

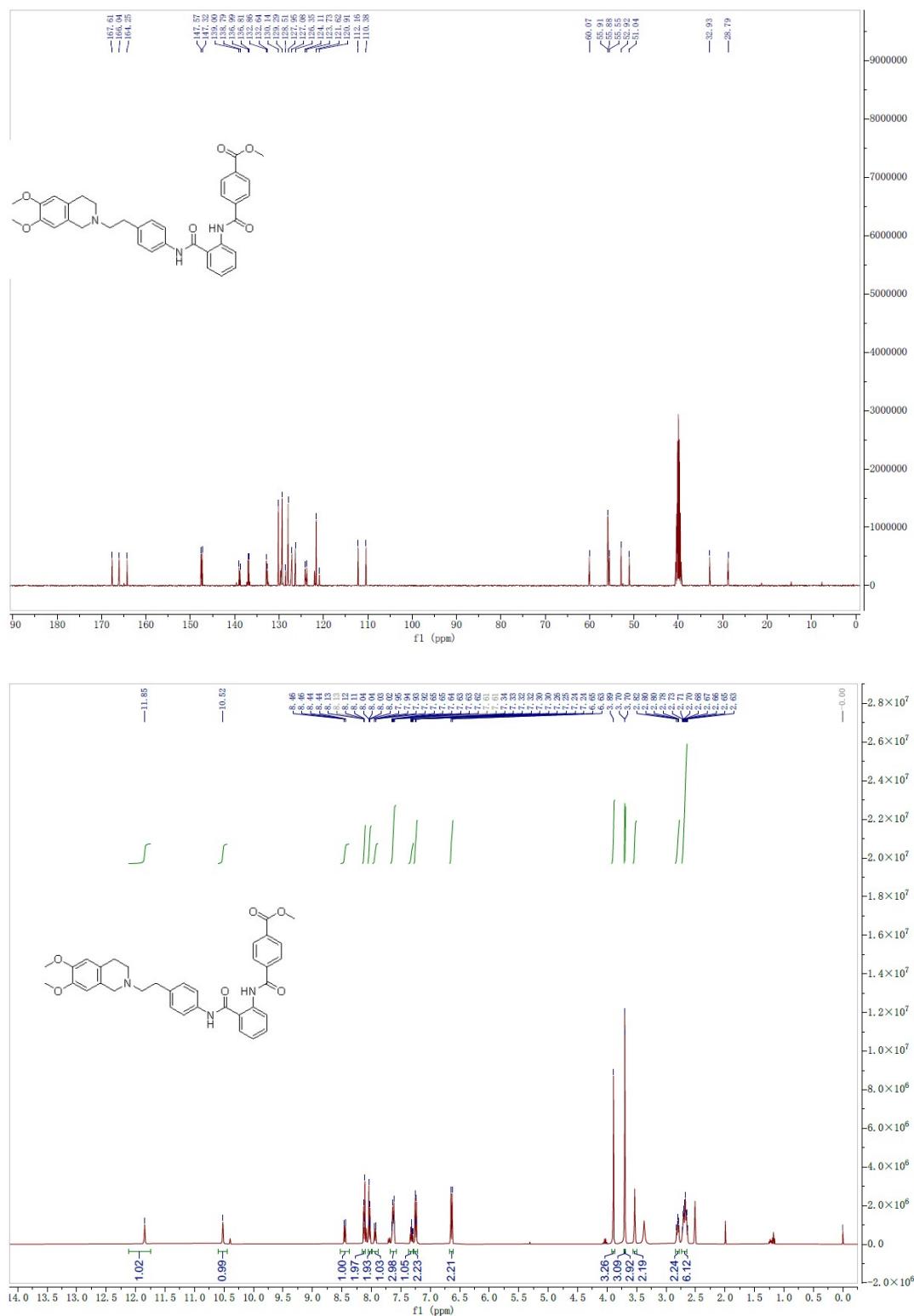
Supporting Information

Synthesis and evaluation of WK-X-34 derivatives as P-glycoprotein (P-gp/ABCB1) inhibitors for reversing multidrug resistance

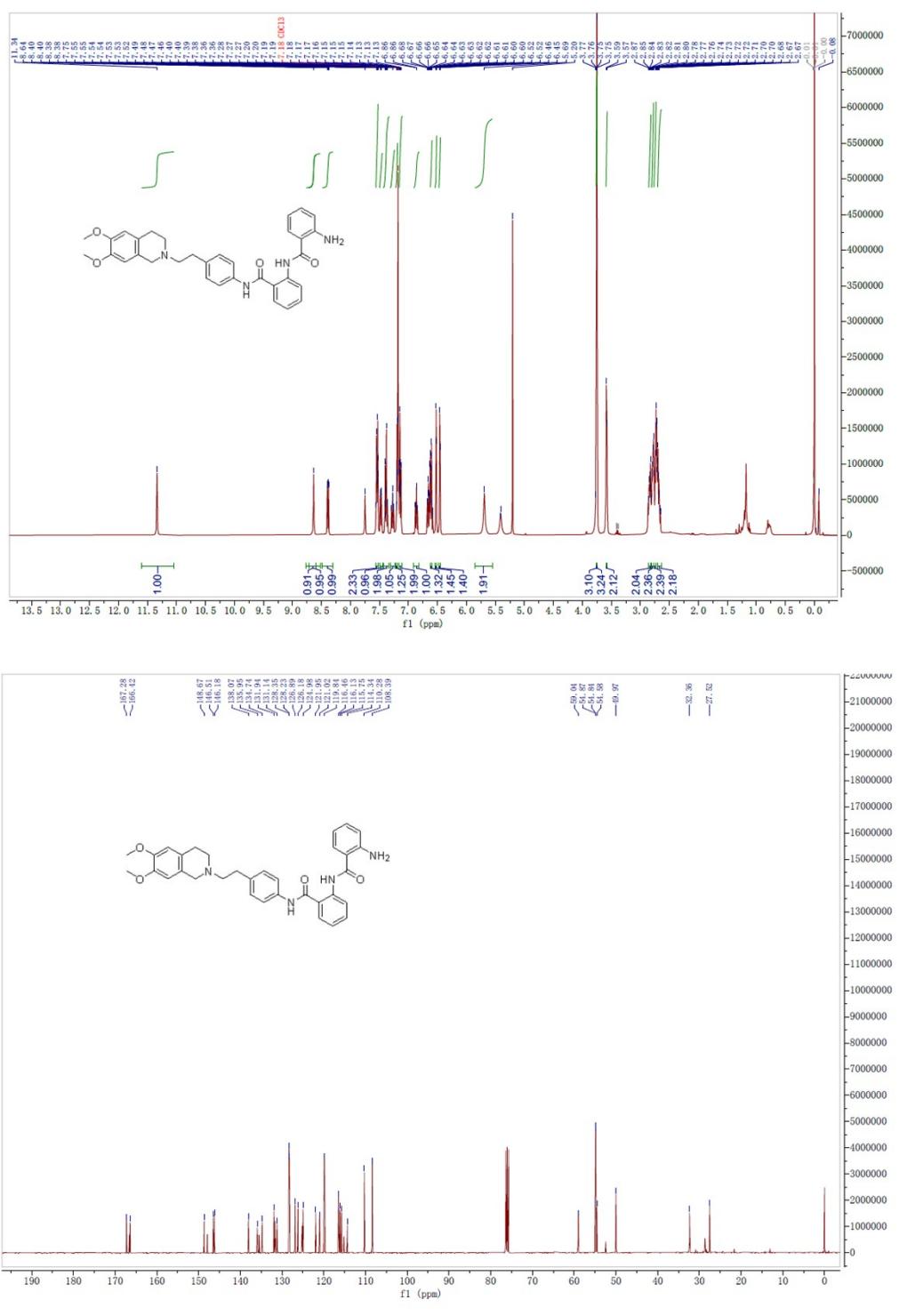
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- e. Key Laboratory of Prevention, Diagnosis and Therapy of Upper Gastrointestinal Cancer of Zhejiang Province, Hangzhou 310022, China

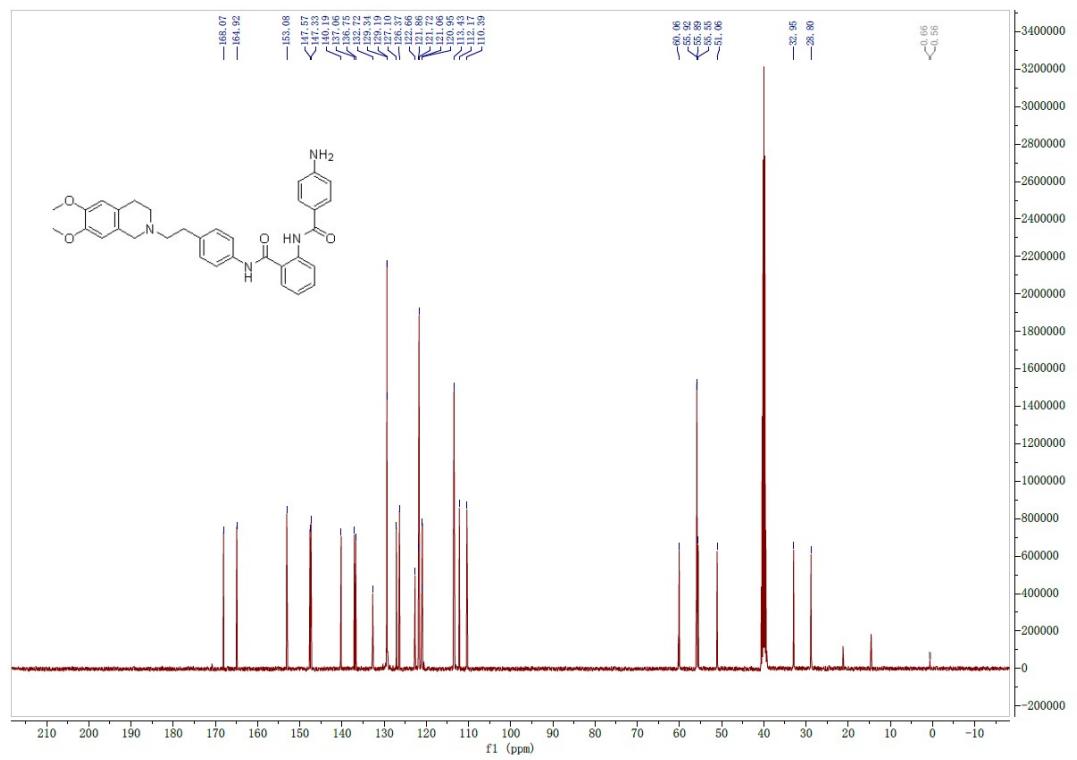
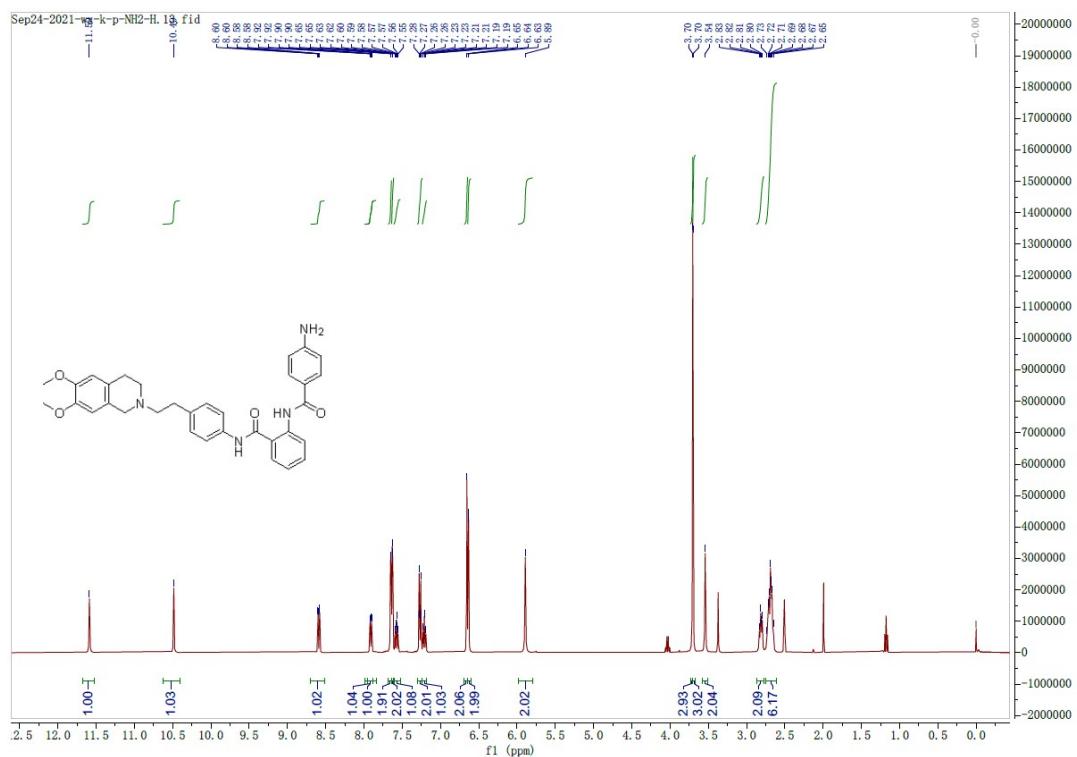
Methyl 4-((2-((4-(2-(6,7-dimethoxy-3,4-dihydroisoquinolin-2(1H)-yl)ethyl)phenyl)carbamoyl)phenyl)carbamoyl)benzoate (PID-1)



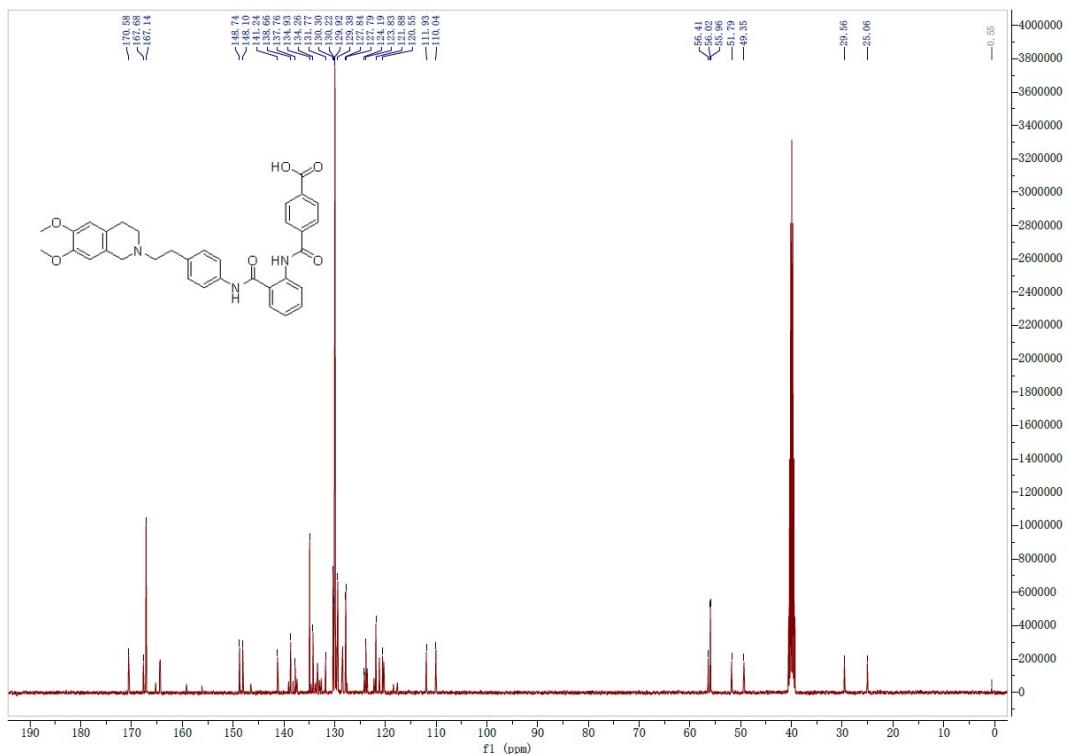
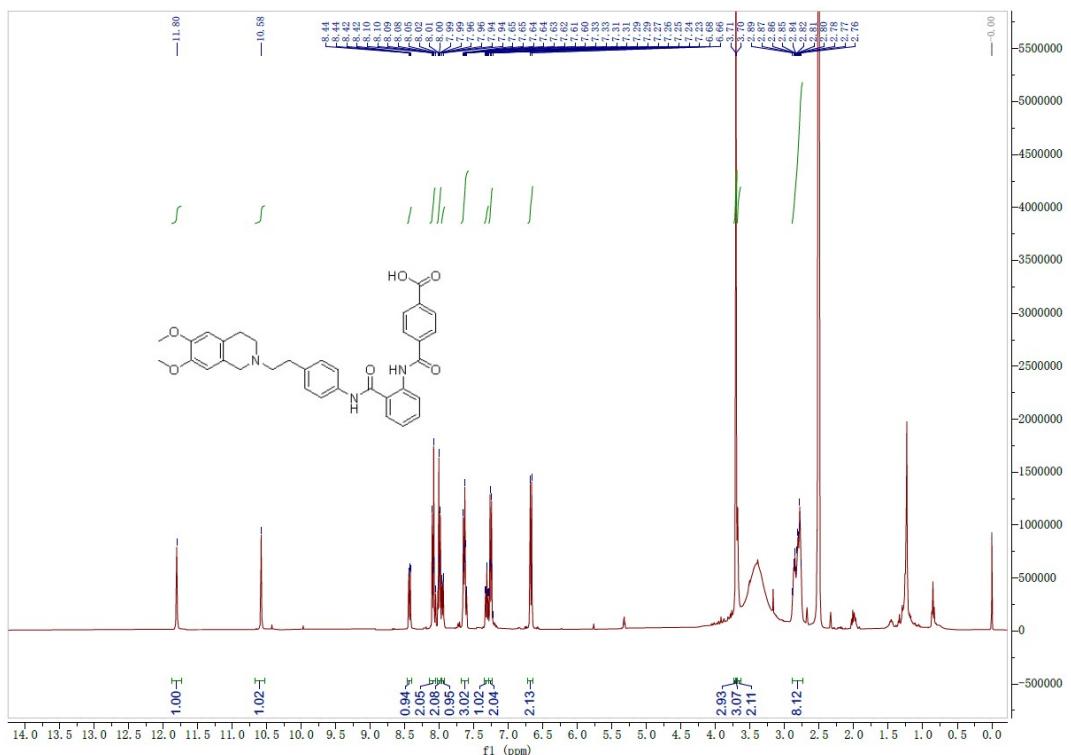
2-Amino-N-(2-((4-(2-(6,7-dimethoxy-3,4-dihydroisoquinolin-2(1H)-yl)ethyl)phenyl)carbamoyl)phenyl)benzamide (PID-2)



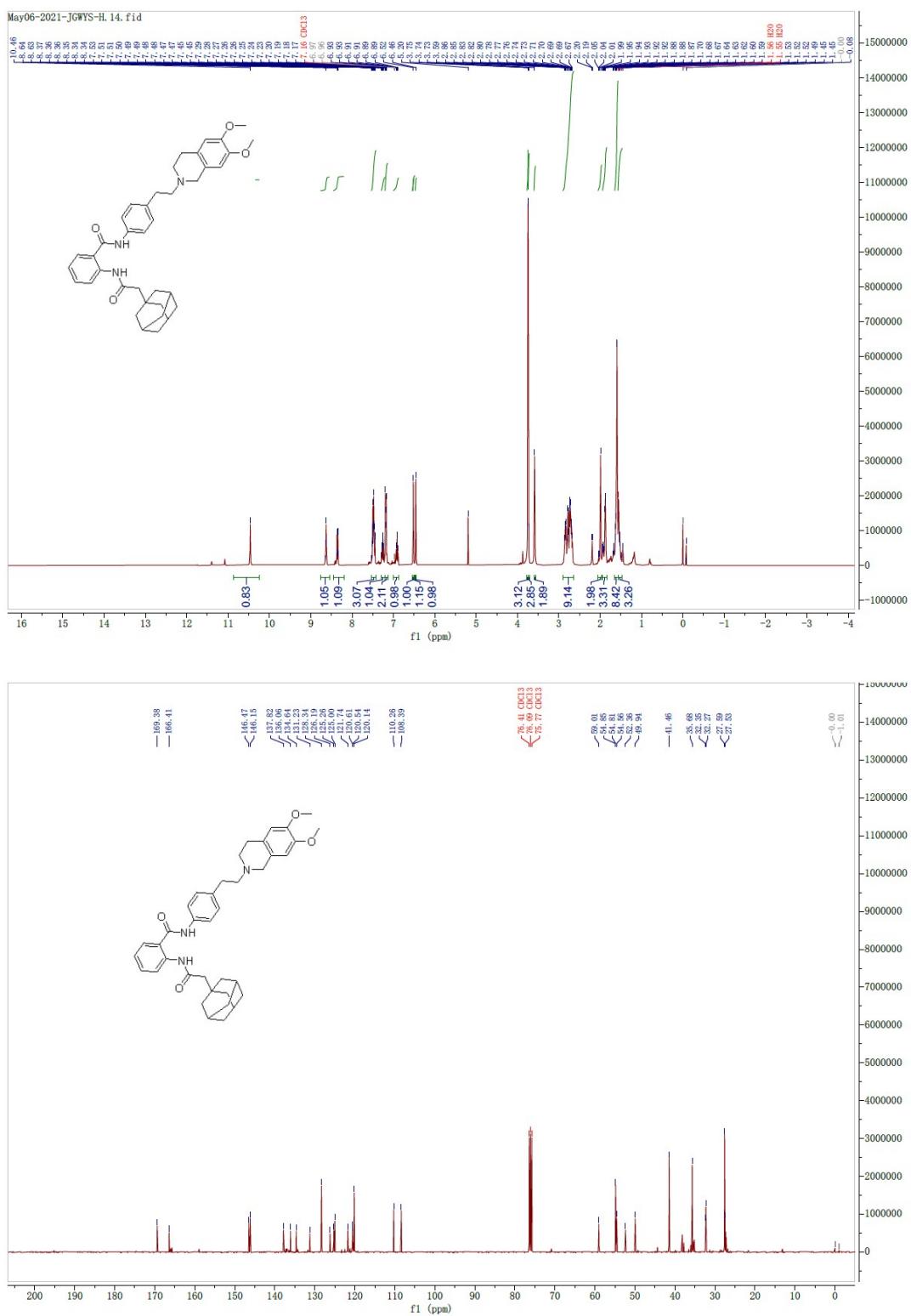
2-(4-Aminobenzamido)-N-(4-(2-(6,7-dimethoxy-3,4-dihydroisoquinolin-2(1H)-yl)ethyl)phenyl)benzamide (PID-3)



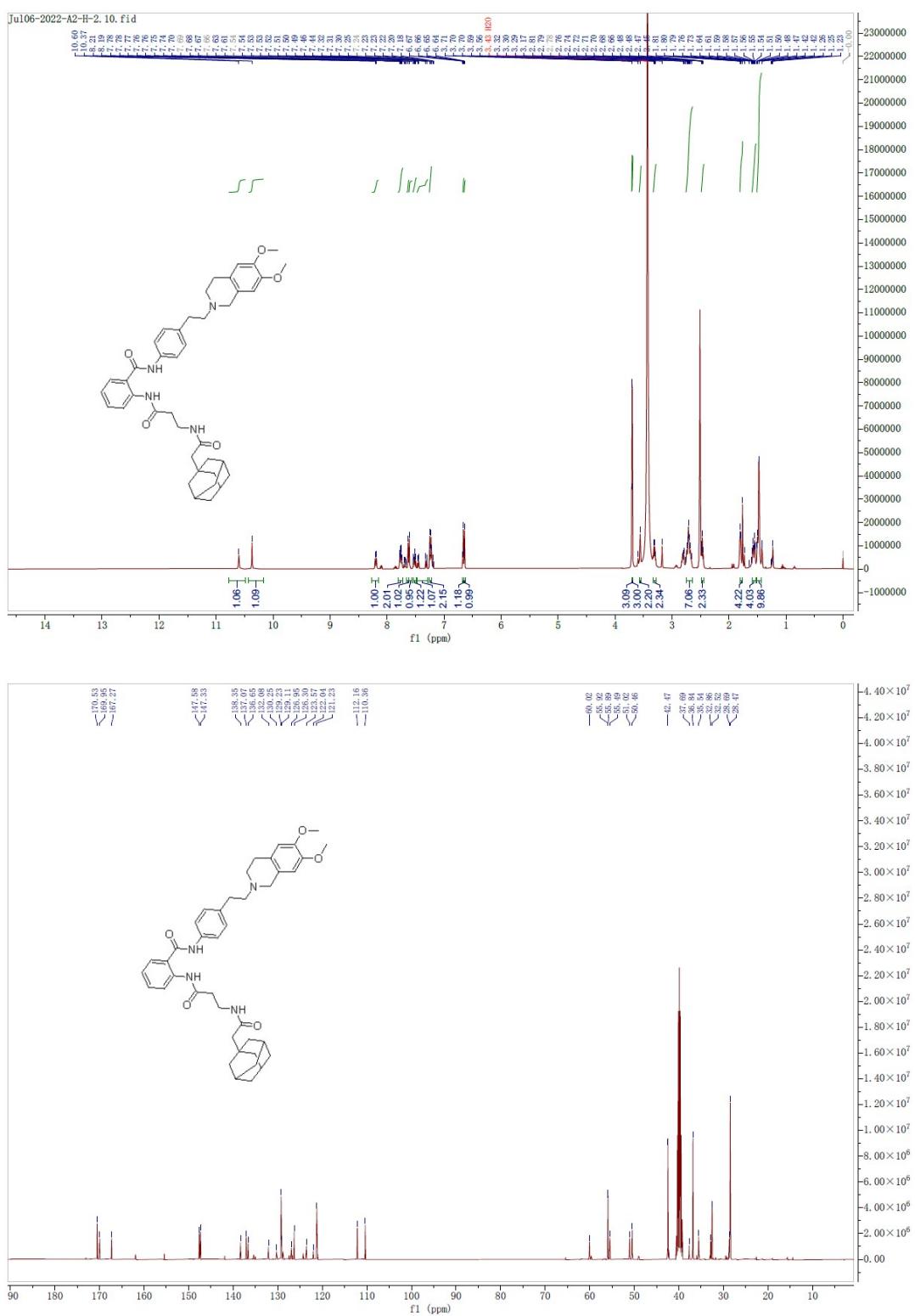
4-((2-((4-(2-(6,7-Dimethoxy-3,4-dihydroisoquinolin-2(1H)yl)ethyl)phenyl)carbamoyl)phenyl)carbamoyl)benzoic acid (PID-4)



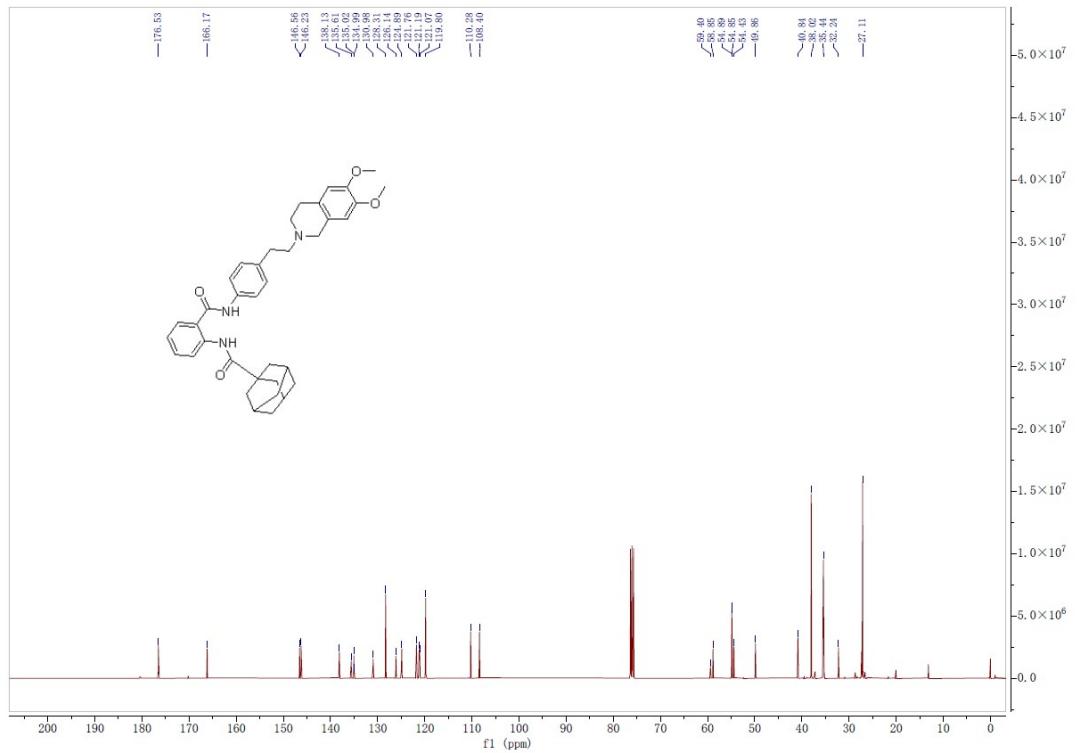
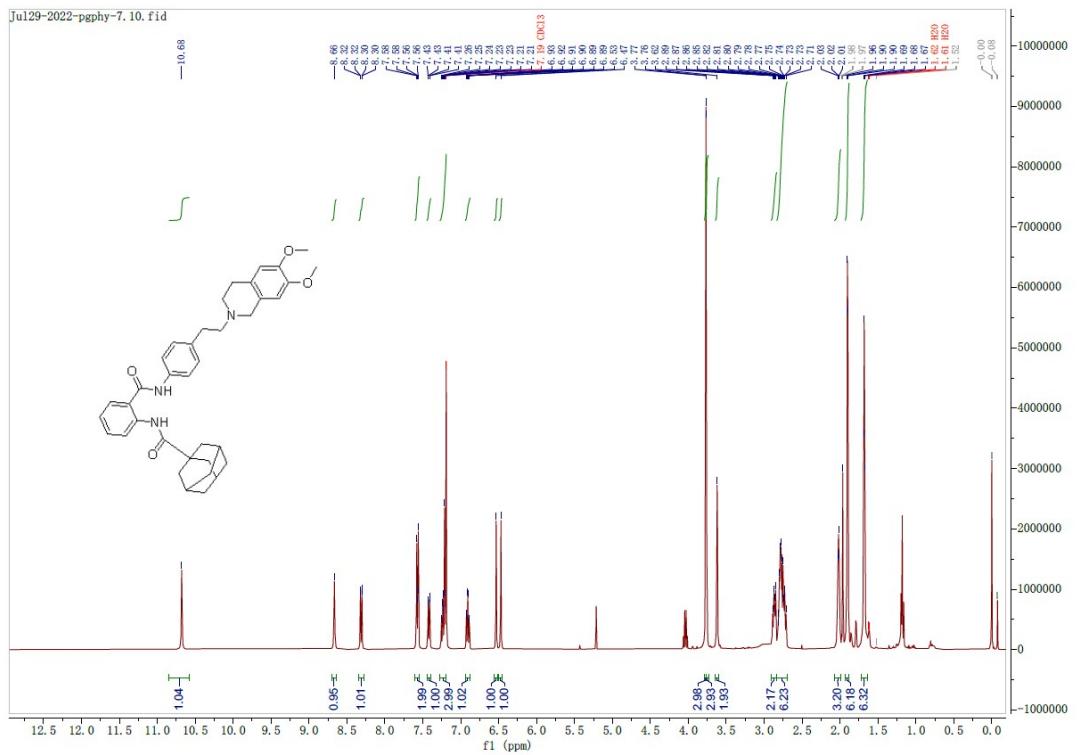
2-(2-(Adamantan-1-yl)acetamido)-N-(4-(2-(6,7-dimethoxy-3,4-dihydroisoquinolin-2(1*H*)-yl)ethyl)phenyl)benzamide (PID-5)



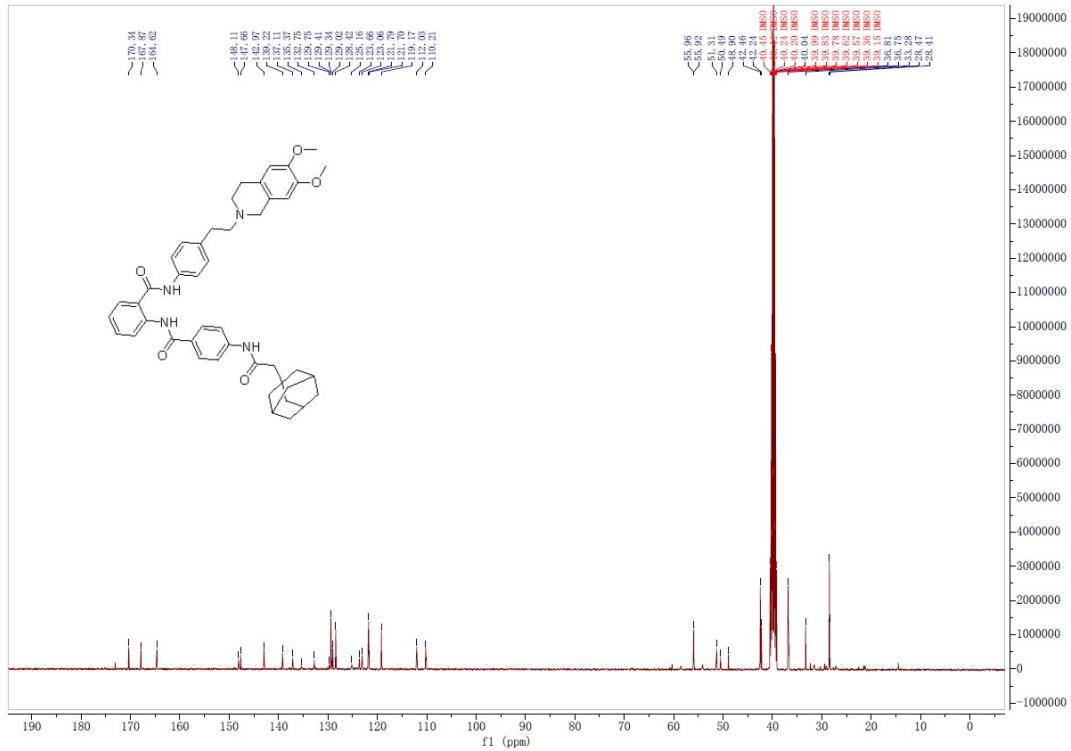
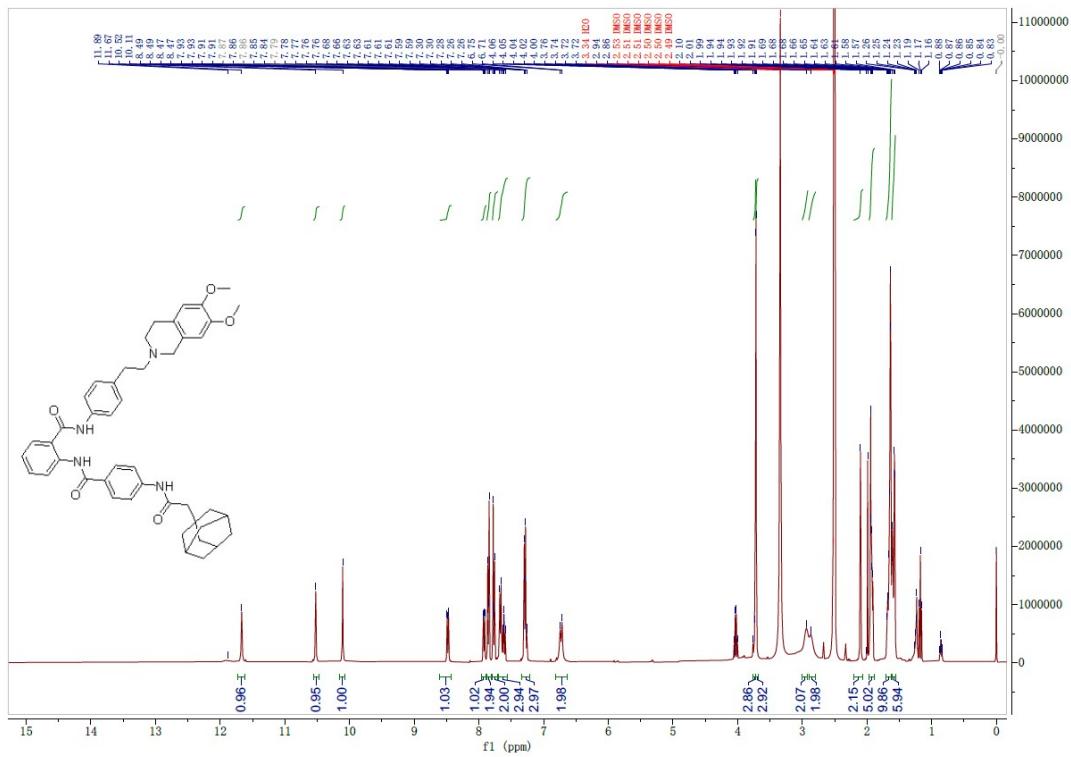
2-(3-(2-(adamantan-1-yl)acetamido)propanamido)-N-(4-(2-(6,7-dimethoxy-3,4-dihydroisoquinolin-2(1H)-yl)ethyl)phenyl)benzamide (PID-6)



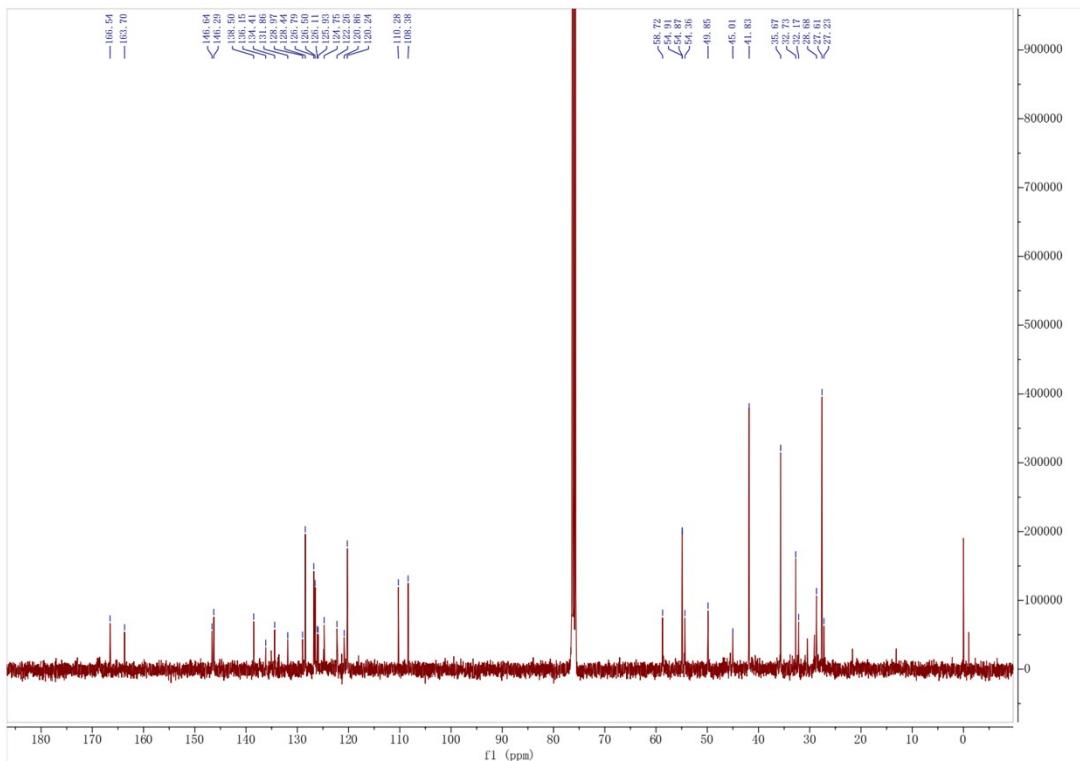
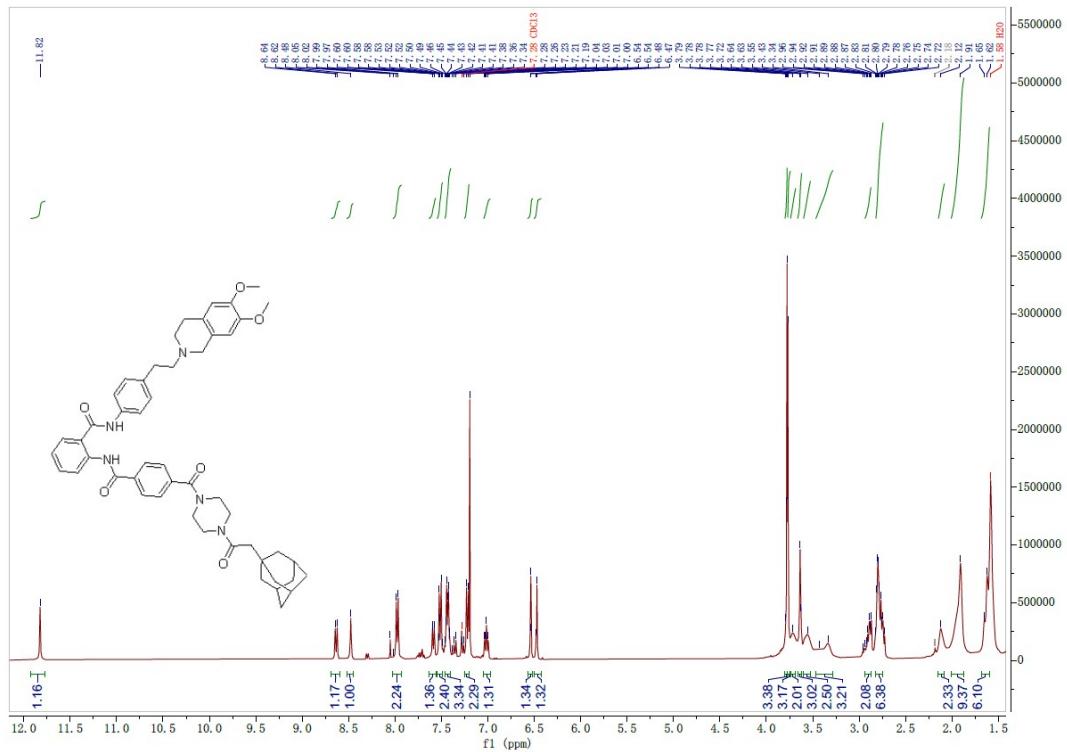
N-(2-((4-(2-(6,7-dimethoxy-3,4-dihydroisoquinolin-2(1*H*)-
yl)ethyl)phenyl)carbamoyl) phenyl)adamantane-1-carboxamide (PID-7)



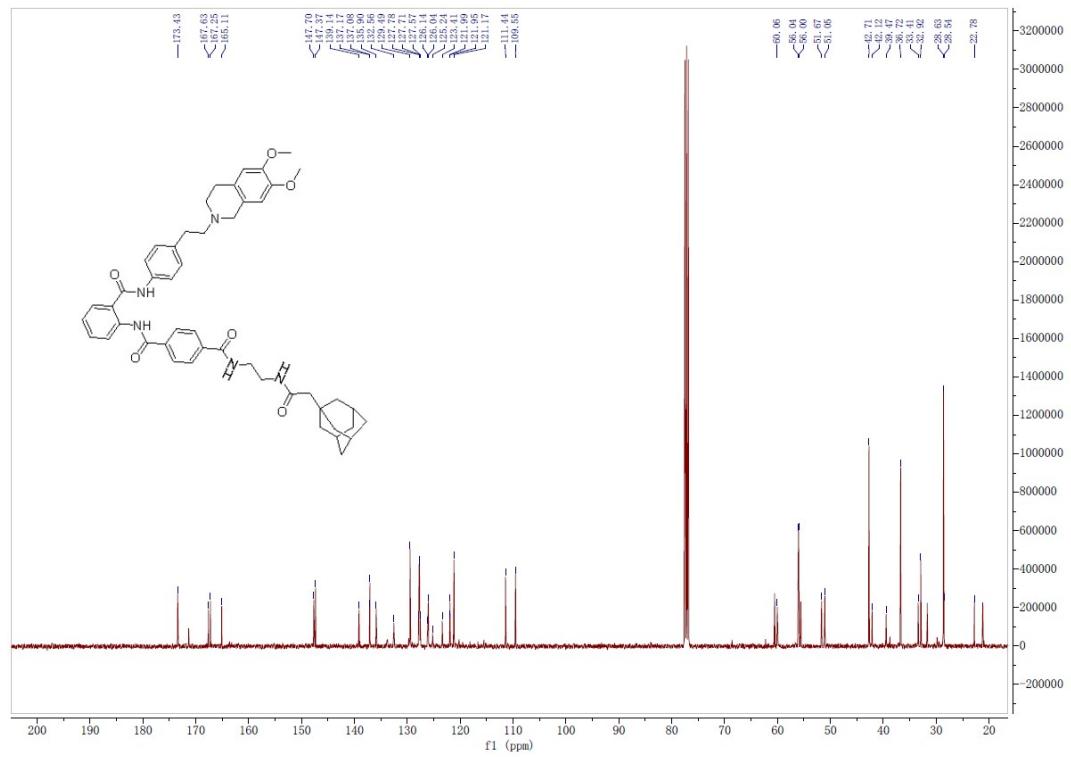
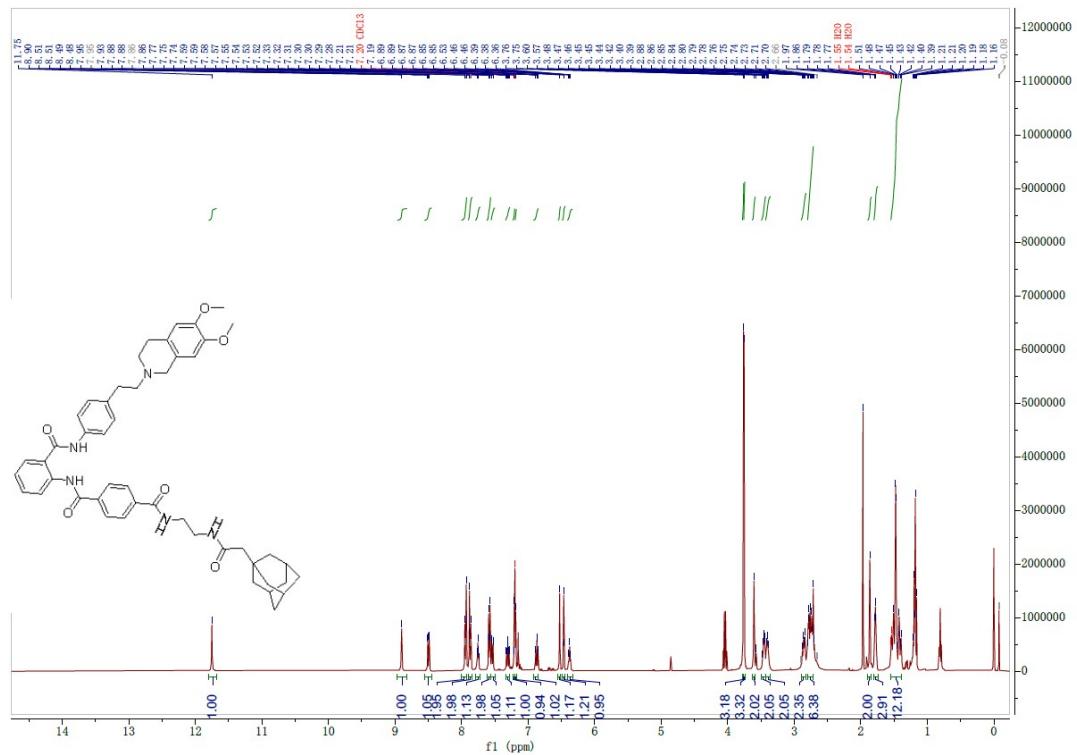
2-(4-(2-(adamantan-1-yl)acetamido)benzamido)-N-(4-(2-(6,7-dimethoxy-3,4-dihydroisoquinolin-2(1*H*)-yl)ethyl)phenyl)benzamide (PID-8)



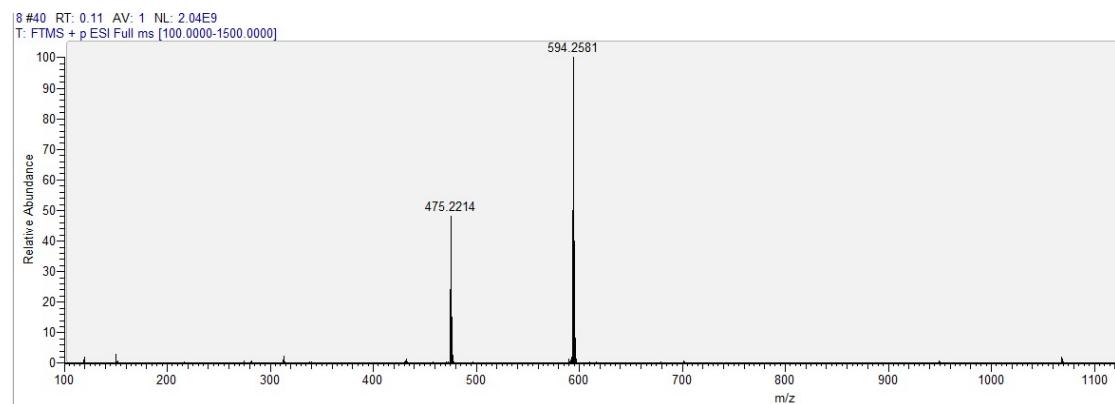
**2-(4-(4-(2-((1S,3S)-adamantan-1-yl)acetyl)piperazine-1-carbonyl)benzamido)-N-(4-(2-(6,7-dimethoxy-3,4-dihydroisoquinolin-2(1H)-yl)ethyl)phenyl)benzamide
(PID-9)**



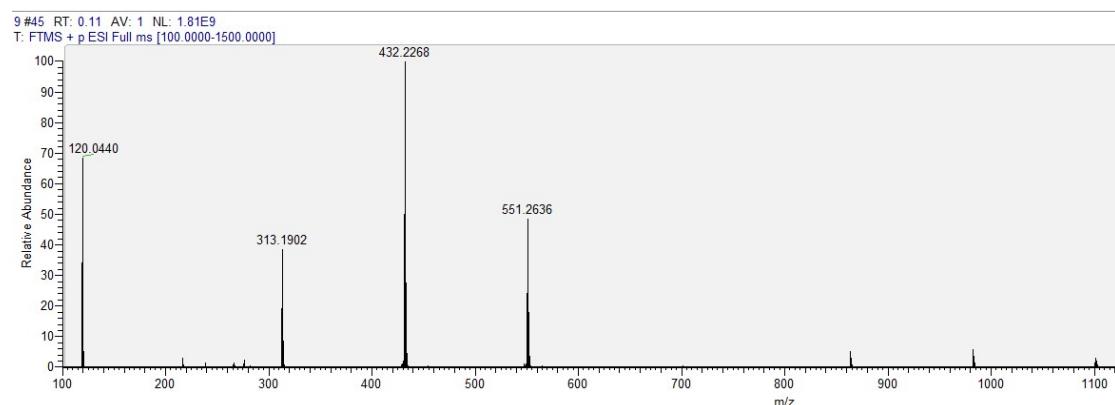
N¹-(2-(2-((1S,3s)-adamantan-1-yl)acetamido)ethyl)-N⁴-(2-((4-(2-(6,7-dimethoxy-3,4-dihydroisoquinolin-2(1H)-yl)ethyl)phenyl)carbamoyl)phenyl)terephthalamide (PID-10)



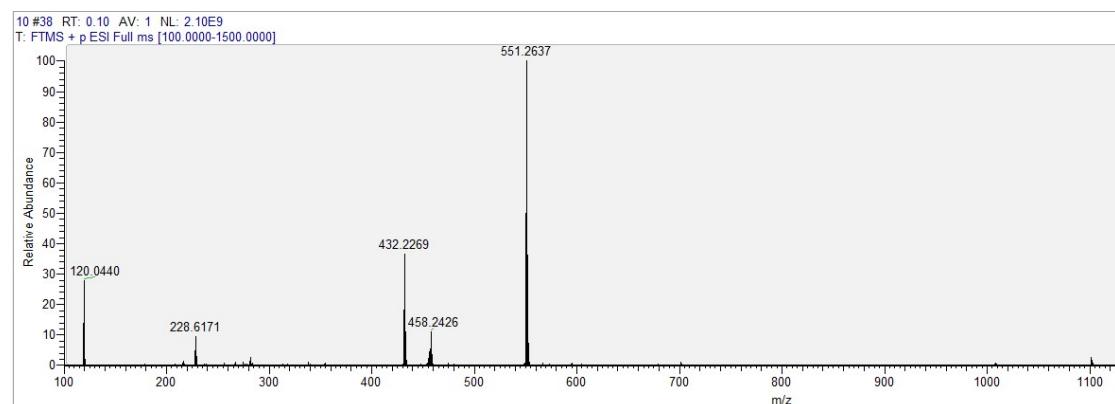
PID-1



PID-2

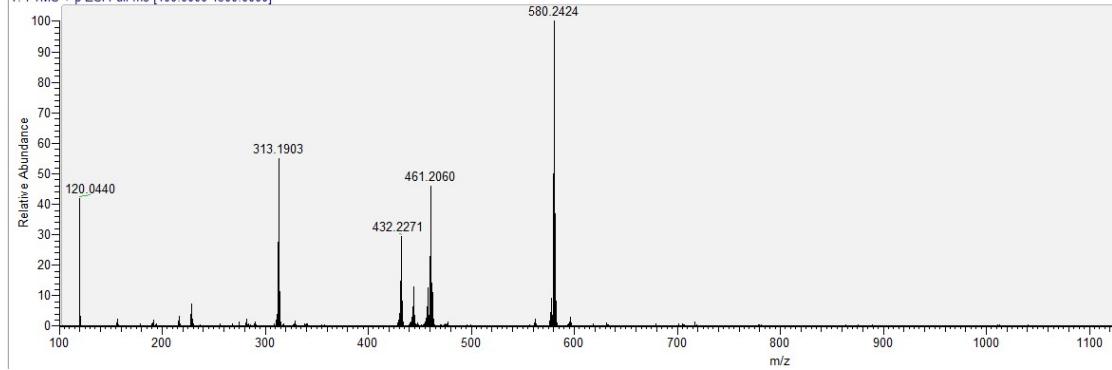


PID-3



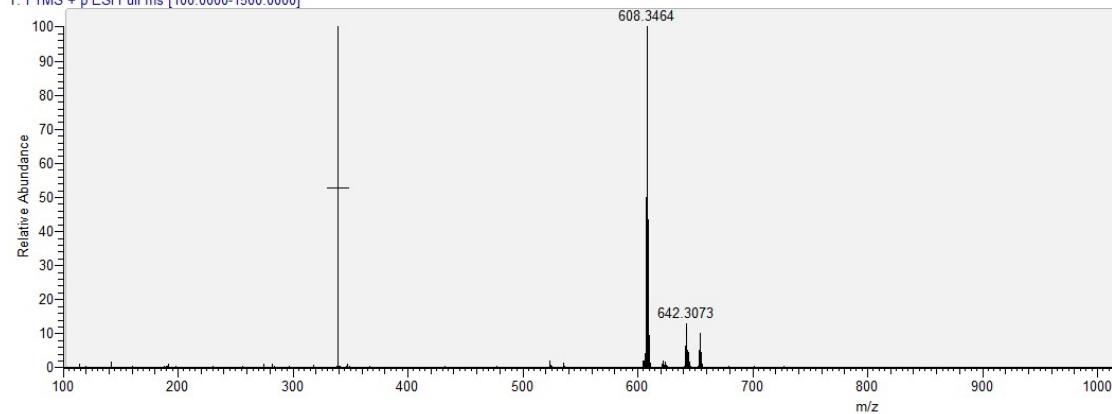
PID-4

11 #31 RT: 0.08 AV: 1 NL: 7.50E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



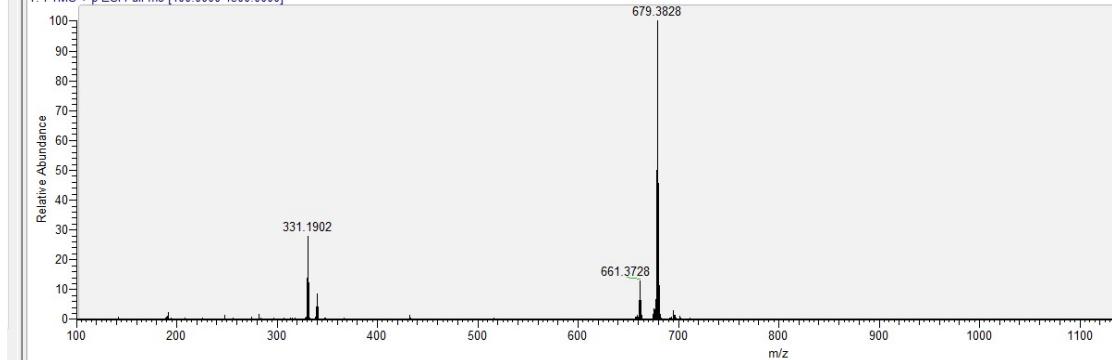
PID-5

1 #30 RT: 0.09 AV: 1 NL: 1.80E9
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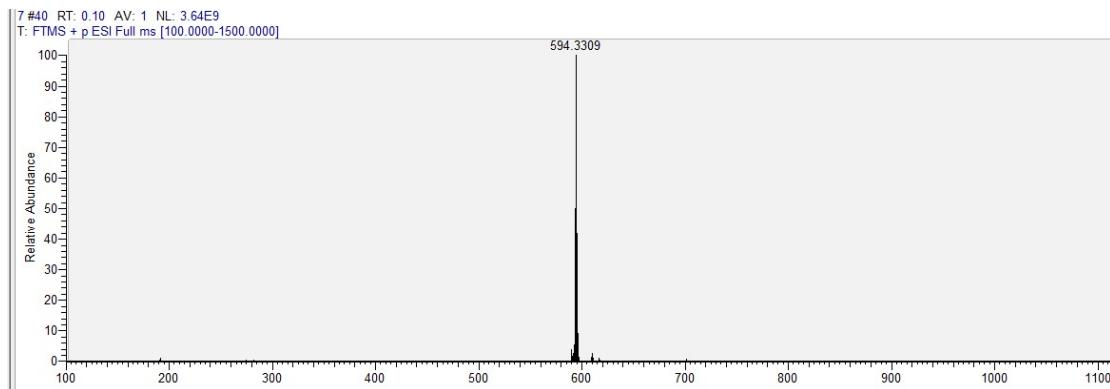


PID-6

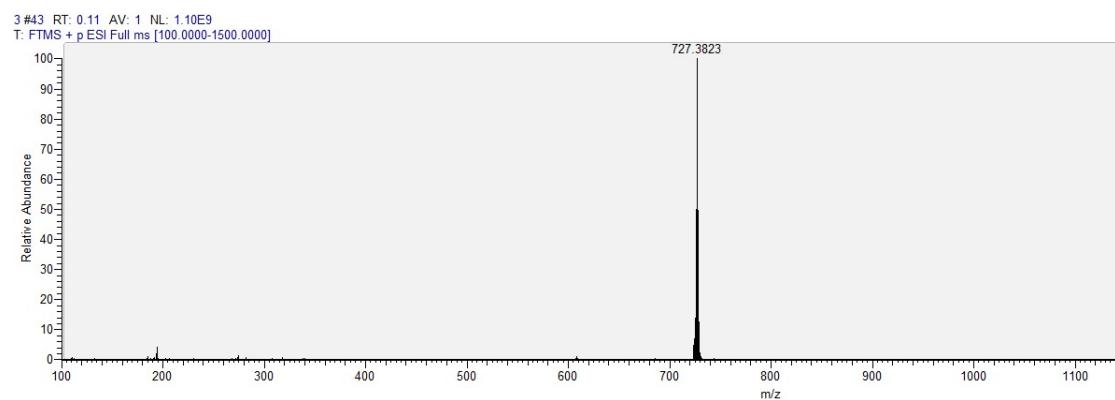
2 #38 RT: 0.10 AV: 1 NL: 1.82E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



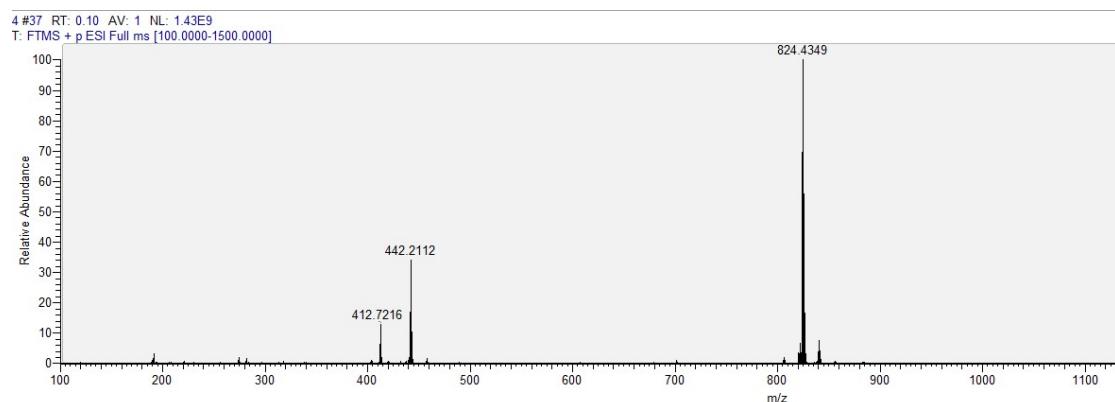
PID-7



PID-8



PID-9



PID-10

