

Supporting Information

Total synthesis of pulmonarin B and design of bromated-phenylacetic acid/tacrine hybrids: marine pharmacophore inspired discovery of new ChE and A β aggregation inhibitors

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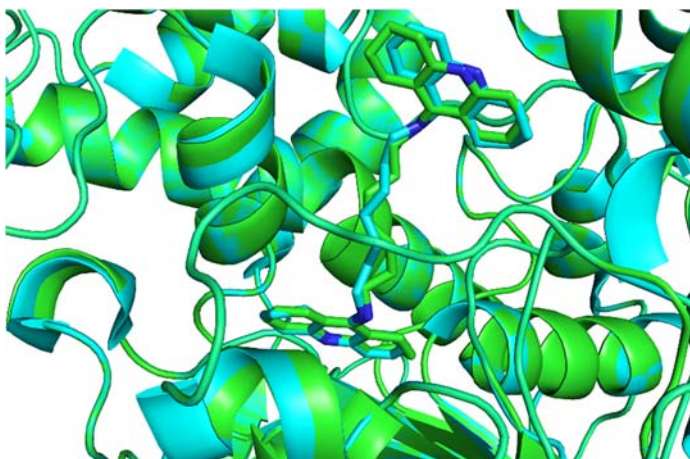
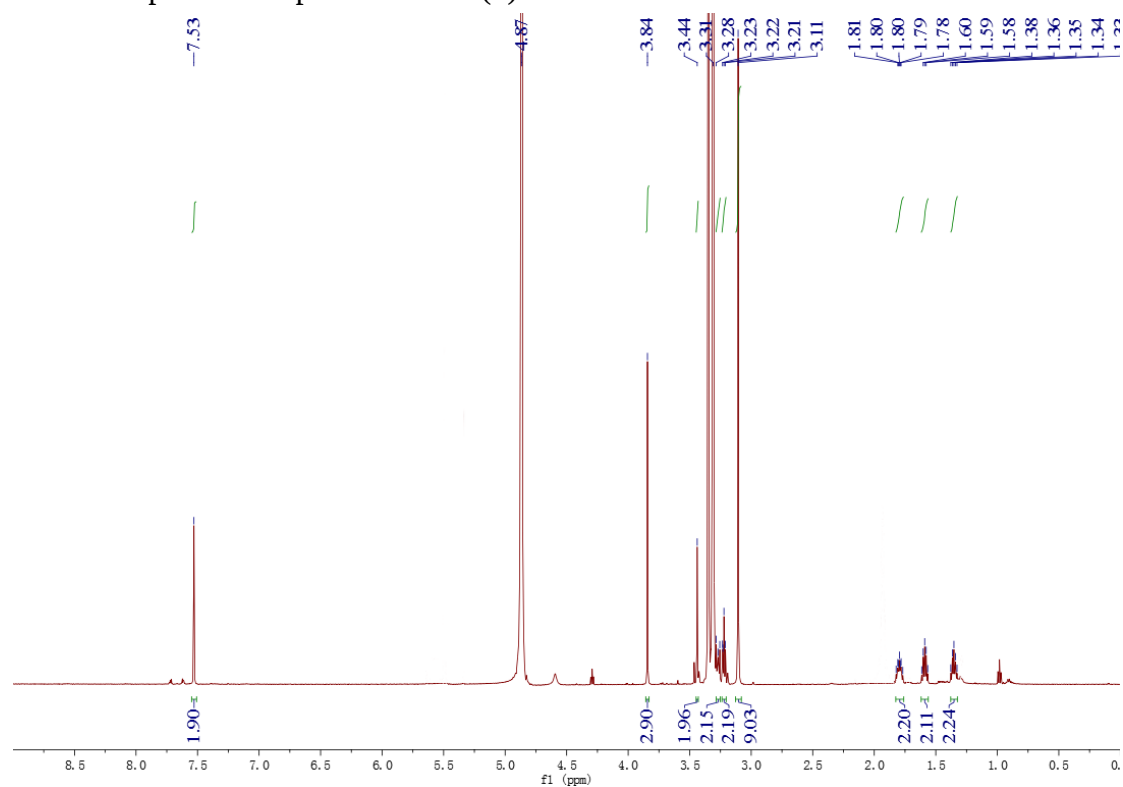
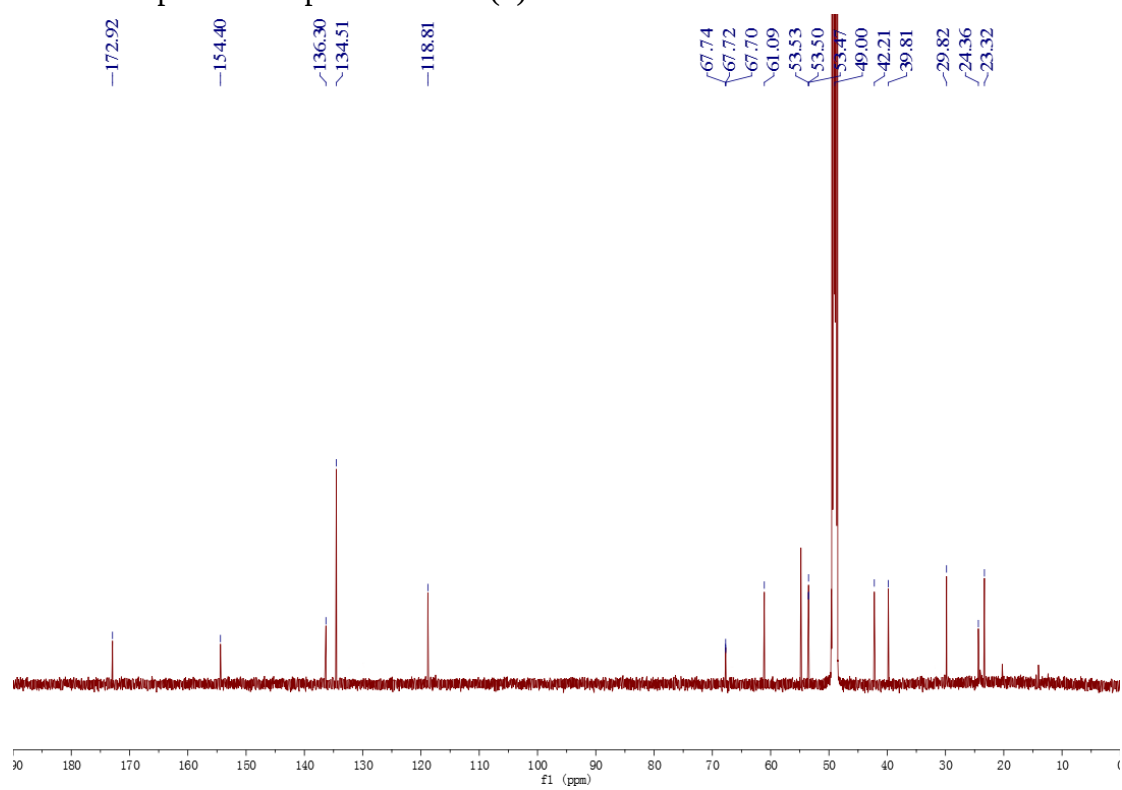


Figure S1. Comparison of the redocked alkylene-linked bis-tacrine to 5EI5 with its original crystal structures. The re-docked ligand was shown in sticks with green color, while the original crystal structure was shown in sticks with cyan color.

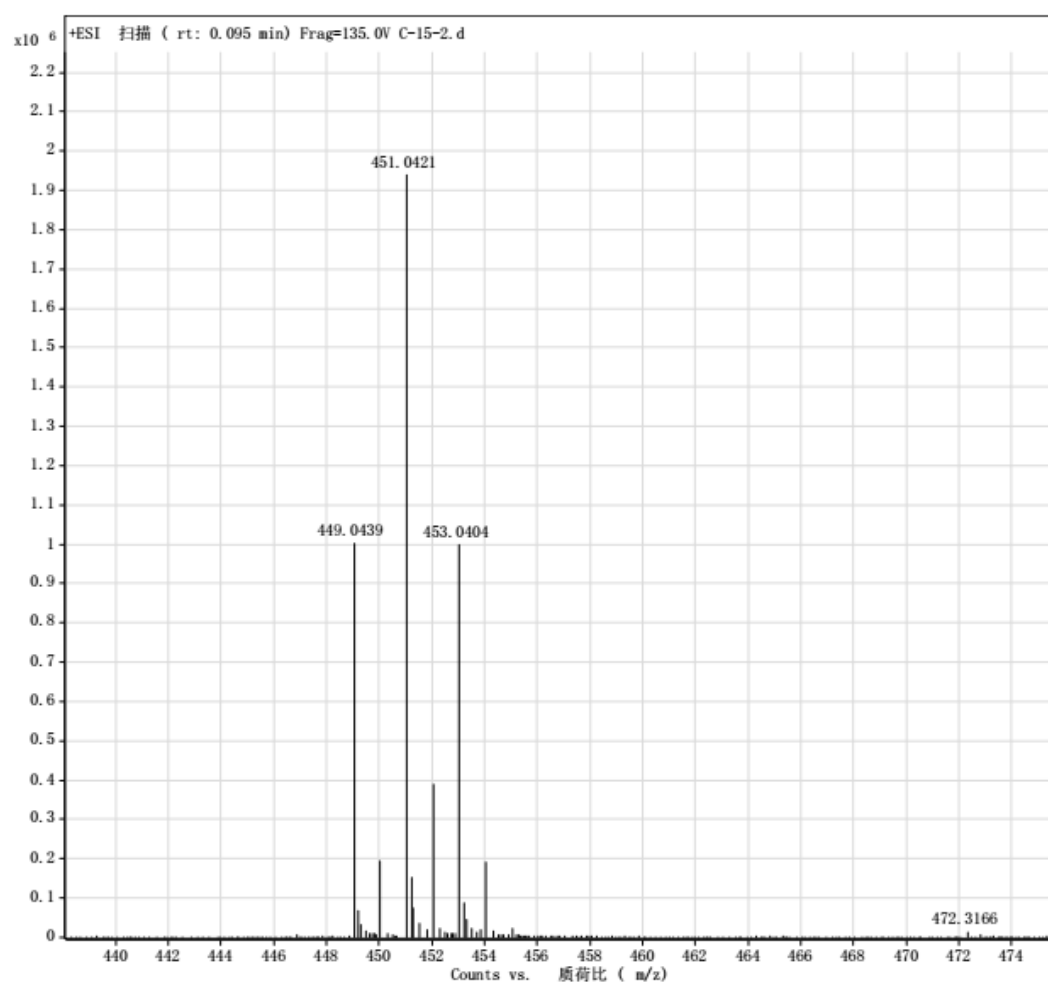
^1H NMR spectrum of pulmonarin B (**1**)



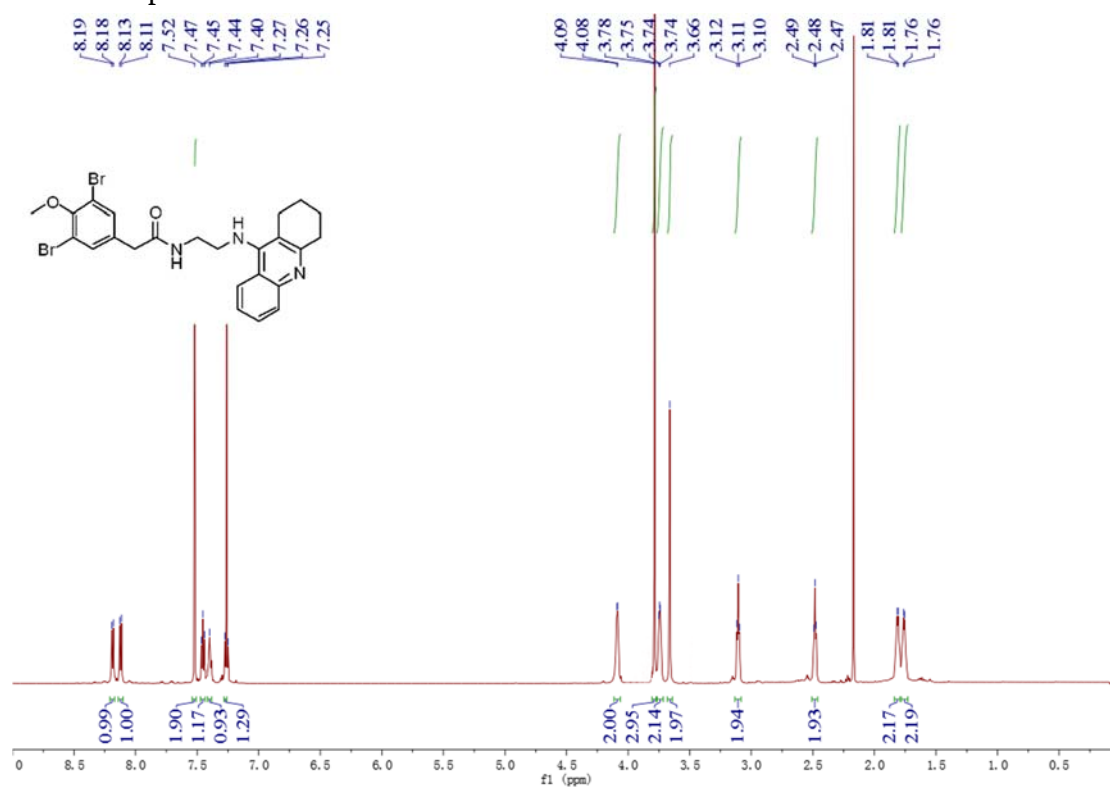
^{13}C NMR spectrum of pulmonarin B (**1**)



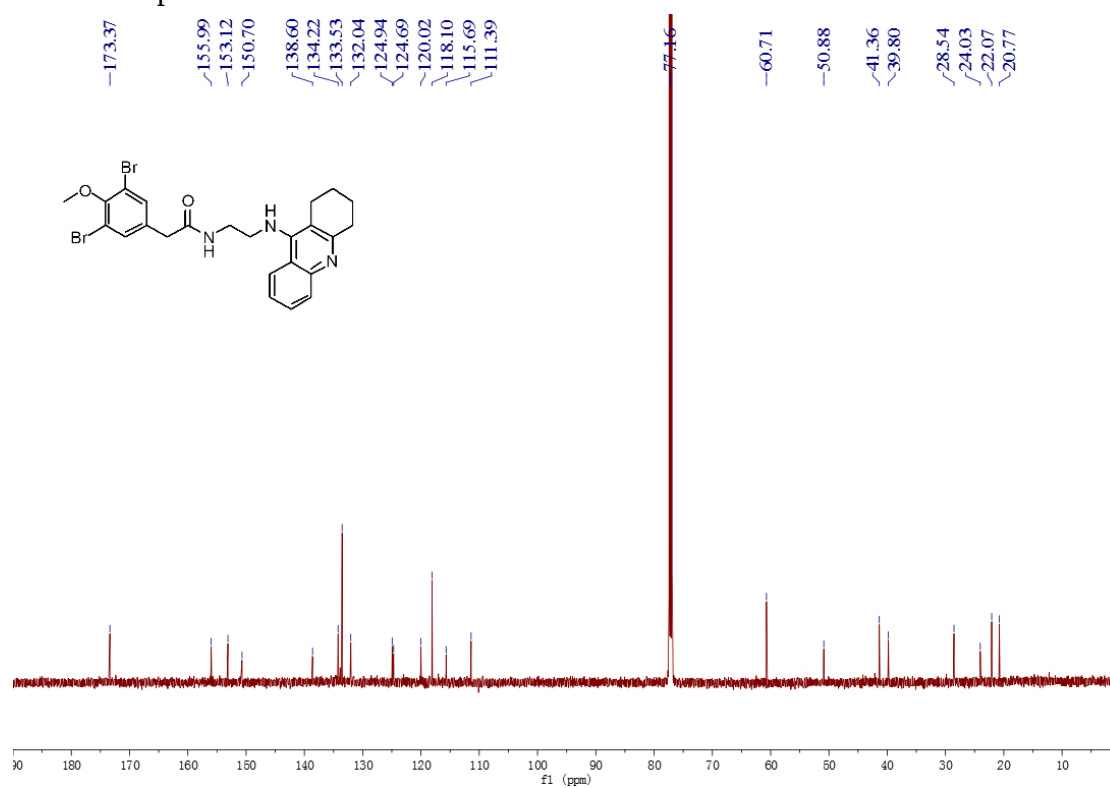
HR-MS (ESI) spectrum of pulmonarin B (1)



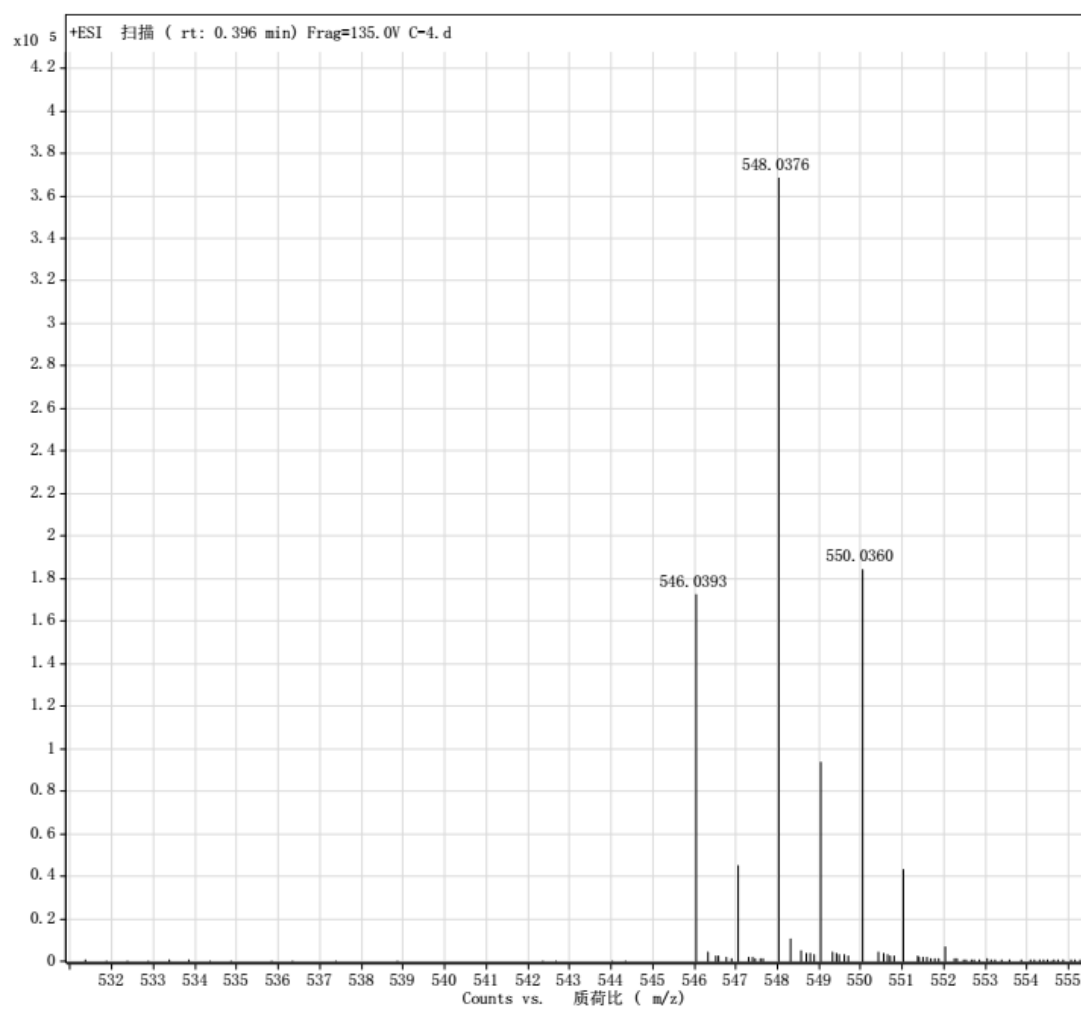
¹H NMR spectrum of **5a**



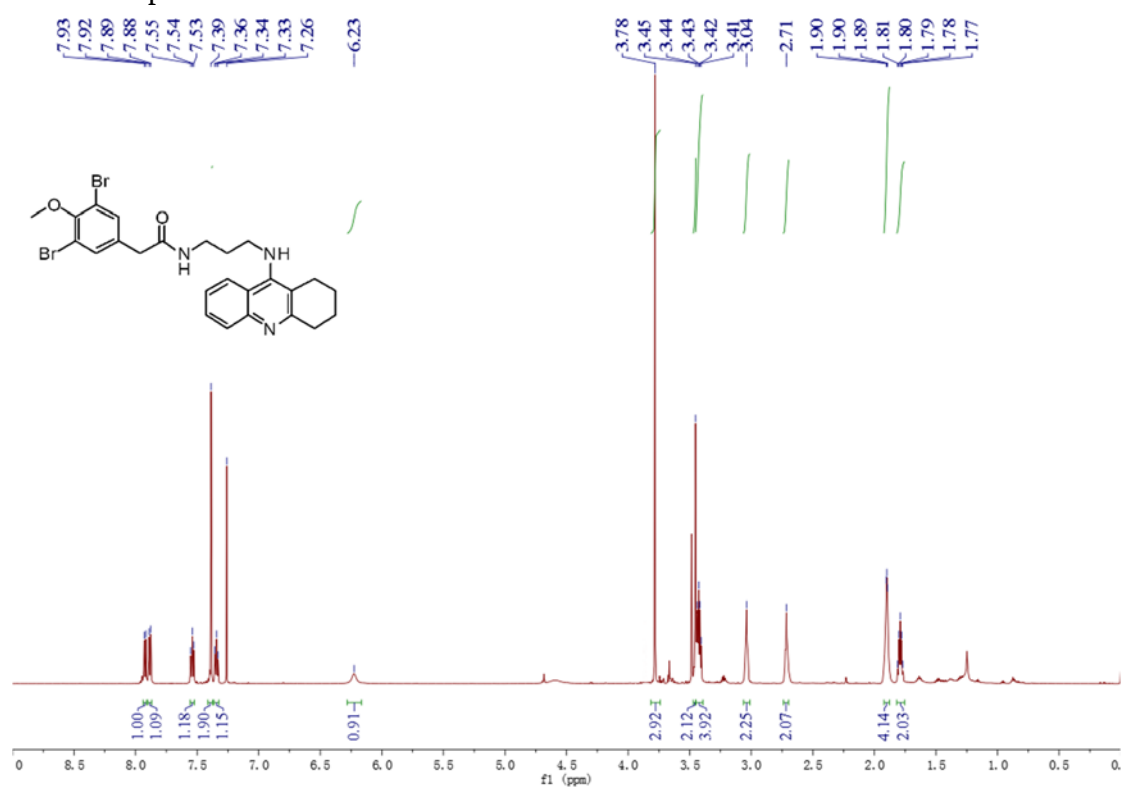
¹³C NMR spectrum of **5a**



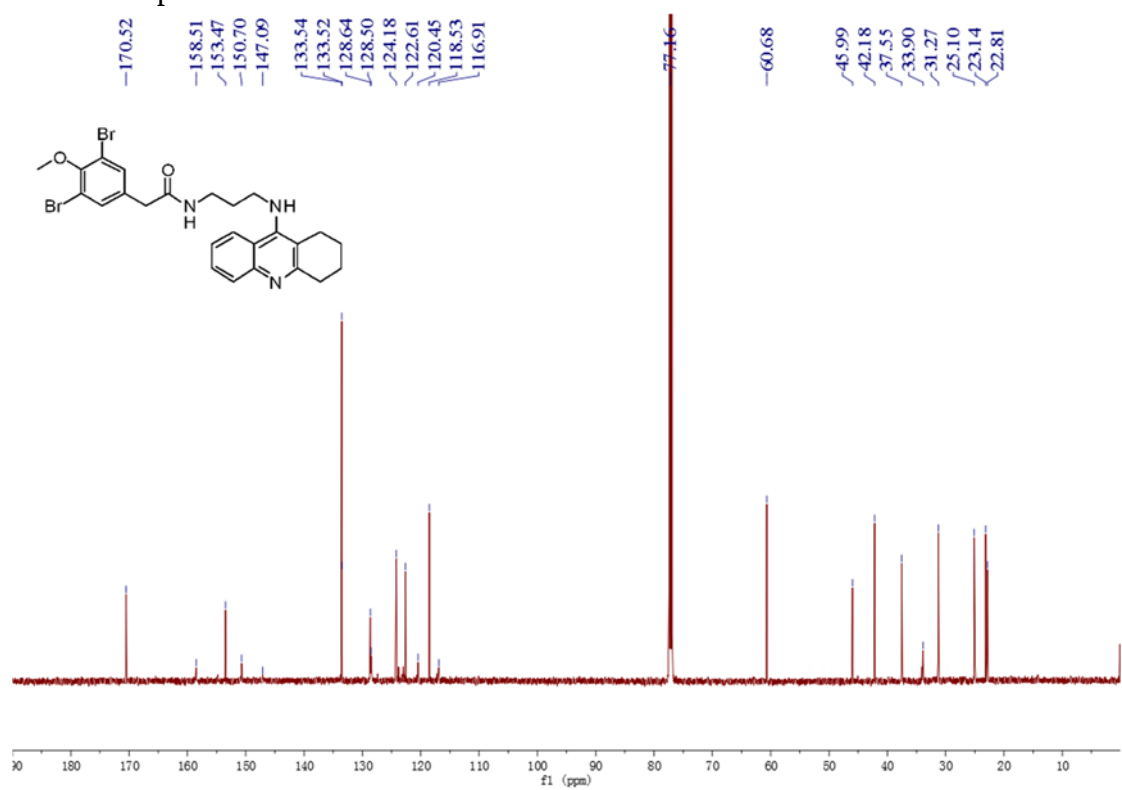
HR-MS (ESI) spectrum of **5a**



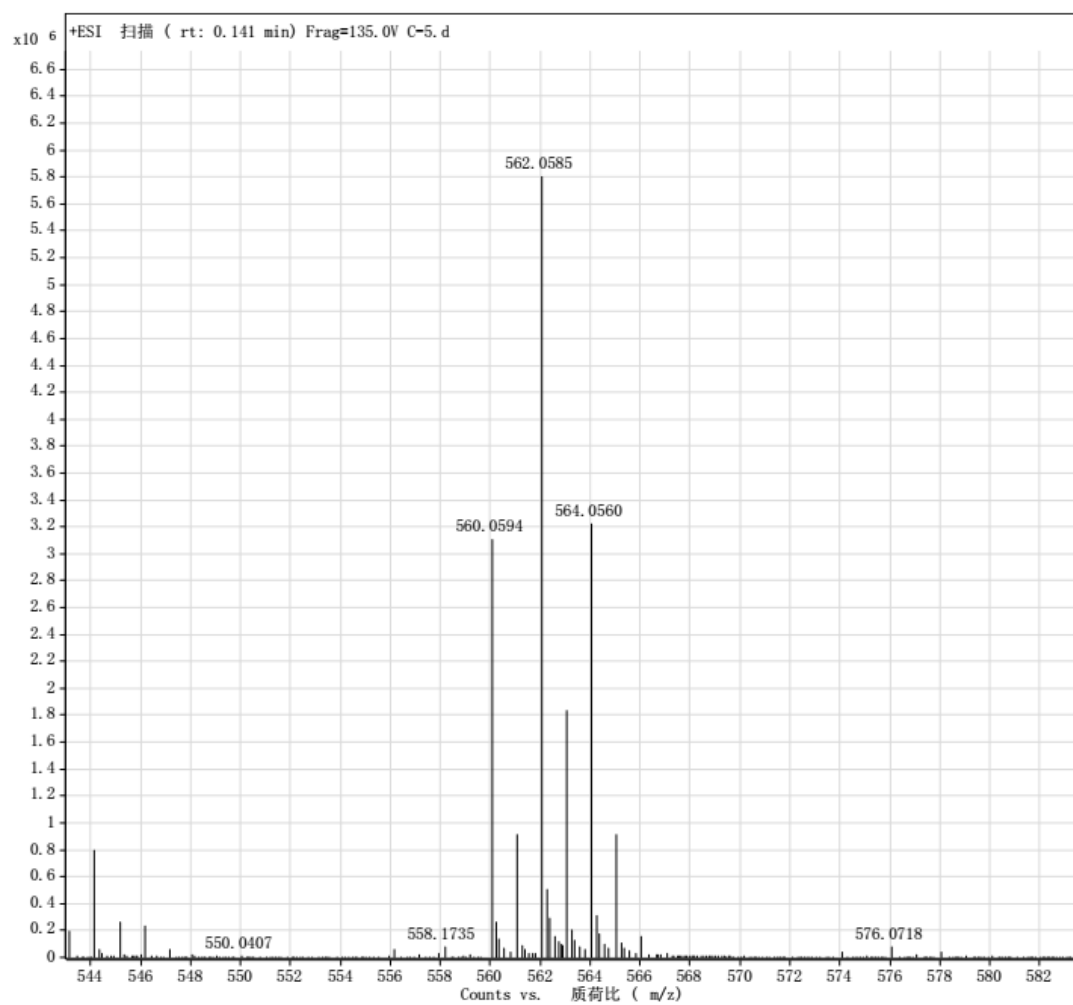
¹H NMR spectrum of **5b**



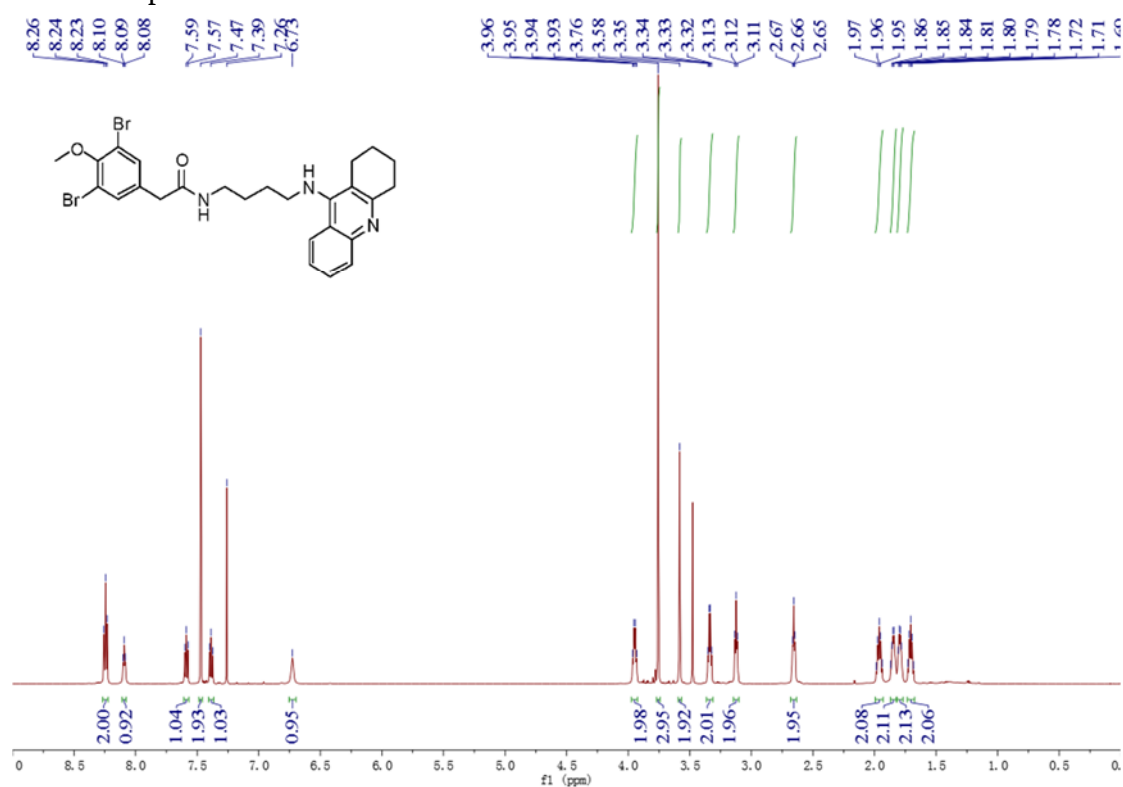
¹³C NMR spectrum of **5b**



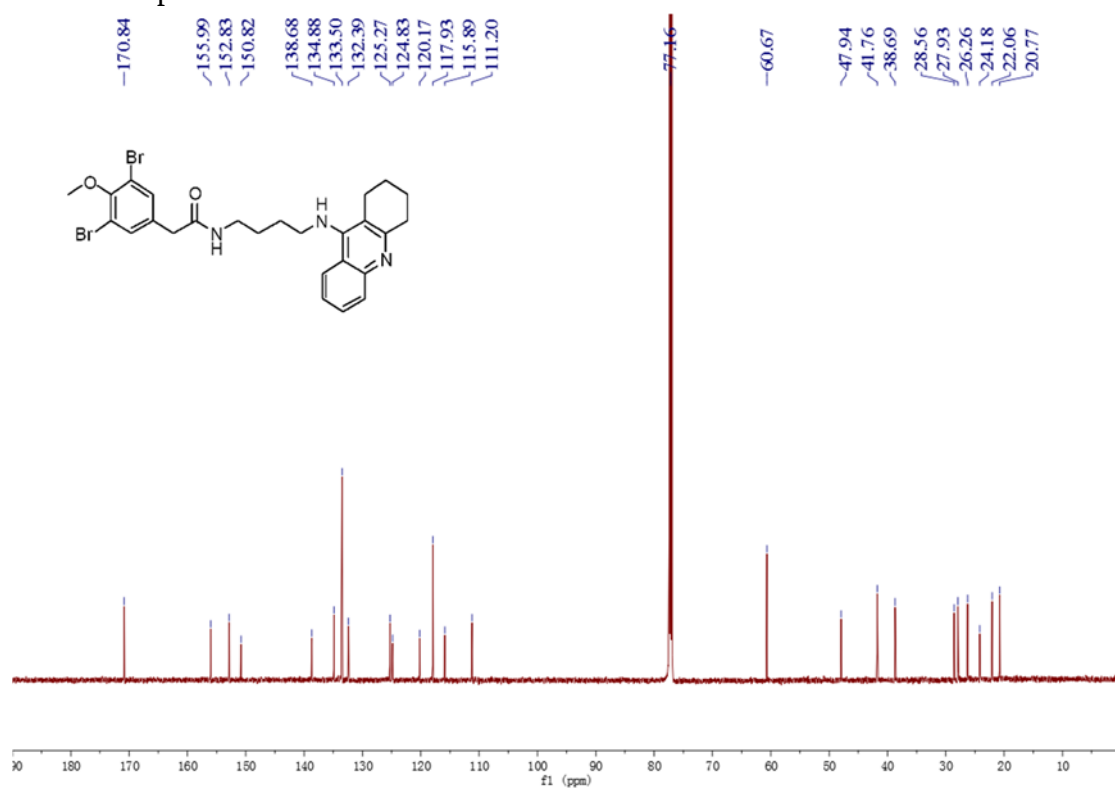
HR-MS (ESI) spectrum of **5b**



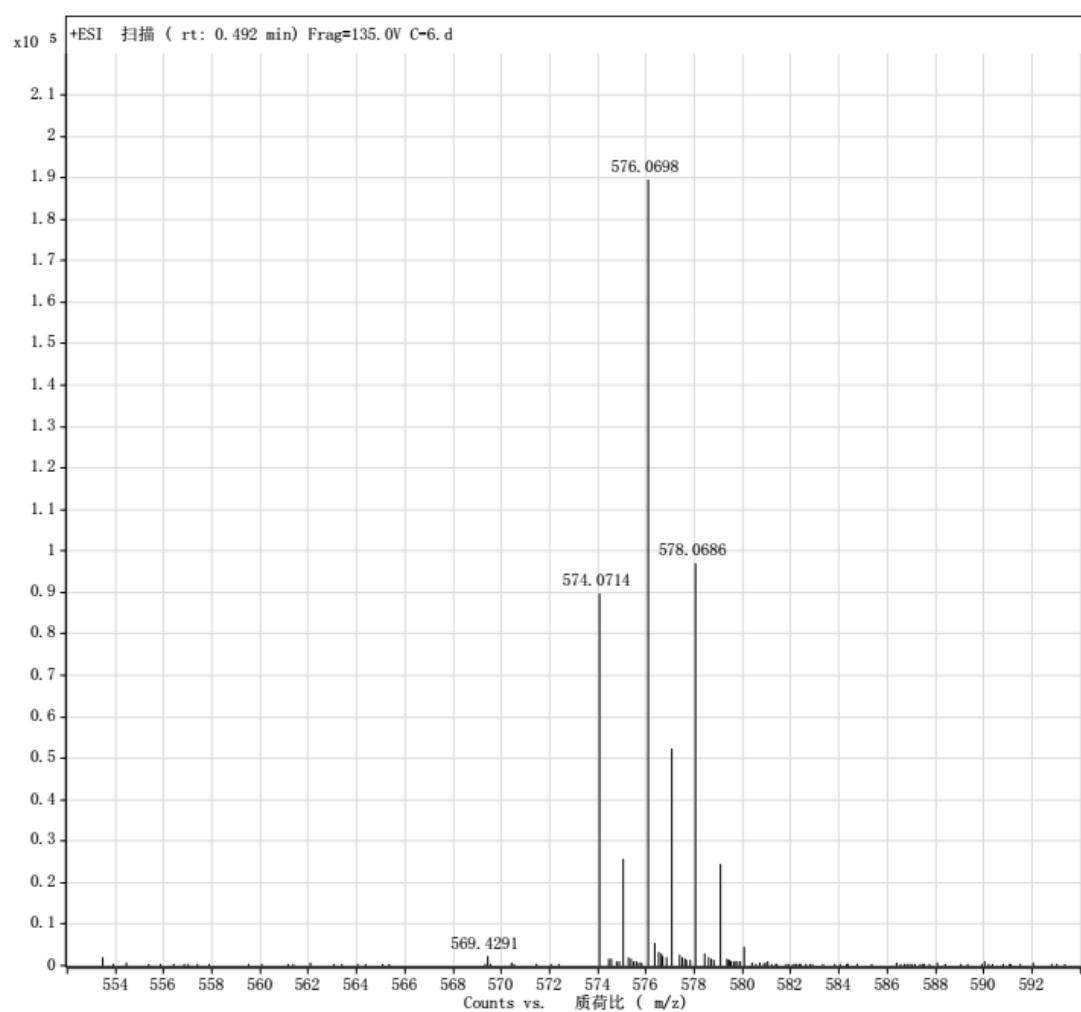
¹H NMR spectrum of **5c**



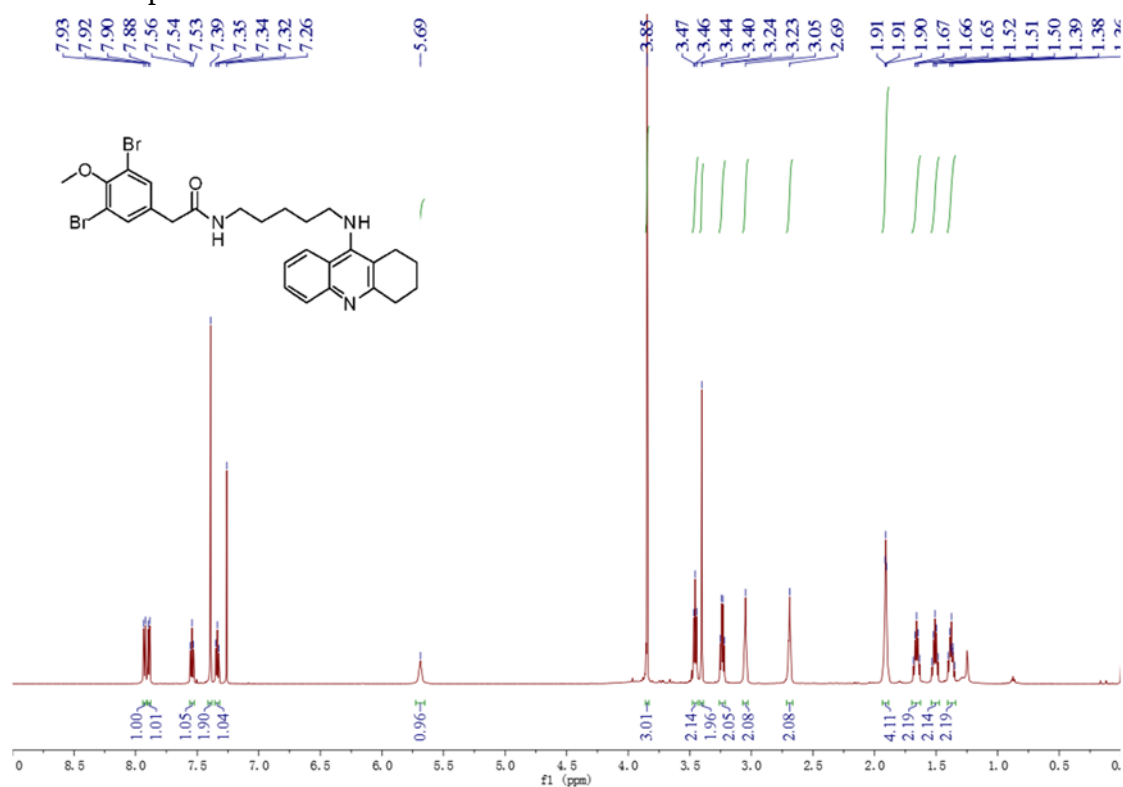
¹³C NMR spectrum of **5c**



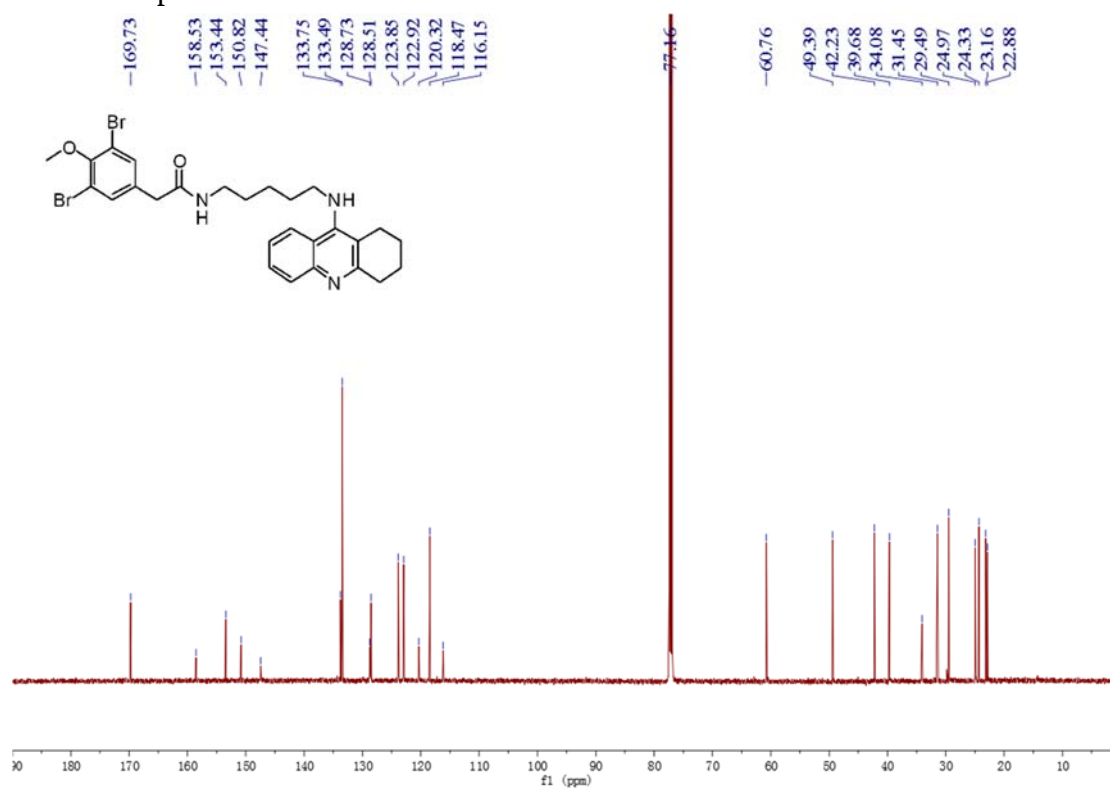
HR-MS (ESI) spectrum of **5c**



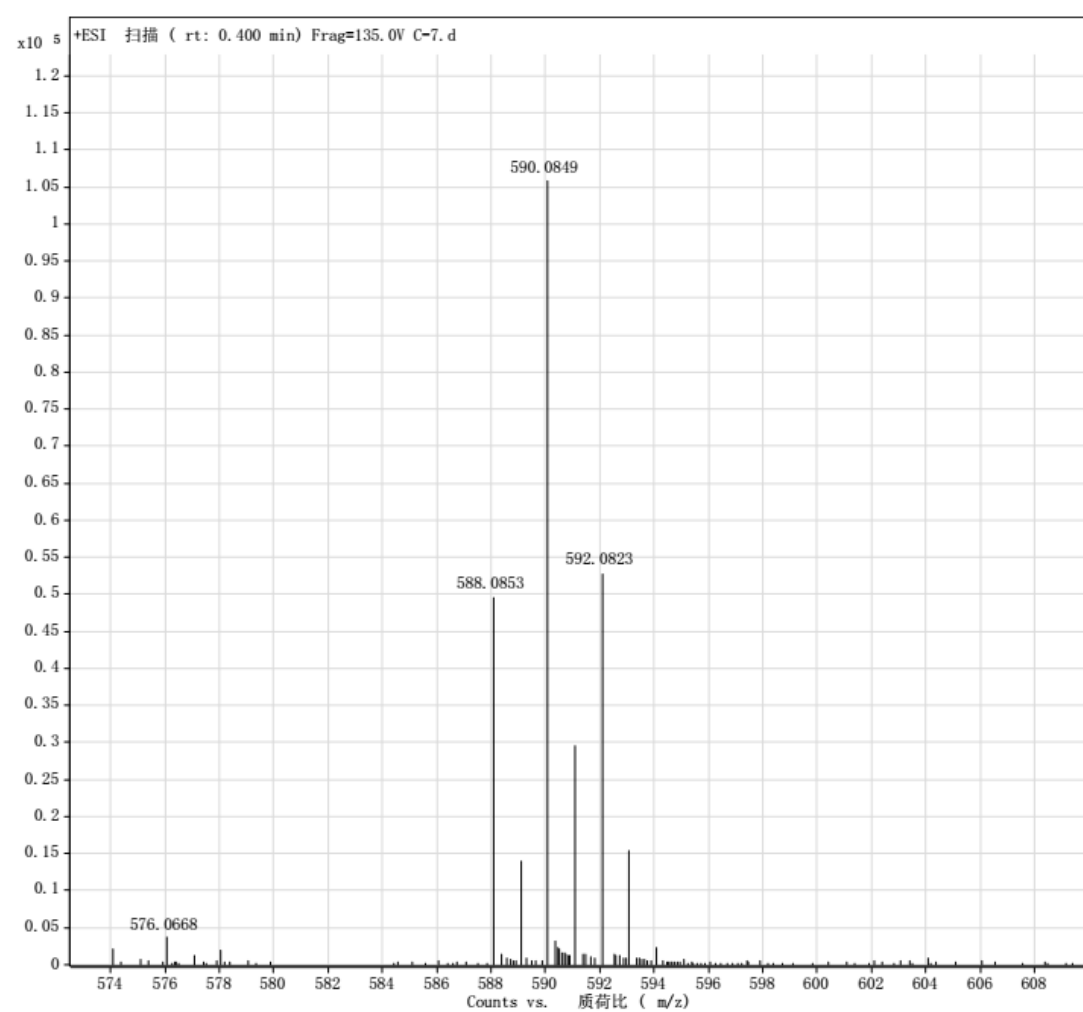
¹H NMR spectrum of **5d**



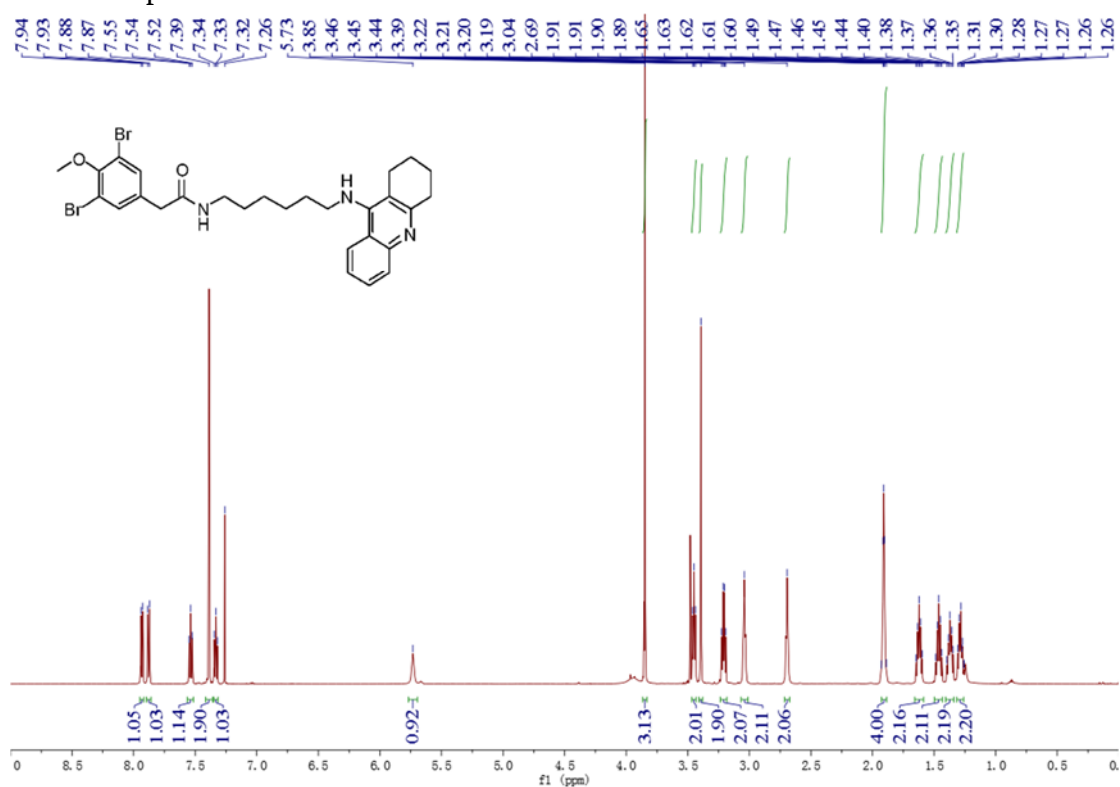
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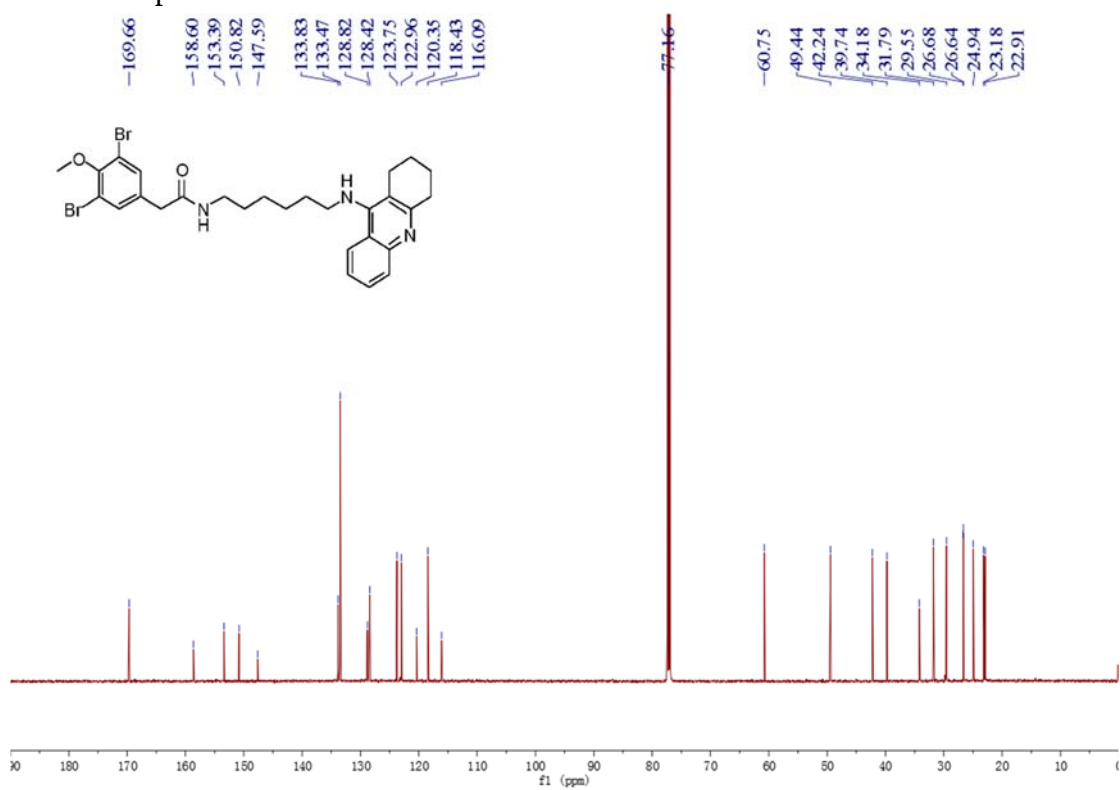
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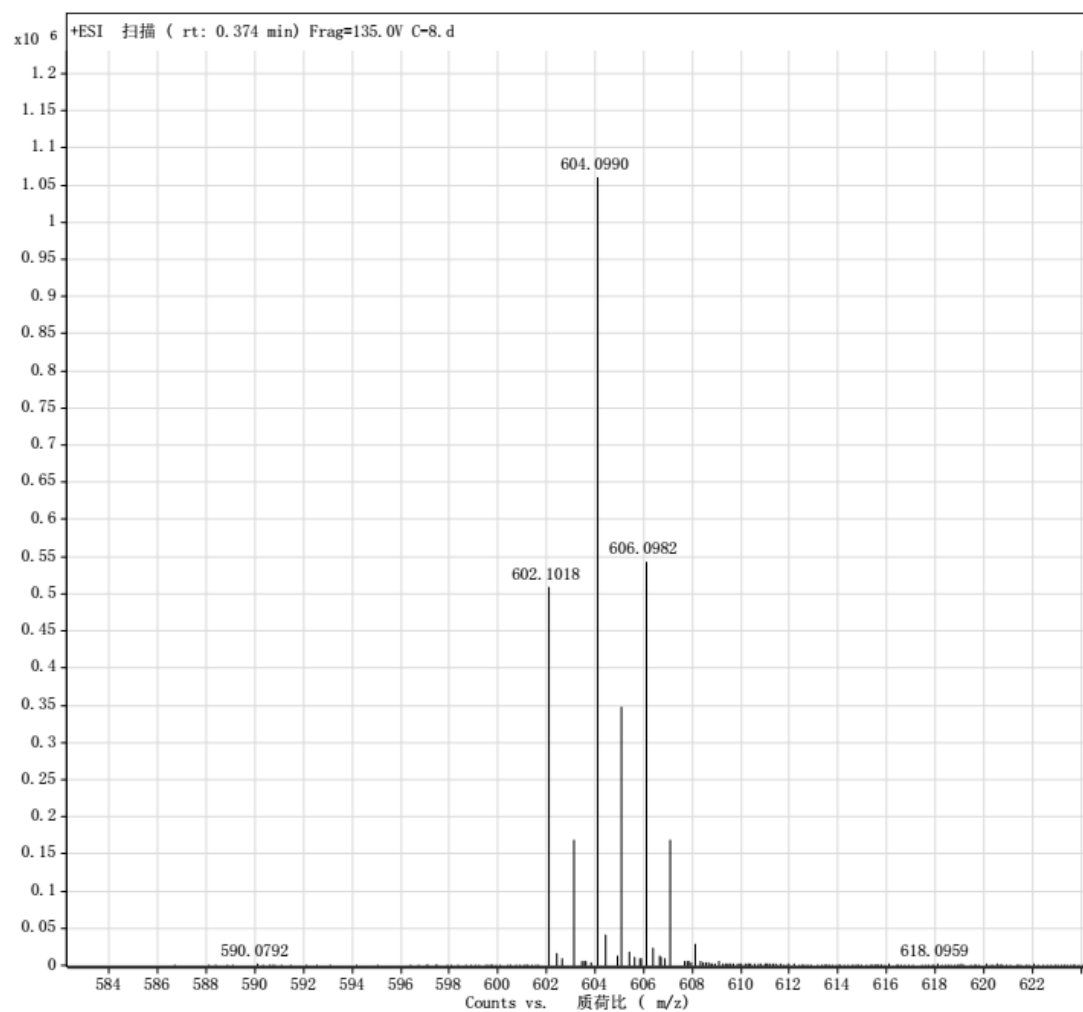
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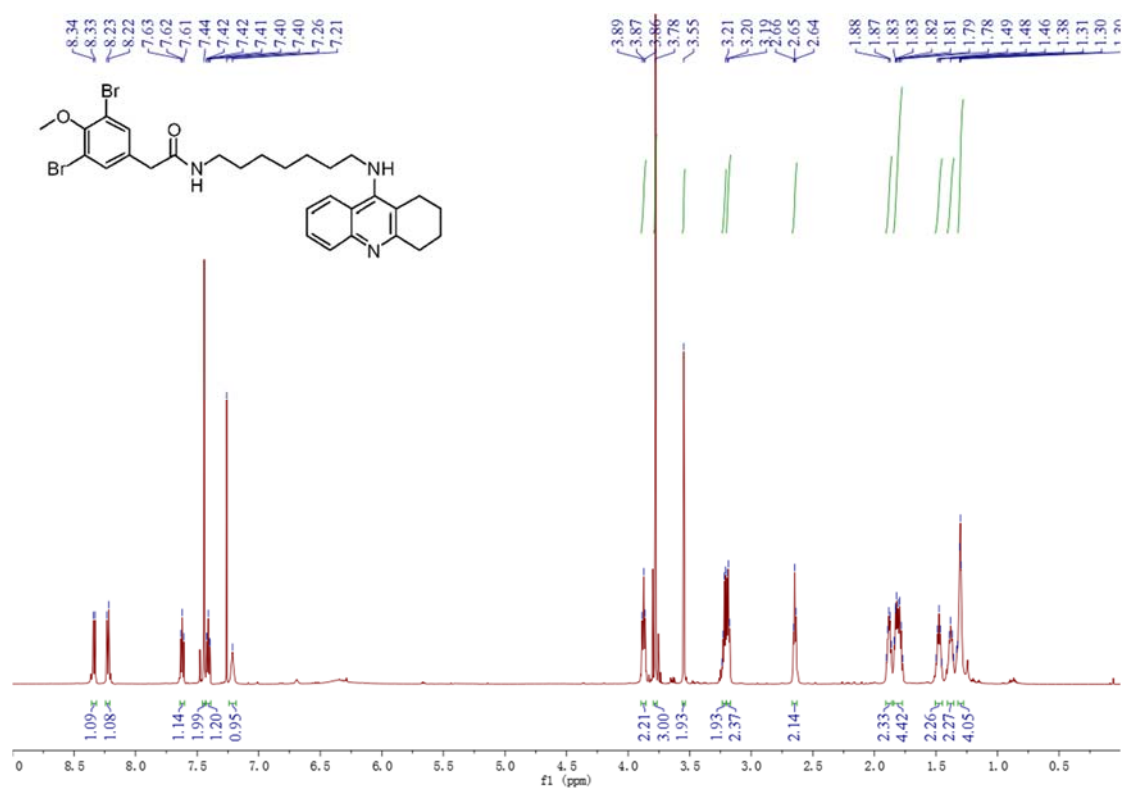
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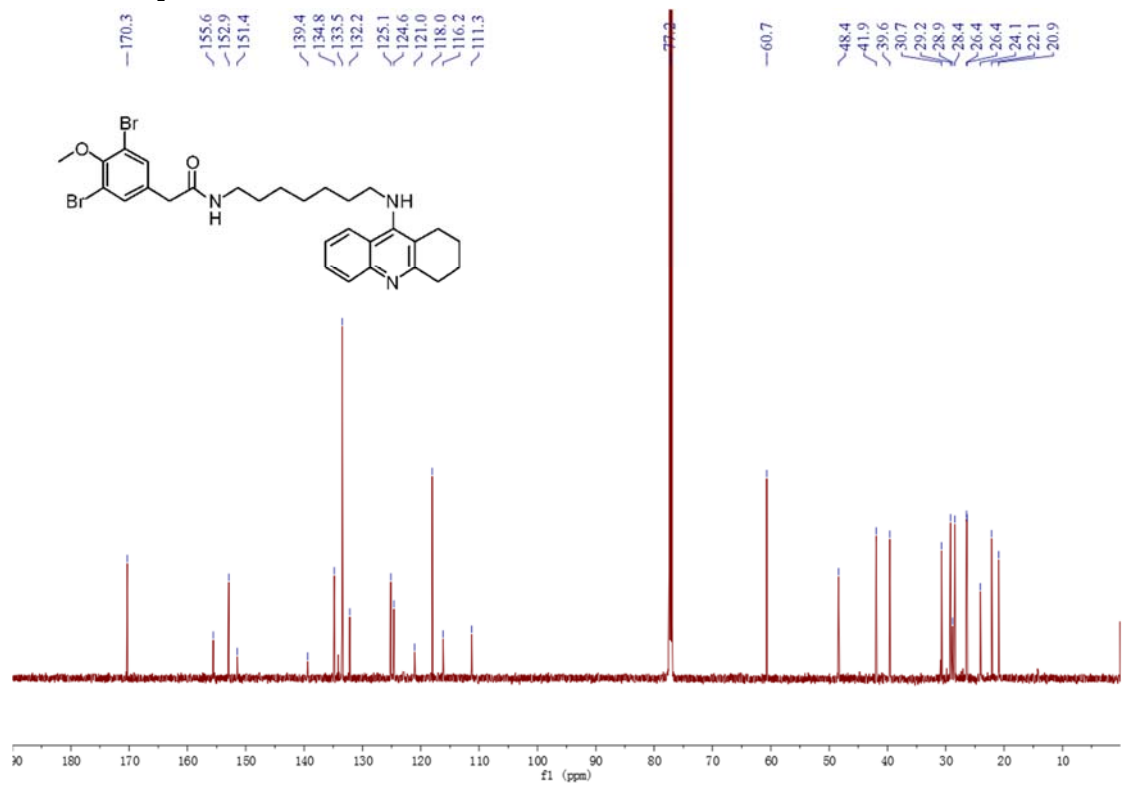
HR-MS (ESI) spectrum of 5e



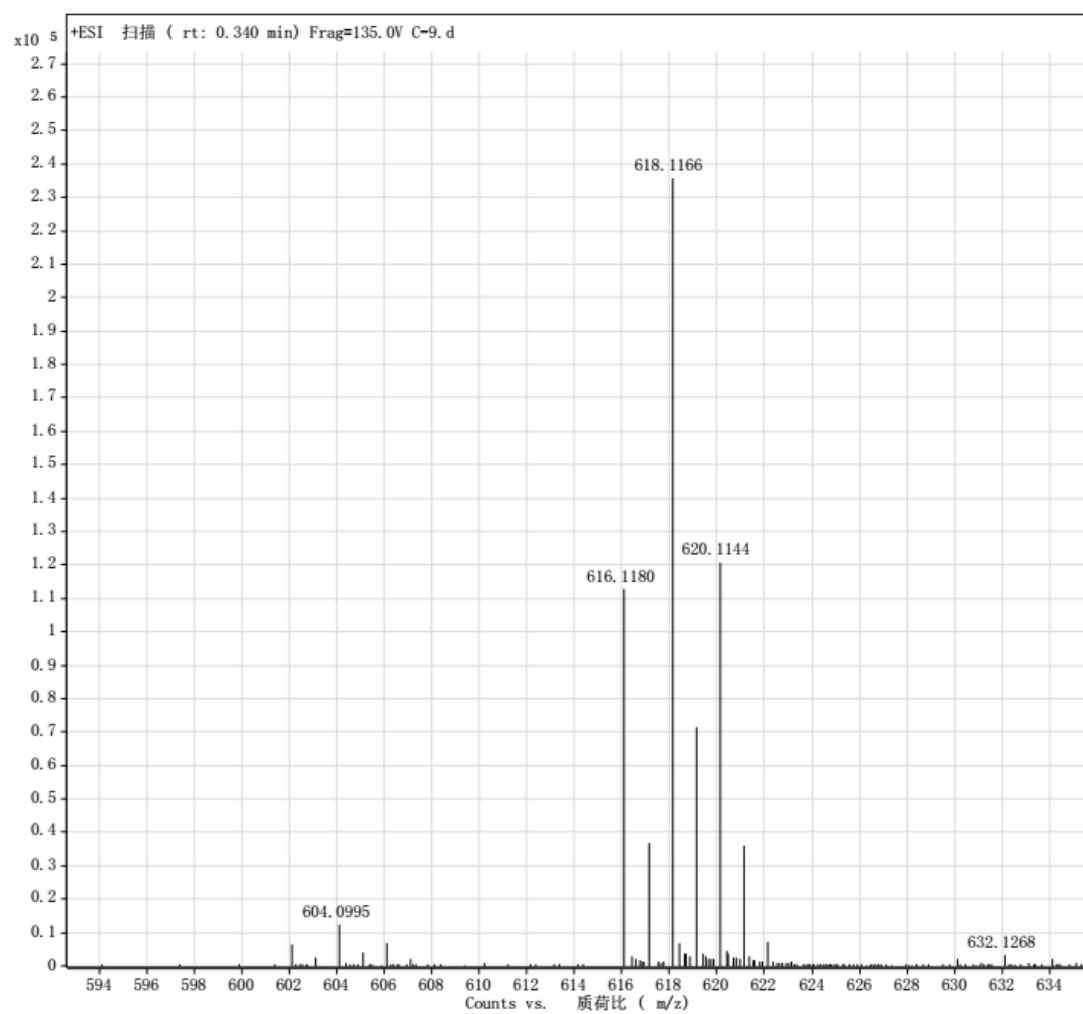
^1H NMR spectrum of **5f**



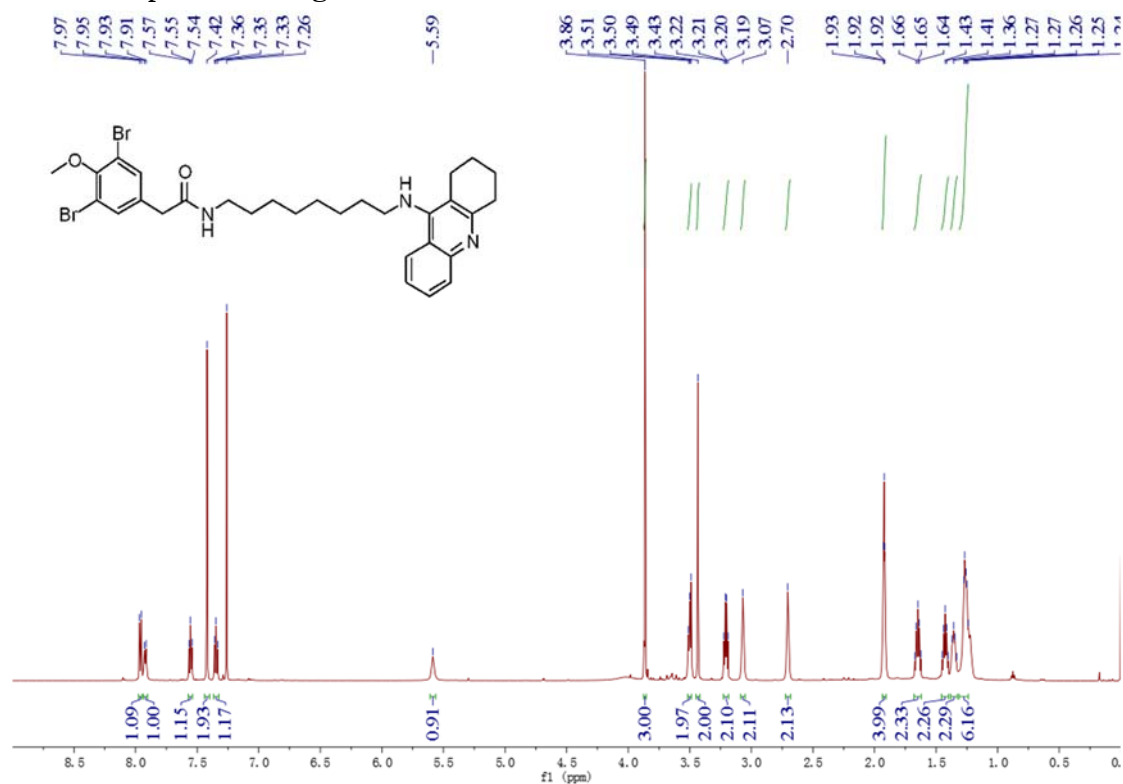
^{13}C NMR spectrum of **5f**



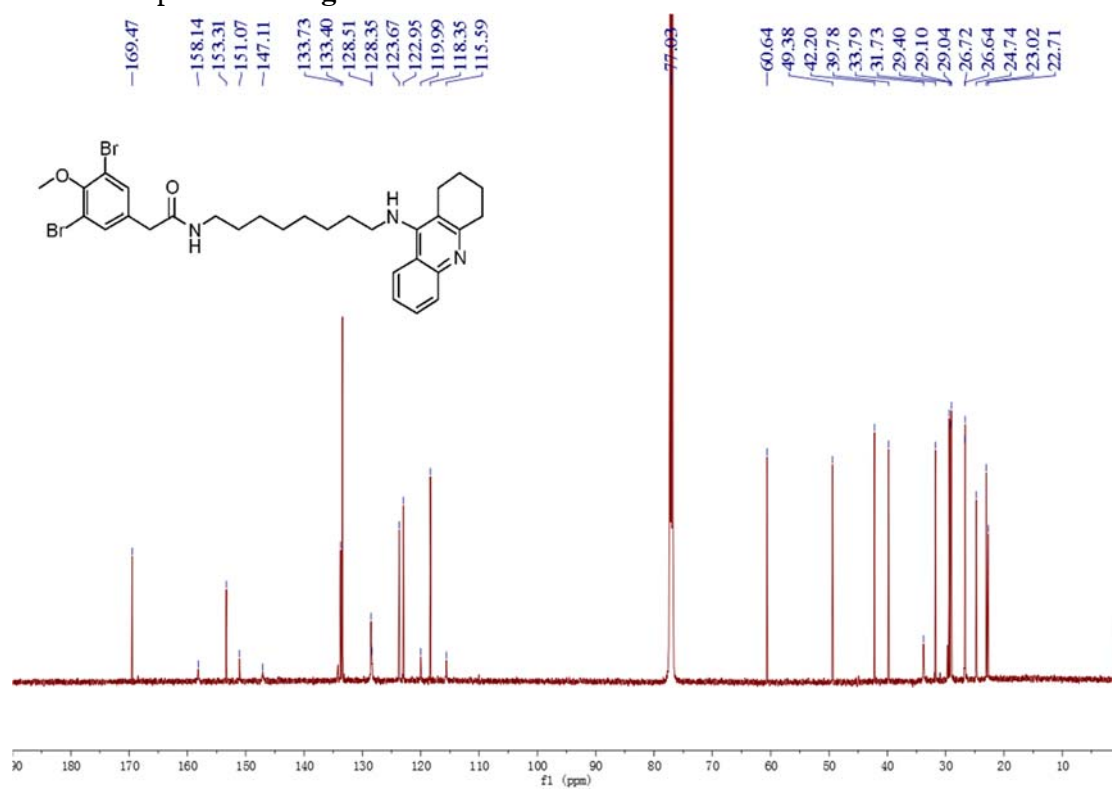
HR-MS (ESI) spectrum of **5f**



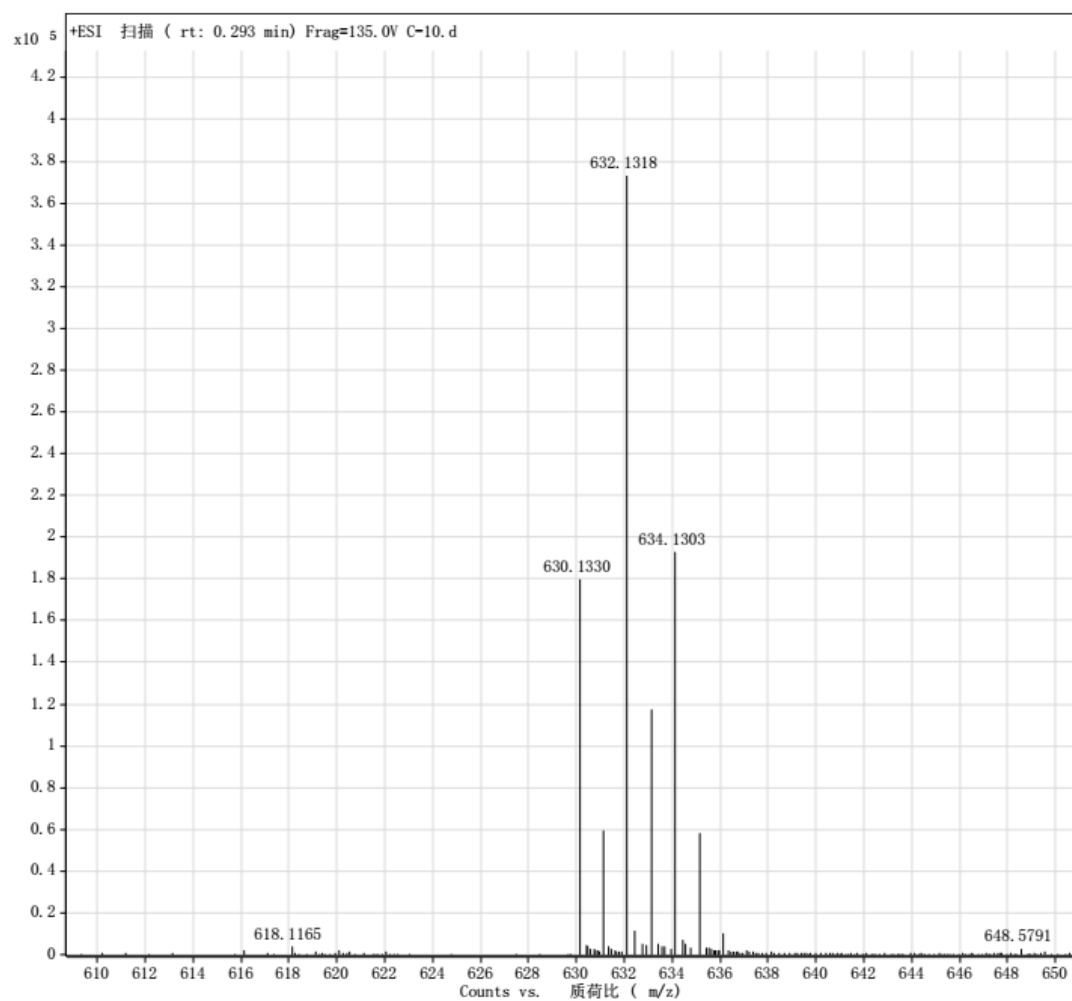
^1H NMR spectrum of **5g**



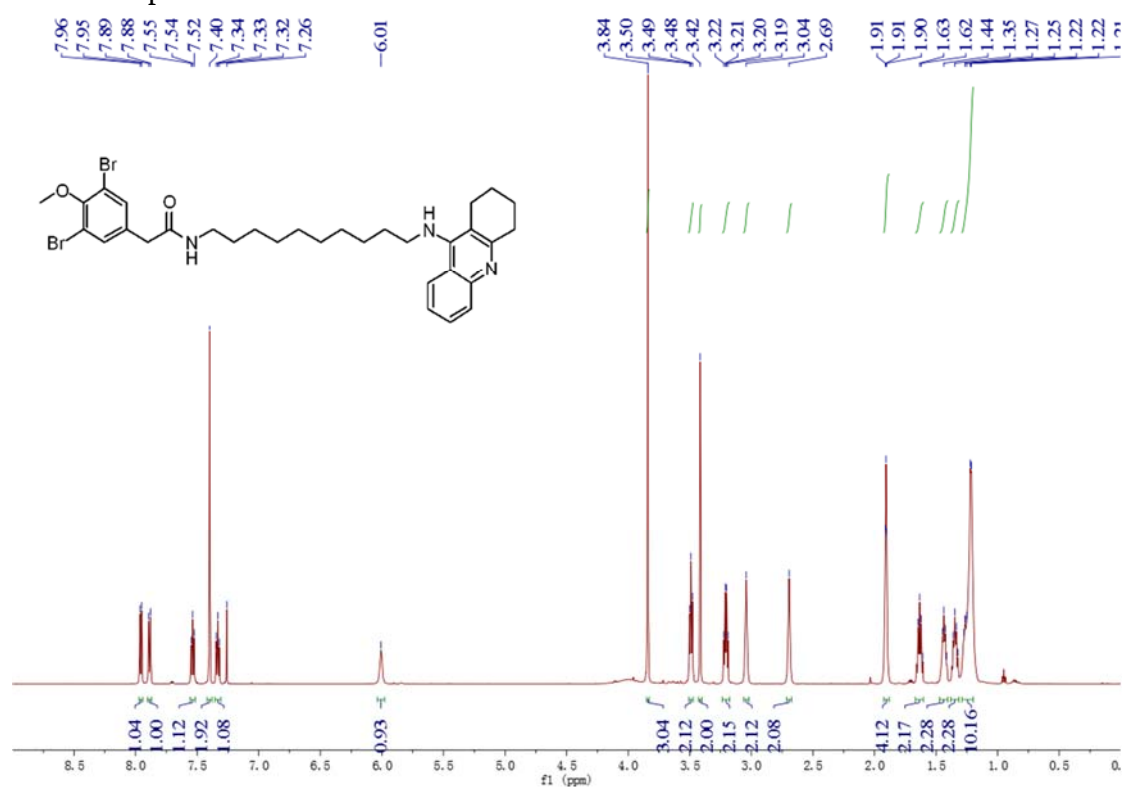
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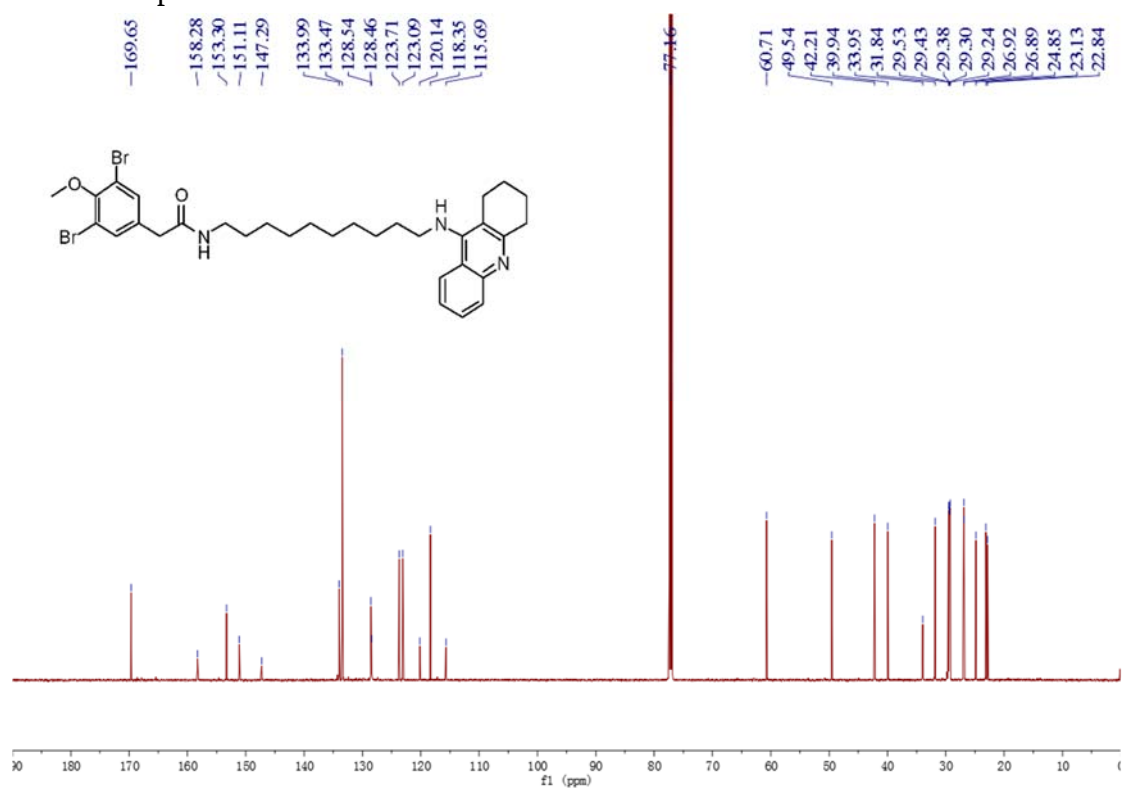
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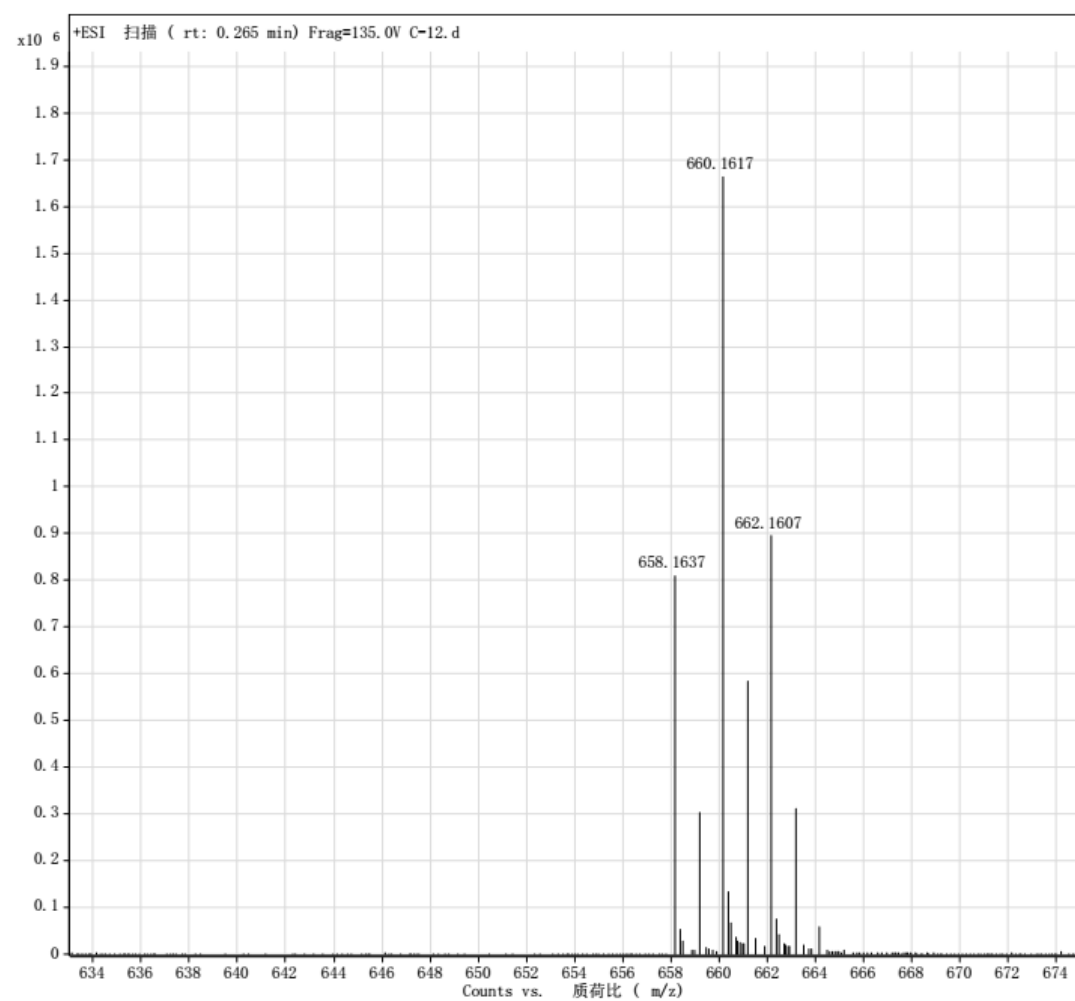
^1H NMR spectrum of **5h**



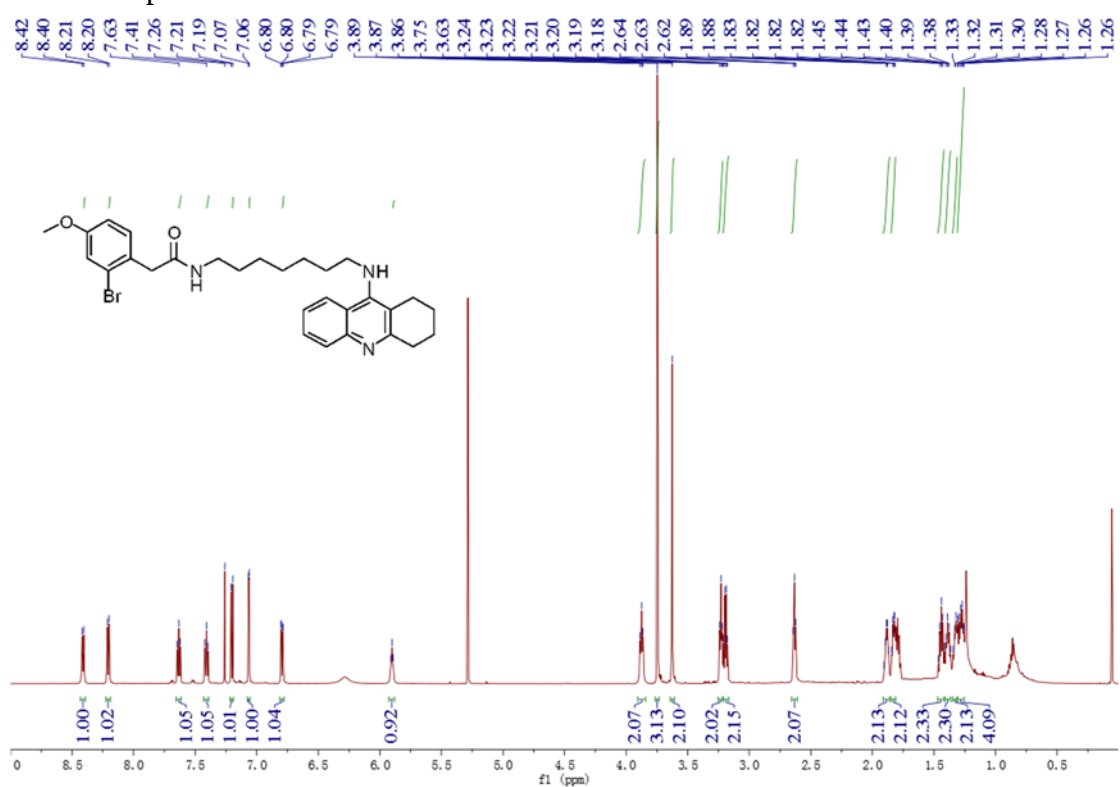
^{13}C NMR spectrum of **5h**



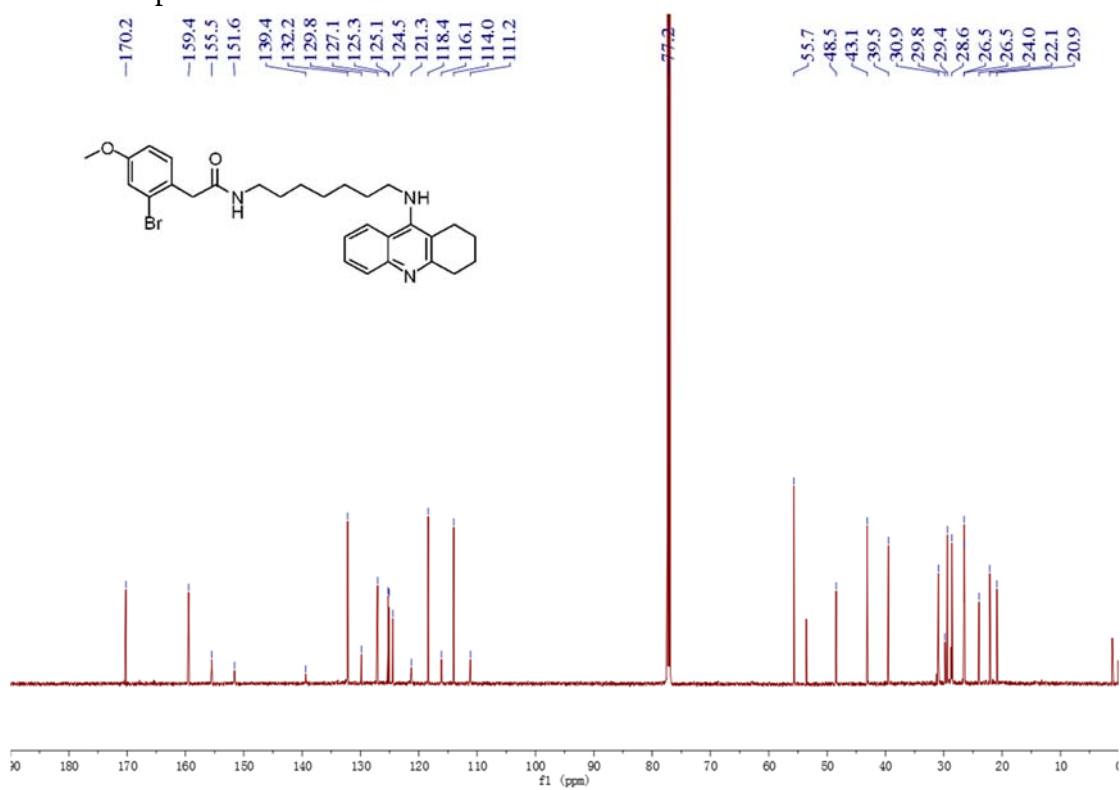
HR-MS (ESI) spectrum of **5h**



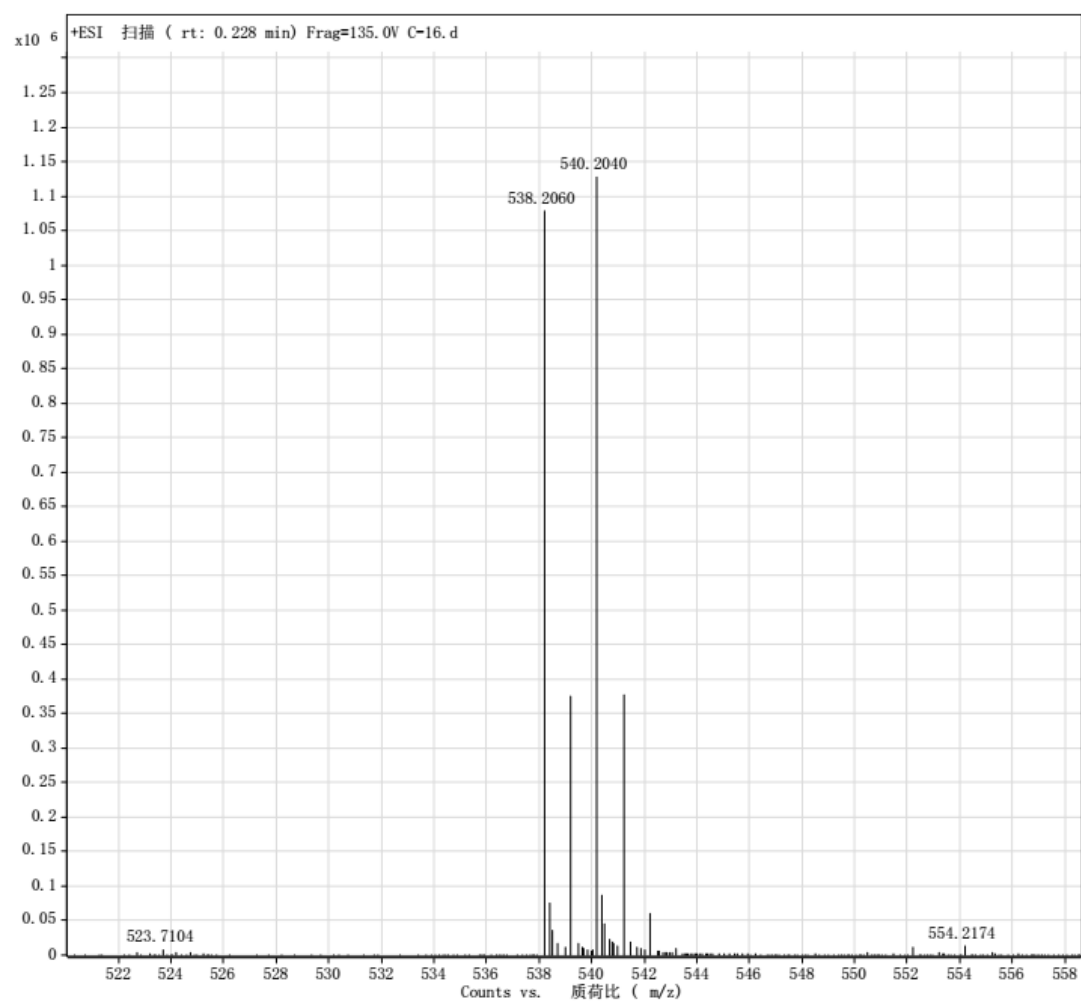
^1H NMR spectrum of **12a**



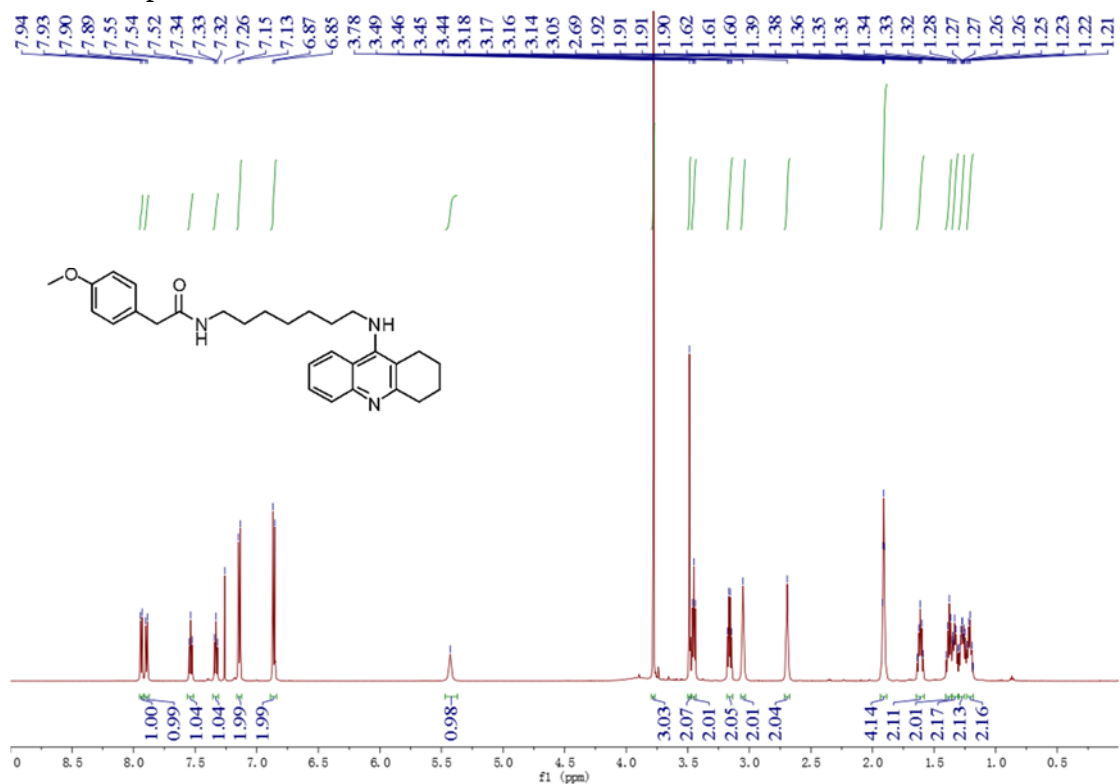
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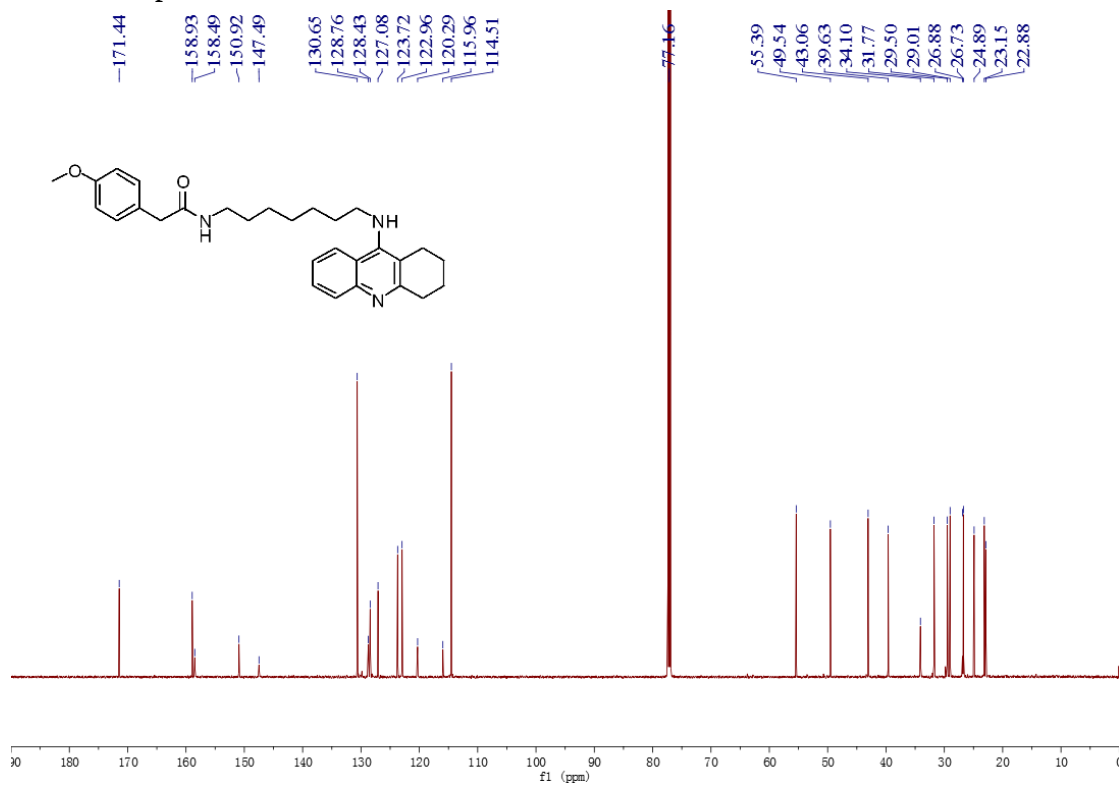
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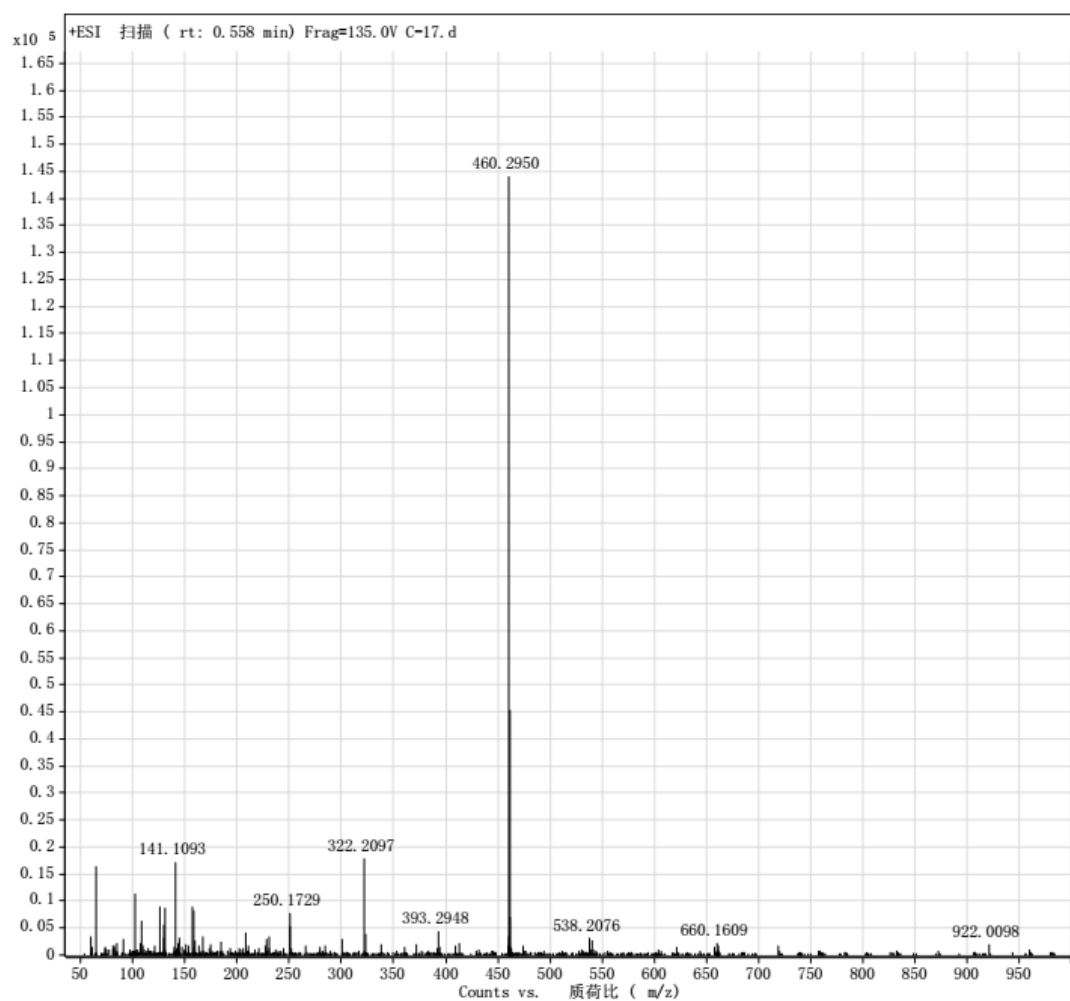
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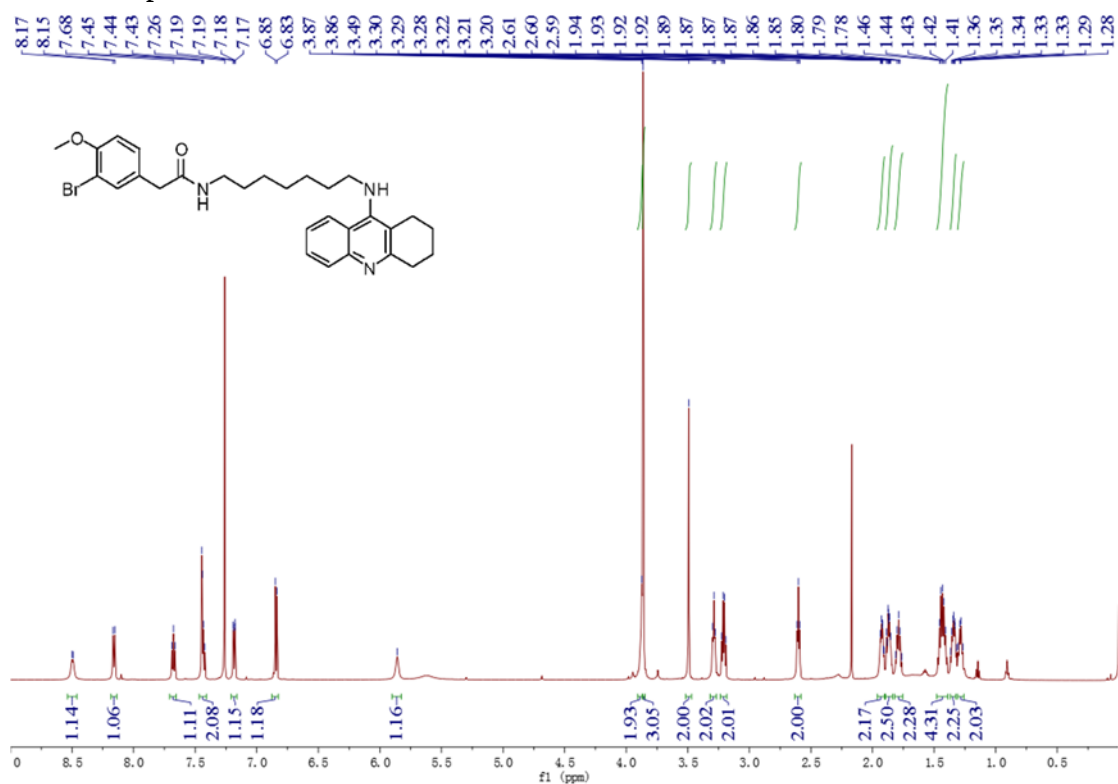
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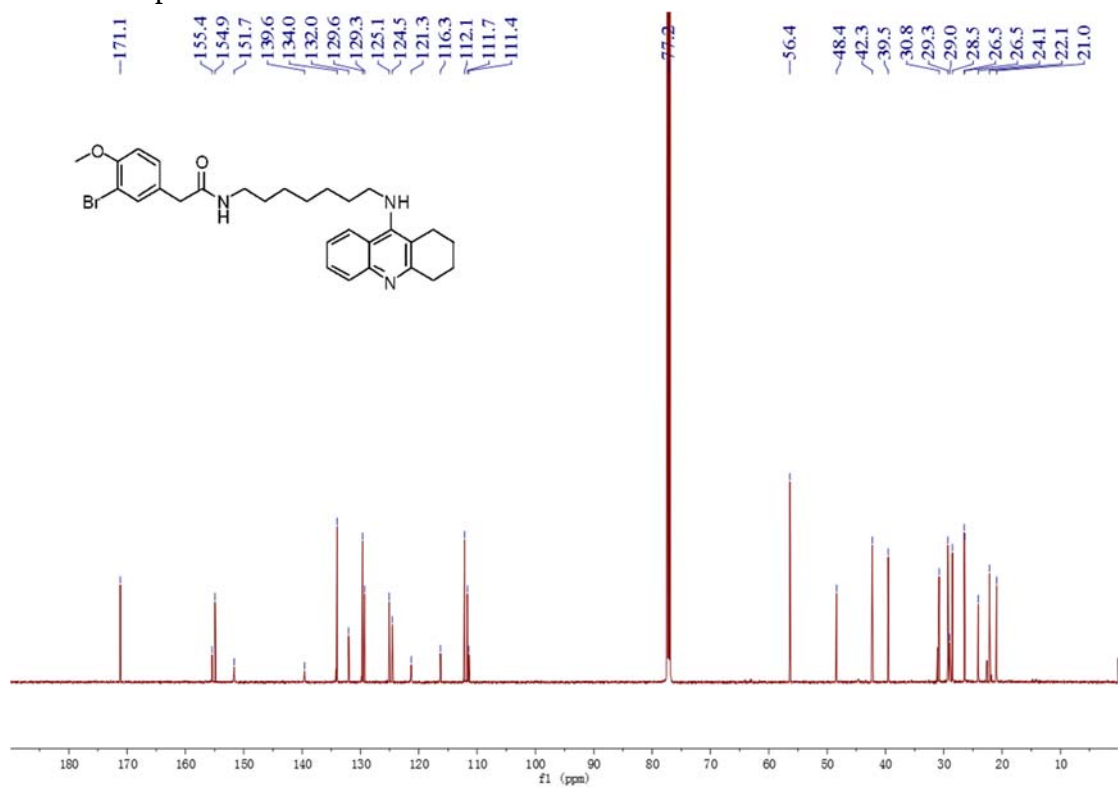
HR-MS (ESI) spectrum of **12b**



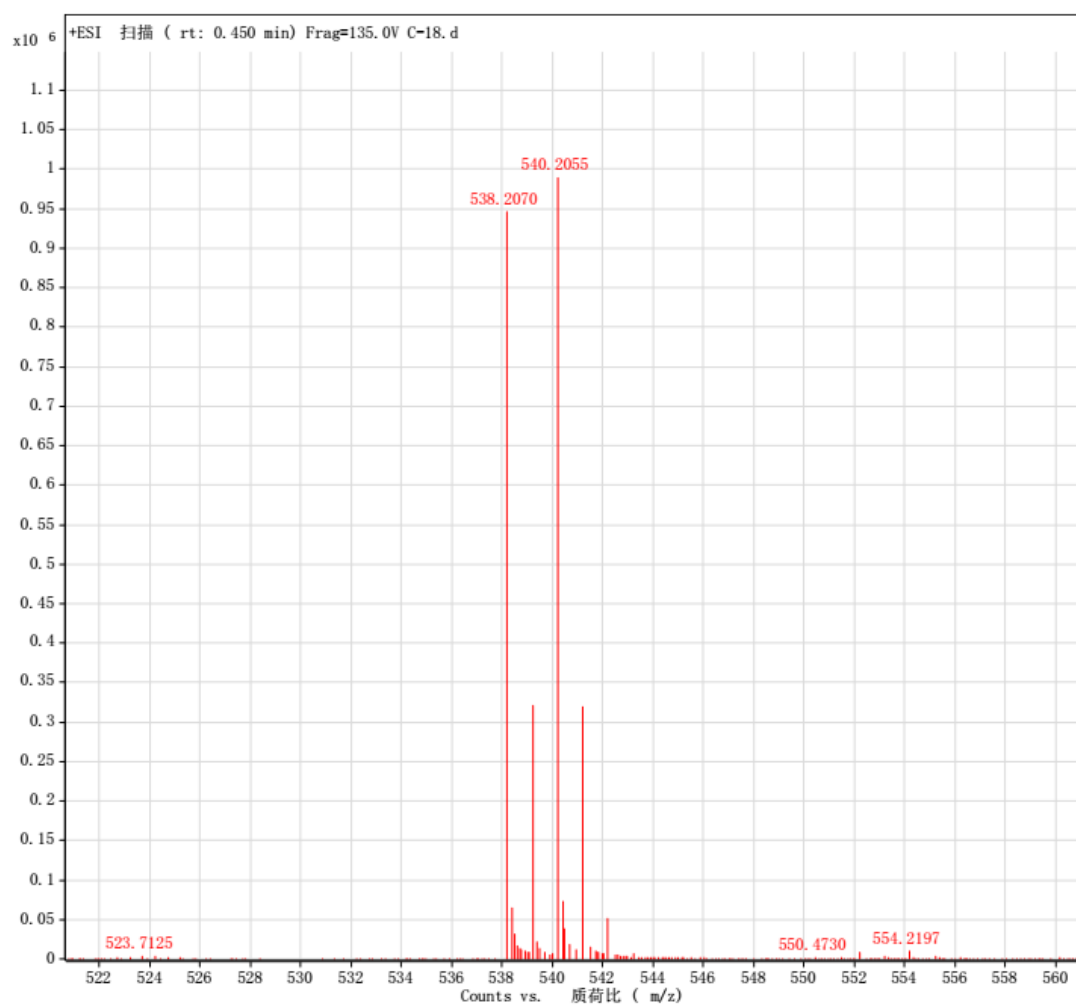
¹H NMR spectrum of **12c**



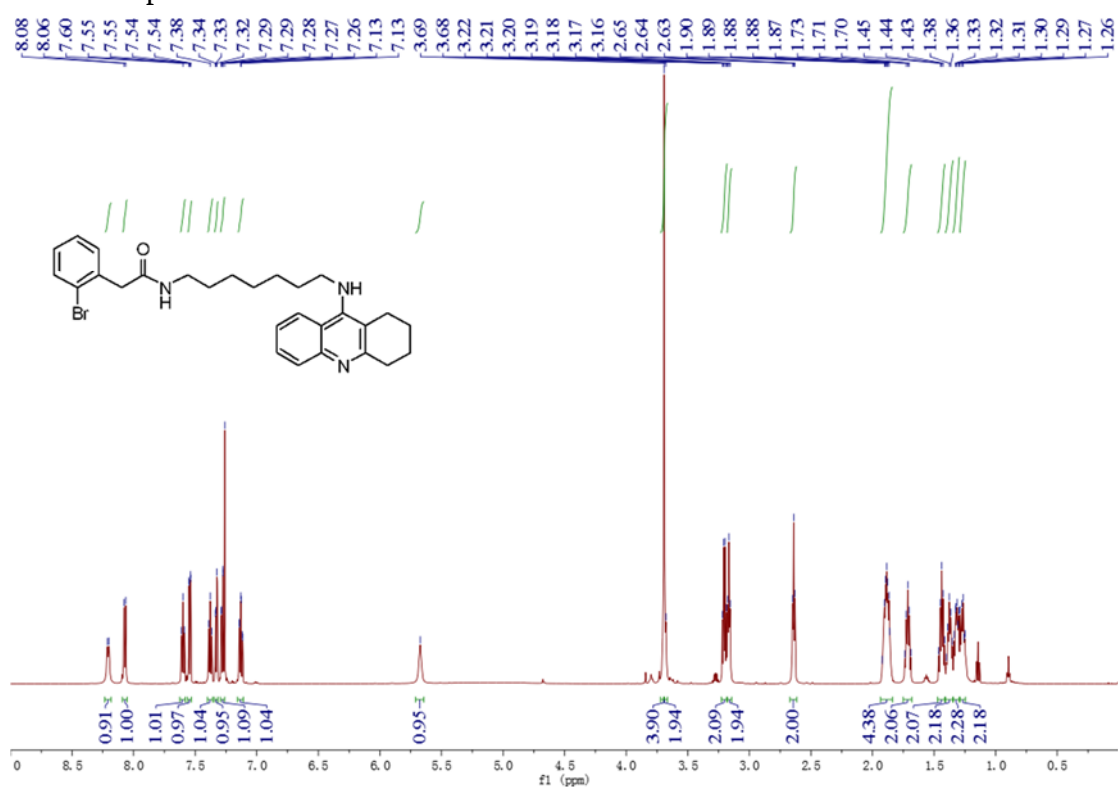
¹³C NMR spectrum of **12c**



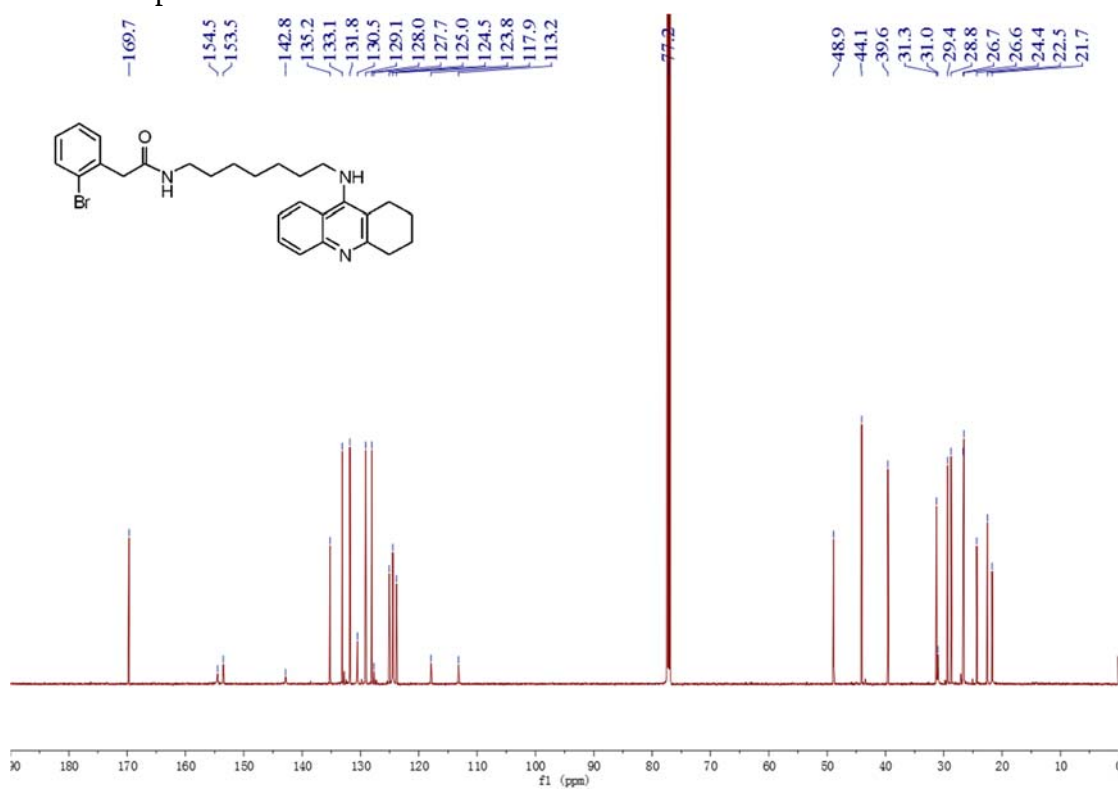
HR-MS (ESI) spectrum of **12c**



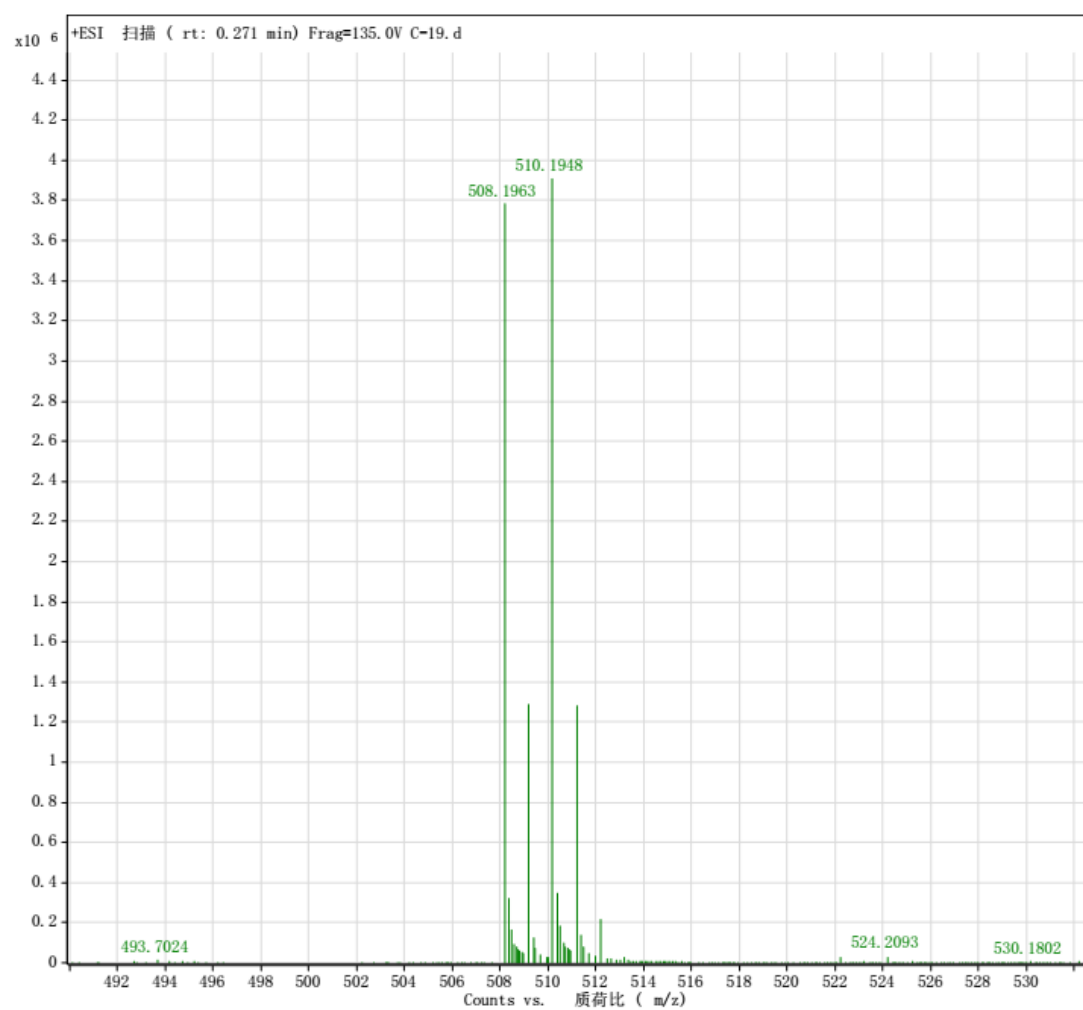
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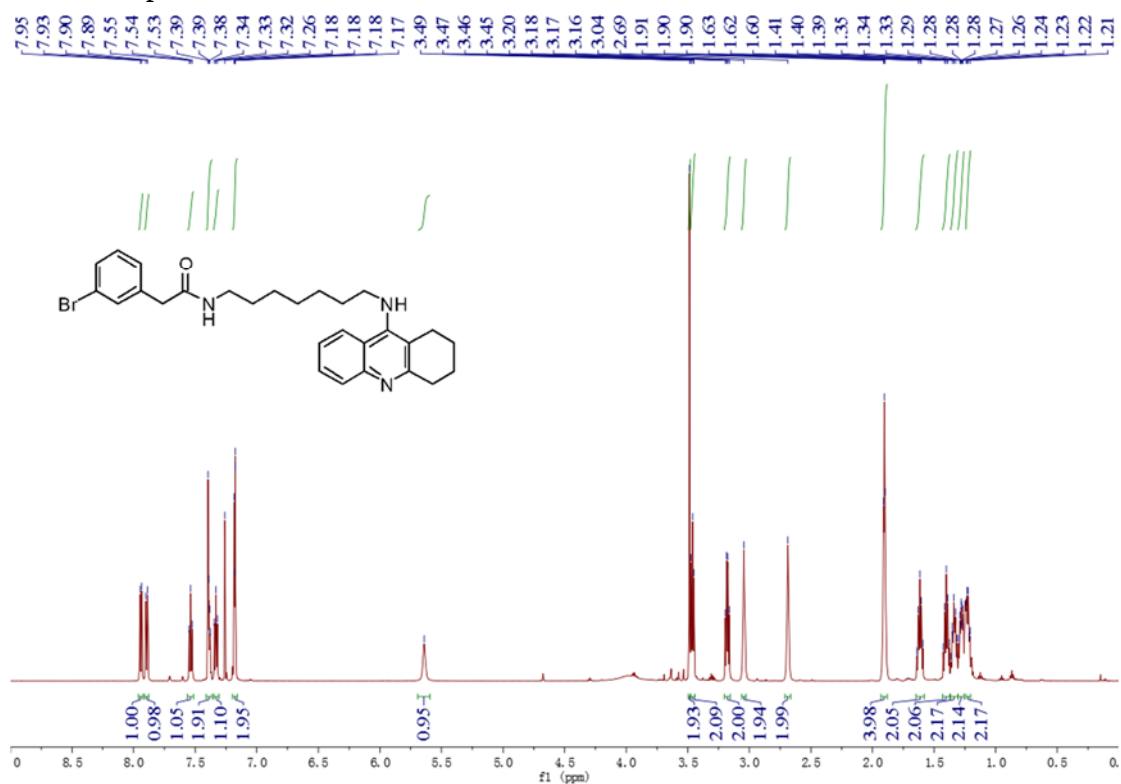
^{13}C NMR spectrum of **12d**



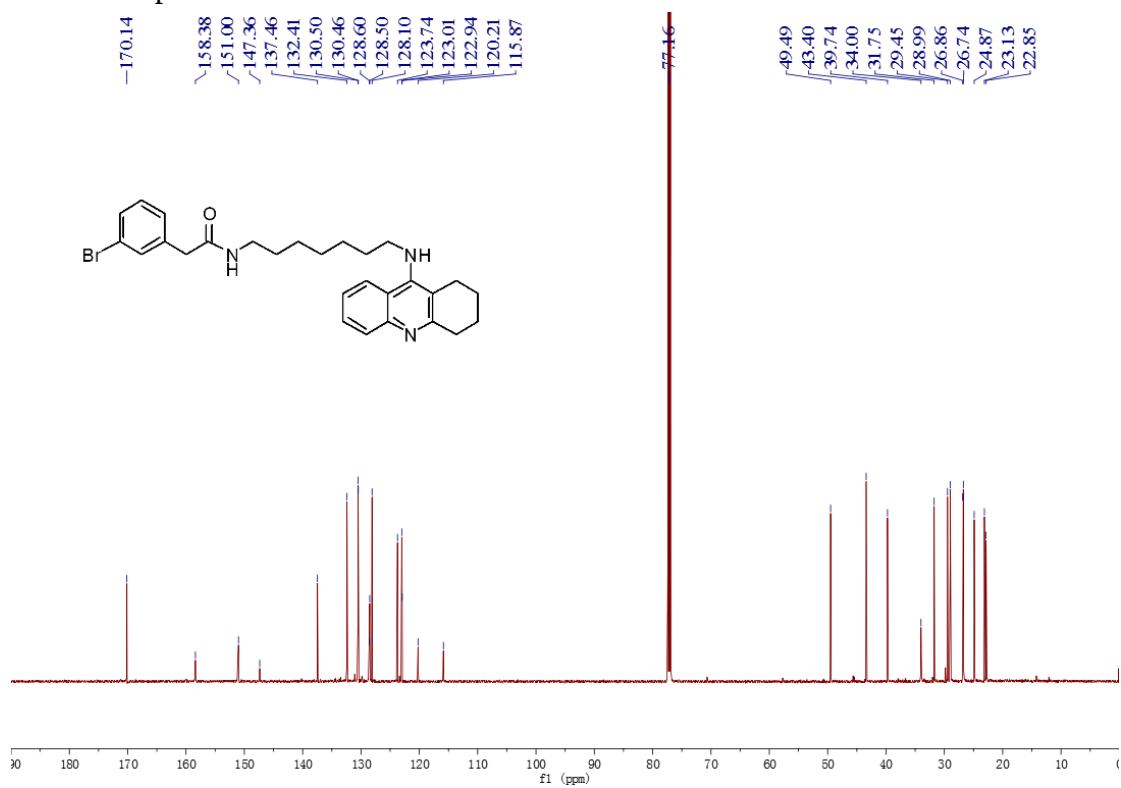
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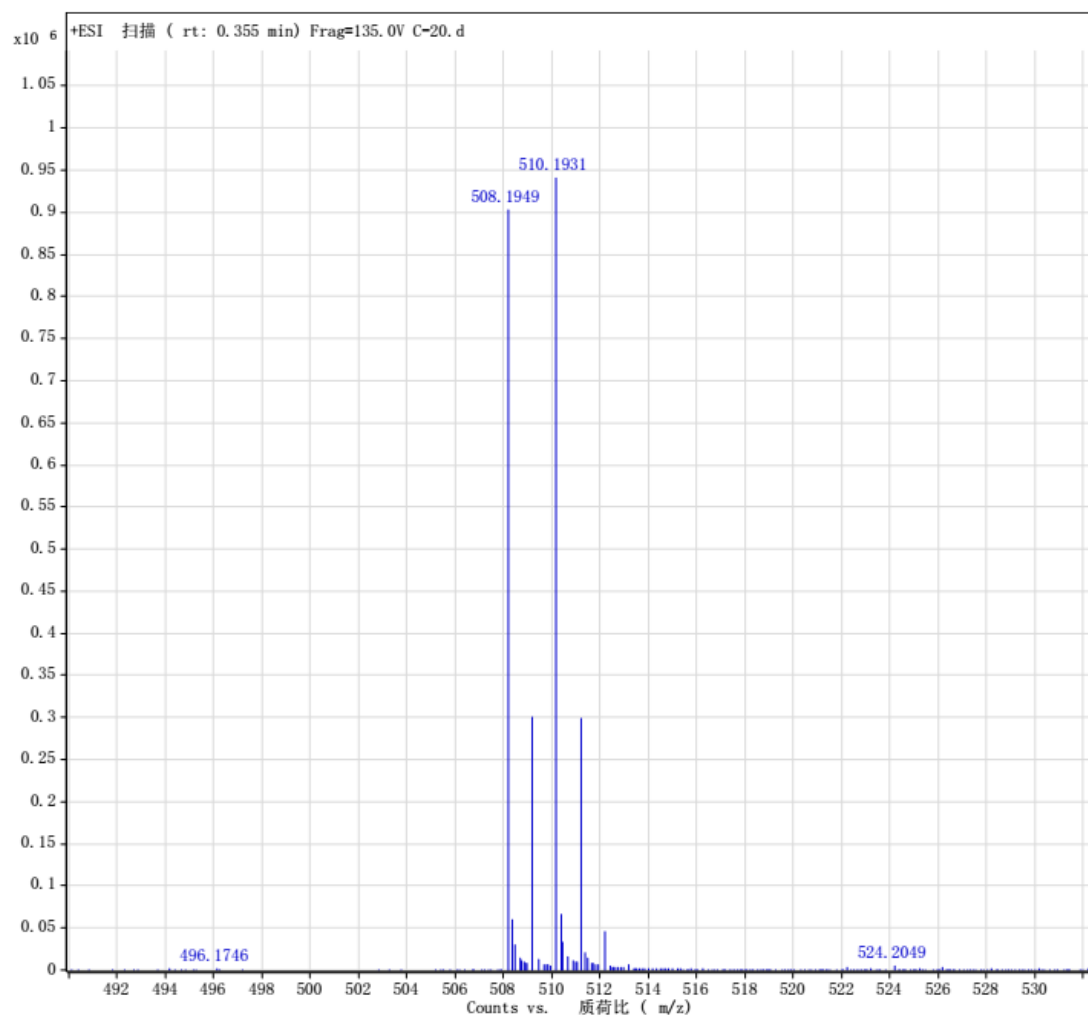
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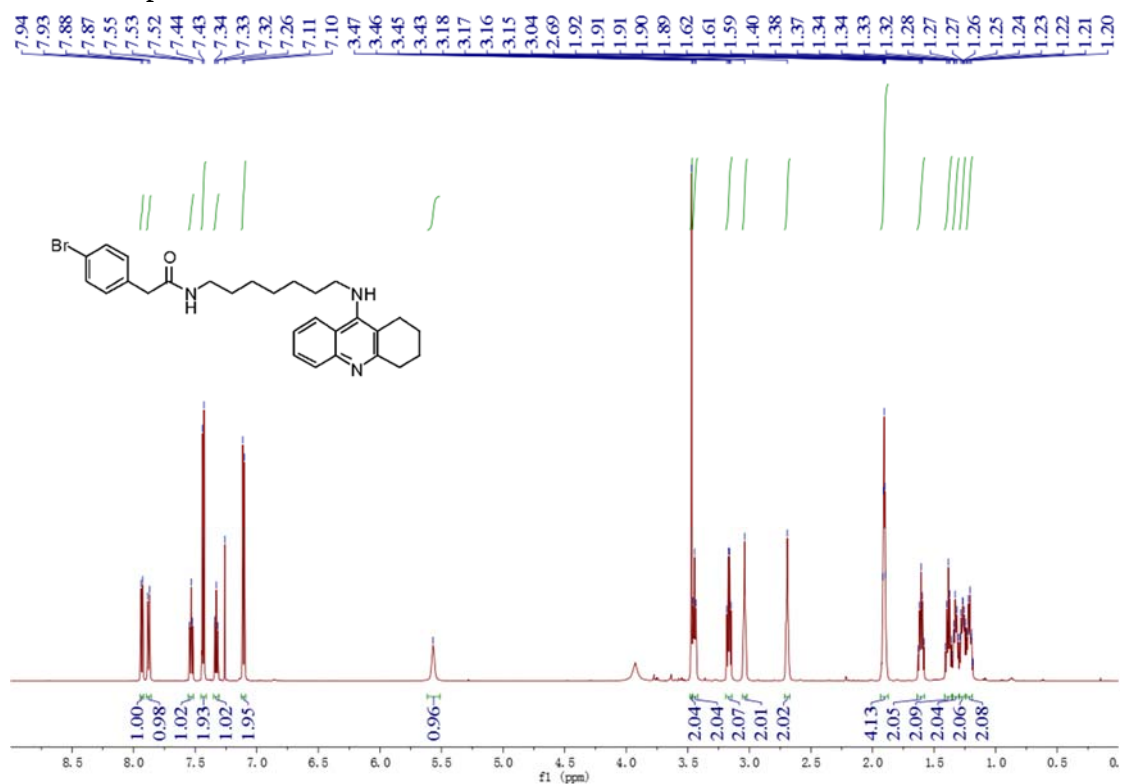
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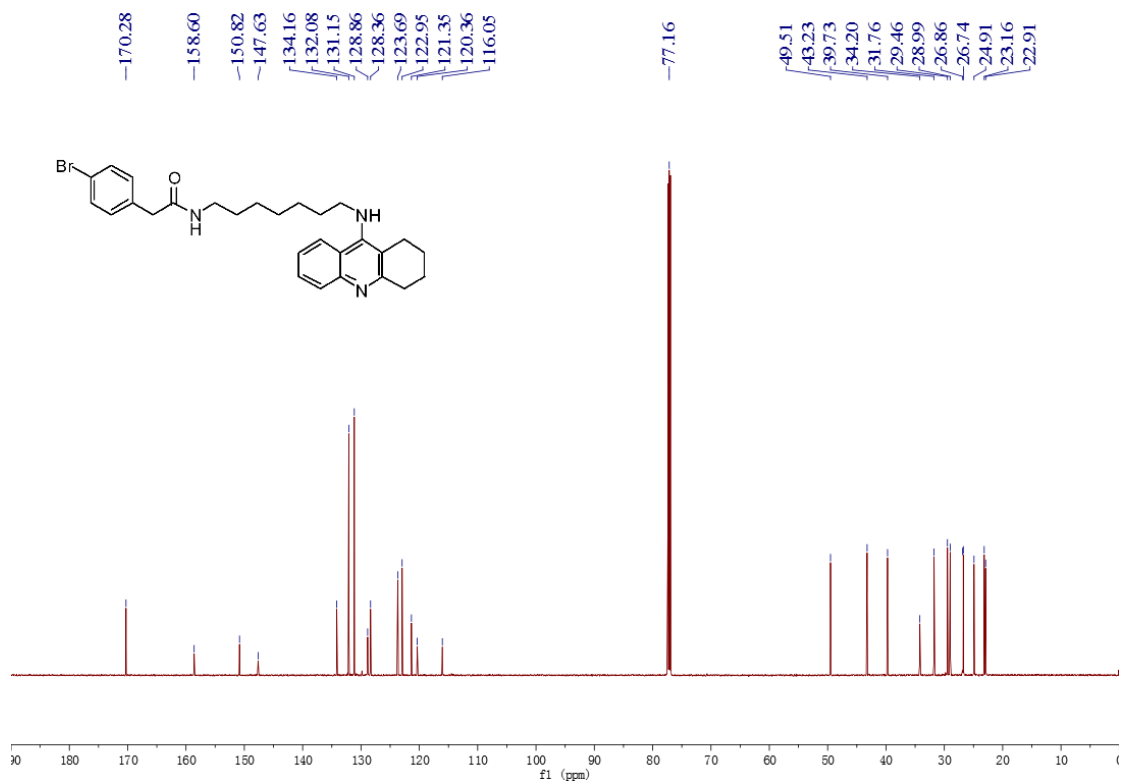
HR-MS (ESI) spectrum of **12e**



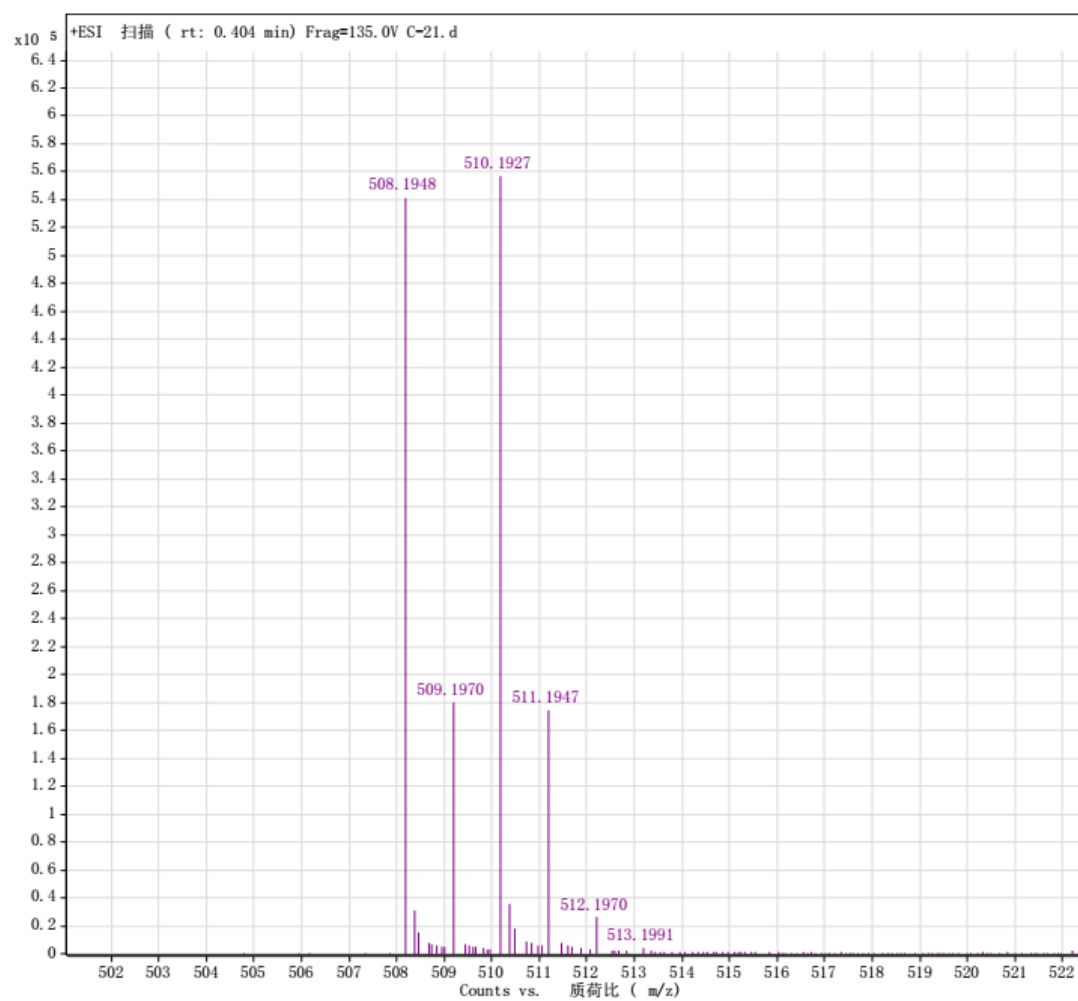
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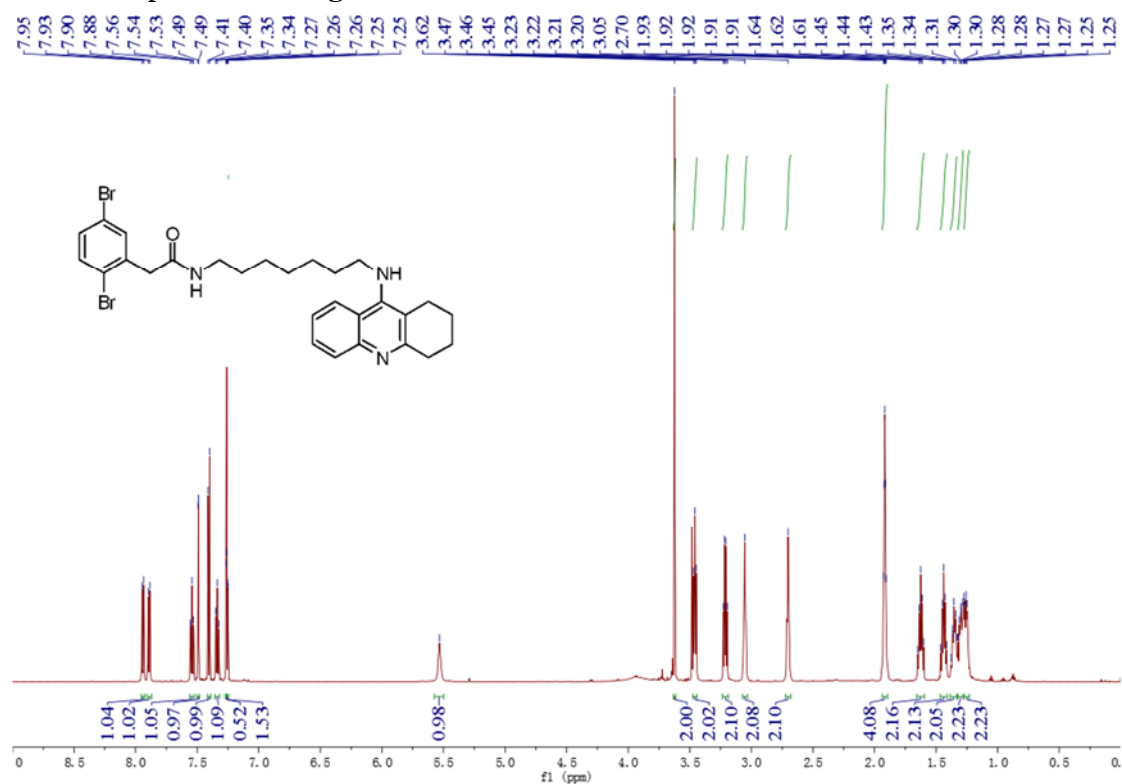
^{13}C NMR spectrum of **12f**



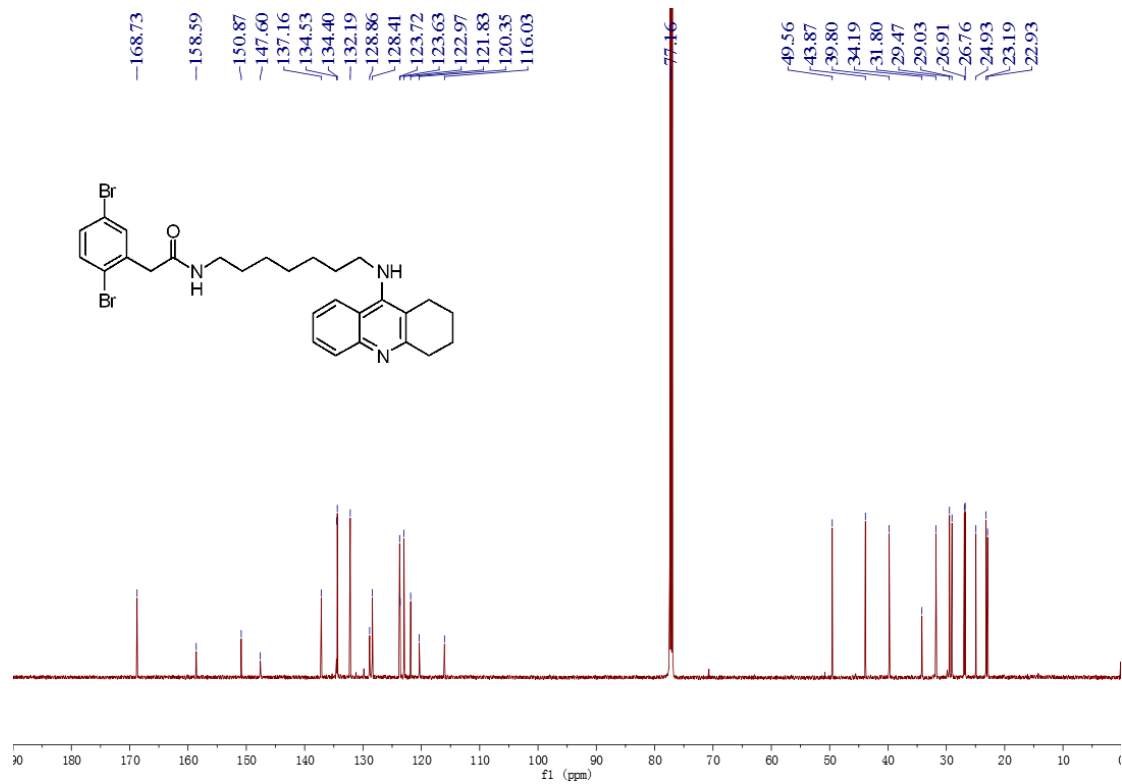
HR-MS (ESI) spectrum of **12f**



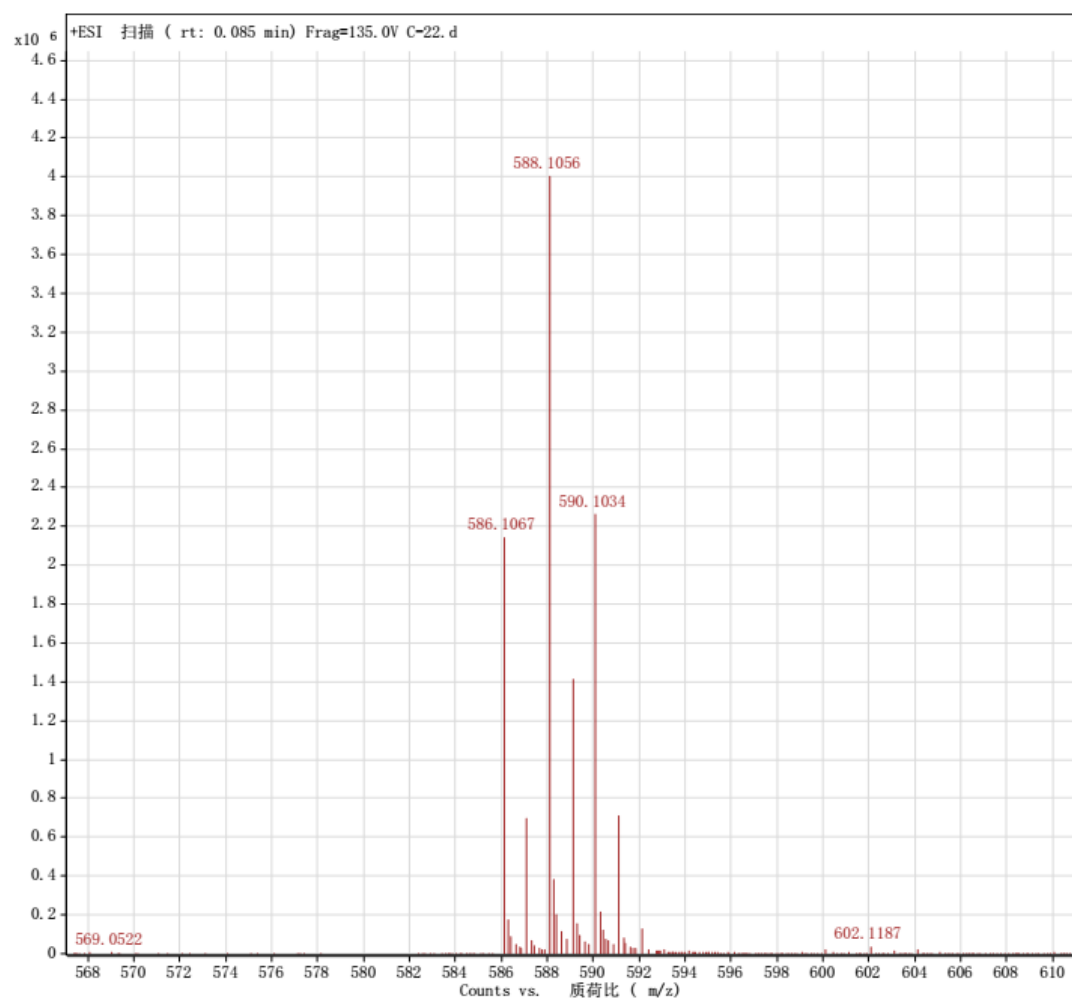
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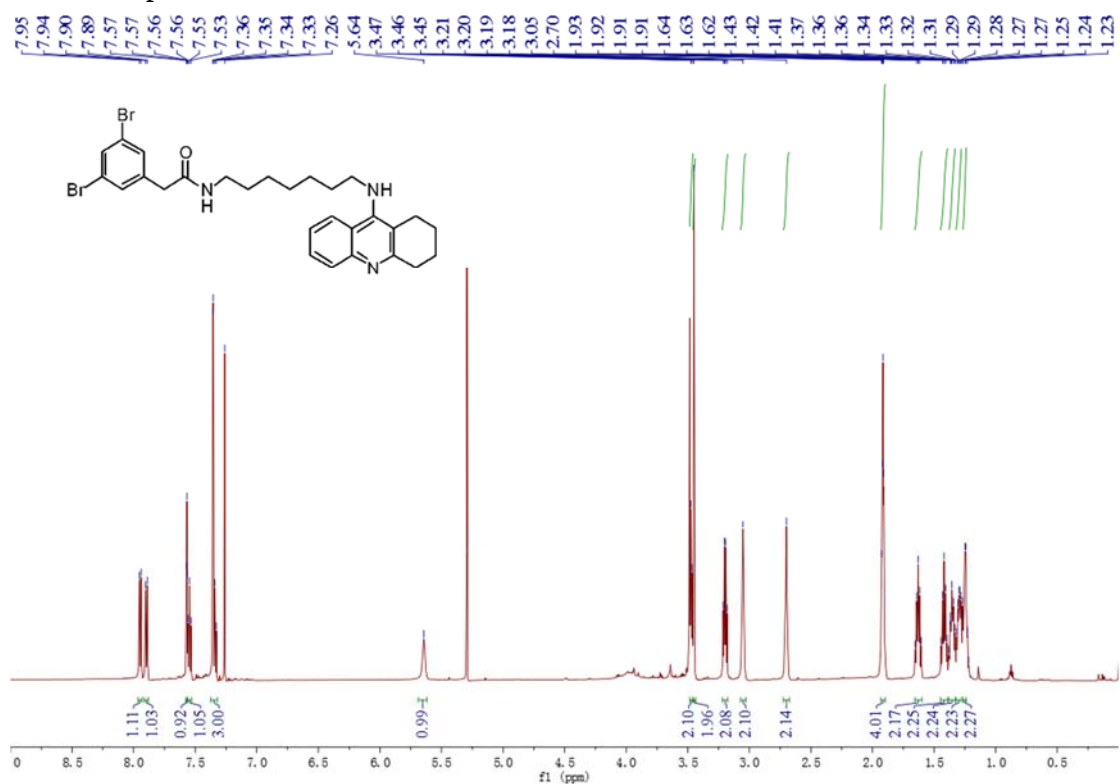
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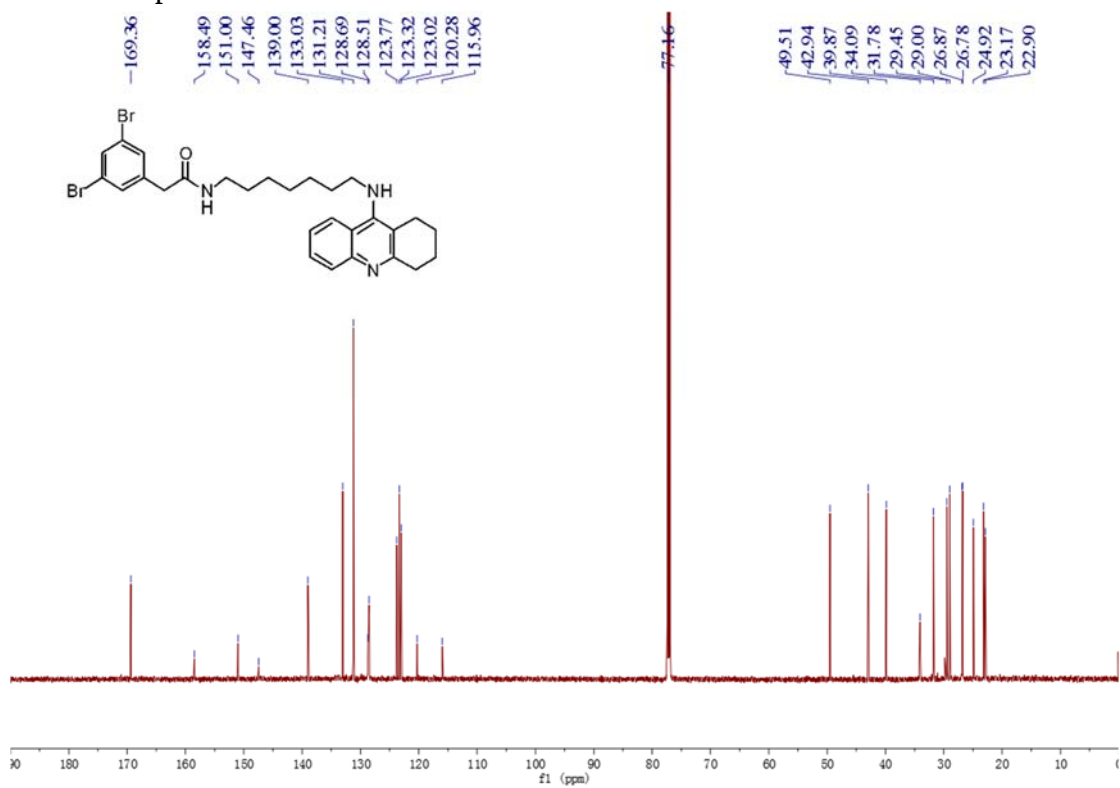
HR-MS (ESI) spectrum of **12g**



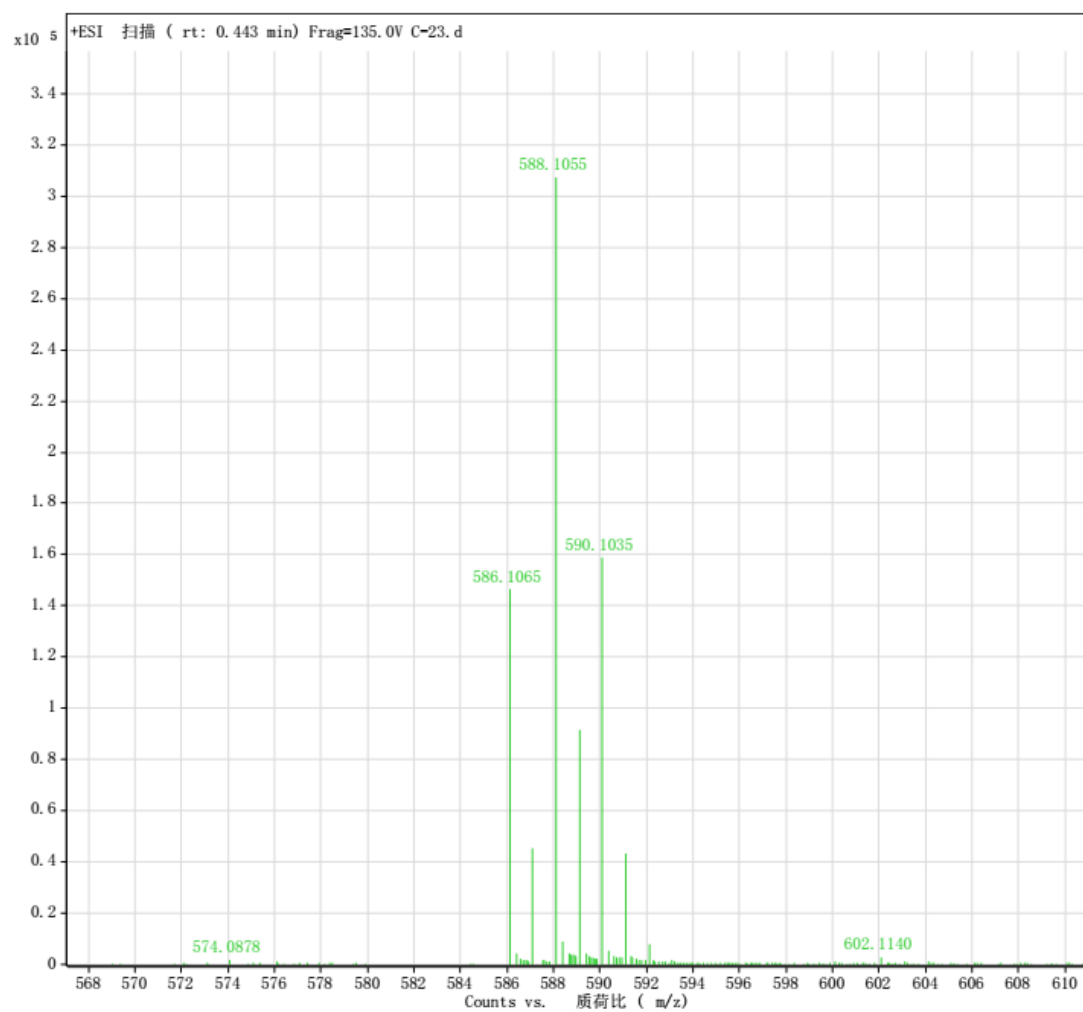
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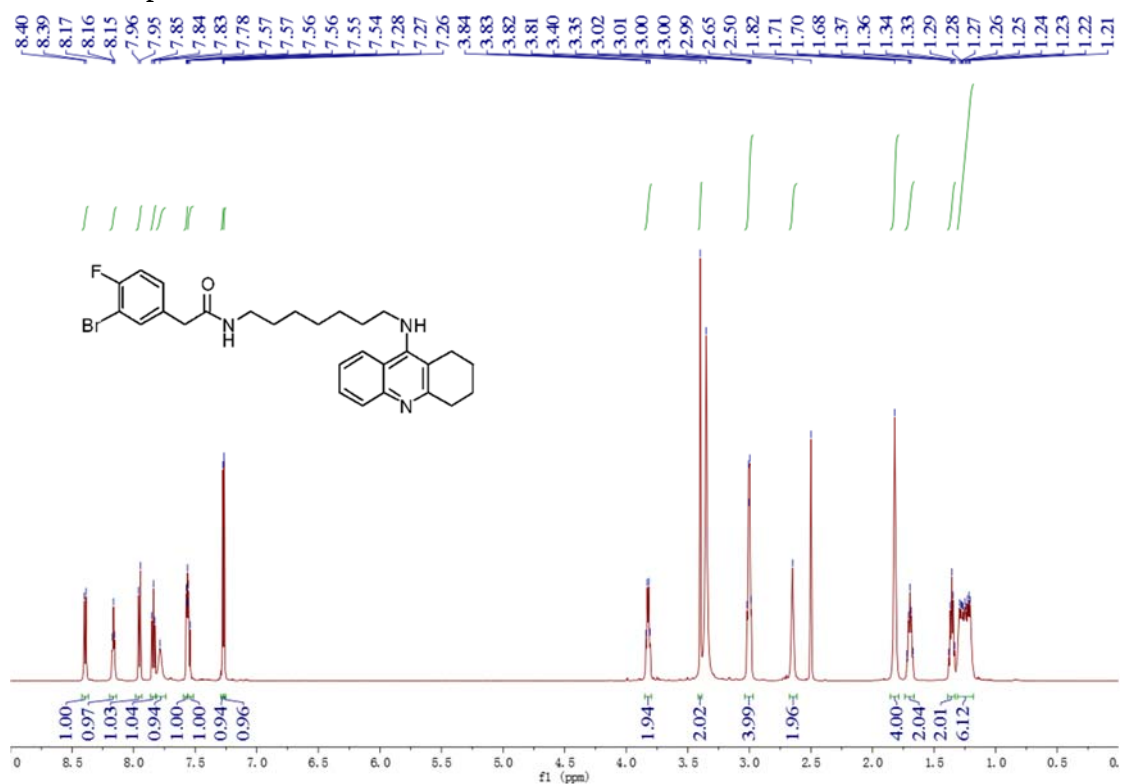
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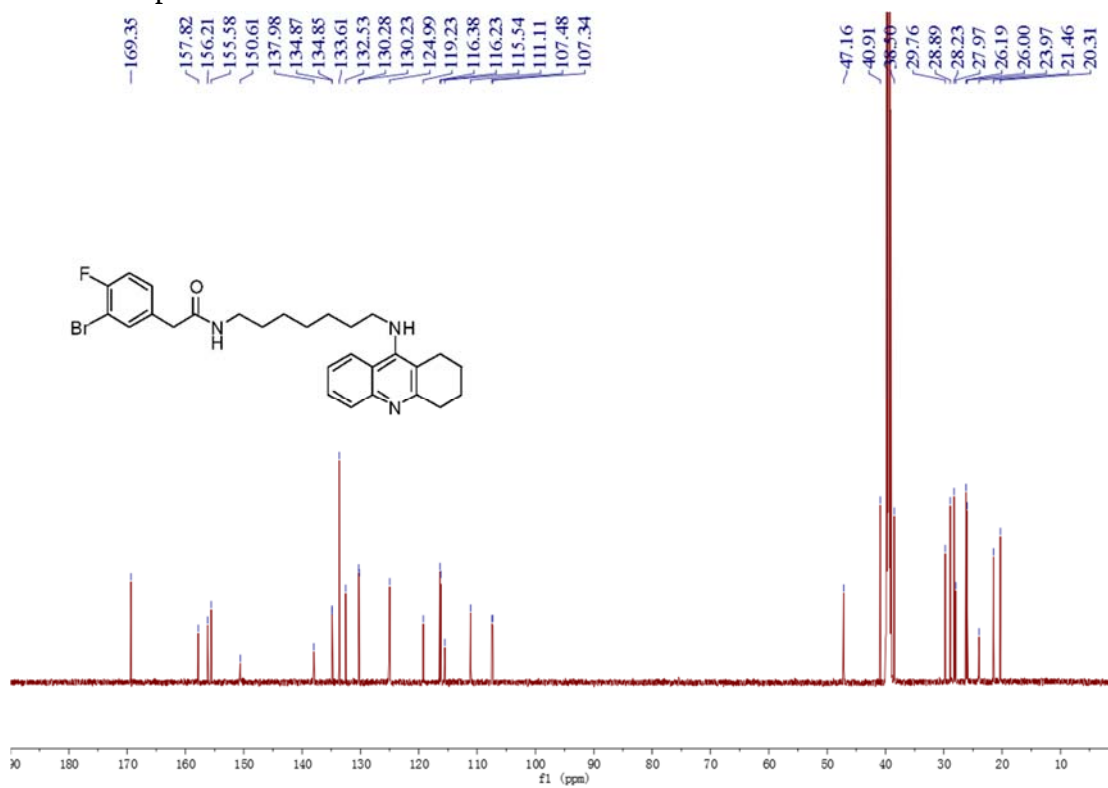
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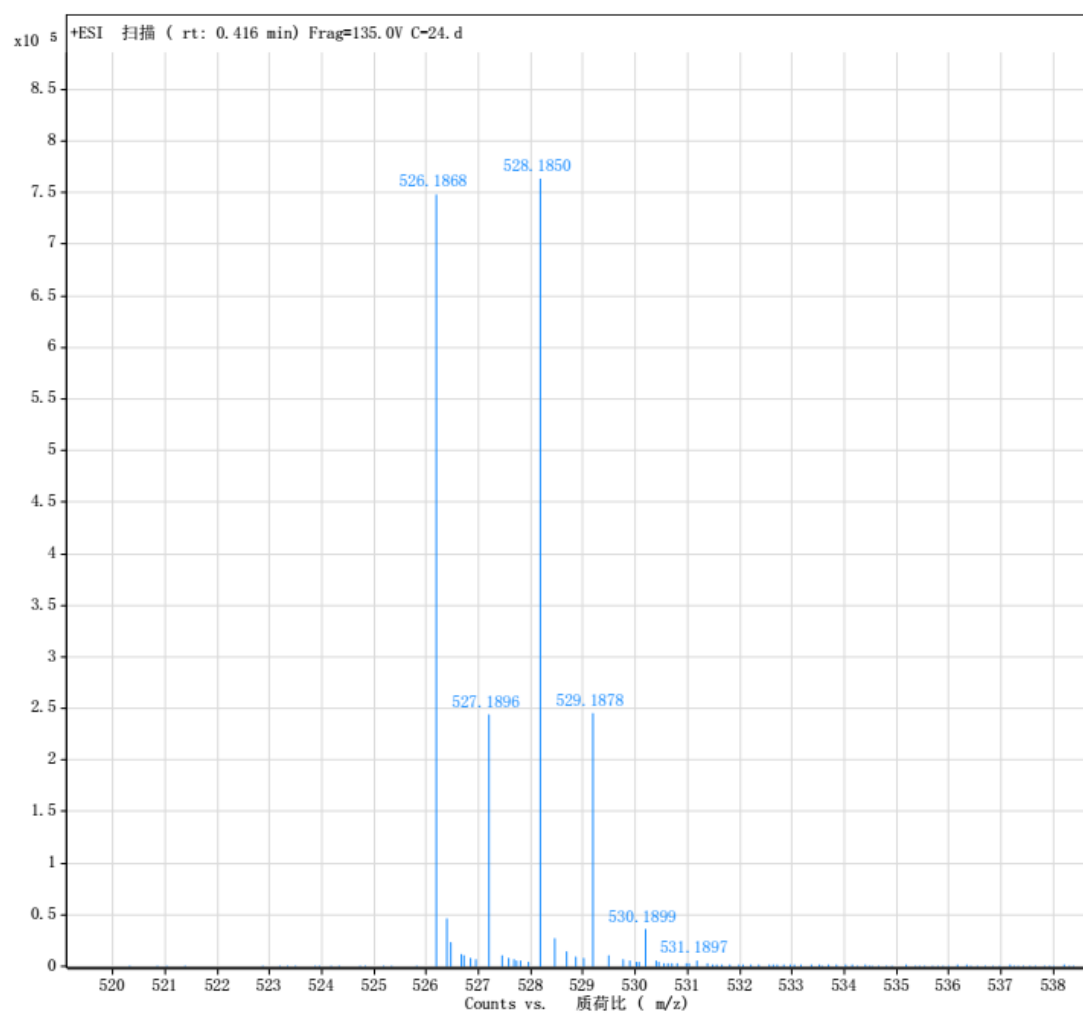
^1H NMR spectrum of **12i**



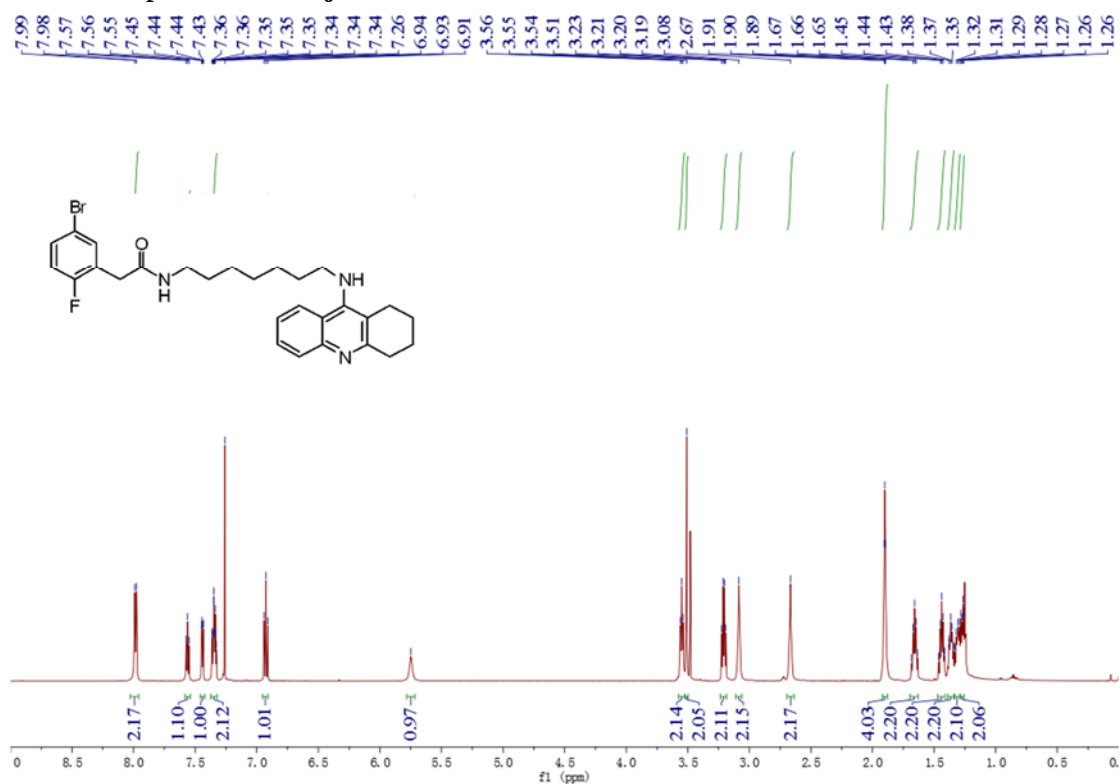
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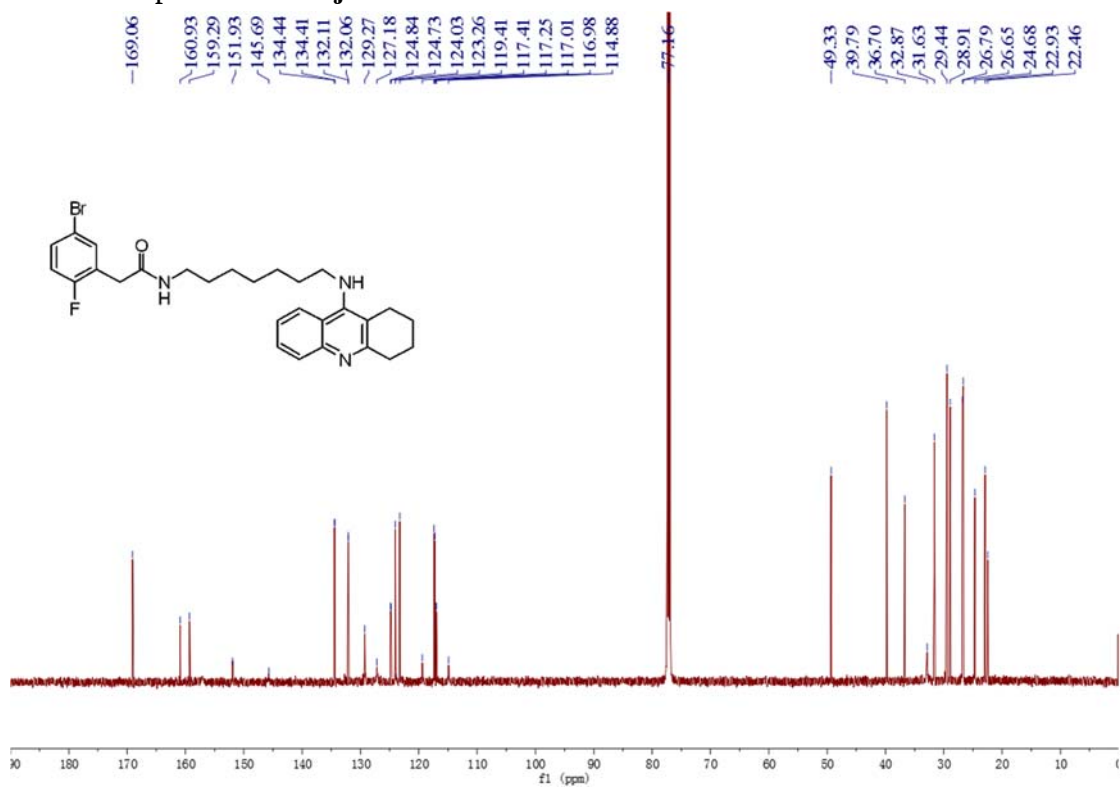
HR-MS (ESI) spectrum of **12i**



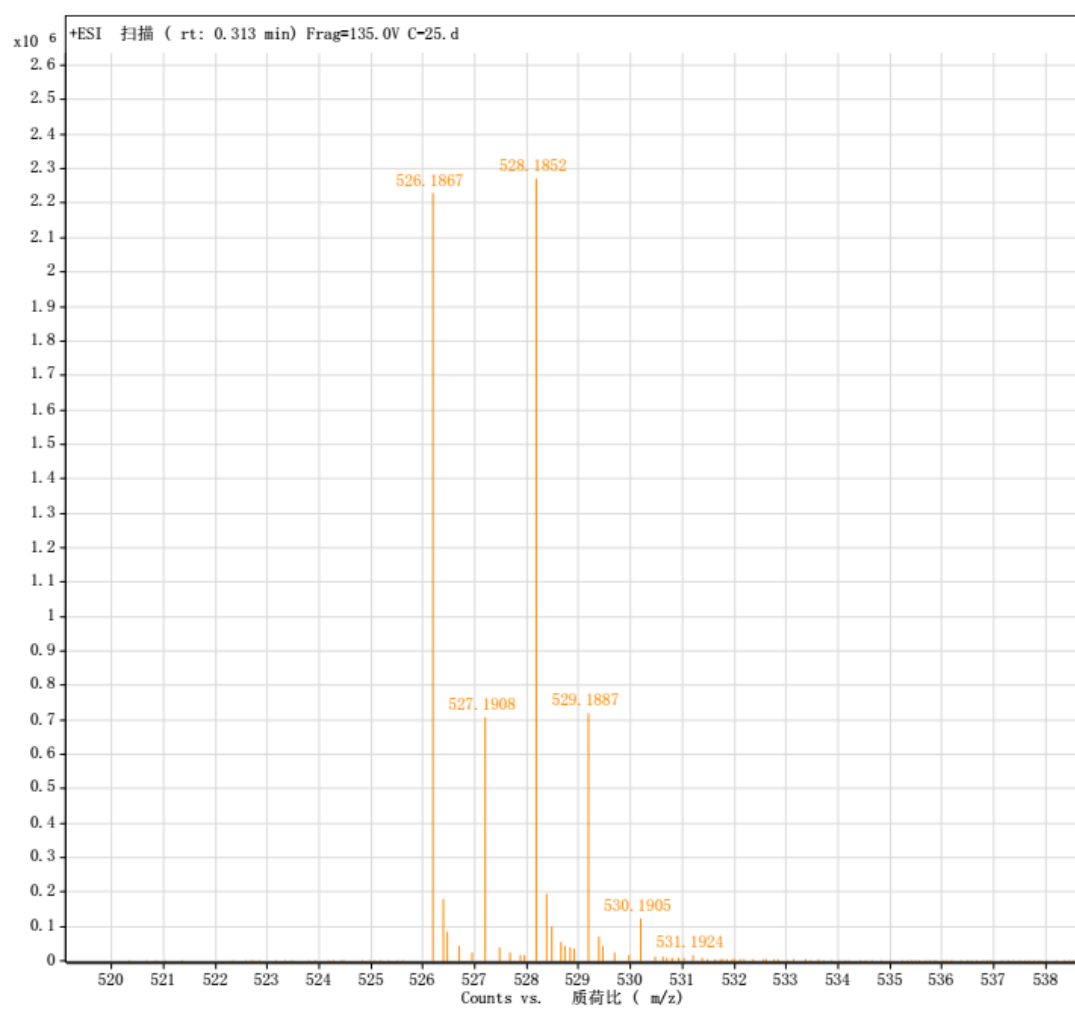
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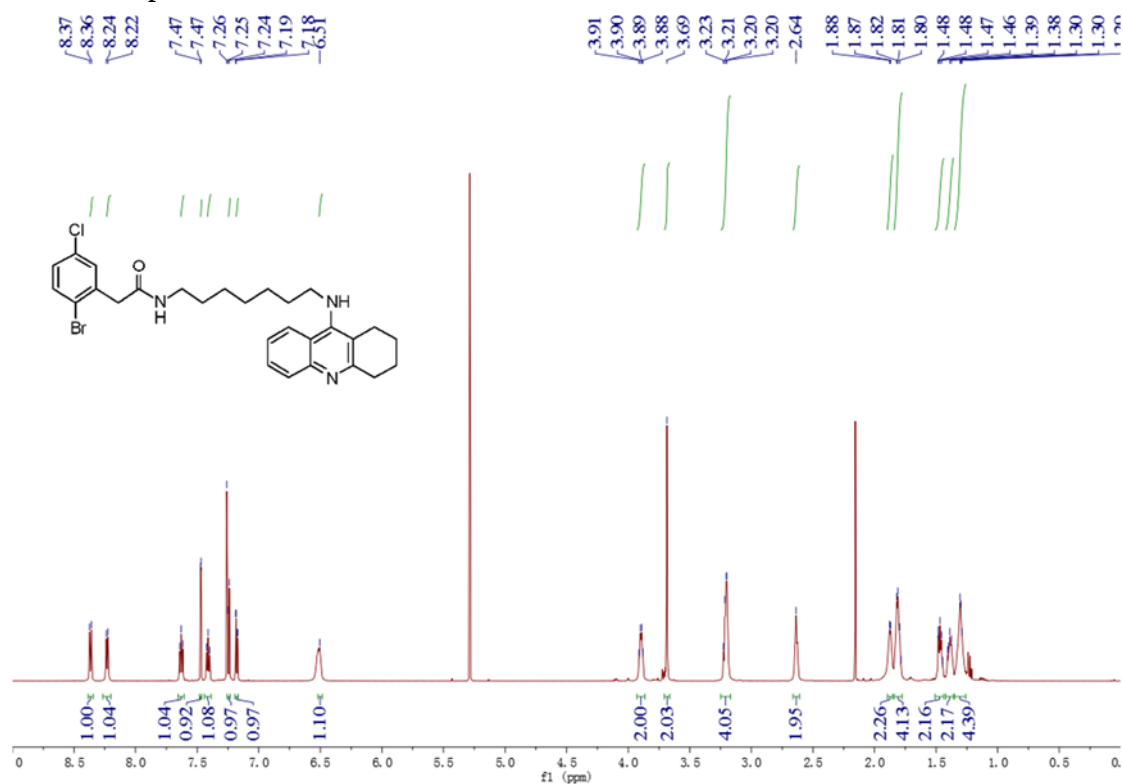
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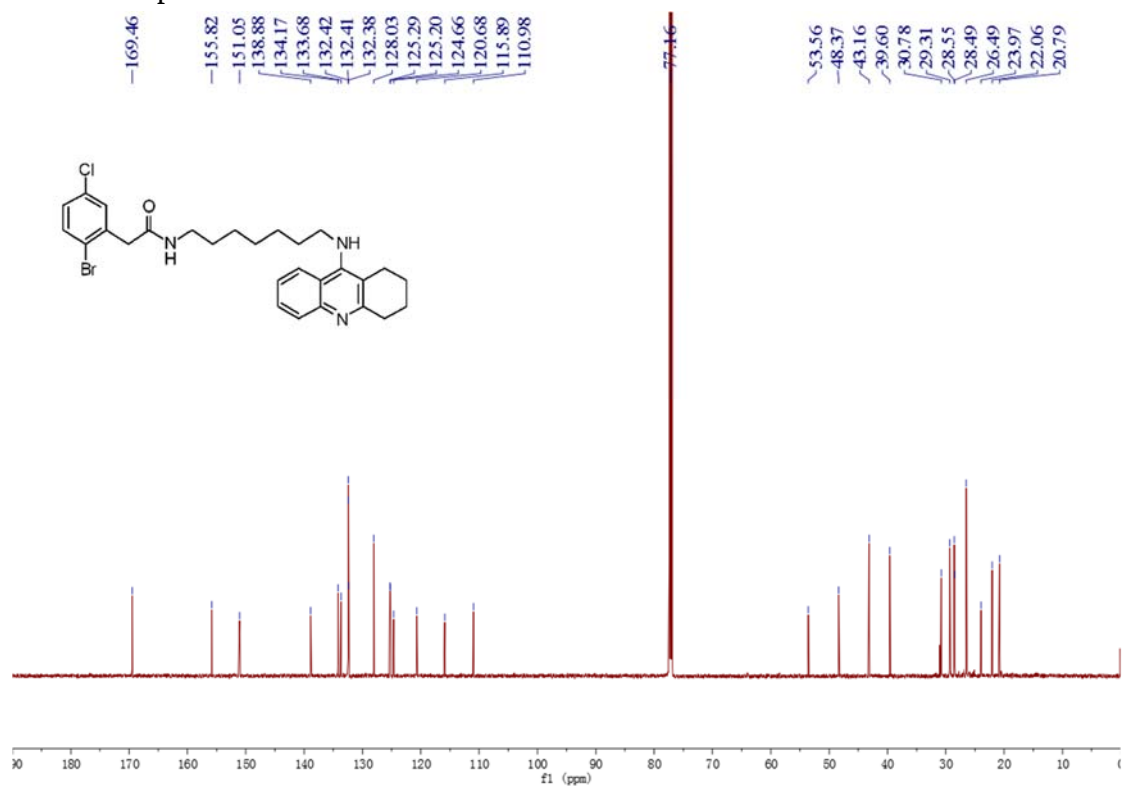
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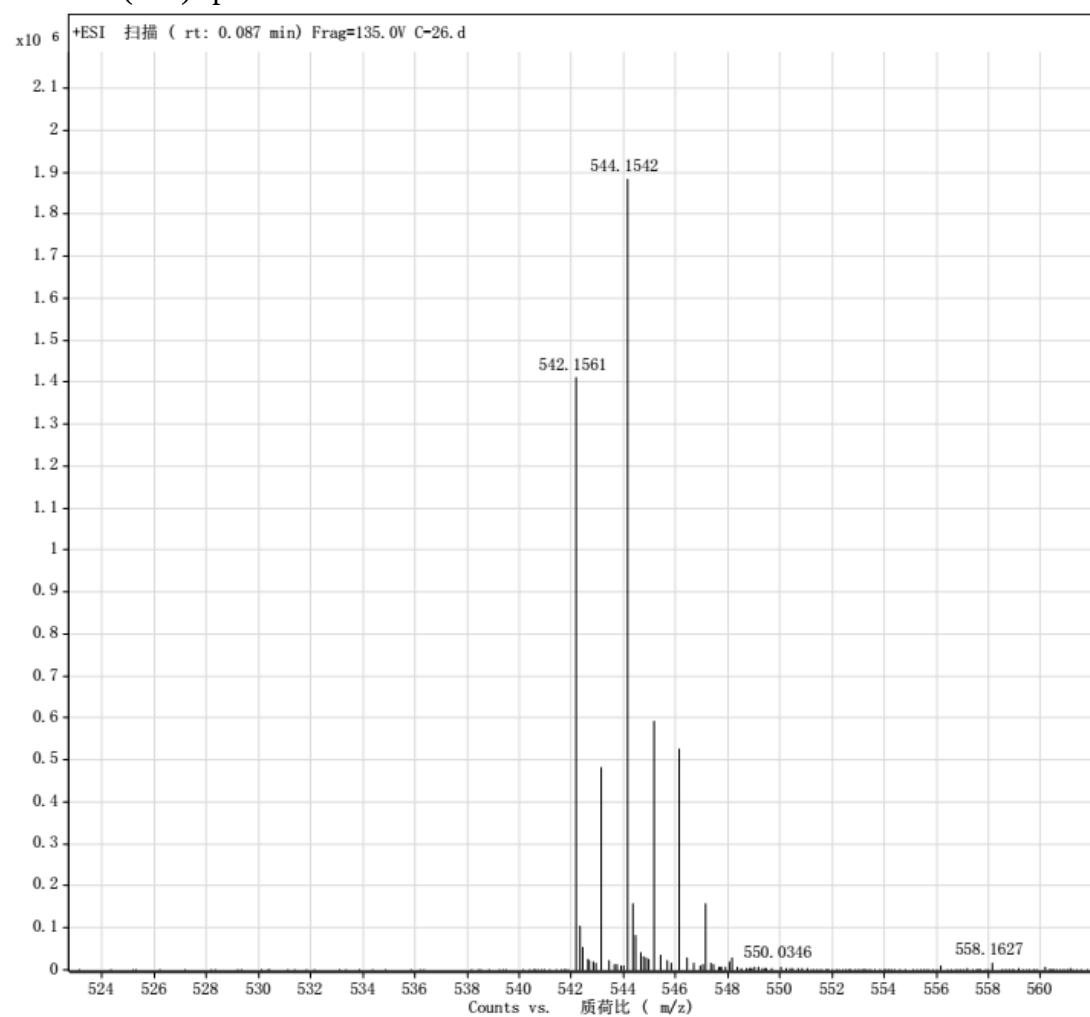
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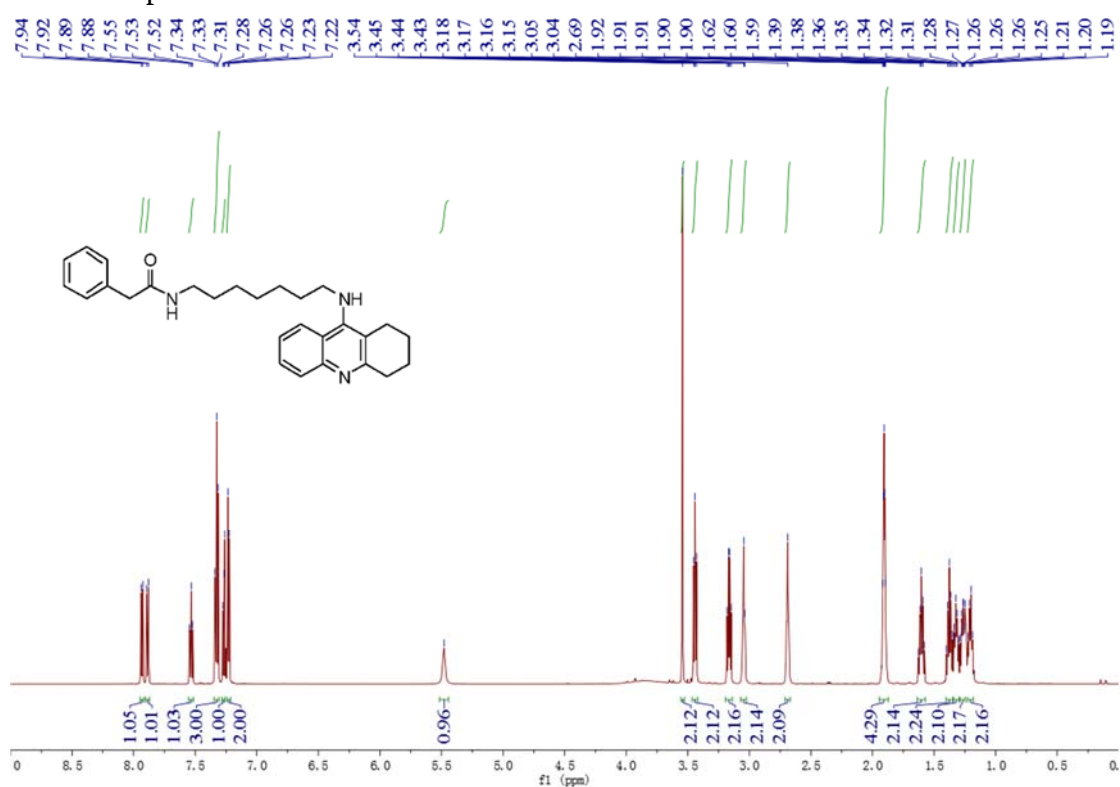
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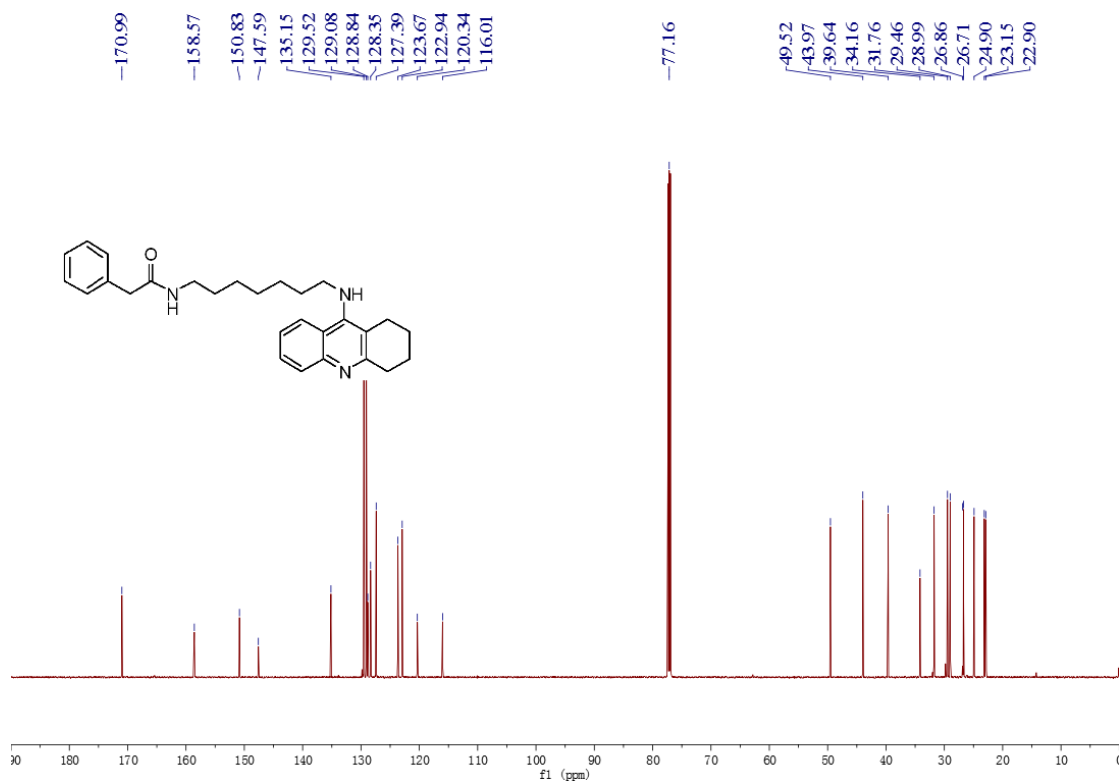
HR-MS (ESI) spectrum of **12k**



¹H NMR spectrum of **121**



¹³C NMR spectrum of **121**



HR-MS (ESI) spectrum of **12I**

