Electronic Supplementary Material (ESI) for New Journal of Chemistry.

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#### Supporting Information

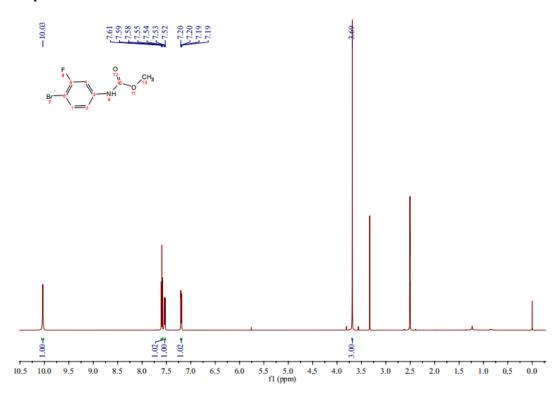
Design, synthesis and antibacterial evaluation of a novel series of biaryloxazolidinone derivatives against antibiotic-susceptible and antibiotic-resistant Gram-positive bacteria

Yinliang Qi <sup>a</sup>, Xiudong Ding <sup>b</sup>, Kun Wang <sup>a</sup>, Pinzhen Yan <sup>a</sup> Xinxin Guo <sup>a</sup>, Shiwei Ma <sup>a</sup>, Mingfei Xiao <sup>a</sup>, Pengrui Sun <sup>b</sup>, Siyu Liu <sup>a</sup>, Yunlei Hou <sup>a</sup>, \*, Yanfang Zhao <sup>a</sup>, \*

- <sup>a</sup> School of Pharmaceutical Engineering, Shenyang Pharmaceutical University, 103 Wenhua Road, Shenhe District, Shenyang, Liaoning, 110016, China.
- <sup>b</sup> Department of Clinical Laboratory, The Eighth Medical Center of PLA General Hospital, Beijing 100091, China

#### 1. <sup>1</sup>H-NMR Spectra

#### Compound 9

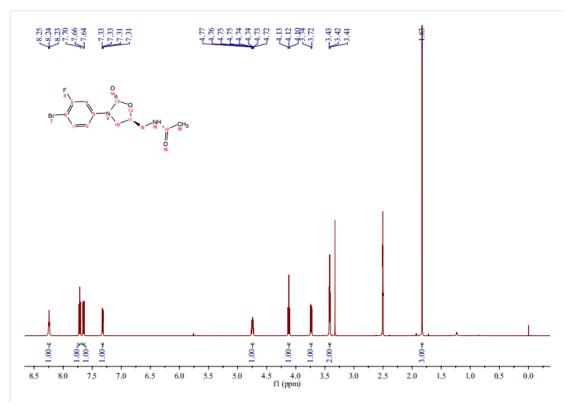


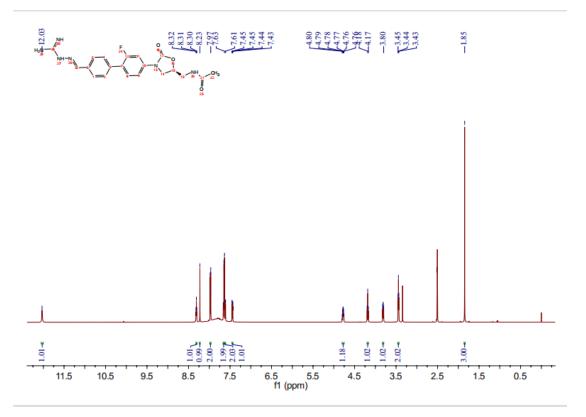
# Compound 10

E-mail addresses: houyunlei901202@163.com (Y. Hou), yanfangzhao@126.com (Y. Zhao).

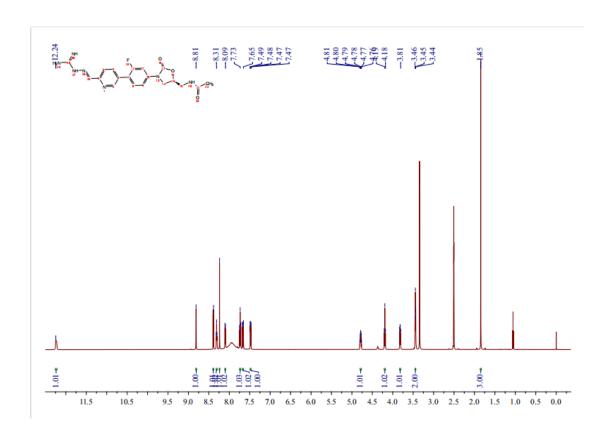
<sup>\*</sup> Corresponding author

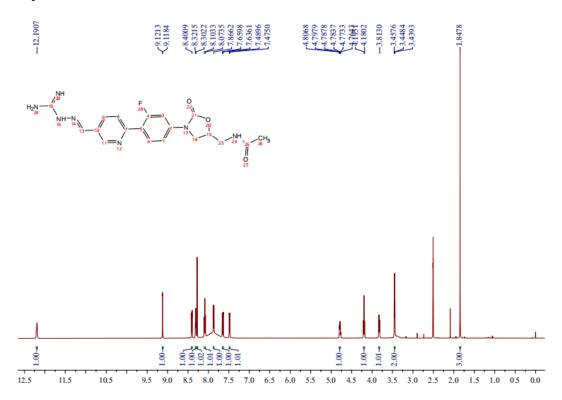
<sup>\*\*</sup> Corresponding author

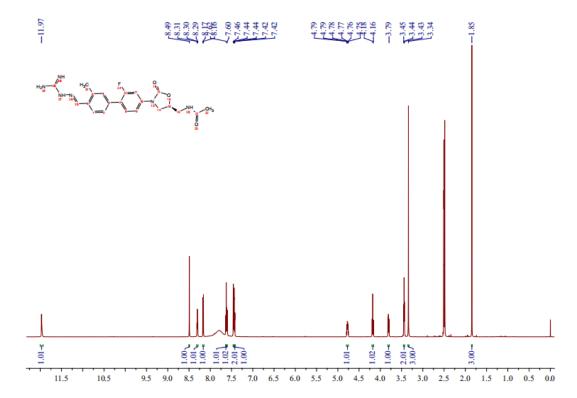


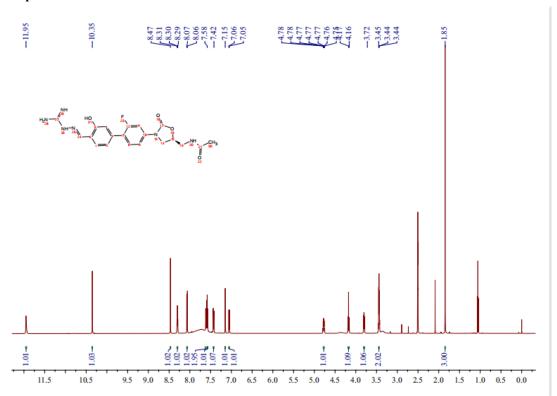


Compound 13a-2

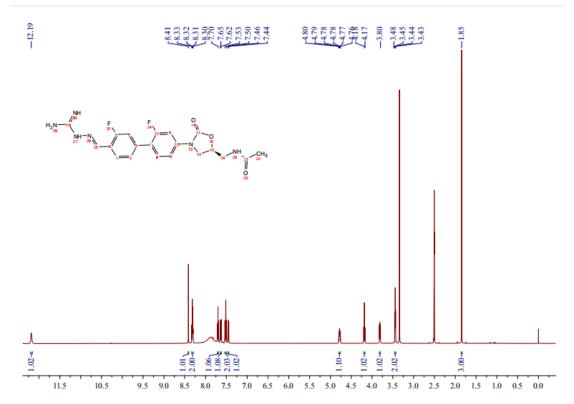


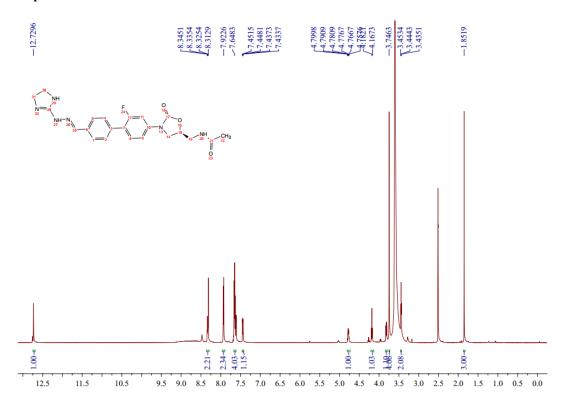




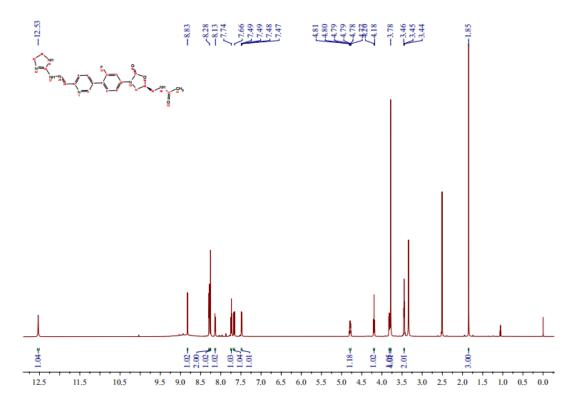


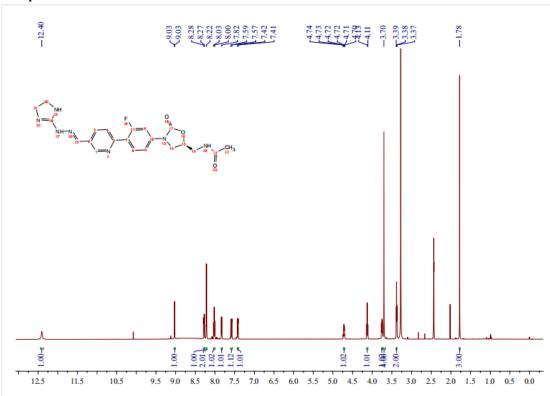
Compound 13a-6



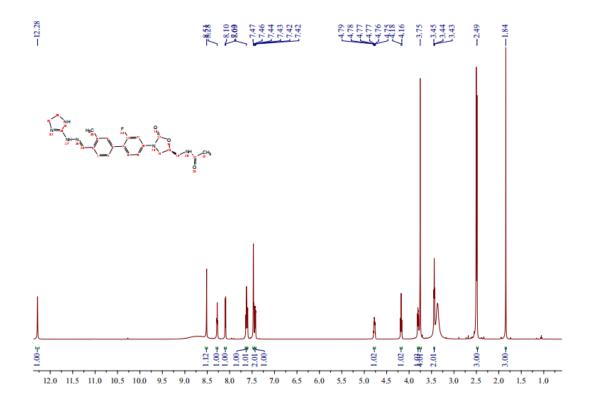


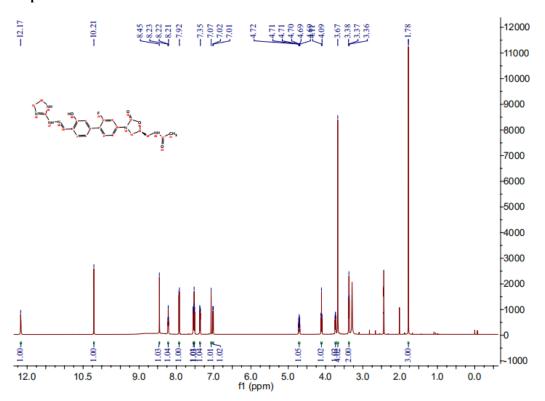
Compound 13b-2



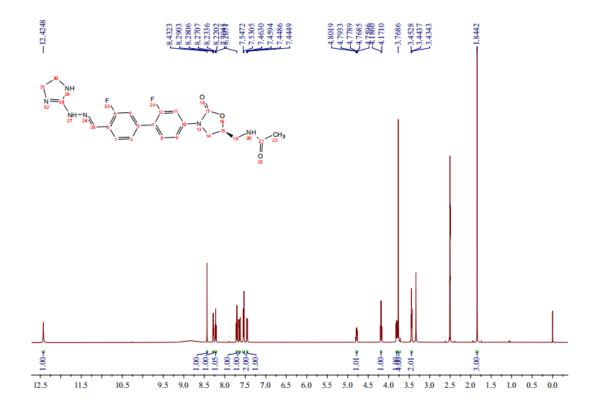


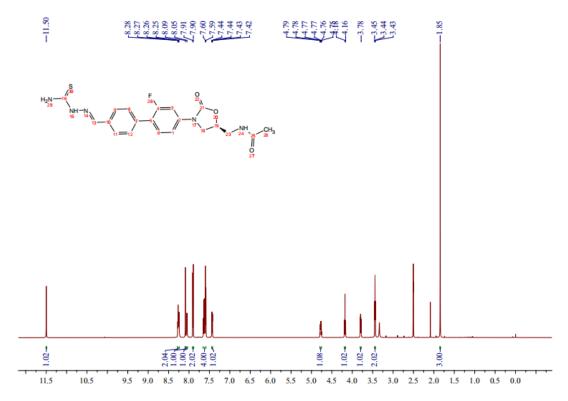
Compound 13b-4



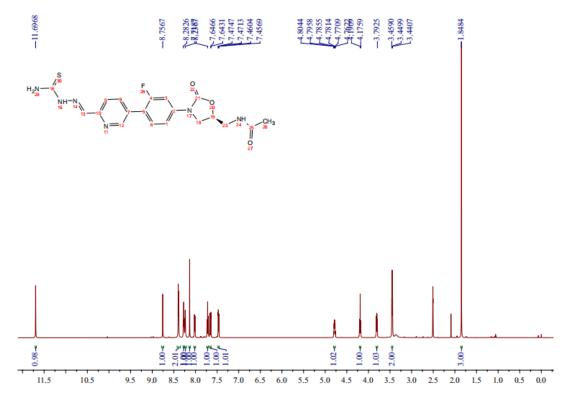


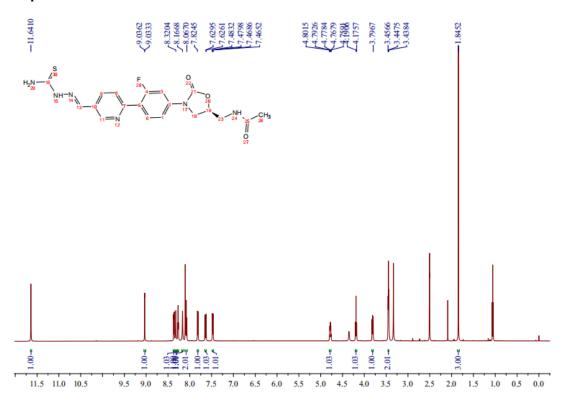
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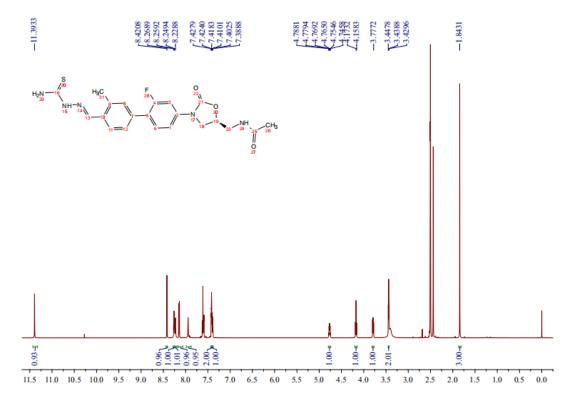


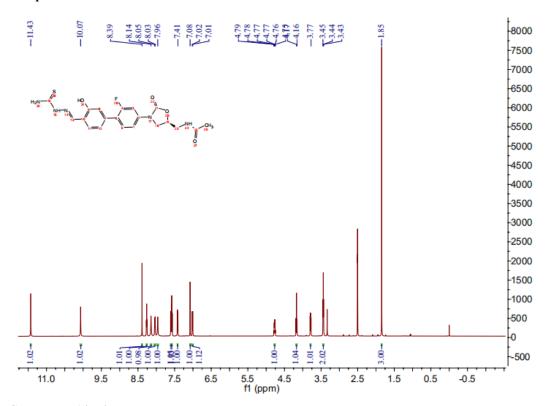
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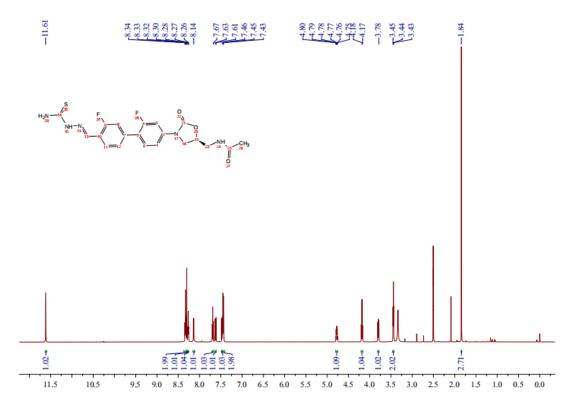


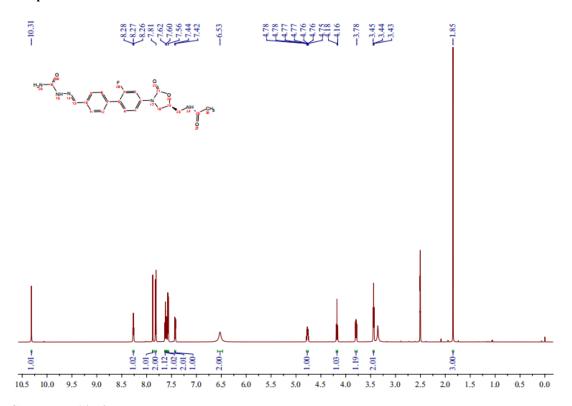
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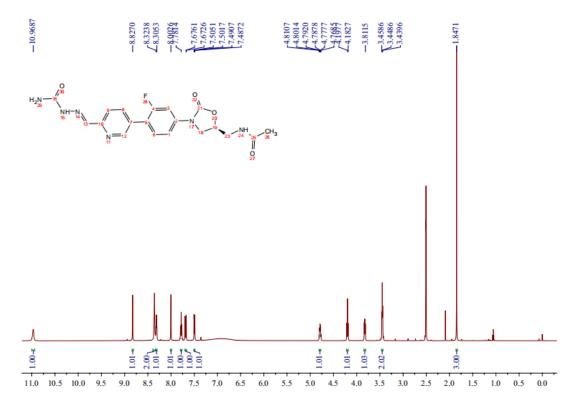


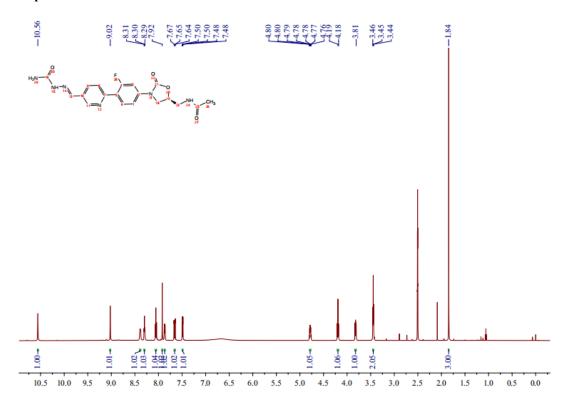
Compound 14a-6



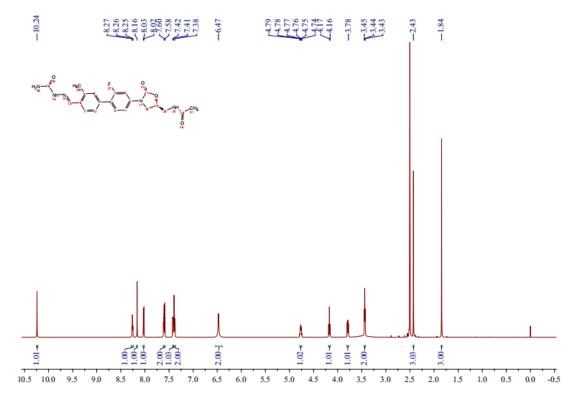


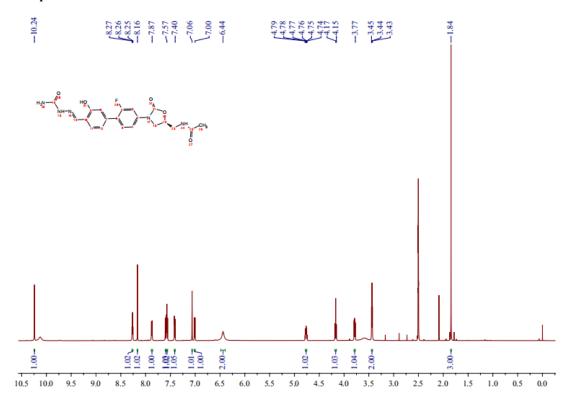
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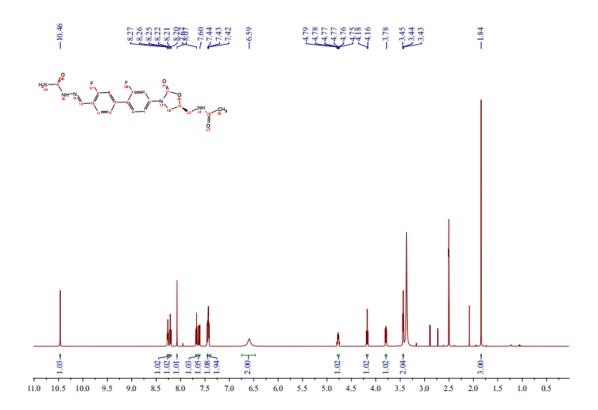


Compound 14b-4

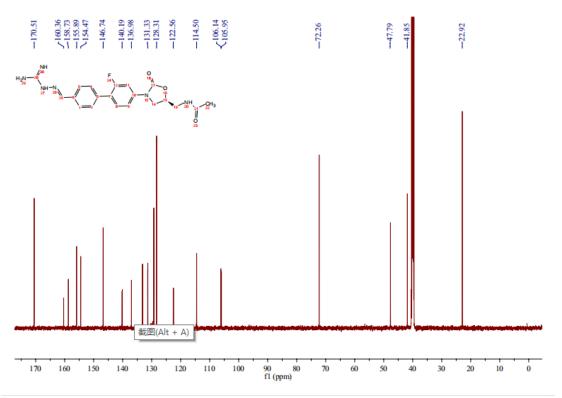




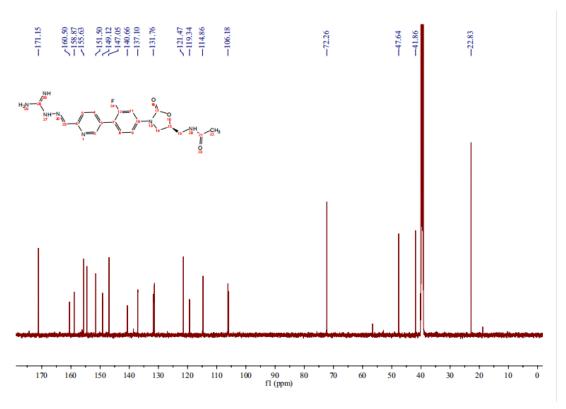
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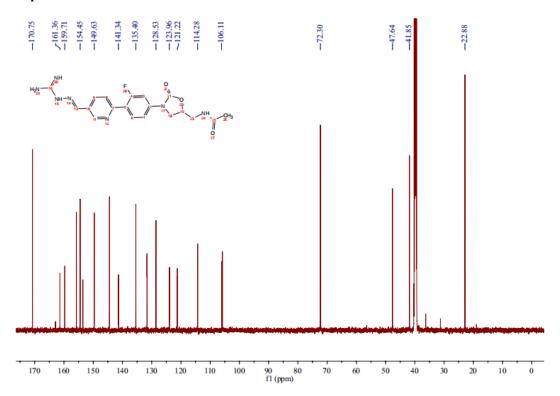


# 2. <sup>13</sup>C-NMR Spectra

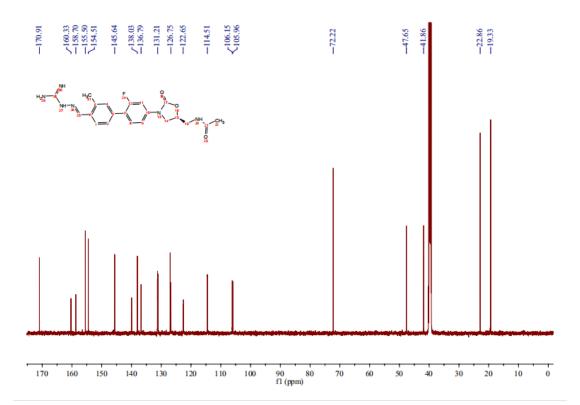


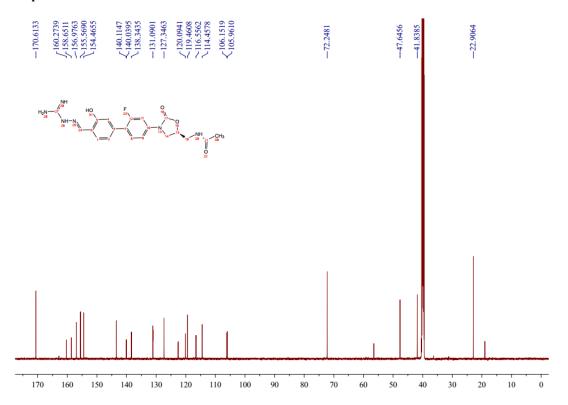
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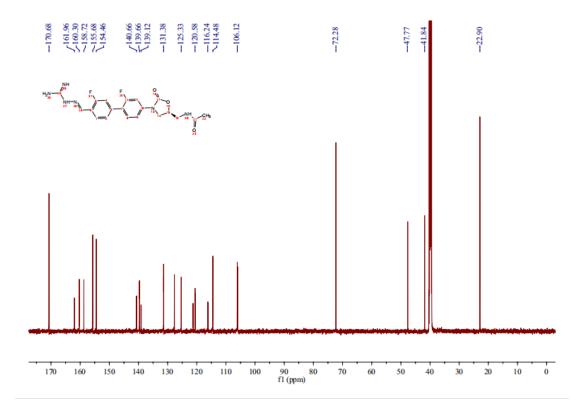


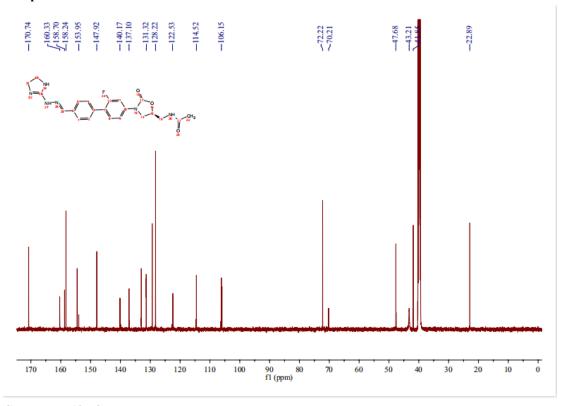
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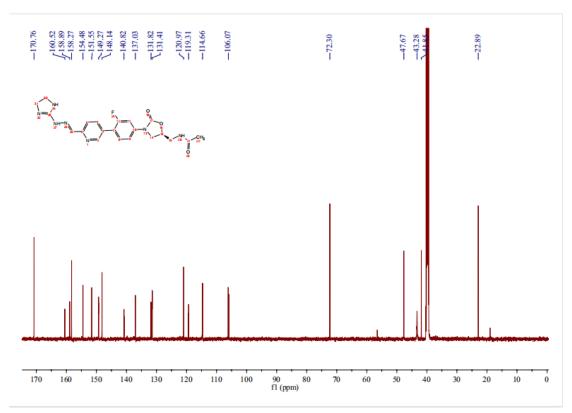


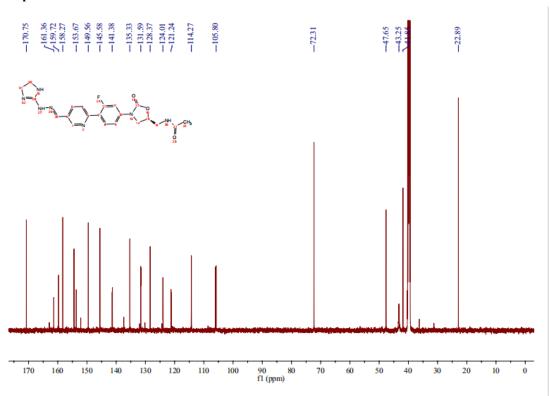
Compound 13a-6



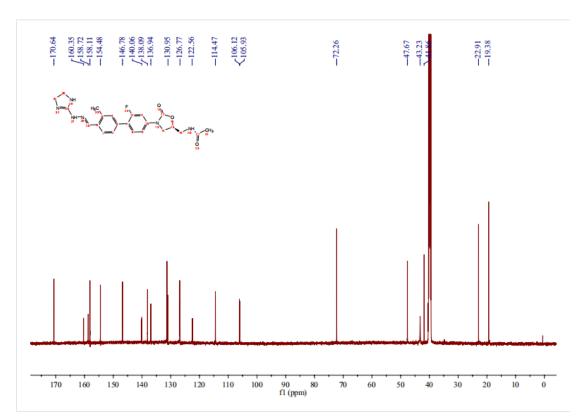


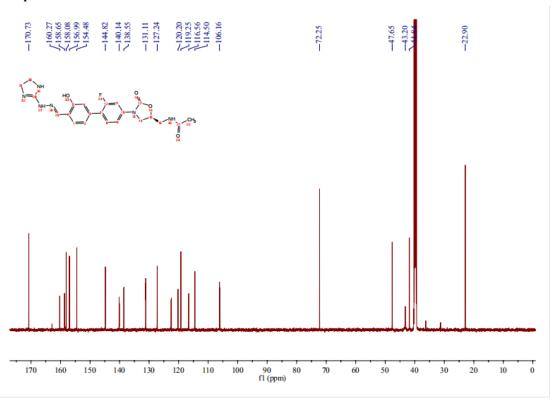
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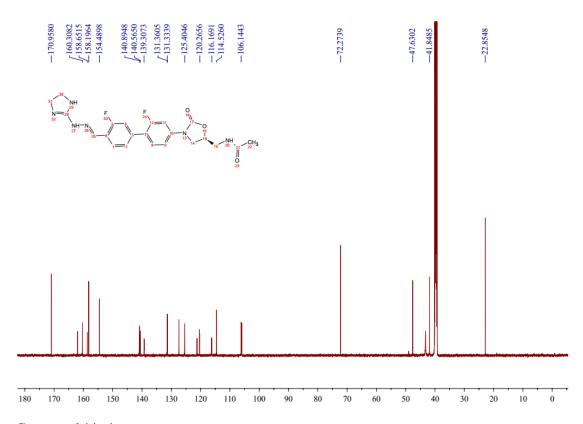


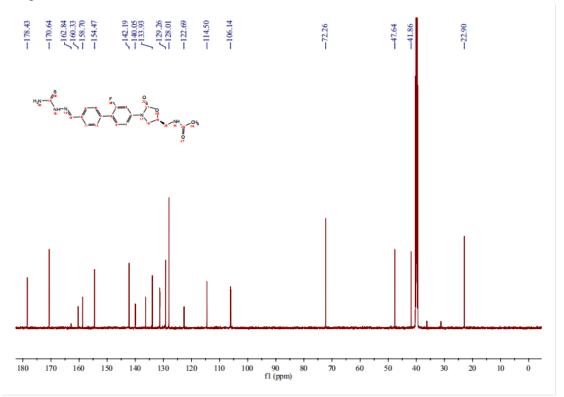
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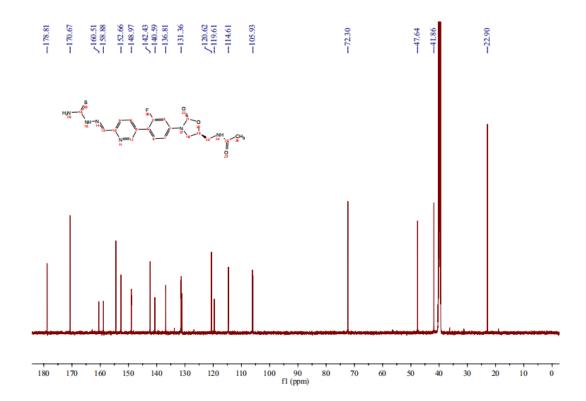


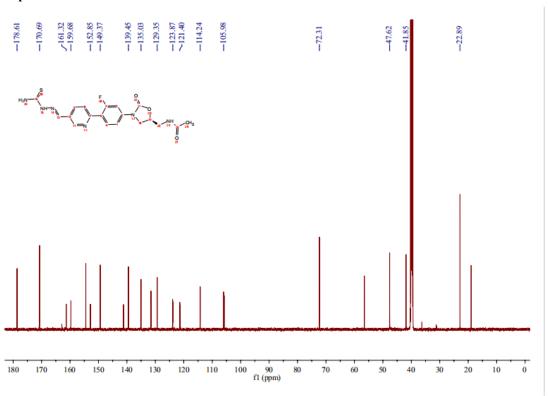
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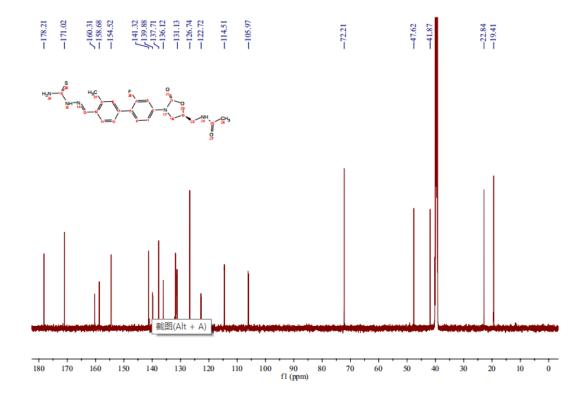


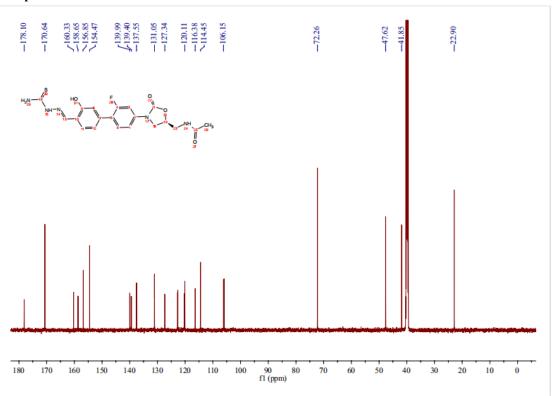
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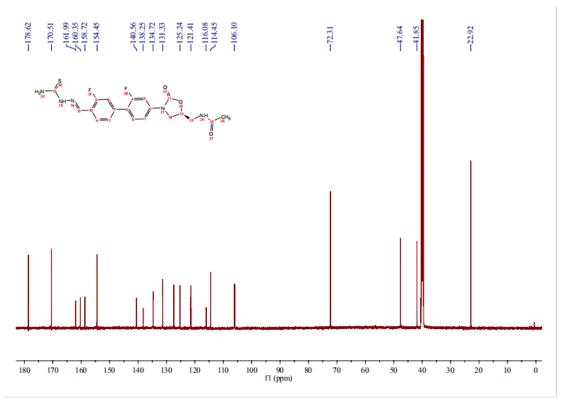


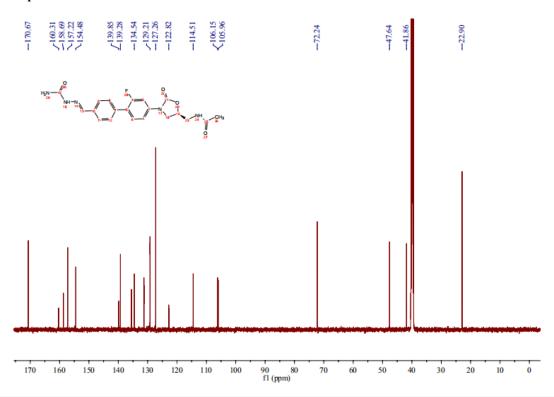
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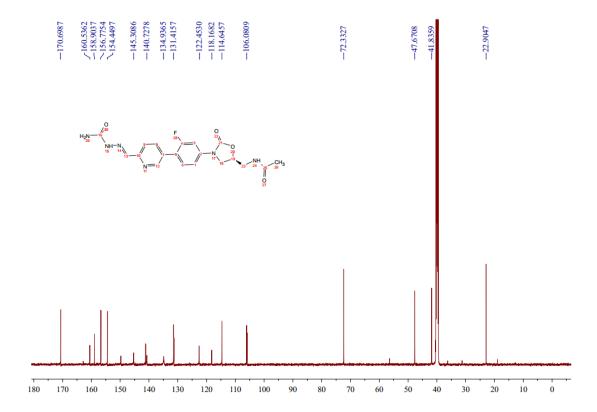


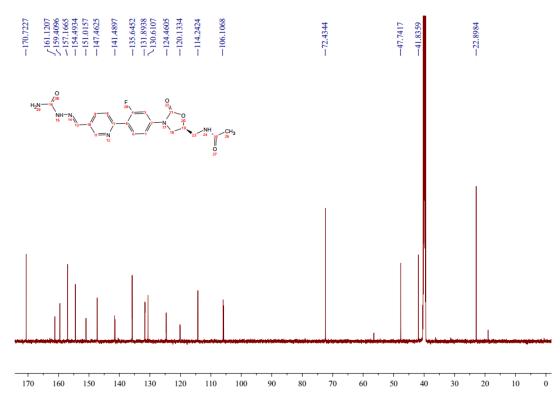
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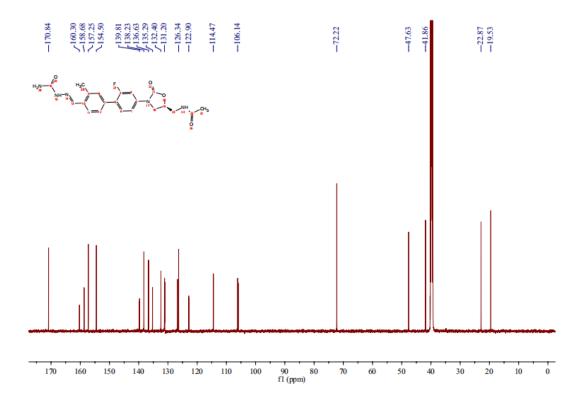


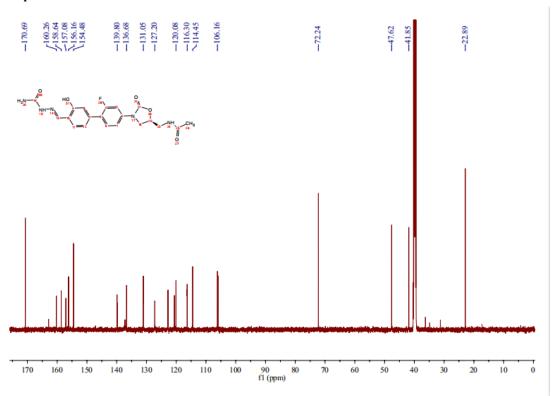
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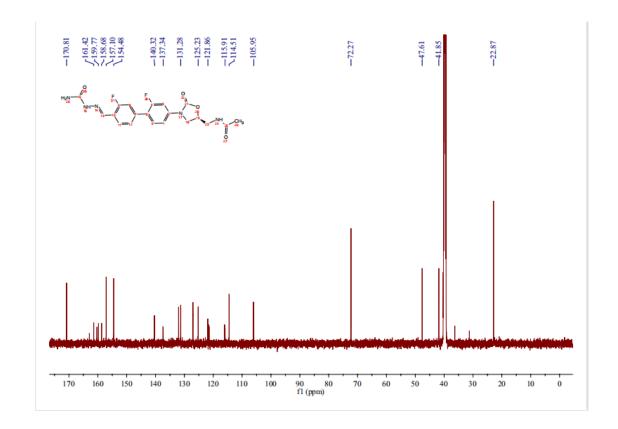


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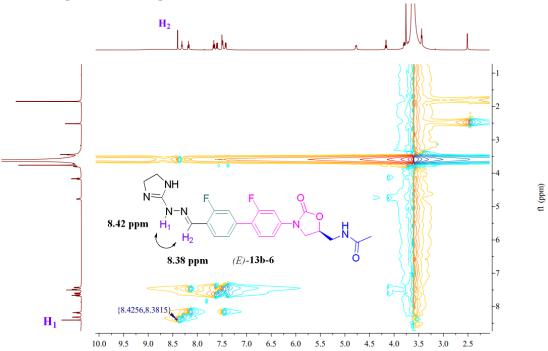




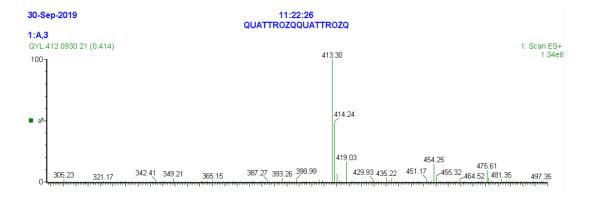
Compound 14b-6

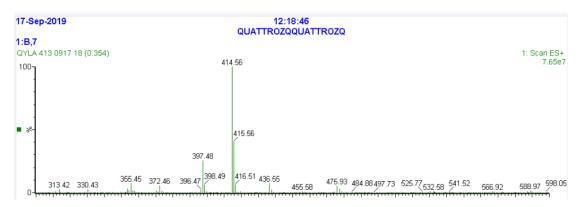


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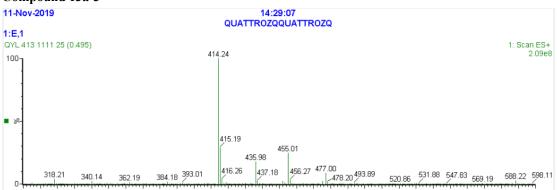


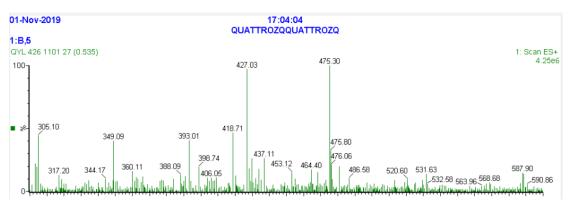
4.MS spectrum Compound 13a-1

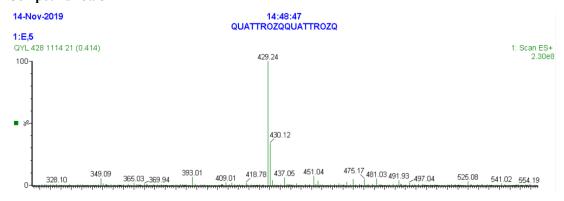




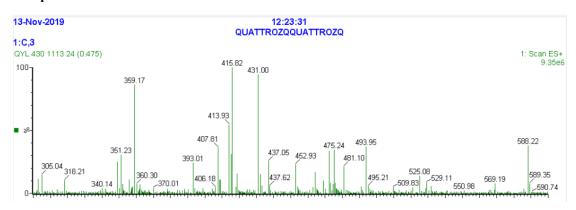
## Compound 13a-3



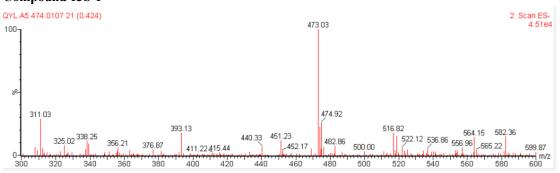


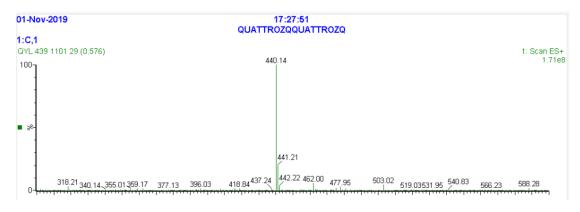


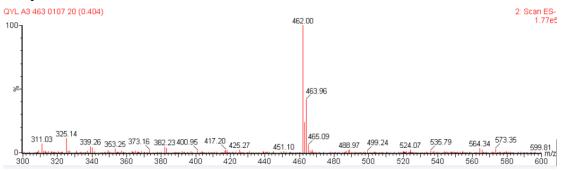
#### Compound 13a-6



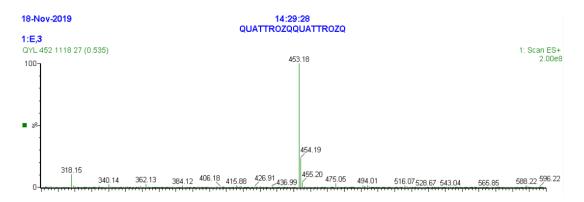
## Compound 13b-1



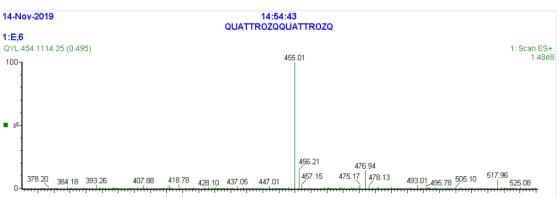




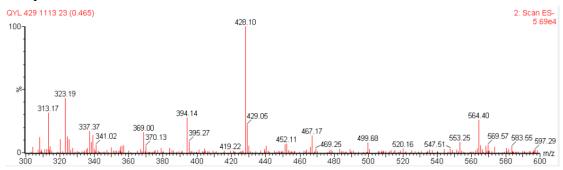
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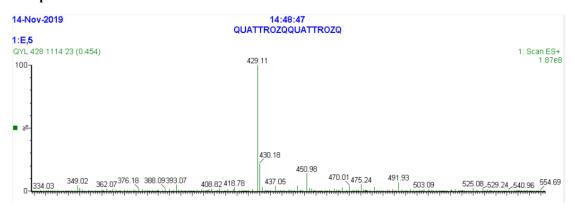
# Compound 13b-5



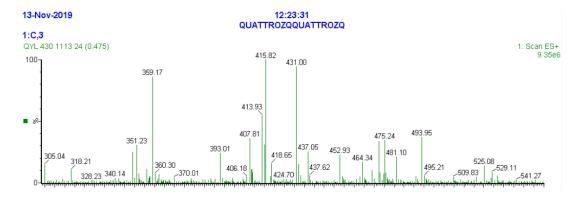


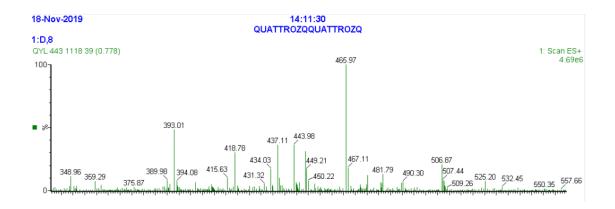


#### Compound 14a-2

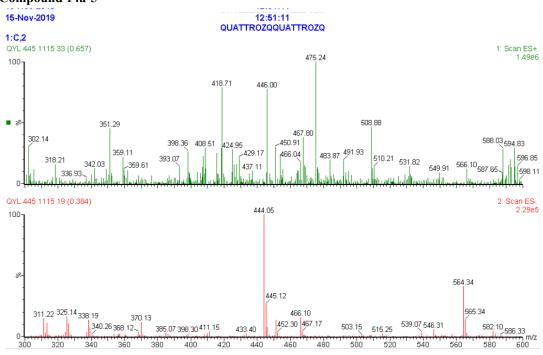


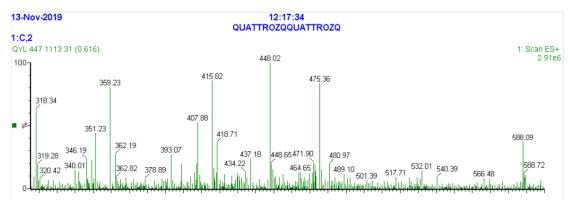
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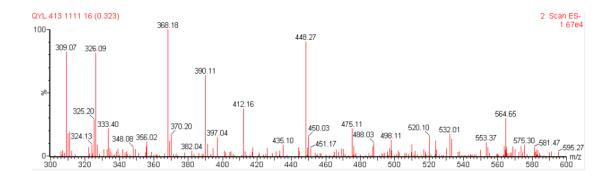


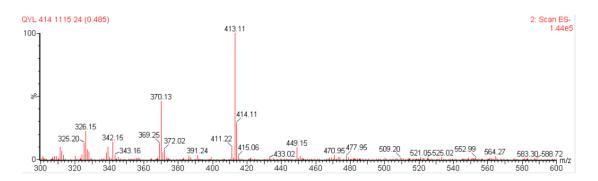




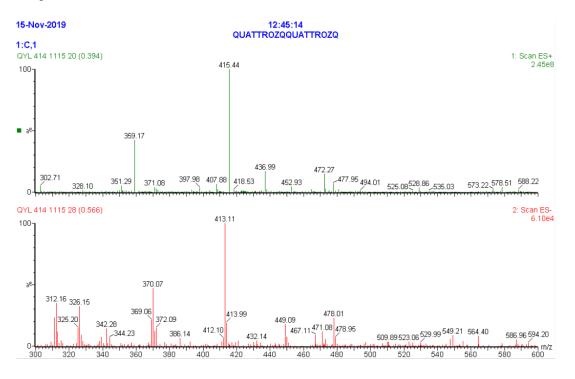


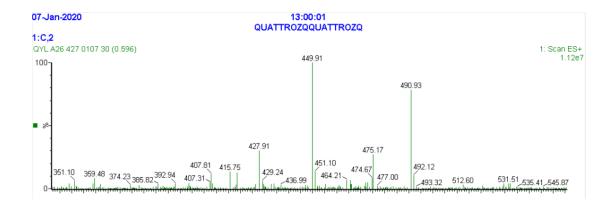


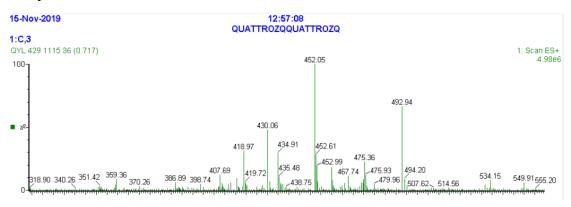


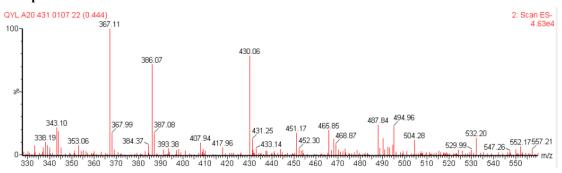


#### Compound 14b-3









# **Qualitative Analysis Report**

Data Filename **Instrument Name** 

Sample Type

13A1.d Sample Instrument 1

13A1 Sample Name Position P1-D6

User Name

12/18/2021 9:07:13 AM

Acq Method **IRM Calibration Status** 

ZHENG100-1000.m Success

**Acquired Time** DA Method

20170311.m

Comment

Sample Group

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

Acquisition SW Version

#### **User Spectra**

Frag	mentor Voltage 200	Collision Energy	Jy Ionization N ESI	lode	
0 6	+ESI Scan (0.		/ 13A1.d Subtract 1750 N6 O3]+H)+		
1.5		([C2011211	No cojy		
25					The second secon
1-		4-45,000			
75-					Park 11 - Property like the park of the pa
0.5 25	130.1592	363.1577	500.2316	701.4950	847.3248

Peak	Hick	

m/z	z Abund		Formula	Ion	
363.1577	. 1	198729.25			
381.168	1	83921.41	Security of the Security	and the	
413.175	1	1737364.88	C20 H21 F N6 O3	(M+H)+	
414,1783	1	405704.5	C20 H21 F N6 O3	(M+H)+	
415.1801	1	49235.4	C20 H21 F N6 O3	(M+H)+	
435.1572	1	189675.69			
701.495	1	60968.27			
825.3427	1	79738.38			
847.3248	1	96803.23			
890.4175	1	63313.89			

Formula Calculator Element Limits

Element	MIN	мах
C	3	60
Н		120
0	160 00	. 30
N	0	30
E	1	1

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C20 H21 F N6 O3 ;	FALSE	412.1678	412.1659	-4.57	C20 H22 F N6 O3	91.32
CZU TIZZ T TIO OS TI						

<sup>---</sup> End Of Report ---

Printed at: 1:09 PM on: 12/18/2021

# **Qualitative Analysis Report**

Data Filename

Sample Type

13A2.d Sample Sample Name Position

P1-D7

**Instrument Name** 

Acq Method **IRM Calibration Status**  Instrument 1 ZHENG100-1000.m

**User Name Acquired Time** DA Method

12/18/2021 9:10:09 AM 20170311.m

Success

Comment

Sample Group

Acquisition SW Version

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

#### **User Spectra**

Frag	mentor \ 200	/oltage	Collision Energy 0	Ion	ization Mode ESI			
10 6	+ESI S	can (0.120	min) Frag=200.0V	13A2.d Sub	tract			
2-			414.1 ([C19 H20 F <sub>i</sub>		53.00 A 17 Y			
1.5-								
0.5	134.11	173	363.1572	500.230	2	701.4948	849.3145	

#### Peak List

m/z	Z	Abund	Formula	Ion
363.1572	1	153184.36		1.
381.1668	1	58807.92	A STATE OF THE STA	4.30 613.2
414.1697	1	1902151.25	C19 H20 F N7 O3	(M+H)+
415.1728	1	432729.94	C19 H20 F N7 O3	(M+H)+
436.1521	1	362744.38		
437.1554	1	75795.52		2 1
701.4948	1	63117.52		The Section
849.3145	1	179315.47		1
850.316	1	77845.45		11 11
985,7147	1	87618.44		127

Formula Calculator Element

Fleurenc	1-11-1	
С	3	60
Н	0	120
0	0	30
N	0	30
-	1	1

Formula Calculator Results

Formula	Best	Mass	Tyc mass	Dili (ppili)	zon species	30010
C19 H20 F N7 O3	TRUE	413.1625	413.1612	-3.1	C19 H21 F N7 O3	95.59

<sup>---</sup> End Of Report ---

Printed at: 1:11 PM on: 12/18/2021

# **Qualitative Analysis Report**

Data Filename

Sample Type

13A3.d Sample

Success

Sample Name Position

13A3 P1-D8

Instrument Name

Acq Method IRM Calibration Status Instrument 1 ZHENG100-1000.m User Name Acquired Time

12/18/2021 9:13:05 AM

DA Method 20170311.m

Comment

Sample Group

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

## User Spectra

rag	mentor Voltage 200	Collision Energy 0	Ionization Mode ESI		
6	+ESI Scan (0.119	min) Frag=200.0V 13A	3.d Subtract	***	
5-		414.1696 ([C19 H20 F <sub>N</sub> 7 C			
5-					
5-					849.3163
5					
5-	134.1173	363.1572	588.4084	701.4944	927.6607

Peak List m/z	Z	Abund	Formula	Ion
363.1572	1	114615.47		
414.1696	1	1763697.63	C19 H20 F N7 O3	(M+H)+
415.1732	1	390626.94	C19 H20 F N7 O3	(M+H)+
436.1522	1	483977.97	19 15 7511	16 600
437.1559	1	99911.38	118 1915 (3)	11.19.
701.4944	1	64110.41		
827.3321	1	135149.81		
849.3163	1	688056.5		
850.3187	1	318098.16		
851.3188	1	70966.66		

Formula Calculator		7.454	Tak Mass	Diff (ppm)	Ion Species	Score
Formula	Best	Mass	Tgt Mass			_
C19 H20 F N7 O3	TRUE	413.1625	413.1612		3.12 C19 H21 F N7 O3	94.65

<sup>---</sup> End Of Report ---

Printed at: 1:12 PM on: 12/18/2021

Data Filename Sample Type Instrument Name 13A4.d Sample

Sample Name 1

13A4 P1-D9

Acq Method IRM Calibration Status Instrument 1 ZHENG100-1000.m Success User Name Acquired Time

12/18/2021 9:16:02 AM

DA Method 20170311.m

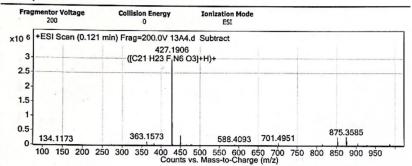
Comment

Sample Group Acquisition SW Version

Info.

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

#### **User Spectra**



Peak List

m/z	Z	Abund	Formula	Ion
363.1573	1	111885.45		
427.1906	1	2973149.75	C21 H23 F N6 O3	(M+H)+
427.3464		200681.03		
428.1942	1	757066.56	C21 H23 F N6 O3	(M+H)+
429.1959	1	97924.82	C21 H23 F N6 O3	(M+H)+
449.173	1	319175.38		
853.3757	1	268360.16		
854.3769	1	127333.49		
875.3585	1	279387.84		
876.36	1	136366.22	The second second second	

070.50			,00,22	
Formula Ca	alculator	Ele	ement Li	mits
Element	Min		Max	]
С		3	60	
Н		0	120	
0	11 350	0	30	
N .		0	30	
F		1	1	

Formula Calculator	or Results					
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C21 H23 F N6 O3	FALSE	426.1835	426.1816	-4.45	C21 H24 F N6 O3	91.32

<sup>---</sup> End Of Report ---

Printed at: 1:13 PM on: 12/18/2021

Data Filename Sample Type **Instrument Name** 

13A5.d Sample Instrument 1 Sample Name Position **User Name Acquired Time** 

DA Method

13A5

**Acq Method IRM Calibration Status**  ZHENG100-1000.m Success

12/18/2021 9:18:56 AM 20170311.m

Comment

Sample Group Acquisition SW Version

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

### User Spectra

Frag	mentor Voltage 200	Collision Energy 0	Ionization Mo ESI	de	
0 6	+ESI Scan (0.122	min) Frag=200.0V 13	A5.d Subtract		
1.2		429.17 ([C20 H21 F N			
0.8			1 1		
0.4	134.1174	363.1579	517.3726	701.4962	879.3169

m/z	Z	Abund	Formula	Ion
363.1579	1	79253.57		
429.171	1	1243426.88	C20 H21 F N6 O4	(M+H)+
429.3247	1	97262.33		1-
430.174	1	282953.06	C20 H21 F N6 O4	(M+H)+
451.153	1	328334.16		
452.1545	1	68005.76		
701.4962	1	63157.16		
857.333	1	70285.61		
879.3169	1	206611.66		
880.3186	1	94164.09		

Formula Calculator Element Limits
Element Min Max

Liement	1.1111	1144
С	3	60
Н	0	120
0	. 0	30
N	0	30
F	1	1

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C20 H21 F N6 O4	FALSE	428.1638	428.1608	-6.85	C20 H22 F N6 O4	82.4

<sup>---</sup> End Of Report ---

Printed at: 1:14 PM on: 12/18/2021

Data Filename Sample Type

13A6.d Sample Sample Name

13A6 P1-E2

**Instrument Name** 

Instrument 1

Position **User Name** 

DA Method

12/18/2021 9:21:53 AM

**Acq Method** IRM Calibration Status ZHENG100-1000.m

**Acquired Time** 

Comment

Success

20170311.m

Sample Group

Info.

Acquisition SW Version

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

#### **User Spectra**

Frag	mentor Ve	oltage	Collision Energy 0		Ionization Mode ESI			
0 6	+ESI Sc	an (0.117 m	min) Frag=200.0V 13A6.d Subtract					
2.5	1		431. ([C20 H20 F	.1660 2 N6 O	3]+H)+			
2-								
1.5								
1	1							
0.5	134.11	73	363.1575	1	588.4094	701.4959	861.3251	

m/z	Z	Abund	Formula	Ion
363.1575	1	81944.73	5	
431.166	1	2232066.75	C20 H20 F2 N6 O3	(M+H)+
432.1696	1	536882.81	C20 H20 F2 N6 O3	(M+H)+
433.1756	1	66417.86	C20 H20 F2 N6 O3	(M+H)+
453.1483	1	230929.38		
861.3251	1	163516.08		
862.3271	1	70253.58	A	

Elamont	Min	May
Formula Ca	culat	or Element Limit
986.7189		75622.13
985.7164	1	117258.66
883.3073	1	110482.97

Element	Litte	MAX
С	3	60
Н	0	120
0	0	30
N	0	30
F	2	2
Formula Ca	Iculator Re	sults

	) Ion Species	t Mass	Mass	Best	Formula
2 N6 O3 85.83	-5.76 C20 H21 F2 N6	430.1565	430.159	FALSE	C20 H20 F2 N6 O3
<u> </u>	-3.70 020 1121	430.1303	430.159	FALSE	C20 H20 F2 N6 O3

--- End Of Report ---

Printed at: 1:15 PM on: 12/18/2021

Data Filename

13B1.d Sample Sample Name Position

13B1 P1-E3

Sample Type **Instrument Name** 

User Name Acquired Time DA Method

12/18/2021 9:24:50 AM

Acq Method

Instrument 1 ZHENG100-1000.m Success

20170311.m

**IRM Calibration Status** Comment

Sample Group

Info.

Acquisition SW Version

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

#### User Spectra

agmentor Voltage 200	Collision Energy 0	1	Ionization Mode ESI			
6 +ESI Scan (0.114	4 min) Frag=200.0V 1		Subtract			
5-	([C22 H23 F	1897 N6 O3]	+H)+			-
					877.	3734
134.1165 231.1	588 363,1557		588.4076	701.4932	814.5773	

m/z	Z	Abund	Formula	Ion
439.1897	1	3637362.75	C22 H23 F N6 O3	(M+H)+
440.1929	1	997847.75	C22 H23 F N6 O3	(M+H)+
441.1998	1	222824.33	C22 H23 F N6 O3	(M+H)+
461.1722	1	284863.44		7 - 7
462.1742	1	64856.43		-12
877.3734	1	1085296.88		7 1
878.3767	1	590897.81	100 100	
879.3806	1	200894.66		
899.3552	1	171019.92		
900.3566	1	86397.9		100

### Formula Calculator Element Limits

Element	Min	Max
С	3	60
Н	0	120
0	0	30
N	0	30
F	1	1

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C22 H23 F N6 O3	TRUE	438.1828	438.1816	-2.72	C22 H24 F N6 O3	92.44

<sup>---</sup> End Of Report ---

Printed at: 1:15 PM on: 12/18/2021

Data Filename Sample Type

13B2.d Sample

Sample Name 13B2 Position

**Instrument Name** Acq Method

Instrument 1 ZHENG100-1000.m **User Name Acquired Time** 

12/18/2021 9:27:46 AM

**IRM Calibration Status** 

Comment

DA Method Info.

20170311.m

Sample Group

Acquisition SW Version

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

#### **User Spectra**

Fragi	mentor Voltage 200	Collision Energy 0	Ionization Mode ESI		
_	+ESI Scan (0.114	min) Frag=200.0V 13B			
3- .5-		440.18 ([C21 H22 F N			
5-		1			
5-	134.1175	363.1565	517.3707	701.4933	901.3470

Peak List				
m/z	Z	Abund	Formula	Ion
440.1854	1	2718939.75	C21 H22 F N7 O3	(M+H)+
441.1892	1	700480.69	C21 H22 F N7 O3	(M+H)+
442.1906	1	90884.5	C21 H22 F N7 O3	(M+H)+
462.1678	1	562085.31		Printer V
463.1698	1	128785.03"		
879.3648	1	410518.78	. Pro Contract	
880.3671	1	202576.11		
901.347	1	424521.16		
902.3493	1	206448.8		
903.3498	1	50881.78		

Formula Calculator Element Limits

Element	Min		мах
С		3	60
Н	4 1175	0	120
0	0. 162	0	30
N		0	30
F straint		1	1
Formula Ca	lculator	Re	sults

Formula	Best	Mass . NOT	Tgt Mass	Diff (ppm)	Ion Species	Score
C21 H22 F N7 O3	FALSE	439.1784	439.1768	-3.51	C21 H23 F N7 O3	93.66

--- End Of Report ---

Printed at: 1:16 PM on: 12/18/2021

.... Data Filename

Sample Type

**Instrument Name** 

Acq Method **IRM Calibration Status** Comment

13B3.d Sample Instrument 1 Sample Name Position

**User Name Acquired Time** DA Method

12/18/2021 9:30:43 AM

20170311.m

P1-E5

Sample Group

Acquisition SW Version

Info. 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

ZHENG100-1000.m

#### **User Spectra**

200	Collision Energy 0	Ionization Mode ESI			
ESI Scan (0.125	min) Frag=200.0V 13	BB3.d Subtract			
1					
	([C21 H22 F	N7 O3]+H)+			
i de	363.1564	588 4092	701 4942	879.3657 819.2796	
		ESI Scan (0.125 min) Frag=200.0V 13 440. ([C21 H22 F	ESI Scan (0.125 min) Frag=200.0V 13B3.d Subtract 440.1861 ([C21 H22 F <sub>1</sub> N7 O3]+H)+	ESI Scan (0.125 min) Frag=200.0V 13B3.d Subtract 440.1861 ([C21 H22 F N7 O3]+H)+	ESI Scan (0.125 min) Frag=200.0V 13B3.d Subtract 440.1861 ([C21 H22 F N7 O3]+H)+

Peak List				
m/z	Z	Abund	Formula	Ion
363.1564	1	82760.33		
440.1861	1	1943522.88	C21 H22 F N7 O3	(M+H)+
441.1893	1	486017.22	C21 H22 F N7 O3	(M+H)+
442.1903	1	63089.89	C21 H22 F N7 O3	(M+H)+
462.1681	1	320570.69	1 2 4 7	
463.1701	1	74666.16		
879.3657	1	277727.31		
880.3679	1	136823.73		1
901.347	1	130375.75	, , , , , , , , , , , , , , , , , , ,	
902 3488	1	62166.71		

Formula Calculator Element Lin						
Element	Min	Max				
С	3	60				
Н	0	120				
0	0	. 30				
N	- 0	30				
-	1	1				

Formula Calculator Results								
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score		
C21 H22 F N7 O3	FALSE	439.1789	439.1768	-4.81	C21 H23 F N7 O3	90.08		

<sup>---</sup> End Of Report ---

Printed at: 1:17 PM on: 12/18/2021

Data Filename

13B4.d

Sample Name

13B4 P1-E6

Sample Type Instrument Name Sample Instrument 1 Position User Name

P1-E6

Acq Method IRM Calibration Status ZHENG100-1000.m Success Acquired Time 12/ DA Method 201

12/18/2021 9:33:39 AM 20170311.m

Comment

Sample Group

.

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

#### User Spectra

Fragmentor Voltage 200	Collision Energy 0	Ionization Mode ESI			
0 6 +ESI Scan (0.12	4 min) Frag=200.0V 13B4 453.20	68			
4-	([C23 H25 F N	6 O3J+H)+			
3-					
2-		-			
1-					905.4081
134.1173	363.1573		701.4935	814.5775	

m/z	Z	Abund	Formula	Ion
363.1573	1	59242.88		
453.2068	1	4113850.5	C23 H25 F N6 O3	(M+H)+
454.2098	1	1158621.5	C23 H25 F N6 O3	(M+H)+
455.2126	1	171343.09	C23 H25 F N6 O3	(M+H)+
475.1892	1	338735.31		
476.1912	1	78905.31		
905.4081	1	886842.19		
906.4108	1	473592.84		
907.4119	1	128916.54		
927.388	1	77905.8		

Formula Ca Element		Max
С	. 3	60
Н	0	120
0	0	30
N	0	30
E .	1	1

Formula Calculator Results							
Formula	Best	Mass	Tgt Mass	Diff (ppm)	1.1	Ion Species	Score
C22 H25 E N6 O3	FALSE	452,1996	452.1972		-5.17	C23 H26 F N6 O3	88.78

<sup>---</sup> End Of Report ---

Printed at: 1:17 PM on: 12/18/2021

**Data Filename** 

Sample Type **Instrument Name**  13B5.d Sample Instrument 1 Sample Name

Position **User Name Acquired Time** 

12/18/2021 9:36:36 AM 20170311.m

**Acq Method IRM Calibration Status** Comment

ZHENG100-1000.m

DA Method

P1-E7

Sample Group Acquisition SW Version

Info.

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

### User Spectra

Fragmentor Voltage 200	Collision Energy 0	Ionization Mode ESI		
0 6 +ESI Scan (0.1	11 min) Frag=200.0V 13B 455.1 ([C22 H23 F <sub> </sub>	855		
25-				
75-				
25-	363.1568	559.1293	701.4912	909.3638

Peak List	
m/z	
363 1568	

m/z	Z	Abund	Formula	Ion
363.1568	1	110080.06	N. C.	
455.1855	1	1679279.75	C22 H23 F N6 O4	(M+H)+
456.1885	1	435122.19	C22 H23 F N6 O4	(M+H)+
457.1891	1	61238.46	C22 H23 F N6 O4	(M+H)+
477.1675	1	400454.44	- 14	120
478.1694	1	95284.05		3
909.3638	1	196912.97		1 2 11
910.3665	1	97425.66	a design and a second	1
931.3461	1	156739.23		L. L. L.
932.3514	1	80171.13		Land Land Till

## Formula Calculator Element Limits

Lien	lenc	i i i i i i	I IUA	
С		3	60	
Н		0	120	
0		0	30	
N		0	30	
E		1	1	

Formula Calculator Results   Mass   Diff (npm)   Ion Species   Score							
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score	
C22 H23 F N6 O4	FALSE	454.1782	454.1765	-3.6	8 C22 H24 F N6 O4	93.68	

<sup>---</sup> End Of Report ---

Printed at: 1:18 PM on: 12/18/2021

Data Filename Sample Type S

13B6.d Sample Sample Name 1386 Position P1-E8

Instrument Name Acq Method Instrument 1 ZHENG100-1000.m

User Name Acquired Time

12/18/2021 9:39:33 AM

IRM Calibration Status

Success

DA Method 20170311.m

Comment

Sample Group

Info.

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

#### User Spectra

Frag	mentor Voltage 200	Collision Energy 0	Ionization Mode ESI		
x10 6	+ESI Scan (0.121	min) Frag=200.0V 13B	6.d Subtract		
2.5		457.1 ([C22 H22 F2		-	
2-					
1.5					288
1-					
0.5	134.1175	363.1573	561.3991	695.4897	913.3557

#### Peak List

m/z	Z	Abund	Formula	Ion
363.1573	1	152427.61		
381.1677	1	63828.09		
457.181	1	2374091.5	C22 H22 F2 N6 O3	(M+H)+
458.1847	1	623355.88	C22 H22 F2 N6 O3	(M+H)+
459.1867	1	82105.44	C22 H22 F2 N6 O3	(M+H)+
479.1637	1	170425.77		*
913.3557	1	222924.61		1
914.3575	1	110910.73		
985.715	1	99292.59		
986.717	1	62713.73		*

## Formula Calculator Element Limits

Element	Min	Max
С	3	60
Н	0	120
0	0	30
N	0	30
_	2	2

F 2 2 Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C22 H22 F2 N6 O3	FALSE	456.1739	456.1721	-3.89	C22 H23 F2 N6 O3	92.65

<sup>---</sup> End Of Report ---

Printed at: 1:19 PM on: 12/18/2021

Data Filename Sample Type

14A1.d Sample

Sample Name Position

P1-A3

**Instrument Name** 

Instrument 1 ZHENG100-1000.m

User Name Acquired Time DA Method

12/17/2021 7:33:21 PM 20170311.m

**Acq Method IRM Calibration Status** 

Comment

Info.

Sample Group Acquisition SW Version

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

#### User Spectra

Frag	mentor Voltage 200	Collision	Energy	Ionization Mode ESI			
10 6	+ESI Scan (0.154	min) Frag=2	00.0V 14A1	.d Subtract			
1-			452.12	239			
0.8							
0.6						881	.2588
0.4							
0.2		363.	1614				
	134.1180 2	74.2772			695.4964	810.2993	

Pe	а	k	Li	st

1	Abund 166778.67
1	166778 67
	100//0.0/
1	62431.75
1	896078.38
1	198570.2
1	54907.35
1	65137.32
1	579139.56
1	274355.19
1	111827.21
1	52005.89
	1 1 1 1 1 1 1

985.725	1 5200	1 52005.89			
Formula Ca	alculator Ele	ement Lir	nits		
Element	Min	Max			
С	3	60			
Н	0	120			
0	0	30			
N	0	30			
F	1	1			
-	1	1	1		

<sup>---</sup> End Of Report ---

Printed at: 1:20 PM on: 12/18/2021

Data Filename Sample Type Instrument Name 14A2.d Sample Instrument 1

Sample Name
Position
User Name
Acquired Time

P1-F1 12/18/2021 9:42:29 AM

Acq Method IRM Calibration Status Comment ZHENG100-1000.m Acquired Tir Success DA Method

20170311.m

Sample Group

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

#### User Spectra

Fragmentor Voltage 200	Collision Energy 0	Ionization Mode ESI			
5 +ESI Scan (0.117	min) Frag=200.0V 14A	2.d Subtract			
4	453.1135 ([C19 H19 F N6 O3 S]+f	Na)+			
2					
8-					
6					
4-					
.2-	- 1				
0	120 120 12	1 155 156	457	458	459
451	452 453 45 Counts	4 455 456 vs. Mass-to-Charge (m/	z) 457	450	400

Pe	ak	L	ist

m/z	Z	Abund
274.2752	1	880201.25
318.3019	1	631956.88
475.3283	2	789562.69
588.4122	1	1445558.13
589.4162	1	501825
701.497	1	2697659.25
702.5001	1	1181877.88
703.5032	1	273883
814.5823	1	1371627.75
815.5858	1	680633.13
Formula Calc	ulate	or Element Limits

Element	Min	Max
C .	3	60
Н	0	120
С . Н	41.0	30
N	0	30
	1	1
S Formula C	1."1	1

Formula Best	Mass	Tgt Mass	Diff (ppm) Ion Species	Score
C19 H19 F N6 O3 S TRU	E 430.124	430.1223	-3.9 C19 H19 F N6 Na O3 S	90.35

<sup>---</sup> End Of Report --- ,

Printed at: 1:22 PM on: 12/18/2021

Data Filename

Sample Type

14A3.d Sample

Sample Name Position

P1-F2

**Instrument Name** 

**Acq Method IRM Calibration Status**  Instrument 1 ZHENG100-1000.m

Info.

User Name **Acquired Time** DA Method

12/18/2021 9:45:24 AM 20170311.m

Success

Comment

Sample Group Acquisition SW Version

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

**User Spectra** 

Fragmentor Voltage 200	Collision Energy 0	Ionization Mode ESI		
x10 4 +ESI Scan (0.118	3 min) Frag=200.0V 14A	3.d Subtract		
8-	453.1131 ([C19 H19 F N6 O3 S]+I	Na)+		
6-				
4-				
2-		1		
0 451	452 453 45	4 455 456	457 4	58 459

Doole	Hick
Peak	LIST

m/z	Z	Abund
274.2752	1	805906.75
318.3016	1	603440.56
475.3277	2	829456.31
588.4116	1	1487310.38
589.4152	1	515069.84
701.4963	1	2830297.75
702.4995	1	1229214.75
703.5029	1	287015.81
814.5816	1	1509447.38
815.5855	1	748071.38

Formula Calculator Element Limits

Element	Min	Max
С	3	60
Н	0	120
0	, 4 . 0	30
N	0	30
F - Char	1	1
S	1	1

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C19 H19 F N6 O3 S	TRUE	430.1238	430.1223	-3.38	C19 H19 F N6 Na O3 S	92.93

--- End Of Report ---

Printed at: 1:22 PM on: 12/18/2021

DA Method

**Data Filename** Sample Type **Instrument Name**  14A4.d Sample Instrument 1 Sample Name Position

P1-F3 **User Name Acquired Time** 

Acq Method IRM Calibration Status ZHENG100-1000.m Success

12/18/2021 9:48:21 AM 20170311.m

Comment Sample Group

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

### User Spectra

Acquisition SW Version

Fragmentor Voltage 200	Collision Energy 0	Ionization Mode ESI	
10 4 +ESI Scan (0.118	8 min) Frag=200.0V 14A4	.d Subtract	
8-	466.1	337	
6-			470.4007
4	1 2 2 3		470.1667
2-		467.1357	472.3217

Do	-1	List
re	aĸ	LIS

reak List		
m/z	Z	Abund
274.2753	1	1013364.5
318.302	1	709357.56
475.3283	2	914926.75
588.4124	1	1628655
589.4164	1	572134.81
701.4973	1	2998258.25
702.5004	1	1313458.38
703.5039	1	306086.88
814.5825	1	1540120.63
815.5864	1	772077.19
Formula Calc	ulate	or Element Limits

Min	Max
3	60
0	120
0	. 30
0	30
1	1
1	. 1
	0

--- End Of Report ---

Printed at: 1:24 PM on: 12/18/2021

Data Filename Sample Type

**Instrument Name** Acq Method

14A5.d Sample Instrument 1 ZHENG100-1000.m

Success

Sample Name Position **User Name** 

DA Method

12/18/2021 9:51:18 AM **Acquired Time** 20170311.m

14A5 P1-F4

**IRM Calibration Status** 

Comment

Sample Group 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) Acquisition SW Version

#### **User Spectra**

Fragmentor Voltage 200	Collision Energy 0	Ionization Mode ESI	
0 5 +ESI Scan (0.117 i	min) Frag=200.0V 14A	5.d Subtract 468.1130	
		([C20 H20 F N5 O4 S]+Na)	+
2-			
1.5-			the process of the second seco
1.			
0.5-			472.3206
0 461 462 4	463 464 465 46	6 467 468 469 4	70 471 472 473 474

Info.

m/z	Z	Abund
274.2752	. 1	999895.94
318.3017	1	665345.69
340.2834	1	304752.38
475.3278	2	741801.88
588.412	1	1374273.25
589.4157	1	472936.34
701.4965	1	2644920.75
702.4997	1	1144999.75
814.5817	1	1319037.13
815.5854	1	651833.63

Element	Min	1	4ax
С		3	60
Н		0	120
0	1.1.7	ī	30
N	- (	)	30
F 4 17 19 1		ı	1
S	100	1	1

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C20 H20 F N5 O4 S	FALSE	445.1236	445.122		3.48 C20 H20 F N5 Na O4 S	91.15

--- End Of Report ---

Printed at: 1:25 PM on: 12/18/2021

Data Filename Sample Type

14A6.d Sample Instrument 1 Sample Name Position User Name

P1-F5

**Instrument Name** Acq Method IRM Calibration Status

ZHENG100-1000.m Success

Acquired Time DA Method

12/18/2021 9:54:15 AM 20170311.m

Comment

Sample Group

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Acquisition SW Version

Fragmentor Voltage 200	Collision Energy 0	Ionization Mode ESI		
10 5 +ESI Scan (0.109	min) Frag=200.0V 14A6	3.d Subtract		_
.75 - 1.5 -		470.1081 0 H19 F2 N5 O3 S]+Na)	•	
1-				
.75- 0.5-				
25-			472.3207	
466	467 468 469 Counts	9 470 471 vs. Mass-to-Charge (m/z	472 473 474	

Peak List							
m/z	Z	Abund					
274.2749	1	952946.69					
318.3015	1	640031.5					
475.3276	2	881883.25					
588.4115	1	1572009.13					
589.4151	1	549769.88					
701.4961	1	3168274.75					
702.4995	1	1379356.88					
814.5813	1	1688069					
815.5851	1	856933.81					
927.6666	1	346751.56					
Formula Cal	culat	or Element Limits					

Min	Max	
3	60	
0	120	
0	30	
0	30	
2	2	
1	1	
	Min 3 0 0 0 0 2 1 1	

I Official Culculator ress	1						
Formula	Best	Mass	Tgt Mass	Diff (ppm)		Ion Species	Score
C20 H19 F2 N5 O3 S	TRUE	447.1187	447.1177		-2.42	C20 H19 F2 N5 Na O3 S	95.05

<sup>---</sup> End Of Report ---

Printed at: 1:26 PM on: 12/18/2021

Data Filename

Sample Type

14B1.d Sample Sample Name Position

P1-F6

**Instrument Name** Acq Method

Instrument 1 ZHENG100-1000.m **IRM Calibration Status** Success User Name **Acquired Time** 

12/18/2021 9:57:11 AM 20170311.m

DA Method

Comment

Sample Group

Acquisition SW Version

Info.

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

#### **User Spectra**

Frag	gmentor Voltage 200	Collision Energy 0	Ionization M ESI	ode	
10 4	+ESI Scan (0.118	min) Frag=200.0V 14B	436	.1407 N5 O4]+Na)+	
3-					
2-		*			
1-					1
0-	435.2	35.4 435.6 435 Counts	.8 436 vs. Mass-to-Ch	436.2 436.4 4	36.6 436.8

Р	-	-	L	ie	٠

m/z	Z	Abund
274.2756	1	940386.5
318.3025	1	640912.25
475.3288	2	921775.19
588.413	1.	1616366.13
589.4169	1	565004.56
701.498	1	3043929.75
702.5012	1	1326821.75
814.5834	1	1599978.88
815.5873	1	799718.94
927.6688	1	314654.5

Element	Min	Max
С	3	60
Н	0	120
Н О	0	30
N	0	30
F	1	1
S	0	0

Formula Calculator Results
Formula Best Mass Tgt Mass Diff (ppm) Ion Species FALSE 413.1515 413.1499 -3.68 C20 H20 F N5 Na O4 C20 H20 F N5 O4 42.35

Printed at: 1:27 PM on: 12/18/2021

<sup>---</sup> End Of Report ---

Data Filename

Sample Type **Instrument Name**  14B2.d Sample Instrument 1

Success

Sample Name Position 14B2 P1-F7

**User Name** 

**Acquired Time** 

12/18/2021 10:00:08 AM 20170311.m

Acq Method **IRM Calibration Status** 

DA Method

Comment

Sample Group

Acquisition SW Version

Info.

ZHENG100-1000.m

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

#### **User Spectra**

Frag	mentor Voltage 200	Collision Energy	Ionization Mode ESI			
10 5	+ESI Scan (0.109	min) Frag=200.0V 14B2.	d Subtract			
1.75-		43	37.2334			
1.5-						
1.25-						
1-		***************************************				
0.75-						
0.5				438.2368		
0.25-						
0-	435.5	436 436.5 437	437.5 43	38 438.5	439 43	39.5

P	ea	k	L	is	t

m/z	Z	Abund
274.2756	1	842026.44
318.3019	1	572126.56
475.3283	2	981313.25
588.4123	1	1740758.38
589.4162	1	615434.06
701.497	1	3221402.75
702.5004	1	1397455
814.5823	1	1725972.75
815.5859	1	882205.88
927.6679	1	362921.09
Formula Cal	culat	or Flement Limits

Element	Min	Max
С	3	60
Н	0	120
0	0	30
N	0	30
F of the	. 1	1
S Formula Ca	0	0

Folilidia Calculator Results								
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score		
C19 H19 F N6 O4	FALSE	414.1487	414.1452	-8.45	C19 H19 F N6 Na O4	71.24		

<sup>---</sup> End Of Report ---

Printed at: 1:29 PM on: 12/18/2021

Data Filename Sample Type **Instrument Name**  14B3.d

Sample Name 14B3 Position **User Name** 

P1-F8

Acq Method IRM Calibration Status Comment

Sample Instrument 1 ZHENG100-1000.m **Acquired Time** DA Method

12/18/2021 10:03:04 AM 20170311.m

Sample Group Acquisition SW Version

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

#### **User Spectra**

Fragr	mentor Voltage 200	Collision Energy 0	Ionization Mode ESI
- 1	+ESI Scan (0.110 r	nin) Frag=200.0V 14B3	3.d Subtract
2.5			7.1374 F N6 O4]+Na)+
1.5-			
.5			438.1394 ([C19 H19 F N6 O4]+Na)+
۰	435.5	136 436.5 43	7 437.5 438 438.5 439 439.5 vs. Mass-to-Charge (m/z)

Peak List				
m/z	Z	Abund		
274.2756	1	733396.81		
318.302	. 1	537000.38		
475.3283	2	842461.13		
588.4124	1	1506011.88		
589.416	1	527113.63		
701.4973	1	2950452.75		
702.5003	1	1297365.5		
814.5826	1	1642104.75		
815.5861	1	829665.94		
927.6681	1	352693.91		

## Formula Calculator Element Limits

Element	PULL	Max
С	3	60
Н	0	120
0	0	30
N	0	30
F	1	1
S	0	0

Formula Calculator Results

Formula	Best	Mass	igt mass	Diff (ppm)	ion Species	Score
C19 H19 F N6 O4	FALSE	414.148	414.1452	-6.89	C19 H19 F N6 Na O4	81.81

<sup>---</sup> End Of Report ---

Printed at: 1:30 PM on: 12/18/2021

Data Filename Sample Type Instrument Name Acq Method 14B6.d Sample Instrument 1 ZHENG100-1000.m Sample Name 1486 Position P1-A2

User Name Acquired Time

12/17/2021 7:30:24 PM 20170311.m

IRM Calibration Status

tus

Success DA Method

Comment

Sample Group Acquisition SW Version

6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

#### User Spectra

Frag	mentor Voltage 200	Collision Energy 0	Ionization Mod ESI	<b>le</b>	
10 5	+ESI Scan (0.170	min) Frag=200.0V 14	B6.d Subtract		
3-	8000	452	2.1406		
2.5					
2-					
1.5-		363.1614			
0.5			550 4000	695.4994	881.2880
		La La Landard Landard	559.1366		

#### Peak List

reak List		
m/z	Z	Abund
339.2349	1	28188.79
363.1614	1	126276.76
381.1713	1	42973.77
452.1406	1	287194.75
453.1437	1	58531.06
695.4994	1	34942.29
881.288	1	33666.73
985.7261	1	145446.08
986.7291	1	94219.14
987.7296	1	30126.18
Formula Cal	culate	or Element Lin

| Formula Calculator Element Limit | Element | Min | Max | C | 3 | 60 | H | 0 | 120 | O | 0 | 30 | N | 0 | 30 | F | 2 | 2 | 2 | 5 | 0 | 0 | 0 |

--- End Of Report ---

Printed at: 1:33 PM on: 12/18/2021

Data Filename Sample Type

ename 1485.d Type Sample Sample Name Position 14B5 P1-A1

Instrument Name
Acq Method

Instrument 1 User Name
ZHENG100-1000.m Acquired Time

Info.

12/17/2021 7:27:27 PM

IRM Calibration Status Success

DA Method

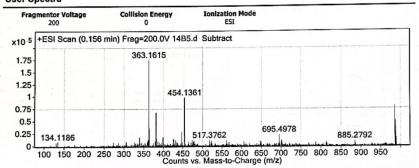
ethod 20170311.m

Comment

Sample Group

Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.2)

User Spectra



D1-	. :
Peak	LIST

m/z	Z	Abund
363.1615	1	175003.34
364.1637	1	35270.89
381.1712	1	68031.12
399.1844	1	18222.71
447.2053	1	28160.41
454.1361	1	97984.98
455.1431	1	23152.24
695.4978	1	22431.54
985.7253	1	79402.95
986.7271	1	50751.21

Formula Calculator Element Limits

Element	Min	Max
С	3	60
Н	. 0	120
0	0	30
N	0	30
F. Mich.	1	1
S		0

--- End Of Report ---

Printed at: 1:32 PM on: 12/18/2021