

## **Supporting Information**

### **Preparation, COX-2 Inhibition and Potent Anticancer Activity of Sclerotiorin Derivatives**

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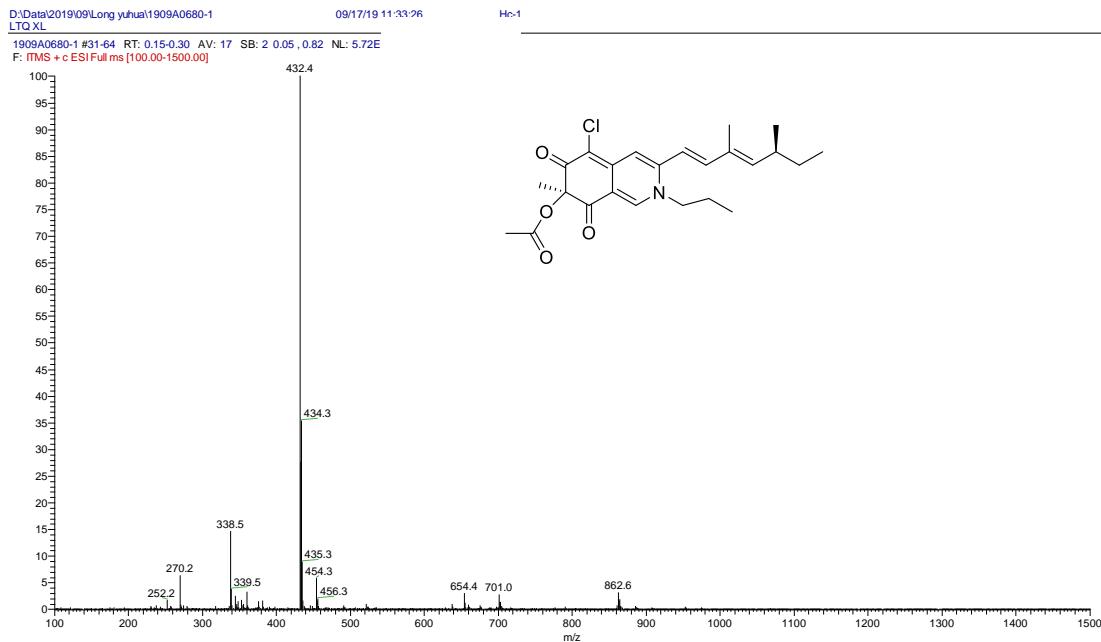
\* Correspondence: [longyh@scnu.edu.cn](mailto:longyh@scnu.edu.cn) (Y.L.); [yuanjie@mail.sysu.edu.cn](mailto:yuanjie@mail.sysu.edu.cn) (J. Y.)

## CONTENT

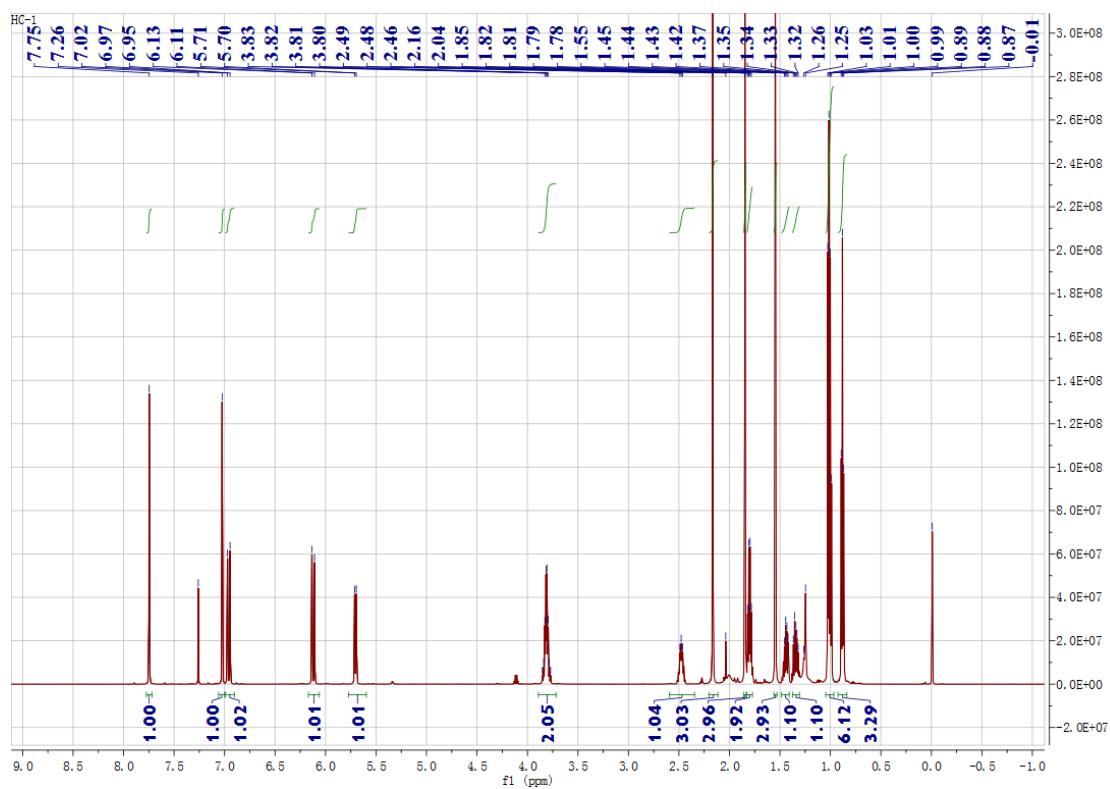
Fig.S1. MS spectrum of compound 1.....	1
Fig.S2. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 1 .....	1
Fig.S3. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 1 .....	2
Fig.S4. MS spectrum of compound 2.....	2
Fig.S5. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 2 .....	3
Fig.S6. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 2 .....	3
Fig.S7. HRMS spectrum of compound 3 .....	4
Fig.S8. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 3 .....	4
Fig.S9. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 3 .....	5
Fig.S10. HRMS spectrum of compound 4 .....	5
Fig.S11. $^1\text{H}$ NMR (600 MHz, $\text{CD}_3\text{OD}$ ) spectrum of compound 4 .....	6
Fig.S12. $^{13}\text{C}$ NMR (150 MHz, $\text{CD}_3\text{OD}$ ) spectrum of compound 4 .....	6
Fig.S13. HRMS spectrum of compound 5 .....	7
Fig.S14. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 5 .....	7
Fig.S15. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 5 .....	8
Fig.S16. HRMS spectrum of compound 6 .....	8
Fig.S17. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 6 .....	9
Fig.S18. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 6 .....	9
Fig.S19. HRMS spectrum of compound 7 .....	10
Fig.S20. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 7 .....	10
Fig.S21. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 7 .....	11
Fig.S22. HRMS spectrum of compound 8 .....	11
Fig.S23. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 8 .....	12
Fig.S24. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 8 .....	12
Fig.S25. MS spectrum of compound 9.....	13
Fig.S26. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 9 .....	13
Fig.S27. HRMS spectrum of compound 10 .....	14
Fig.S28. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 10 .....	14
Fig.S29. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 10.....	15
Fig.S30. HRMS spectrum of compound 11 .....	15
Fig.S31. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 11 .....	16
Fig.S32. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 11 .....	16
Fig.S33. MS spectrum of compound 12.....	17

Fig.S34. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 12 .....	17
Fig.S35. HRMS spectrum of compound 13 .....	18
Fig.S36. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 13 .....	18
Fig.S37. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 13 .....	19
Fig.S38. HRMS spectrum of compound 14 .....	19
Fig.S39. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 14 .....	20
Fig.S40. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 14 .....	20
Fig.S41. MS spectrum of compound 15.....	21
Fig.S42. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 15 .....	21
Fig.S43. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 15 .....	22
Fig.S44. MS spectrum of compound 16.....	22
Fig.S45. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 16 .....	23
Fig.S46. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 16.....	23
Fig.S47. HRMS spectrum of compound 17 .....	24
Fig.S48. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 17 .....	24
Fig.S49. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 17 .....	25
Fig.S50. HRMS spectrum of compound 18 .....	25
Fig.S51. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 18 .....	26
Fig.S52. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 18 .....	26
Fig.S53. HRMS spectrum of compound 19 .....	27
Fig.S54. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 19 .....	27
Fig.S55. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 19 .....	28
Fig.S56. HRMS spectrum of compound 20 .....	28
Fig.S57. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 20 .....	29
Fig.S58. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 20 .....	29
Fig.S59. HRMS spectrum of compound 21 .....	30
Fig.S60. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 21 .....	30
Fig.S61. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 21 .....	31
Fig.S62. MS spectrum of compound 22.....	31
Fig.S63. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 22 .....	32
Fig.S64. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 22 .....	32
Fig.S65. HRMS spectrum of compound 23 .....	33
Fig.S66. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 23 .....	33
Fig.S67. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 23 .....	34

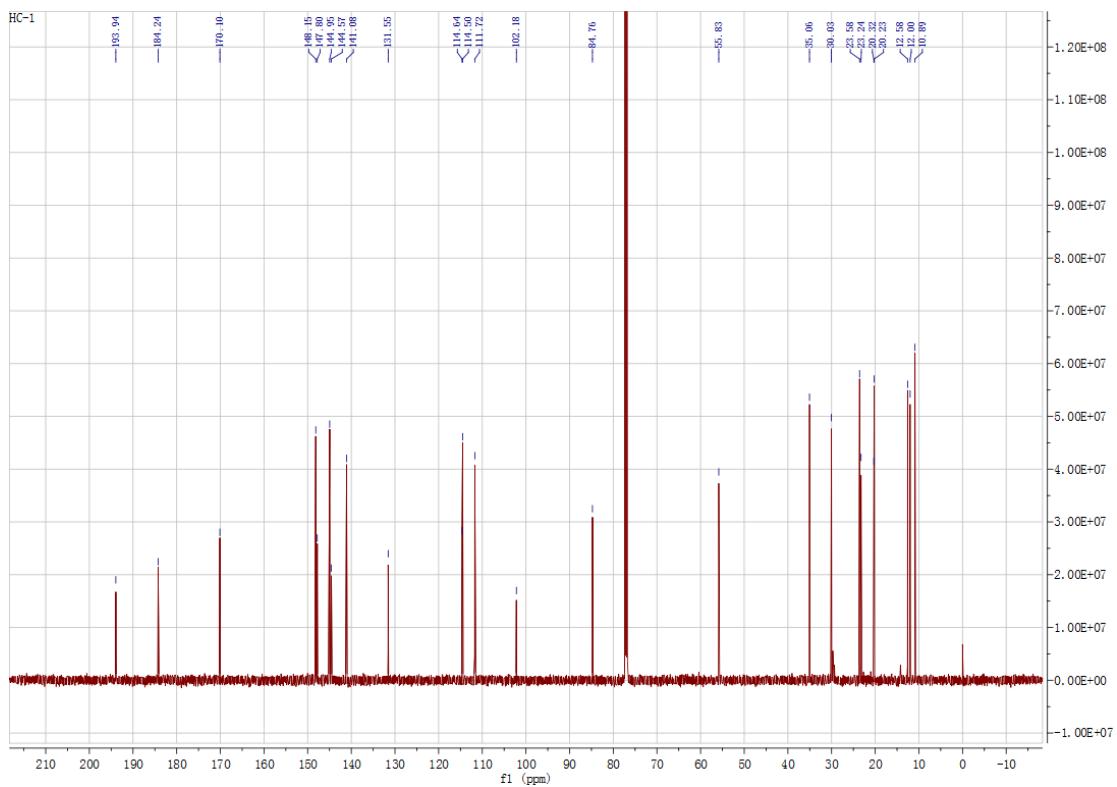
Fig.S68. HRMS spectrum of compound 24 .....	34
Fig.S69. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 24 .....	35
Fig.S70. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 24 .....	35
Fig.S71. HRMS spectrum of compound 25 .....	36
Fig.S72. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 25 .....	36
Fig.S73. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 25 .....	37
Fig.S74. HRMS spectrum of compound 26 .....	38
Fig.S75. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 26 .....	38
Fig.S76. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 26 .....	38
Fig.S77. HRMS spectrum of compound 27 .....	39
Fig.S78. $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of compound 27 .....	40
Fig.S79. $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of compound 27 .....	40



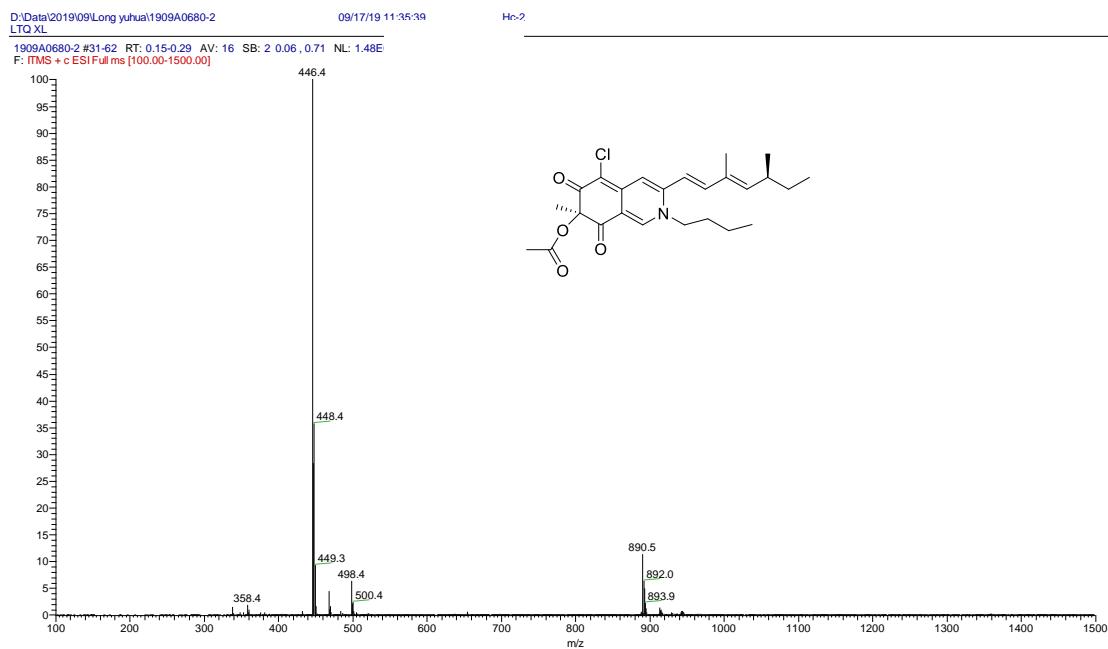
**Fig.S1.** MS spectrum of compound 1



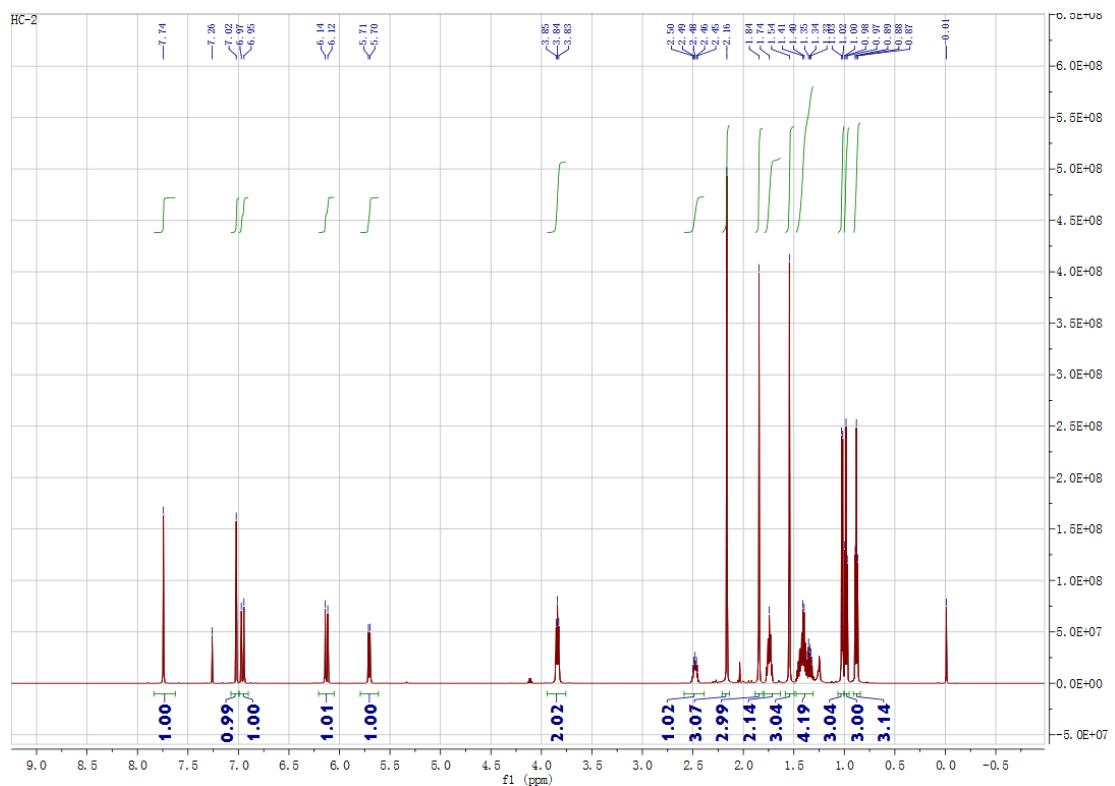
**Fig.S2.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound 1



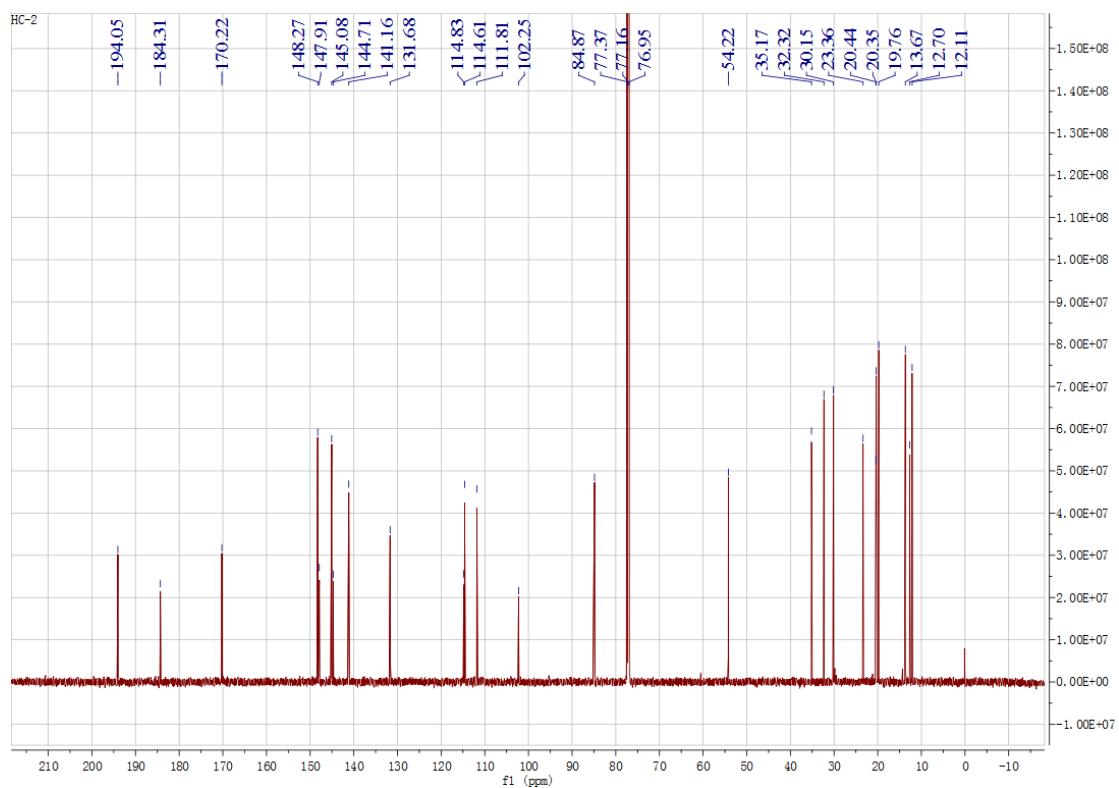
**Fig.S3.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 1



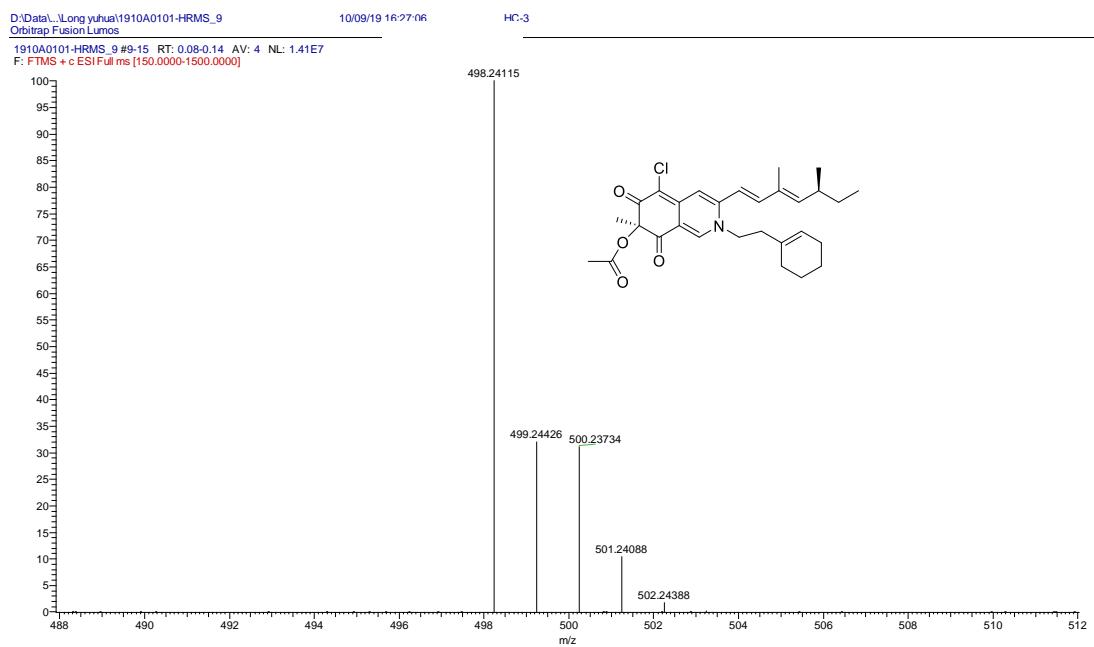
**Fig.S4.** MS spectrum of compound 2



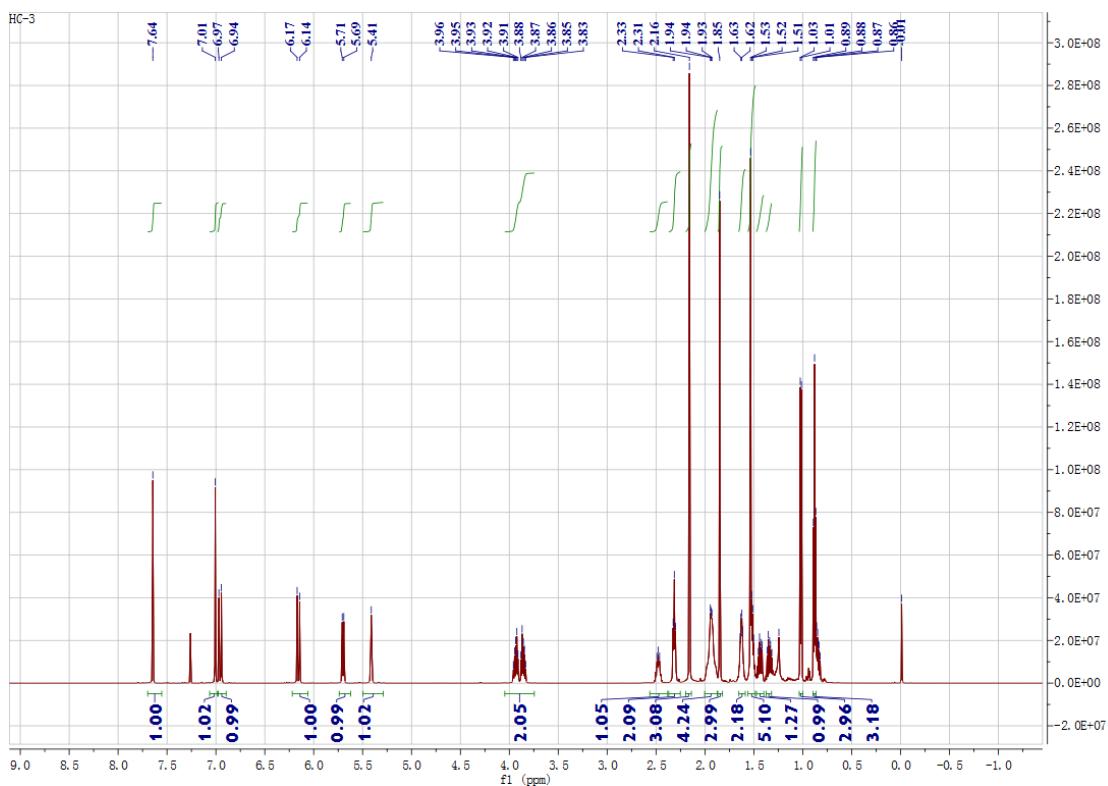
**Fig.S5.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound 2



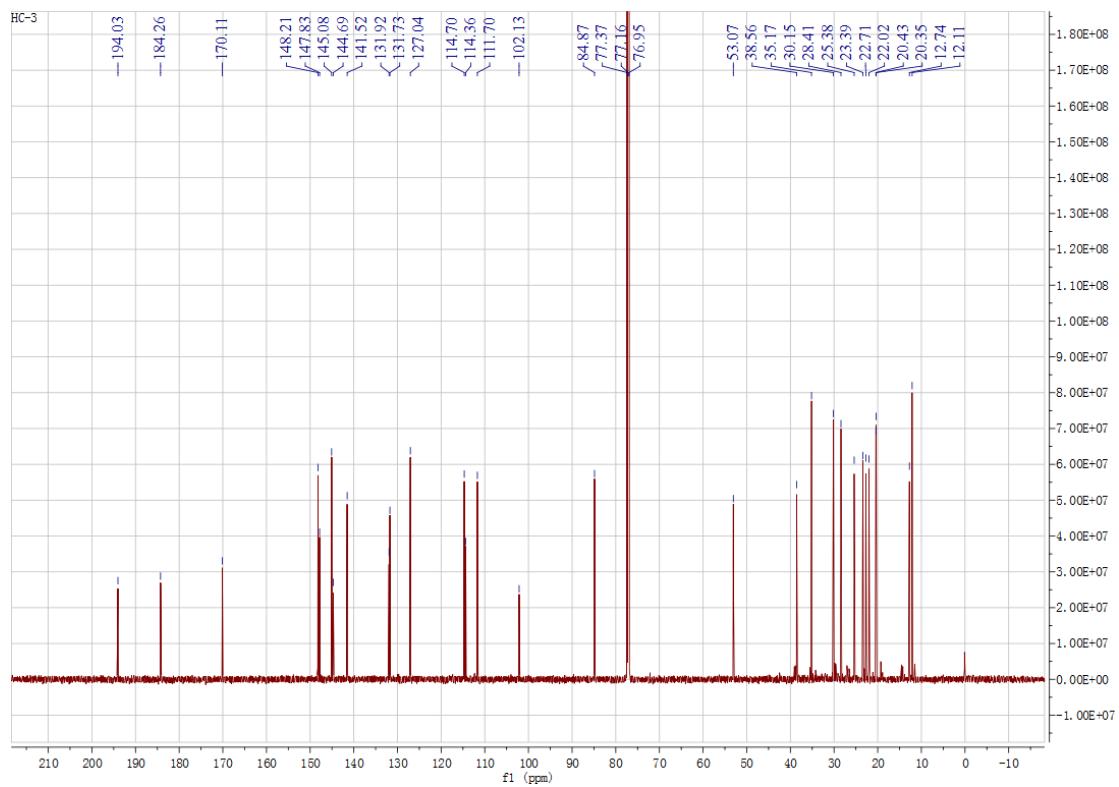
**Fig.S6.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 2



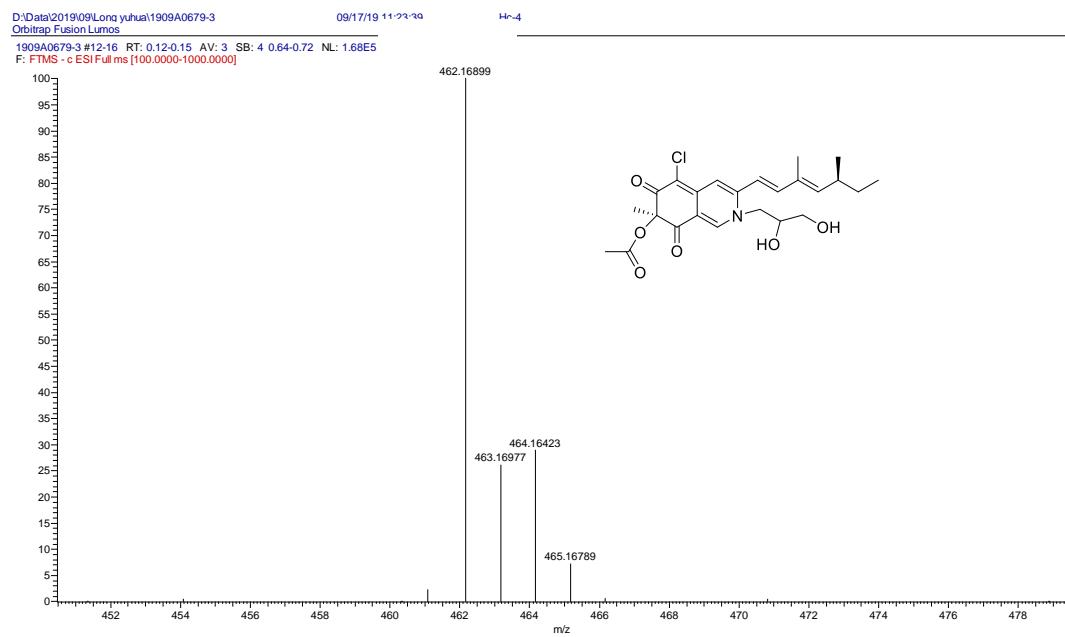
**Fig.S7.** HRMS spectrum of compound 3



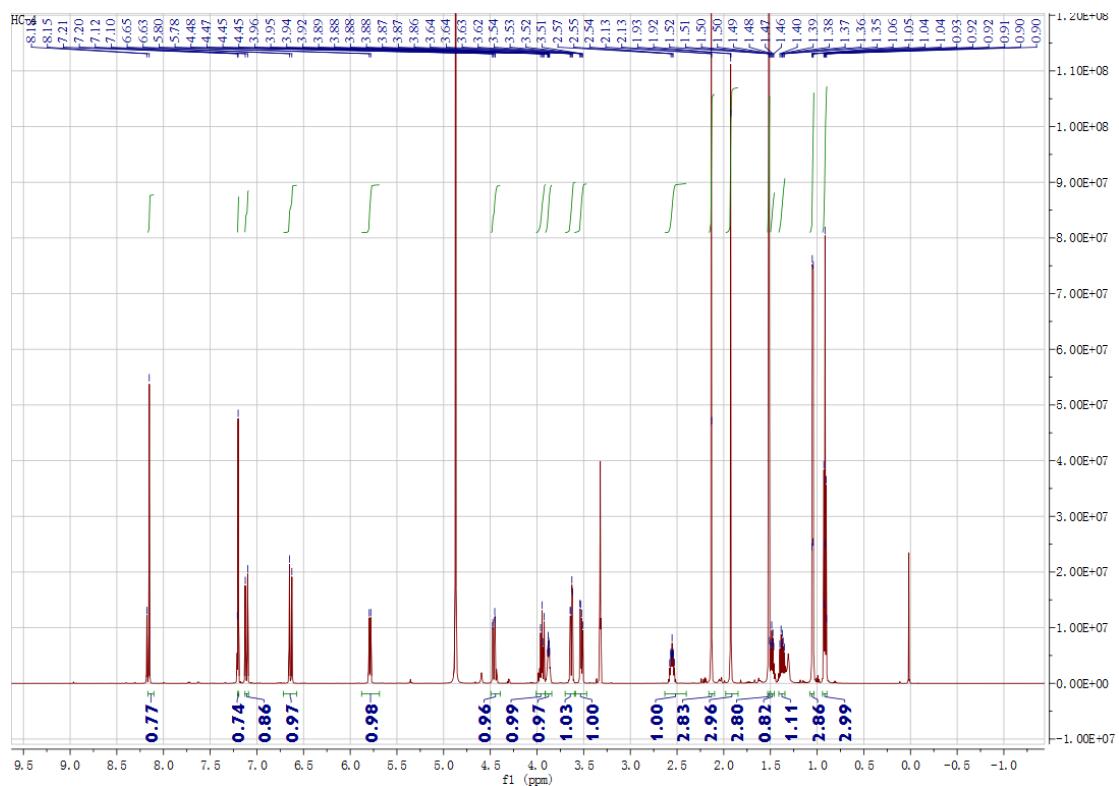
**Fig.S8.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3



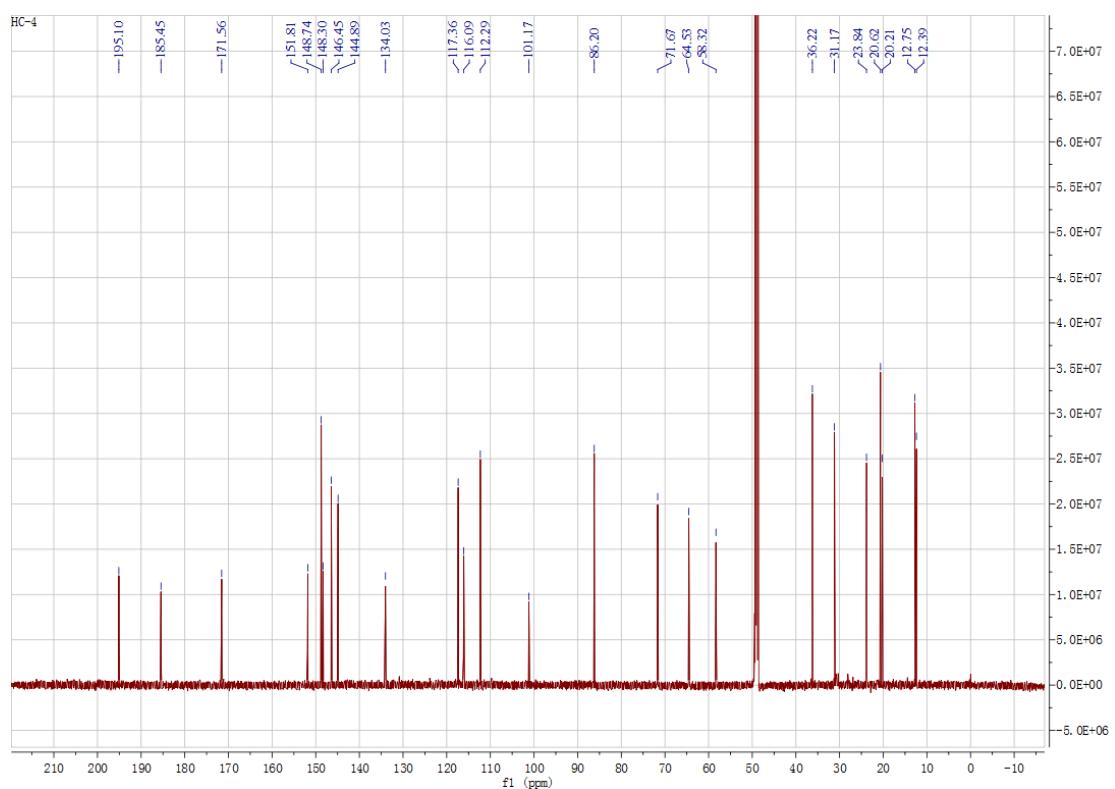
**Fig.S9.**<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) spectrum of compound 3



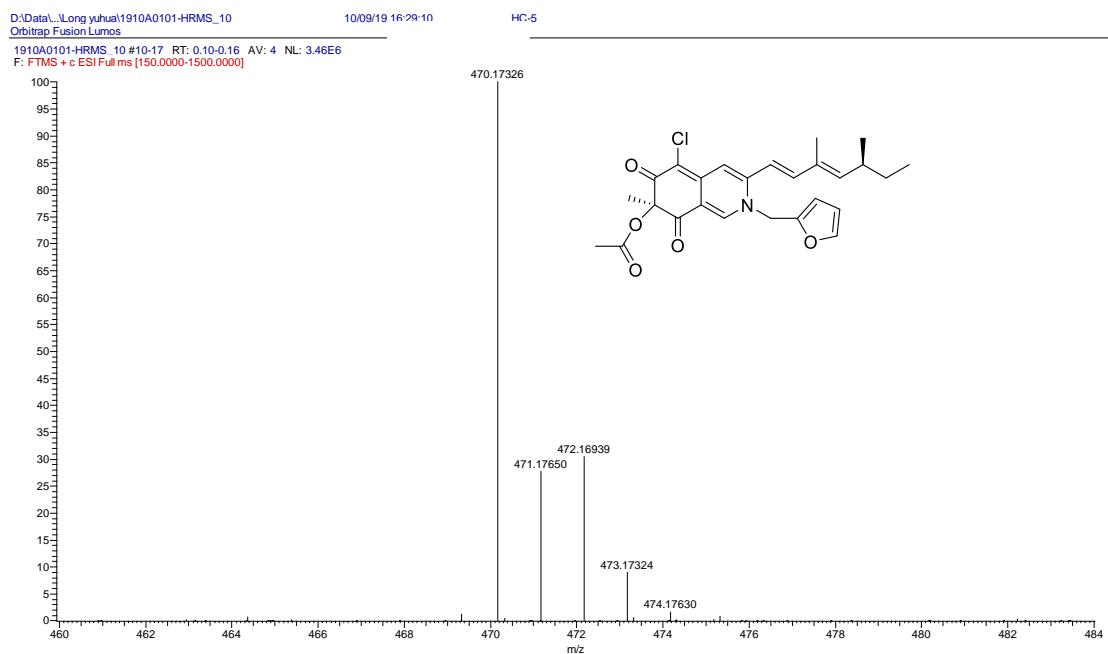
**Fig.S10.** HRMS spectrum of compound 4



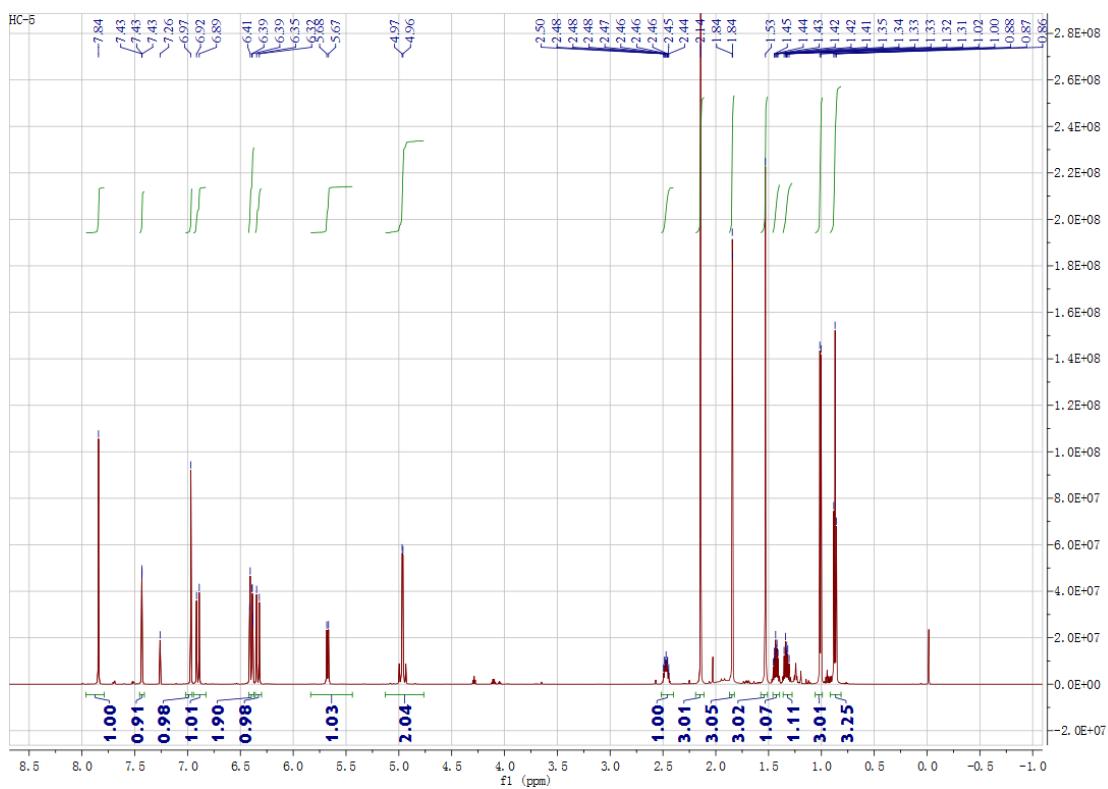
**Fig.S11.**  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 4



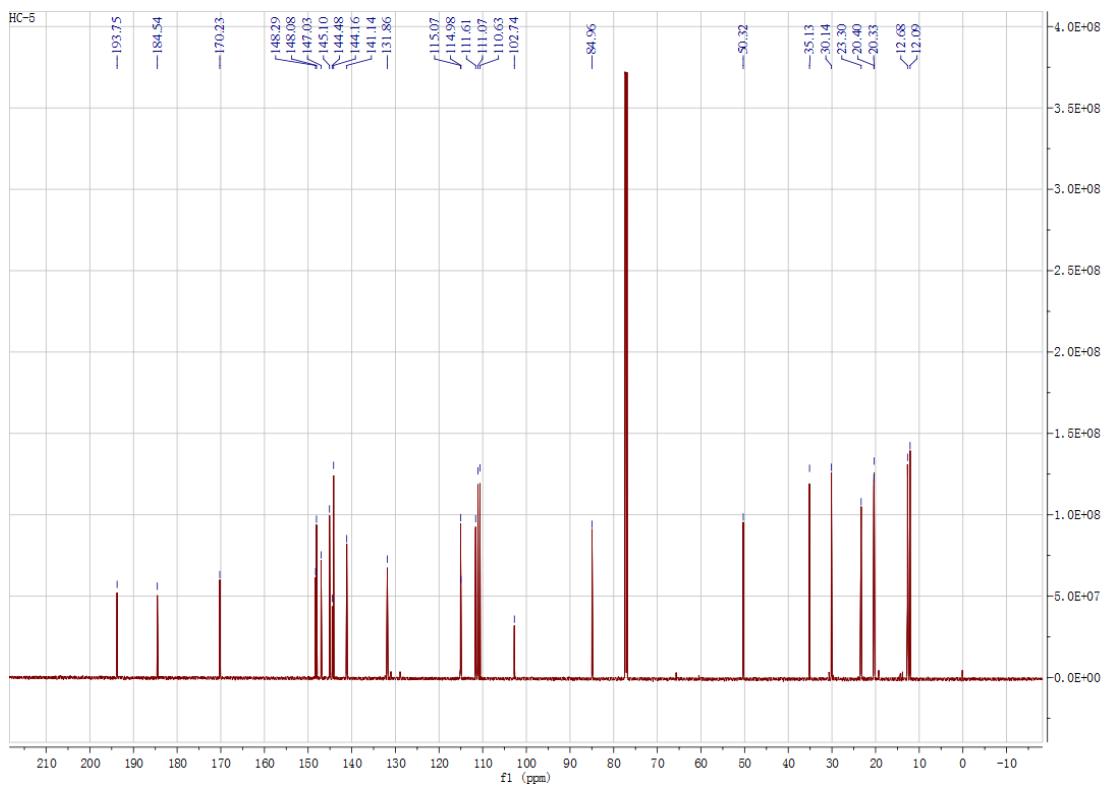
**Fig.S12.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 4



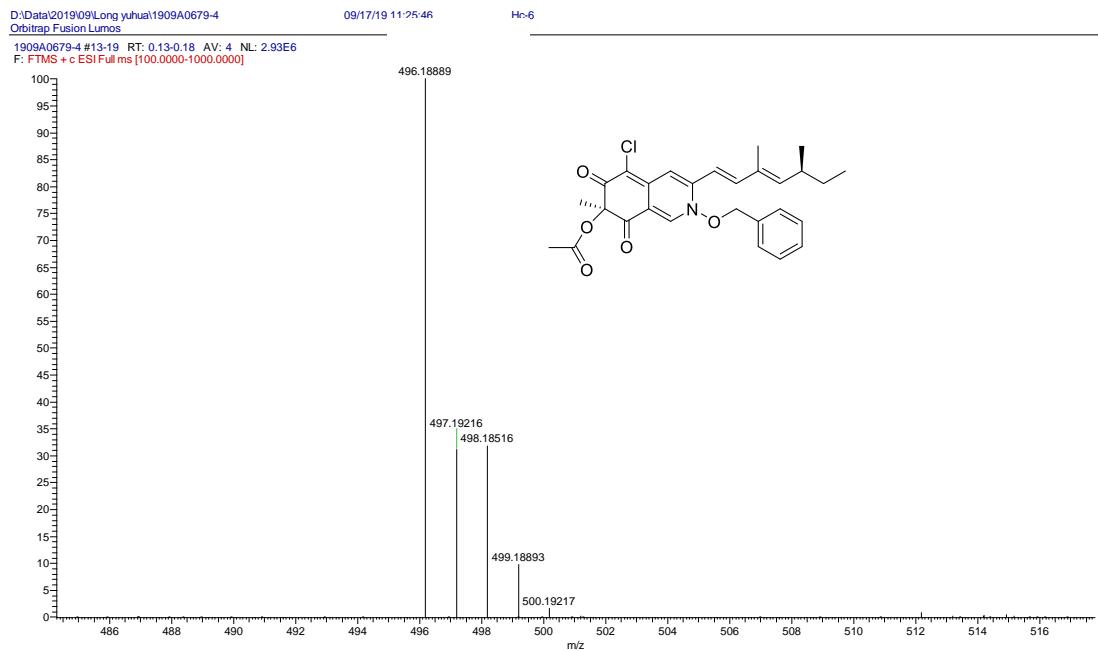
**Fig.S13.** HRMS spectrum of compound 5



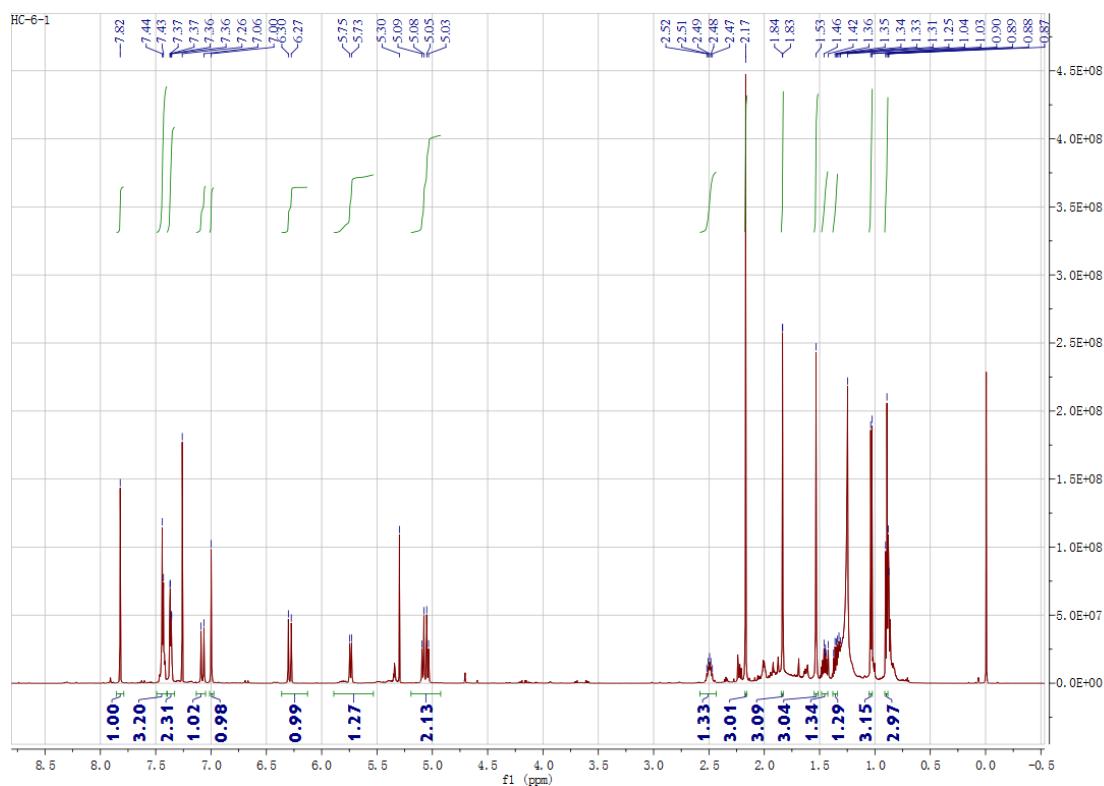
**Fig.S14.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound 5



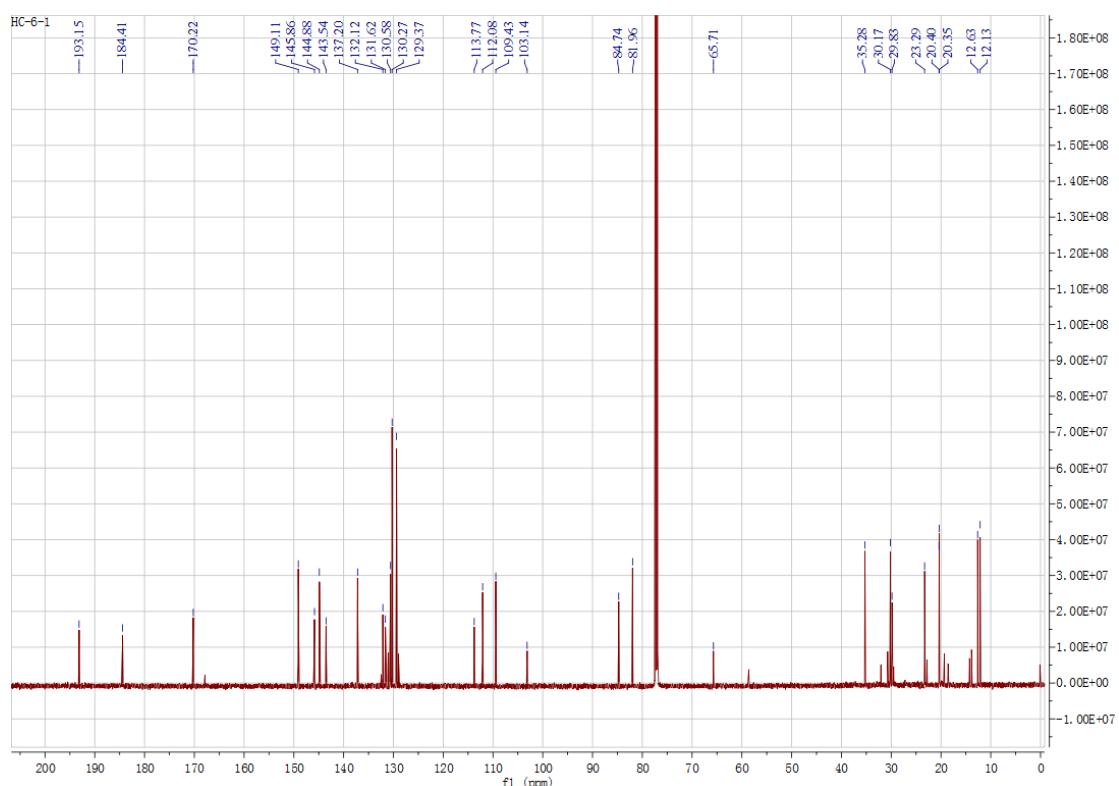
**Fig.S15.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound **5**



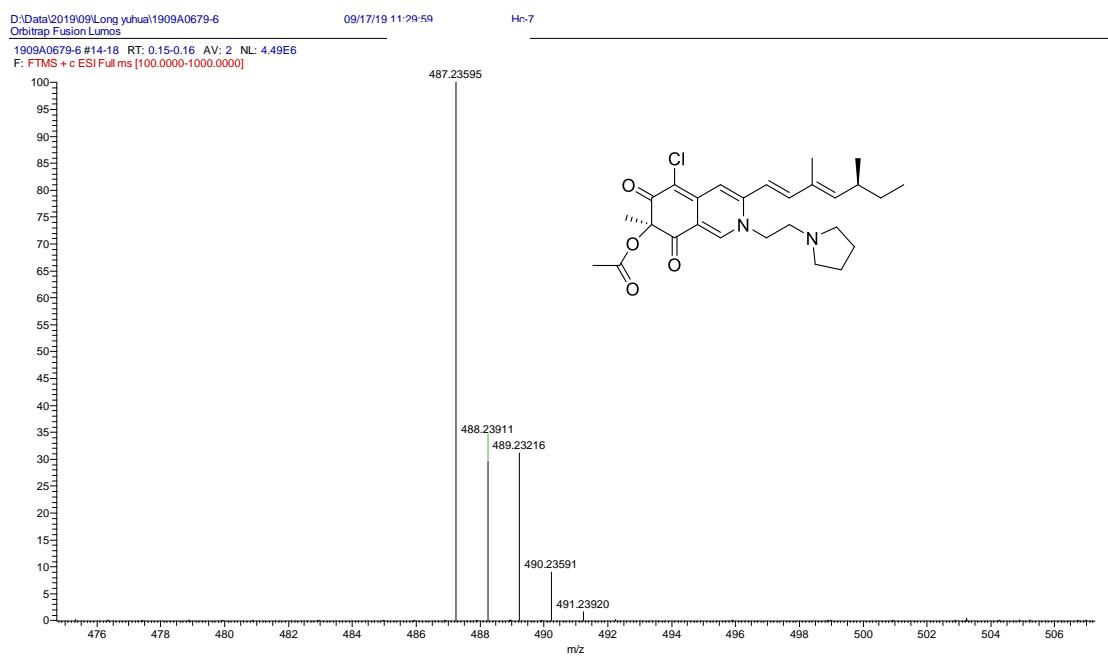
**Fig.S16.** HRMS spectrum of compound **6**



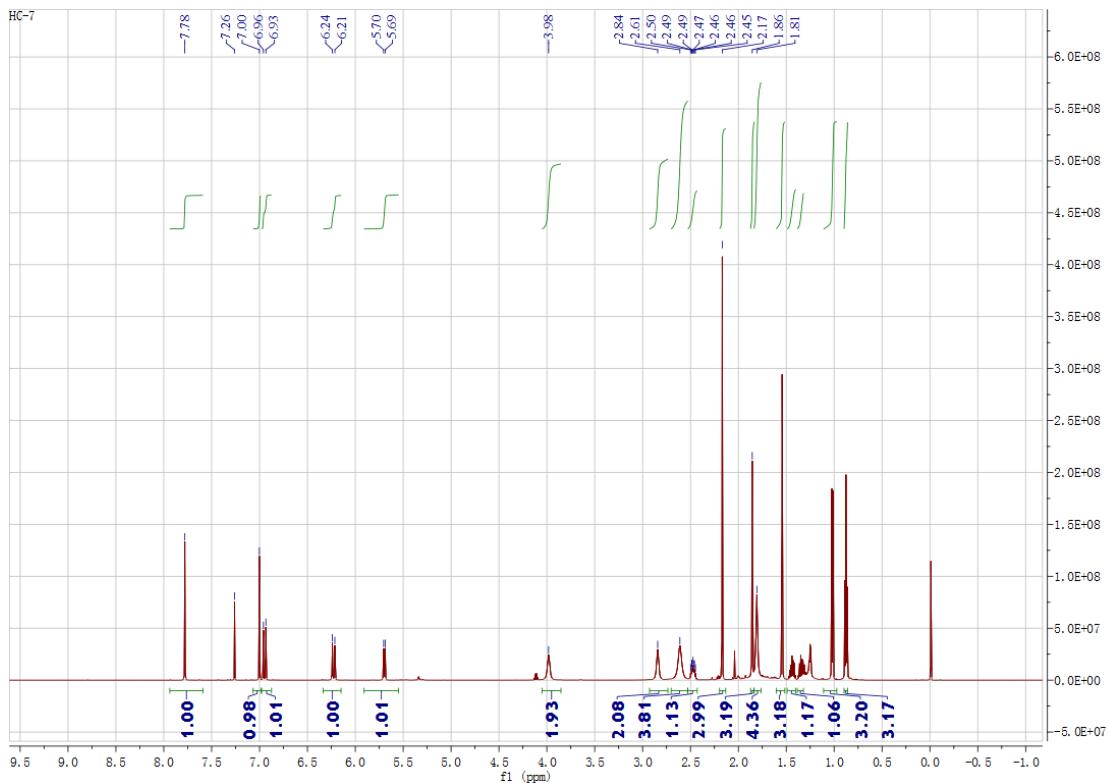
**Fig.S17.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **6**



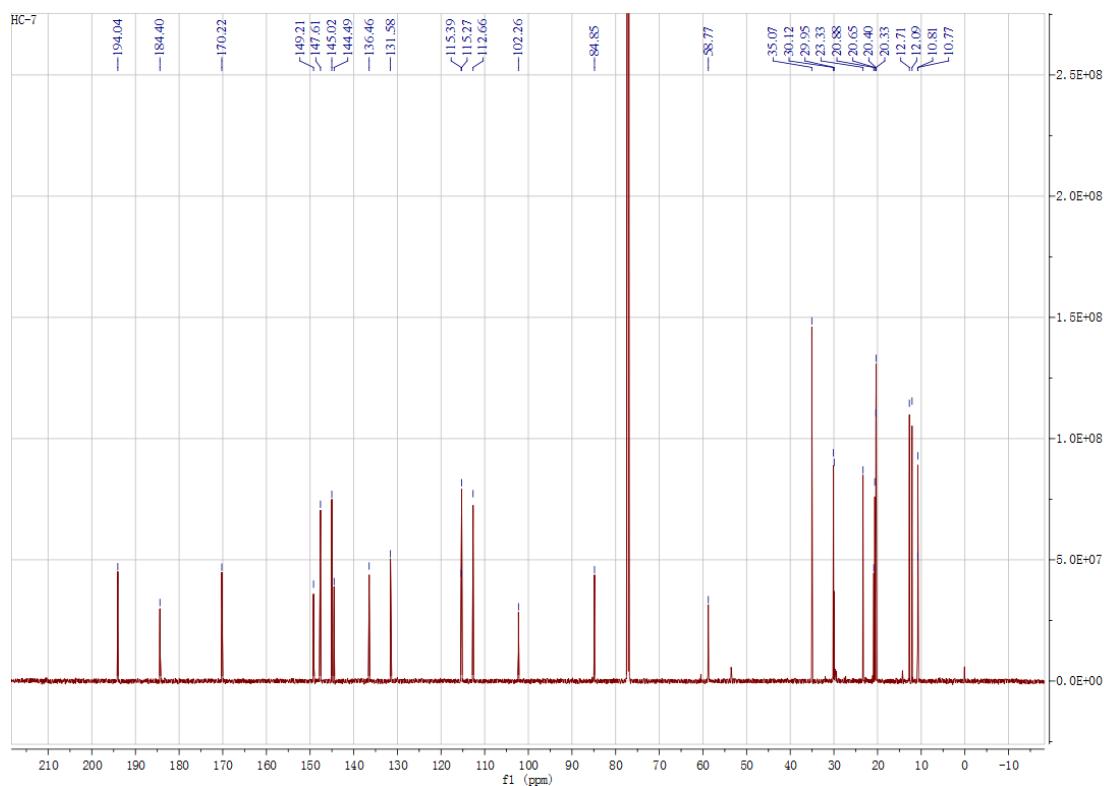
**Fig.S18.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound **6**



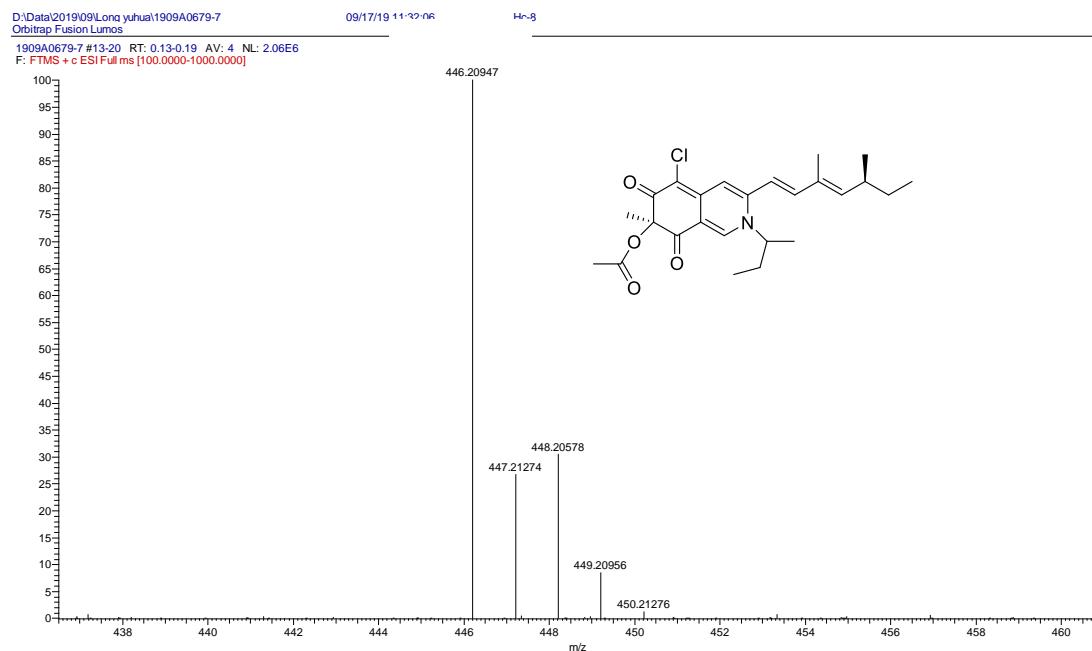
**Fig.S19.** HRMS spectrum of compound 7



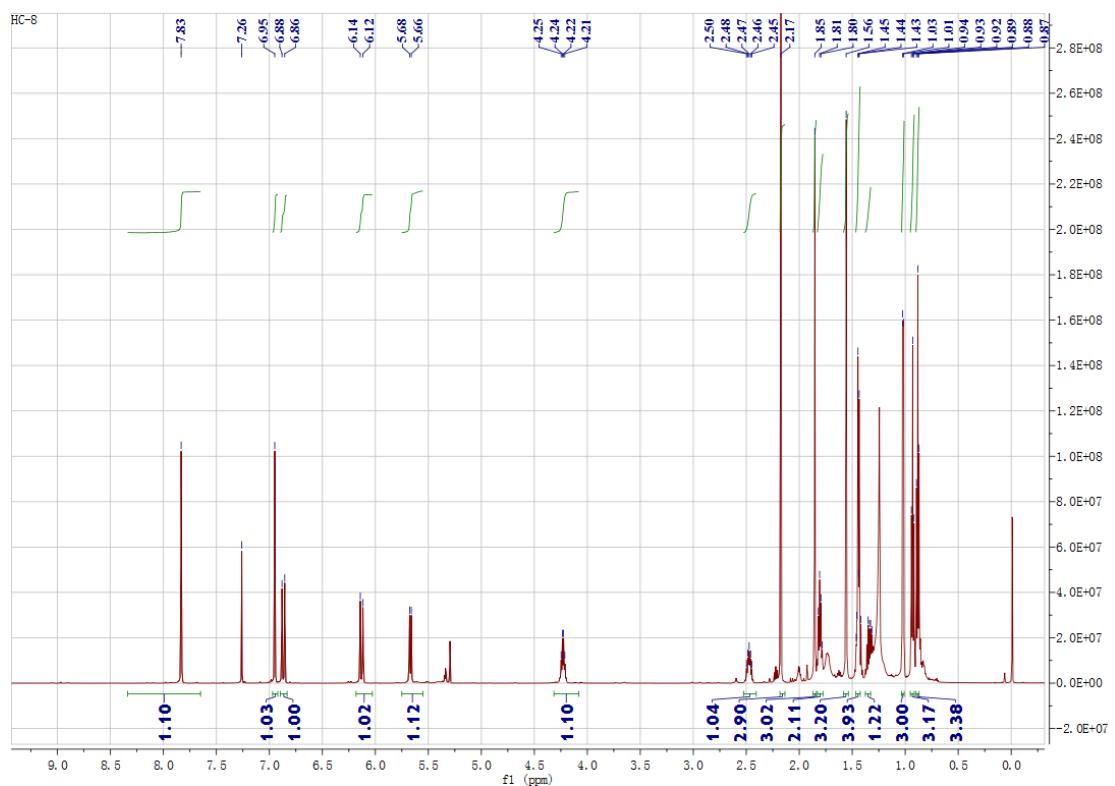
**Fig.S20.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound 7



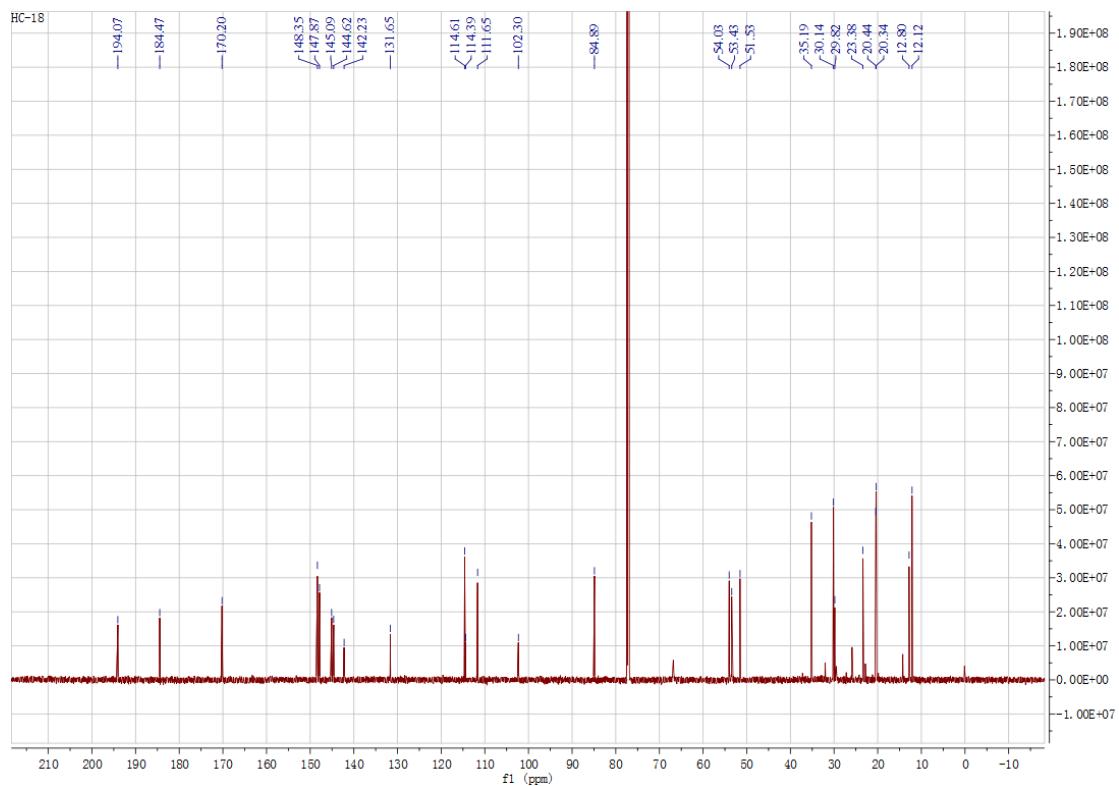
**Fig.S21.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 7



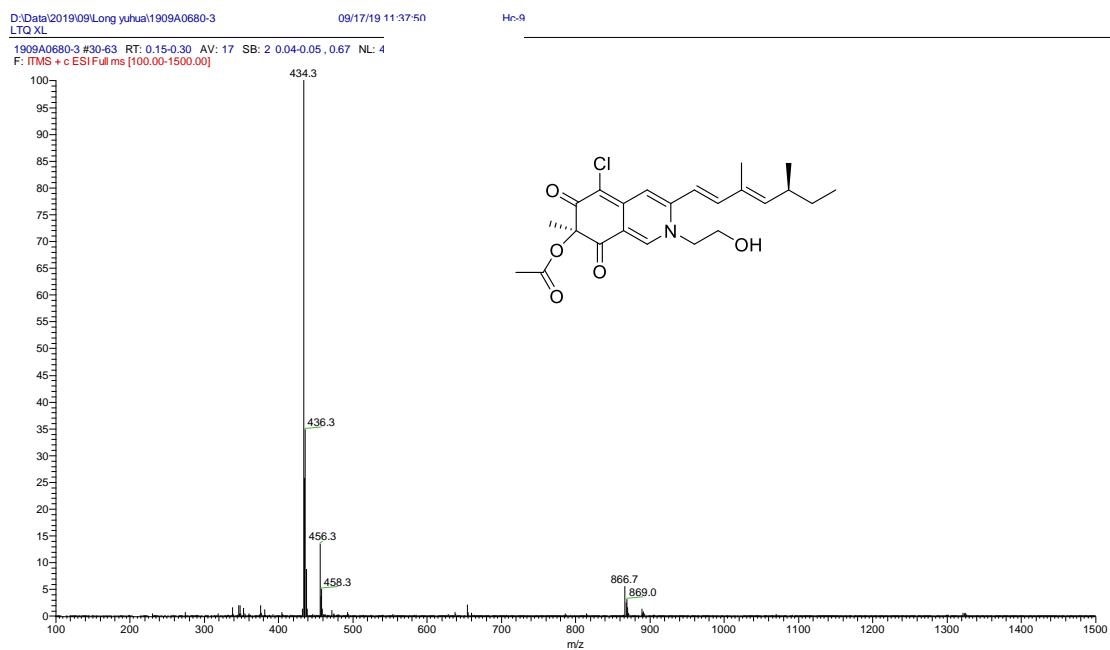
**Fig.S22.** HRMS spectrum of compound 8



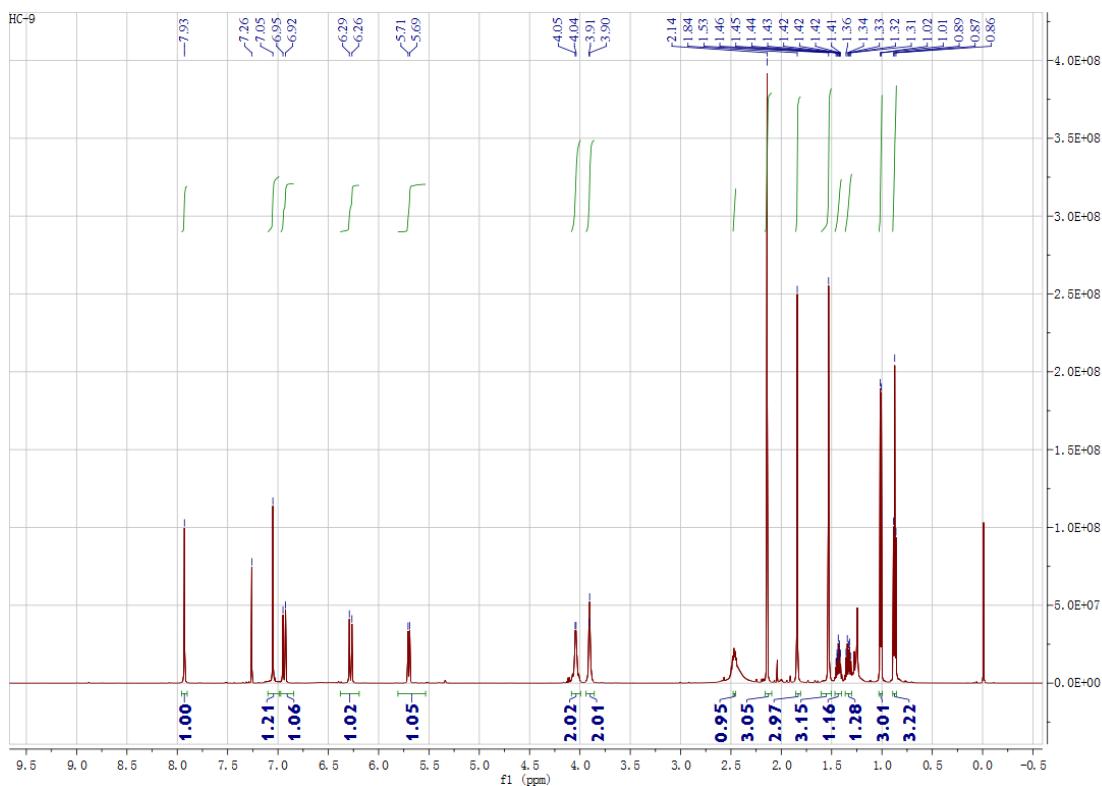
**Fig.S23.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **8**



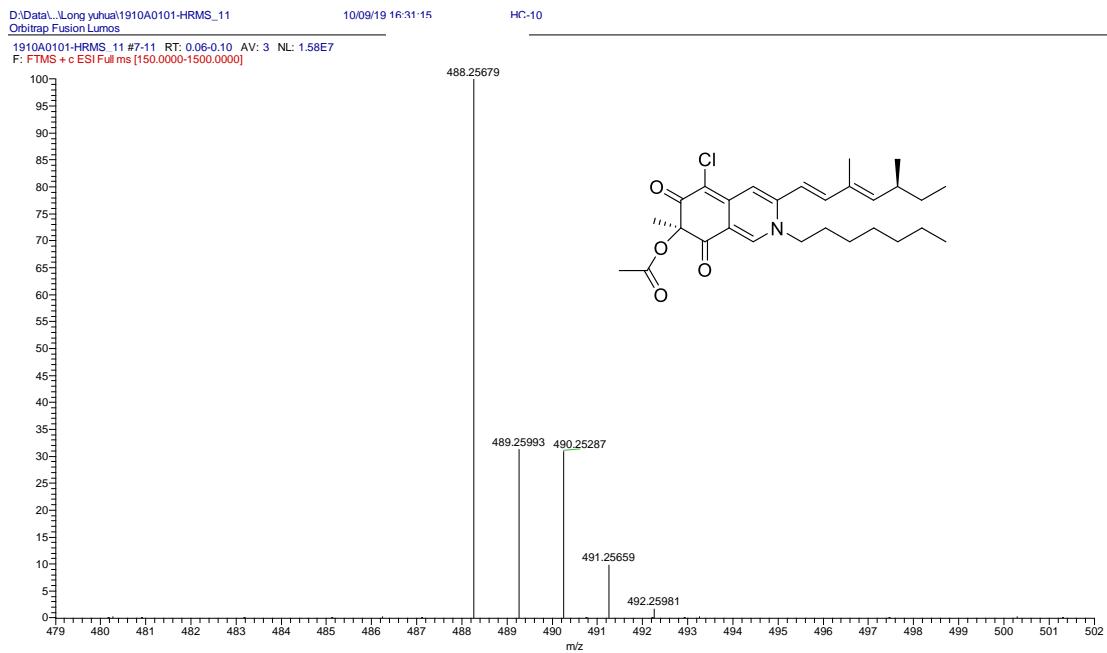
**Fig.S24.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound **8**



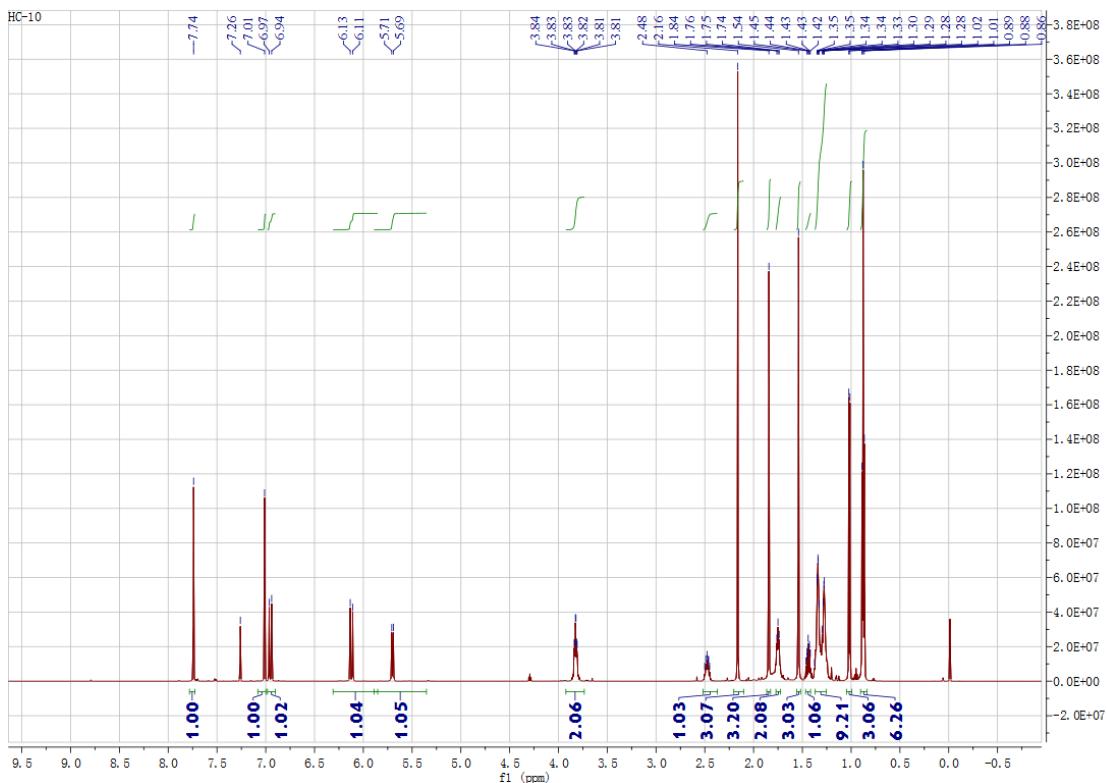
**Fig.S25.** MS spectrum of compound **9**

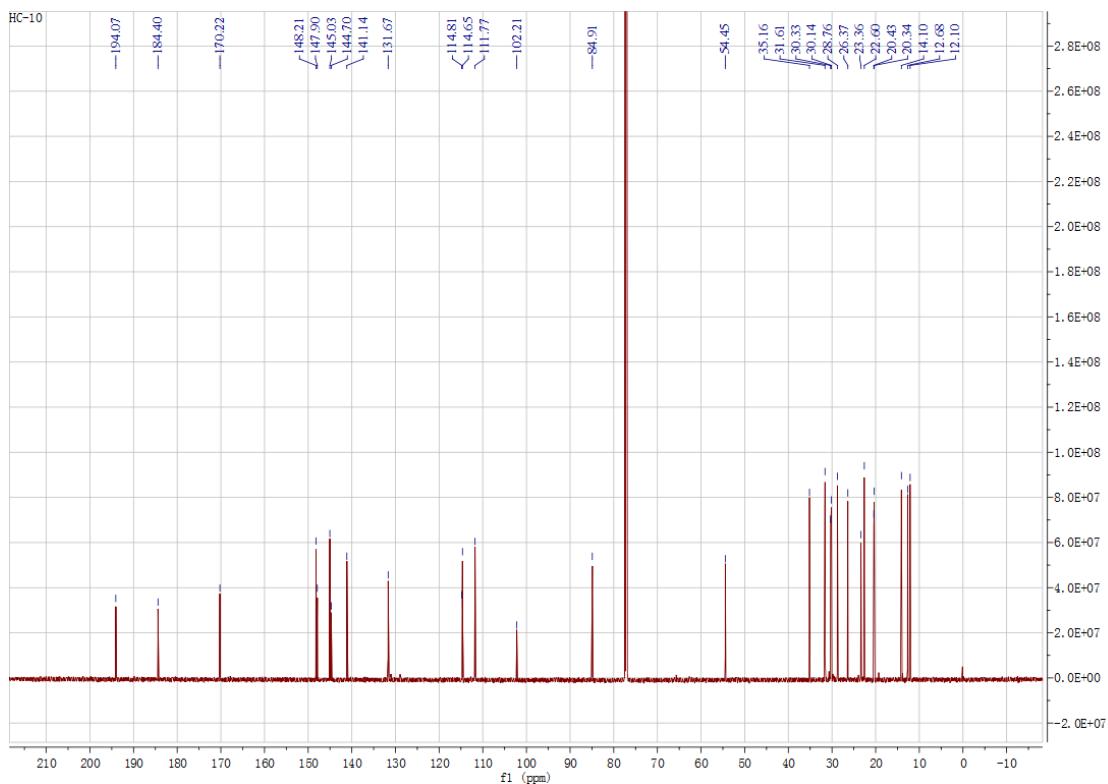


**Fig.S26.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **9**

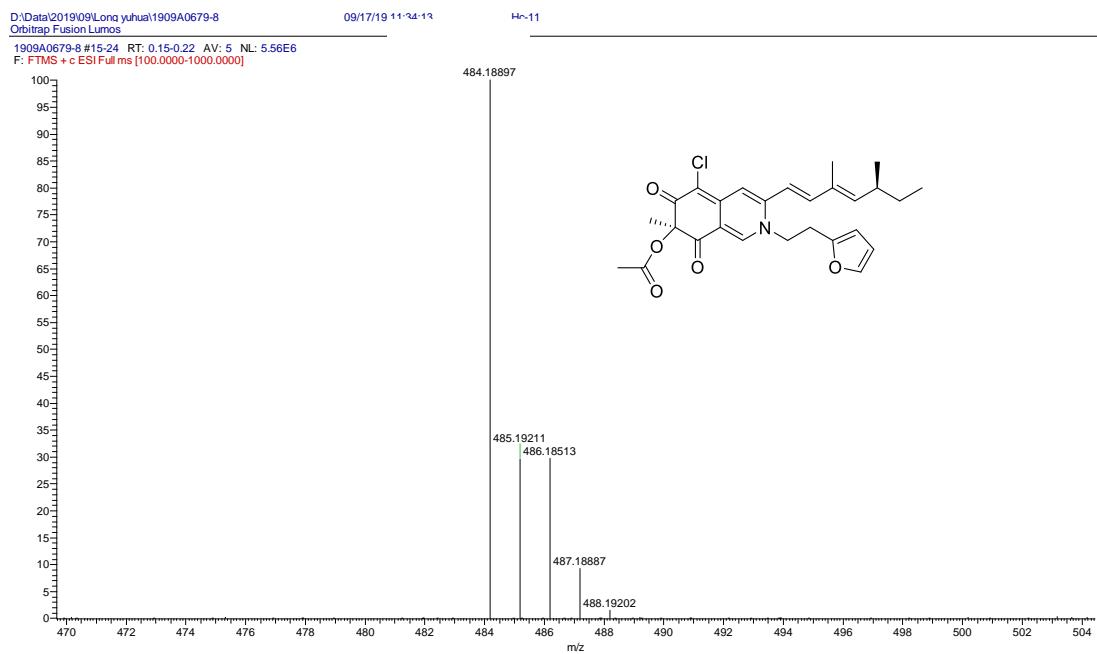


**Fig.S27.** HRMS spectrum of compound **10**

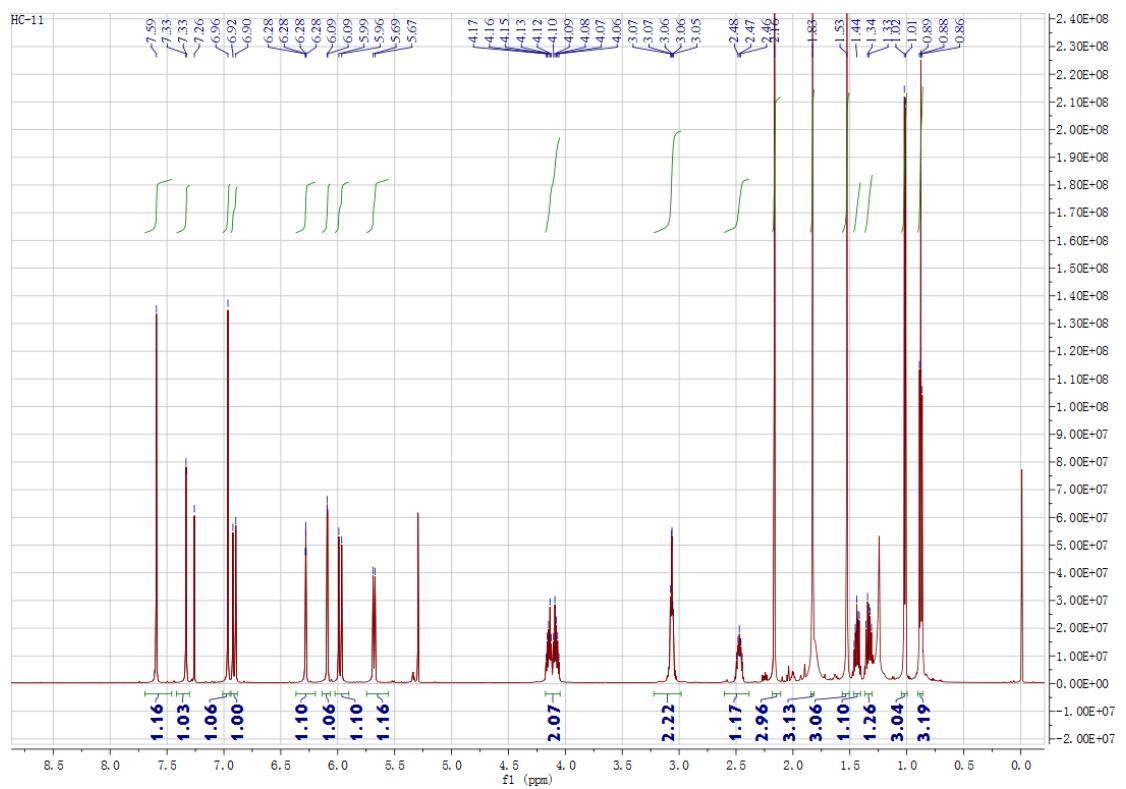




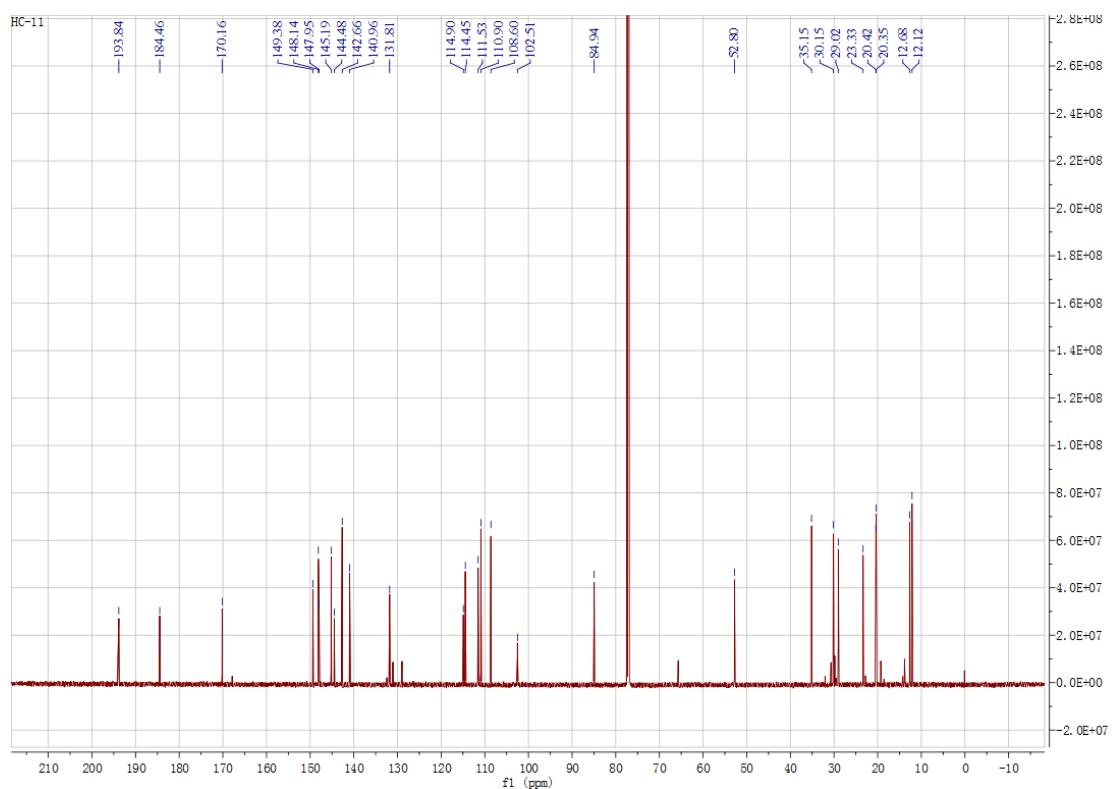
**Fig.S29.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound **10**



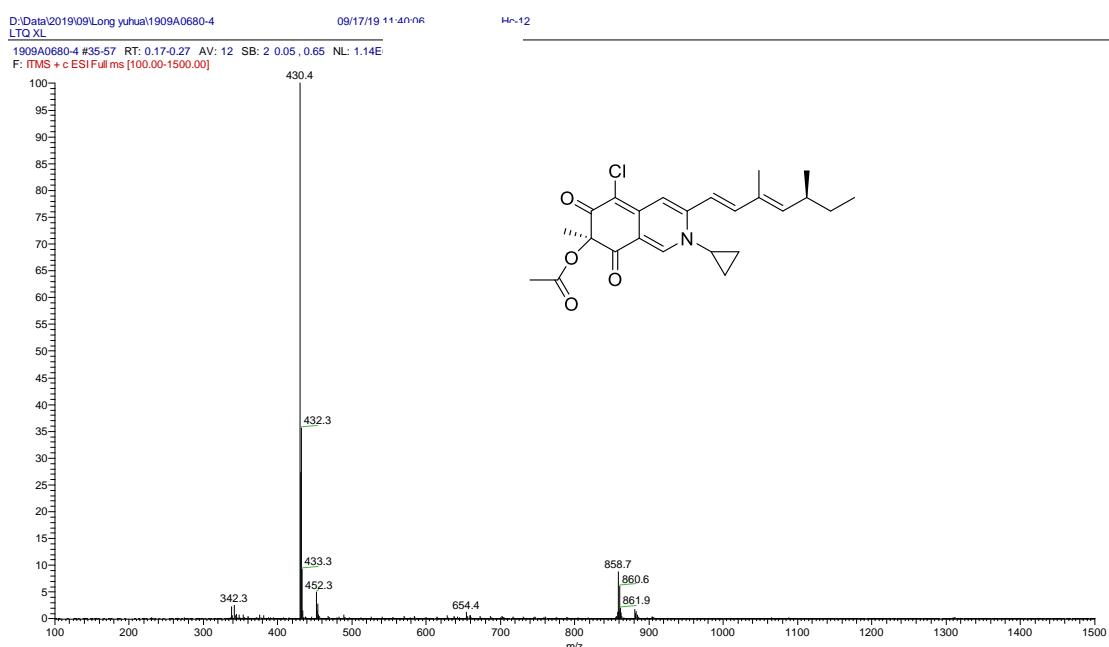
**Fig.S30.** HRMS spectrum of compound **11**



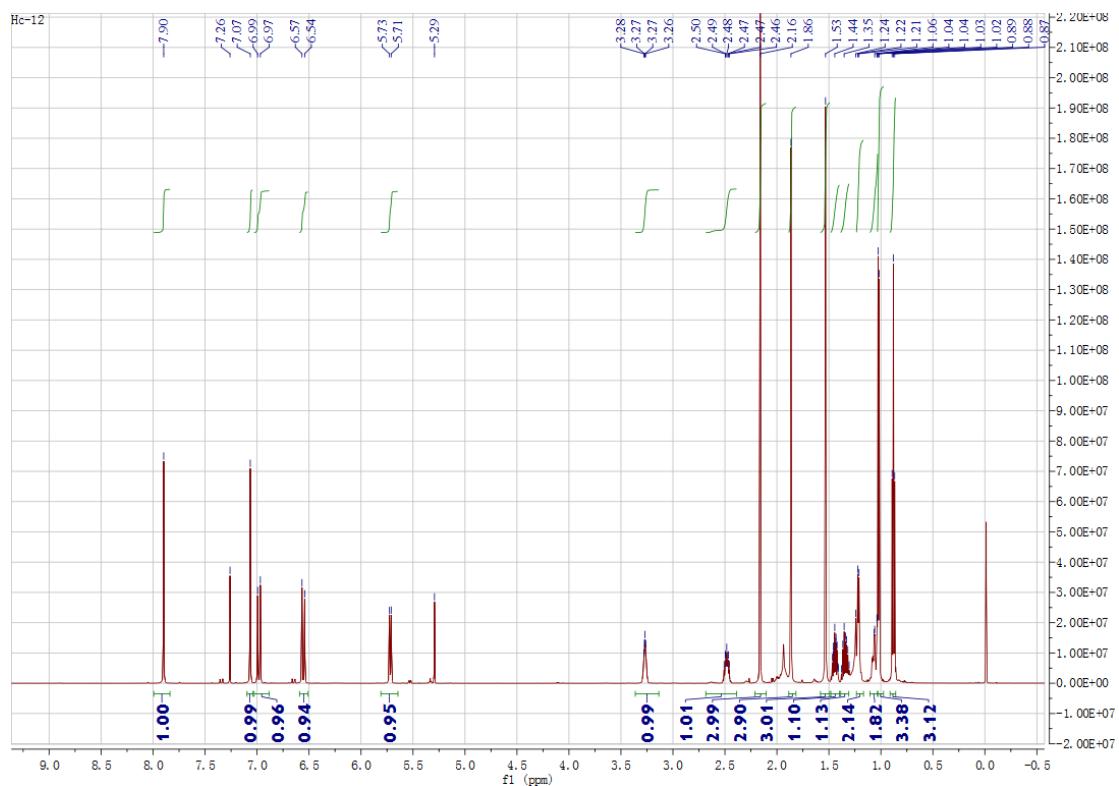
**Fig.S31.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **11**



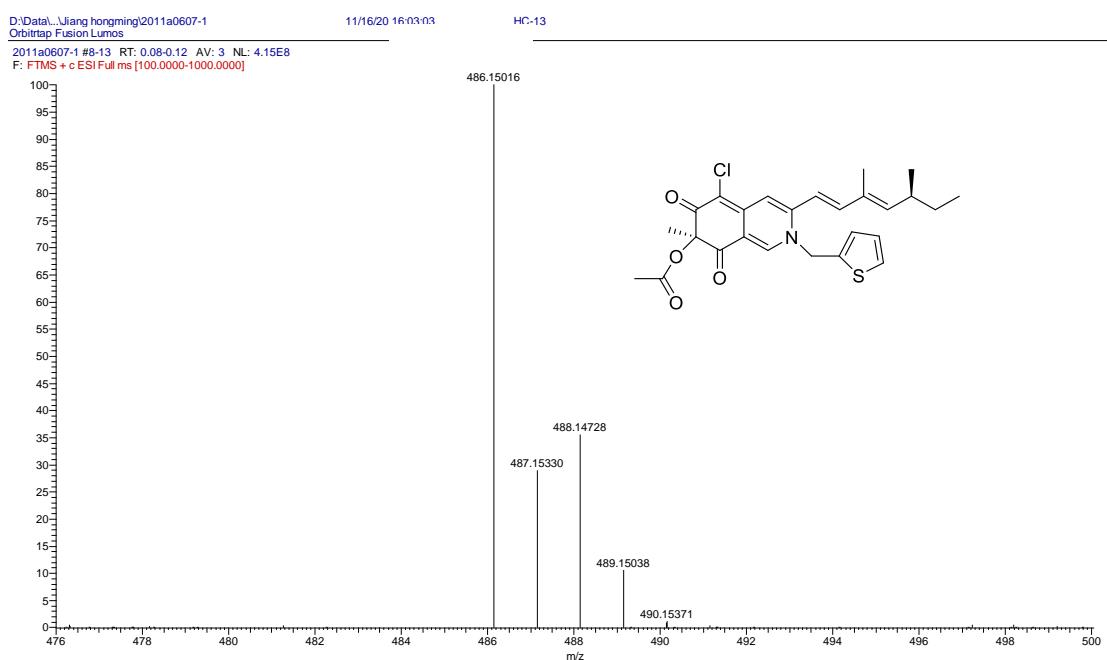
**Fig.S32.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound **11**



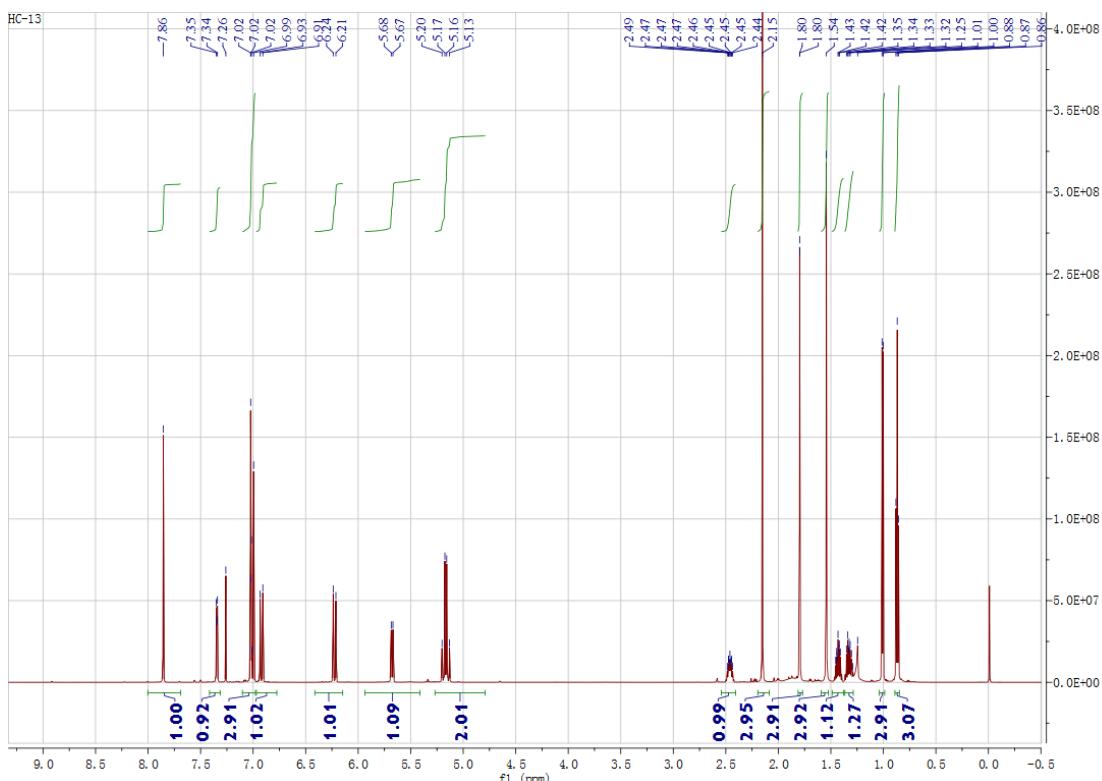
**Fig.S33.** MS spectrum of compound **12**



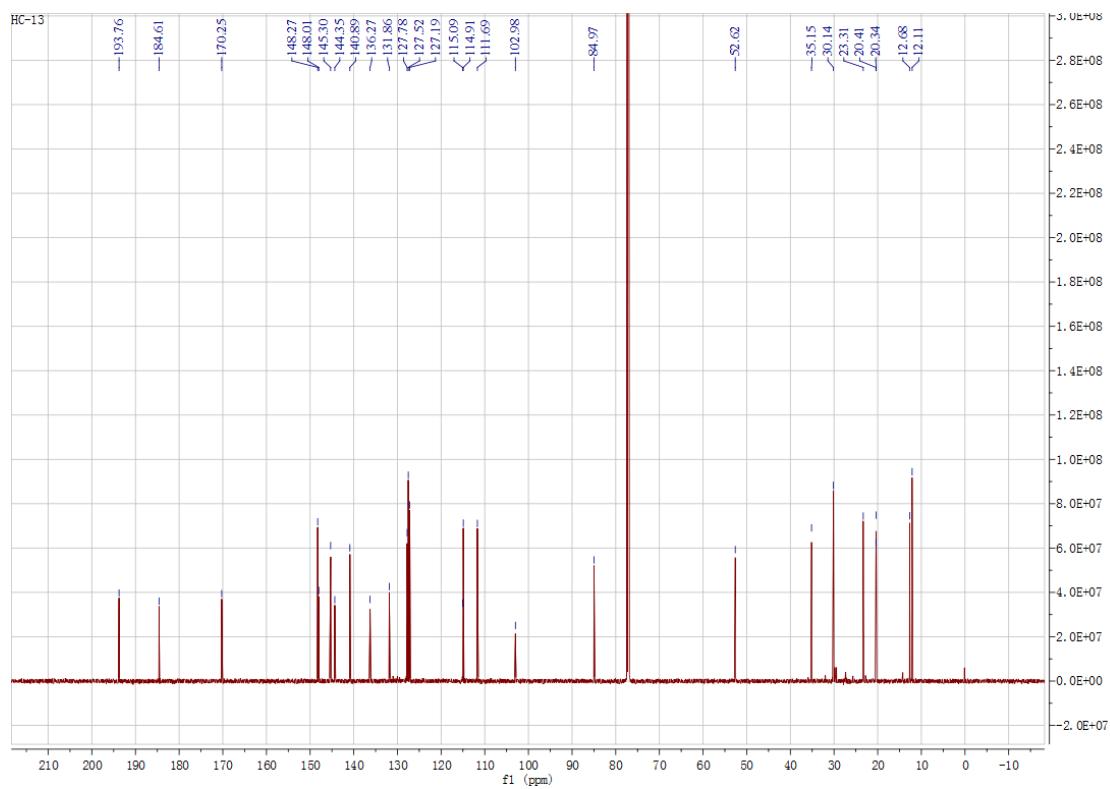
**Fig.S34.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **12**



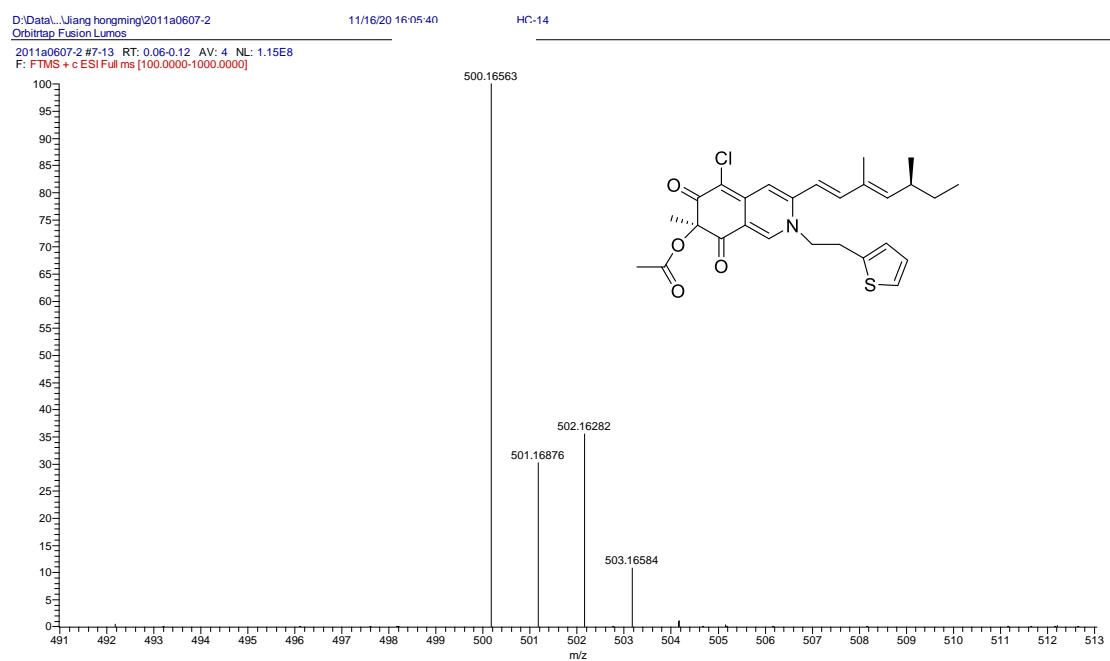
**Fig.S35.** HRMS spectrum of compound **13**



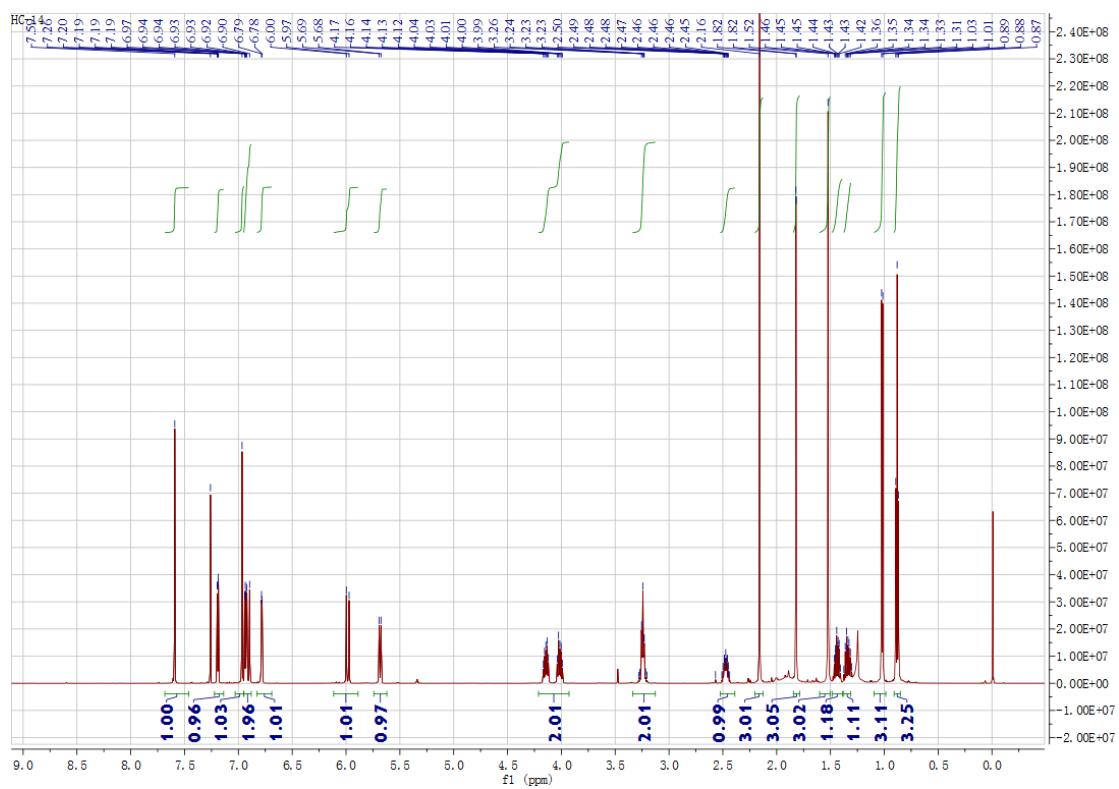
**Fig.S36.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **13**



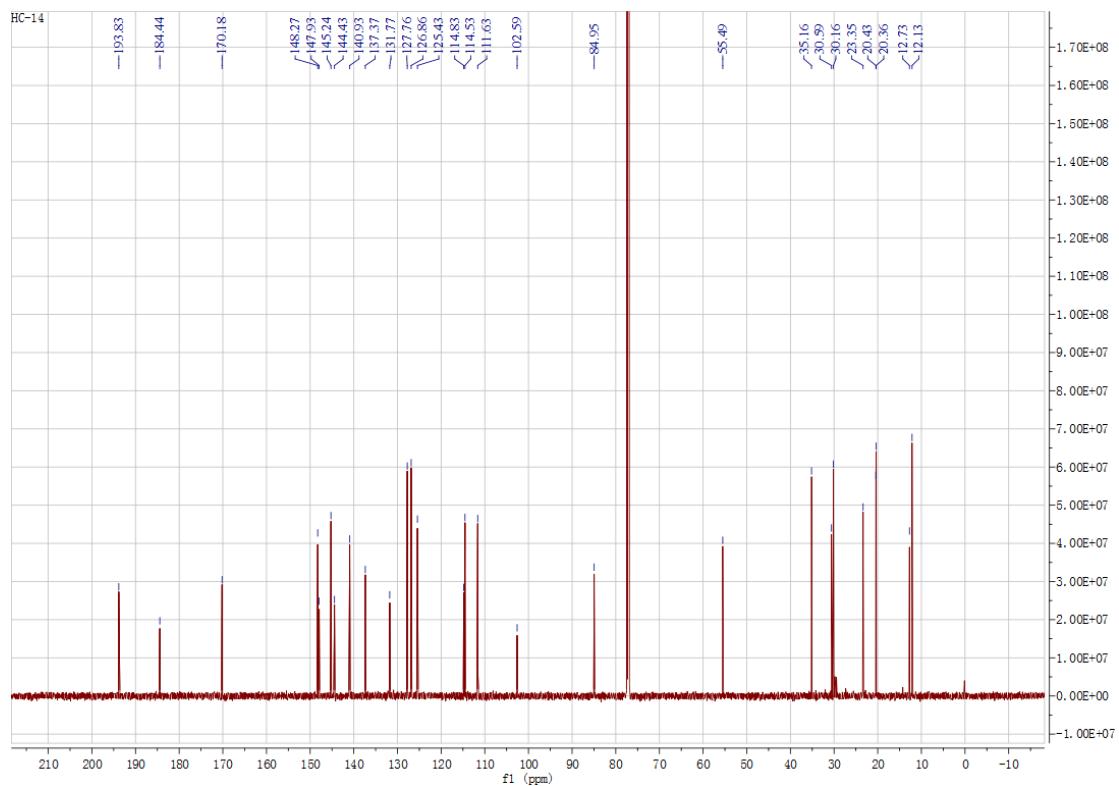
**Fig.S37.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 13



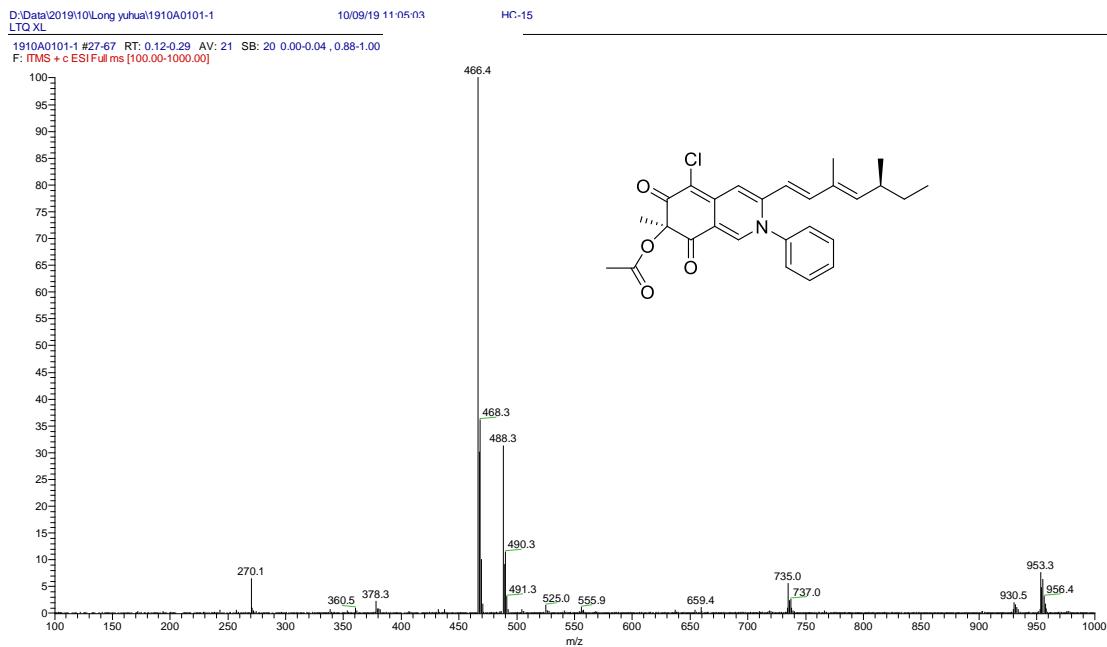
**Fig.S38.** HRMS spectrum of compound 14



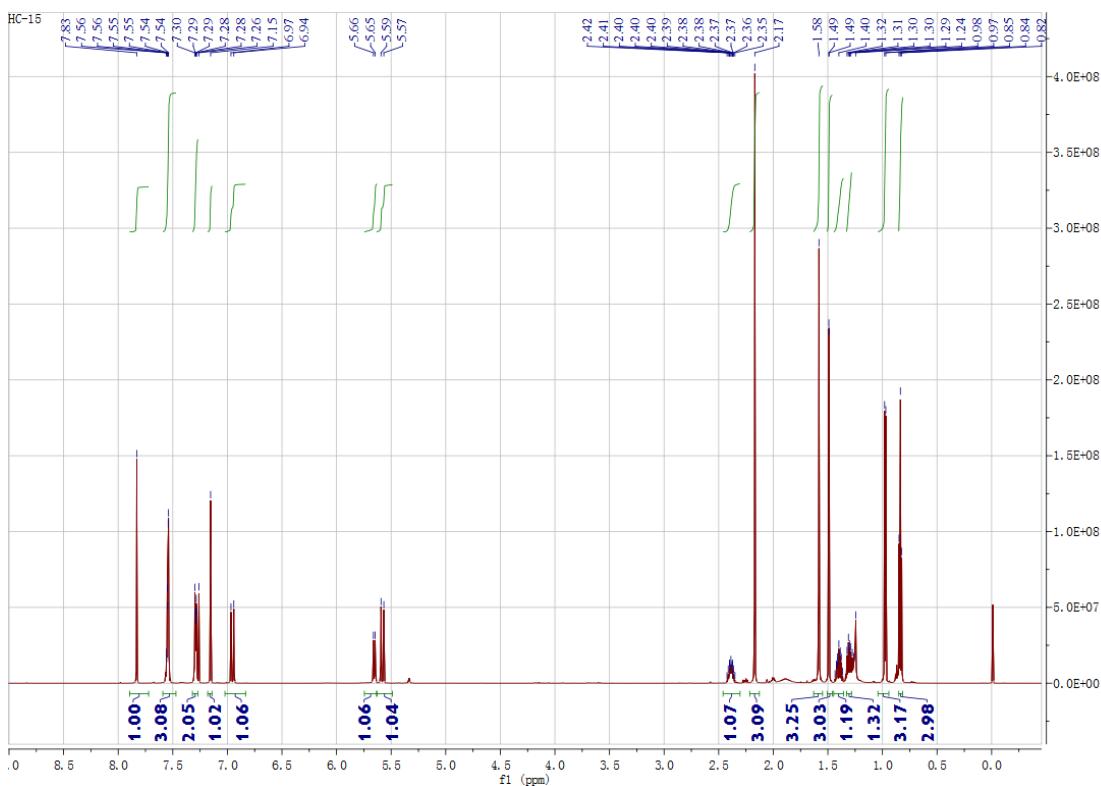
**Fig.S39.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **14**



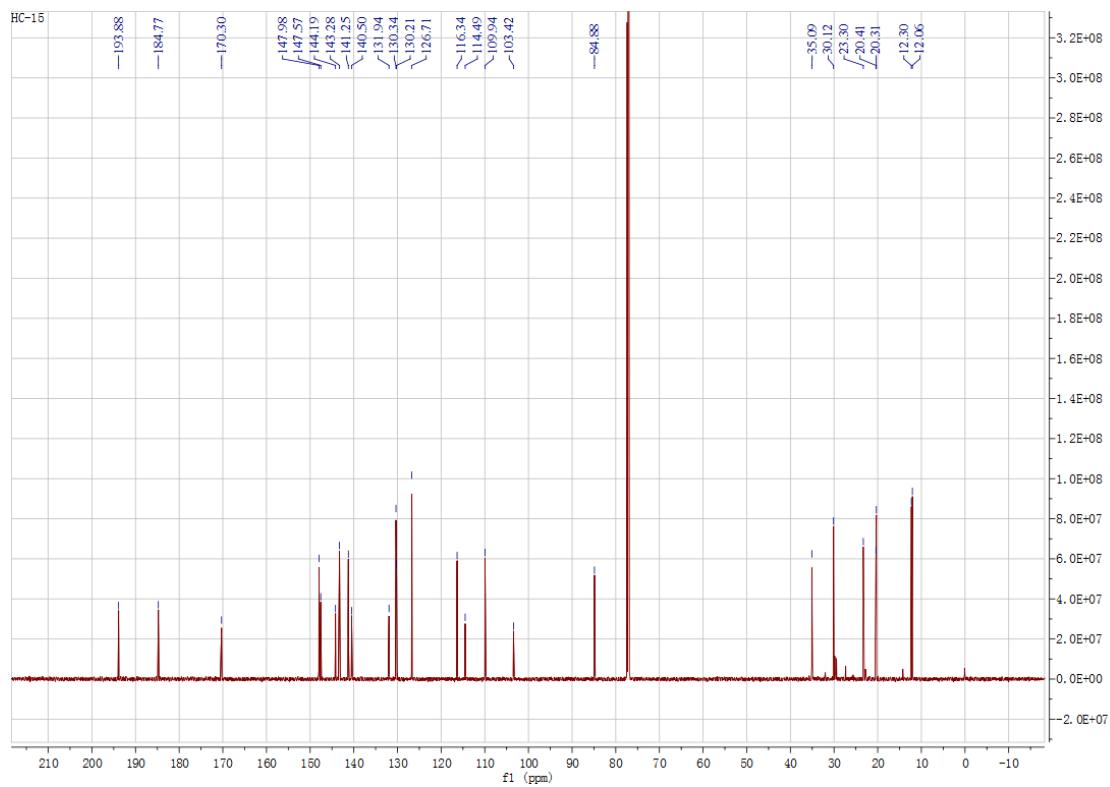
**Fig.S40.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound **14**



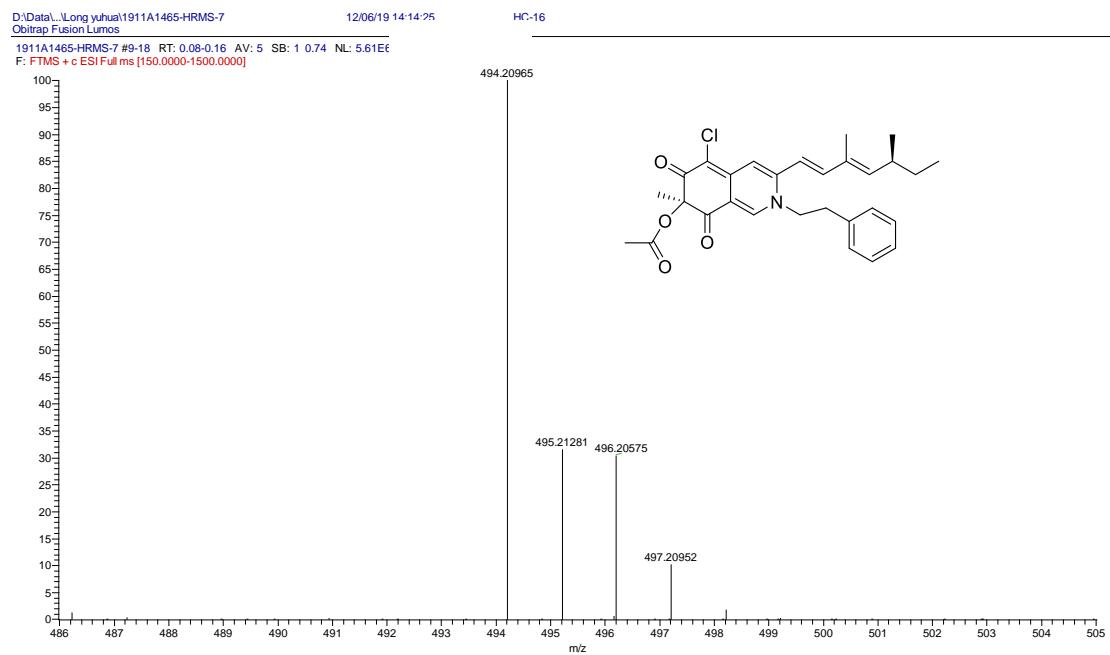
**Fig.S41.** MS spectrum of compound **15**



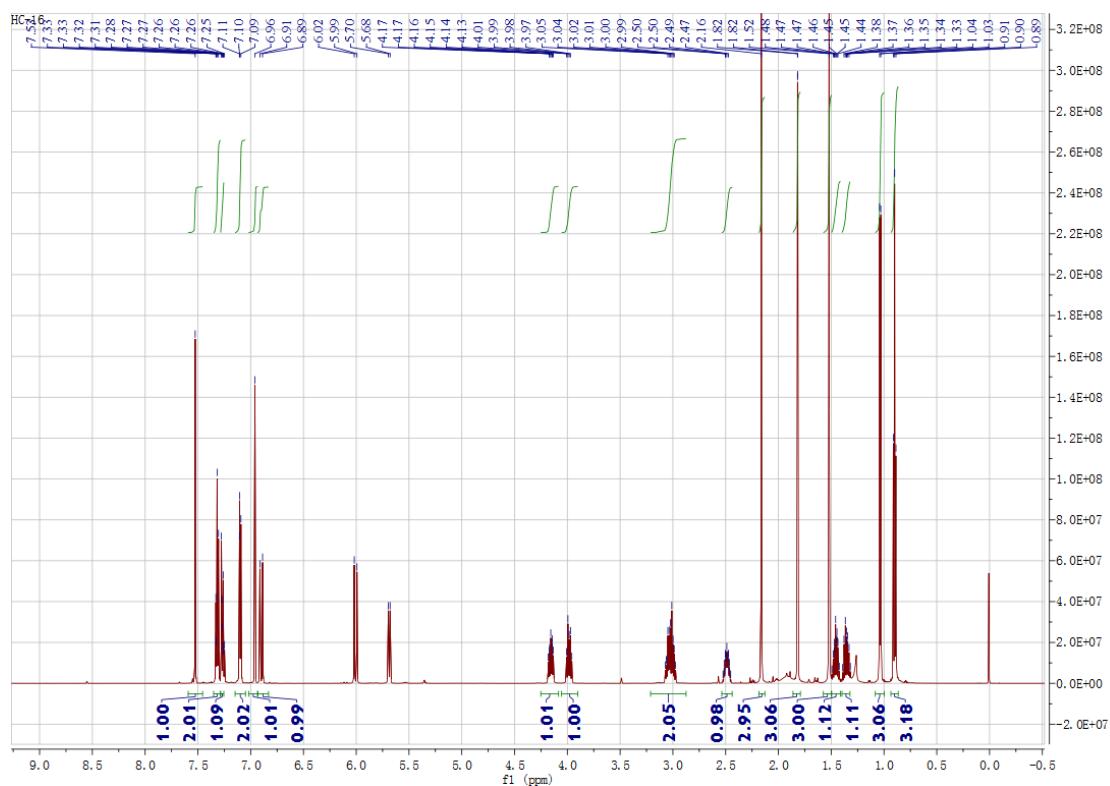
**Fig.S42.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **15**



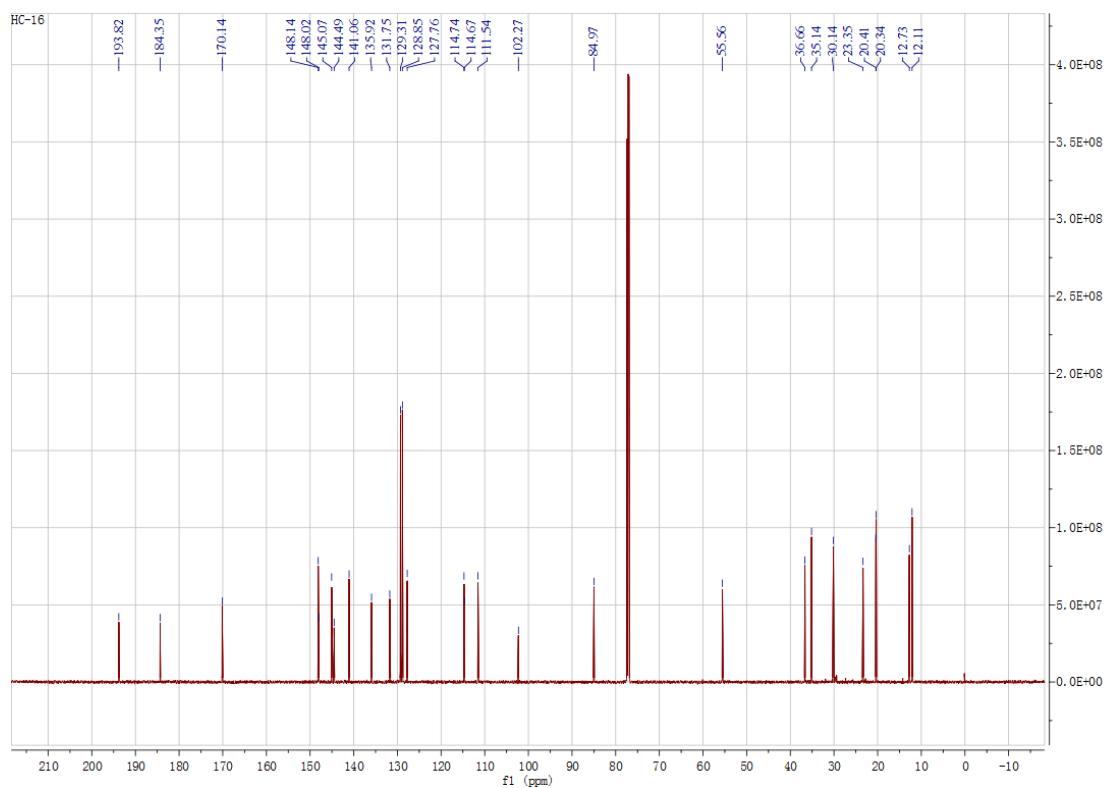
**Fig.S43.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 15



**Fig.S44.** MS spectrum of compound 16

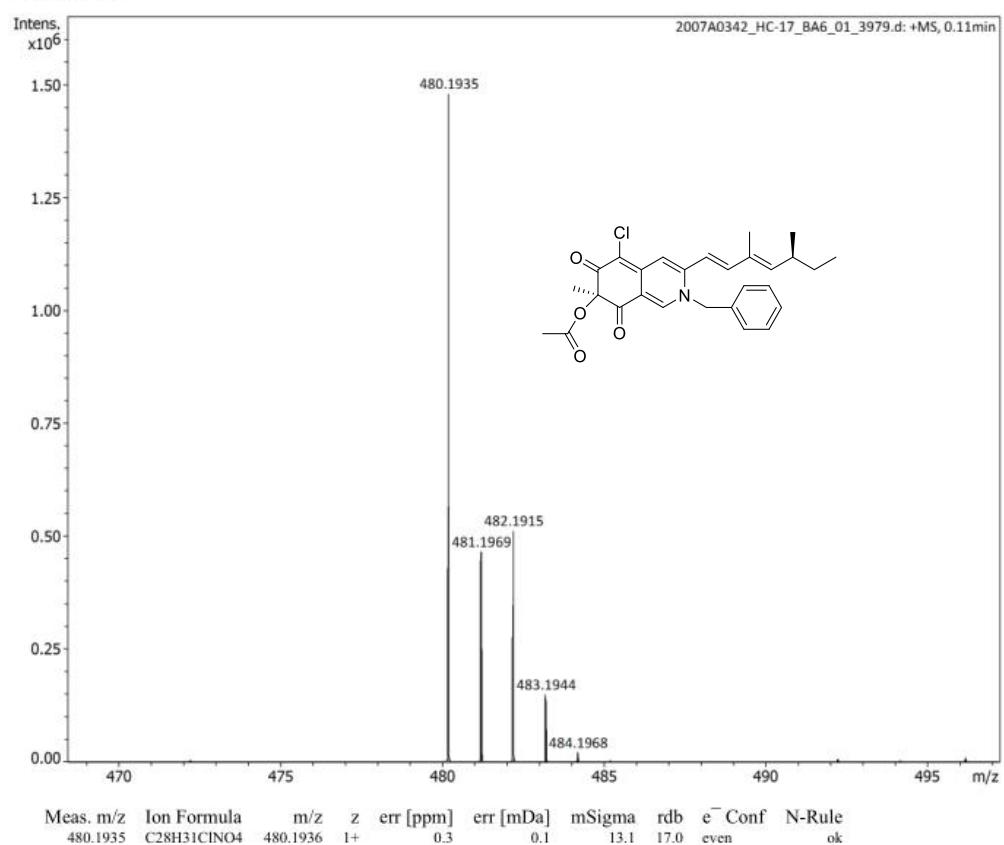


**Fig.S45.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **16**

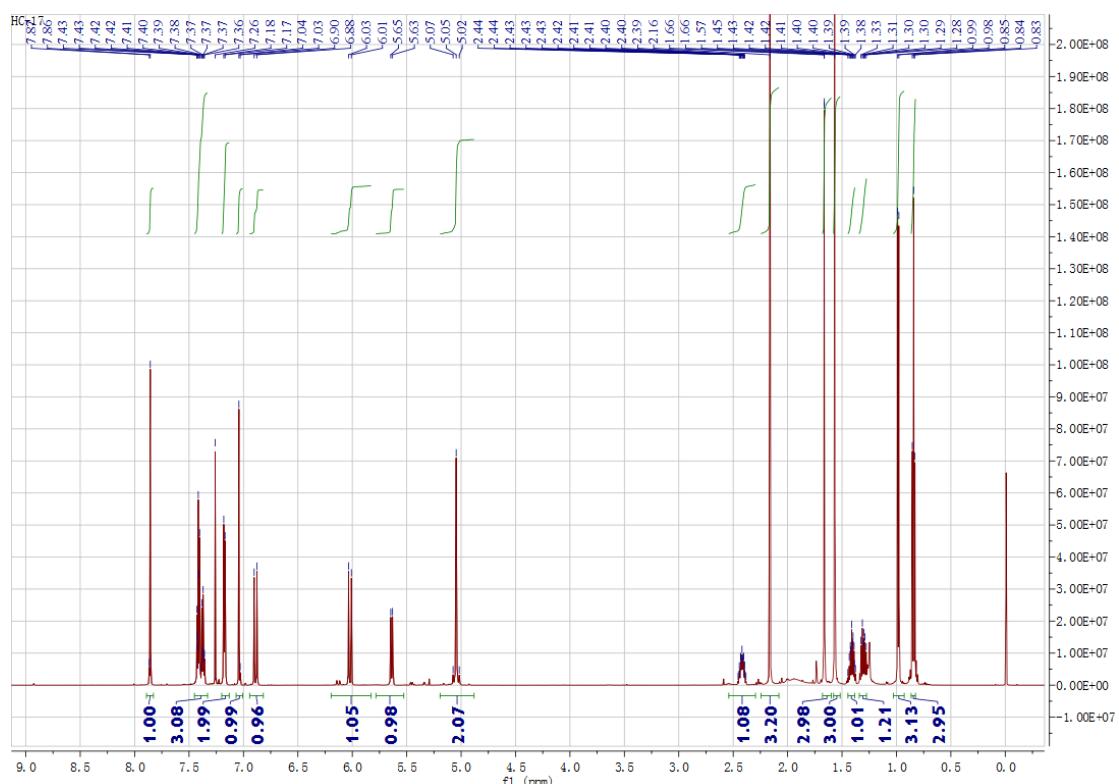


**Fig.S46.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound **16**

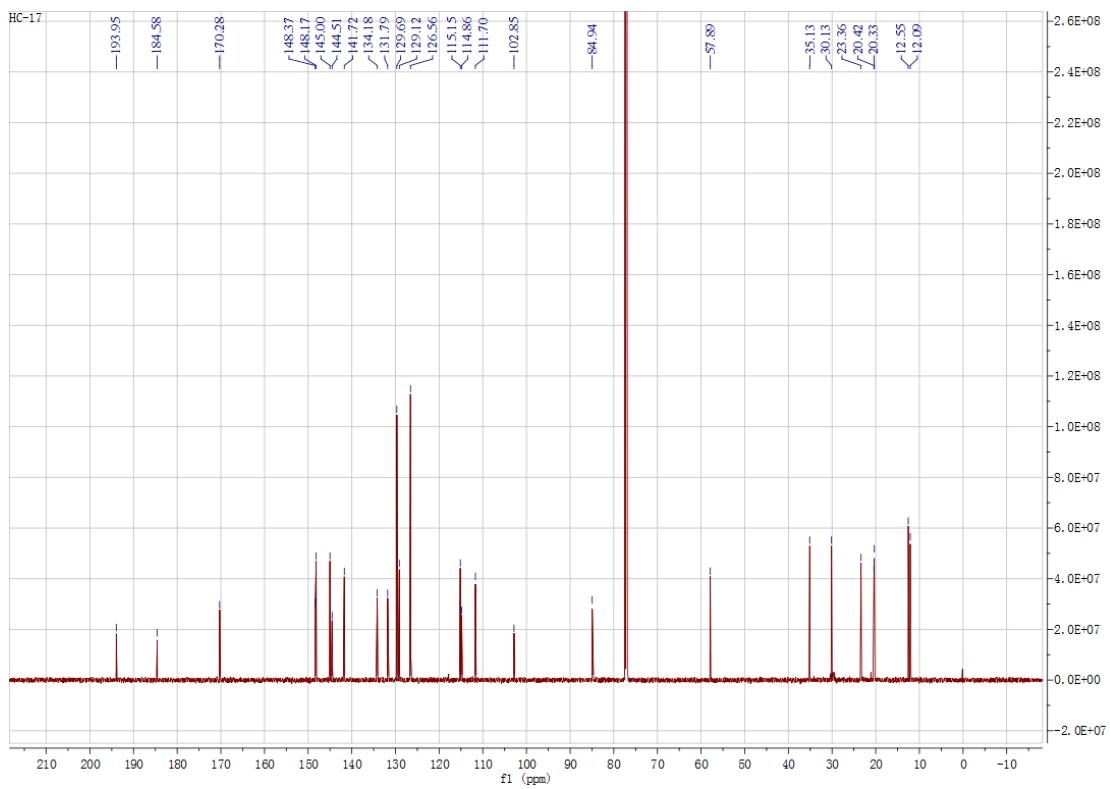
+MS, 0.11min



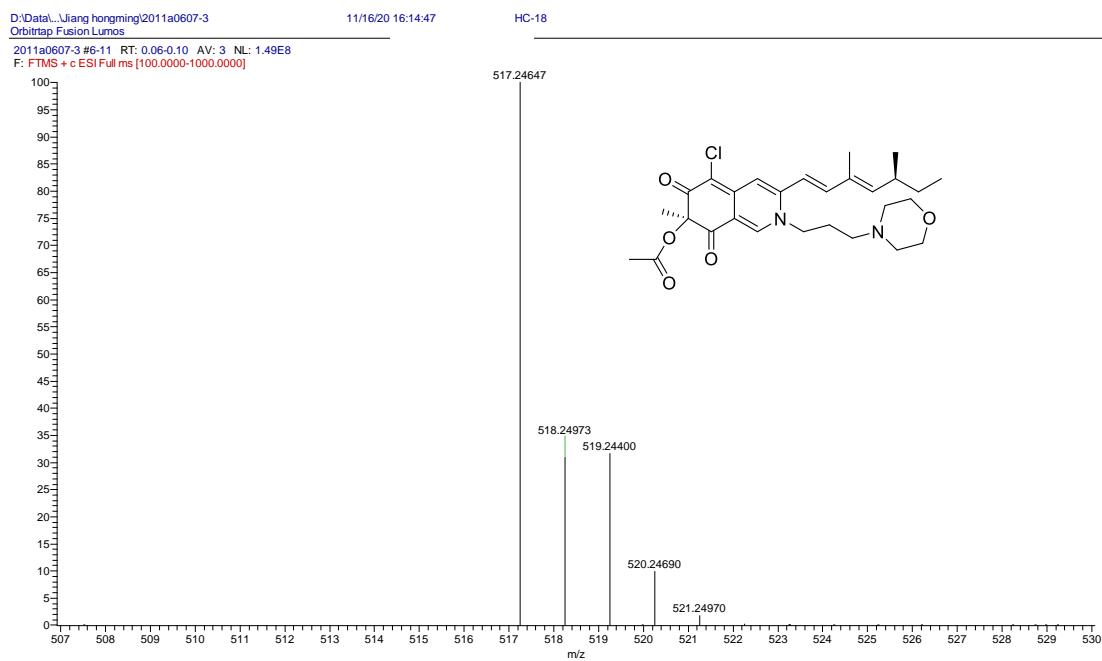
**Fig.S47.** HRMS spectrum of compound 17



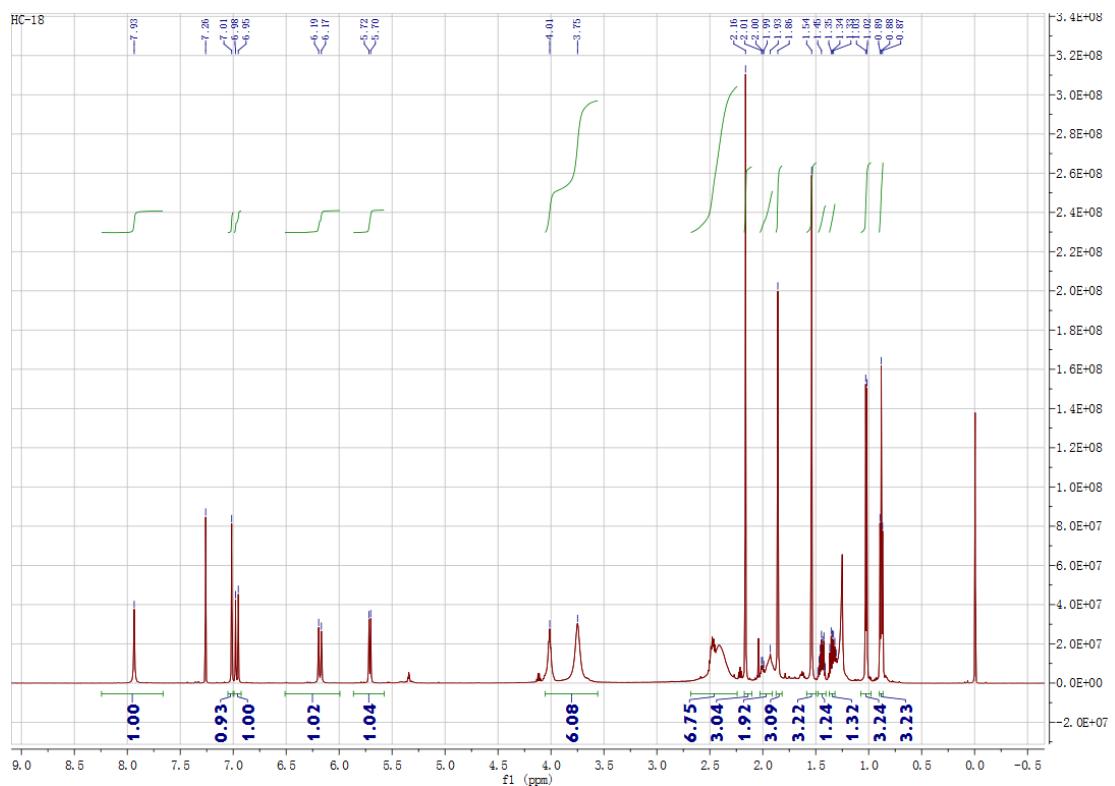
**Fig.S48.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound 17



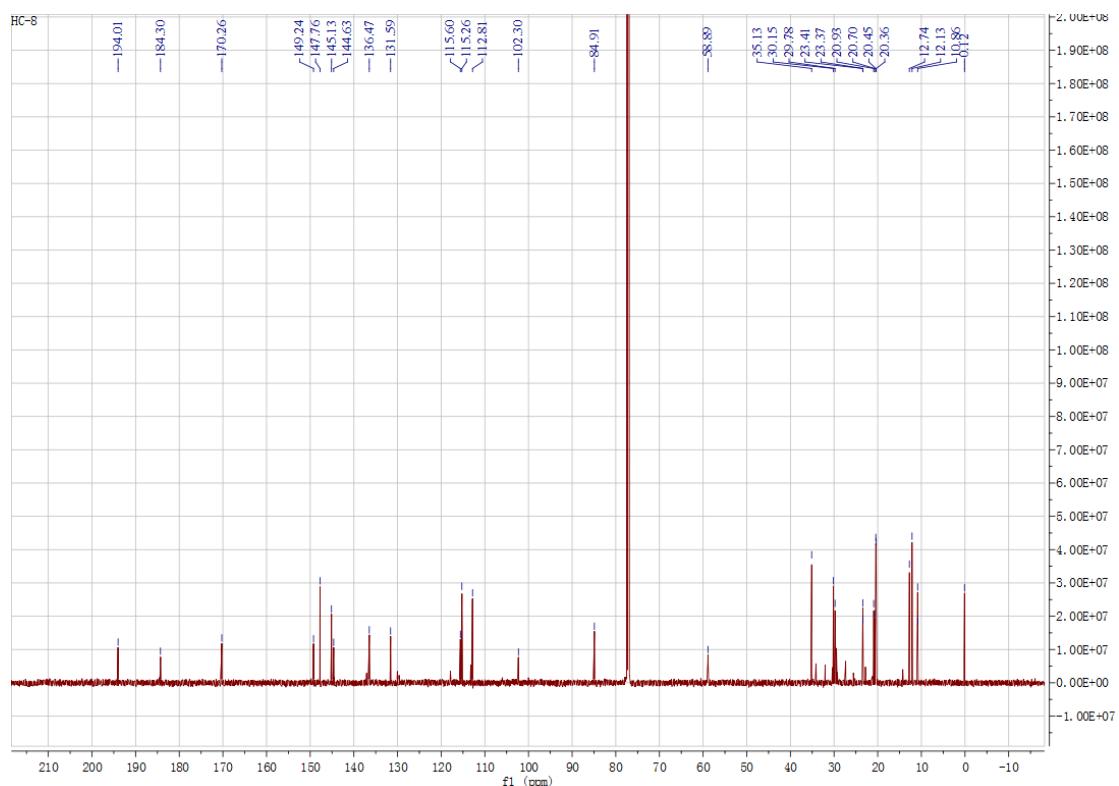
**Fig.S49.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 17



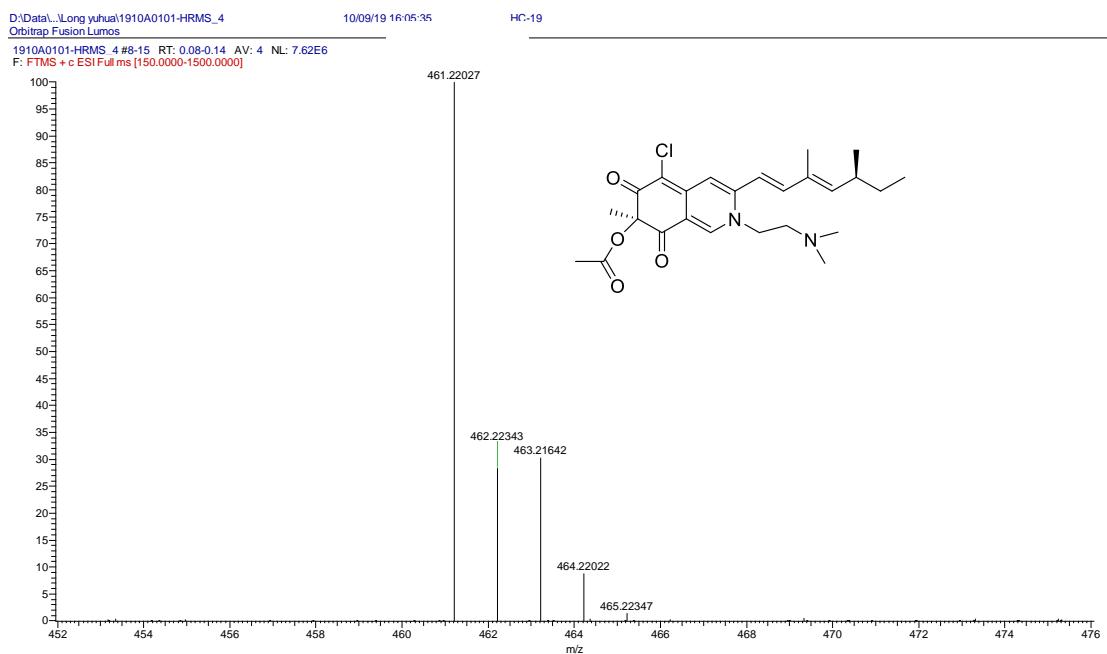
**Fig.S50.** HRMS spectrum of compound 18



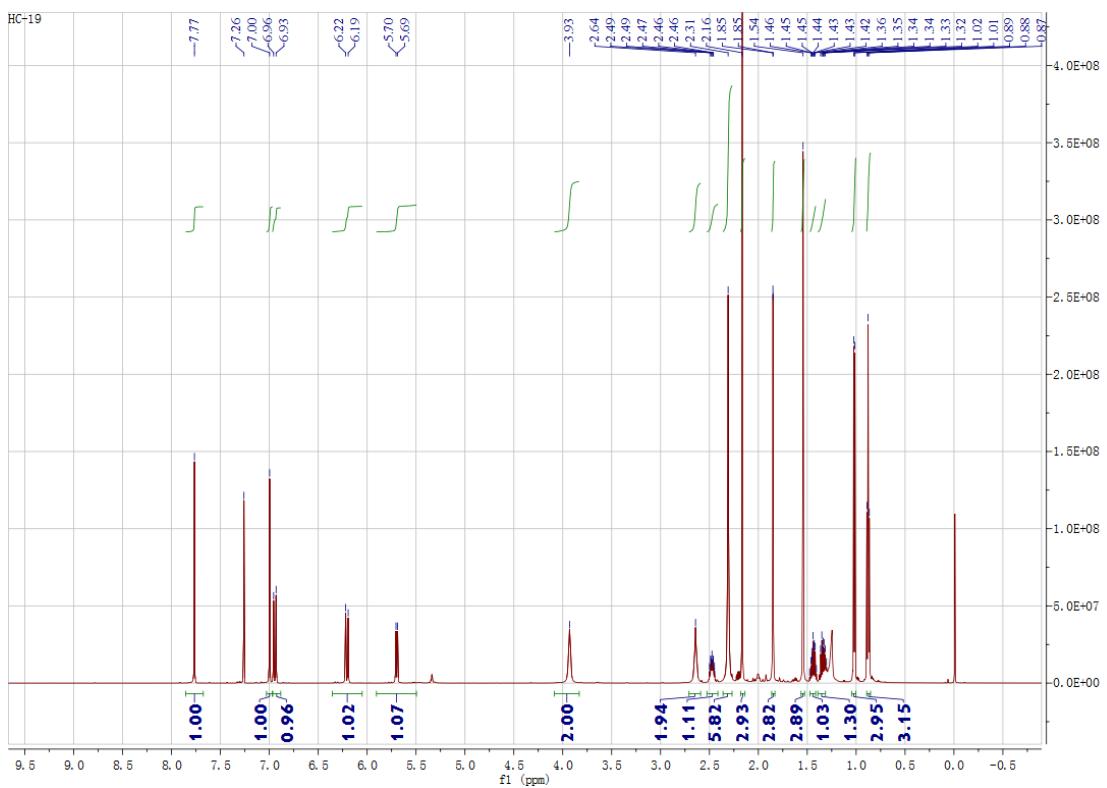
**Fig.S51.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **18**



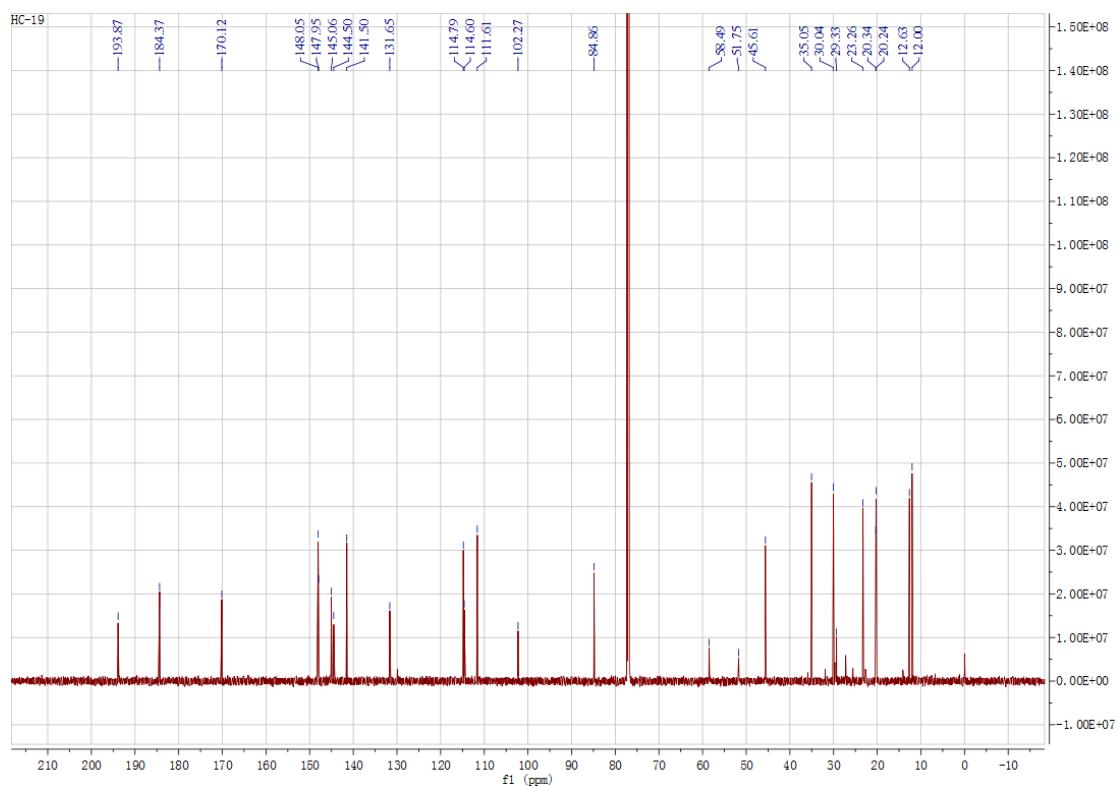
**Fig.S52.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound **18**



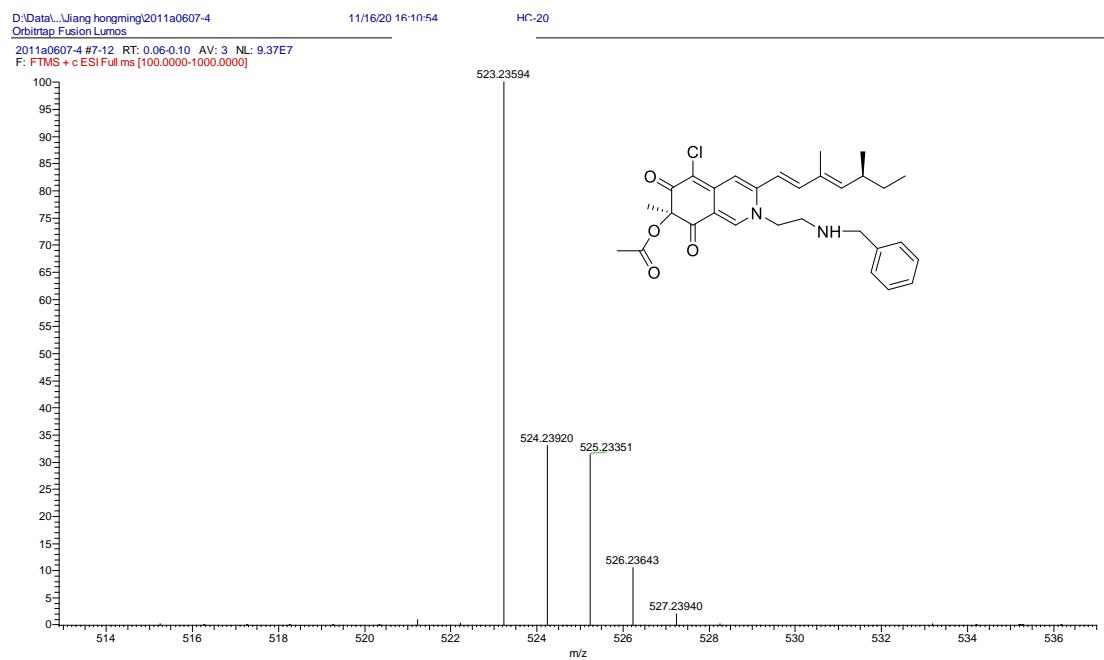
**Fig.S53.** HRMS spectrum of compound 19



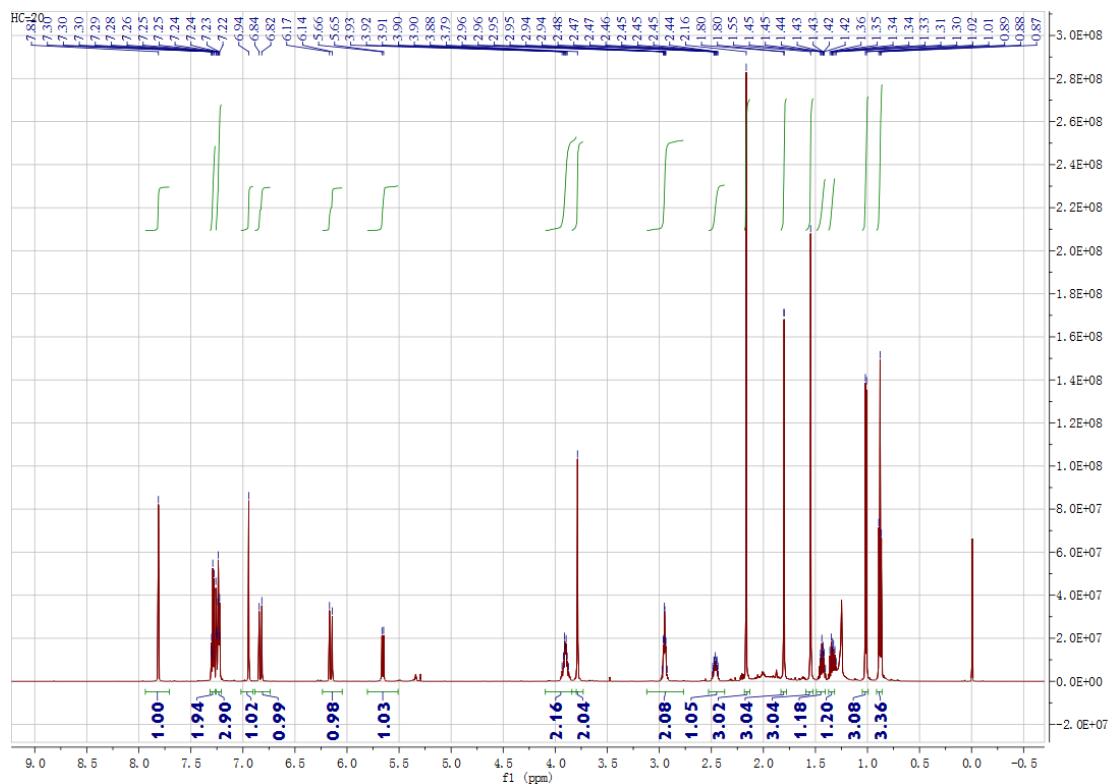
**Fig.S54.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound 19



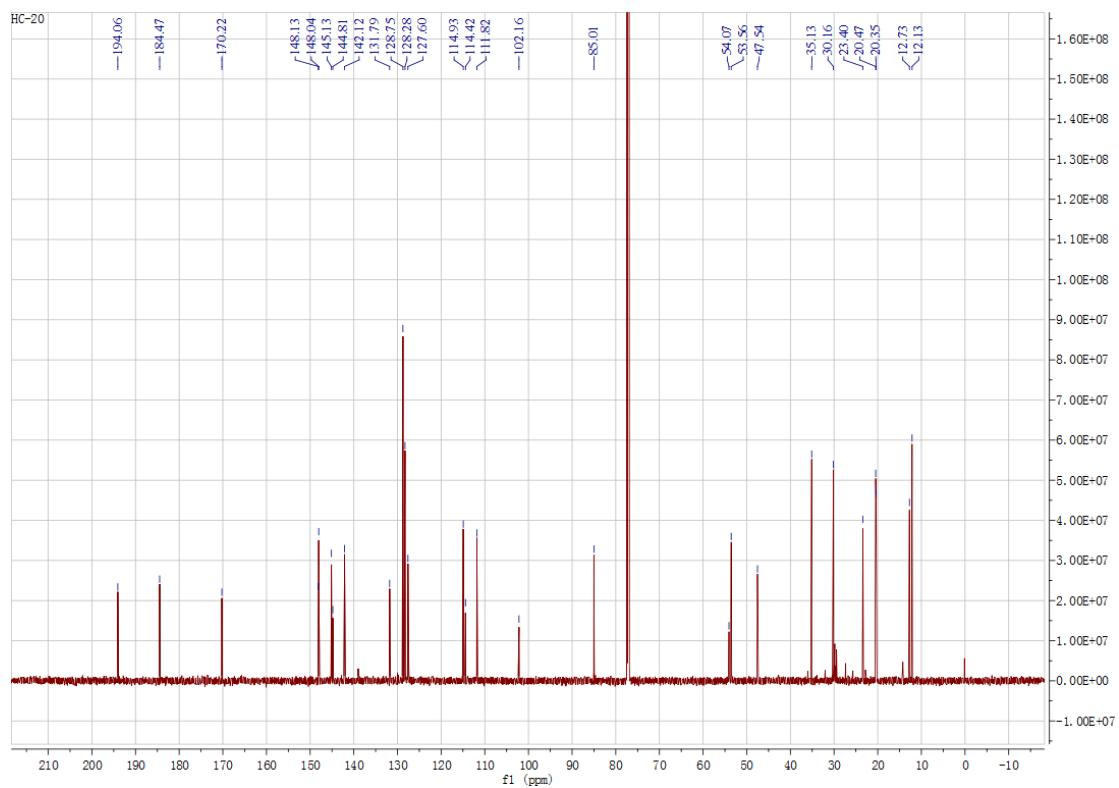
**Fig.S55.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 19



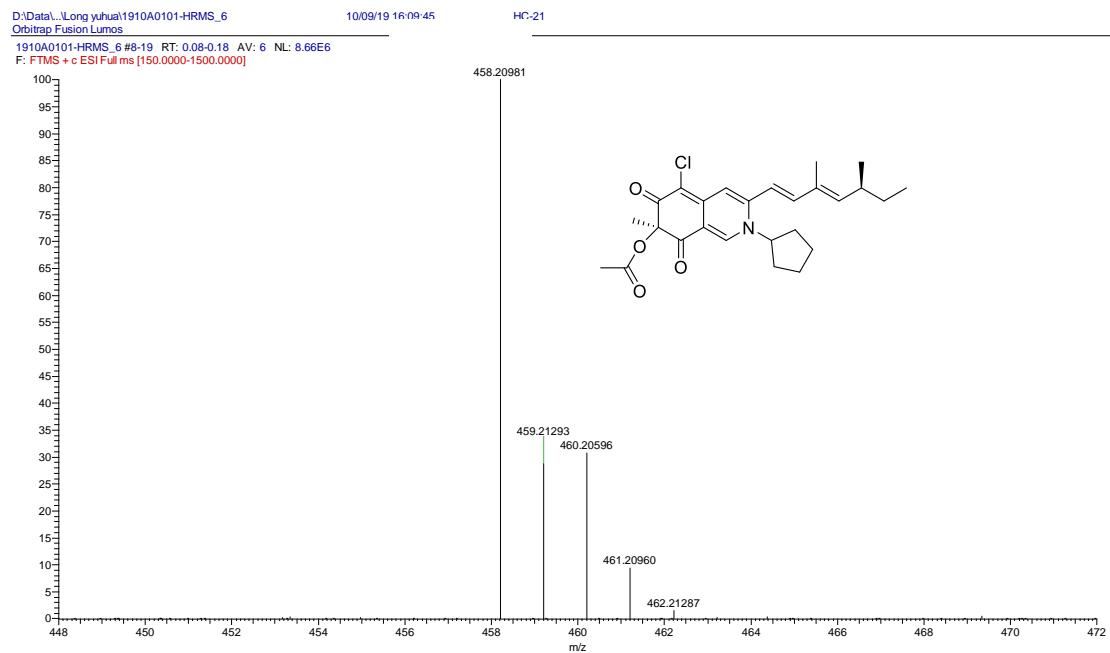
**Fig.S56.** HRMS spectrum of compound 20



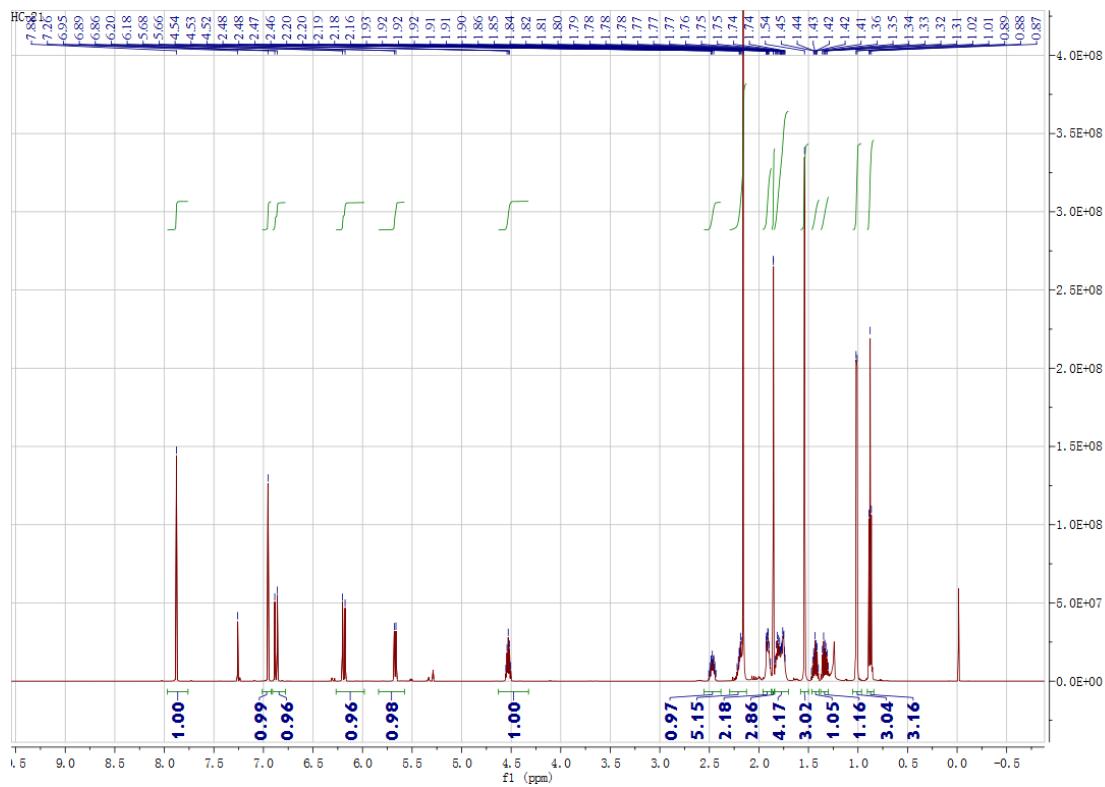
**Fig.S57.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **20**



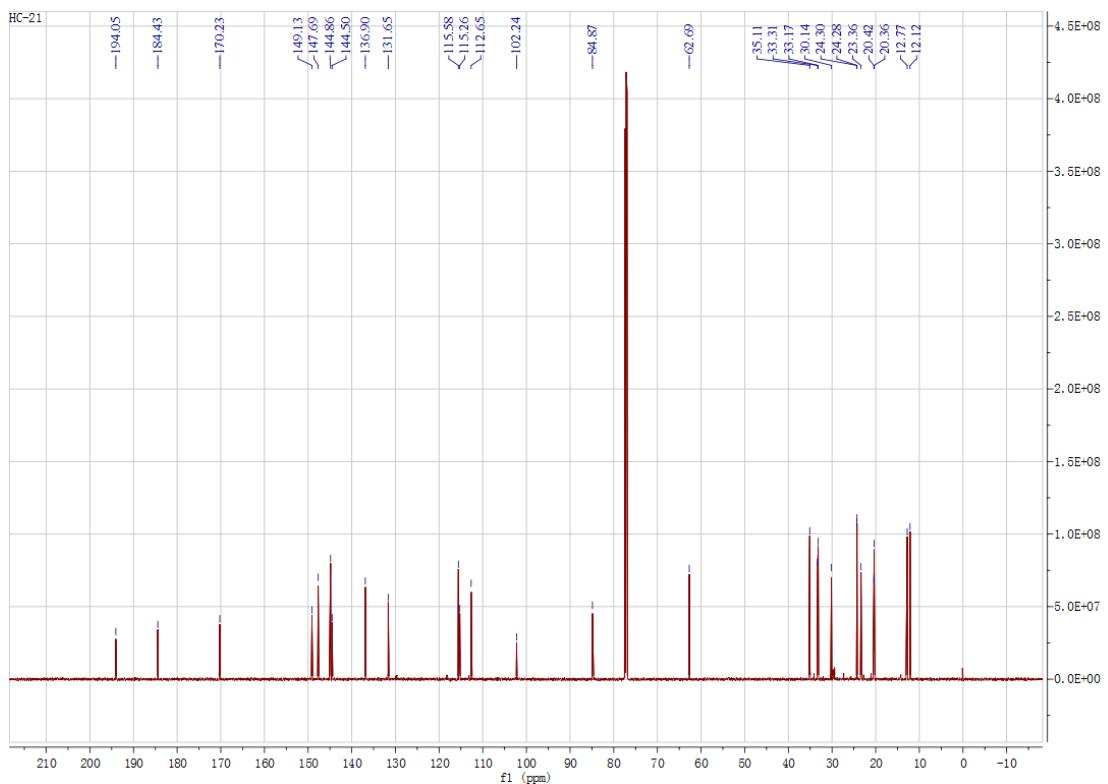
**Fig.S58.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound **20**



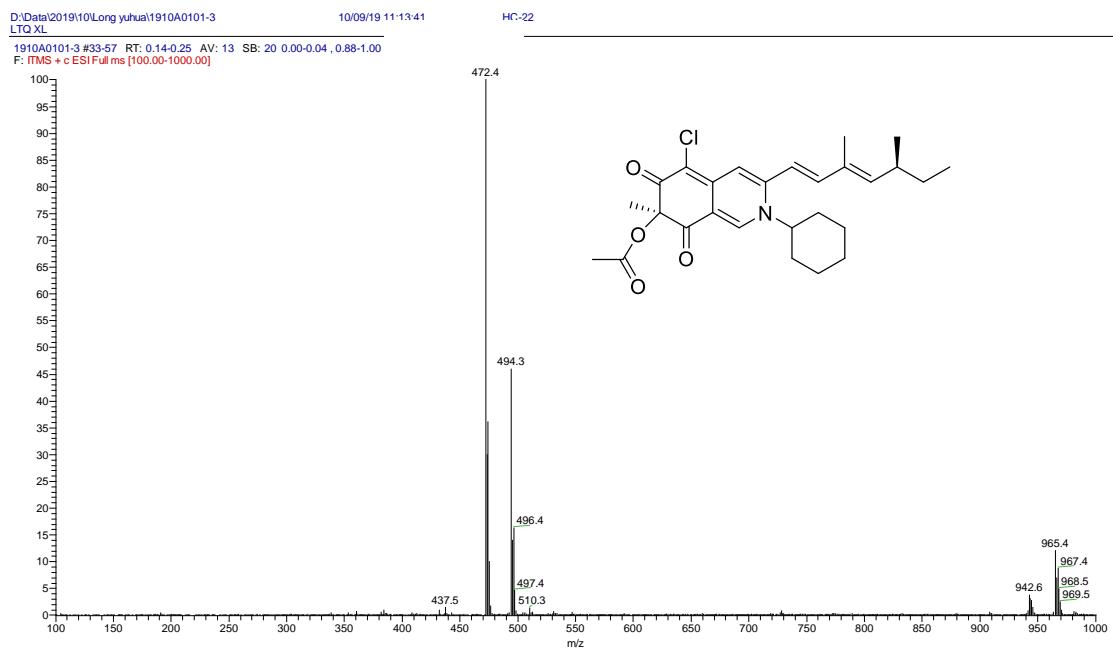
**Fig.S59.** HRMS spectrum of compound 21



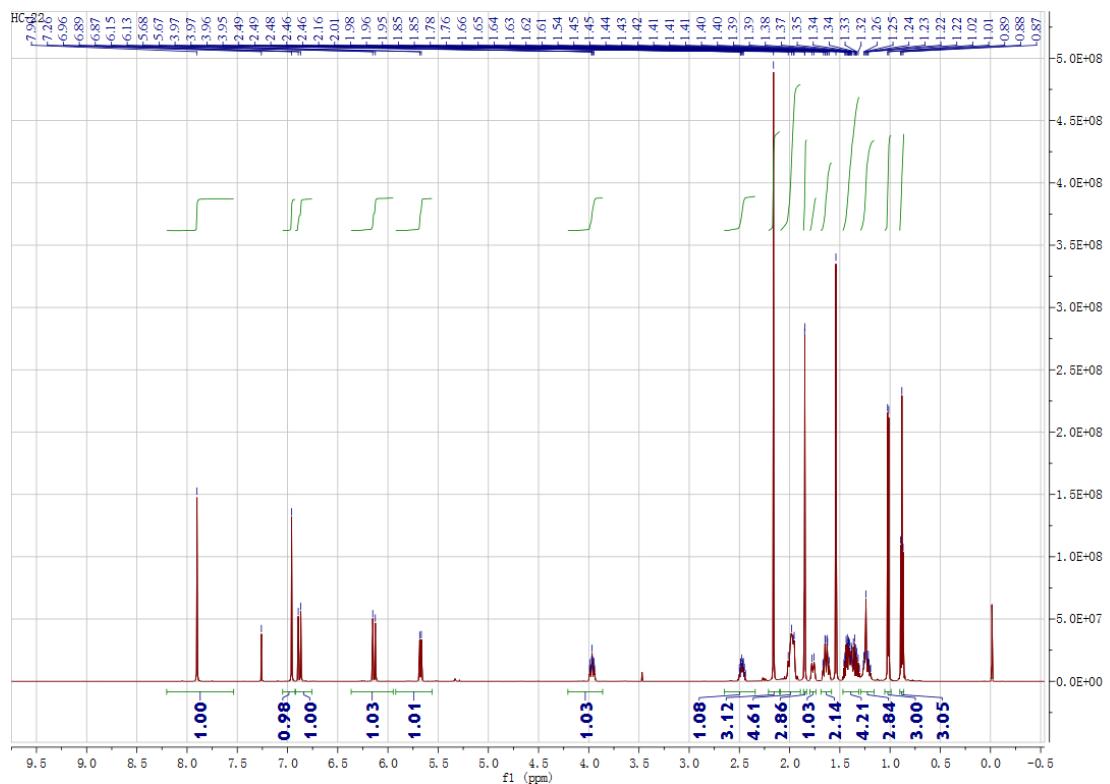
**Fig.S60.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound 21



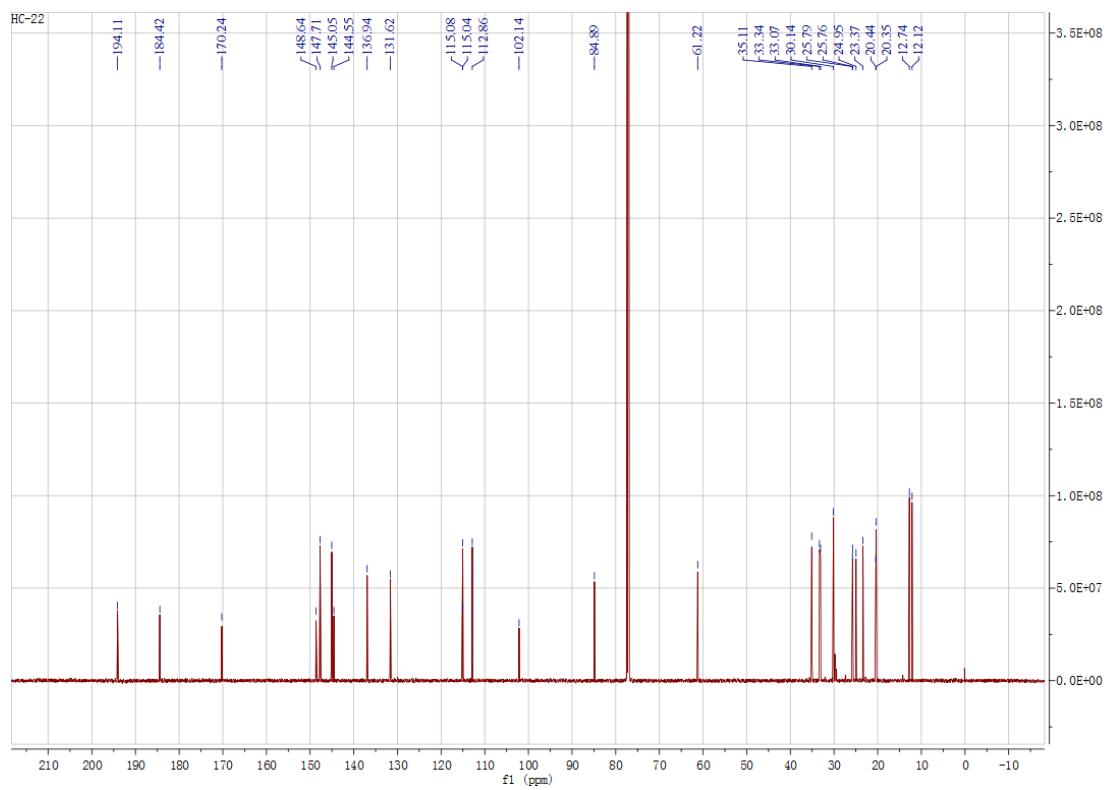
**Fig.S61.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 21



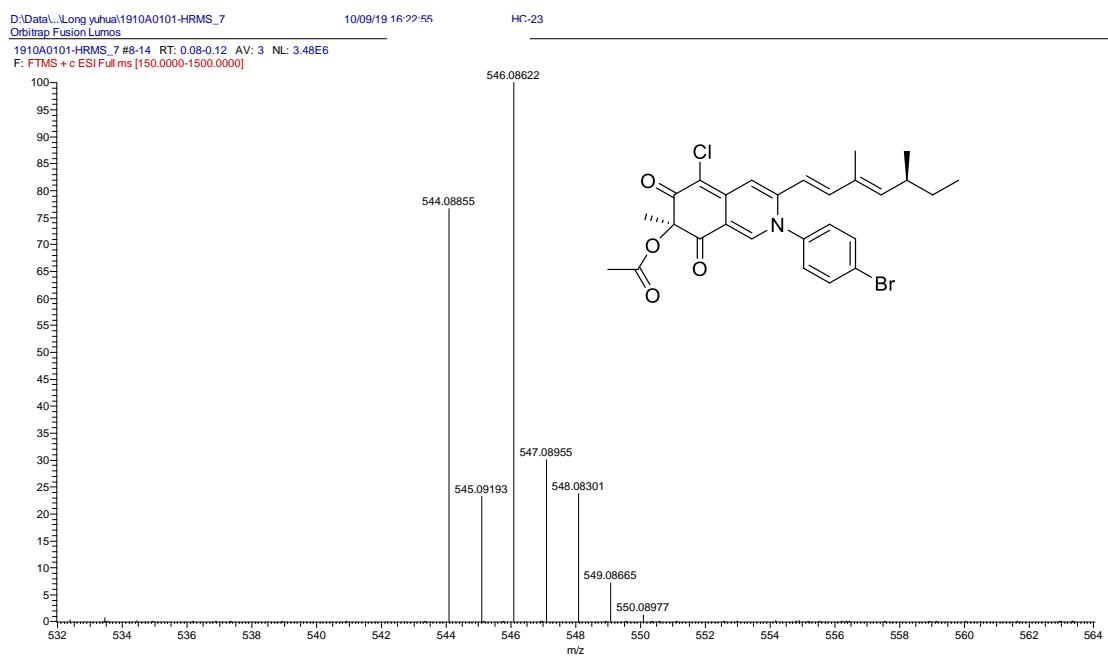
**Fig.S62.** MS spectrum of compound 22



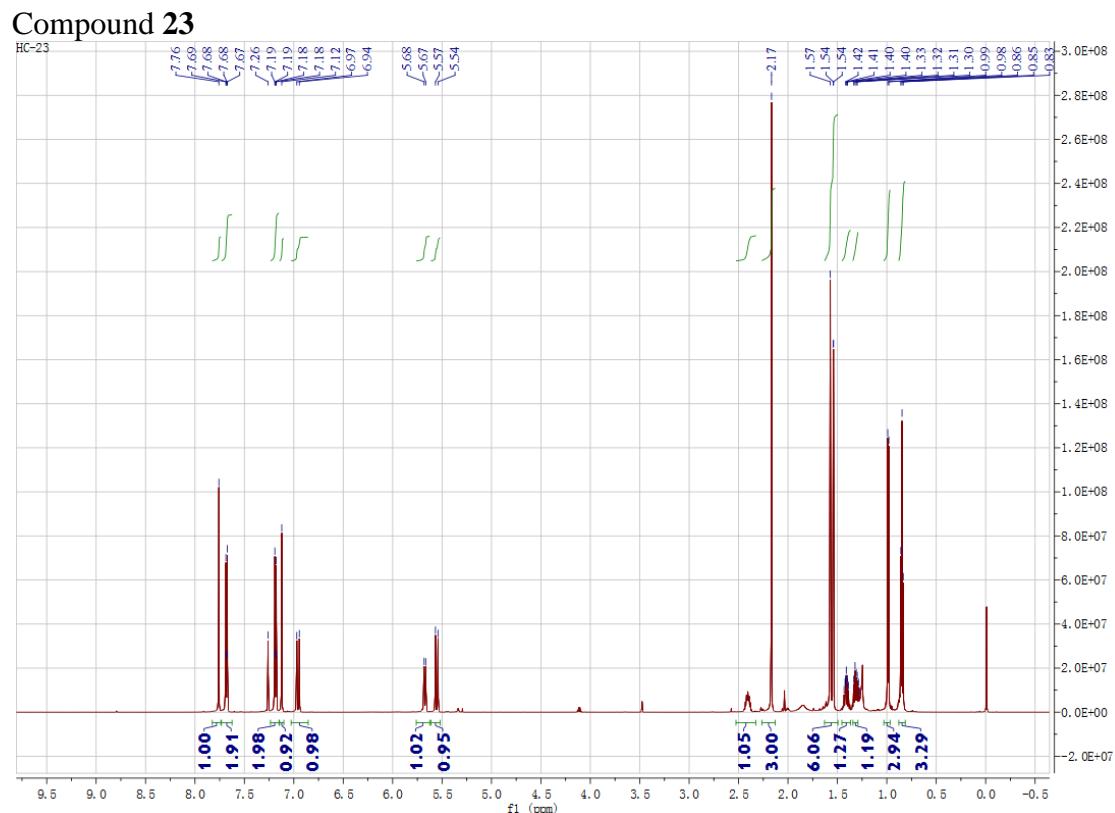
**Fig.S63.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound 22



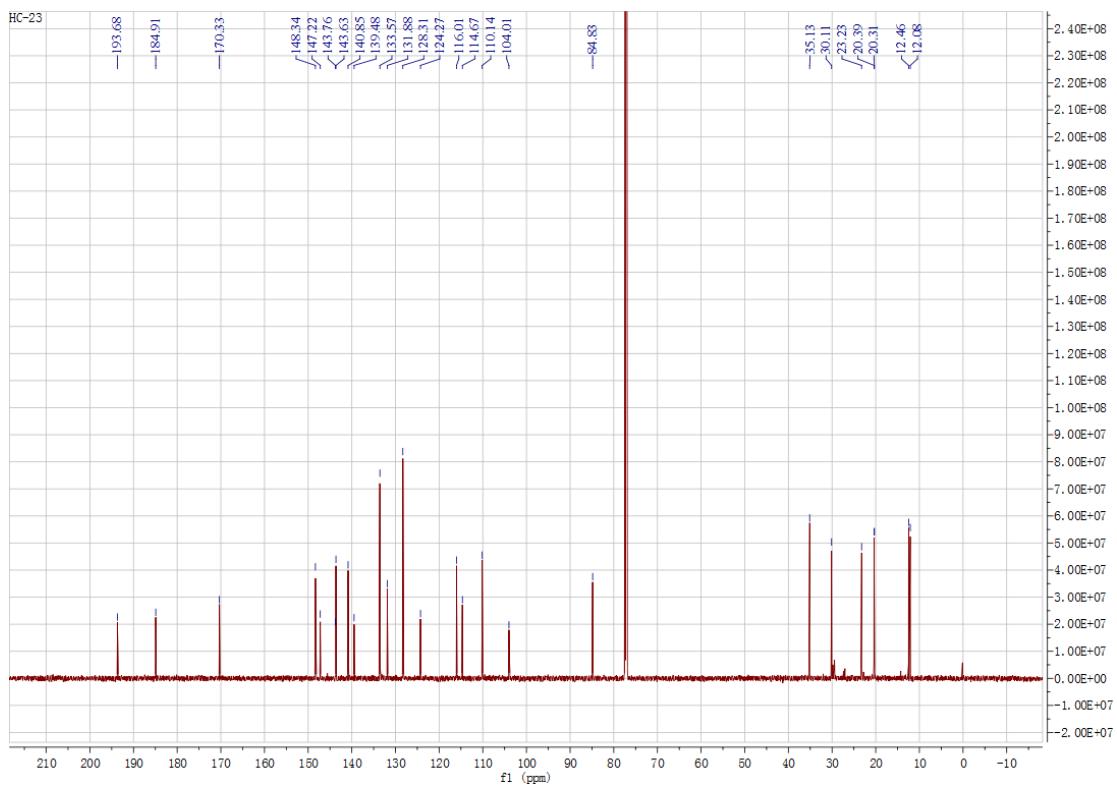
**Fig.S64.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 22



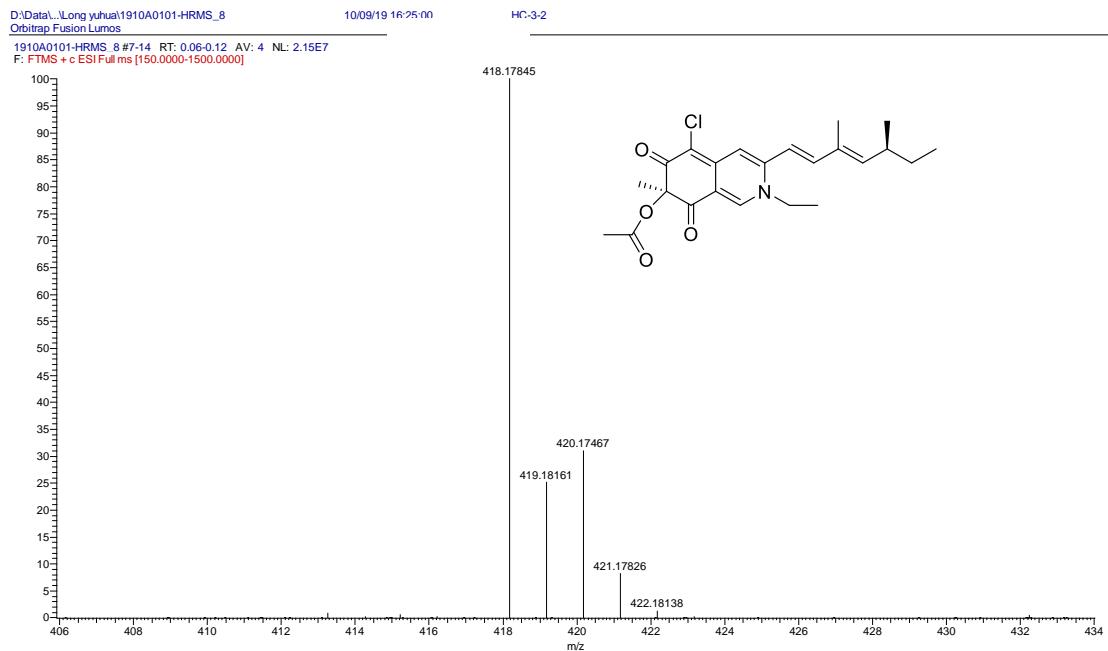
**Fig.S65.** HRMS spectrum of compound 23



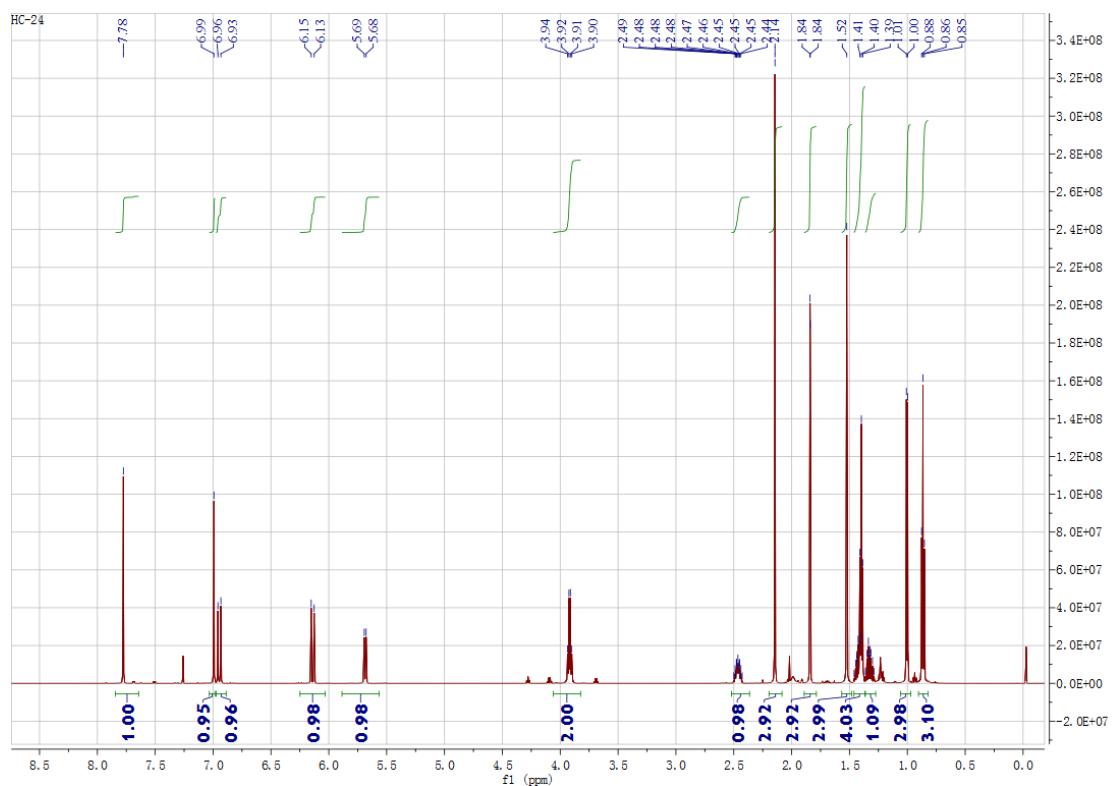
**Fig.S66.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound 23



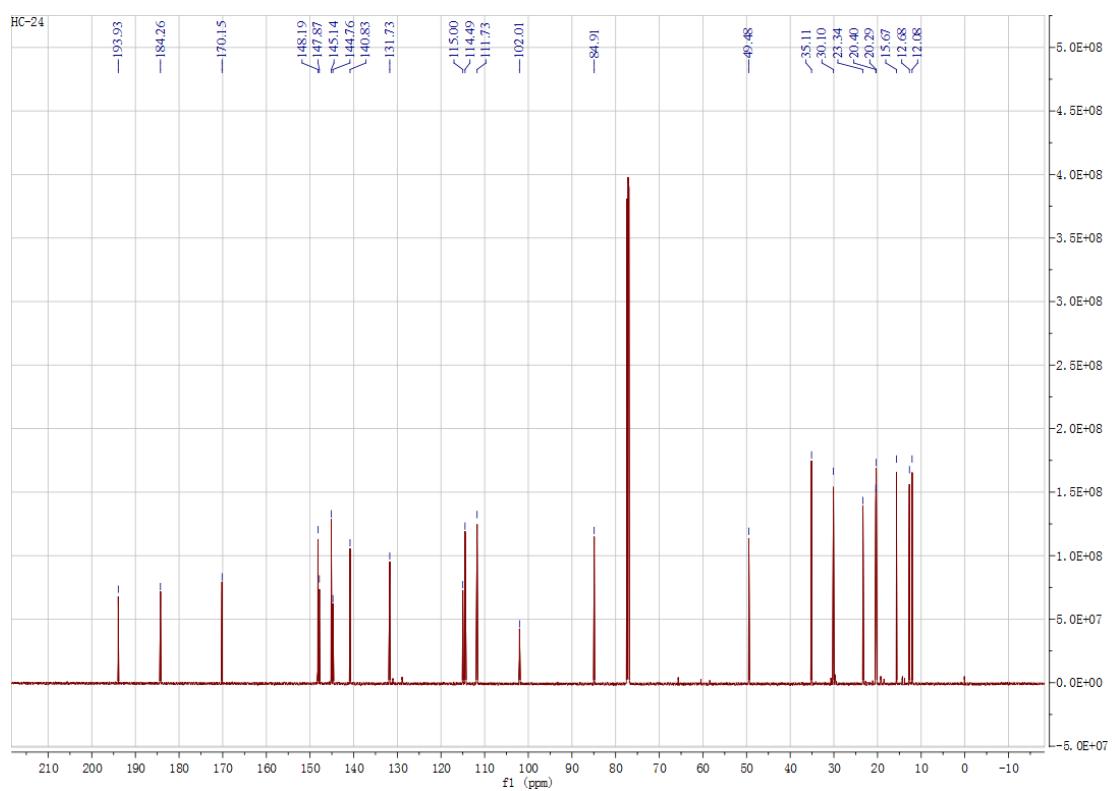
**Fig.S67.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 23



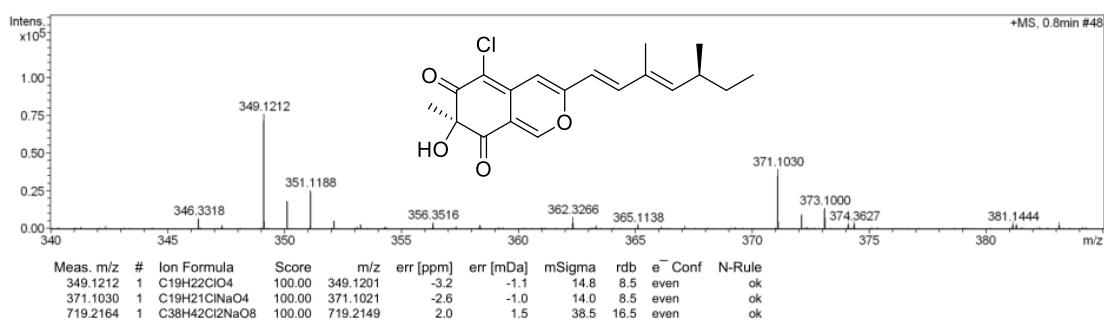
**Fig.S68.** HRMS spectrum of compound 24



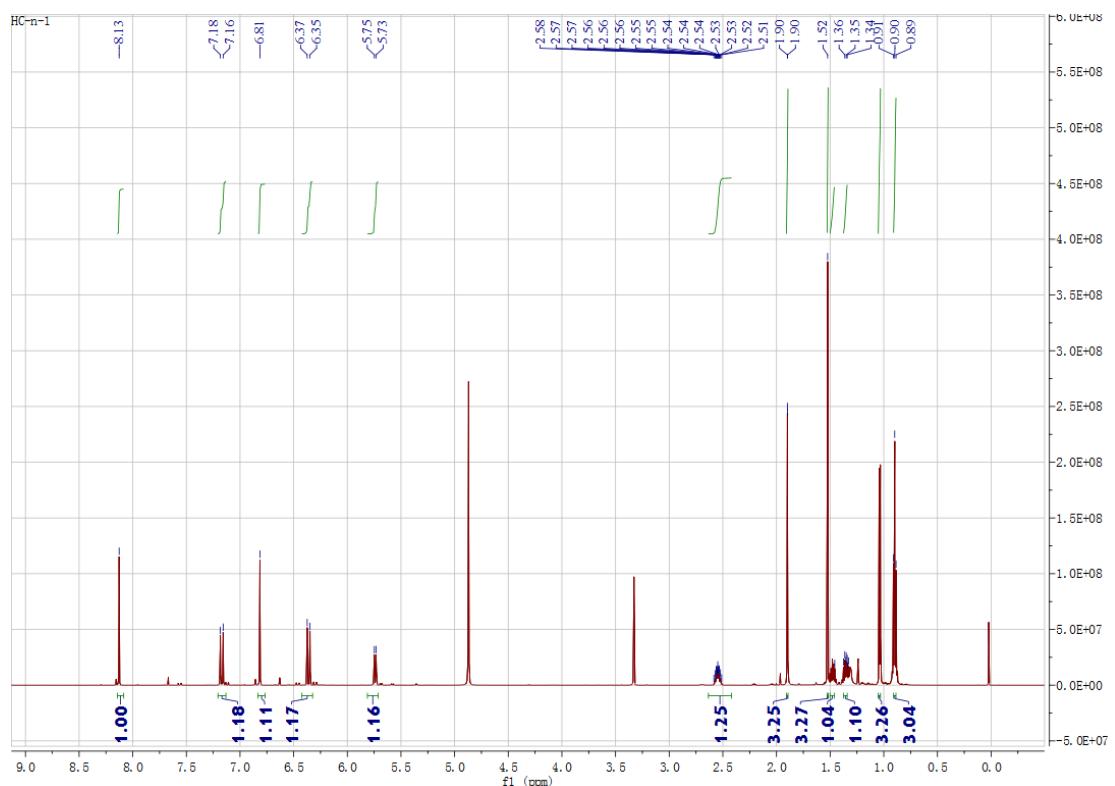
**Fig.S69.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound 24



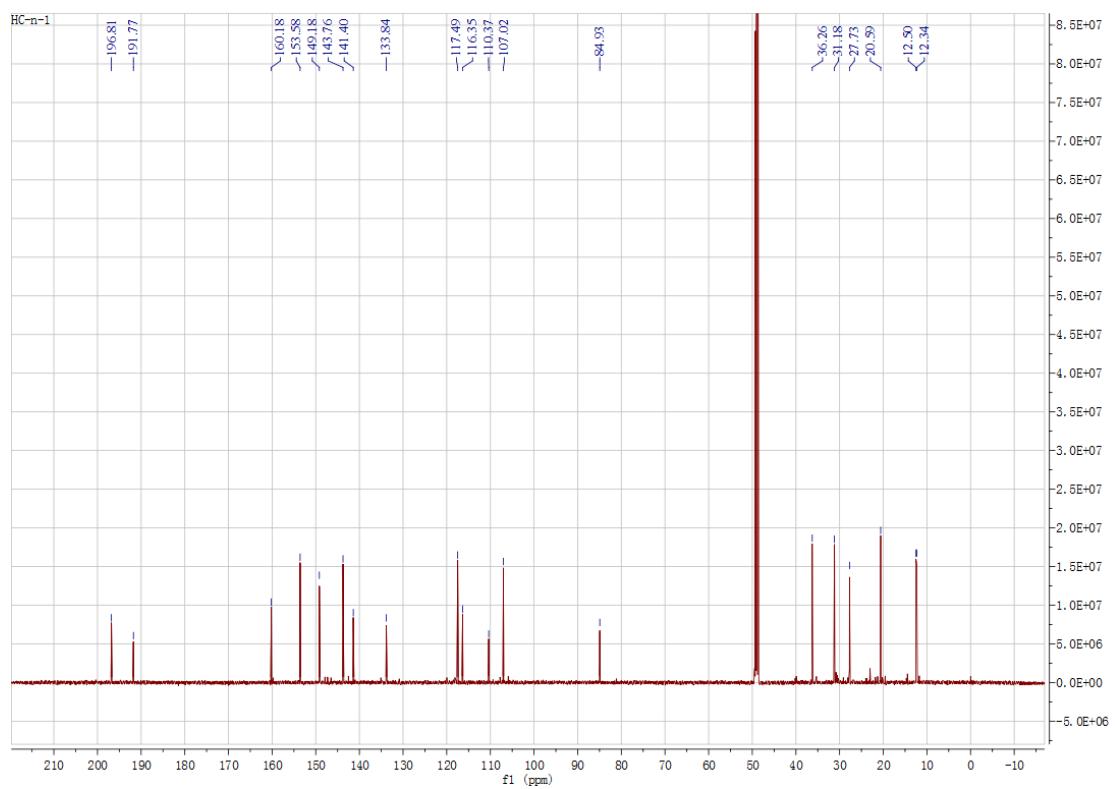
**Fig.S70.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 24



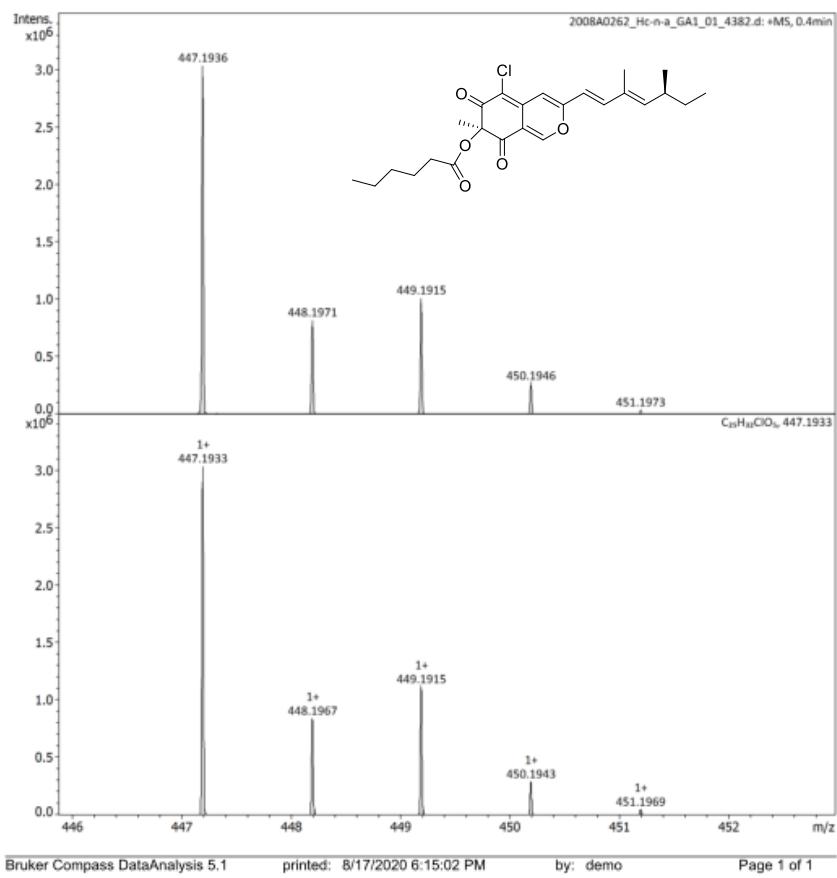
**Fig.S71. HRMS spectrum of compound 25**



**Fig.S72.  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound 25**

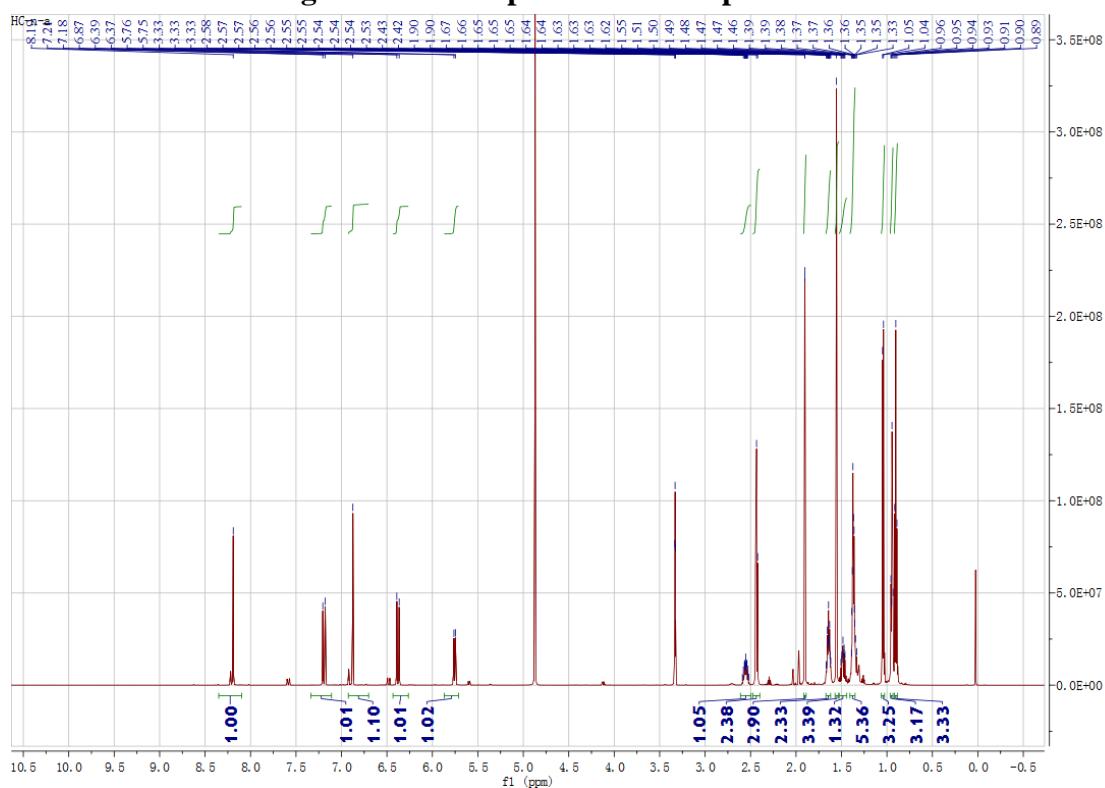


**Fig.S73.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 25

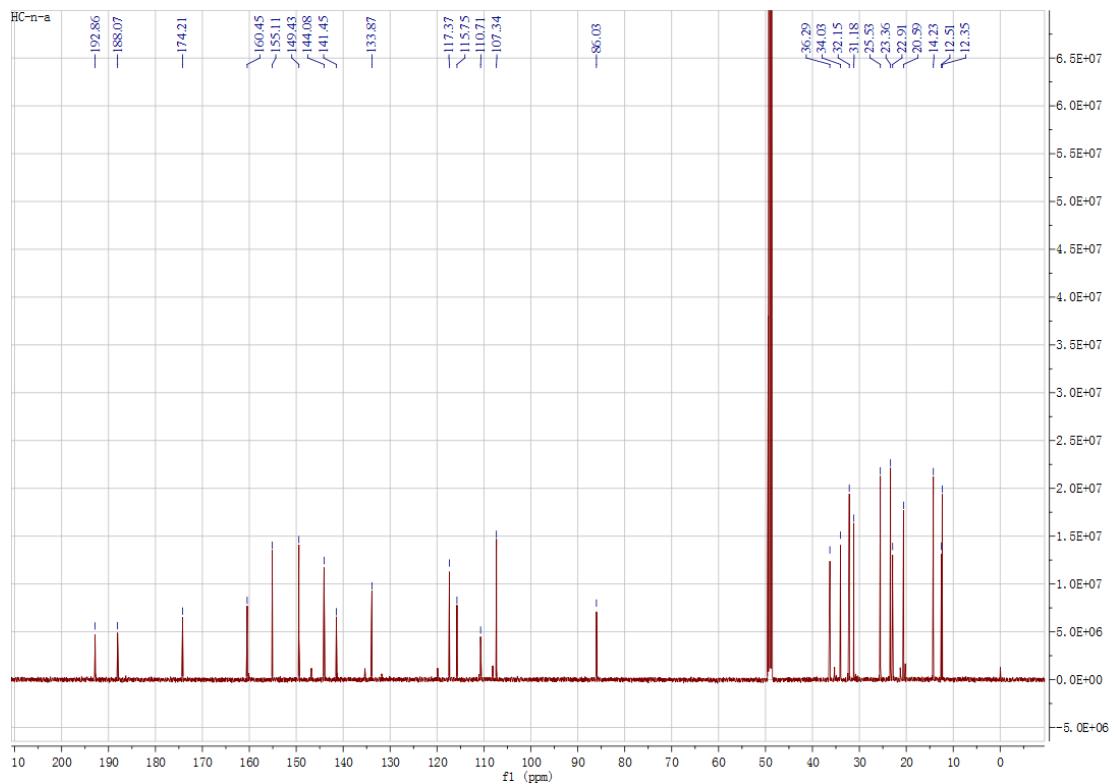


Bruker Compass DataAnalysis 5.1 printed: 8/17/2020 6:15:02 PM by: demo Page 1 of 1

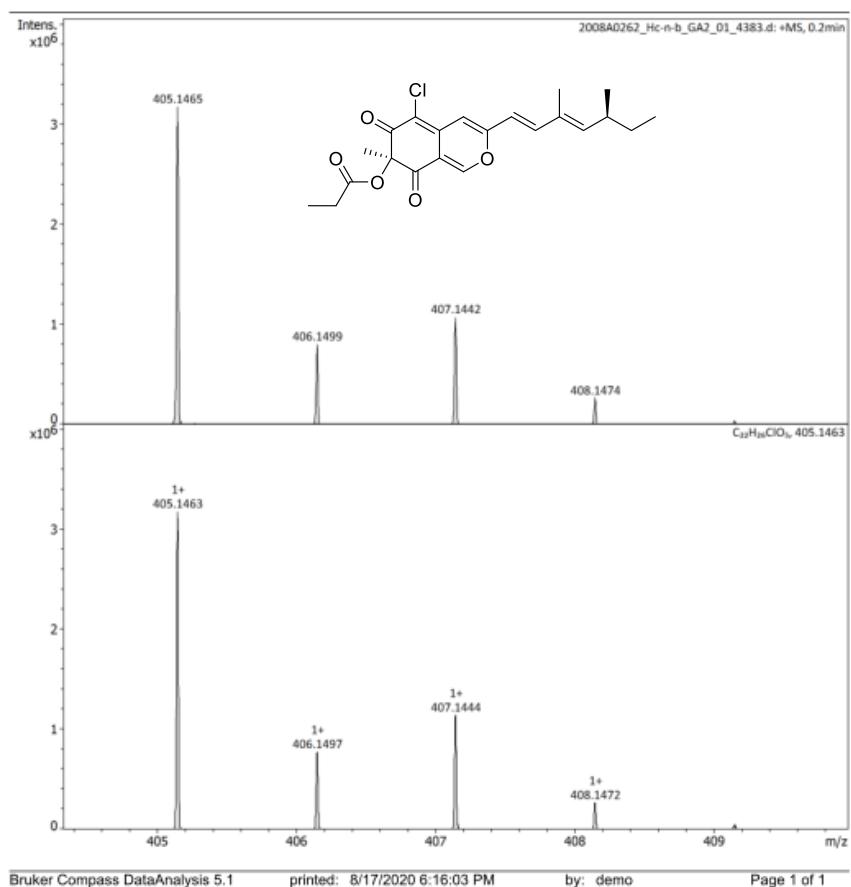
**Fig.S74.** HRMS spectrum of compound **26**



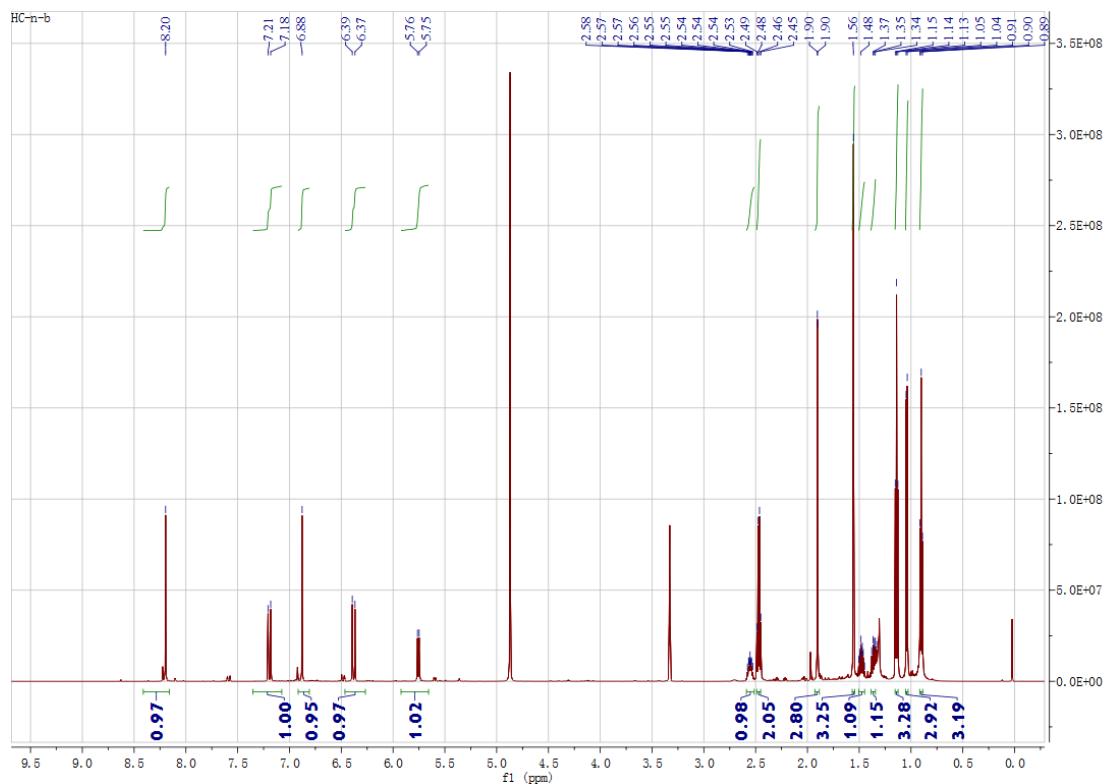
**Fig.S75.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **26**



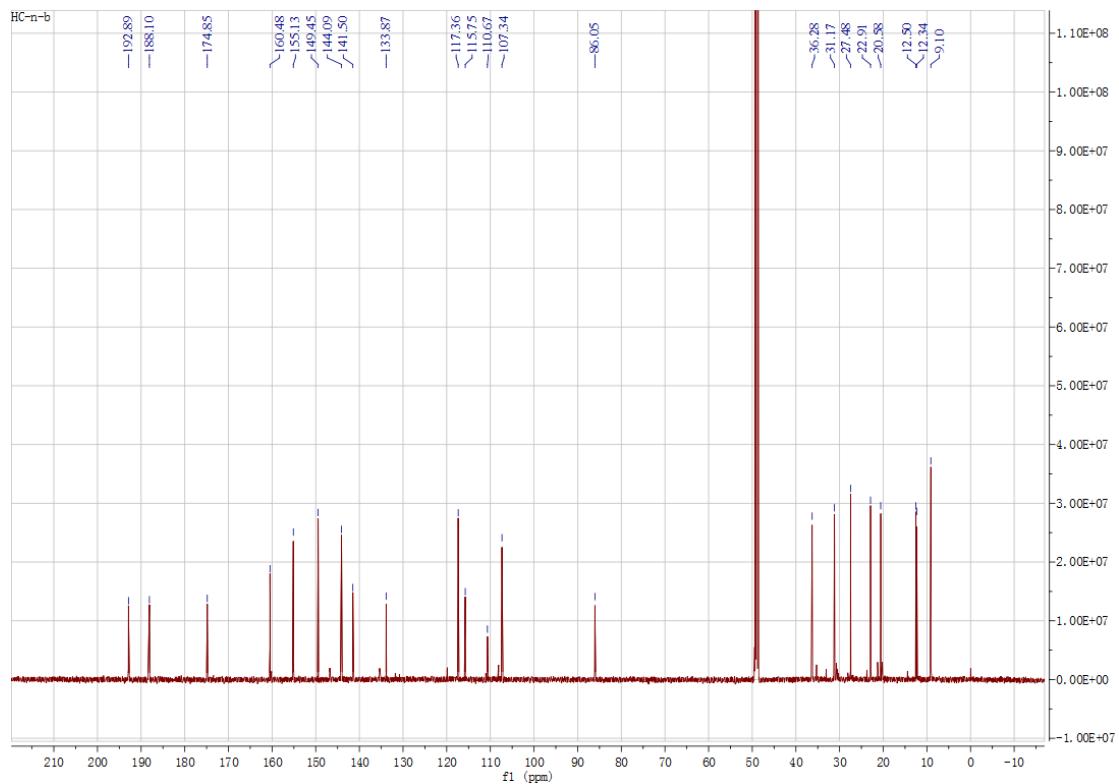
**Fig.S76.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound **26**



**Fig.S77. HRMS spectrum of compound 27**



**Fig.S78.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **27**



**Fig.S79.**  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound **27**