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

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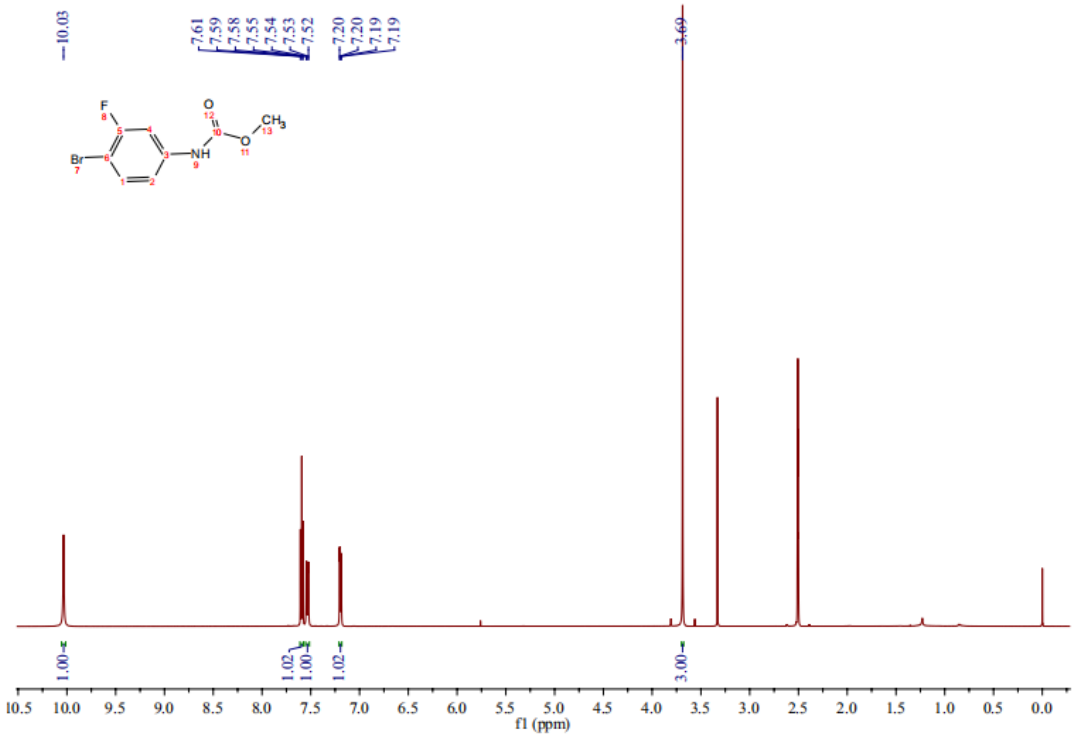
[b] *Department of Clinical Laboratory, The Eighth Medical Center of PLA General Hospital, Beijing 100091, China*

1. ^{1}H-NMR Spectra

Compound 9



Compound 10

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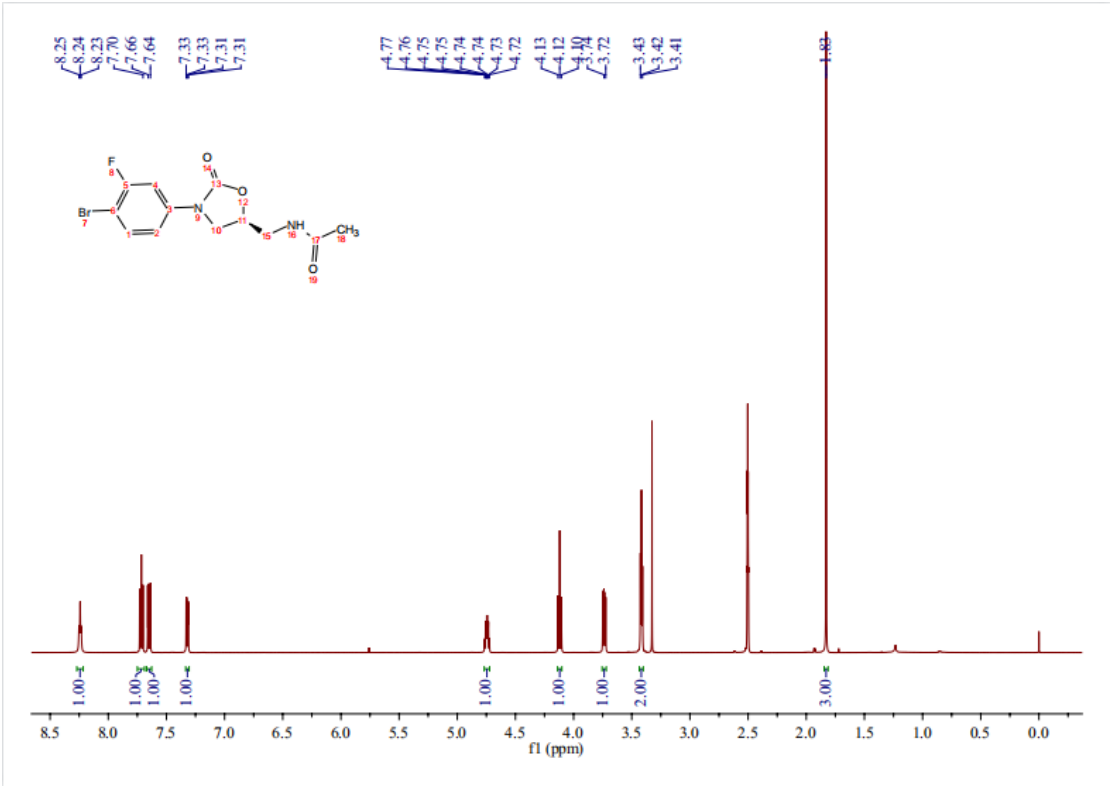
E-mail addresses: houyunlei901202@163.com (Y. Hou), yanfangzhao@126.com (Y. Zhao).



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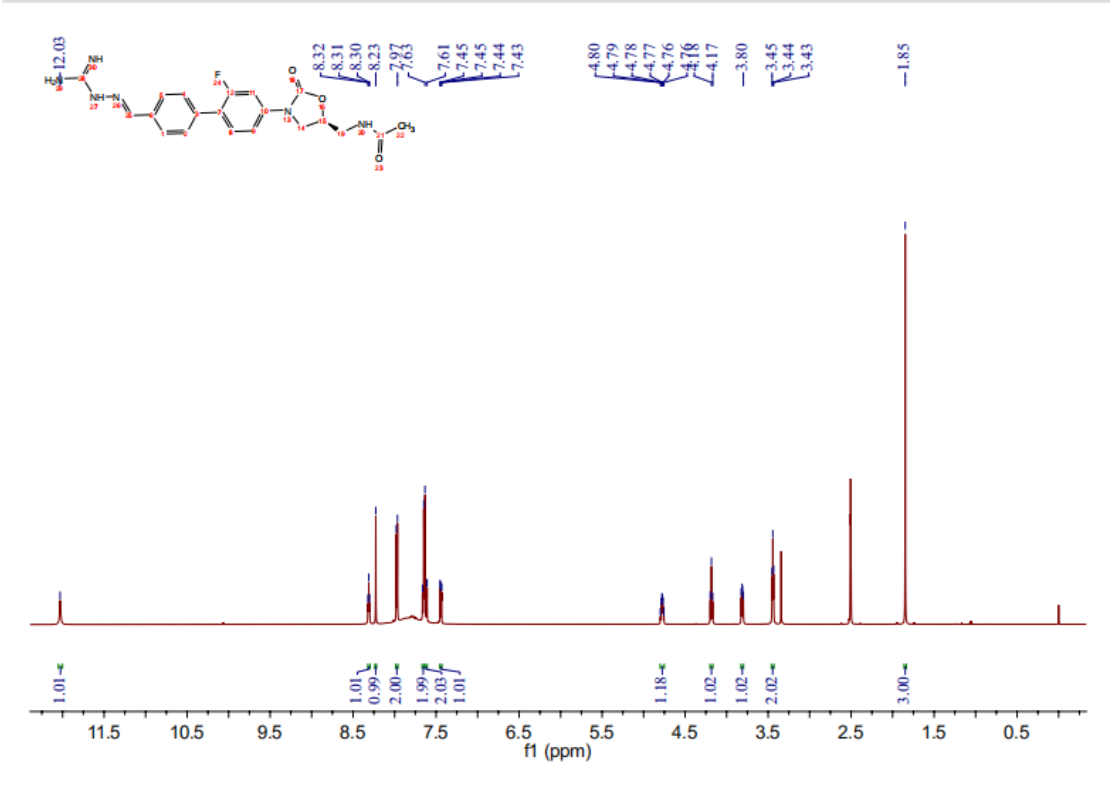

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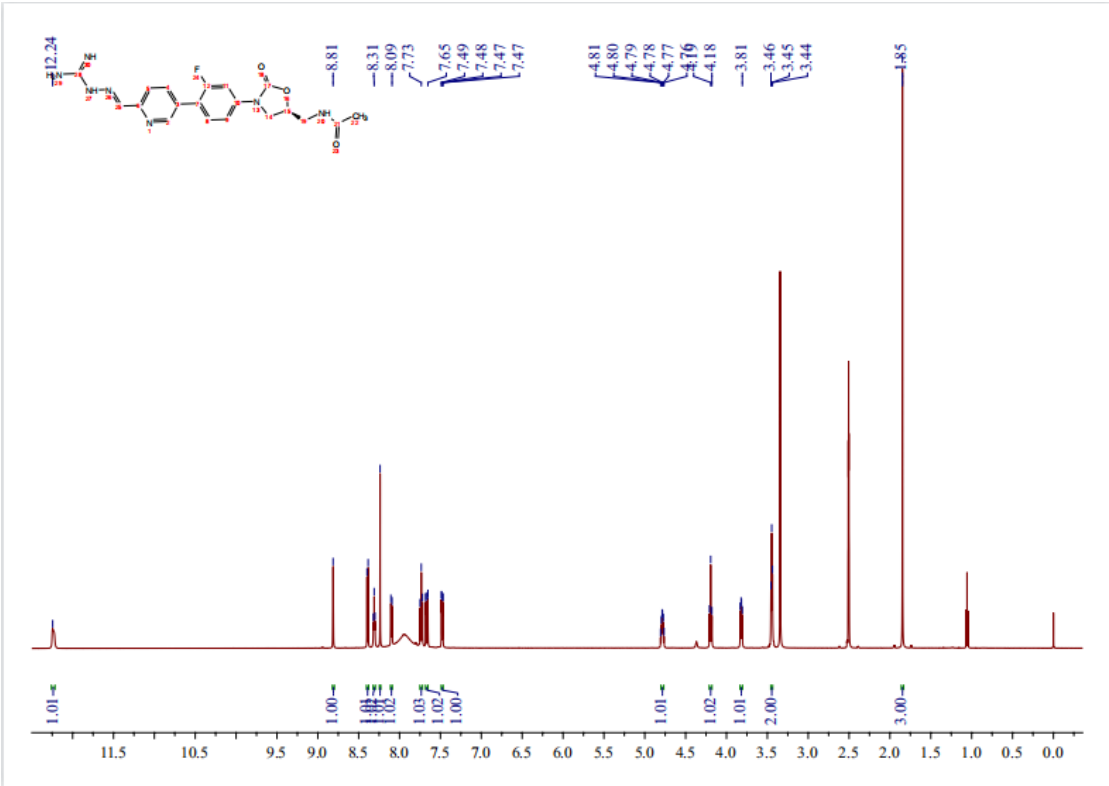

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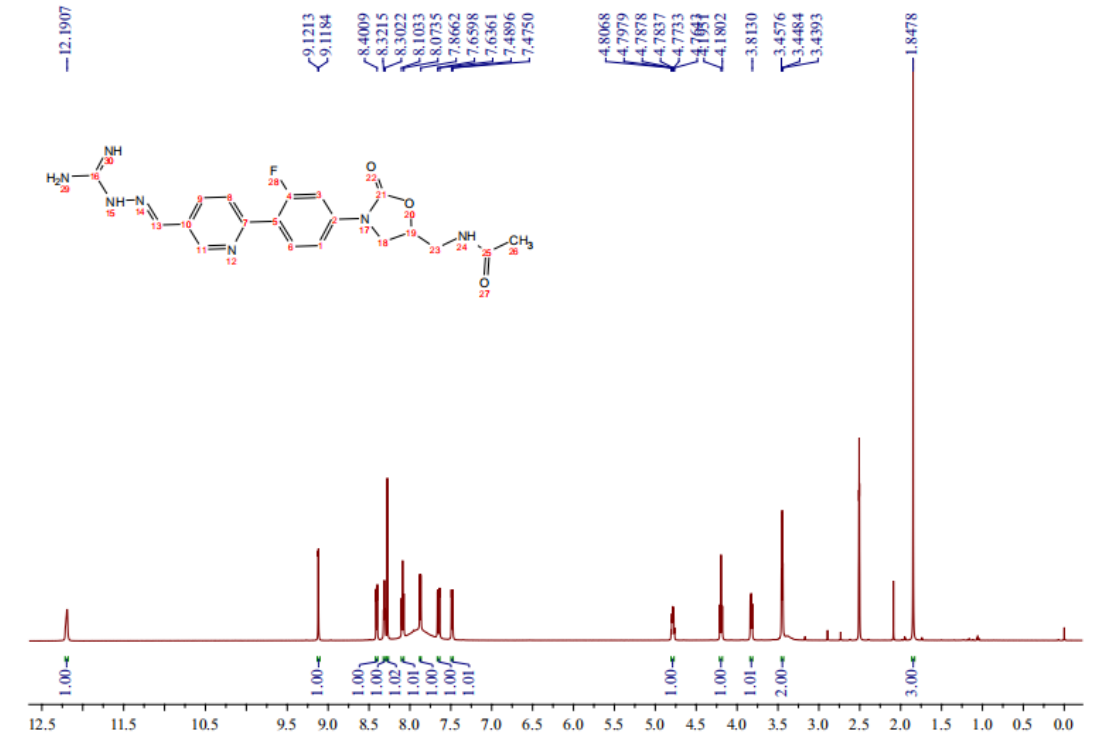

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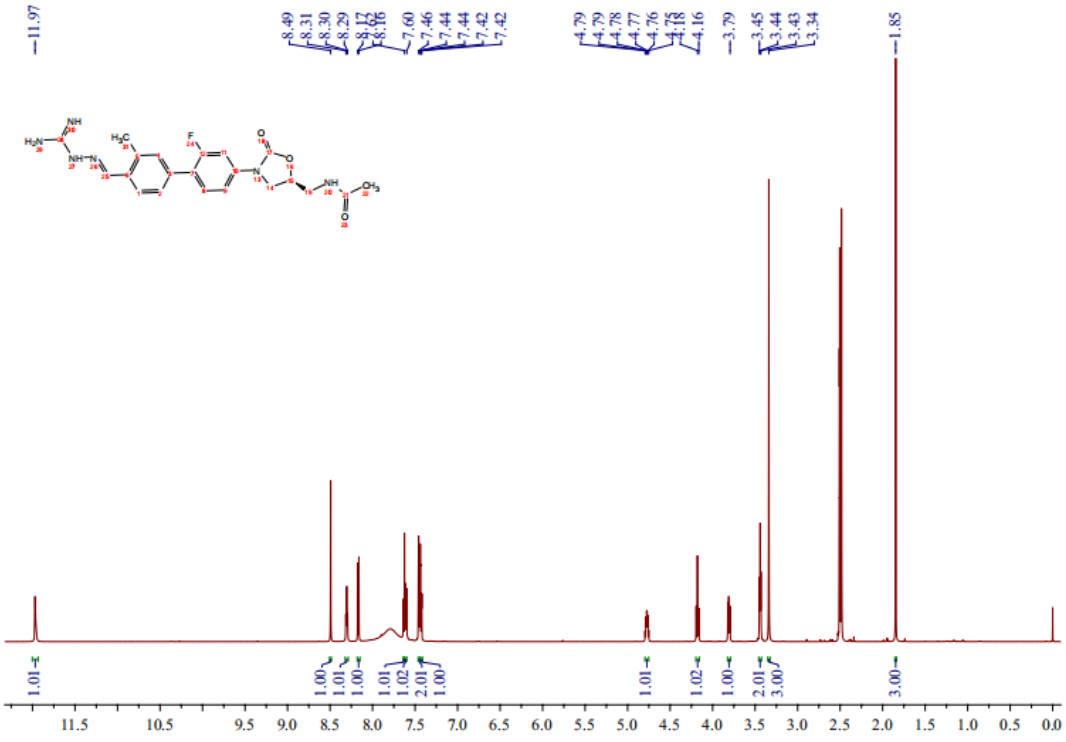

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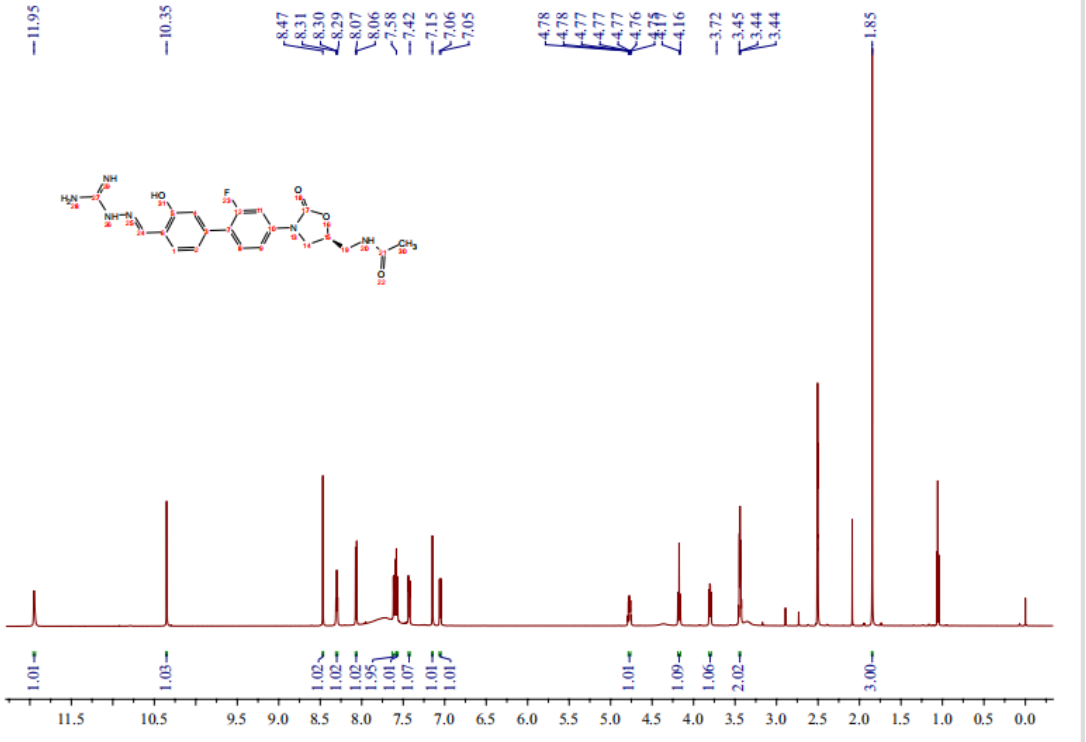
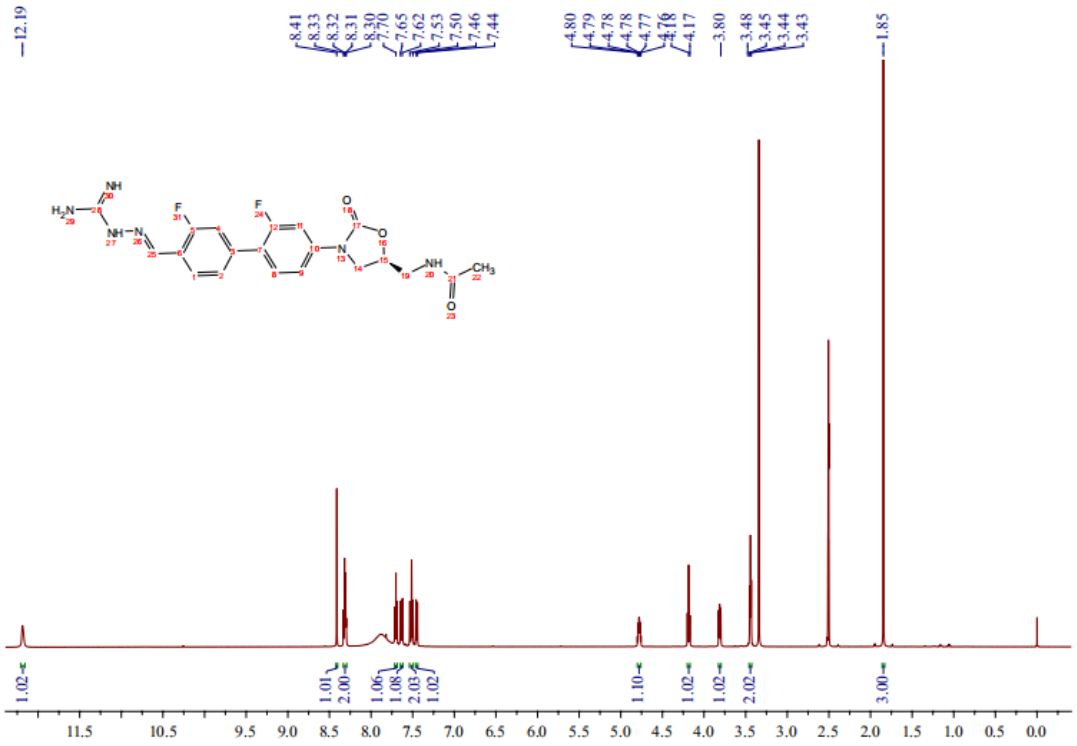


Compound 13a-6



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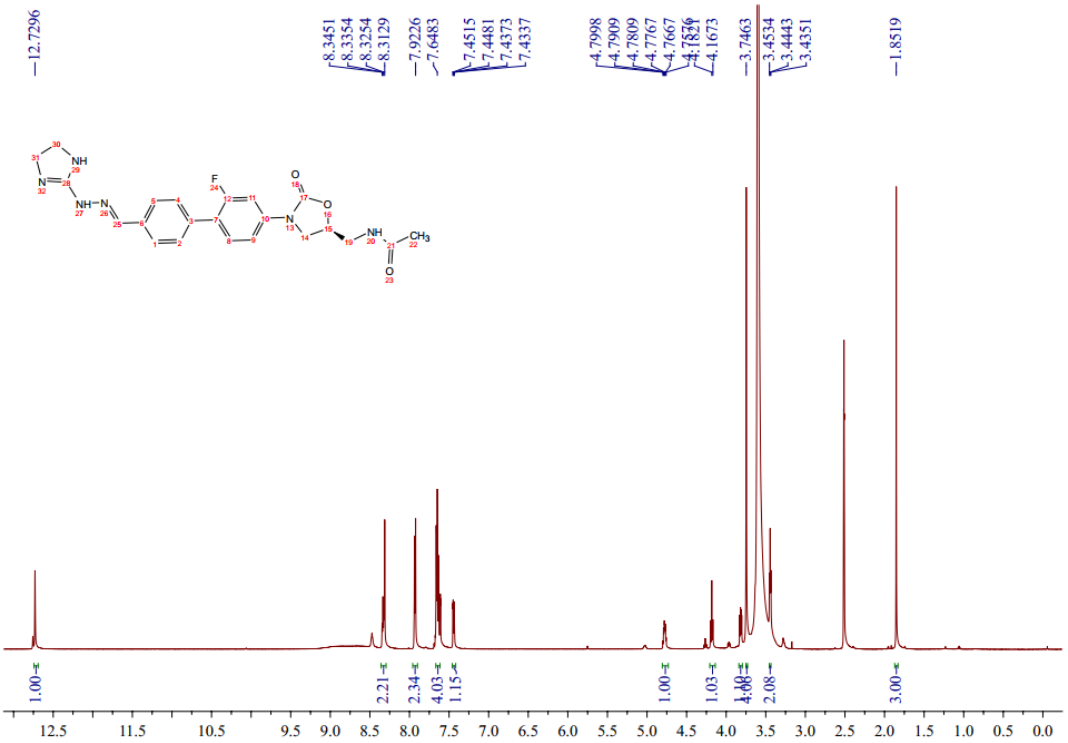

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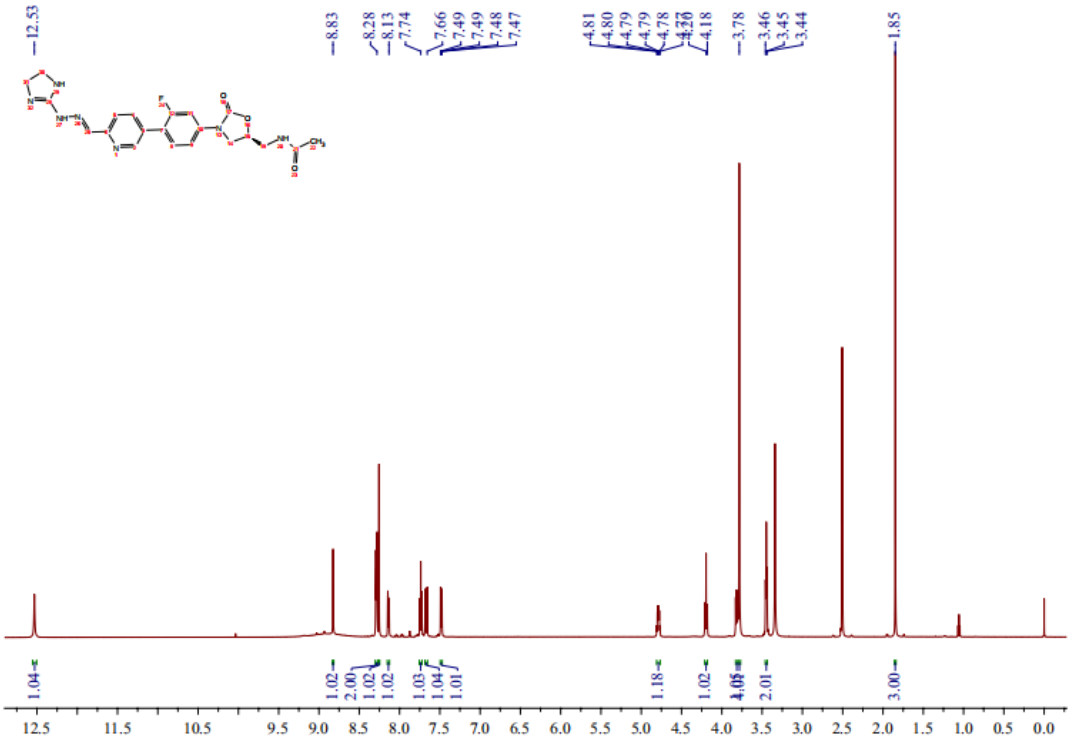

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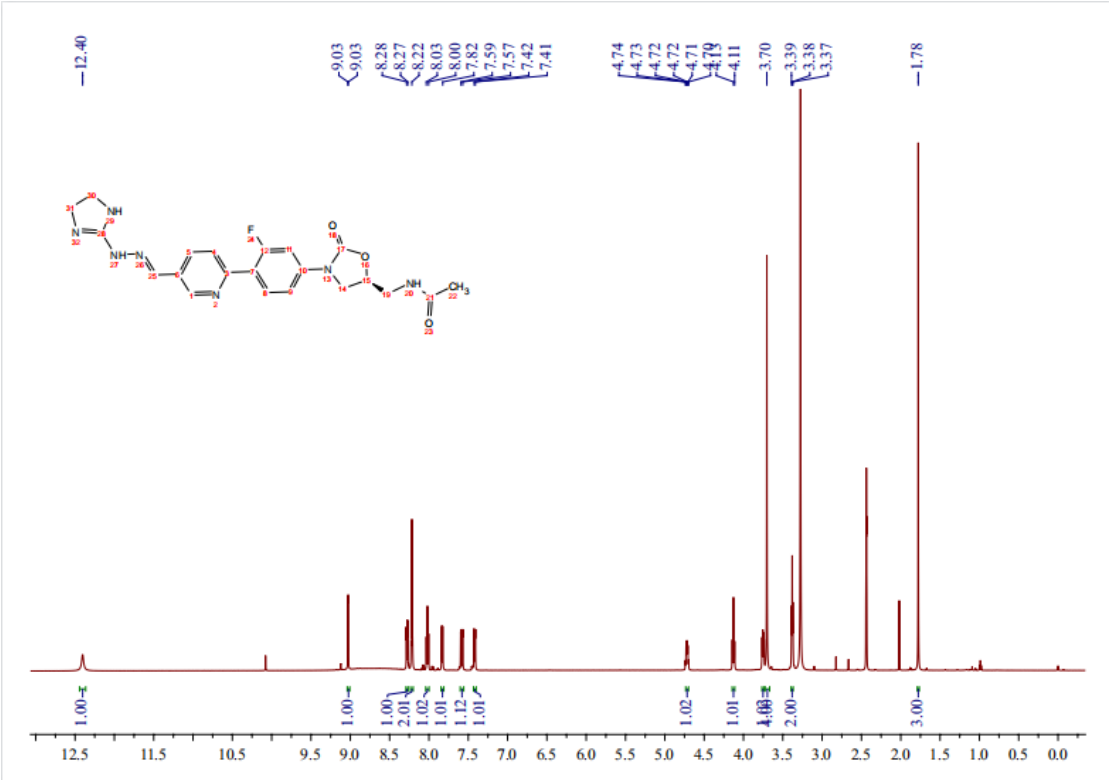

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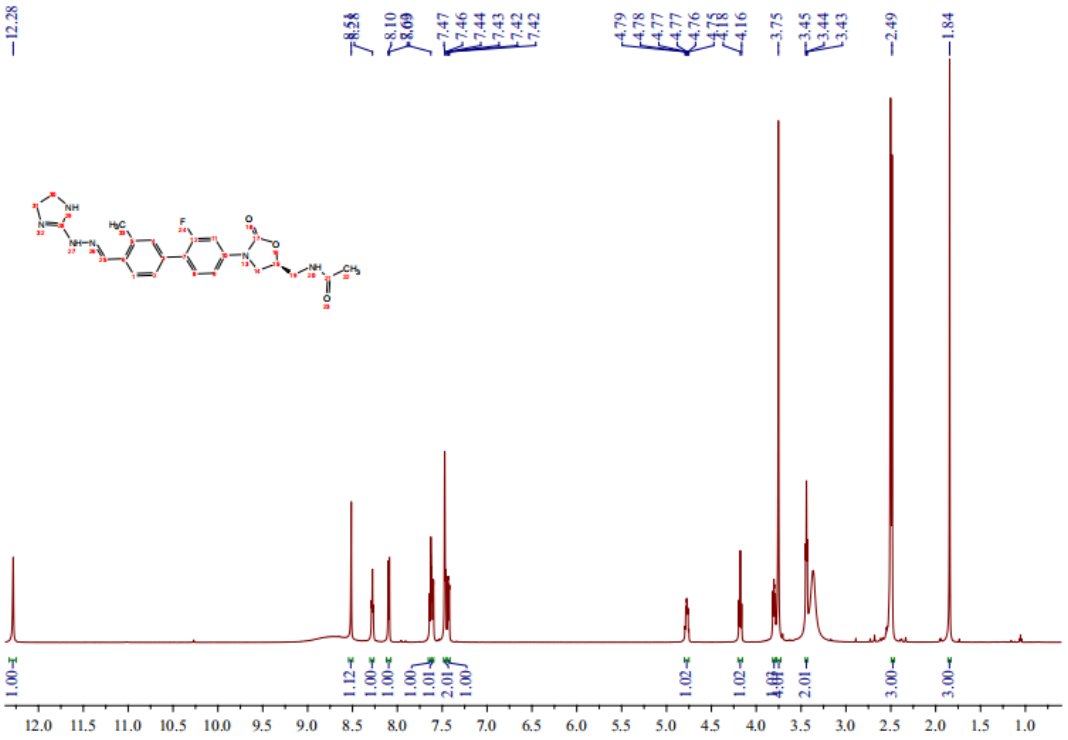

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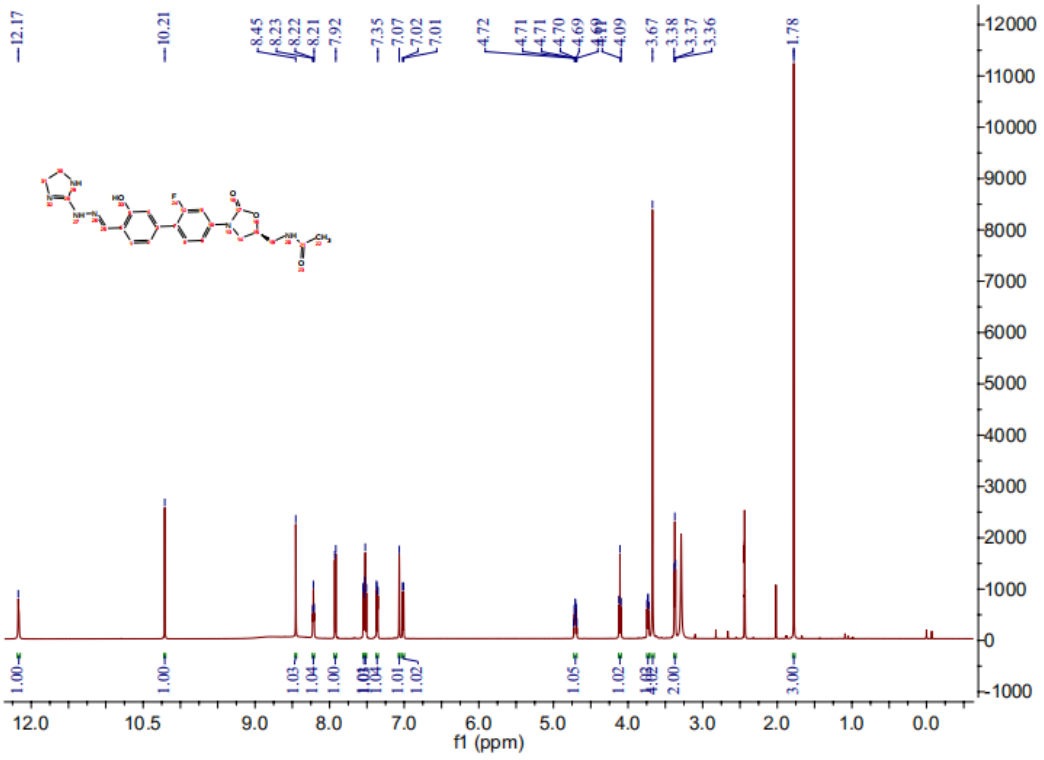

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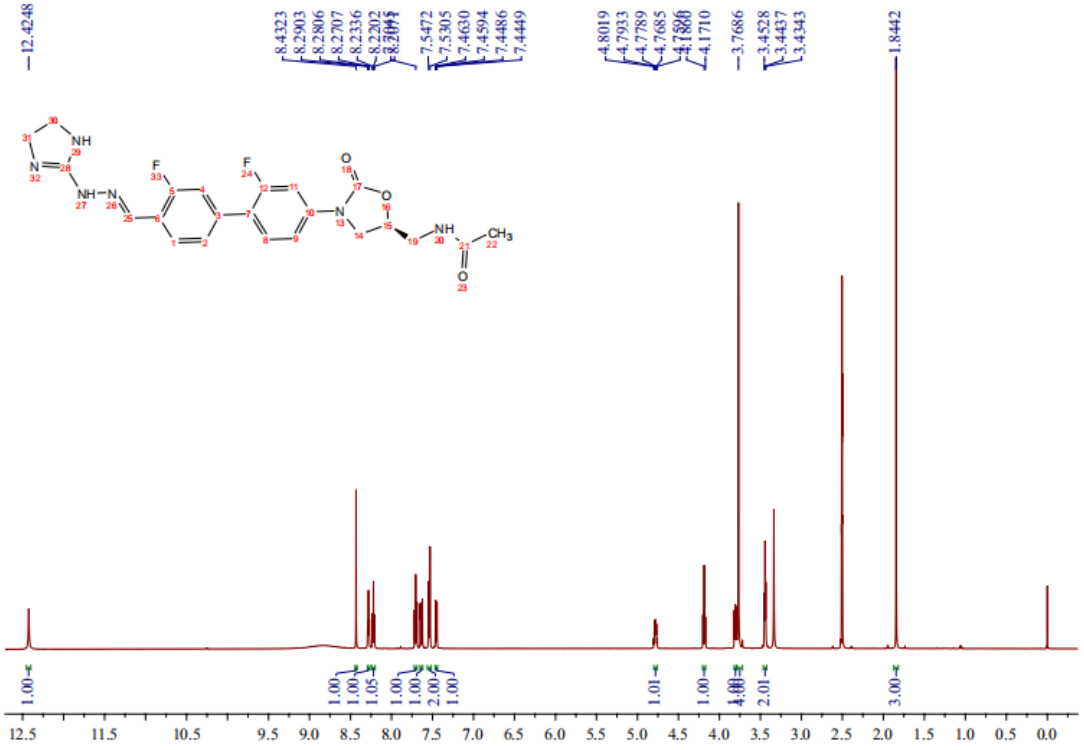

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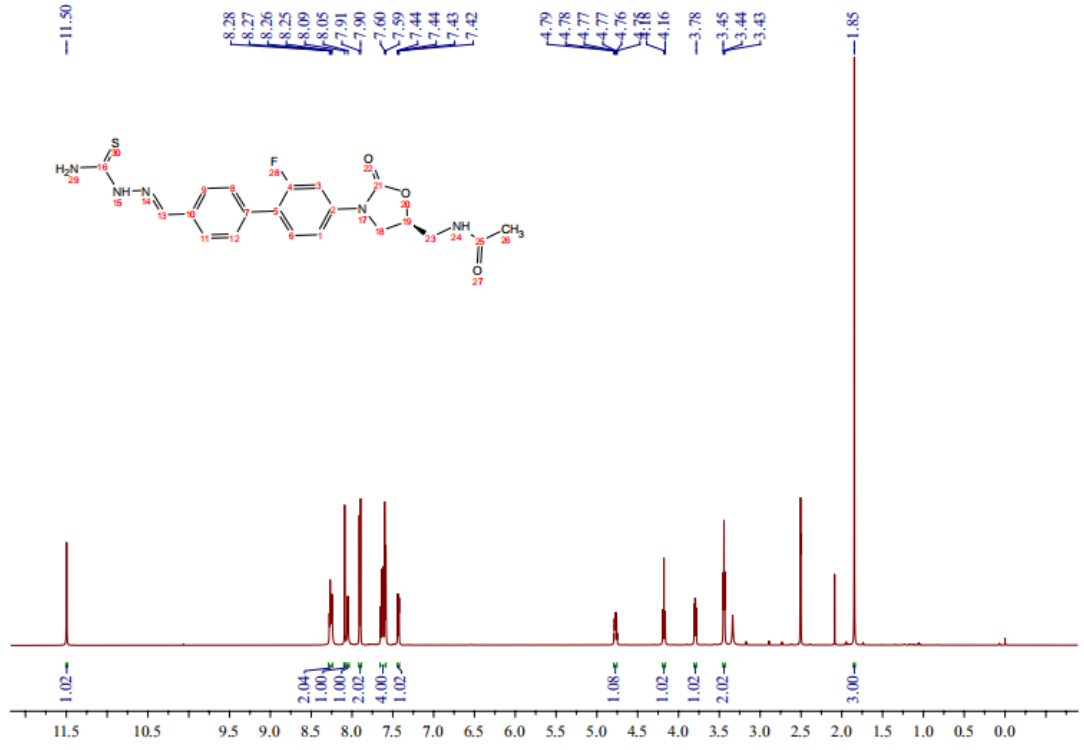

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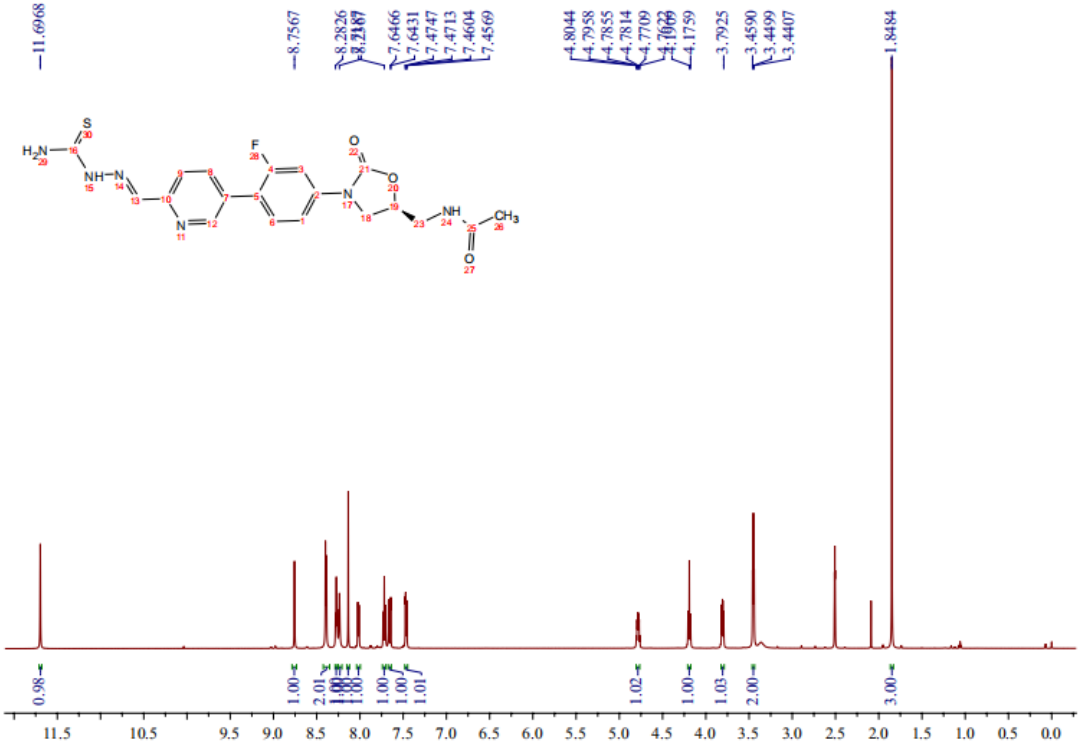

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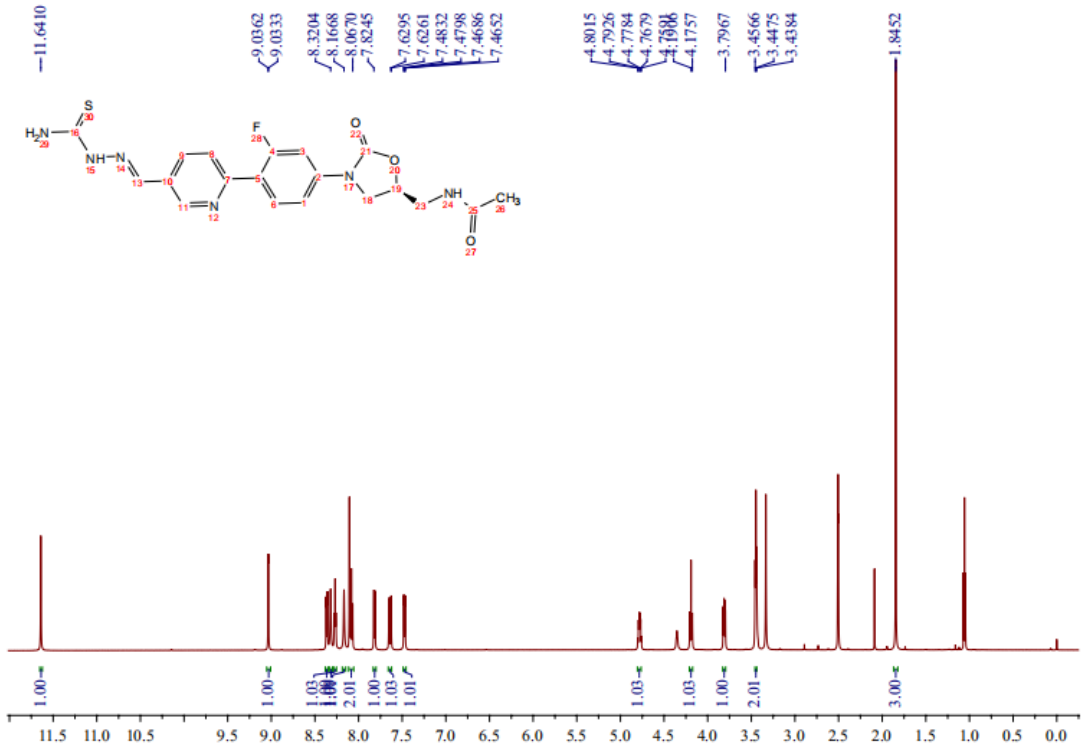

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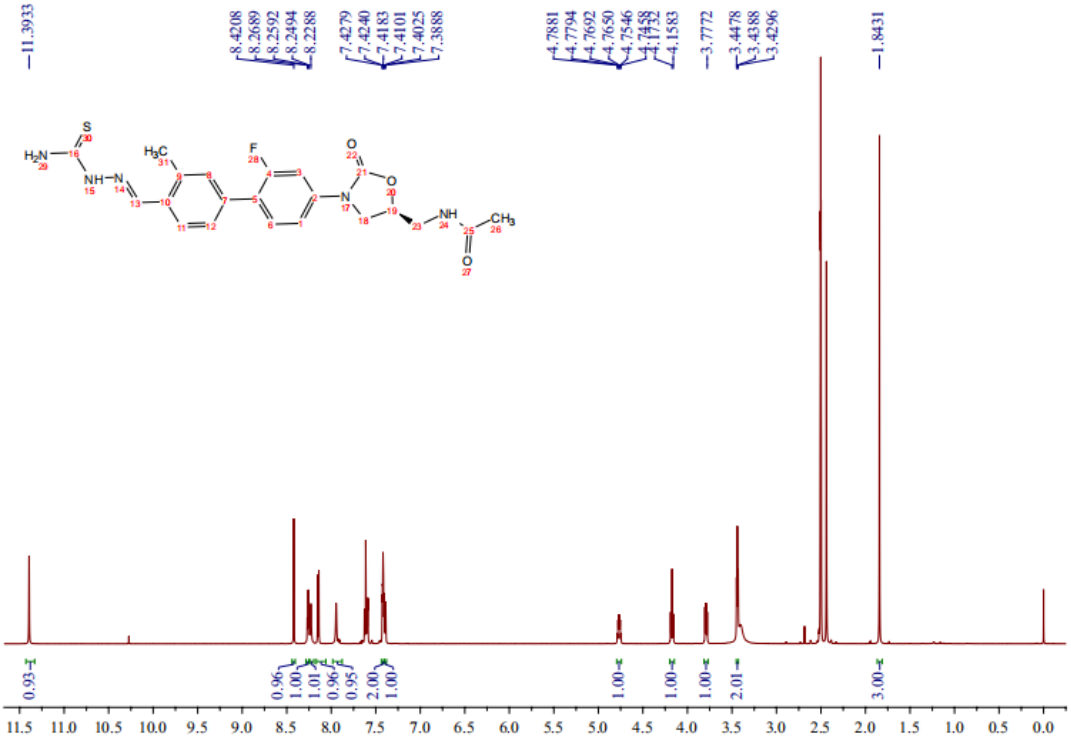

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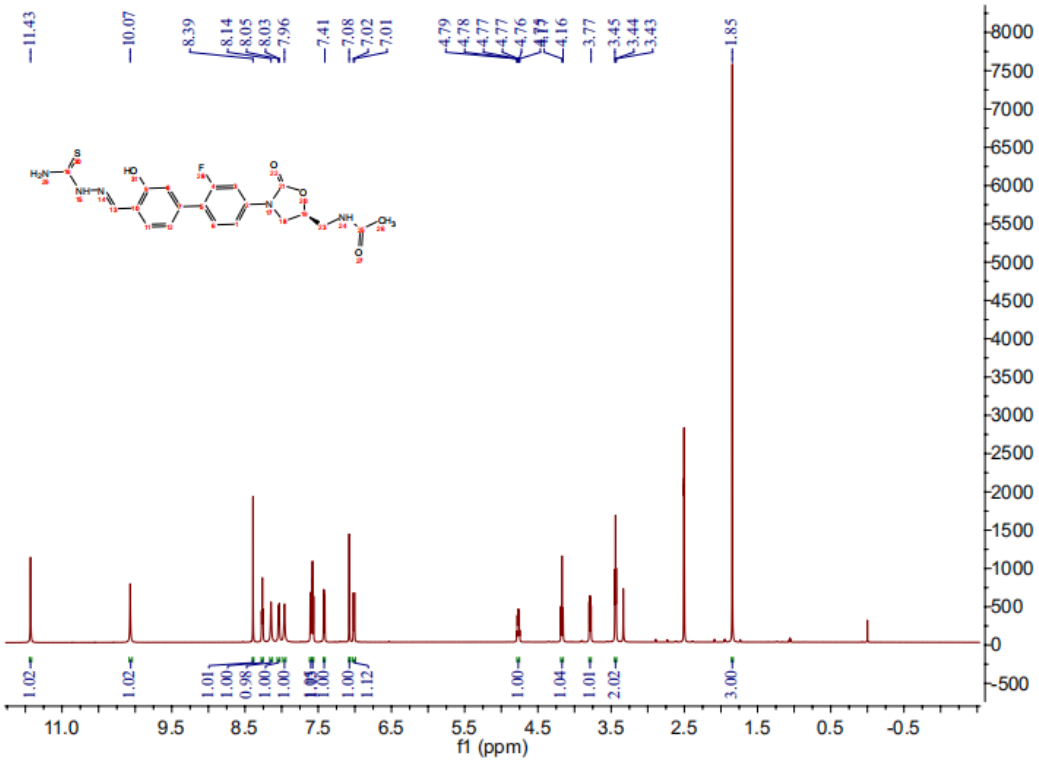

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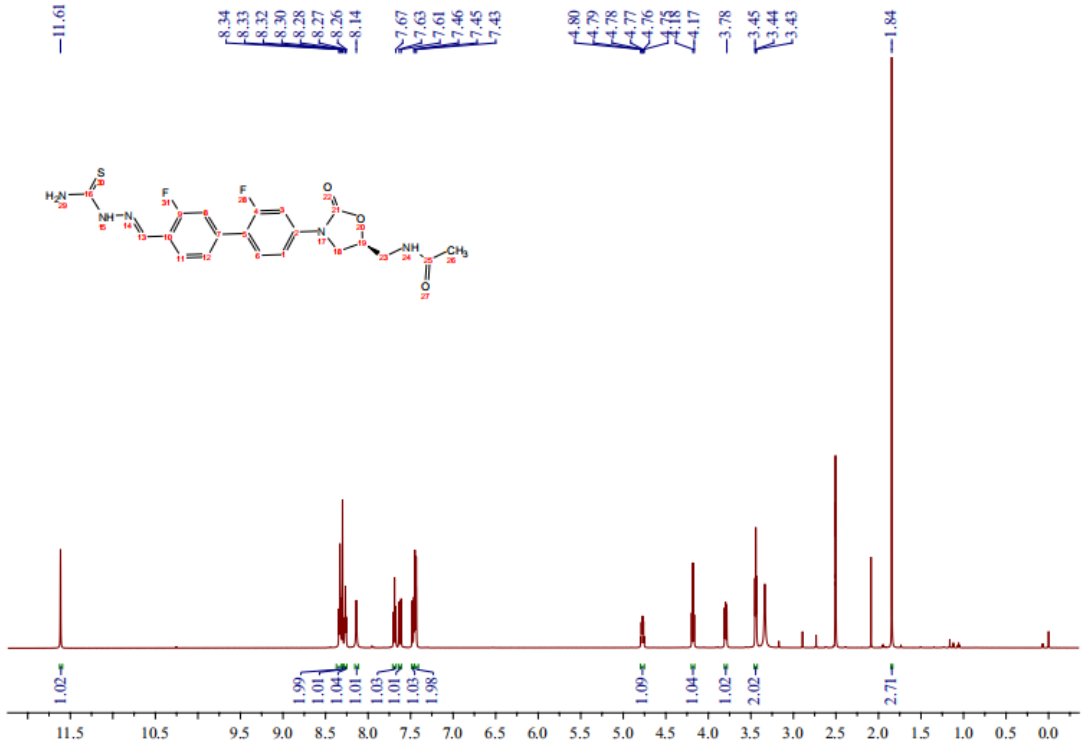

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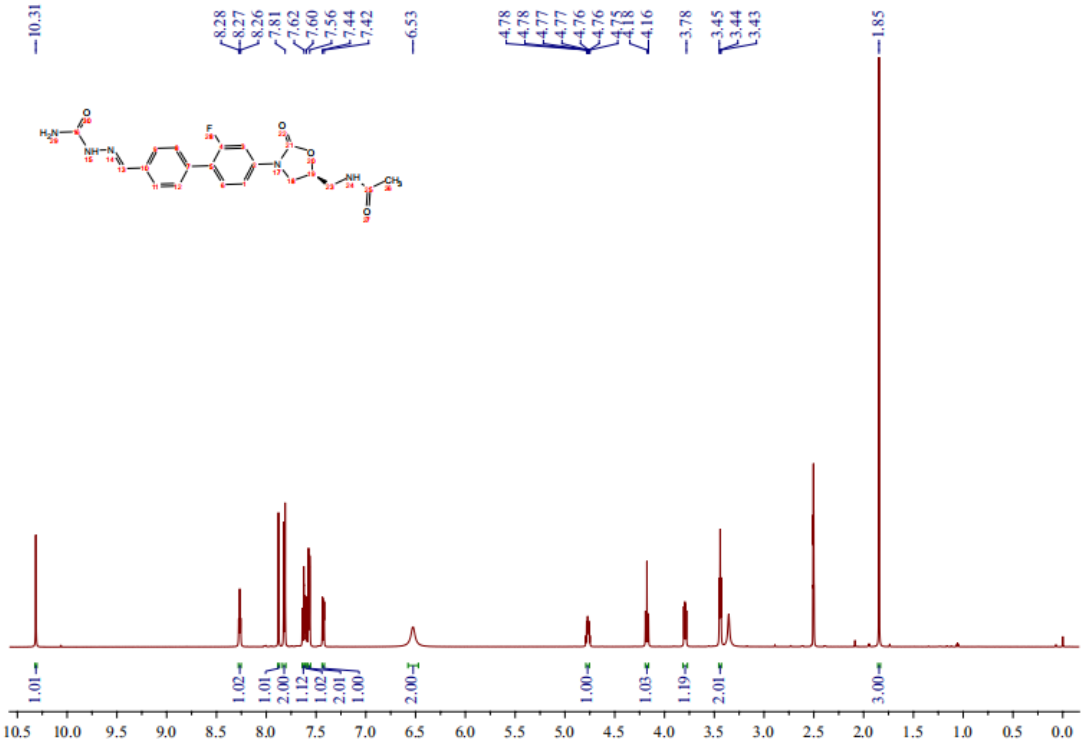

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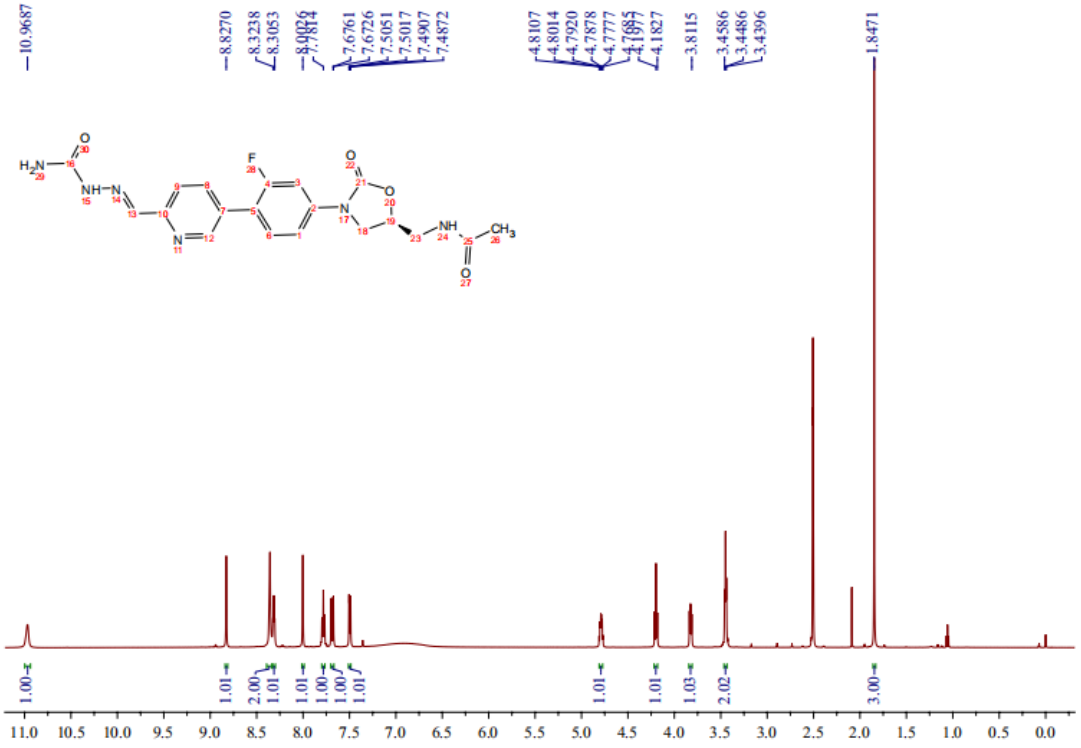

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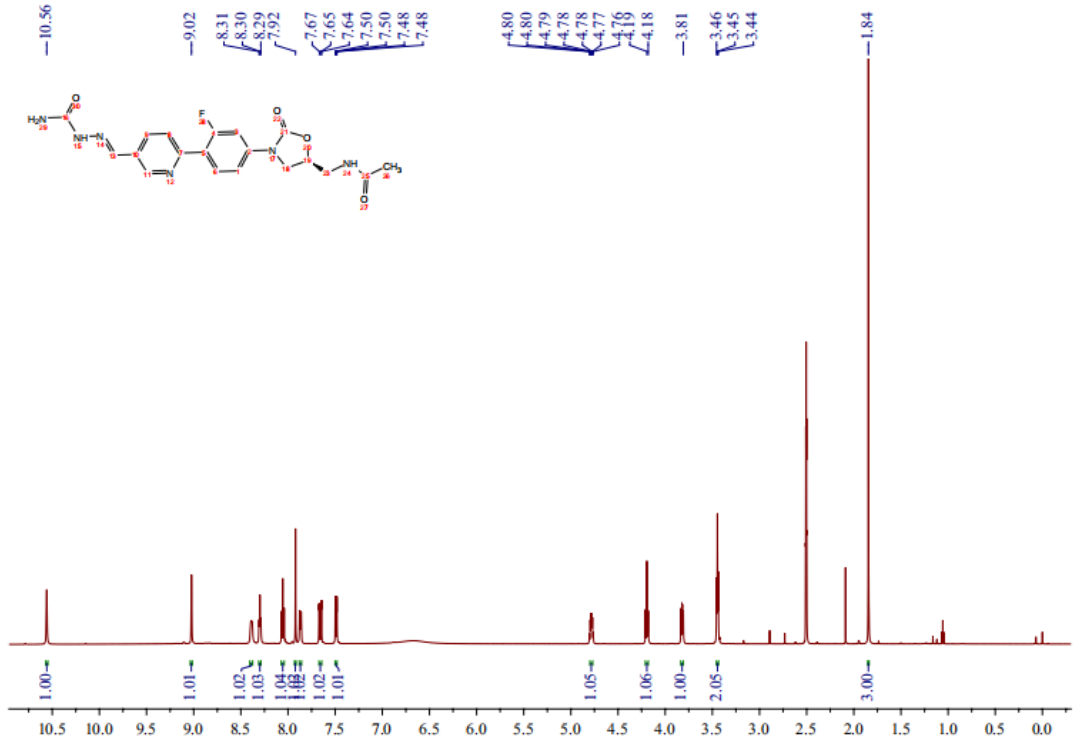

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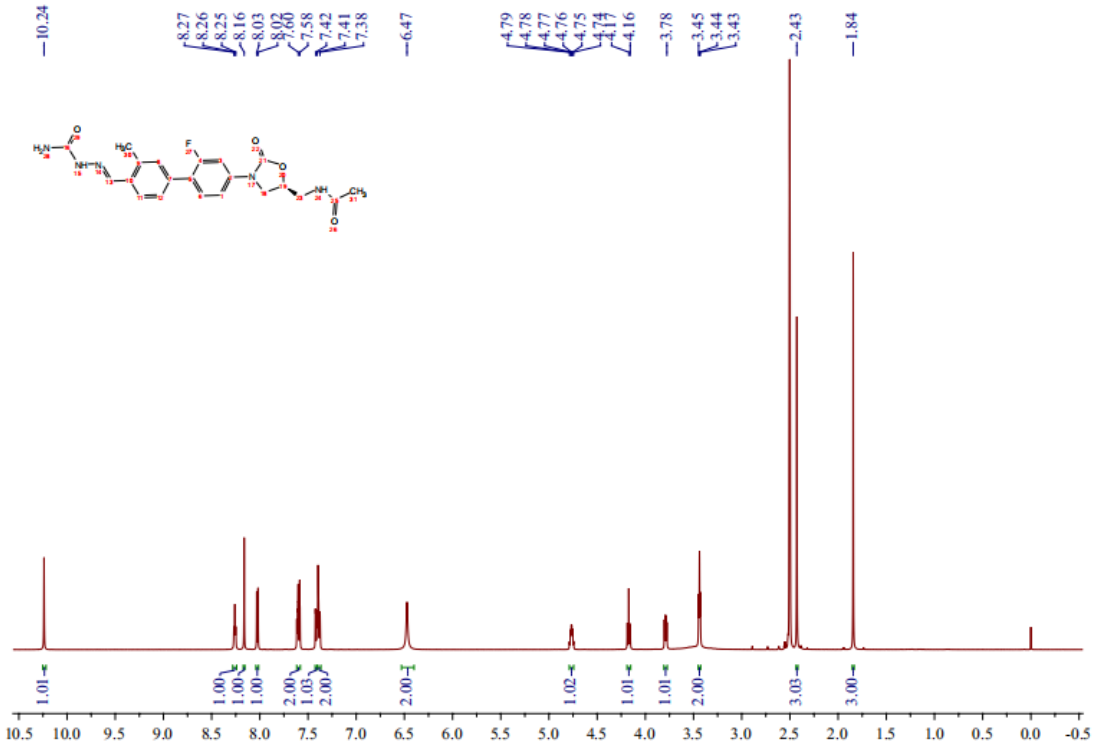

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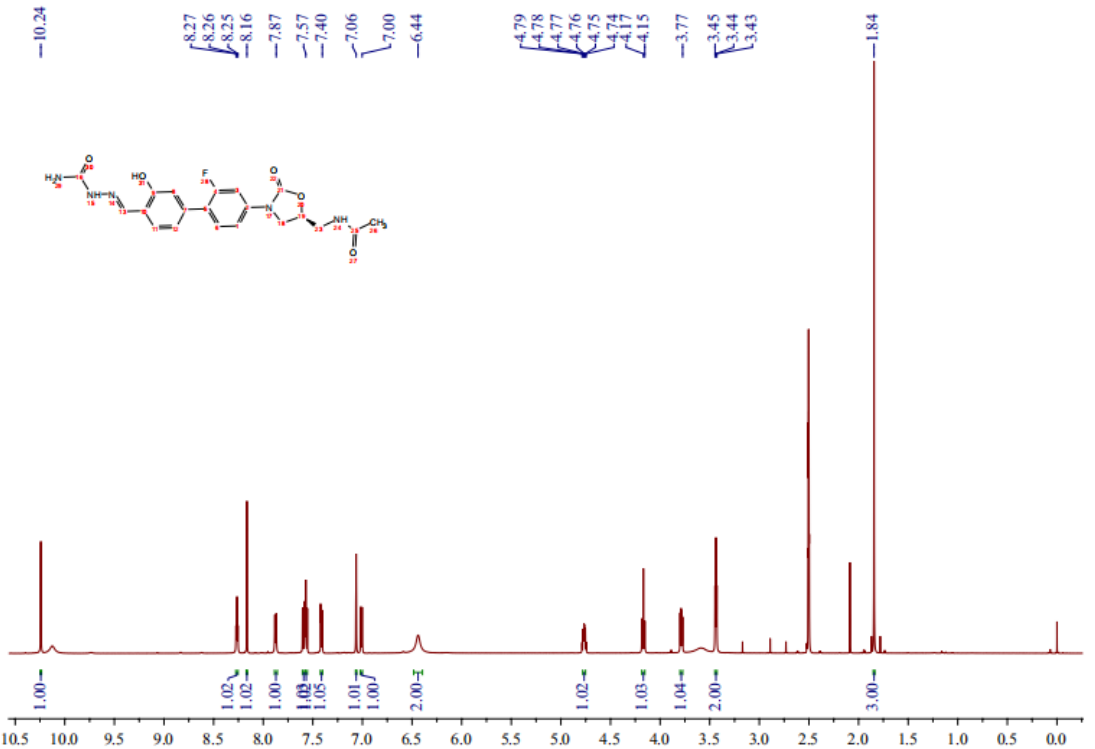

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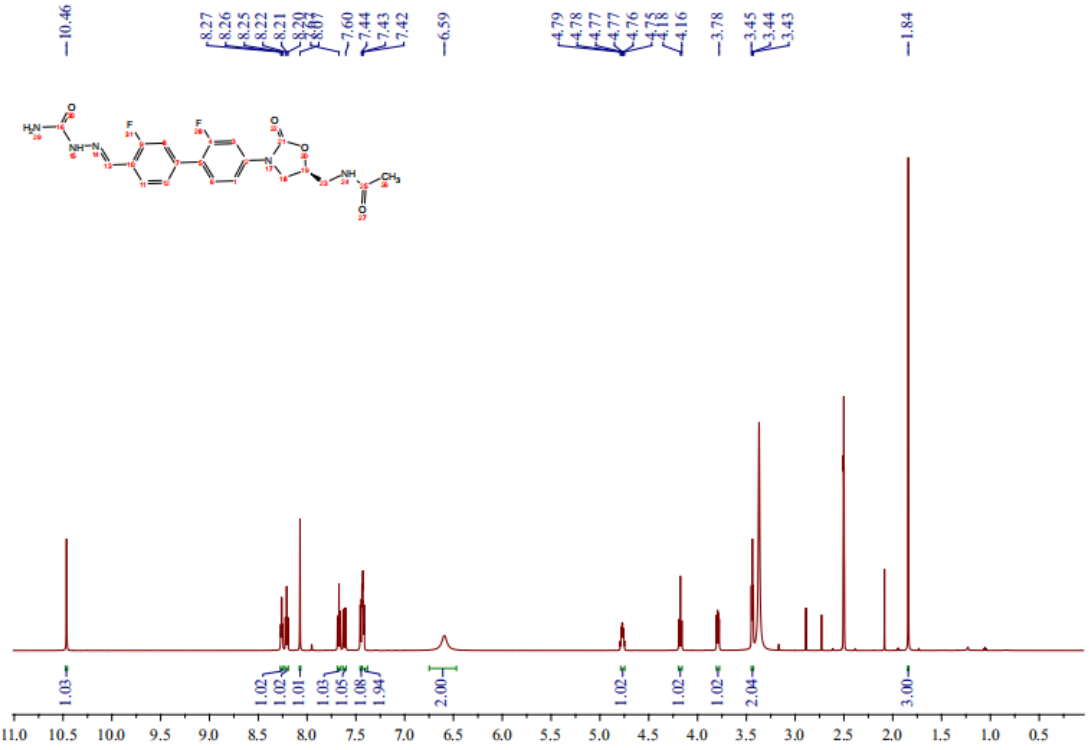

2. ^{13}C-NMR Spectra

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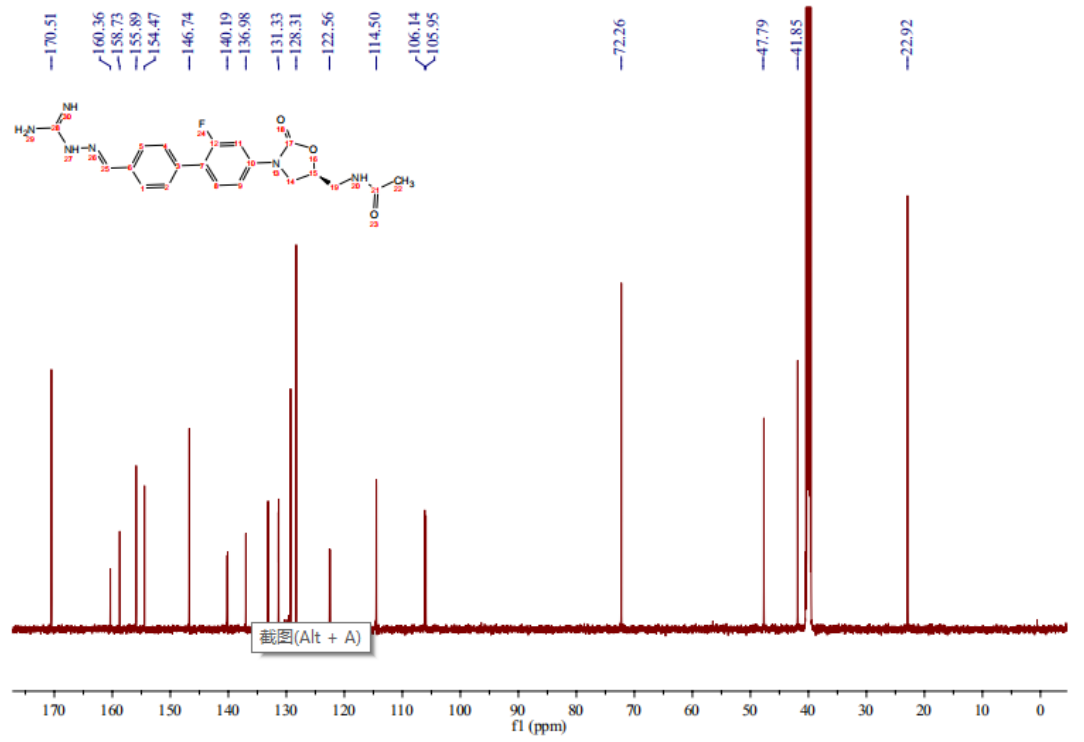

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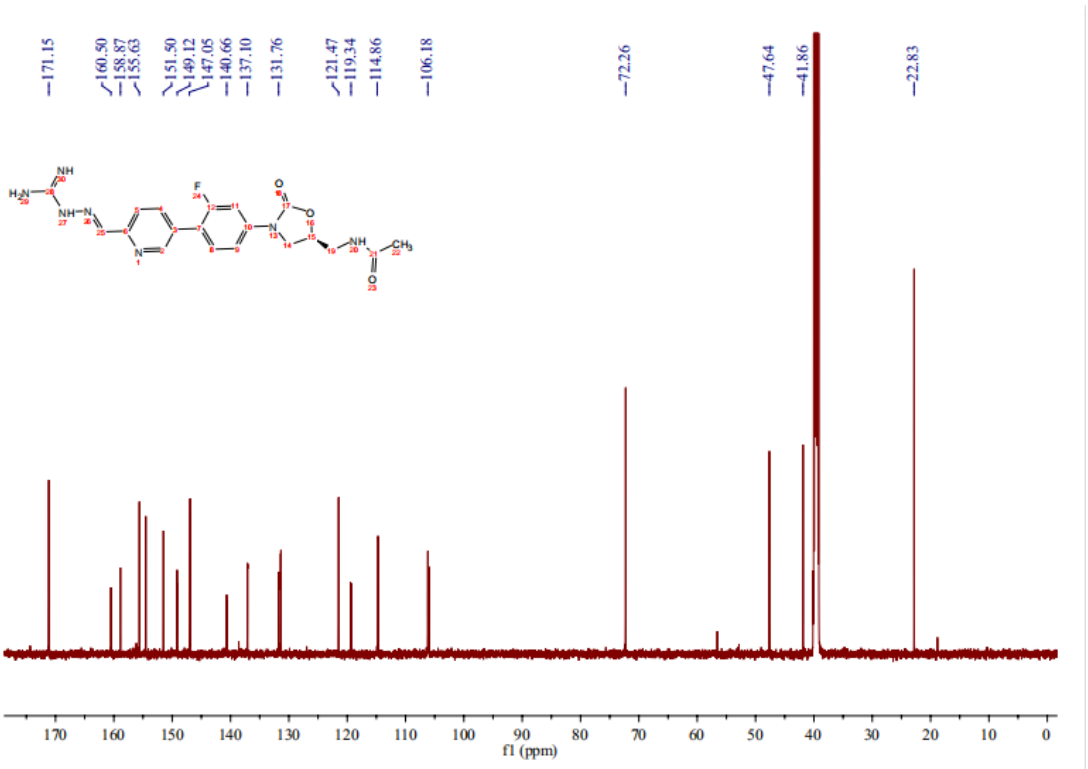

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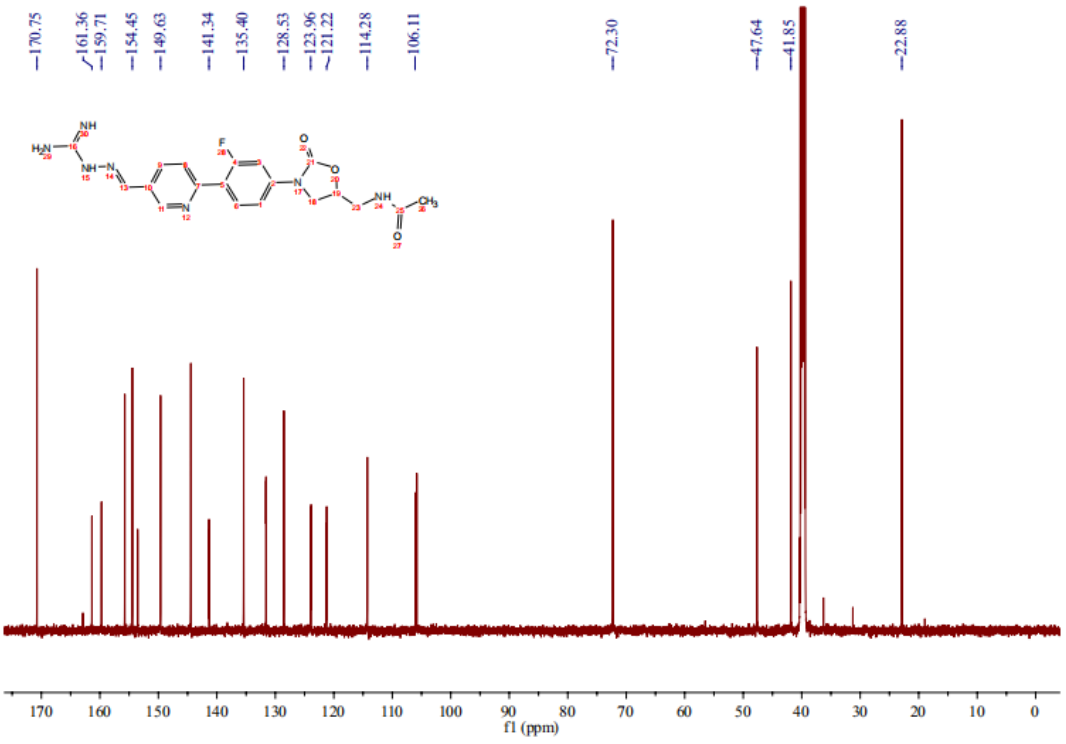

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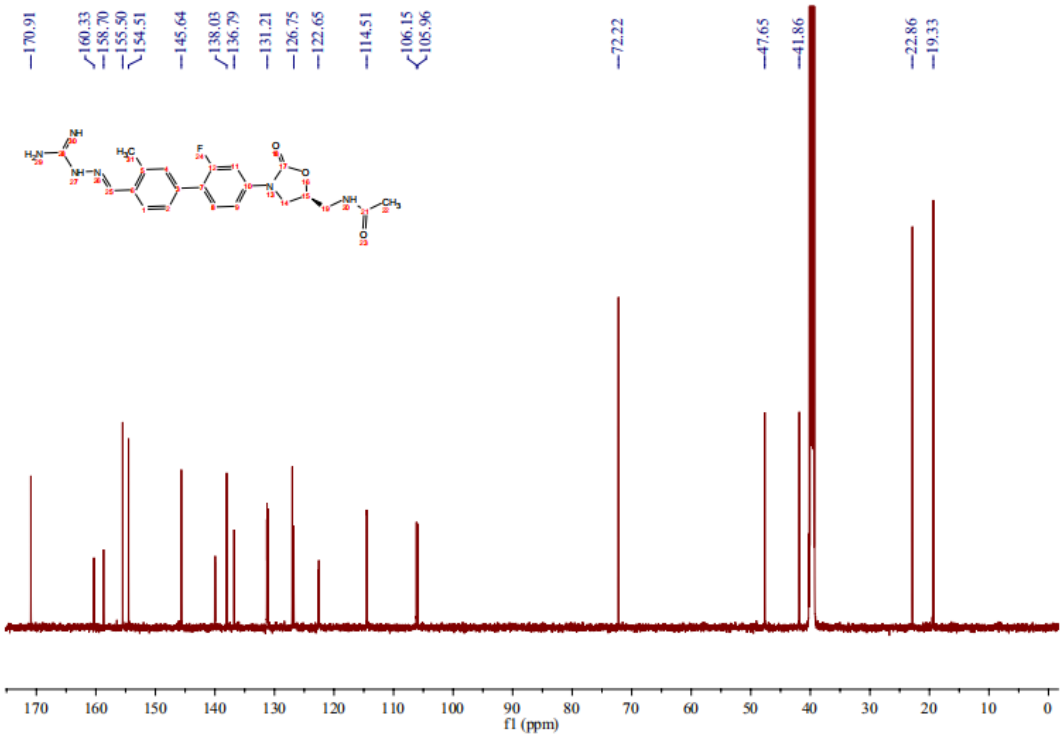

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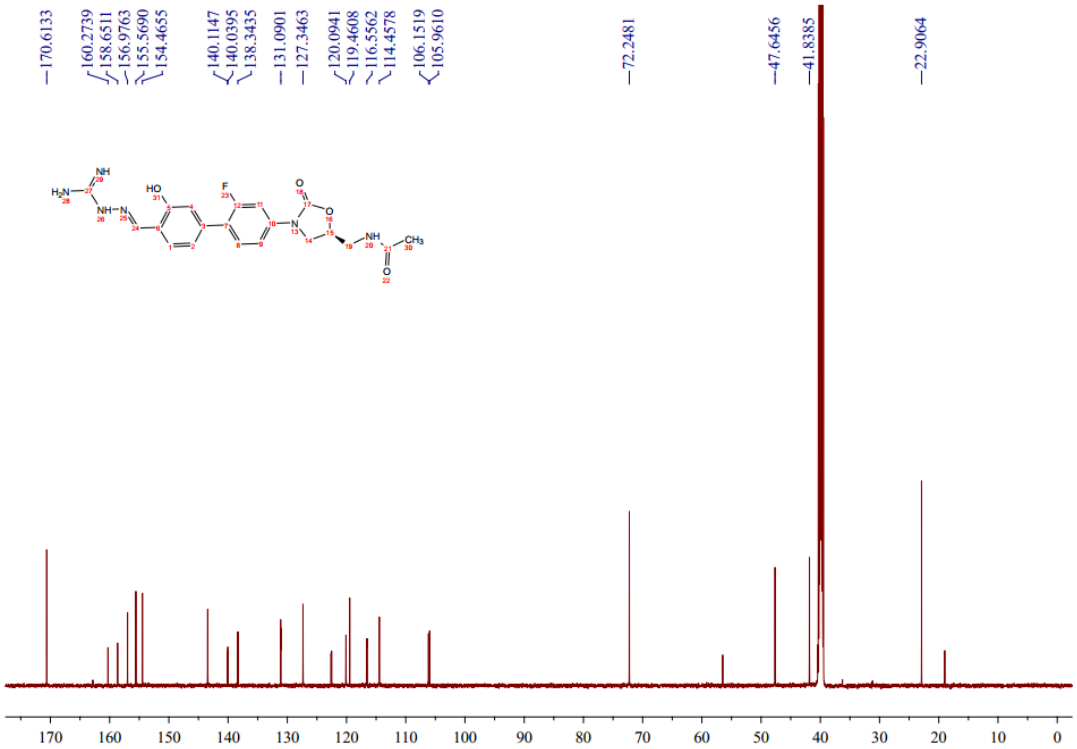
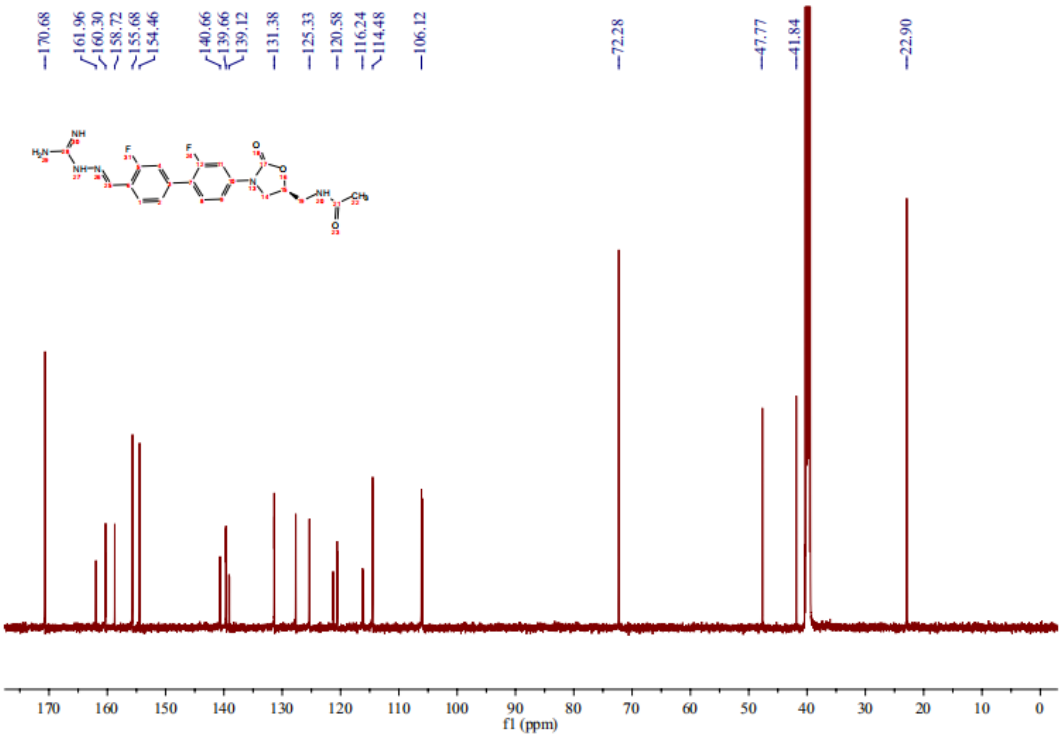


Compound 13a-6



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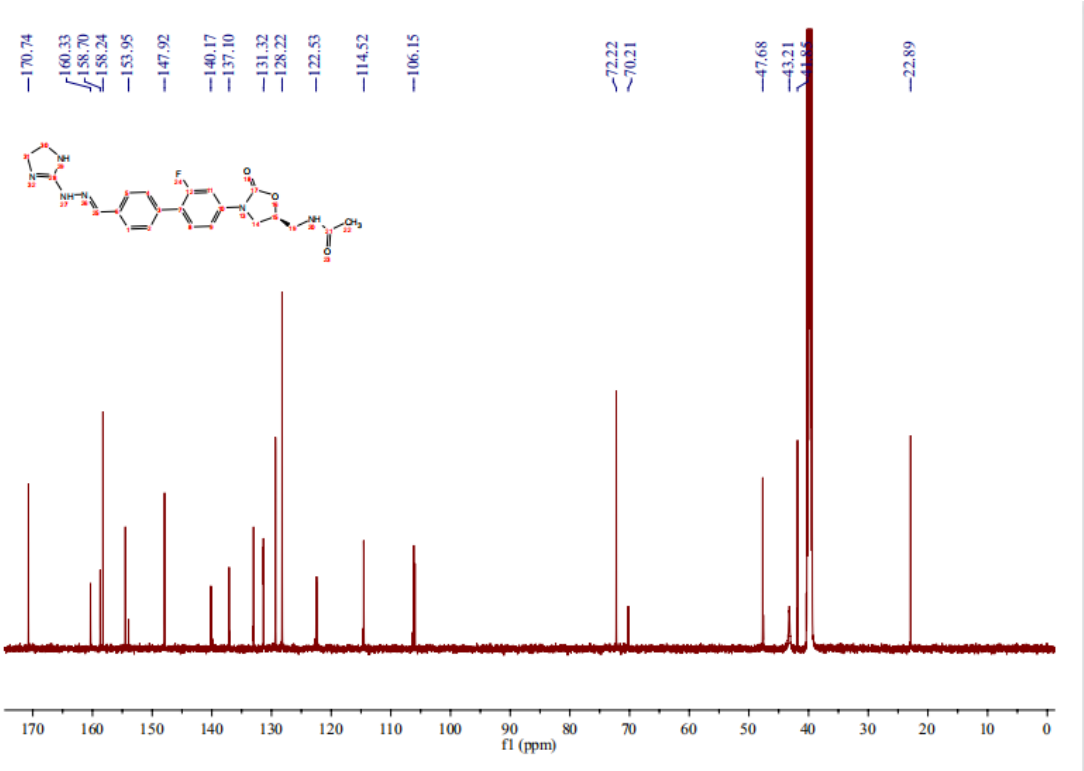

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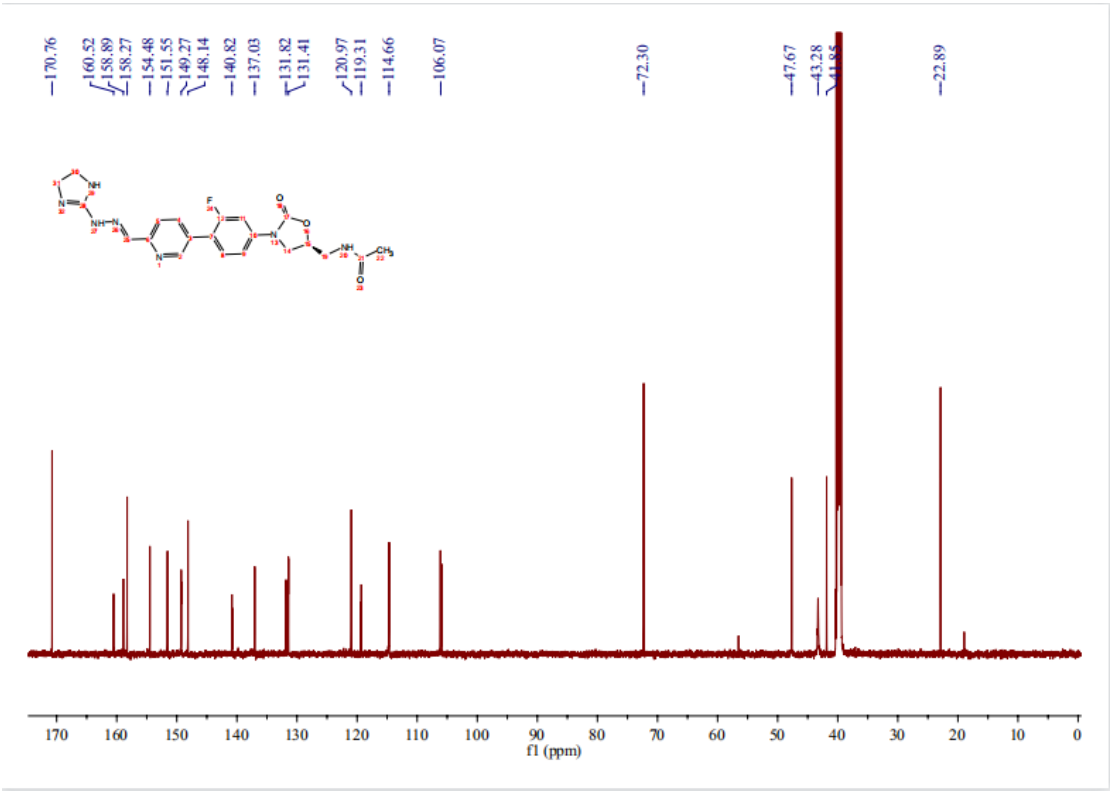

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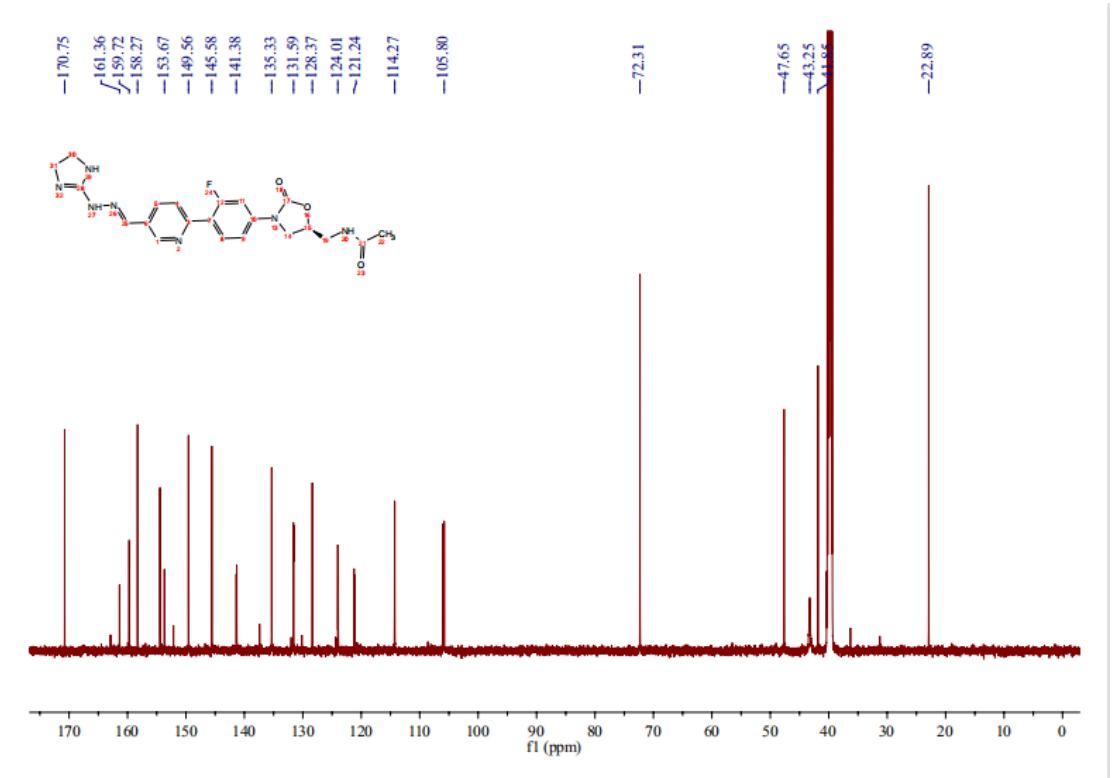

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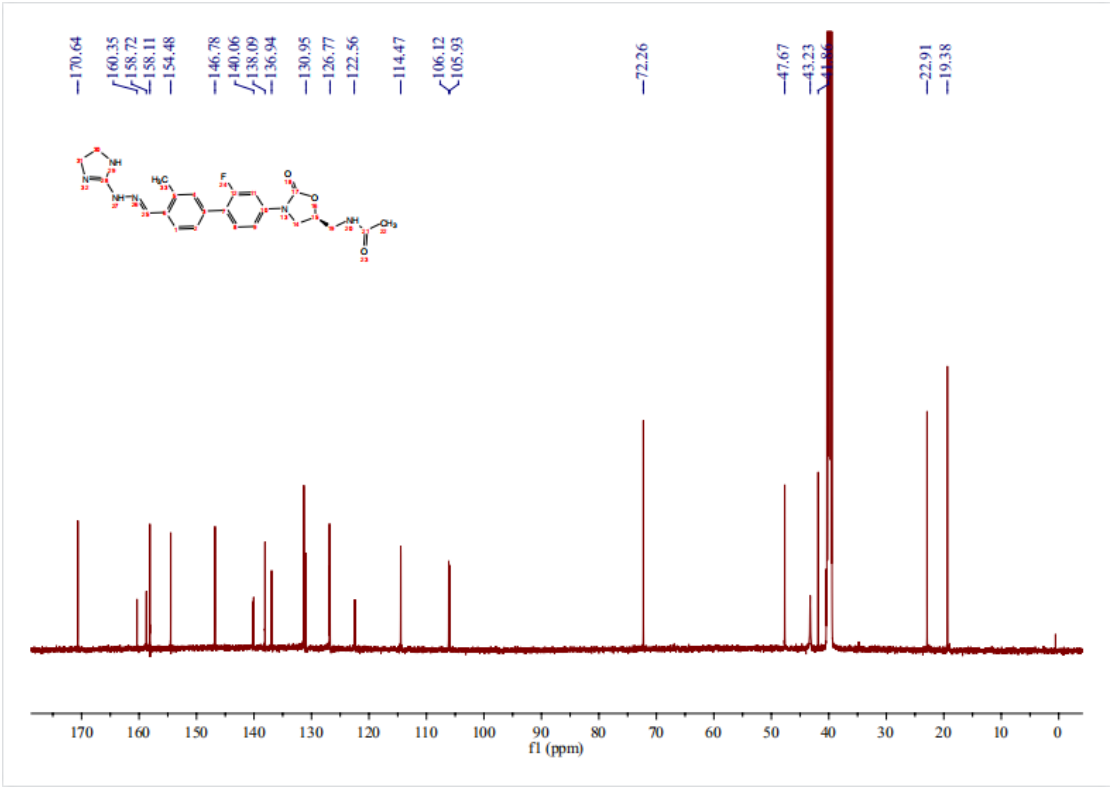

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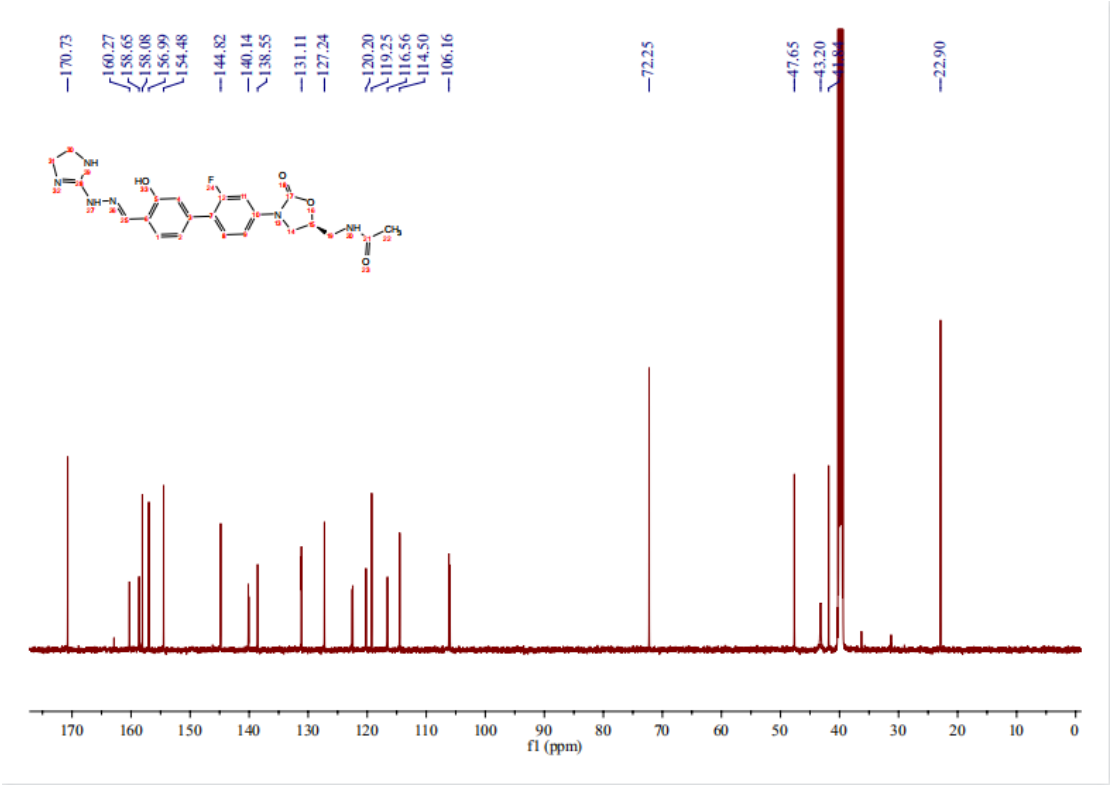

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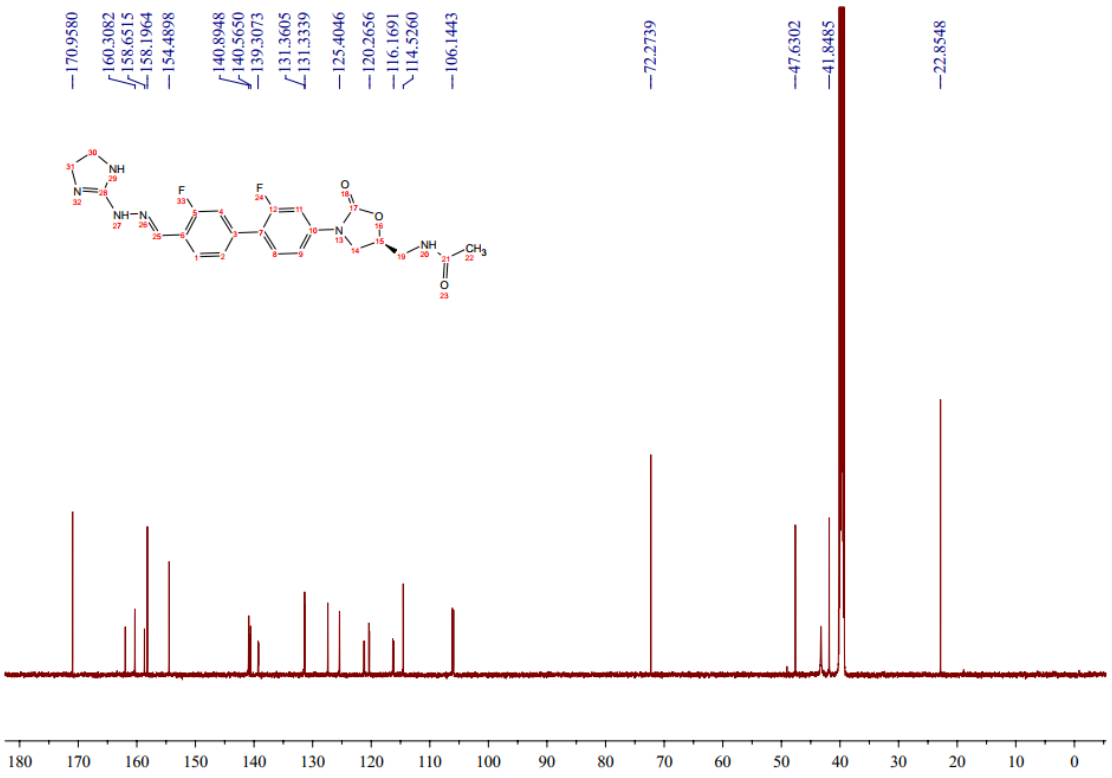

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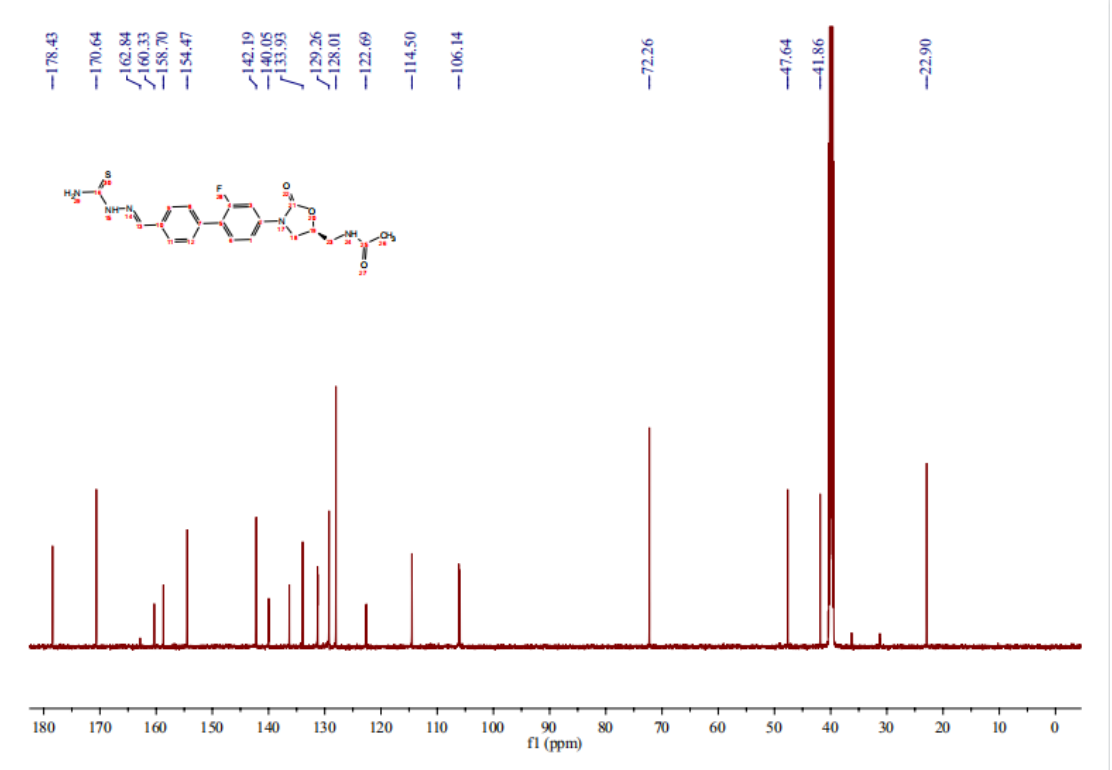

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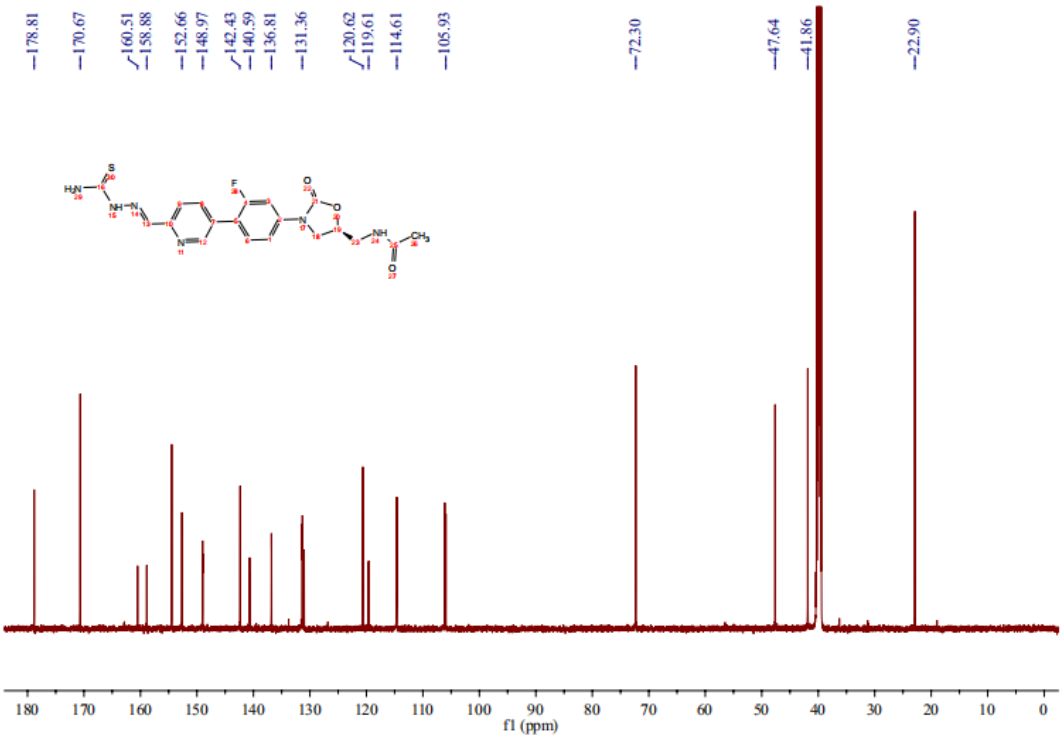

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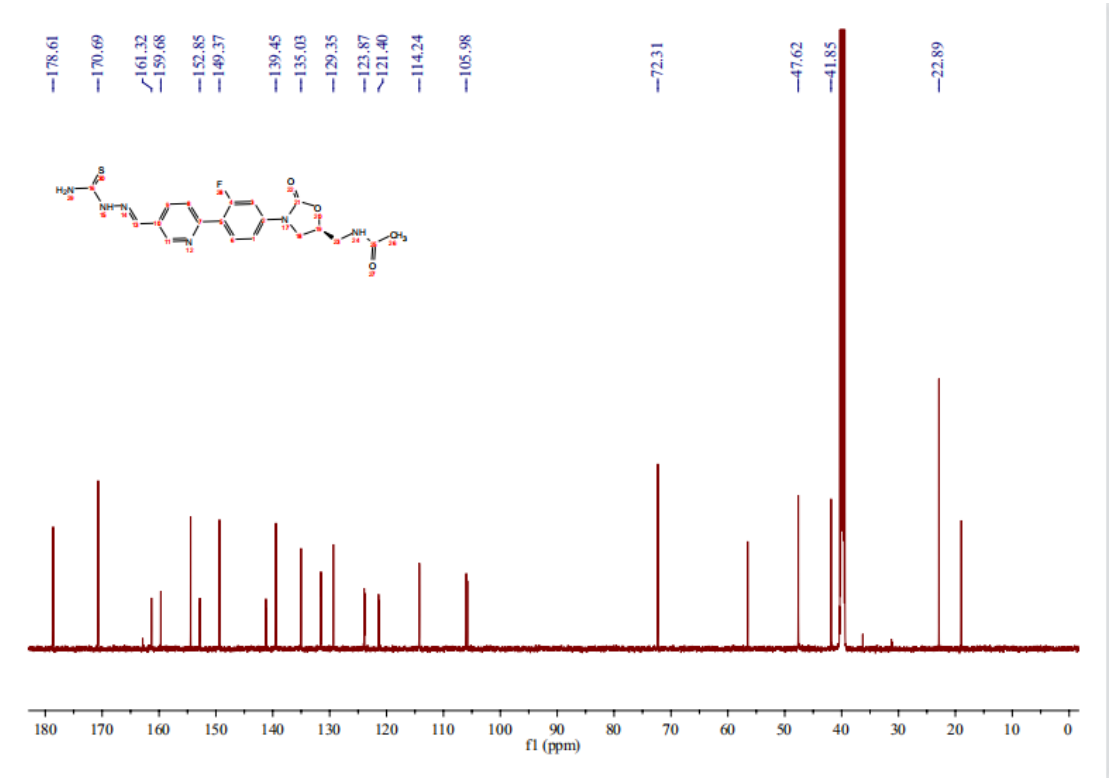

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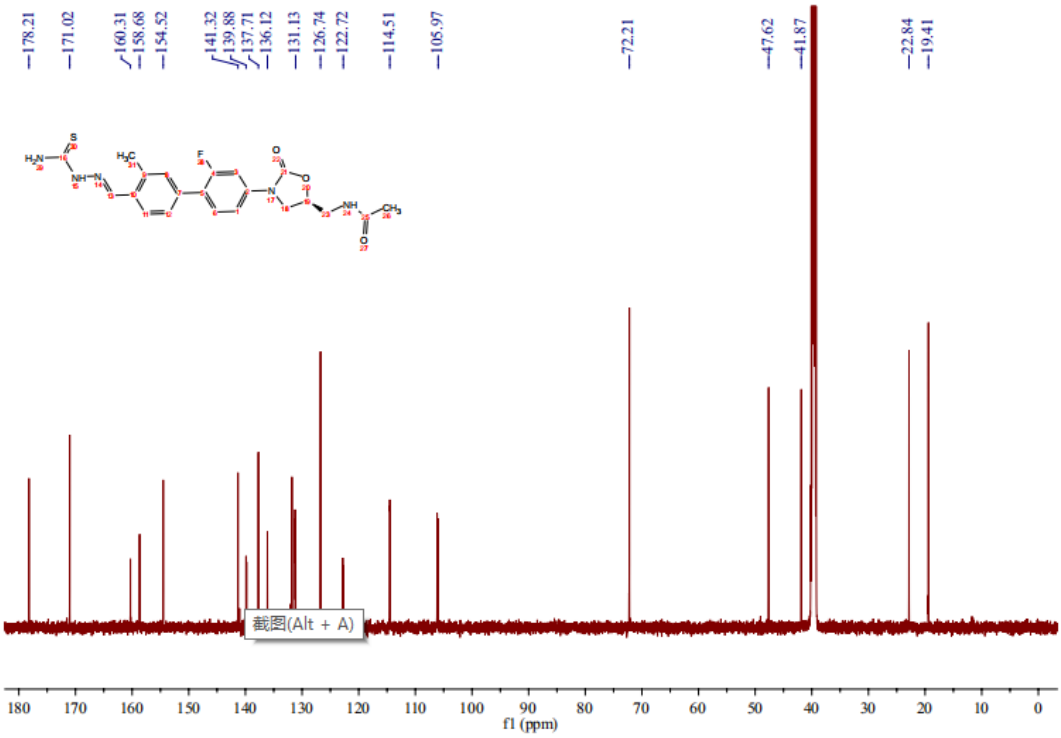

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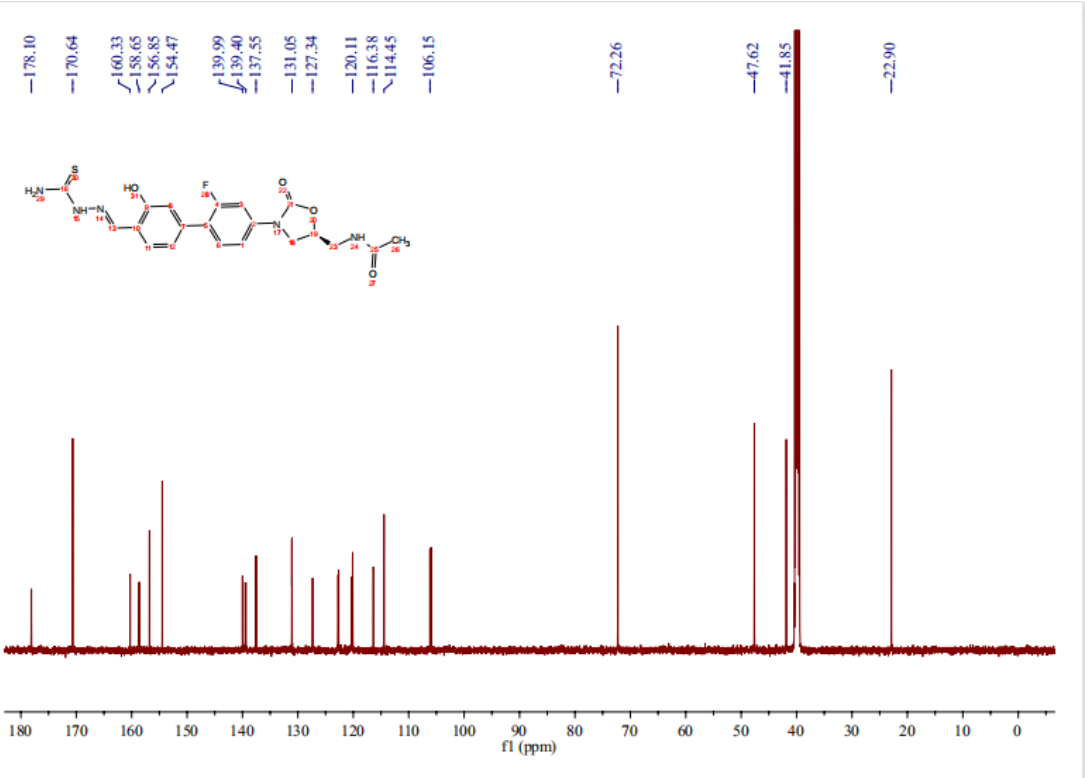
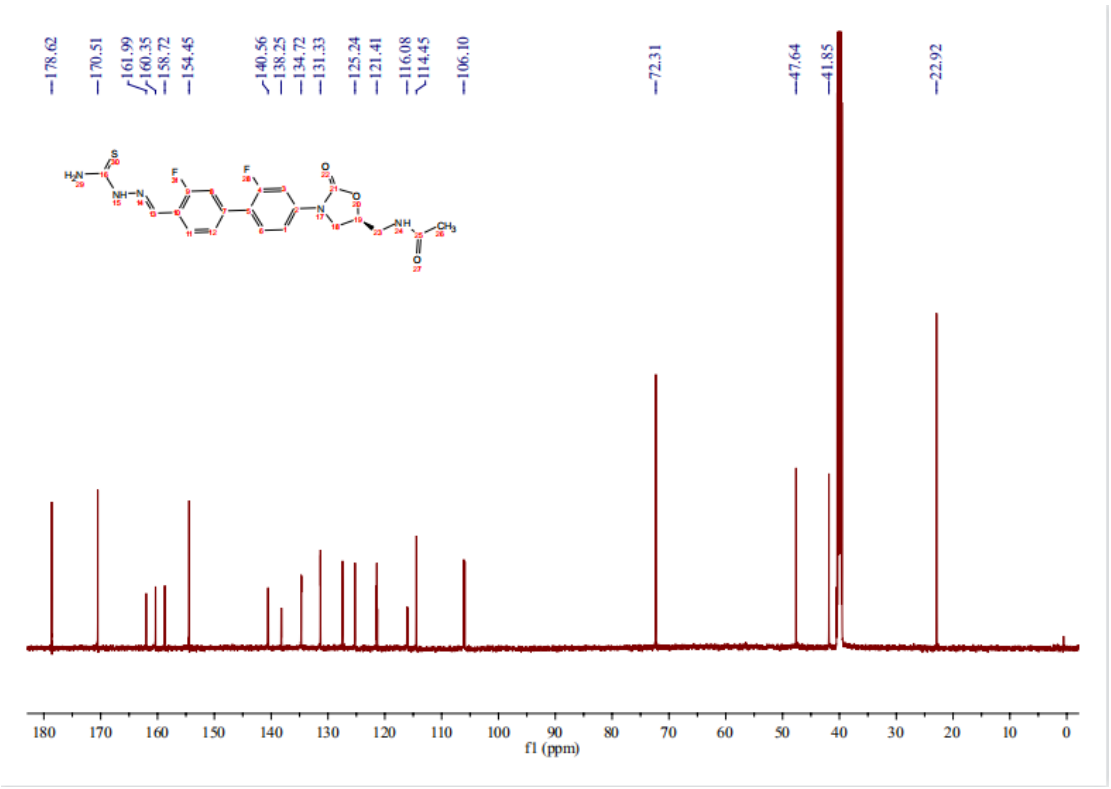
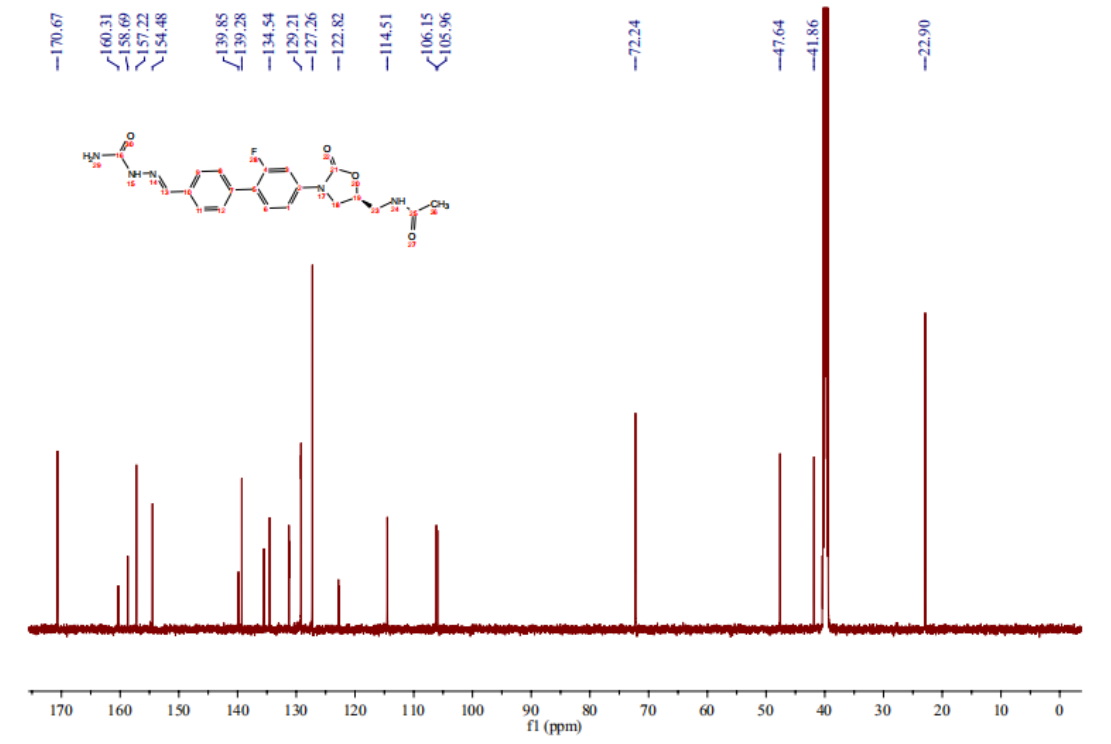


Compound 14a-6



Compound 14b-1



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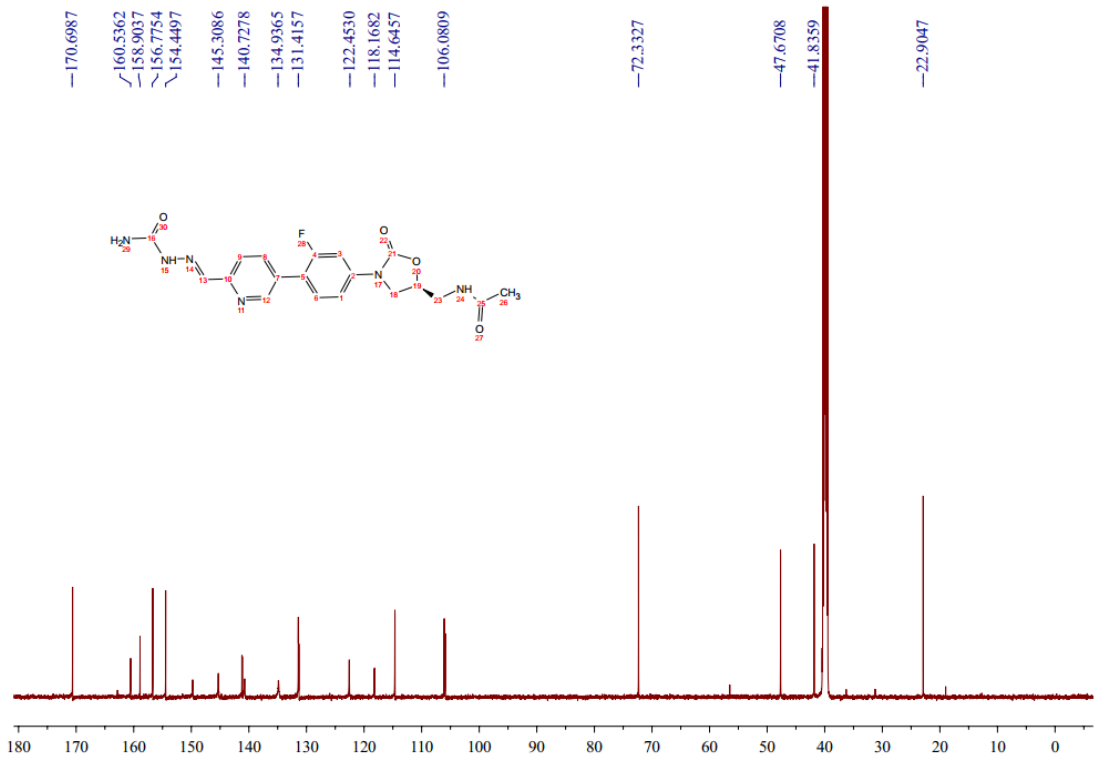

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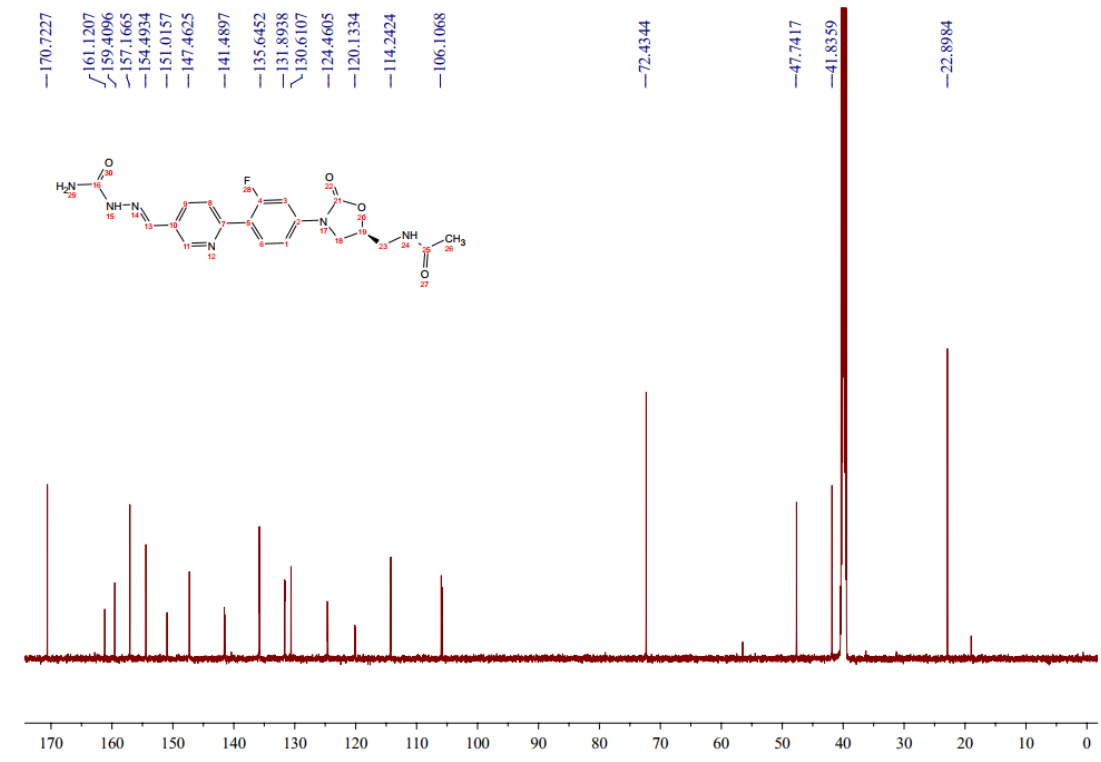

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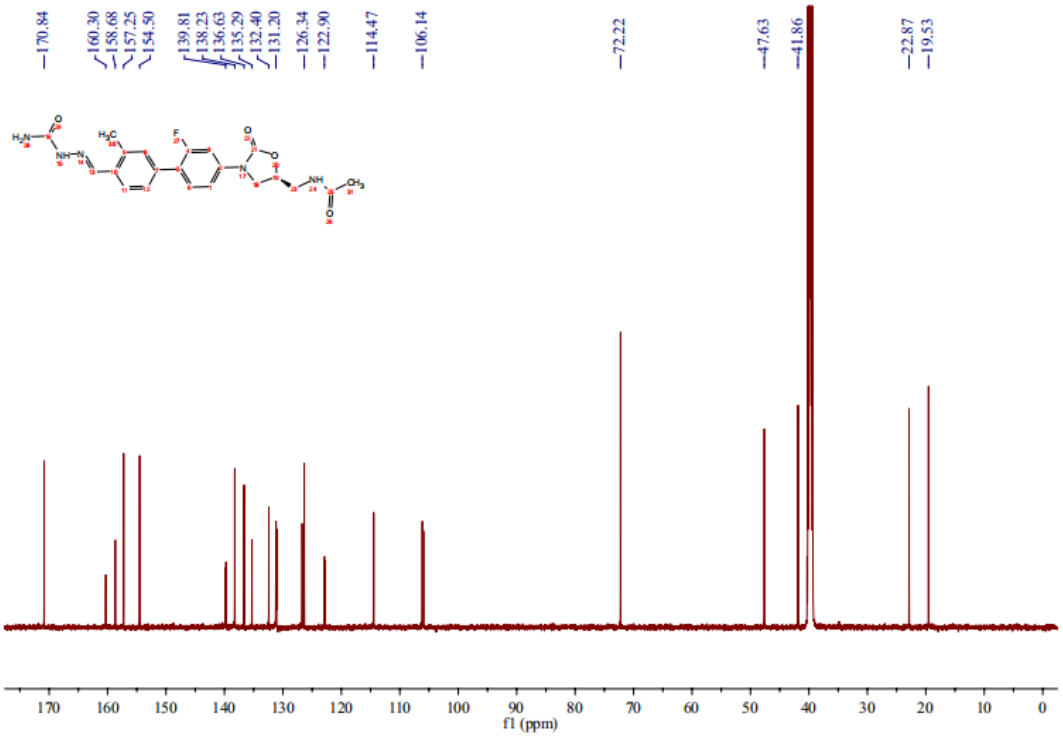

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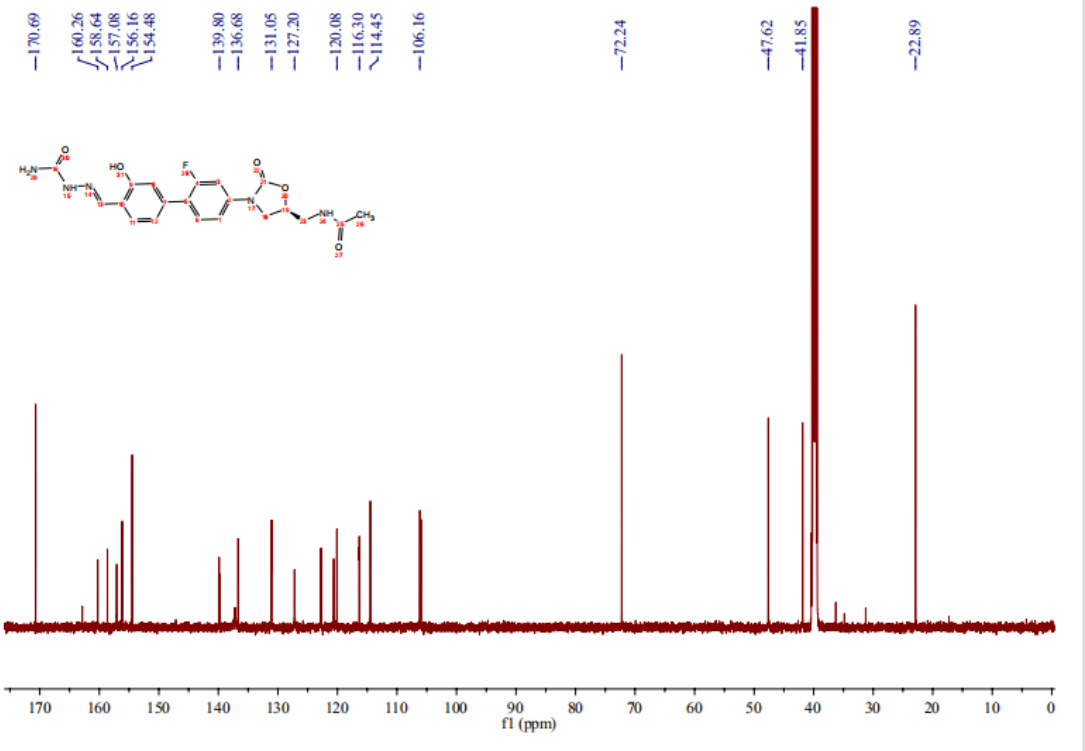
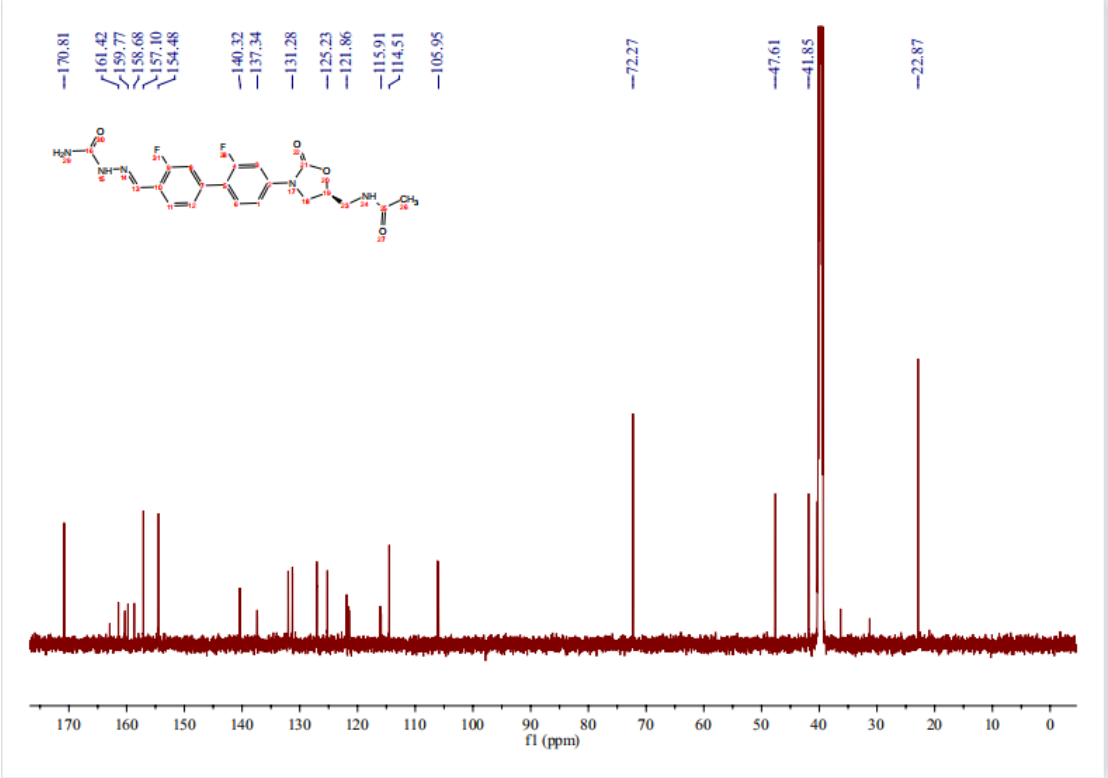
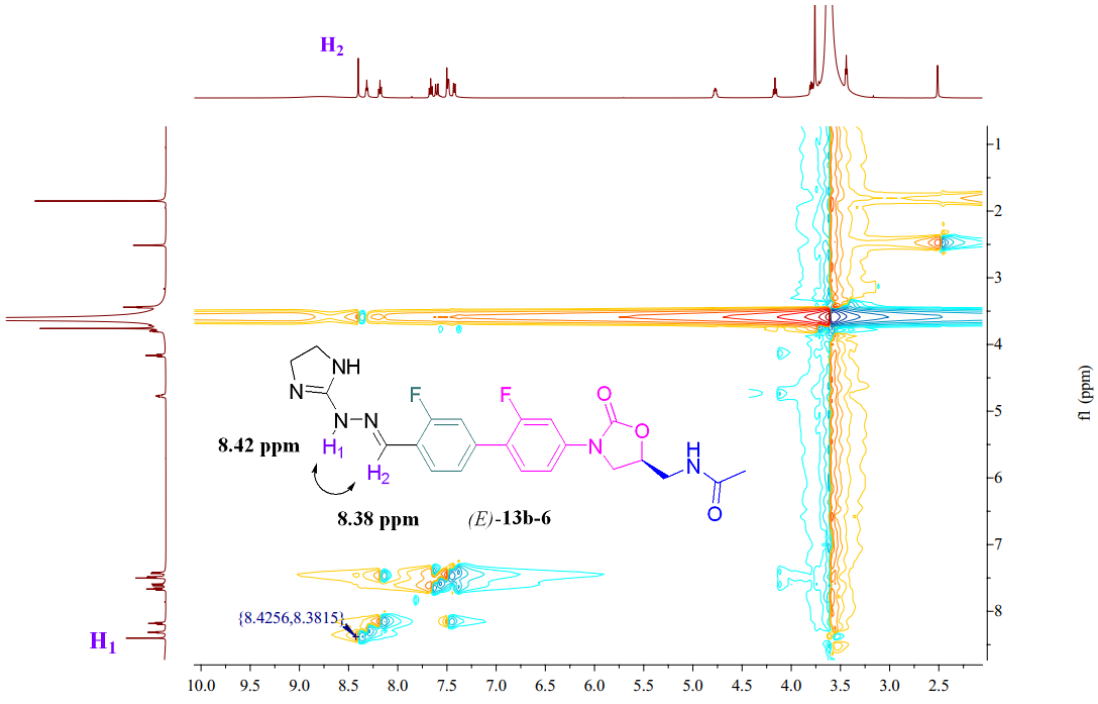


Compound 14b-6

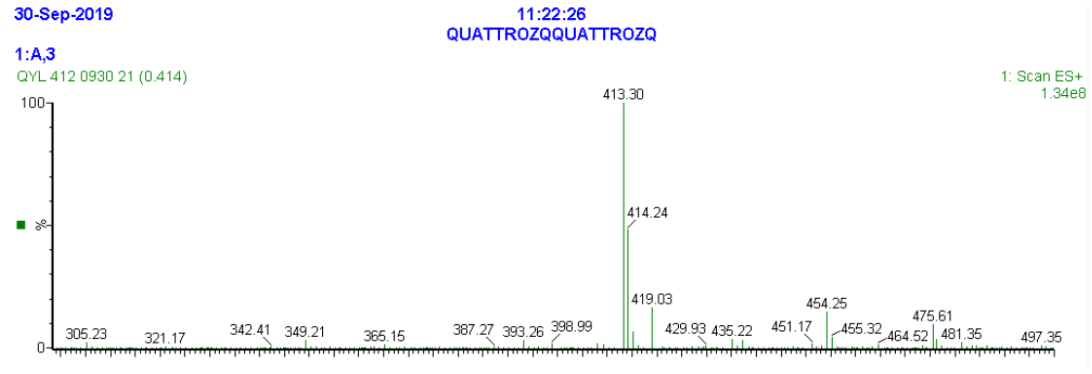


3. NOESY spectrum of compound **13b-6**

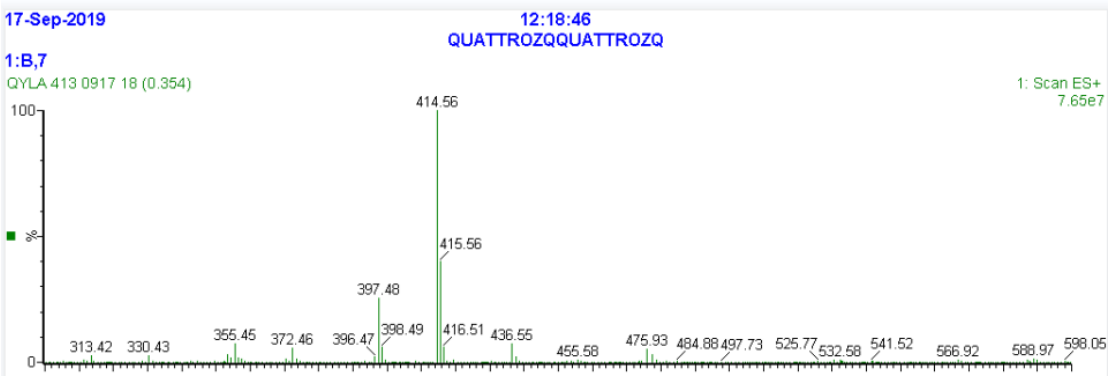


4.MS spectrum

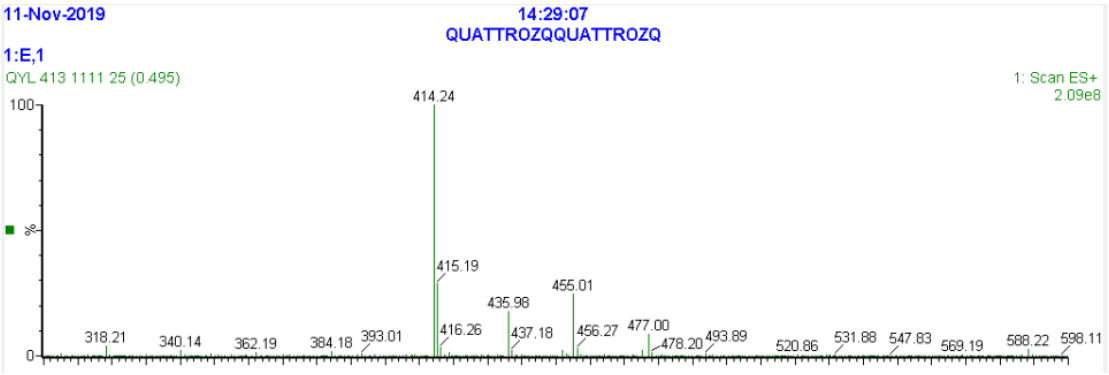
Compound 13a-1



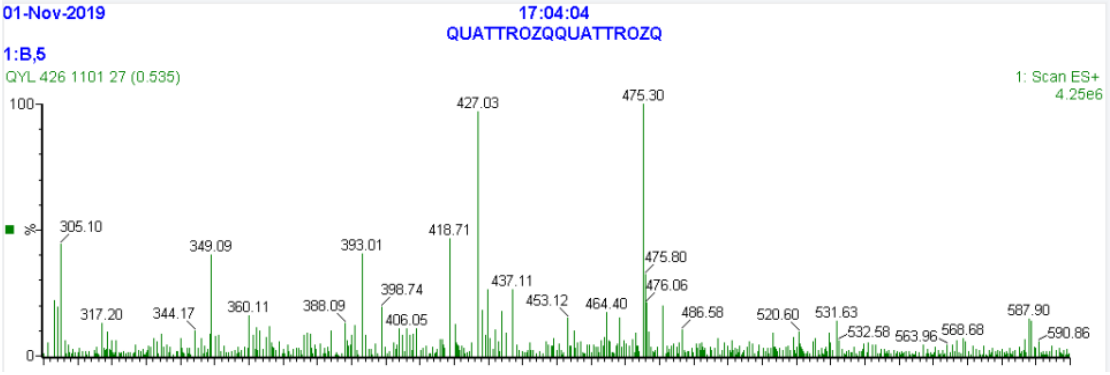
Compound 13a-2



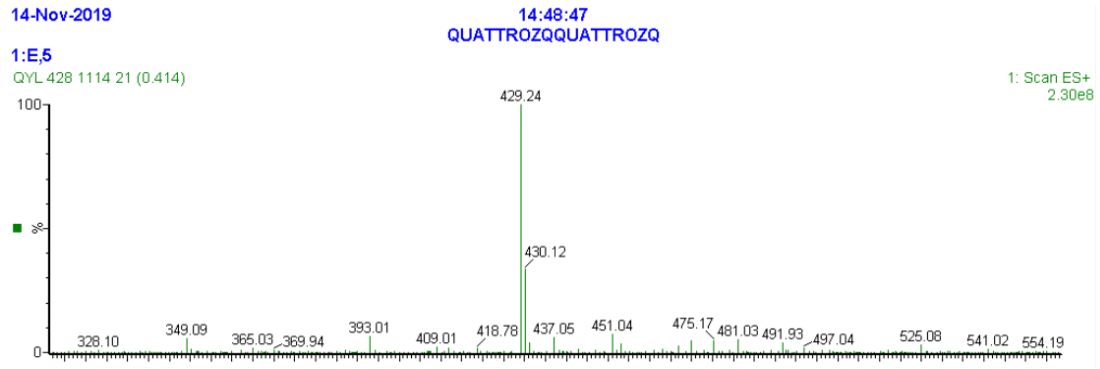
Compound 13a-3



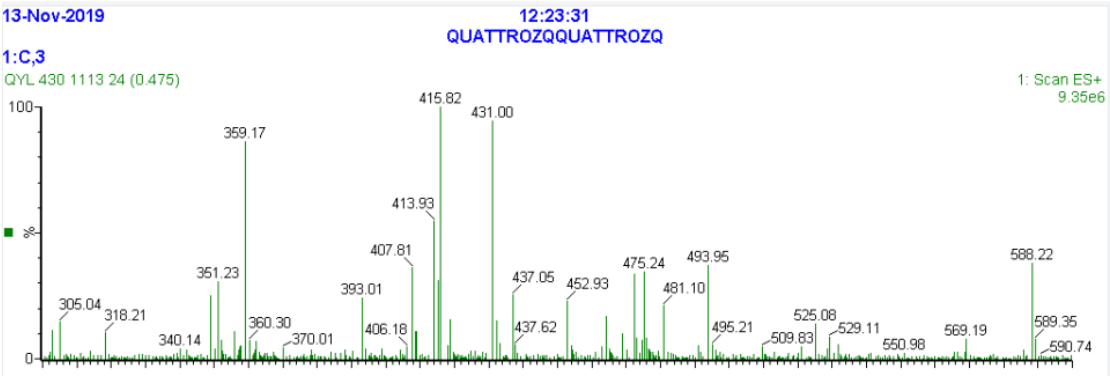
Compound 13a-4



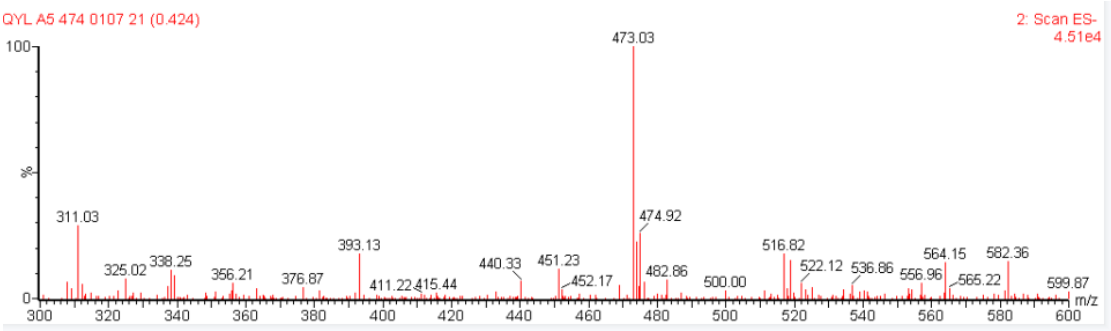
Compound 13a-5



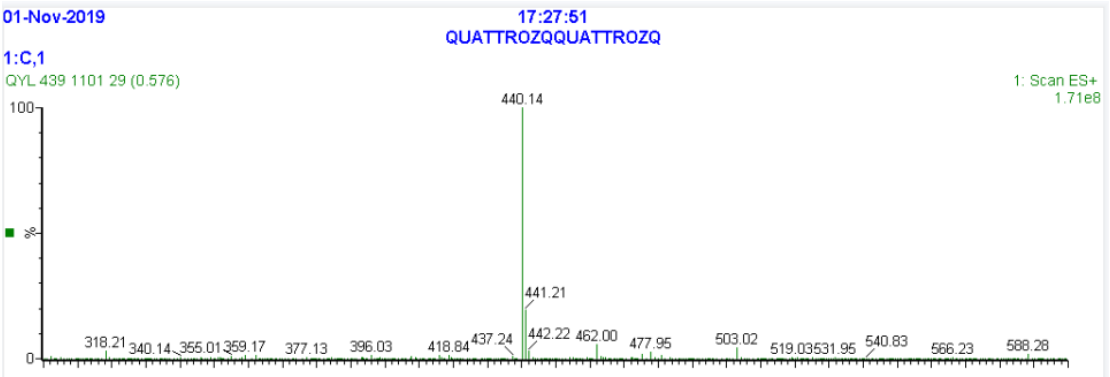
Compound 13a-6



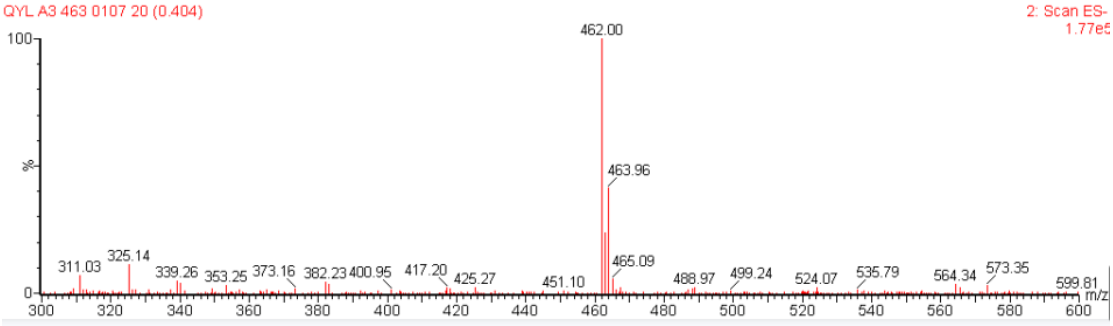
Compound 13b-1



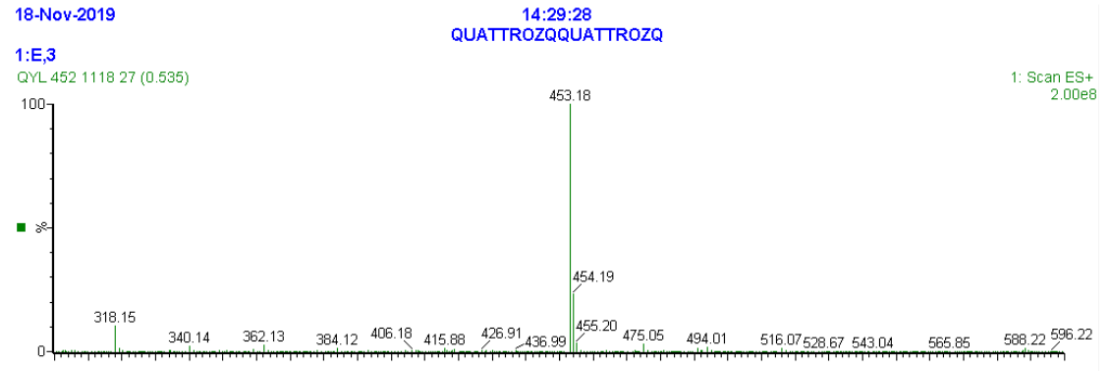
Compound 13b-2



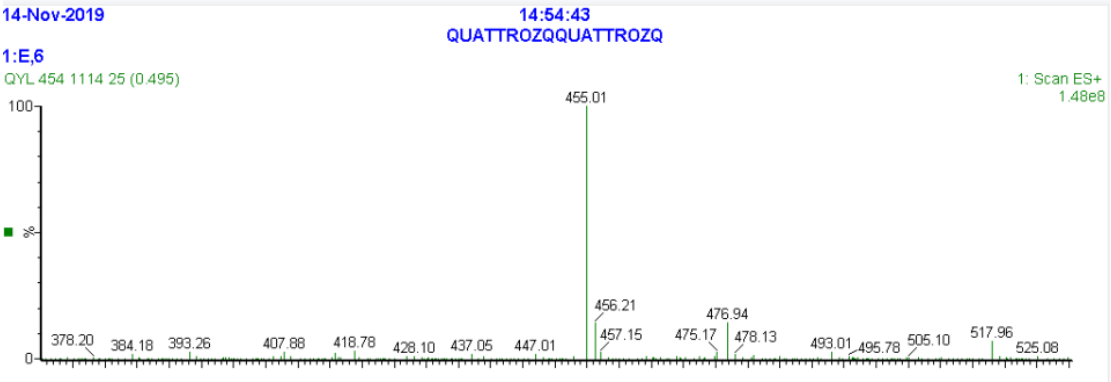
Compound 13b-3



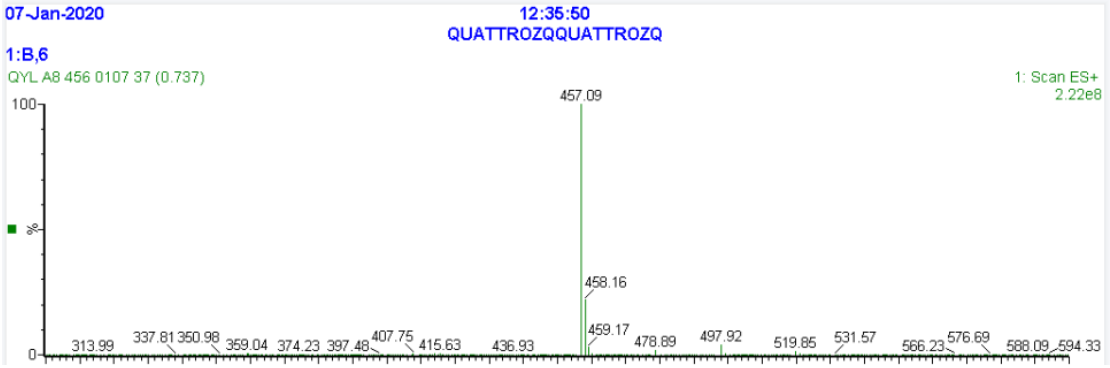
Compound 13b-4



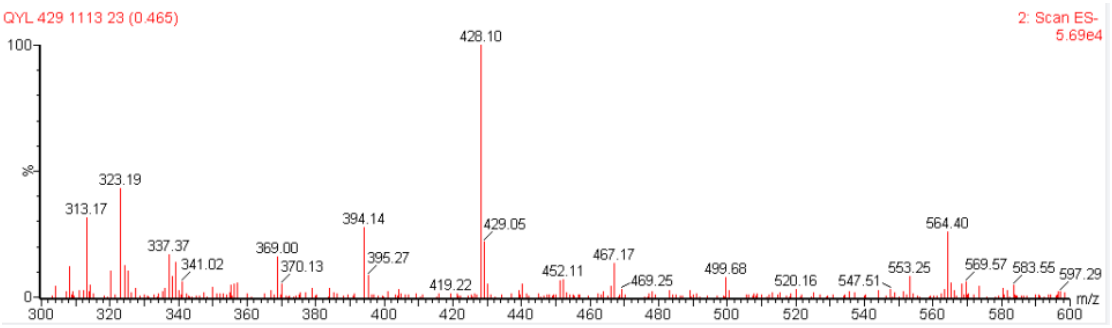
Compound 13b-5



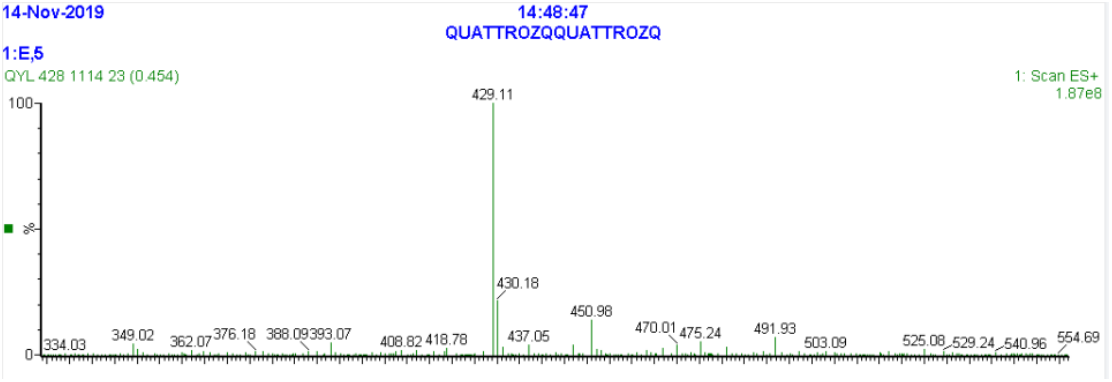
Compound 13b-6



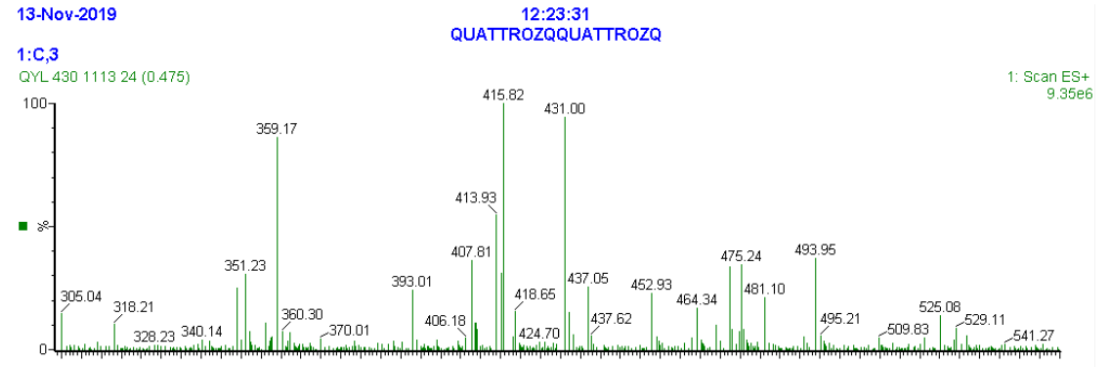
Compound 14a-1



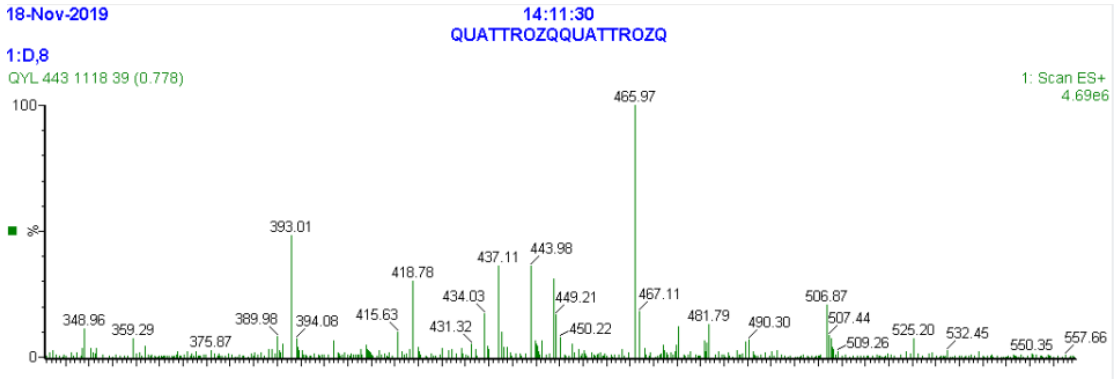
Compound 14a-2



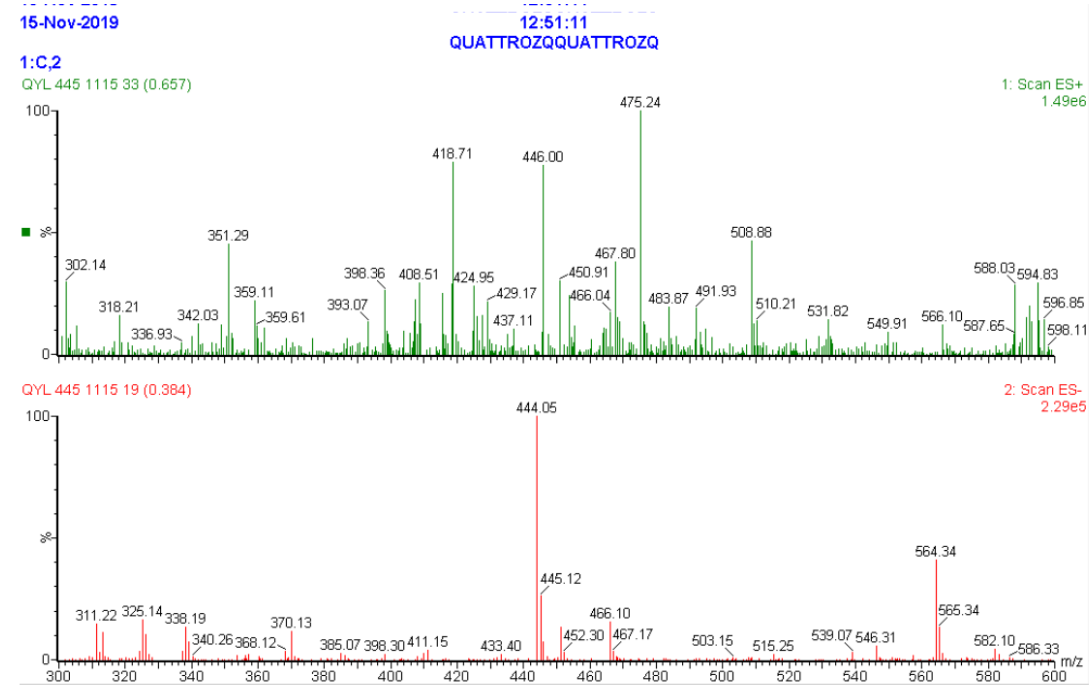
Compound 14a-3



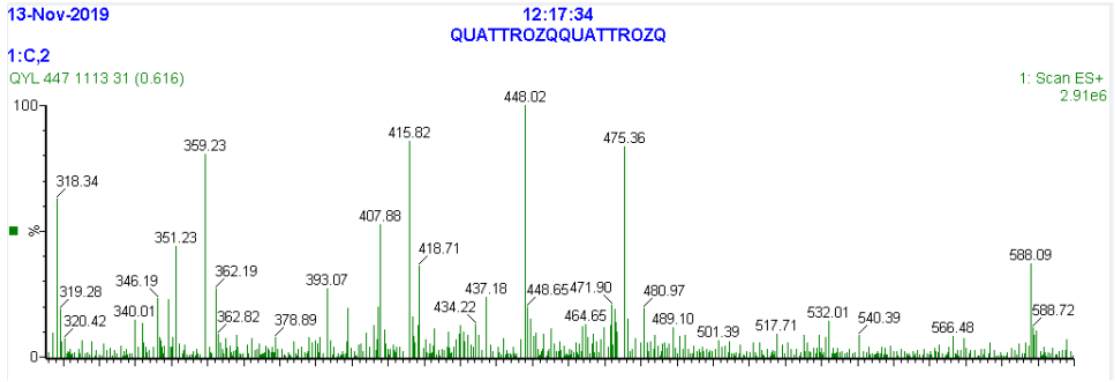
Compound 14a-4



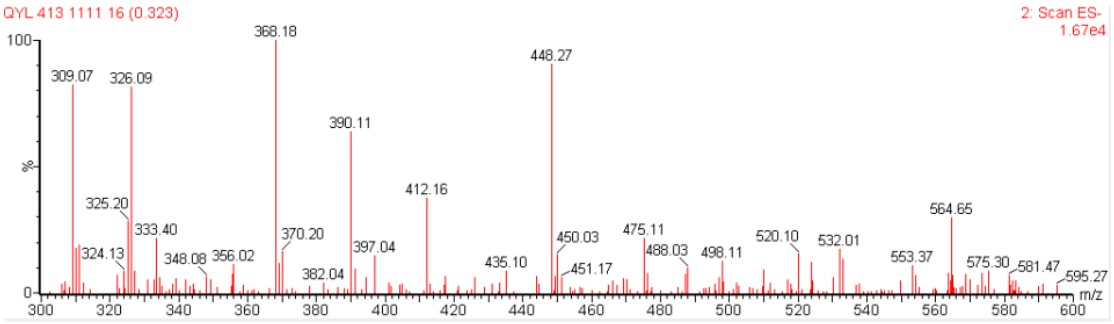
Compound 14a-5



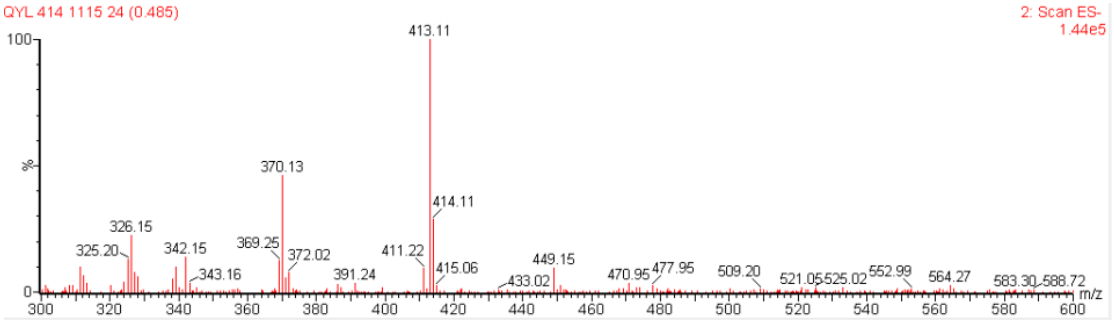
Compound 14a-6



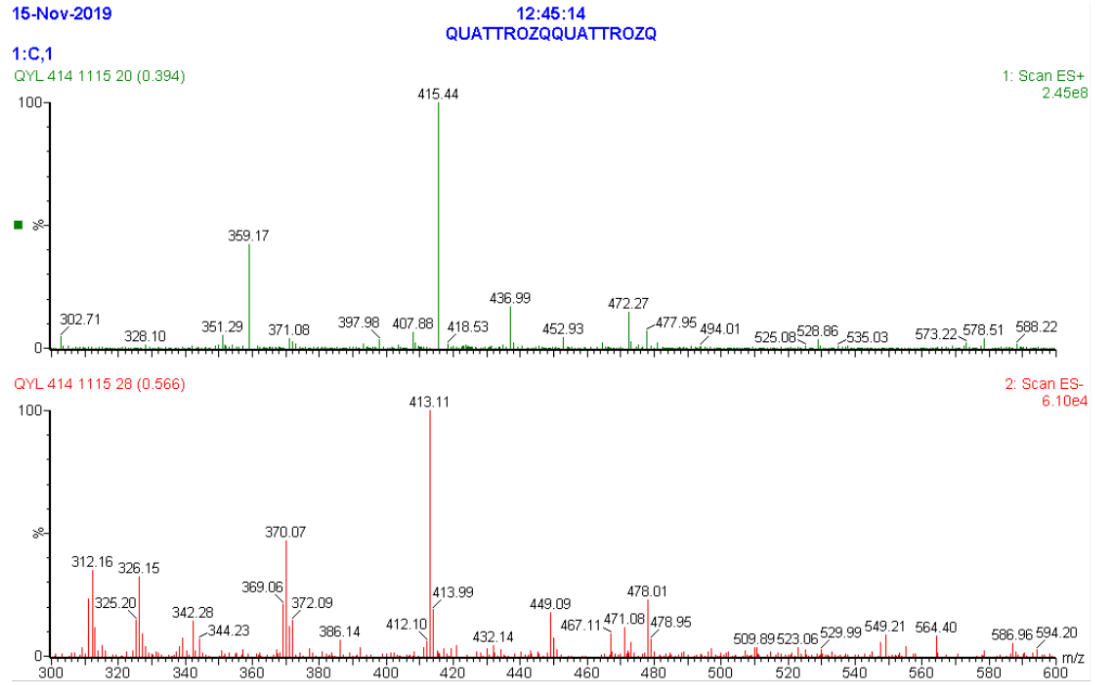
Compound 14b-1



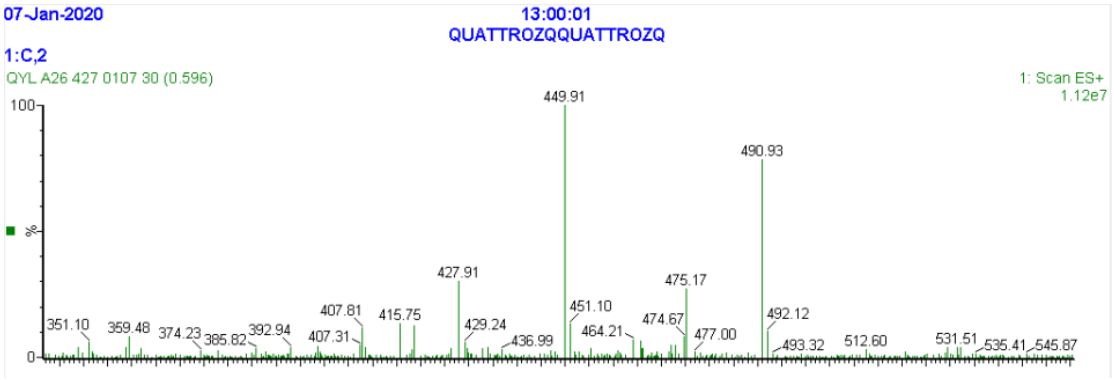
Compound 14b-2



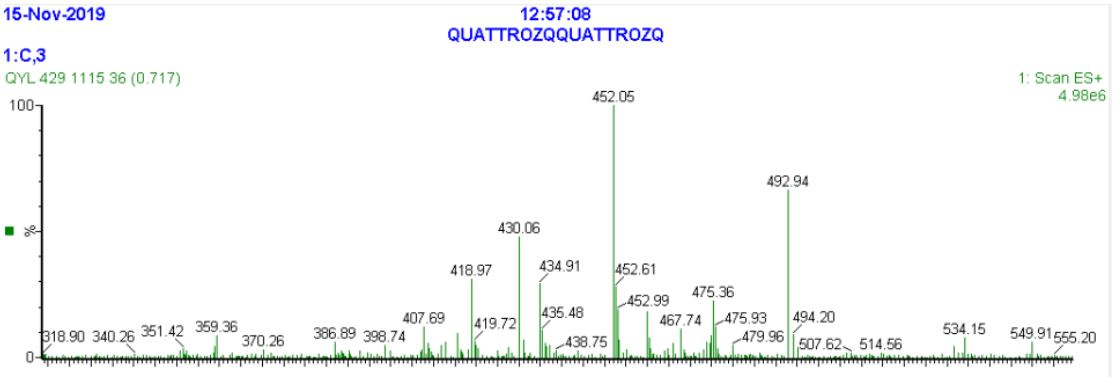
Compound 14b-3



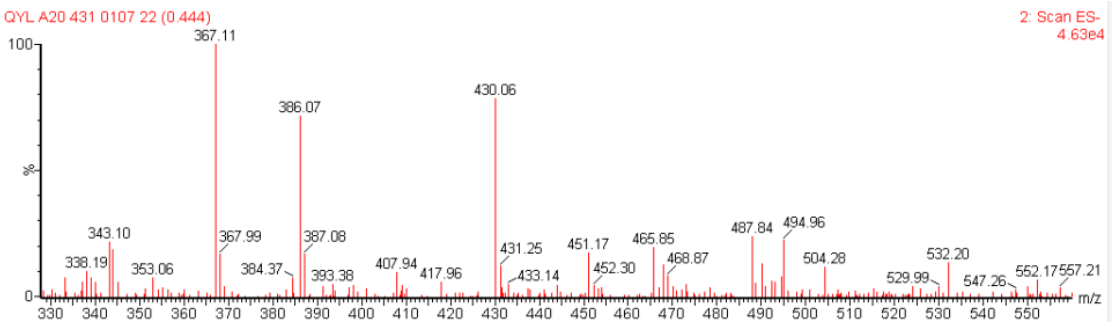
Compound 14b-4



Compound 14b-5



Compound 14b-6



Compound 13a-1

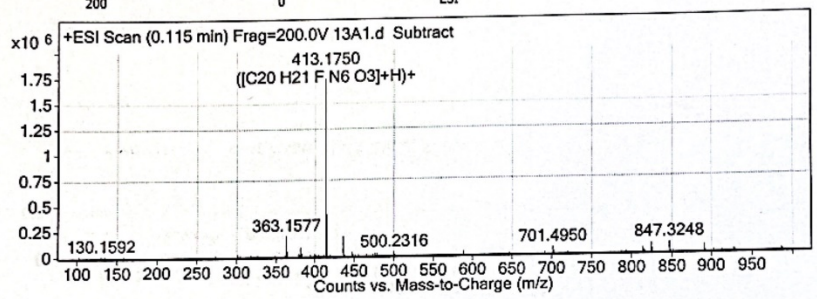
Qualitative Analysis Report

Data Filename	13A1.d	**Sample Name**	13A1
Sample Type	Sample	**Position**	P1-D6
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:07:13 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
363.1577	1	198729.25		
381.168	1	83921.41		
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	Max
C	3	60
H	0	120
O	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 O3	FALSE	412.1678	412.1659	-4.57	C20 H22 F N6 O3	91.32

--- End Of Report ---

Compound 13a-2

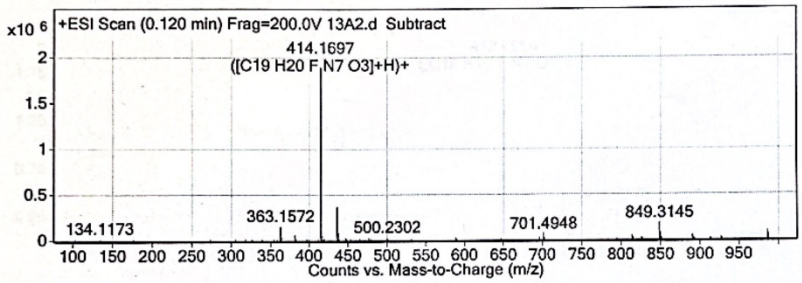
Qualitative Analysis Report

Data Filename	13A2.d	**Sample Name**	13A2
Sample Type	Sample	**Position**	P1-D7
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:10:09 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
363.1572	1	153184.36		
381.1668	1	58807.92		
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		
701.4948	1	63117.52		
849.3145	1	179315.47		
850.316	1	77845.45		
985.7147	1	87618.44		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	1	1

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C19 H20 F N7 O3	TRUE	413.1625	413.1612	-3.12	C19 H21 F N7 O3	95.59

--- End Of Report ---

Compound 13a-3

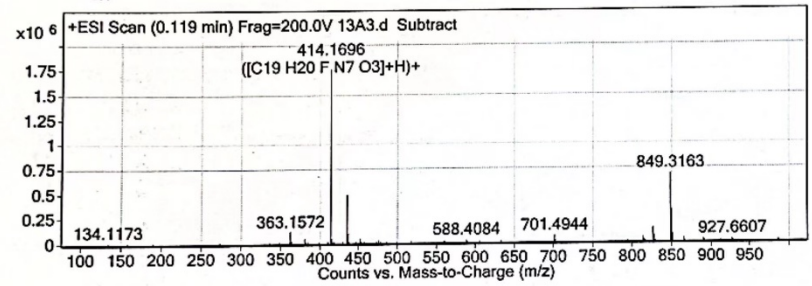
Qualitative Analysis Report

Data Filename	13A3.d	**Sample Name**	13A3
Sample Type	Sample	**Position**	P1-D8
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:13:05 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



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		
437.1559	1	99911.38		
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 Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	1	1

Formula Calculator Results

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

--- End Of Report ---

Compound 13a-4

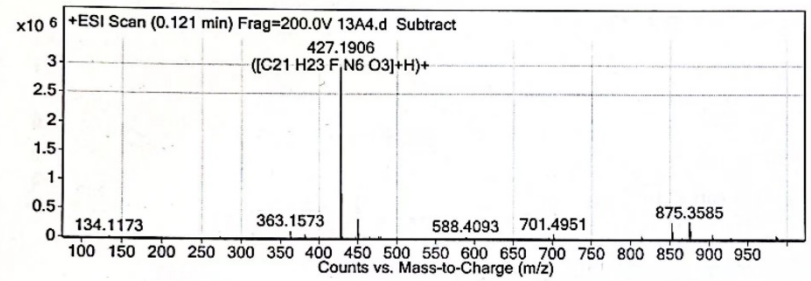
Qualitative Analysis Report

Data Filename	13A4.d	**Sample Name**	13A4
Sample Type	Sample	**Position**	P1-D9
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:16:02 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



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		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	1	1

Formula Calculator 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

--- End Of Report ---

Compound 13a-5

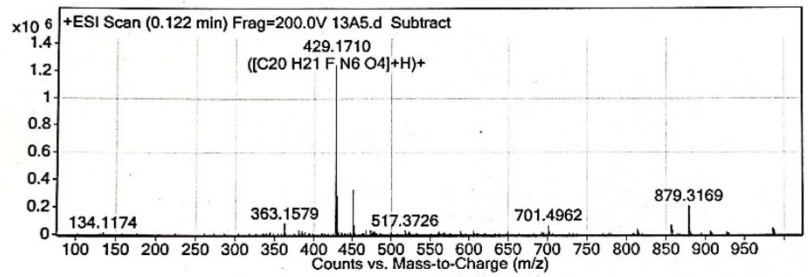
Qualitative Analysis Report

Data Filename	13A5.d	**Sample Name**	13A5
Sample Type	Sample	**Position**	P1-E1
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:18:56 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

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		
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
C	3	60
H	0	120
O	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

--- End Of Report ---

Compound 13a-6

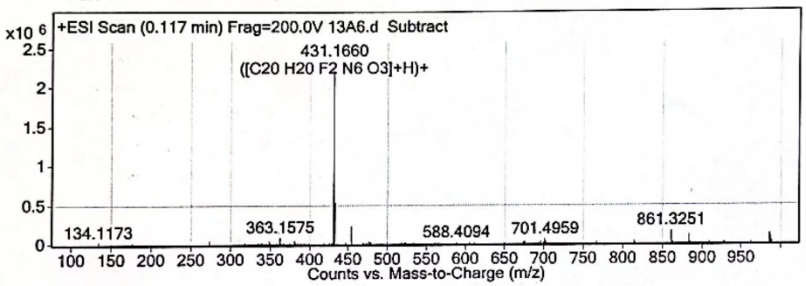
Qualitative Analysis Report

Data Filename	13A6.d	**Sample Name**	13A6
Sample Type	Sample	**Position**	P1-E2
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:21:53 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
363.1575	1	81944.73		
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		
883.3073	1	110482.97		
985.7164	1	117258.66		
986.7189	1	75622.13		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	2	2

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C20 H20 F2 N6 O3	FALSE	430.159	430.1565	-5.76	C20 H21 F2 N6 O3	85.83

--- End Of Report ---

Compound 13b-1

Qualitative Analysis Report

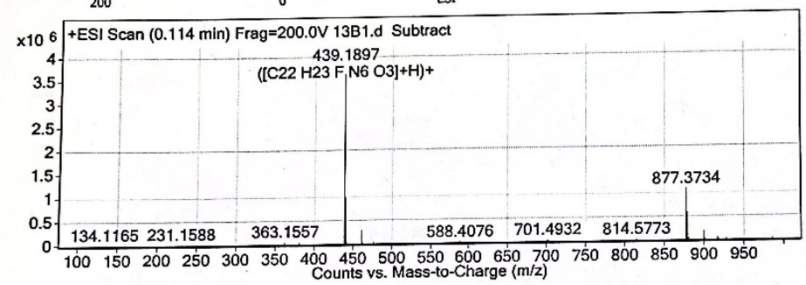
Data Filename	13B1.d	**Sample Name**	13B1
Sample Type	Sample	**Position**	P1-E3
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:24:50 AM
IRM Calibration Status	Success	**DA Method**	20170311.m
Comment			

Sample Group **Info.**

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

User Spectra

Fragmentor Voltage 200 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

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		
462.1742	1	64856.43		
877.3734	1	1085296.88		
878.3767	1	590897.81		
879.3806	1	200894.66		
899.3552	1	171019.92		
900.3566	1	86397.9		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	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

--- End Of Report ---

Compound 13b-2

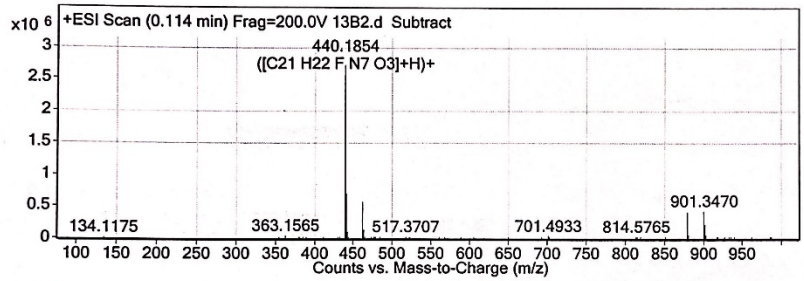
Qualitative Analysis Report

Data Filename	13B2.d	**Sample Name**	13B2
Sample Type	Sample	**Position**	P1-E4
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:27:46 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



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		
463.1698	1	128785.03		
879.3648	1	410518.78		
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	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	1	1

Formula Calculator Results

Formula	Best	Mass	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 ---

Compound 13b-3

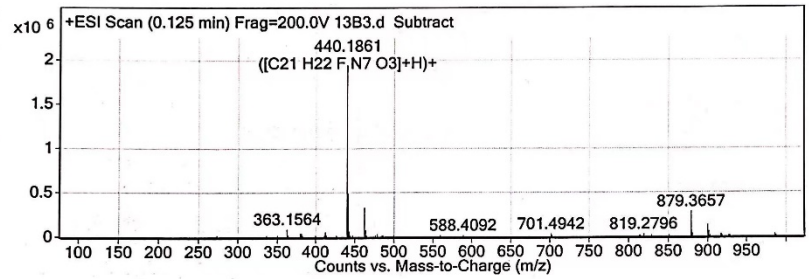
Qualitative Analysis Report

Data Filename	13B3.d	**Sample Name**	13B3
Sample Type	Sample	**Position**	P1-E5
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:30:43 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



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		
463.1701	1	74666.16		
879.3657	1	277727.31		
880.3679	1	136823.73		
901.347	1	130375.75		
902.3488	1	62166.71		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	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

--- End Of Report ---

Compound 13b-4

Qualitative Analysis Report

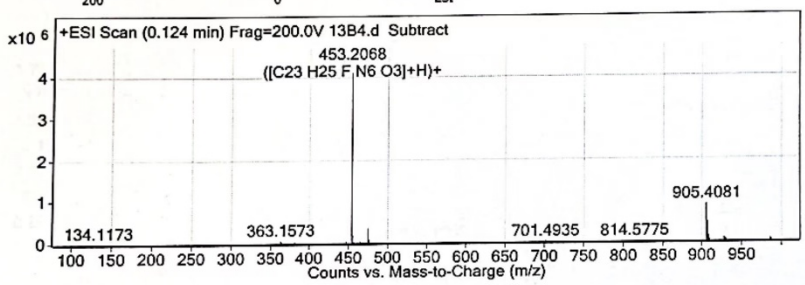
Data Filename	13B4.d	**Sample Name**	13B4
Sample Type	Sample	**Position**	P1-E6
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:33:39 AM
IRM Calibration Status	Success	**DA Method**	20170311.m
Comment			

Sample Group **Info.**

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

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 Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	1	1

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C23 H25 F N6 O3	FALSE	452.1996	452.1972	-5.17	C23 H26 F N6 O3	88.78

--- End Of Report ---

Compound 13b-5

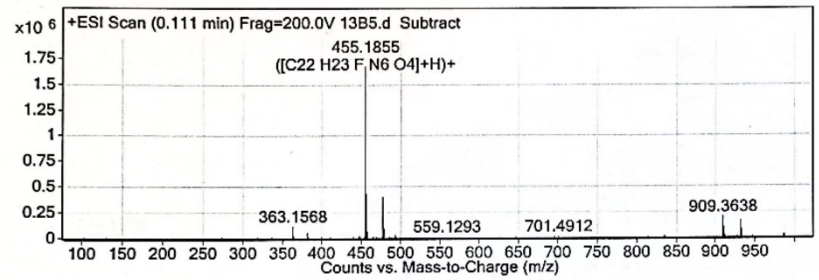
Qualitative Analysis Report

Data Filename	13B5.d	**Sample Name**	13B5
Sample Type	Sample	**Position**	P1-E7
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:36:36 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
363.1568	1	110080.06		
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		
478.1694	1	95284.05		
909.3638	1	196912.97		
910.3665	1	97425.66		
931.3461	1	156739.23		
932.3514	1	80171.13		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	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 O4	FALSE	454.1782	454.1765	-3.68	C22 H24 F N6 O4	93.68

--- End Of Report ---

Compound 13b-6

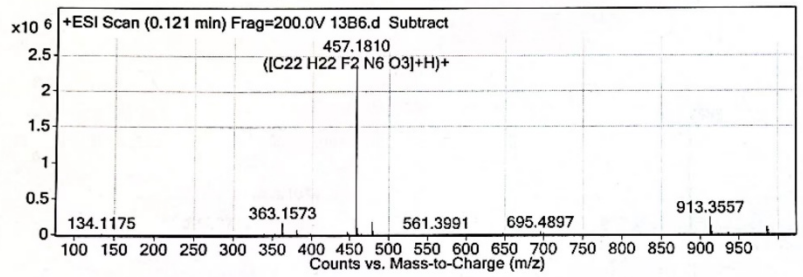
Qualitative Analysis Report

Data Filename	13B6.d	**Sample Name**	13B6
Sample Type	Sample	**Position**	P1-E8
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



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		
914.3575	1	110910.73		
985.715	1	99292.59		
986.717	1	62713.73		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
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

--- End Of Report ---

Compound 14a-1

Qualitative Analysis Report

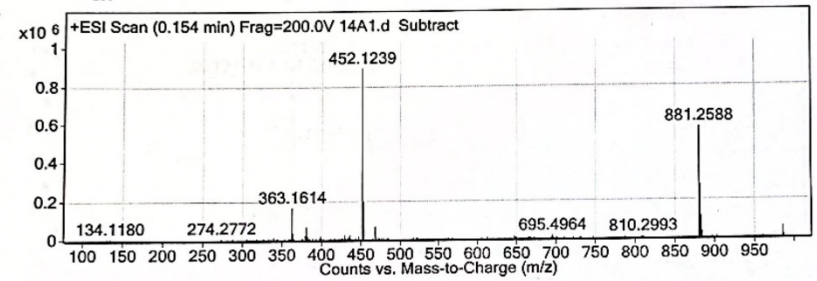
Data Filename	14A1.d	**Sample Name**	14A1
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/17/2021 7:33:21 PM
IRM Calibration Status	Success	**DA Method**	20170311.m
Comment			

Sample Group **Info.**

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund
363.1614	1	166778.67
381.171	1	62431.75
452.1239	1	896078.38
453.1267	1	198570.2
454.1231	1	54907.35
468.0965	1	65137.32
881.2588	1	579139.56
882.261	1	274355.19
883.2587	1	111827.21
985.725	1	52005.89

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	1	1
S	1	1

--- End Of Report ---

Compound 14a-2

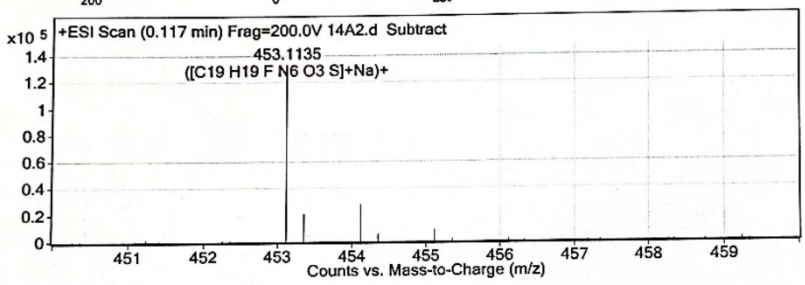
Qualitative Analysis Report

Data Filename	14A2.d	**Sample Name**	14A2
Sample Type	Sample	**Position**	P1-F1
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:42:29 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

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 Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	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	430.124	430.1223	-3.9	C19 H19 F N6 Na O3 S	90.35

--- End Of Report ---

Compound 14a-3

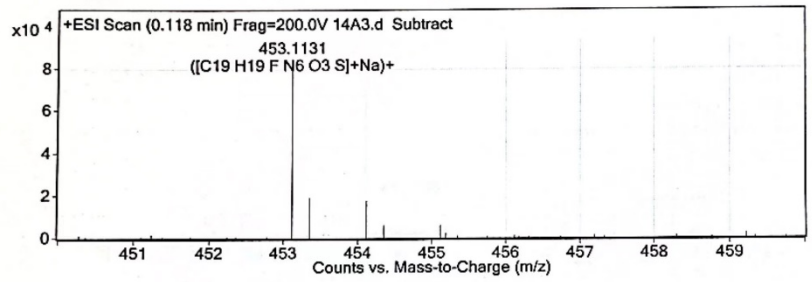
Qualitative Analysis Report

Data Filename	14A3.d	**Sample Name**	14A3
Sample Type	Sample	**Position**	P1-F2
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:45:24 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



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
C	3	60
H	0	120
O	0	30
N	0	30
F	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 ---

Compound 14a-4

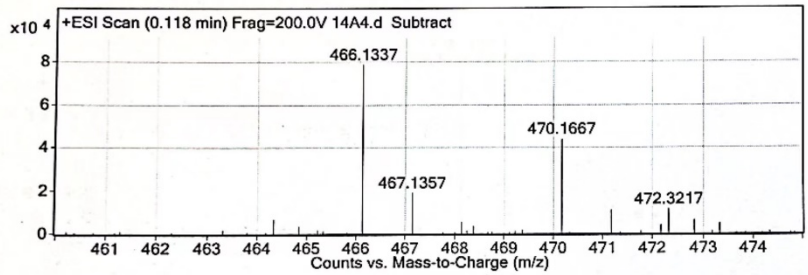
Qualitative Analysis Report

Data Filename	14A4.d	**Sample Name**	14A4
Sample Type	Sample	**Position**	P1-F3
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:48:21 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak 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 Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	1	1
S	1	1

--- End Of Report ---

Compound 14a-5

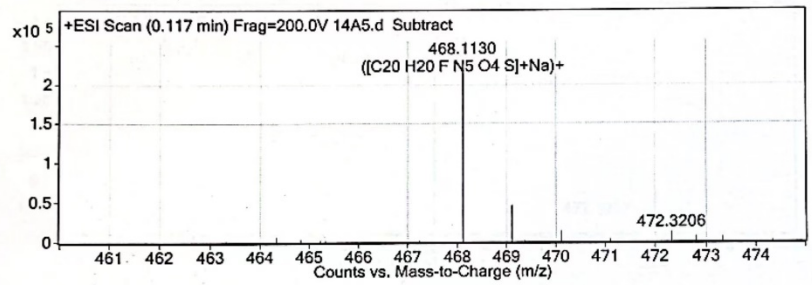
Qualitative Analysis Report

Data Filename	14A5.d	**Sample Name**	14A5
Sample Type	Sample	**Position**	P1-F4
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:51:18 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

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

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	1	1
S	1	1

Formula Calculator Results

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 ---

Compound 14a-6

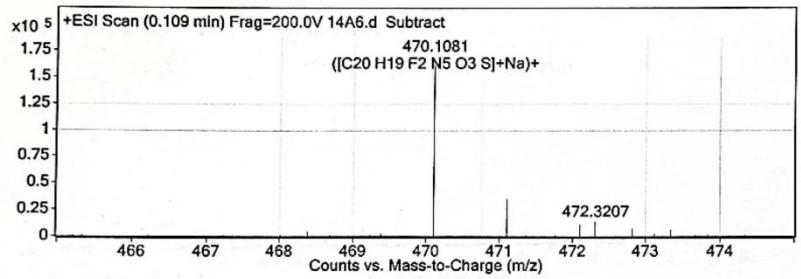
Qualitative Analysis Report

Data Filename	14A6.d	**Sample Name**	14A6
Sample Type	Sample	**Position**	P1-F5
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:54:15 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



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 Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	2	2
S	1	1

Formula Calculator Results

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

--- End Of Report ---

Compound 14b-1

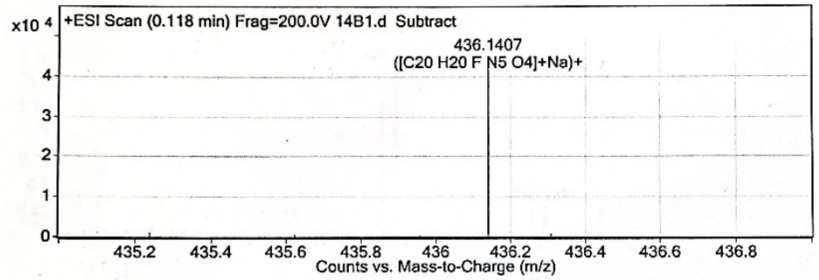
Qualitative Analysis Report

Data Filename	14B1.d	**Sample Name**	14B1
Sample Type	Sample	**Position**	P1-F6
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 9:57:11 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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

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

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	1	1
S	0	0

Formula Calculator Results

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

--- End Of Report ---

Compound 14b-2

Qualitative Analysis Report

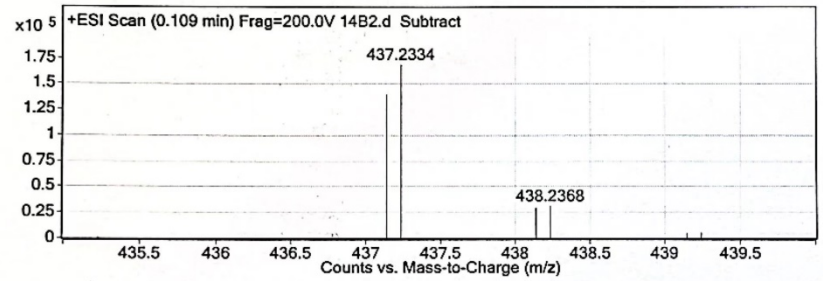
Data Filename	14B2.d	**Sample Name**	14B2
Sample Type	Sample	**Position**	P1-F7
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 10:00:08 AM
IRM Calibration Status	Success	**DA Method**	20170311.m
Comment			

Sample Group **Info.**

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

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 Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	1	1
S	0	0

Formula 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

--- End Of Report ---

Compound 14b-3

Qualitative Analysis Report

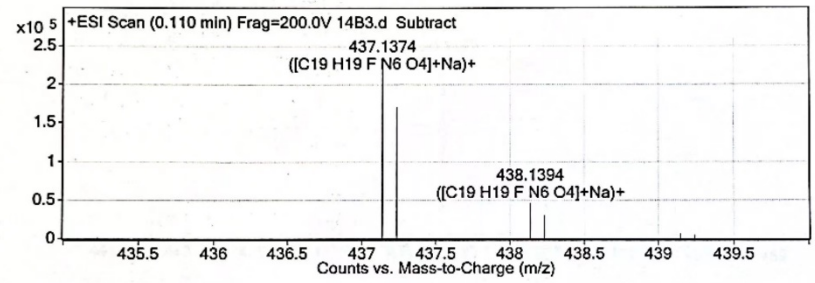
Data Filename	14B3.d	**Sample Name**	14B3
Sample Type	Sample	**Position**	P1-F8
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/18/2021 10:03:04 AM
IRM Calibration Status	Success	**DA Method**	20170311.m
Comment			

Sample Group **Info.**

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



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	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	1	1
S	0	0

Formula Calculator Results

Formula	Best	Mass	Tgt 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

--- End Of Report ---

Compound 14b-5

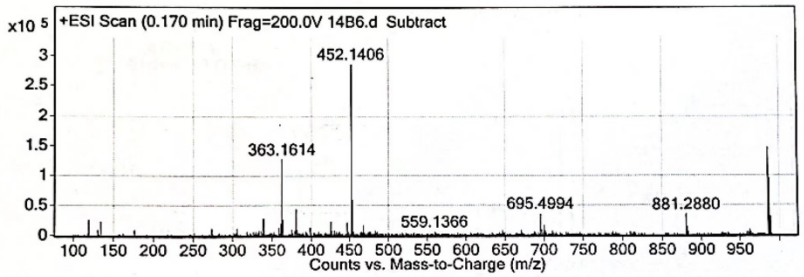
Qualitative Analysis Report

Data Filename	14B6.d	**Sample Name**	14B6
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/17/2021 7:30:24 PM
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

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak 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 Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	2	2
S	0	0

--- End Of Report ---

Compound 14b-6

Qualitative Analysis Report

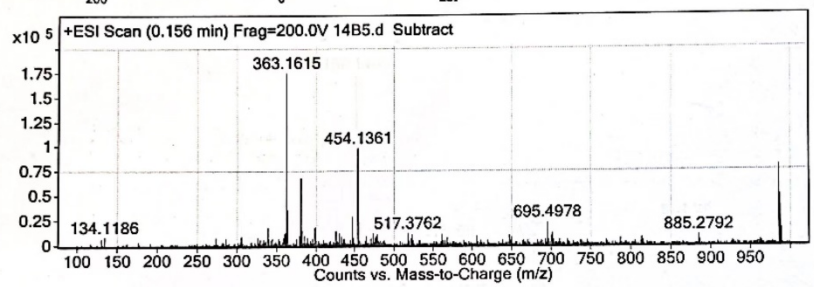
Data Filename	14B5.d	**Sample Name**	14B5
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	ZHENG100-1000.m	**Acquired Time**	12/17/2021 7:27:27 PM
IRM Calibration Status	Success	**DA Method**	20170311.m
Comment			

Sample Group **Info.**

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



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
C	3	60
H	0	120
O	0	30
N	0	30
F	1	1
S	0	0

--- End Of Report ---