

Optimization and Antibacterial Evaluation of Novel 3-(5-Fluoropyridine-3-yl)-2-oxazolidinone Derivatives Containing a Pyrimidine Substituted Piperazine

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1. Compounds spectral data

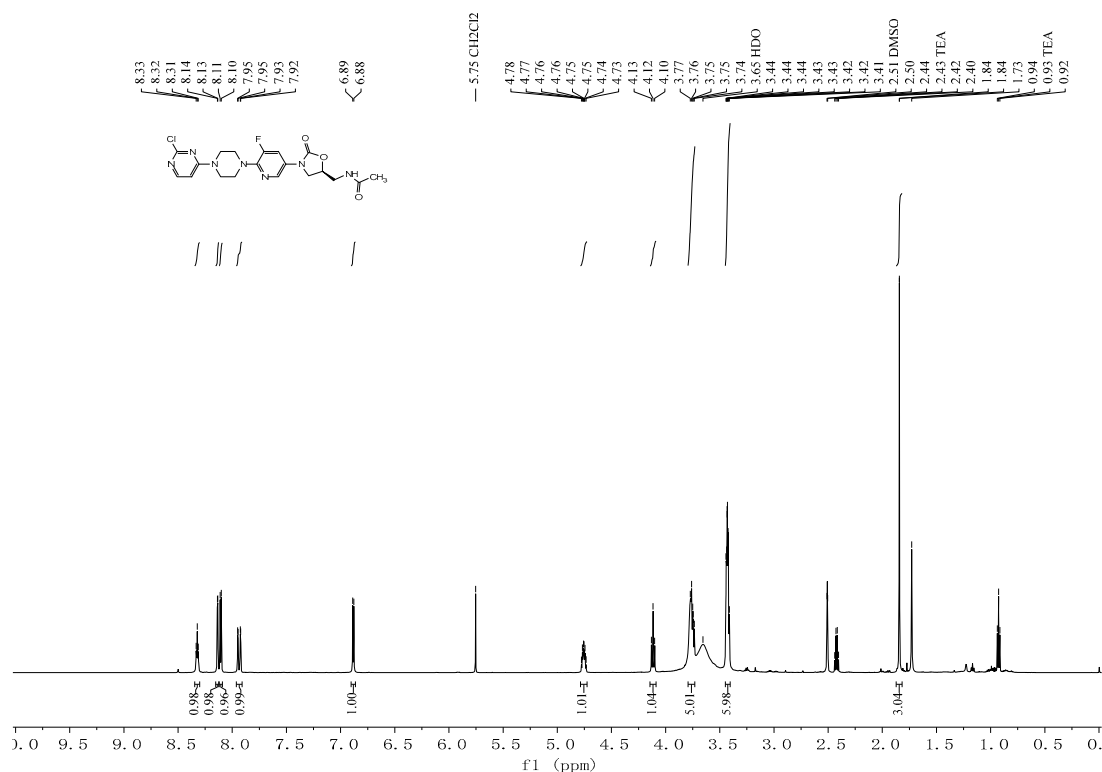


Figure S1. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of 5.

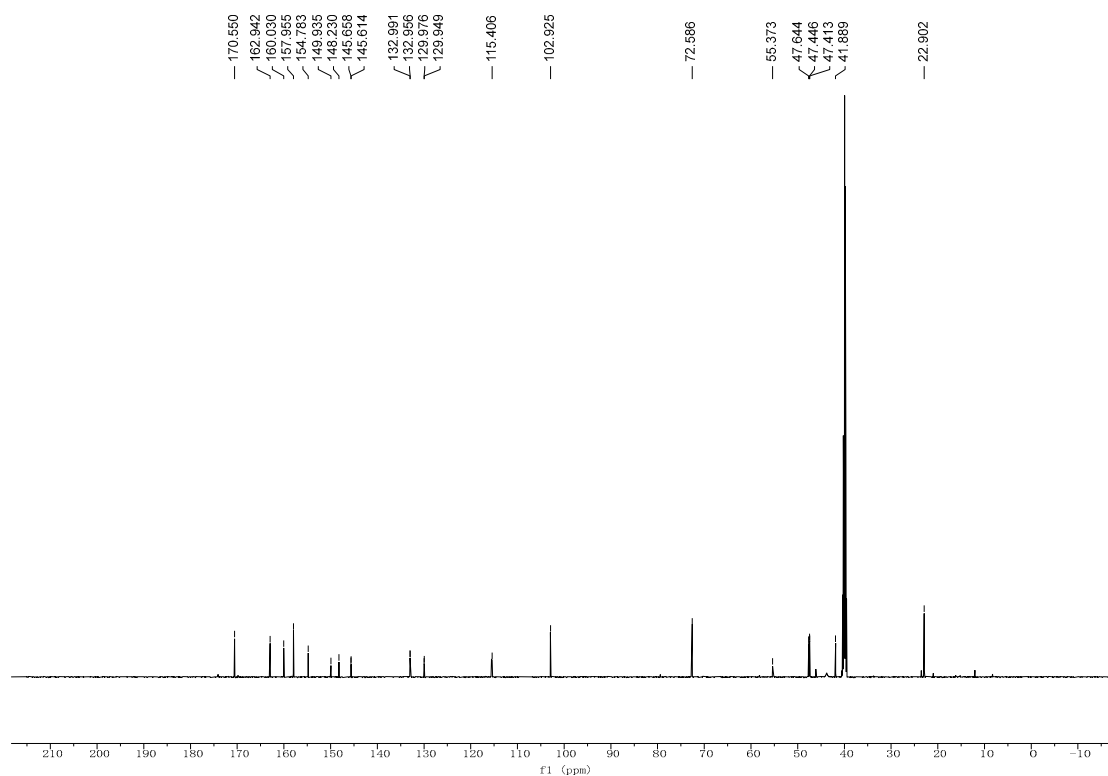


Figure S2. ^{13}C NMR Spectrum (DMSO- d_6 , 150 MHz) of **5**.

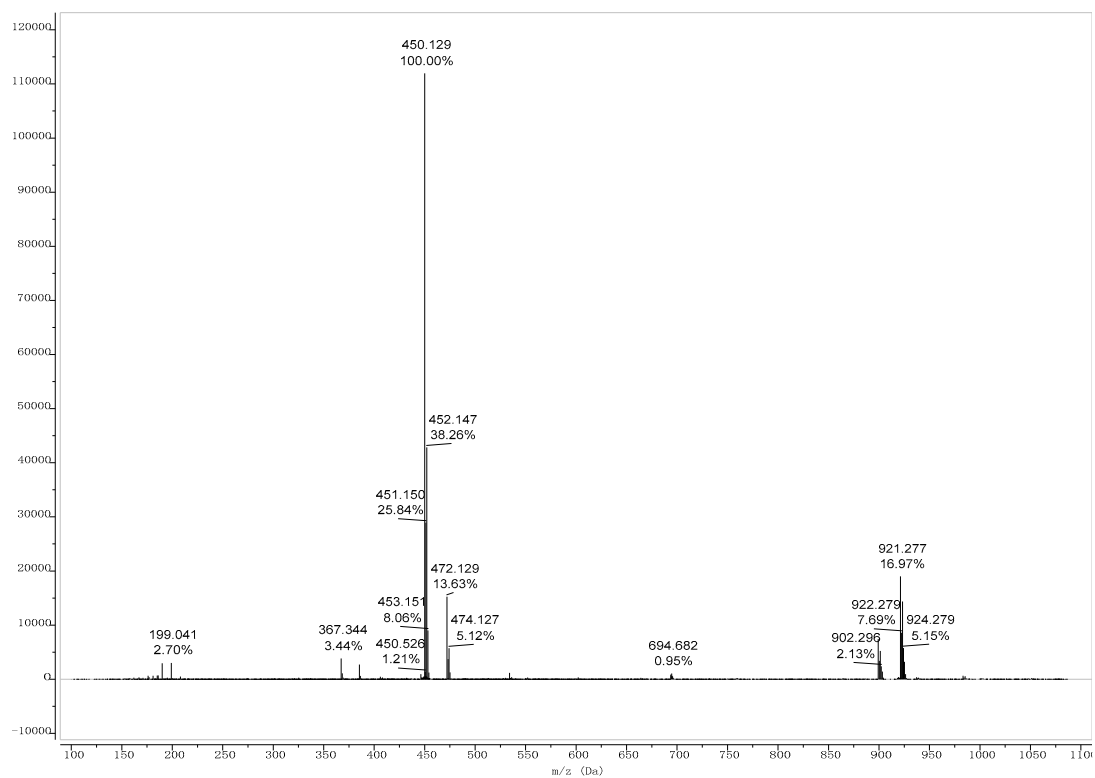


Figure S3. MS for $\text{C}_{19}\text{H}_{21}\text{ClFN}_7\text{O}_3$ (Mwt.: 449.87): m/z 450.129 ($[\text{M}+\text{H}]^+$, bp) of **5**.

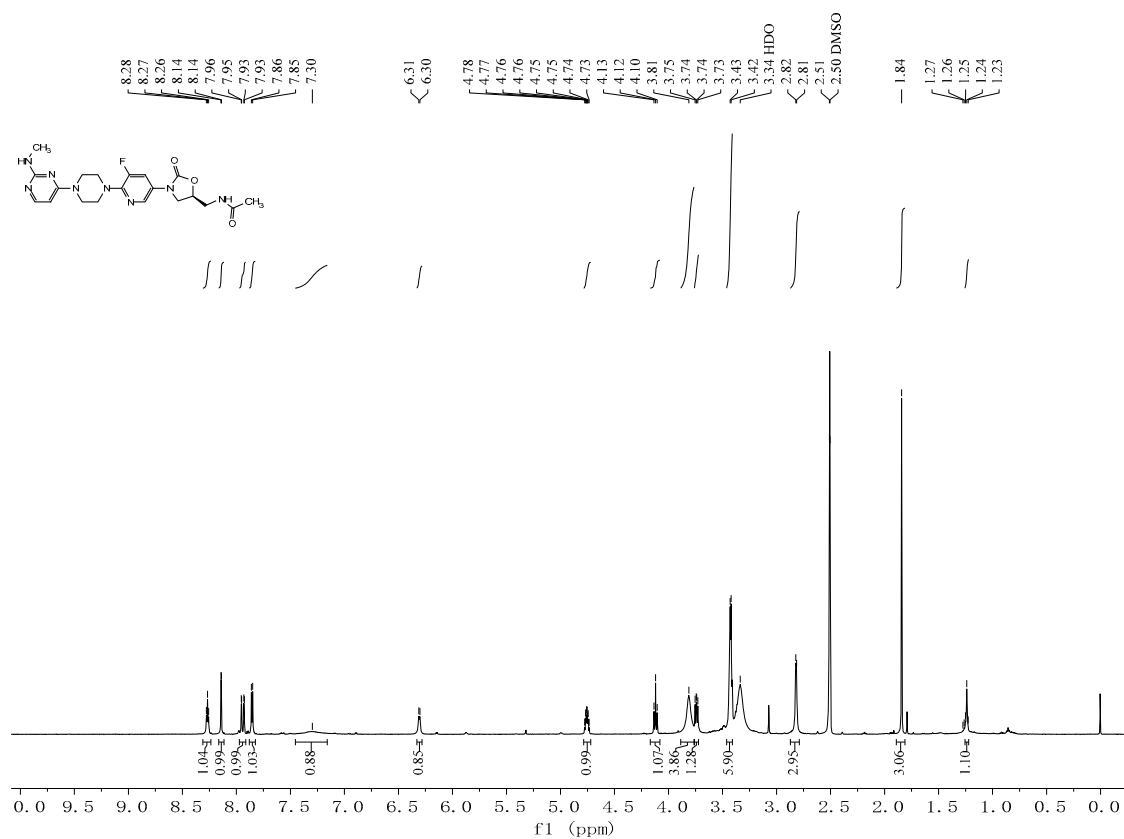


Figure S4. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of **6a**.

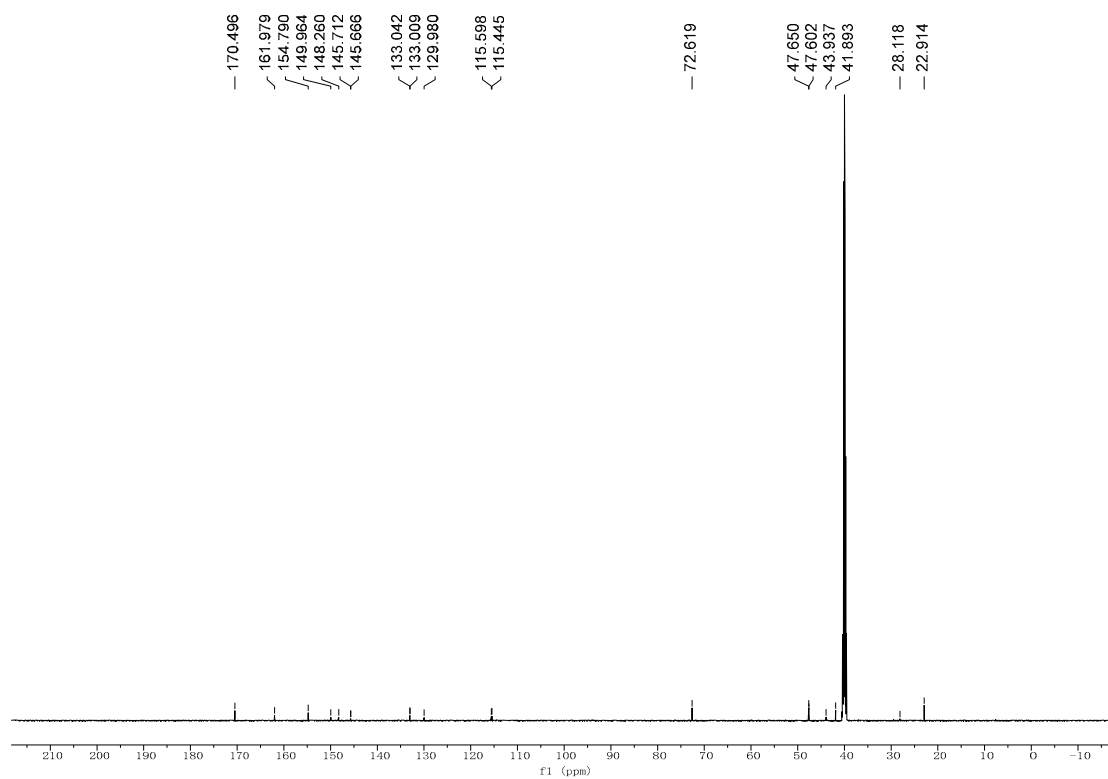
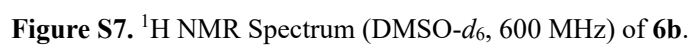
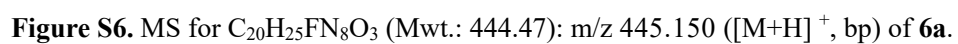


Figure S5. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **6a**.



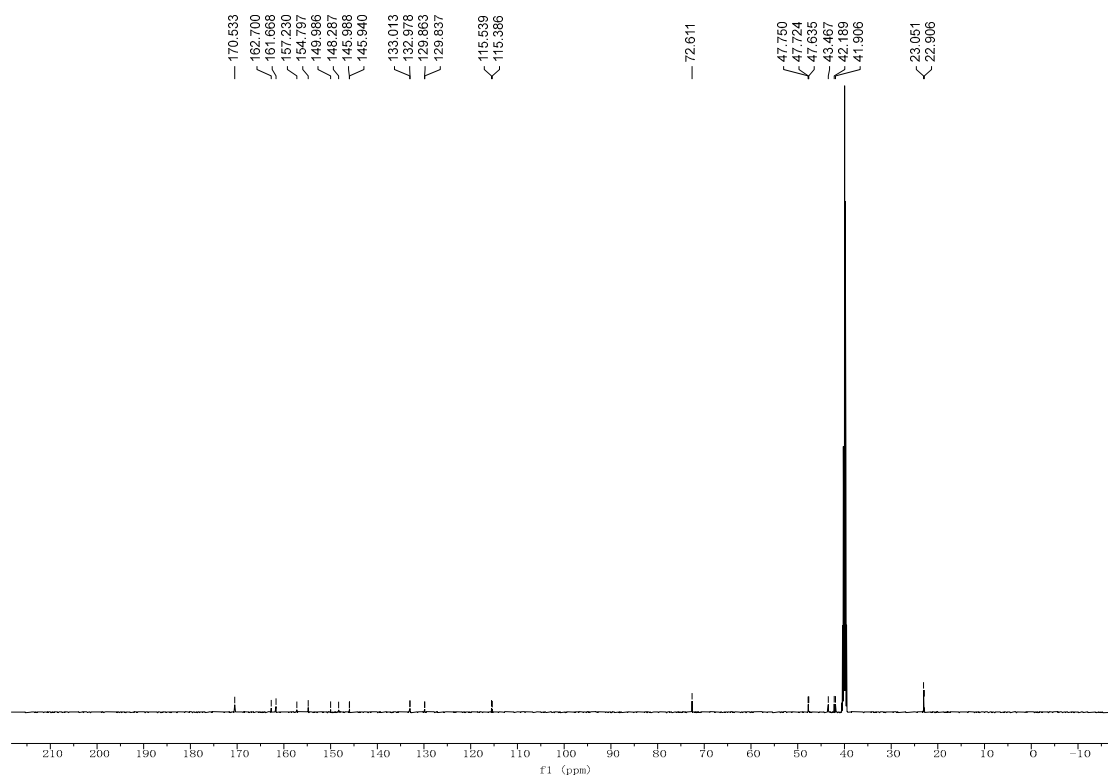


Figure S8. ^{13}C NMR Spectrum (DMSO- d_6 , 150 MHz) of **6b**.

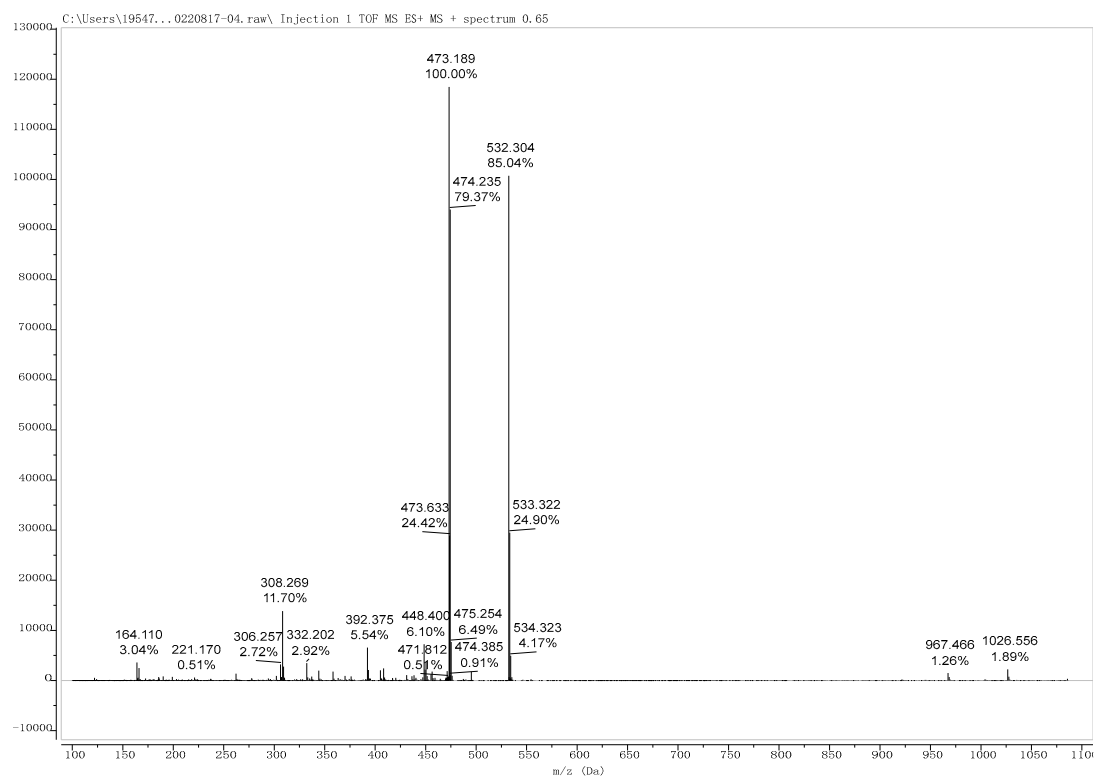


Figure S9. MS for $\text{C}_{22}\text{H}_{29}\text{FN}_8\text{O}_3$ (Mwt.: 472.53): m/z 473.189 ($[\text{M}+\text{H}]^+$, bp) of **6b**.

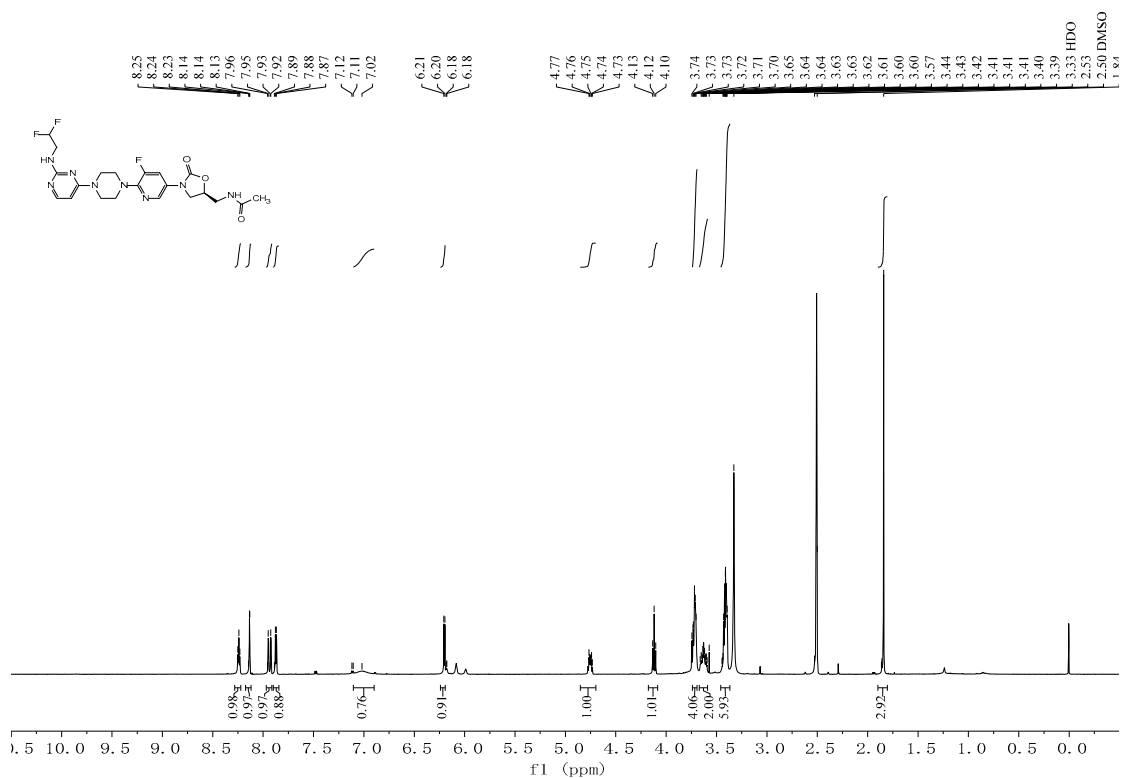


Figure S10. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of **6c**.

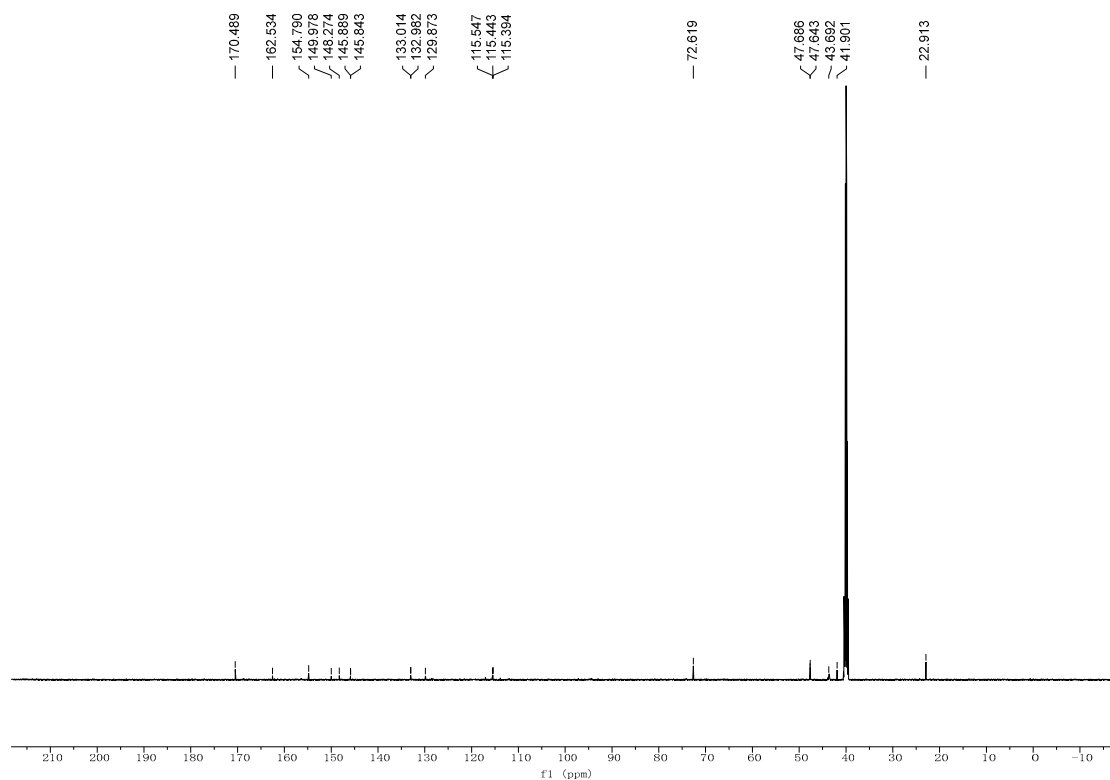


Figure S11. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **6c**.

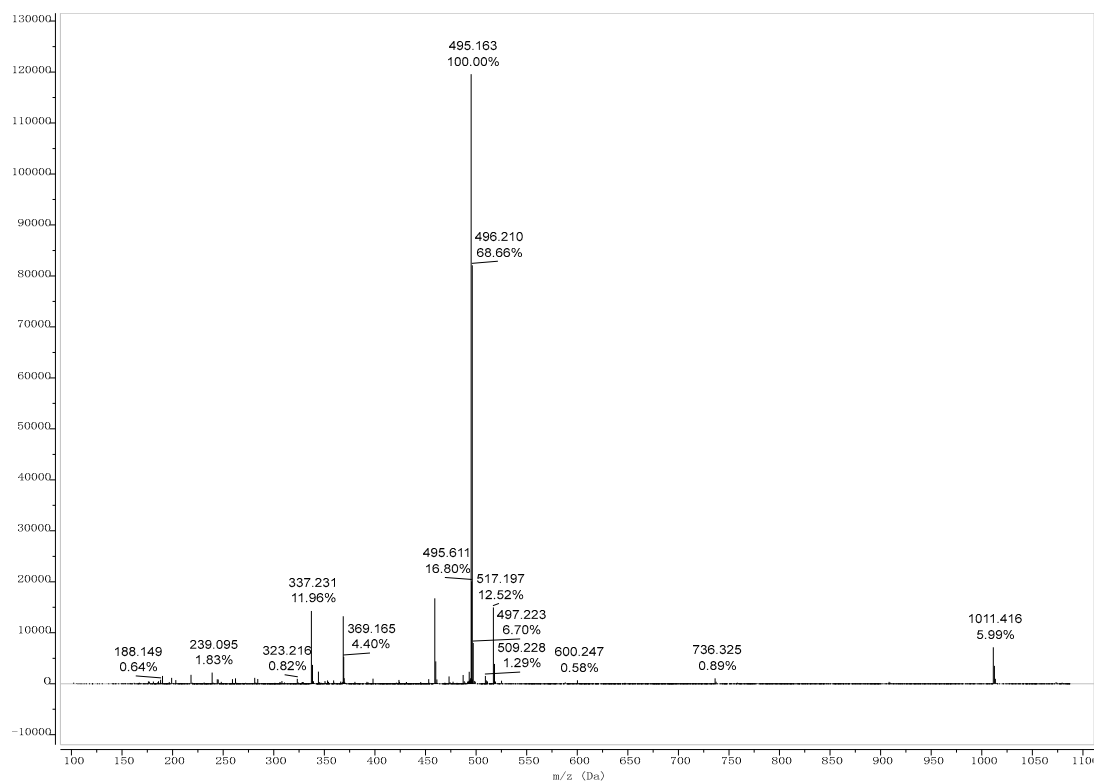
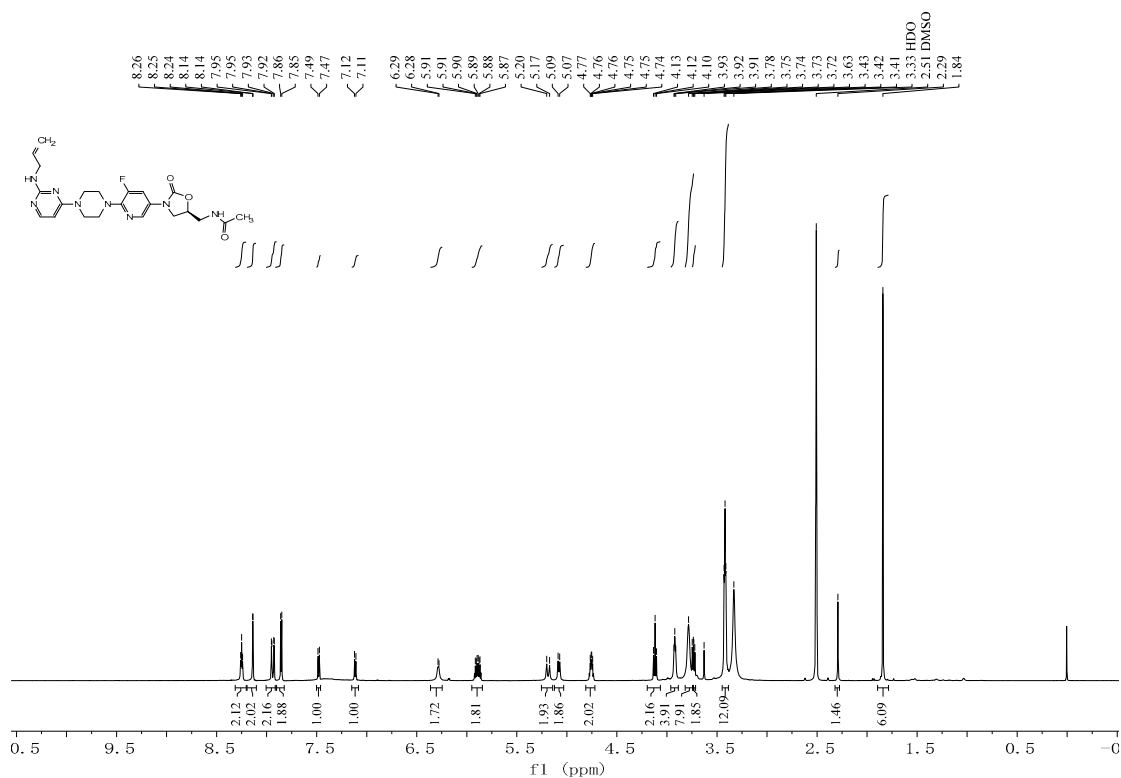


Figure S12. MS for $C_{21}H_{25}F_3N_8O_3$ (Mwt.: 494.48): m/z 495.163 ($[M+H]^+$, bp) of **6c**.



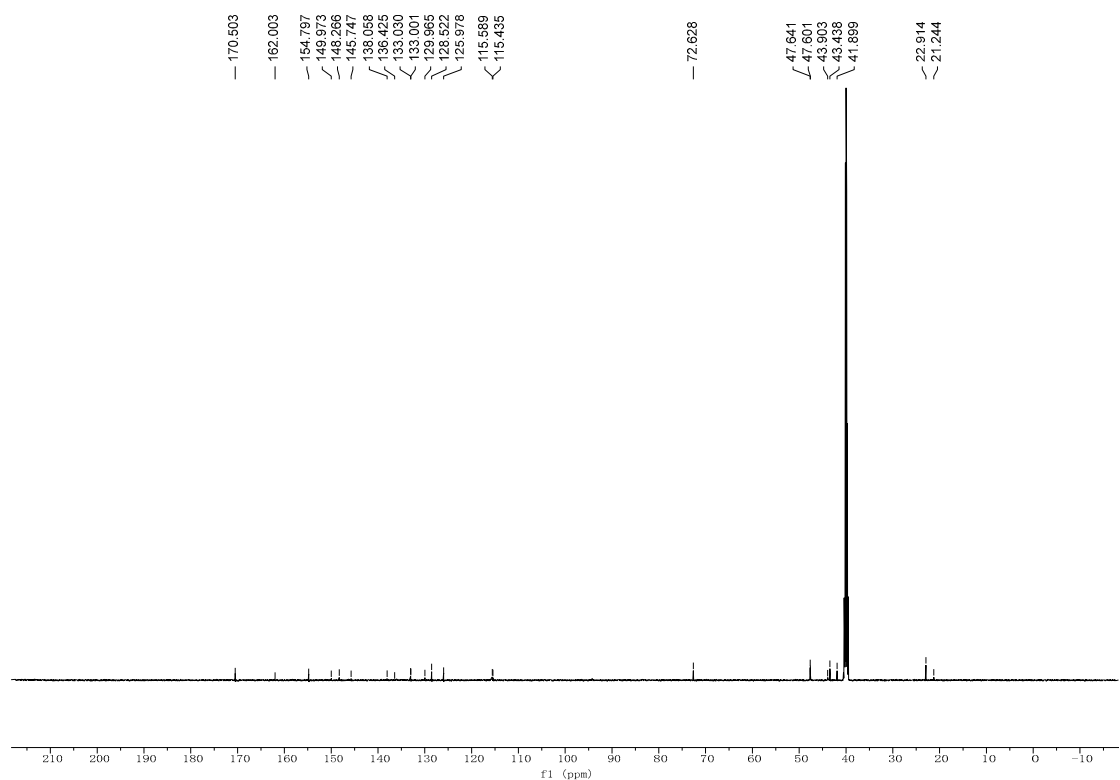


Figure S14. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **6d**.

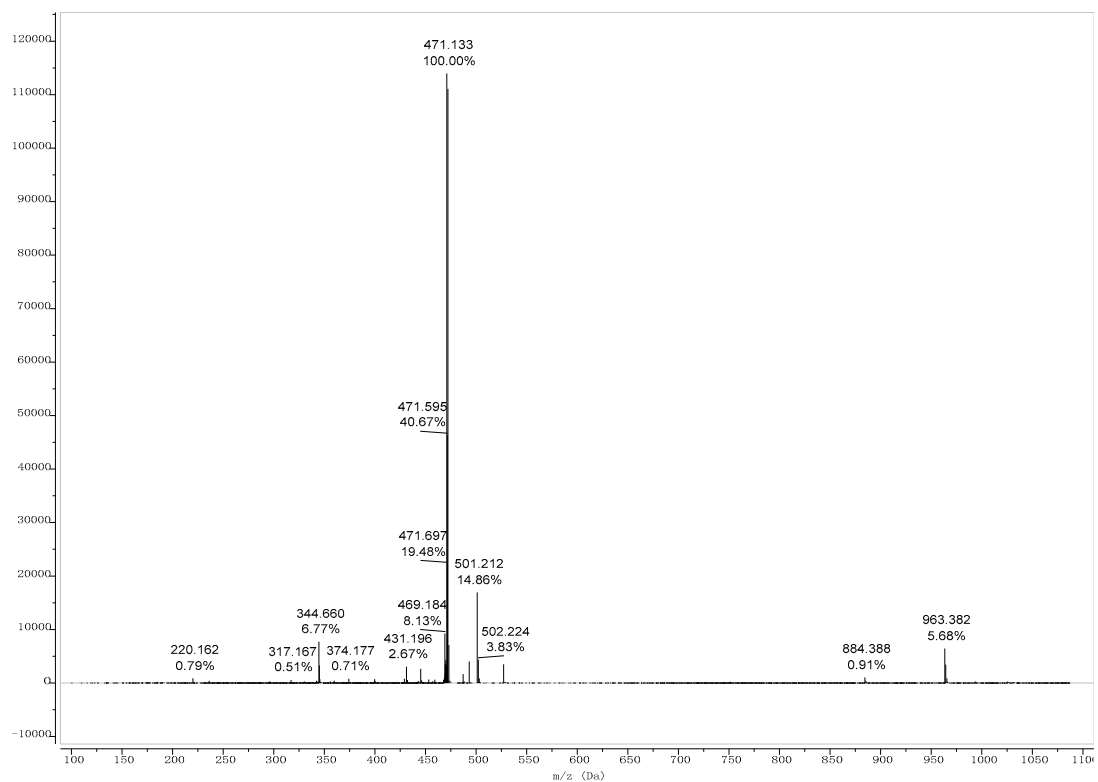


Figure S15. MS for C₂₂H₂₇FN₈O₃ (Mwt.: 470.51): m/z 471.133 ([M+H]⁺, bp) of **6d**.

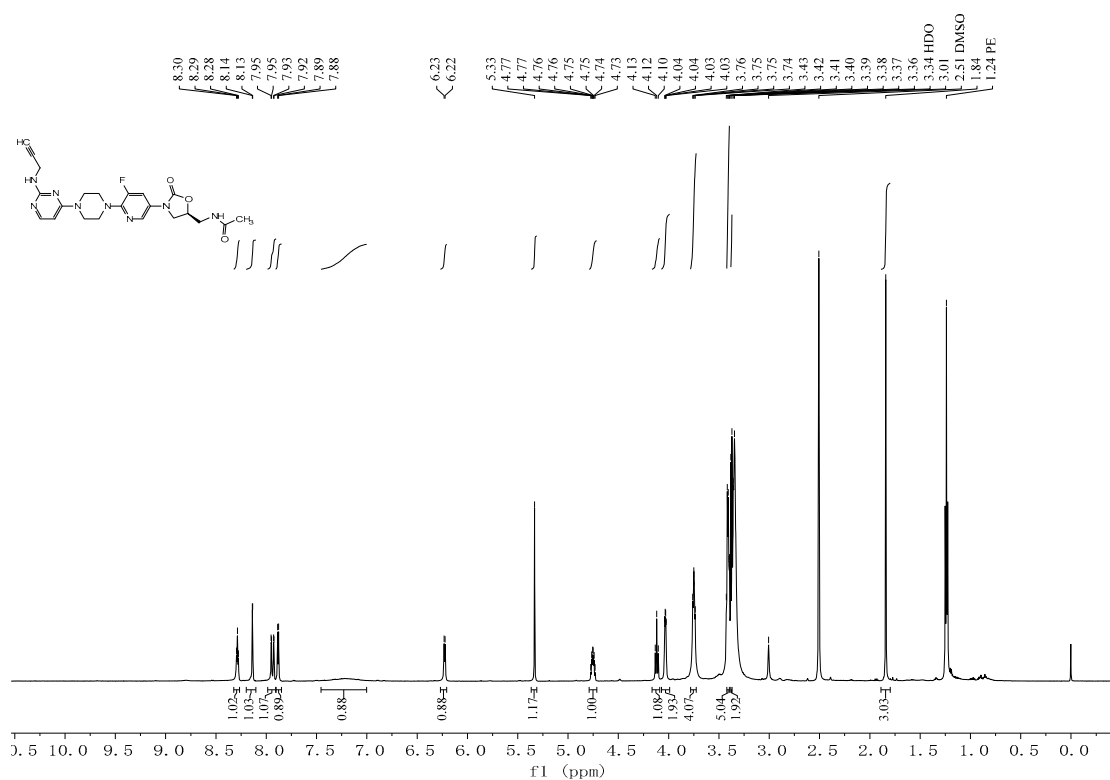


Figure S16. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of **6e**.

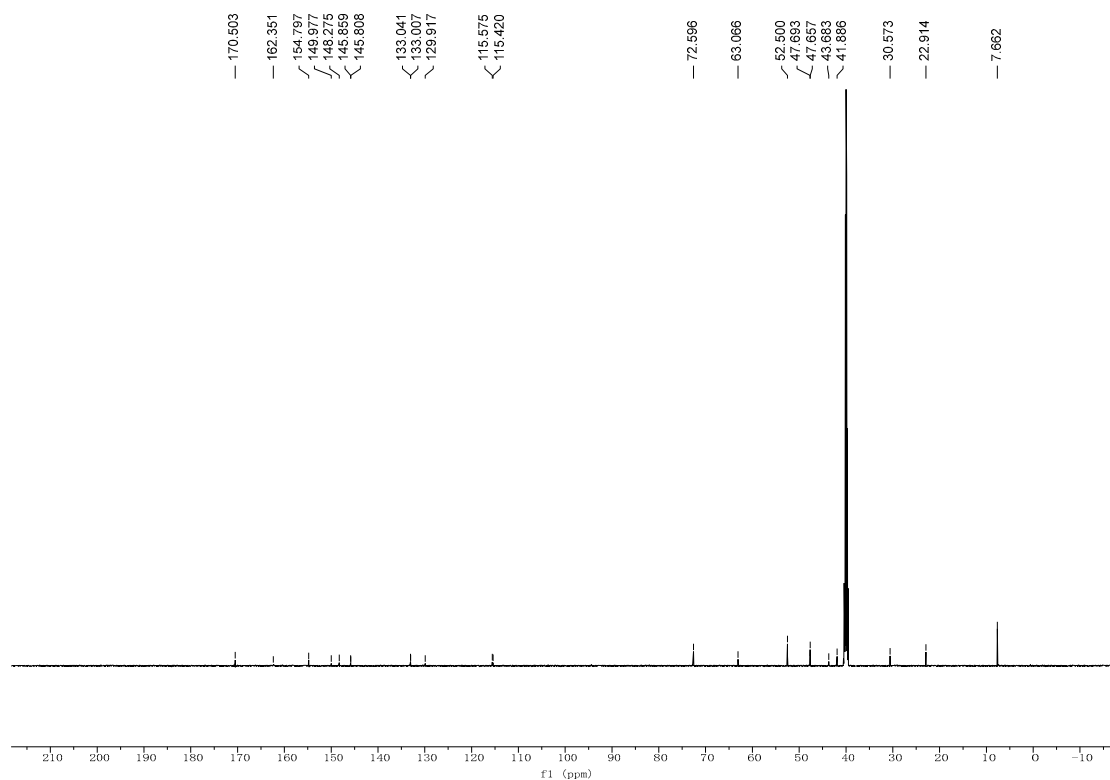
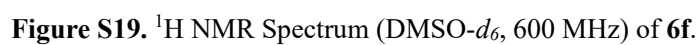
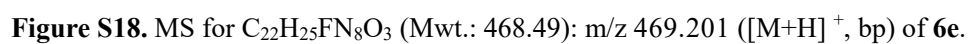


Figure S17. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **6e**.



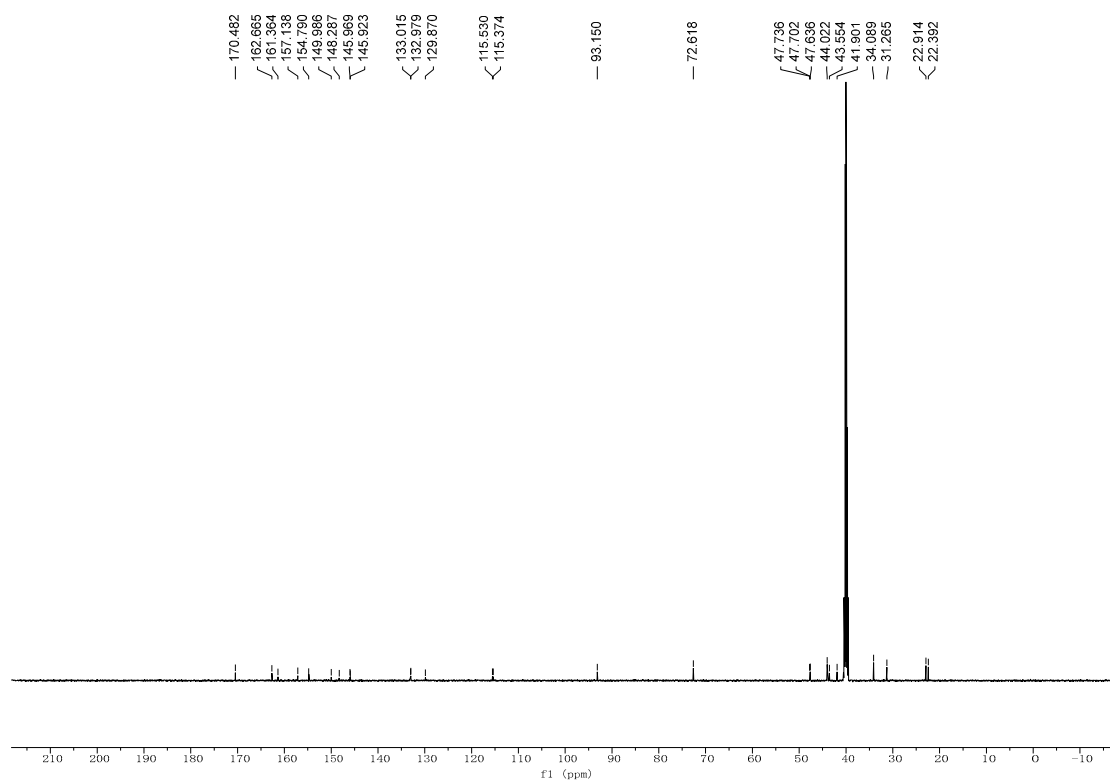


Figure S20. ^{13}C NMR Spectrum ($\text{DMSO-}d_6$, 150 MHz) of **6f**.

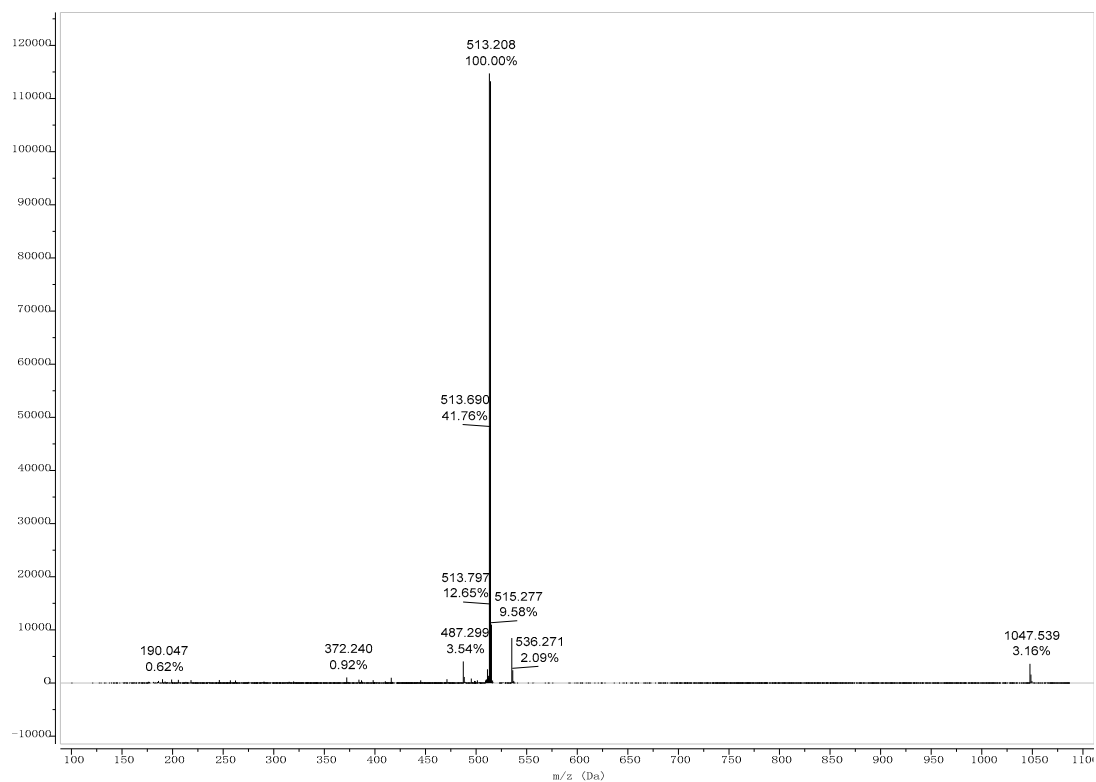


Figure S21. MS for $\text{C}_{25}\text{H}_{33}\text{FN}_8\text{O}_3$ (Mwt.: 512.59): m/z 513.208 ($[\text{M}+\text{H}]^+$, bp) of **6f**.

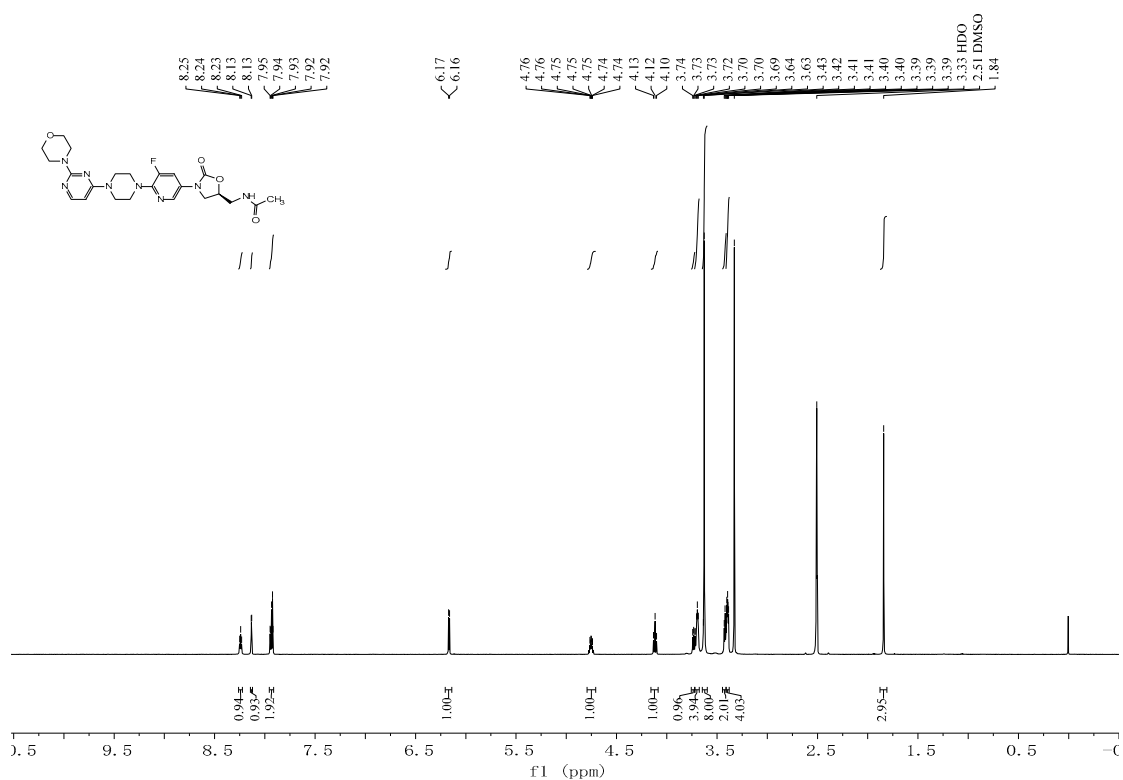


Figure S22. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of **6g**.

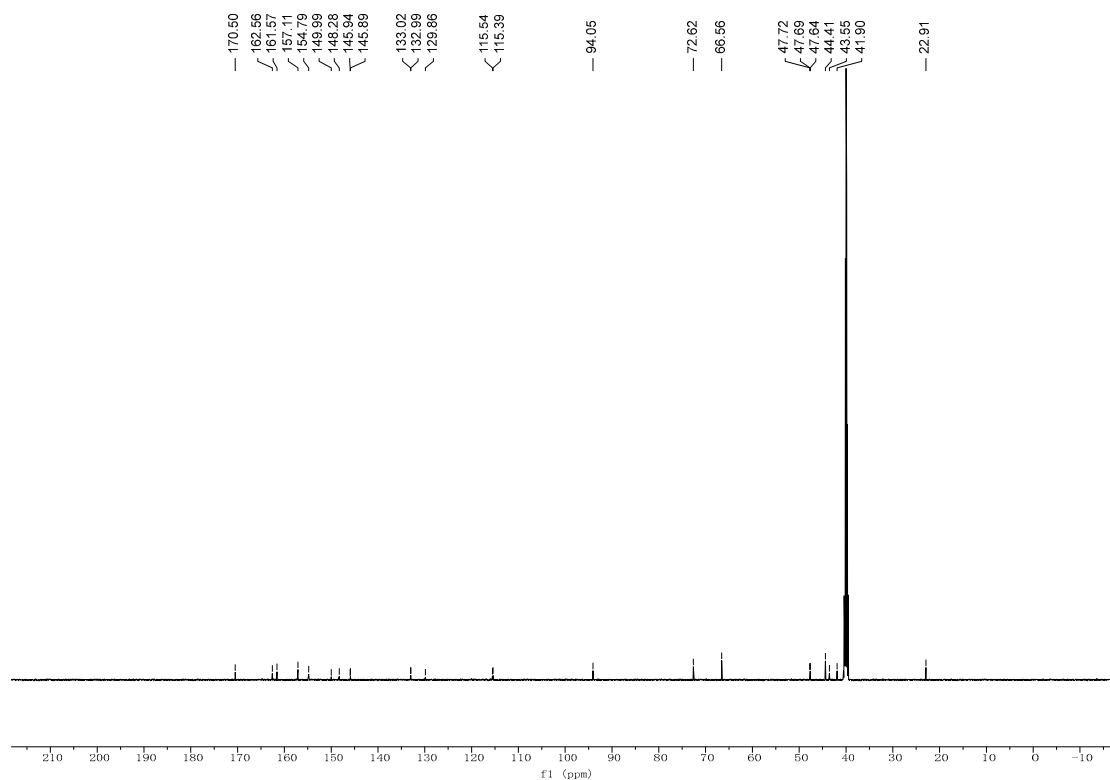


Figure S23. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **6g**.

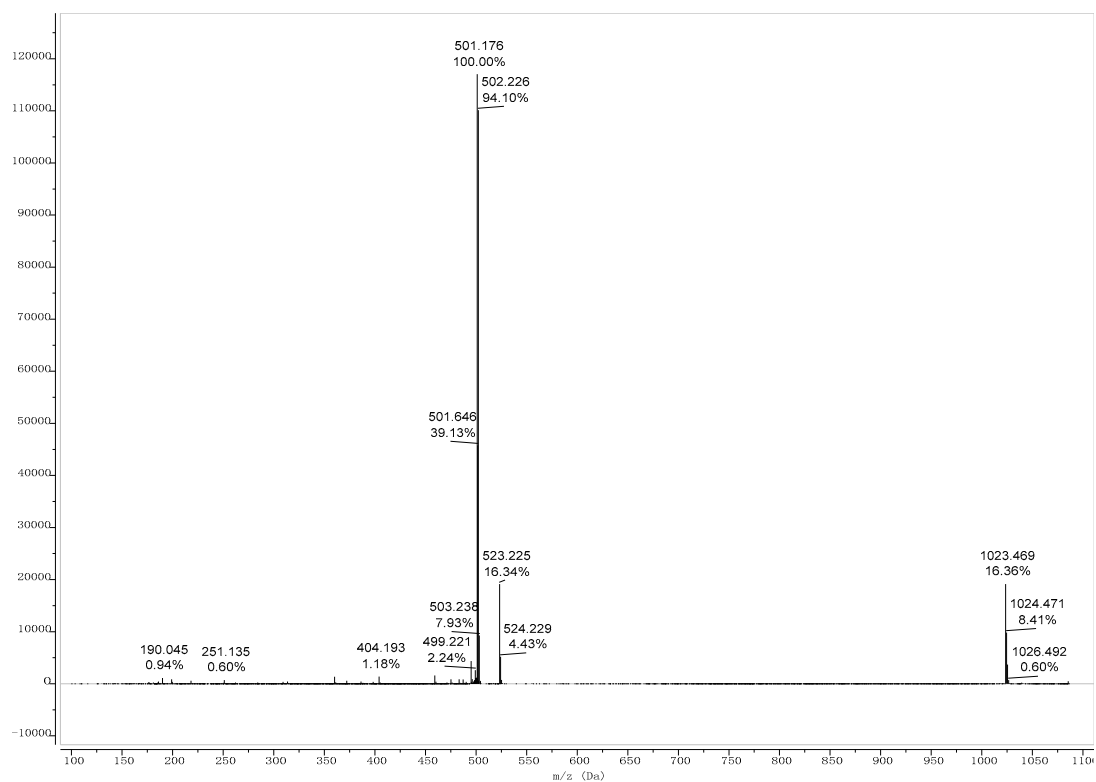


Figure S24. MS for $C_{23}H_{29}FN_8O_4$ (Mwt.: 500.54): m/z 501.176 ($[M+H]^+$, bp) of **6g**.

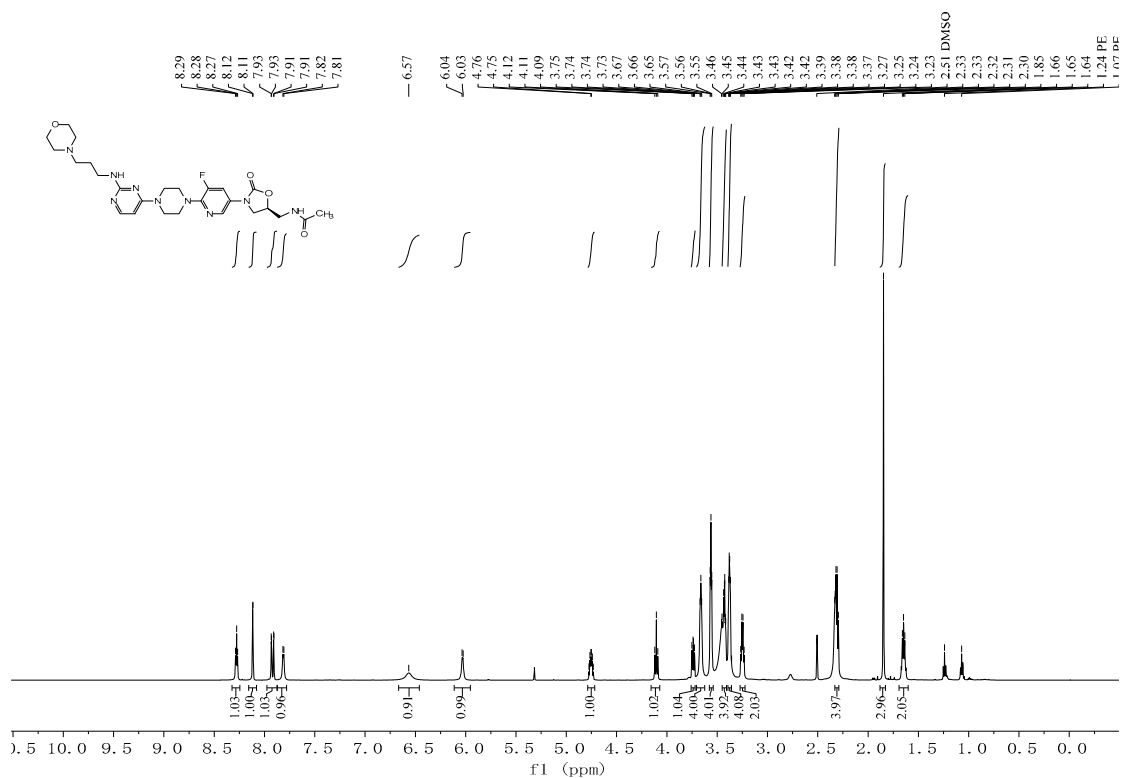


Figure S25. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of **6h**.

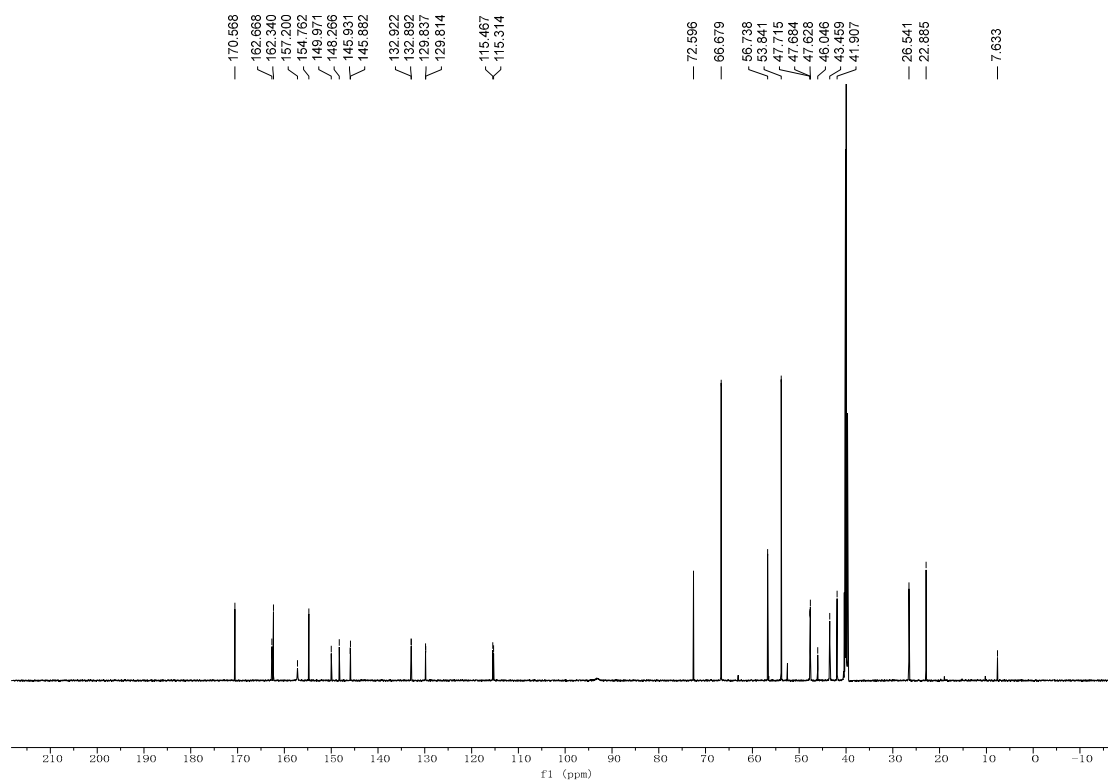


Figure S26. ^{13}C NMR Spectrum ($\text{DMSO-}d_6$, 150 MHz) of **6h**.

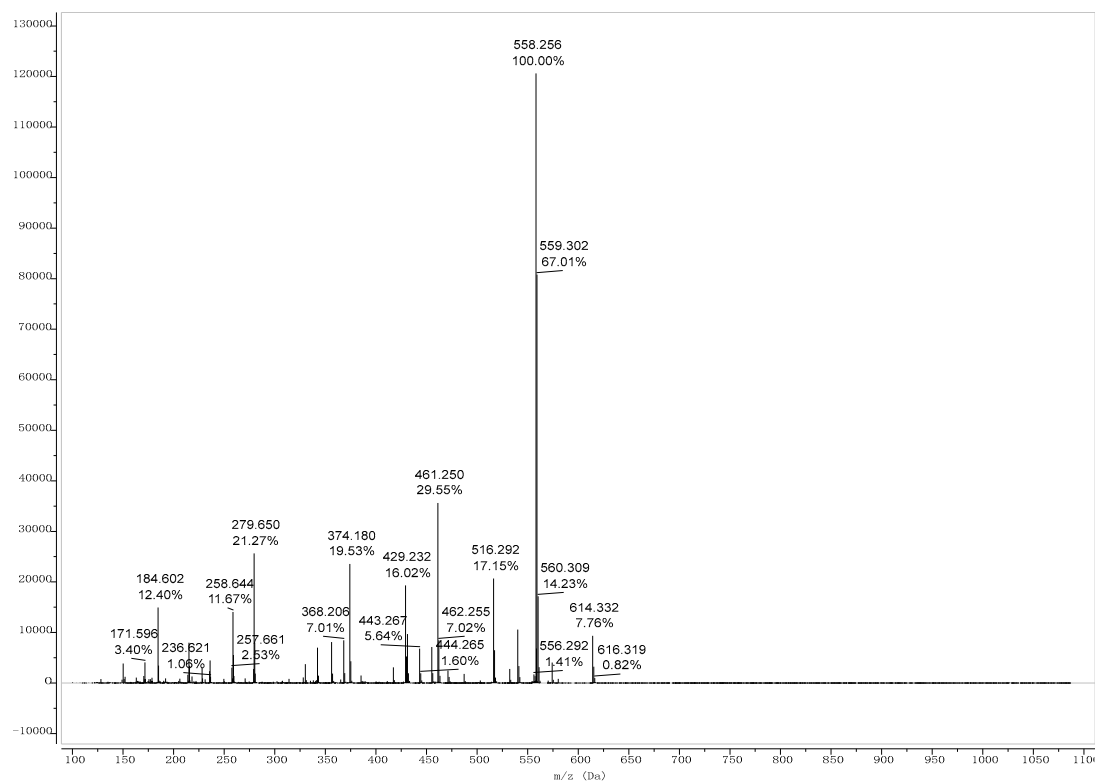


Figure S27. MS for $\text{C}_{26}\text{H}_{35}\text{FN}_8\text{O}_4$ (Mwt.: 557.63): m/z 558.256 ($[\text{M}+\text{H}]^+$, bp) of **6h**.

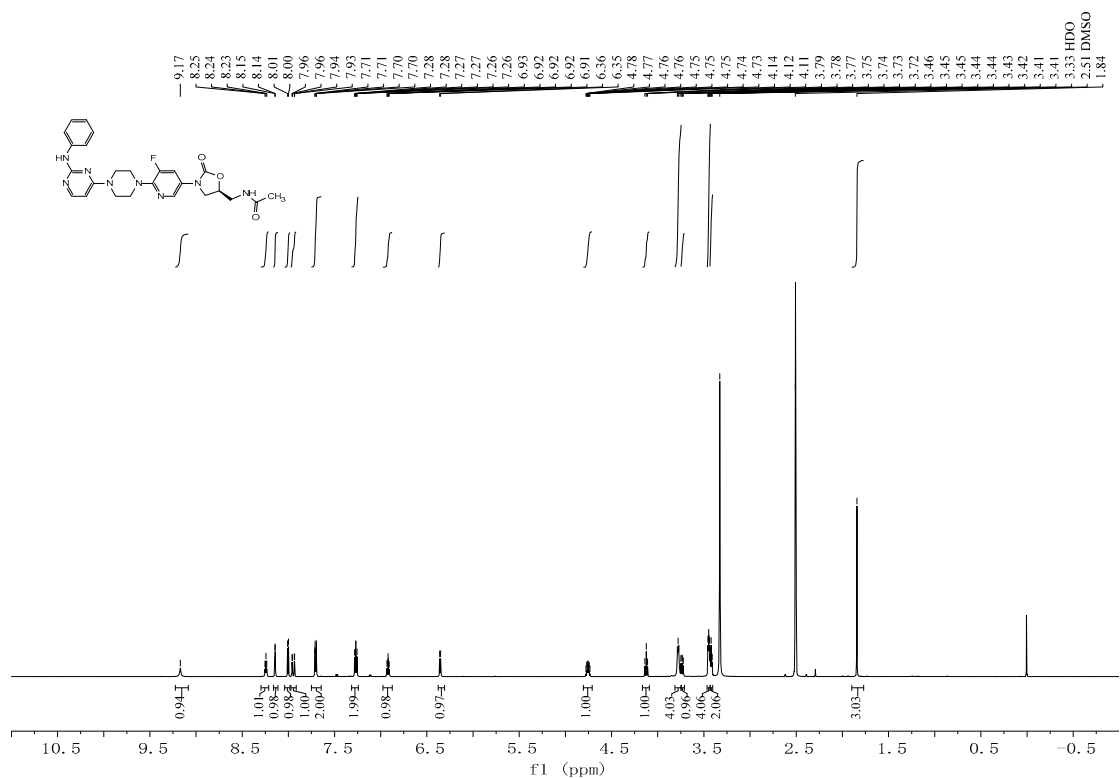


Figure S28. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of **6i**.

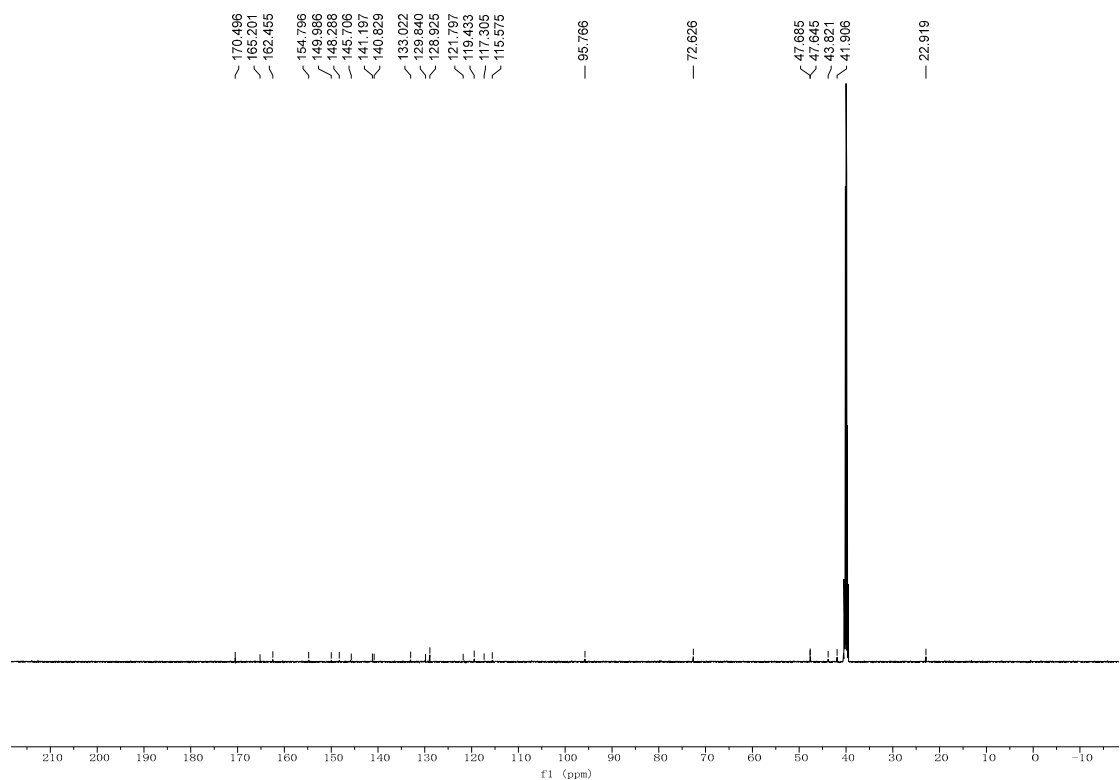


Figure S29. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **6i**.

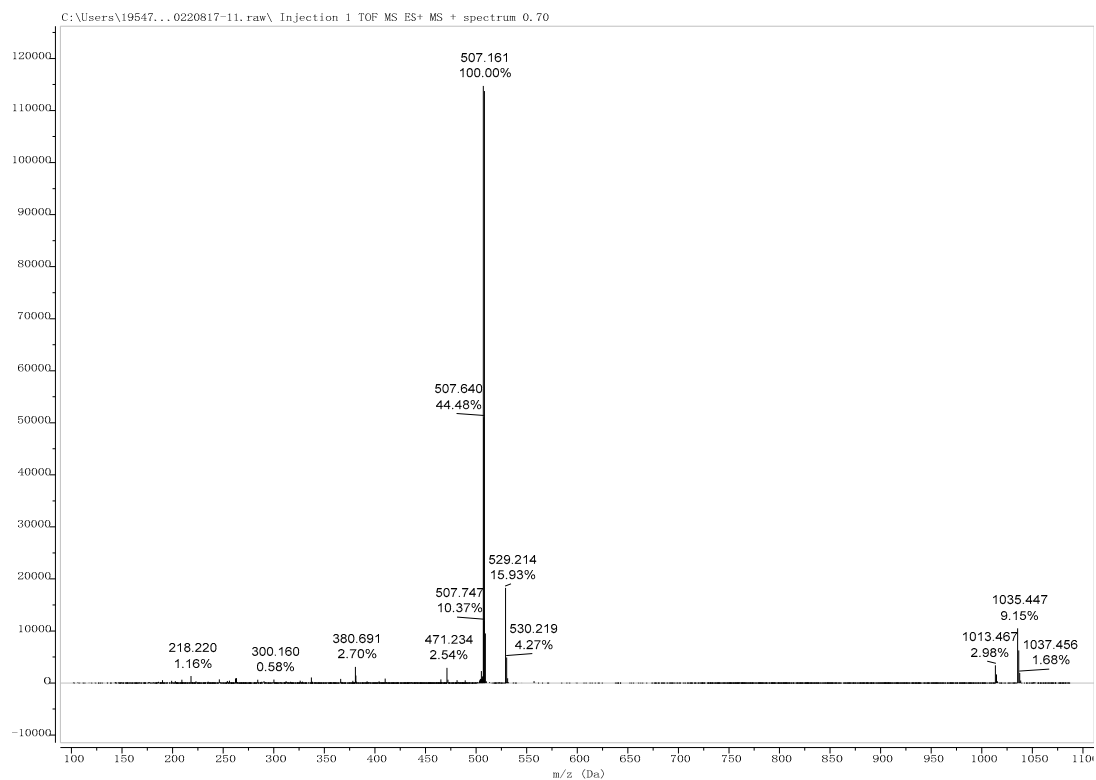


Figure S30. MS for $C_{25}H_{27}FN_8O_3$ (Mwt.: 506.54): m/z 507.161 ($[M+H]^+$, bp) of **6i**.

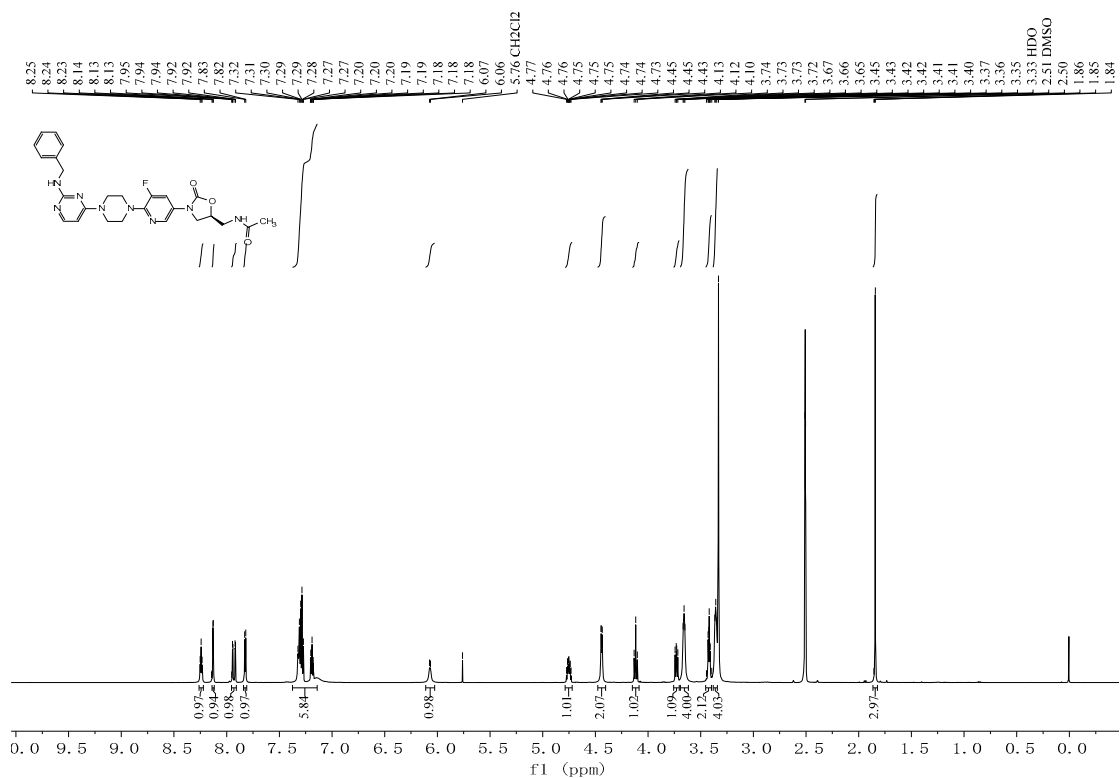


Figure S31. ^1H NMR Spectrum ($DMSO-d_6$, 600 MHz) of **6j**.

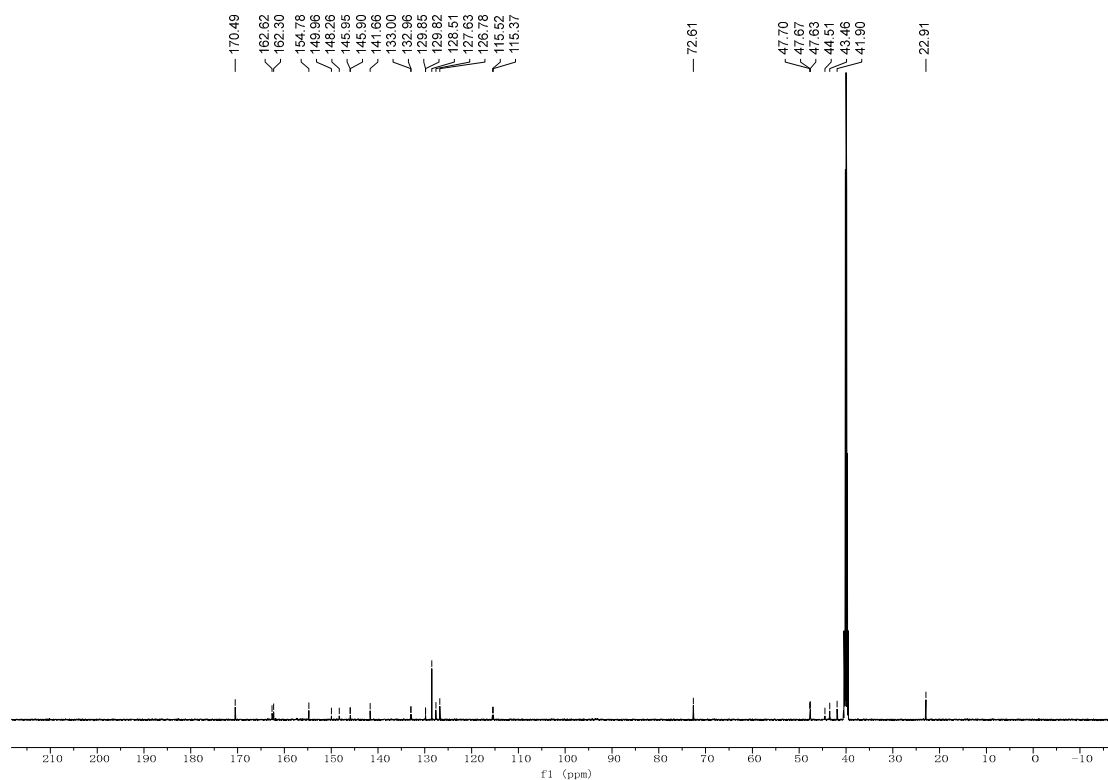


Figure S32. ^{13}C NMR Spectrum ($\text{DMSO-}d_6$, 150 MHz) of **6j**.

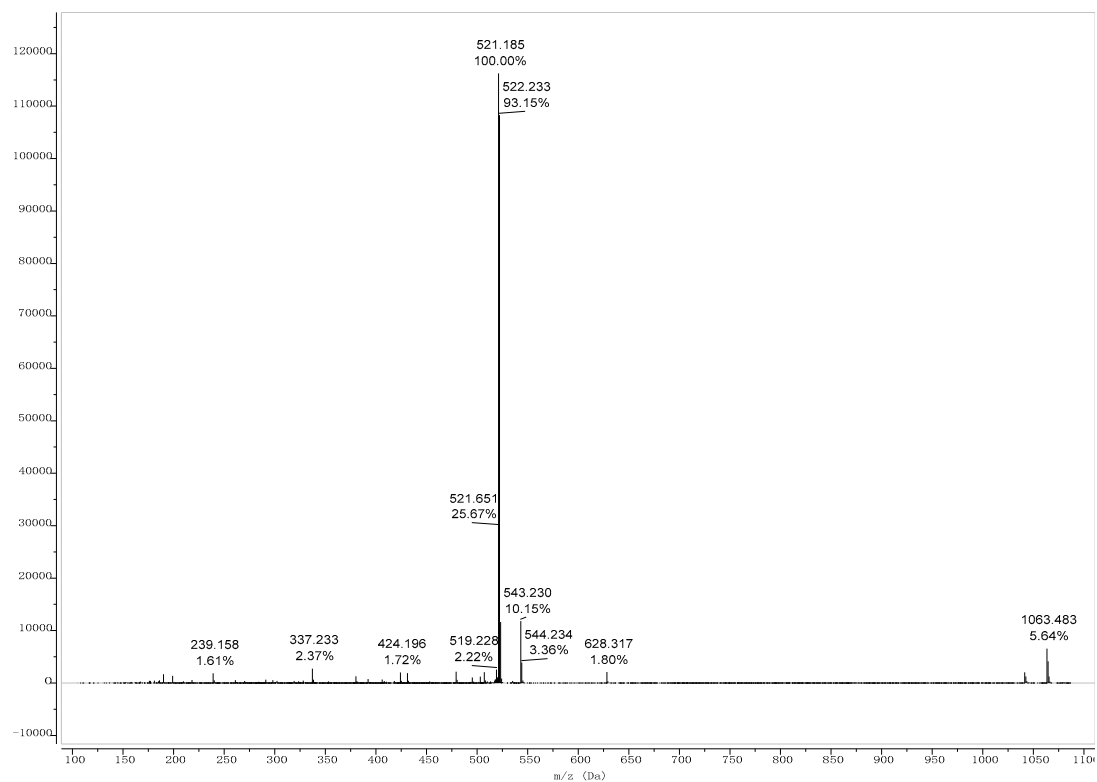


Figure S33. MS for $\text{C}_{26}\text{H}_{29}\text{FN}_8\text{O}_3$ (Mwt.: 520.57): m/z 521.185 ($[\text{M}+\text{H}]^+$, bp) of **6j**.

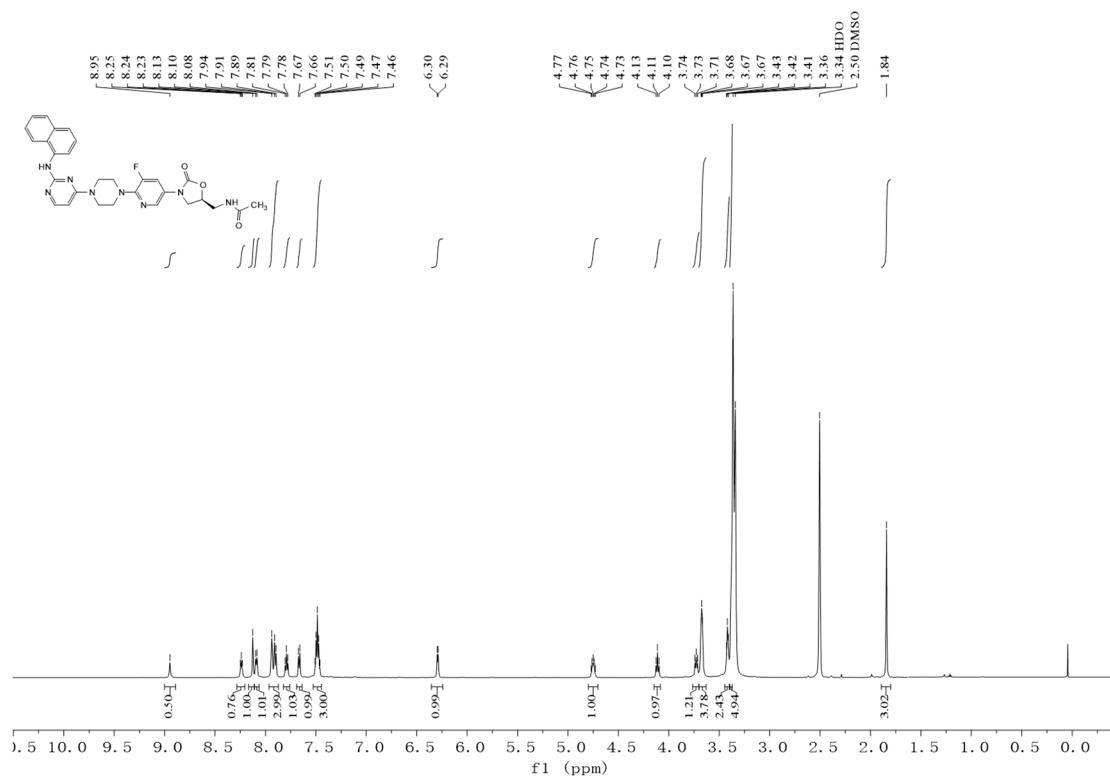


Figure S34. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of **6k**.

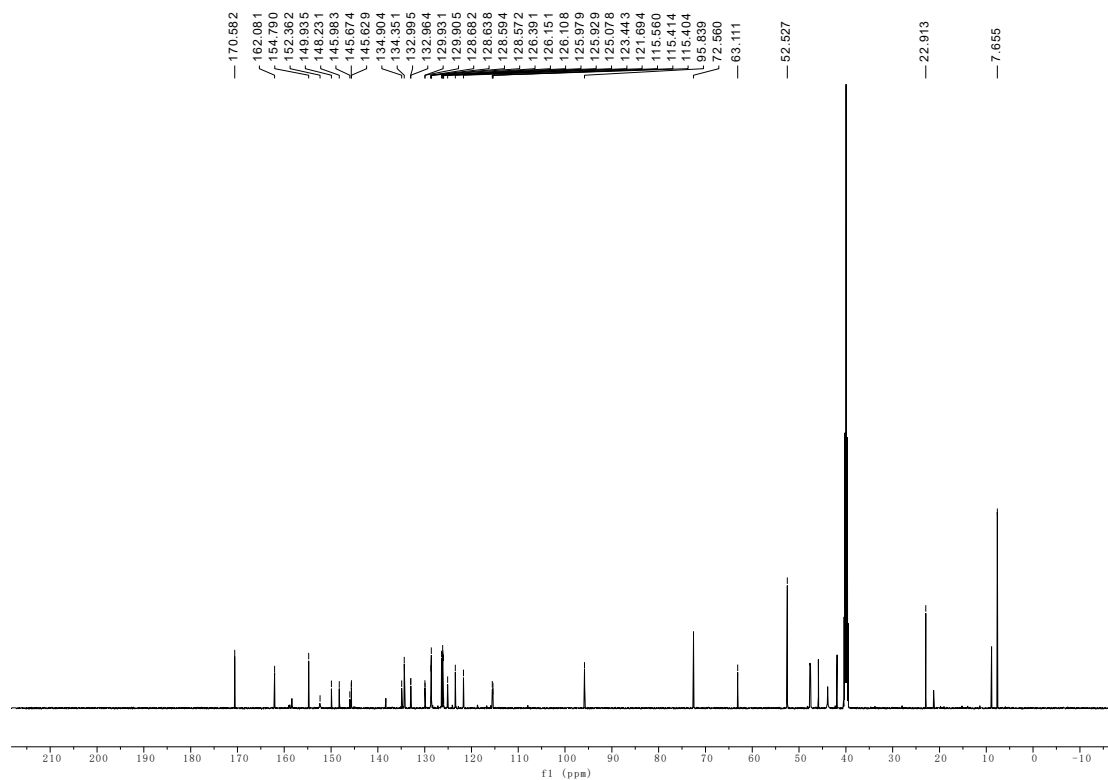


Figure S35. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **6k**.

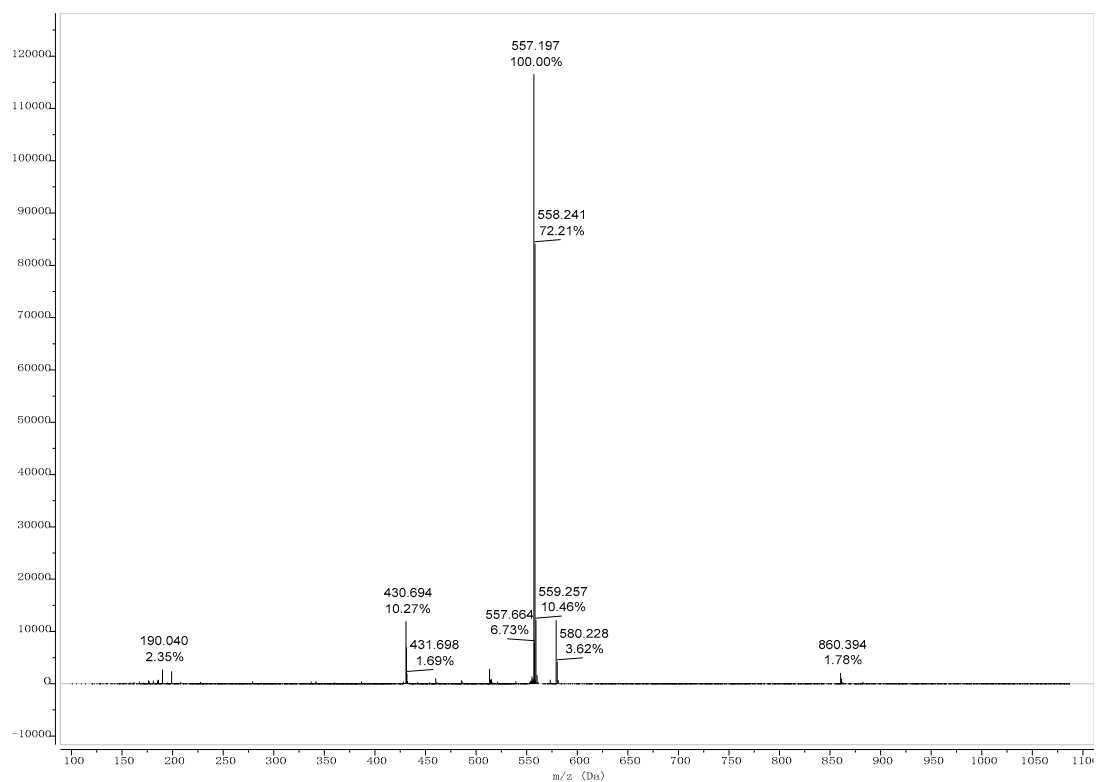


Figure S36. MS for $C_{29}H_{29}FN_8O_3$ (Mwt.: 556.60): m/z 557.197 ($[M+H]^+$, bp) of **6k**.

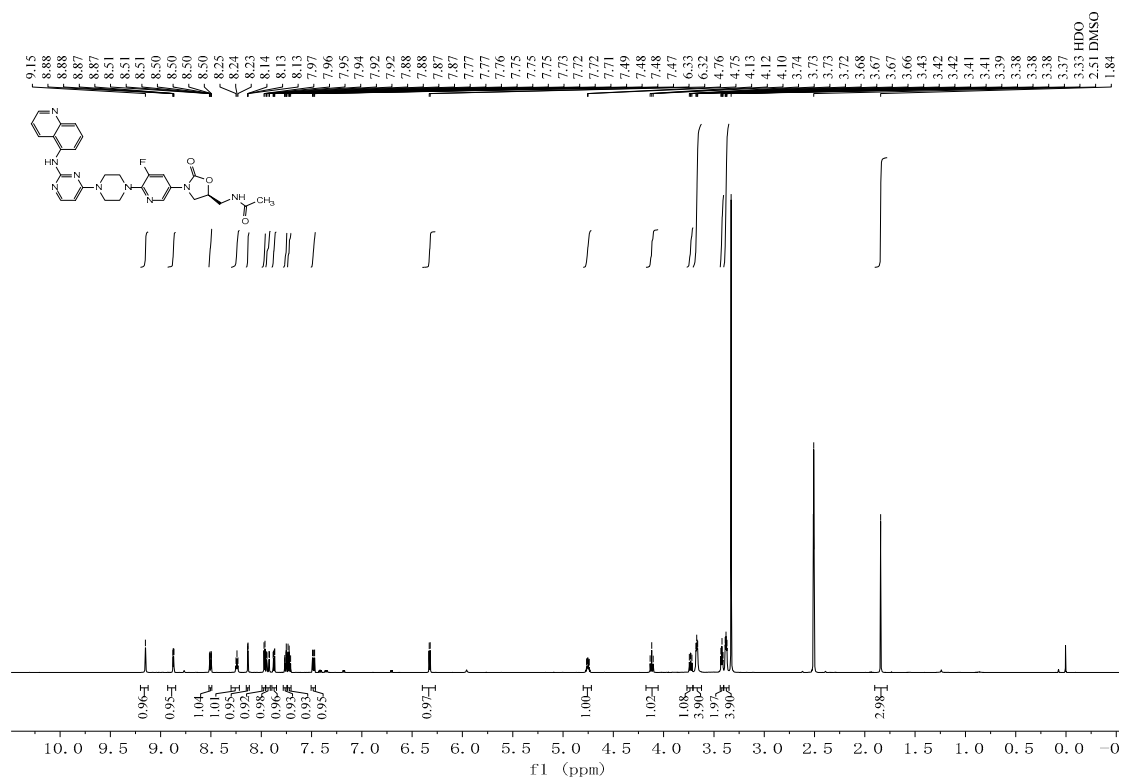


Figure S37. ^1H NMR Spectrum ($DMSO-d_6$, 600 MHz) of **6l**.

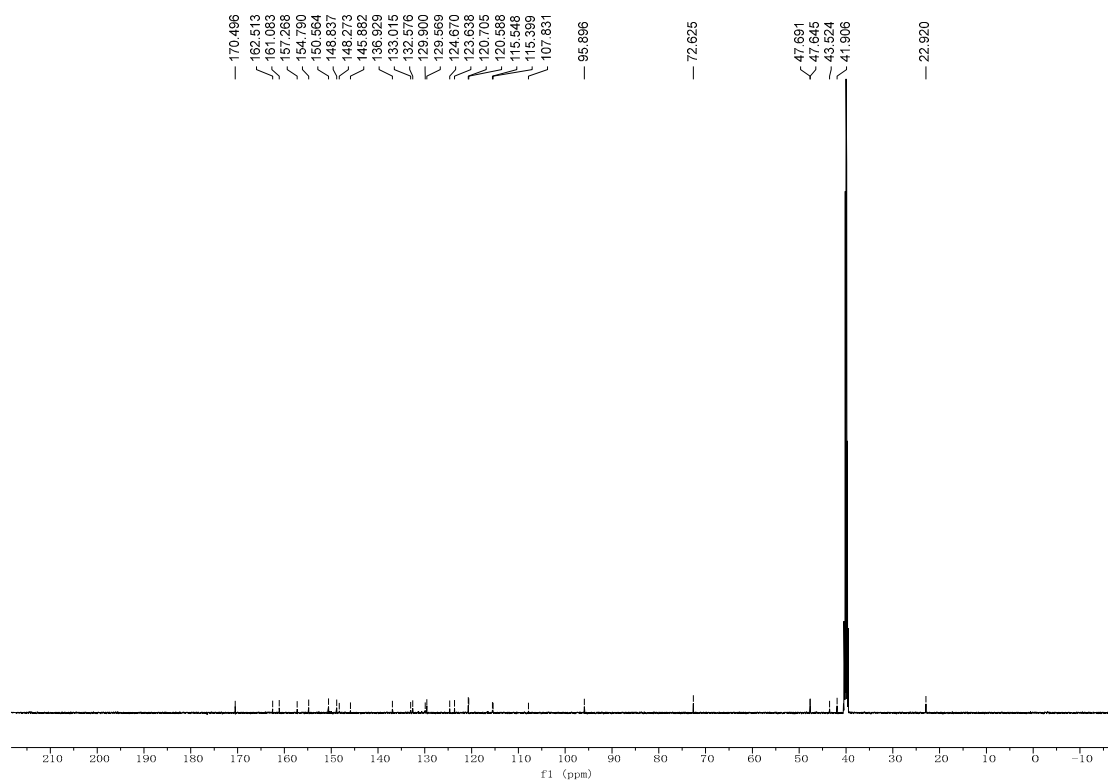


Figure S38. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **6l**.

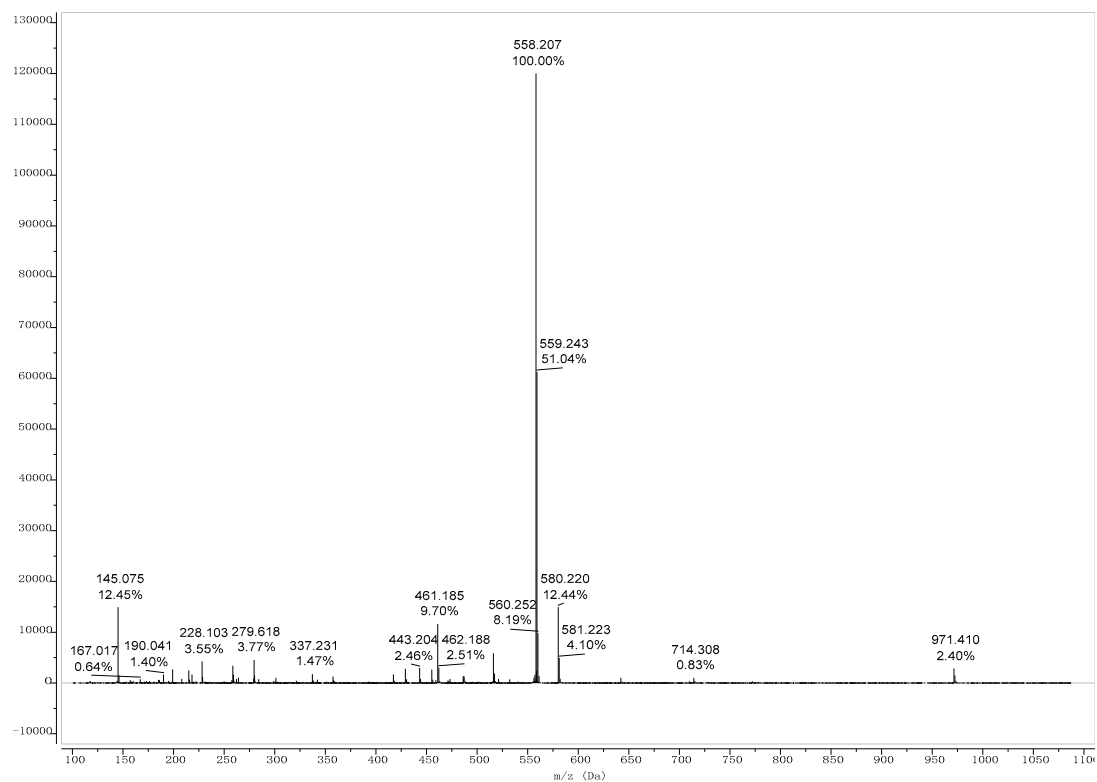


Figure S39. MS for C₂₈H₂₈FN₉O₃ (Mwt.: 557.59): *m/z* 558.207 ([M+H]⁺, bp) of **6l**.

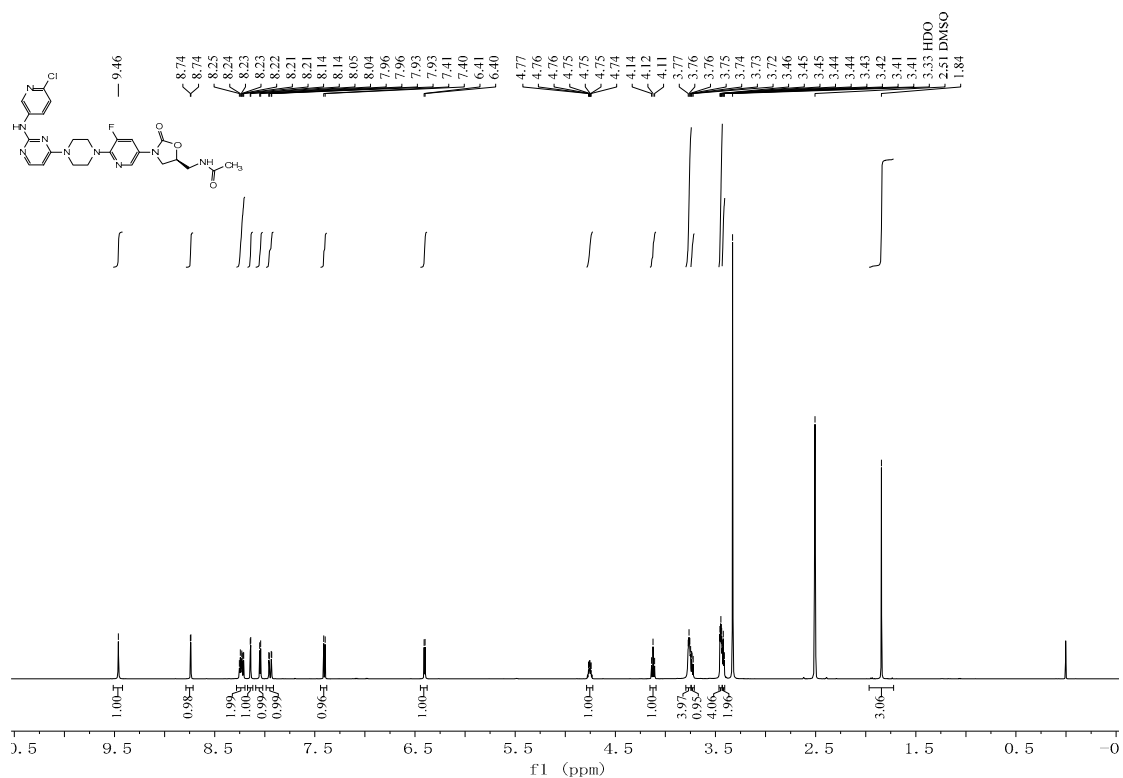


Figure S40. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of **6m**.

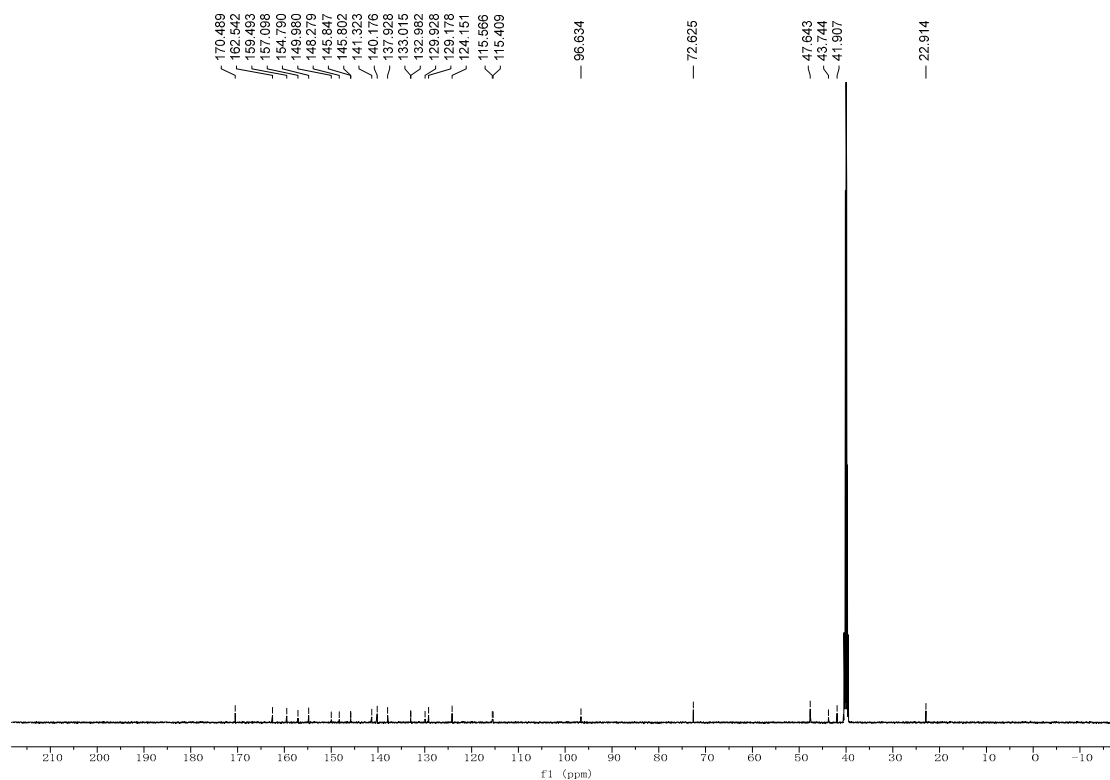


Figure S41. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **6m**.

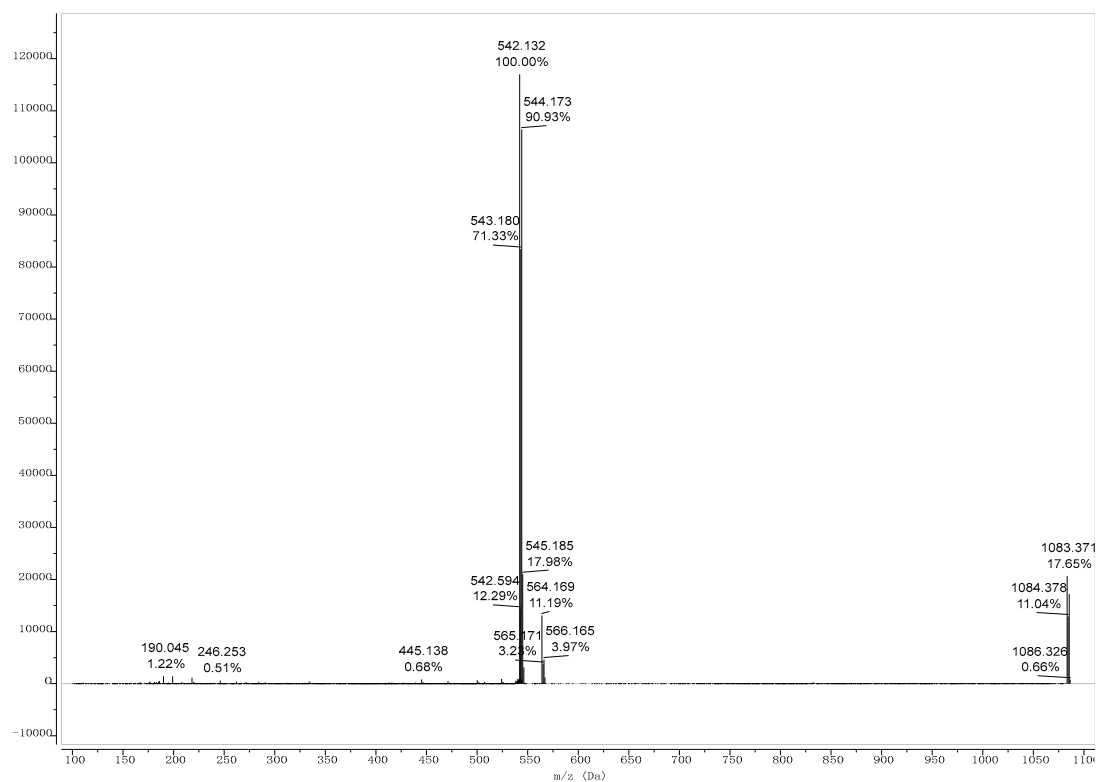


Figure S42. MS for $C_{24}H_{25}ClFN_9O_3$ (Mwt.: 541.97): m/z 542.132 ($[M+H]^+$, bp) of **6m**.

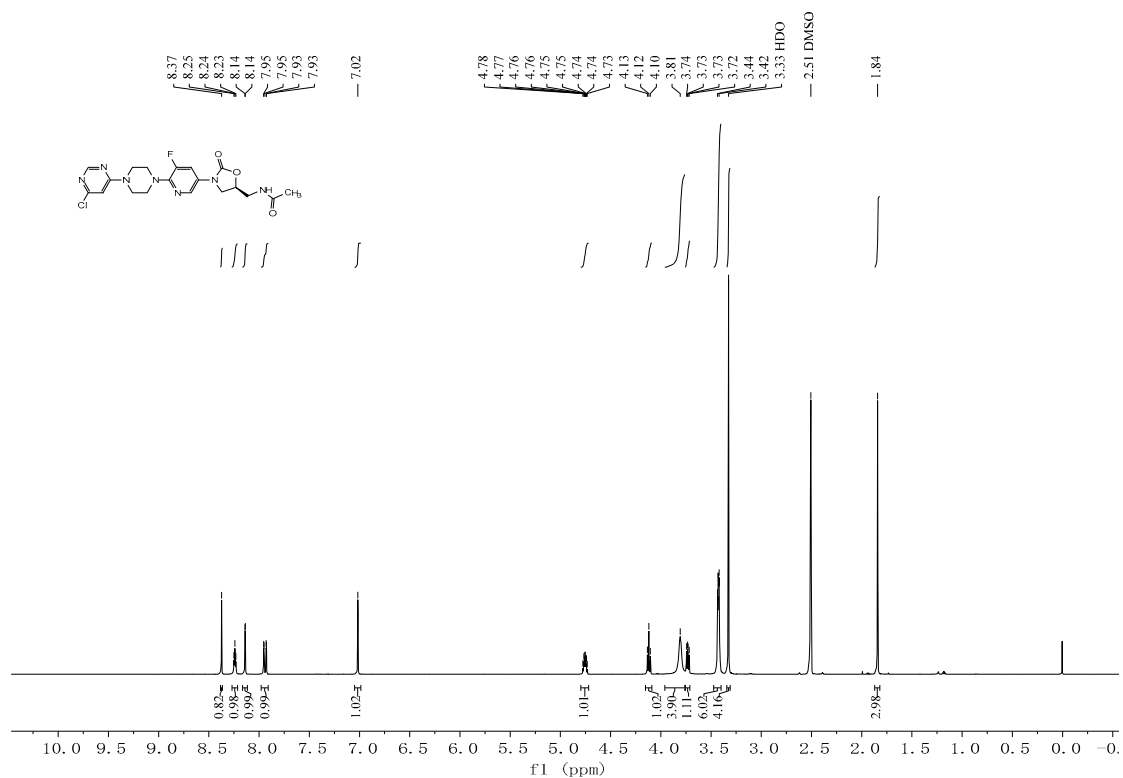


Figure S43. ^1H NMR Spectrum ($DMSO-d_6$, 600 MHz) of **7a**.

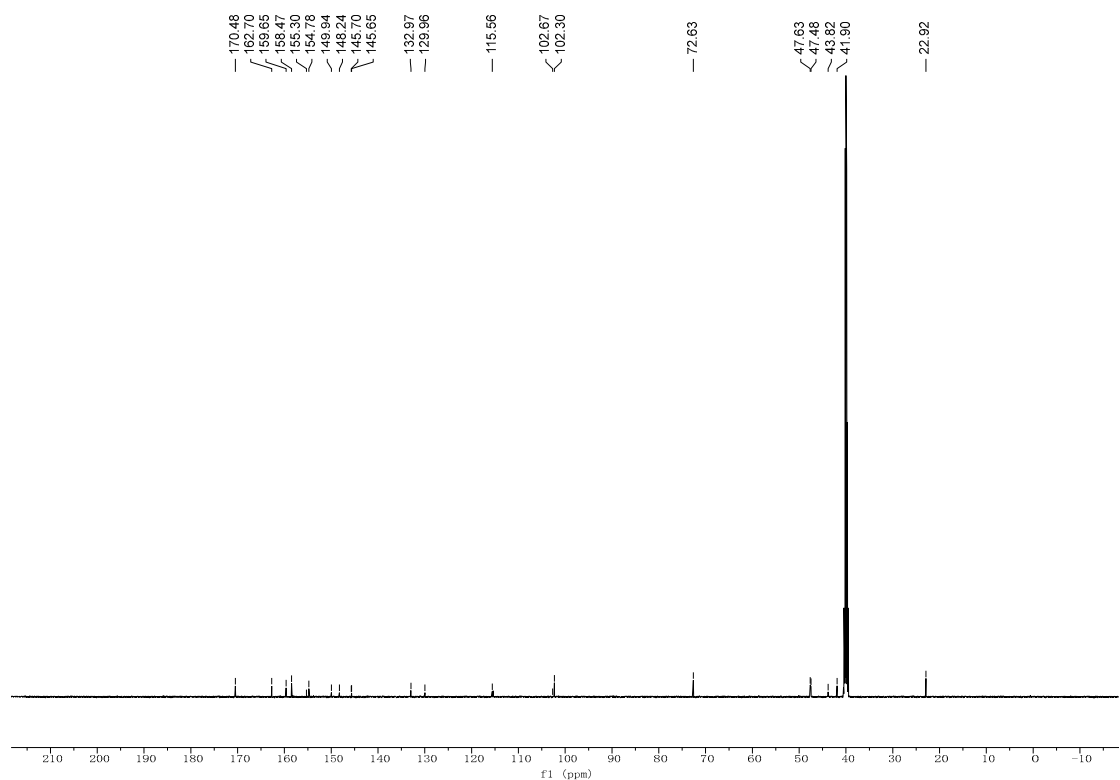


Figure S44. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **7a**.

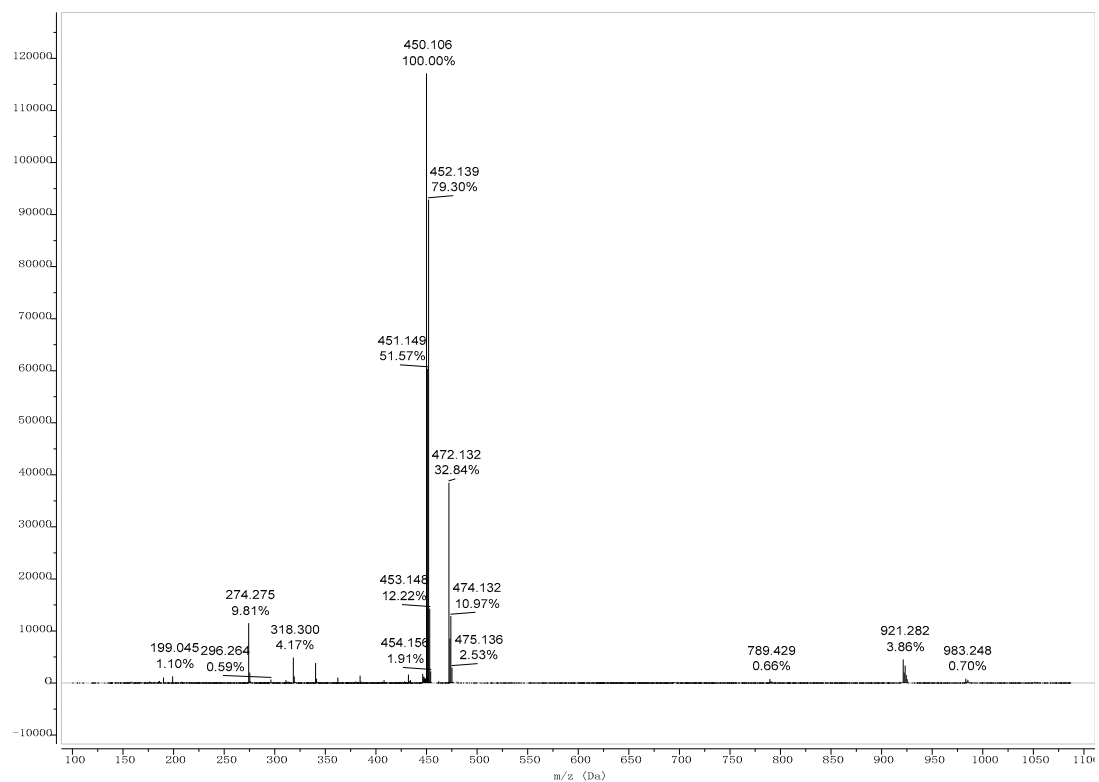


Figure S45. MS for C₁₉H₂₁ClFN₇O₃ (Mwt.: 449.87): m/z 450.106 ([M+H]⁺, bp) of **7a**.

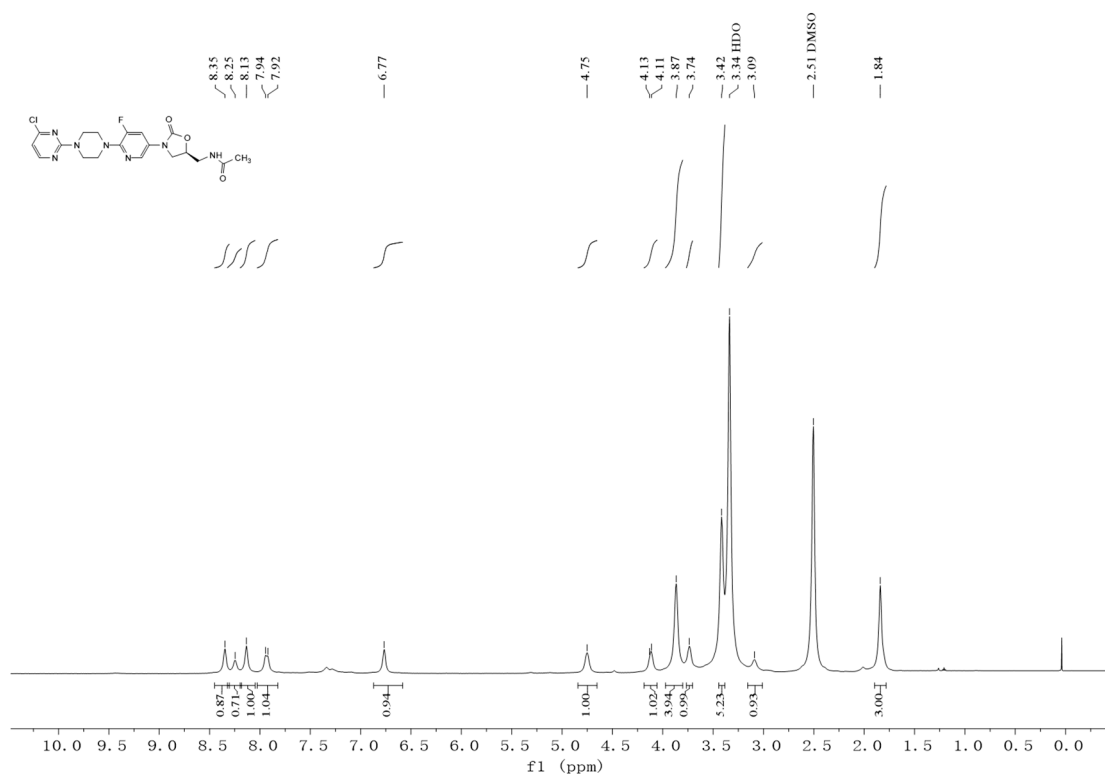


Figure S46. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of **7b**.

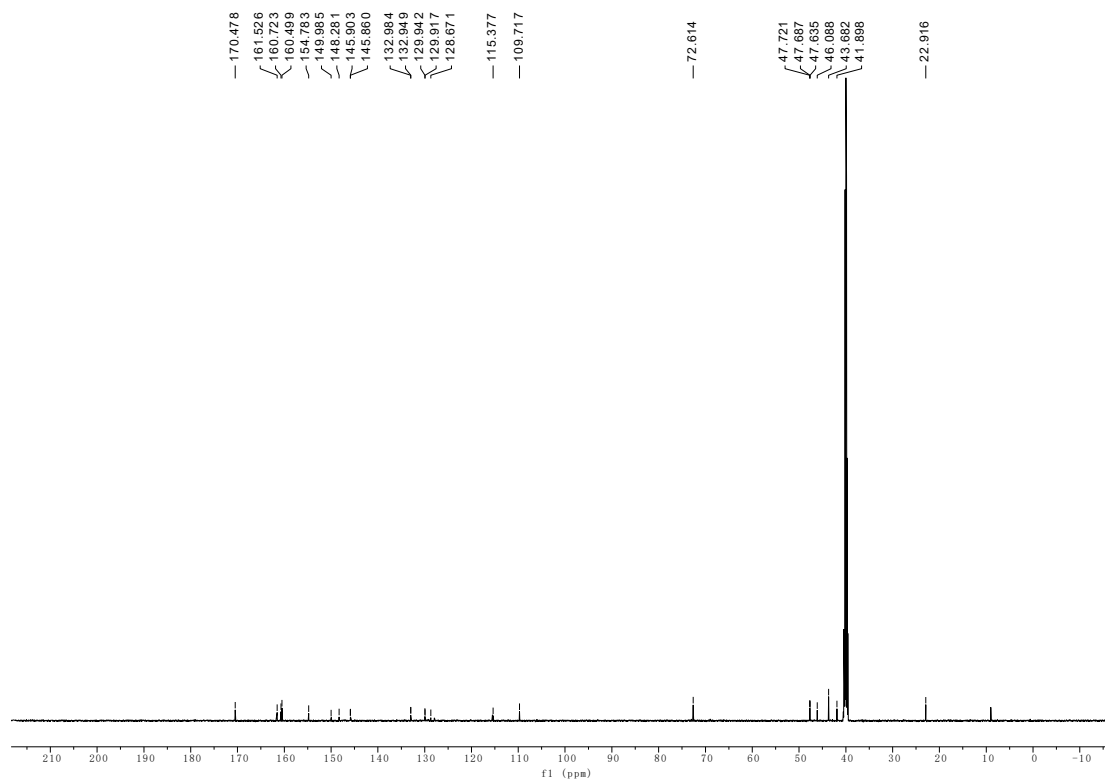


Figure S47. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **7b**.

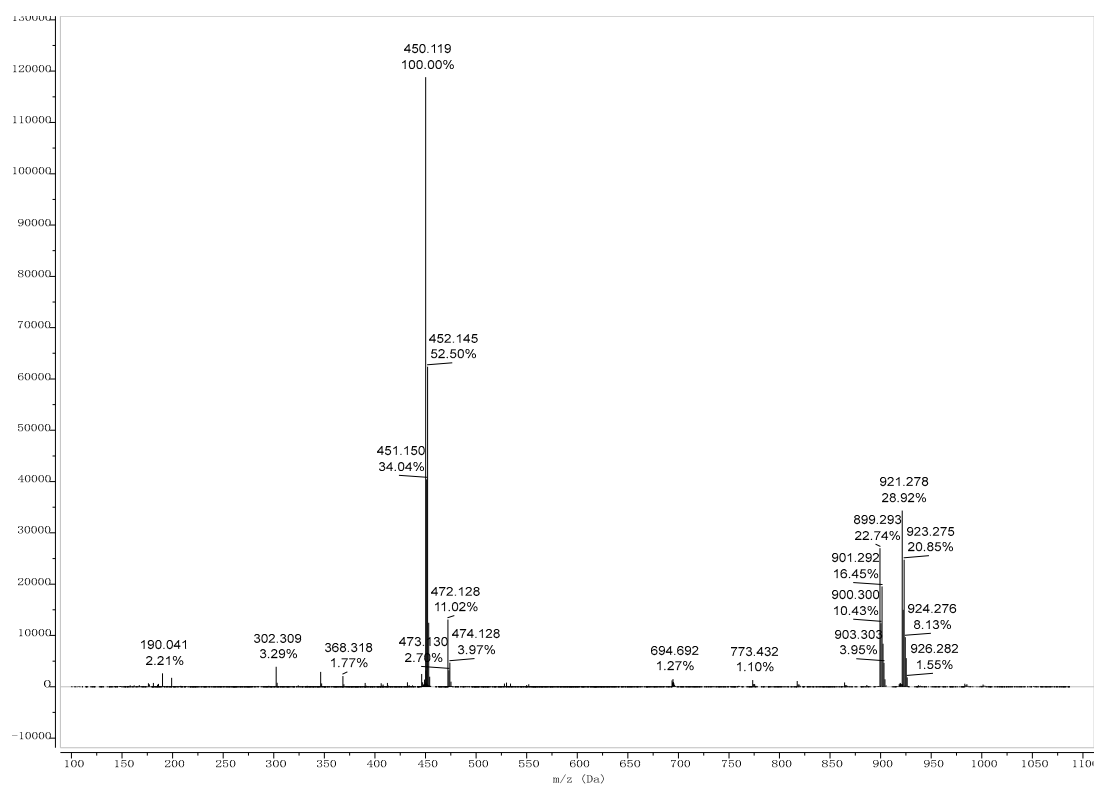


Figure S48. MS for C₁₉H₂₁ClFN₇O₃ (Mwt.: 449.87): m/z 450.119 ([M+H]⁺, bp) of **7b**.

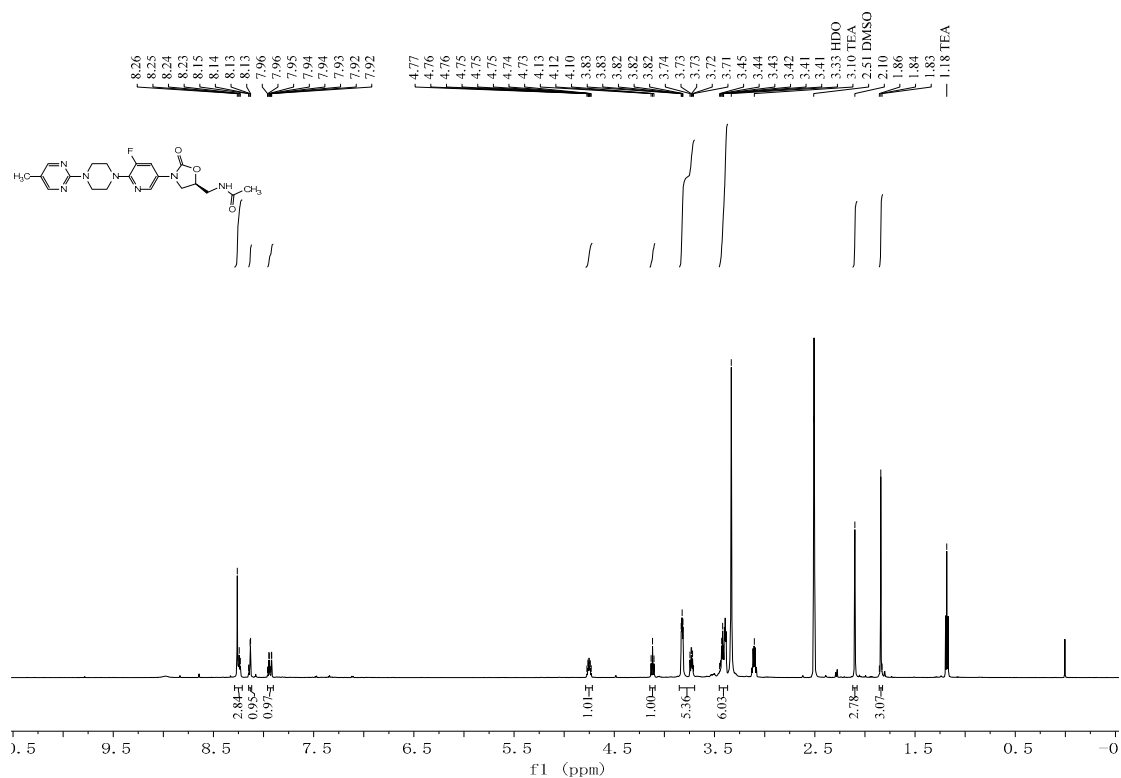


Figure S49. ¹H NMR Spectrum (DMSO-d₆, 600 MHz) of **7c**.

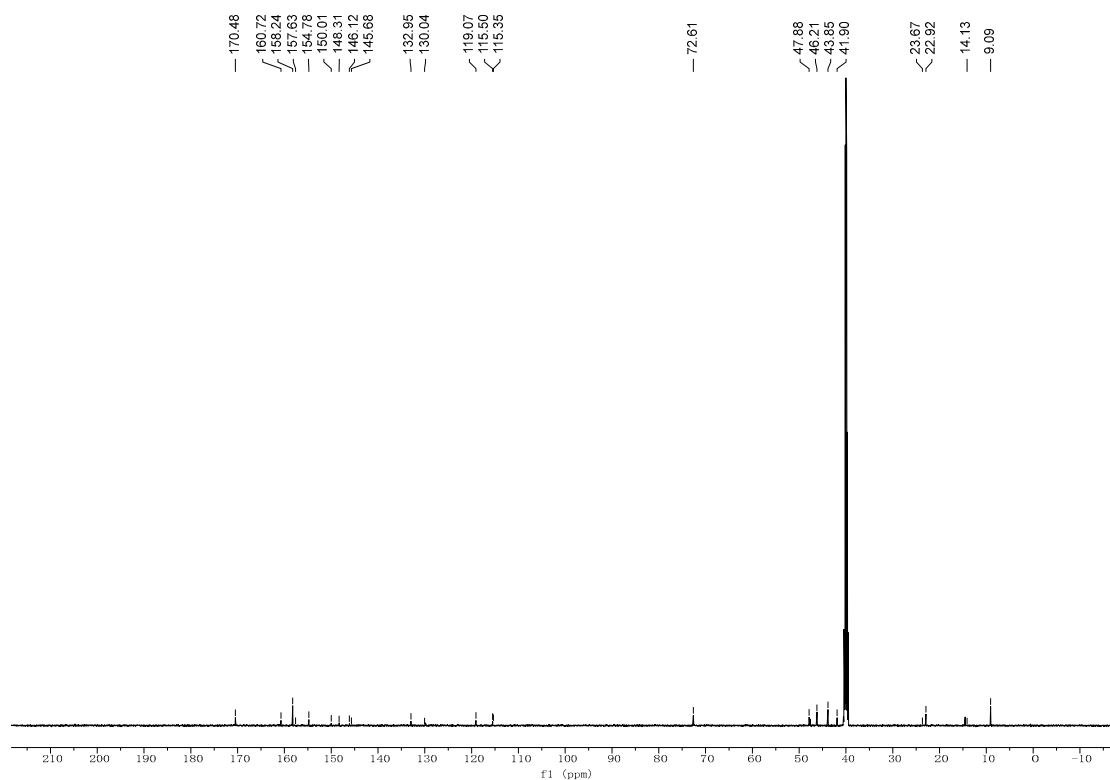


Figure S50. ^{13}C NMR Spectrum ($\text{DMSO-}d_6$, 150 MHz) of **7c**.

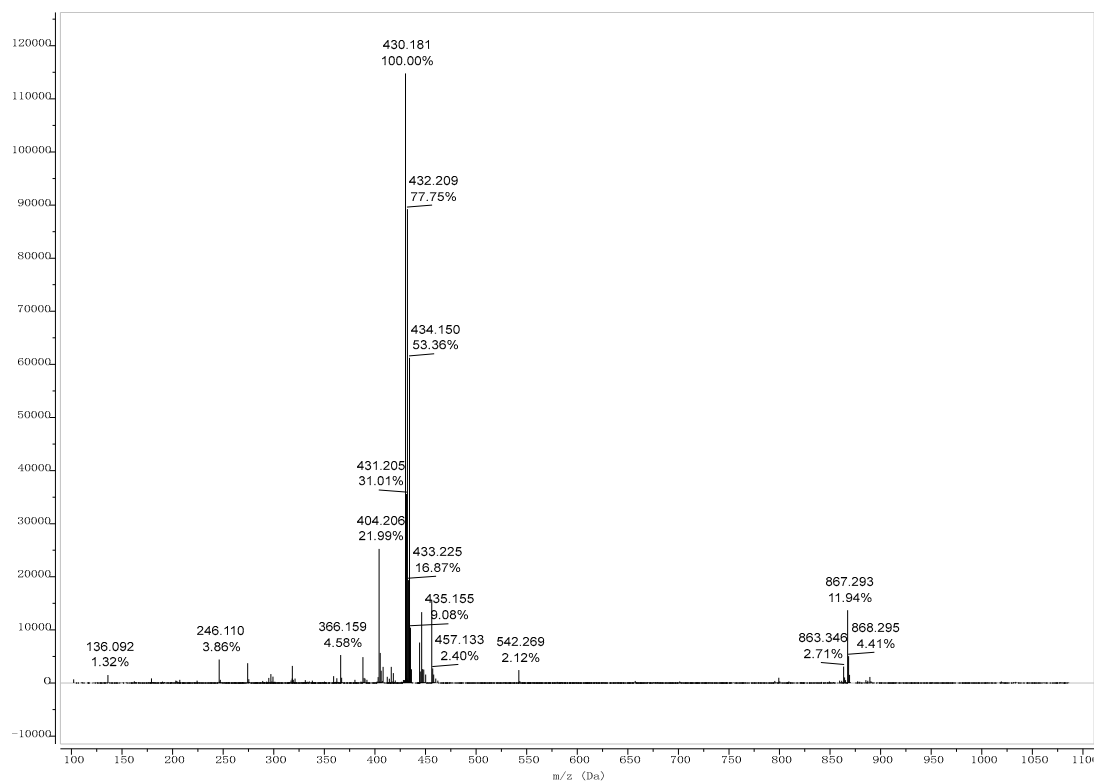


Figure S51. MS for $\text{C}_{20}\text{H}_{24}\text{FN}_7\text{O}_3$ (Mwt.: 429.46): m/z 430.181 ($[\text{M}+\text{H}]^+$, bp) of **7c**.

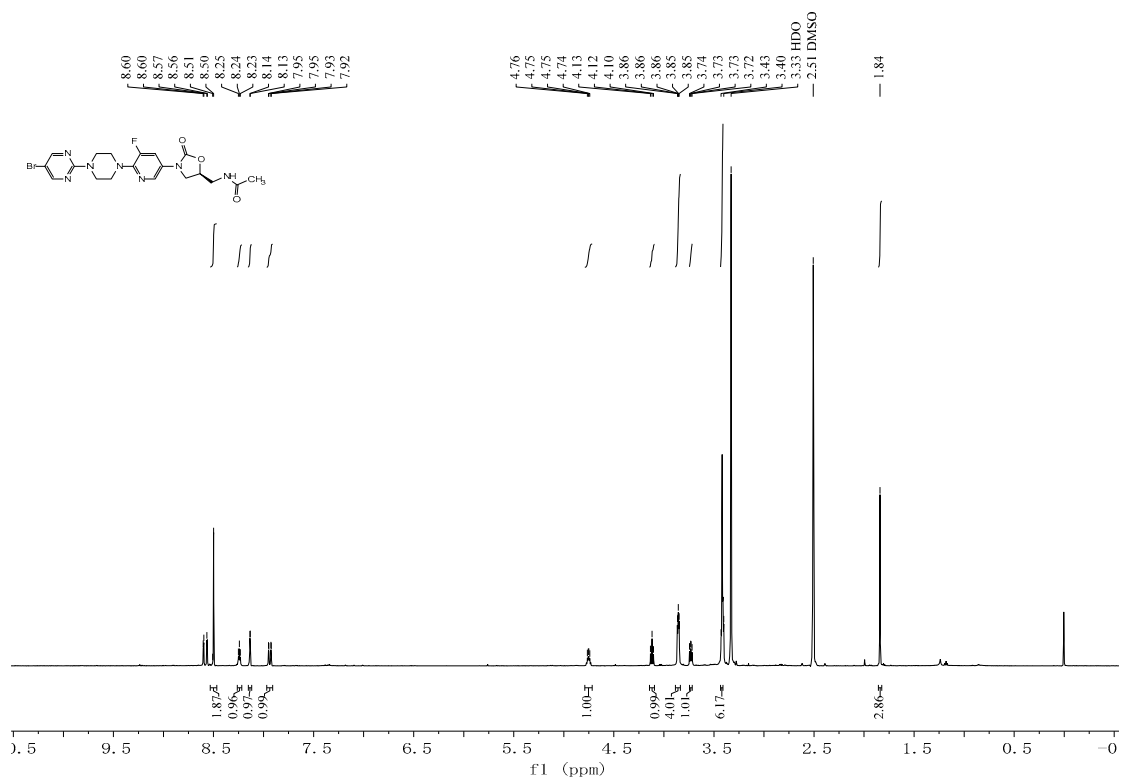


Figure S52. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of 7d.

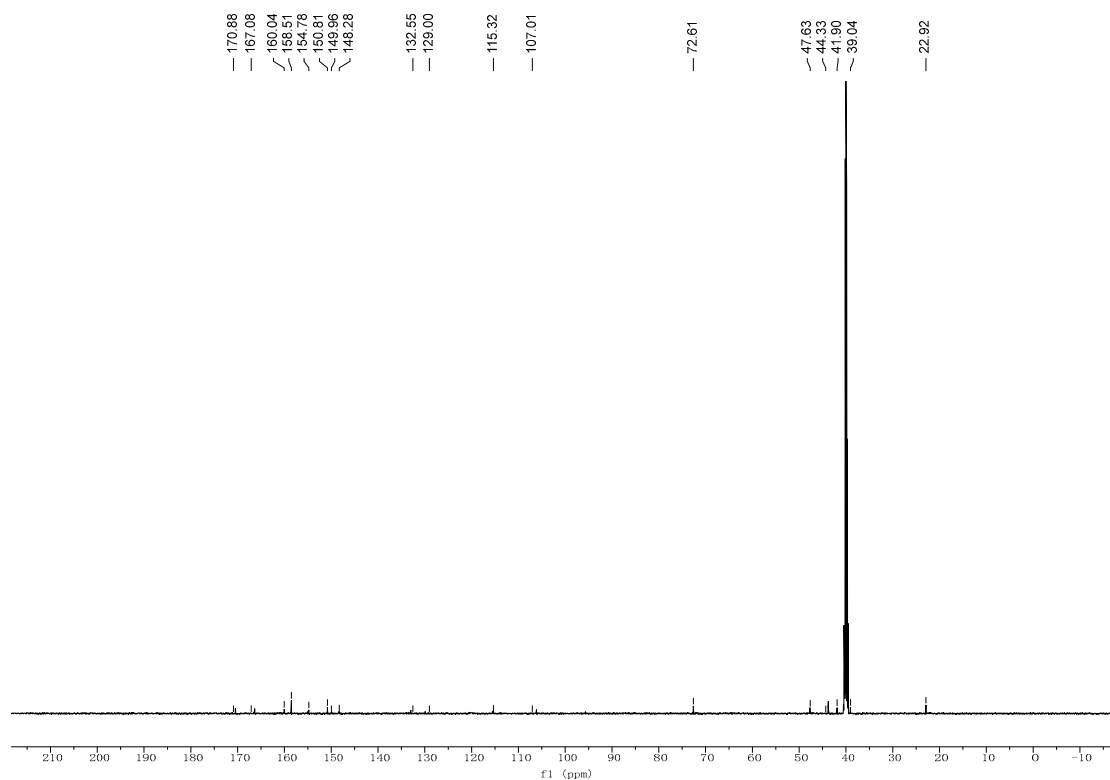


Figure S53. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of 7d.

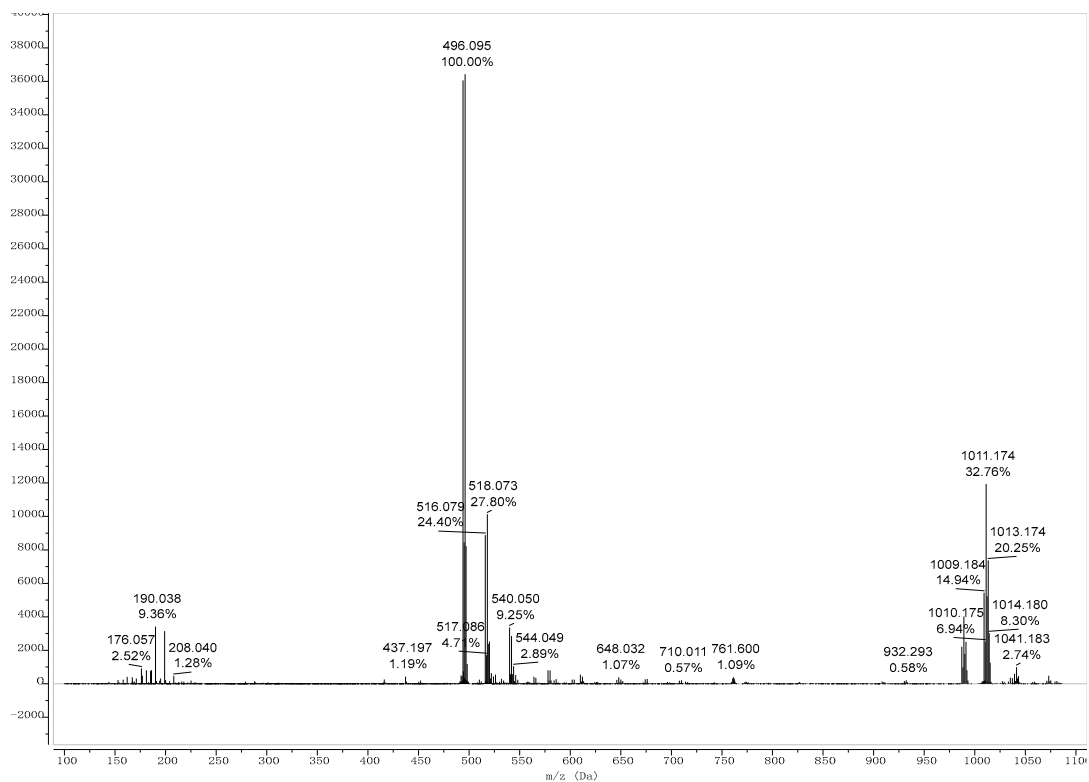


Figure S54. MS for $C_{19}H_{21}BrFN_7O_3$ (Mwt.: 494.33): m/z 496.095 ($[M+H]^+$, bp) of **7d**.

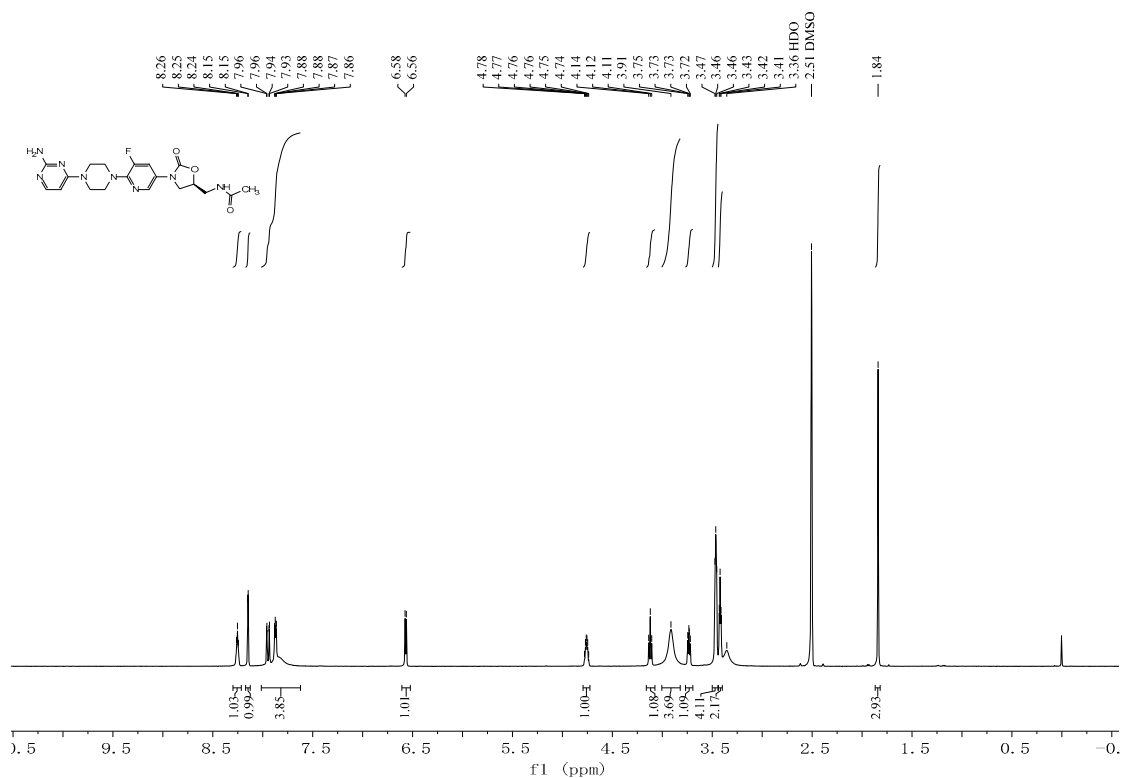


Figure S55. ^1H NMR Spectrum ($DMSO-d_6$, 600 MHz) of **7e**.

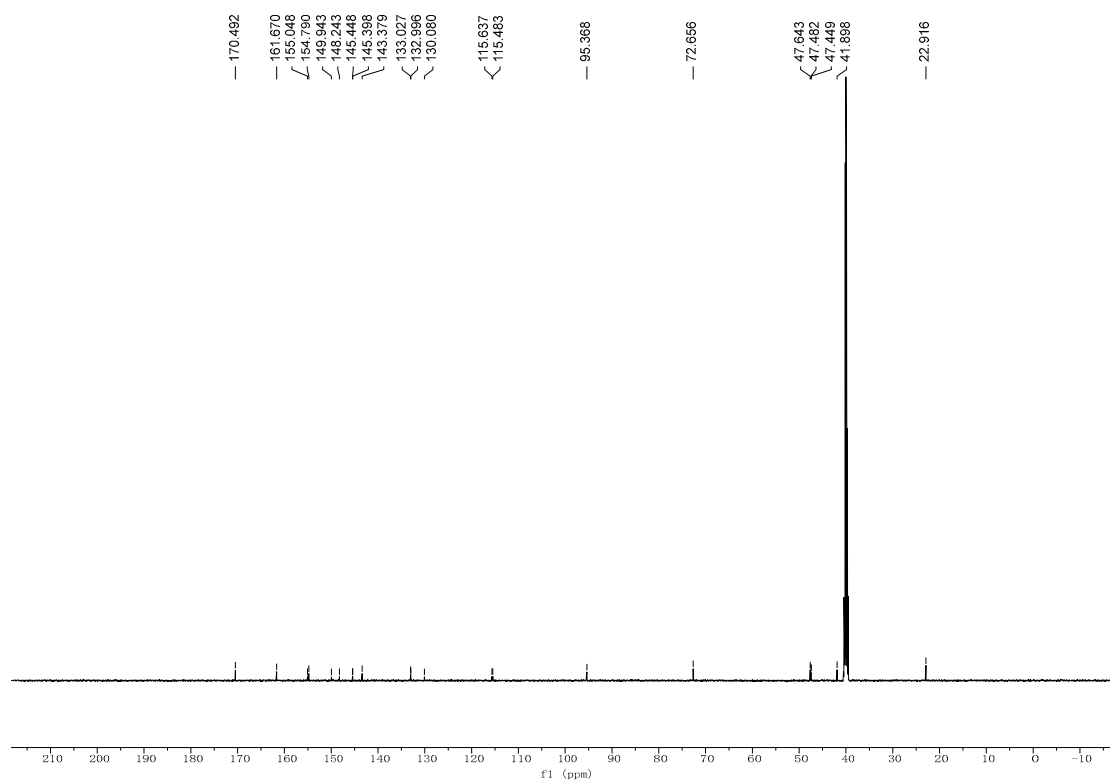


Figure S56. ^{13}C NMR Spectrum (DMSO- d_6 , 150 MHz) of **7e**.

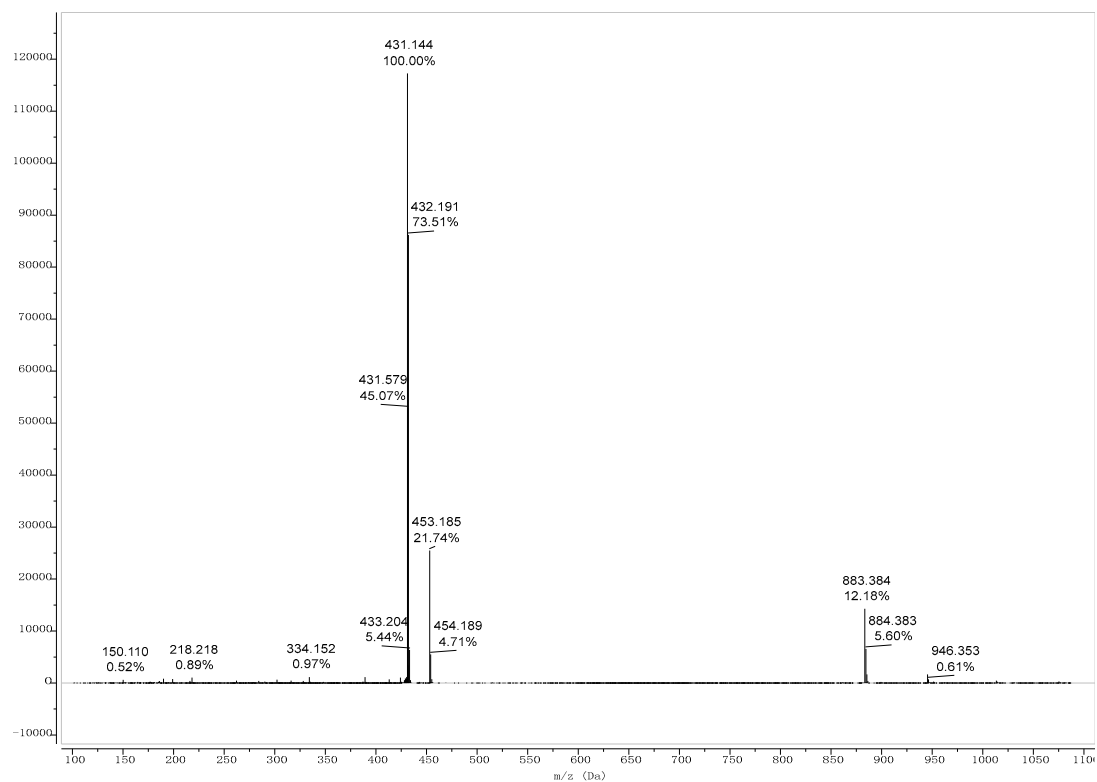


Figure S57. MS for $\text{C}_{19}\text{H}_{23}\text{FN}_8\text{O}_3$ (Mwt.: 430.44): m/z 431.144 ($[\text{M}+\text{H}]^+$, bp) of **7e**.

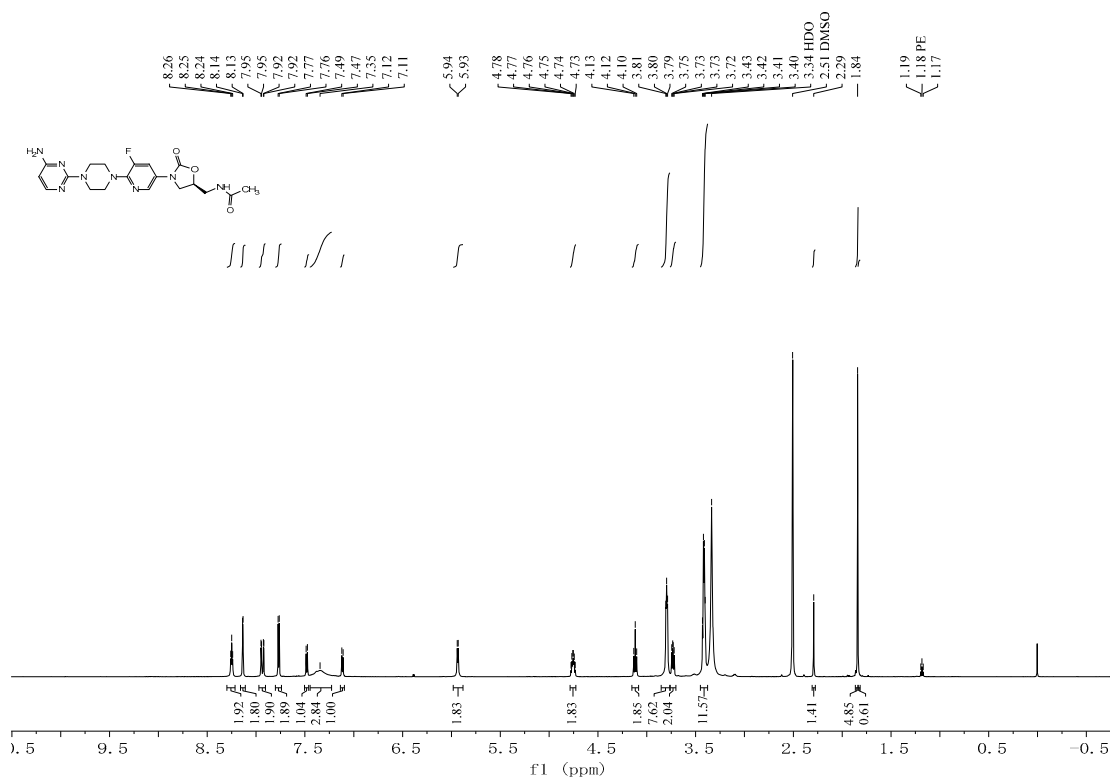


Figure S58. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of **7f**.

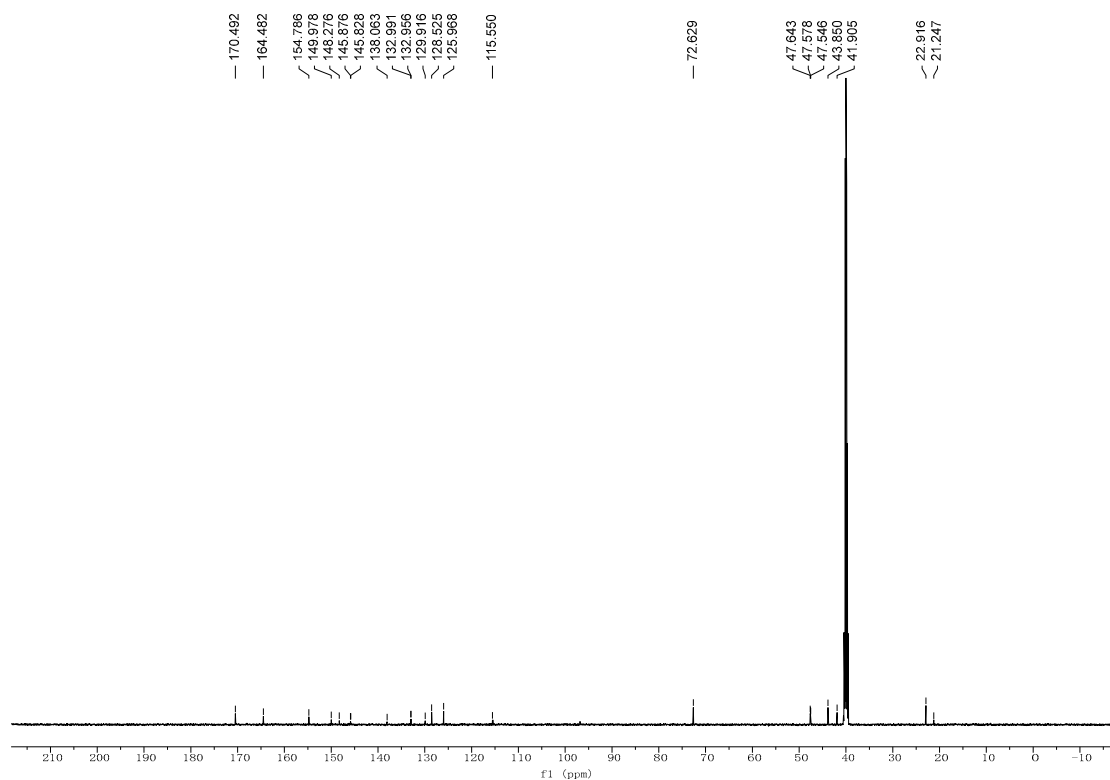


Figure S59. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **7f**.

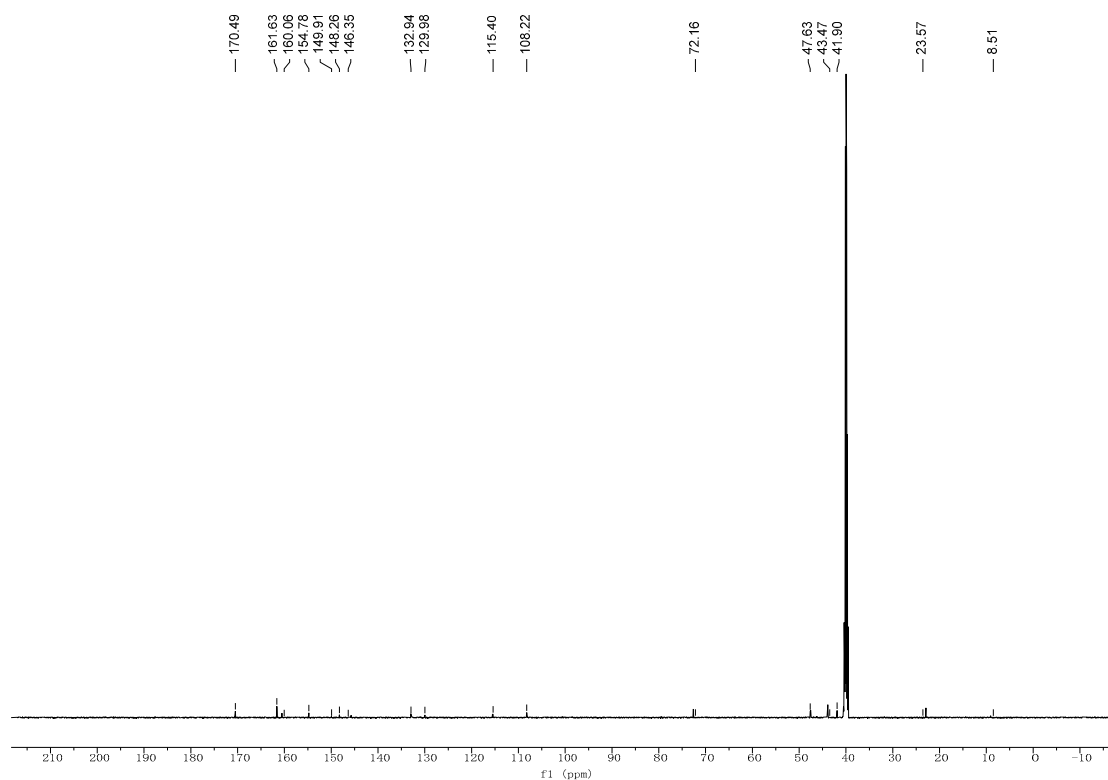


Figure S62. ^{13}C NMR Spectrum ($\text{DMSO-}d_6$, 150 MHz) of **7g**.

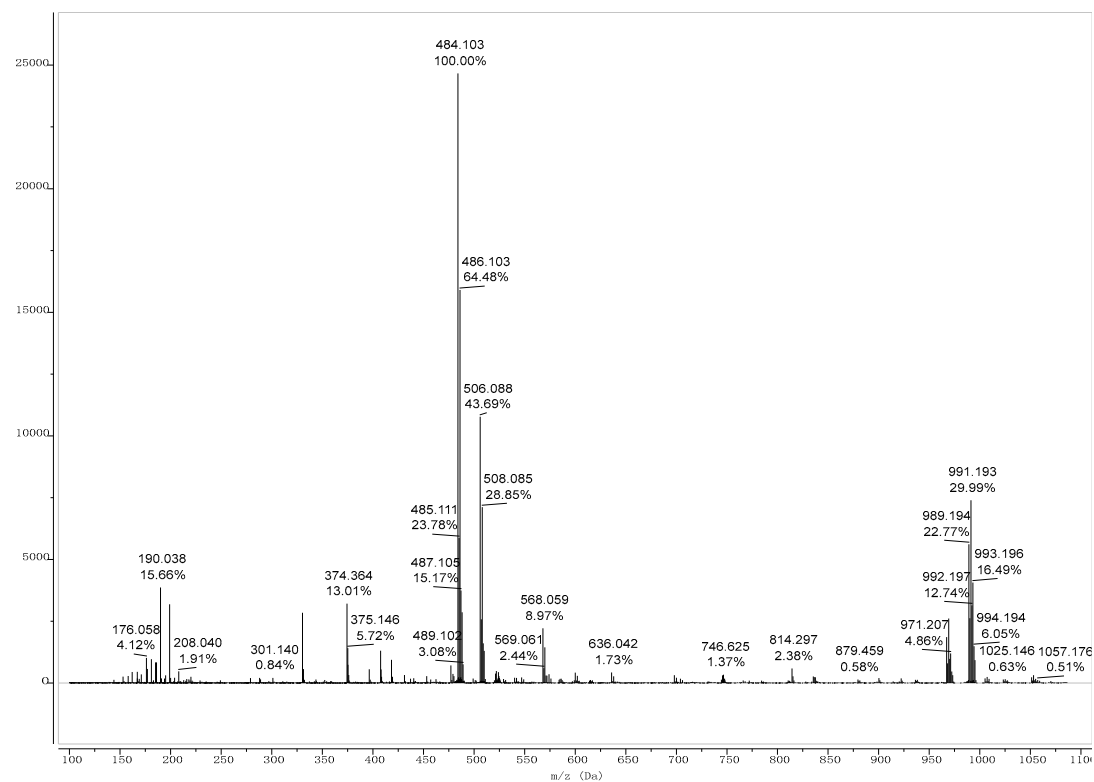


Figure S63. MS for $\text{C}_{19}\text{H}_{20}\text{Cl}_2\text{FN}_7\text{O}_3$ (Mwt.: 483.10): m/z 484.103 ($[\text{M}+\text{H}]^+$, bp) of **7g**.

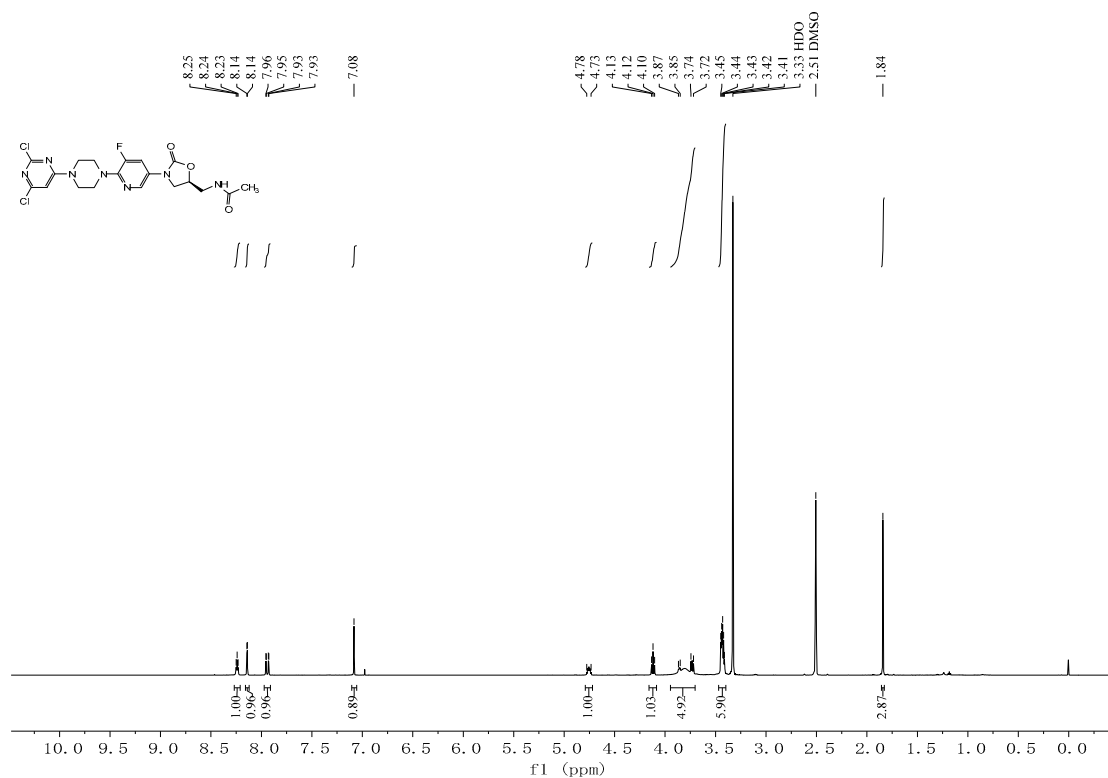


Figure S64. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of **7h**.

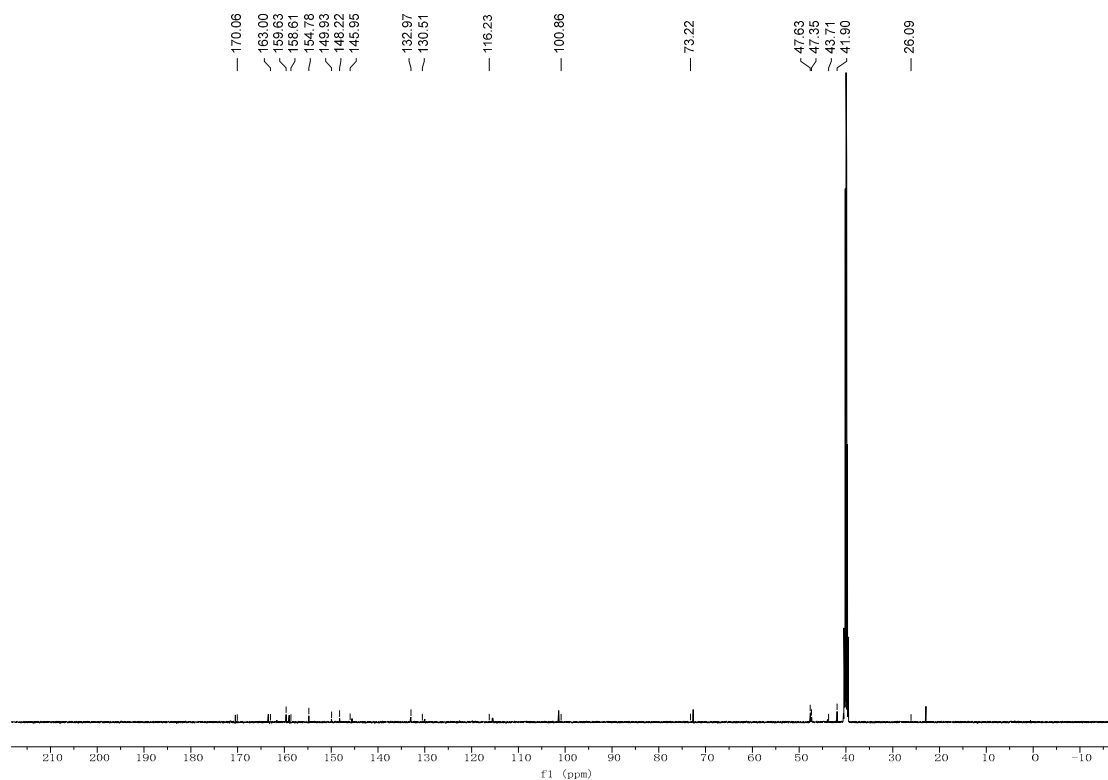


Figure S65. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **7h**.

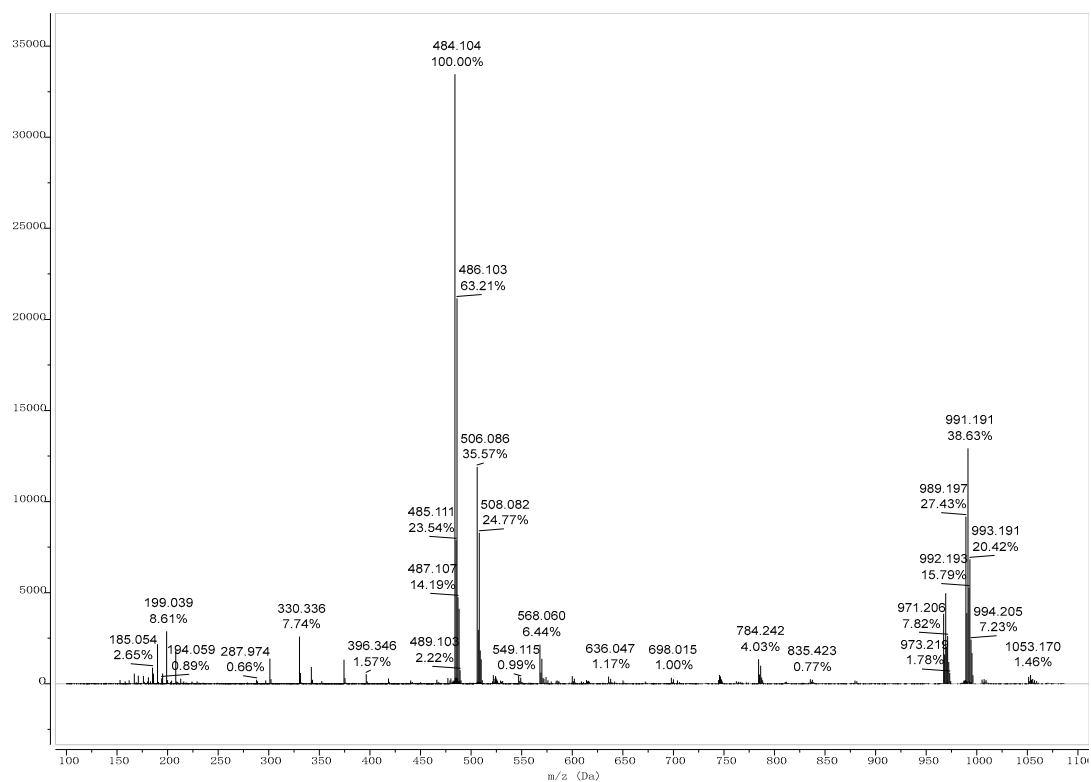


Figure S66. MS for $C_{19}H_{20}Cl_2FN_7O_3$ (Mwt.: 483.10): m/z 484.104 ($[M+H]^+$, bp) of **7h**.

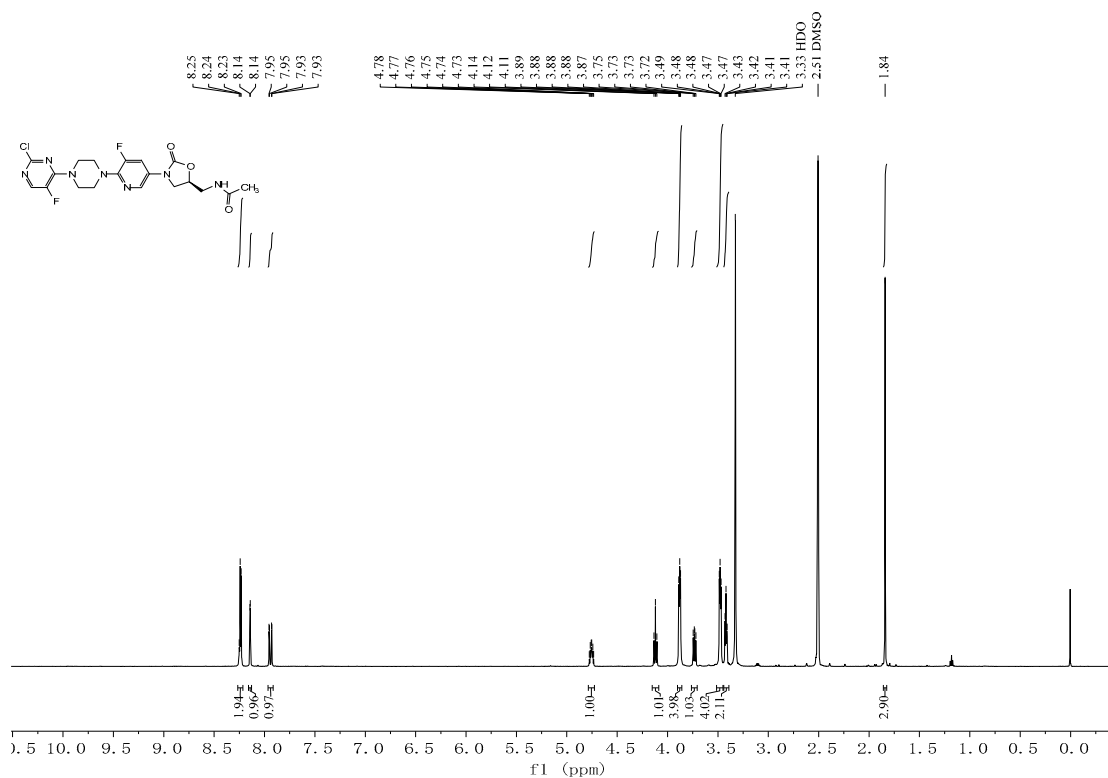


Figure S67. ^1H NMR Spectrum ($DMSO-d_6$, 600 MHz) of **7i**.

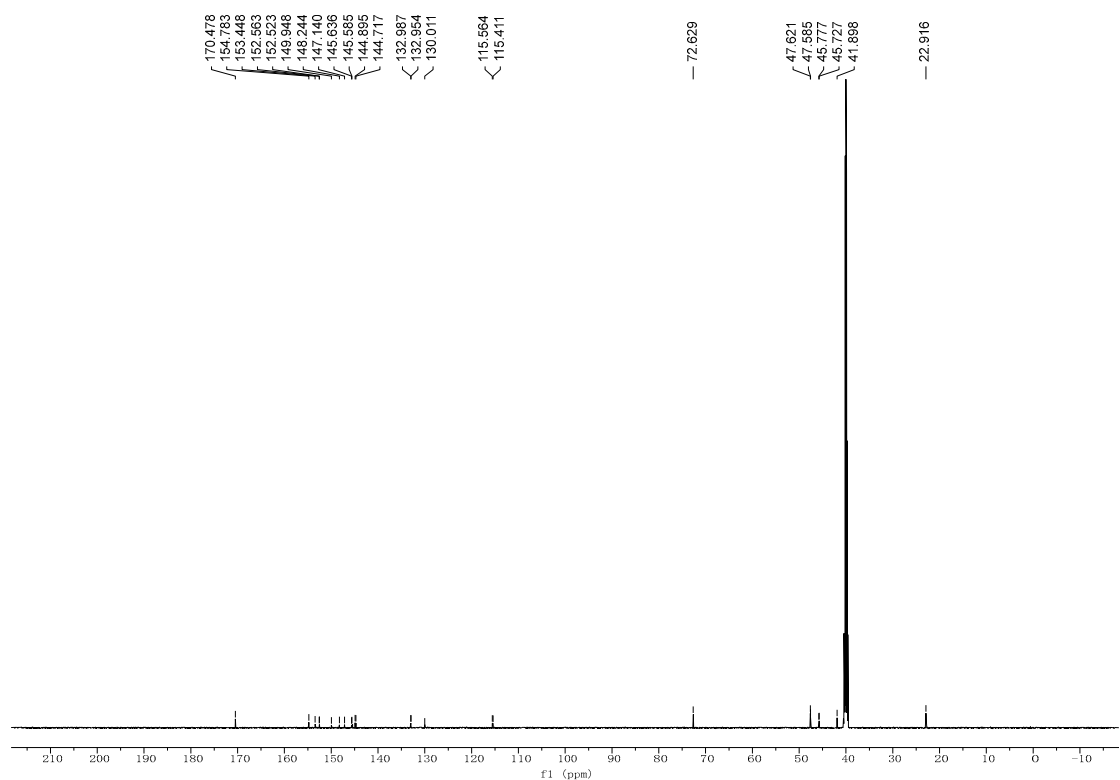


Figure S68. ^{13}C NMR Spectrum ($\text{DMSO-}d_6$, 150 MHz) of **7i**.

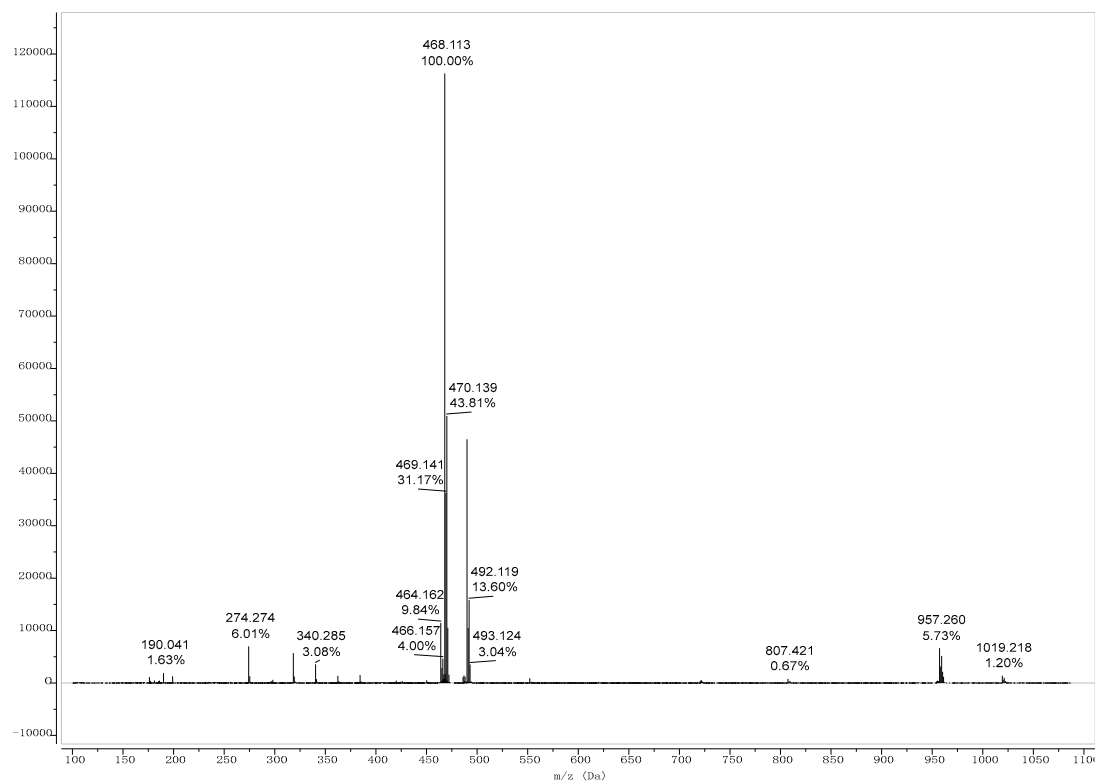


Figure S69. MS for $\text{C}_{19}\text{H}_{20}\text{ClF}_2\text{N}_7\text{O}_3$ (Mwt.: 467.86): m/z 468.113 ($[\text{M}+\text{H}]^+$, bp) of **7i**.

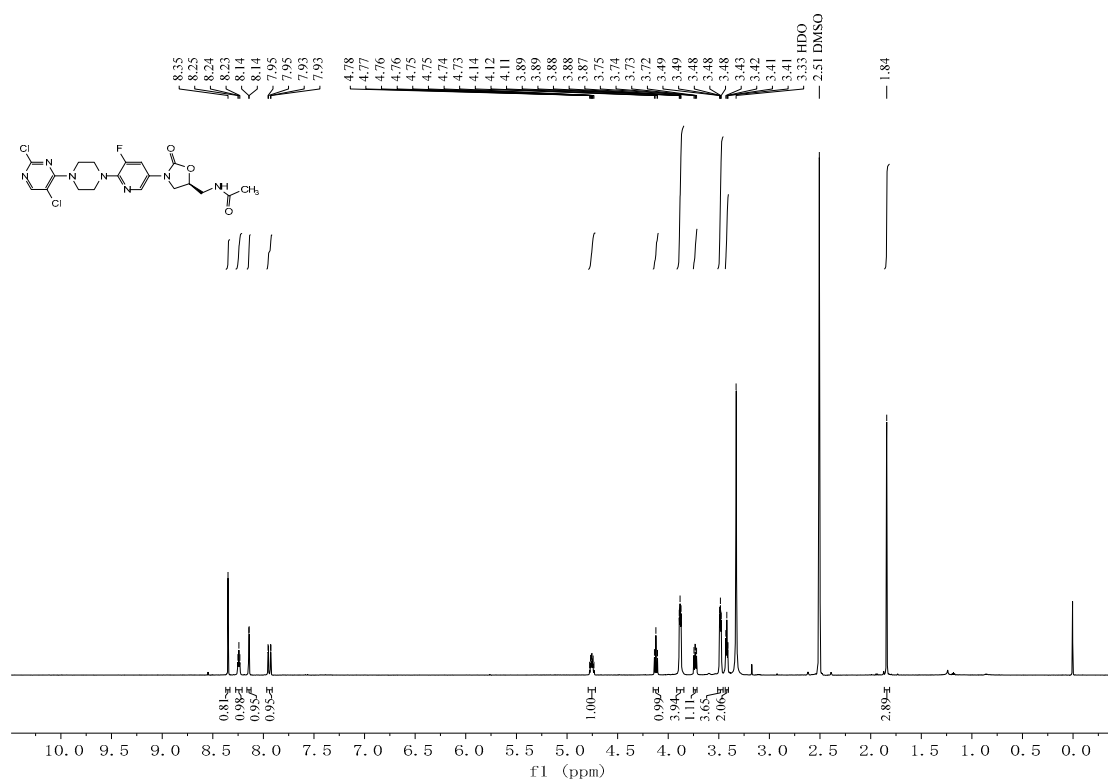


Figure S70. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of **7j**.

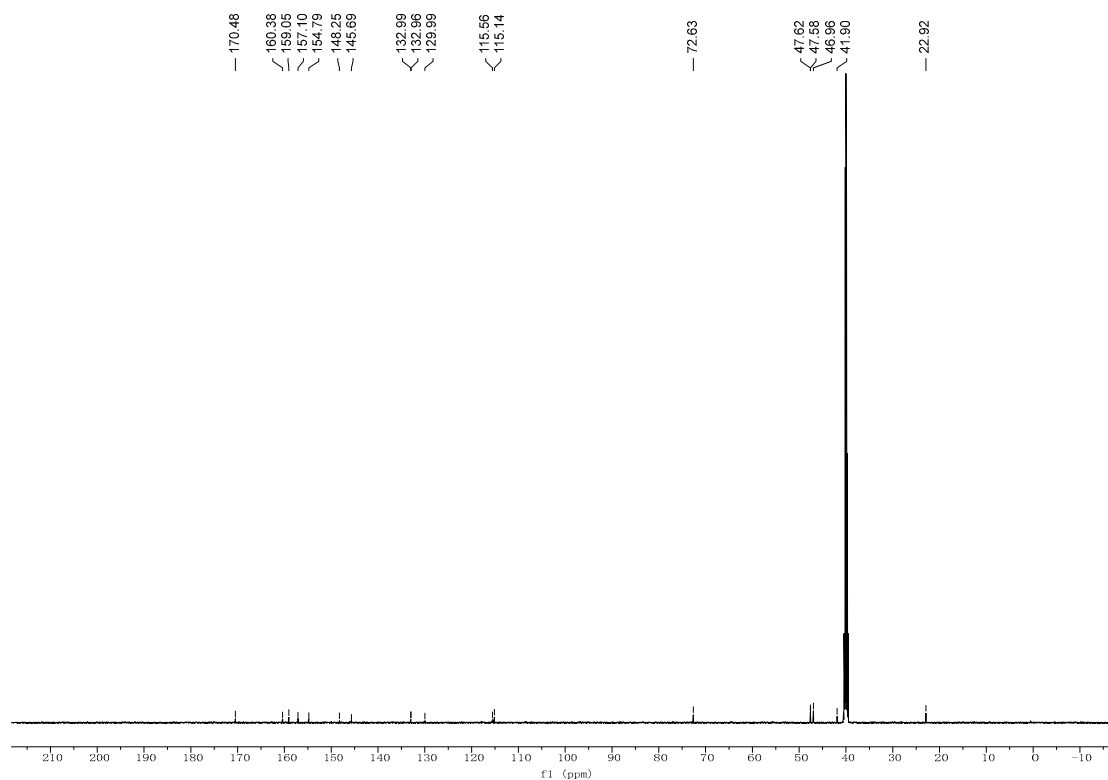


Figure S71. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **7j**.

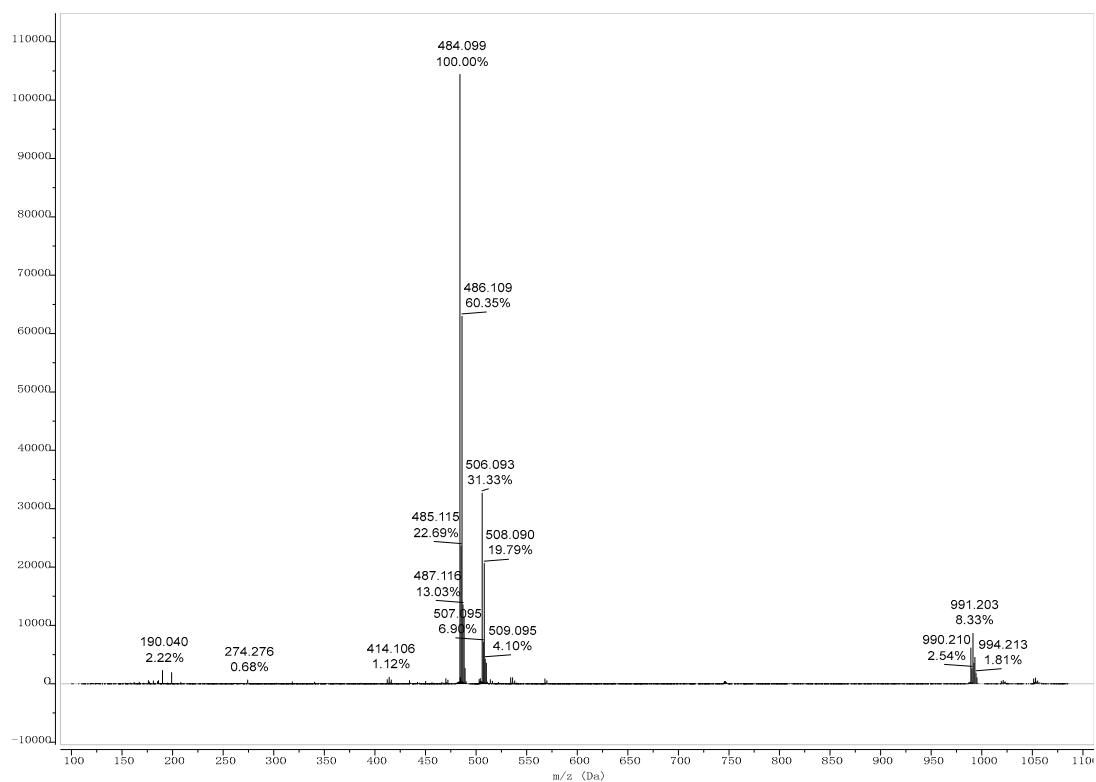


Figure S72. MS for $C_{19}H_{20}Cl_2FN_7O_3$ (Mwt.: 483.10): m/z 484.099 ($[M+H]^+$, bp) of **7j**.

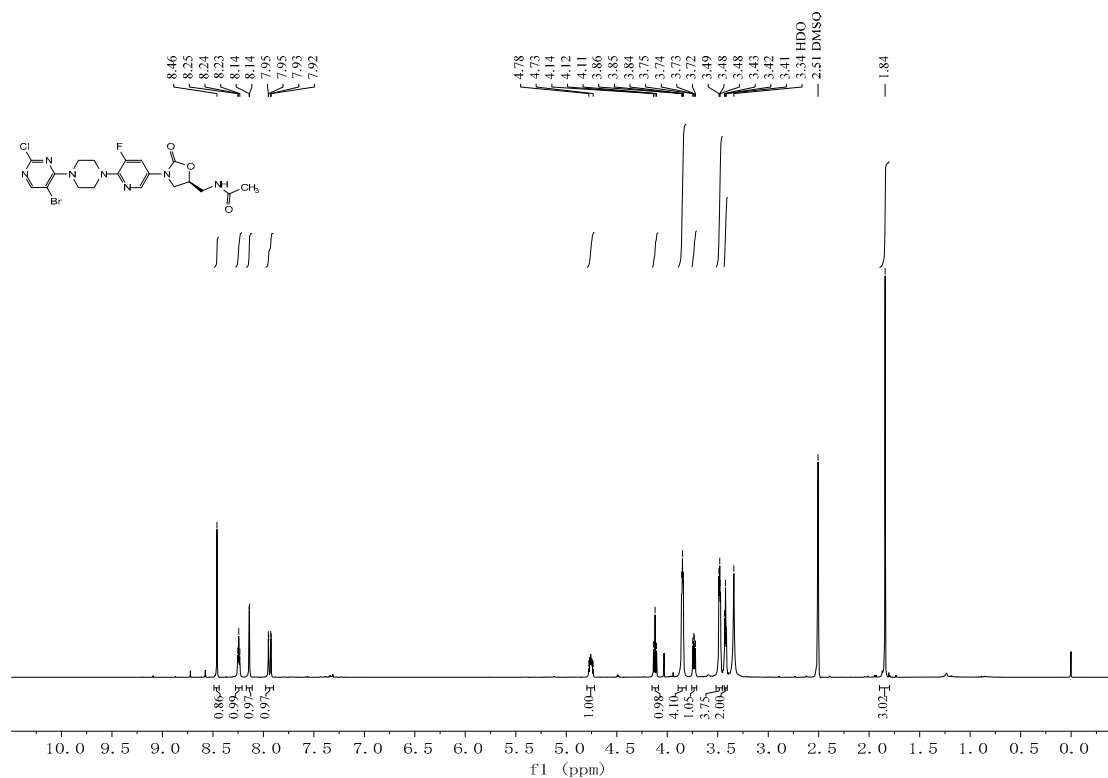


Figure S73. ^1H NMR Spectrum ($DMSO-d_6$, 600 MHz) of **7k**.

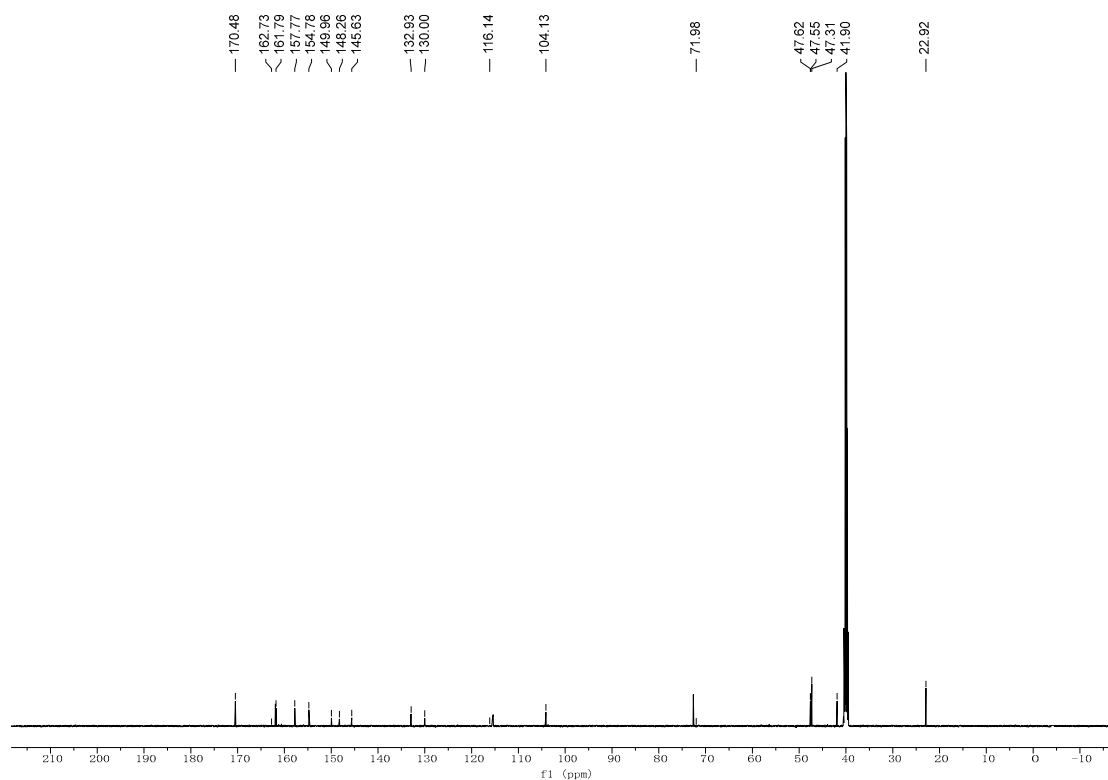


Figure S74. ^{13}C NMR Spectrum ($\text{DMSO-}d_6$, 150 MHz) of **7k**.

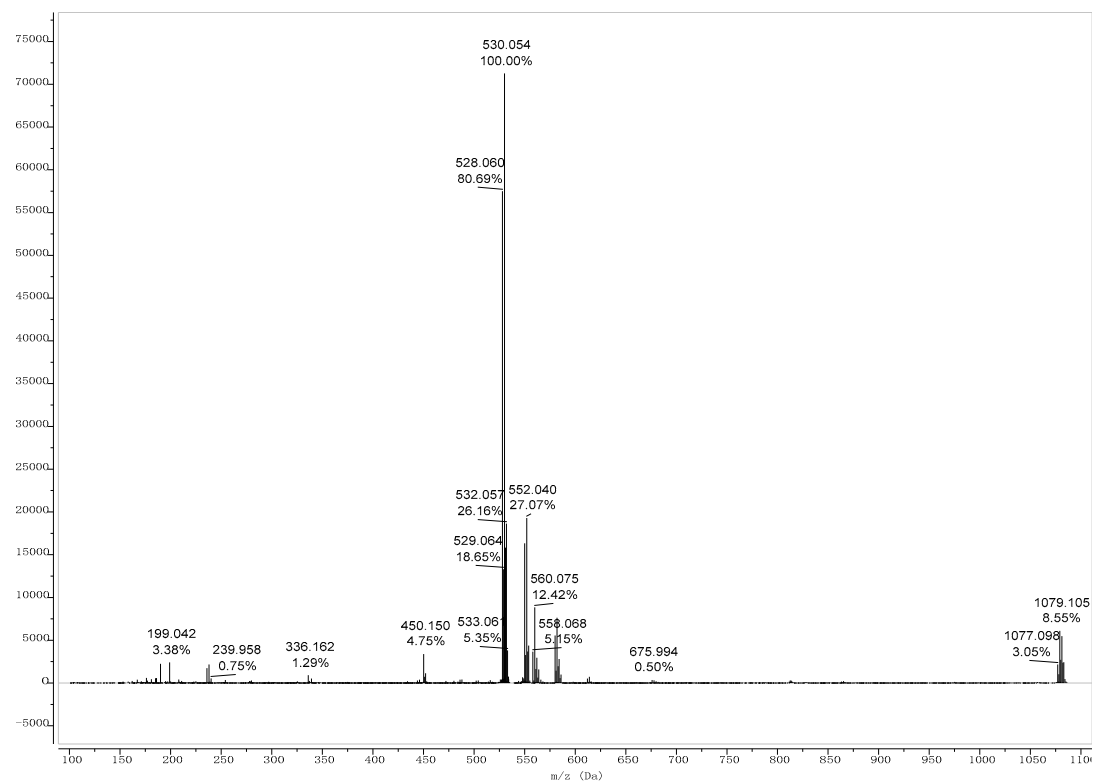


Figure S75. MS for $\text{C}_{19}\text{H}_{20}\text{BrClFN}_7\text{O}_3$ (Mwt.: 528.77): m/z 530.054 ($[\text{M}+\text{H}]^+$, bp) of **7k**.

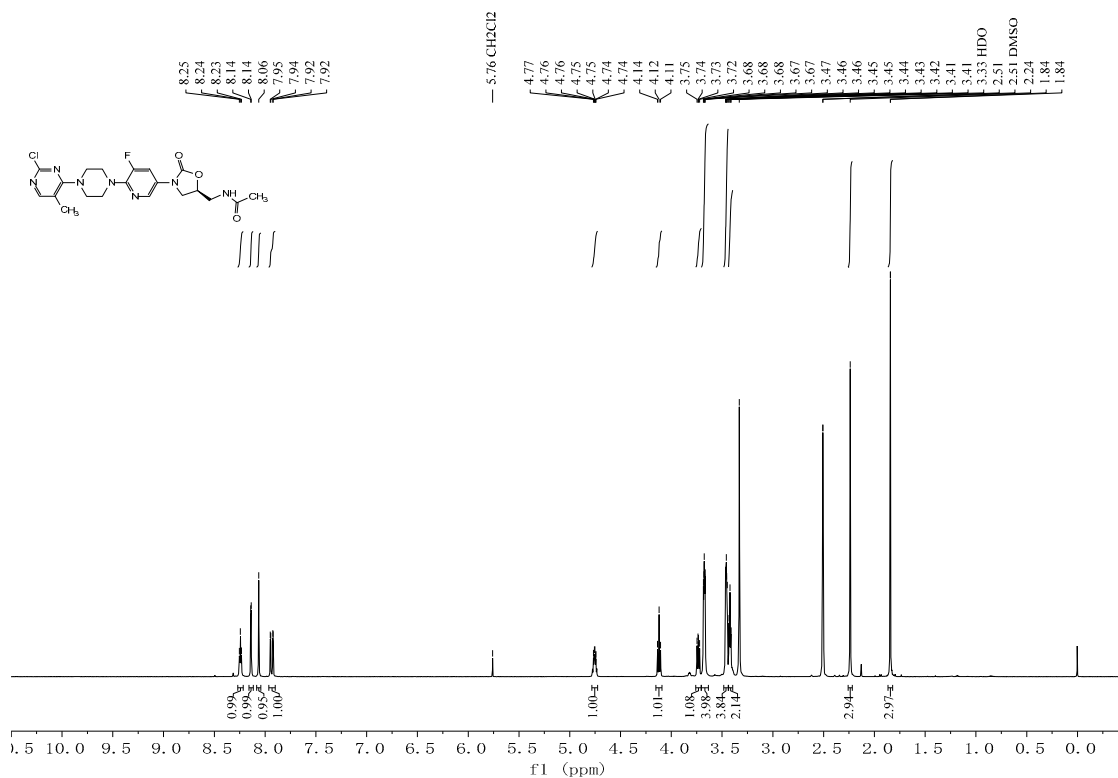


Figure S76. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of 7l.

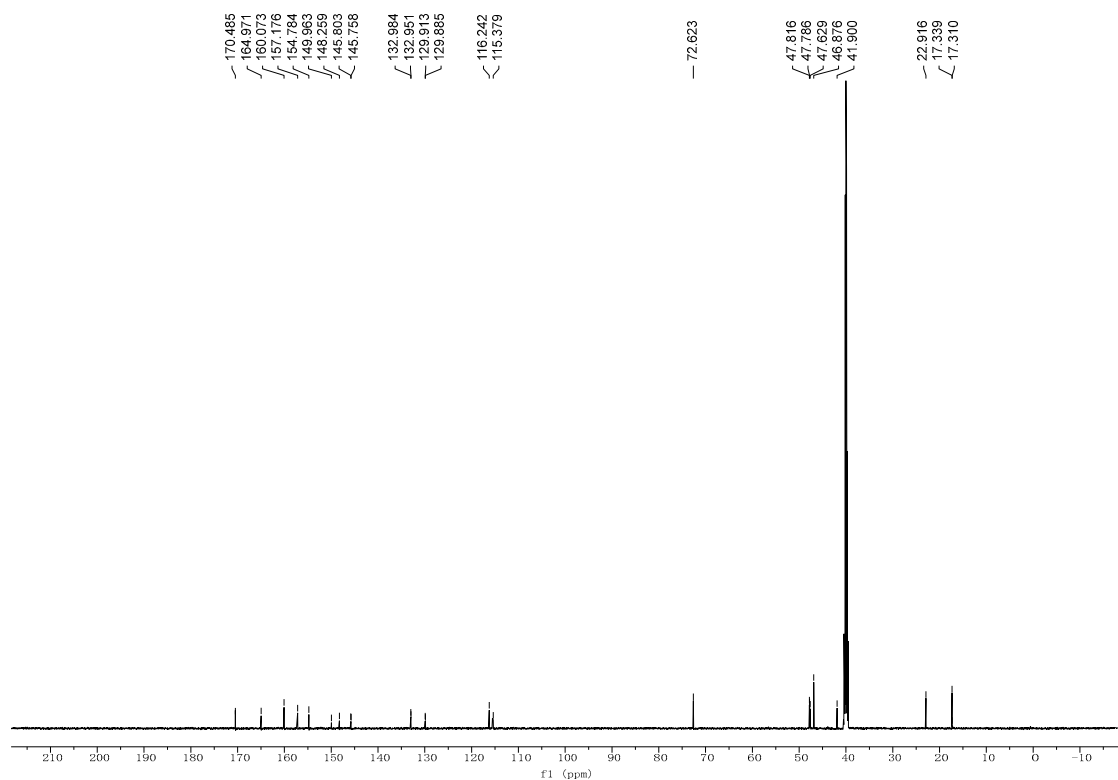


Figure S77. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of 7l.

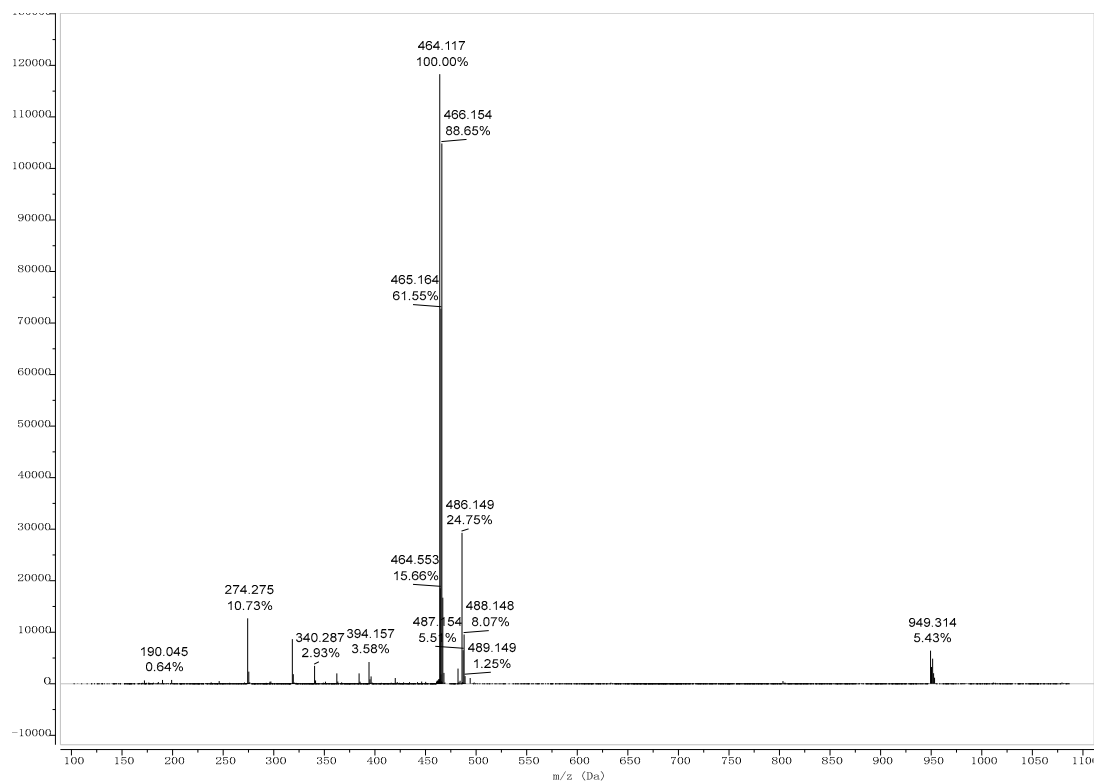


Figure S78. MS for $C_{20}H_{23}ClFN_7O_3$ (Mwt.: 463.90): m/z 464.117 ($[M+H]^+$, bp) of **7l**.

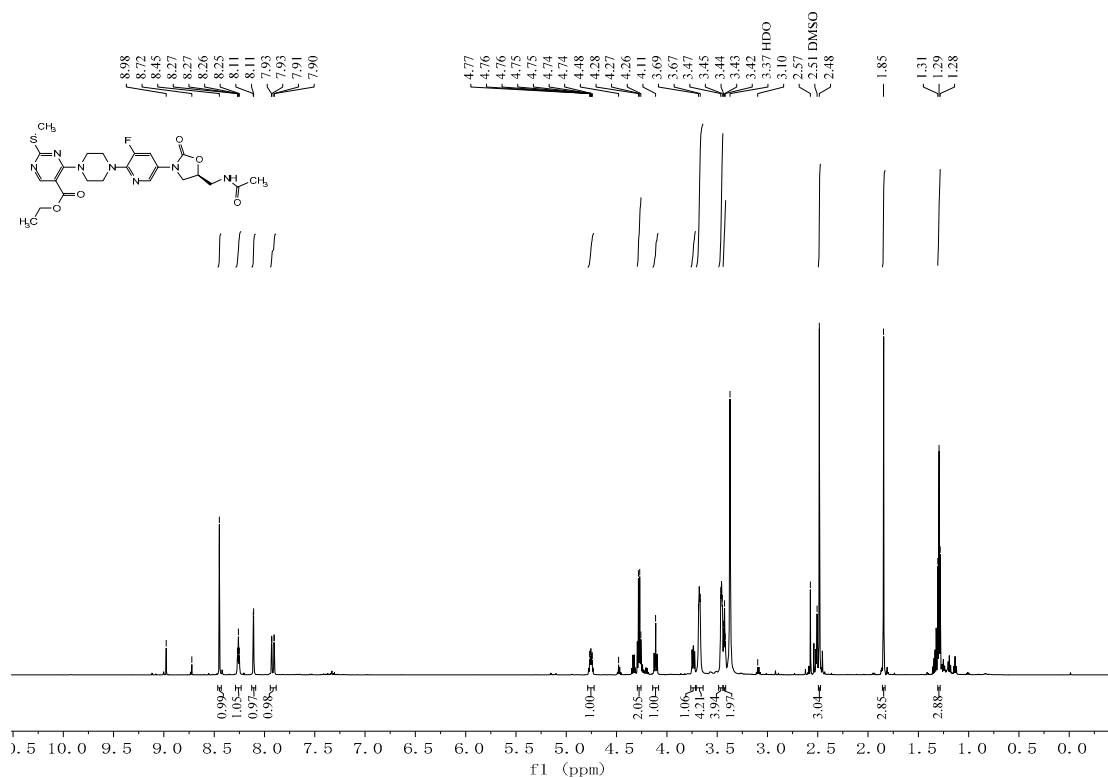


Figure S79. ^1H NMR Spectrum ($DMSO-d_6$, 600 MHz) of **7m**.

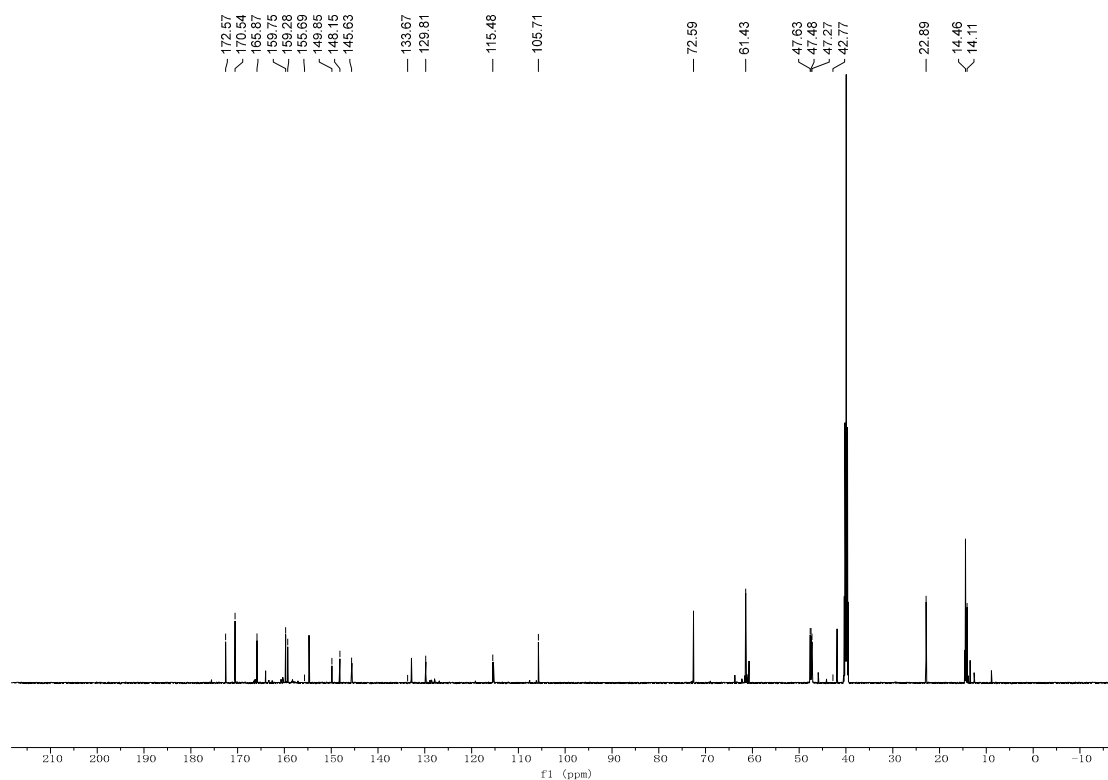


Figure S80. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of **7m**.

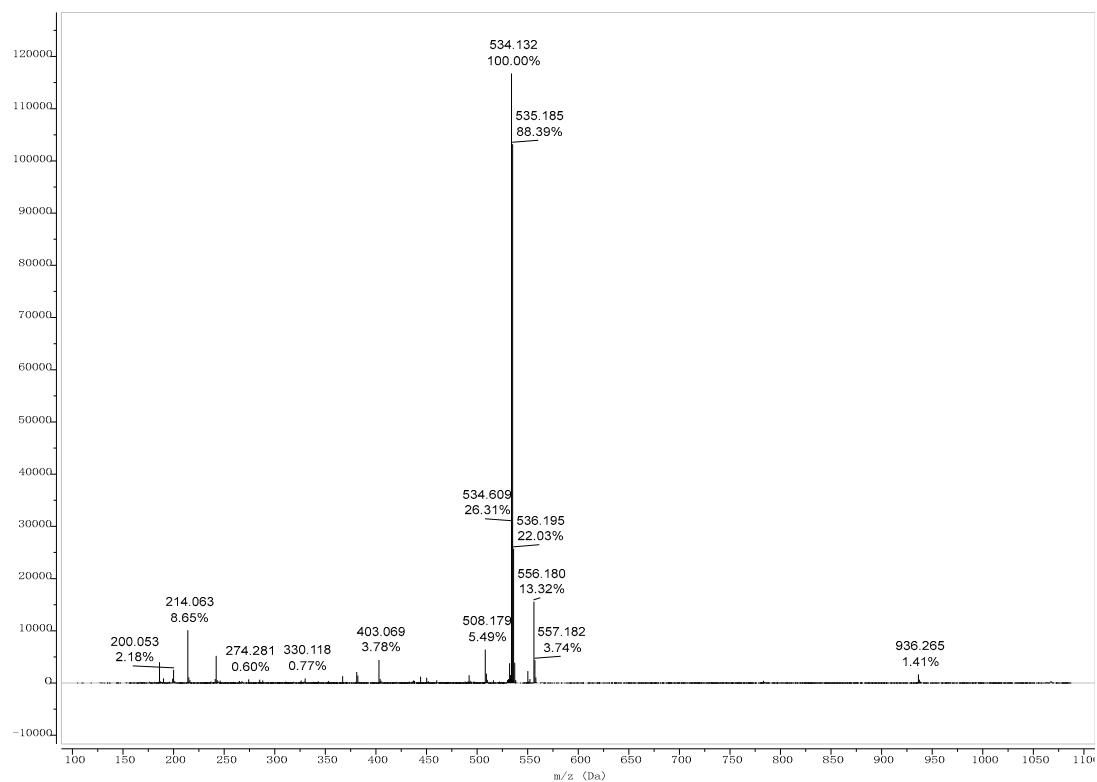


Figure S81. MS for C₂₃H₂₈FN₇O₅S (Mwt.: 533.58): *m/z* 534.132 ([M+H]⁺, bp) of **7m**.

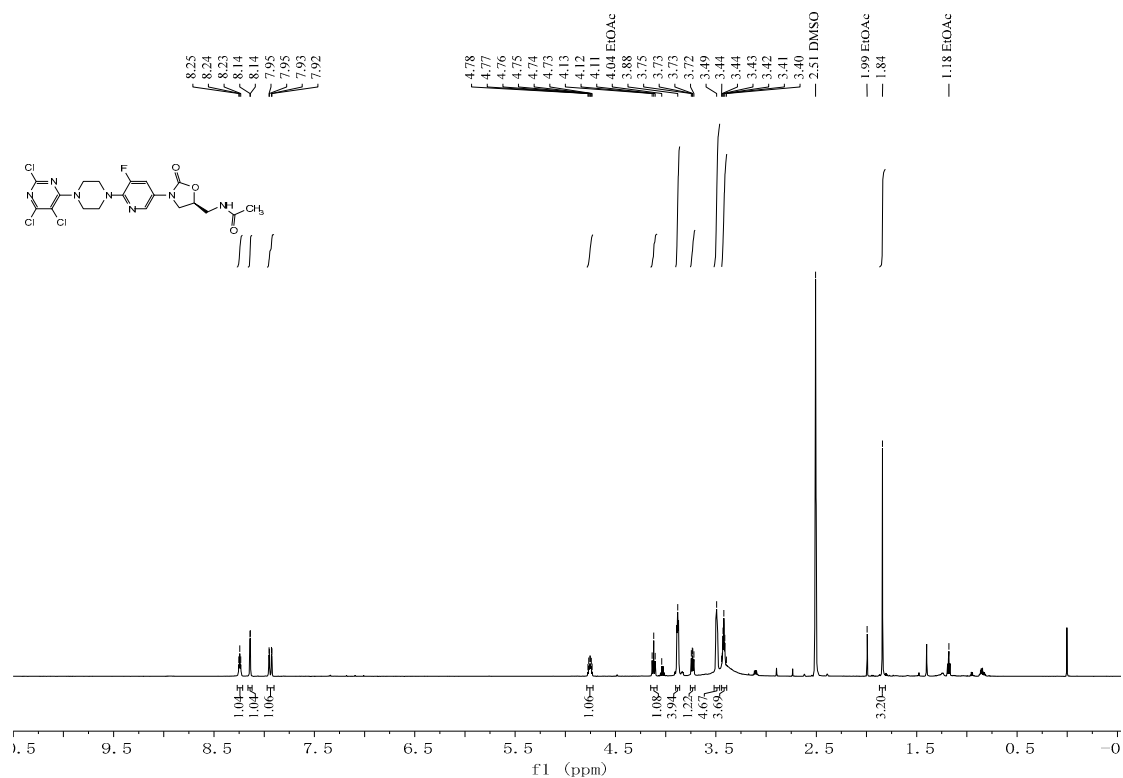


Figure S82. ¹H NMR Spectrum (DMSO-*d*₆, 600 MHz) of 7n.

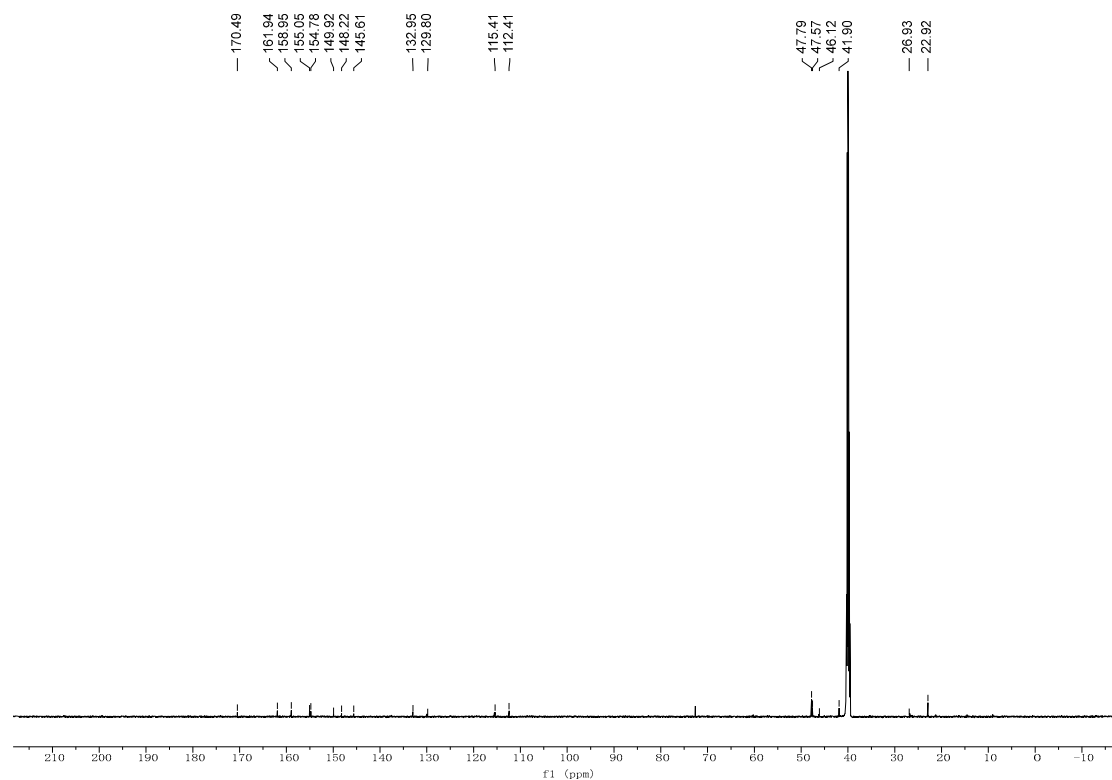


Figure S83. ¹³C NMR Spectrum (DMSO-*d*₆, 150 MHz) of 7n.

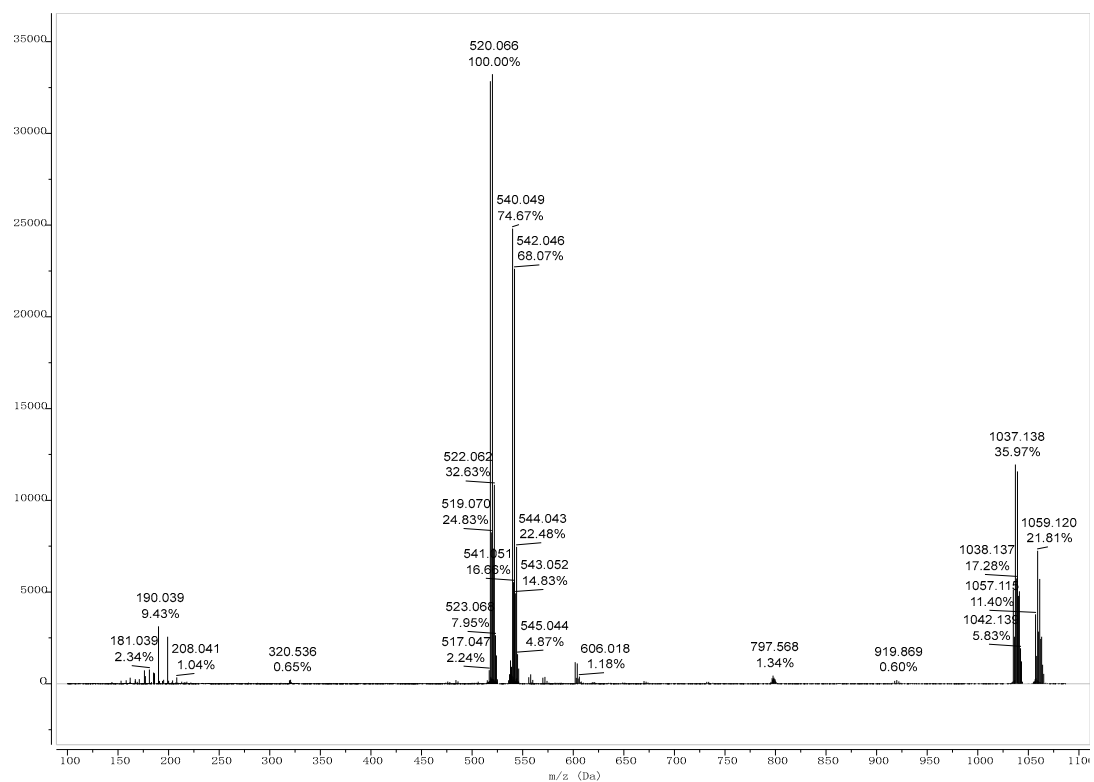


Figure S84. MS for $C_{19}H_{19}C_{13}FN_7O_3$ (Mwt.: 518.76): m/z 520.066 ($[M+H]^+$, bp) of **7n**.