

Supporting Information

Discovery of novel small-molecule inhibitors of PD-1/PD-L1 interaction via structural simplification strategy

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I. Supplementary Table

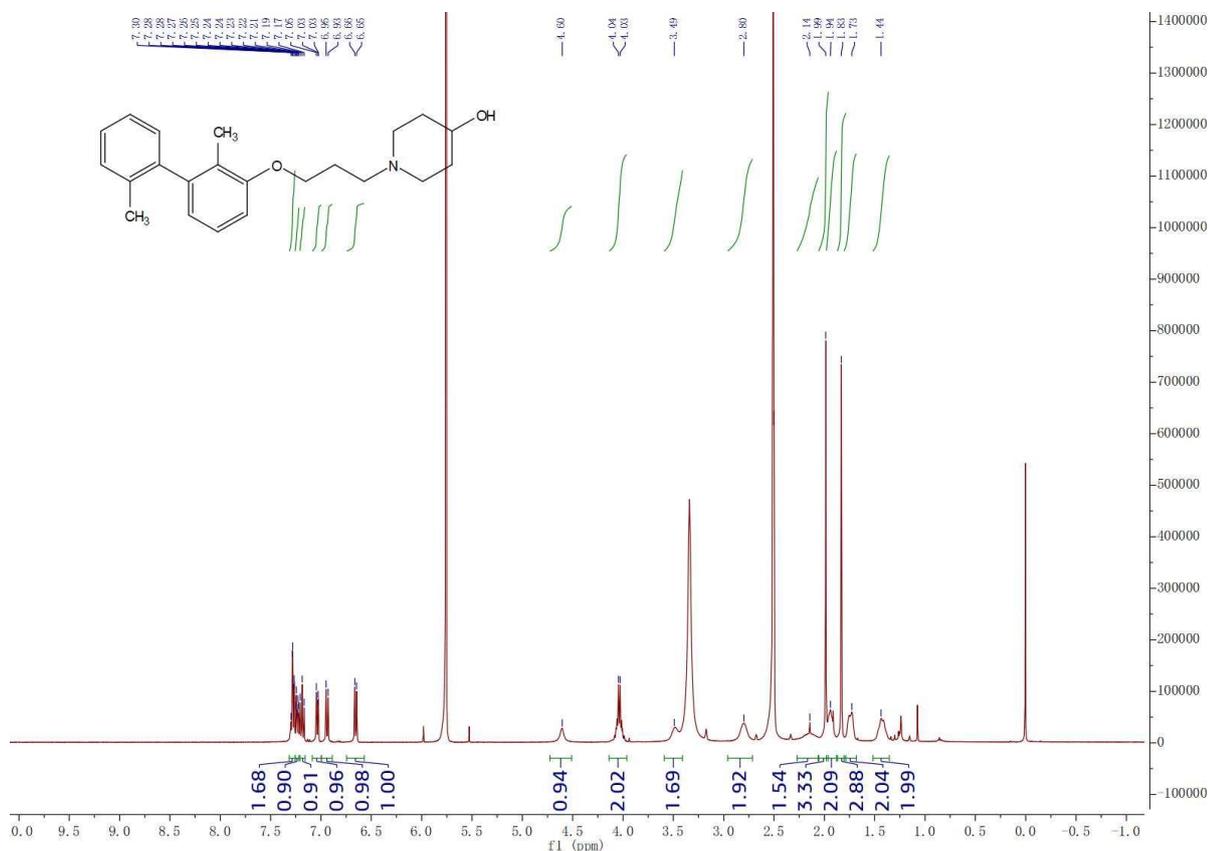
Table S1. The Kinetic Parameters and Binding Affinities of compounds with hPD-L1.

Compound	K_a ($M^{-1}s^{-1}$)	K_d (s^{-1})	K_D (M)	LE ^a
A7	7.89×10^5	6.38×10^{-3}	8.09×10^{-9}	0.35
A9	5.38×10^5	1.96×10^{-3}	3.64×10^{-9}	0.40
A11	5.76×10^5	3.68×10^{-3}	6.39×10^{-9}	0.39
A15	5.05×10^5	1.01×10^{-2}	1.99×10^{-8}	0.36

^a The result is calculated by the equation: $LE = -1.35 \log K_D / N_{\text{heavy atoms}}$, $N_{\text{heavy atoms}}$ is the number of non-H atoms.

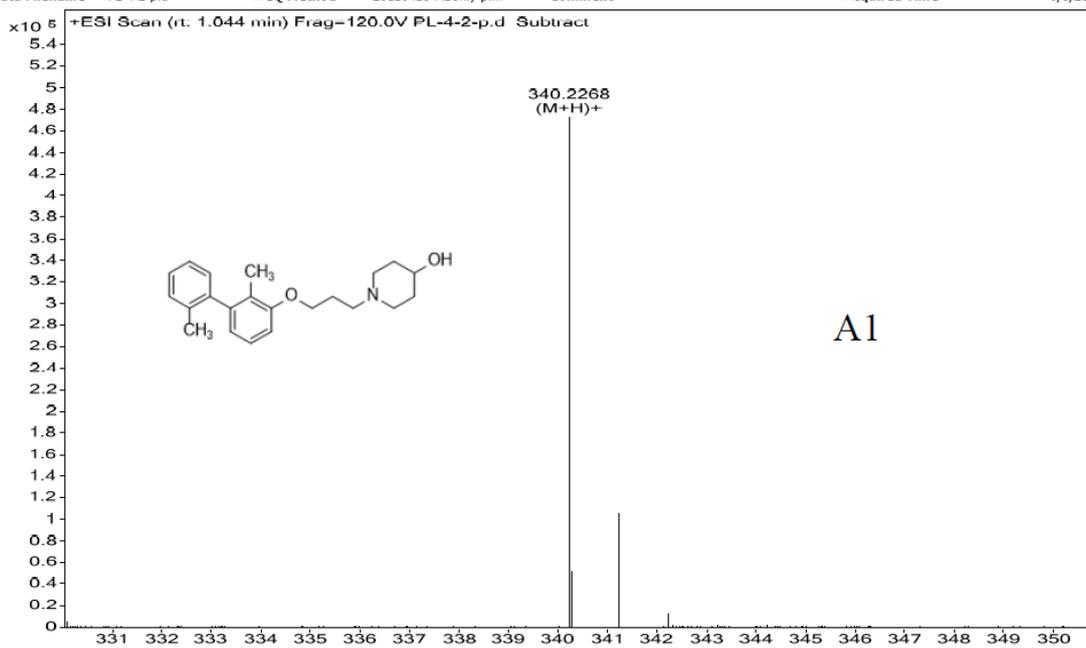
II. Spectroscopic data of compounds A1-18

¹H NMR Spectra for Compound A1

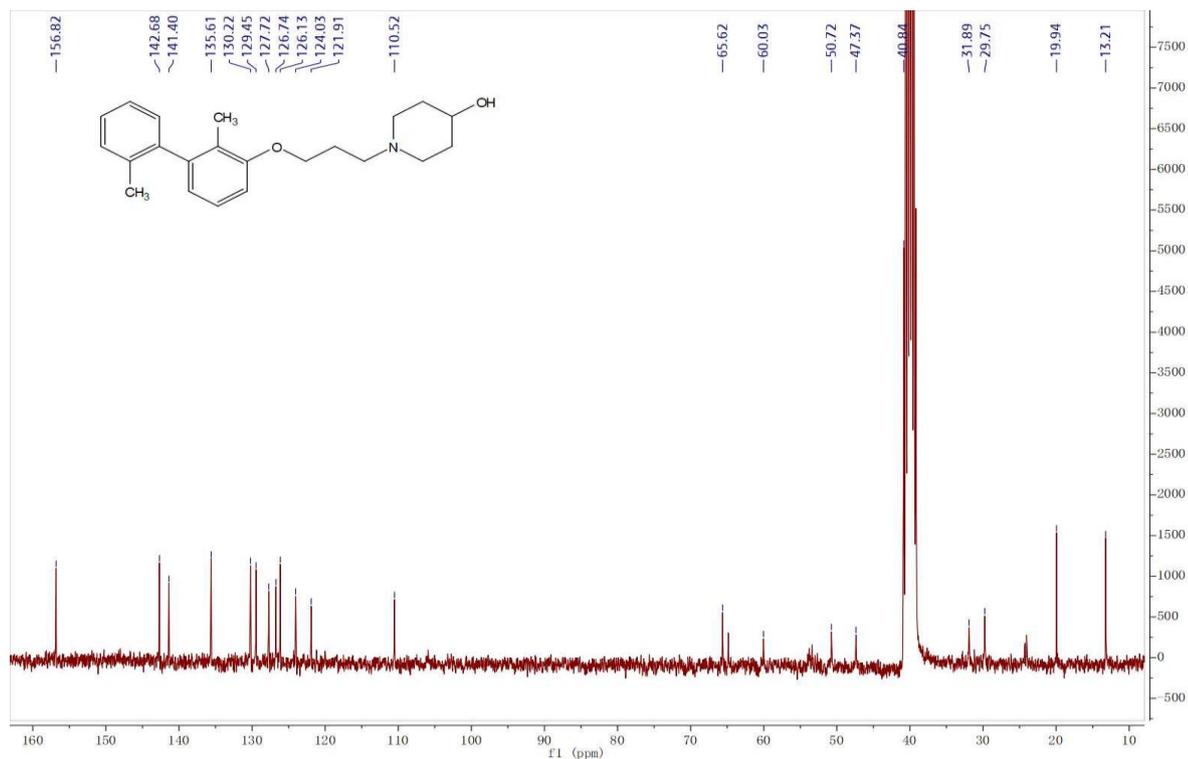


LCMS Spectra for Compound A1

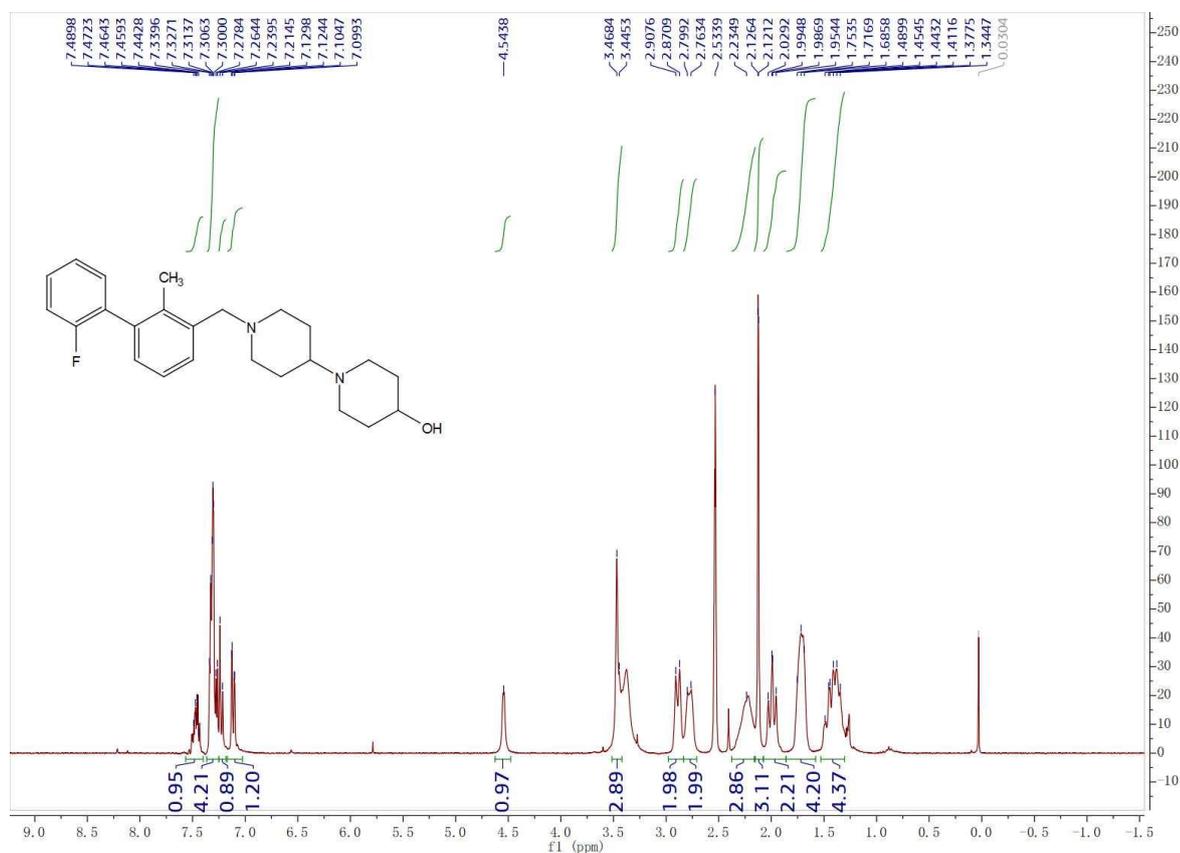
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¹³C NMR Spectra for Compound A1

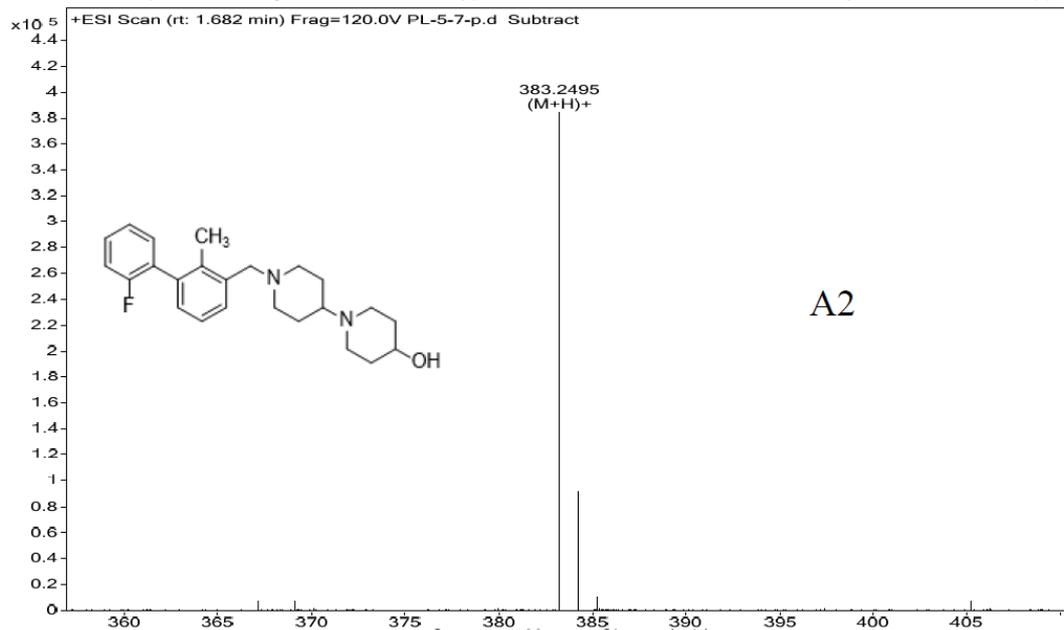


¹H NMR Spectra for Compound A2

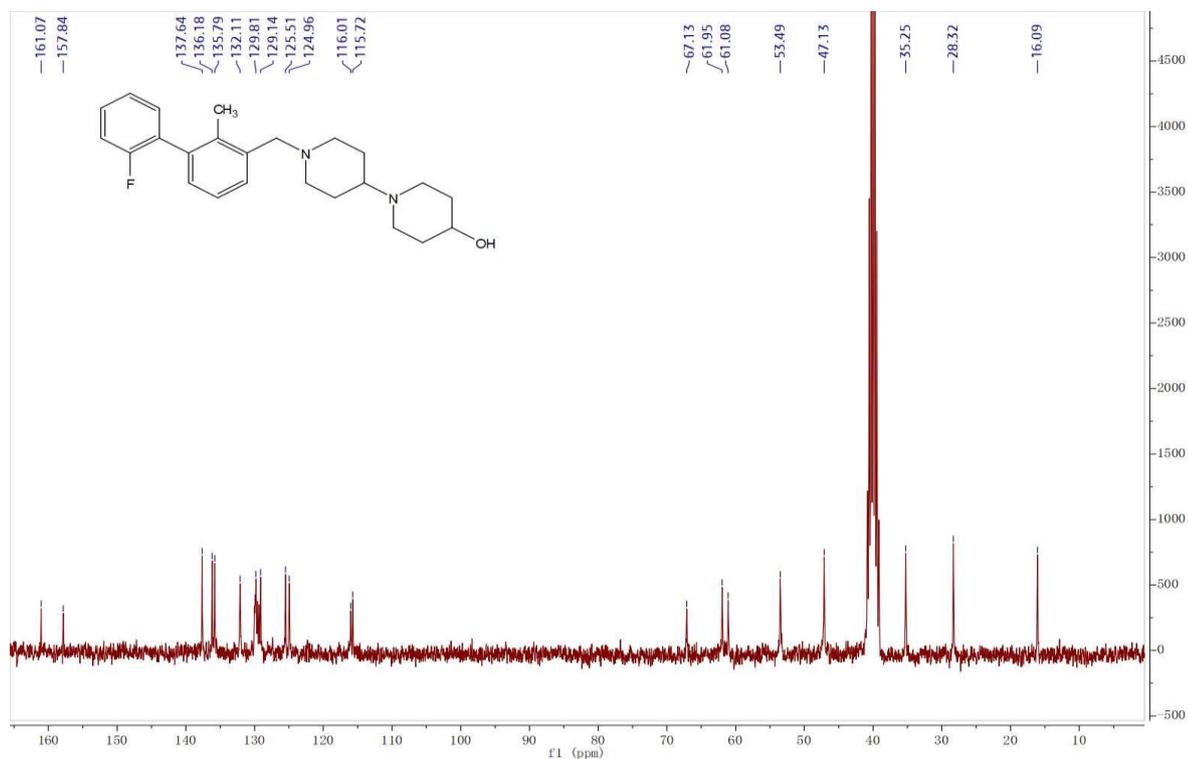


LCMS Spectra for Compound A2

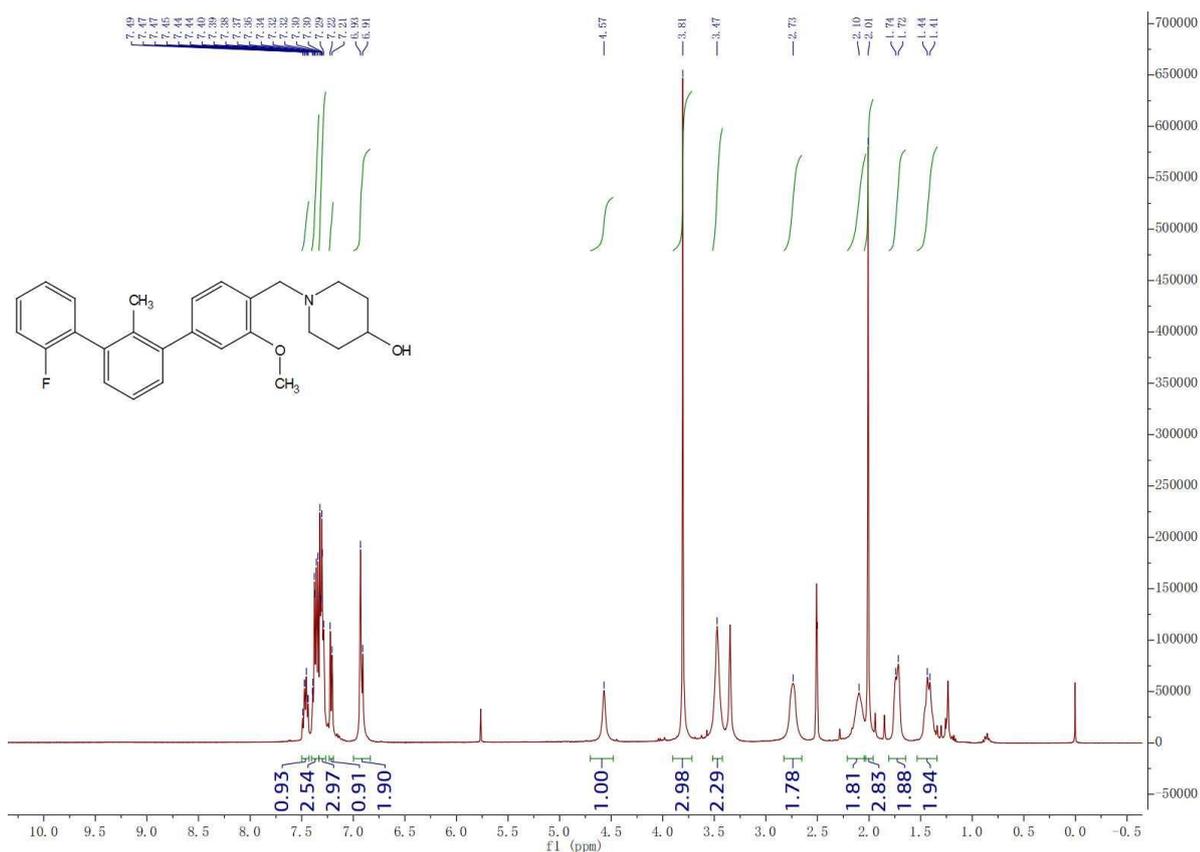
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¹³C NMR Spectra for Compound A2

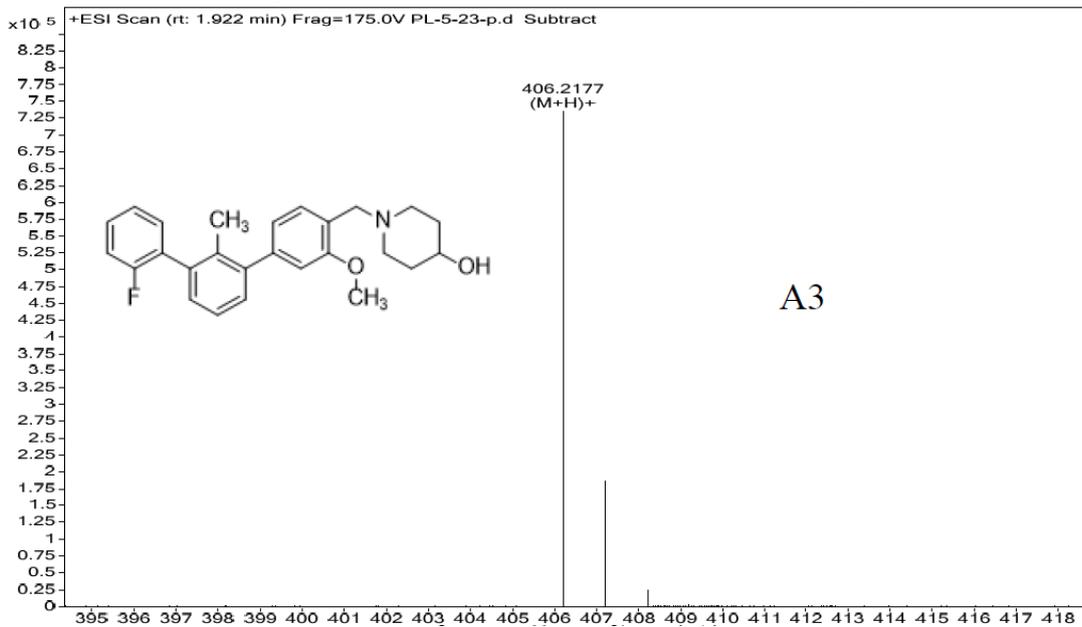


¹H NMR Spectra for Compound A3

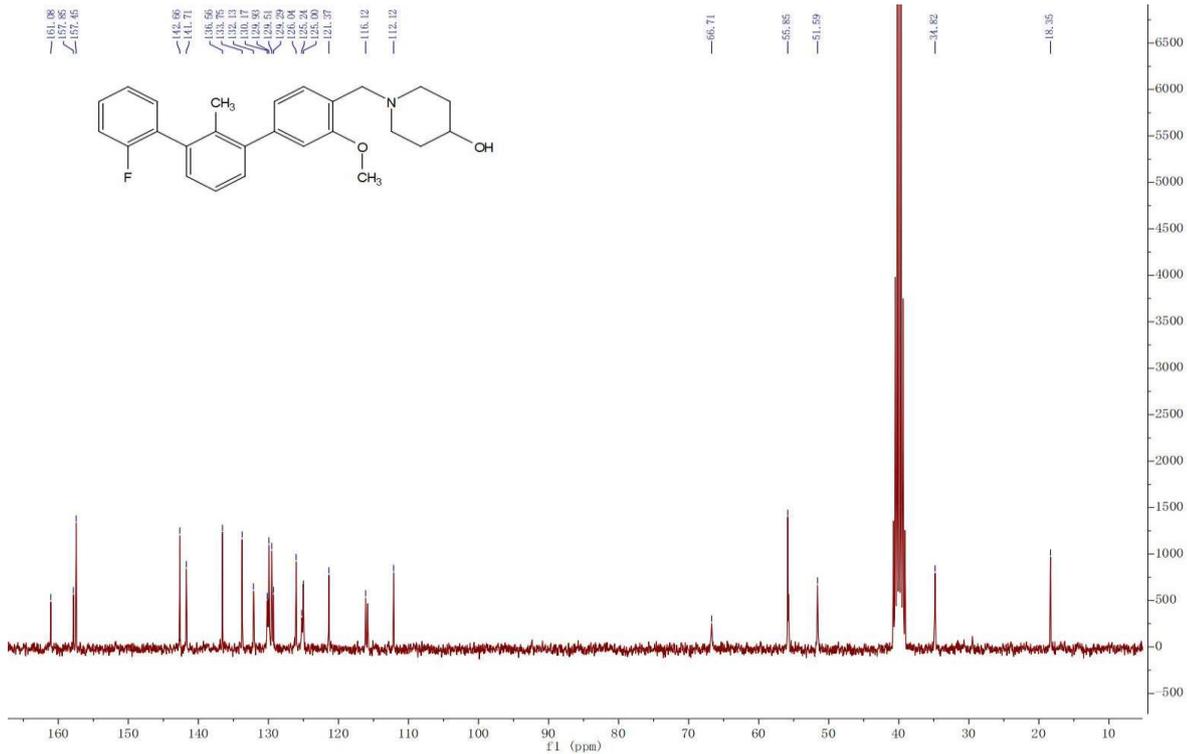


LCMS Spectra for Compound A3

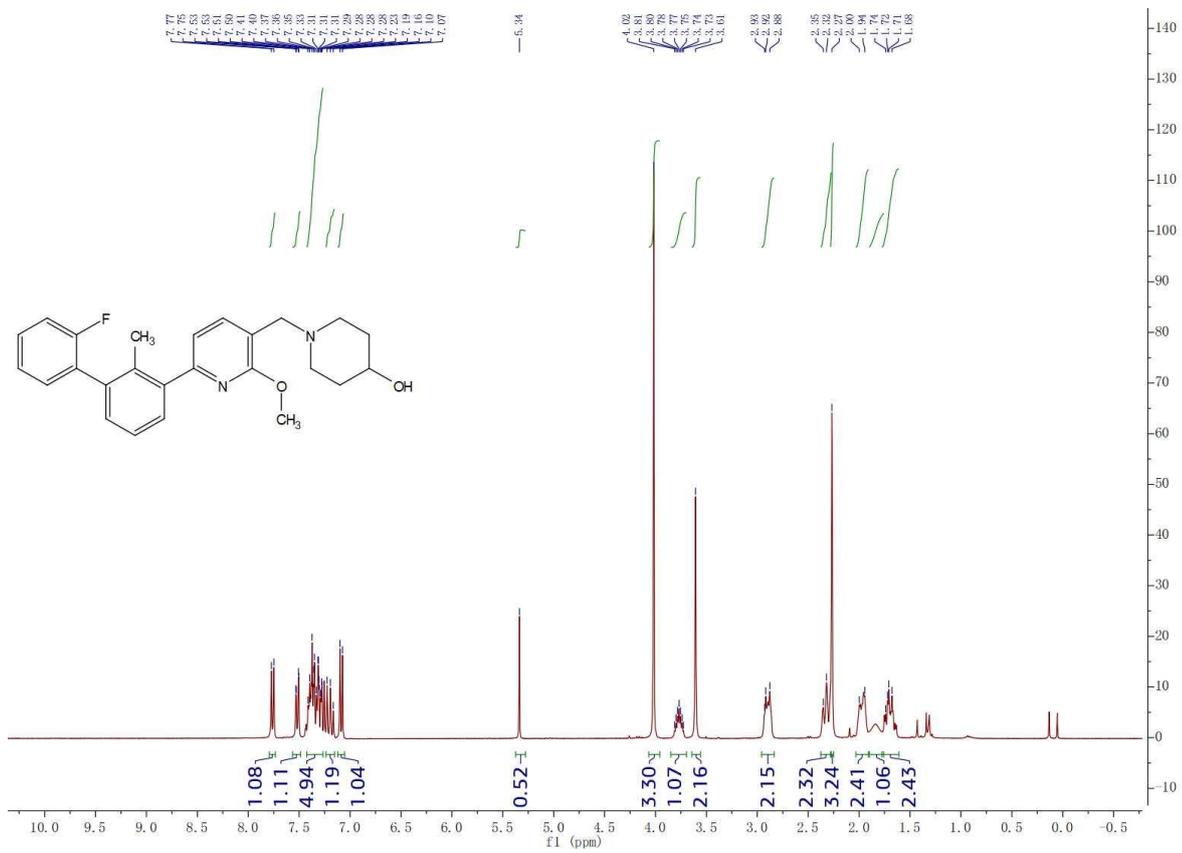
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¹³C NMR Spectra for Compound A3

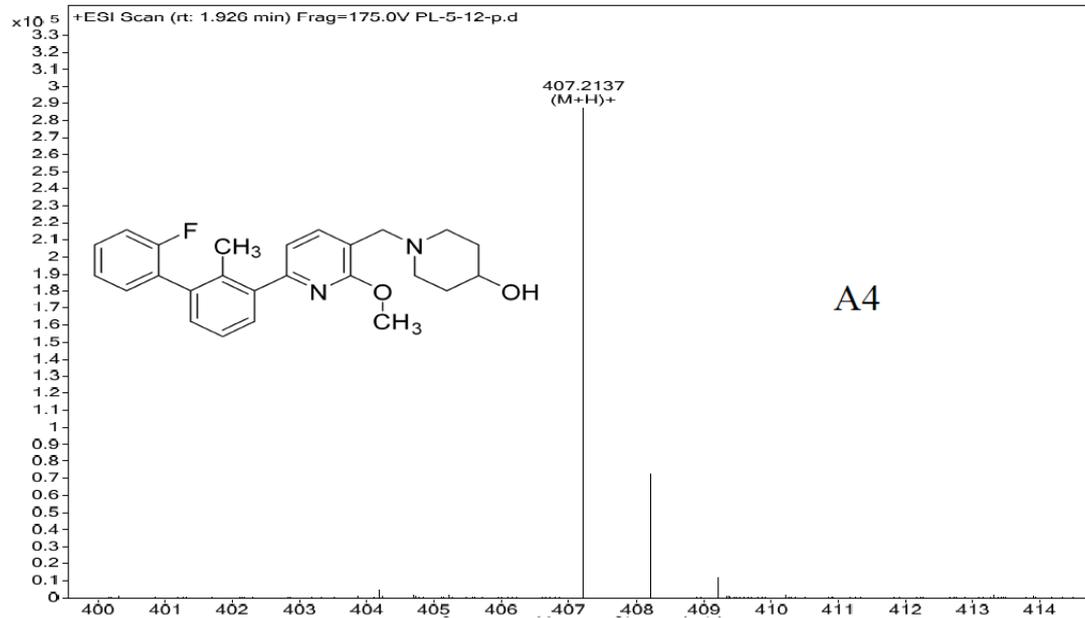


¹H NMR Spectra for Compound A4

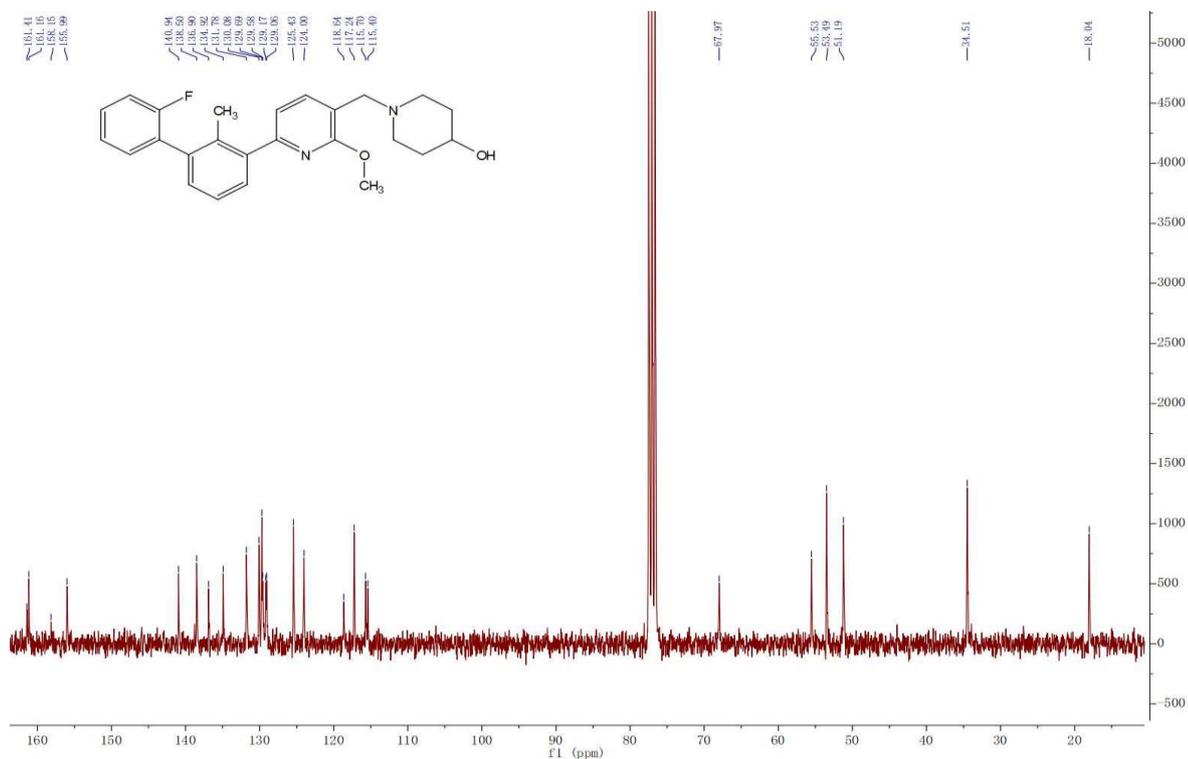


LCMS Spectra for Compound A4

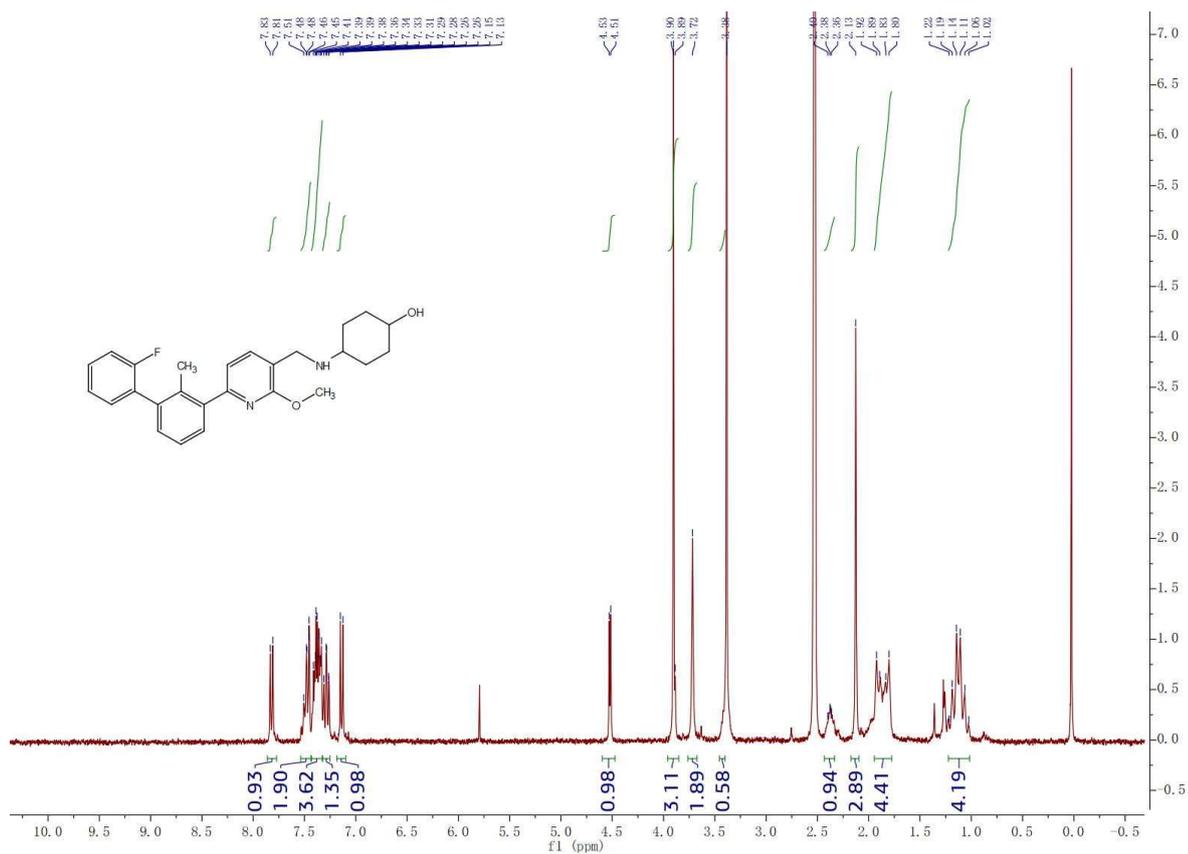
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¹³C NMR Spectra for Compound A4

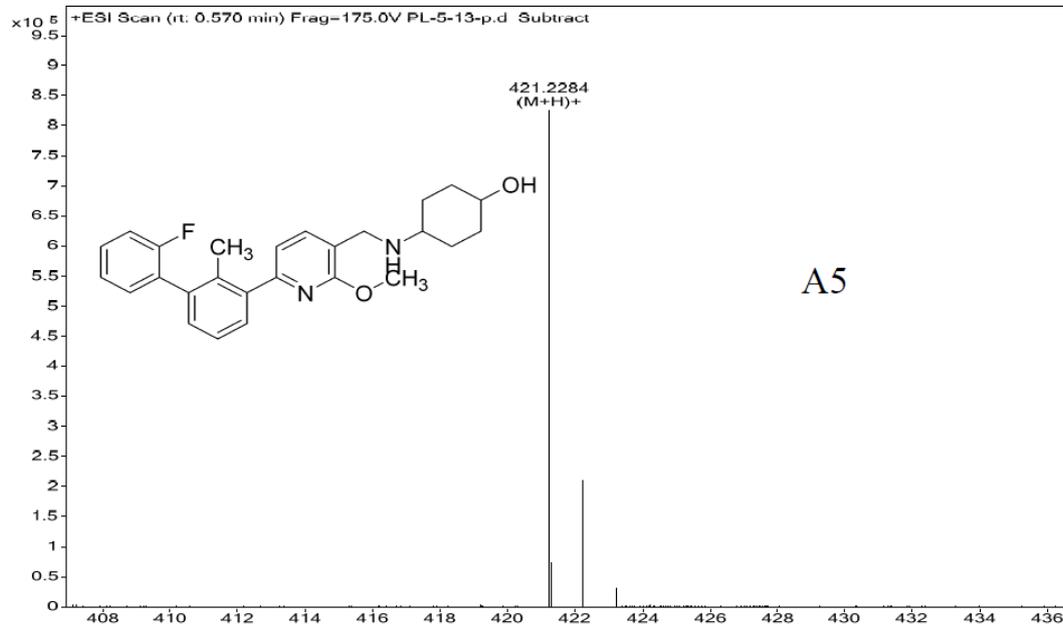


¹H NMR Spectra for Compound A5



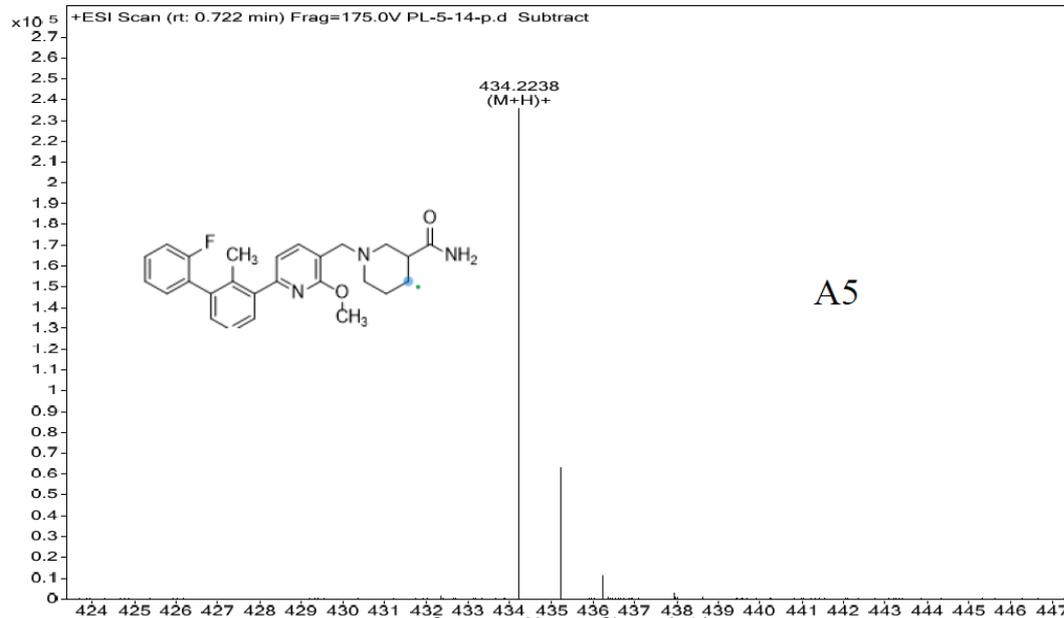
LCMS Spectra for Compound A5

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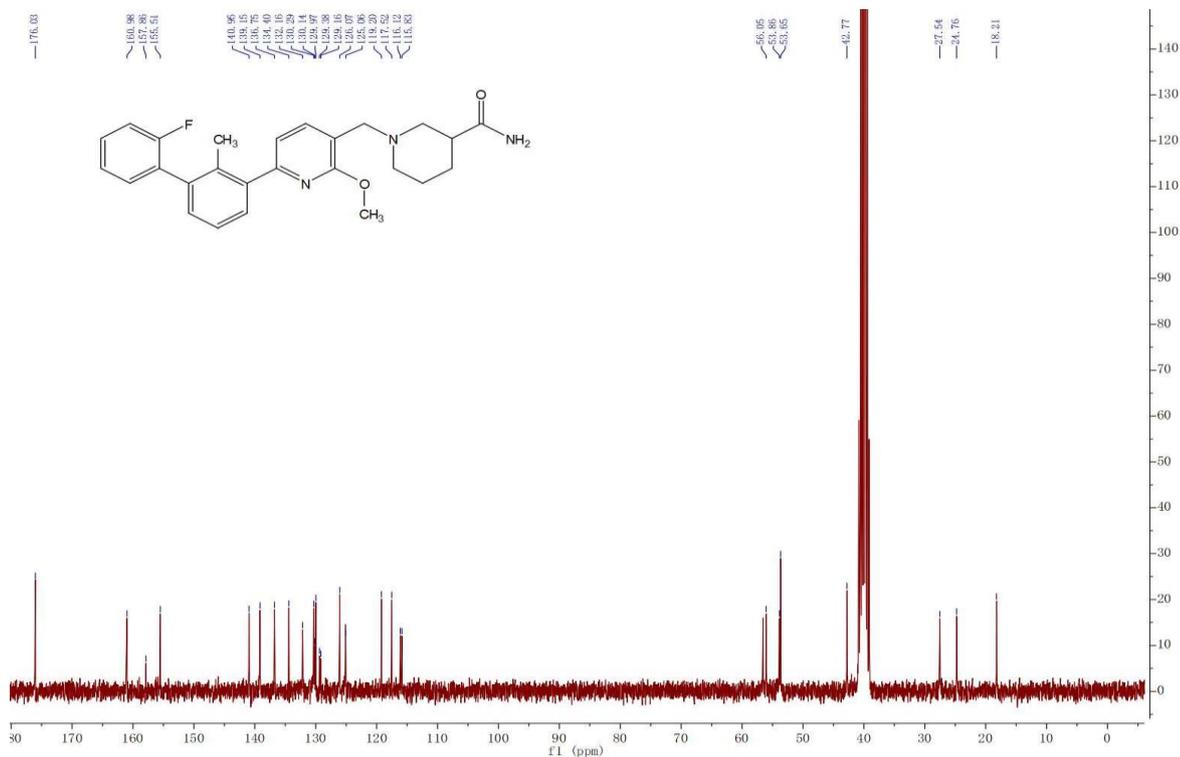


¹³C NMR Spectra for Compound A5

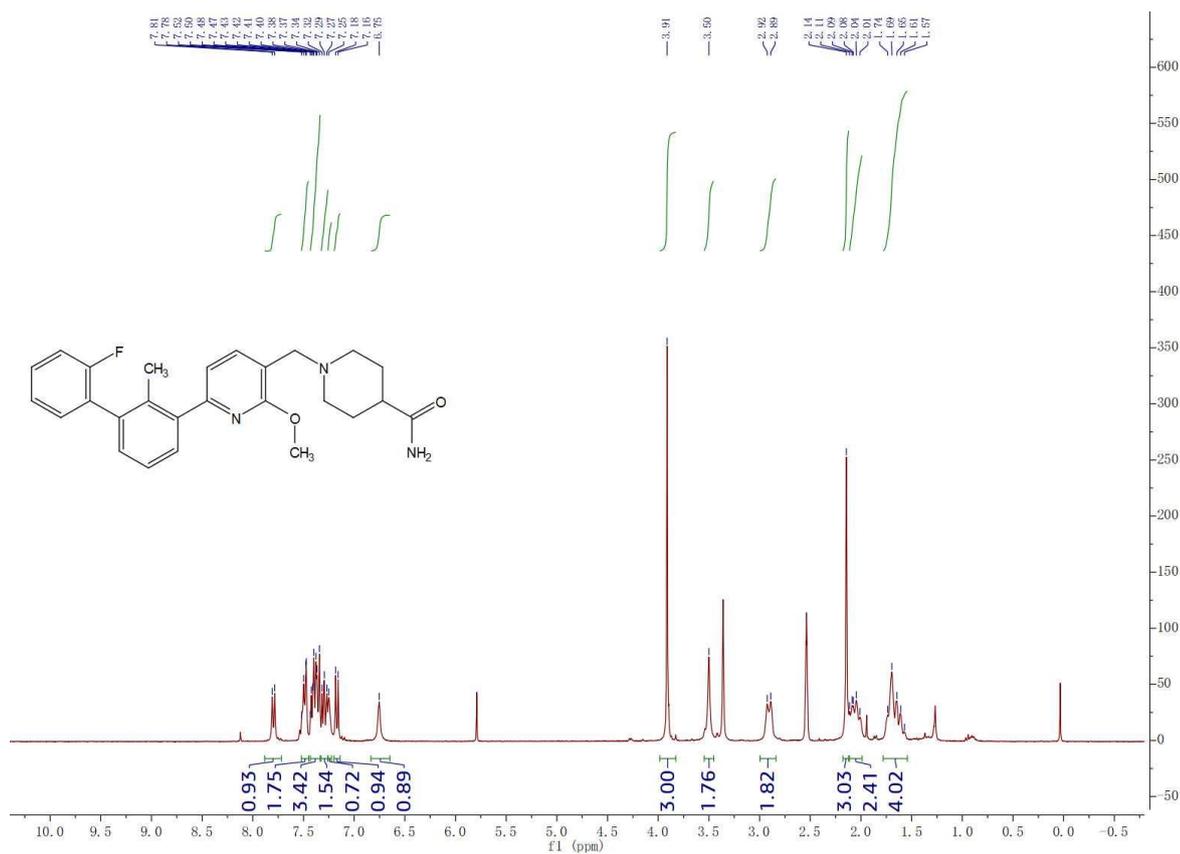
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¹³C NMR Spectra for Compound A6

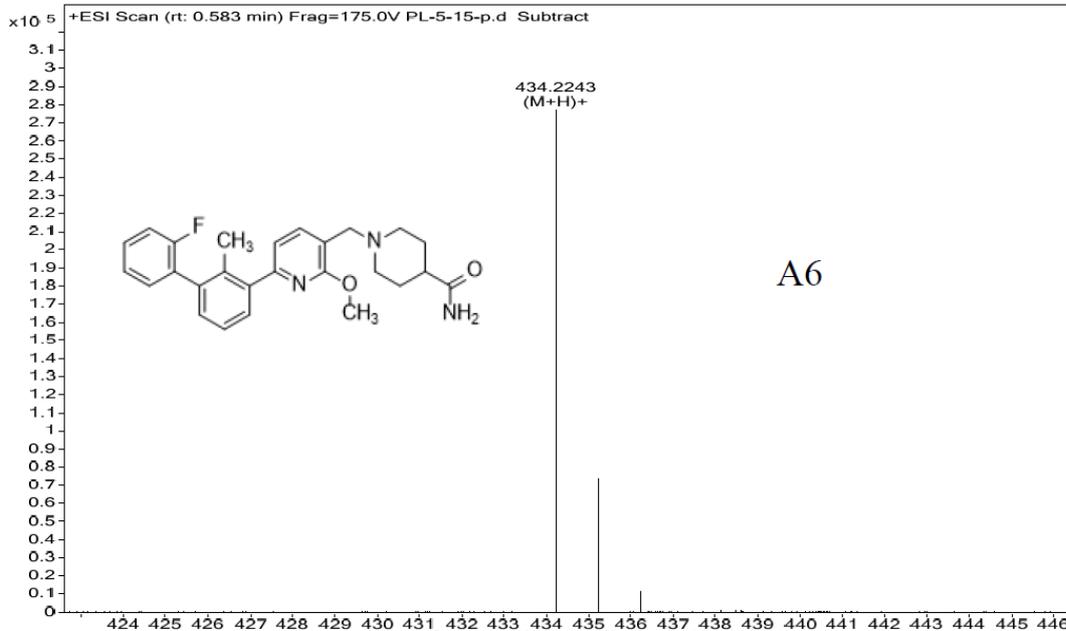


¹H NMR Spectra for Compound A7

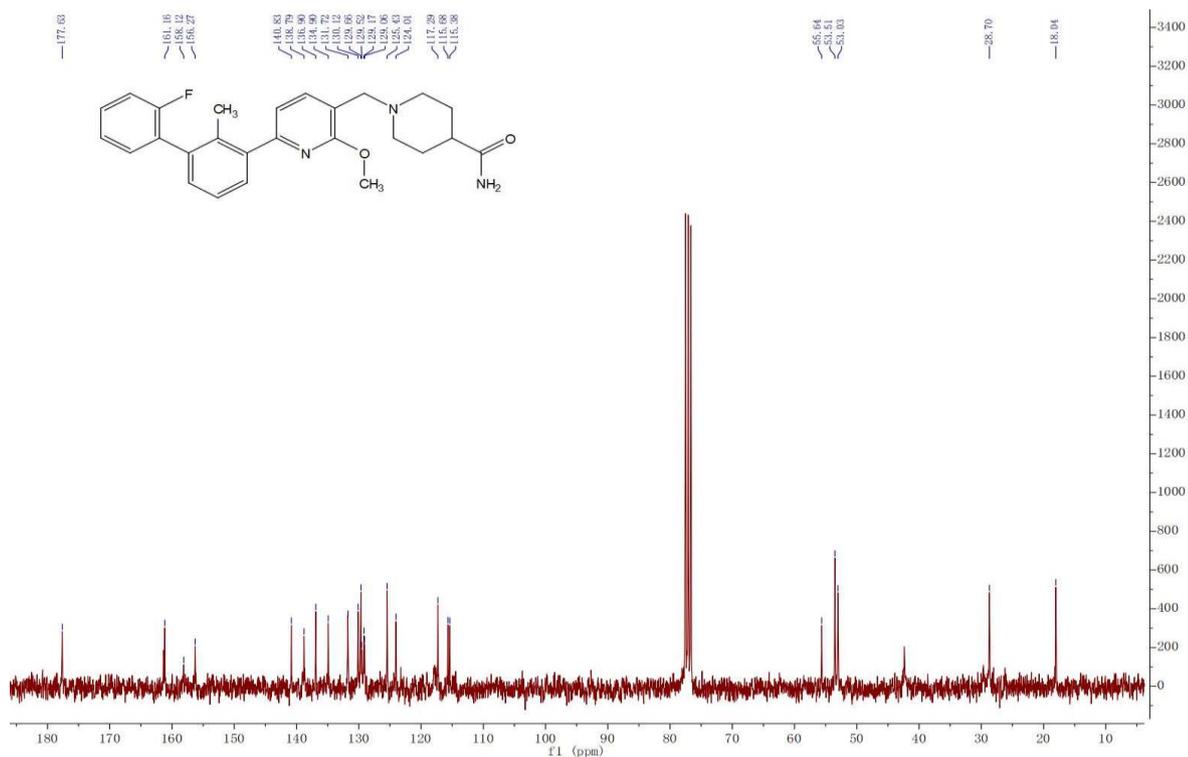


LCMS Spectra for Compound A7

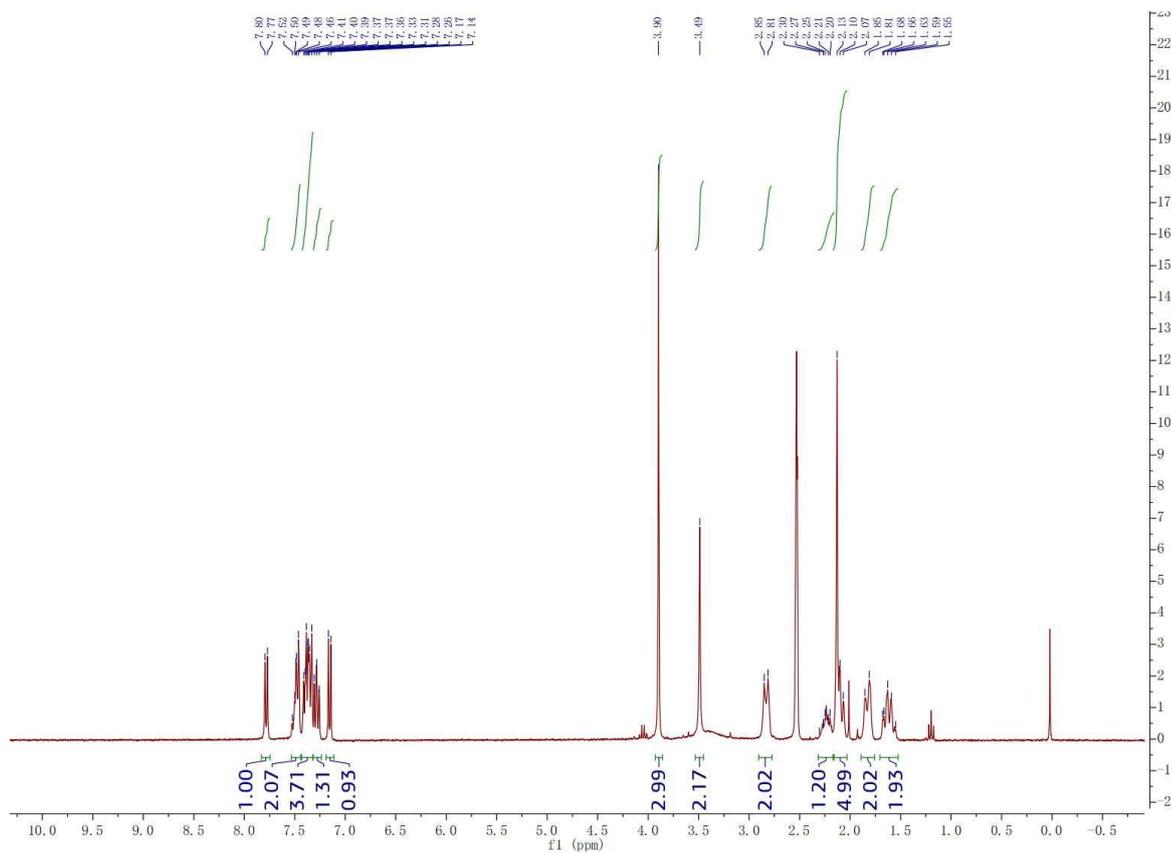
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¹³C NMR Spectra for Compound A7

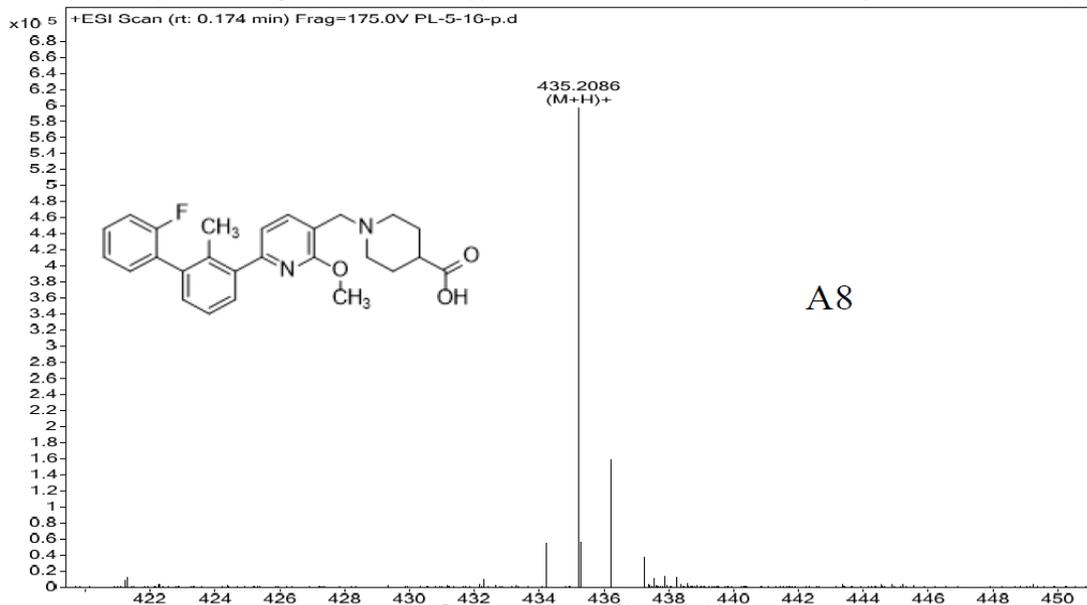


¹H NMR Spectra for Compound A8

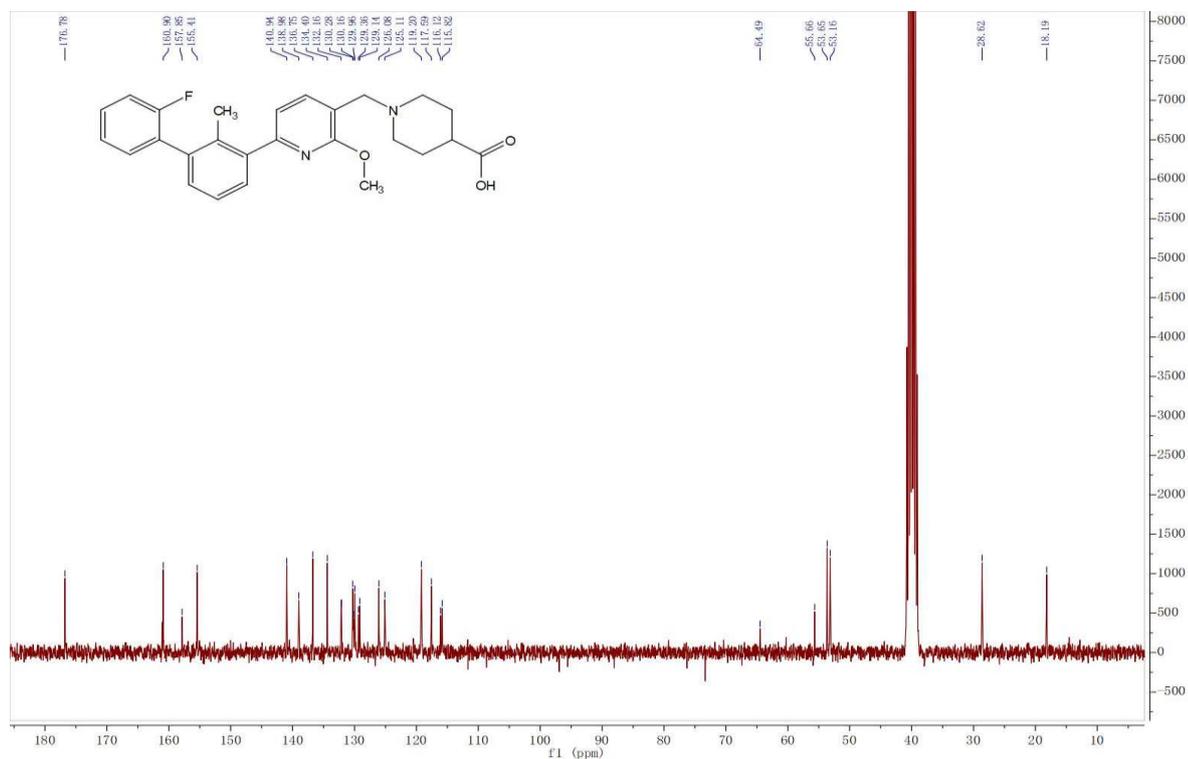


LCMS Spectra for Compound A8

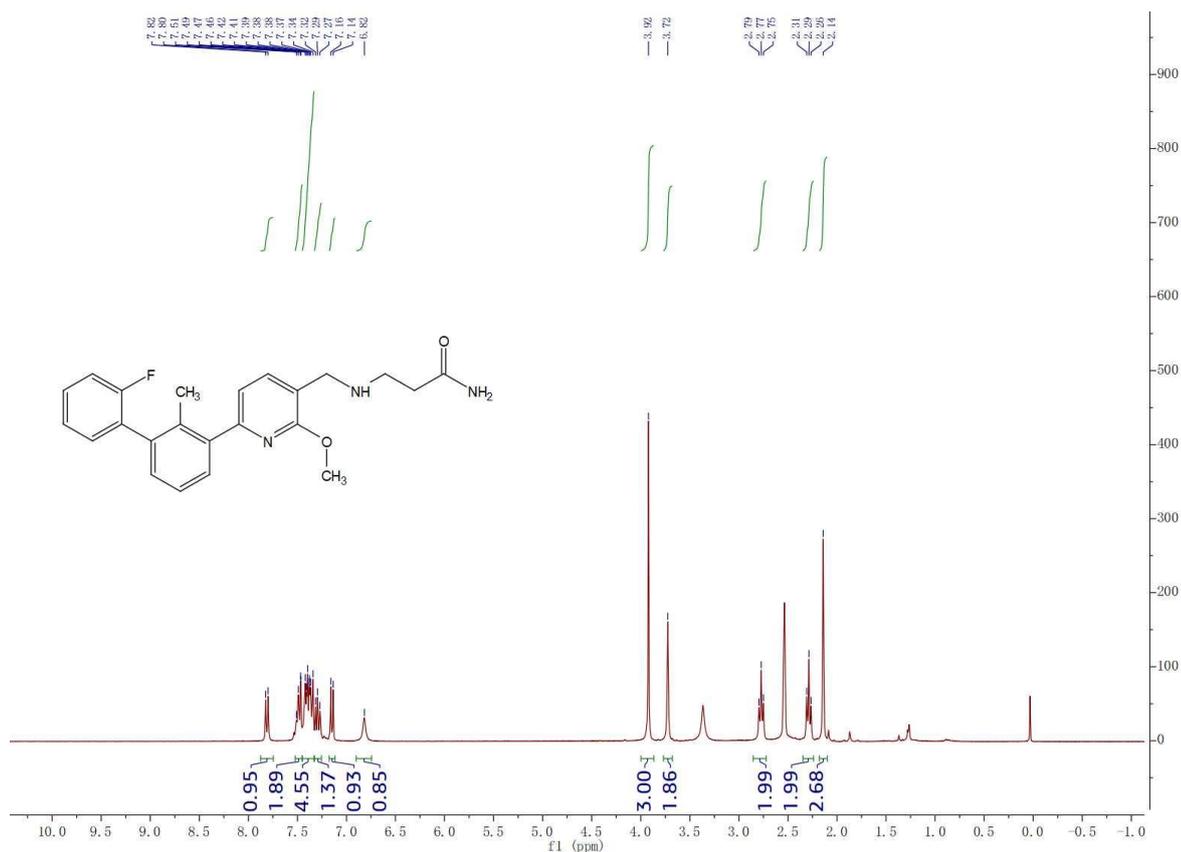
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¹³C NMR Spectra for Compound A8

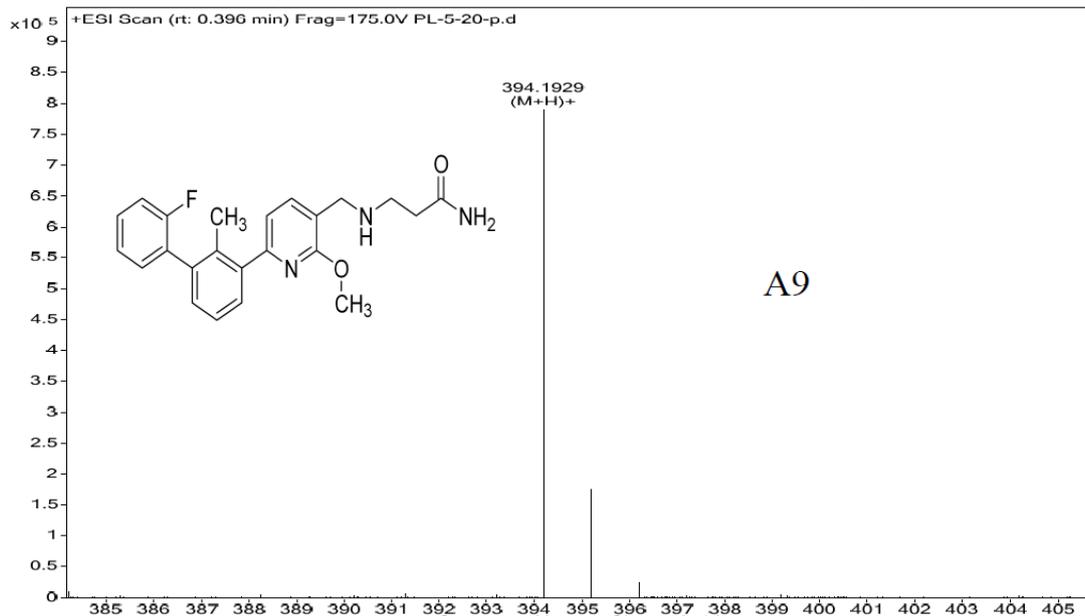


¹H NMR Spectra for Compound A9

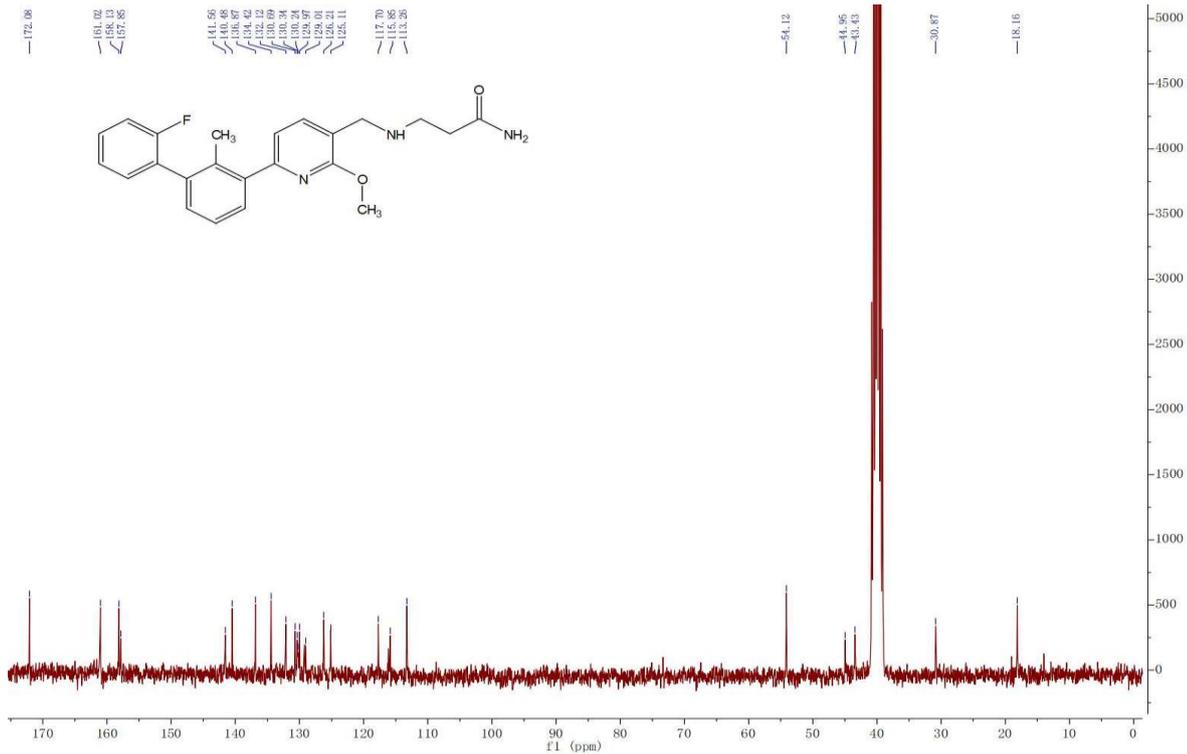


LCMS Spectra for Compound A9

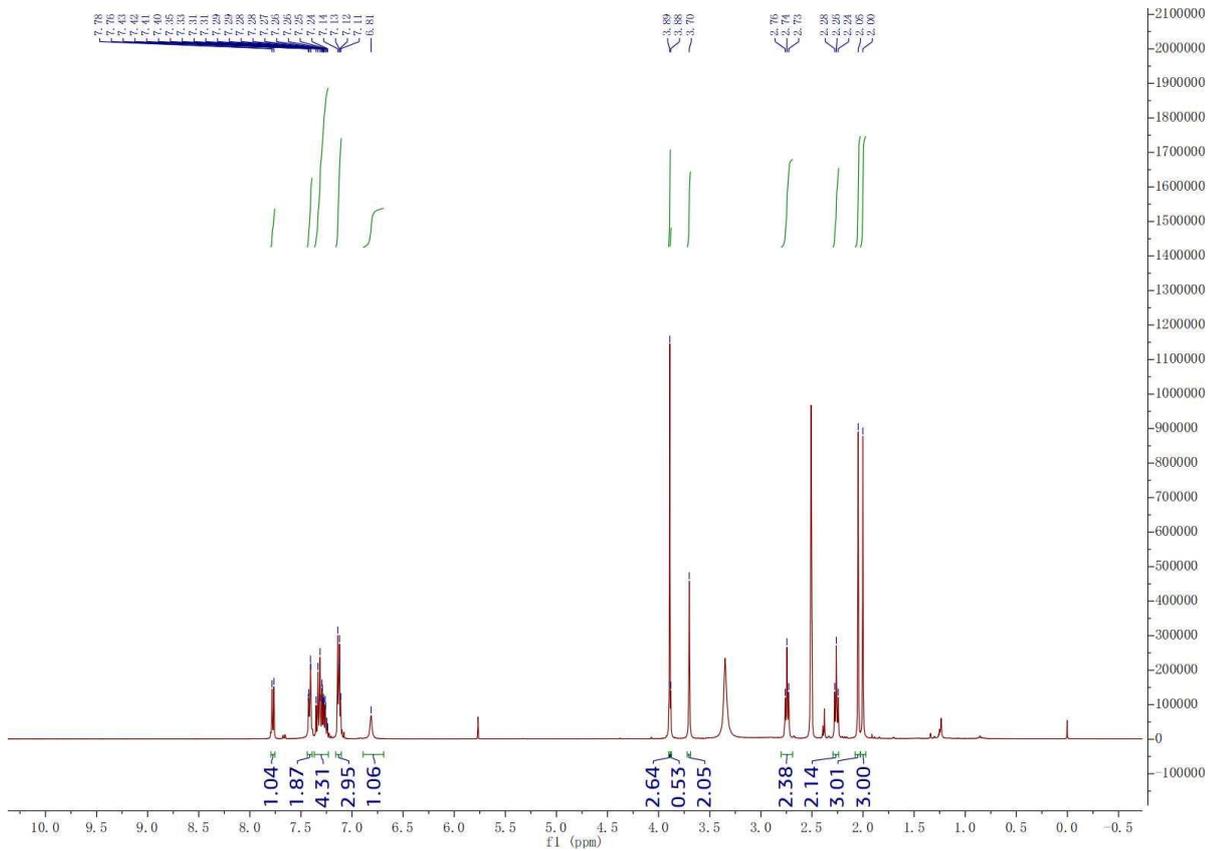
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¹³C NMR Spectra for Compound A9

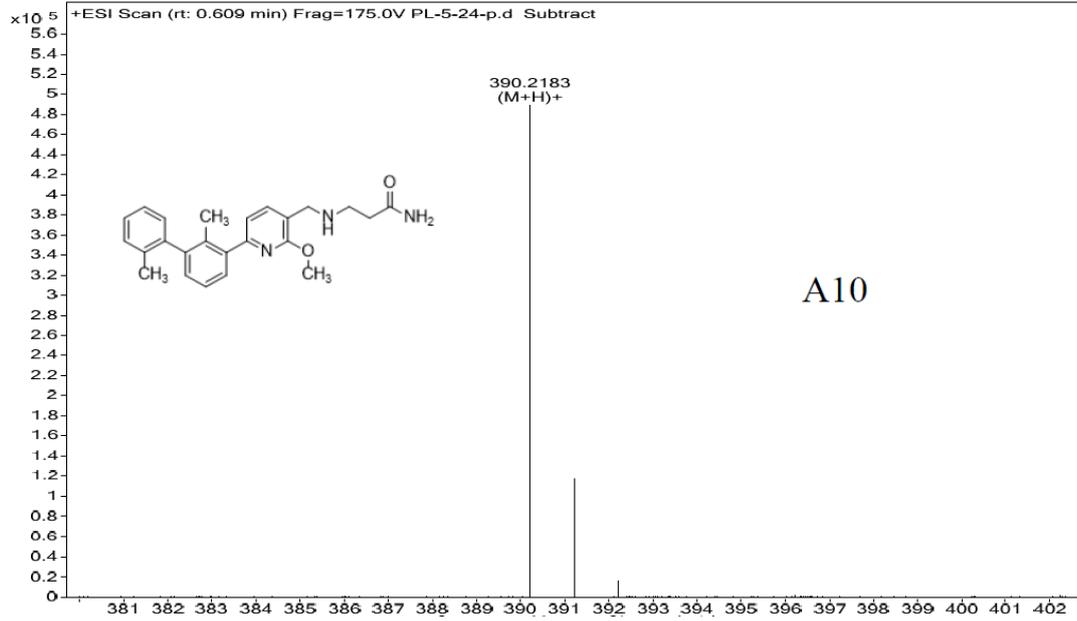


¹H NMR Spectra for Compound A10

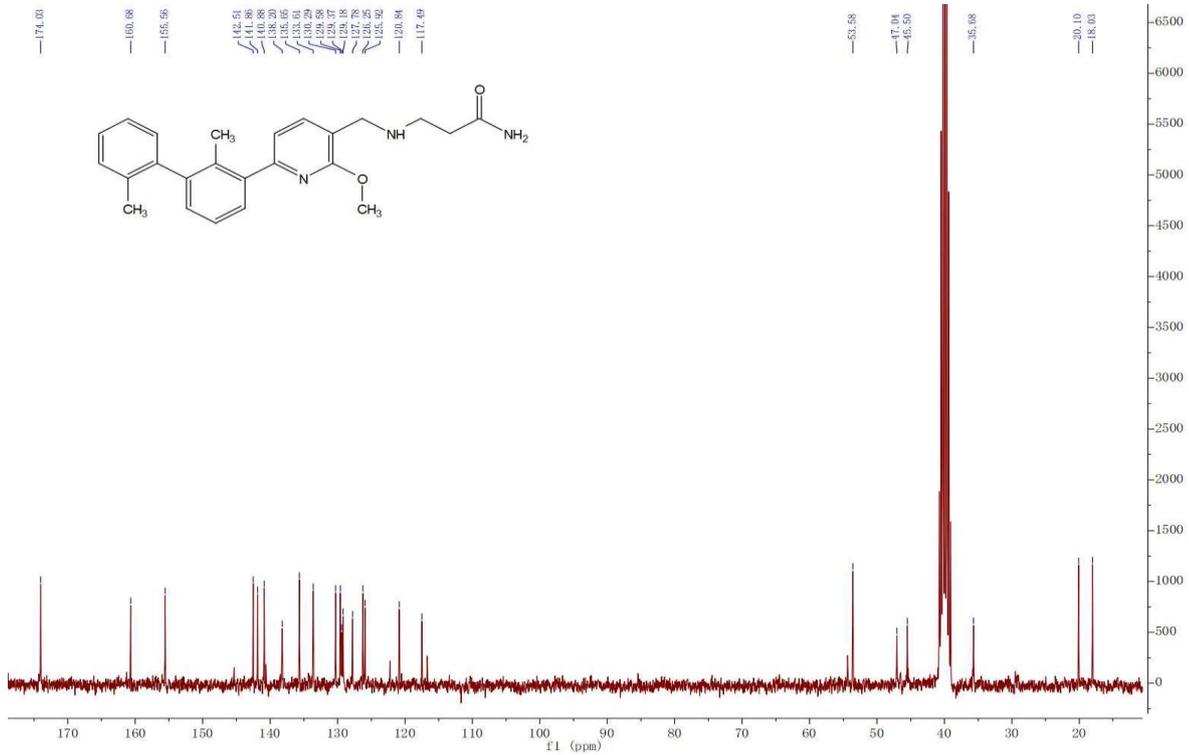


LCMS Spectra for Compound A10

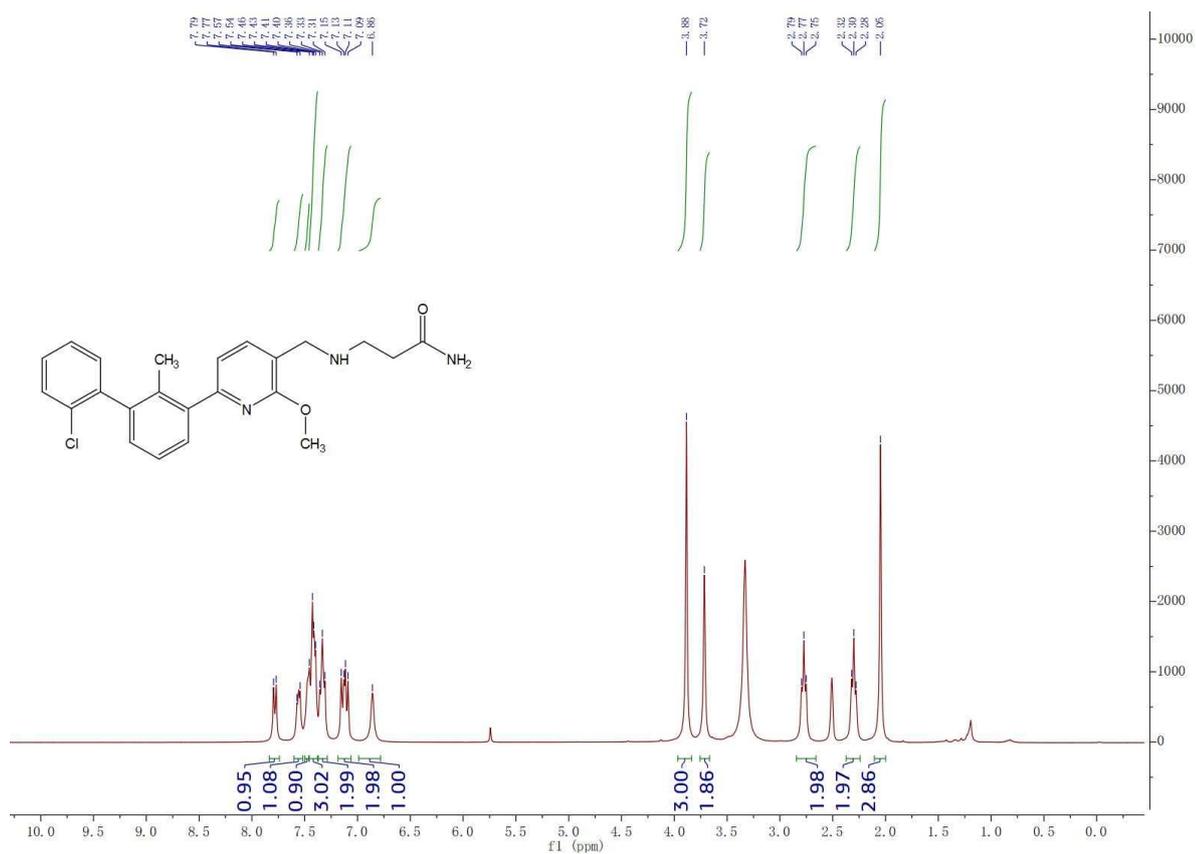
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¹³C NMR Spectra for Compound A10

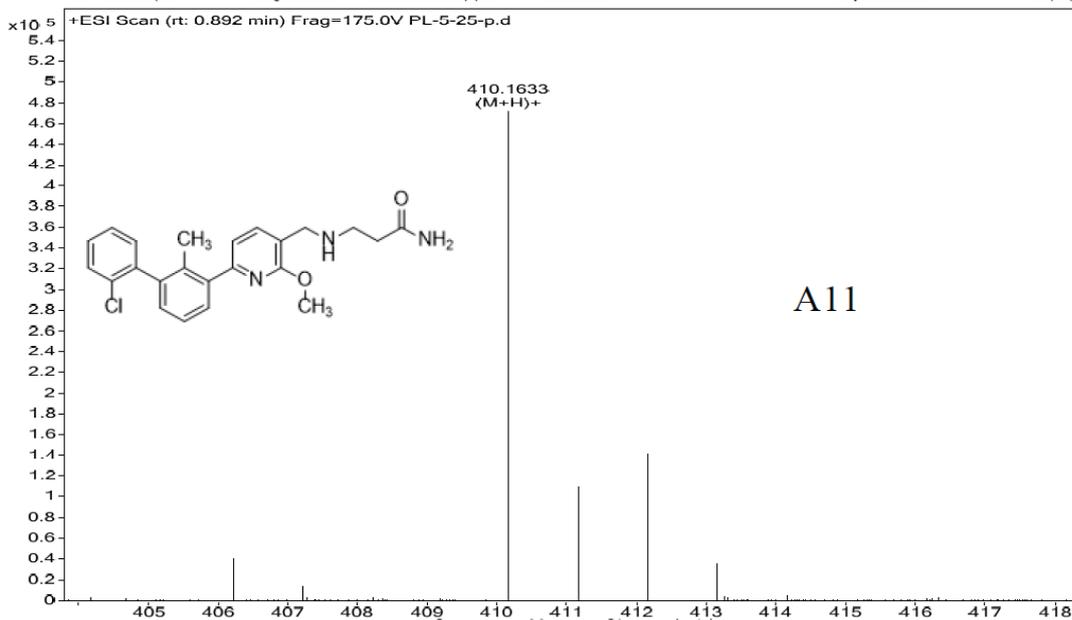


¹H NMR Spectra for Compound A11

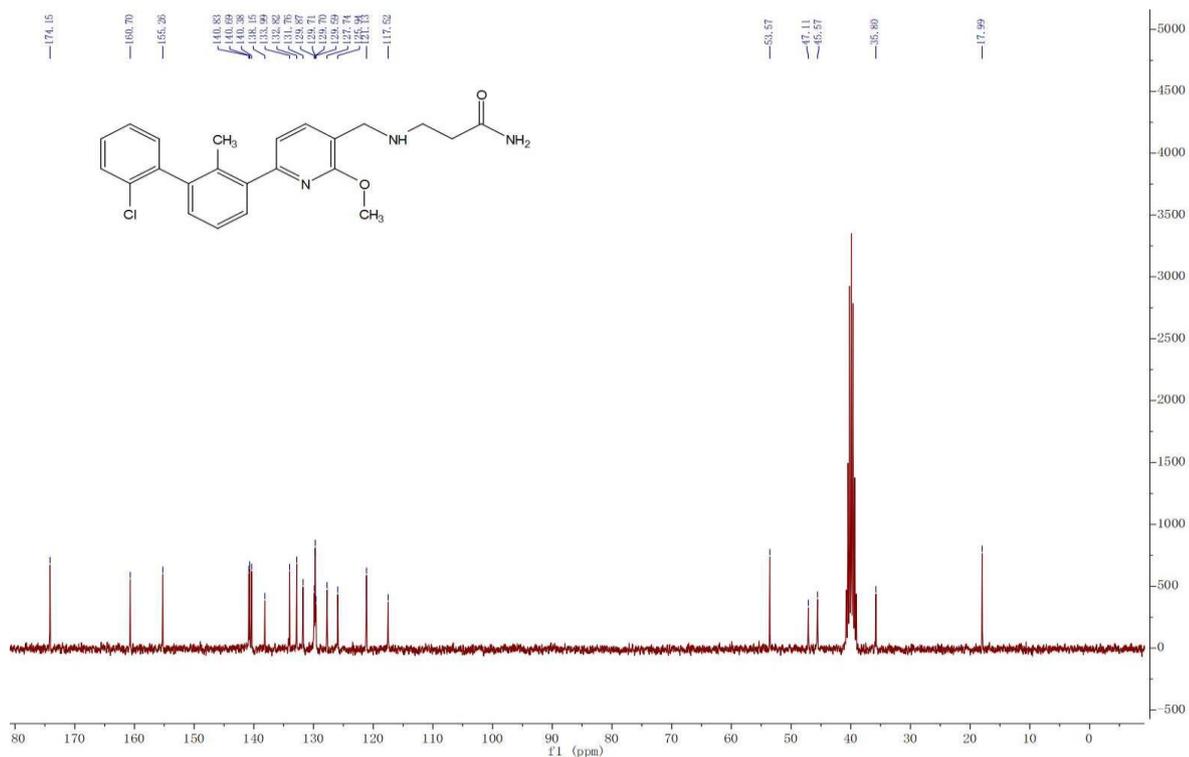


LCMS Spectra for Compound A11

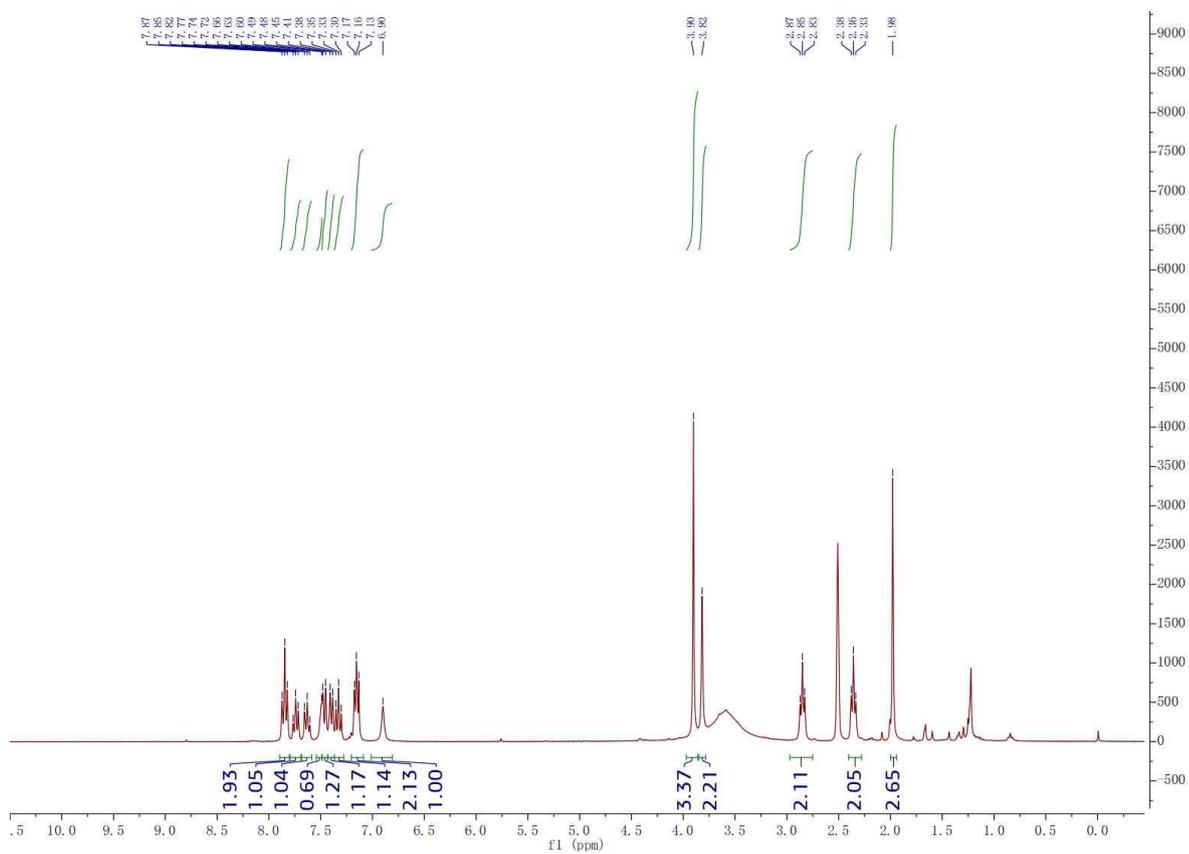
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¹³C NMR Spectra for Compound A11

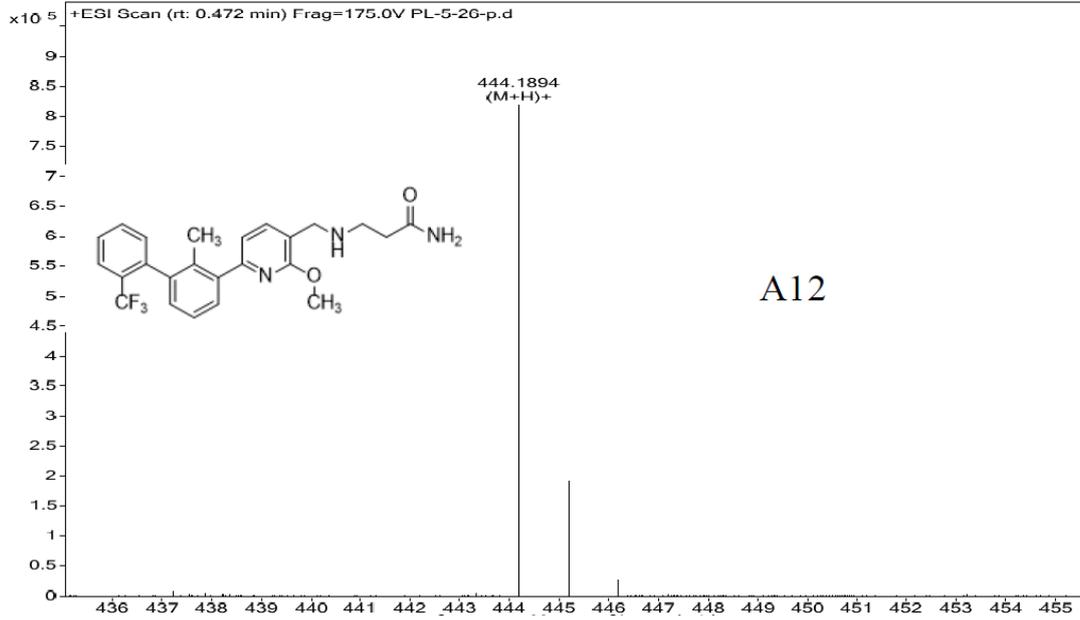


¹H NMR Spectra for Compound A12

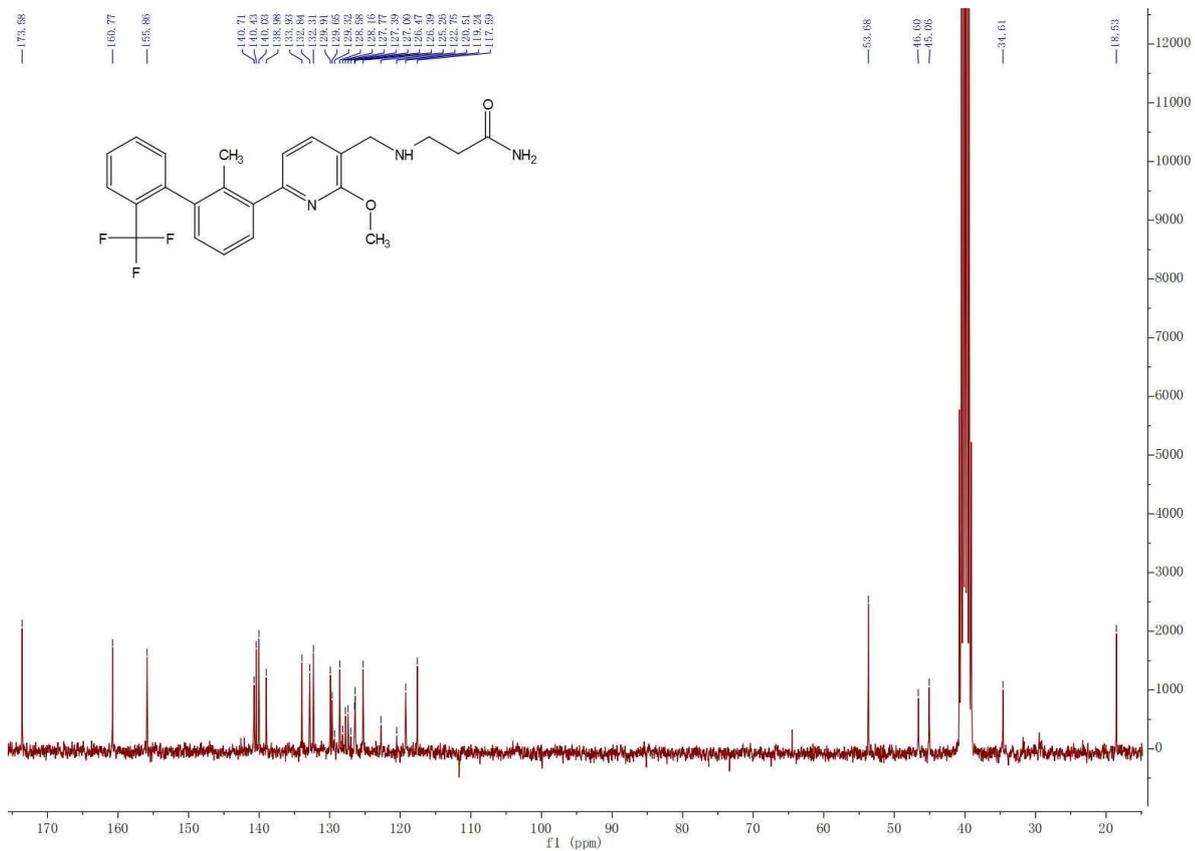


LCMS Spectra for Compound A12

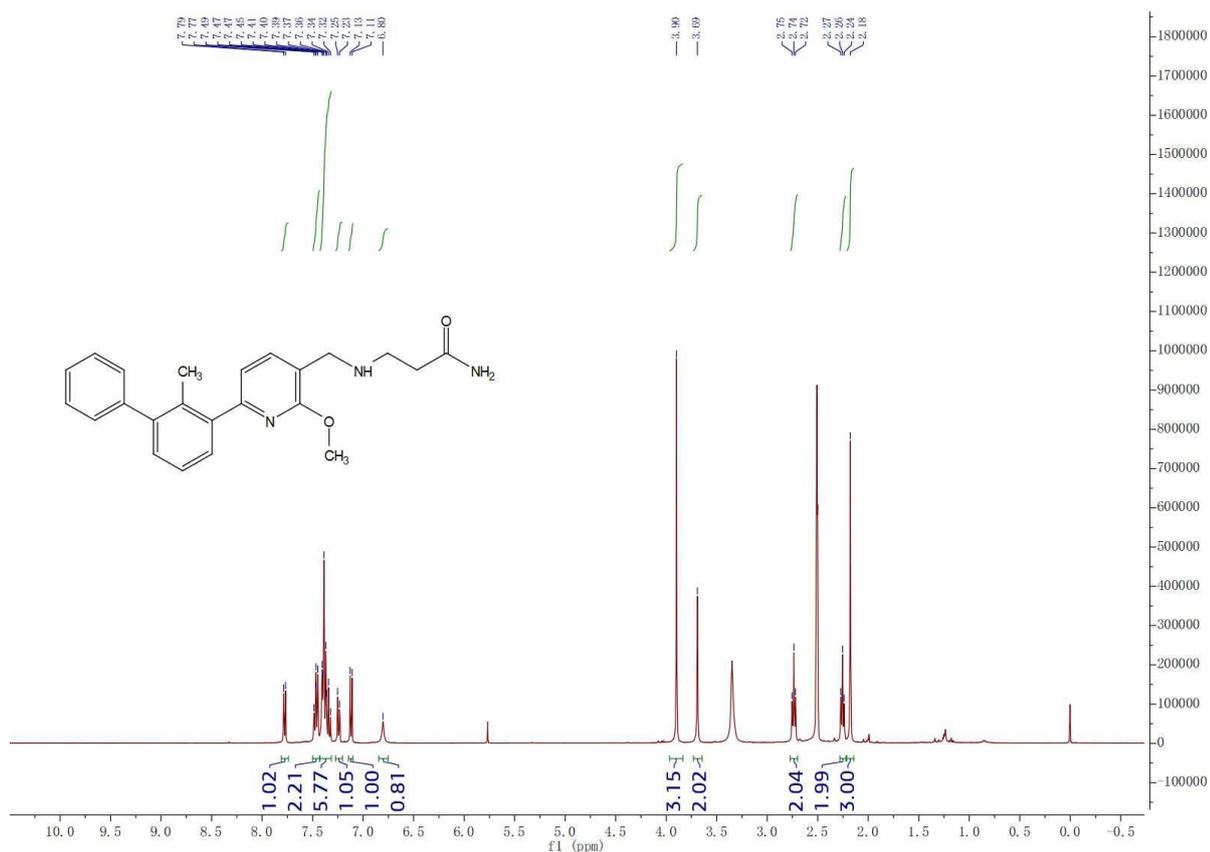
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¹³C NMR Spectra for Compound A12

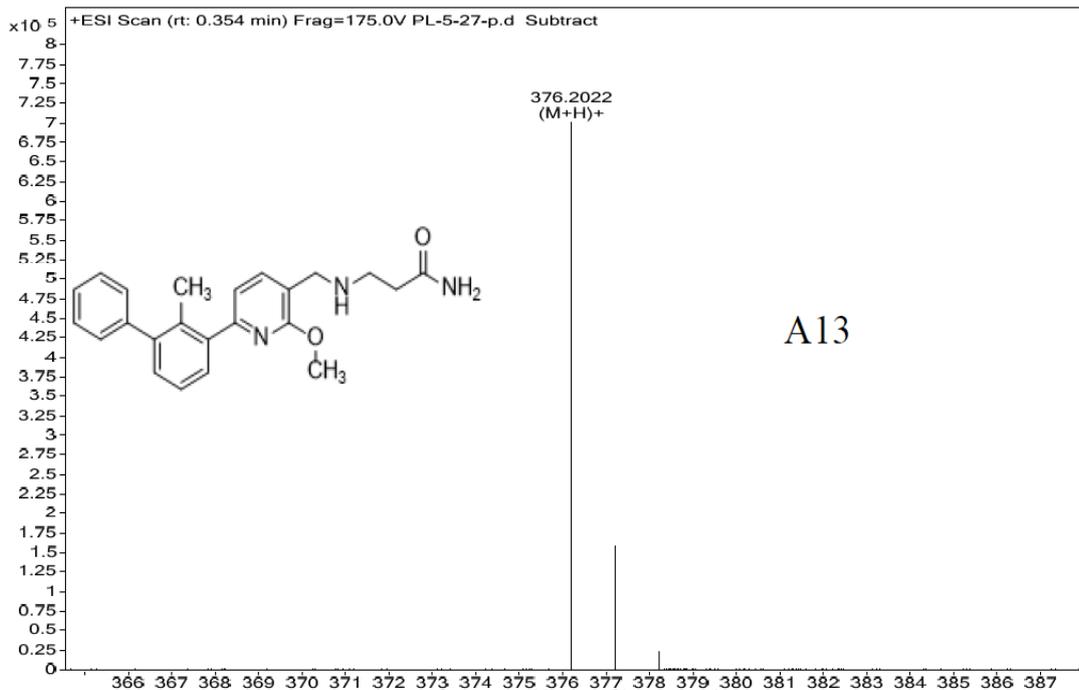


¹H NMR Spectra for Compound A13



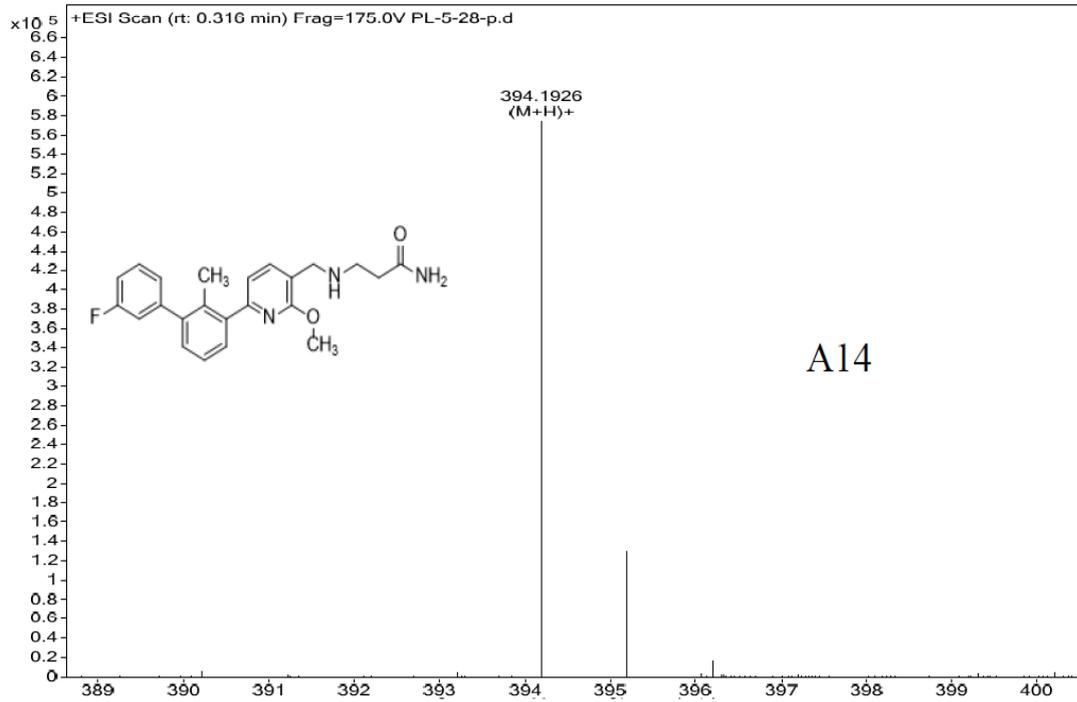
LCMS Spectra for Compound A13

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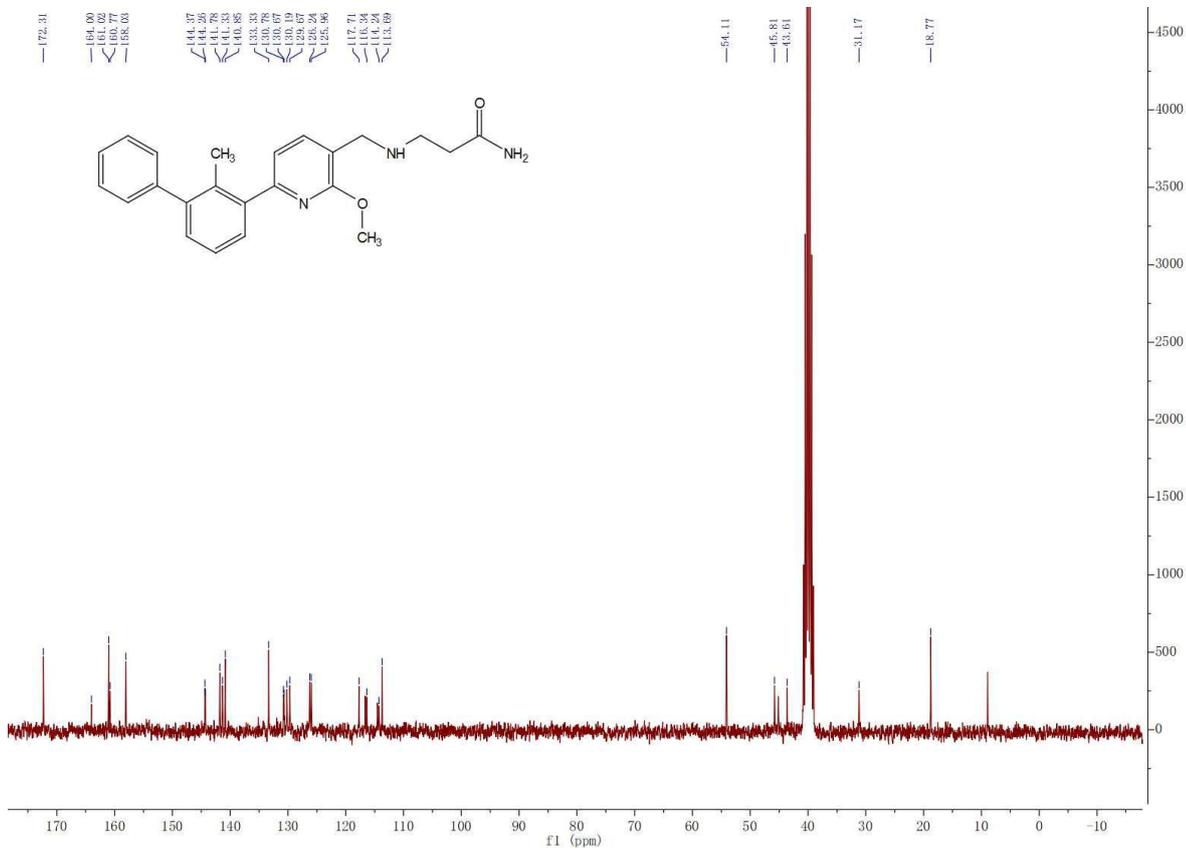


¹³C NMR Spectra for Compound A13

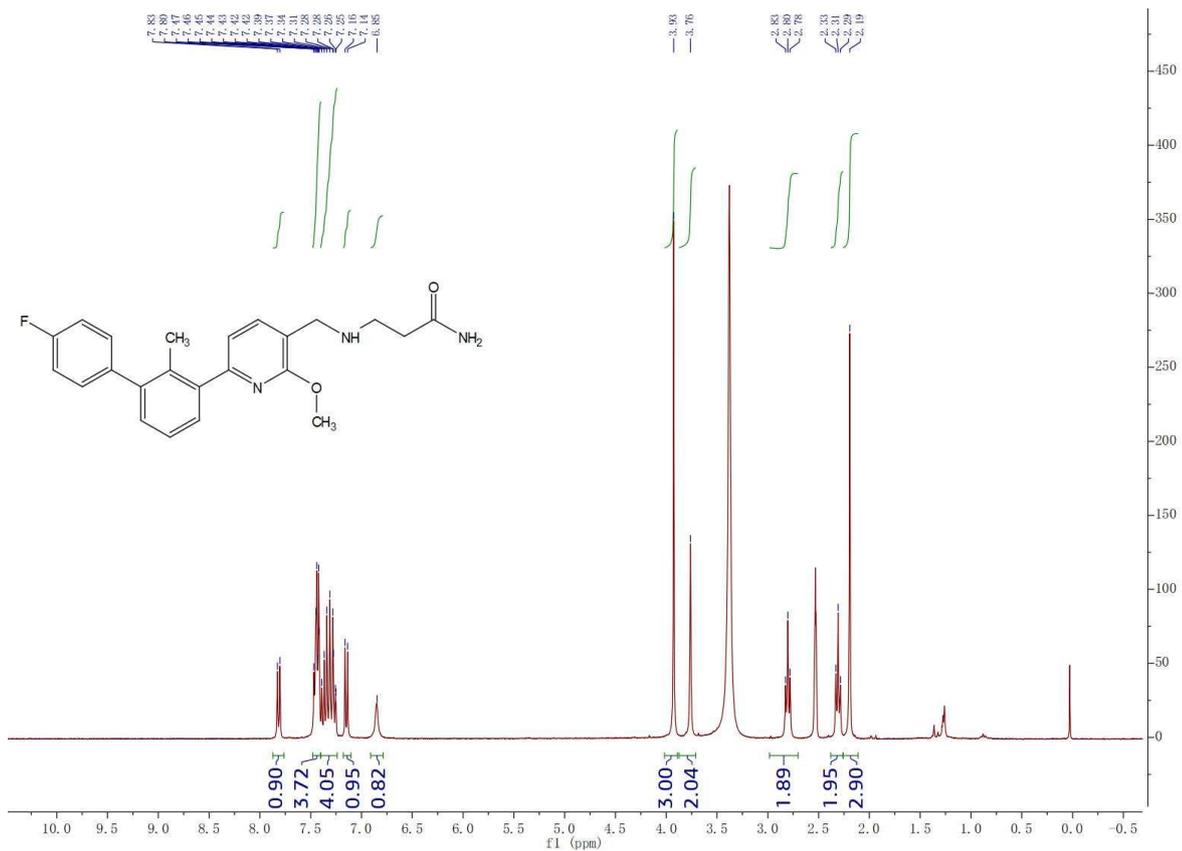
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¹³C NMR Spectra for Compound A14

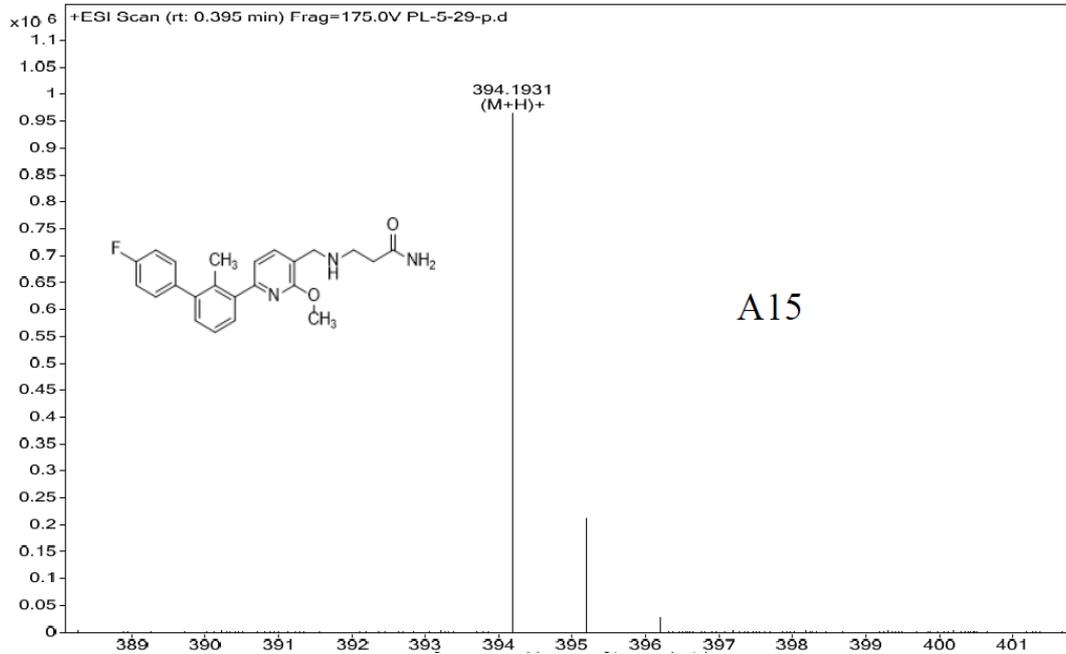


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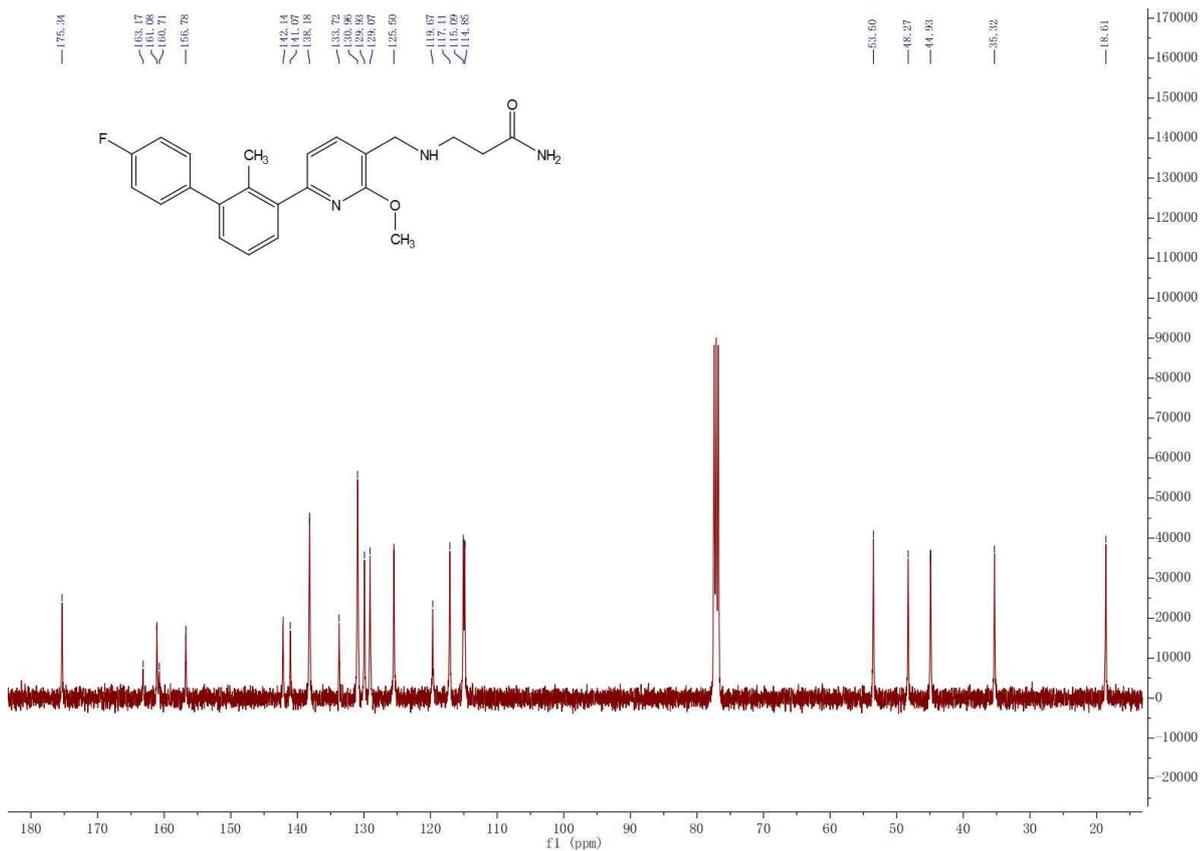


LCMS Spectra for Compound A15

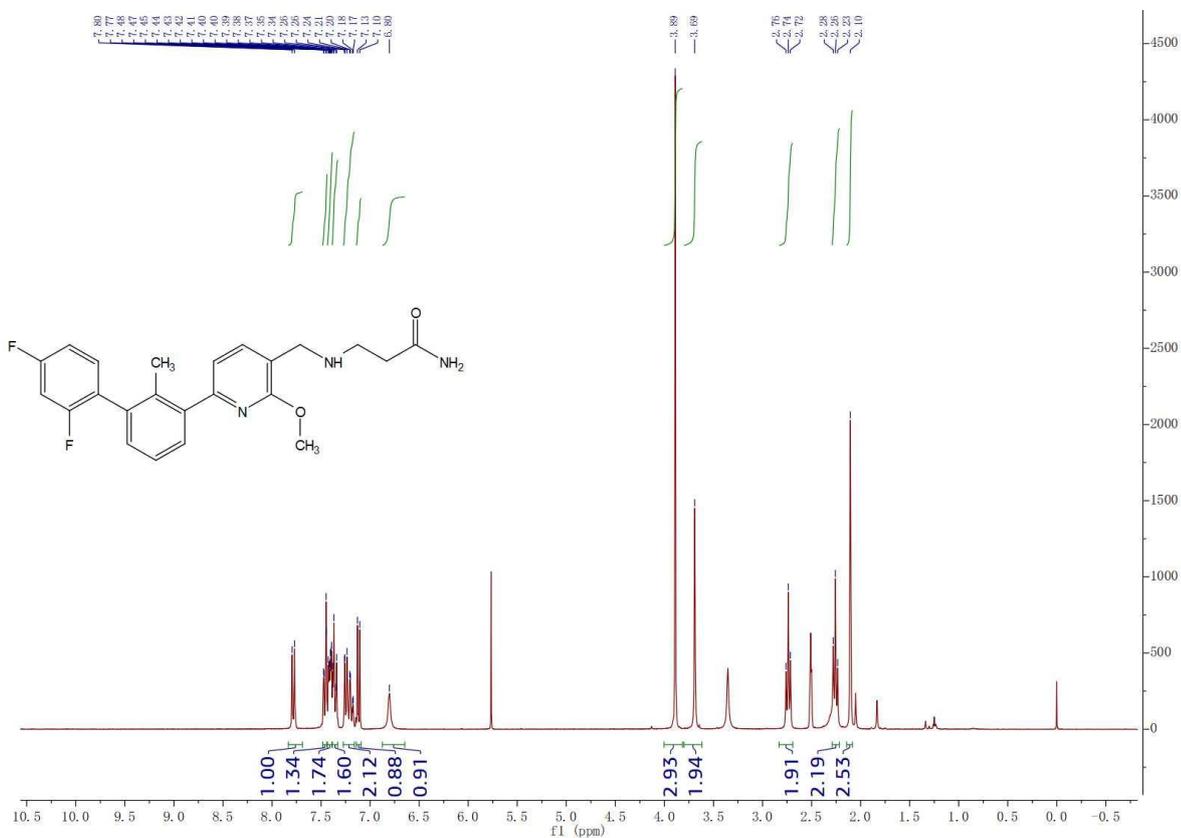
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¹³C NMR Spectra for Compound A15

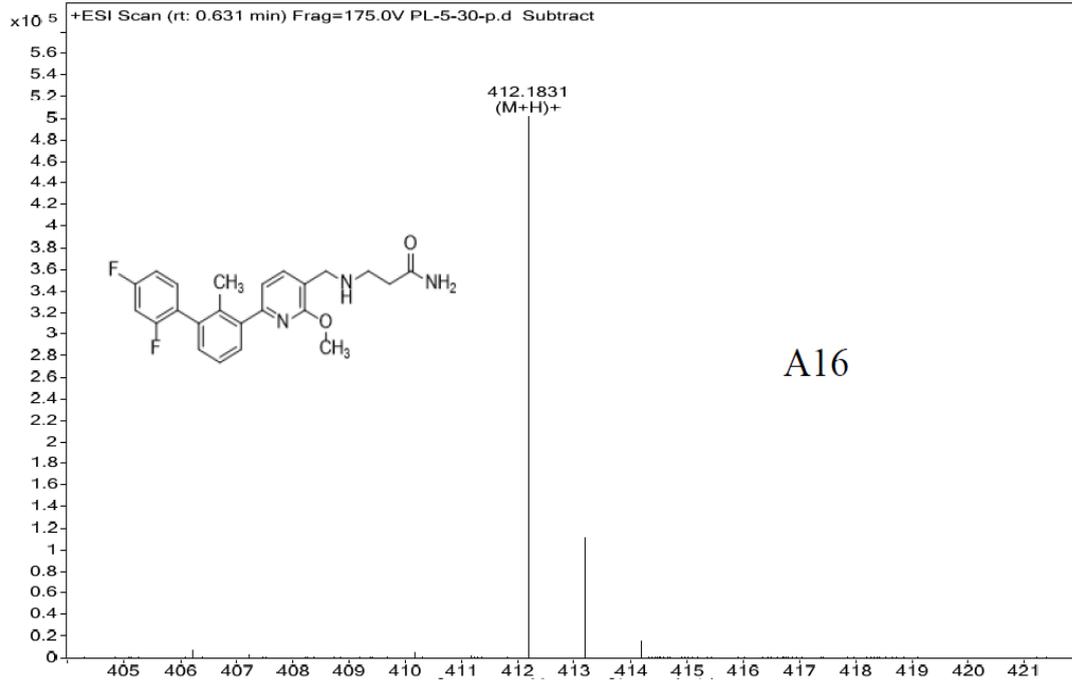


¹H NMR Spectra for Compound A16

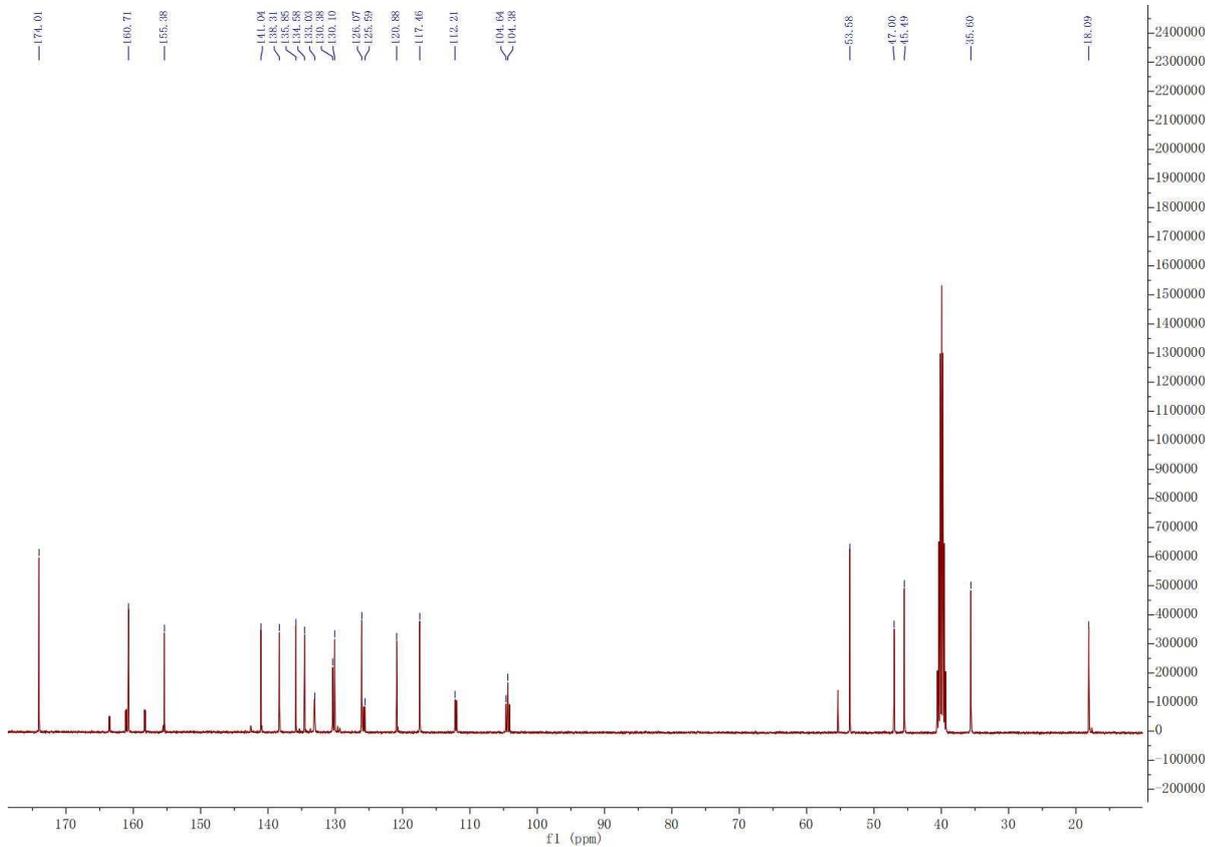


LCMS Spectra for Compound A16

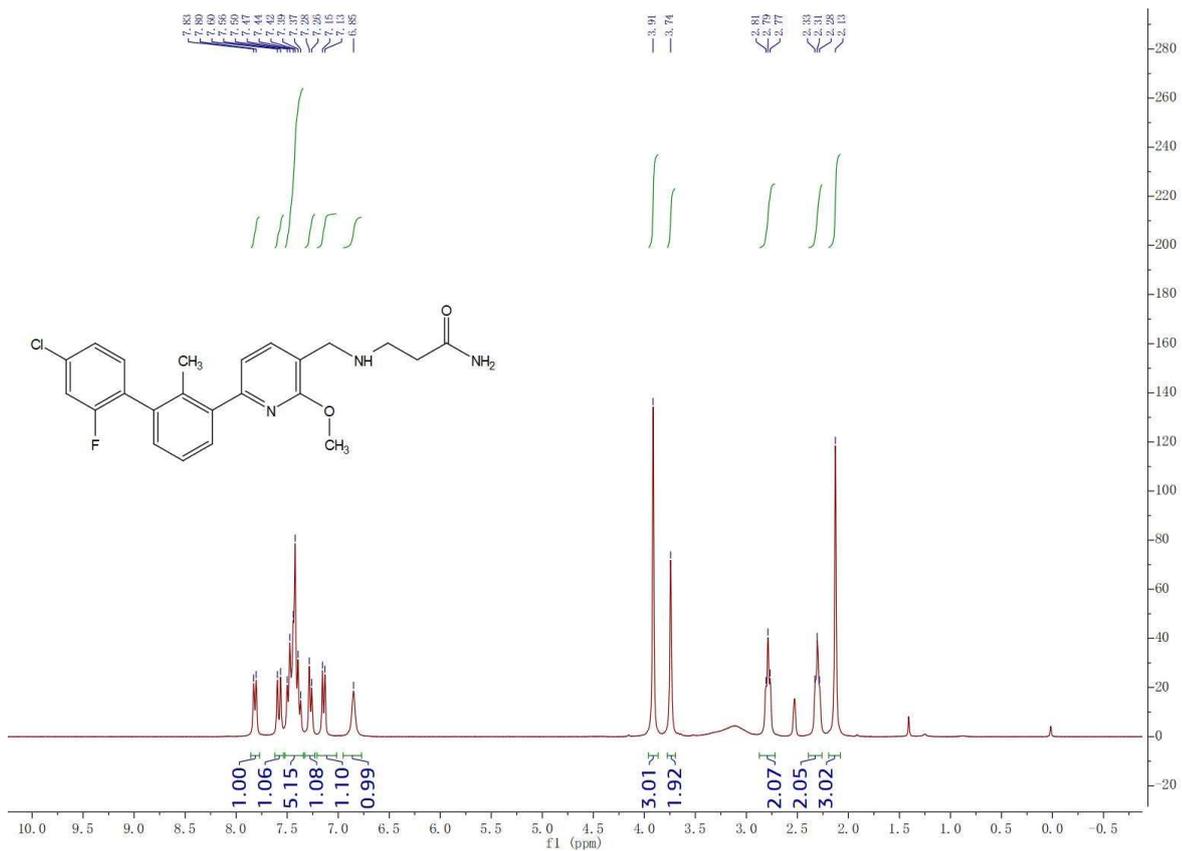
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¹³C NMR Spectra for Compound A16

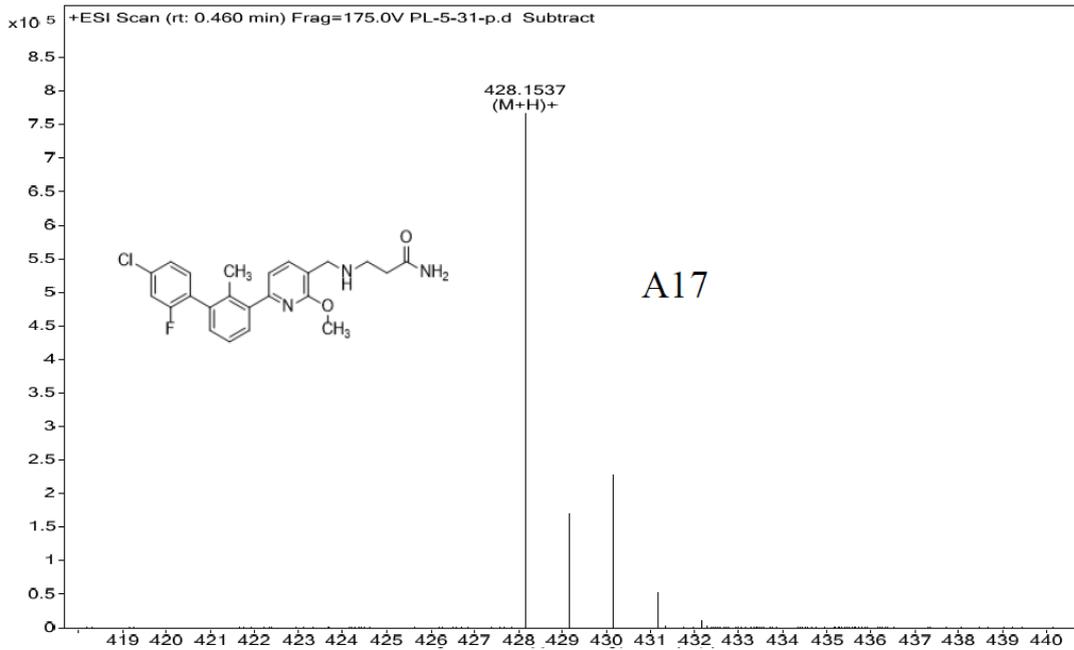


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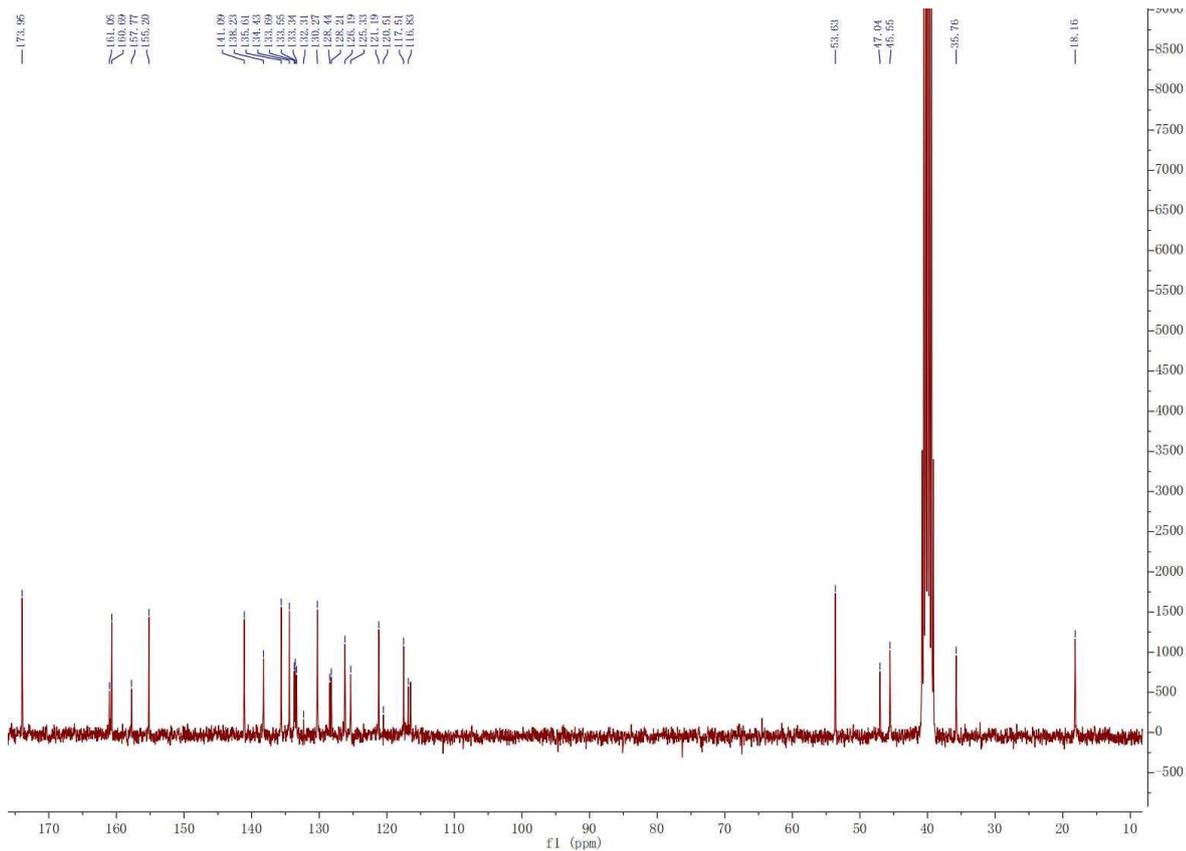


LCMS Spectra for Compound A17

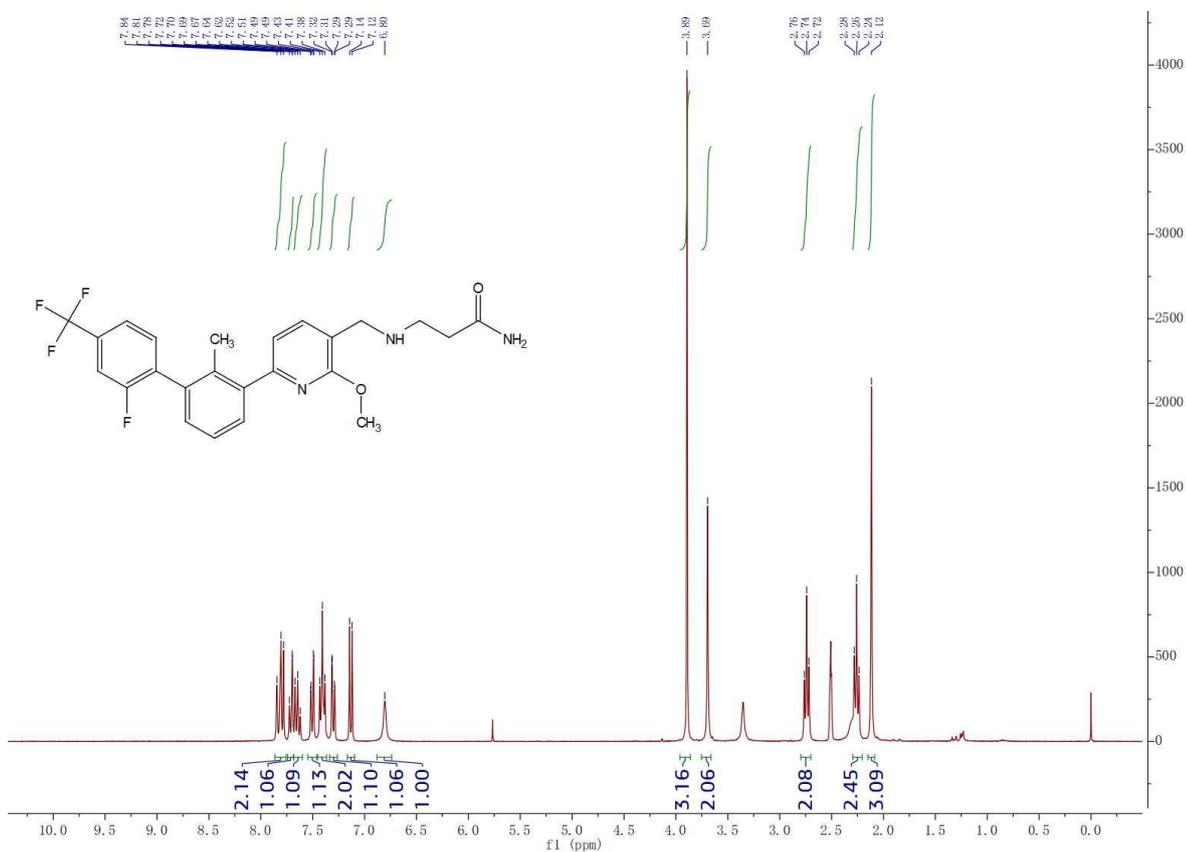
Sample Name	Position	p2e9	Instrument Name	Instrument 1	User Name	G6520B-PC\Admin
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¹³C NMR Spectra for Compound A17

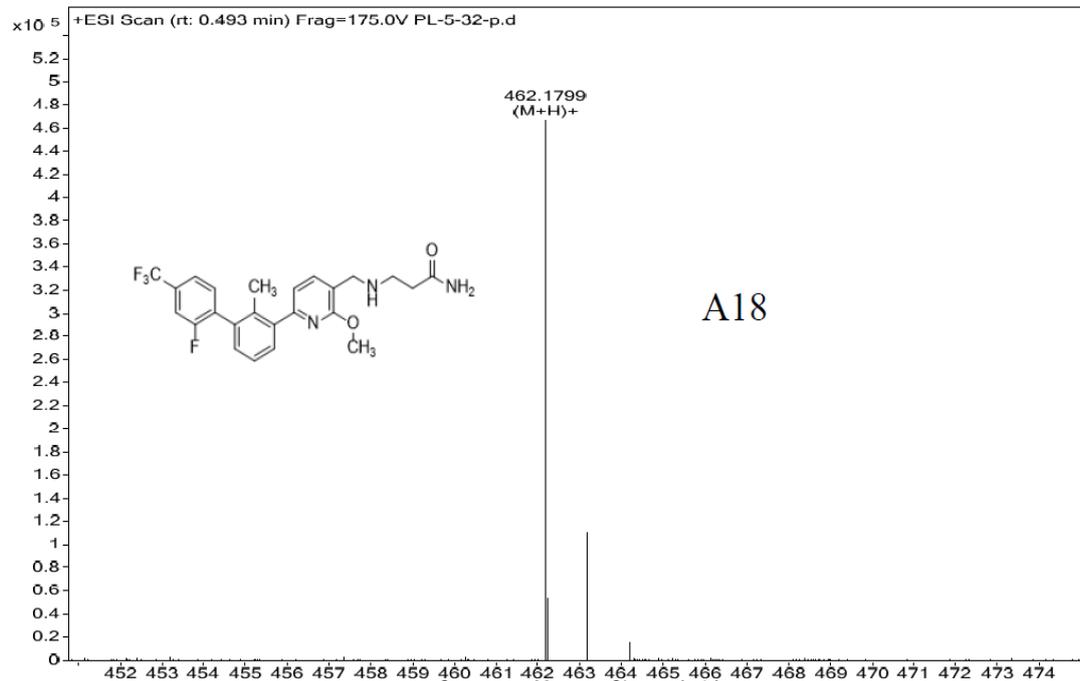


¹H NMR Spectra for Compound A18

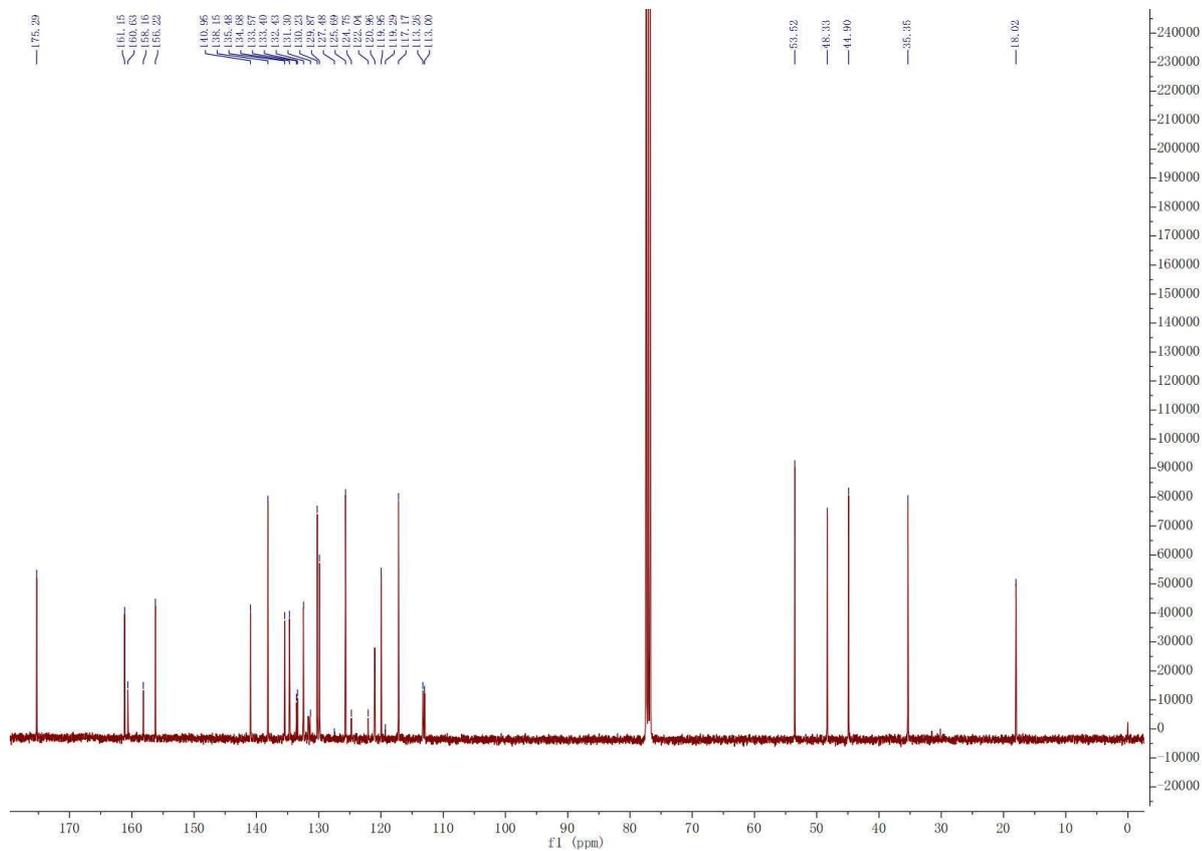


LCMS Spectra for Compound A18

Sample Name	Position	p2f1	Instrument Name	Instrument 1	User Name	G6520B-PCAdmin
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¹³C NMR Spectra for Compound A18



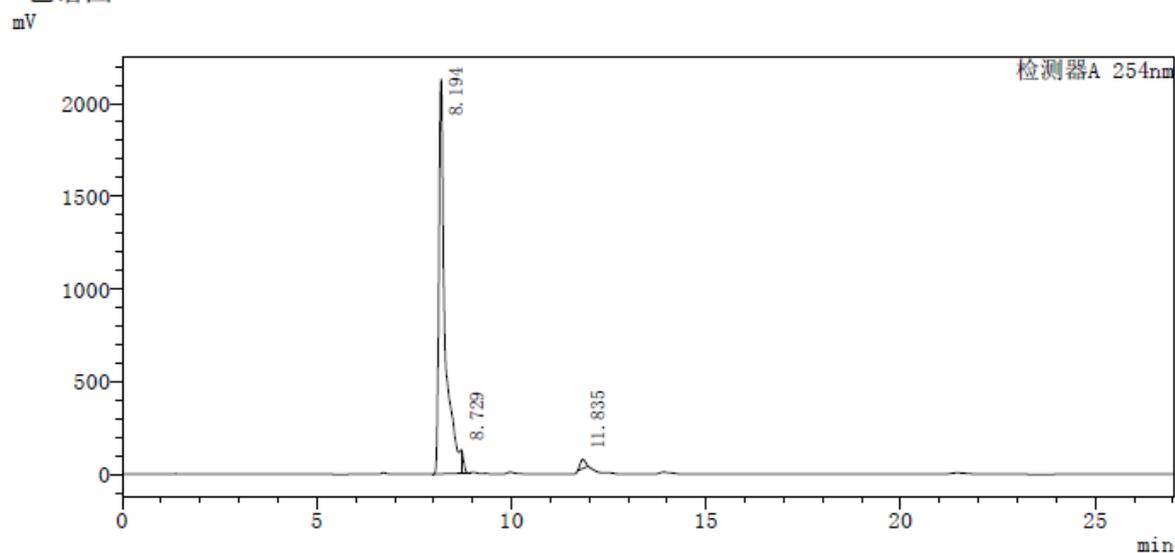
III. HPLC Spectroscopic data for A9



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进样体积 : 10 uL
分析日期 : 2021/1/14 15:34:51
处理日期 : 2021/1/14 16:01:59
样品类型 : 未知
分析者 : System Administrator
处理者 : System Administrator

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<峰表>

检测器A 254nm

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