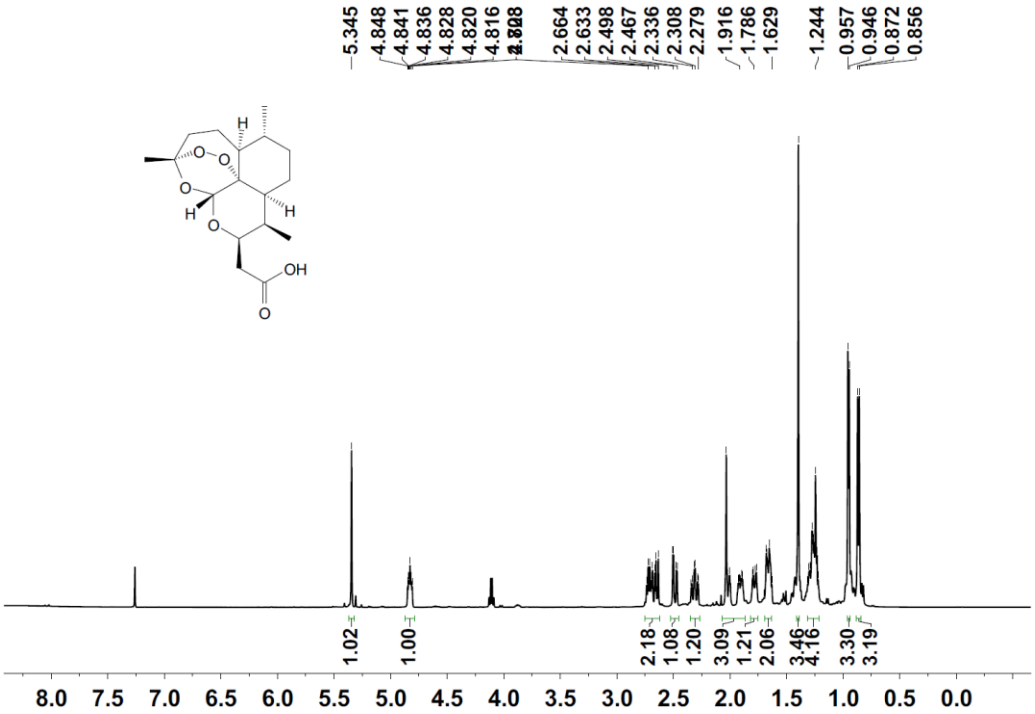
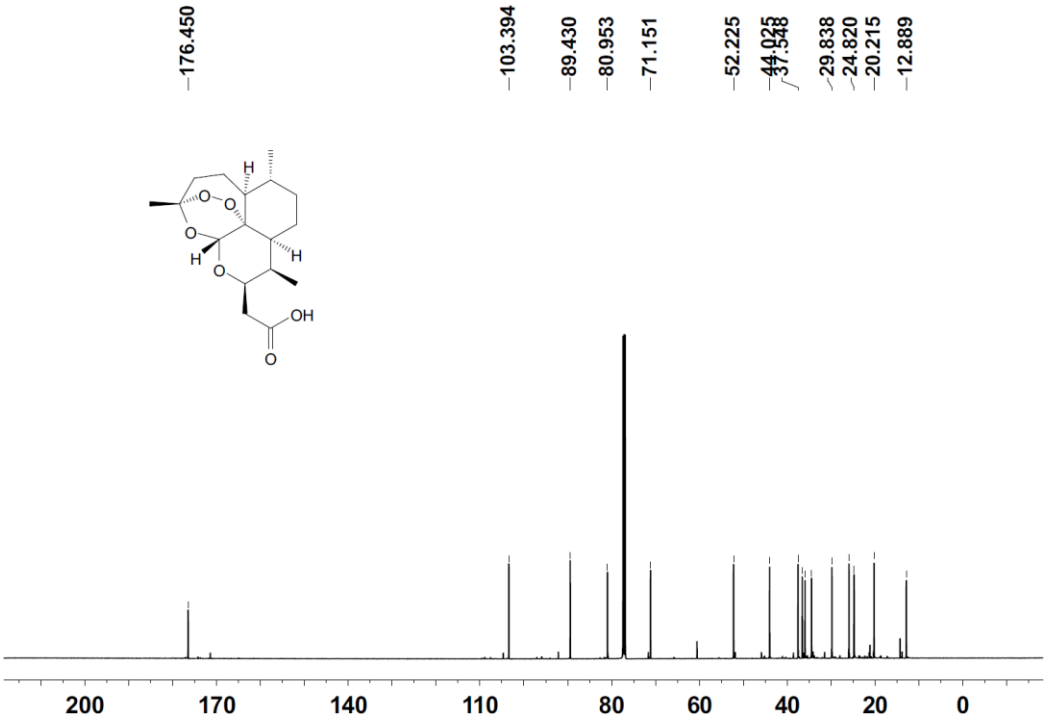
Data S1. Characterization of compounds and extended raw data. Related to "Compound synthesis and characterization" section in STAR Methods.

NMR

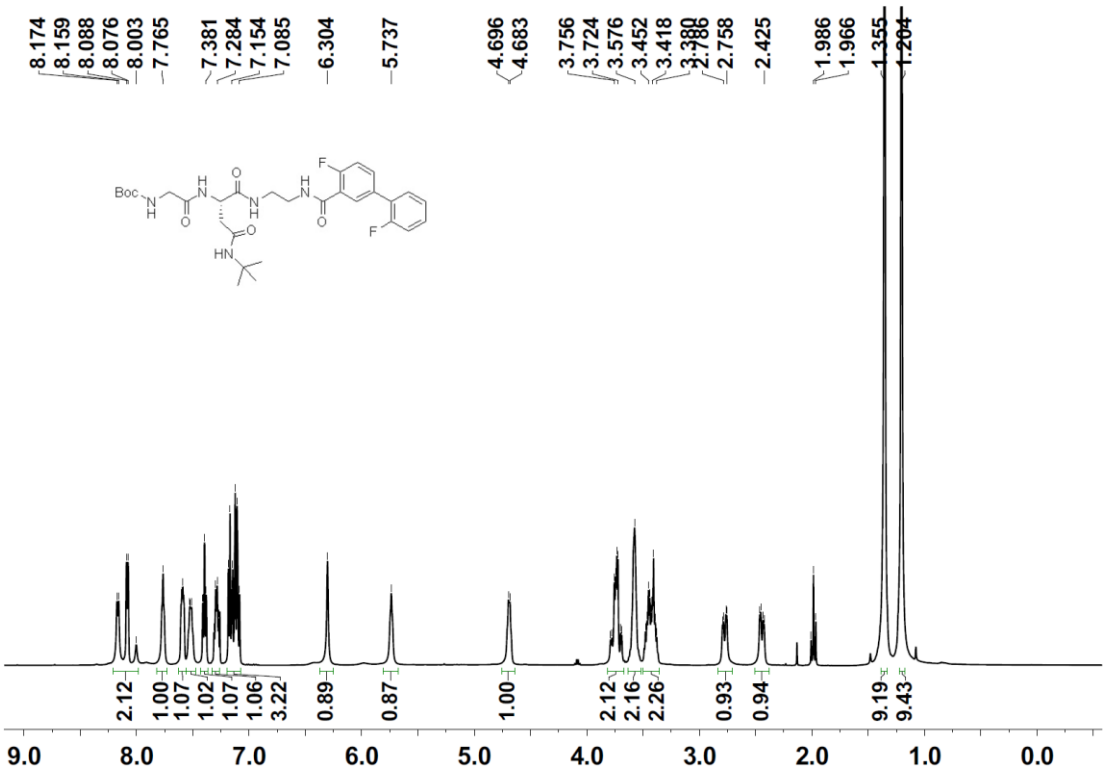
^{1}H NMR of compound 9



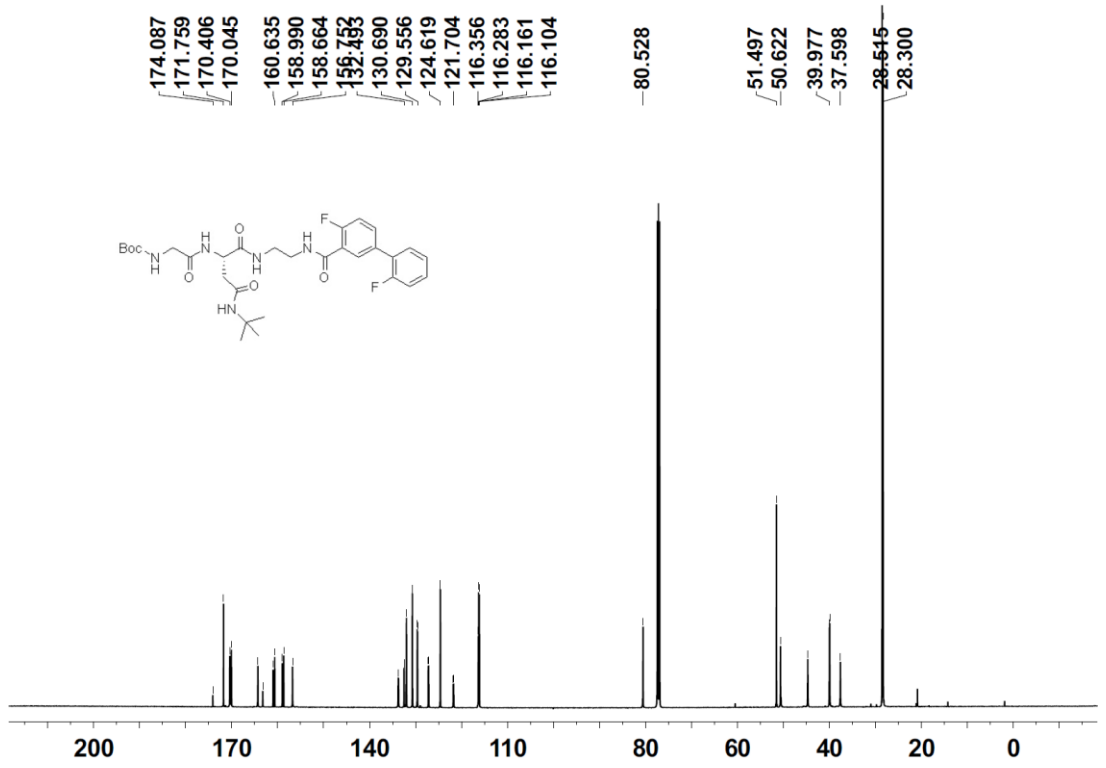
^{13}C NMR of compound 9



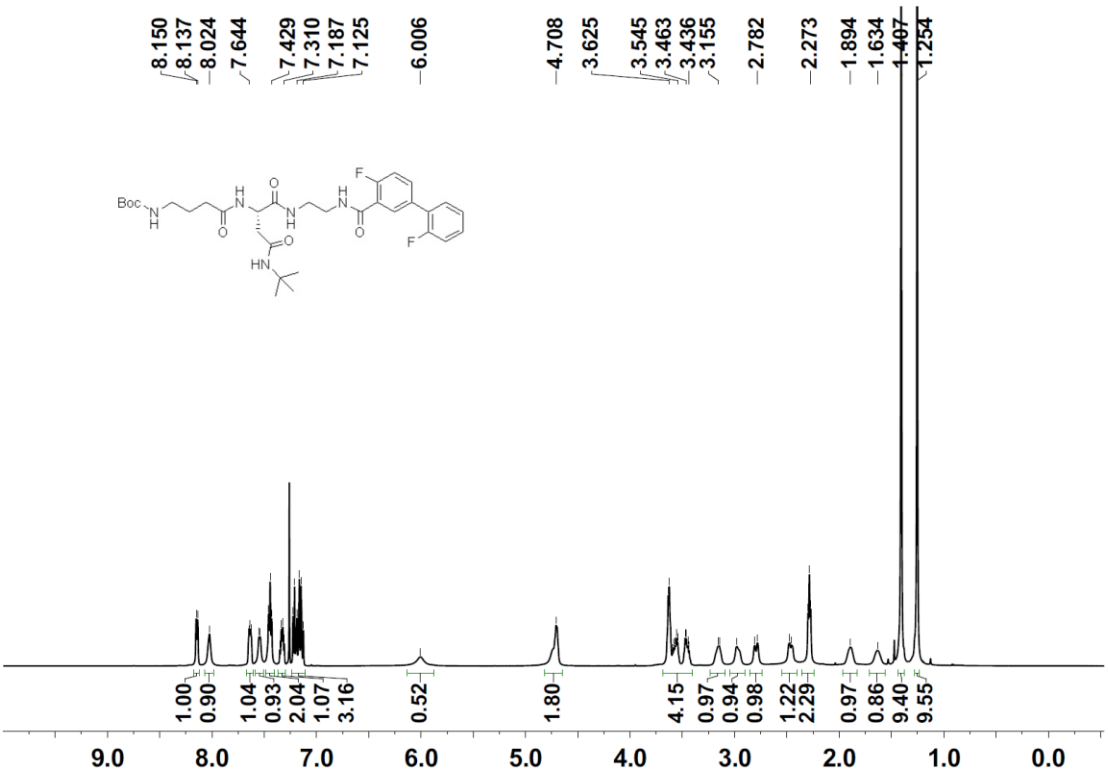
^{1}H NMR of compound WZ-0917



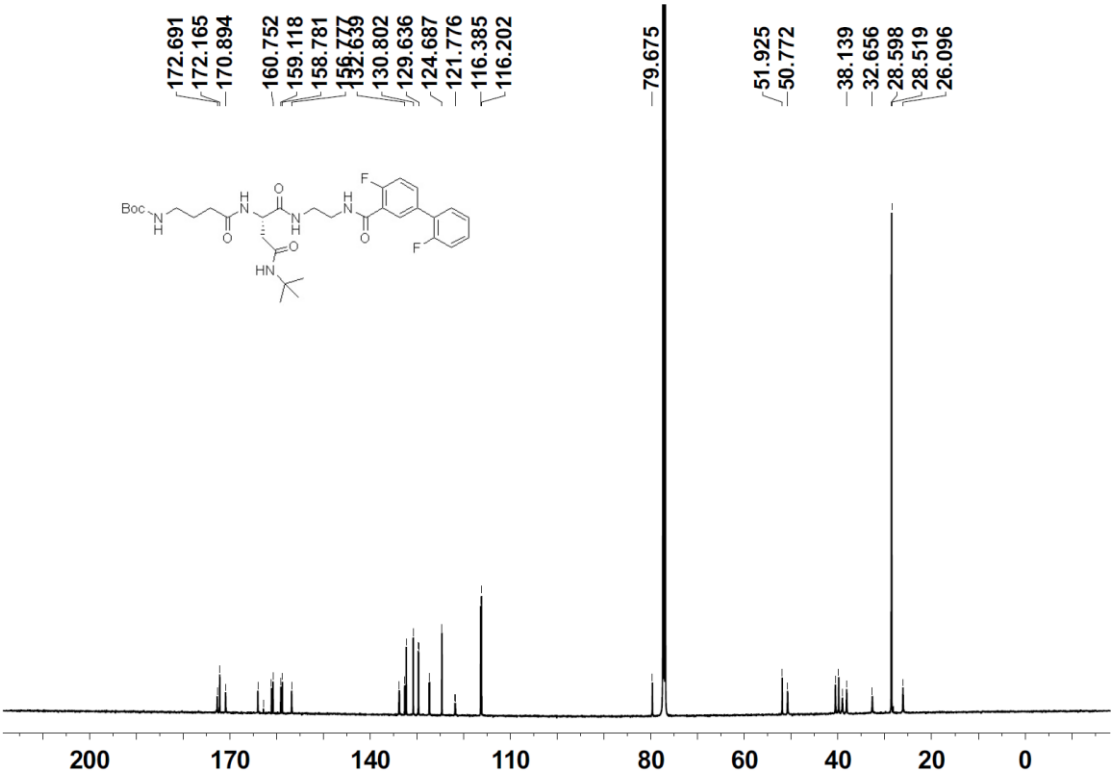
^{13}C NMR of compound WZ-0917



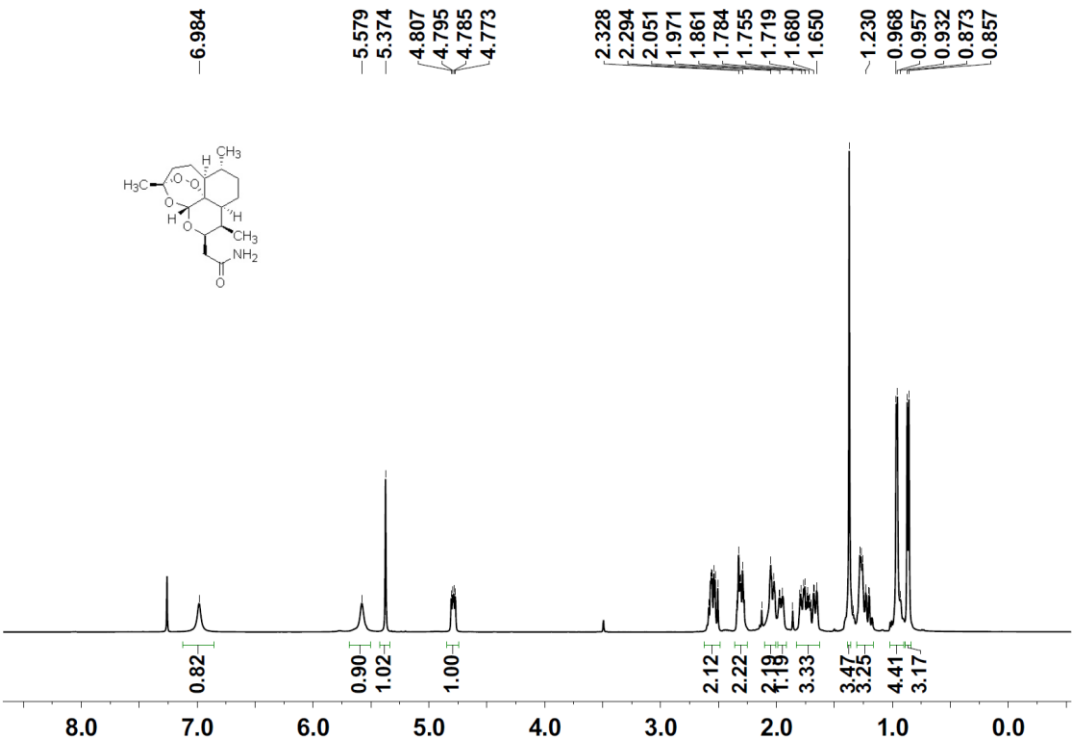
^{1}H NMR of compound WZ-183 (PI01)



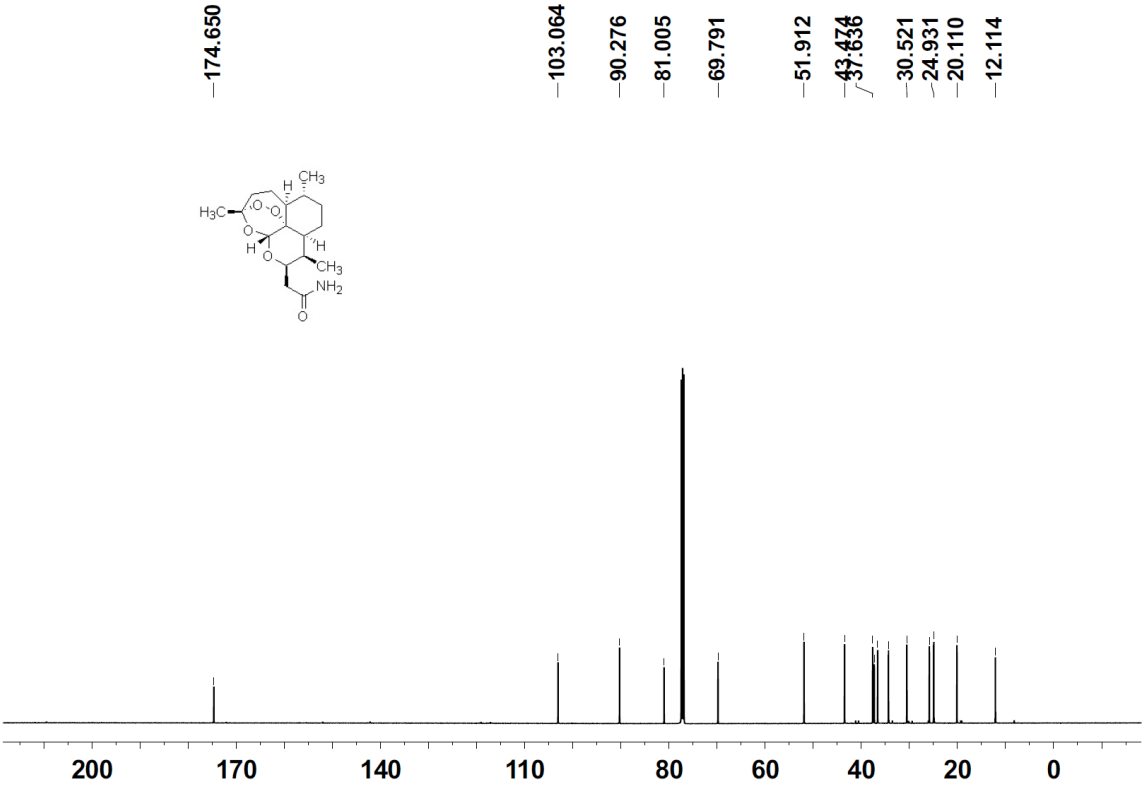
^{13}C NMR of compound WZ-183 (PI01)



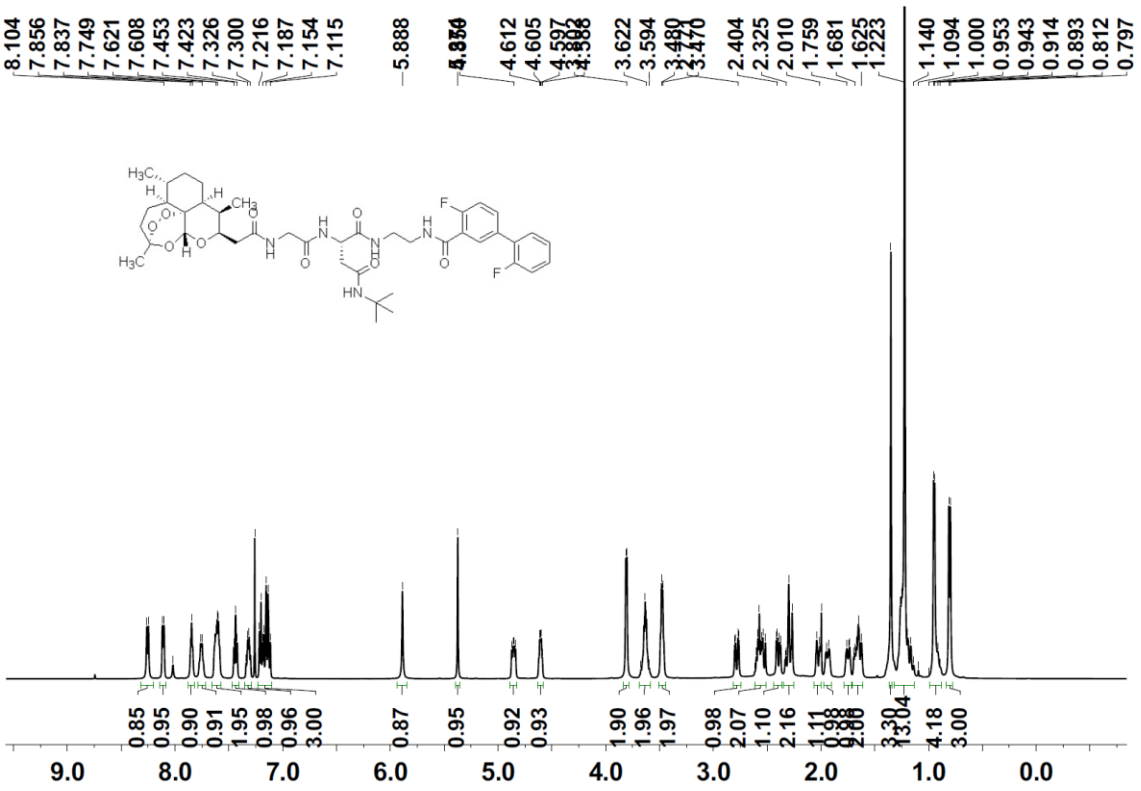
^{1}H NMR of ART1



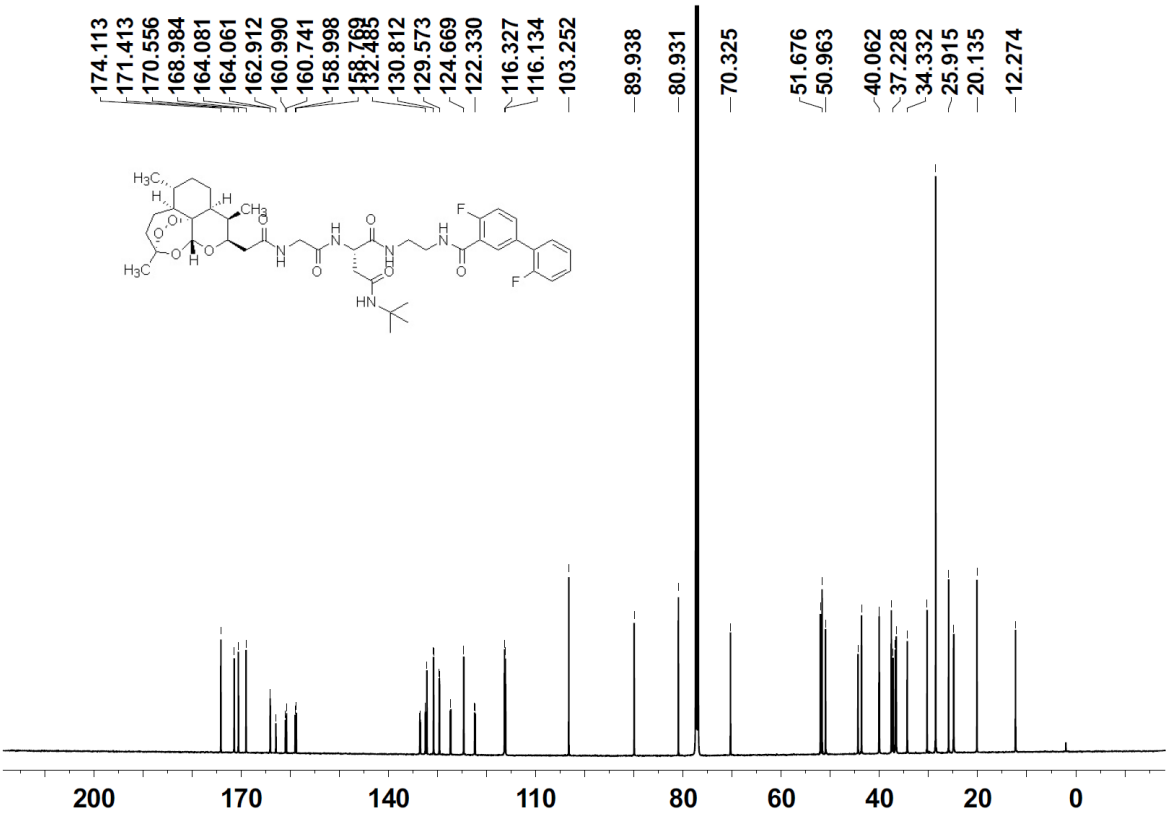
^{13}C NMR of ART1



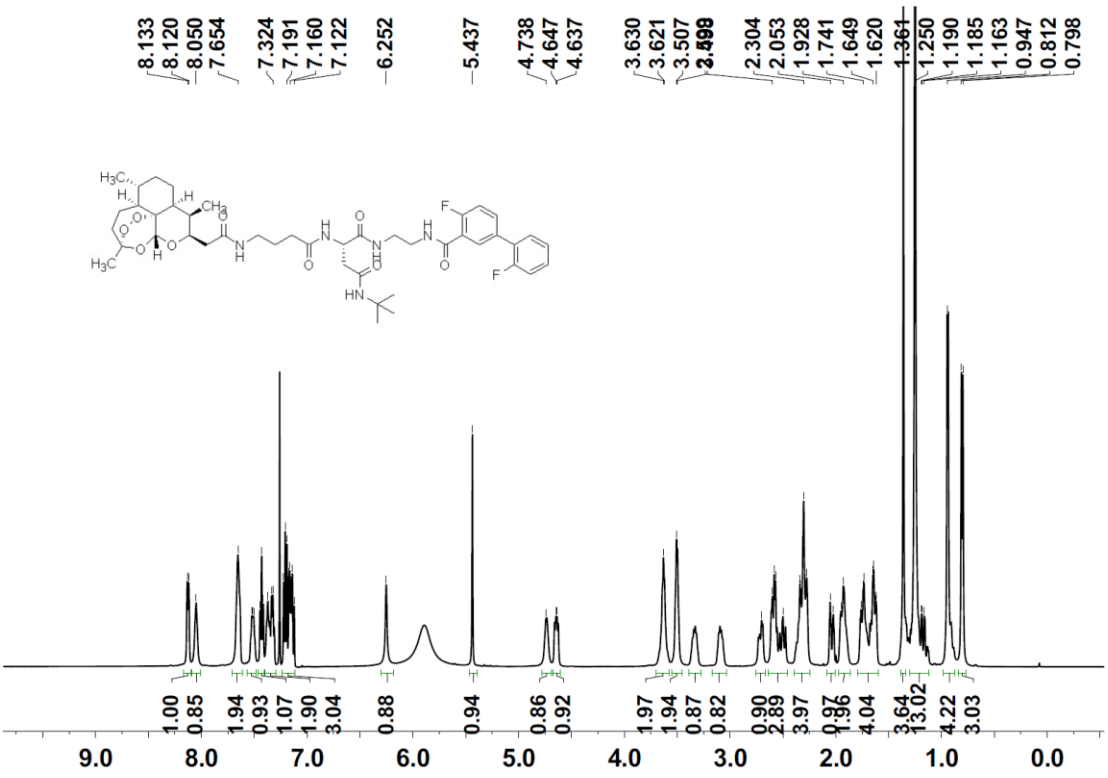
^{1}H NMR of ATZ2



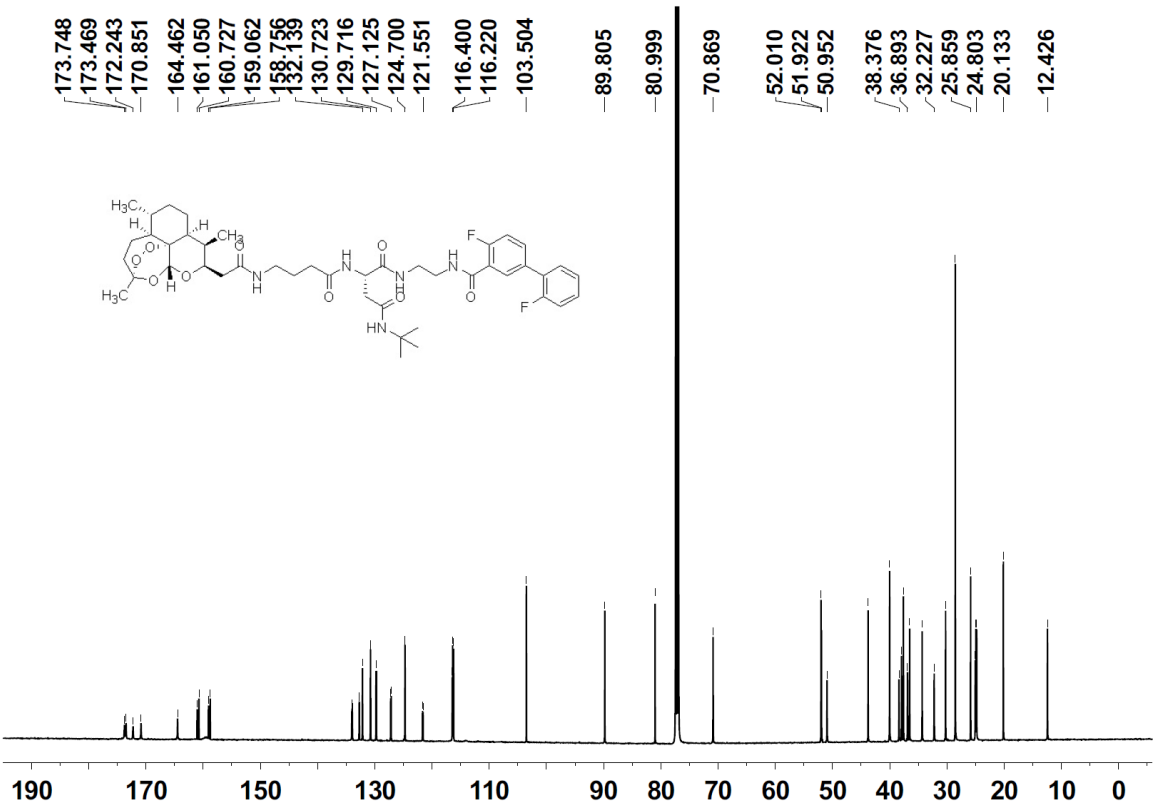
^{13}C NMR of ATZ2



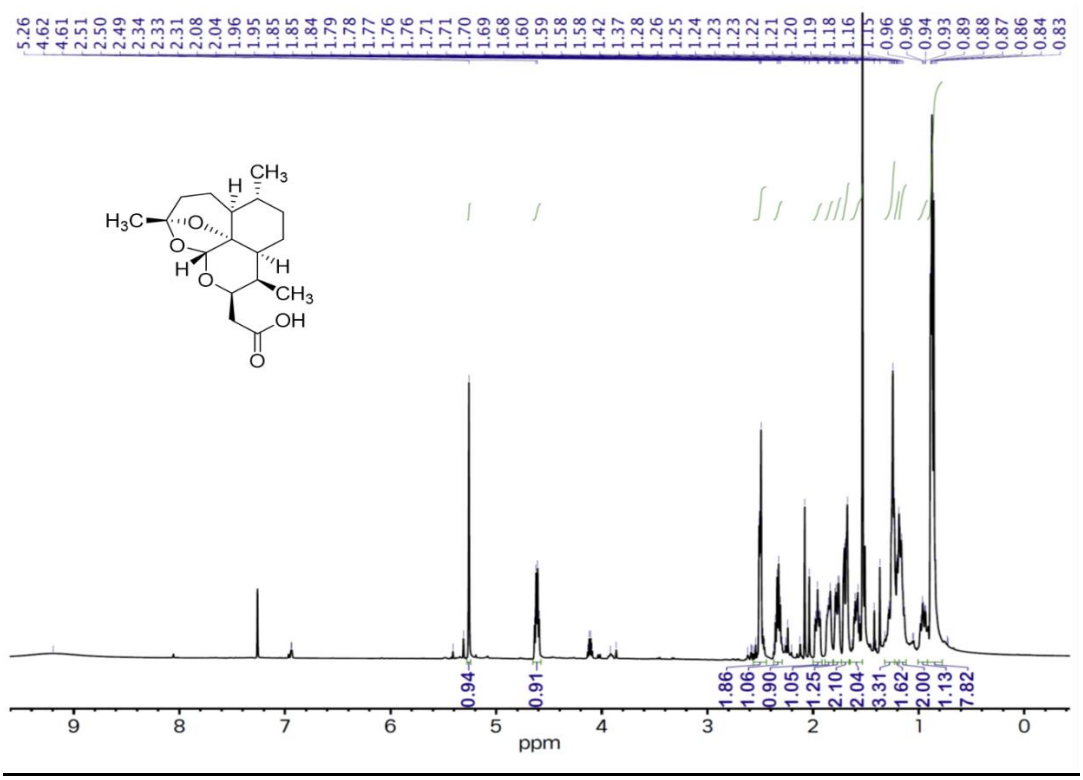
^{1}H NMR of ATZ4



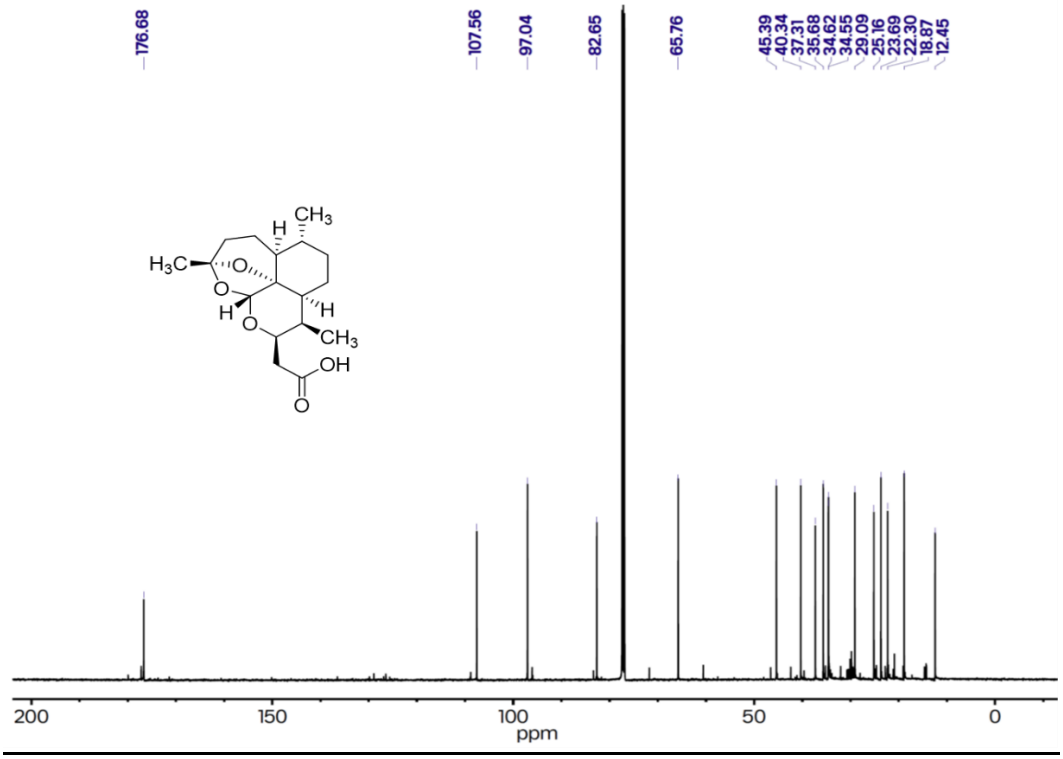
^{13}C NMR of ATZ4



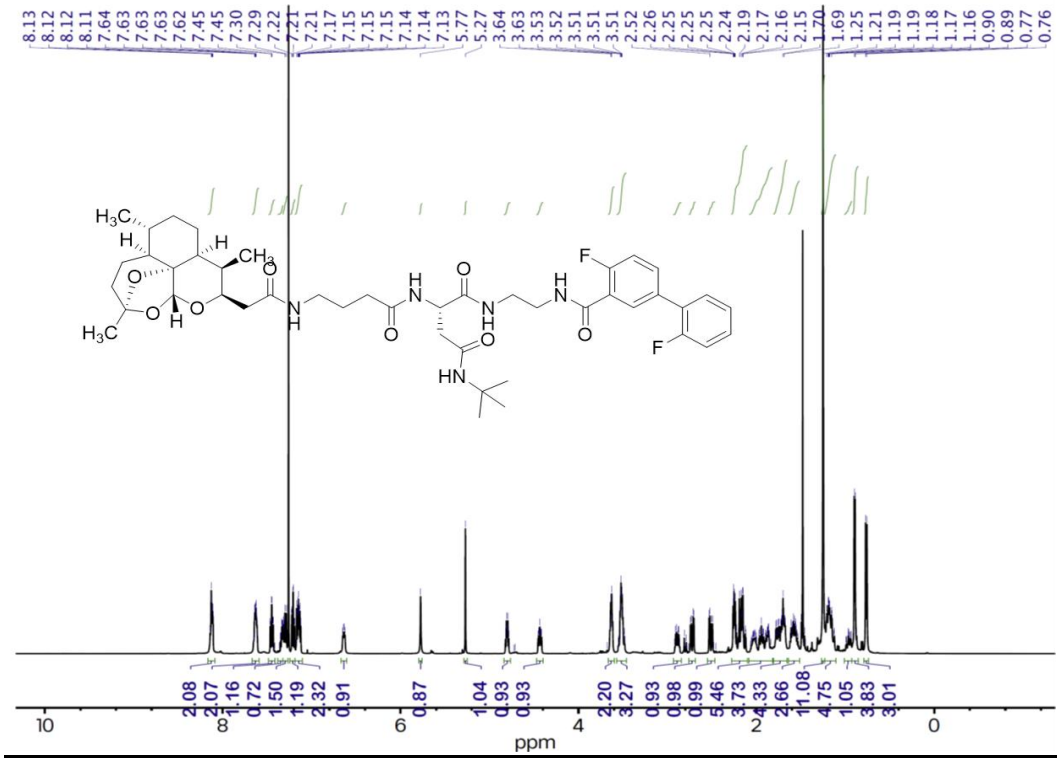
^{1}H NMR of compound 10 (deoxy-ART-AcOH)



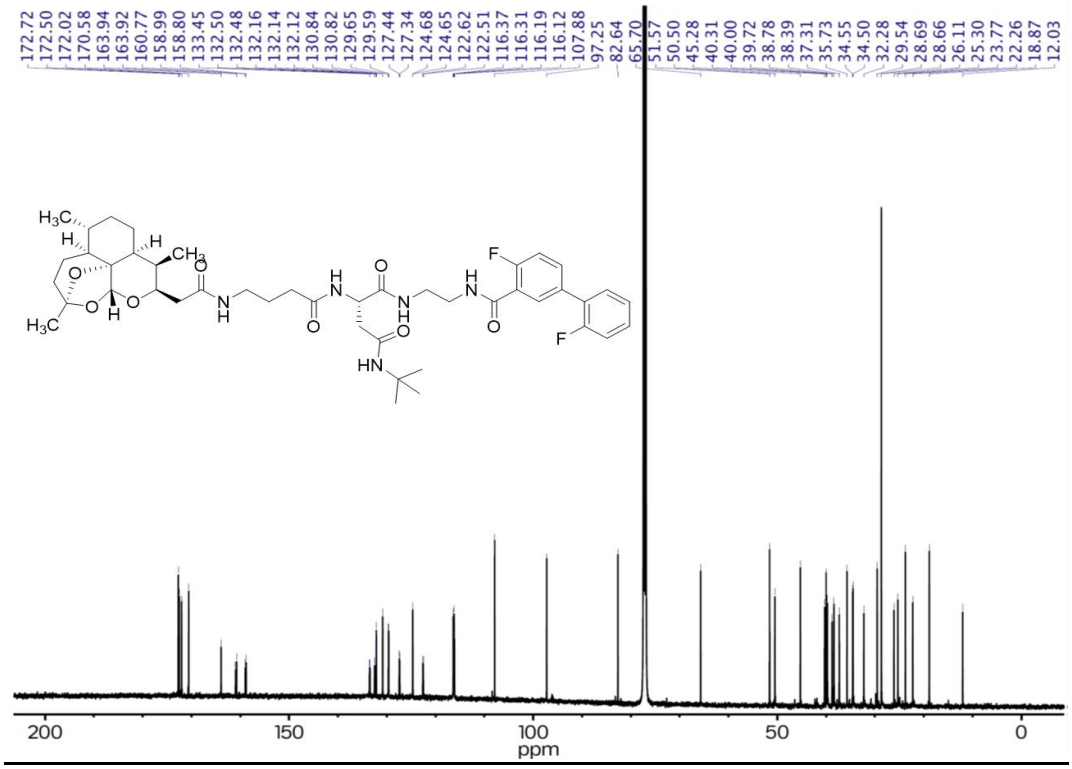
^{13}C NMR of compound 10 (deoxy-ART-AcOH)



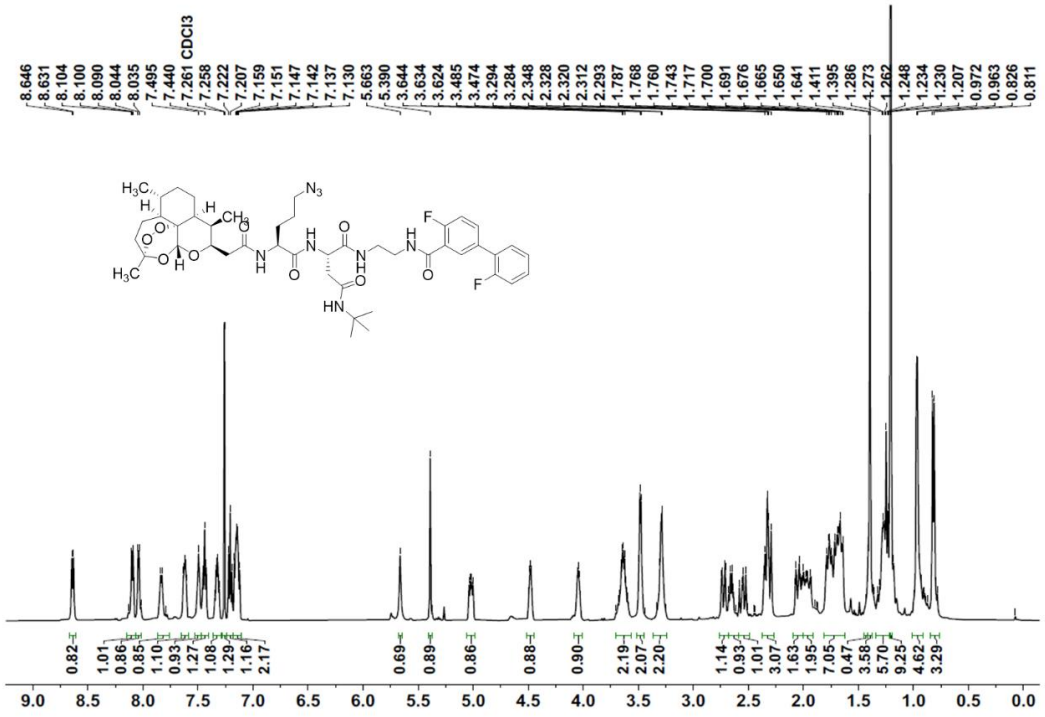
^{1}H NMR of deoxy-ATZ4



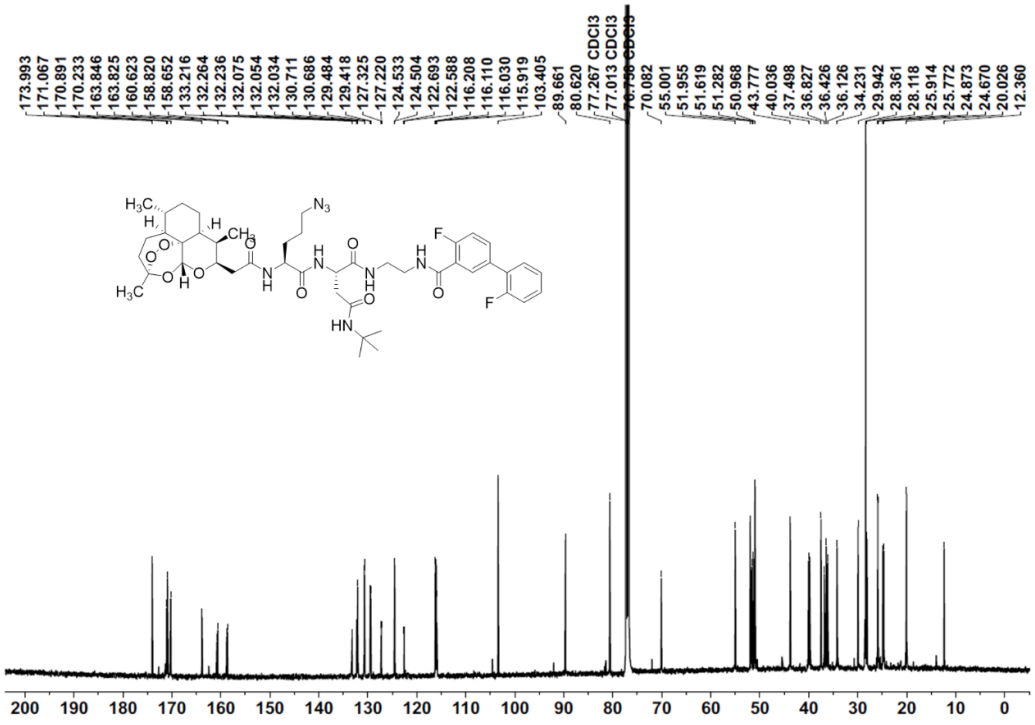
^{13}C NMR of deoxy-ATZ4



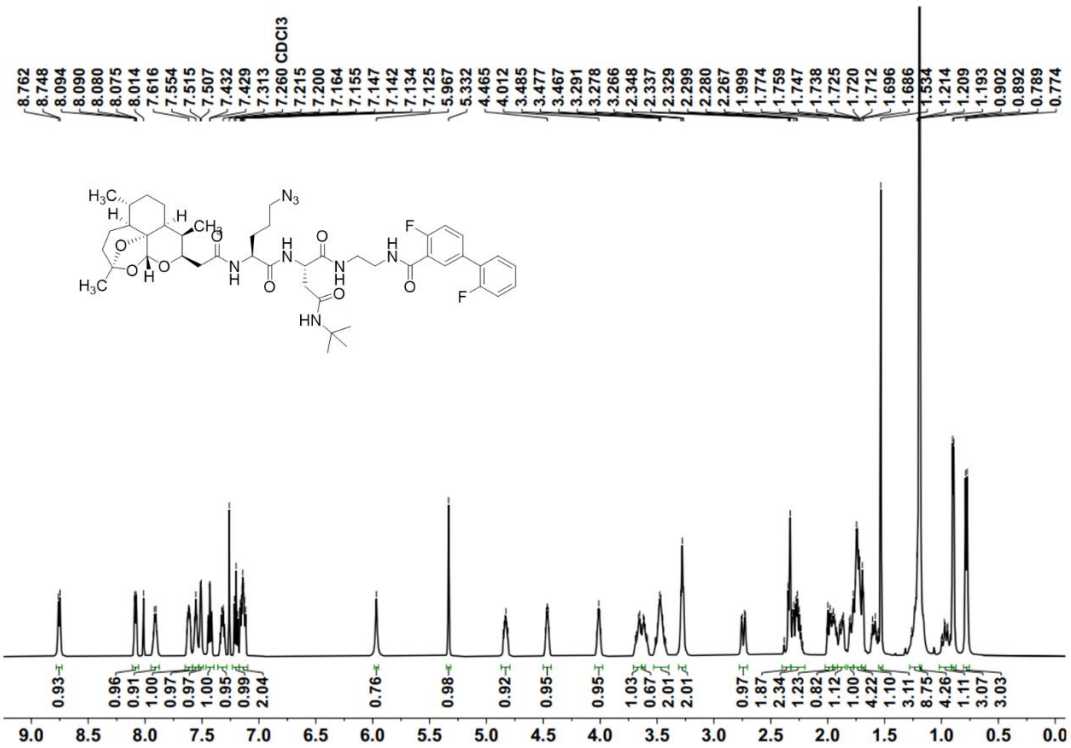
^{1}H NMR of ATZ-P1



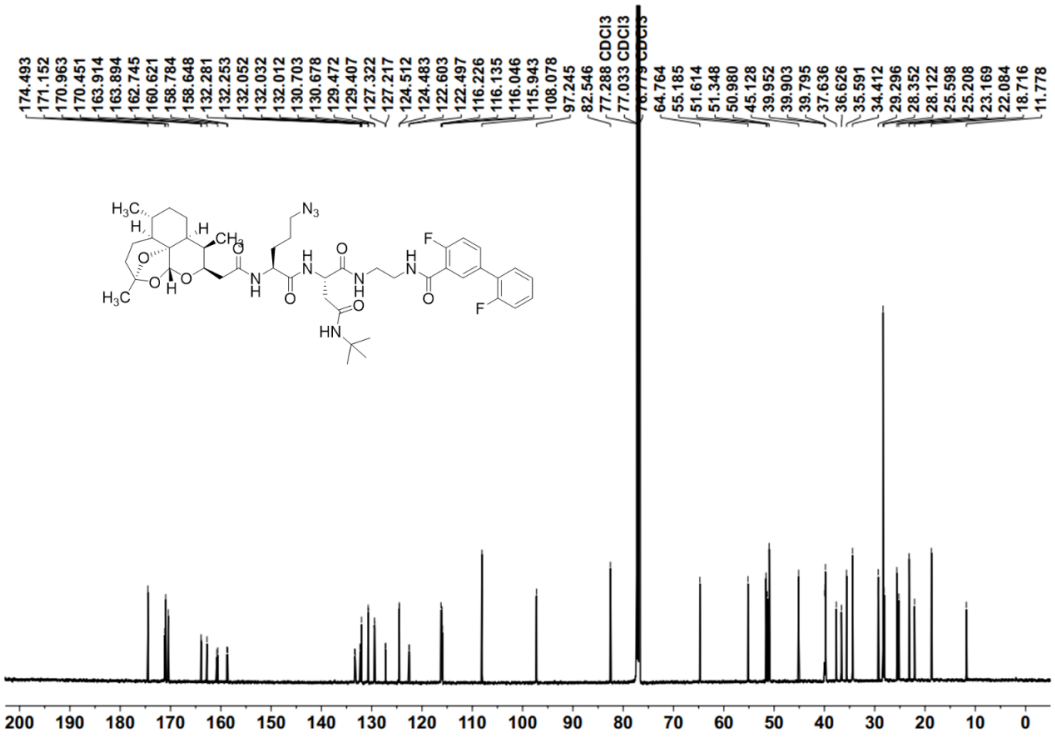
^{13}C NMR of ATZ-P1



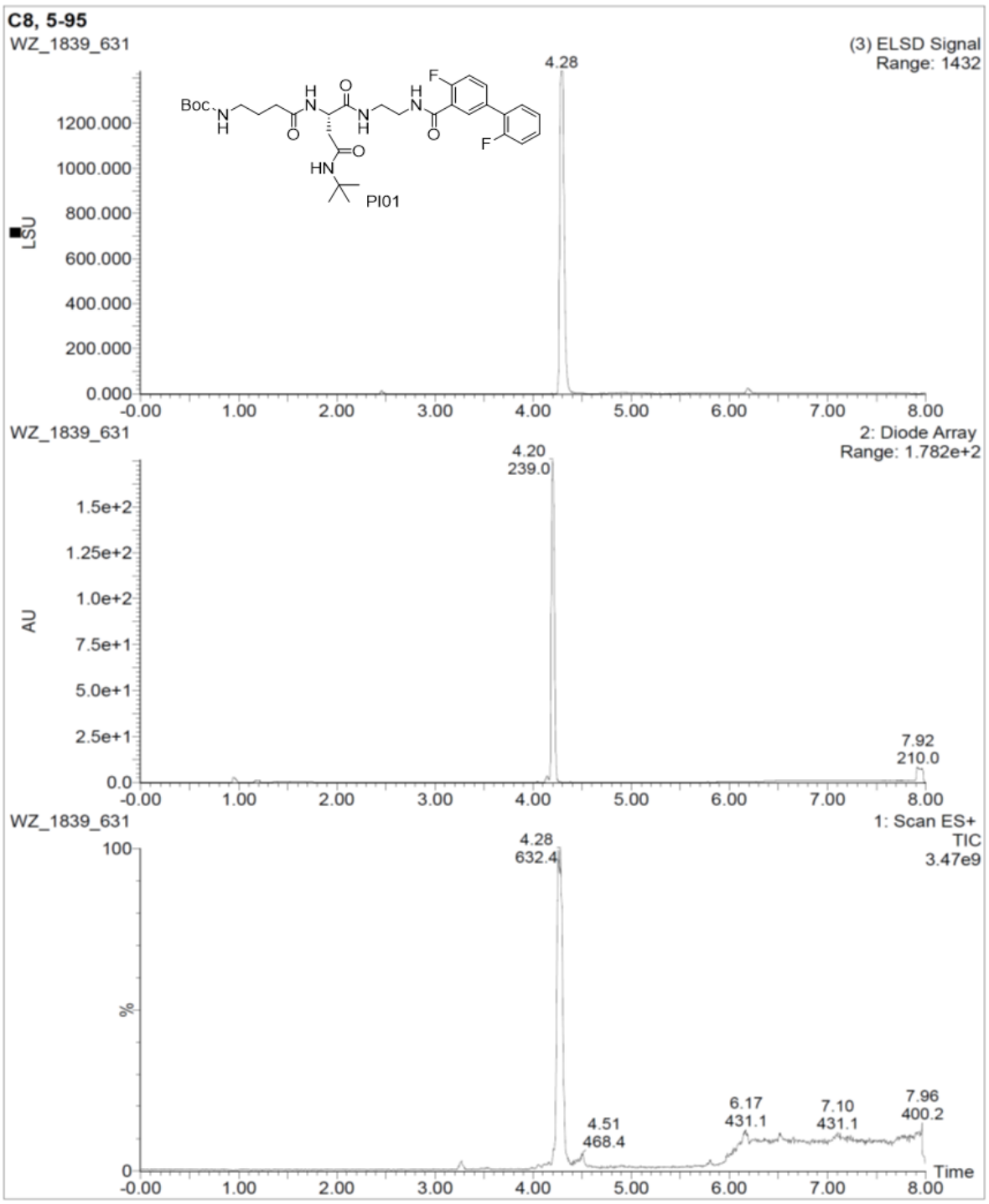
^{1}H NMR of deoxy-ATZ-P1

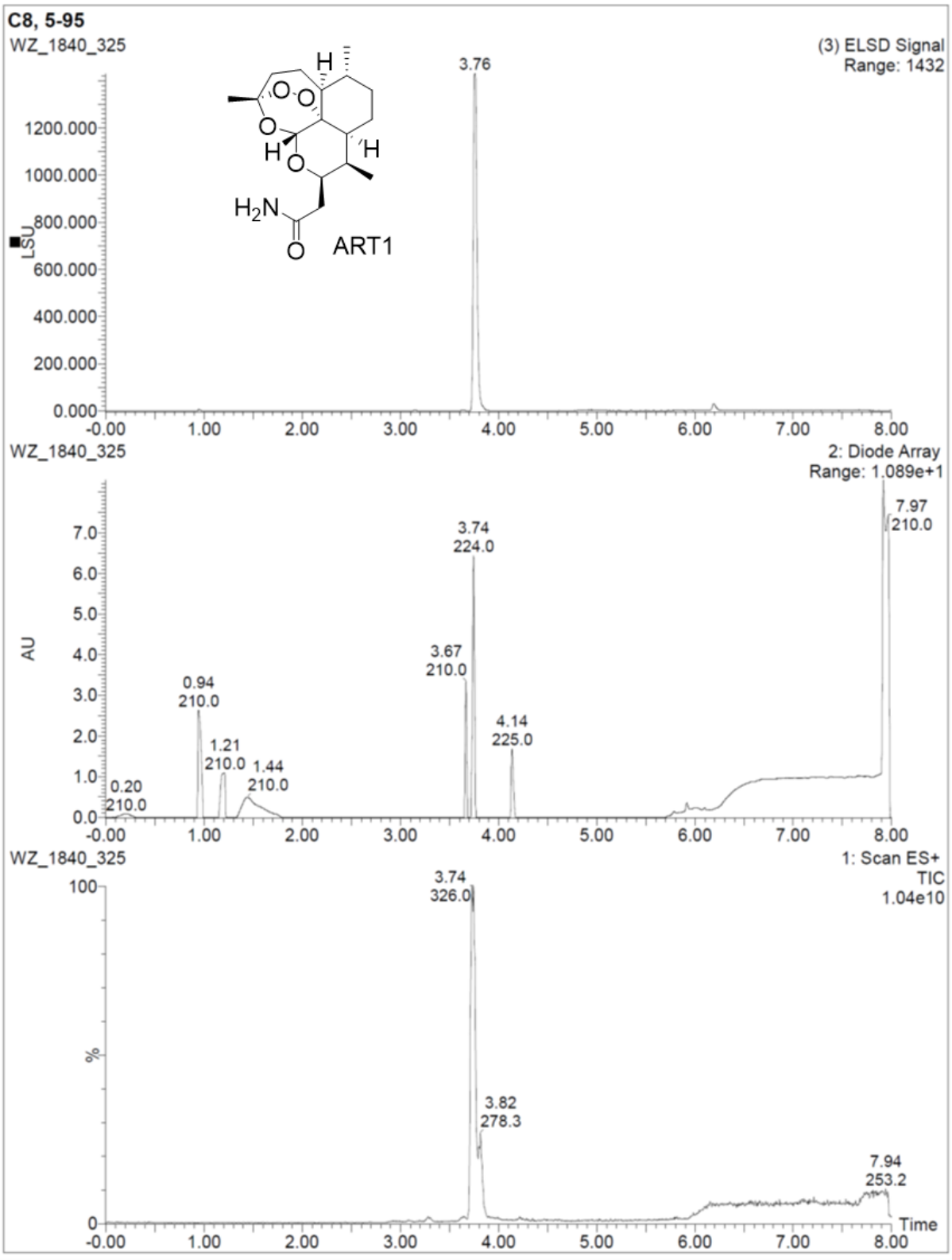


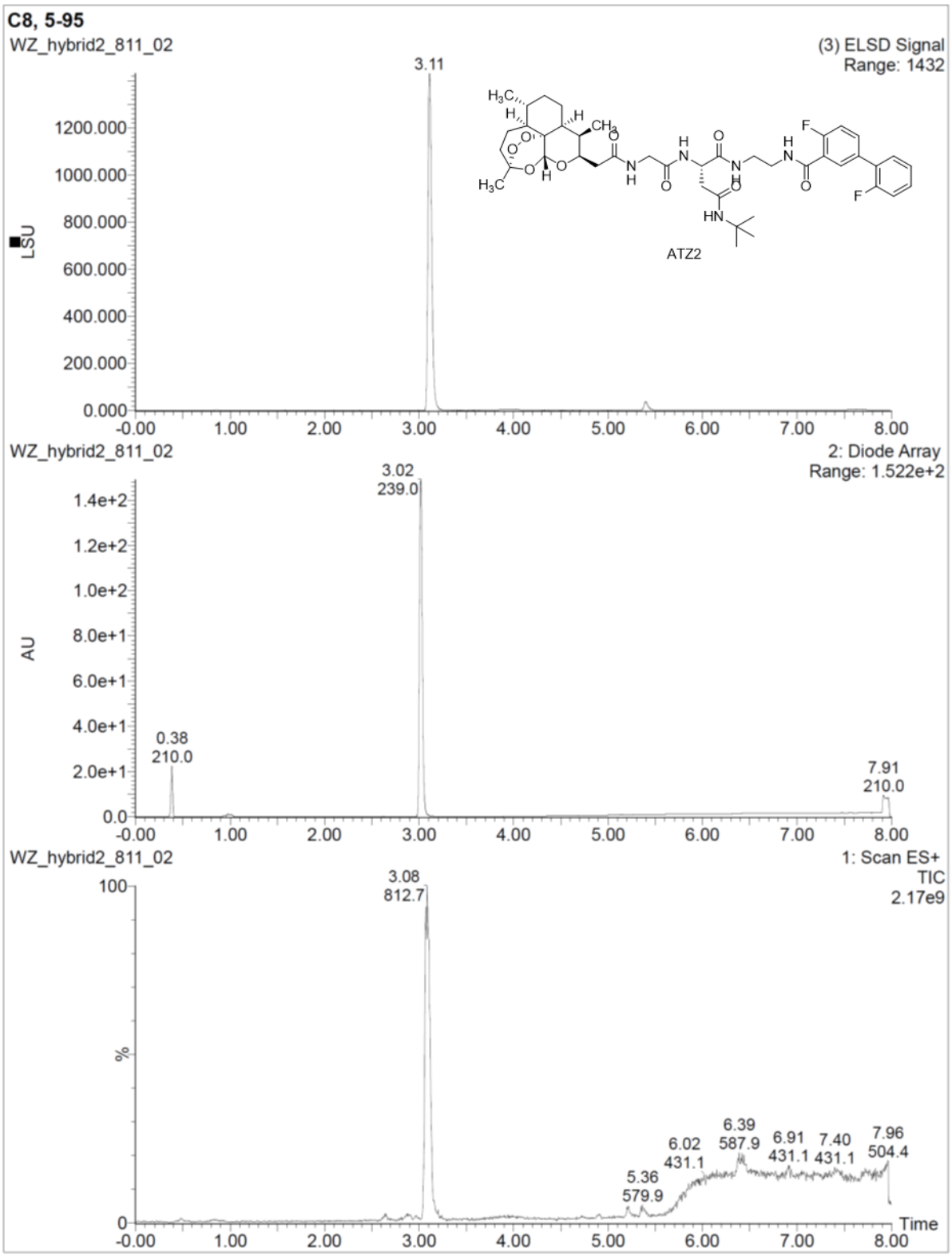
^{13}C NMR of deoxy-ATZ-P1

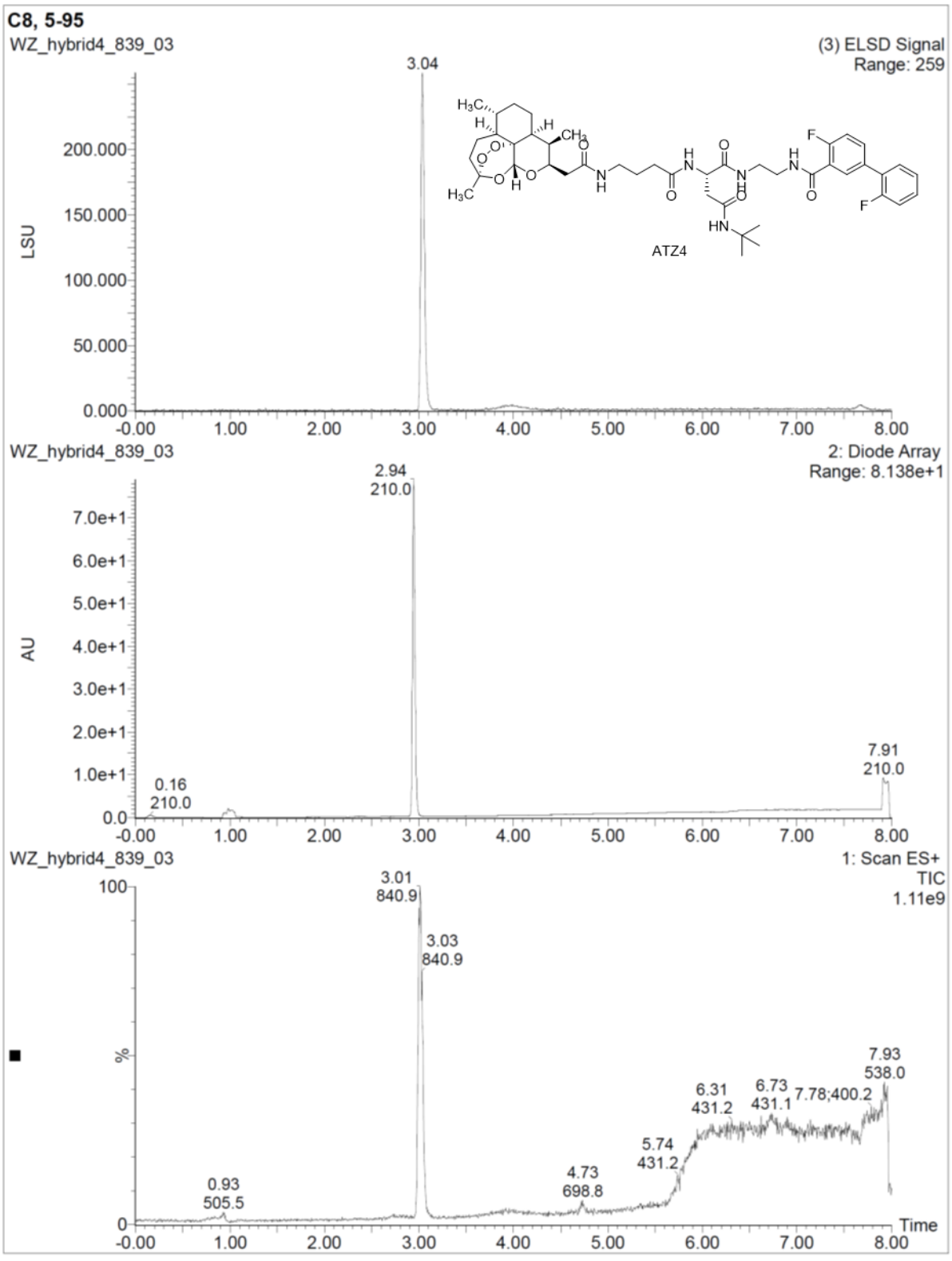


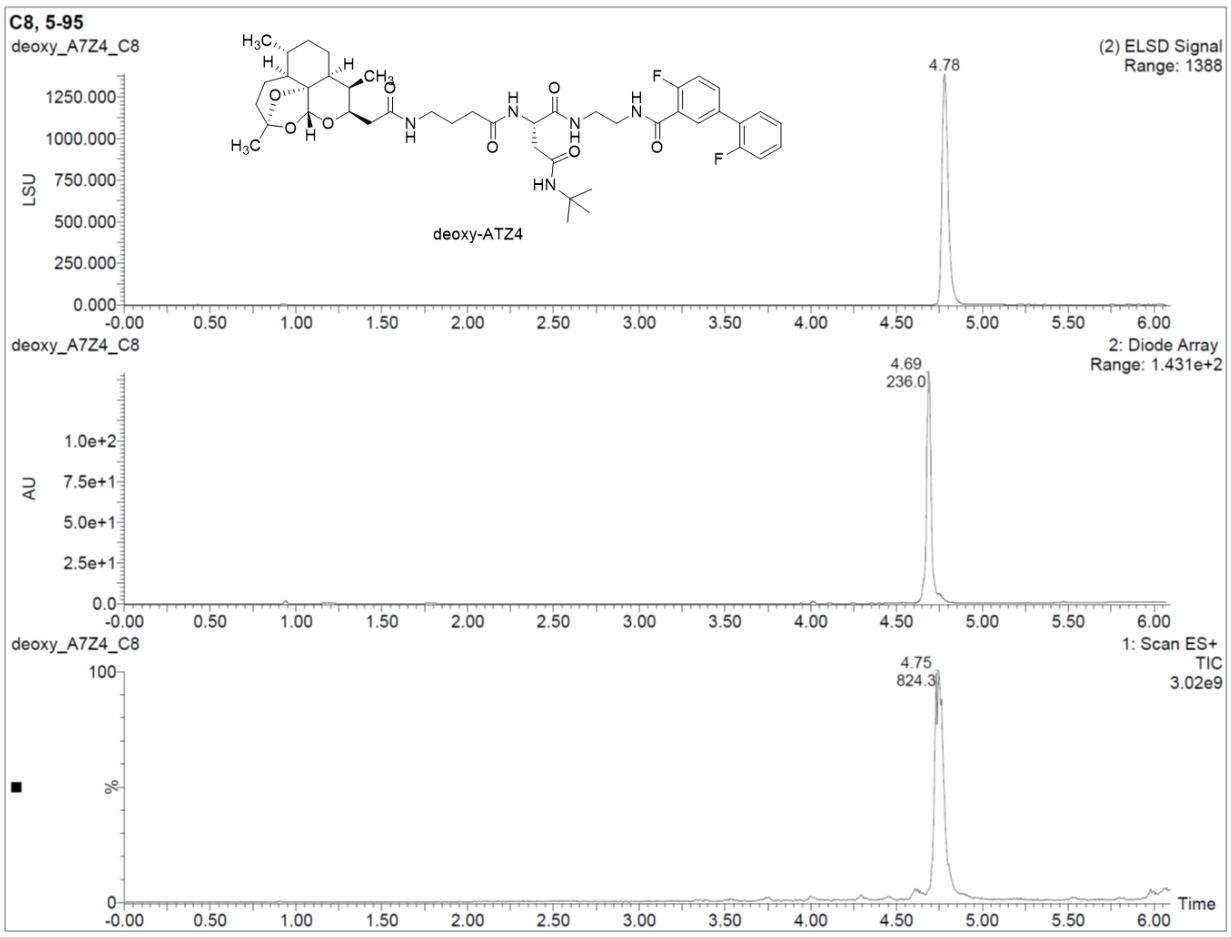
LCMS

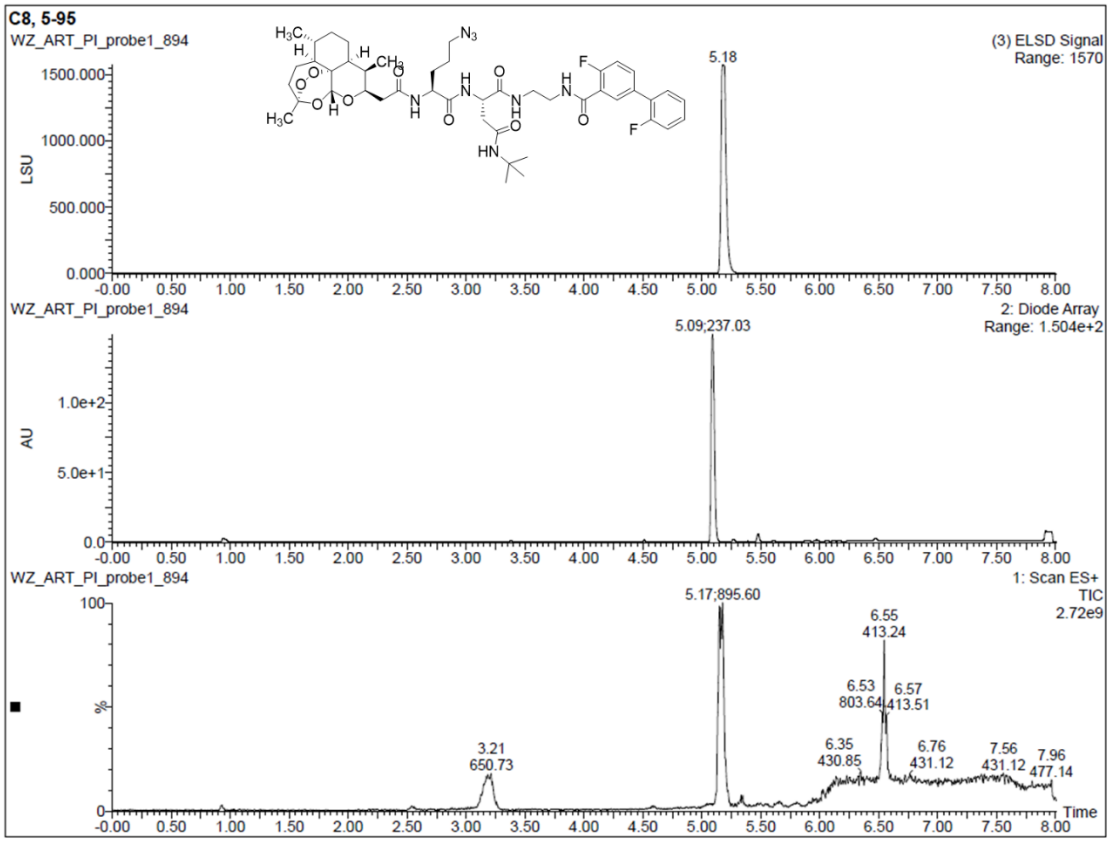

C8, 5-95
WZ_1839_631
(3) ELSD Signal
Range: 1432
4.28
Boc
PI01
LSU
1200.000
1000.000
800.000
600.000
400.000
200.000
0.000
-0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
WZ_1839_631
2: Diode Array
Range: 1.782e+2
4.20
239.0
7.92
210.0
AU
1.5e+2
1.25e+2
1.0e+2
7.5e+1
5.0e+1
2.5e+1
0.0
WZ_1839_631
1: Scan ES+
TIC
3.47e9
4.28
632.4
4.51
468.4
6.17
431.1
7.10
431.1
7.96
400.2
%
100
0
Time

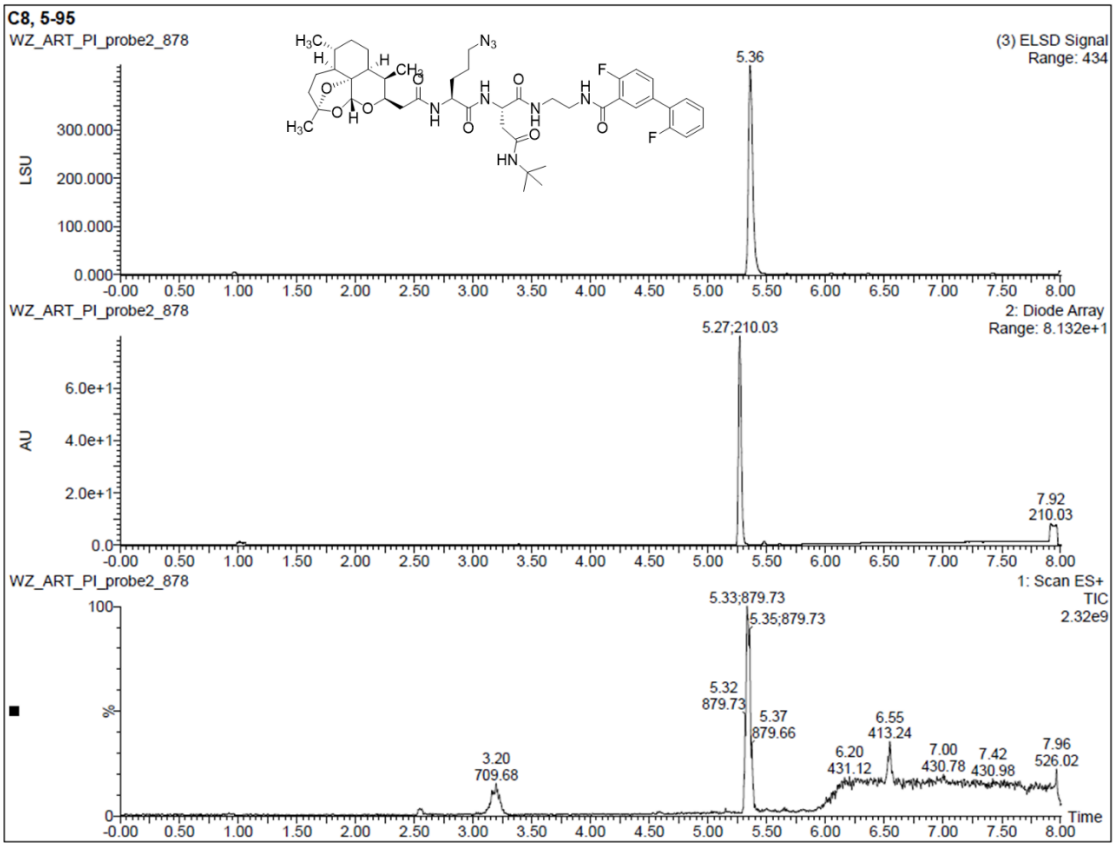

C8, 5-95
WZ_1840_325
(3) ELSD Signal
Range: 1432
3.76
LSU
ART1
WZ_1840_325
2: Diode Array
Range: 1.089e+1
7.97
210.0
3.74
224.0
3.67
210.0
0.94
210.0
1.21
210.0
1.44
210.0
4.14
225.0
0.20
210.0
AU
WZ_1840_325
1: Scan ES+
TIC
1.04e10
3.74
326.0
3.82
278.3
7.94
253.2
%
Time


C8, 5-95
WZ_hybrid2_811_02
(3) ELSD Signal
Range: 1432
3.11
LSU
ATZ2
WZ_hybrid2_811_02
2: Diode Array
Range: 1.522e+2
3.02
239.0
AU
0.38
210.0
7.91
210.0
WZ_hybrid2_811_02
1: Scan ES+
TIC
2.17e9
3.08
812.7
%
5.36
579.9
6.02
431.1
6.39
587.9
6.91
431.1
7.40
431.1
7.96
504.4
Time


C8, 5-95
WZ_hybrid4_839_03
(3) ELSD Signal
Range: 259
3.04
LSU
200.000
150.000
100.000
50.000
0.000
-0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
ATZ4
WZ_hybrid4_839_03
2: Diode Array
Range: 8.138e+1
2.94
210.0
AU
7.0e+1
6.0e+1
5.0e+1
4.0e+1
3.0e+1
2.0e+1
1.0e+1
0.0
0.16
210.0
7.91
210.0
WZ_hybrid4_839_03
1: Scan ES+
TIC
1.11e9
100
%
0
3.01
840.9
3.03
840.9
0.93
505.5
4.73
698.8
5.74
431.2
6.31
431.2
6.73
431.1
7.78;400.2
7.93
538.0
Time


C8, 5-95
deoxy_A7Z4_C8
(2) ELSD Signal
Range: 1388
4.78
LSU
1250.000
1000.000
750.000
500.000
250.000
0.000
deoxy-ATZ4
deoxy_A7Z4_C8
2: Diode Array
Range: 1.431e+2
4.69
236.0
AU
1.0e+2
7.5e+1
5.0e+1
2.5e+1
0.0
deoxy_A7Z4_C8
1: Scan ES+
TIC
3.02e9
4.75
824.3
100
%
0
Time
-0.00
0.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
5.00
5.50
6.00


C8, 5-95
WZ_ART_PI_probe1_894
(3) ELSD Signal
Range: 1570
LSU
5.18
2: Diode Array
Range: 1.504e+2
AU
5.09;237.03
1: Scan ES+
TIC
2.72e9
%
5.17;895.60
6.55
413.24
6.53
803.64
6.57
413.51
3.21
650.73
6.35
430.85
6.76
431.12
7.56
431.12
7.96
477.14
Time


C8, 5-95
WZ_ART_PI_probe2_878
(3) ELSD Signal
Range: 434
LSU
5.36
2: Diode Array
Range: 8.132e+1
AU
5.27;210.03
7.92
210.03
1: Scan ES+
TIC
2.32e9
%
5.33;879.73
5.35;879.73
5.32
879.73
5.37
879.66
6.55
413.24
3.20
709.68
6.20
431.12
7.00
430.78
7.42
430.98
7.96
526.02
Time

HRMS:

Elemental Composition Report **Page 1**

HRMS of PI01

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

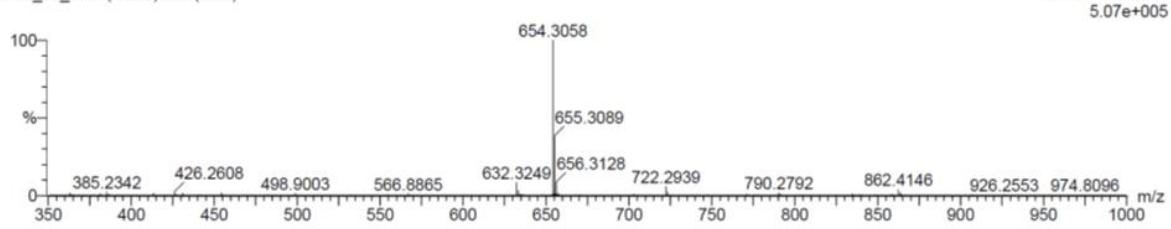
Monoisotopic Mass, Even Electron Ions
243 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-32 H: 0-45 N: 0-5 O: 0-6 F: 0-2 Na: 0-1

Rong
Rong
C32H43F2N5O6
WZ_18_39 9 (0.208) Cm (9:16)

NMR Analytical Core Facility
LCT Premier XE

28-Sep-2018
2::1::3

1: TOF MS ES+
5.07e+005



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
654.3058	654.3079	-2.1	-3.2	12.5	520.8	0.0	C32 H43 N5 O6 F2 Na

Elemental Composition Report **Page 1**

HRMS of ART1

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

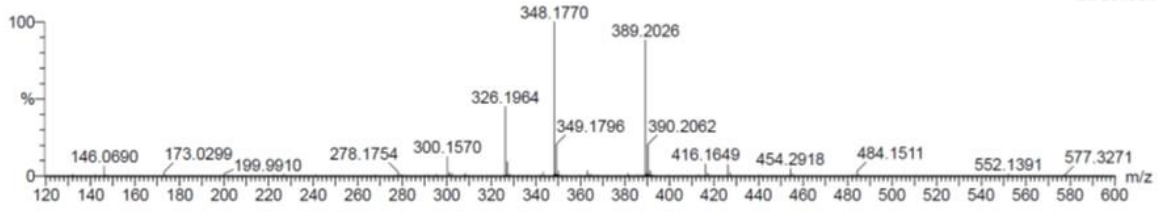
Monoisotopic Mass, Even Electron Ions
32 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-17 H: 0-45 N: 0-1 O: 0-6 Na: 0-1

Rong
Rong
C17H27NO5
WZ_18_40 25 (0.570) Cm (25:31)

NMR Analytical Core Facility
LCT Premier XE

28-Sep-2018
2::4::2

1: TOF MS ES+
8.79e+004



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
348.1770	348.1787	-1.7	-4.9	4.5	545.8	0.0	C17 H27 N O5 Na

Elemental Composition Report Page 1

HRMS of ATZ2

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

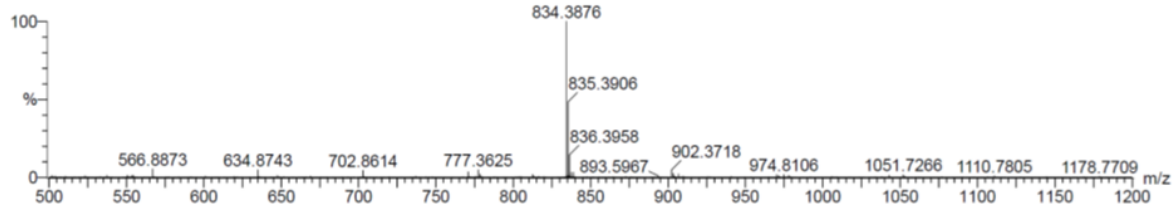
Monoisotopic Mass, Even Electron Ions
347 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-42 H: 0-56 N: 0-5 O: 0-9 F: 0-2 Na: 0-1

Rong
Rong
C42H55F2N5O9
WZ_Hybrid2_811 16 (0.350) Cm (11:16)

NMR Analytical Core Facility
LCT Premier XE

28-Sep-2018
2::8::0

1: TOF MS ES+
1.49e+005



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
834.3876	834.3866	1.0	1.2	16.5	370.2	0.0	C42 H55 N5 O9 F2 Na

Elemental Composition Report Page 1

HRMS of ATZ4

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

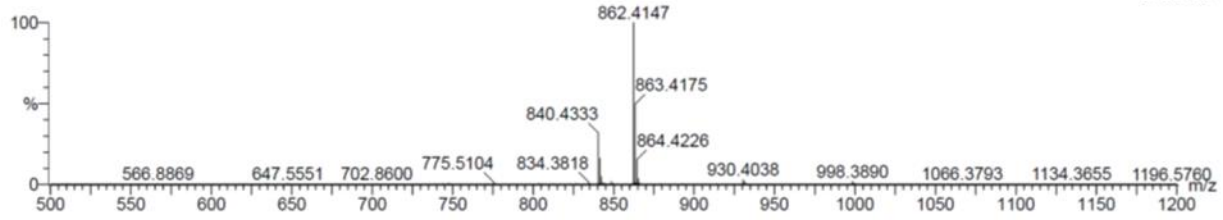
Monoisotopic Mass, Even Electron Ions
347 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-44 H: 0-60 N: 0-5 O: 0-9 F: 0-2 Na: 0-1

Rong
Rong
C44H59F2N5O9
WZ_Hybrid4_839 28 (0.622) Cm (28:33)

NMR Analytical Core Facility
LCT Premier XE

28-Sep-2018
2::8::8

1: TOF MS ES+
9.78e+004



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
862.4147	862.4179	-3.2	-3.7	16.5	327.2	0.0	C44 H59 N5 O9 F2 Na

Elemental Composition Report

HRMS of Deoxy-ATZ4

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

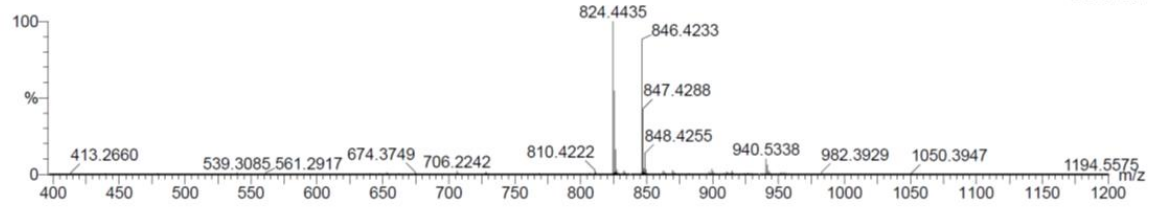
Monoisotopic Mass, Even Electron Ions
199 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-44 H: 0-60 N: 0-5 O: 0-8 F: 0-3

Gang
Gang
C44H59F2N5O8
deoxy_A7Z4 11 (0.244) Cm (9:11)

NMR Analytical Core Facility
LCT Premier XE

17-Feb-2021
3::8::2

1: TOF MS ES+
2.97e+004



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
824.4435	824.4410	2.5	3.0	16.5	138.2	0.0	C44 H60 N5 O8 F2

HRMS of ATZ-P1

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

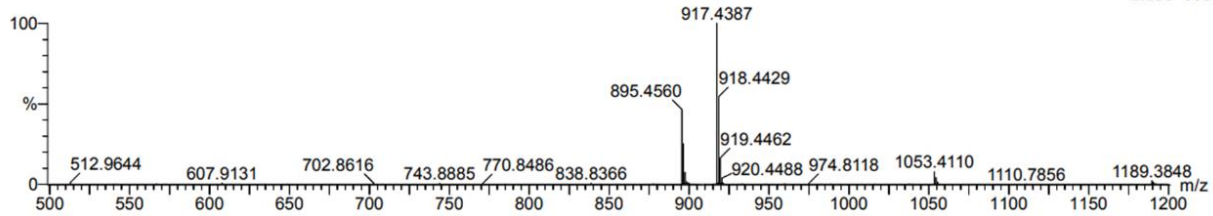
Monoisotopic Mass, Even Electron Ions
524 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-45 H: 0-61 N: 0-8 O: 0-9 F: 0-2 Na: 0-1

Gang
Wenfu
C45H60F2N8O9
WZ_ART_PI_probe1_894 63 (1.420) Cm (62:66)

NMR Analytical Core Facility
LCT Premier XE

15-Apr-2019
11:59:18

1: TOF MS ES+
2.23e+005



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
917.4387	917.4349	3.8	4.1	18.5	190.6	0.0	C45 H60 N8 O9 F2 Na

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

HRMS of Deoxy-ATZ-P1

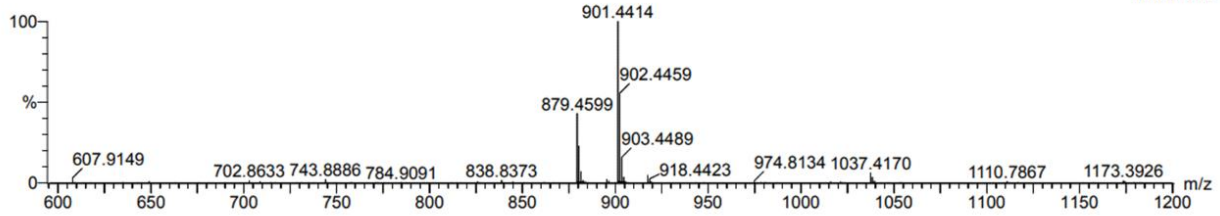
Monoisotopic Mass, Even Electron Ions
510 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-45 H: 0-61 N: 0-8 O: 0-9 F: 0-2 Na: 0-1

Gang
Wenfu
C45H60F2N8O8
WZ_ART_PI_probe2_878 35 (0.786) Cm (30:35)

NMR Analytical Core Facility
LCT Premier XE

15-Apr-2019
12:05:09

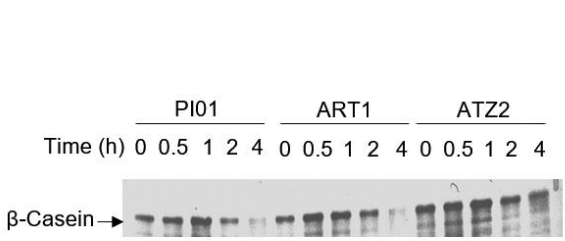
1: TOF MS ES+
1.52e+005

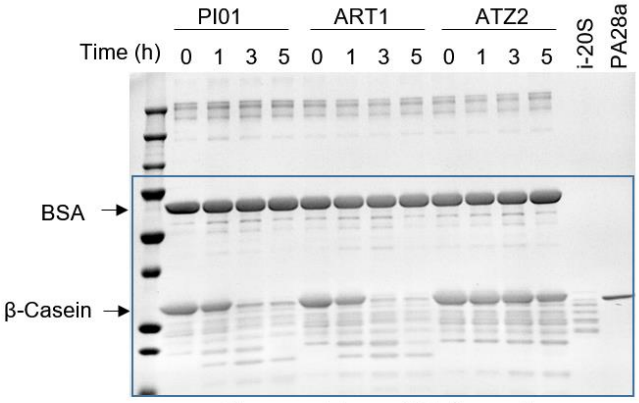


Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
901.4414	901.4400	1.4	1.6	18.5	195.3	0.0	C45 H60 N8 O8 F2 Na

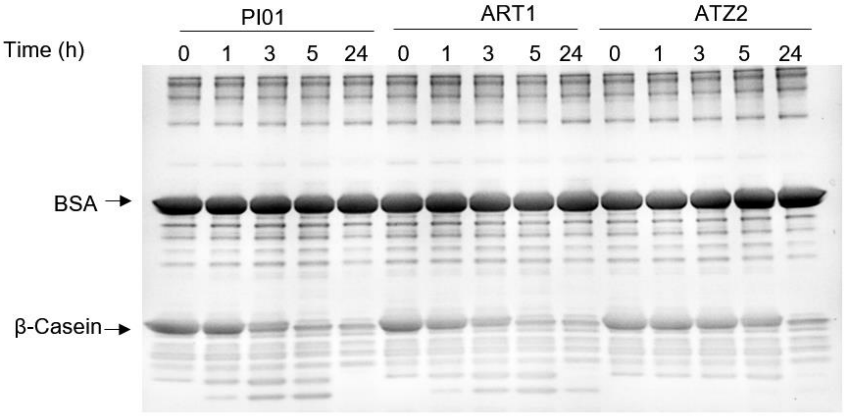
Extended Raw Data

a. Extended data for Figure 2. Triplicate β-casein degradation with dialysis.

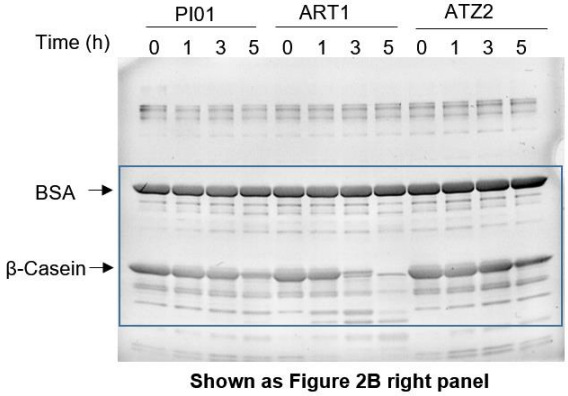




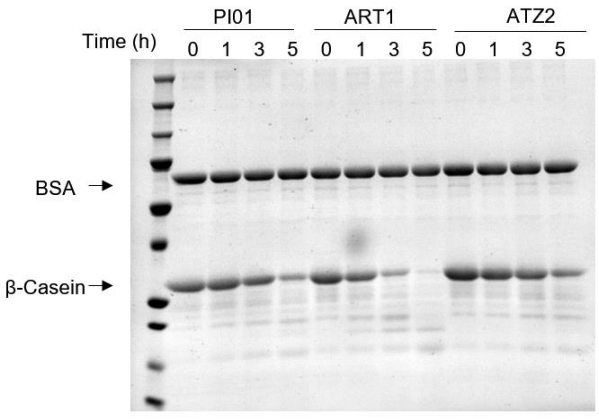
Shown as Figure 2B left panel



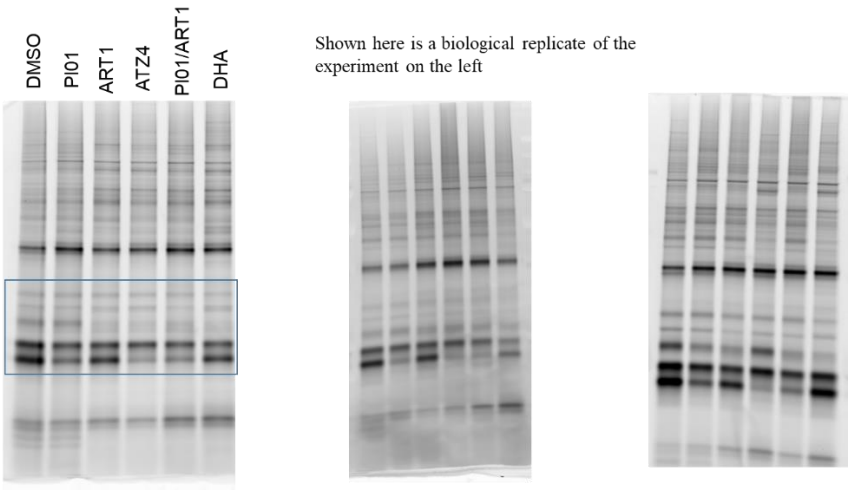
b. Extended data for Figure 2. Duplicate β-casein degradation without dialysis



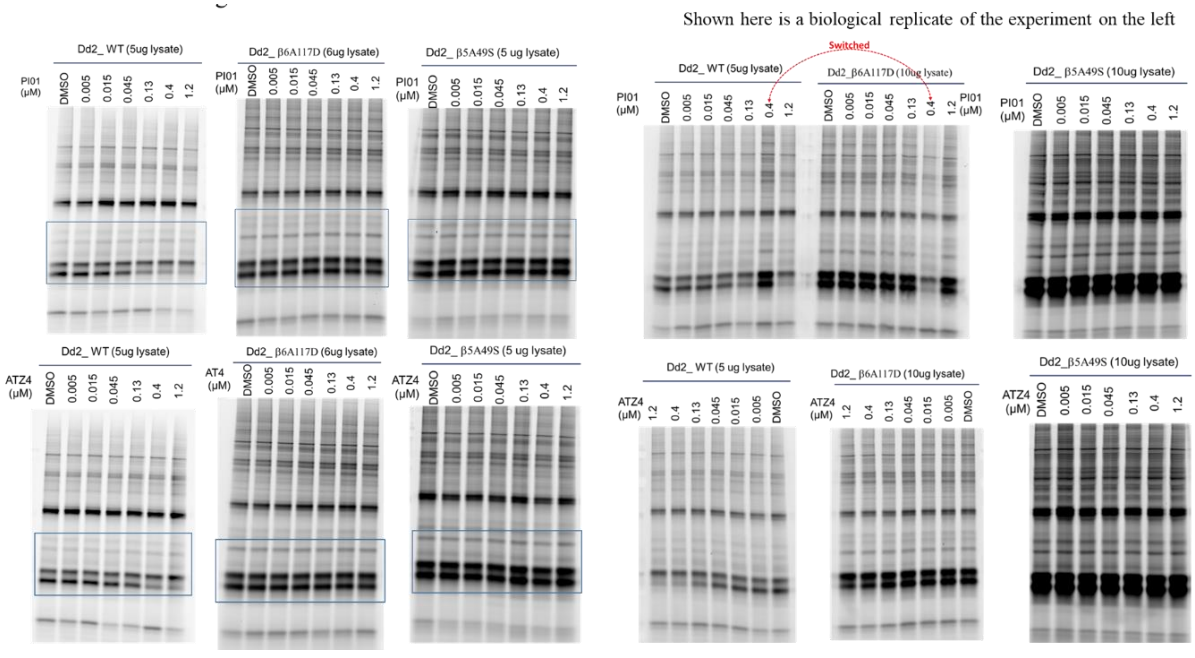
Shown as Figure 2B right panel



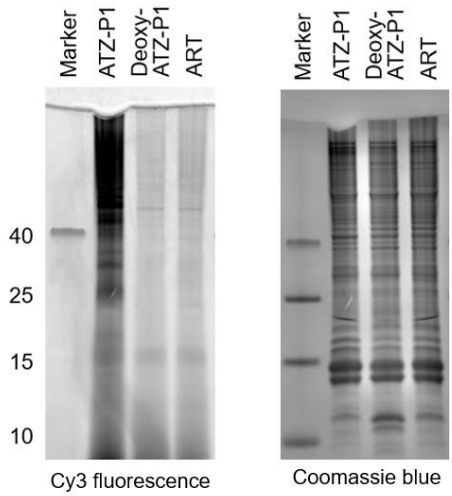
c. Extended Data for Figure S2



d. Extended Data for Figure 4 (switched samples indicated by red arrow were recorded in notebook)



e. Extended data for Figure 5B. Repeat of ATZ-P1 labeling experiment.


Marker
ATZ-P1
Deoxy-ATZ-P1
ART
40
25
15
10
Cy3 fluorescence
Marker
ATZ-P1
Deoxy-ATZ-P1
ART
Coomassie blue

f. Extended data for Figure 5D. Triplicate experiments.