

Supporting Information

Integrating amino acids into Bcr-Abl inhibitors: Design, synthesis, biological evaluation, and *in silico* studies

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Figure S1. The Western blot results of compounds TL3, TL8, TL10, BS3, BS4, BS7, BS10, SR2, SR5 and SR10.

The nomenclature, chemical structure, HPLC, HRMS, ¹H-NMR and ¹³C-NMR spectra data of title compounds.

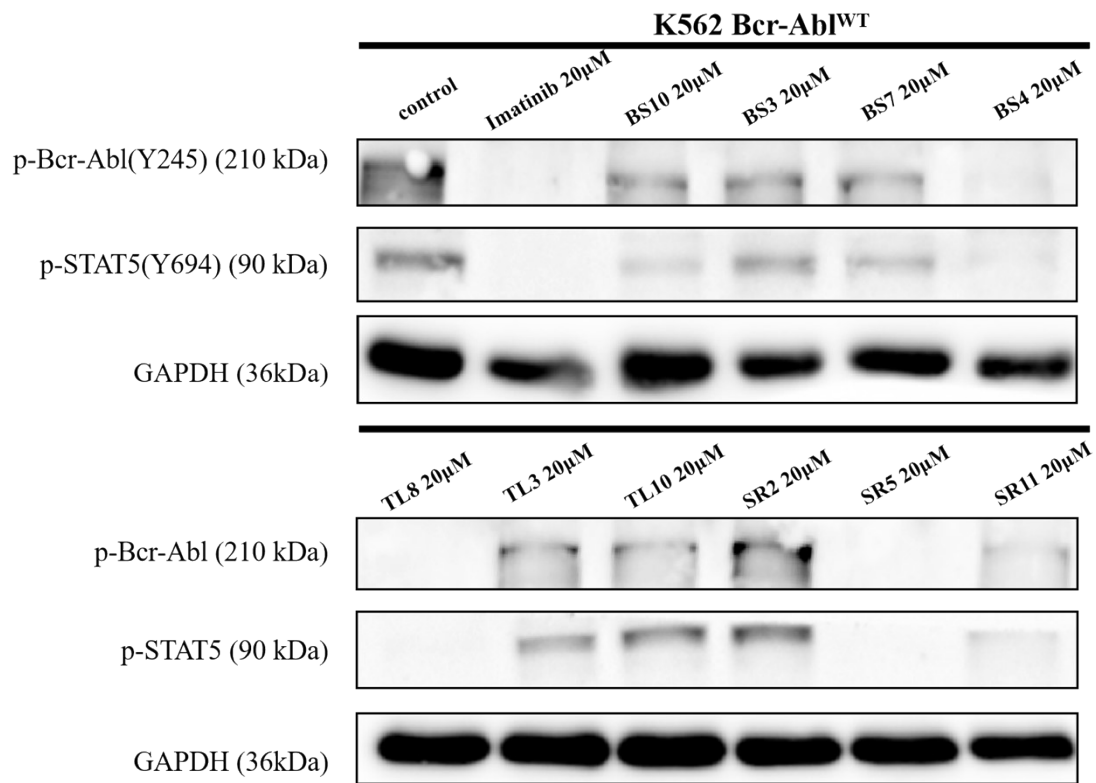
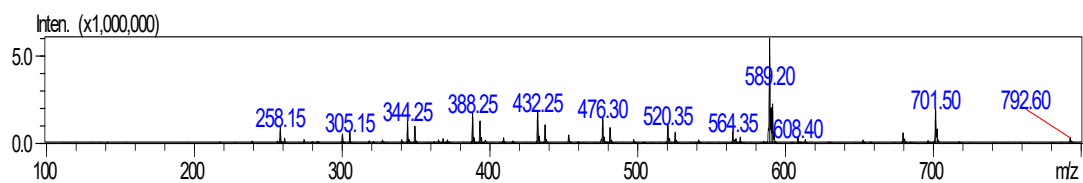
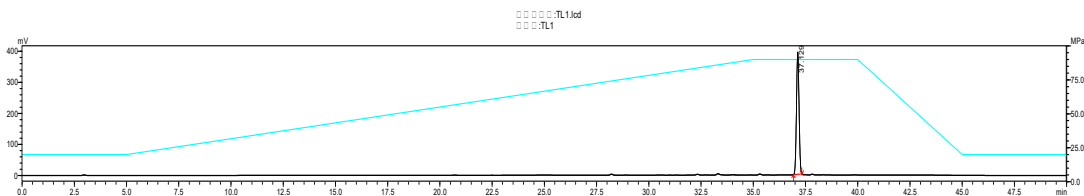
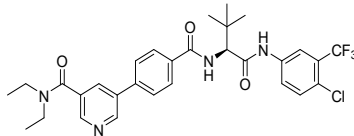


Figure S1. The effect of compounds **TL3**, **TL8**, **TL10**, **BS3**, **BS4**, **BS7**, **BS10**, **SR2**, **SR5** and **SR10** on phosphorylation level of Bcr-Abl and STAT5 in CML cells. K562 cells were treated with DMSO (0.1%), and compounds at 20 μM for 48 h, respectively. The cells were lysed by RIPA (Radio Immunoprecipitation assay buffer) containing protease and phosphatase inhibitor, and p-Bcr-Abl, p-STAT5 and GAPDH levels were analyzed by Western blot.

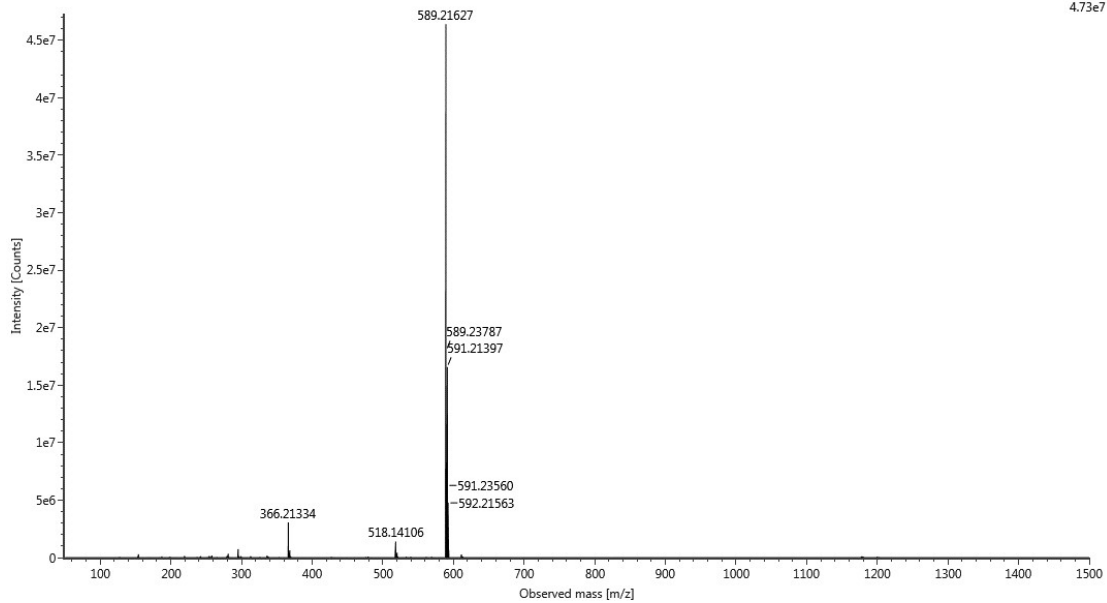
(S)-5-(4-((1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3,3-dimethyl-1-oxobutan-2-yl)carbamoyl)phenyl)-N,N-diethylnicotinamide (TL1)

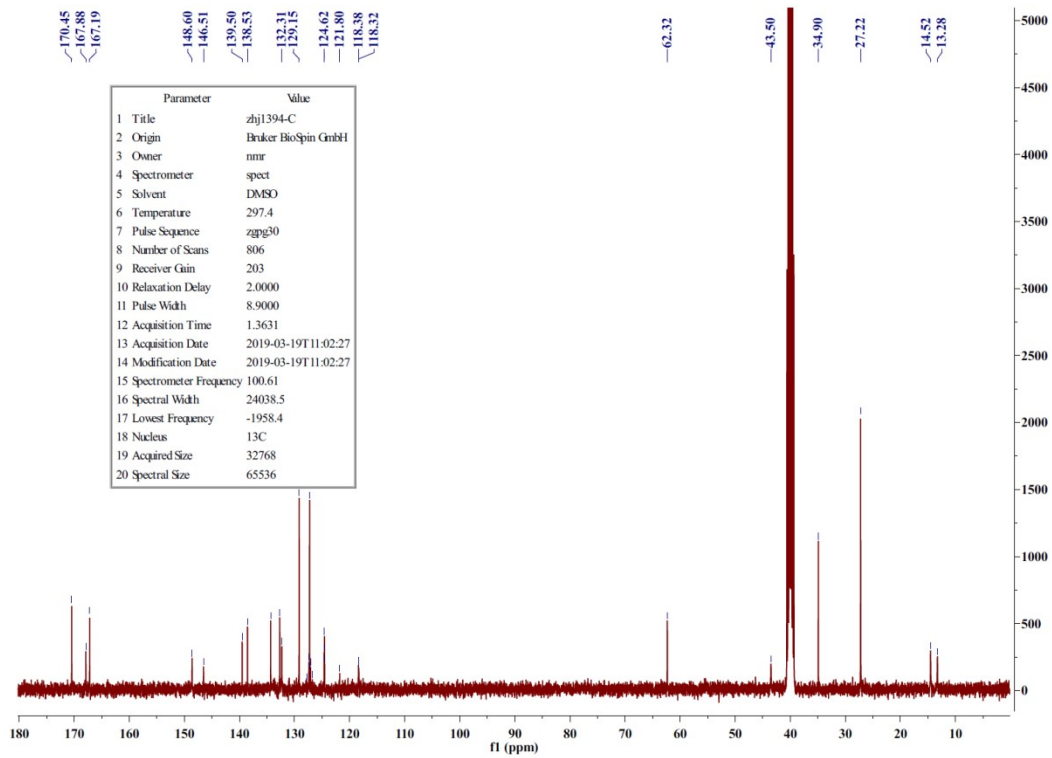
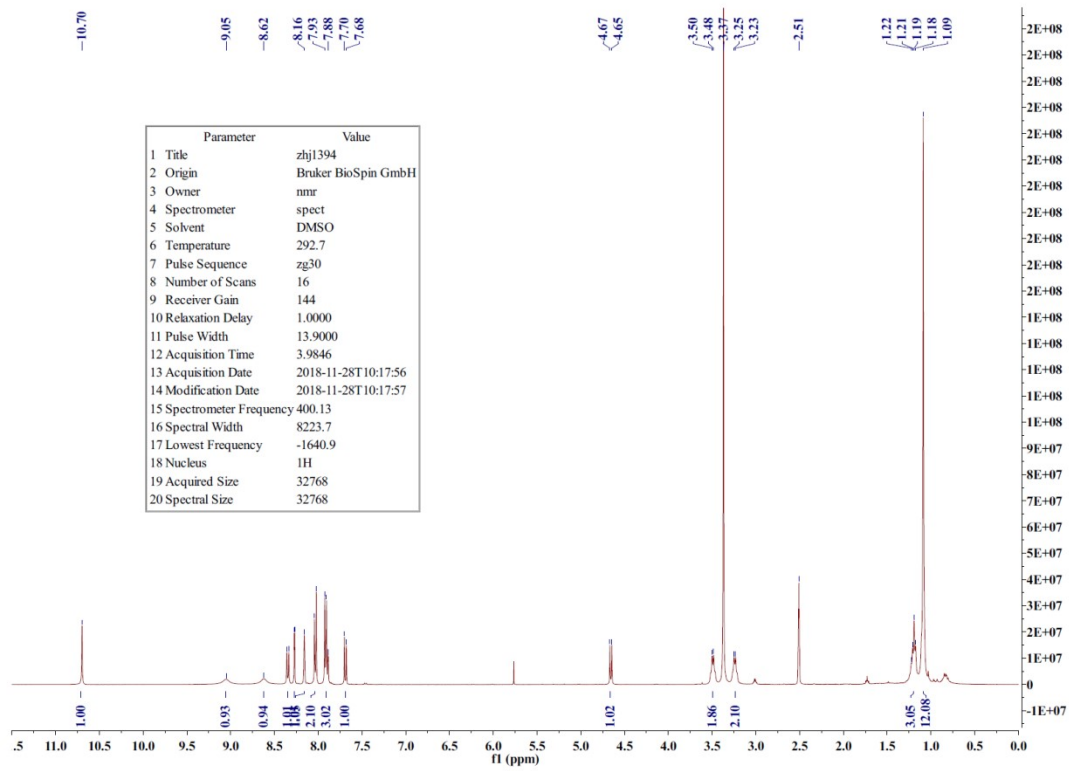


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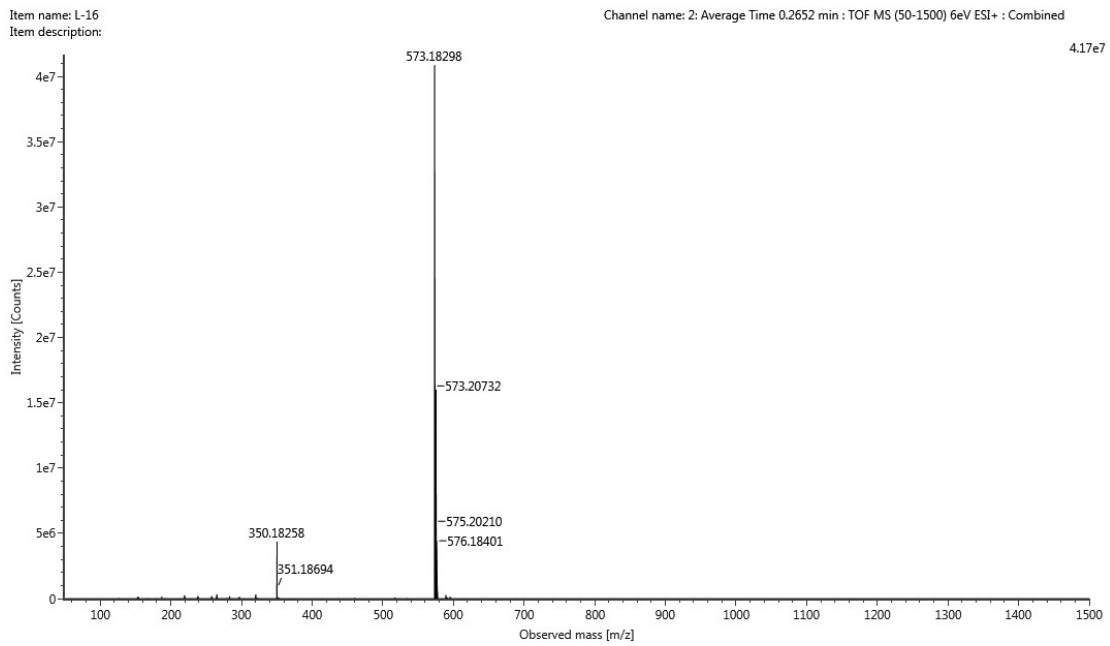
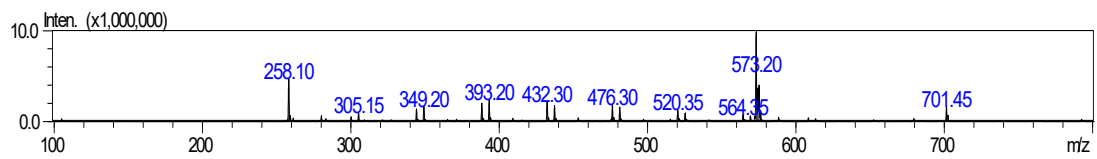
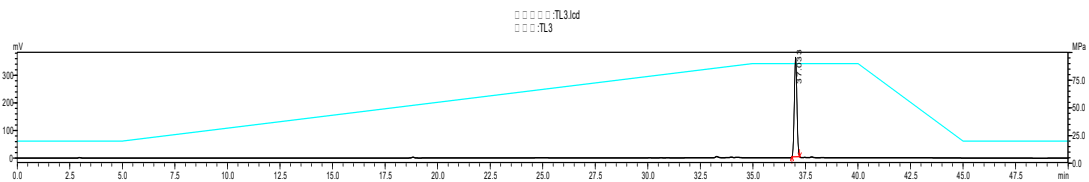
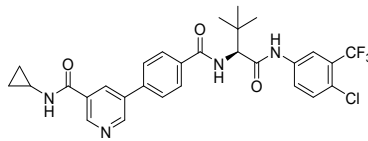
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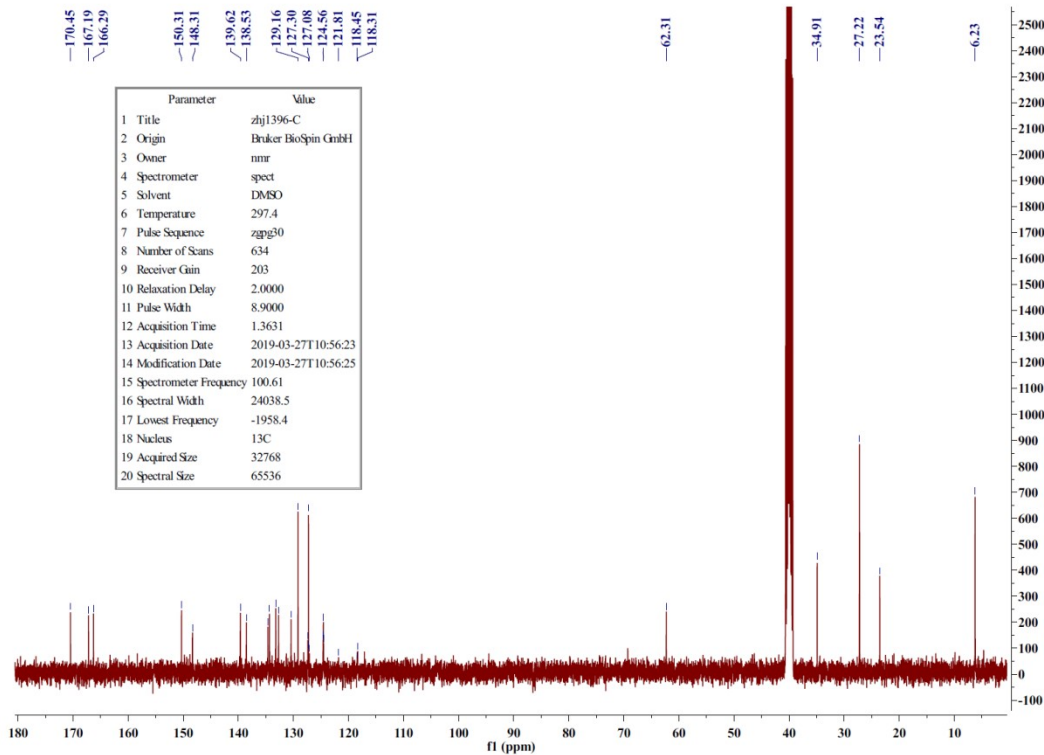
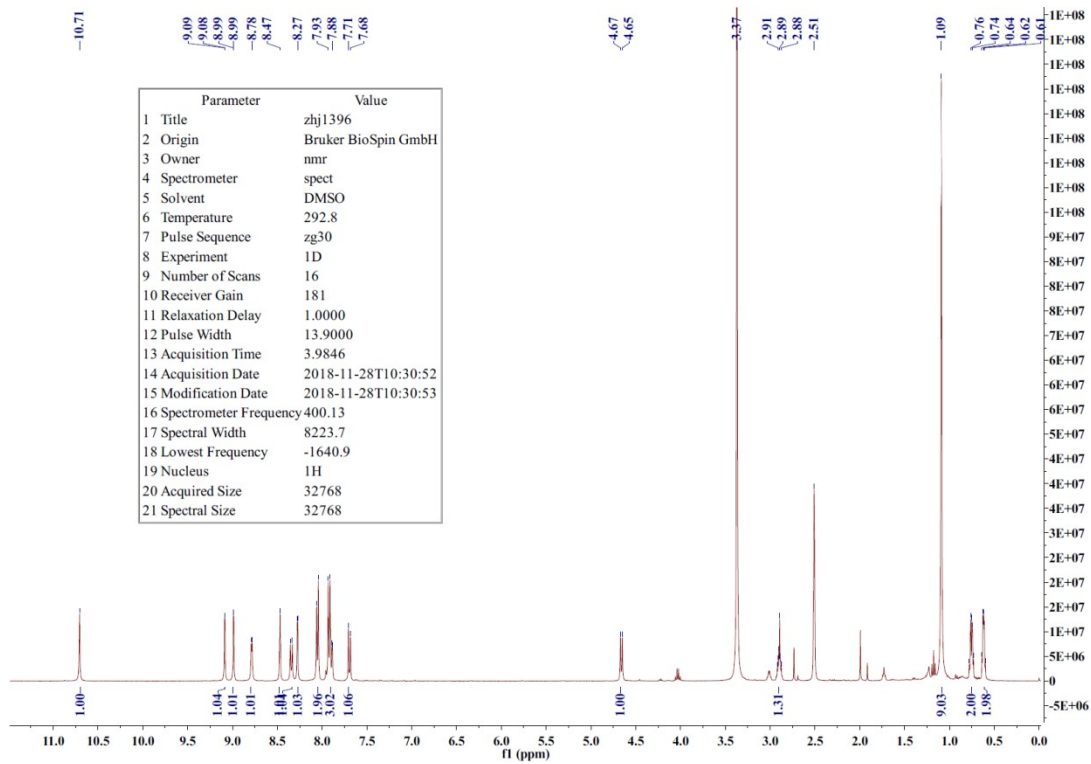
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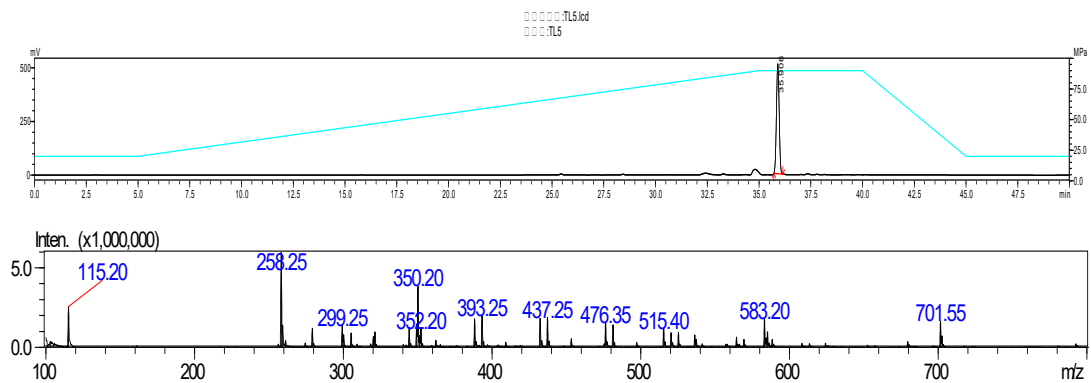
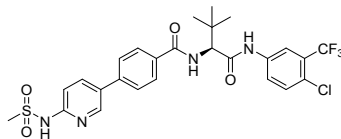


(S)-5-(4-((1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3,3-dimethyl-1-oxobutan-2-yl)carbamoyl)phenyl)-N-cyclopropylnicotinamide (TL2)





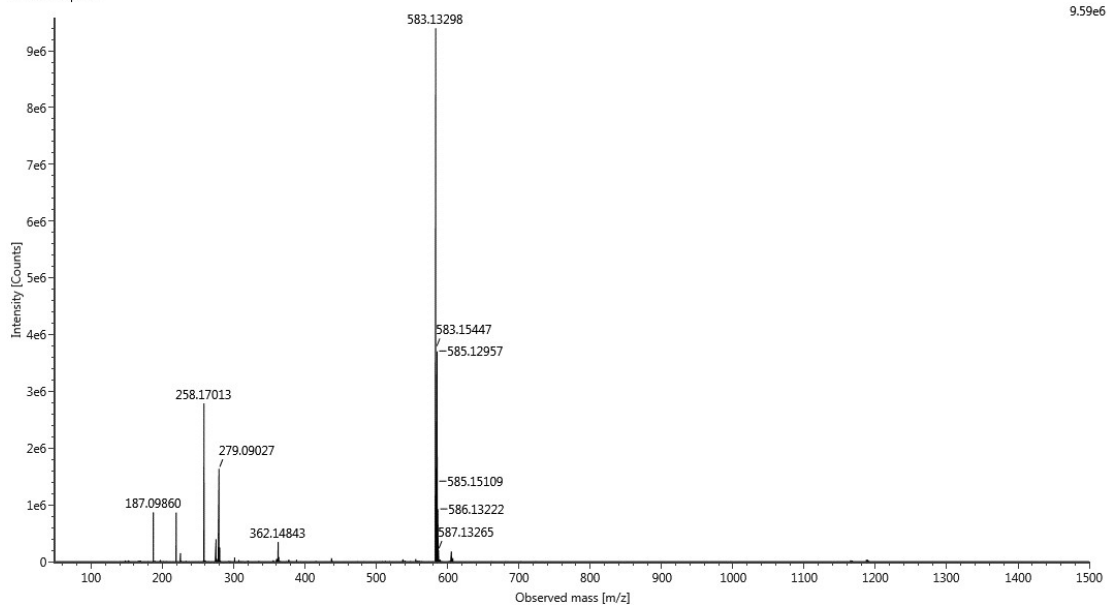
(S)-N-(1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3,3-dimethyl-1-oxobutan-2-yl)-4-(6-(methylsulfonamido)pyridin-3-yl)benzamide (TL3)

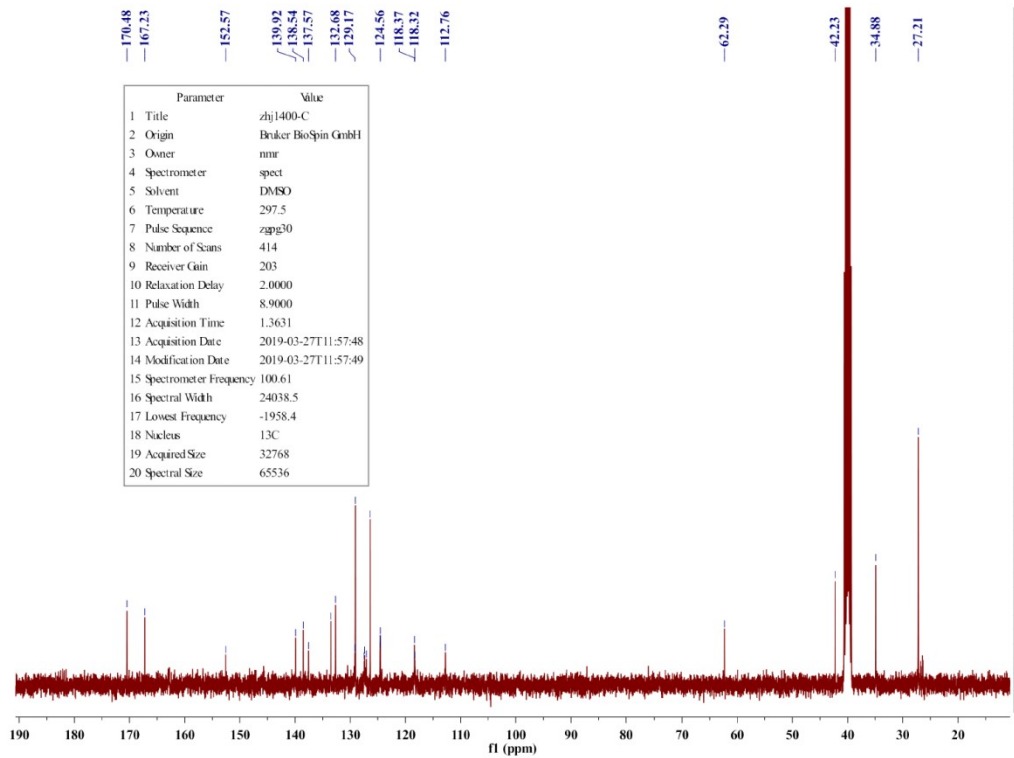
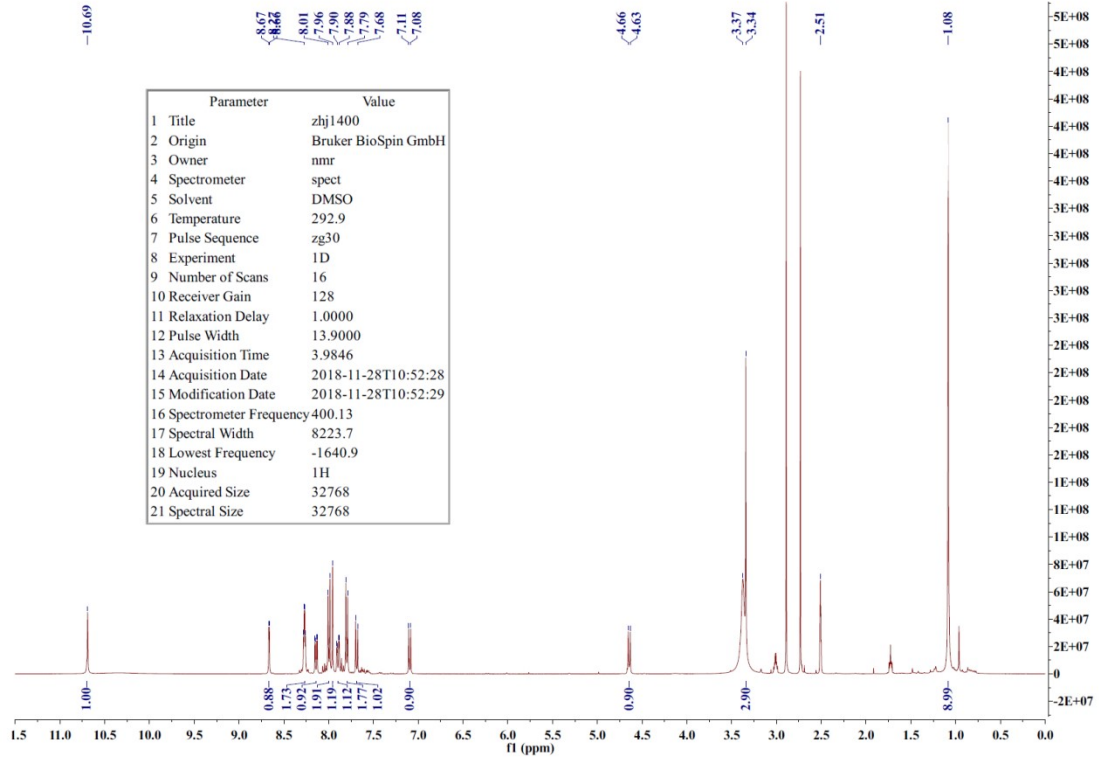


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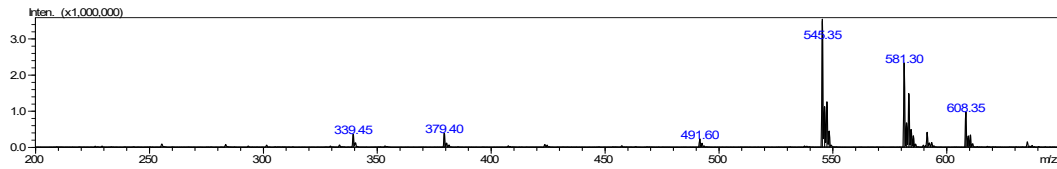
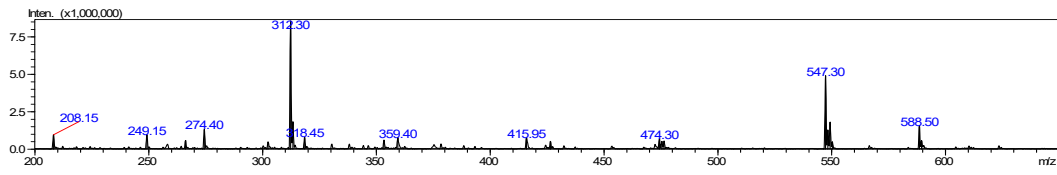
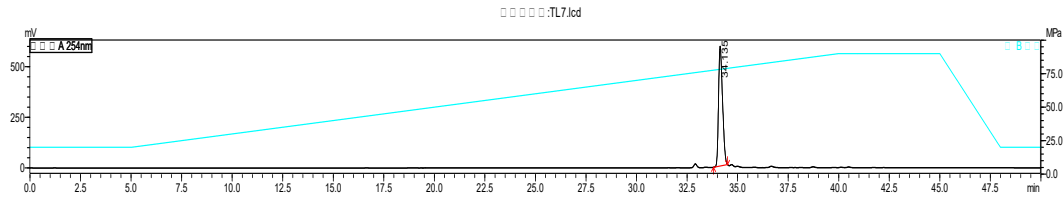
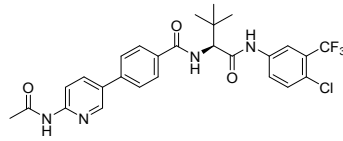
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9.59e6





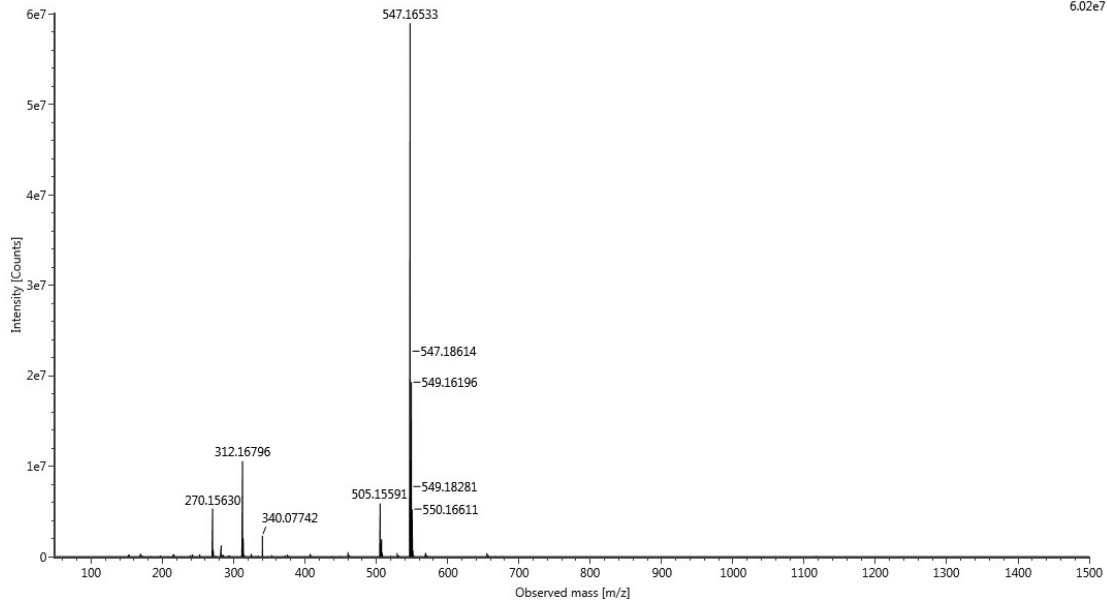
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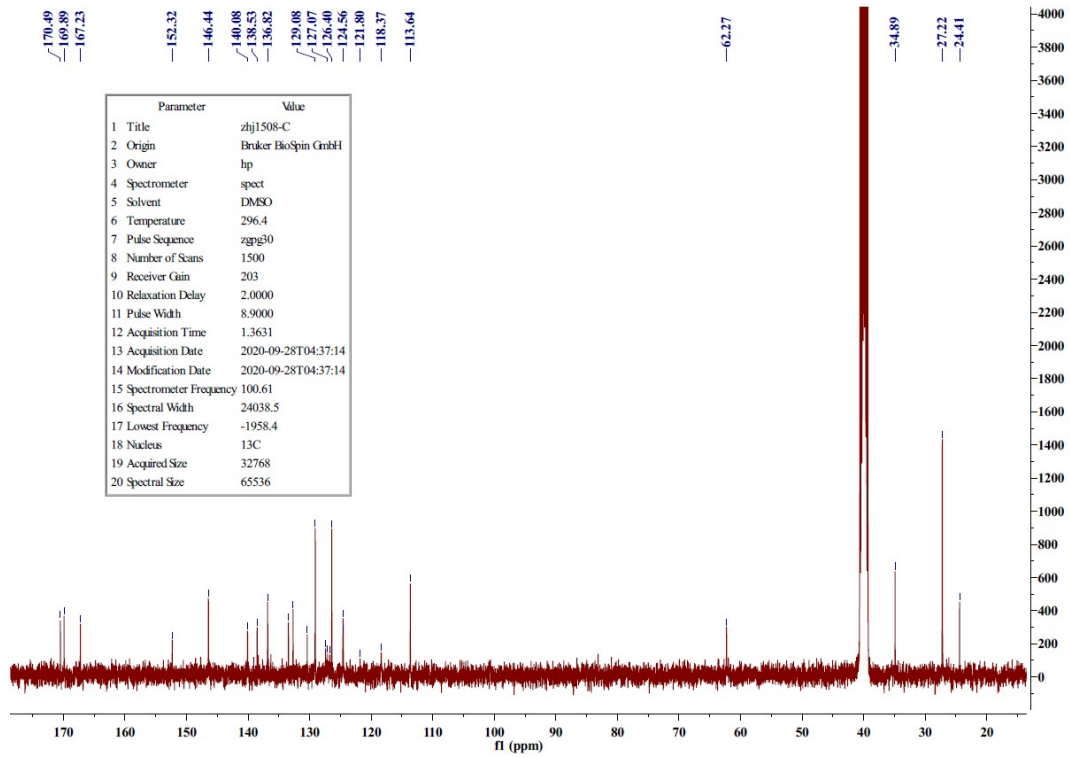
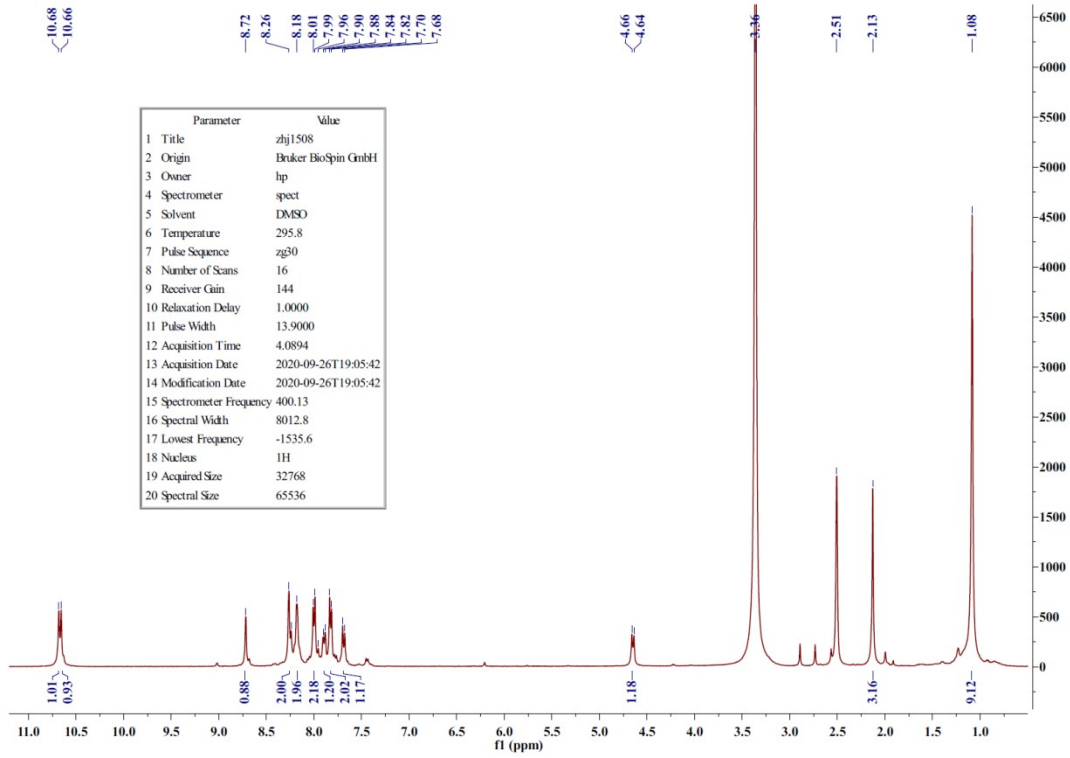


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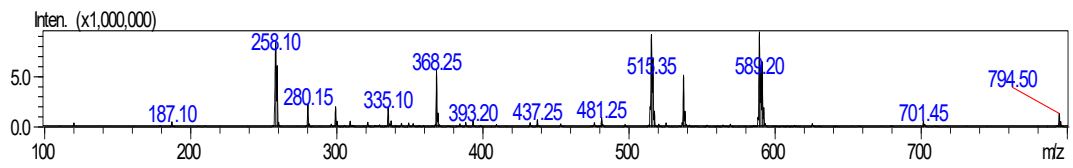
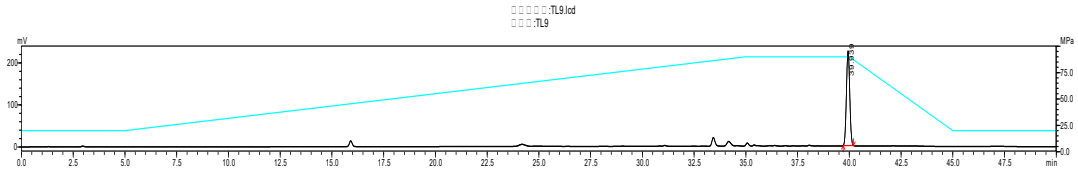
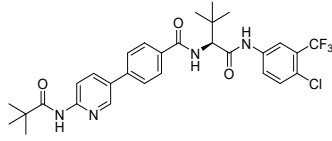
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6.02e7





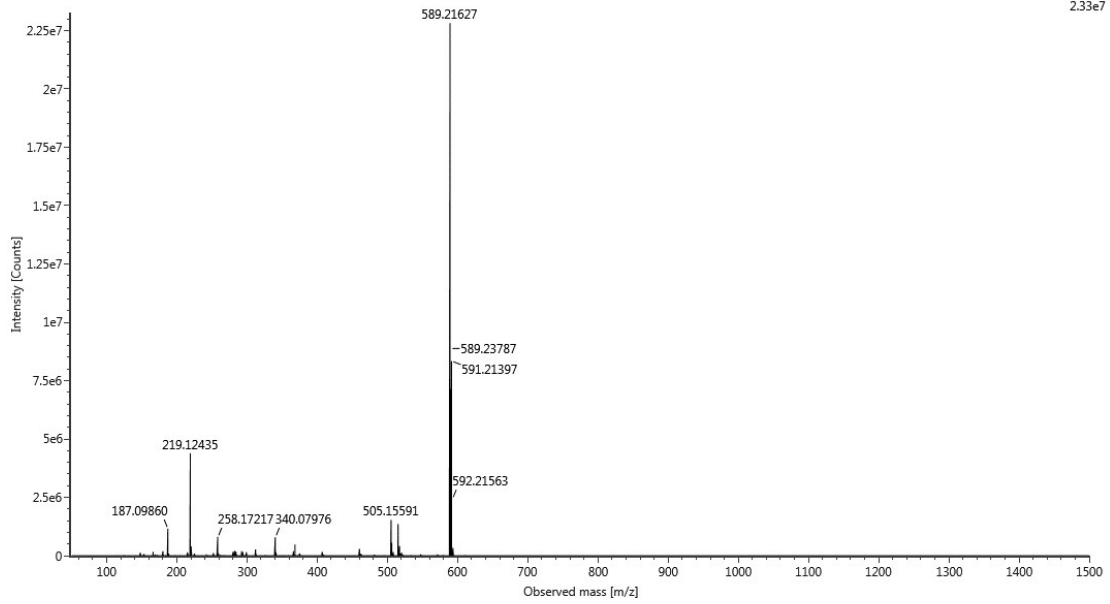
(S)-N-(1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3,3-dimethyl-1-oxobutan-2-yl)-4-(6-pivalamidopyridin-3-yl)benzamide (TL5)

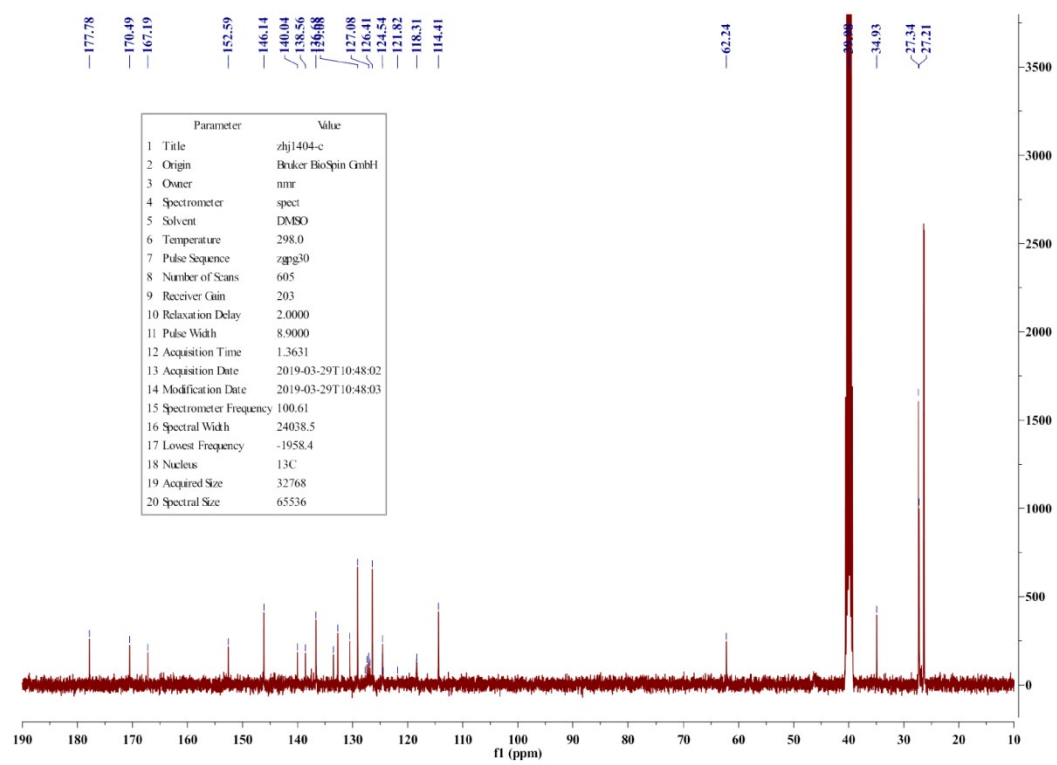
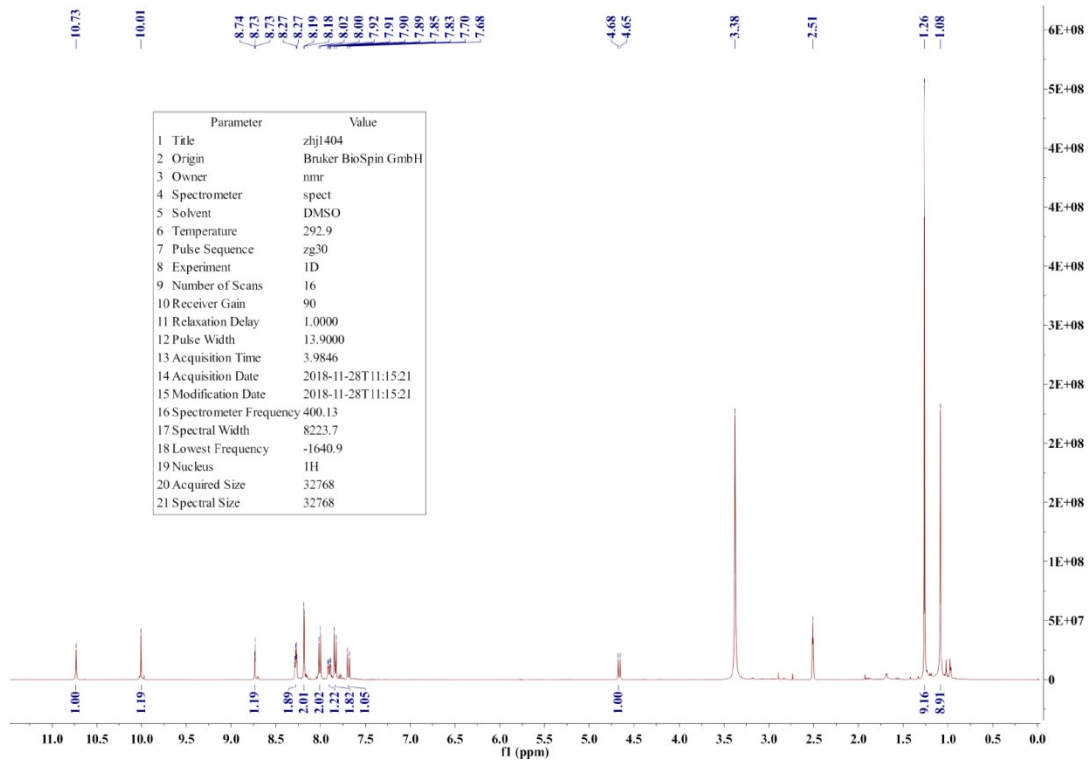


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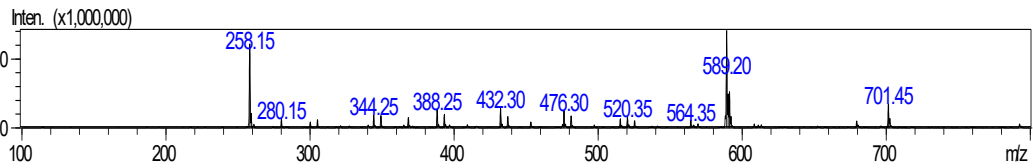
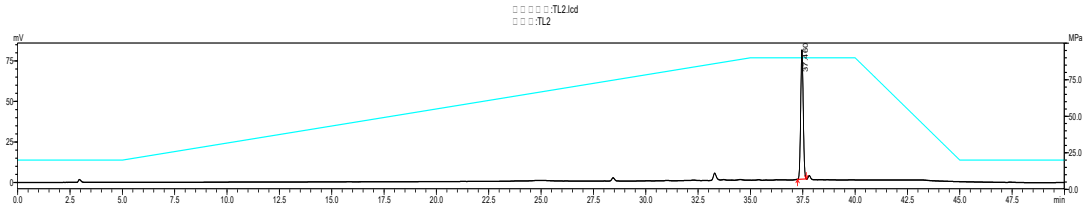
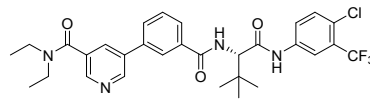
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2.33e7



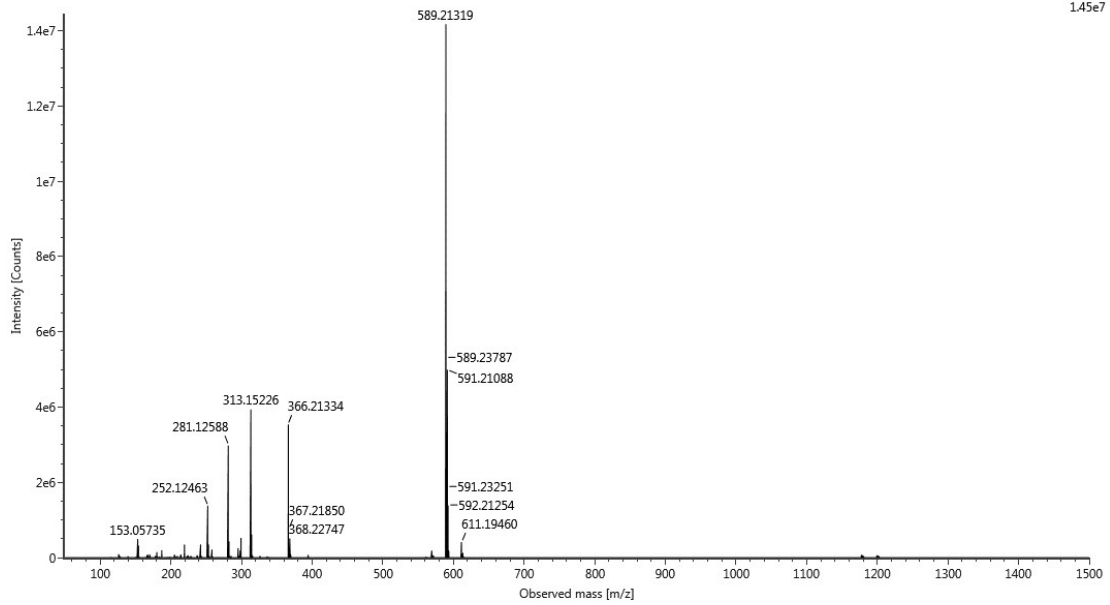


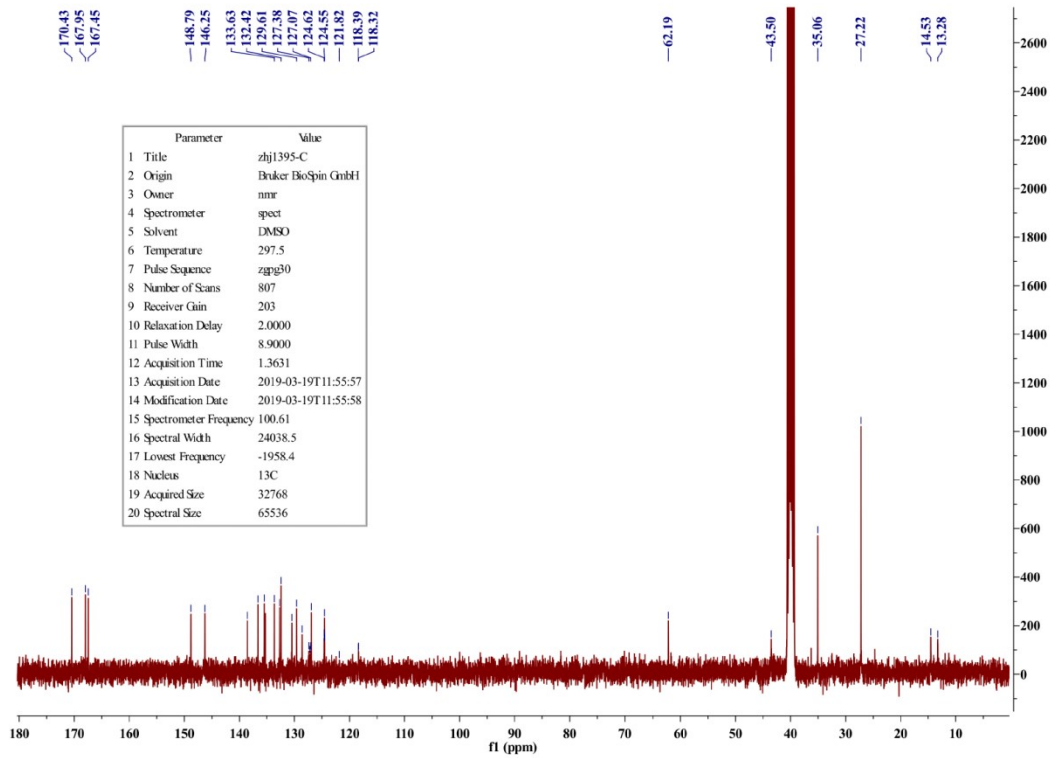
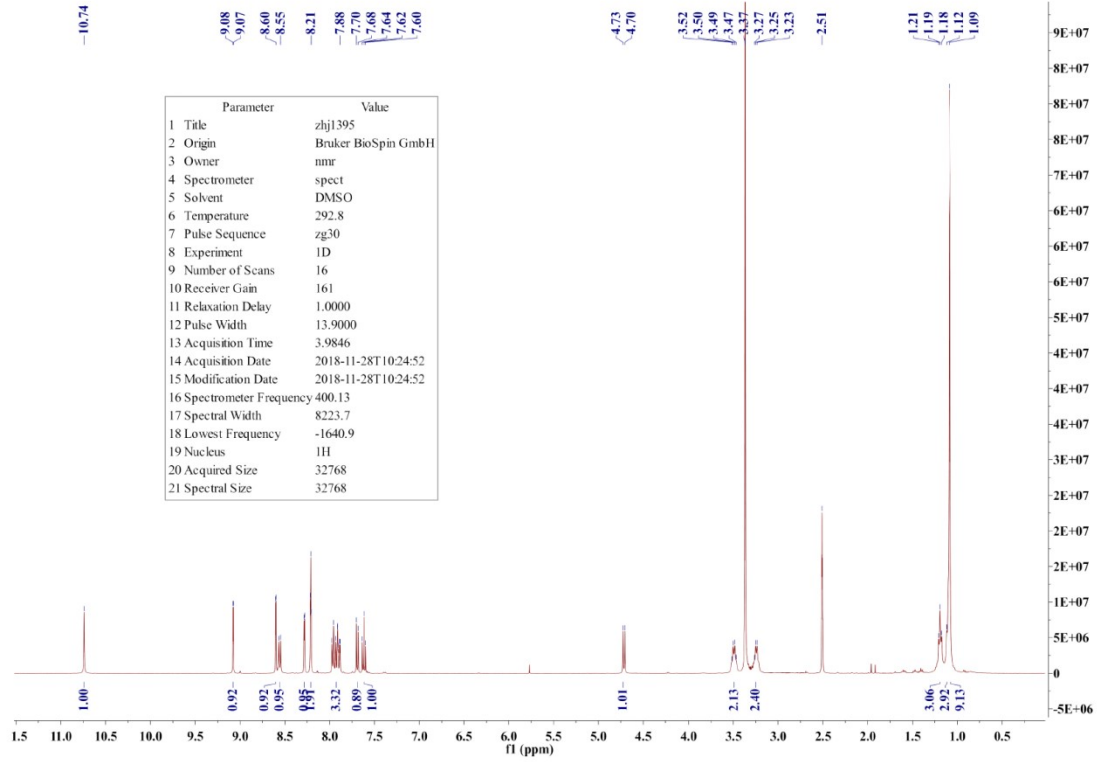
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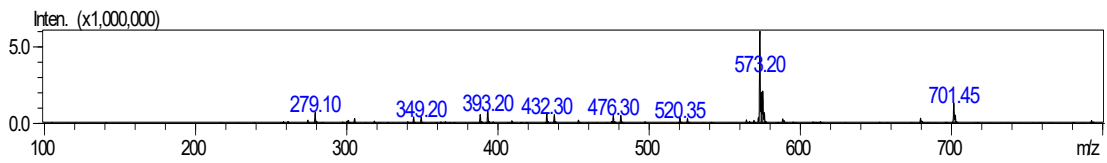
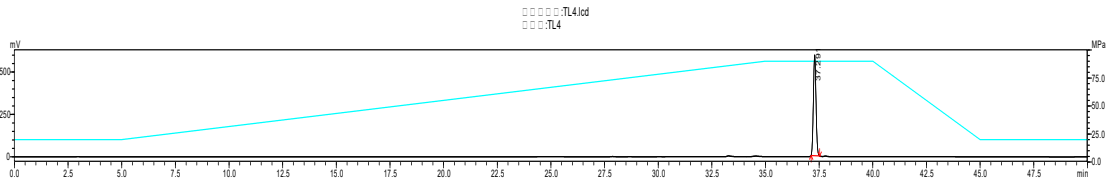
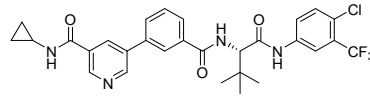
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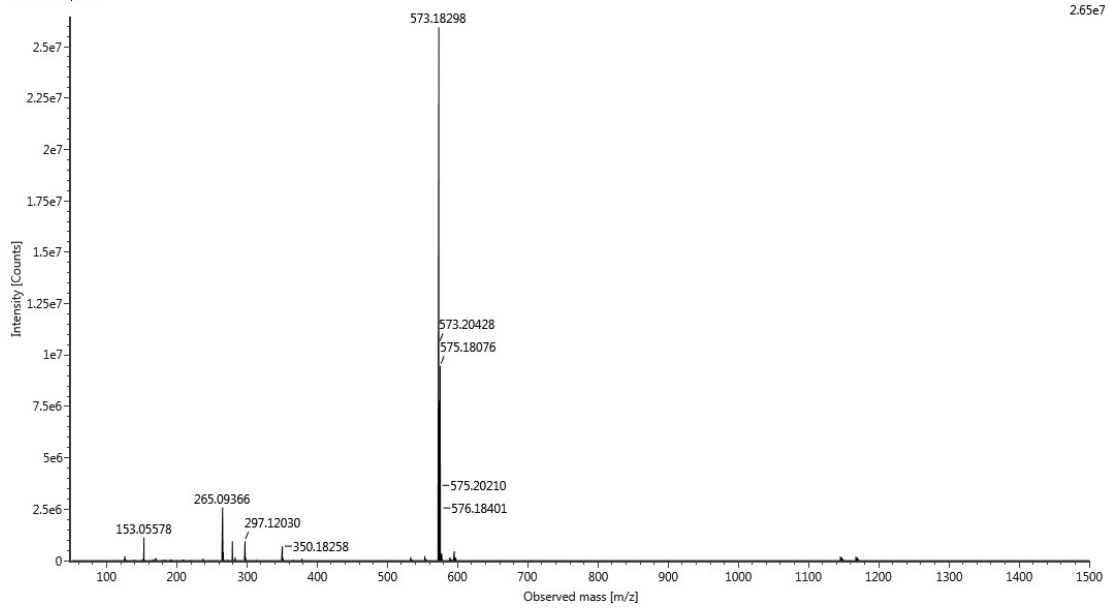


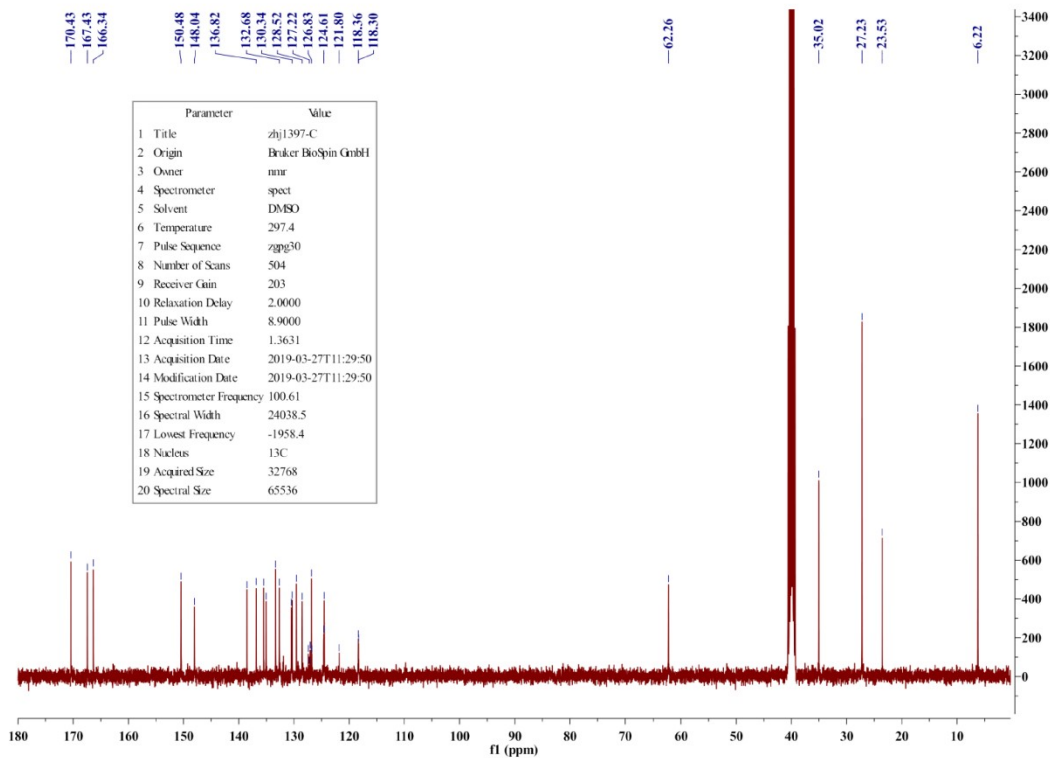
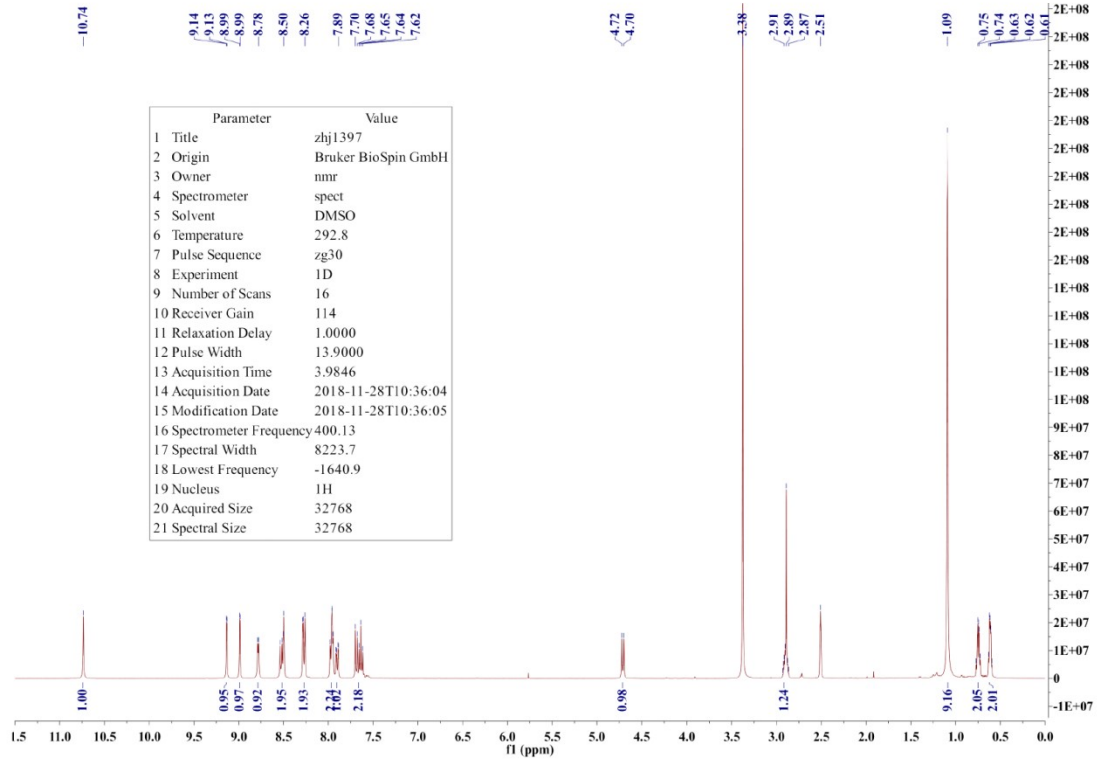
(S)-5-(3-((1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3,3-dimethyl-1-oxobutan-2-yl)carbamoyl)phenyl)-N-cyclopropylnicotinamide (TL7)



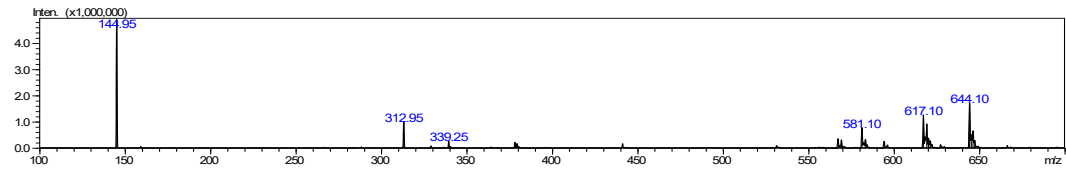
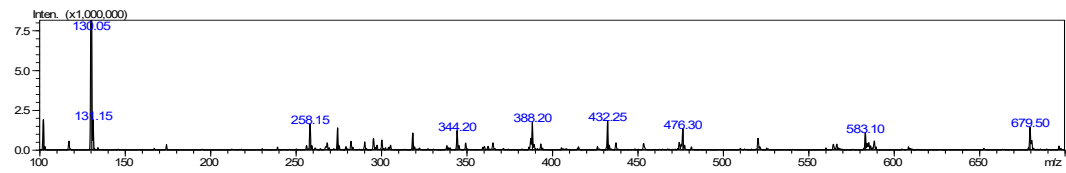
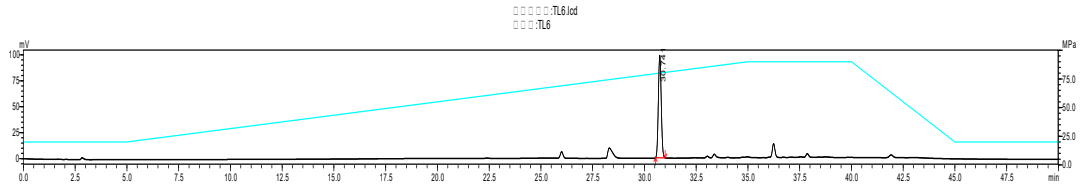
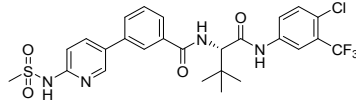
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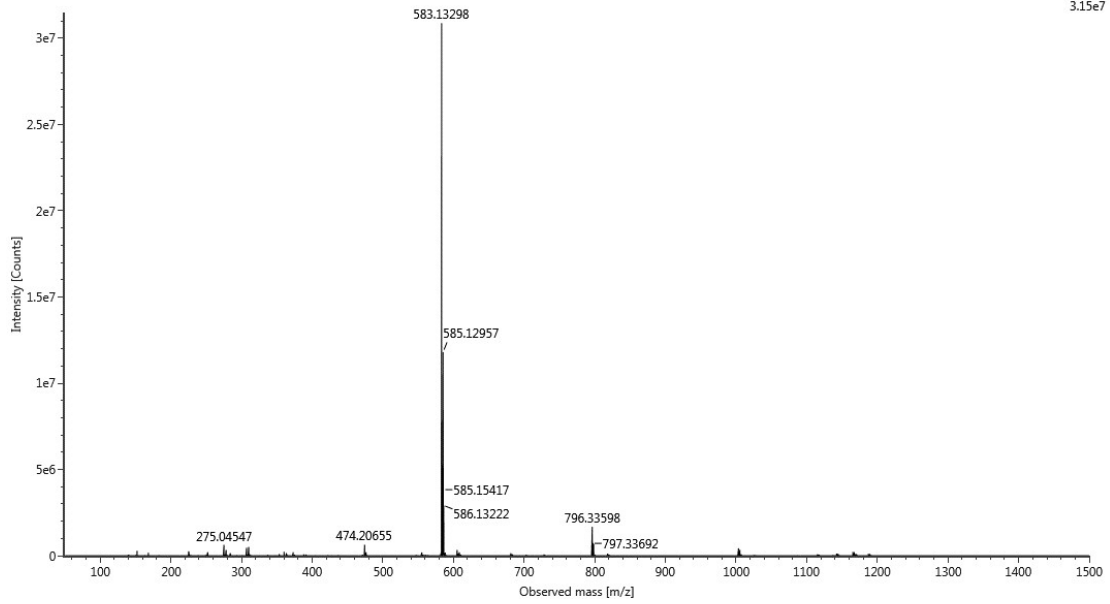
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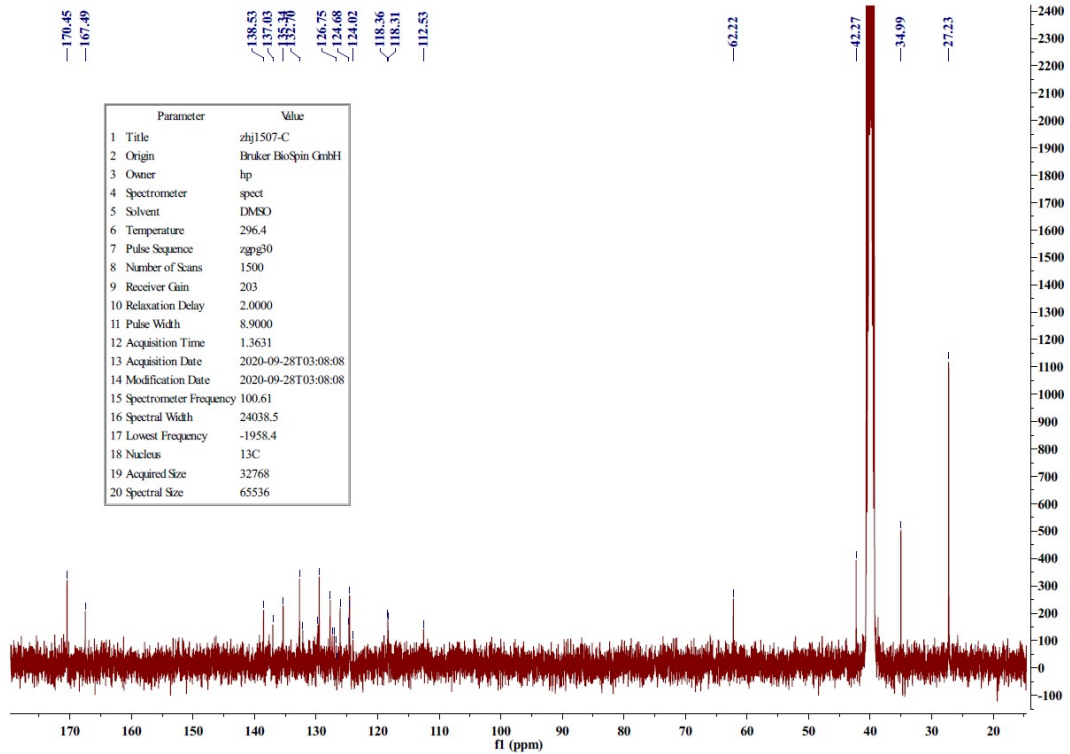
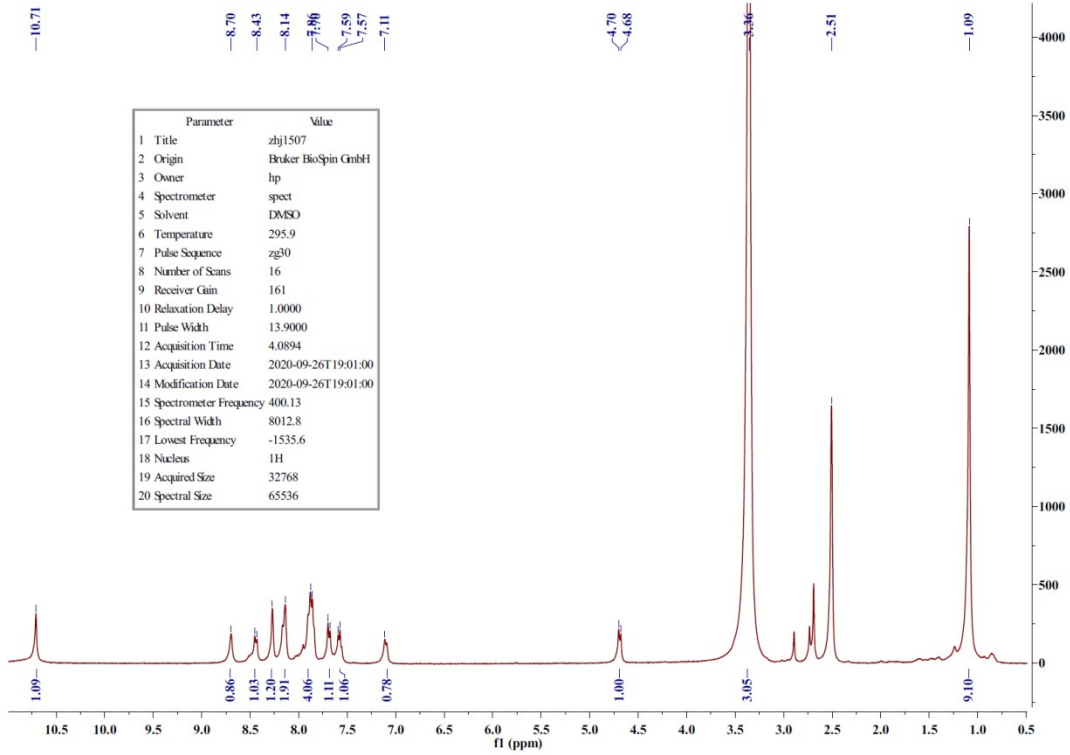


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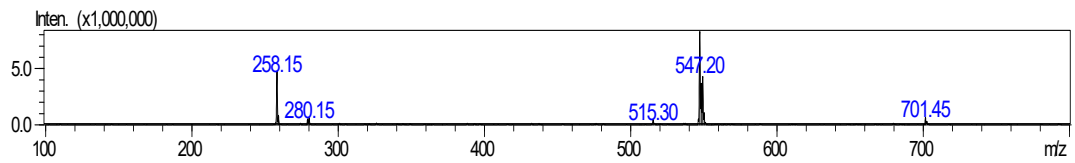
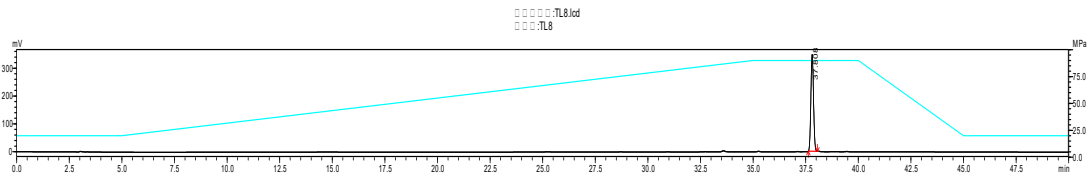
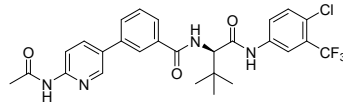
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3.15e7





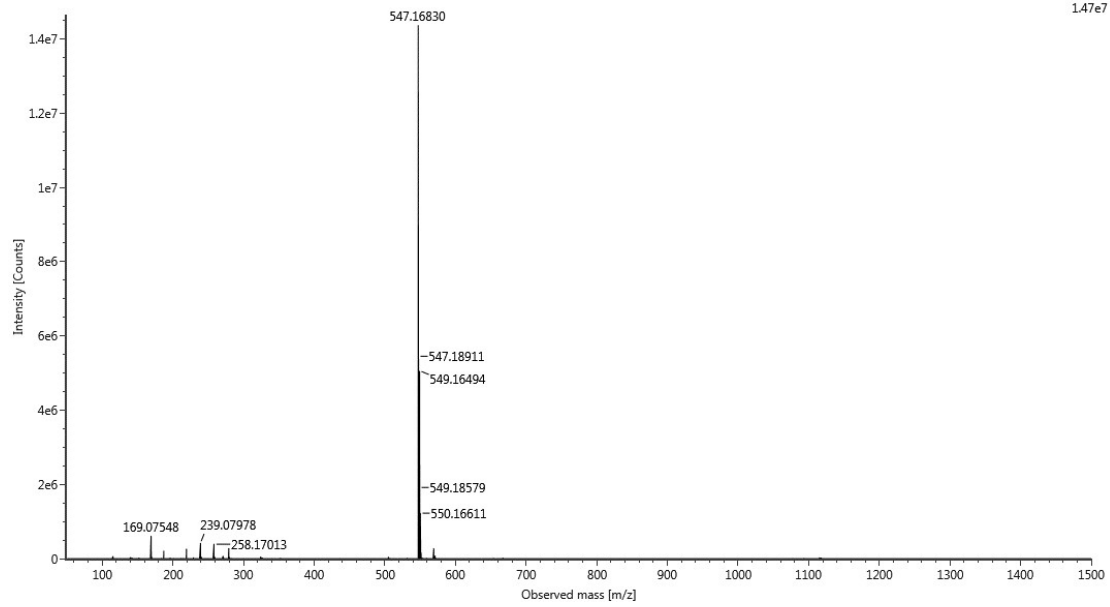
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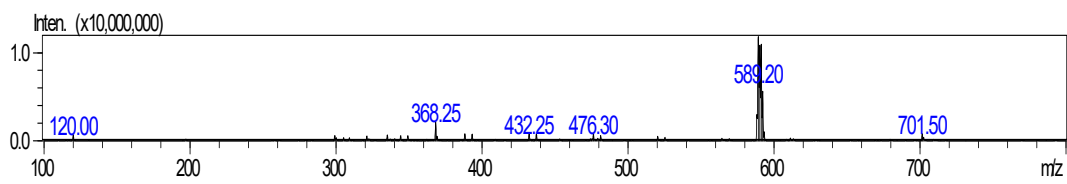
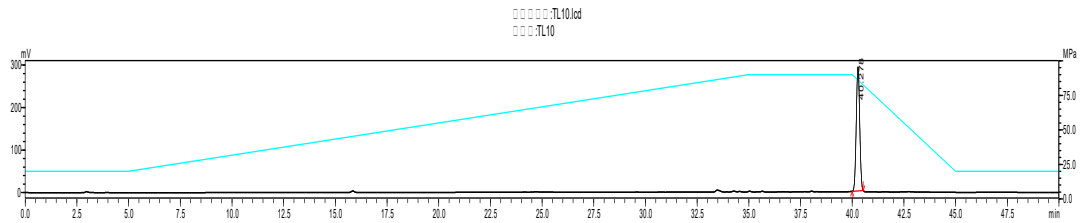
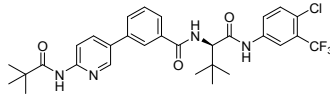
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1.47e7



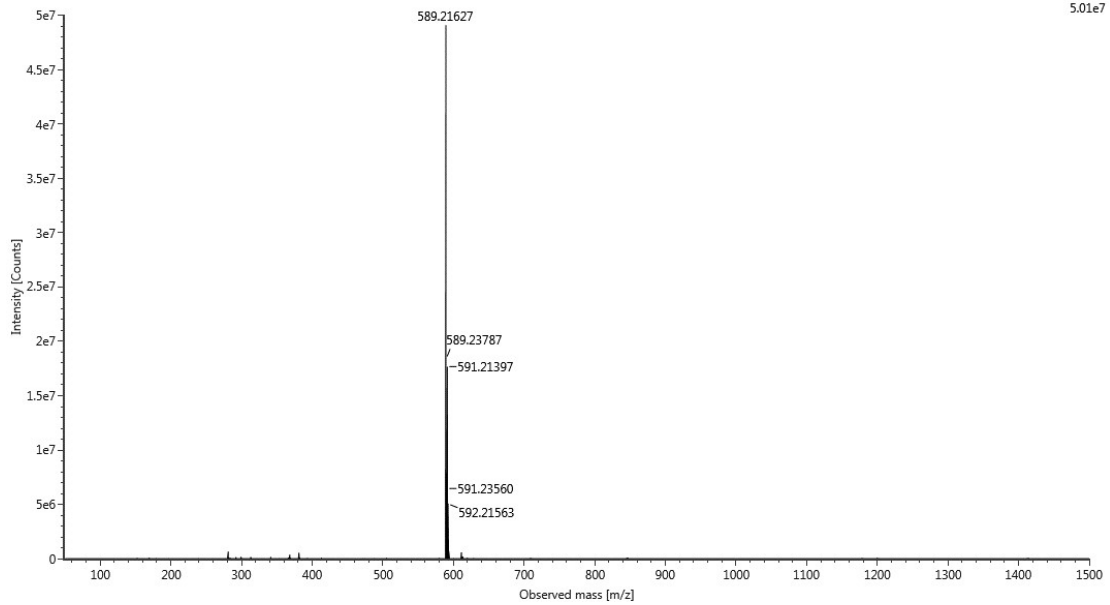
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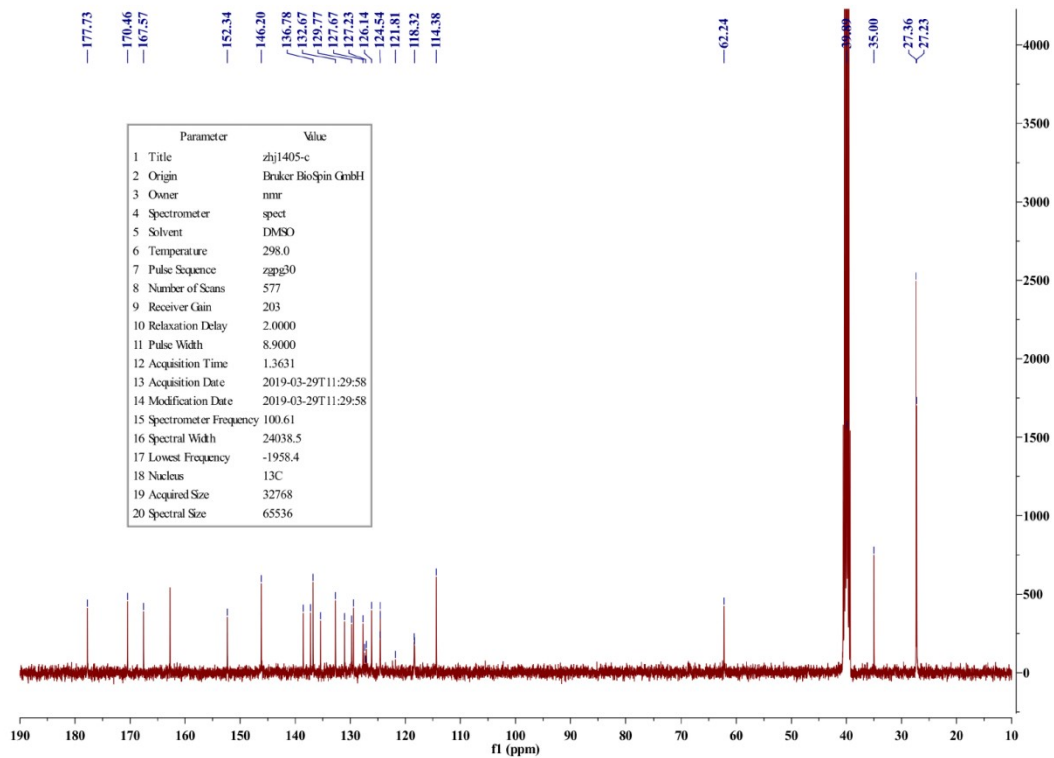
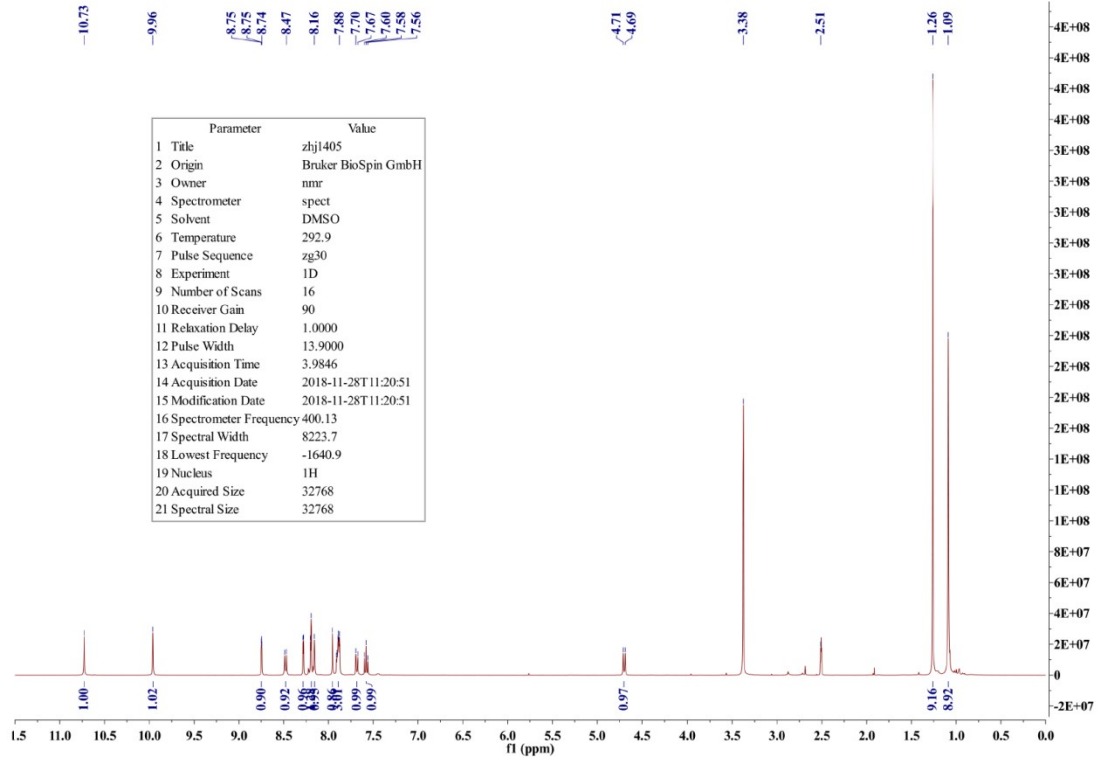


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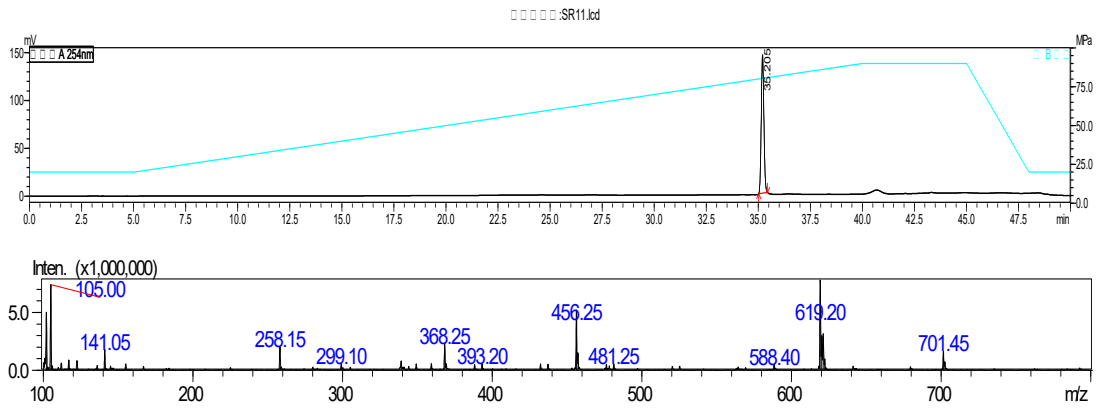
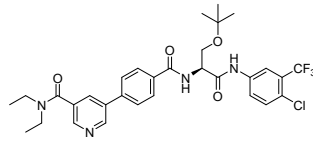
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5.01e7





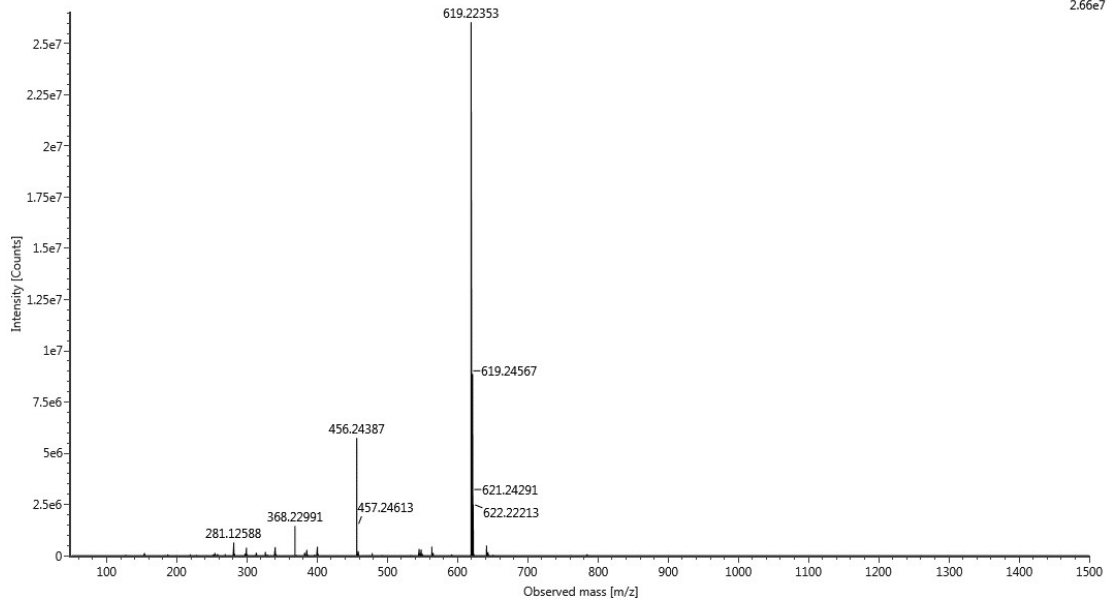
(S)-5-(4-((3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)carbamoyl)phenyl)-N,N-diethylnicotinamide (BS1)

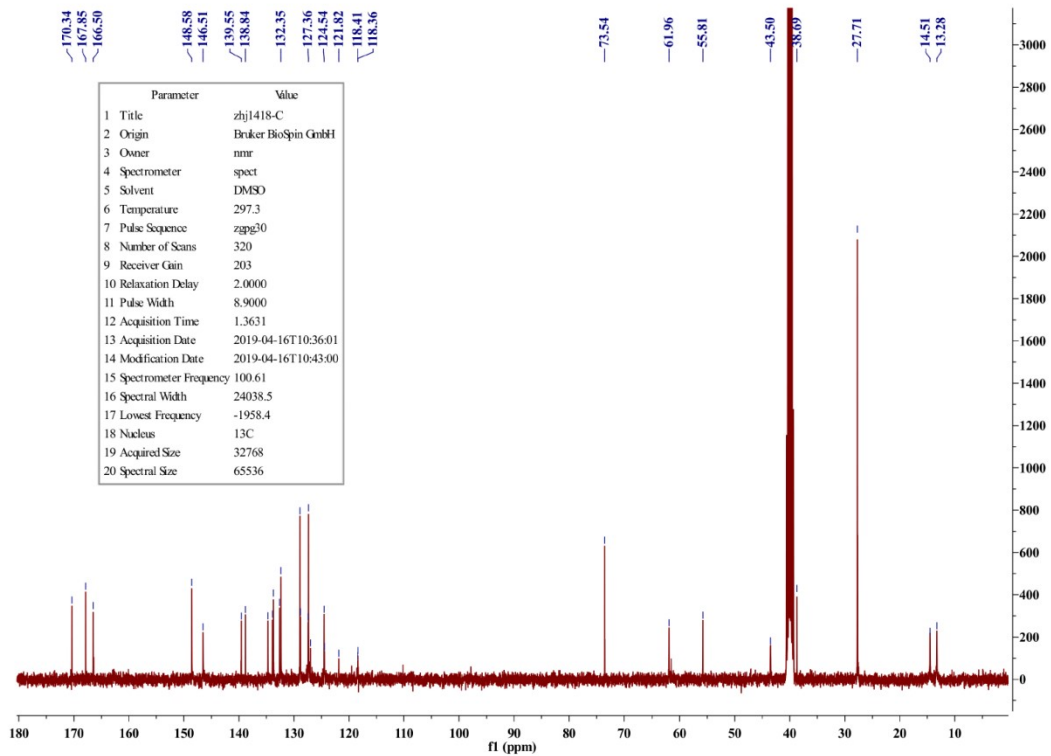
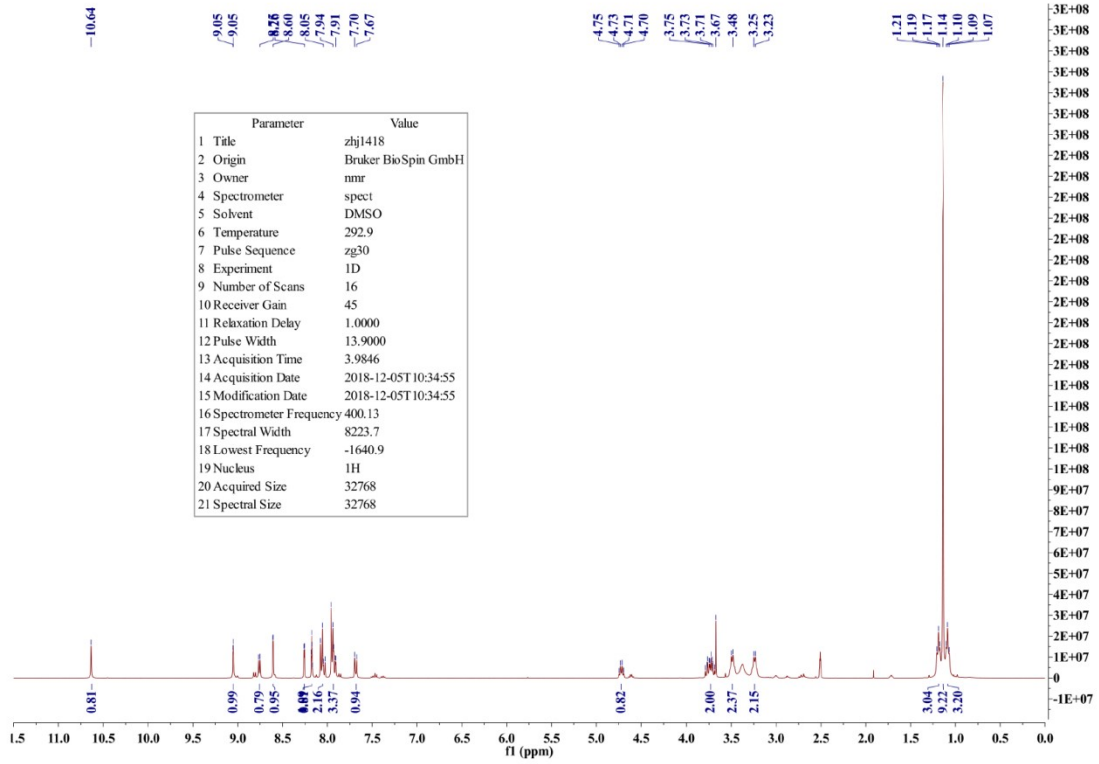


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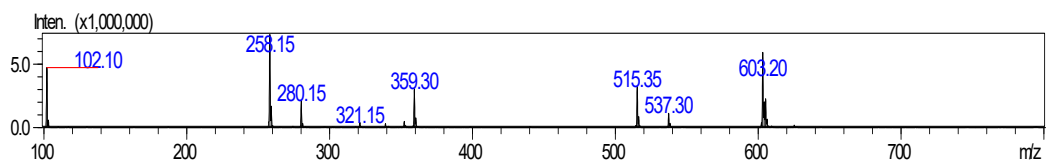
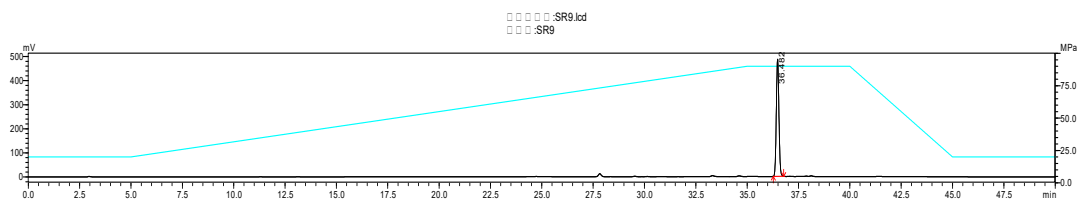
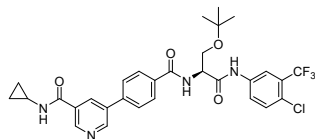
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2.66e7





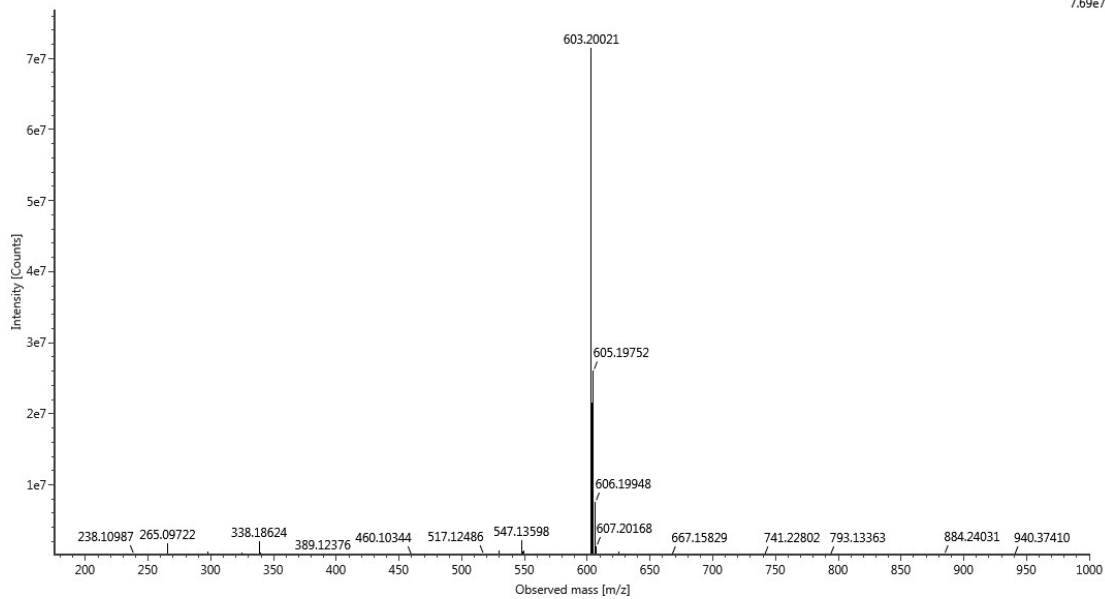
(S)-5-(4-((3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)carbamoyl)phenyl)-N-cyclopropylnicotinamide (**BS2**)

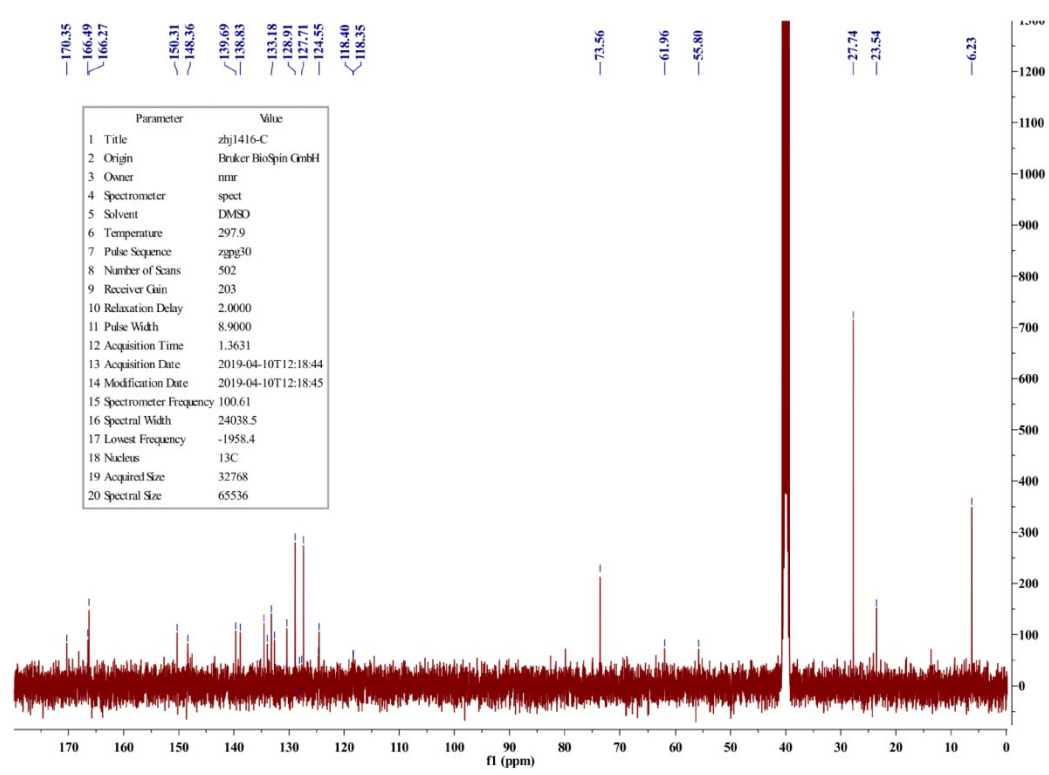
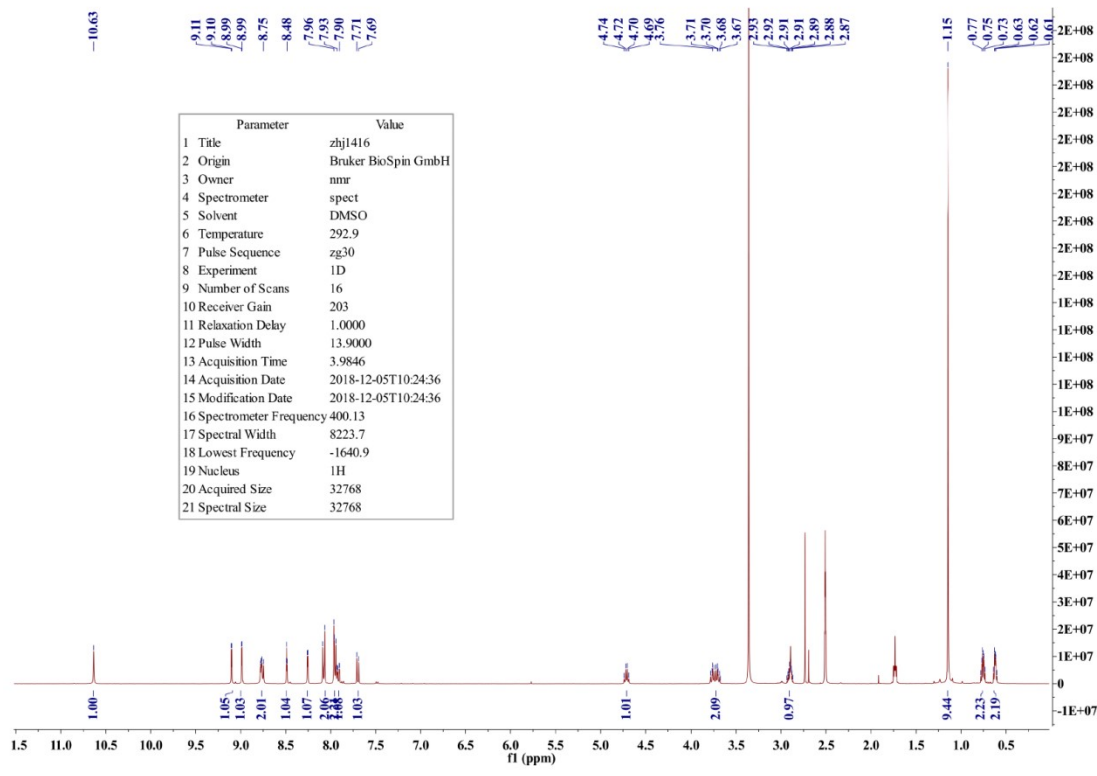


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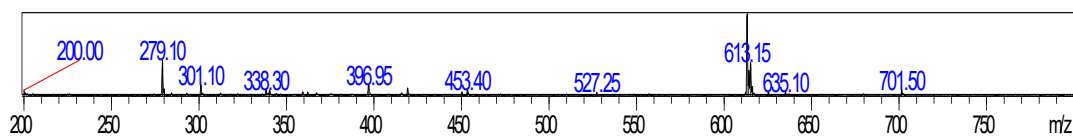
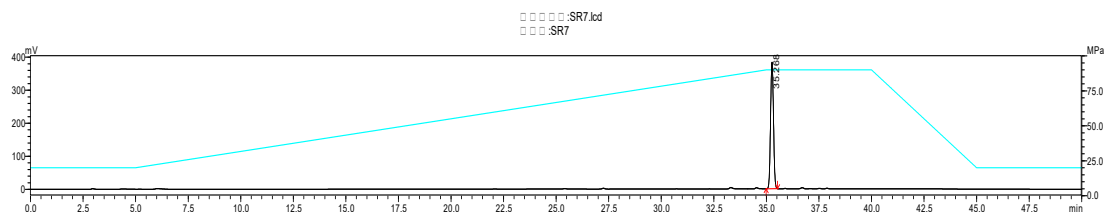
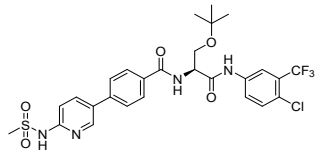
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7.69e7





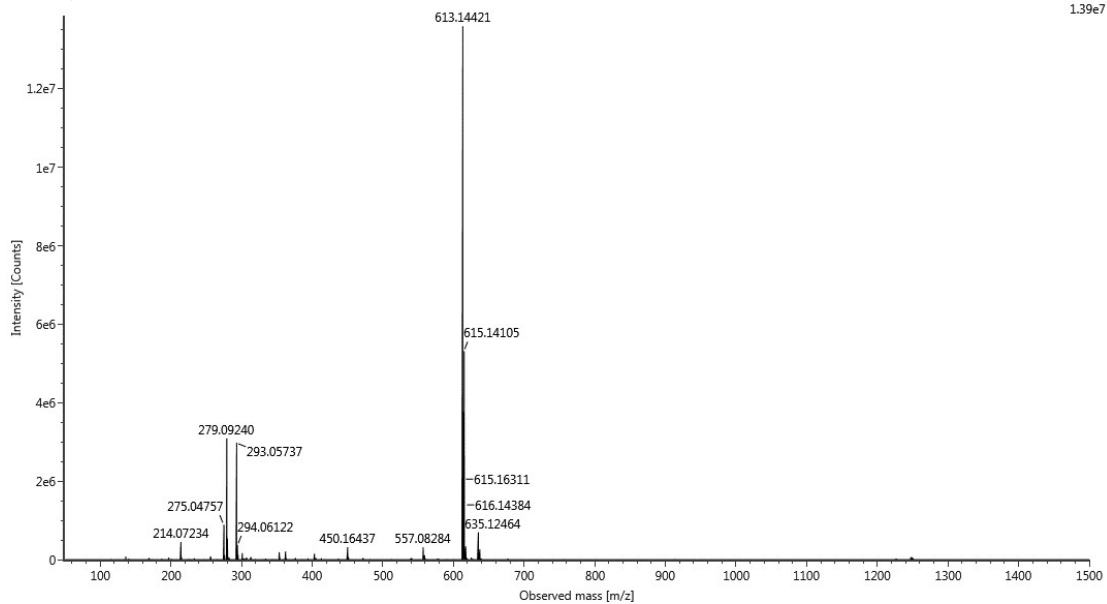
(S)-N-(3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)-4-(6-(methylsulfonamido)pyridin-3-yl)benzamide (BS3)

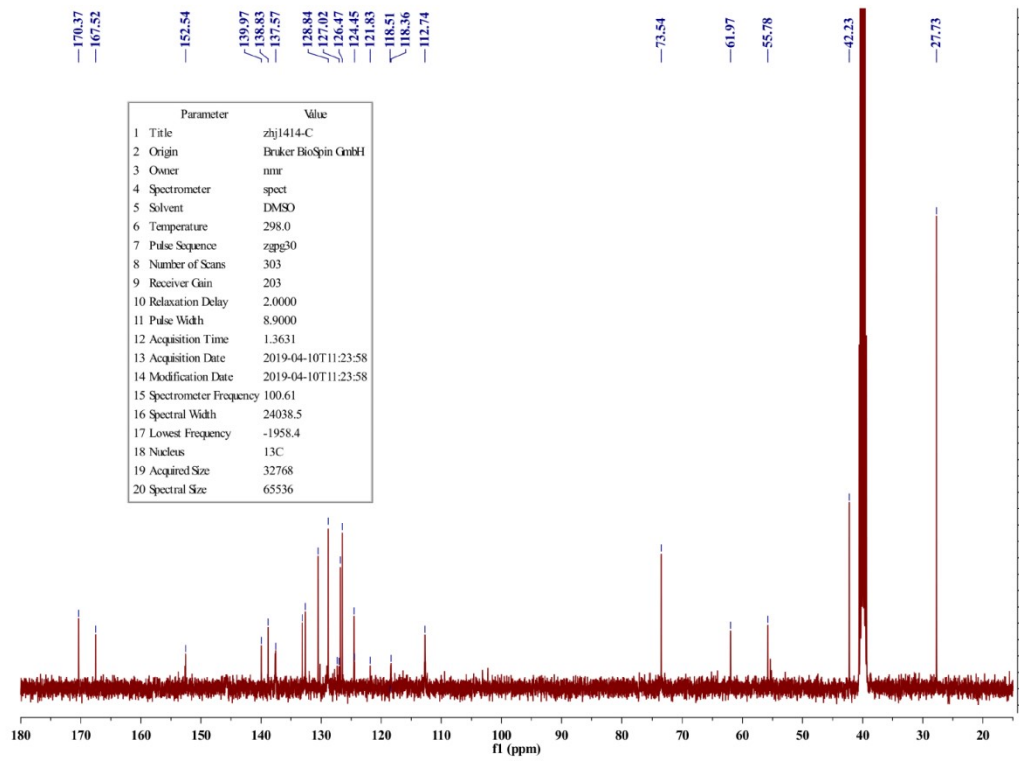
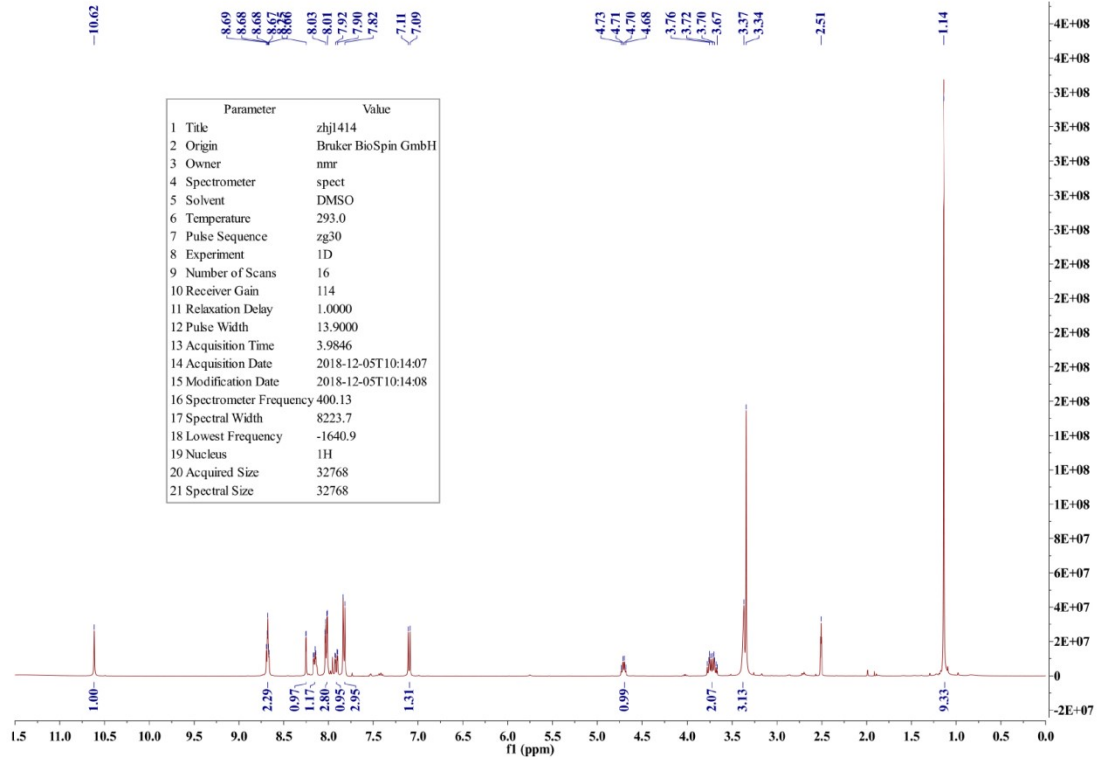


Item name: L-26
Item description:

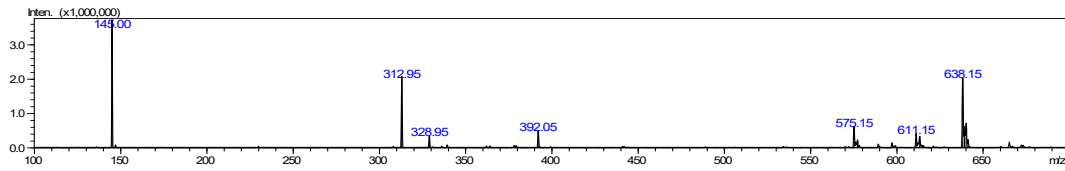
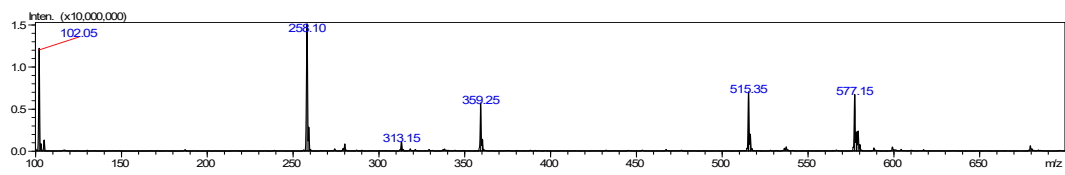
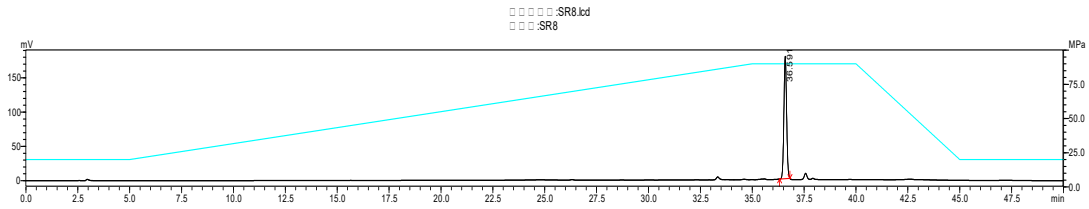
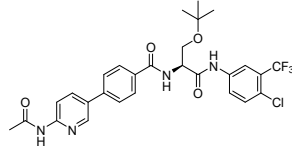
Channel name: 2: Average Time 0.3181 min : TOF MS (50-1500) 6eV ESI+ : Combined

1.39e7





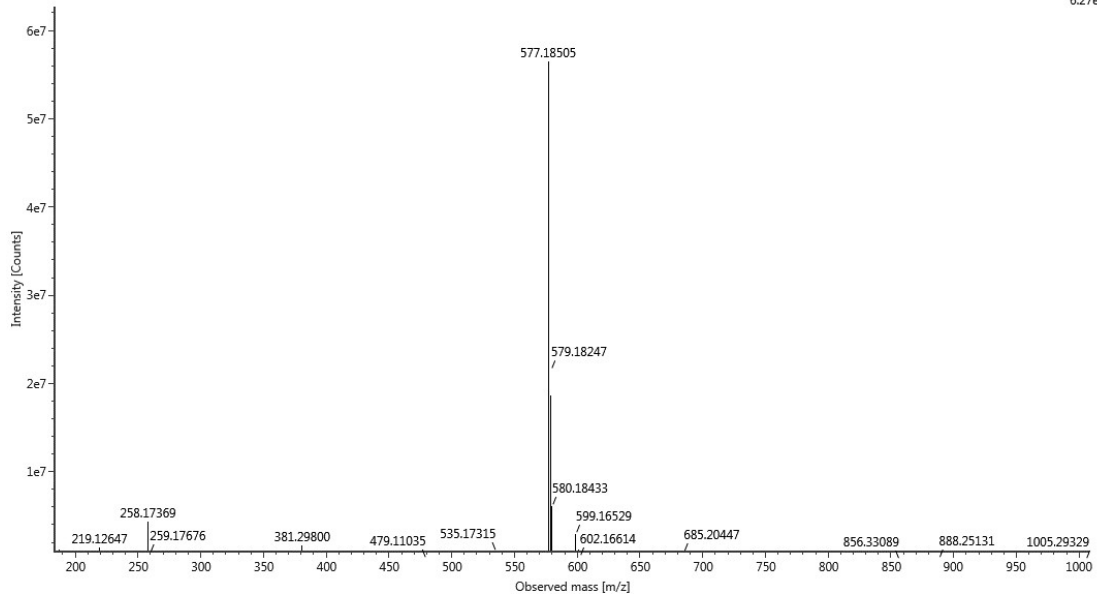
(S)-4-(6-acetamidopyridin-3-yl)-N-(3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)benzamide (BS4)

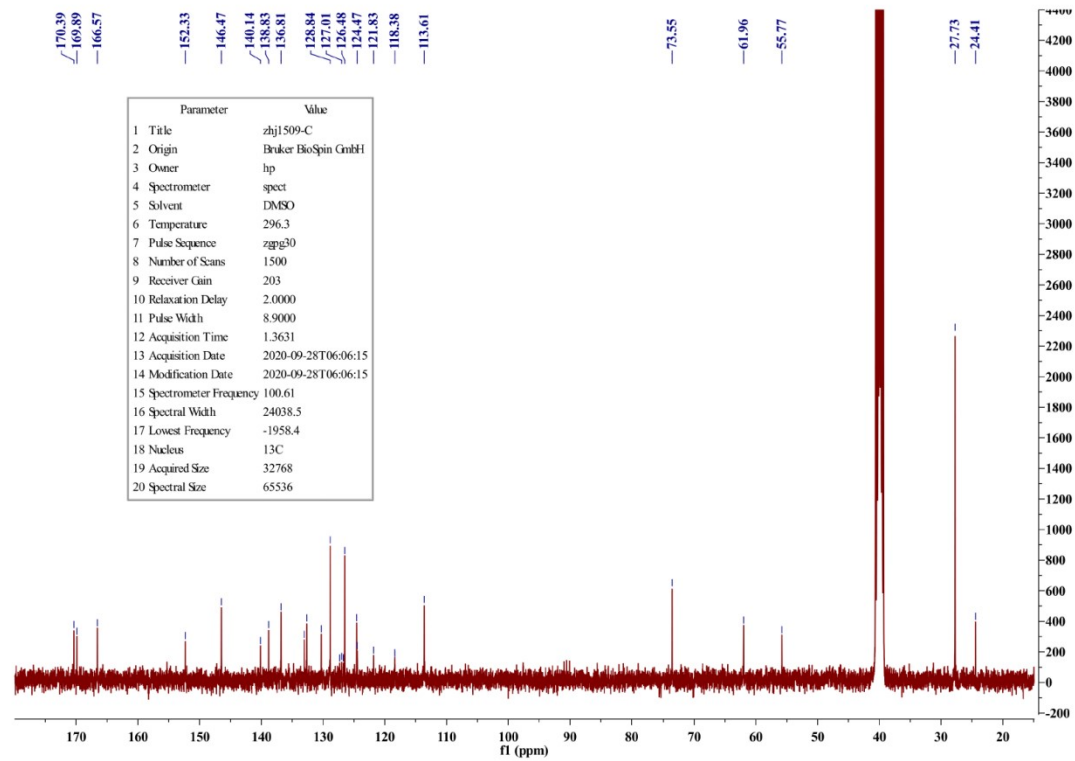
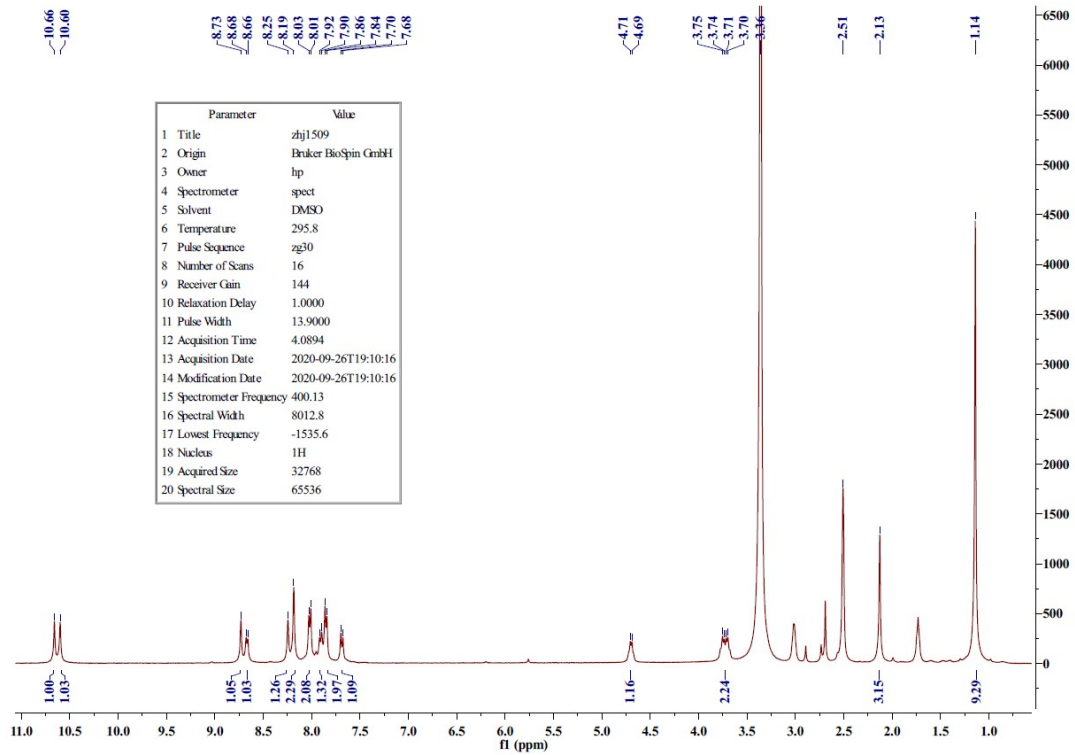


Item name: L-8
Item description:

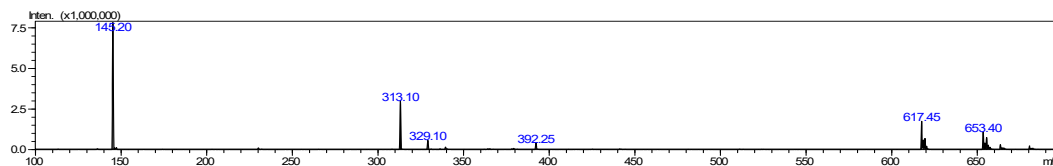
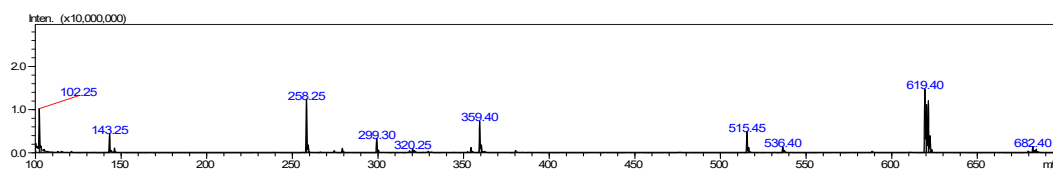
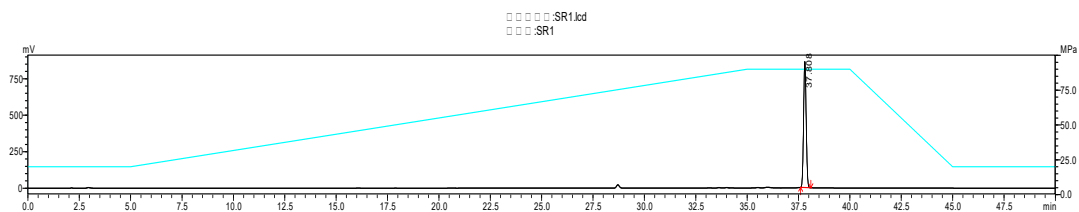
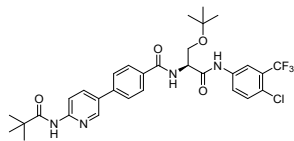
Channel name: 2: Average Time 0.3000 min : TOF MSe (50-2000) 6eV ESI+ : Centroided : Combined

6.27e7





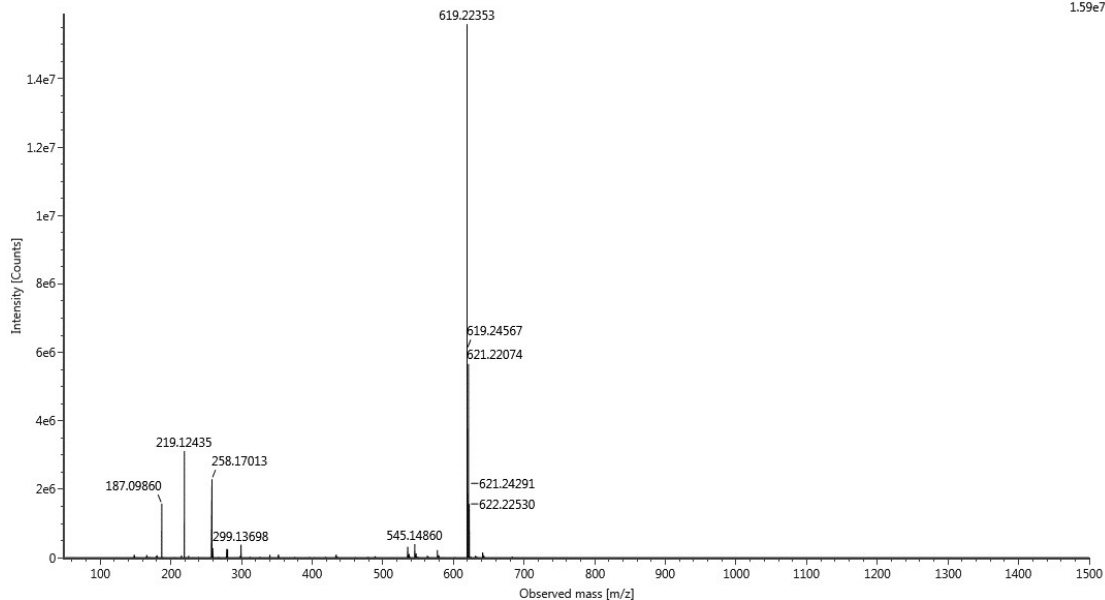
(S)-N-(3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)-4-(6-pivalamidopyridin-3-yl)benzamide (BS5)

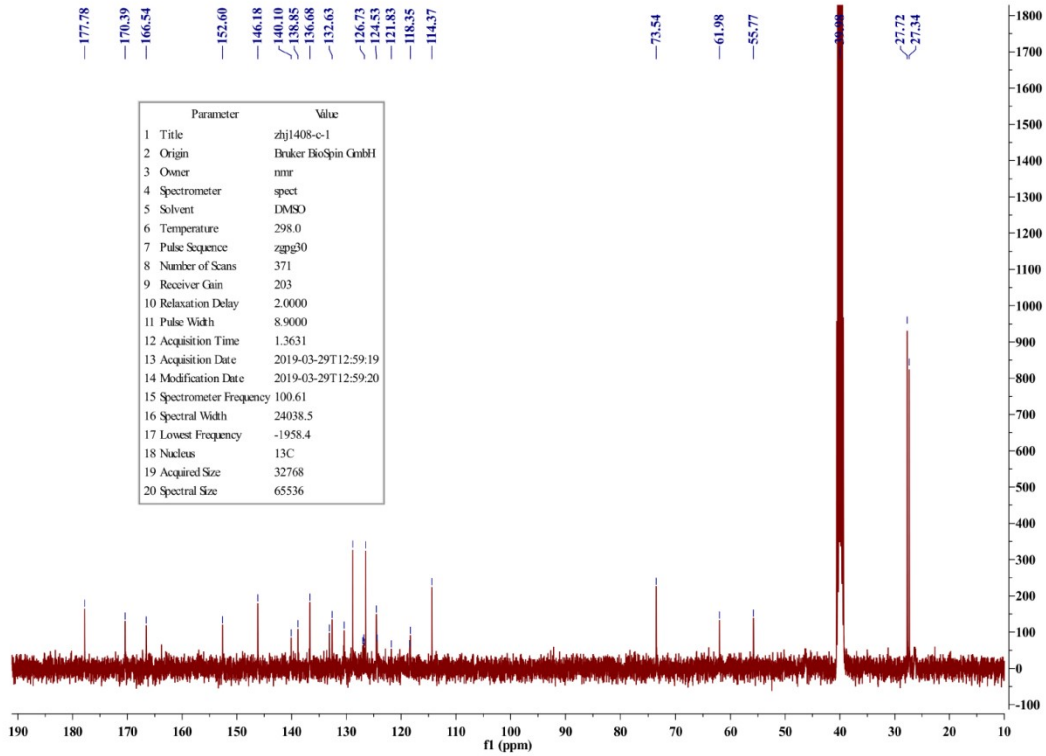
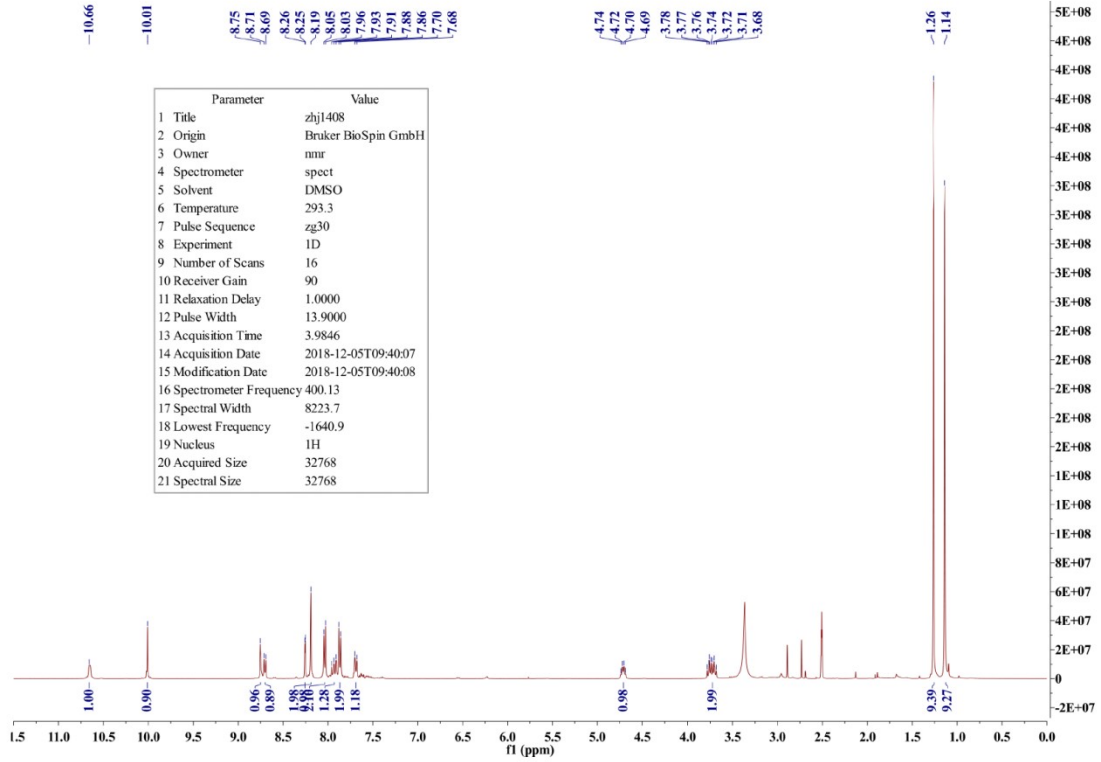


Item name: L-23
Item description:

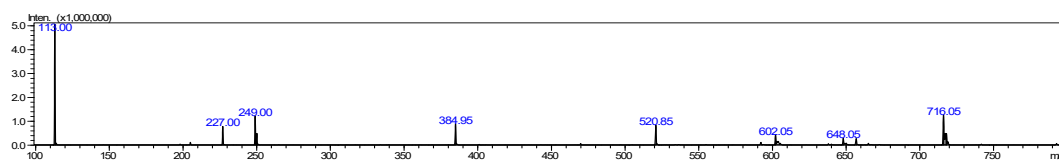
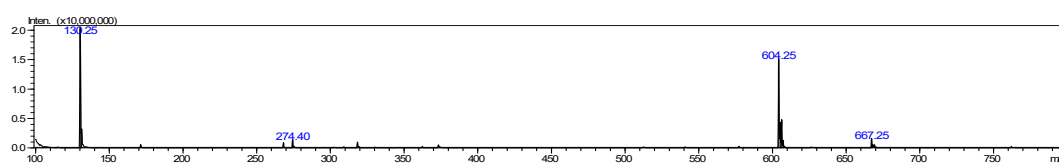
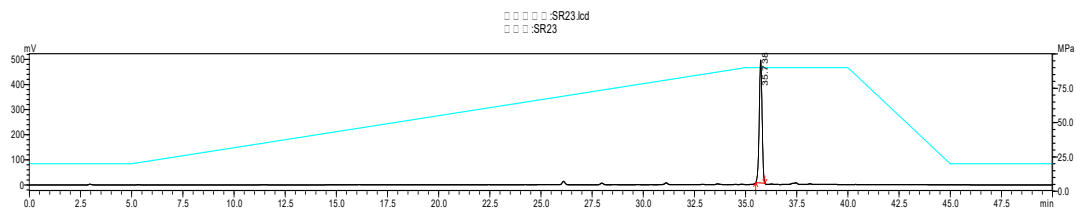
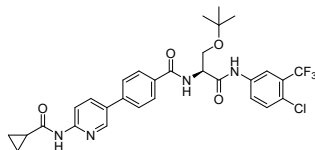
Channel name: 2: Average Time 0.2929 min : TOF MS (50-1500) 6eV ESI+ : Combined

1.59e7





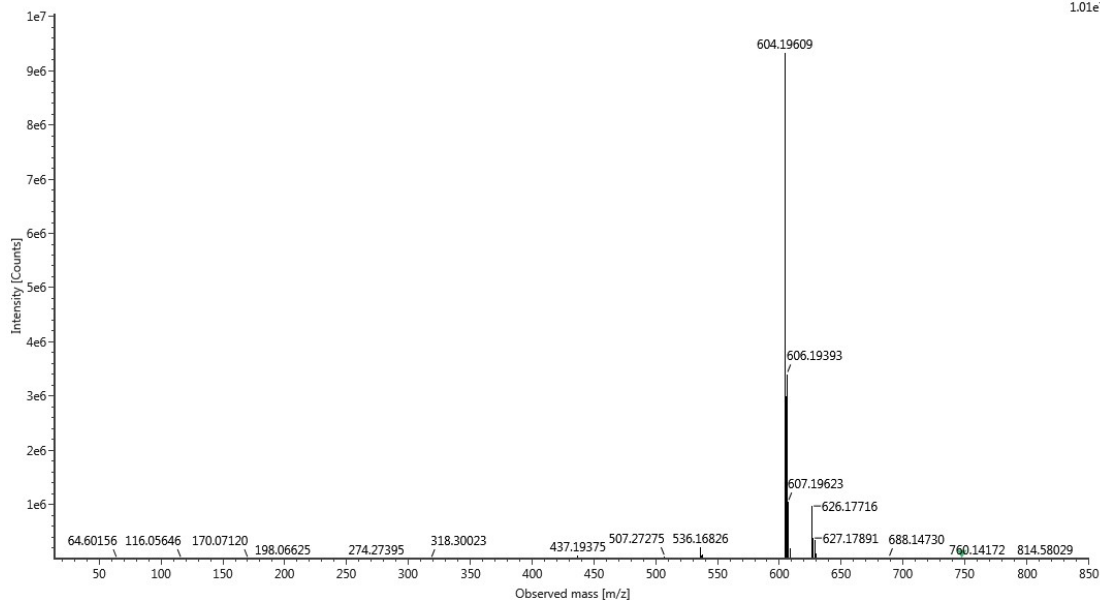
(S)-N-(3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)-4-(6-(cyclopropanecarboxamido)pyridin-3-yl)benzamide (**BS6**)

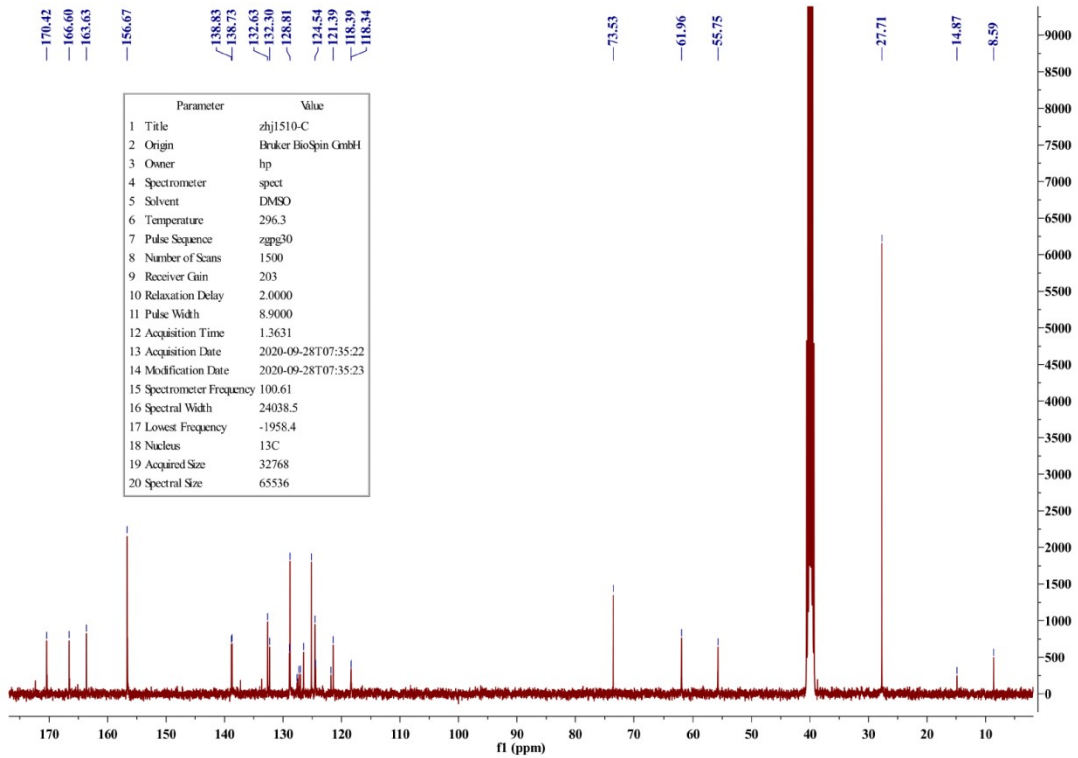
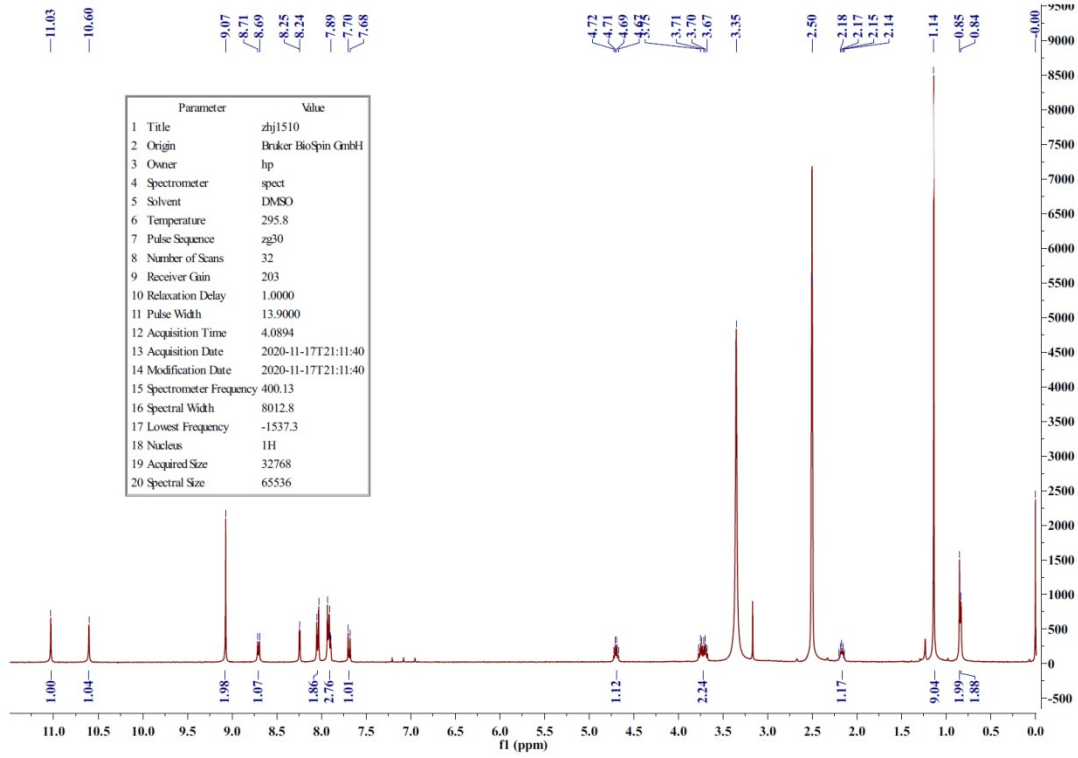


Item name: L5
Item description:

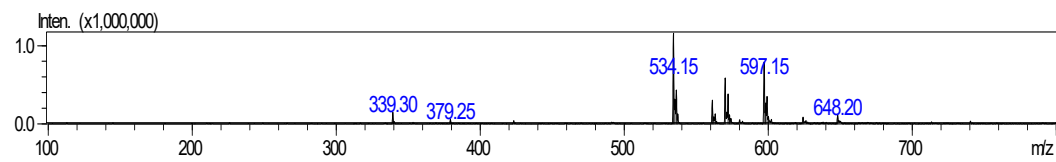
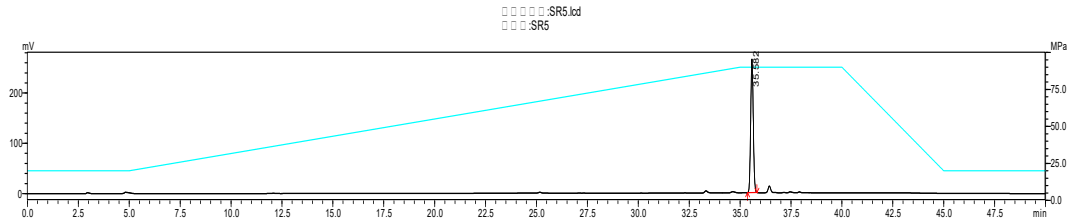
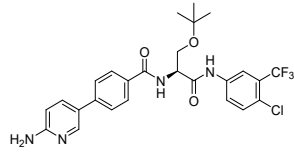
Channel name: 2: Average Time 0.1839 min : TOF MSe (50-2000) 6eV ESI+ : Centroided : Combined

1.01e7



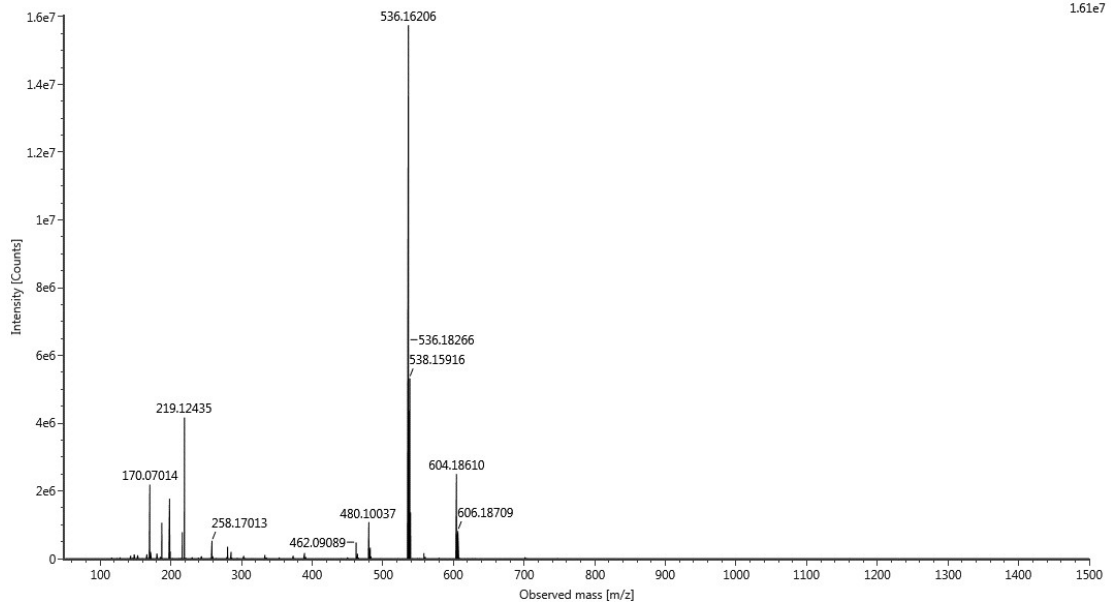


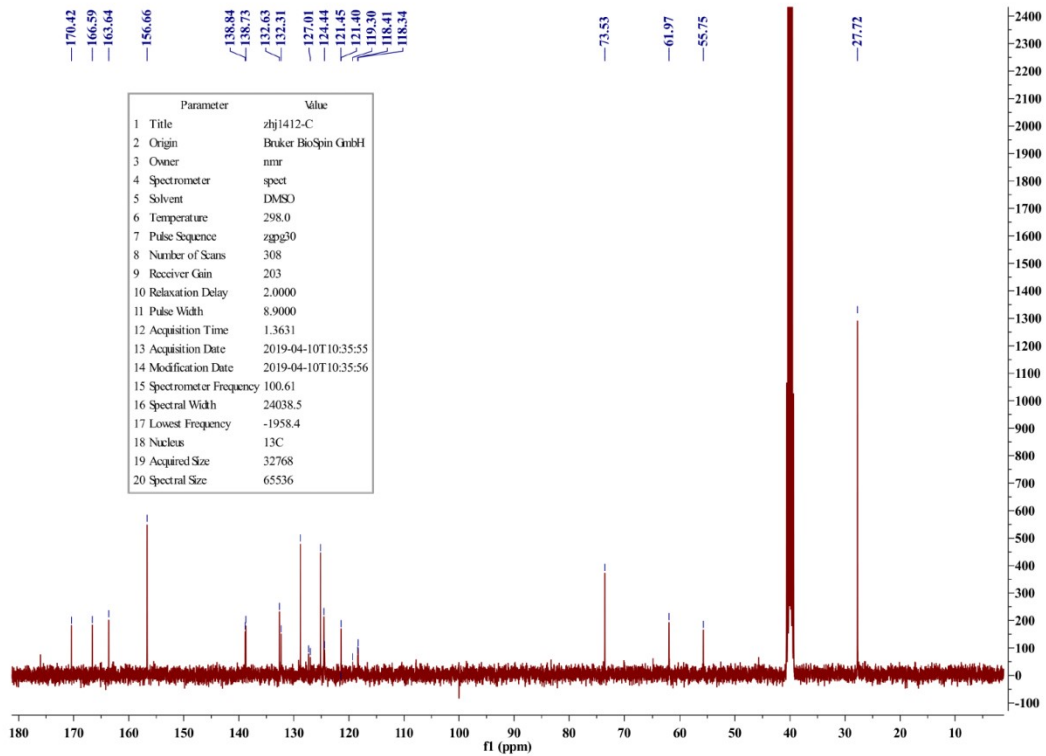
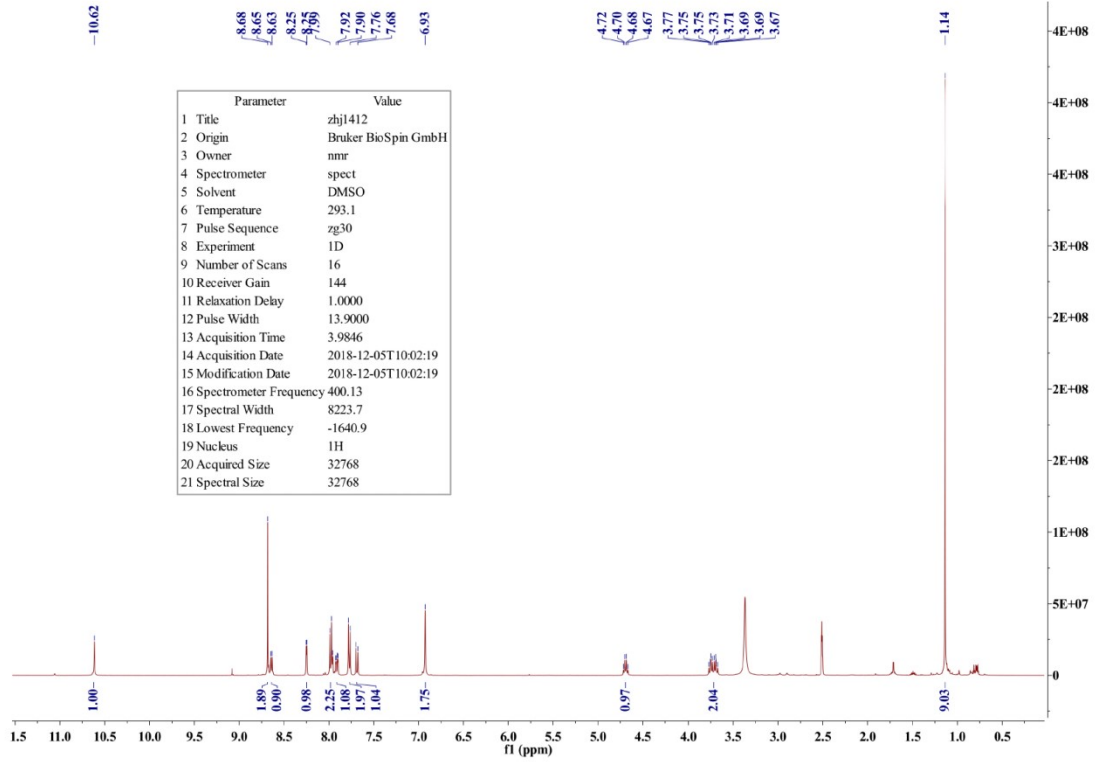
(S)-4-(6-aminopyridin-3-yl)-N-(3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)benzamide (BS7)



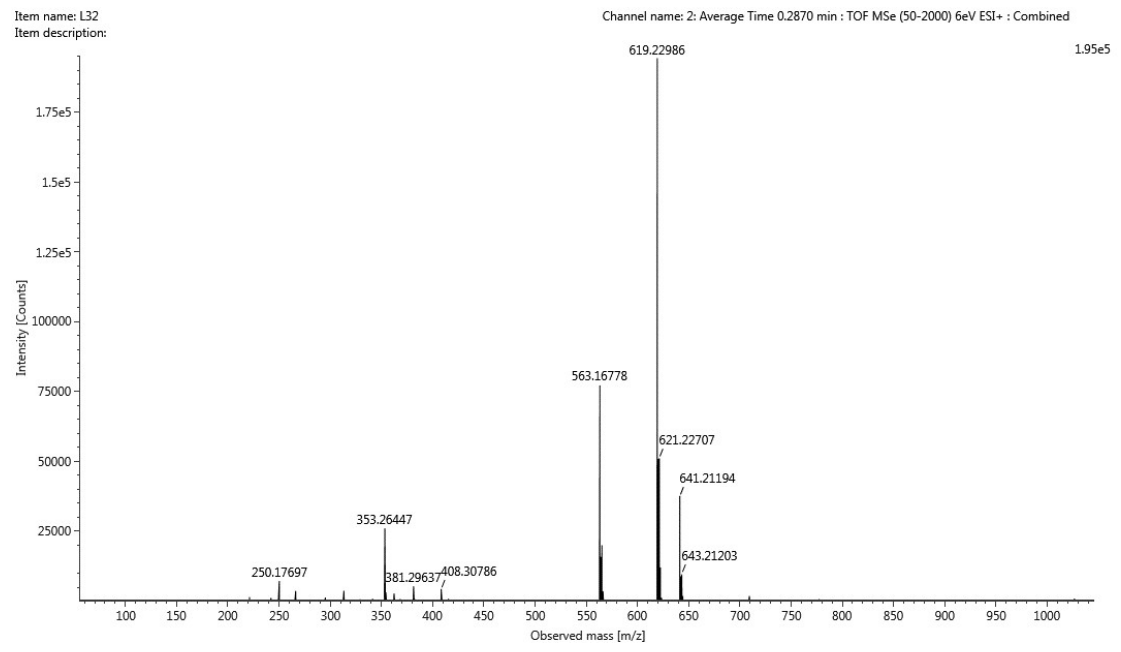
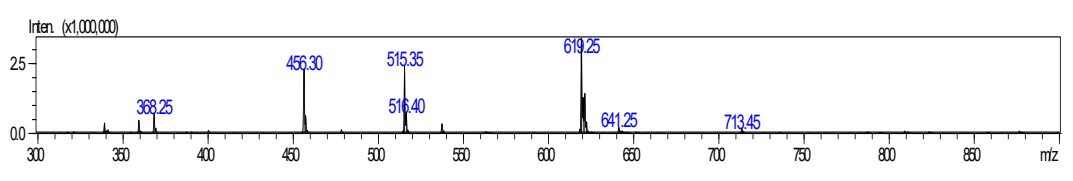
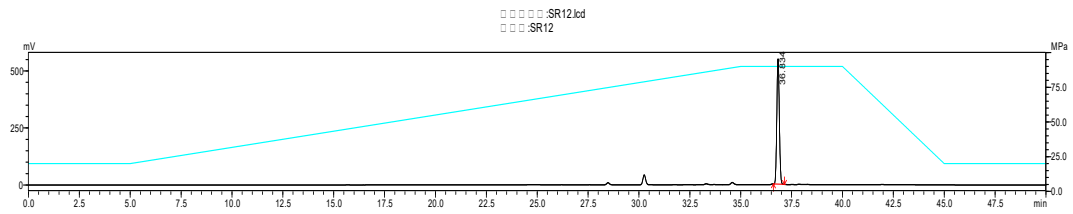
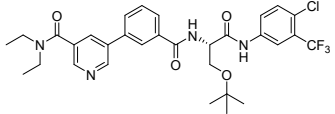
Item name: L-24
Item description:

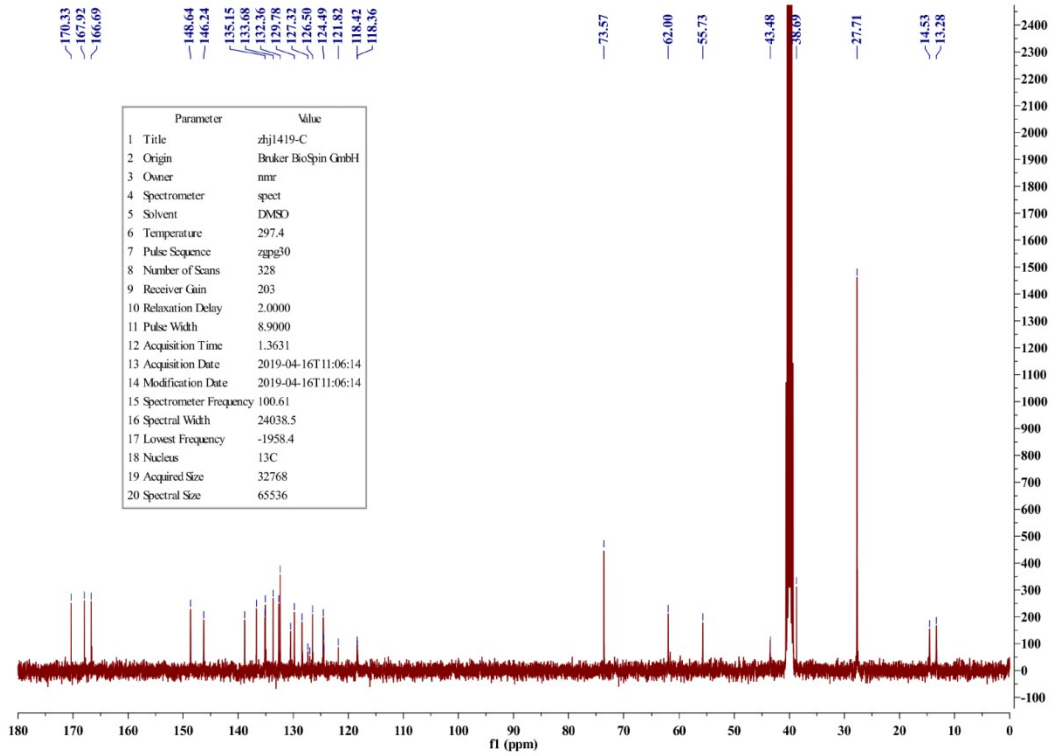
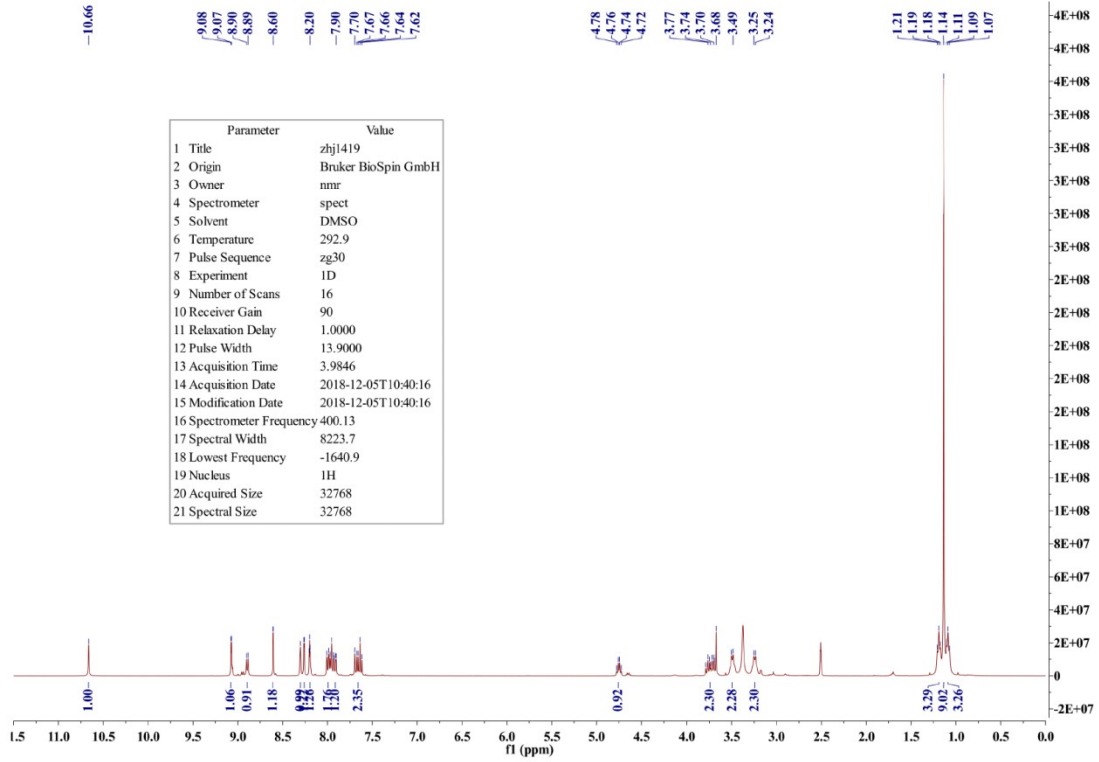
Channel name: 2: Average Time 0.2317 min : TOF MS (50-1500) 6eV ESI+ : Combined



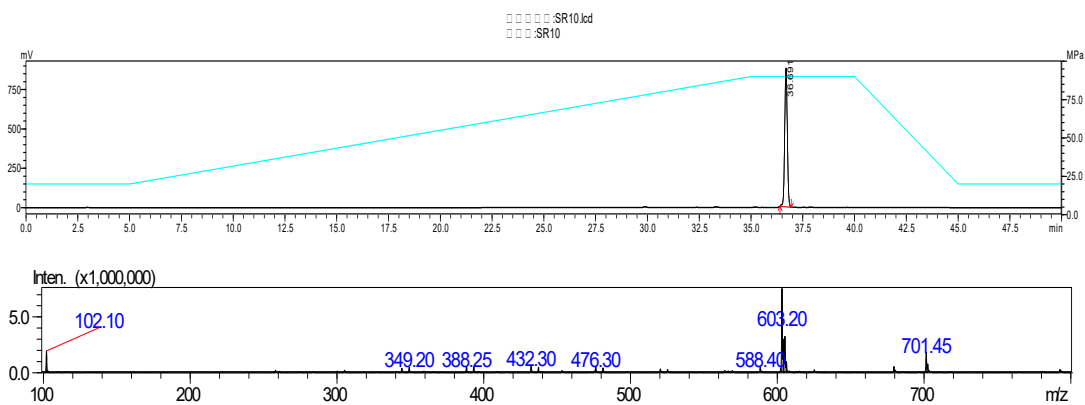
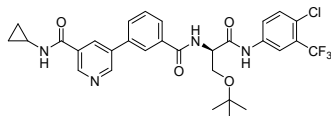


(S)-5-(3-((3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)carbamoyl)phenyl)-N,N-diethylnicotinamide (BS8)



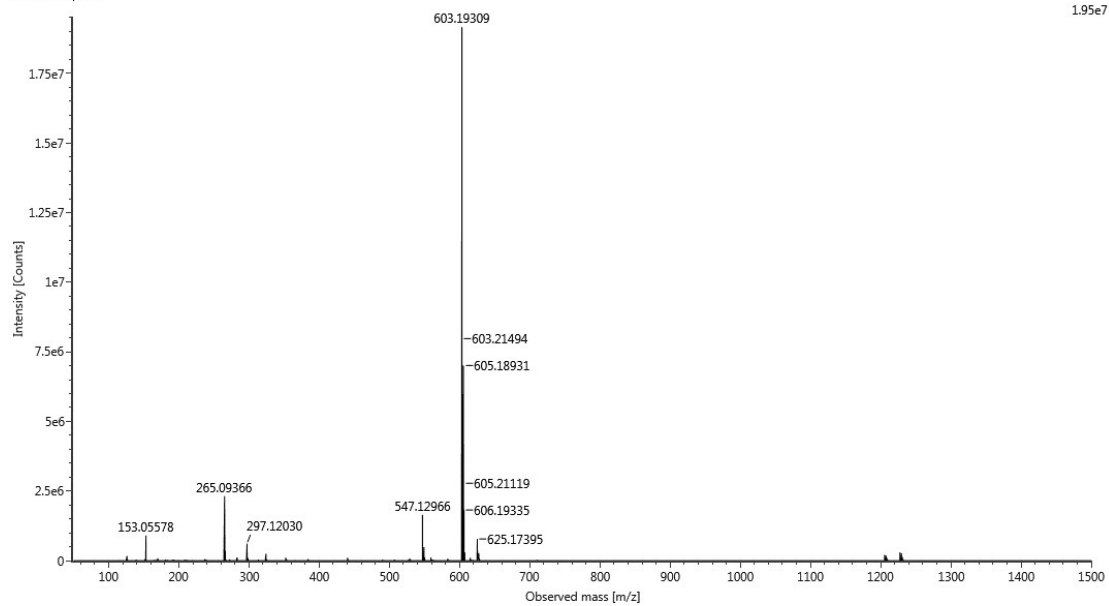


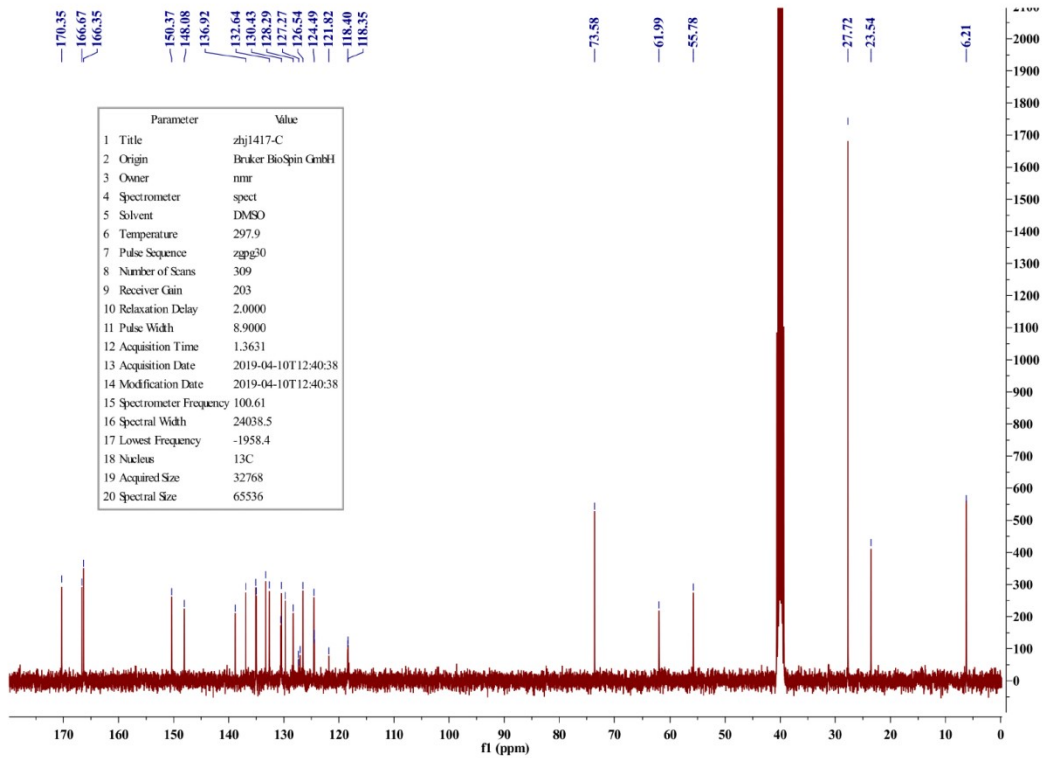
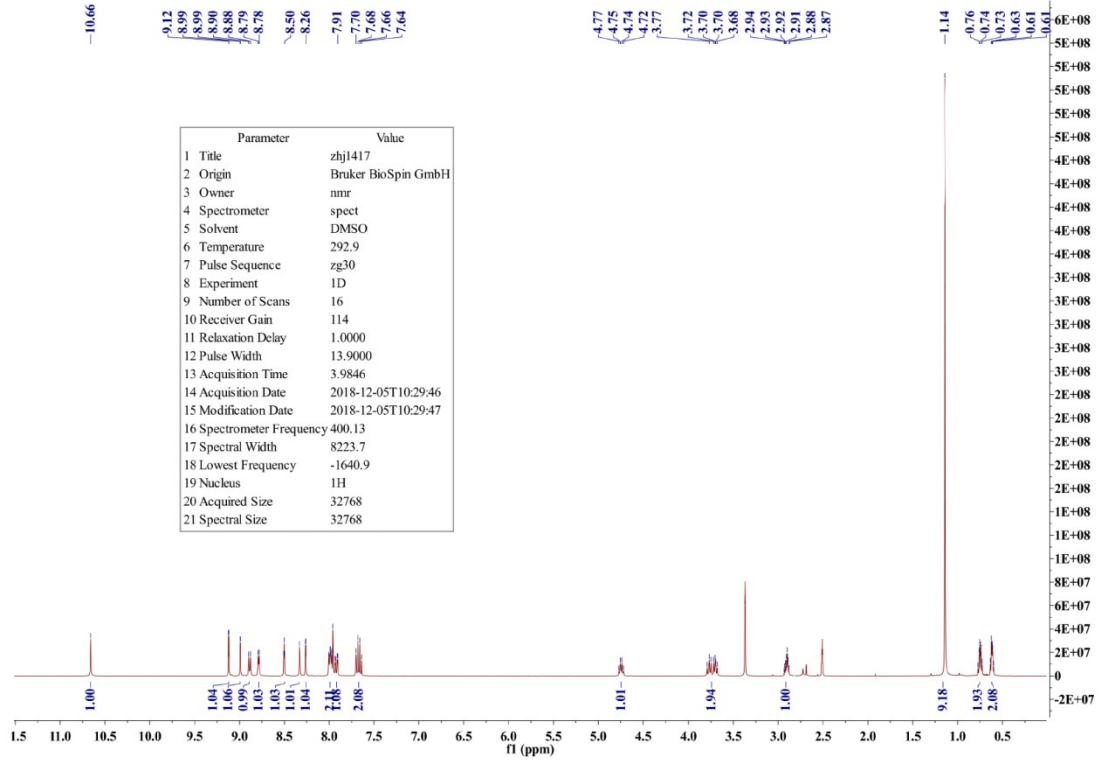
(S)-5-(3-((3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)carbamoyl)phenyl)-N-cyclopropylnicotinamide (BS9)



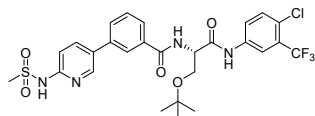
Item name: L-33
Item description:

Channel name: 2: Average Time 0.3013 min : TOF MS (50-1500) 6eV ESI+ : Combined

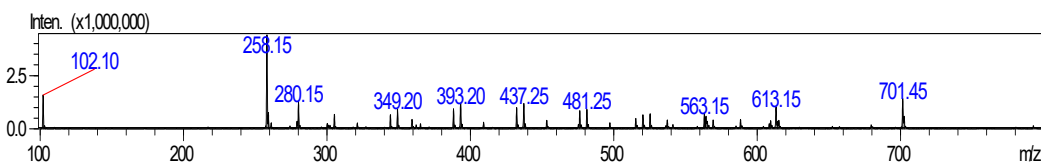
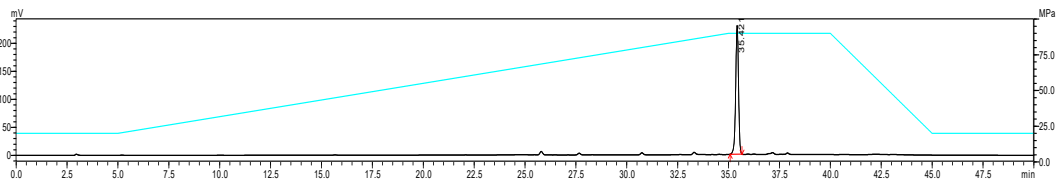




(S)-N-(3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)-3-(6-(methylsulfonamido)pyridin-3-yl)benzamide (BS10)



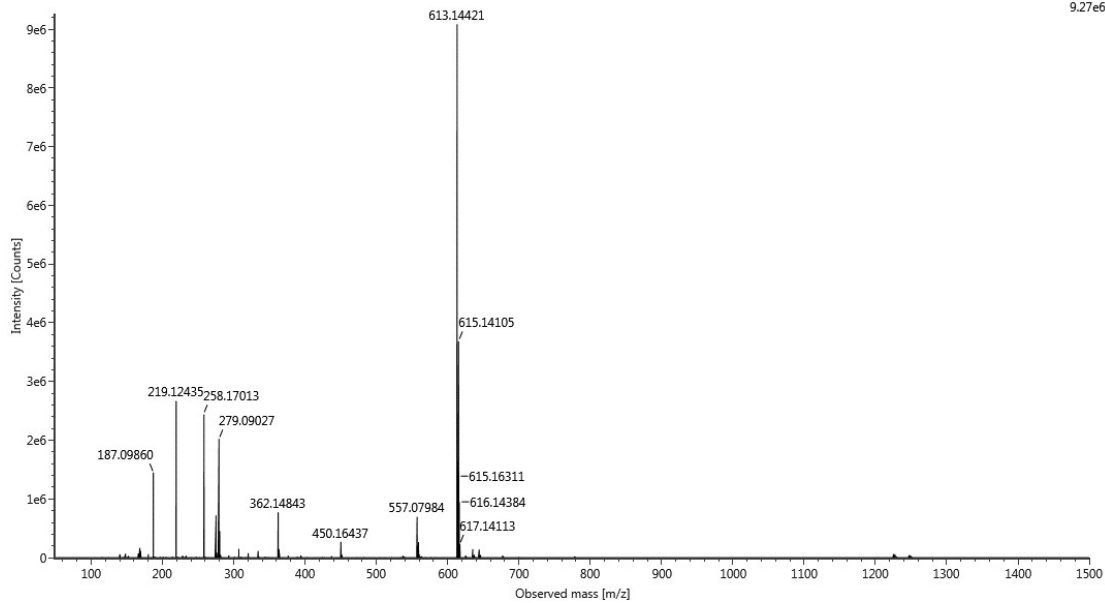
SR6.td
SR6

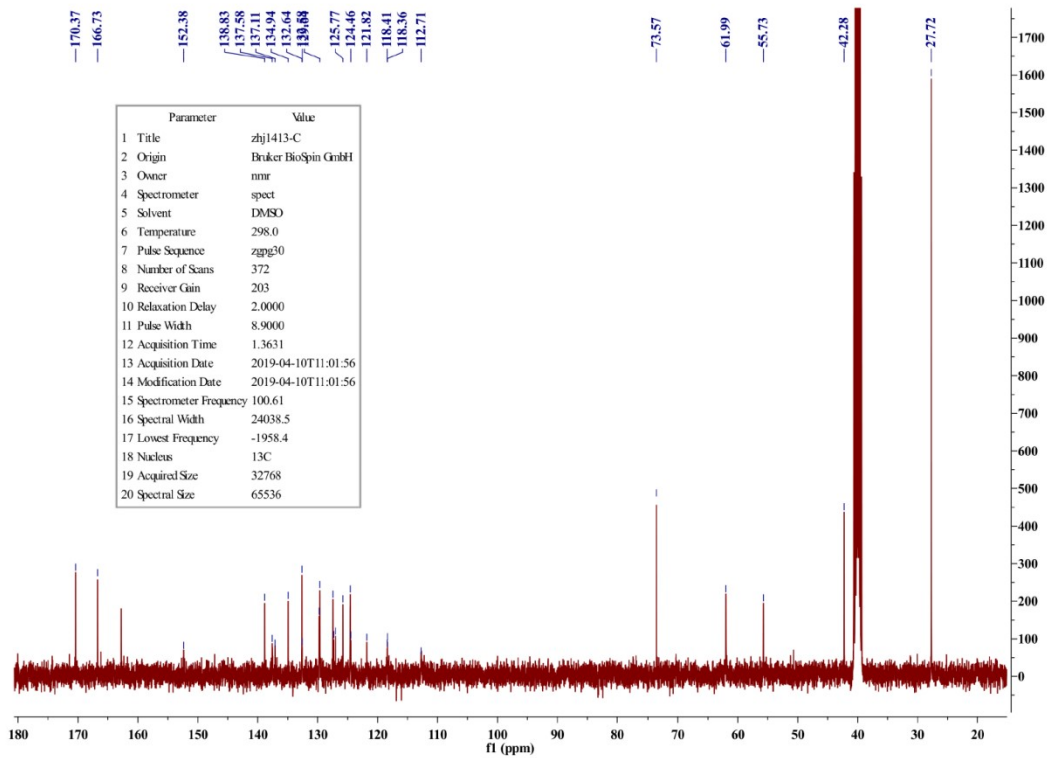
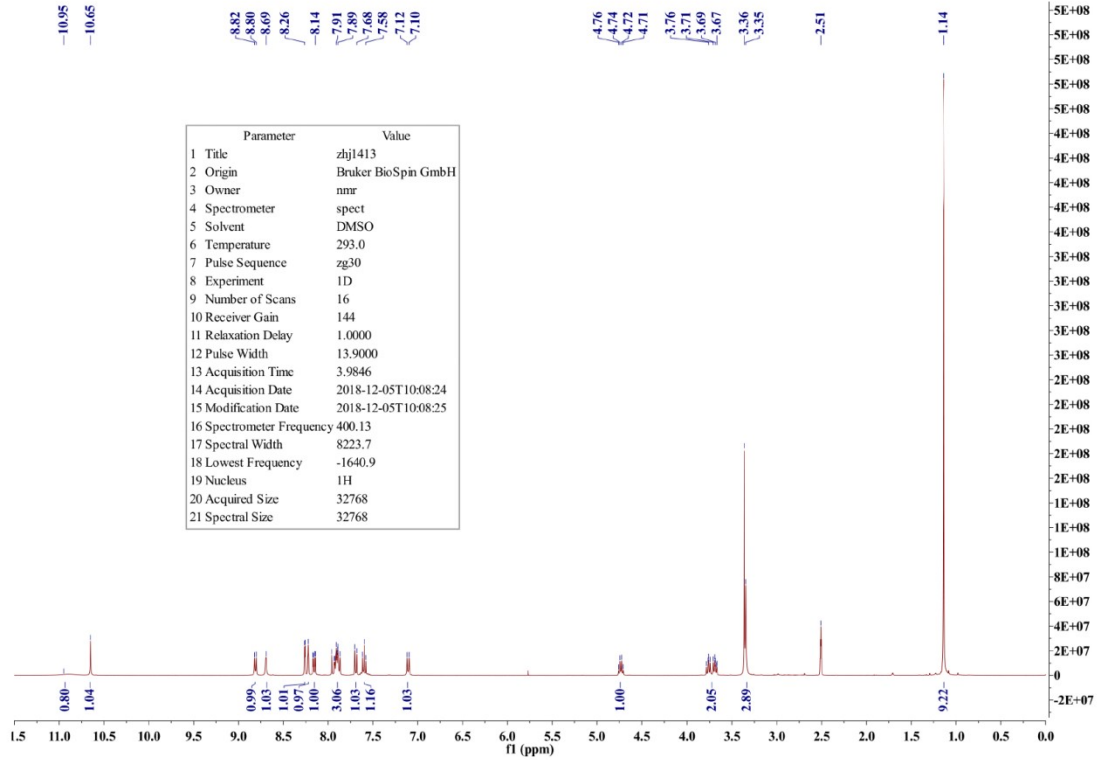


Item name: L-31
Item description:

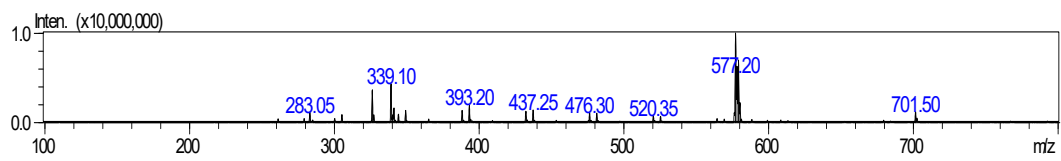
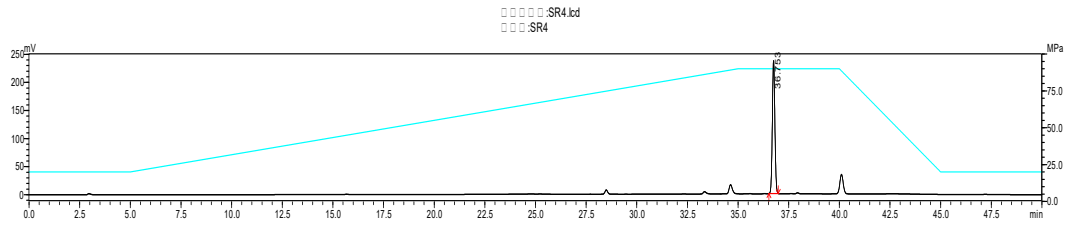
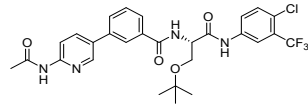
Channel name: 2: Average Time 0.2736 min : TOF MS (50-1500) 6eV ESI+ : Combined

9.27e6





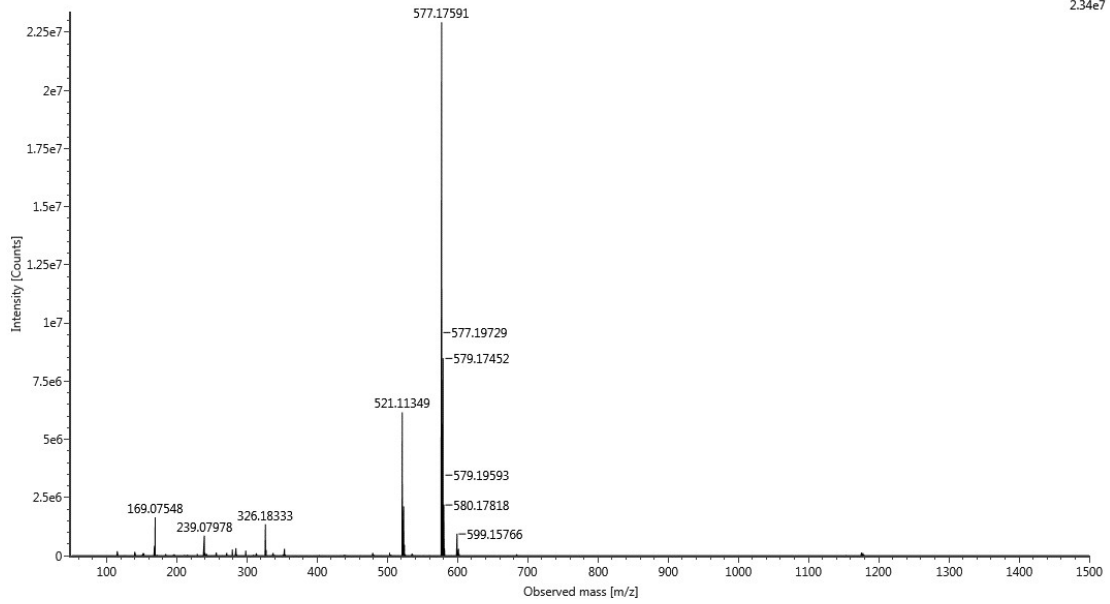
(S)-3-(6-acetamidopyridin-3-yl)-N-(3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)benzamide (BS11)

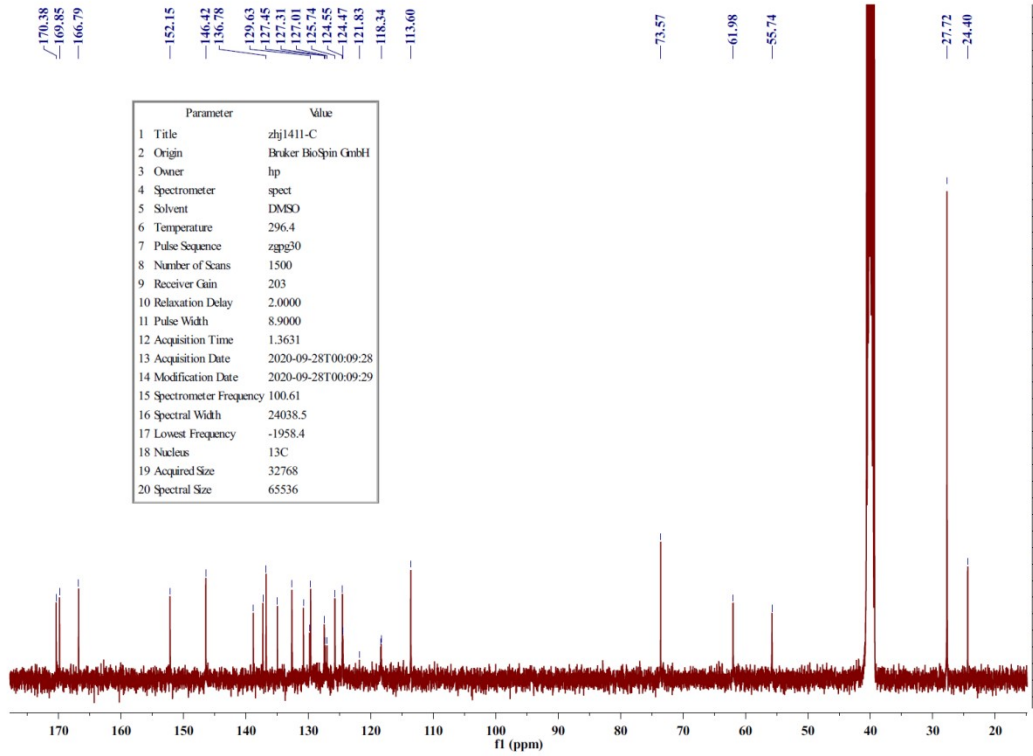
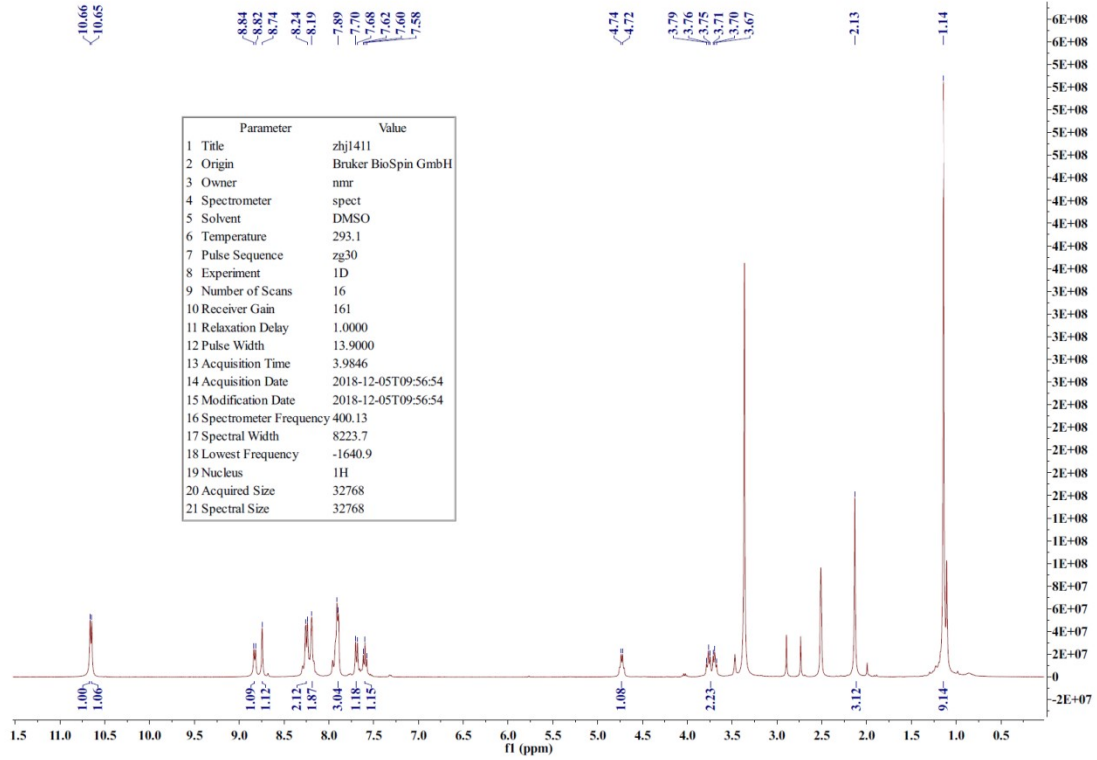


Item name: L-34
Item description:

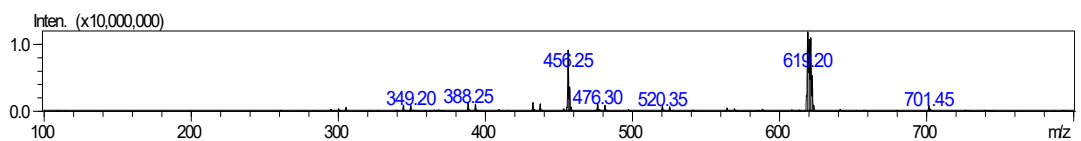
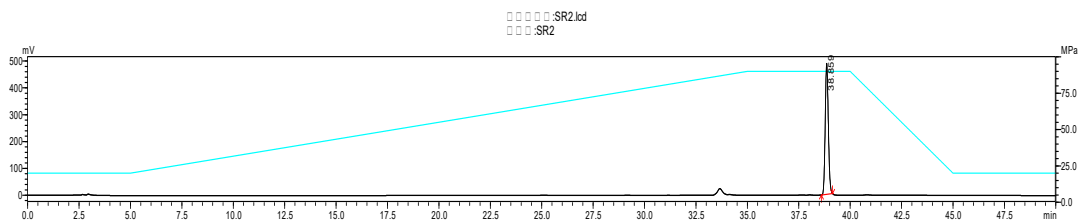
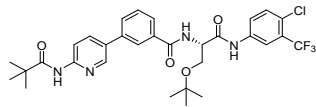
Channel name: 2: Average Time 0.3097 min : TOF MS (50-1500) 6eV ESI+ : Combined

2.34e7





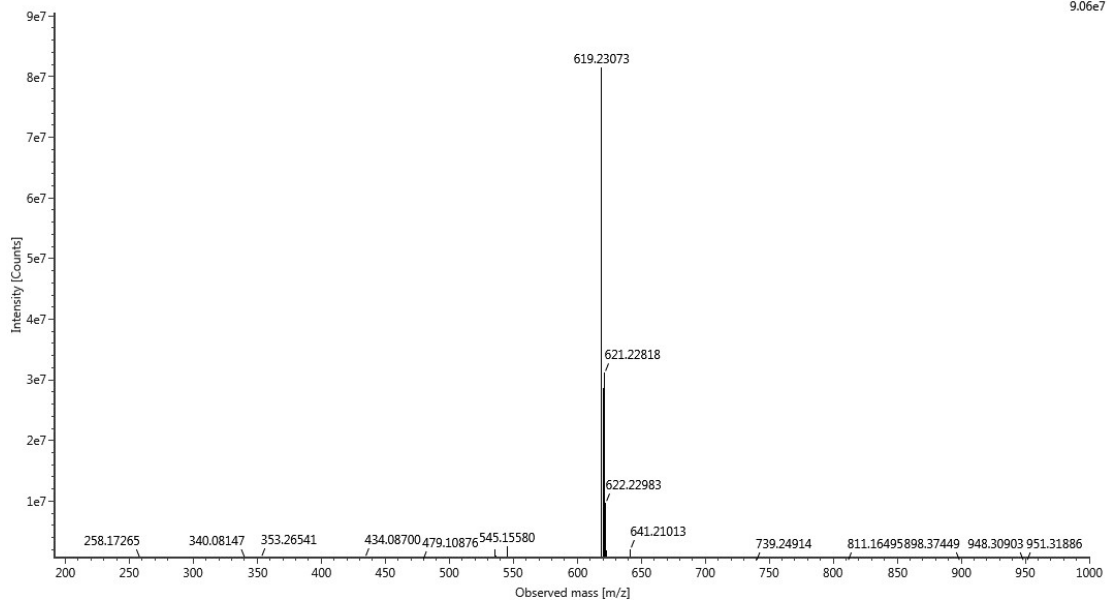
(S)-N-(3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)-3-(6-pivalamidopyridin-3-yl)benzamide (BS12)

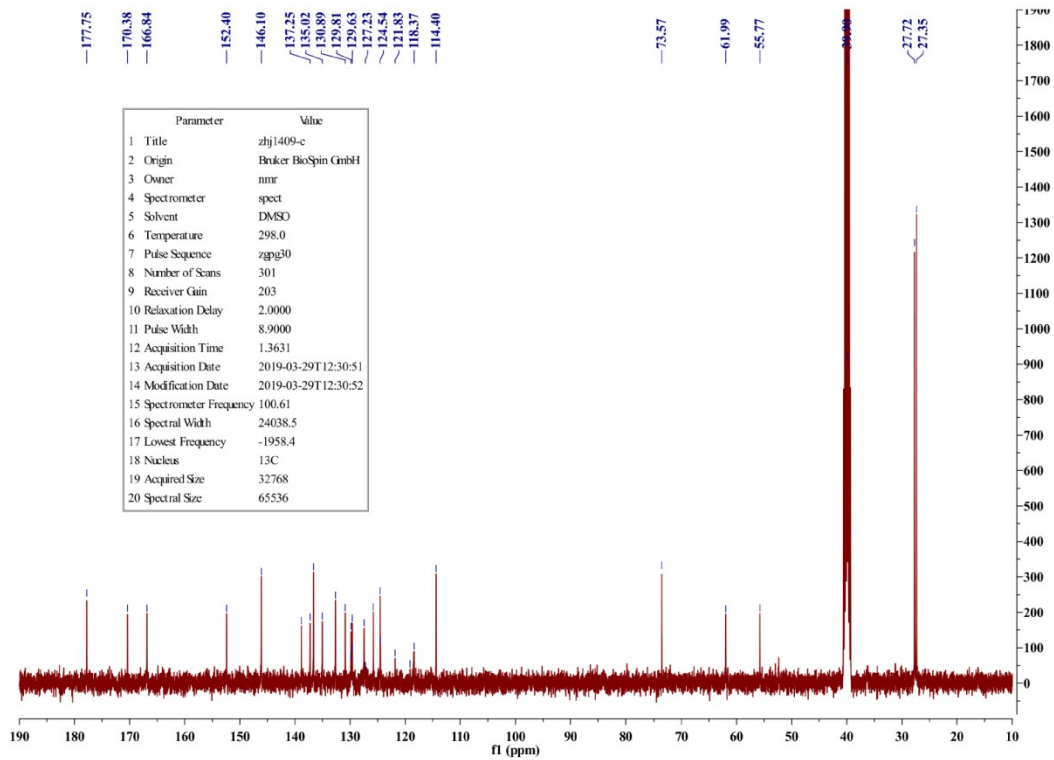
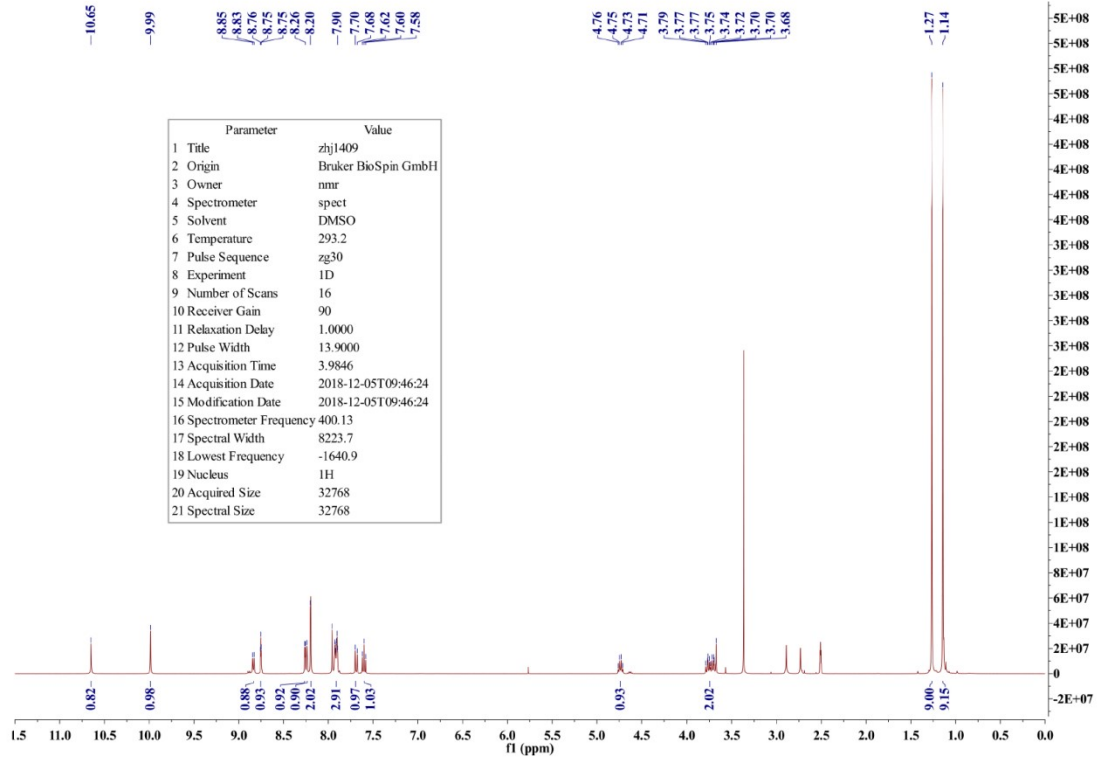


Item name: L-2
Item description:

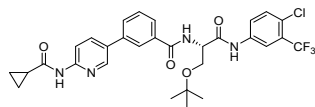
Channel name: 2: Average Time 0.2080 min : TOF MSe (50-2000) 6eV ESI+ : Centroided : Combined

9.06e7

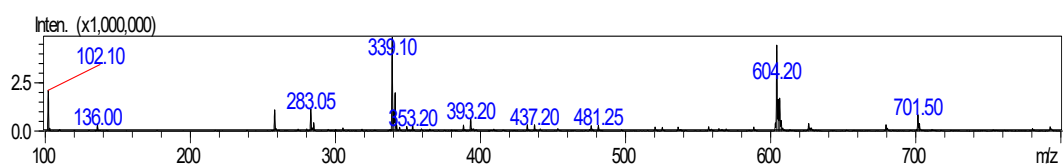
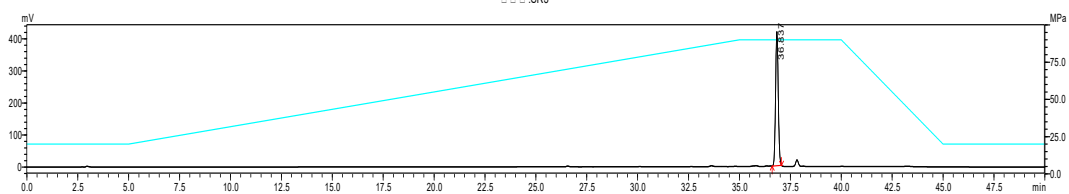




(S)-N-(3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)-3-(6-(cyclopropanecarboxamido)pyridin-3-yl)benzamide (BS13)



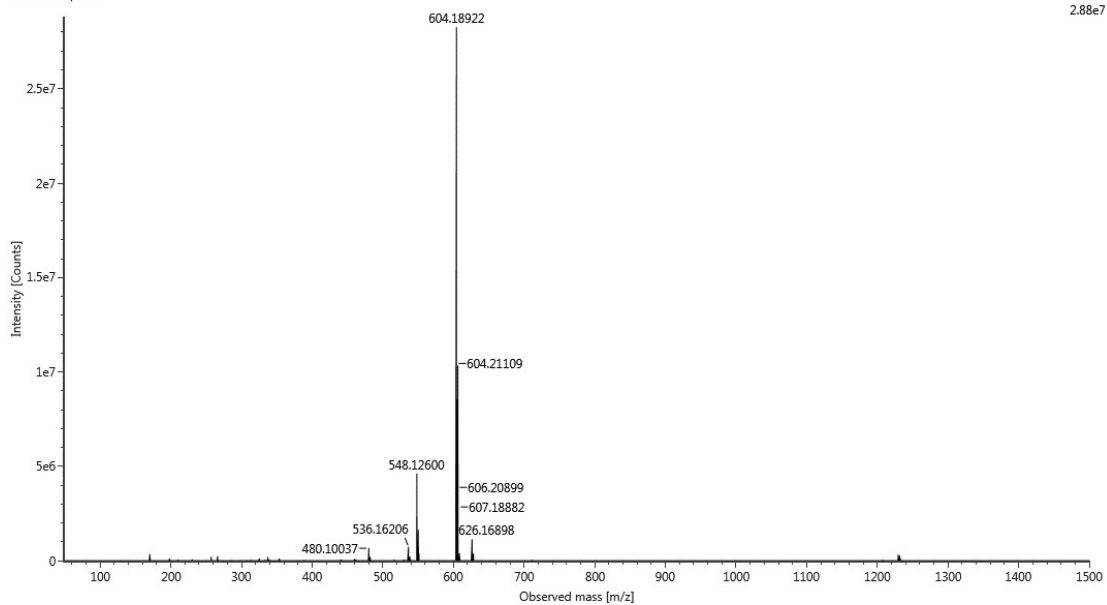
SR3.td
SR3

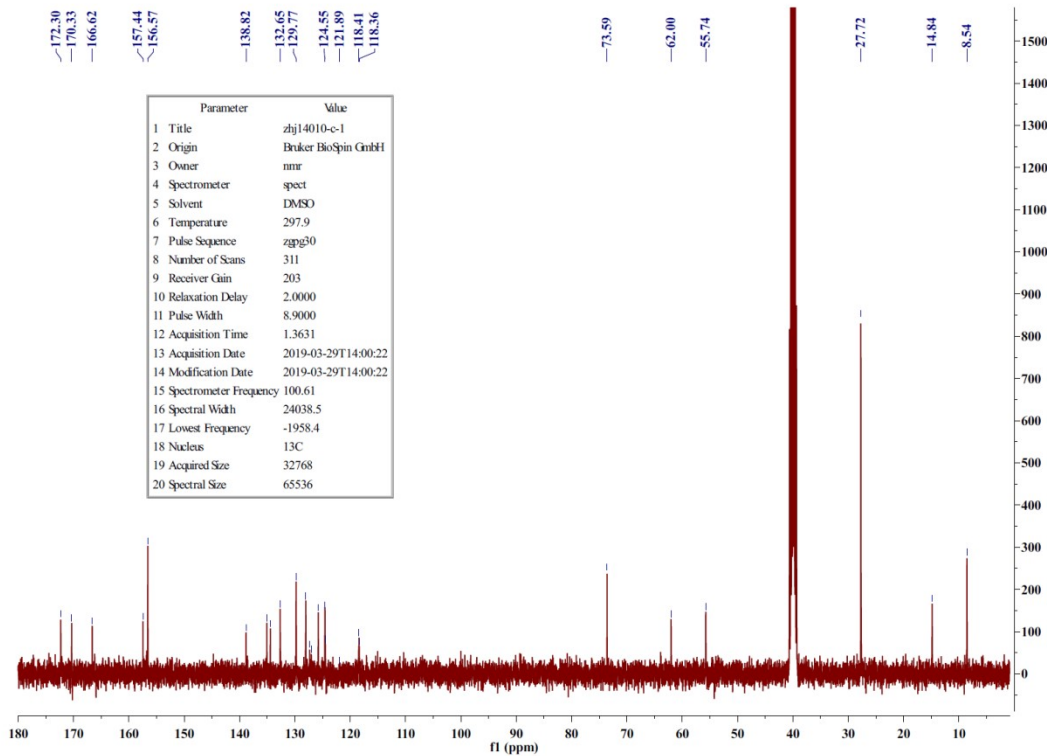
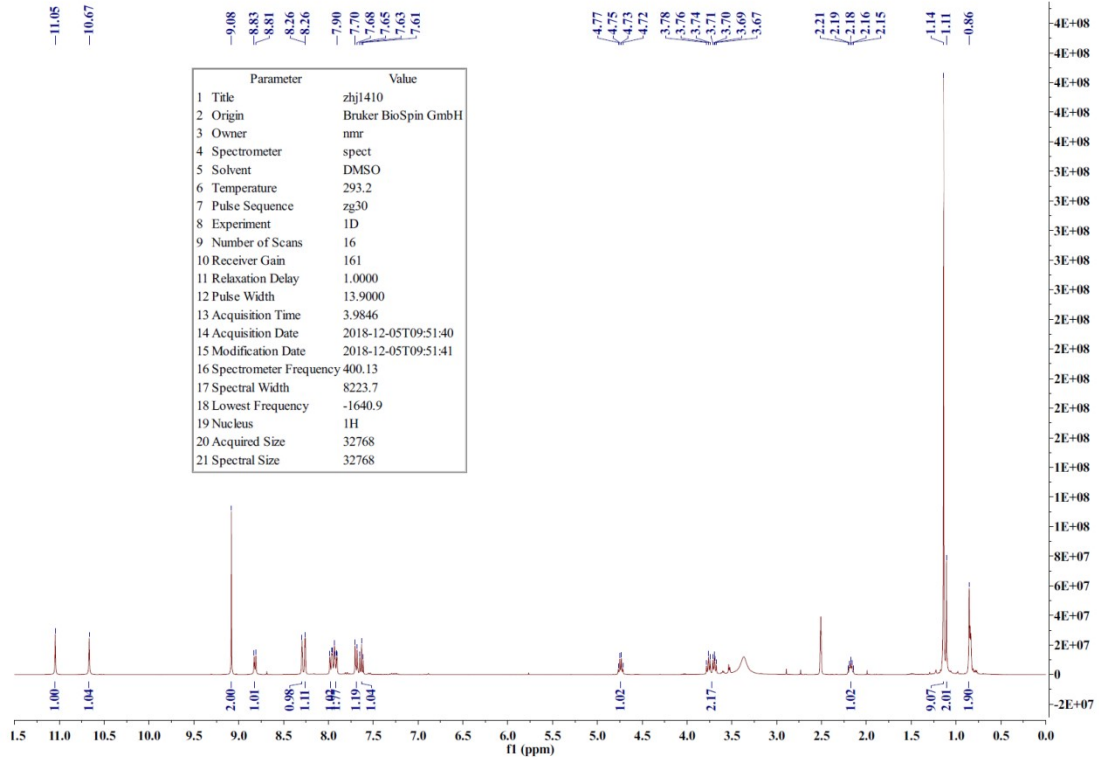


Item name: L-21
Item description:

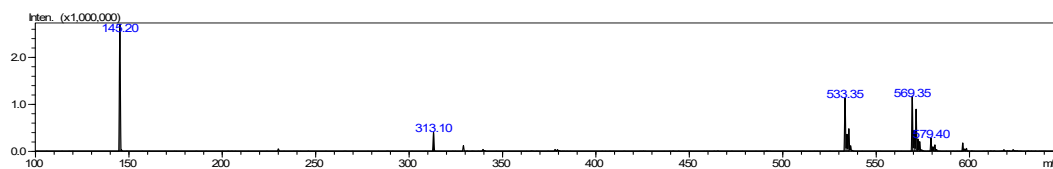
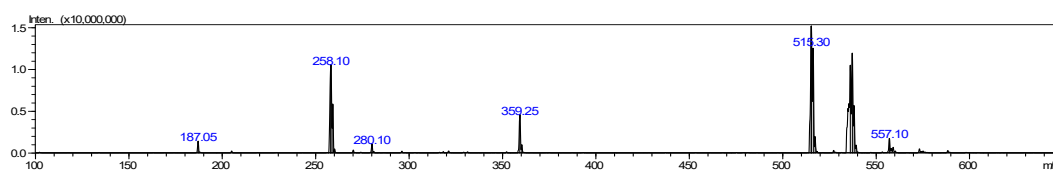
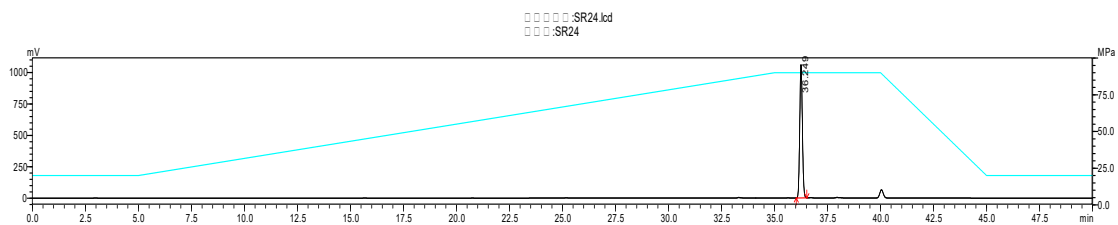
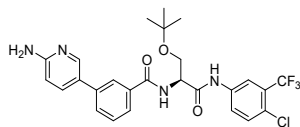
Channel name: 2: Average Time 0.3183 min : TOF MS (50-1500) 6eV ESI+ : Combined

2.88e7





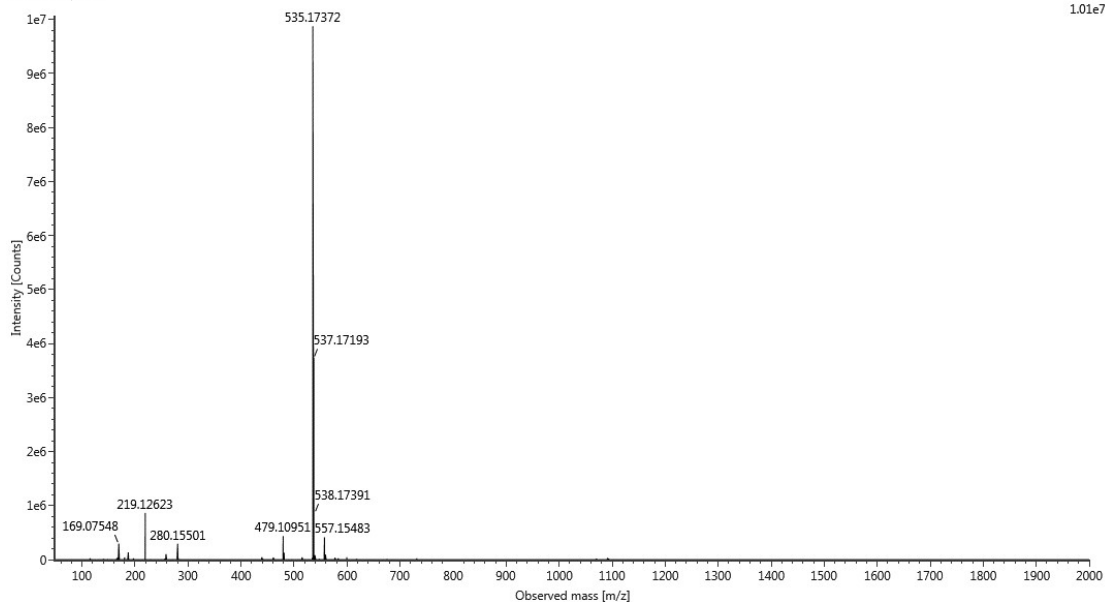
(S)-3-(6-aminopyridin-3-yl)-N-(3-(tert-butoxy)-1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-1-oxopropan-2-yl)benzamide (BS14)

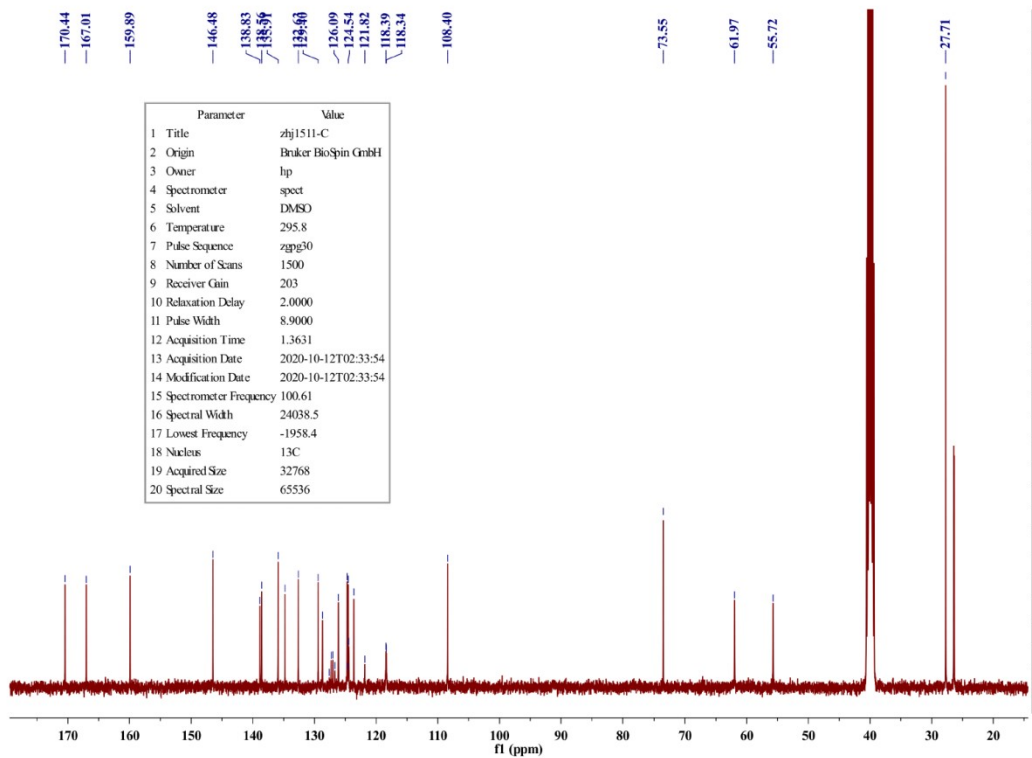
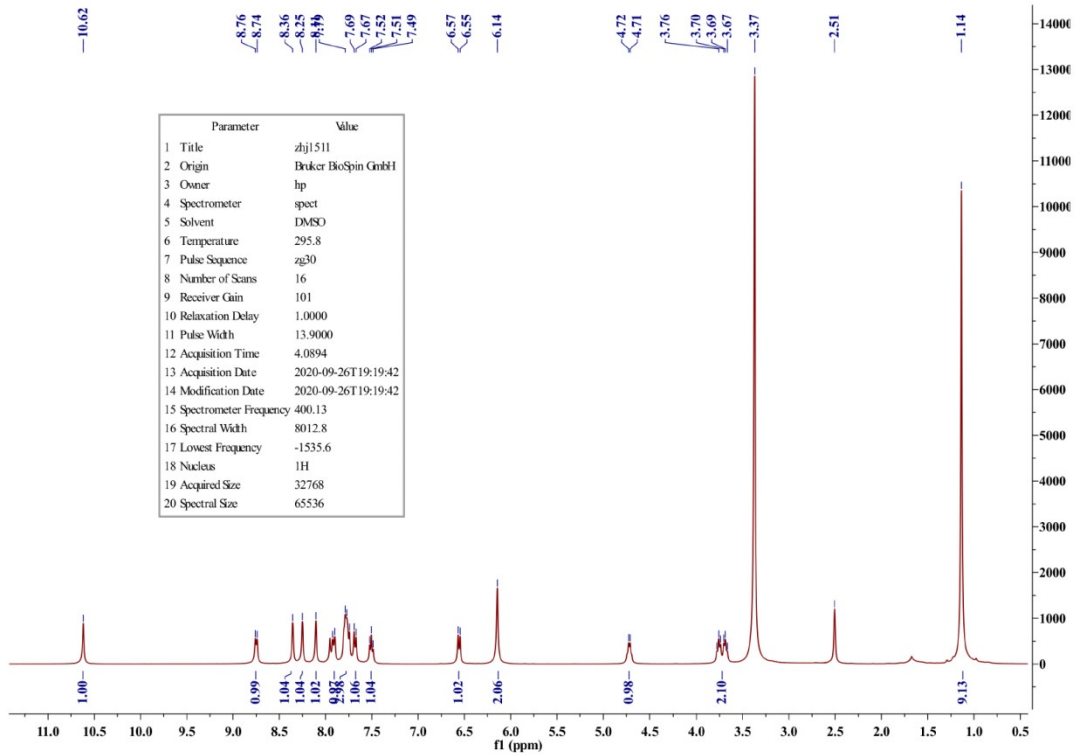


Item name: L3
Item description:

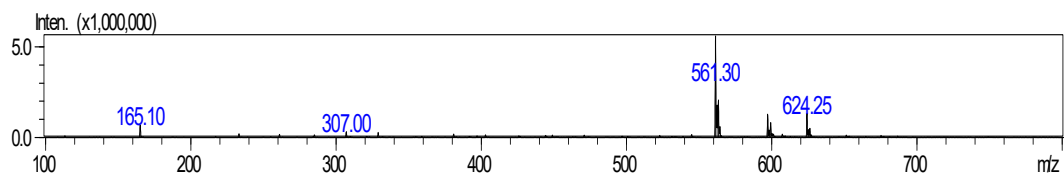
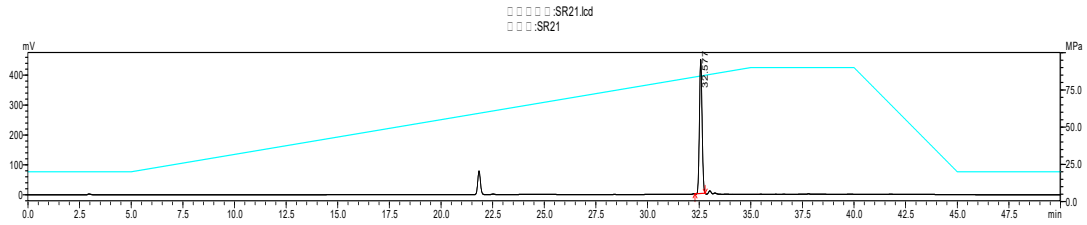
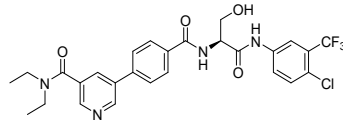
Channel name: 2: Average Time 0.1701 min : TOF MSe (50-2000) 6eV ESI+ : Combined

1.01e7





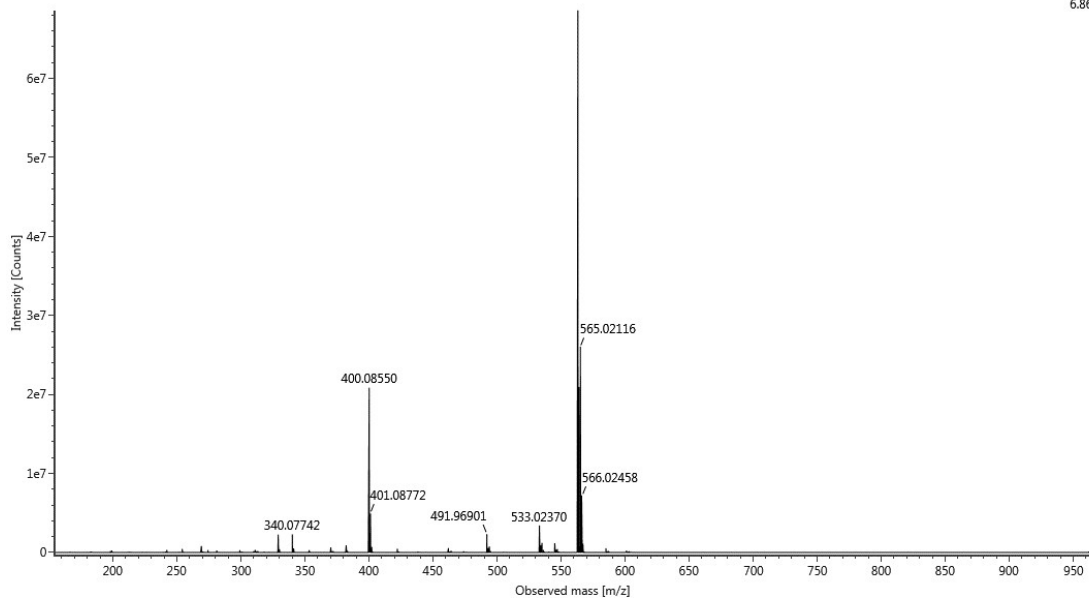
(S)-5-(4-((1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3-hydroxy-1-oxopropan-2-yl)carbamoyl)phenyl)-N,N-diethylnicotinamide (SR1)

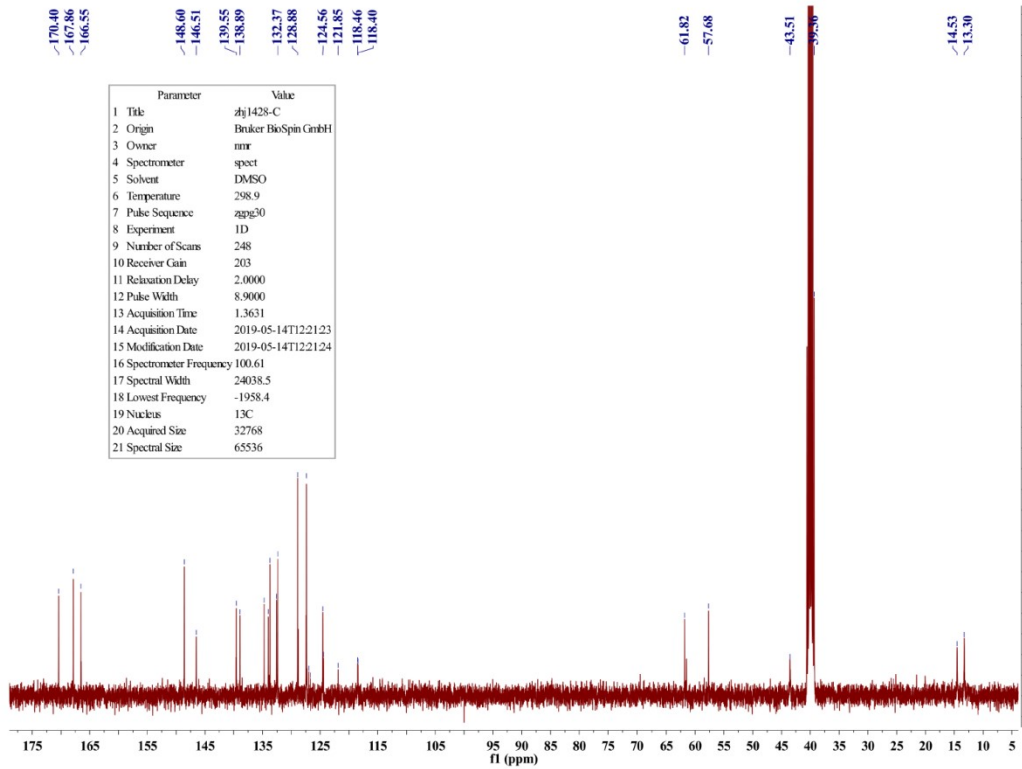
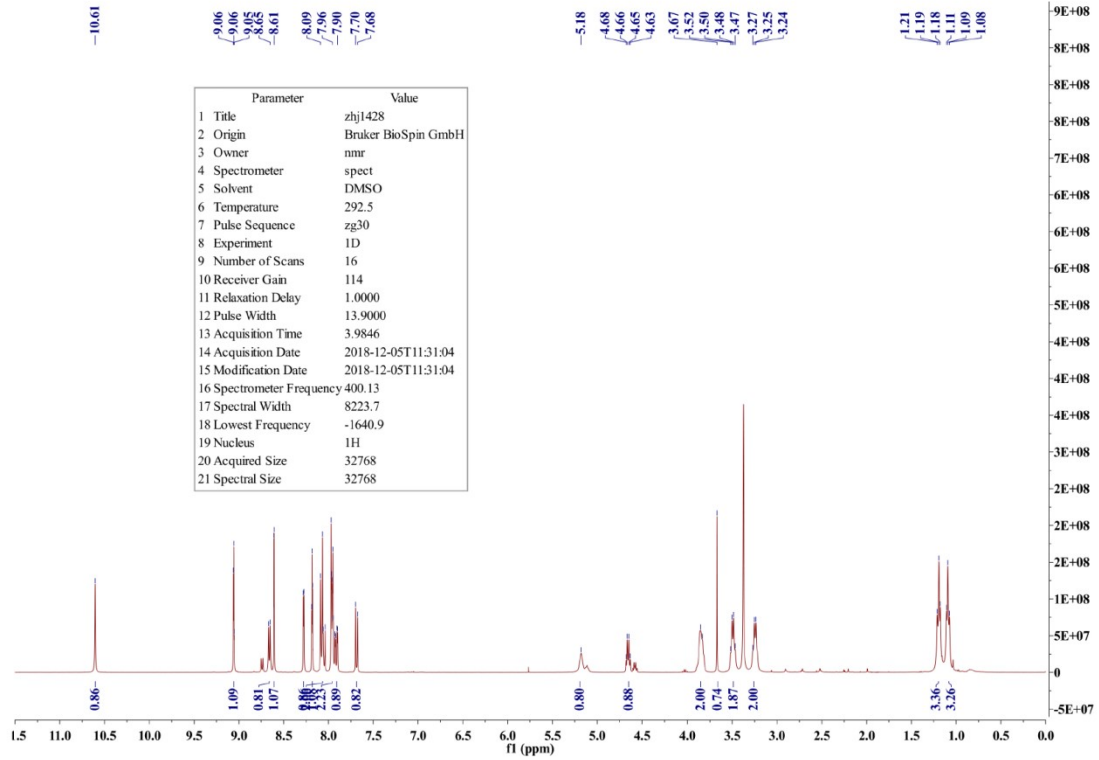


Item name: L39
Item description:

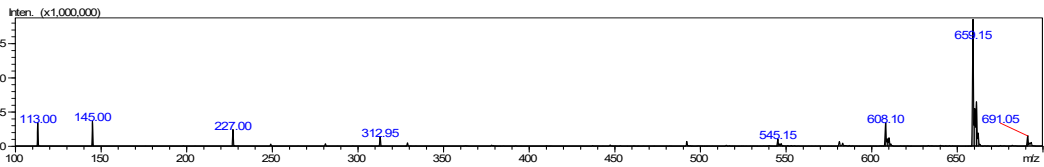
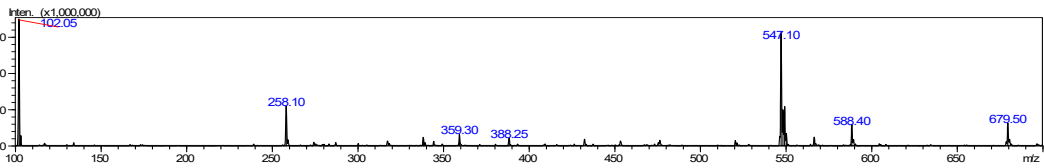
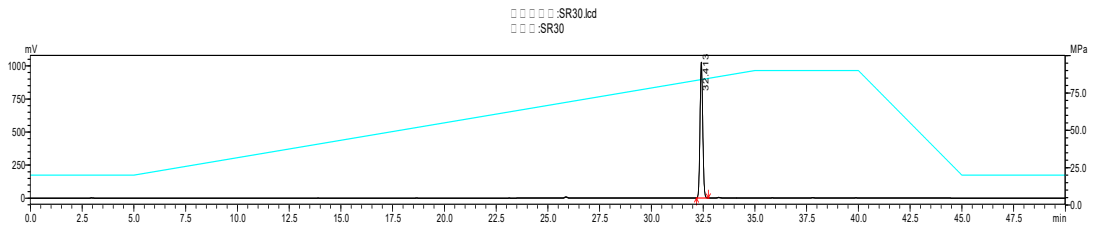
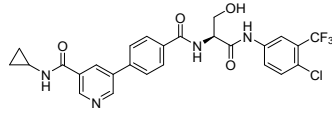
563.02905 Channel name: 2: Average Time 0.1463 min : TOF MS (50-3000) 6eV ESI+ : Combined

6.86e7





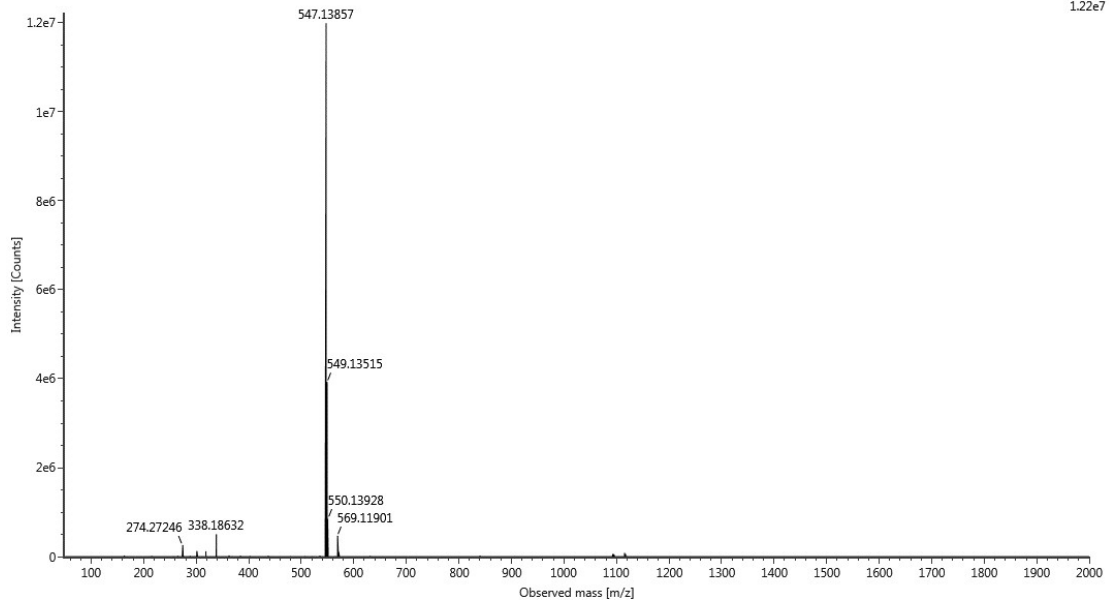
(S)-5-(4-((1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3-hydroxy-1-oxopropan-2-yl)carbamoyl)phenyl)-N-cyclopropylnicotinamide (SR2)

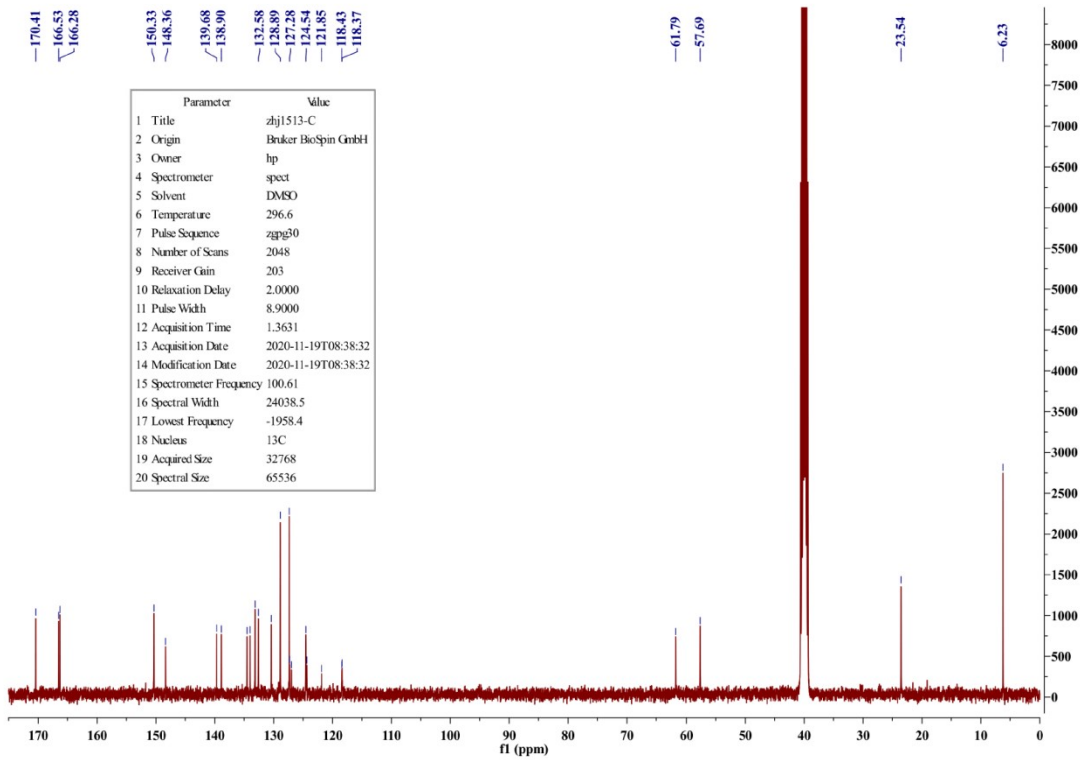
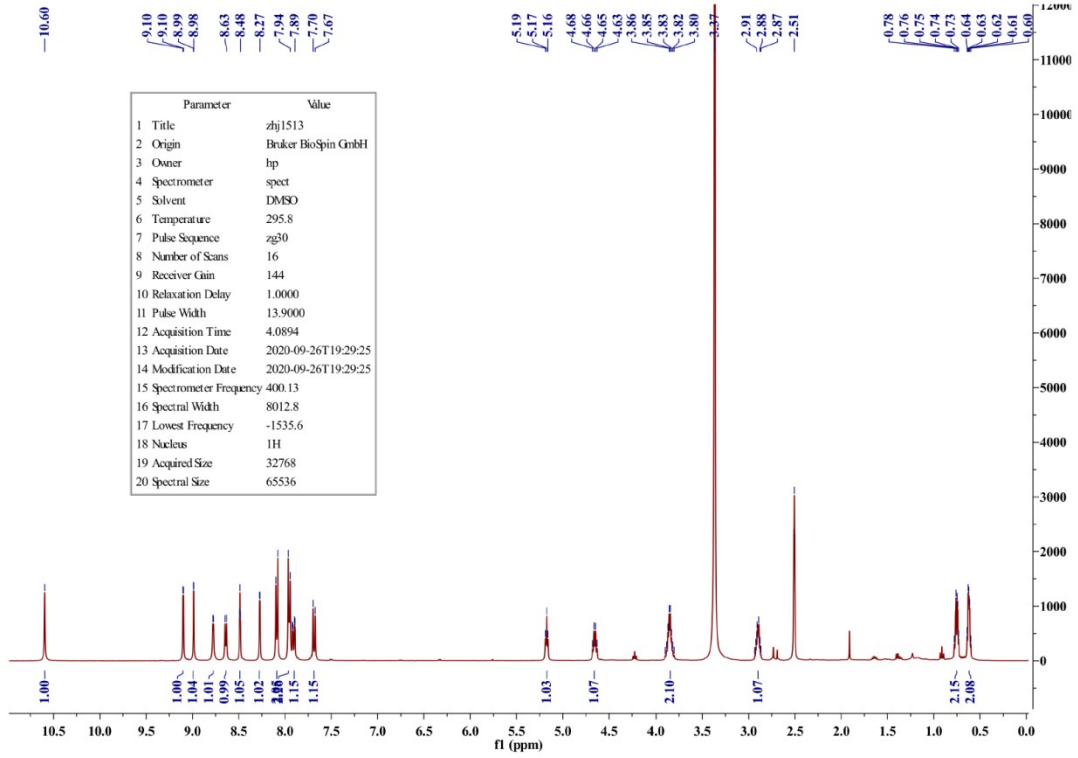


Item name: L6
Item description:

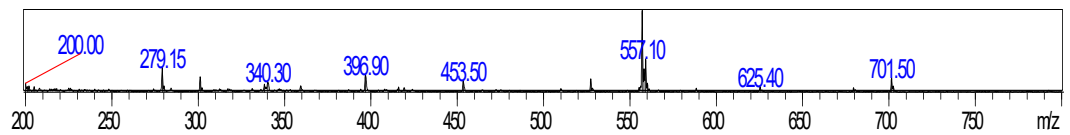
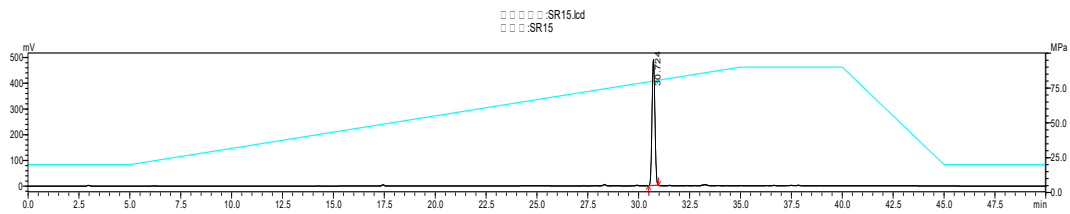
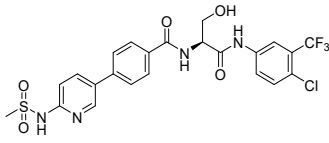
Channel name: 2: Average Time 0.1527 min : TOF MSe (50-2000) 6eV ESI+ : Combined

1.22e7



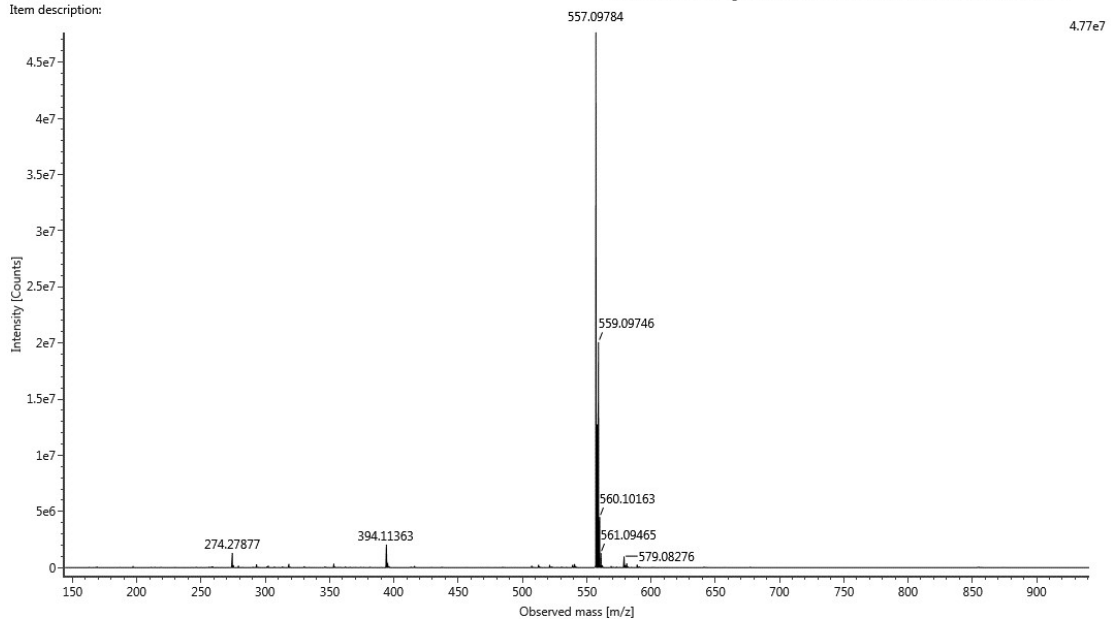


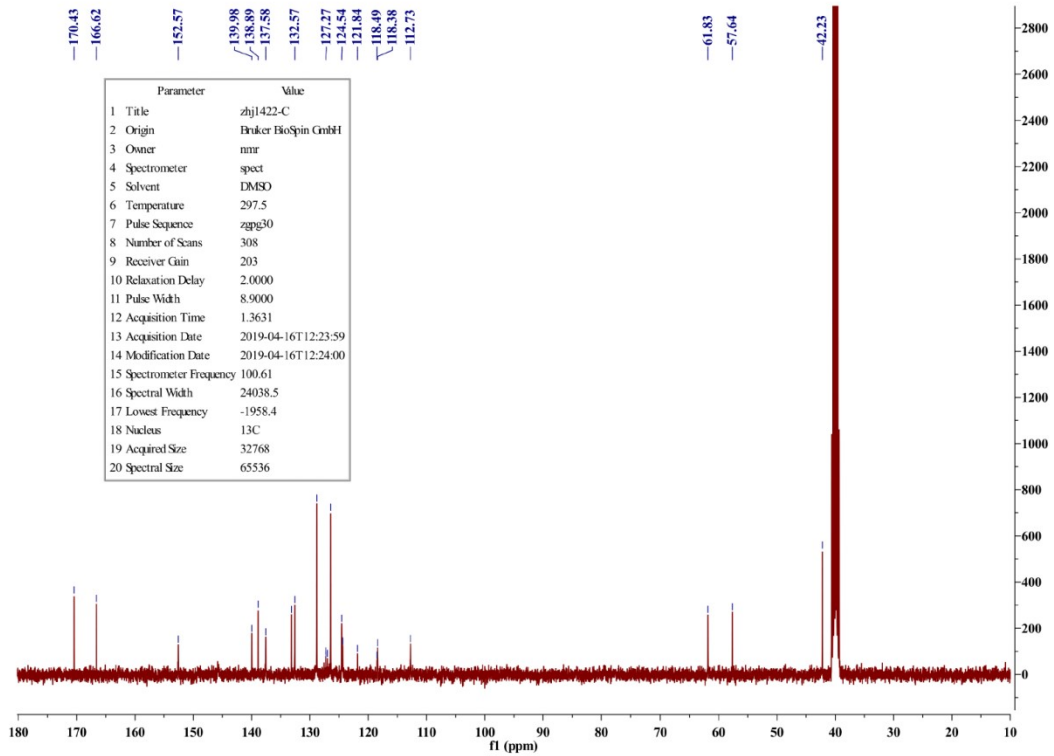
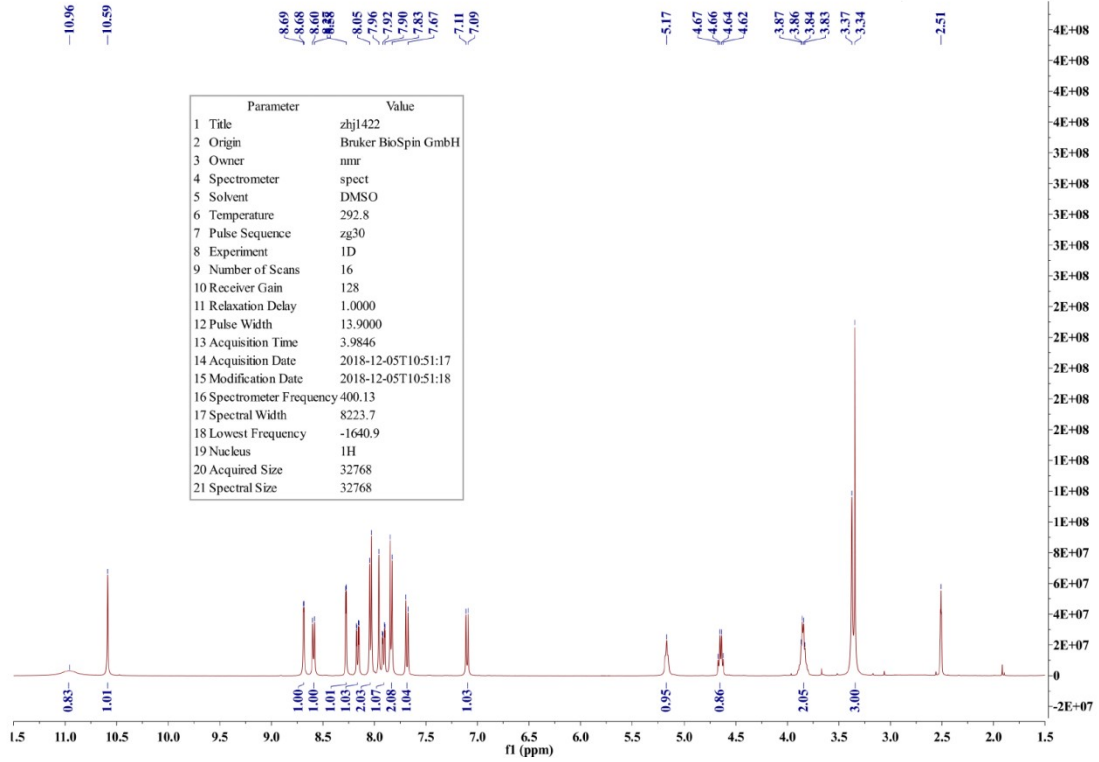
(S)-N-(1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3-hydroxy-1-oxopropan-2-yl)-4-(6-(methylsulfonamido)pyridin-3-yl)benzamide (SR3)



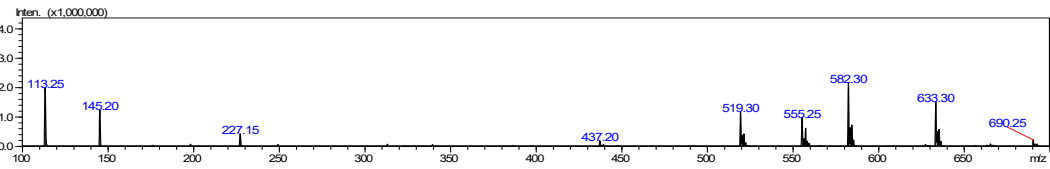
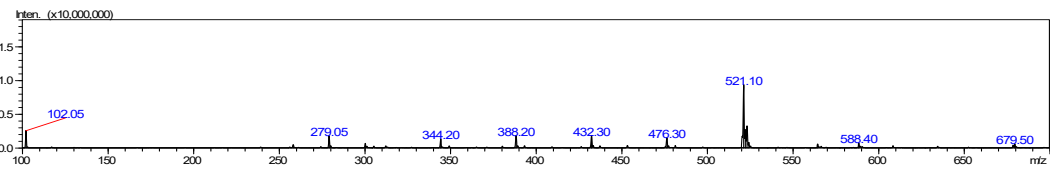
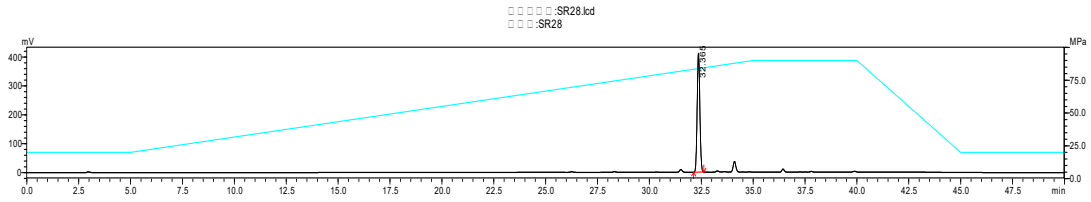
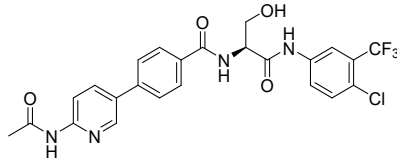
Item name: L40
Item description:

Channel name: 2: Average Time 0.1582 min : TOF MS (50-3000) 6eV ESI+ : Combined





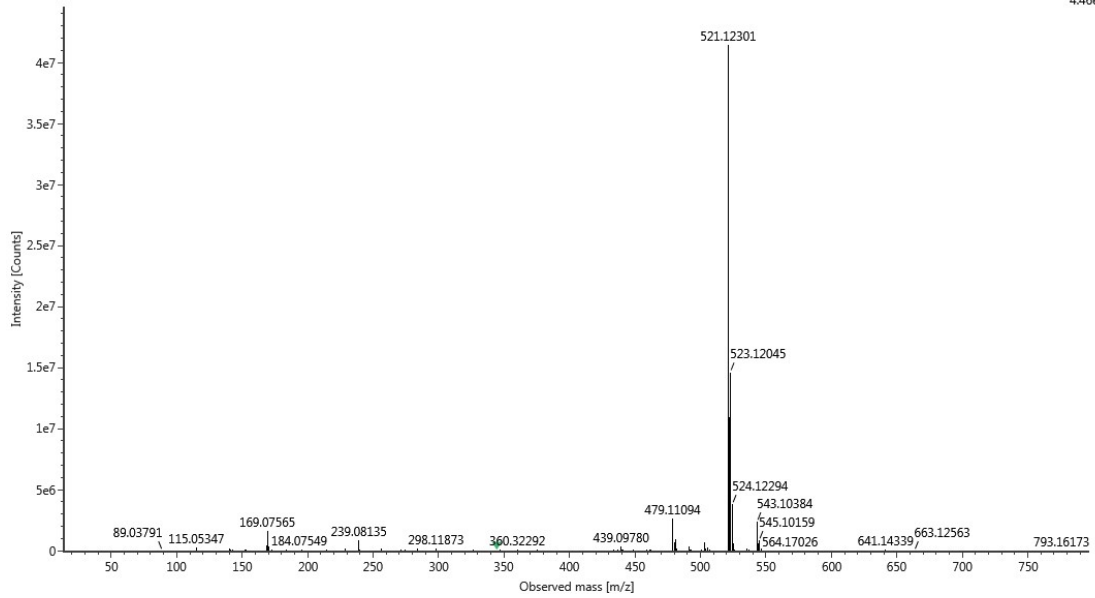
(S)-4-(6-acetamidopyridin-3-yl)-N-(1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3-hydroxy-1-oxopropan-2-yl)benzamide (SR4)

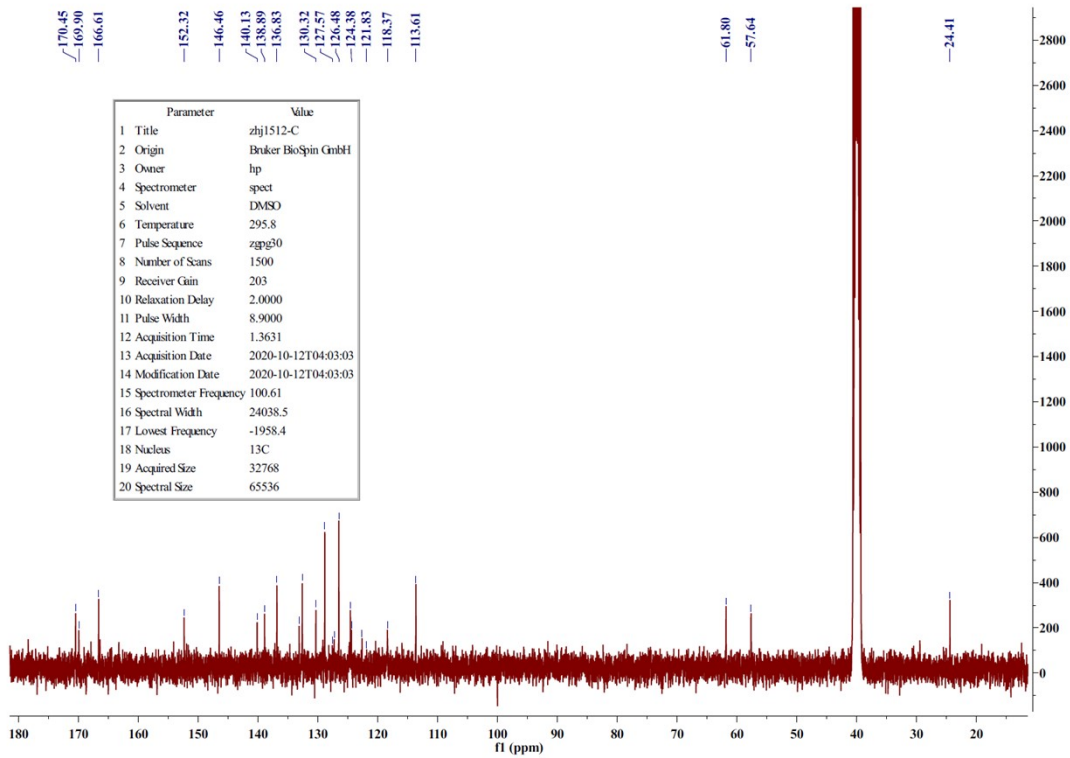
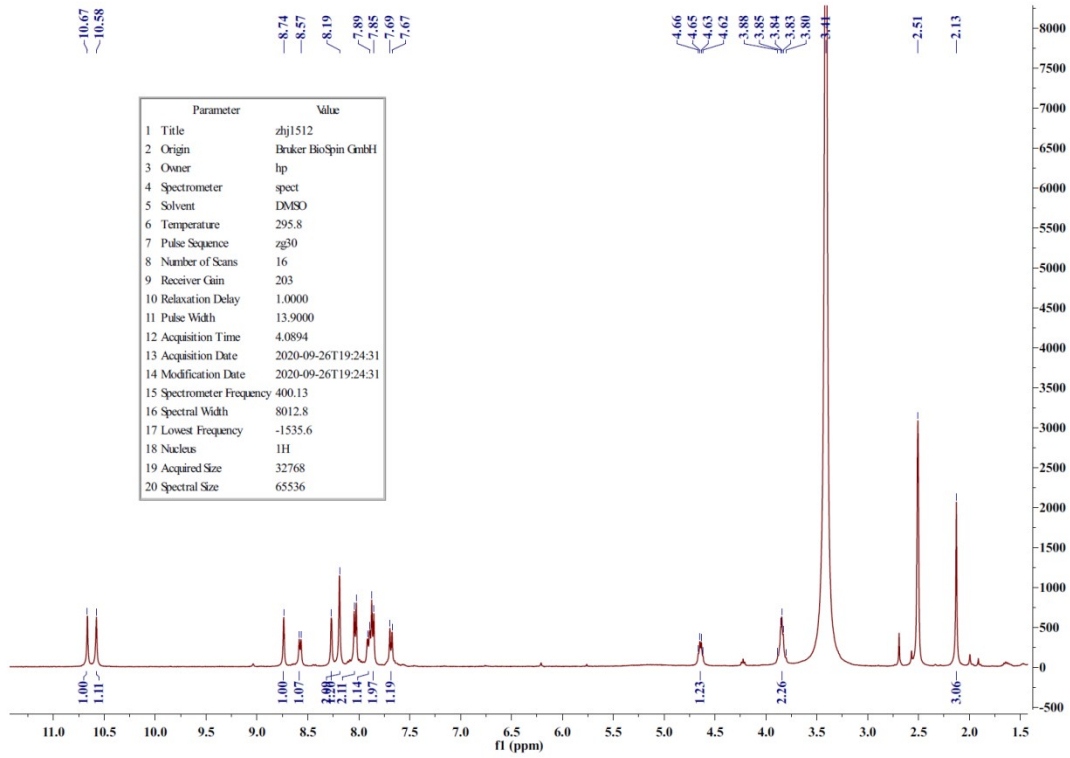


Item name: L4
Item description:

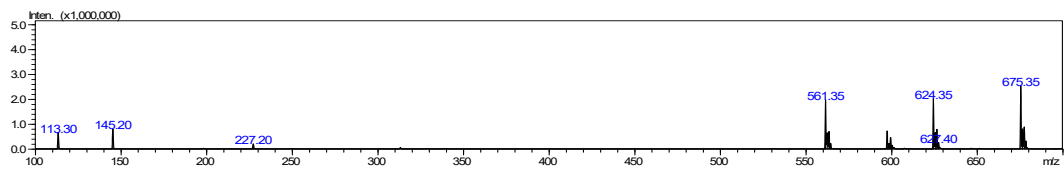
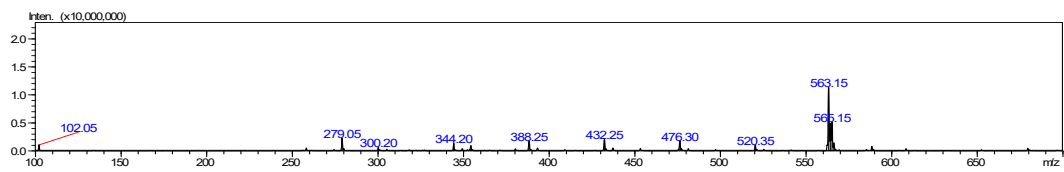
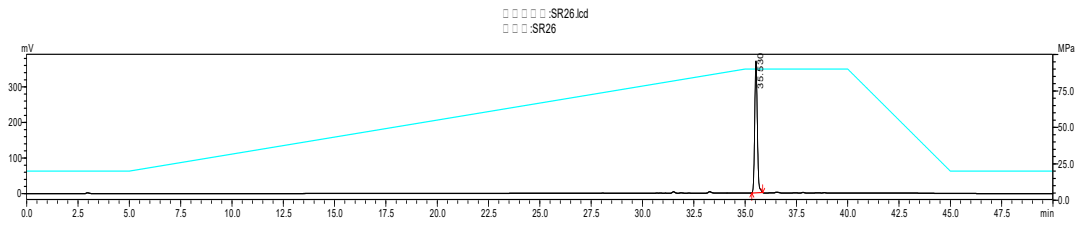
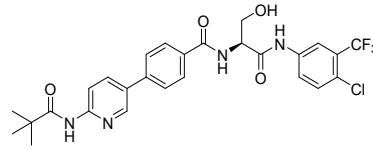
Channel name: 2: Average Time 0.1497 min : TOF MSe (50-2000) 6eV ESI+ : Centroided : Combined

4.46e7





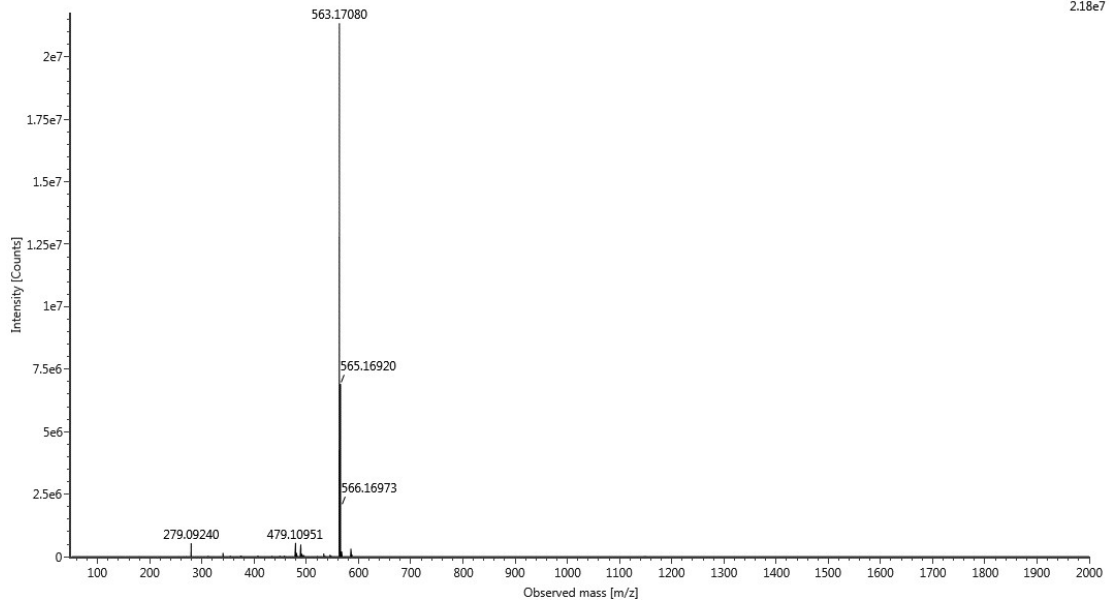
(S)-N-(1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3-hydroxy-1-oxopropan-2-yl)-4-(6-pivalamidopyridin-3-yl)benzamide (SR5)

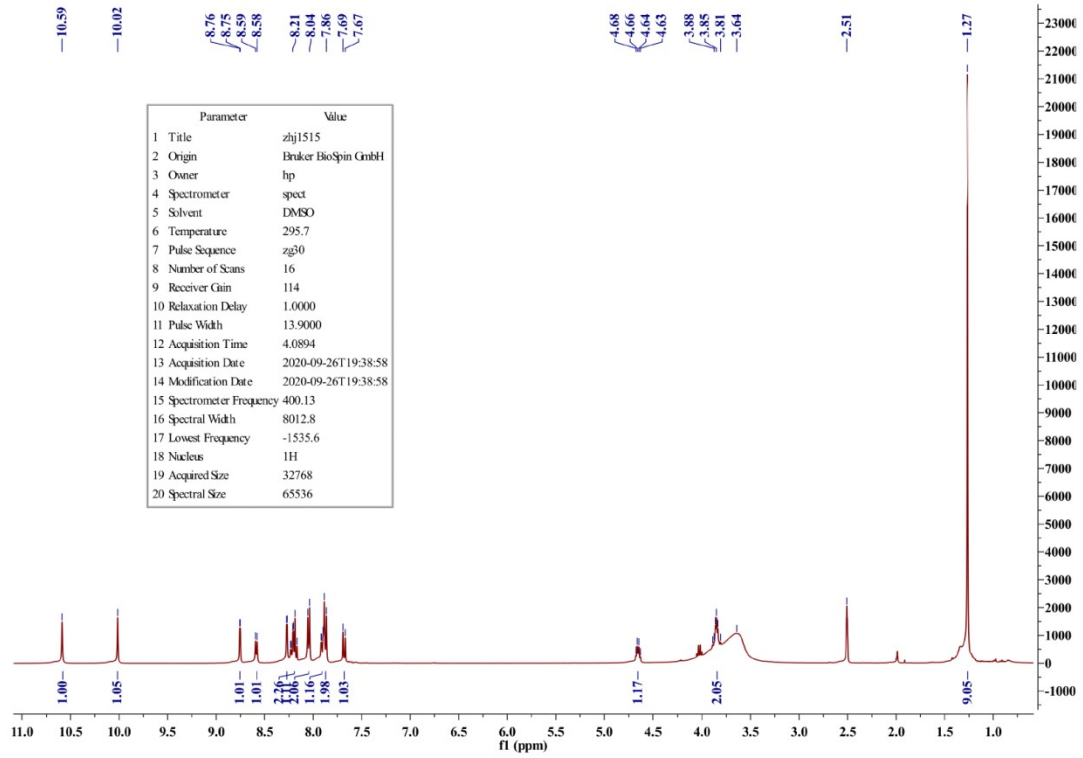


Item name: L9
Item description:

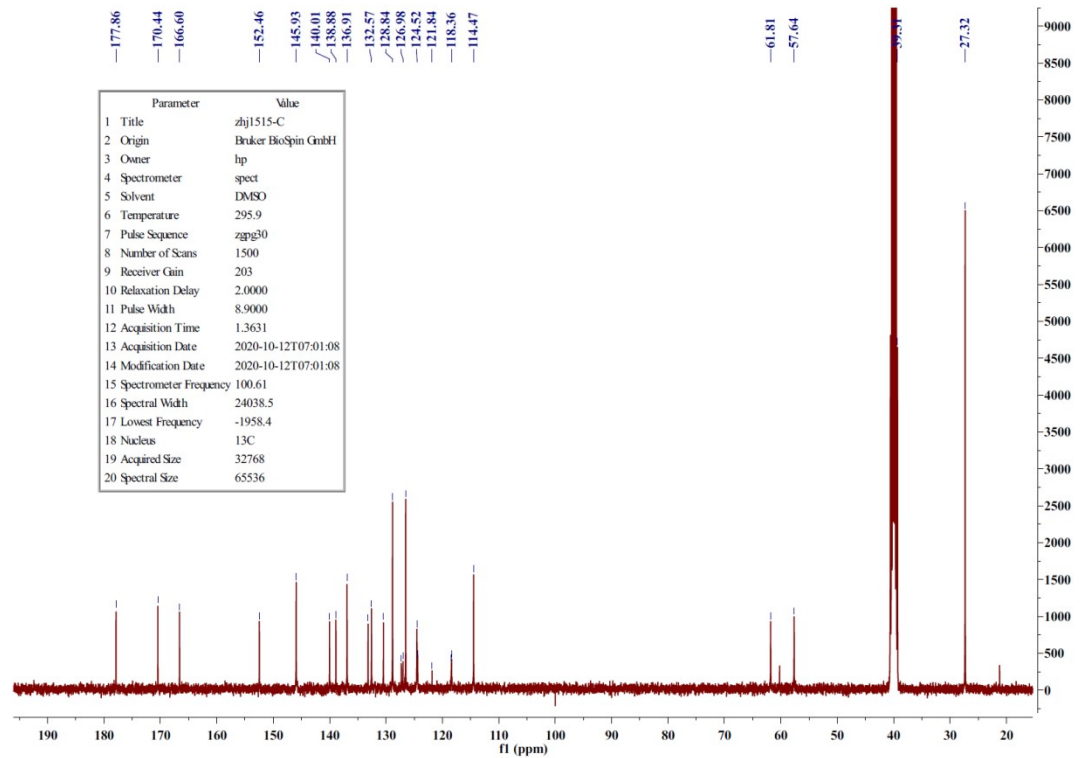
Channel name: 2: Average Time 0.1774 min : TOF MSe (50-2000) 6eV ESI+ : Combined

2.18e7



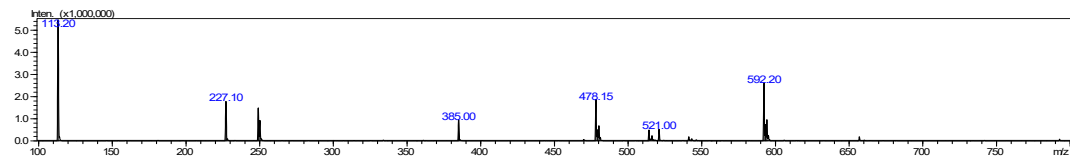
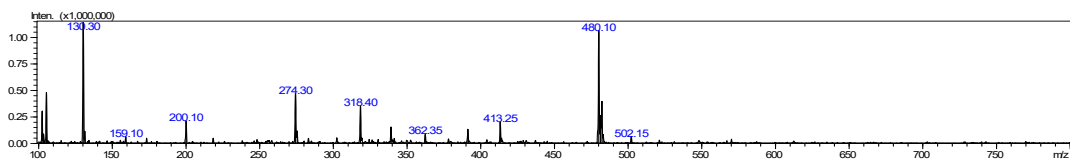
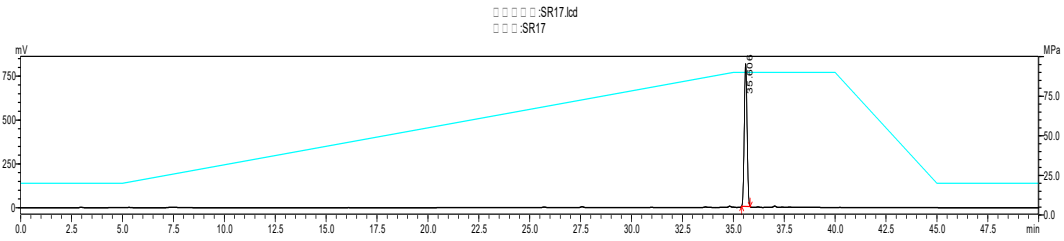
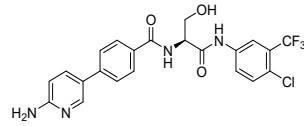


Parameter	Value
1 Title	zhj1515
2 Origin	Bruker BioSpin GmbH
3 Owner	hp
4 Spectrometer	spect
5 Solvent	DMSO
6 Temperature	295.7
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Receiver Gain	114
10 Relaxation Delay	1.0000
11 Pulse Width	13.9000
12 Acquisition Time	4.0894
13 Acquisition Date	2020-09-26T19:38:58
14 Modification Date	2020-09-26T19:38:58
15 Spectrometer Frequency	400.13
16 Spectral Width	8012.8
17 Lowest Frequency	-1535.6
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536



Parameter	Value
1 Title	zhj1515-C
2 Origin	Bruker BioSpin GmbH
3 Owner	hp
4 Spectrometer	spect
5 Solvent	DMSO
6 Temperature	295.9
7 Pulse Sequence	zgpg30
8 Number of Scans	1500
9 Receiver Gain	203
10 Relaxation Delay	2.0000
11 Pulse Width	8.9000
12 Acquisition Time	1.3631
13 Acquisition Date	2020-10-12T07:01:08
14 Modification Date	2020-10-12T07:01:08
15 Spectrometer Frequency	100.61
16 Spectral Width	24038.5
17 Lowest Frequency	-1958.4
18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536

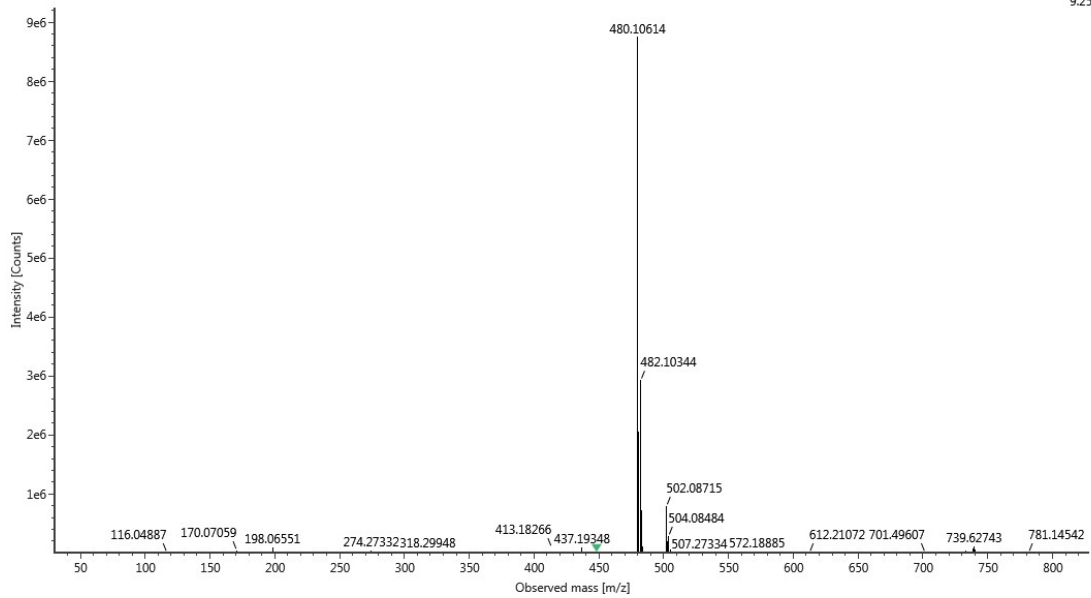
(S)-4-(6-aminopyridin-3-yl)-N-(1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3-hydroxy-1-oxopropan-2-yl)benzamide (SR6)

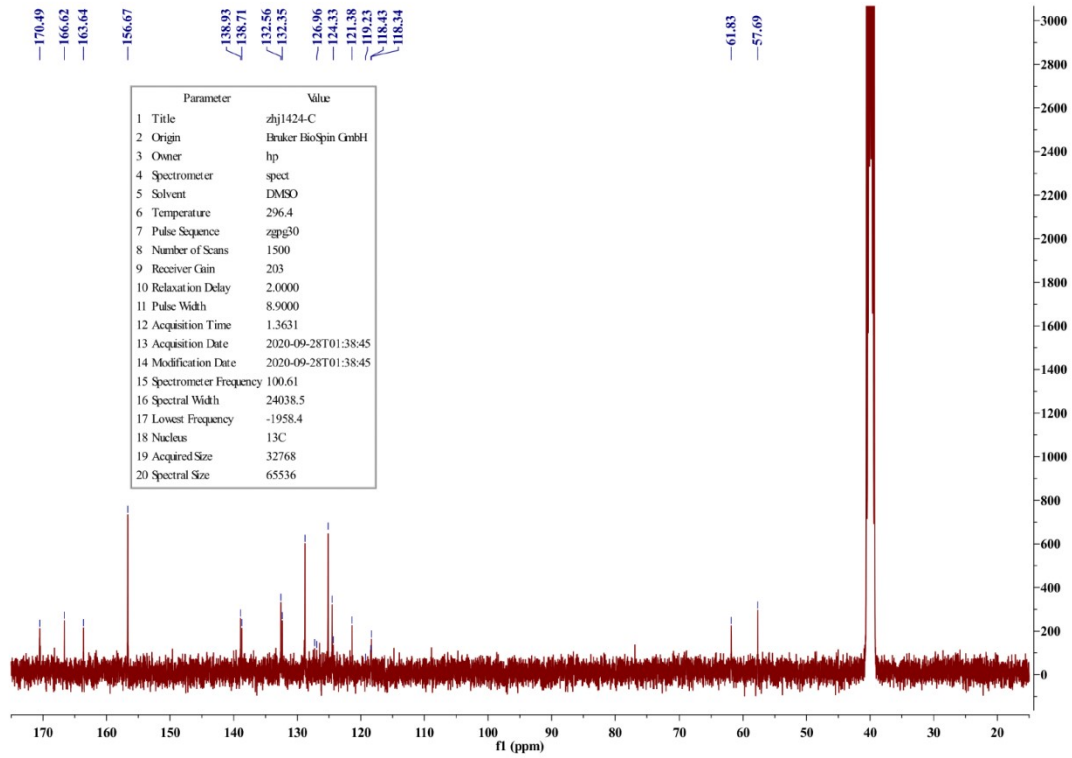
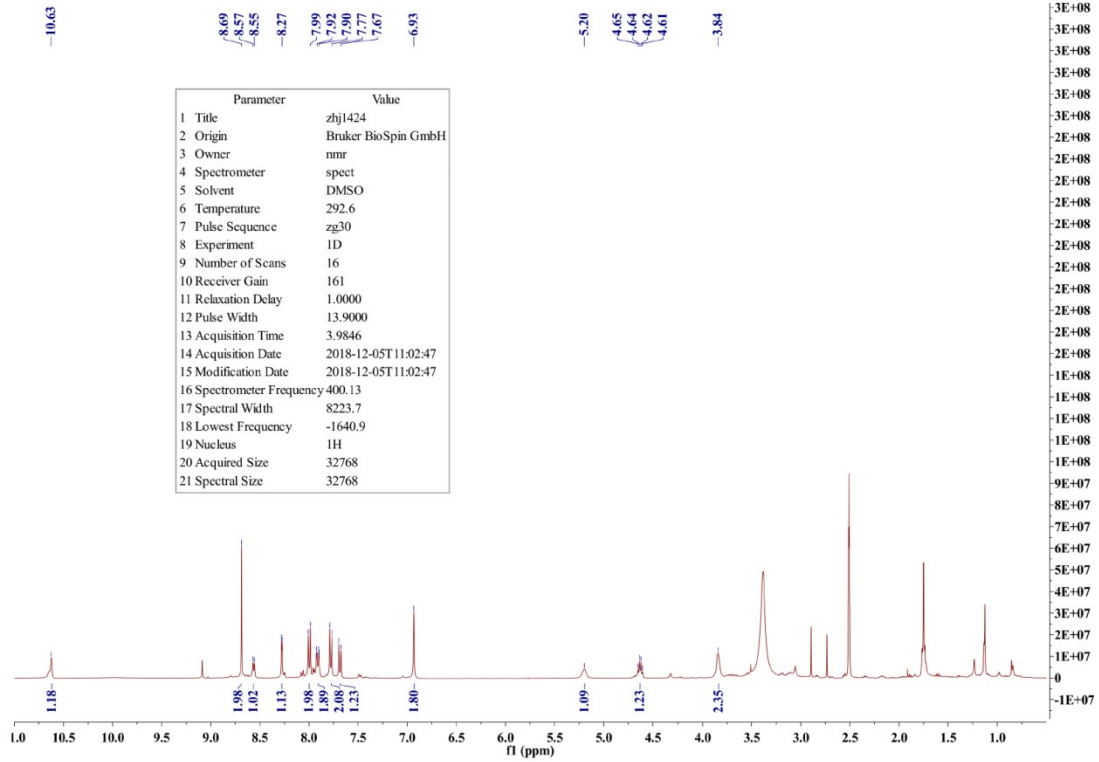


Item name: L22
Item description:

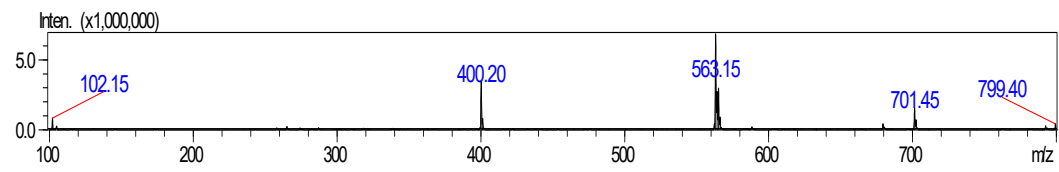
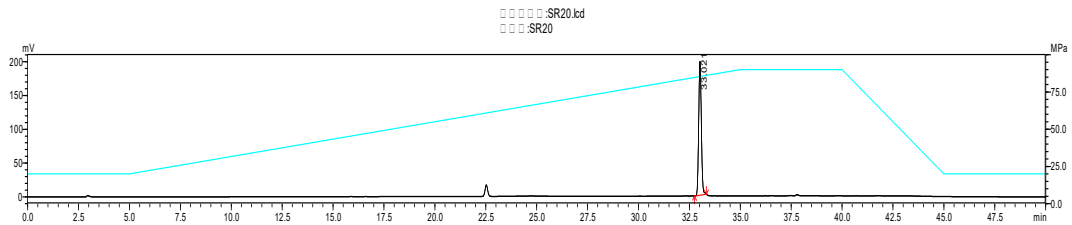
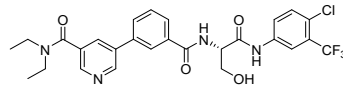
Channel name: 2: Average Time 0.1462 min : TOF MSe (50-2000) 6eV ESI+ : Centroided : Combined

9.25e6



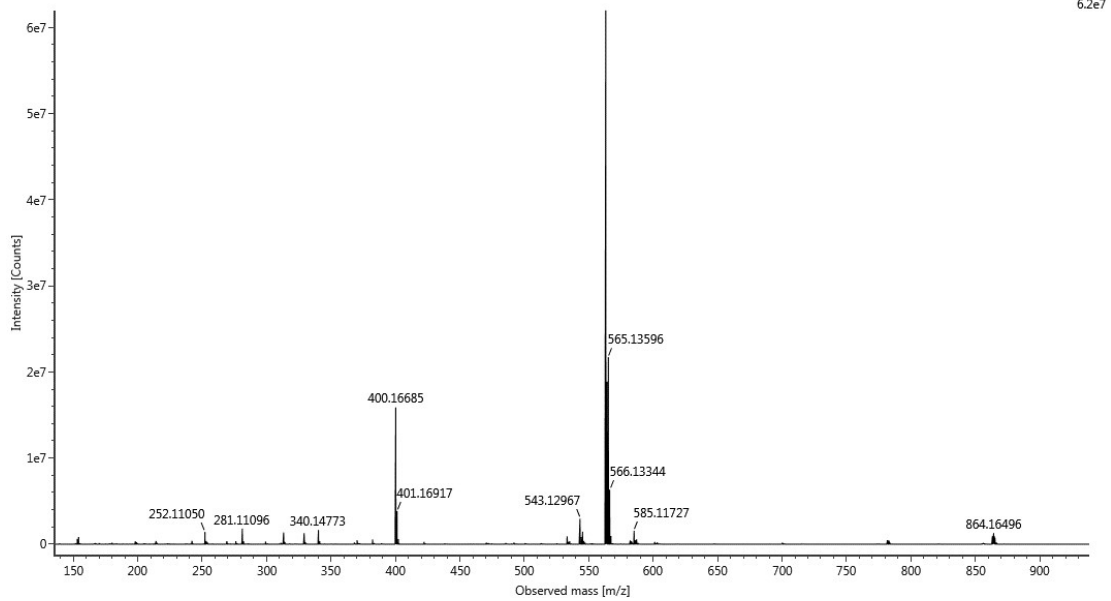


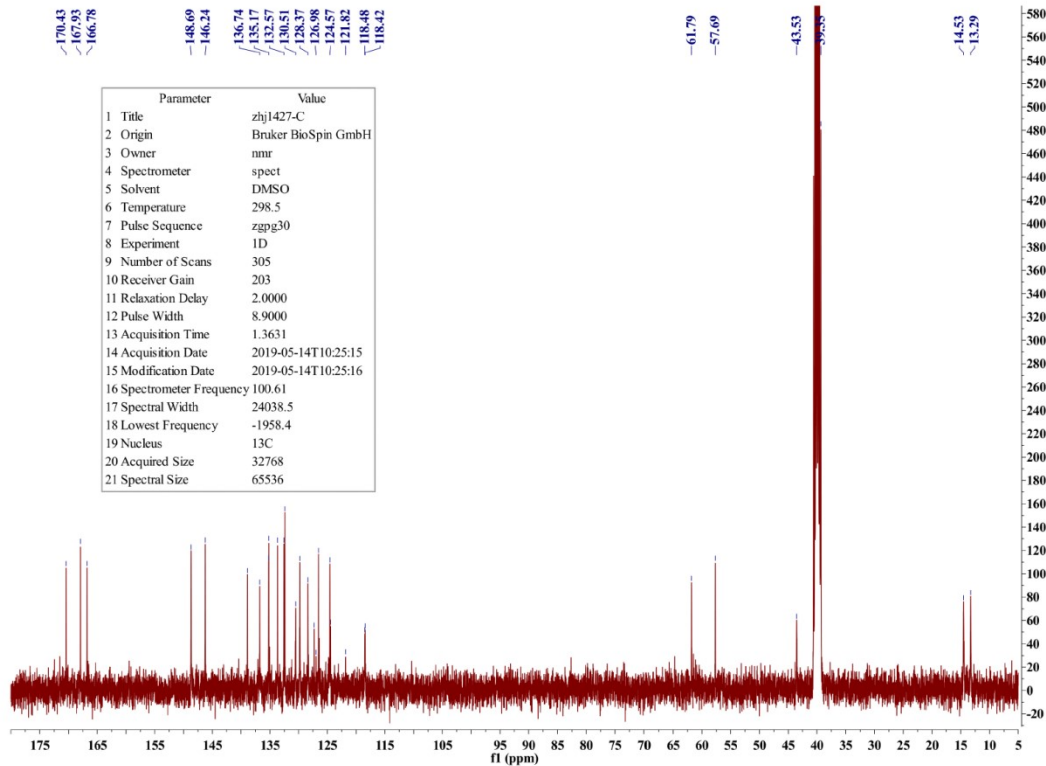
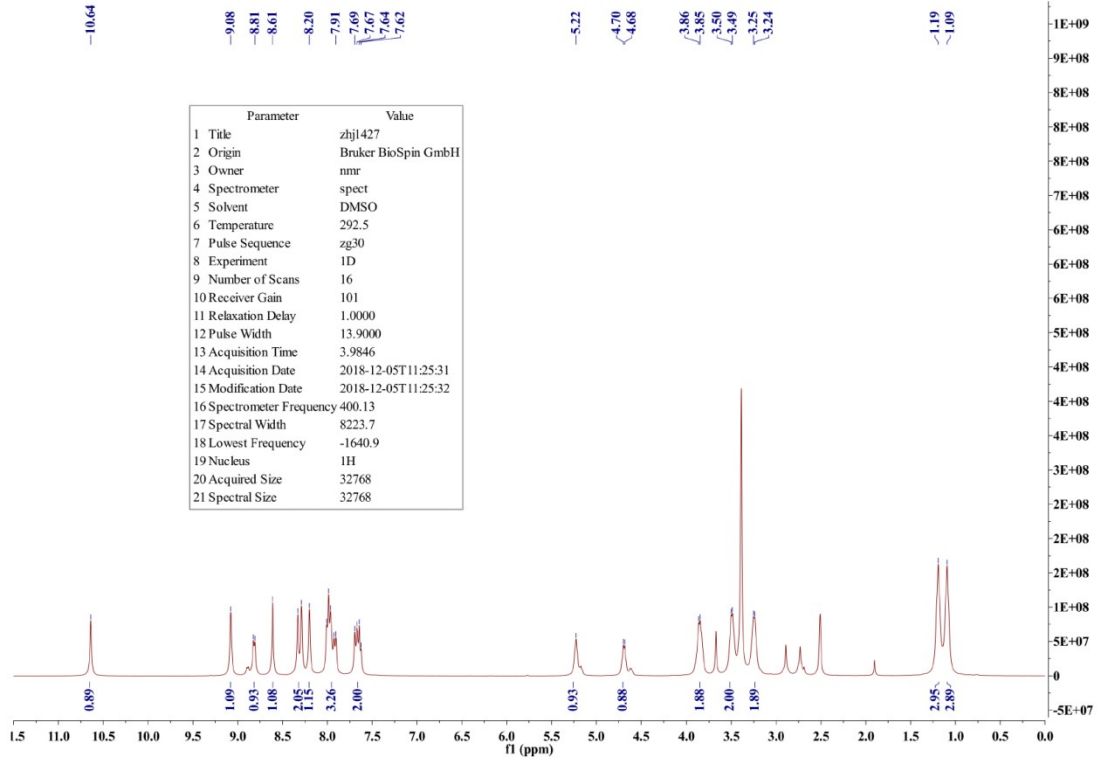
(S)-5-(3-((1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3-hydroxy-1-oxopropan-2-yl)carbamoyl)phenyl)-N,N-diethylnicotinamide (SR7)



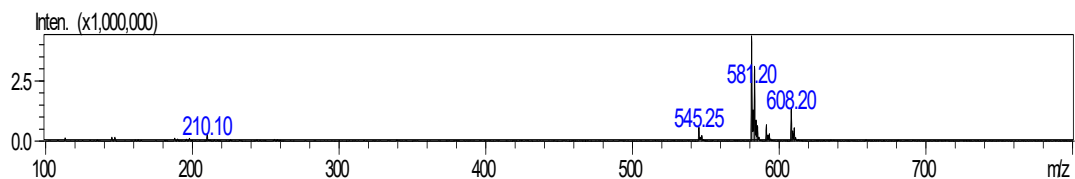
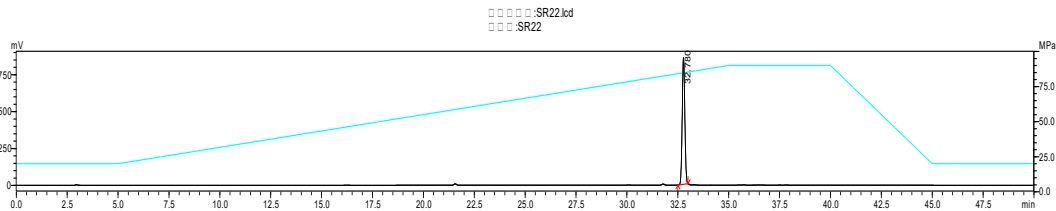
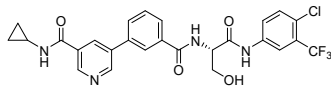
Item name: L35
Item description:

Channel name: 2: Average Time 0.1581 min : TOF MS (50-3000) 6eV ESI+ : Combined



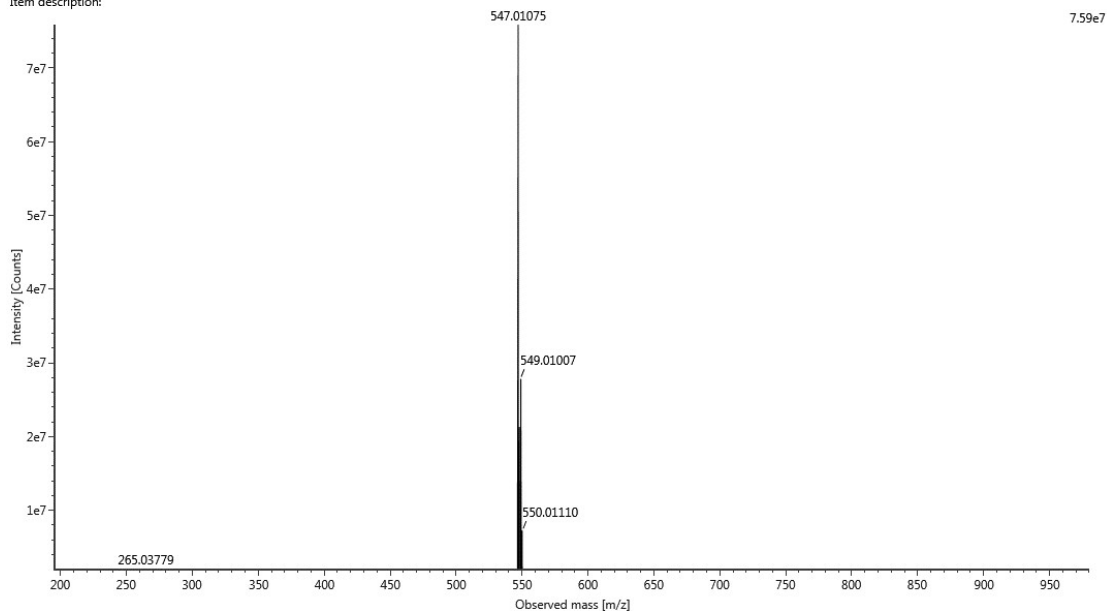


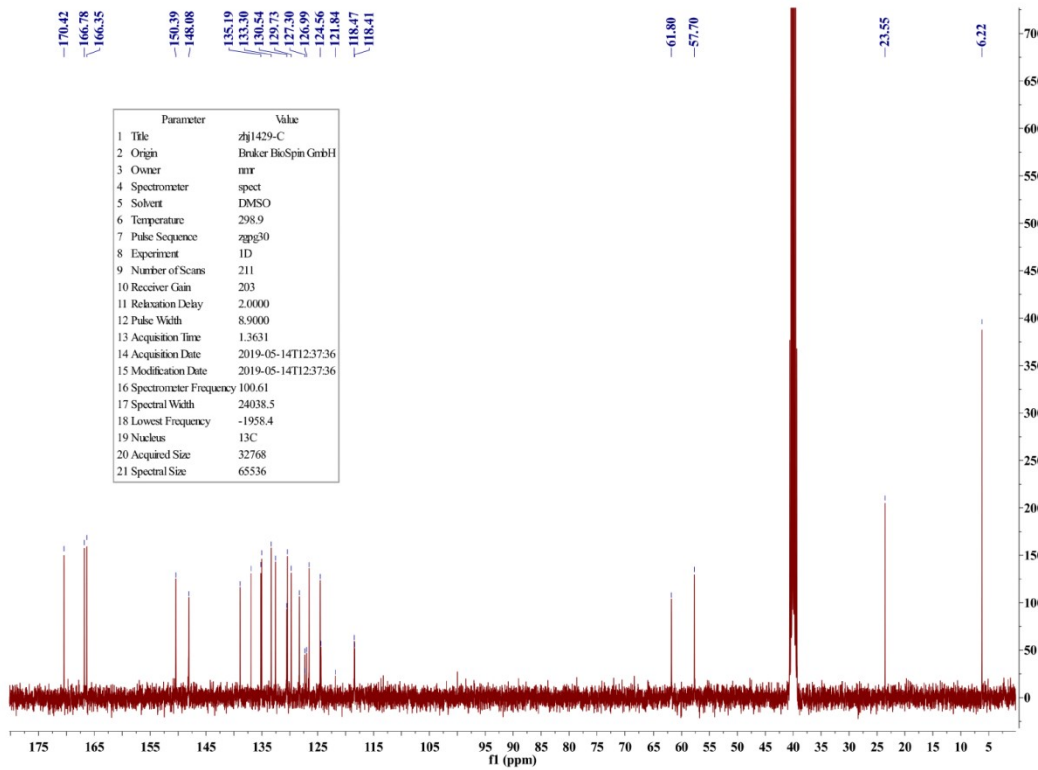
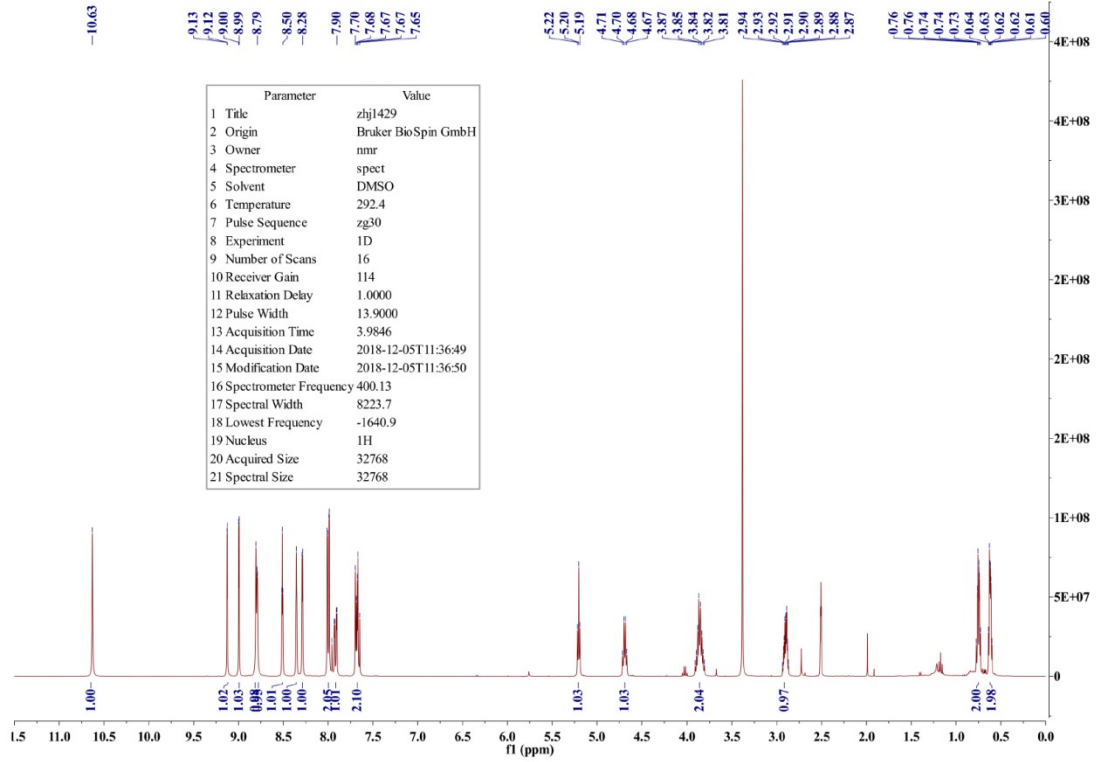
(S)-5-(3-((1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3-hydroxy-1-oxopropan-2-yl)carbamoyl)phenyl)-N-cyclopropylnicotinamide (SR8)



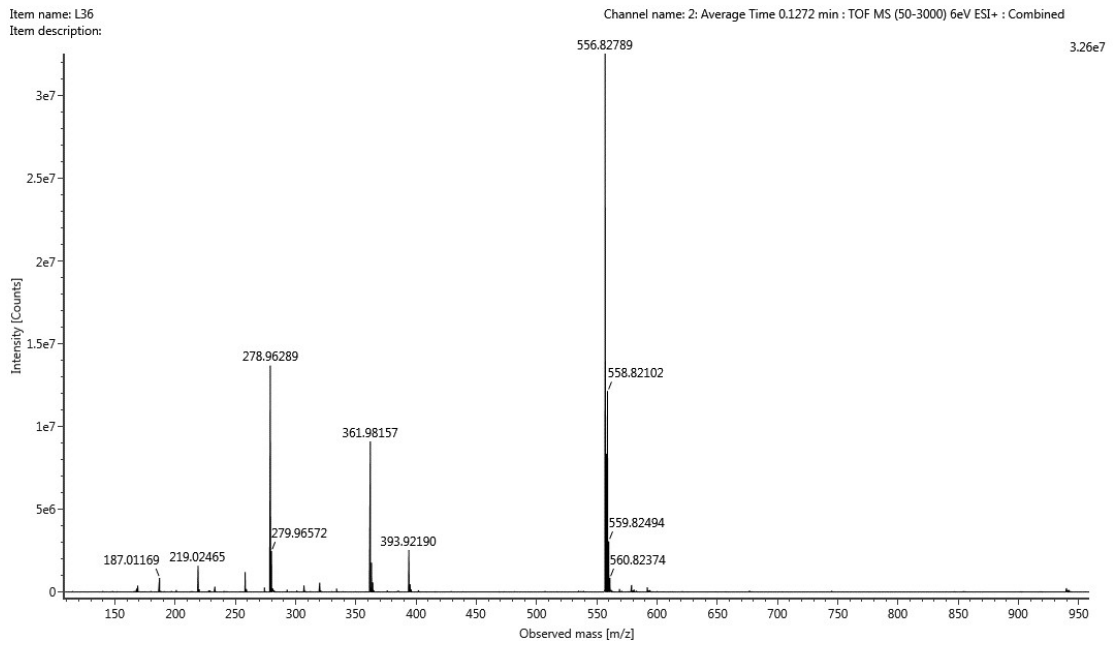
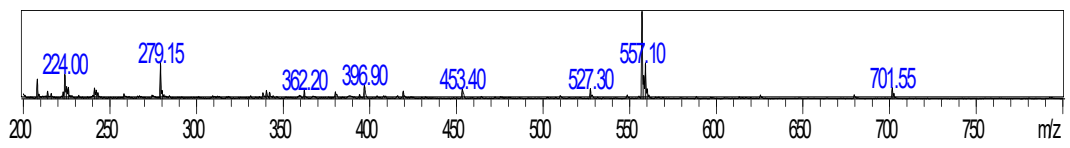
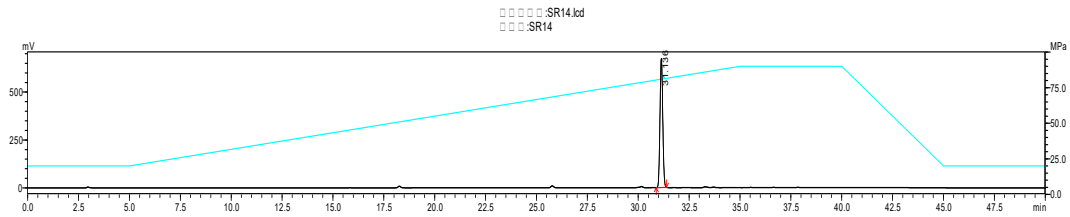
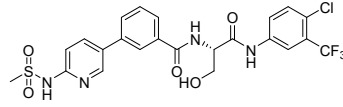
Item name: L38
Item description:

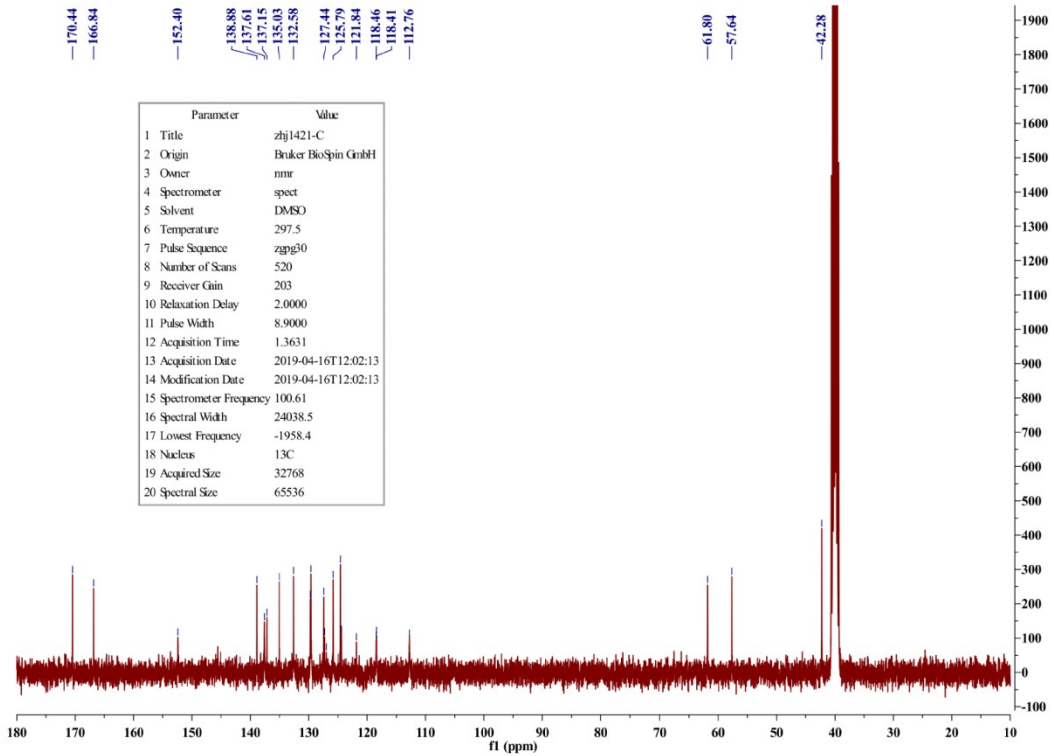
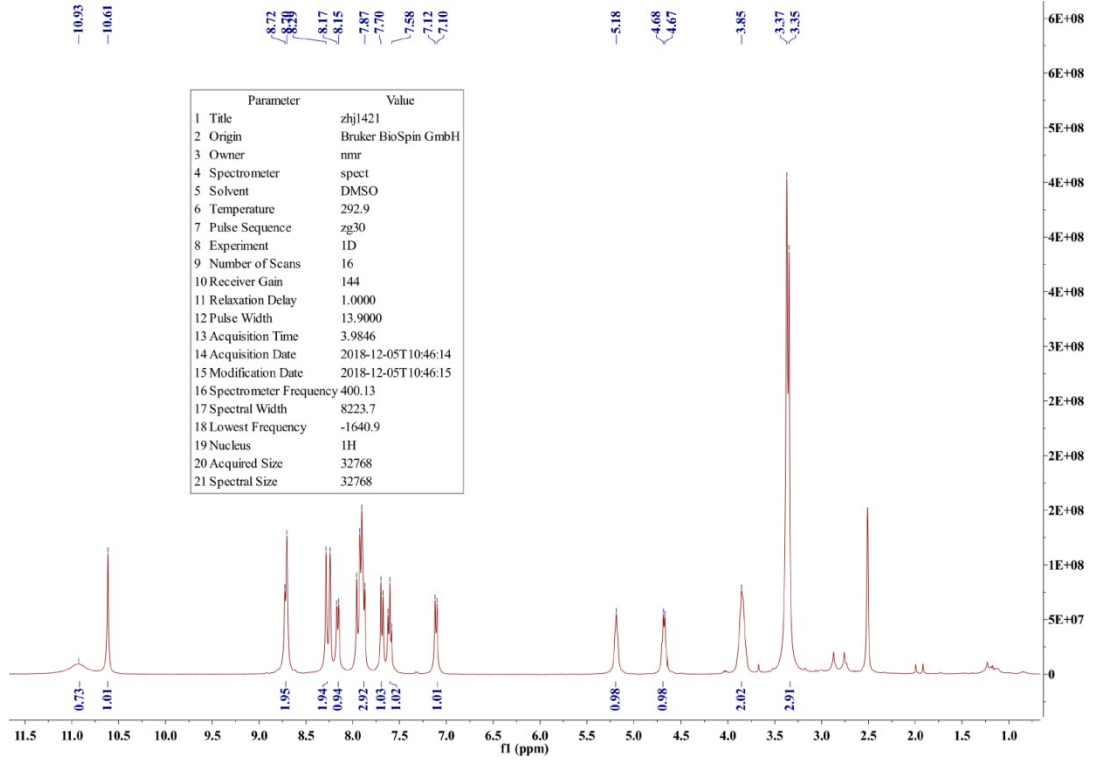
Channel name: 2: Average Time 0.1460 min : TOF MS (50-3000) 6eV ESI+ : Combined



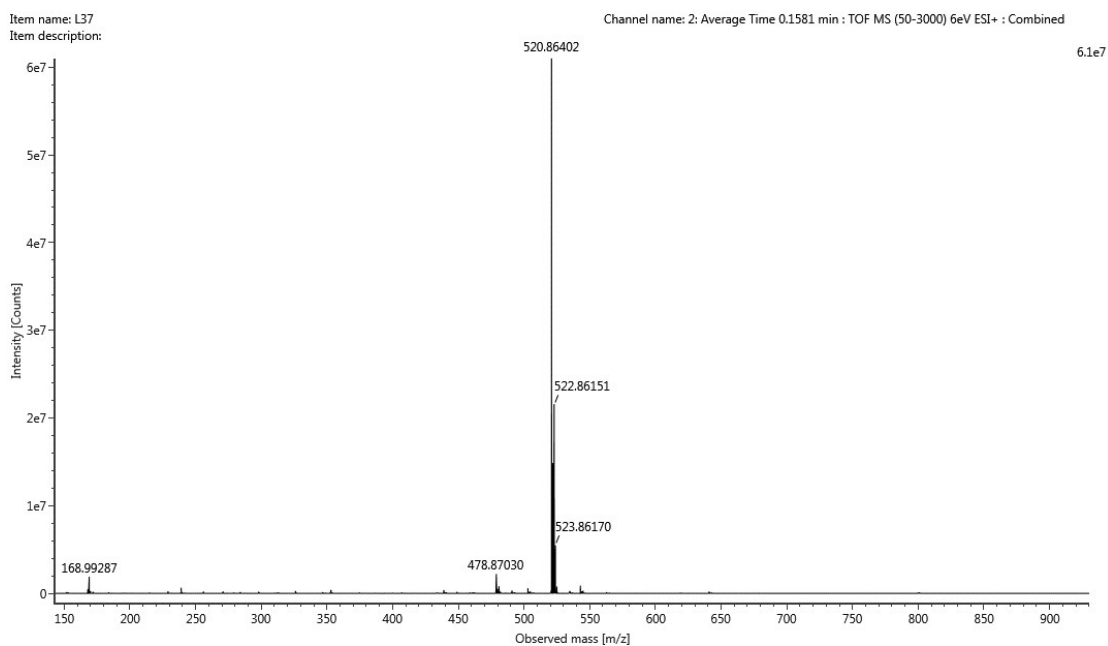
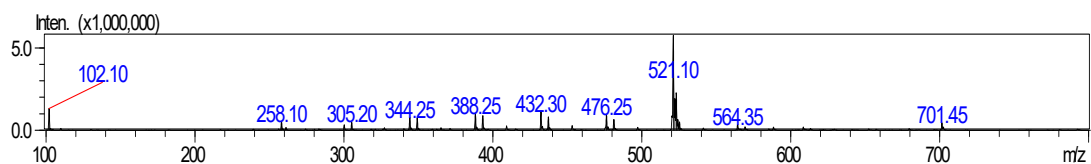
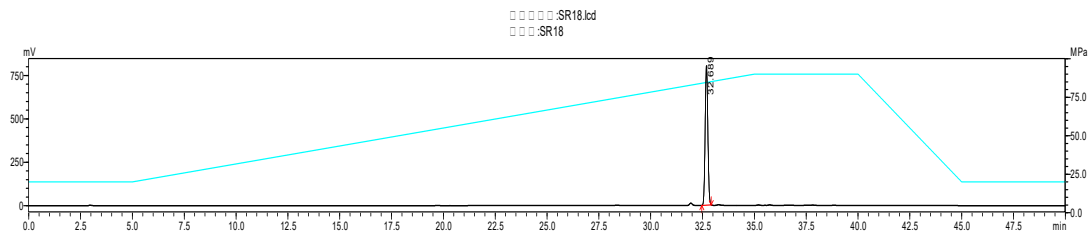
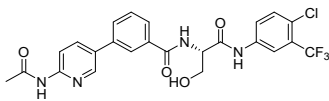


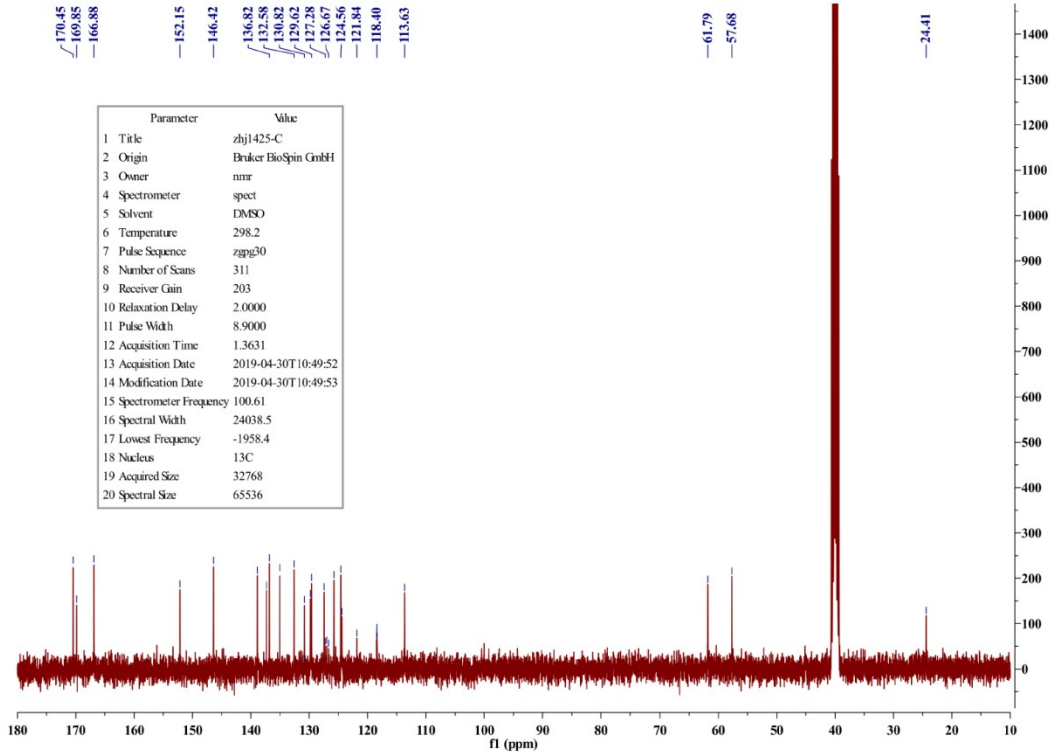
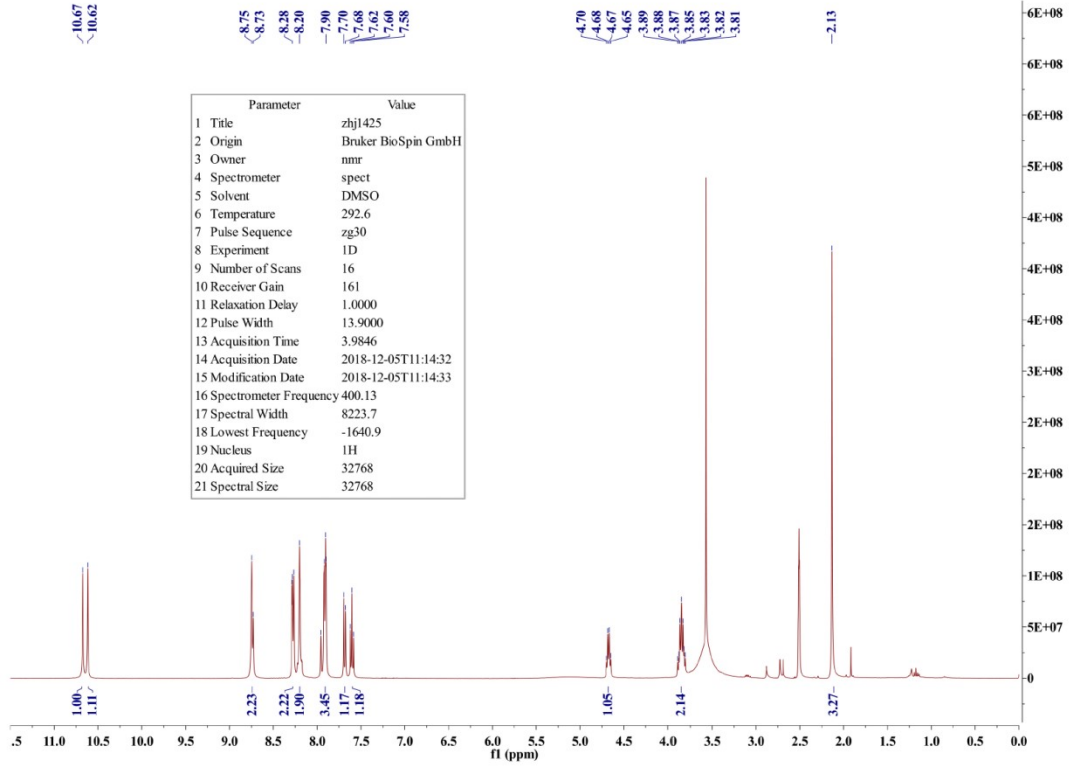
(S)-N-(1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3-hydroxy-1-oxopropan-2-yl)-3-(6-(methylsulfonamido)pyridin-3-yl)benzamide (SR9)



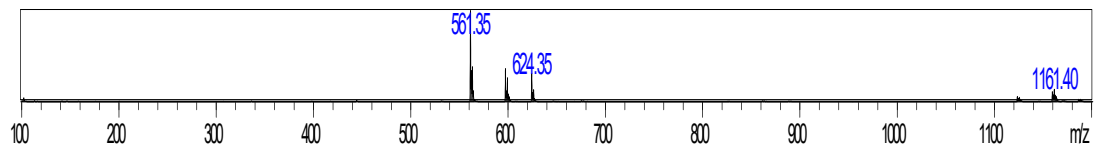
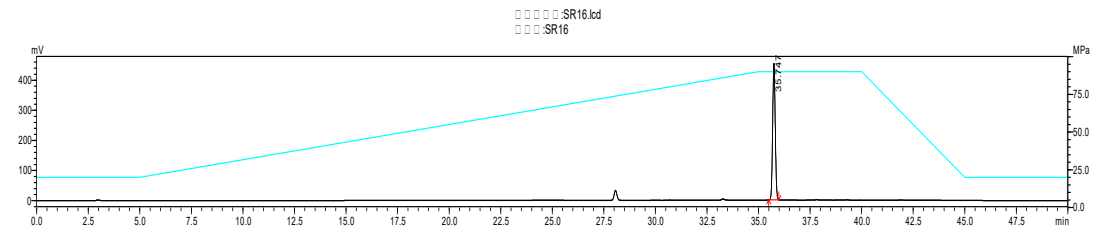
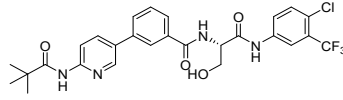


(S)-3-(6-acetamidopyridin-3-yl)-N-(1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3-hydroxy-1-oxopropan-2-yl)benzamide (SR10)



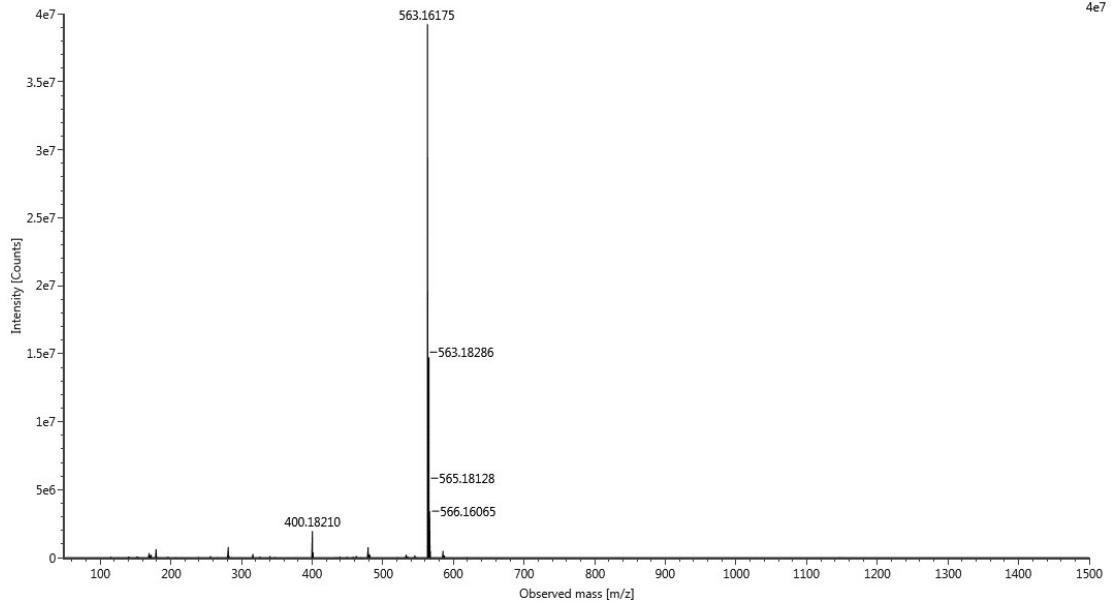


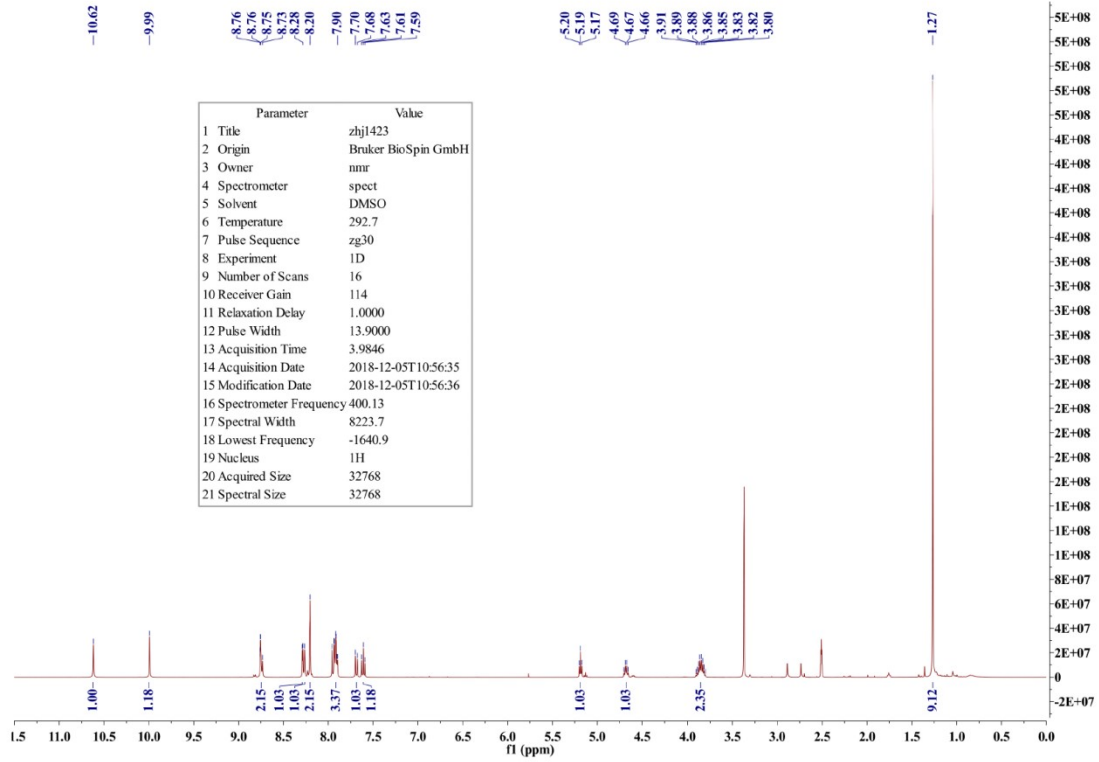
(S)-N-(1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3-hydroxy-1-oxopropan-2-yl)-3-(6-pivalamidopyridin-3-yl)benzamide (SR11)



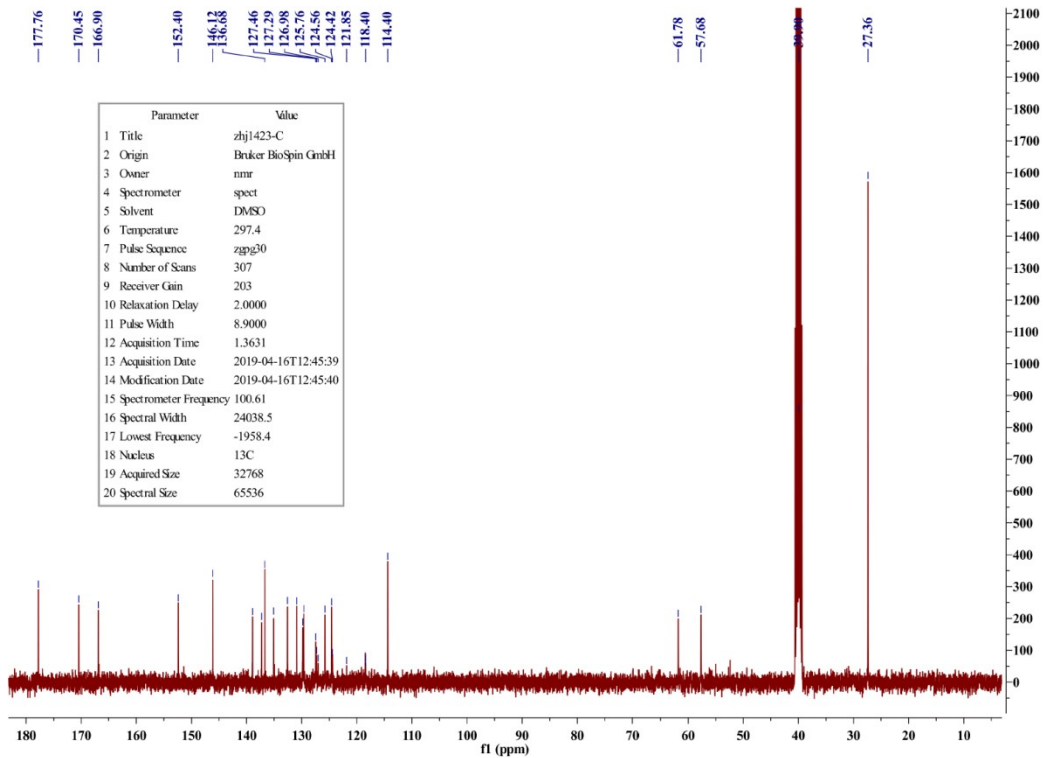
Item name: L-30
Item description:

Channel name: 2: Average Time 0.2845 min : TOF MS (50-1500) 6eV ESI+ : Combined



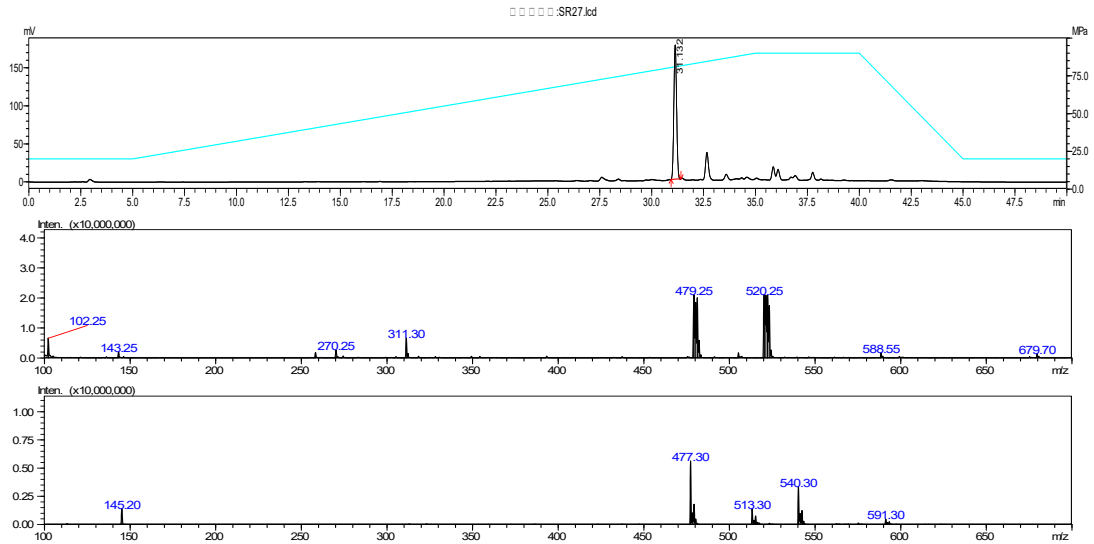
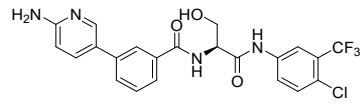


Parameter	Value
1 Title	zhj1423
2 Origin	Bruker BioSpin GmbH
3 Owner	nmr
4 Spectrometer	spect
5 Solvent	DMSO
6 Temperature	292.7
7 Pulse Sequence	zg30
8 Experiment	1D
9 Number of Scans	16
10 Receiver Gain	114
11 Relaxation Delay	1.0000
12 Pulse Width	13.9000
13 Acquisition Time	3.9846
14 Acquisition Date	2018-12-05T10:56:35
15 Modification Date	2018-12-05T10:56:36
16 Spectrometer Frequency	400.13
17 Spectral Width	8223.7
18 Lowest Frequency	-1640.9
19 Nucleus	1H
20 Acquired Size	32768
21 Spectral Size	32768



Parameter	Value
1 Title	zhj1423-C
2 Origin	Bruker BioSpin GmbH
3 Owner	nmr
4 Spectrometer	spect
5 Solvent	DMSO
6 Temperature	297.4
7 Pulse Sequence	zgpg30
8 Number of Scans	307
9 Receiver Gain	203
10 Relaxation Delay	2.0000
11 Pulse Width	8.9000
12 Acquisition Time	1.3631
13 Acquisition Date	2019-04-16T12:45:39
14 Modification Date	2019-04-16T12:45:40
15 Spectrometer Frequency	100.61
16 Spectral Width	24038.5
17 Lowest Frequency	-1958.4
18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536

(S)-3-(6-aminopyridin-3-yl)-N-(1-((4-chloro-3-(trifluoromethyl)phenyl)amino)-3-hydroxy-1-oxopropan-2-yl)benzamide (SR12)



Item name: L7
Item description:

Channel name: 2: Average Time 0.1632 min : TOF MSe (50-2000) 6eV ESI+ : Combined

1.94e7

