**Supplementary Materials**

**Synthesis and Biochemical Evaluation of 8*H*-Indeno[1,2-*d*]thiazole Derivatives as Novel SARS-CoV-2 3CL Protease Inhibitors**

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## <sup>1</sup>H NMR of compound **4**



## <sup>13</sup>C NMR of compound **4**



## MS of compound **4**



Peak#:1  R.Time:1.316(Scan#:105)
MassPeaks:484
Spectrum Mode:Averaged 1.275-1.325(103-107)
BG Mode:Calc  Segment 1 - Event 1

MS Spectrum

Exact Mass: 382.10
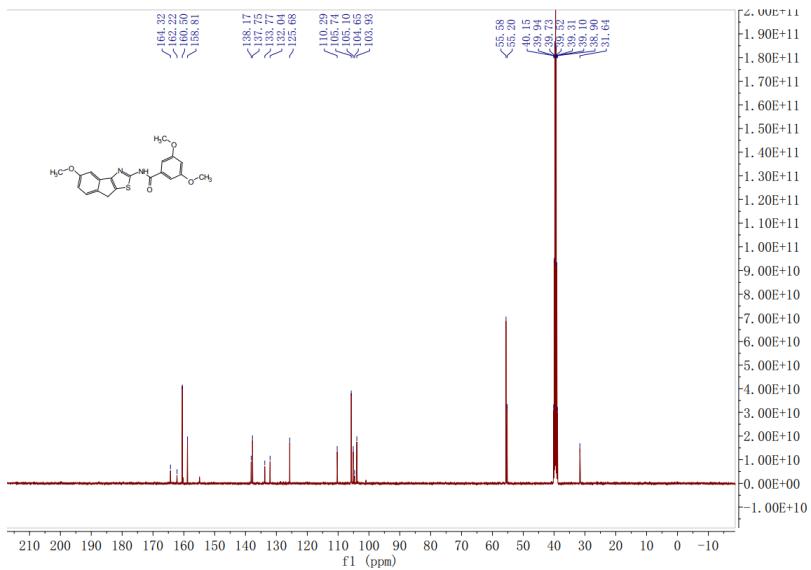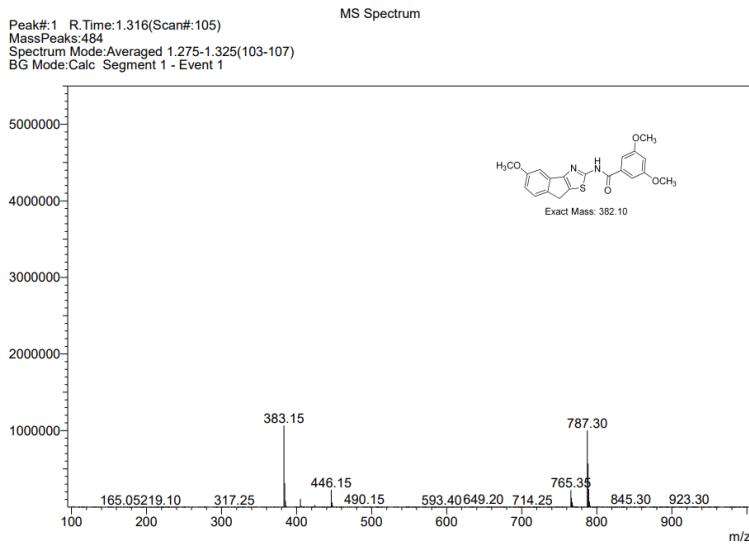
## ^{1}H NMR of compound 7a
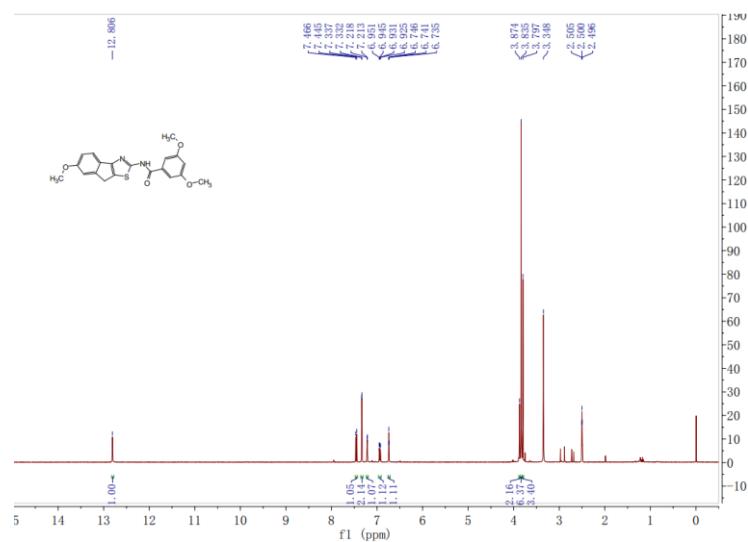


## ^{13}C NMR of compound 7a



## MS of compound 7a

Peak#:1  R.Time:1.450(Scan#:115)
MassPeaks:479
Spectrum Mode:Averaged 1.400-1.450(113-117)
BG Mode:Calc  Segment 1 - Event 1

MS Spectrum

Exact Mass: 382.10
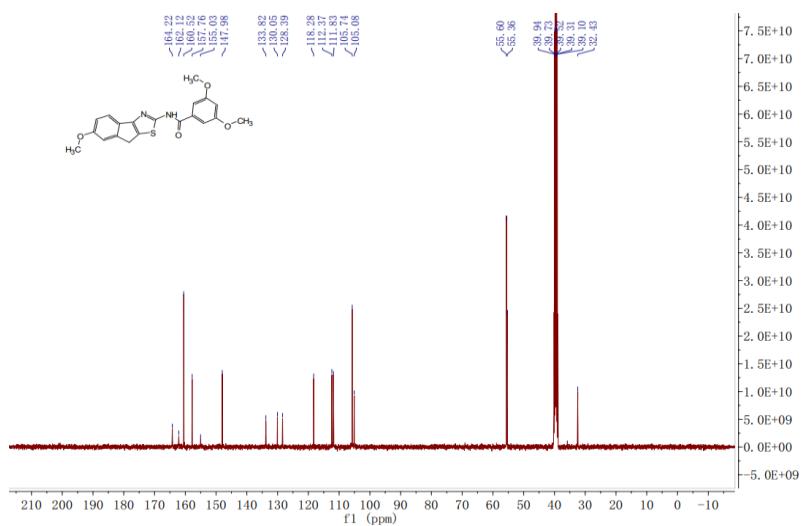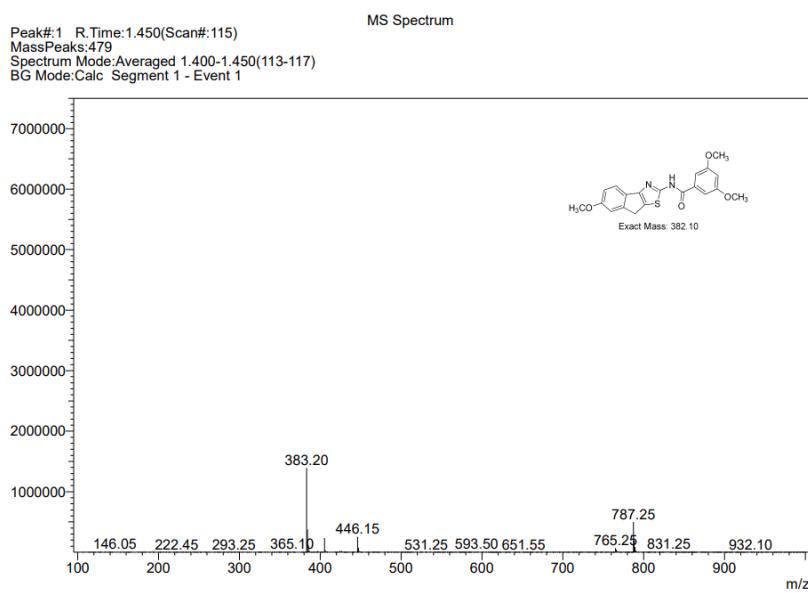
## <sup>1</sup>H NMR of compound **7b**
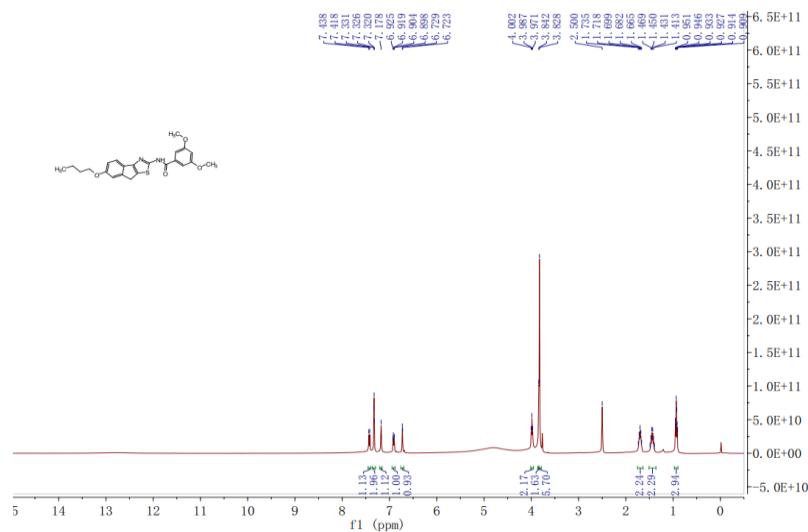


## <sup>13</sup>C NMR of compound **7b**



## MS of compound **7b**

Peak#:1    R.Time:1.526(Scan#:123)
MassPeaks:453
Spectrum Mode:Averaged 1.500-1.550(121-125)
BG Mode:Calc  Segment 1 - Event 1

MS Spectrum



Exact Mass: 424.15
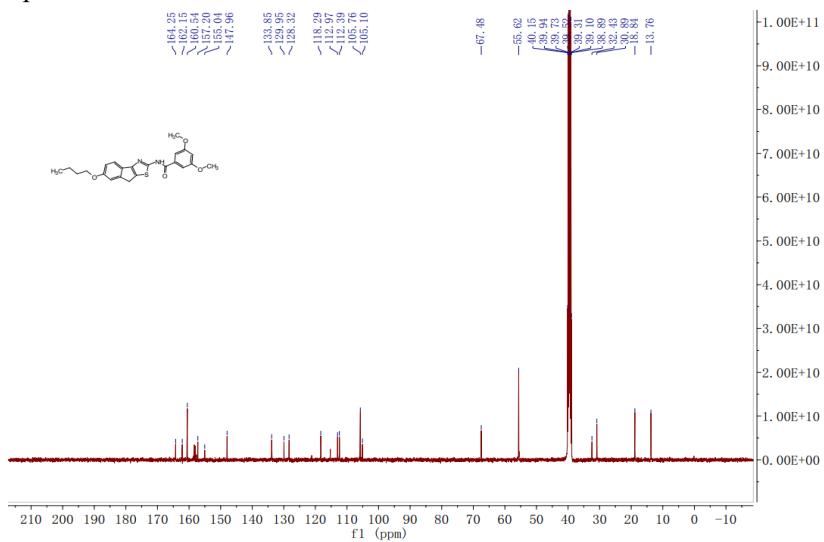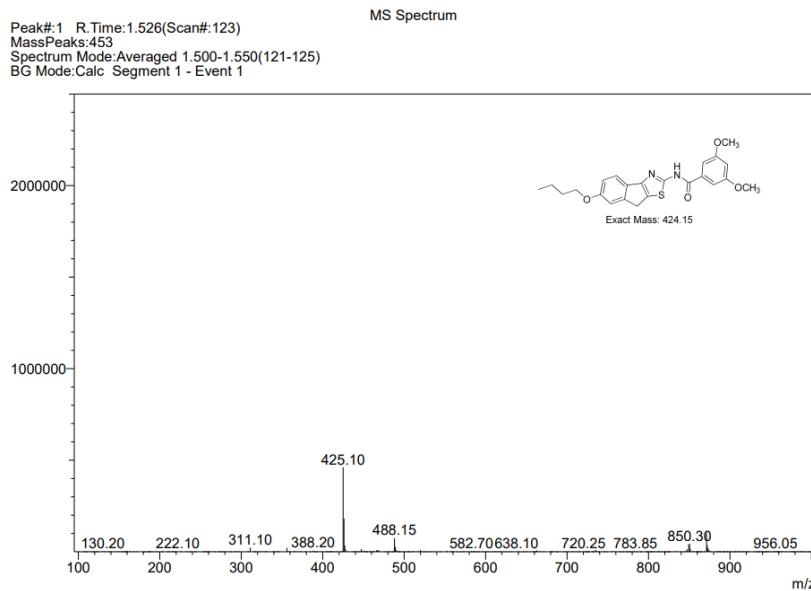
## $^1$H NMR of compound **7c**
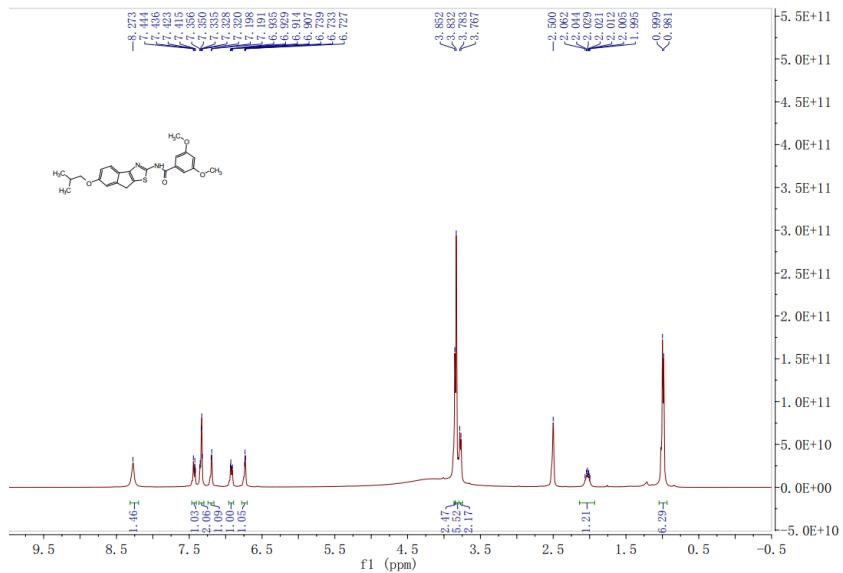


## $^{13}$C NMR of compound **7c**



## MS of compound **7c**



Peak#:1  R.Time:1.677(Scan#:135)
MassPeaks:487
Spectrum Mode:Averaged 1.650-1.700(133-137)
BG Mode:Calc  Segment 1 - Event 1

MS Spectrum

Exact Mass: 424.15

6
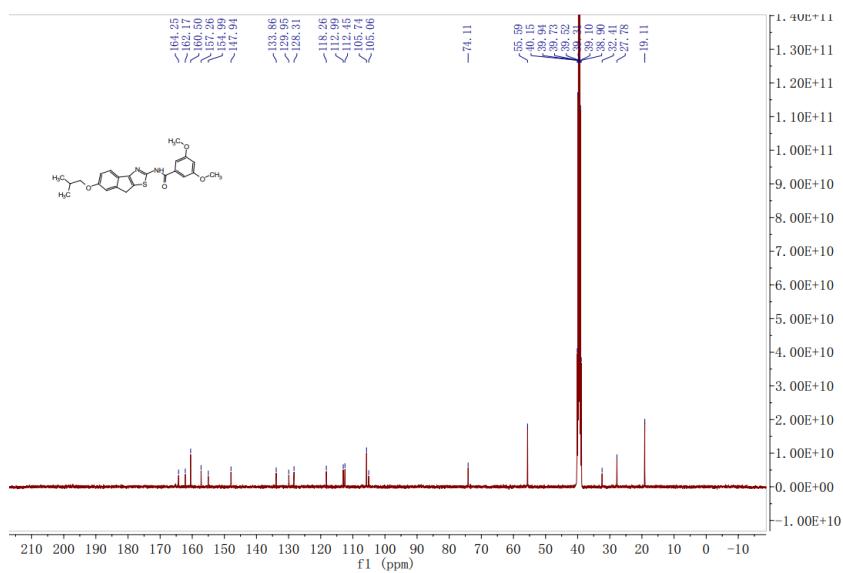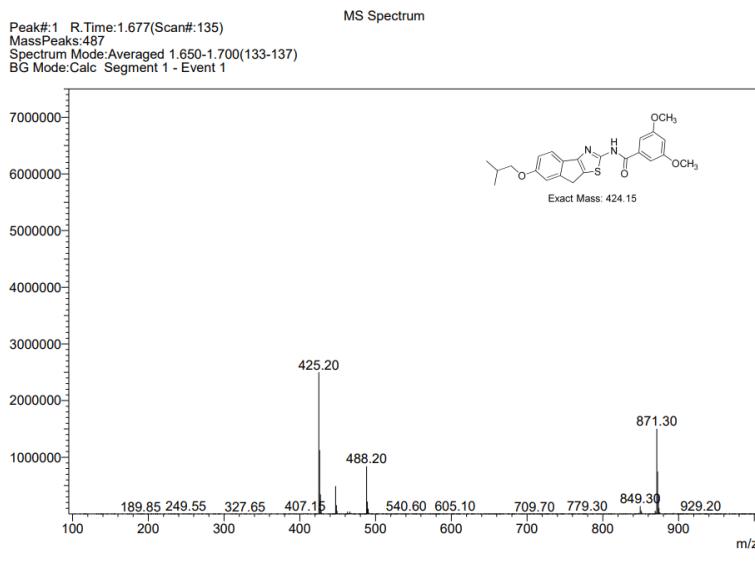
## $^1$H NMR of compound 7d
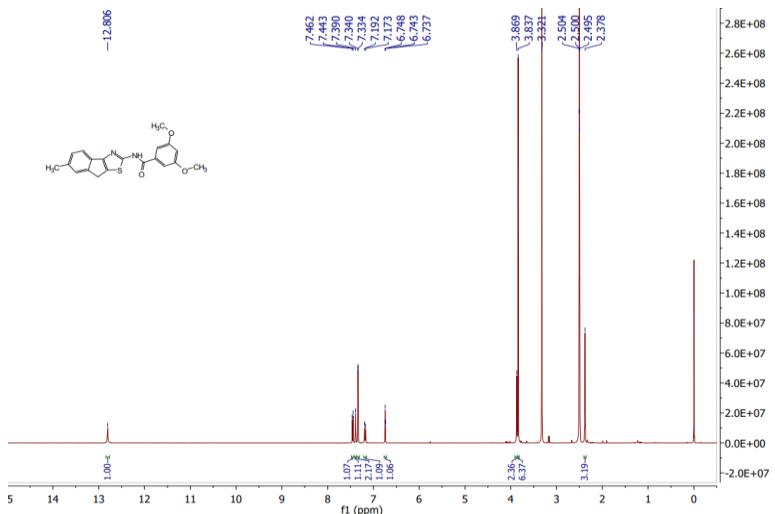


## $^{13}$C NMR of compound 7d



## MS of compound 7d



Peak#:1  R.Time:1.561(Scan#:125)
MassPeaks:439
Spectrum Mode:Averaged 1.525-1.575(123-127)
BG Mode:Calc  Segment 1 - Event 1

MS Spectrum

Exact Mass: 366.10

7
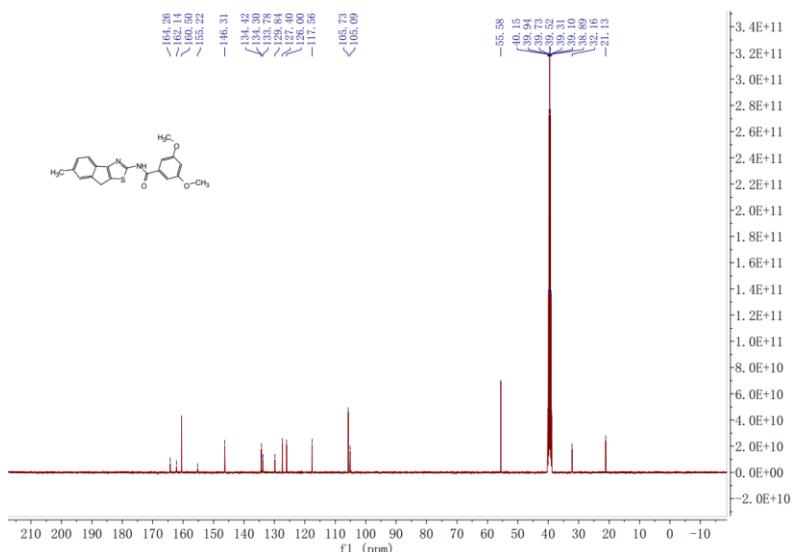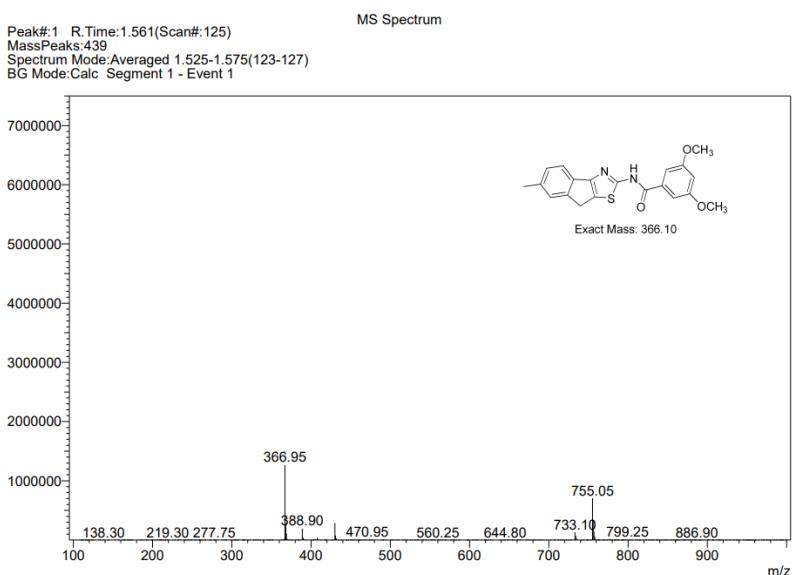
# $^1$H NMR of compound 7e
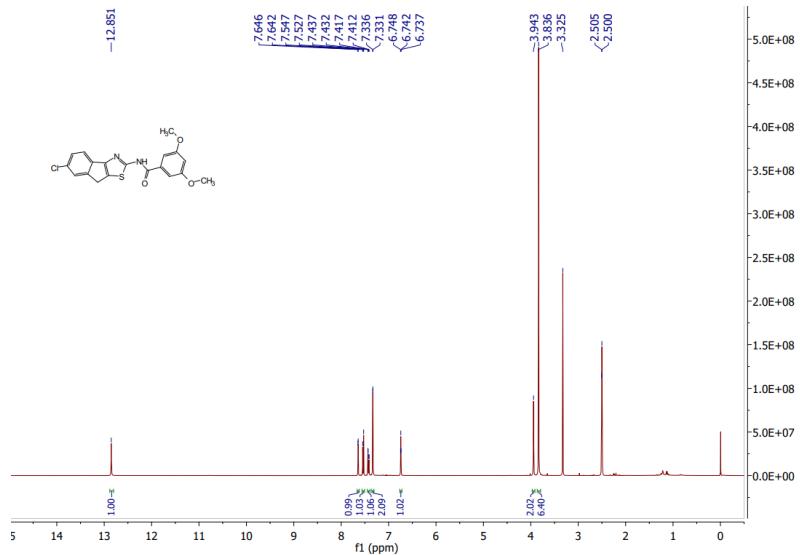


# $^{13}$CNMR of compound 7e



# MS of compound 7e



Peak#:1  R.Time:1.561(Scan#:125)
MassPeaks:453
Spectrum Mode:Averaged 1.525-1.575(123-127)
BG Mode:Calc  Segment 1 - Event 1

MS Spectrum

Exact Mass: 386.05
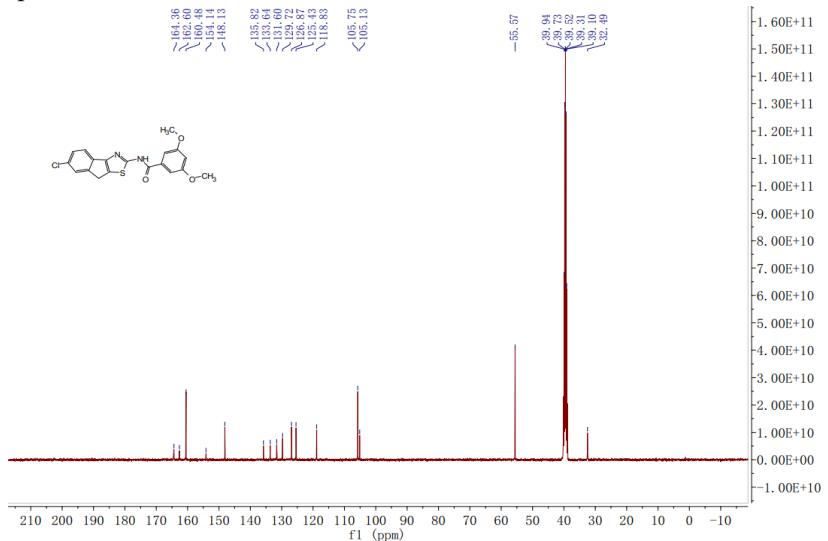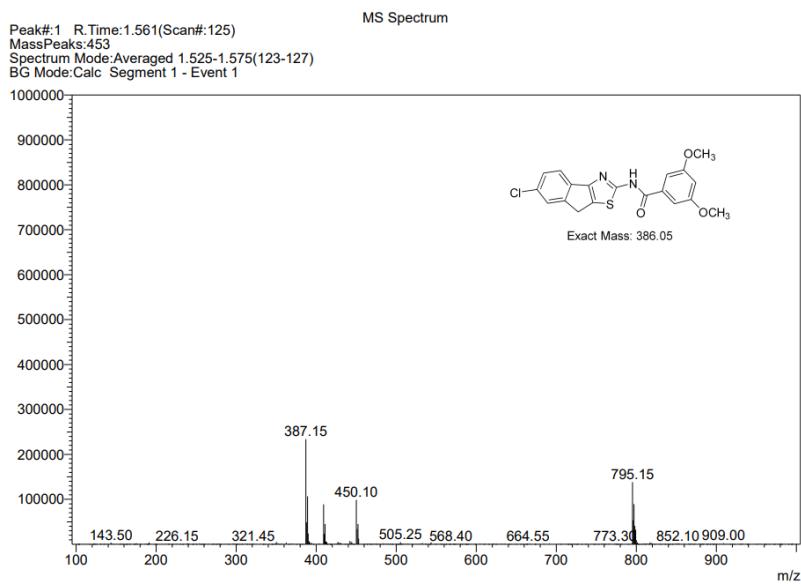
## $^1$H NMR of compound **7f**
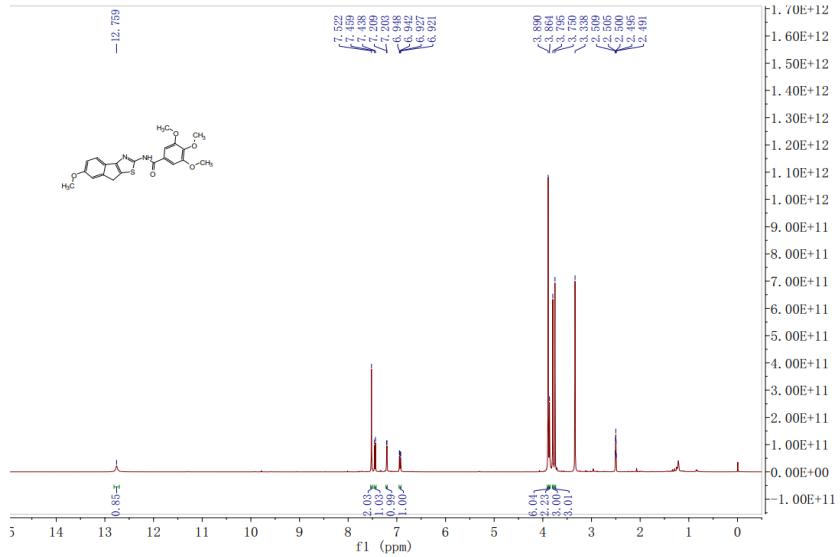


## $^{13}$C NMR of compound **7f**
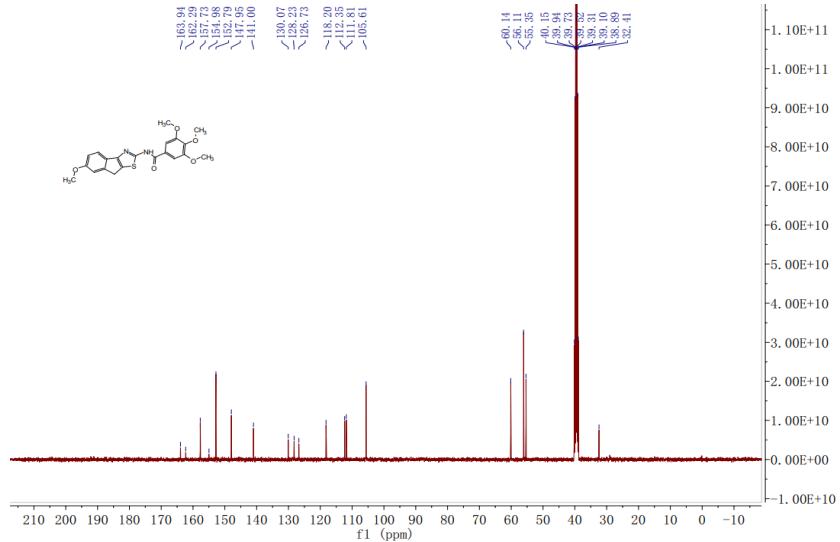


## MS of compound **7f**



Peak#:1  R.Time:1.246(Scan#:99)
MassPeaks:439
Spectrum Mode:Averaged 1.200-1.250(97-101)
BG Mode:Calc  Segment 1 - Event 1

MS Spectrum

Exact Mass: 412.11
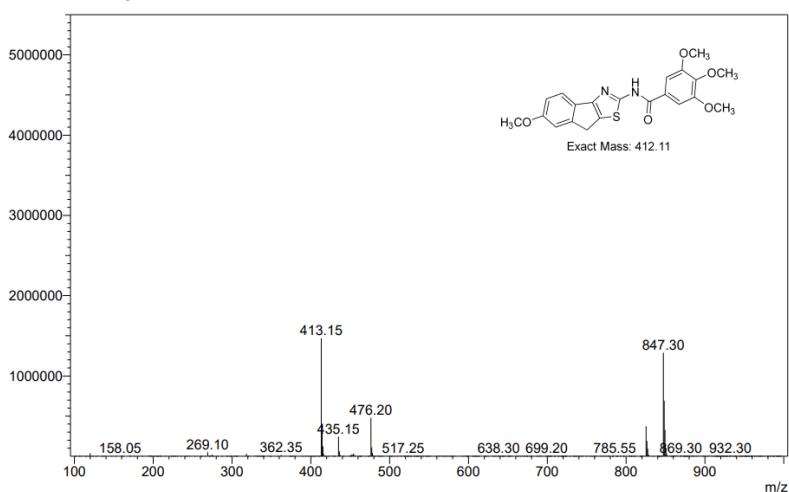
# $^1$H NMR of compound 7g
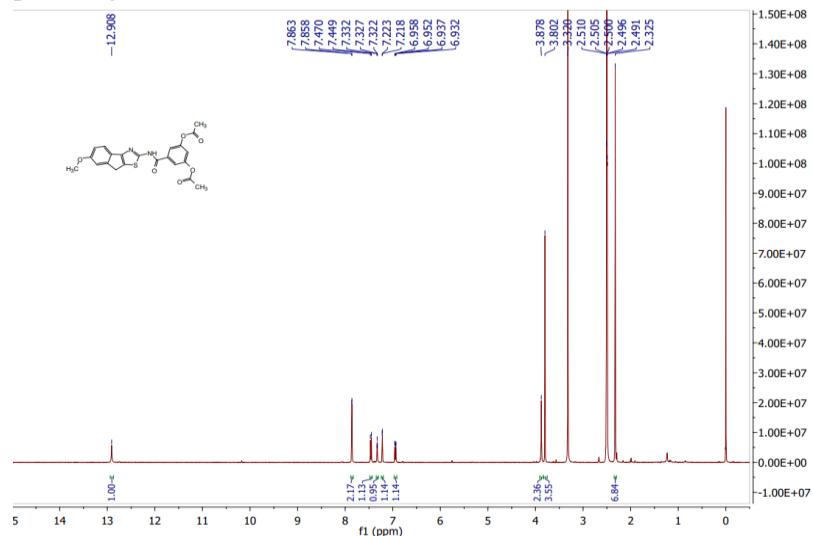


# $^{13}$C NMR of compound 7g



# MS of compound 7g

Peak#:1   R.Time:1.350(Scan#:107)
MassPeaks:442
Spectrum Mode:Averaged 1.300-1.350(105-109)
BG Mode:Calc  Segment 1 - Event 1

MS Spectrum

Exact Mass: 438.09
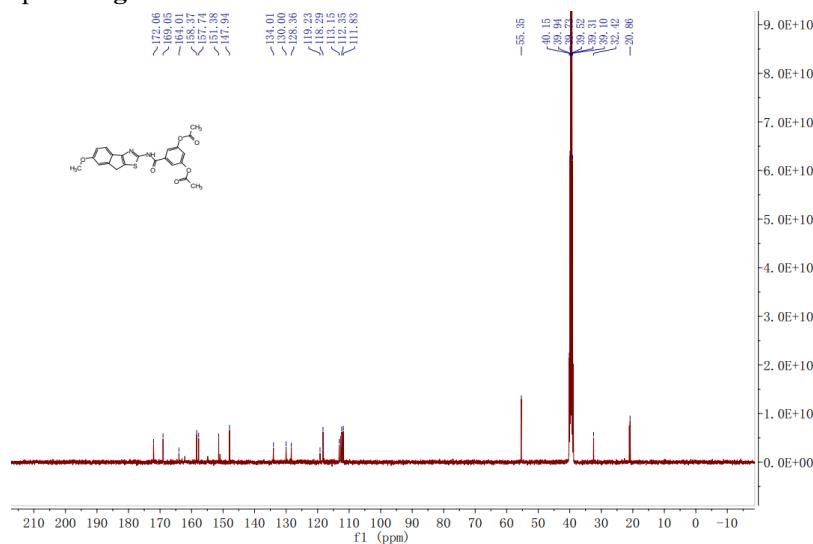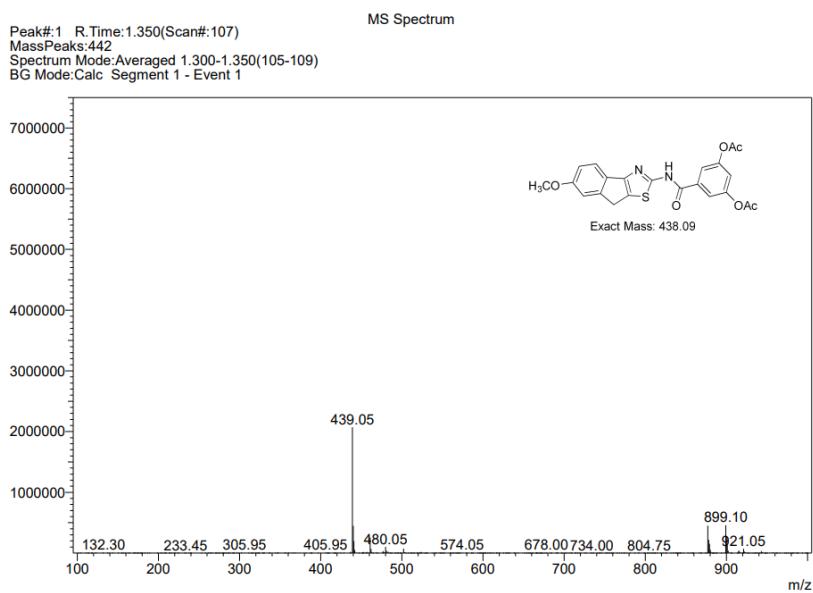
# $^1$H NMR of compound 7h
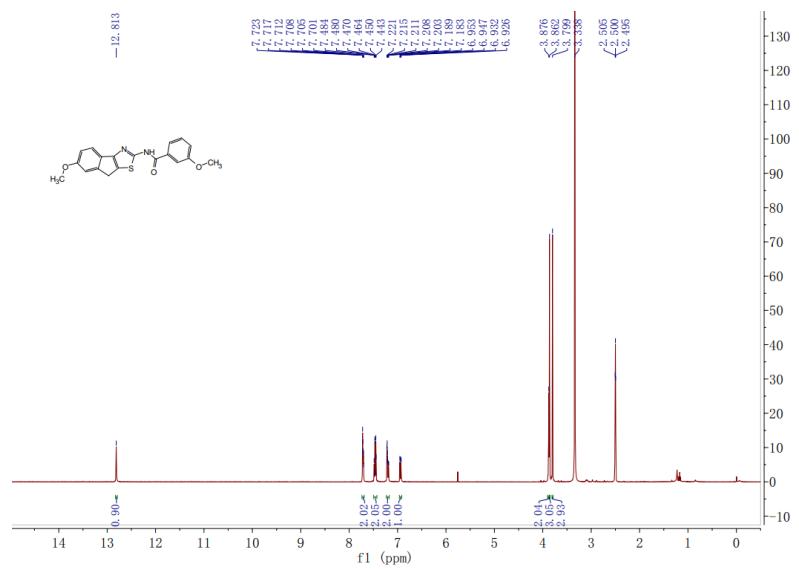


# $^{13}$C NMR of compound 7h
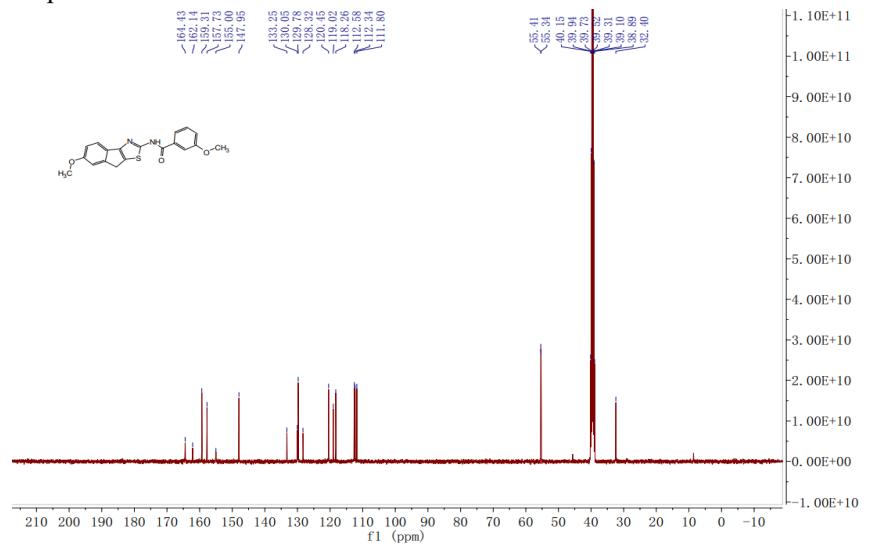


# MS of compound 7h



Peak#:1  R.Time:1.267(Scan#:101)
MassPeaks:525
Spectrum Mode:Averaged 1.225-1.275(99-103)
BG Mode:Calc  Segment 1 - Event 1

MS Spectrum

Exact Mass: 352.09
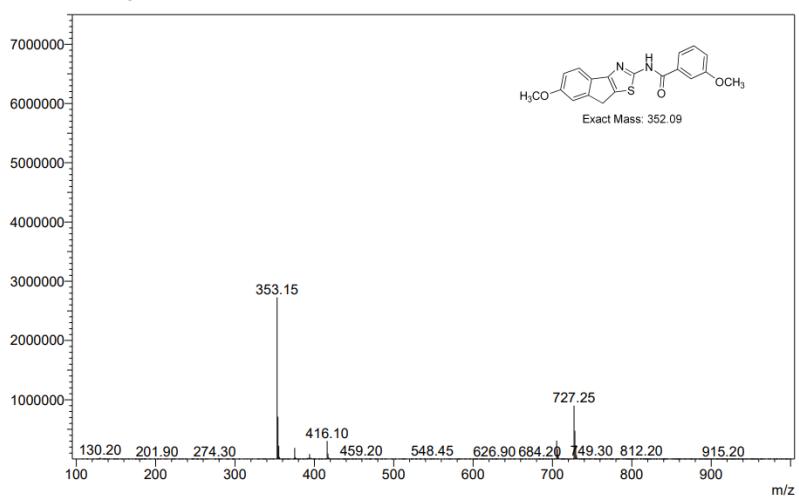
## ¹H NMR of compound 7i
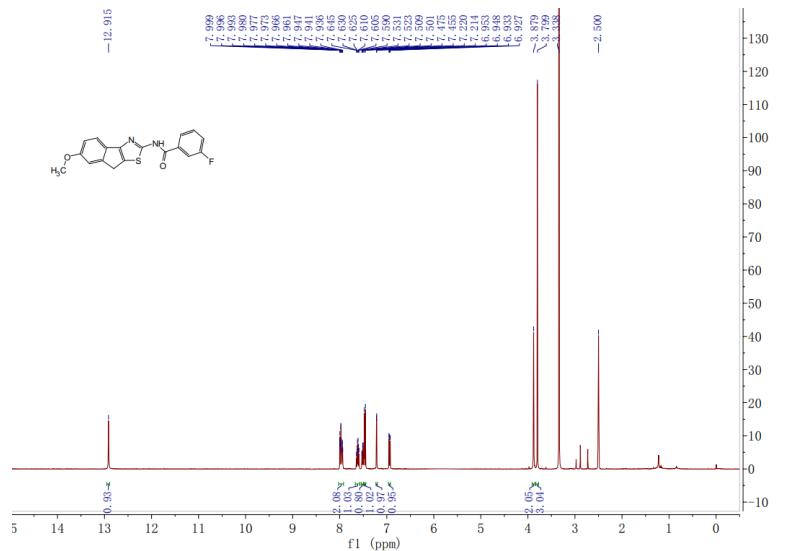


## ¹³C NMR of compound 7i



## MS of compound 7i

Peak#:1  R.Time:1.459(Scan#:117)
MassPeaks:440
Spectrum Mode:Averaged 1.425-1.475(115-119)
BG Mode:Calc  Segment 1 - Event 1

MS Spectrum

Exact Mass: 340.07



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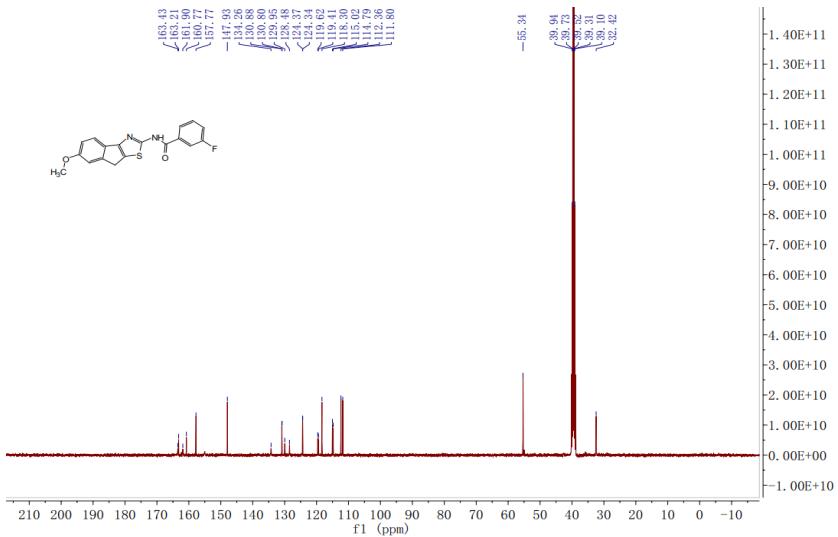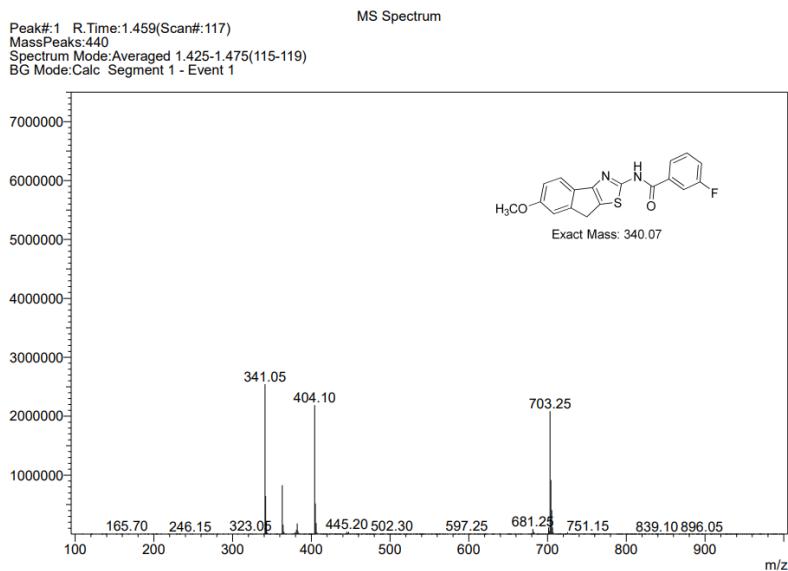
## $^1$H NMR of compound 7j
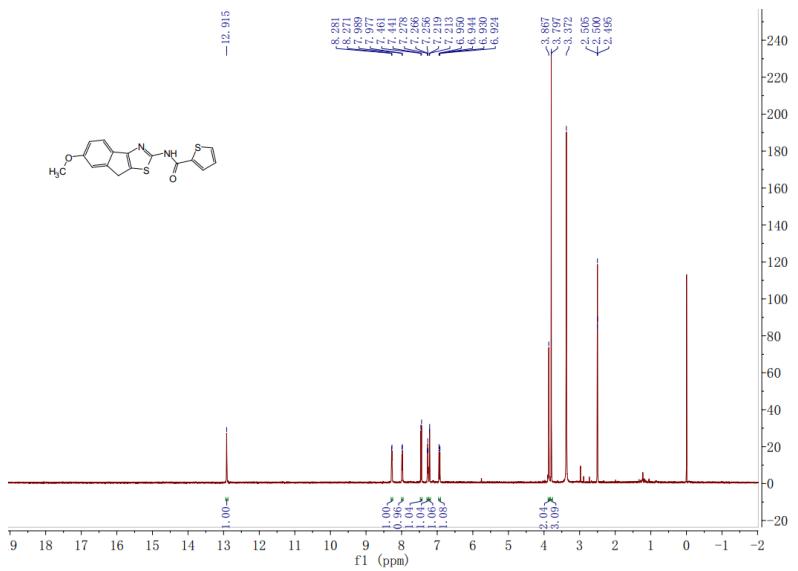


## $^{13}$C NMR of compound 7j
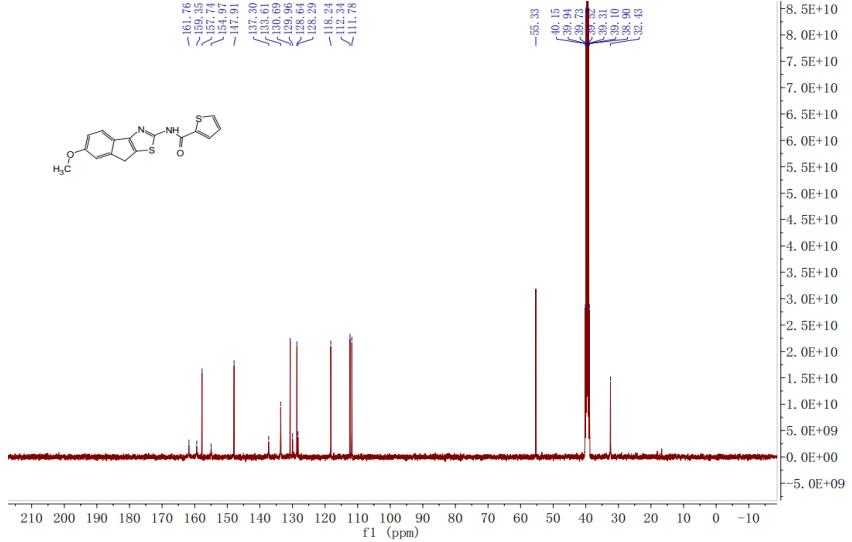


## MS of compound 7j

Peak#:1   R.Time:1.192(Scan#:95)
MassPeaks:548
Spectrum Mode:Averaged 1.150-1.200(93-97)
BG Mode:Calc  Segment 1 - Event 1

MS Spectrum

Exact Mass: 328.03



13
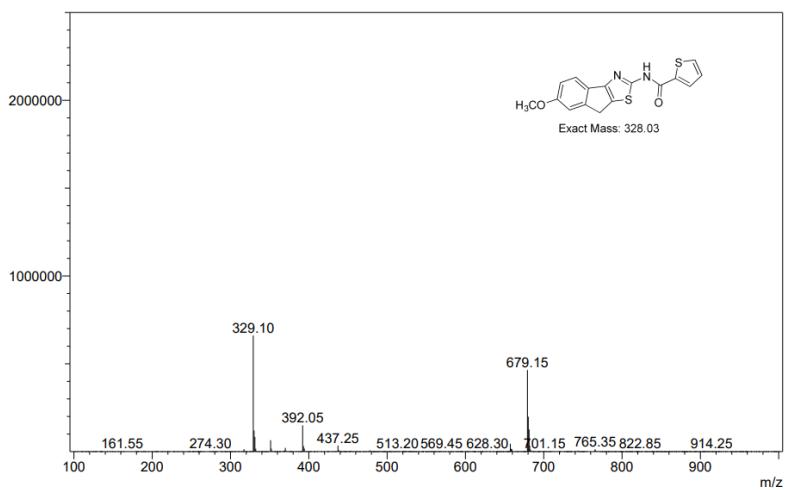
# <sup>1</sup>H NMR of compound **7k**
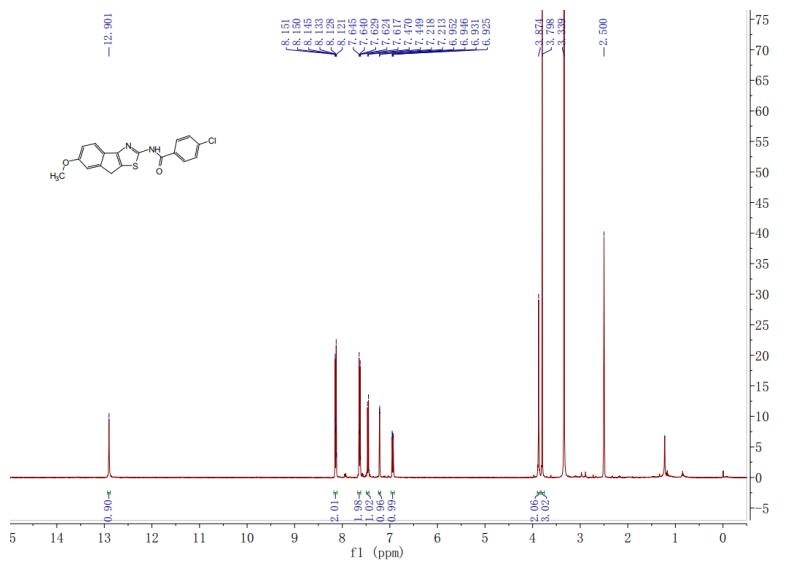


# <sup>13</sup>C NMR of compound **7k**



# MS of compound **7k**



MS Spectrum

Peak#:1  R.Time:1.505(Scan#:121)
MassPeaks:444
Spectrum Mode:Averaged 1.475-1.525(119-123)
BG Mode:Calc  Segment 1 - Event 1

Exact Mass: 356.04
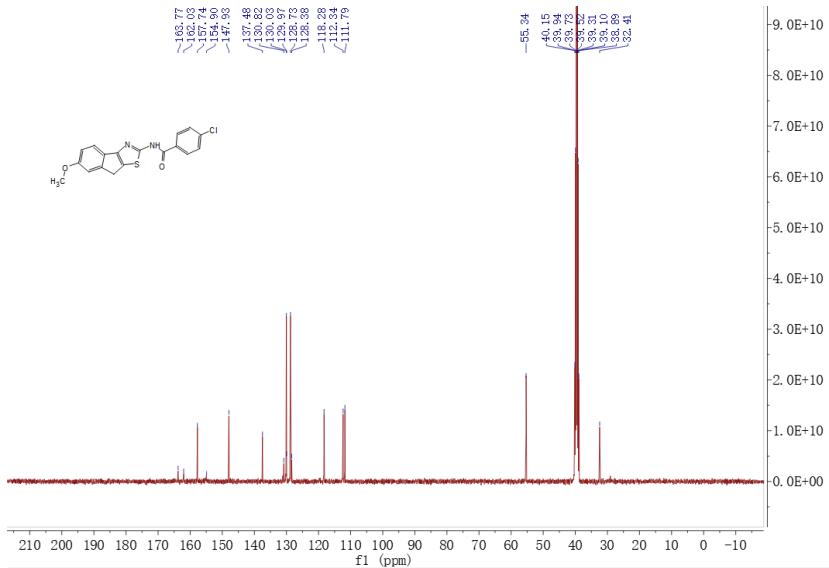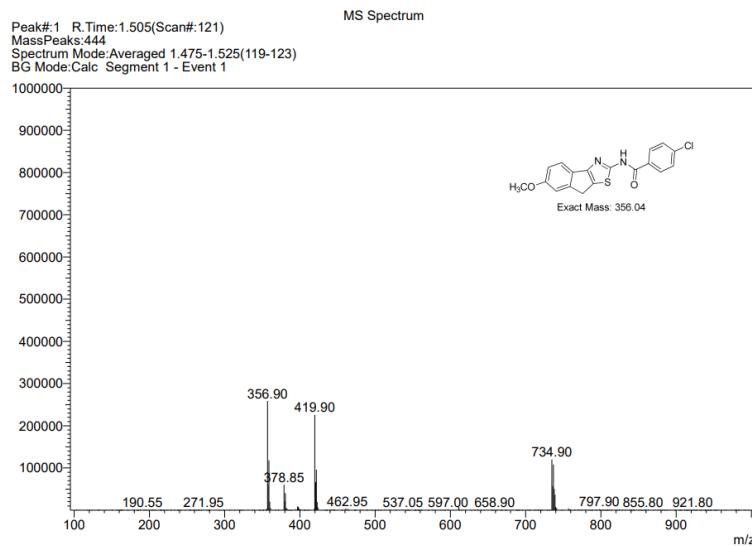
## ¹H NMR of compound **7l**
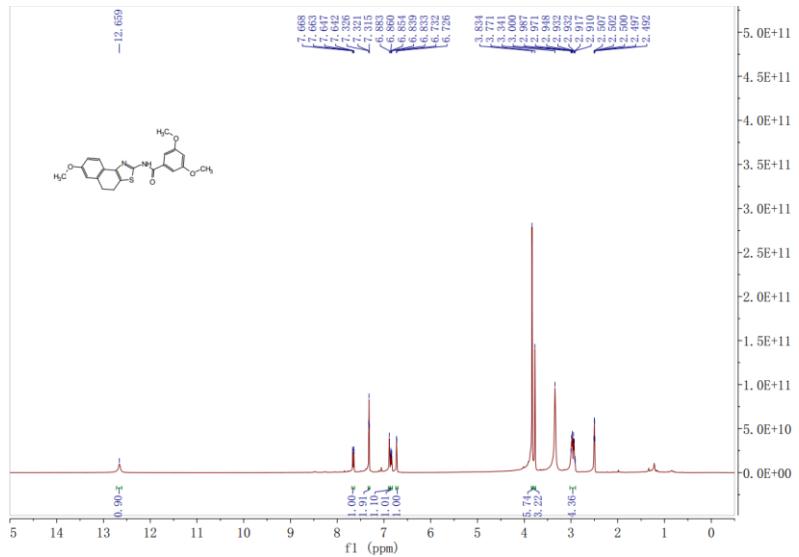


## ¹³C NMR of compound **7l**



## MS of compound **7l**

Peak#:1   R.Time:1.528(Scan#:123)
MassPeaks:431
Spectrum Mode:Averaged 1.500-1.550(121-125)
BG Mode:Calc  Segment 1 - Event 1

MS Spectrum

Exact Mass: 396.11



15
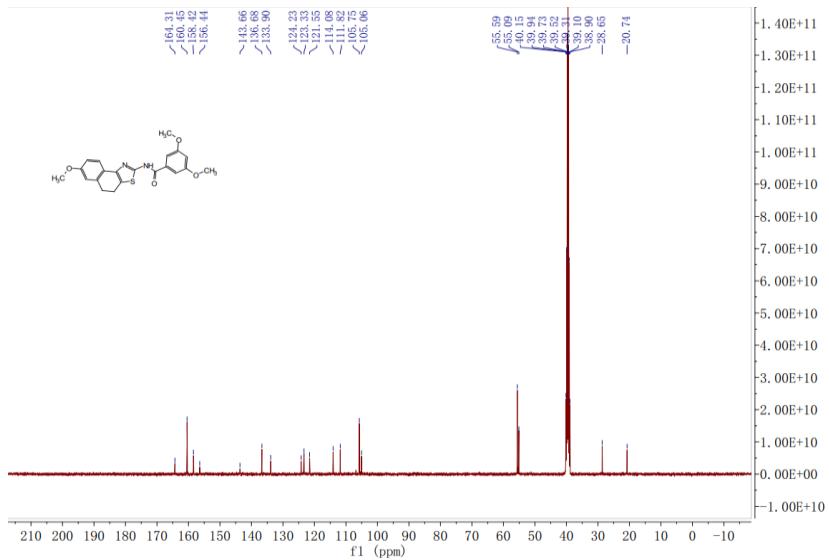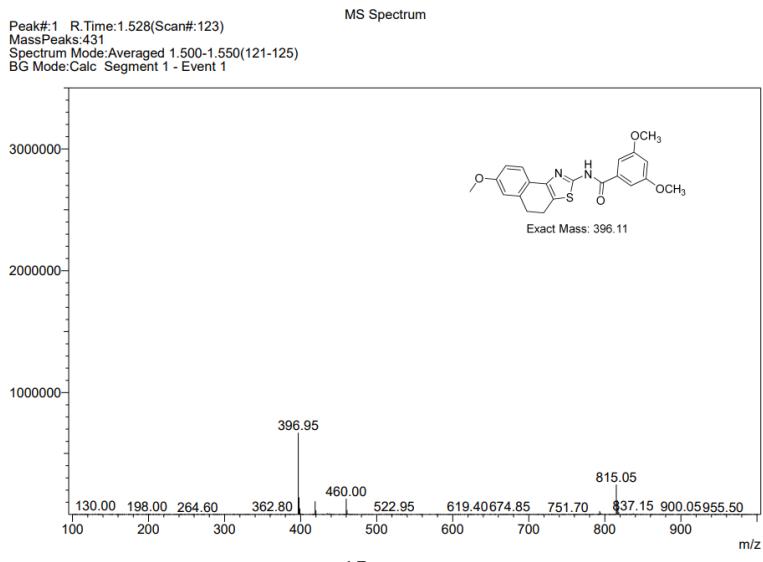
## ¹H NMR of compound 10a
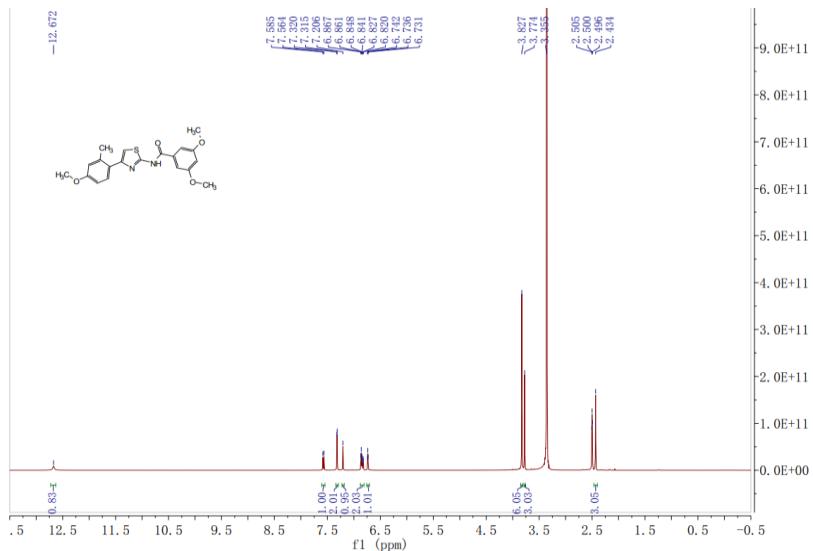


## ¹³C NMR of compound 10a



## MS of compound 10a



Peak#:1   R.Time:1.500(Scan#:121)
MassPeaks:499
Spectrum Mode:Averaged 1.475-1.525(119-123)
BG Mode:Calc  Segment 1 - Event 1

MS Spectrum

Exact Mass: 384.11

16
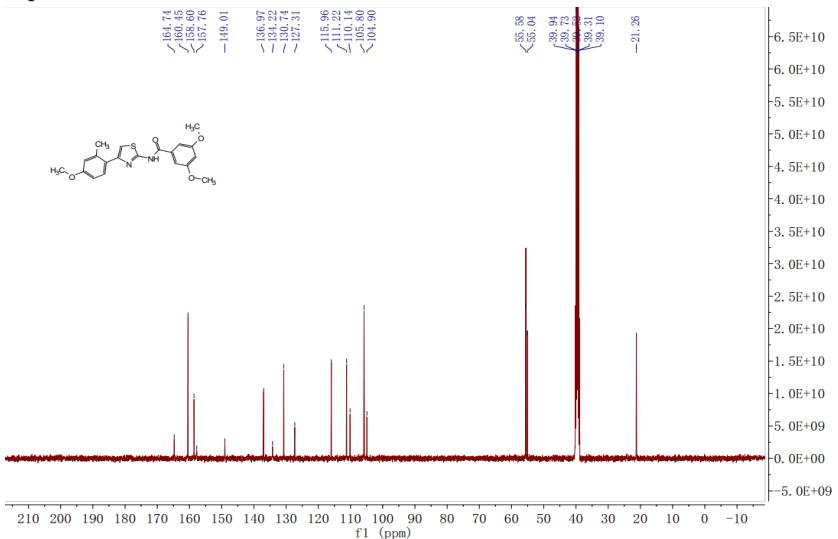
## <sup>1</sup>H NMR of compound **10b**
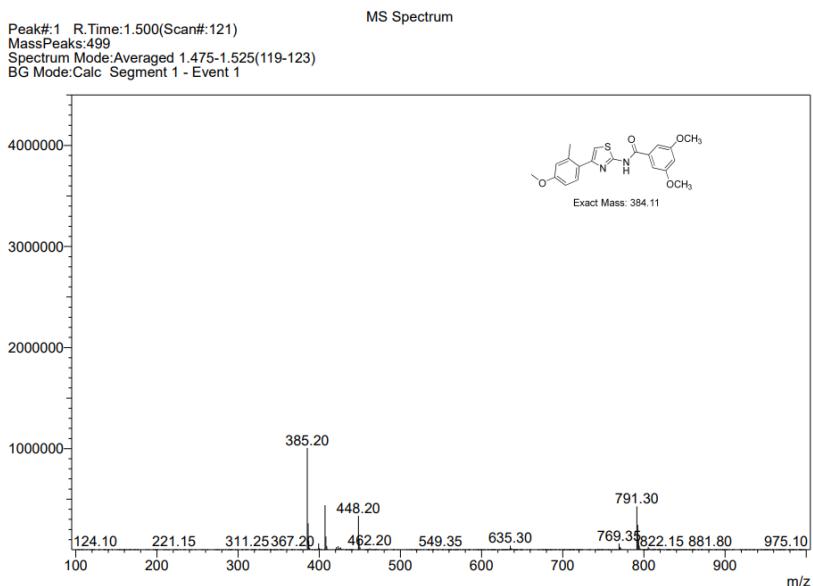
¹H NMR of compound **10b**
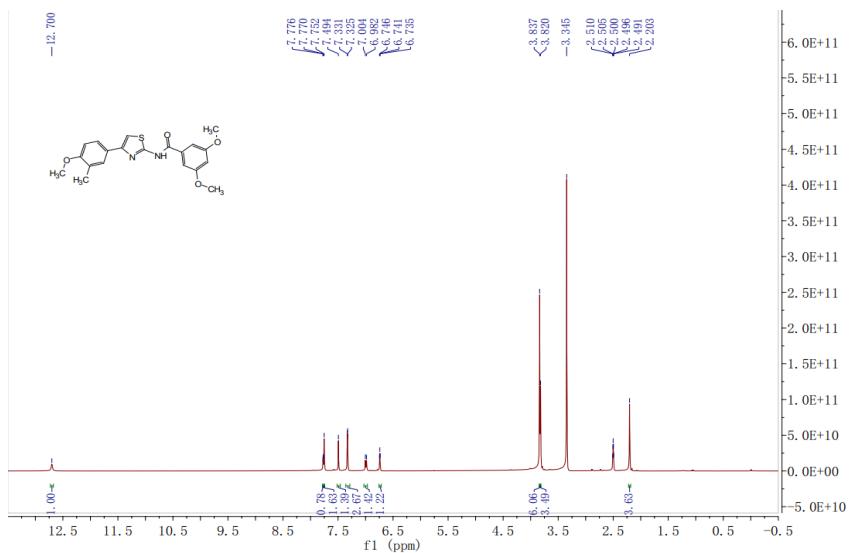


## ¹³C NMR of compound **10b**
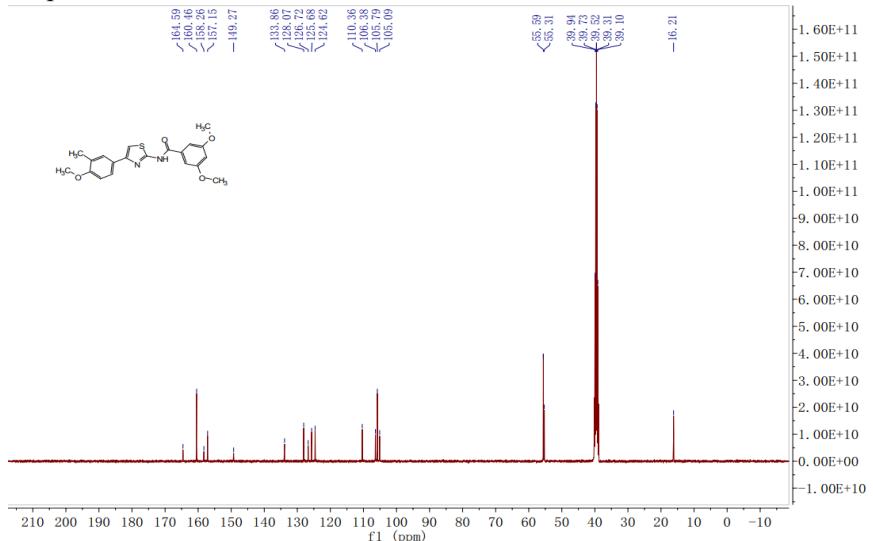


## MS of compound **10b**

Peak#:1　R.Time:1.531(Scan#:123)
MassPeaks:481
Spectrum Mode:Averaged 1.500-1.550(121-125)
BG Mode:Calc　Segment 1 - Event 1

MS Spectrum

Exact Mass: 384.11



17
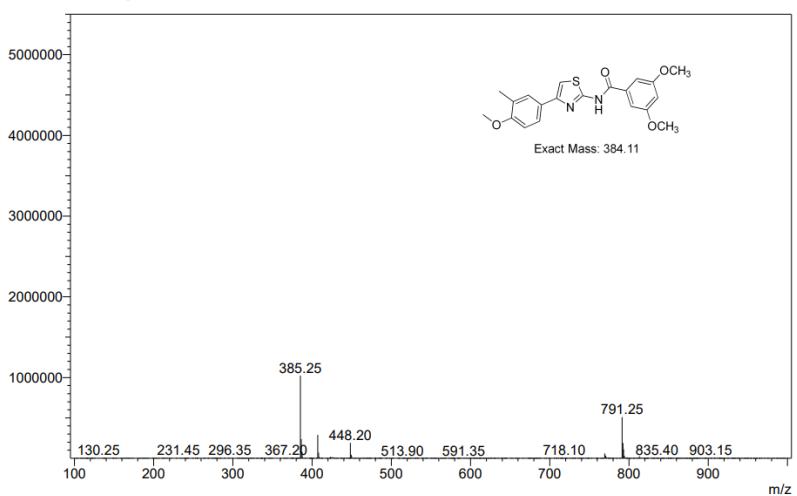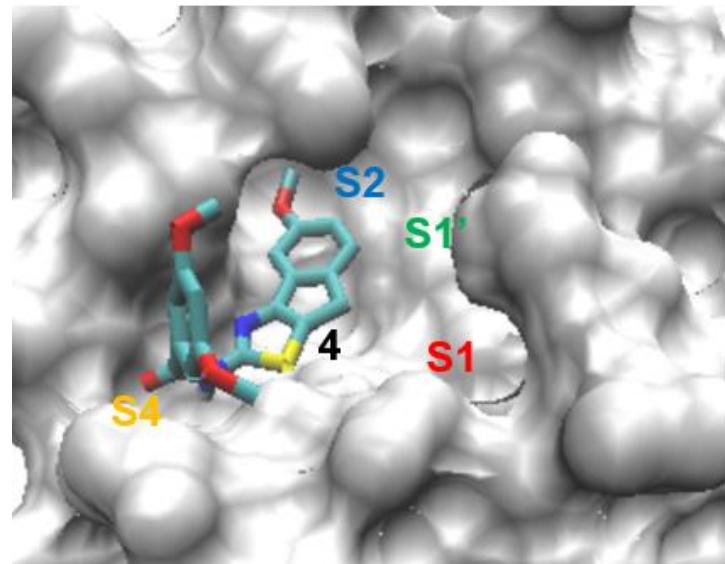
**Figure S1.** surf representation of the compound **4** (bonds representation) in the 3CL<sup>pro</sup> S1(red), S2(blue), S1'(green), S4(orange) binding pocket
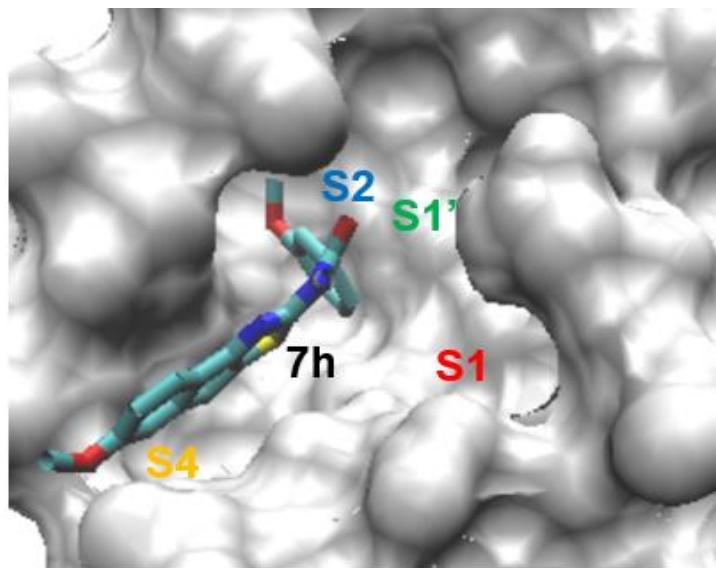


**Figure S2.** surf representation of the compound **7h** (bonds representation) in the 3CL<sup>pro</sup> S1(red), S2(blue), S1'(green), S4(orange) binding pocket