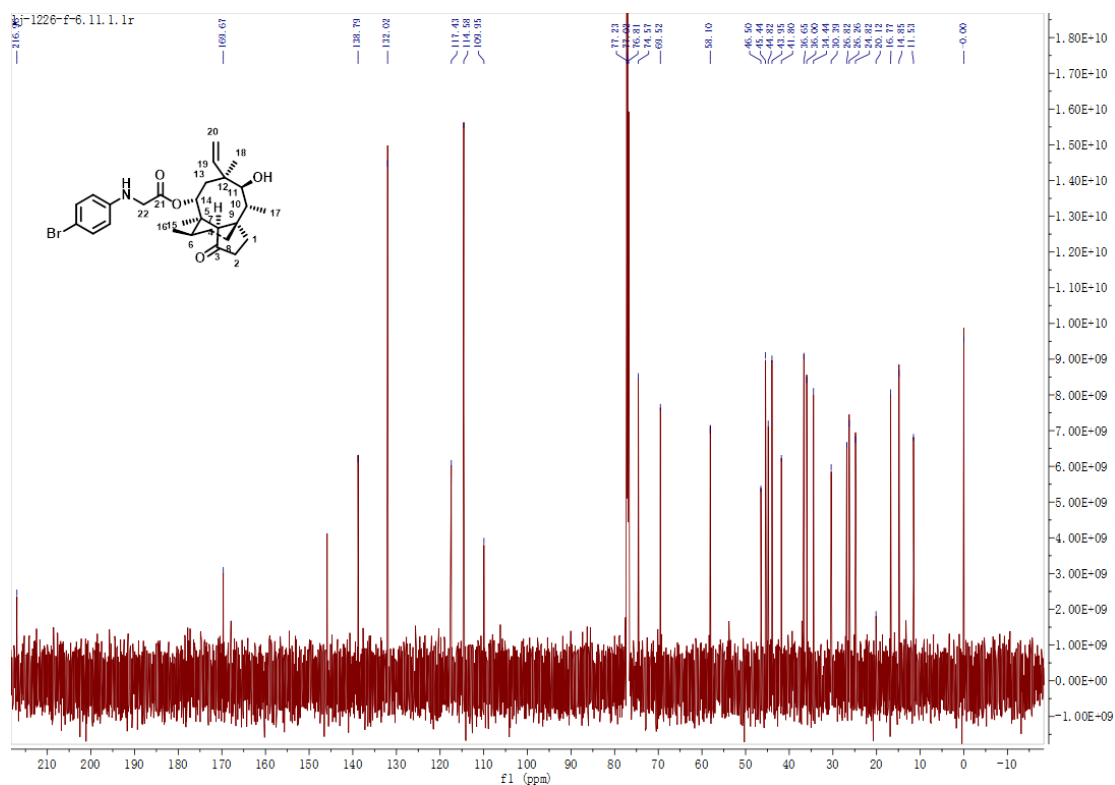


Figure SI 6-2. ^{13}C -NMR spectrum (CDCl₃, 101MHz) of compound 13.

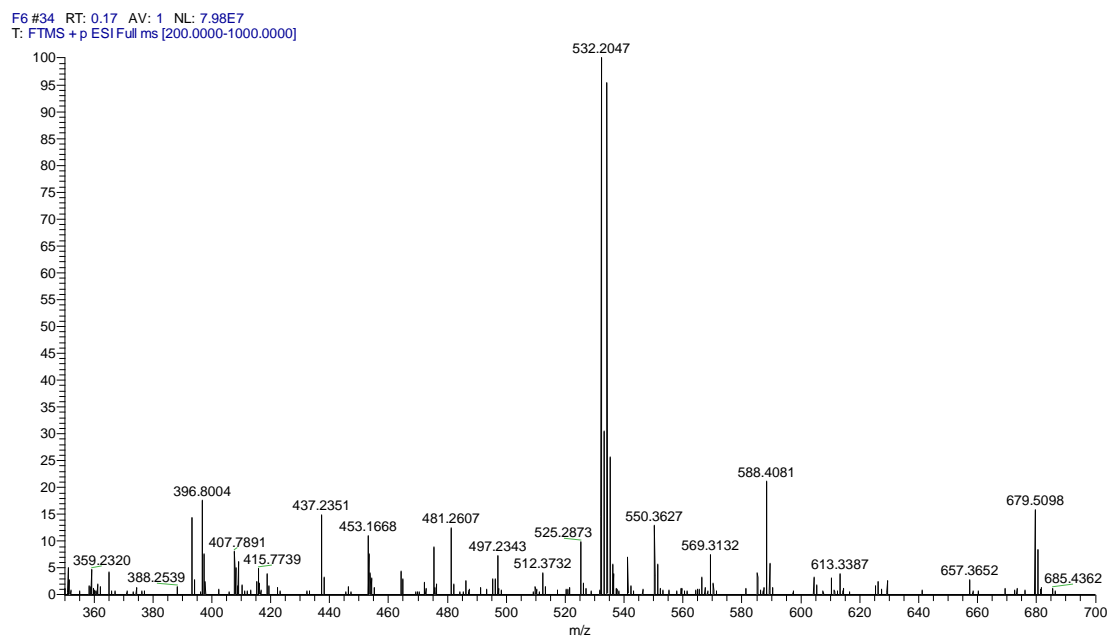


Figure SI 6-3. HR Mass spectrum (ESI) of compound 13.

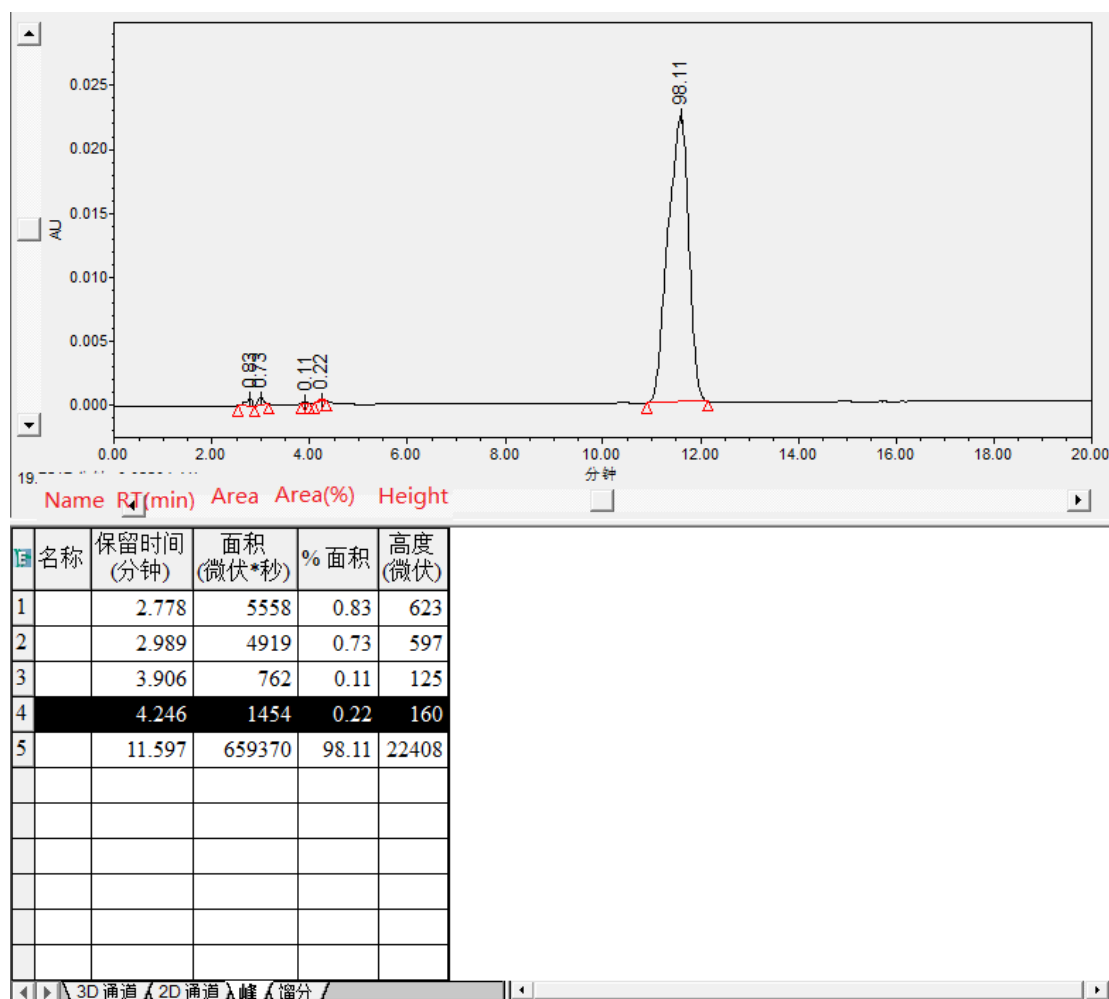


Figure SI 6-4. HPLC of compound 13.

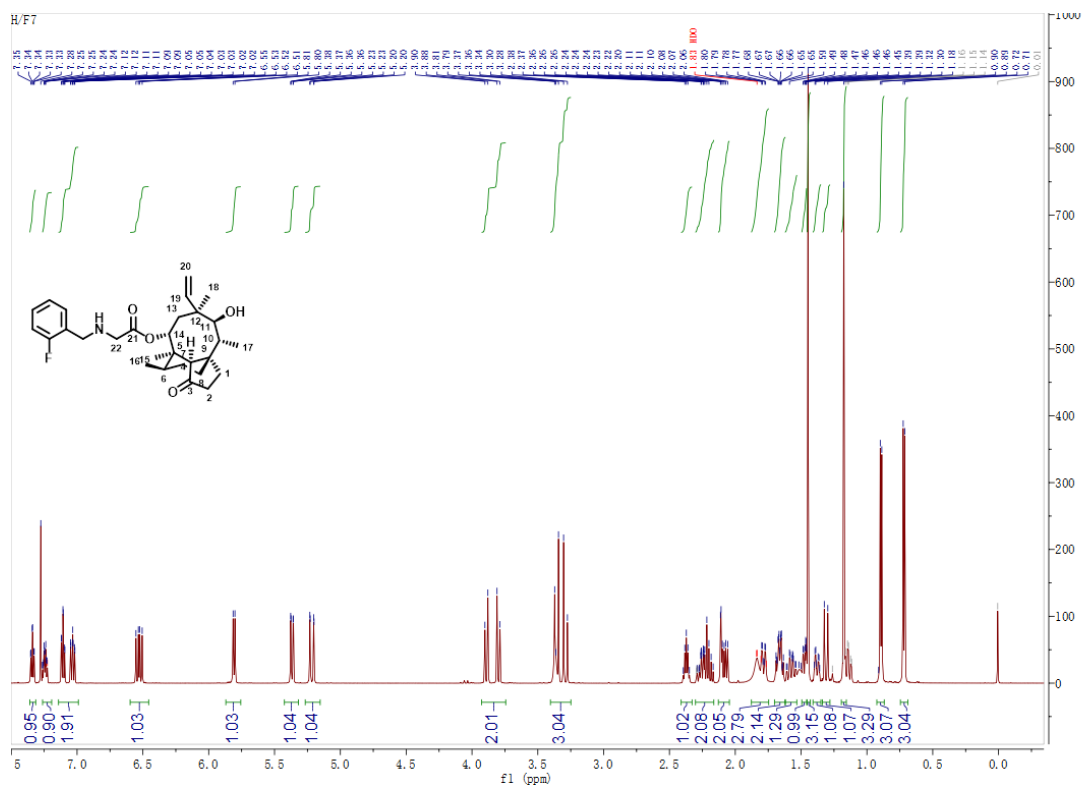


Figure SI 7-1. ¹H-NMR spectrum (CDCl₃, 400MHz) of compound 14.

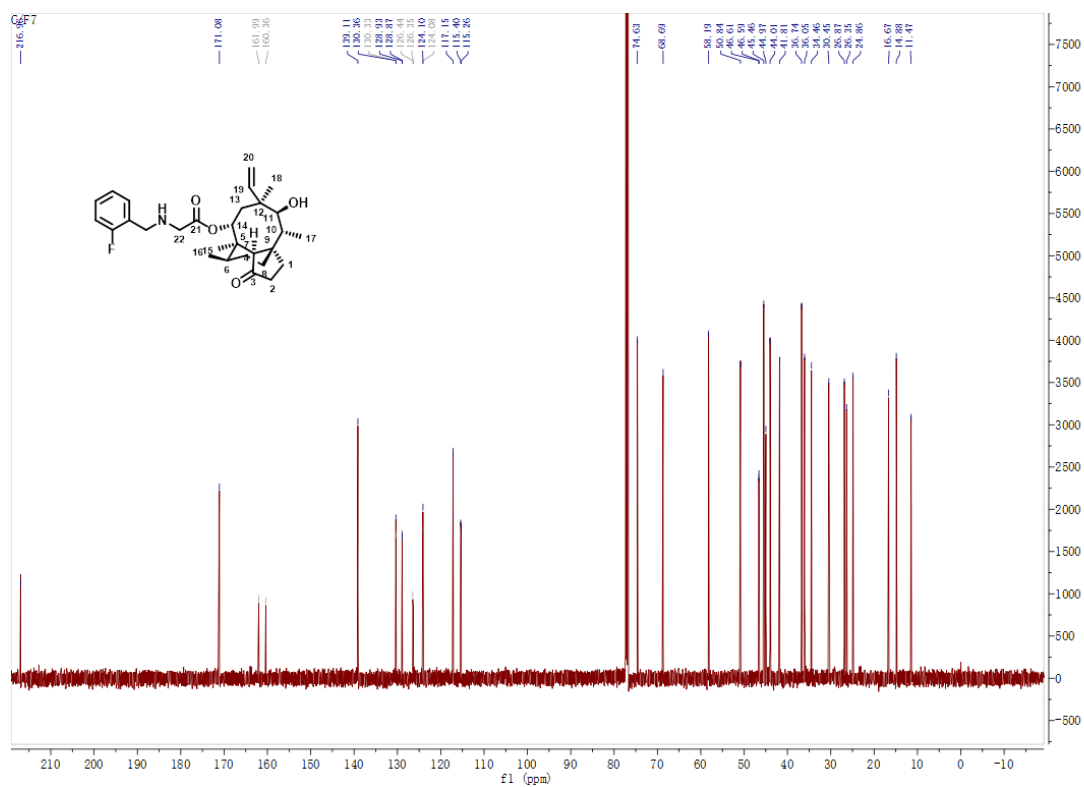


Figure SI 7-2. ¹³C-NMR spectrum (CDCl₃, 101MHz) of compound 14.

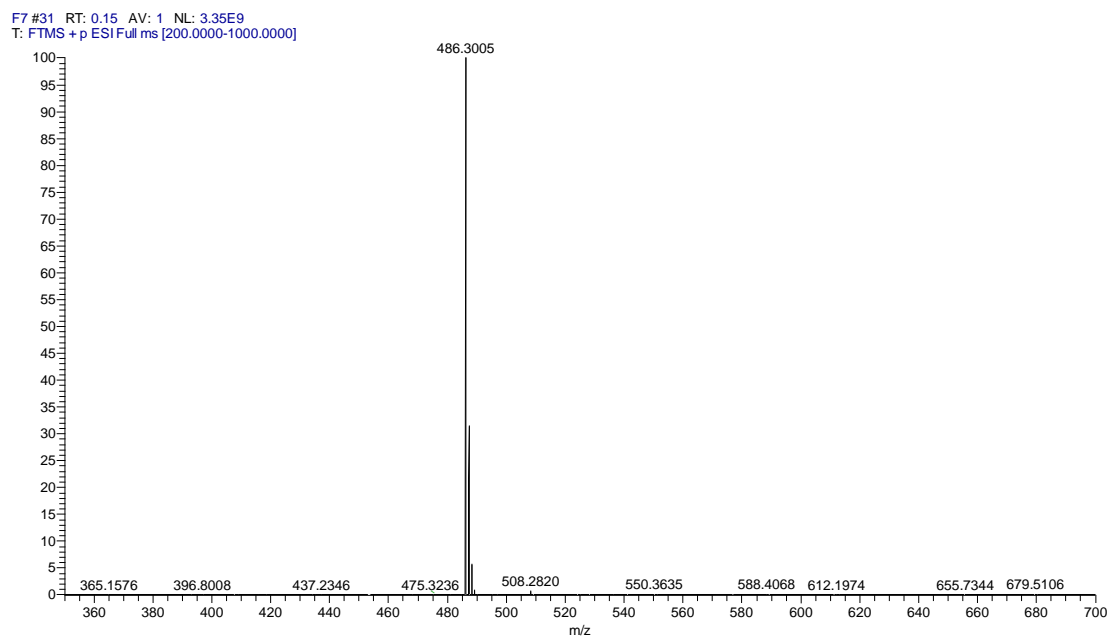


Figure SI 7-3. HR Mass spectrum (ESI) of compound 14.

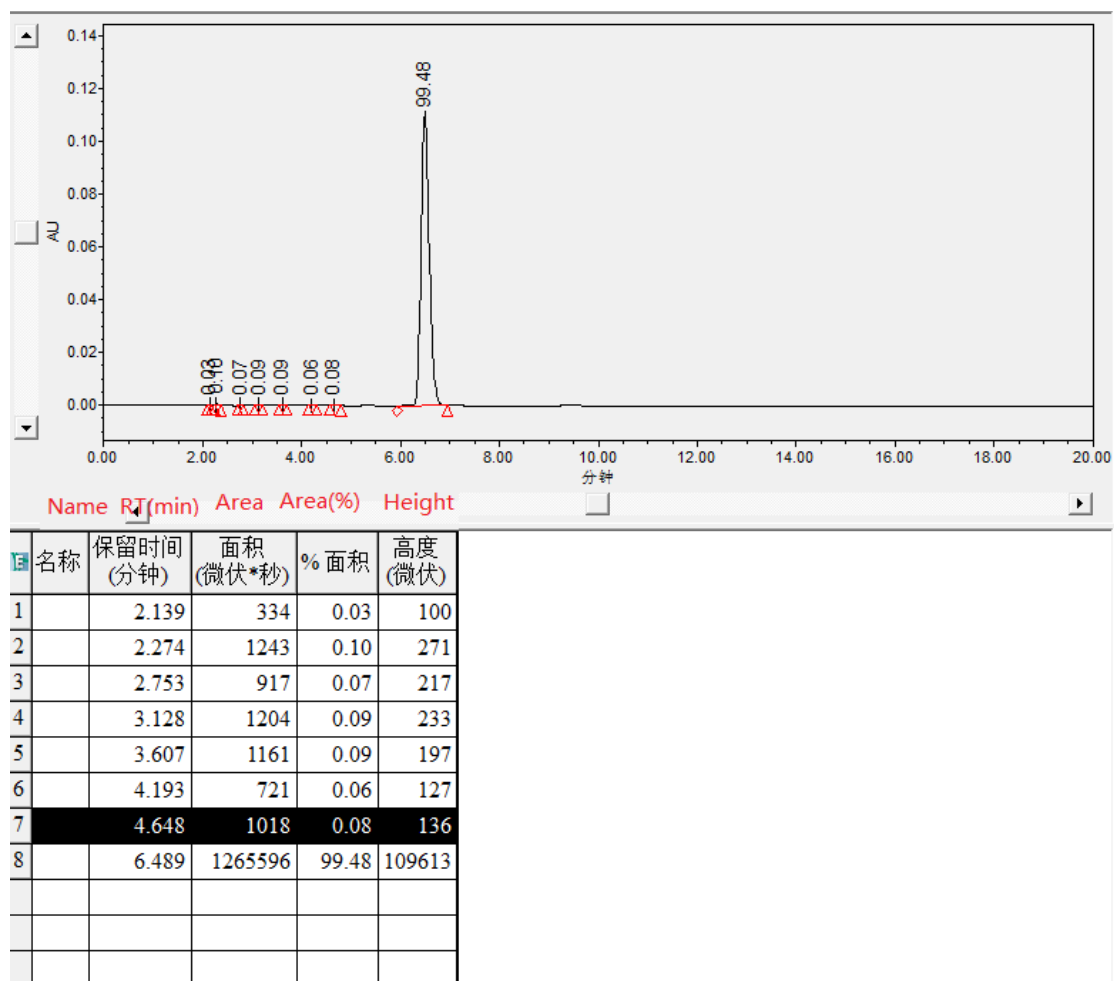


Figure SI 7-4. HPLC of compound 14.

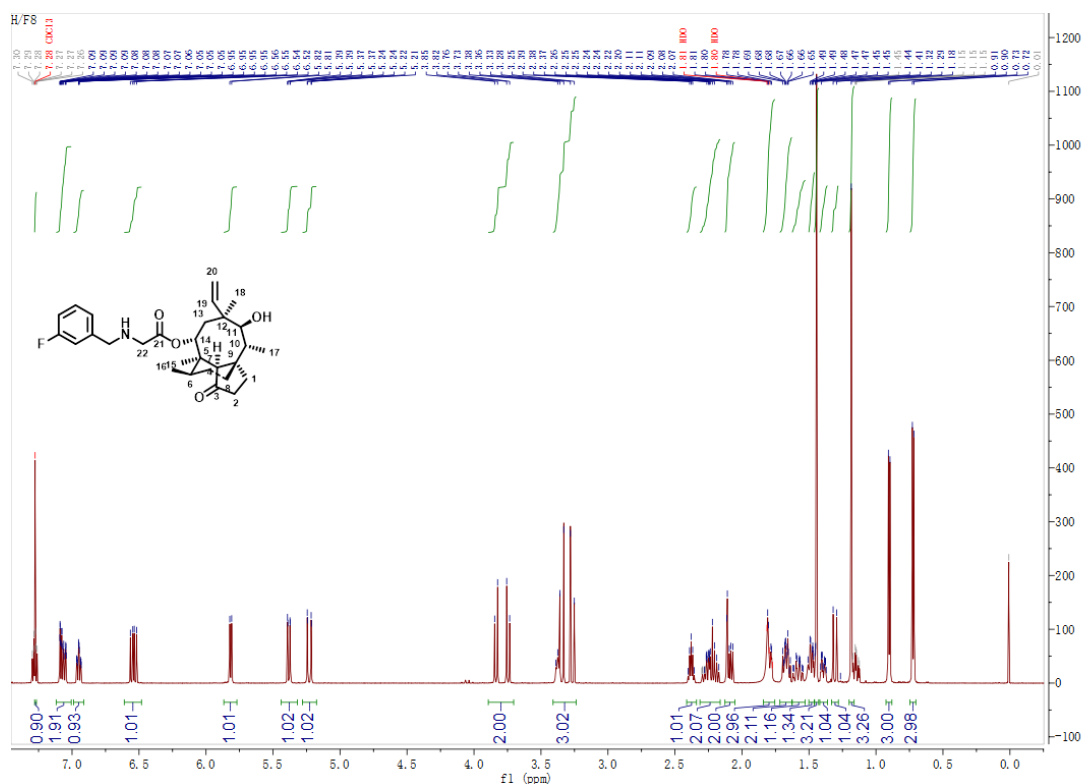


Figure SI 8-1. ¹H-NMR spectrum (CDCl₃, 400MHz) of compound 15.

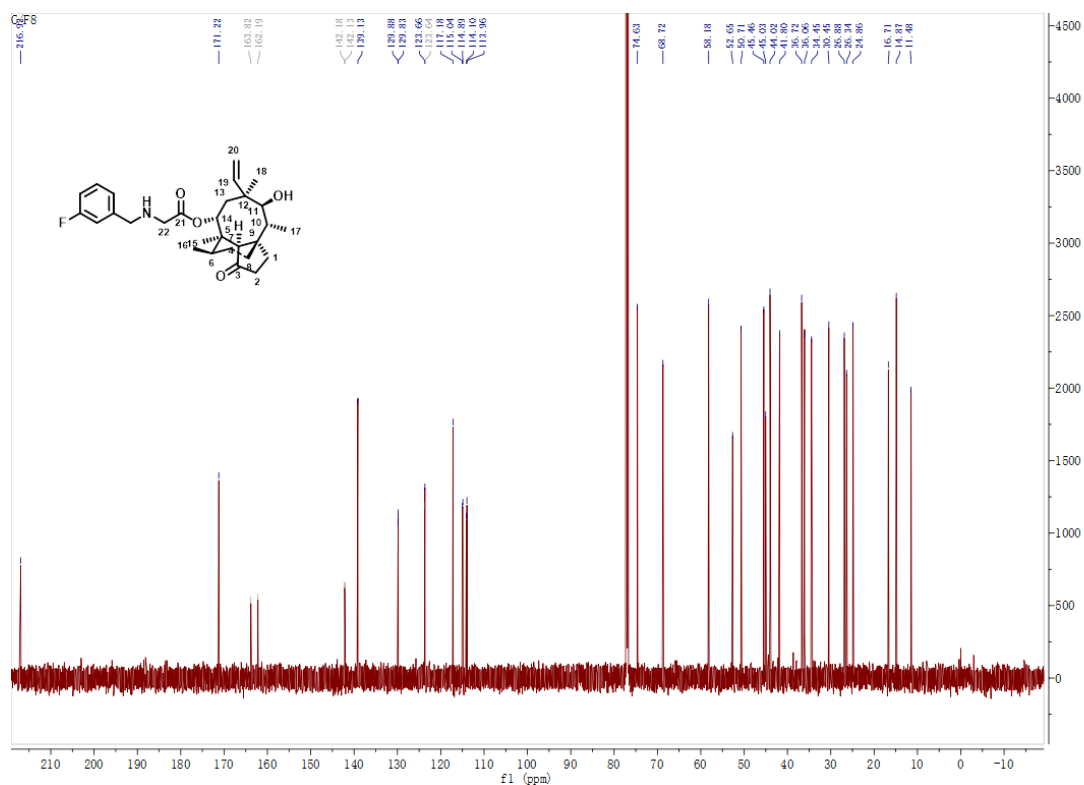


Figure SI 8-2. ¹³C-NMR spectrum (CDCl₃, 101MHz) of compound 15.

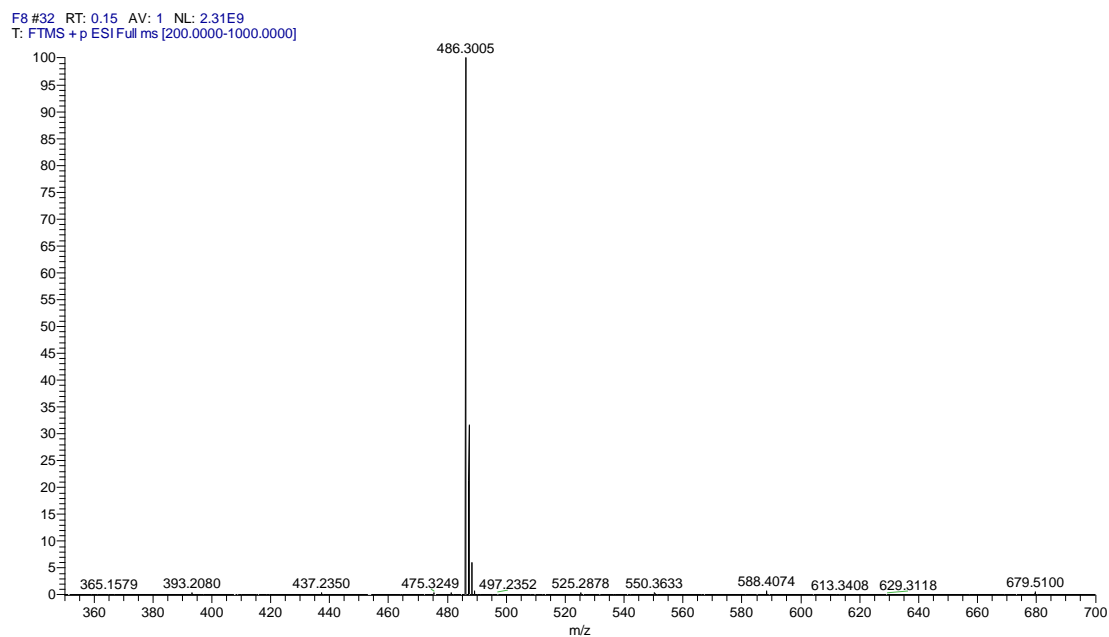


Figure SI 8-3. HR Mass spectrum (ESI) of compound 15.

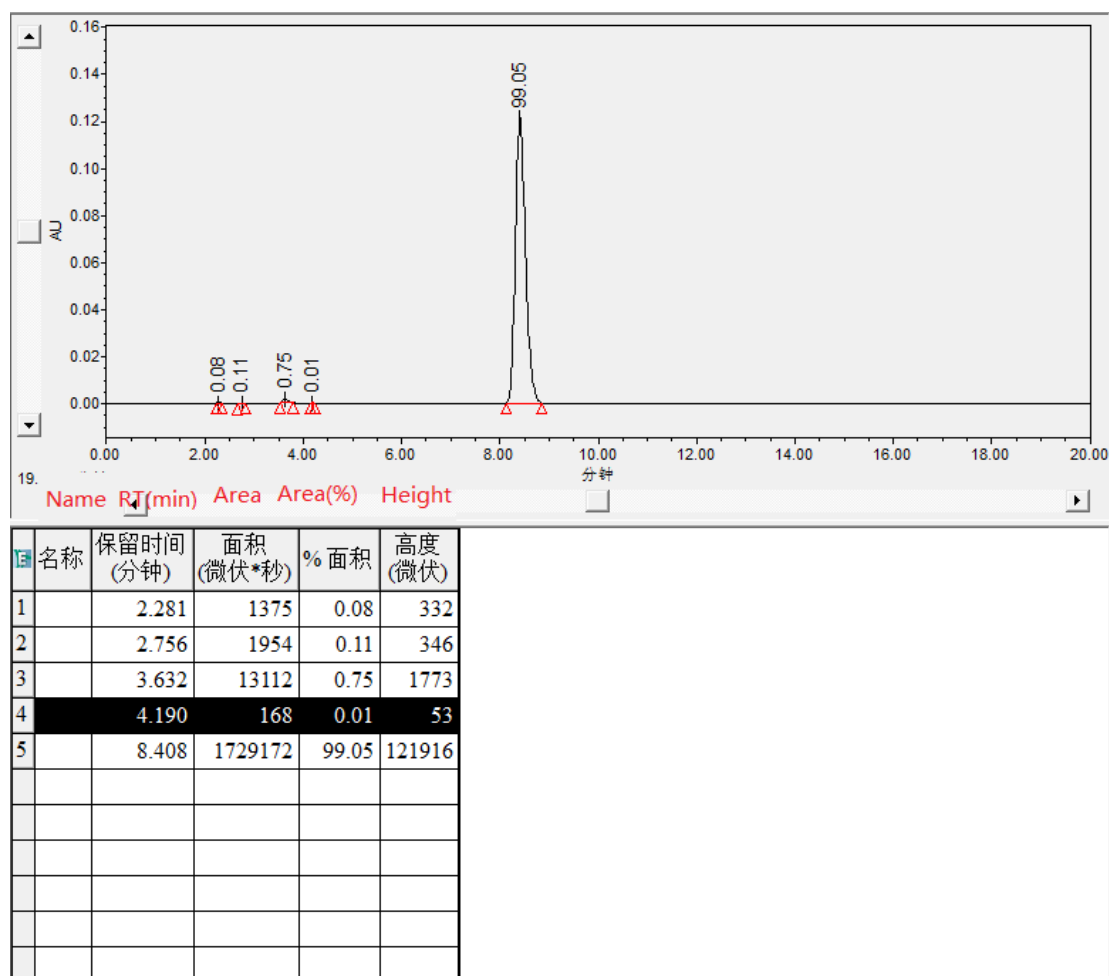


Figure SI 8-4. HPLC of compound 15.

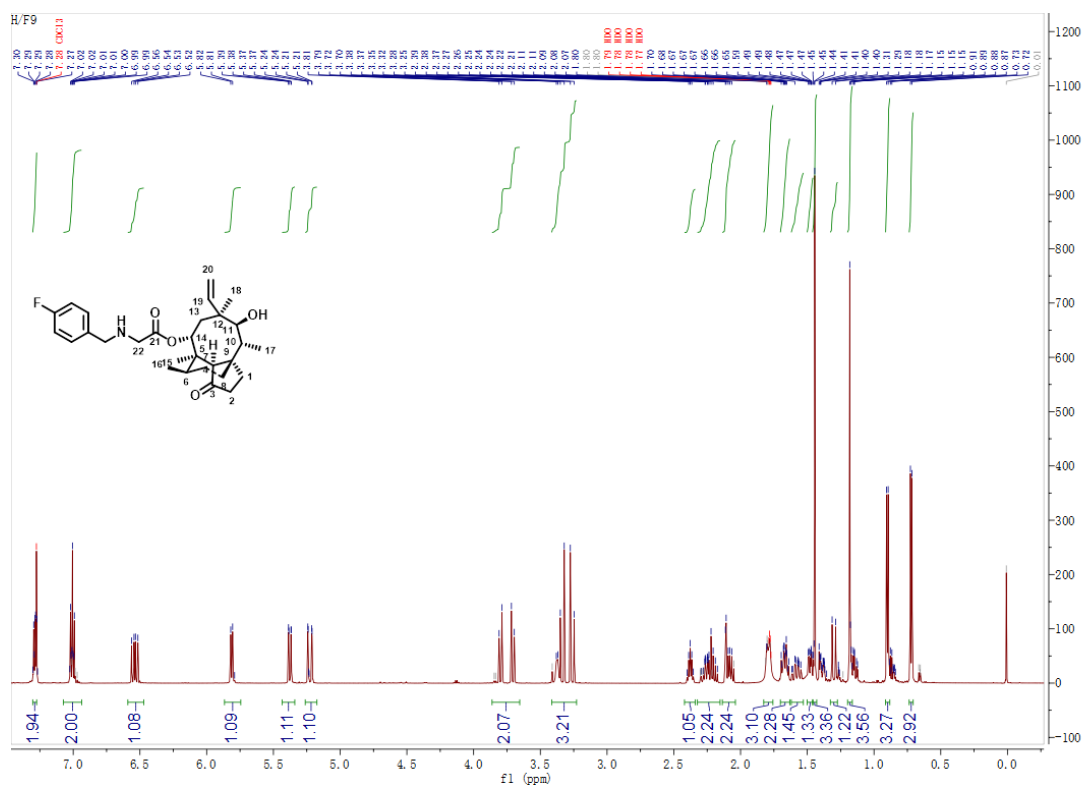


Figure SI 9-1. ¹H-NMR spectrum (CDCl₃, 400MHz) of compound 16.

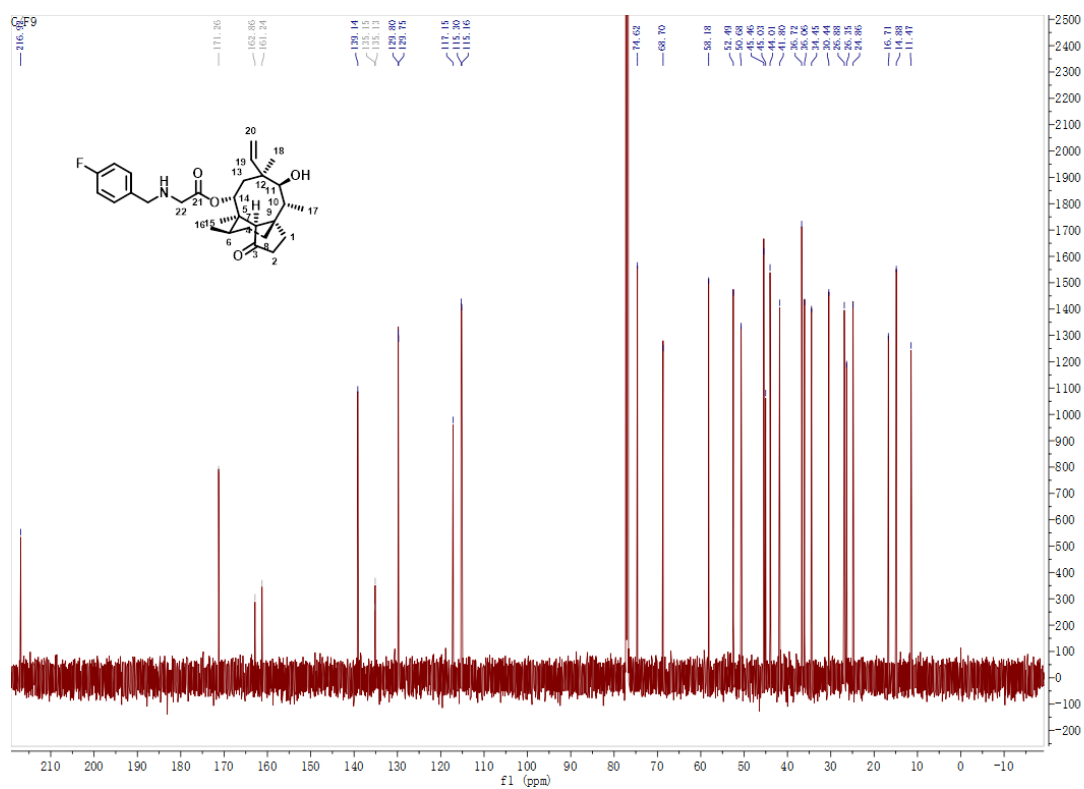


Figure SI 9-2. ¹³C-NMR spectrum (CDCl₃, 101MHz) of compound 16.

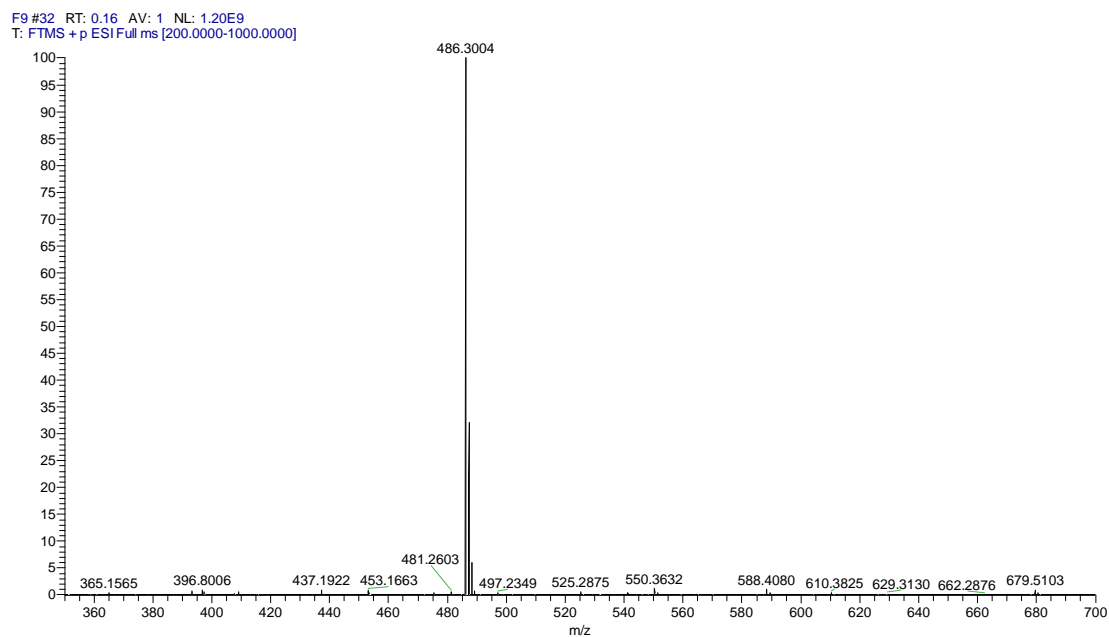


Figure SI 9-3. HR Mass spectrum (ESI) of compound 16.

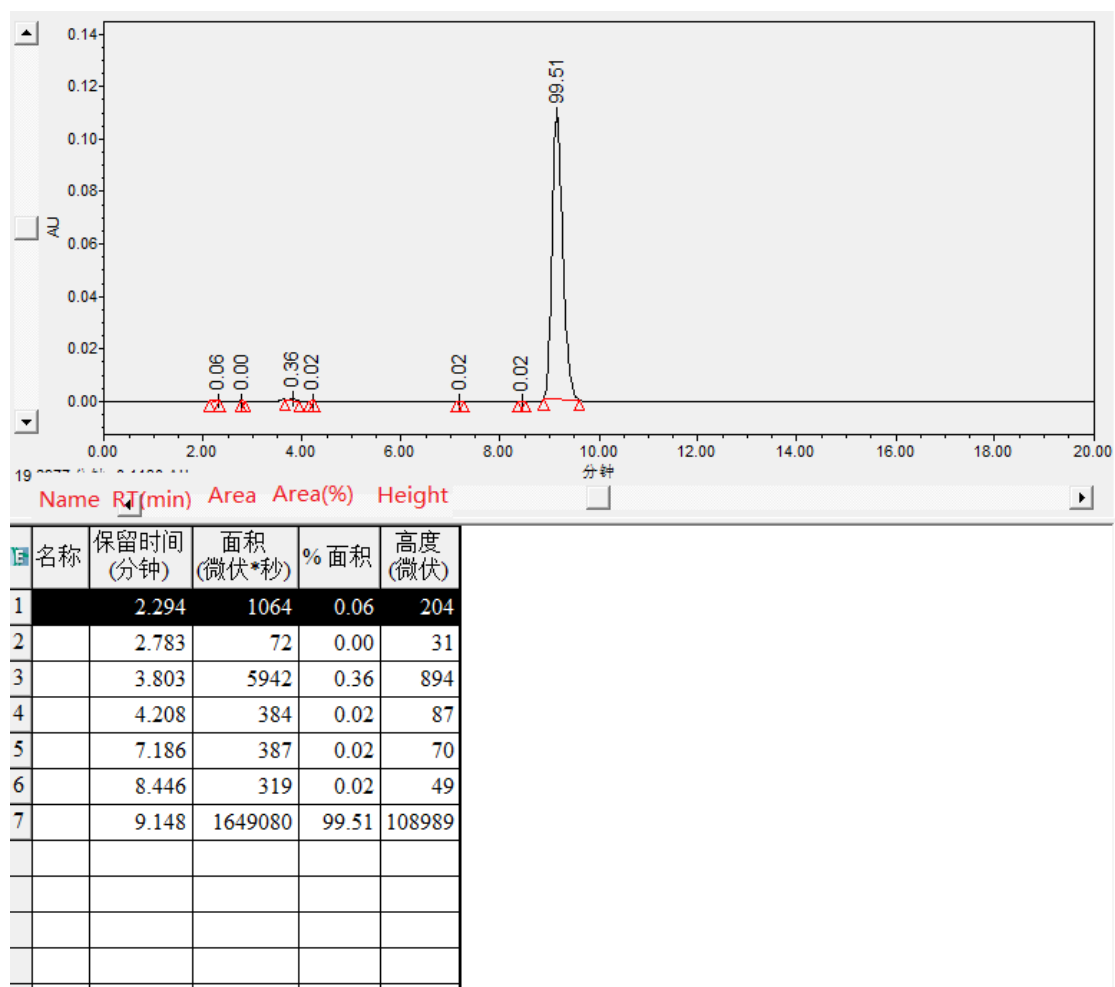


Figure SI 9-4. HPLC of compound 16.

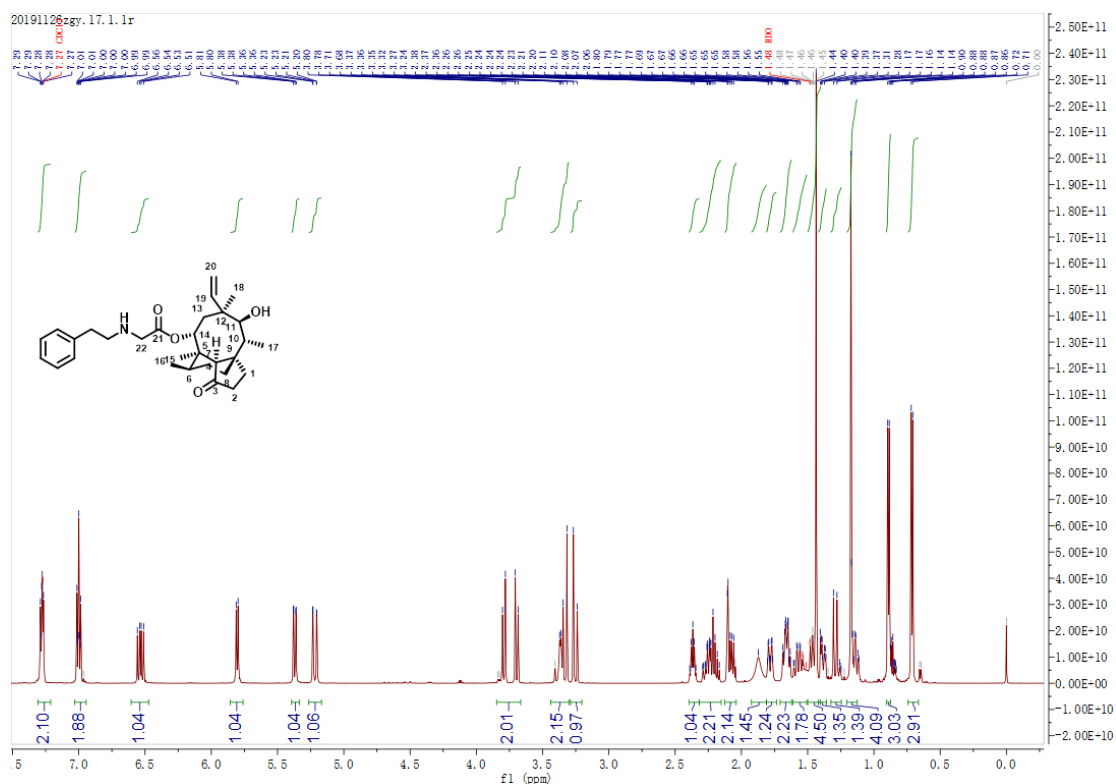


Figure SI 10-1. ^1H -NMR spectrum (CDCl₃, 400MHz) of compound 17.

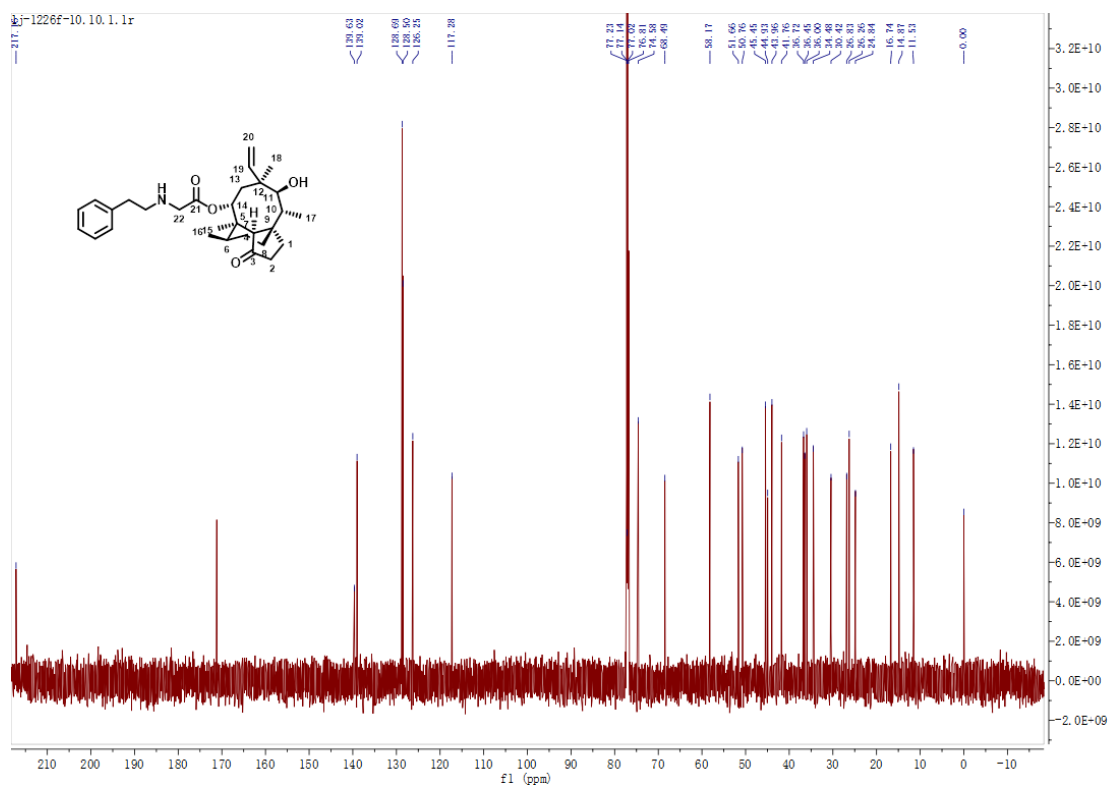


Figure SI 10-2. ^{13}C -NMR spectrum (CDCl₃, 101MHz) of compound 17.

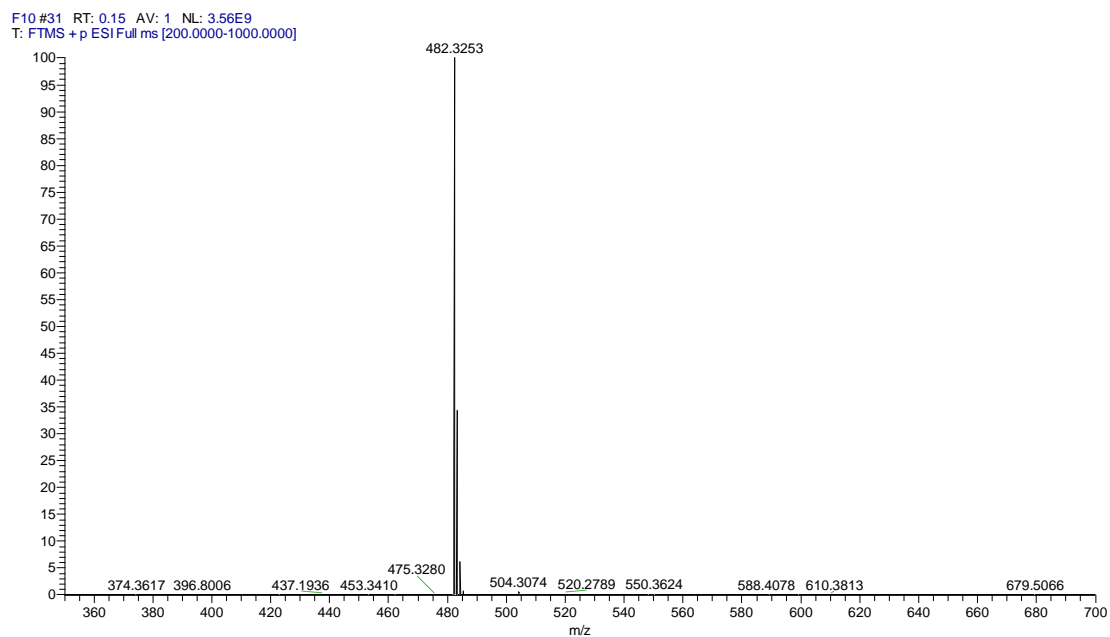


Figure SI 10-3. HR Mass spectrum (ESI) of compound 17.

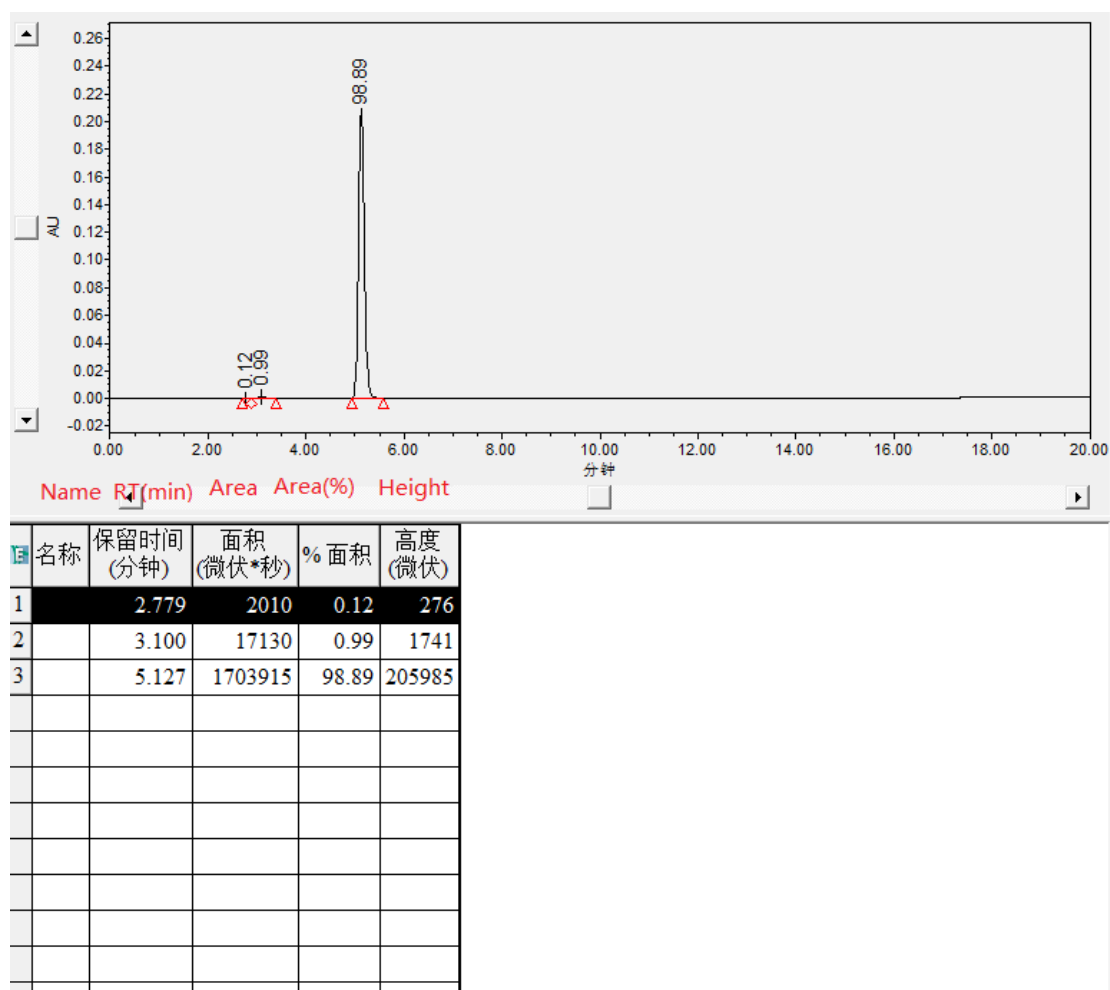


Figure SI 10-4. HPLC of compound 17.

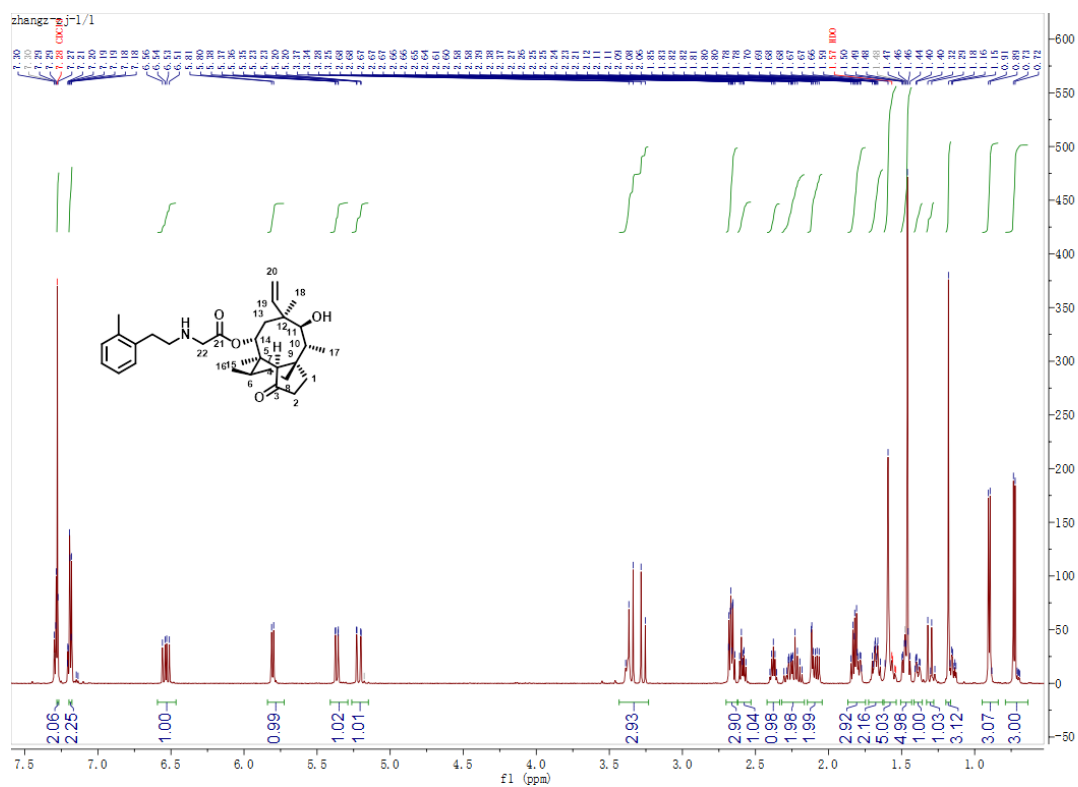


Figure SI 11-1. ^1H -NMR spectrum (CDCl_3 , 400MHz) of compound **18**.

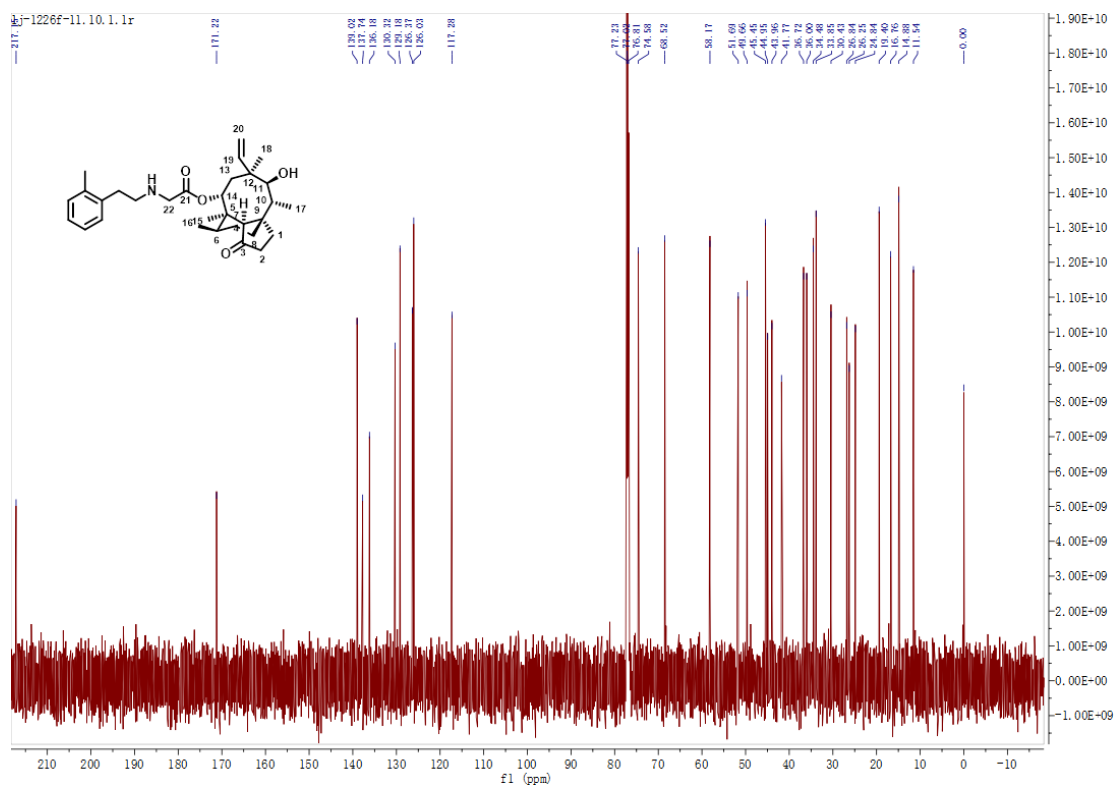


Figure SI 11-2. ^{13}C -NMR spectrum (CDCl_3 , 101MHz) of compound **18**.

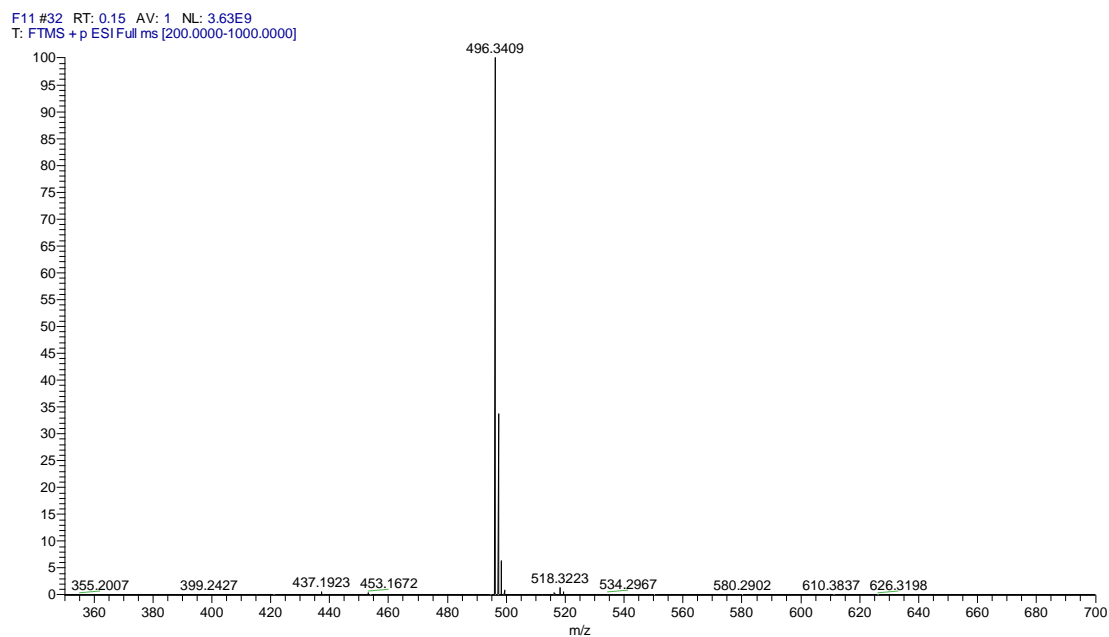


Figure SI 11-3. HR Mass spectrum (ESI) of compound 18.

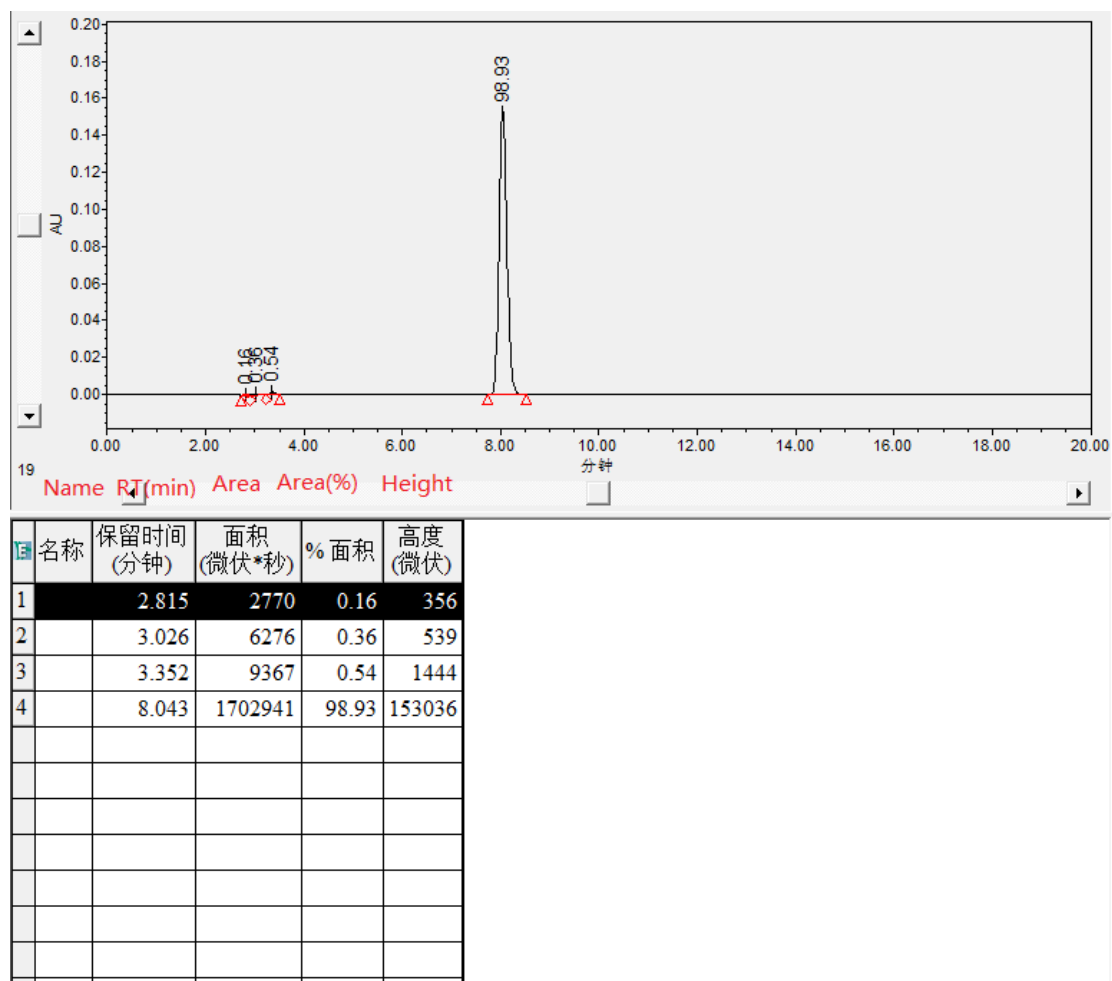


Figure SI 11-4. HPLC of compound 18.

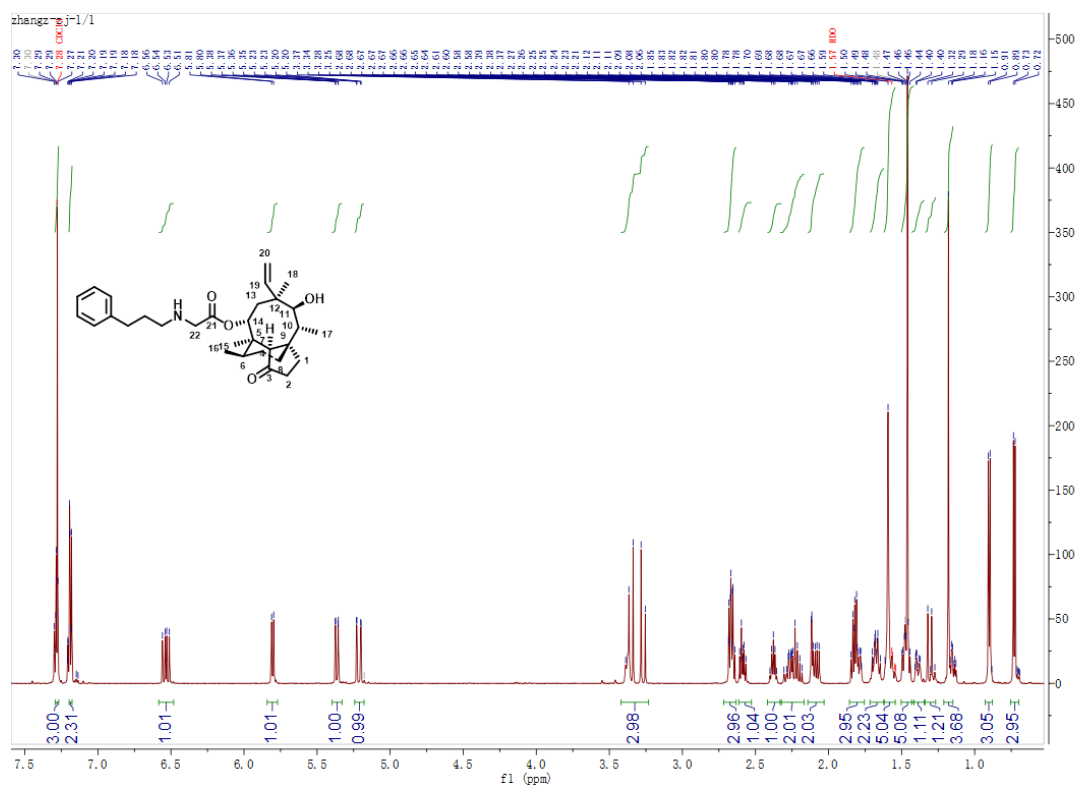


Figure SI 12-1. ^1H -NMR spectrum (CDCl_3 , 400MHz) of compound 19.

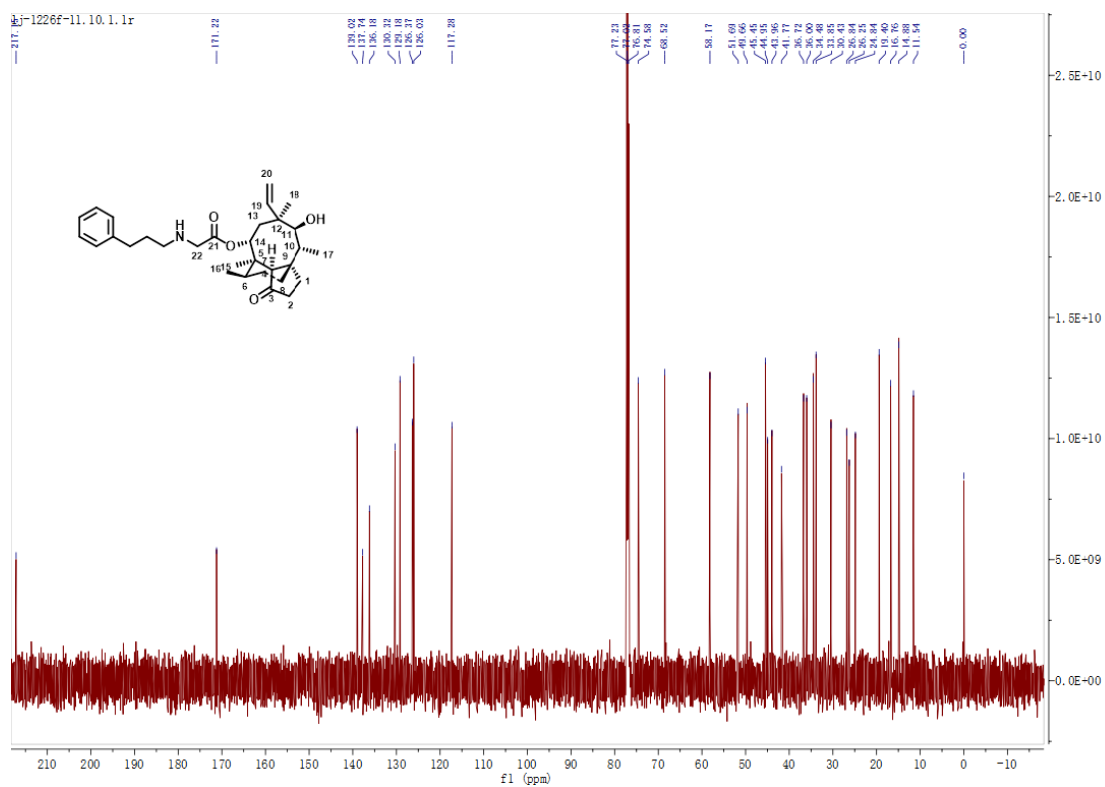


Figure SI 12-2. ^{13}C -NMR spectrum (CDCl_3 , 101MHz) of compound 19.

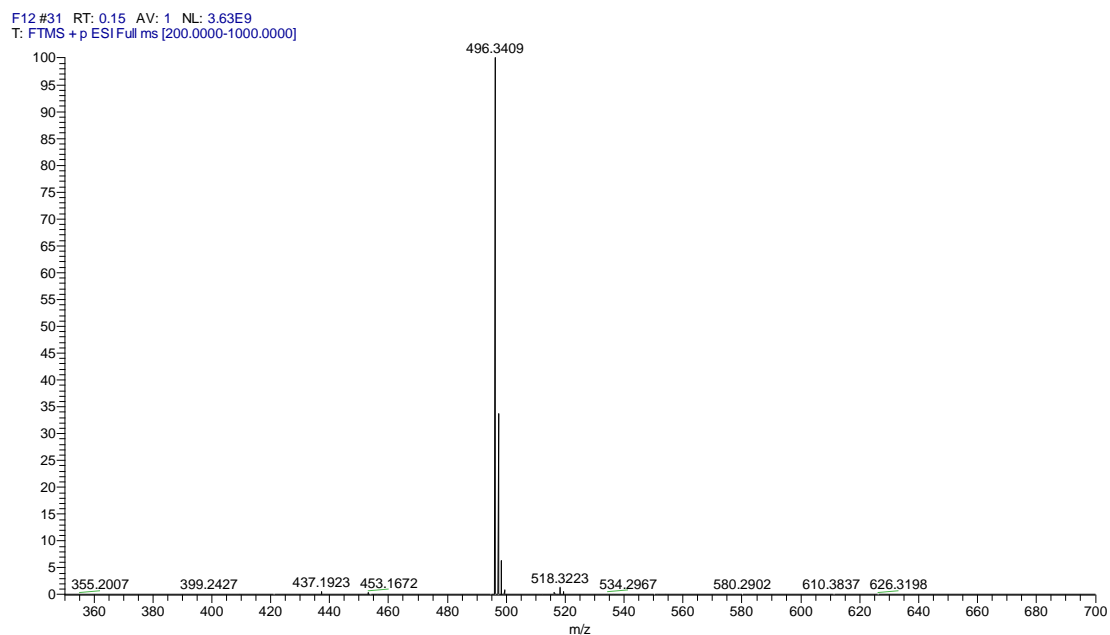


Figure SI 12-3. HR Mass spectrum (ESI) of compound 19.

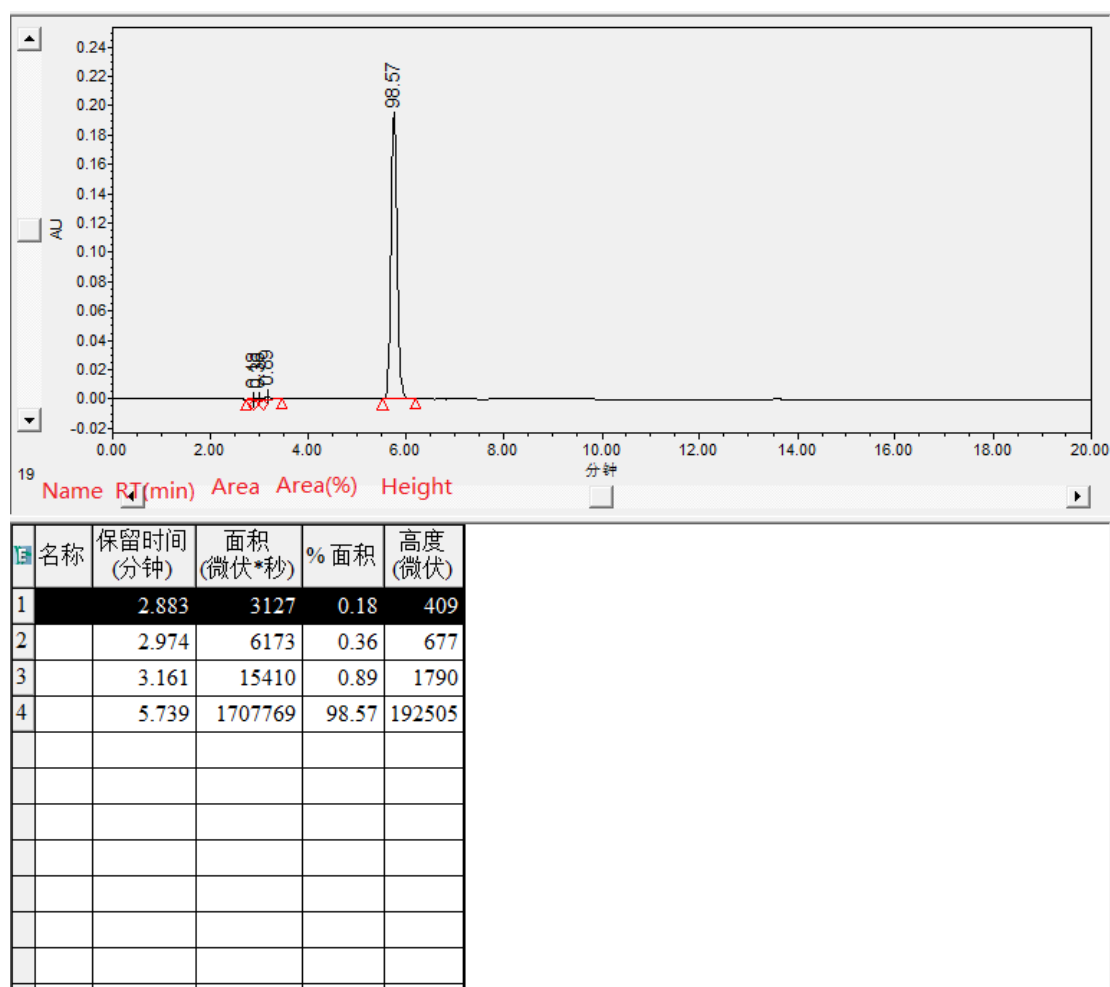


Figure SI 12-4. HPLC of compound 19.

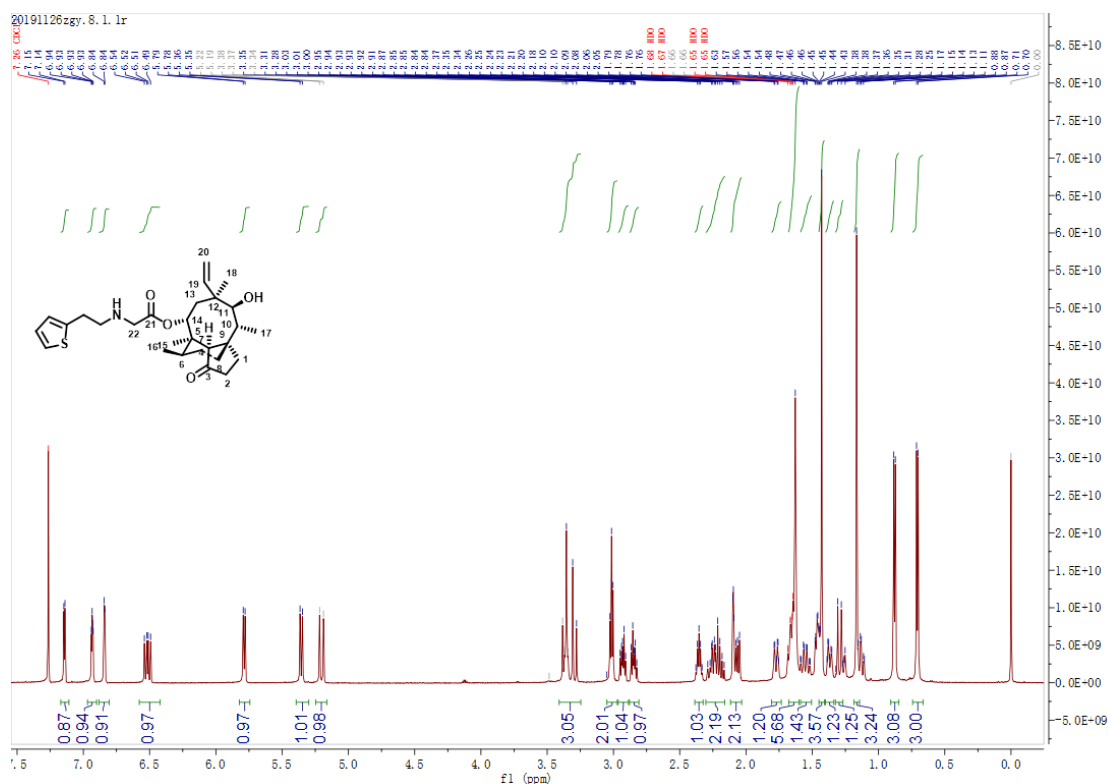


Figure SI 13-1. ^1H -NMR spectrum (CDCl_3 , 400MHz) of compound **20**.

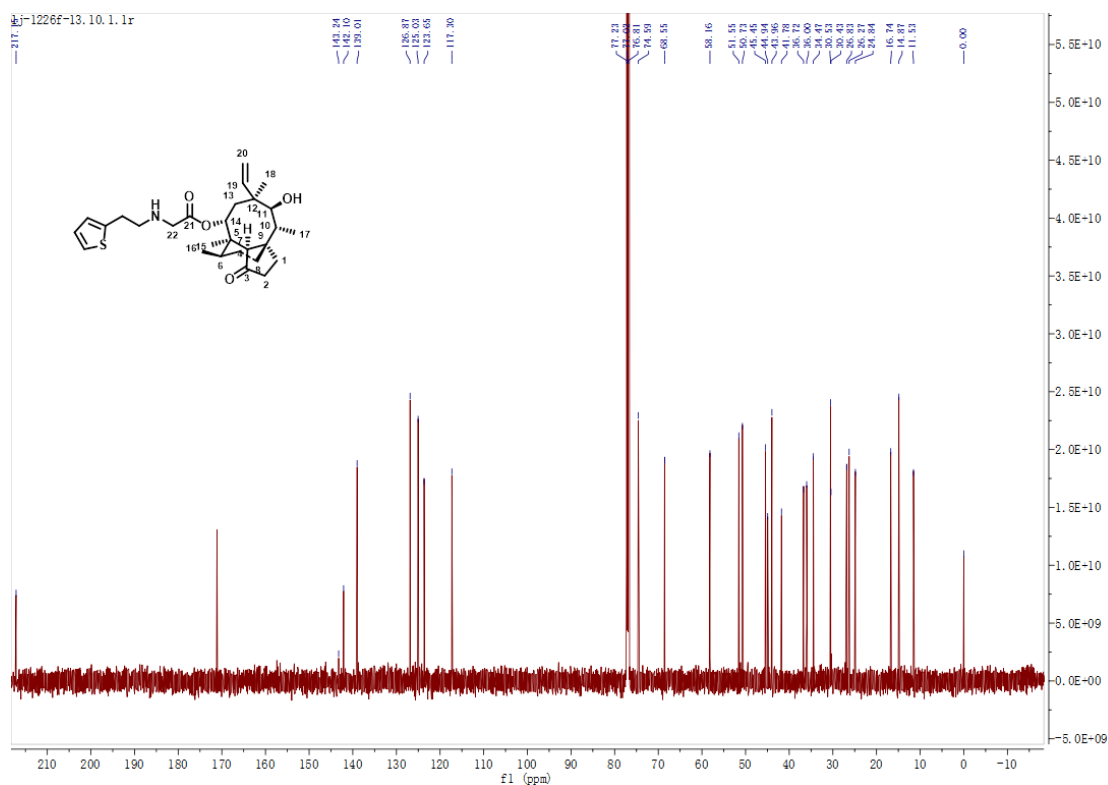


Figure SI 13-2. ^{13}C -NMR spectrum (CDCl_3 , 101MHz) of compound **20**.

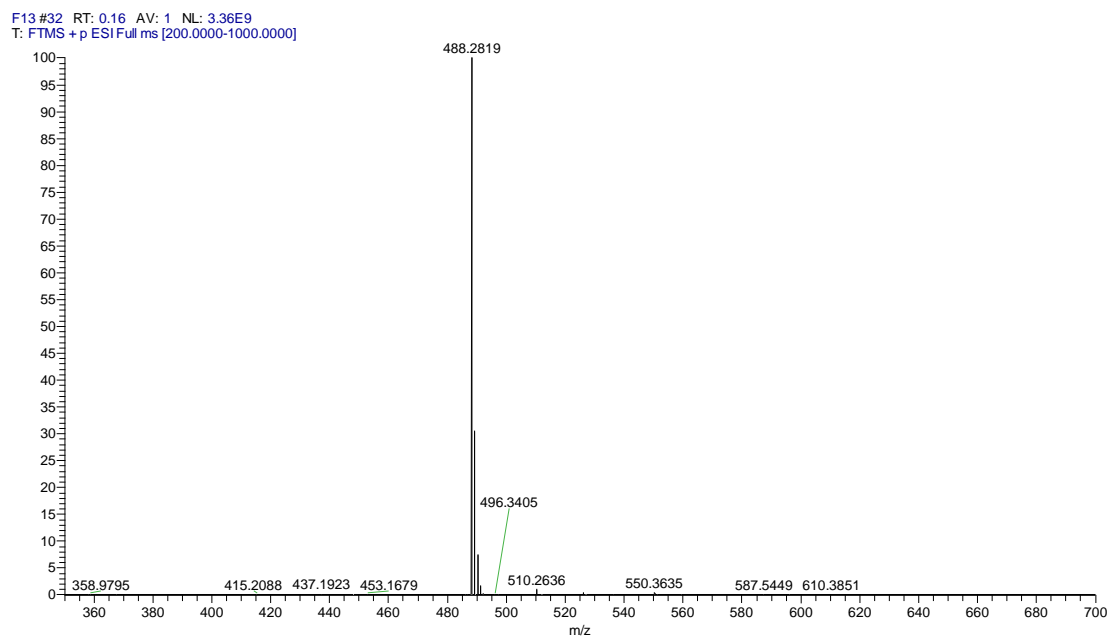


Figure SI 13-3. HR Mass spectrum (ESI) of compound 20.

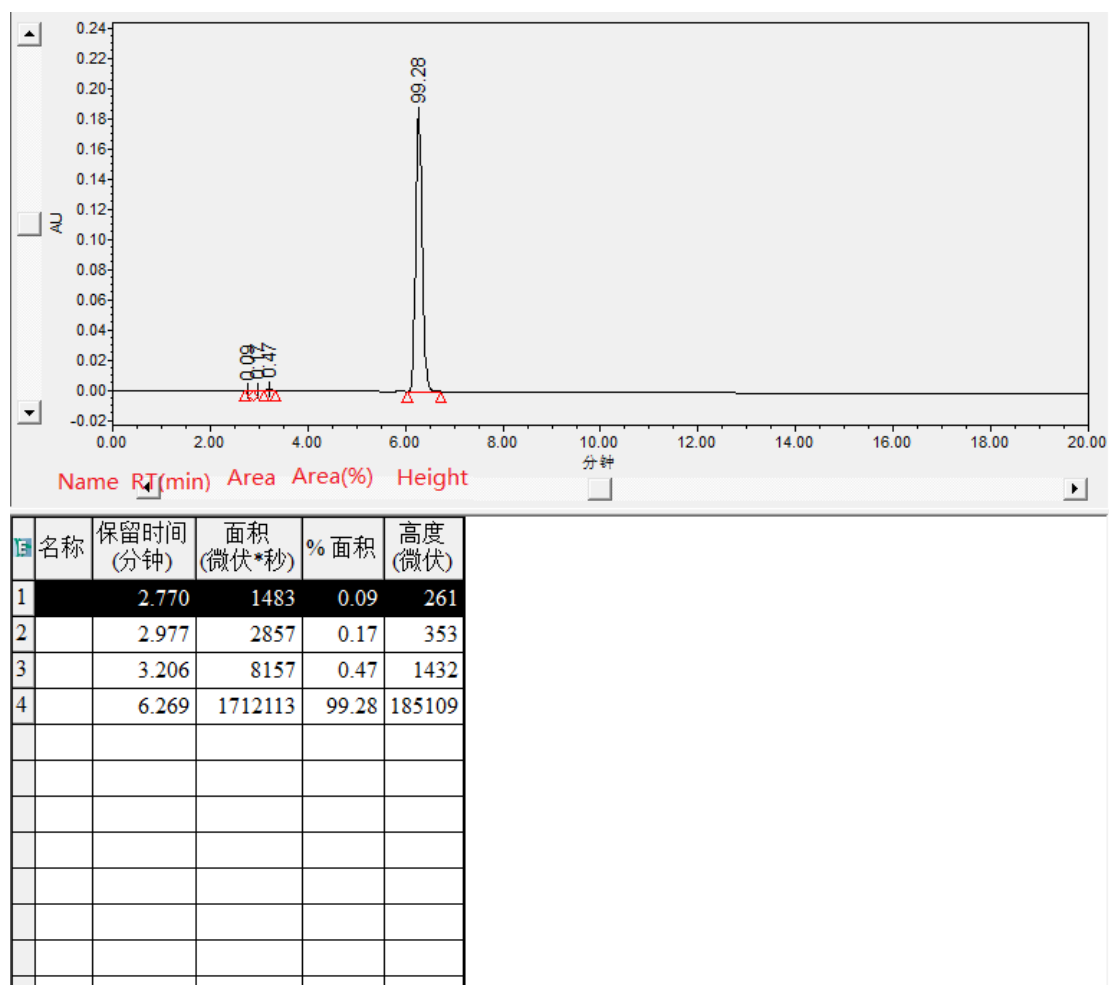


Figure SI 13-4. HPLC of compound 20.

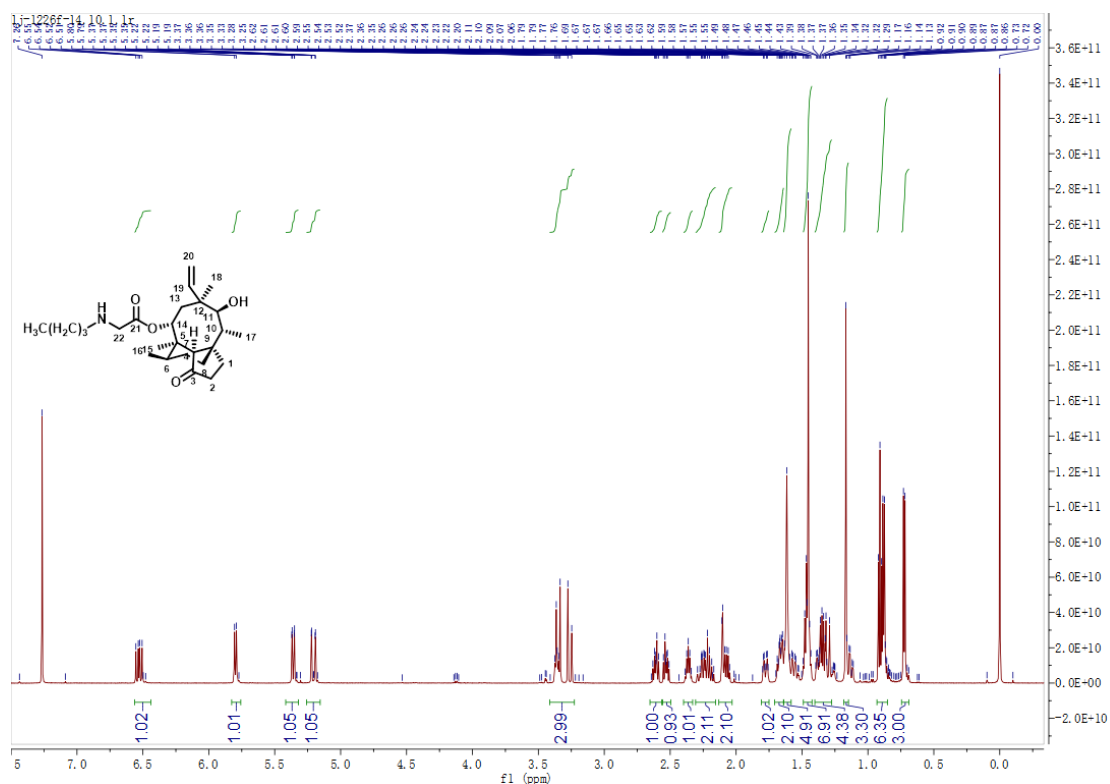


Figure SI 14-1. ¹H-NMR spectrum (CDCl₃, 400MHz) of compound 21.

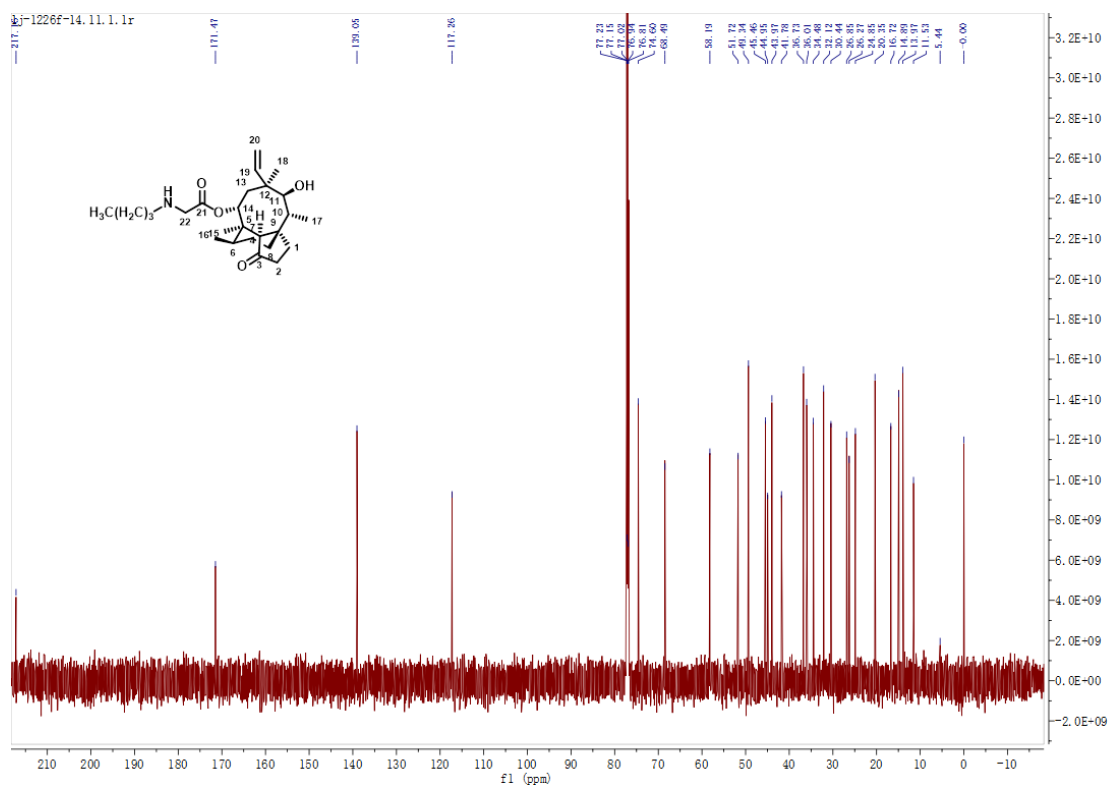


Figure SI 14-2. ¹³C-NMR spectrum (CDCl₃, 101MHz) of compound 21.

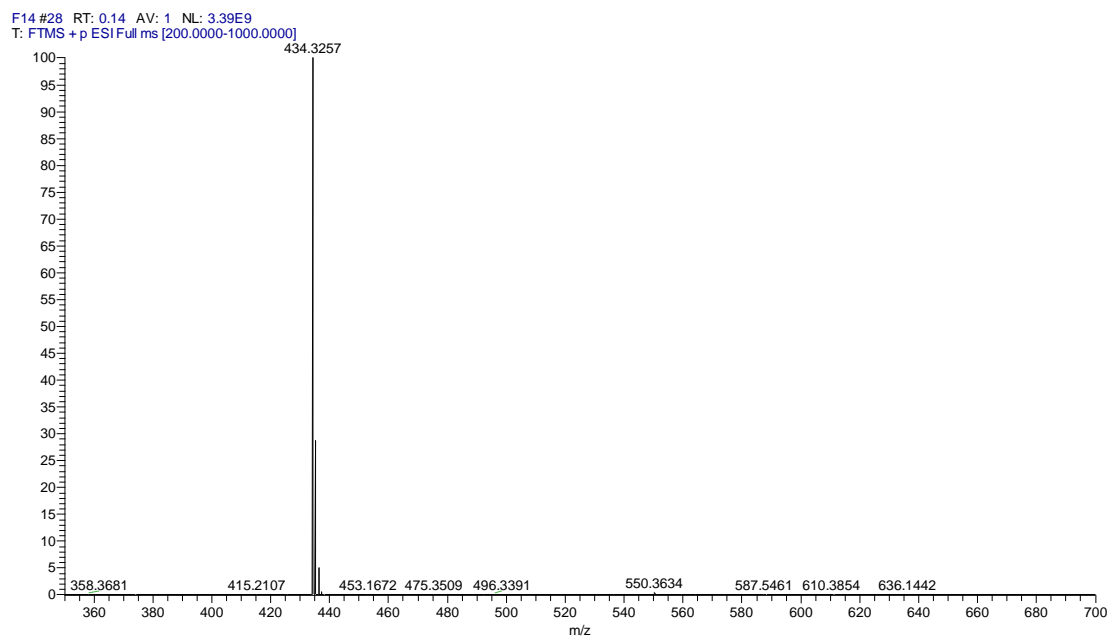


Figure SI 14-3. HR Mass spectrum (ESI) of compound 21.

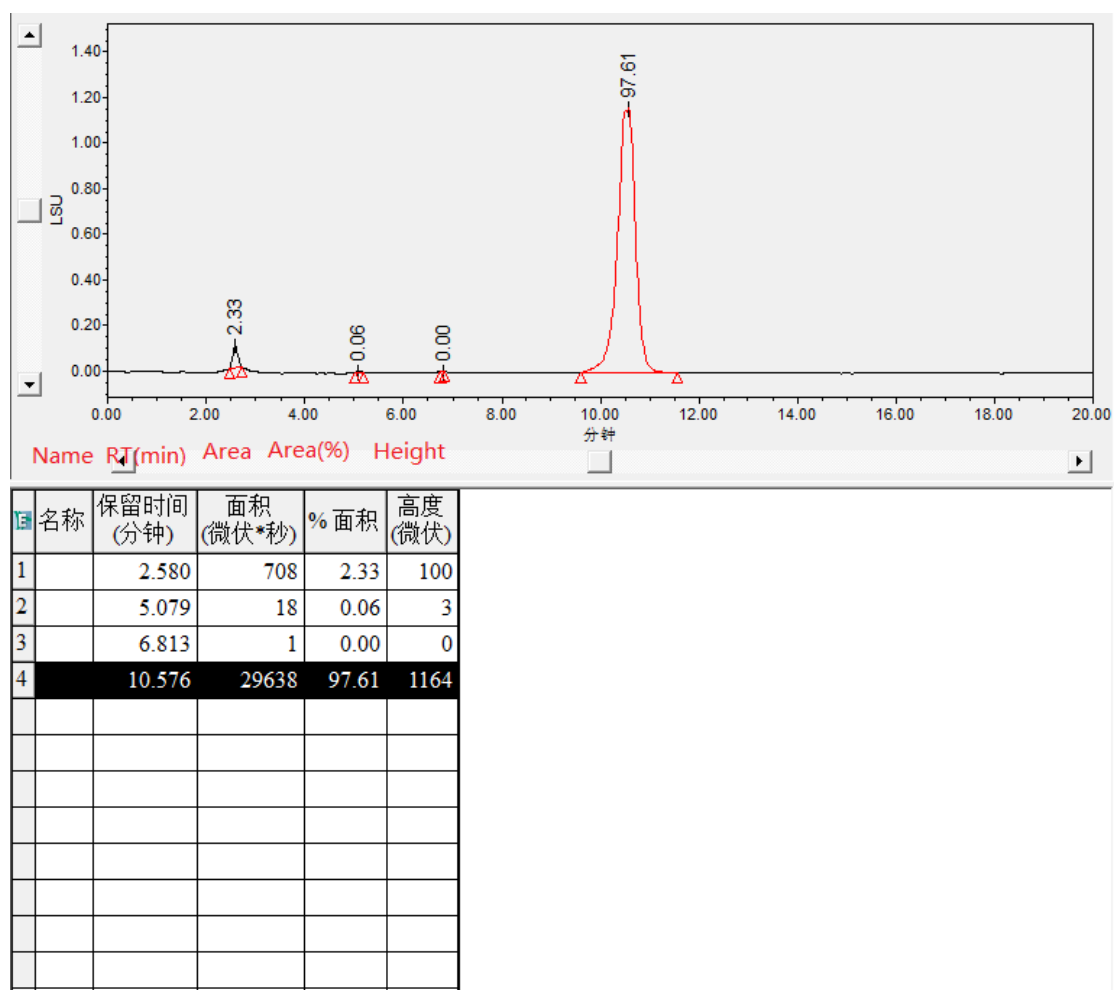
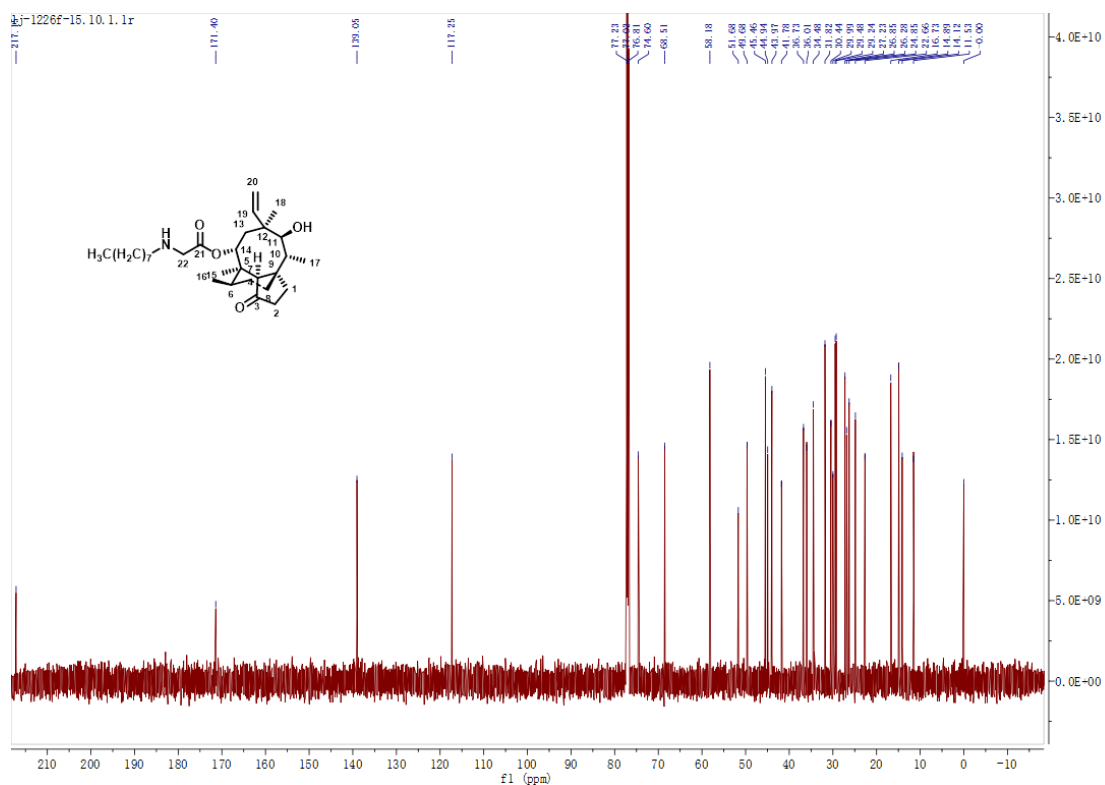
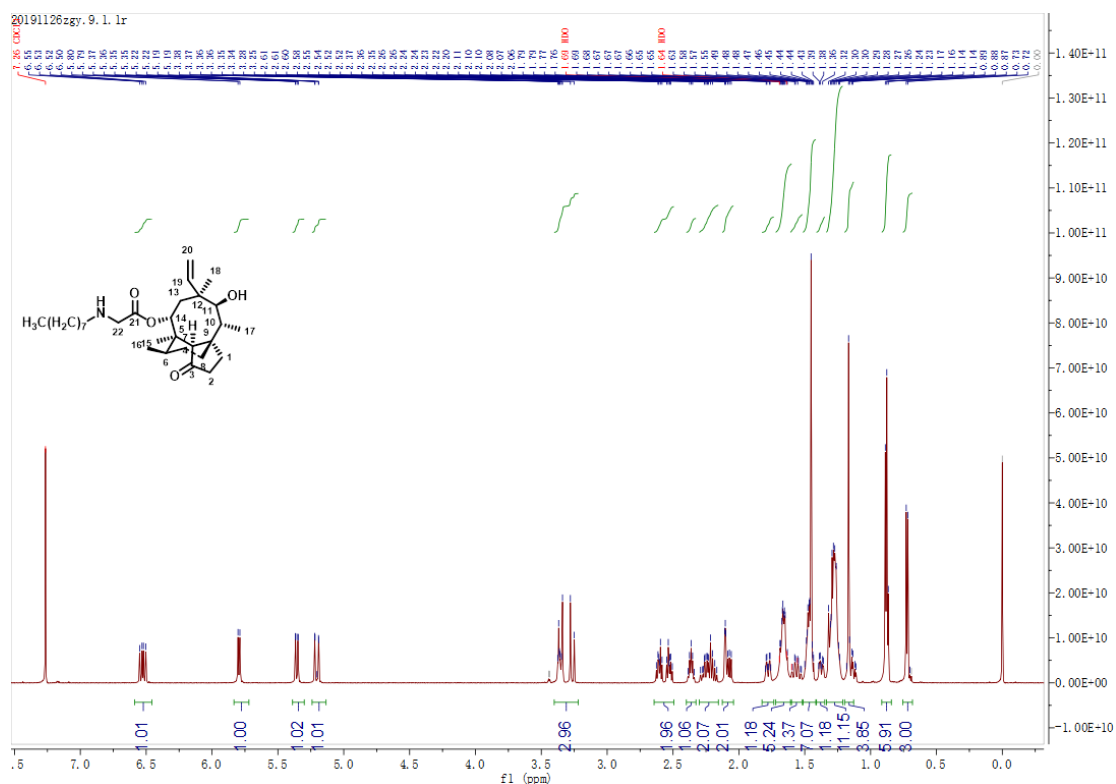


Figure SI 14-4. HPLC of compound 21.



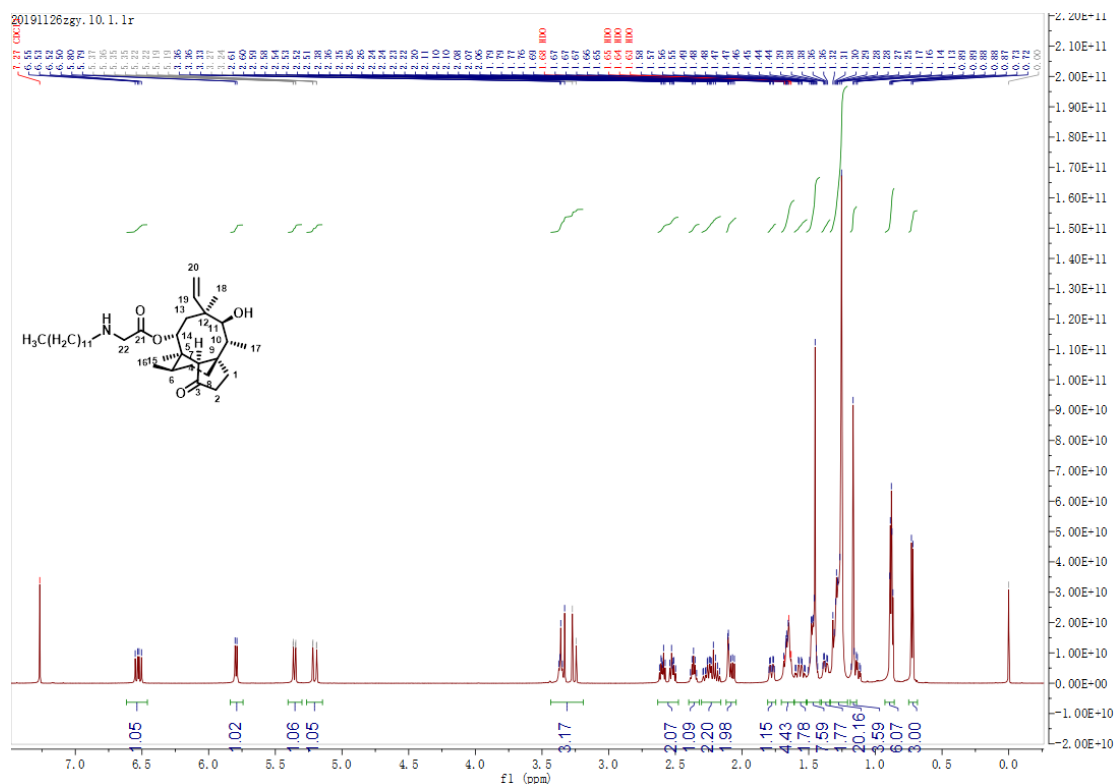


Figure SI 16-1. ¹H-NMR spectrum (CDCl₃, 400MHz) of compound 23.

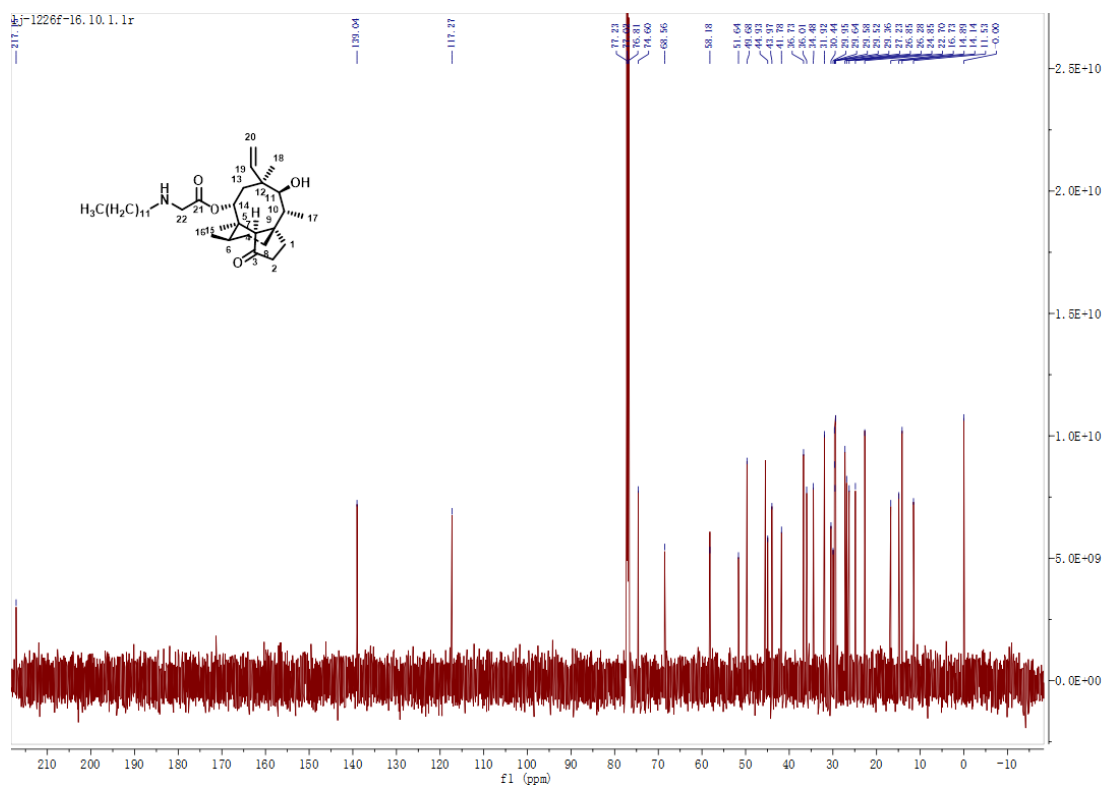
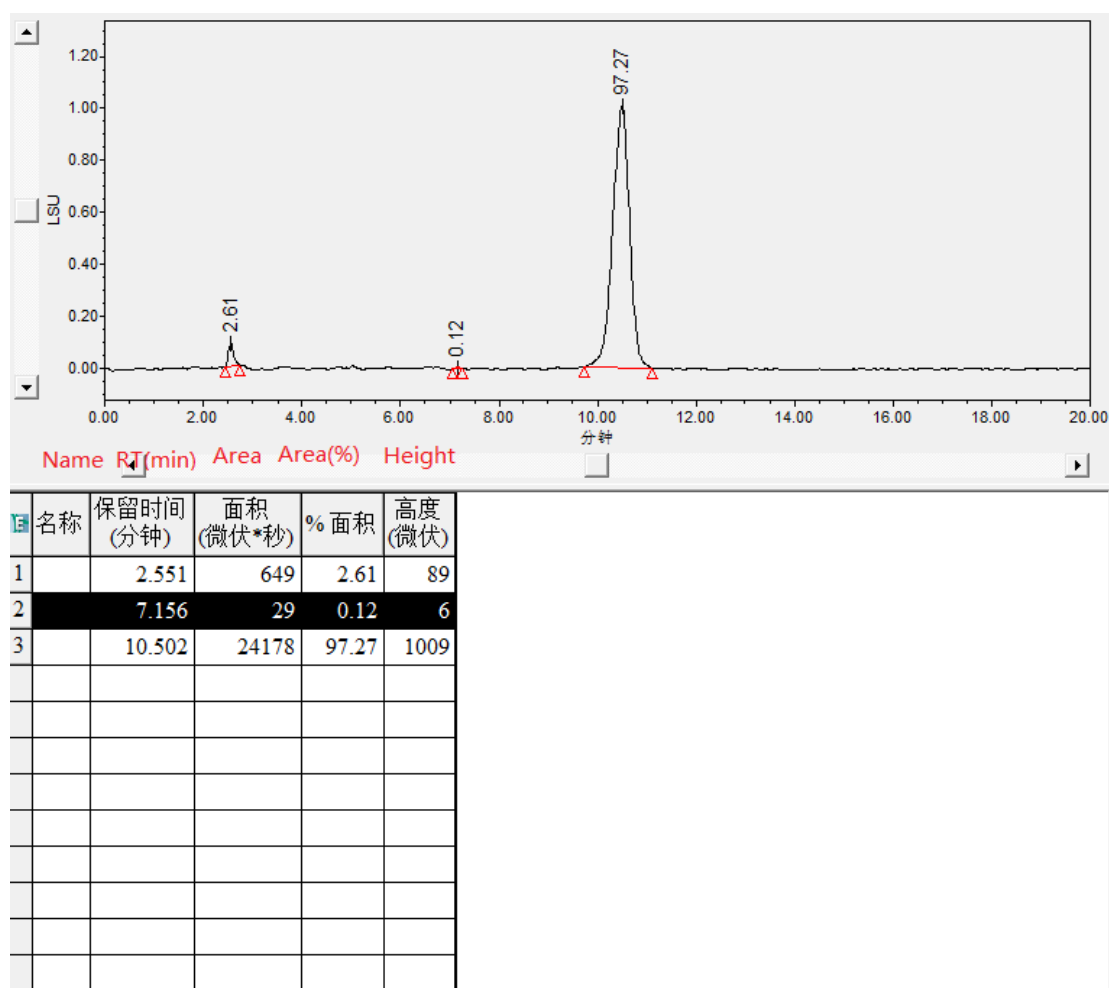
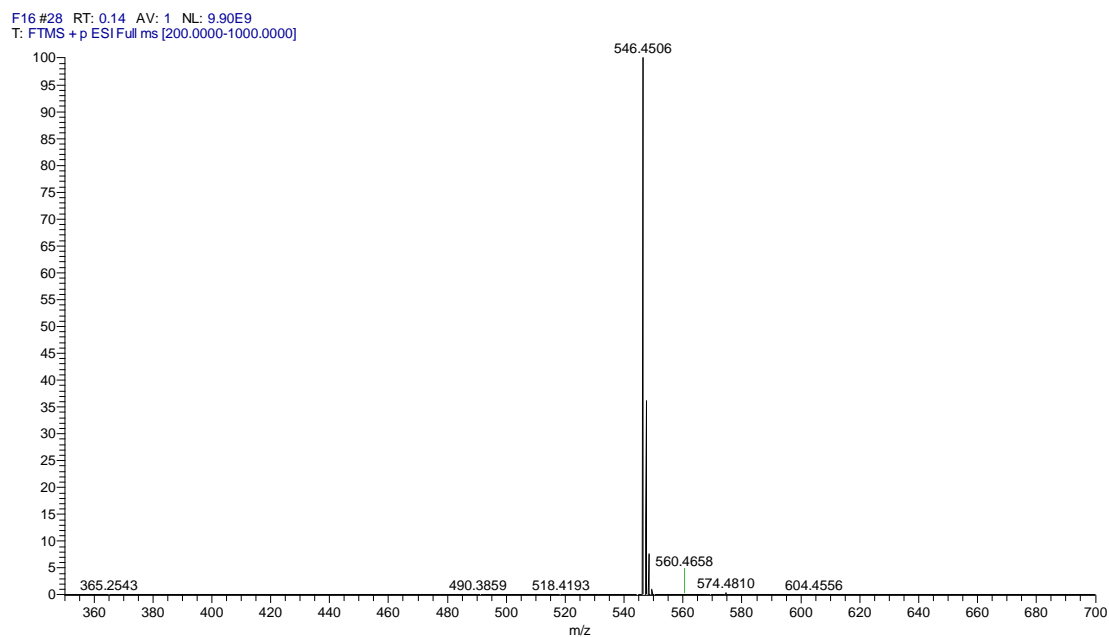


Figure SI 16-2. ¹³C-NMR spectrum (CDCl₃, 101MHz) of compound 23.



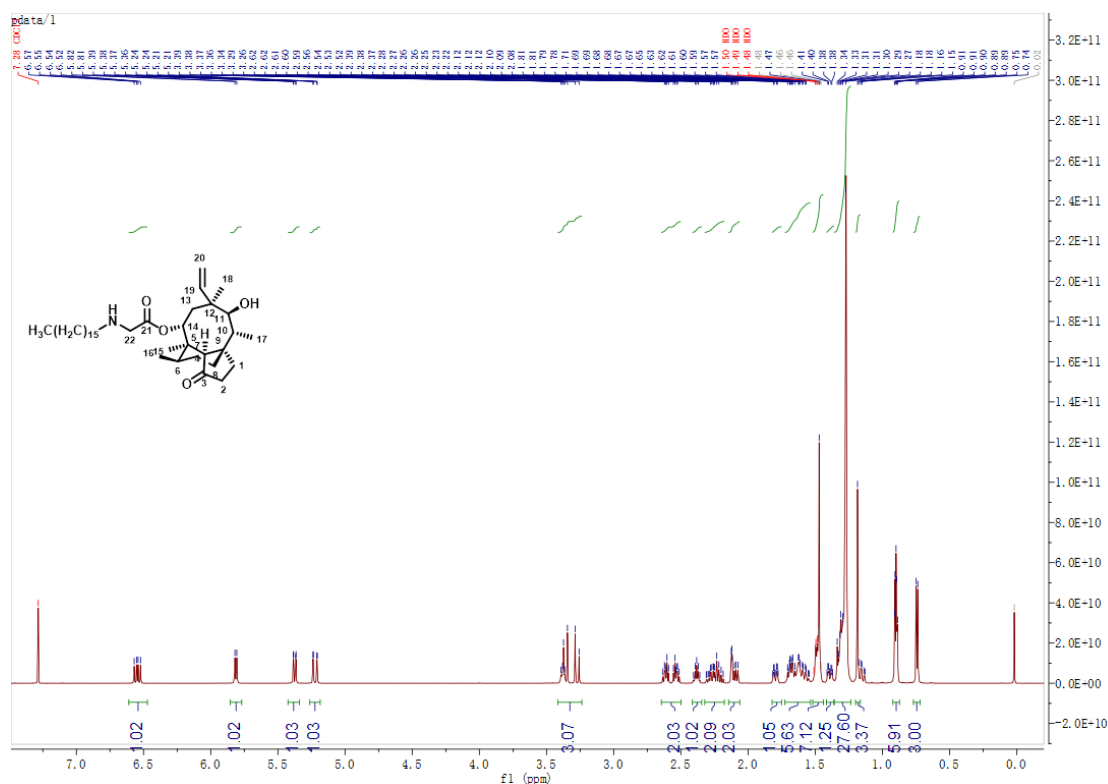


Figure SI 17-1. ^1H -NMR spectrum (CDCl₃, 400MHz) of compound 24.

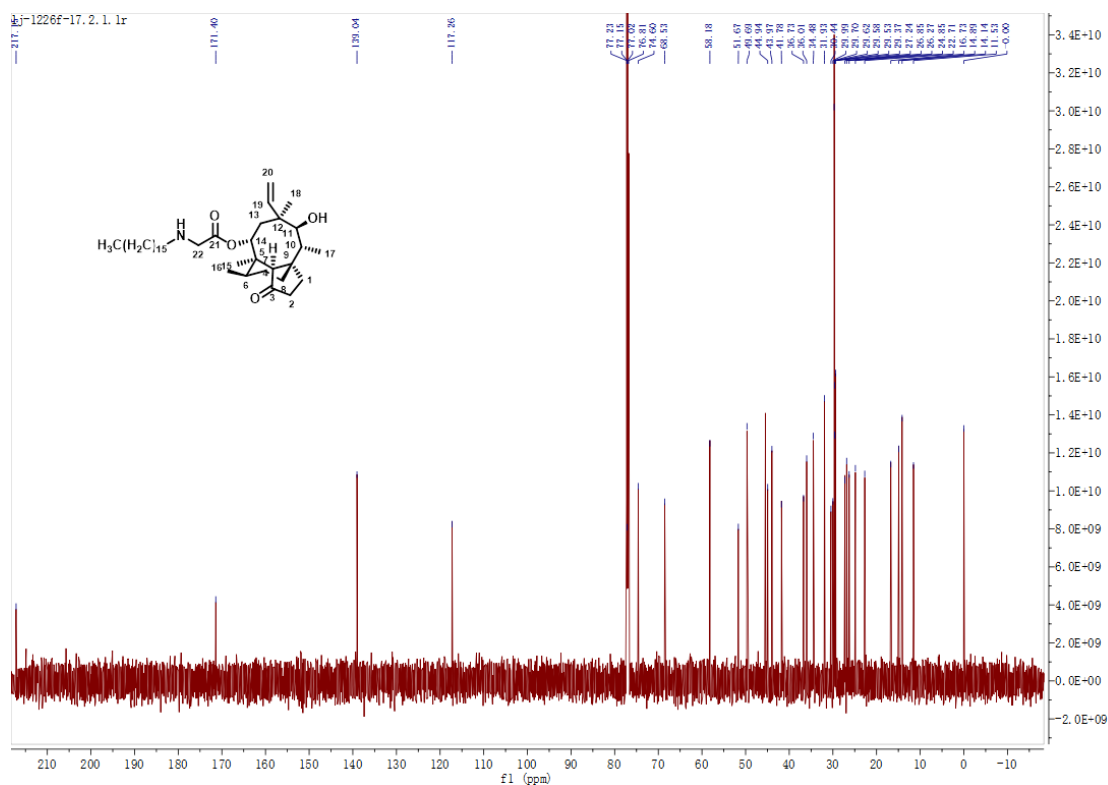


Figure SI 17-2. ^{13}C -NMR spectrum (CDCl₃, 101MHz) of compound 24.

Mass spectrum plot showing relative intensity versus m/z . The x-axis ranges from 360 to 700 m/z , and the y-axis ranges from 0 to 100 relative intensity. The base peak is at m/z 602.5128. Other labeled peaks include 383.1214, 437.1909, 499.4761, 546.4489, 574.4813, 588.4976, 617.5400, and 630.5439.

Name	RT(min)	Area	Area(%)	Height
1	2.580	887	2.60	103
2	6.760	19	0.06	4
3	10.509	33198	97.34	1370

35

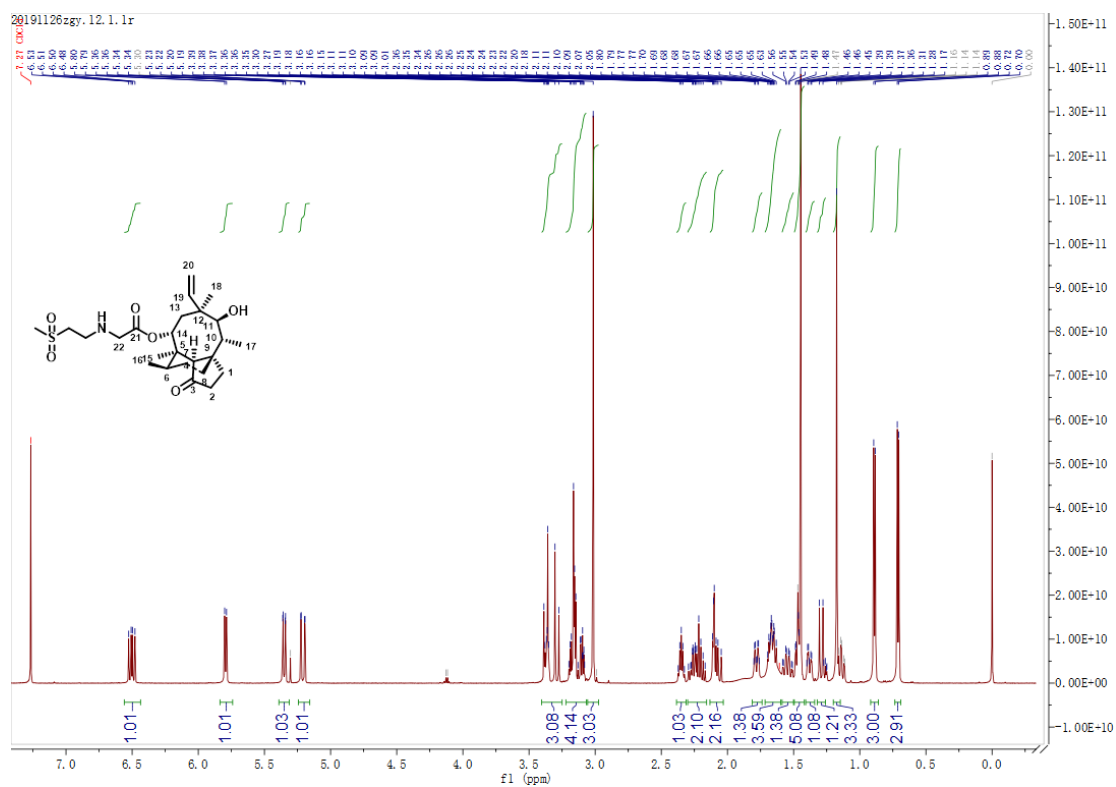


Figure SI 18-1. ^1H -NMR spectrum (CDCl_3 , 400MHz) of compound **25**.

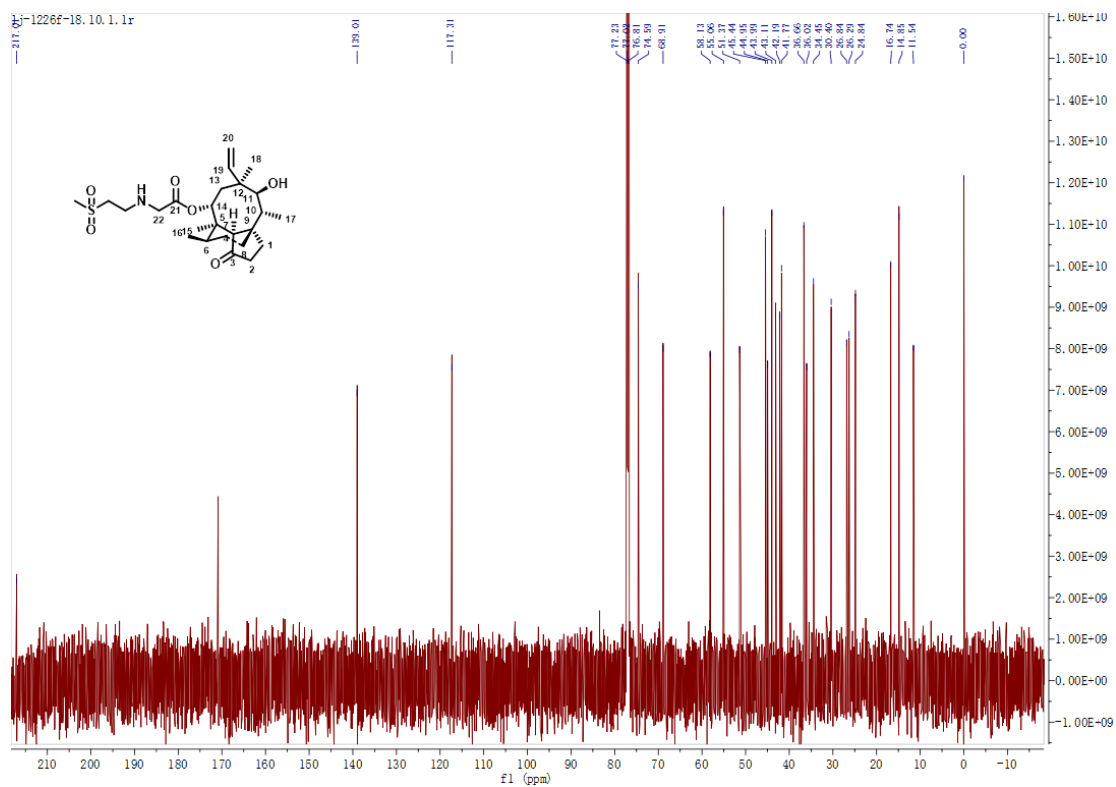


Figure SI 18-2. ^{13}C -NMR spectrum (CDCl_3 , 101MHz) of compound **25**.

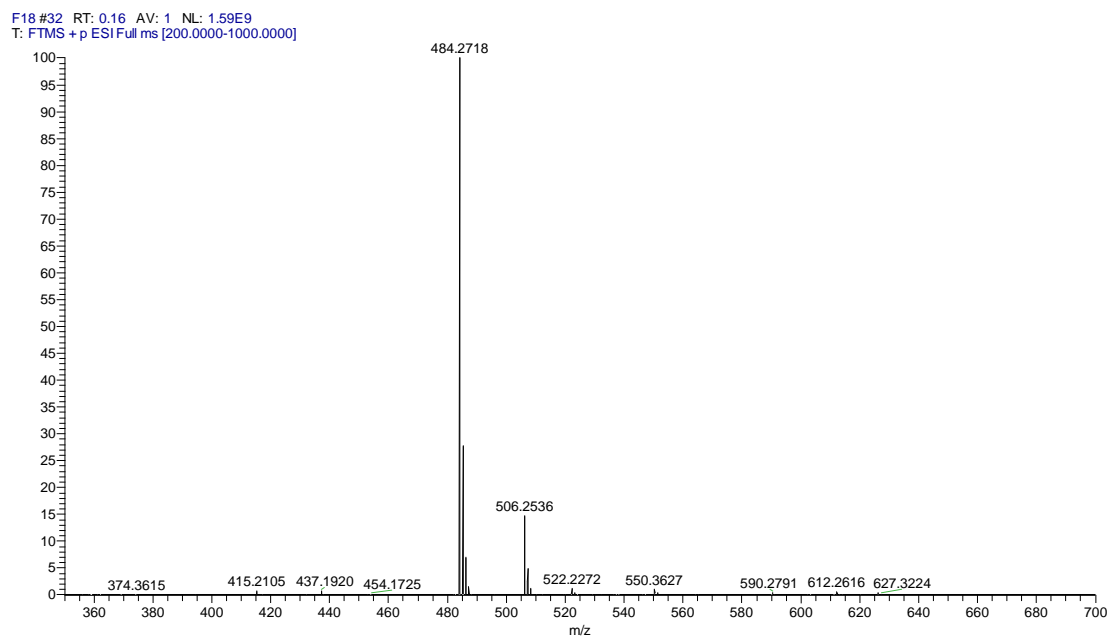


Figure SI 18-3. HR Mass spectrum (ESI) of compound 25.

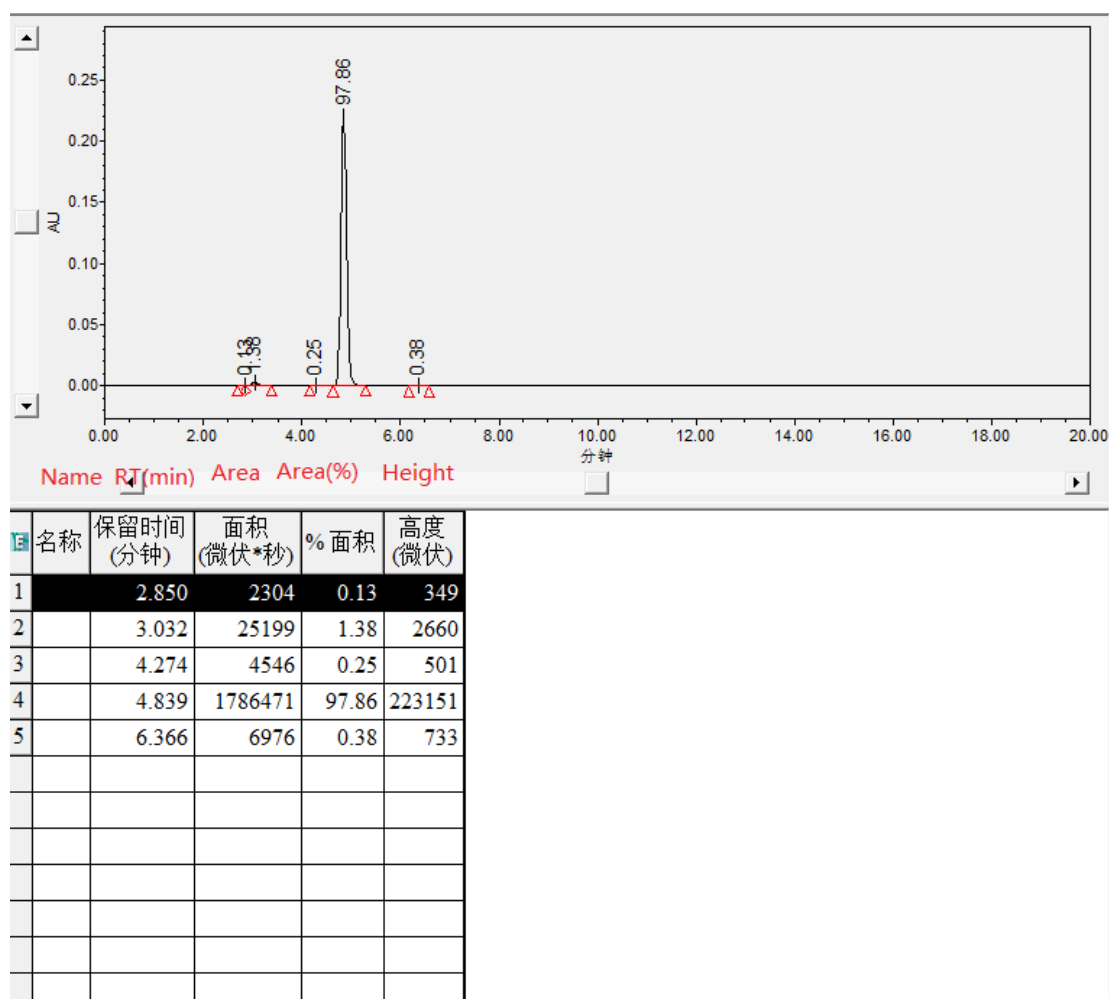


Figure SI 18-4. HPLC of compound 25.

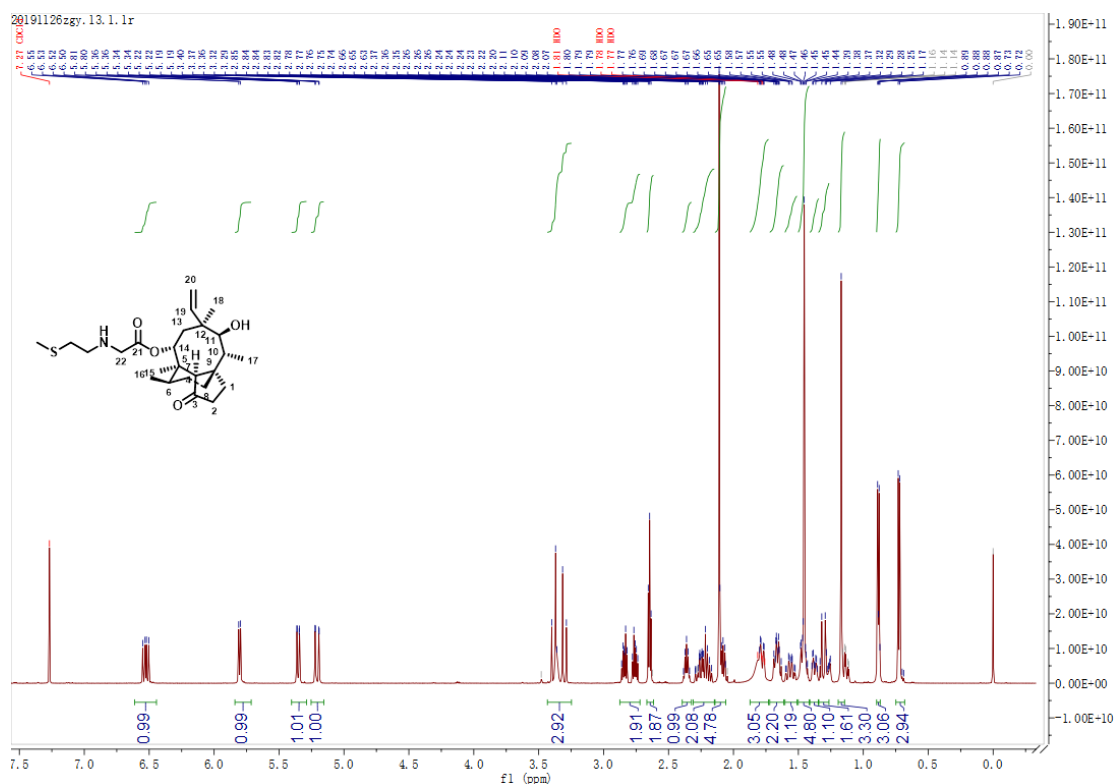


Figure SI 19-1. ^1H -NMR spectrum (CDCl_3 , 400MHz) of compound 26.

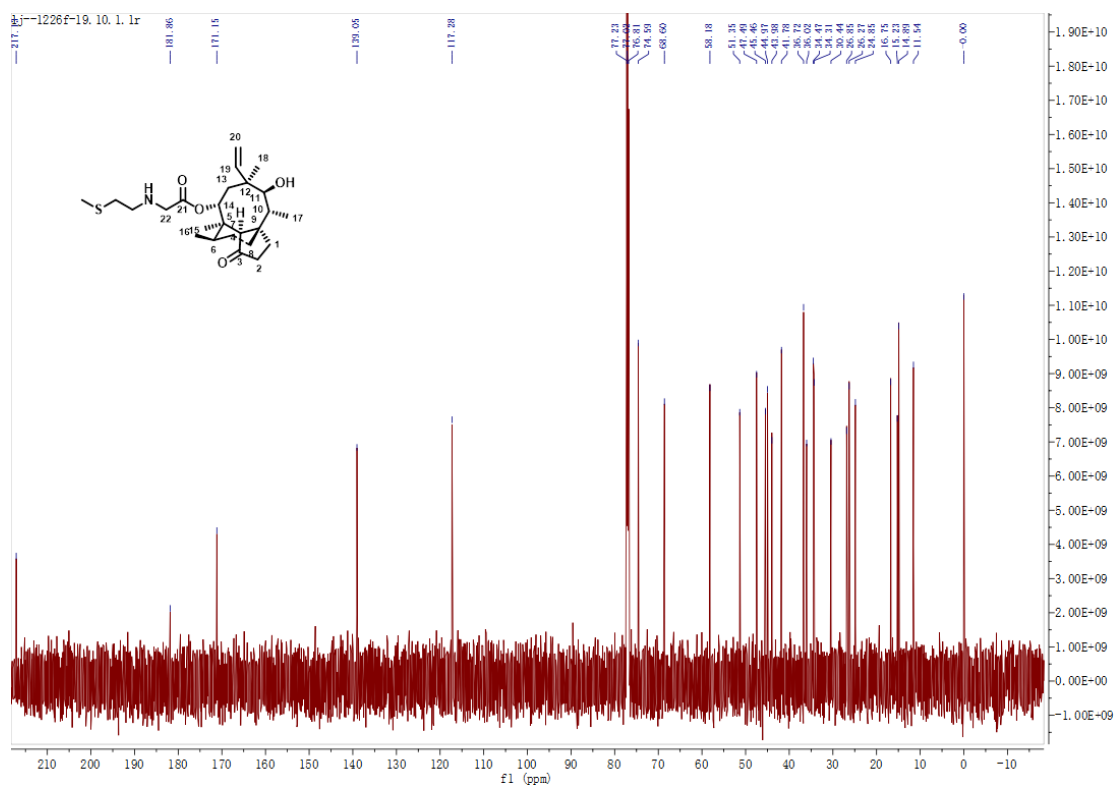


Figure SI 19-2. ^{13}C -NMR spectrum (CDCl_3 , 101MHz) of compound 26.

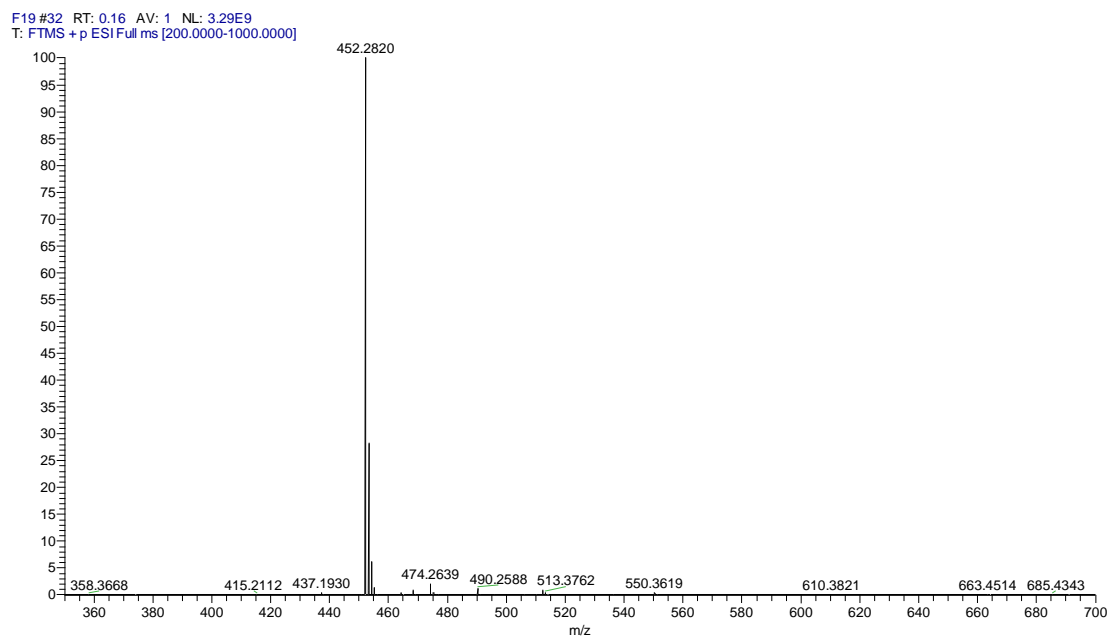


Figure SI 19-3. HR Mass spectrum (ESI) of compound 26.

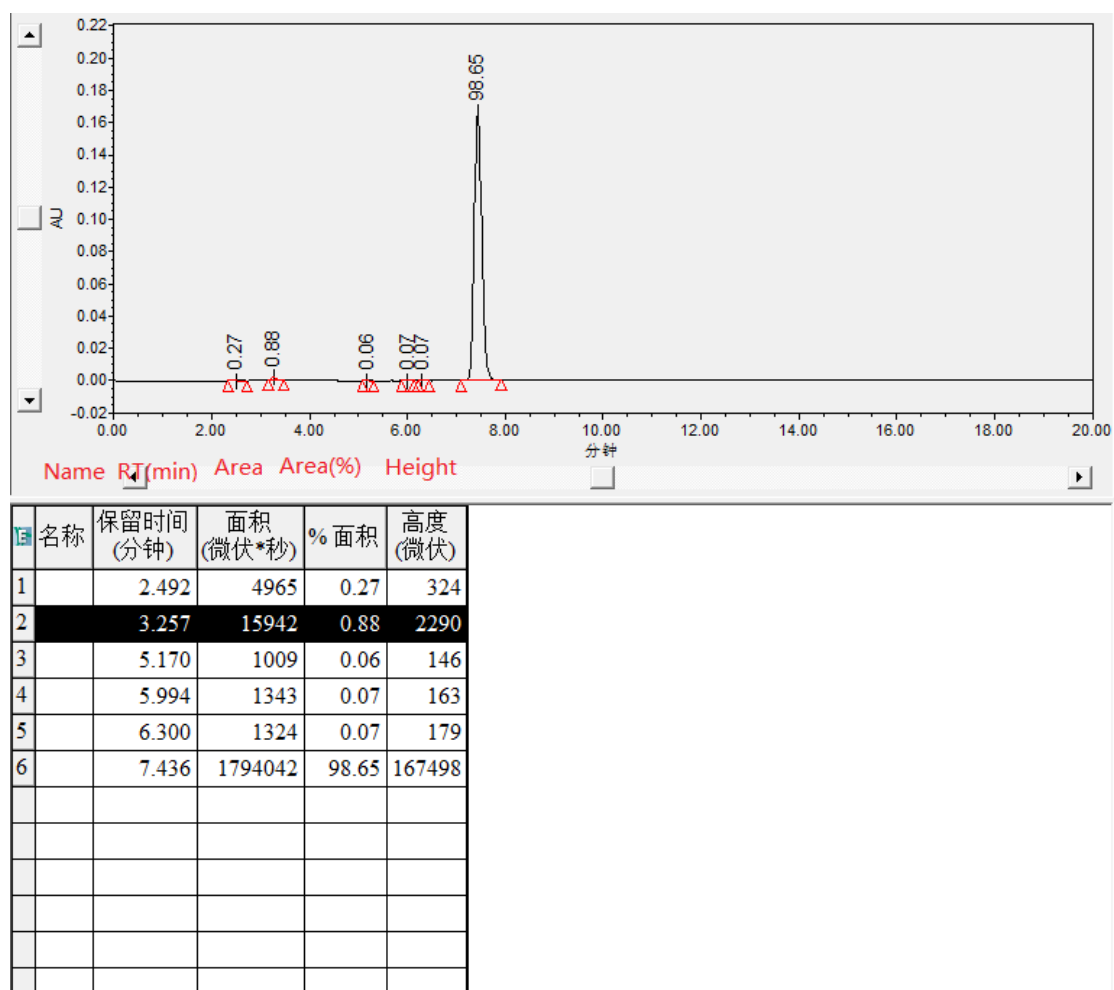


Figure SI 19-4. HPLC of compound 26.

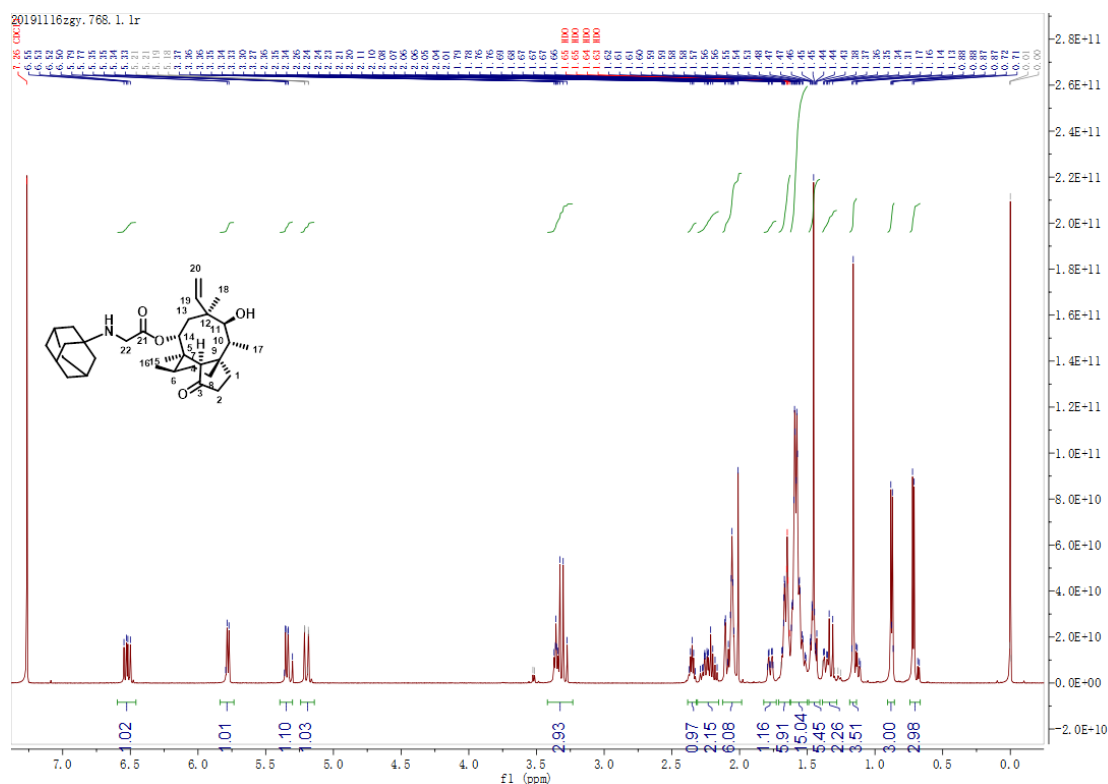


Figure SI 20-1. ^1H -NMR spectrum (CDCl_3 , 400MHz) of compound 27.

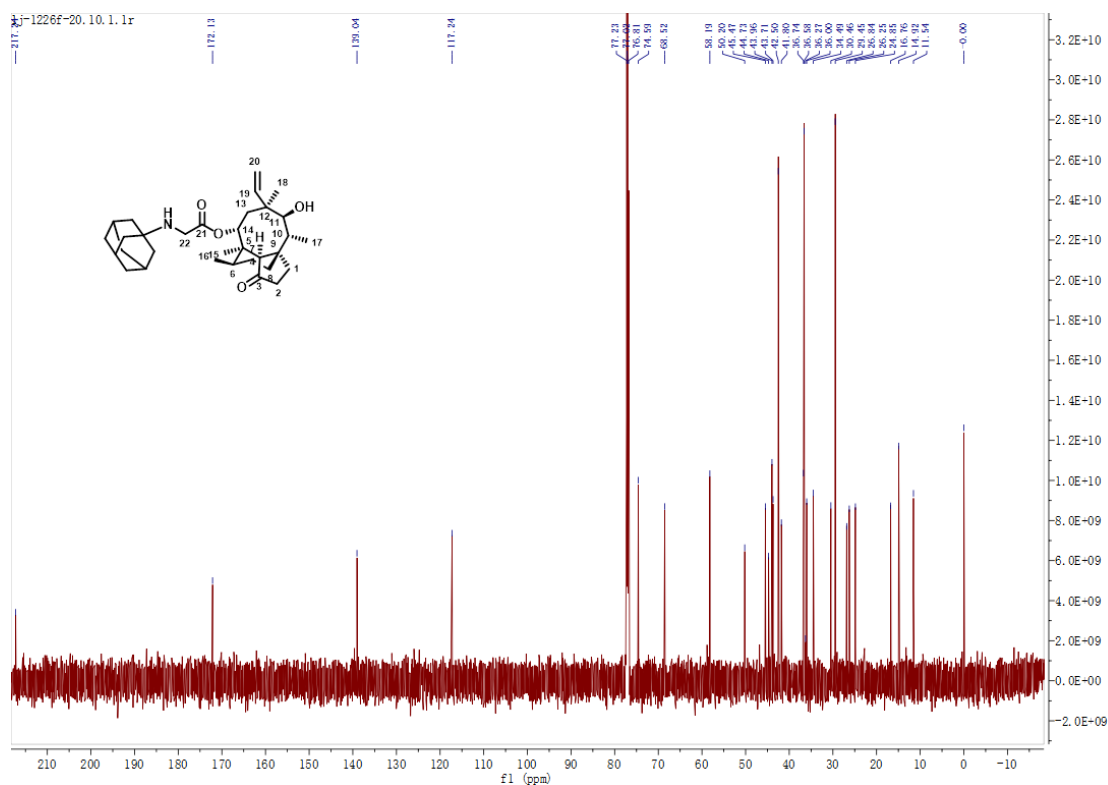


Figure SI 20-2. ^{13}C -NMR spectrum (CDCl_3 , 101MHz) of compound 27.

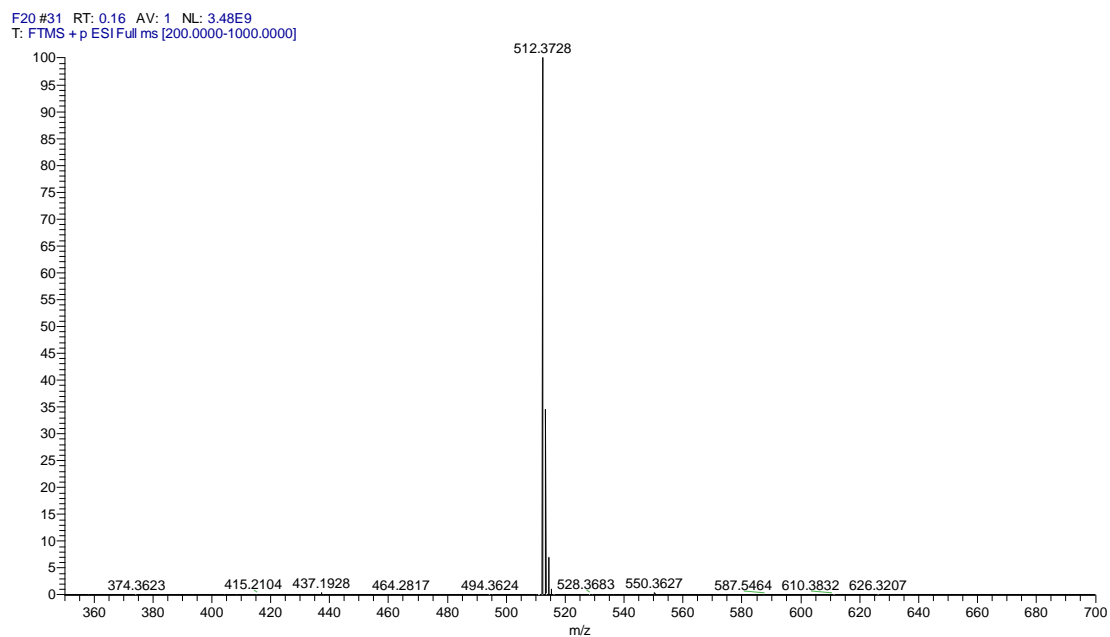


Figure SI 20-3. HR Mass spectrum (ESI) of compound 27.

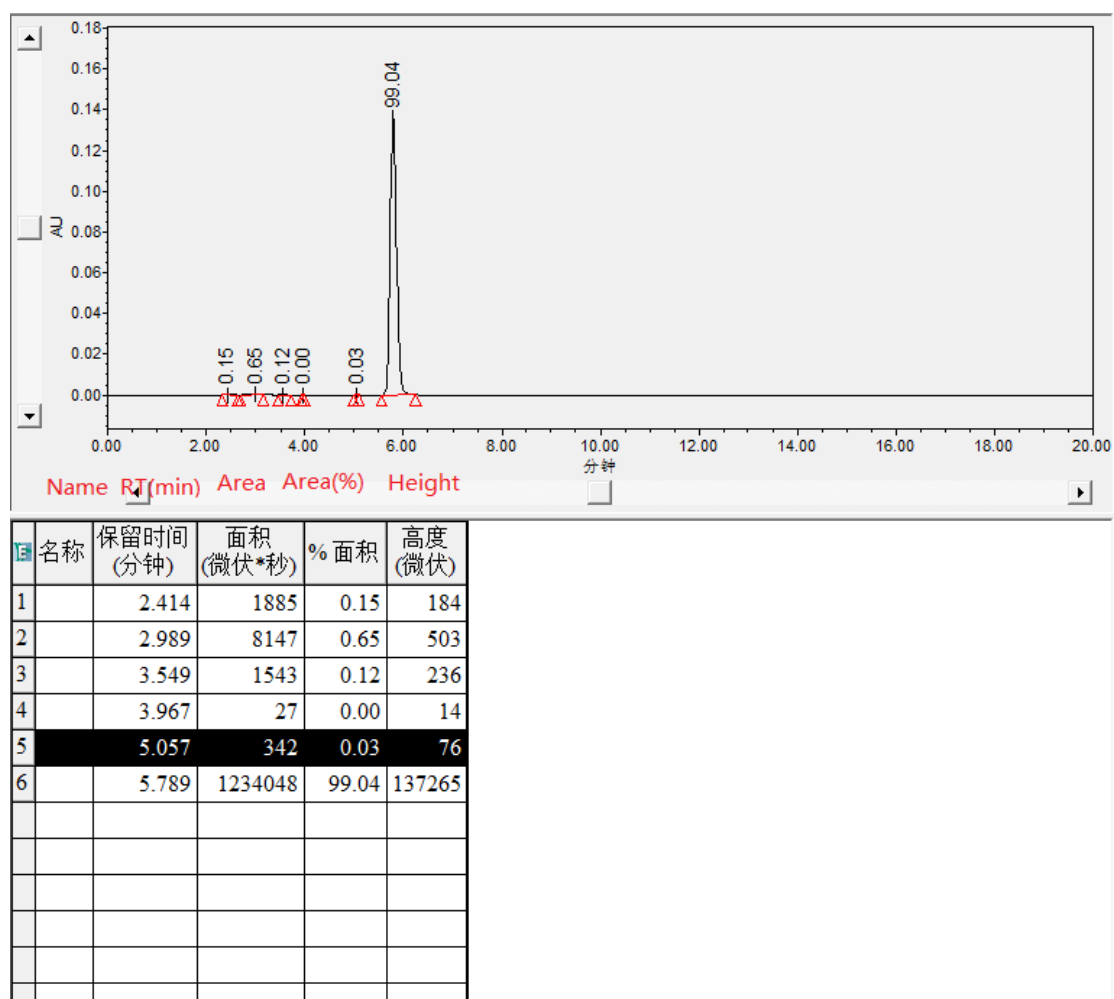
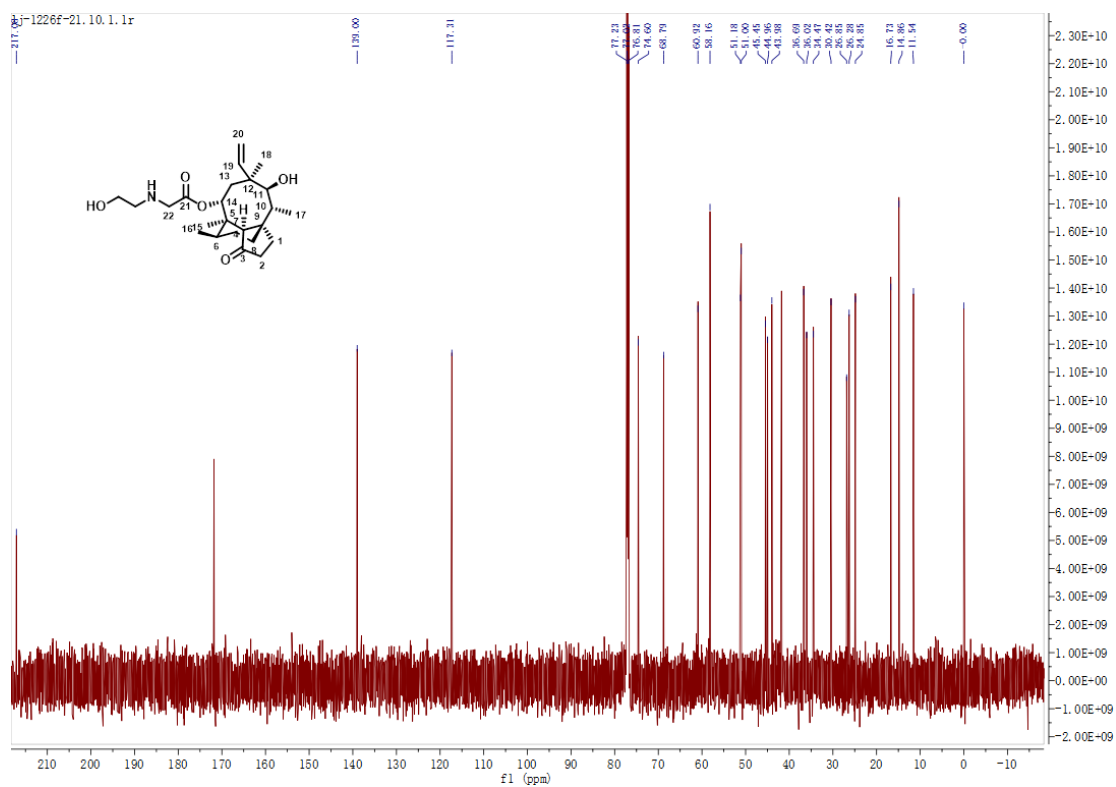
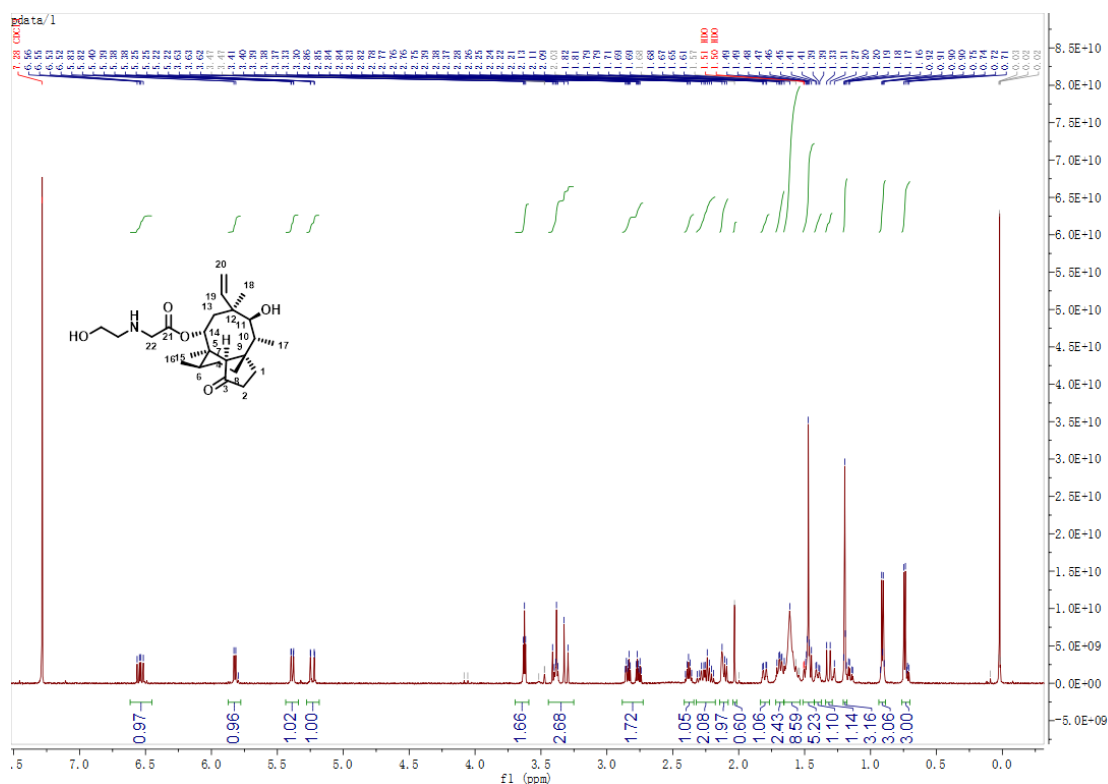


Figure SI 20-4. HPLC of compound 27.



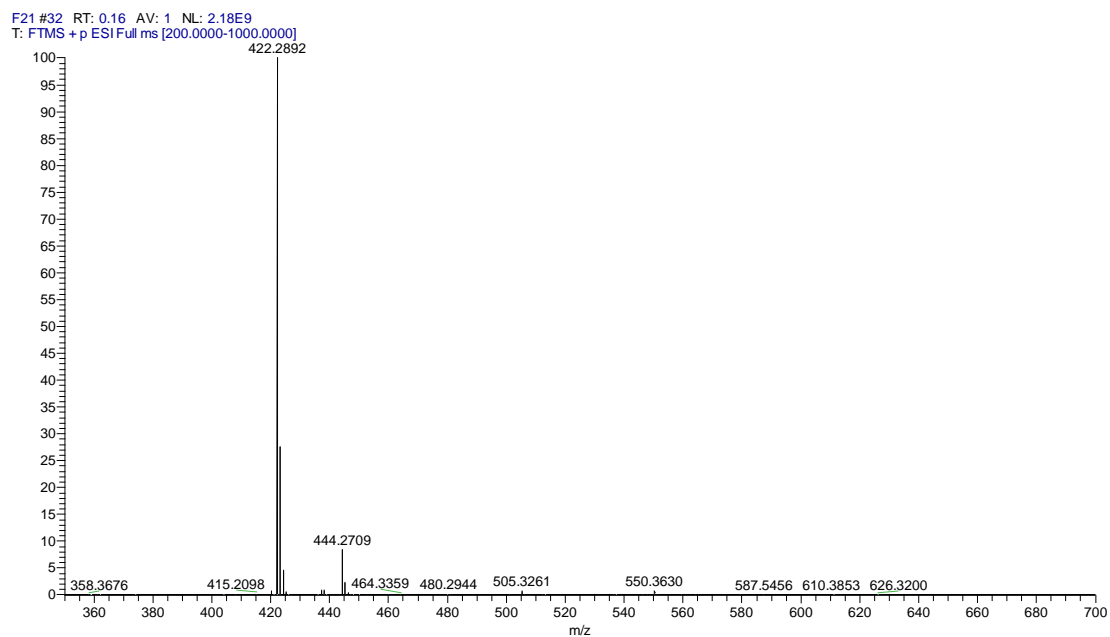


Figure SI 21-3. HR Mass spectrum (ESI) of compound 28.

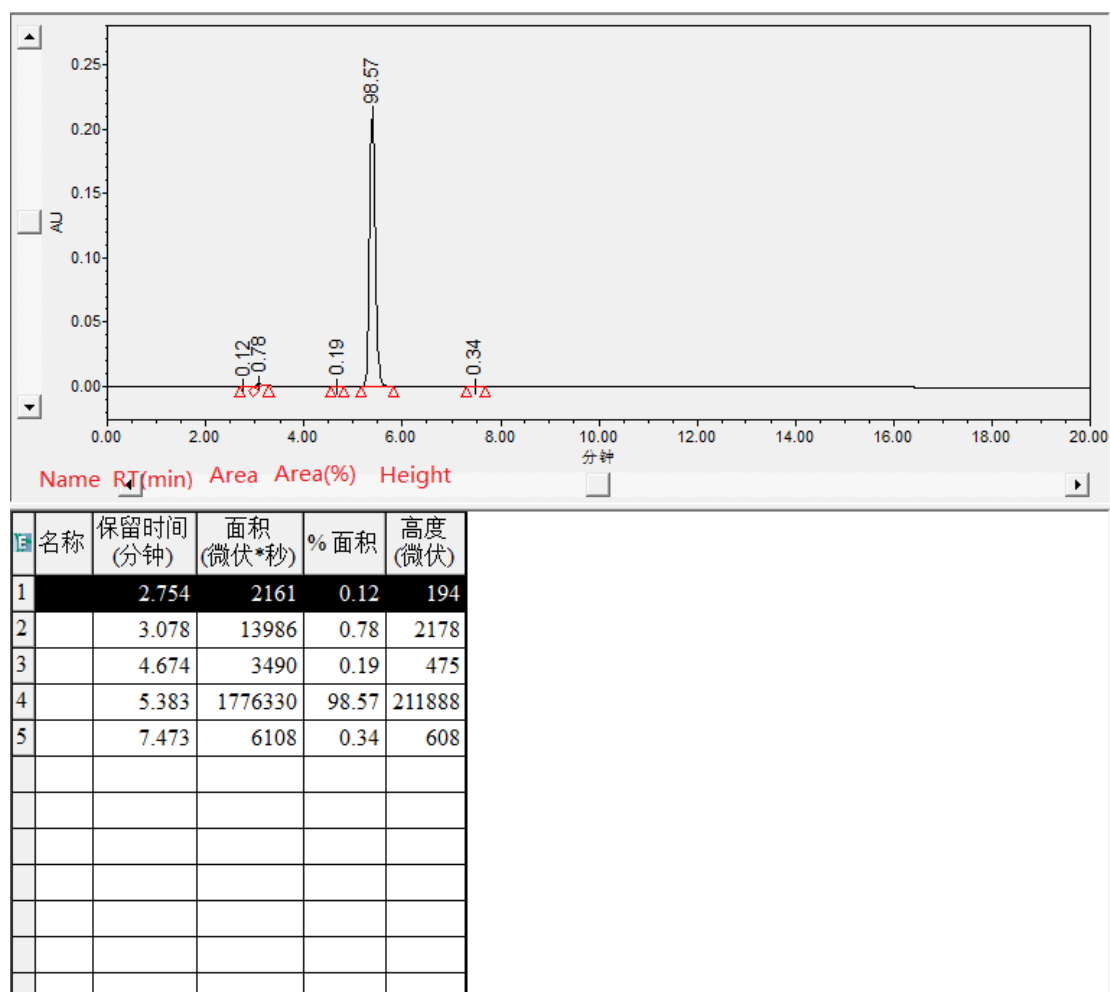


Figure SI 21-4. HPLC of compound 28.

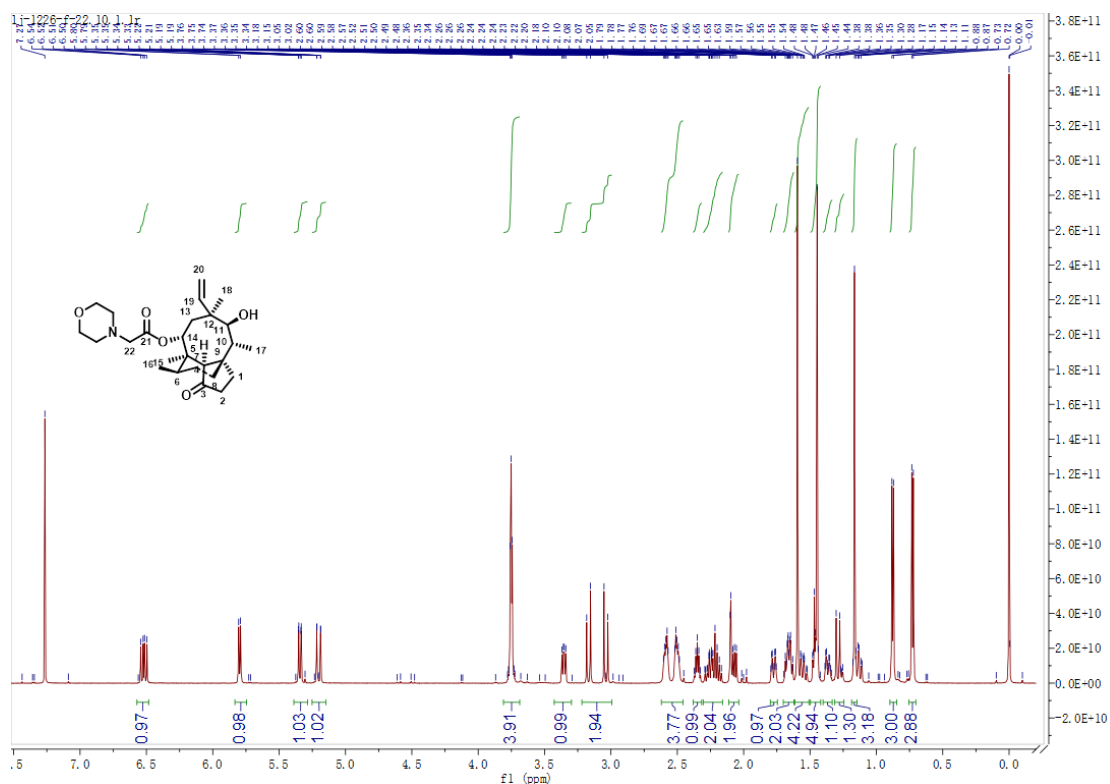


Figure SI 22-1. ^1H -NMR spectrum (CDCl₃, 400MHz) of compound **29**.

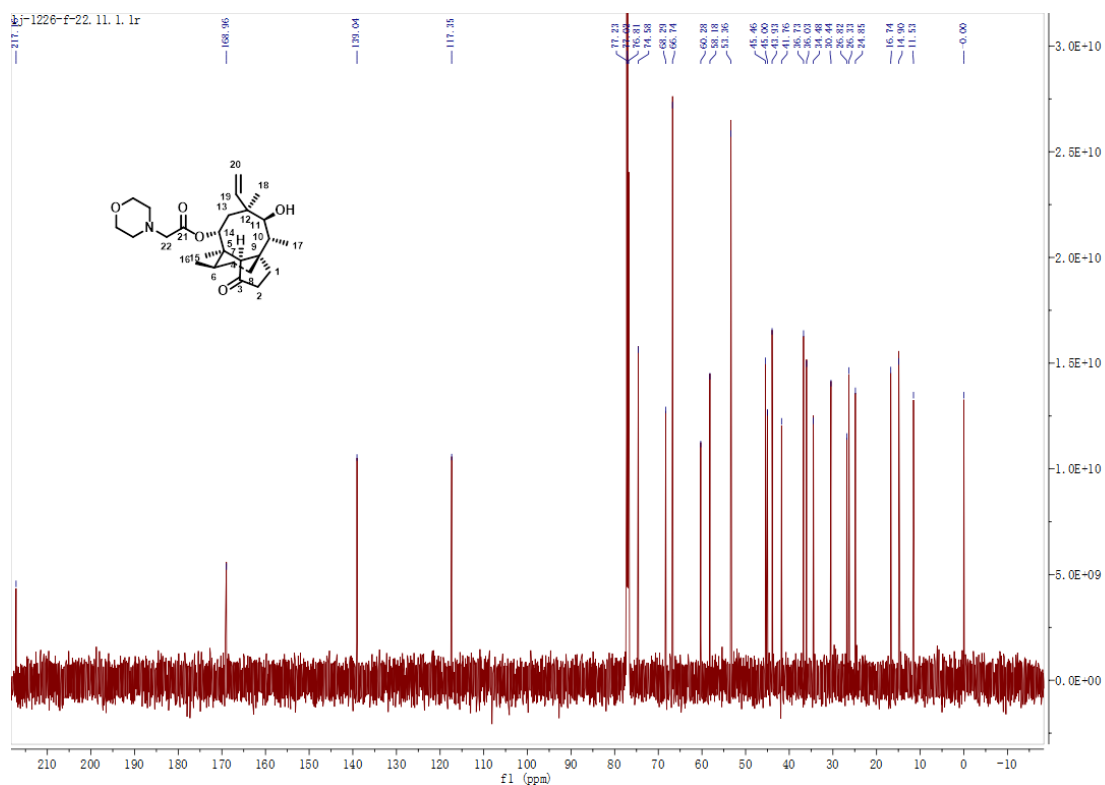


Figure SI 22-2. ^{13}C -NMR spectrum (CDCl₃, 101MHz) of compound **29**.

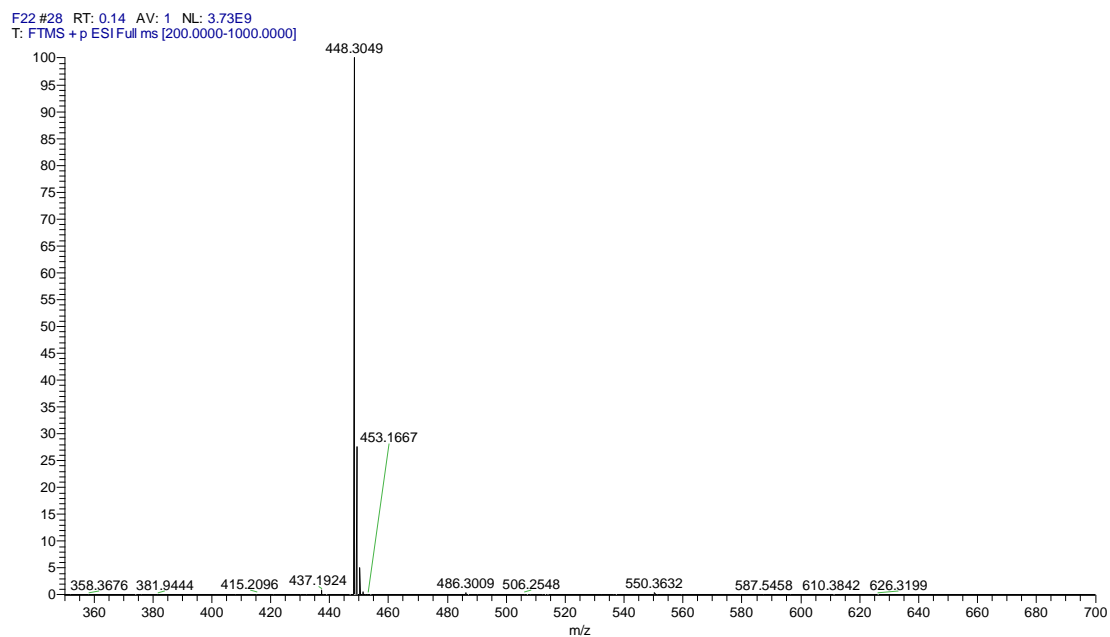


Figure SI 22-3. HR Mass spectrum (ESI) of compound 29.

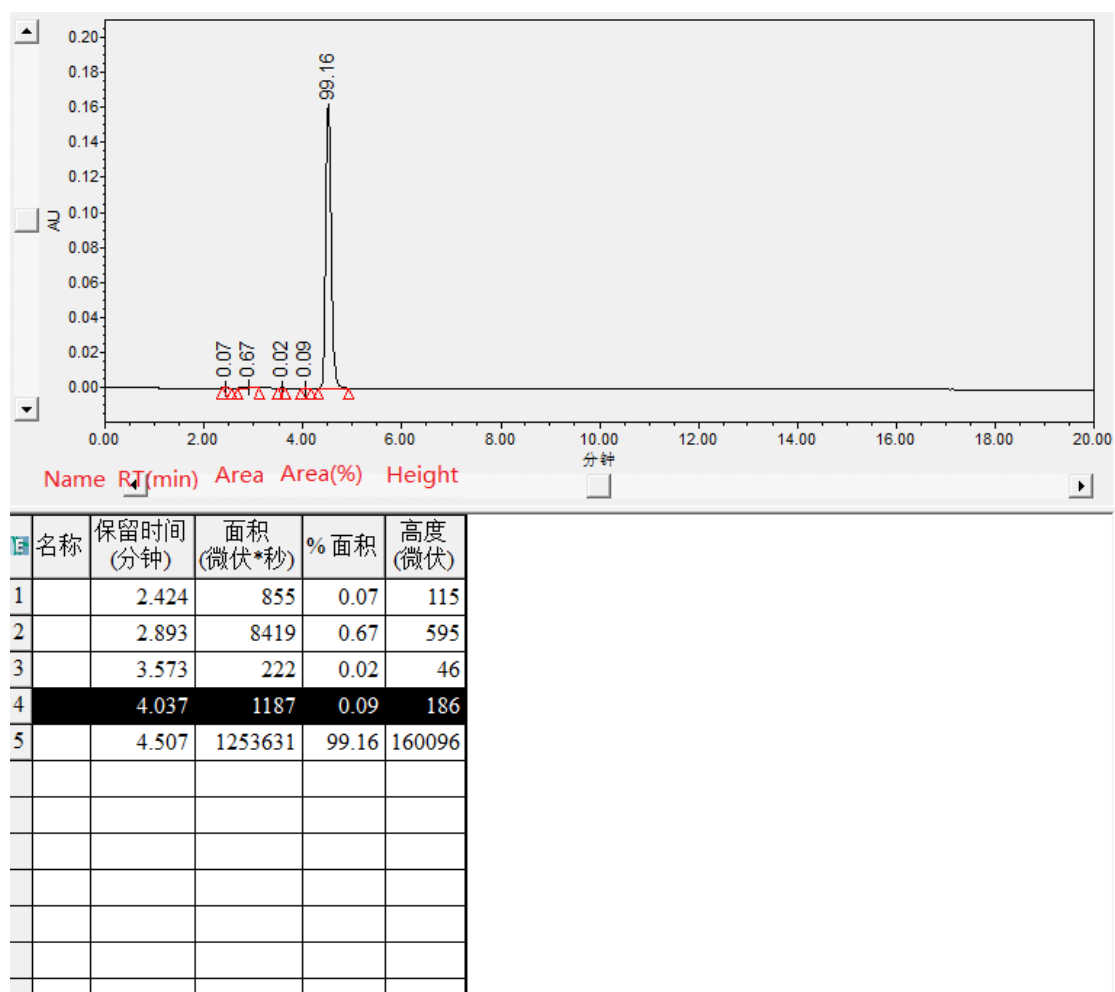
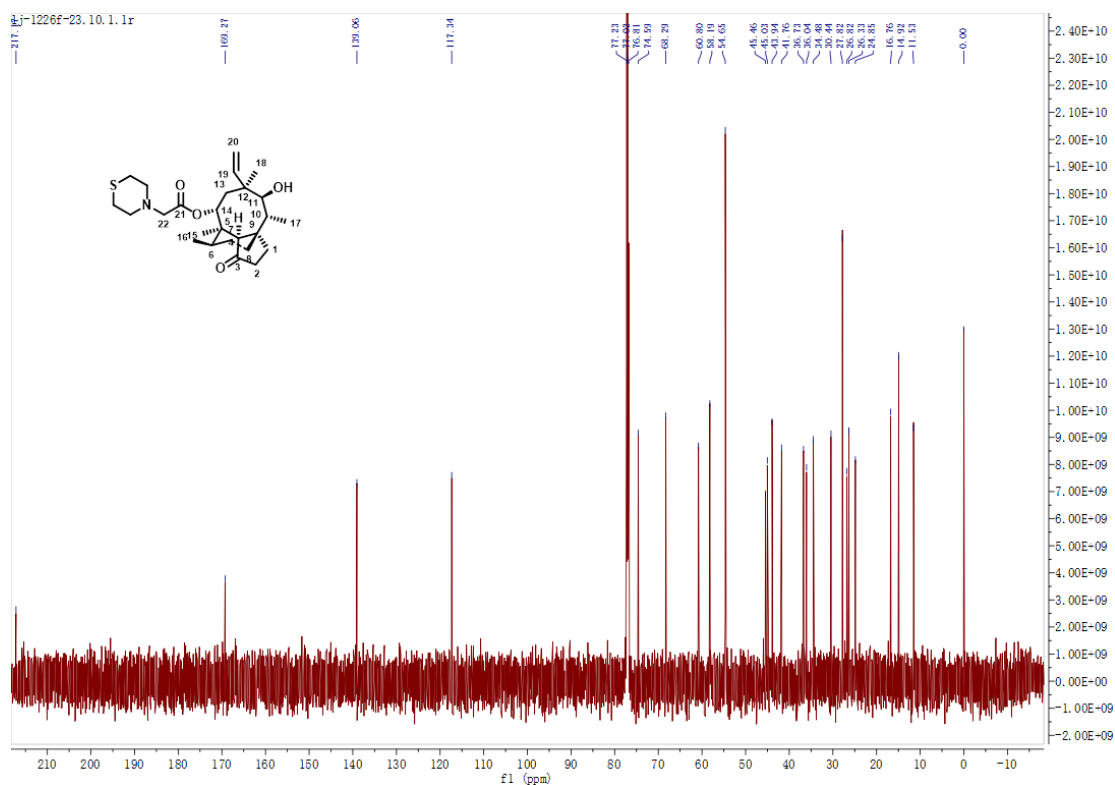
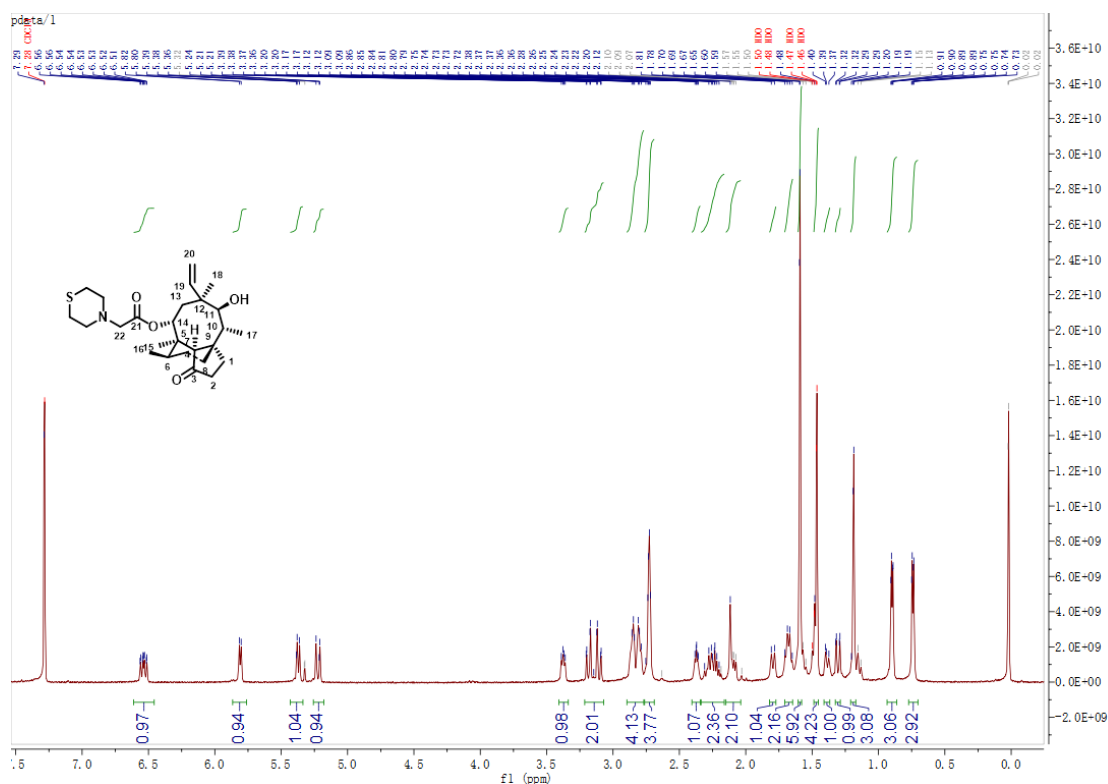


Figure SI 22-4. HPLC of compound 29.



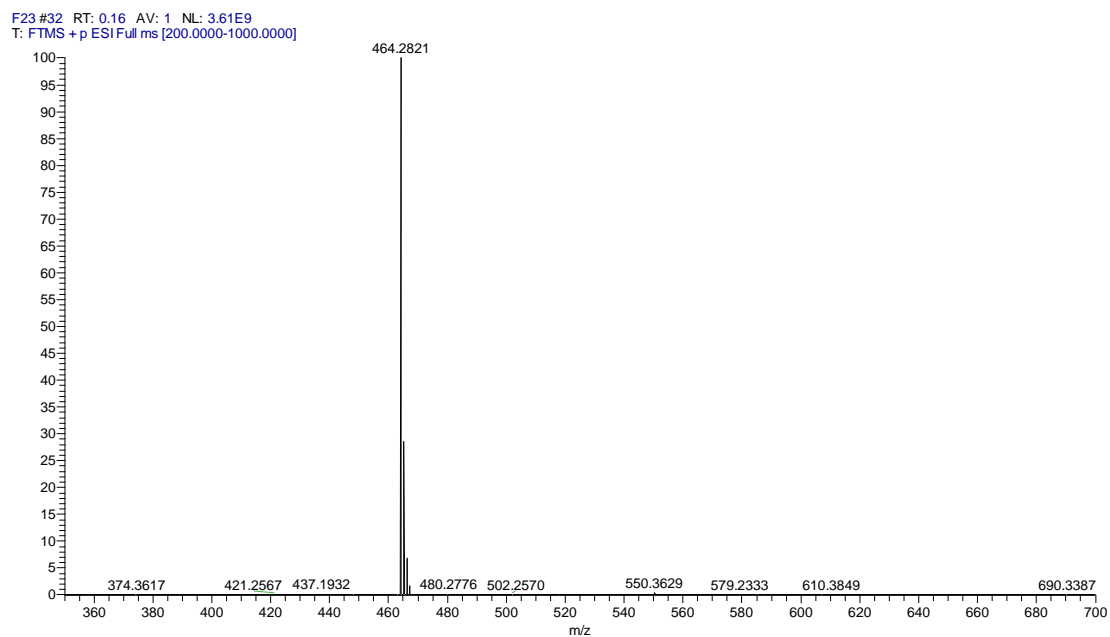


Figure SI 23-3. HR Mass spectrum (ESI) of compound 30.

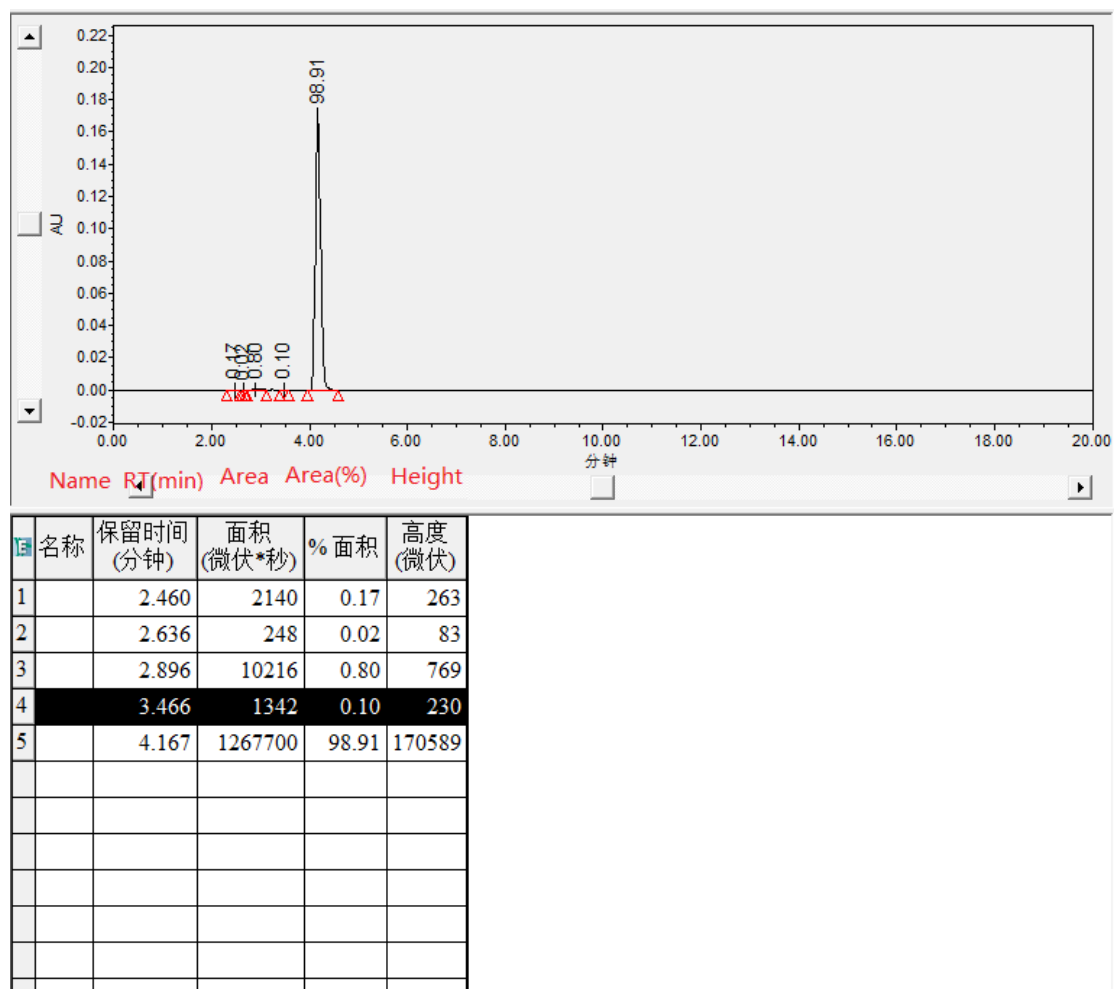


Figure SI 23-4. HPLC of compound 30.

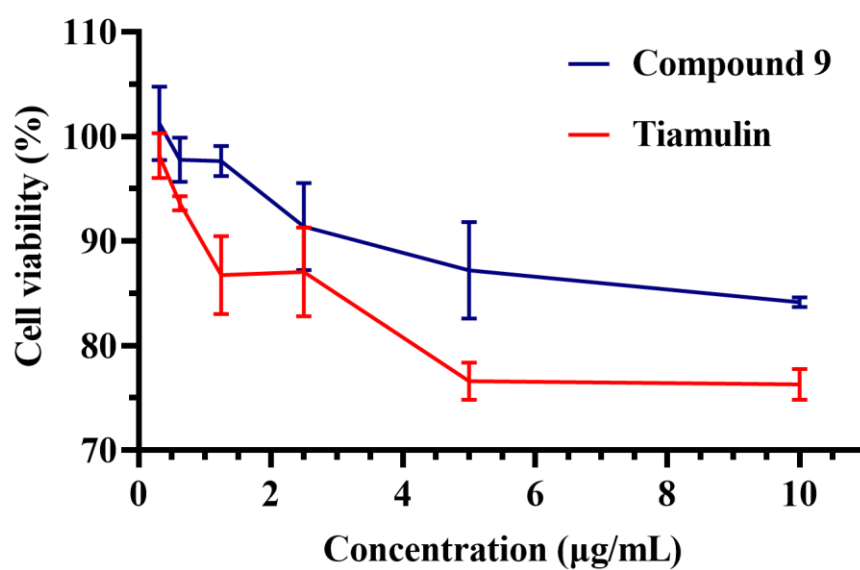


Figure SI 24. The cytotoxicity assay of compound **9** and tiamulin to RAW 264.7 cells.