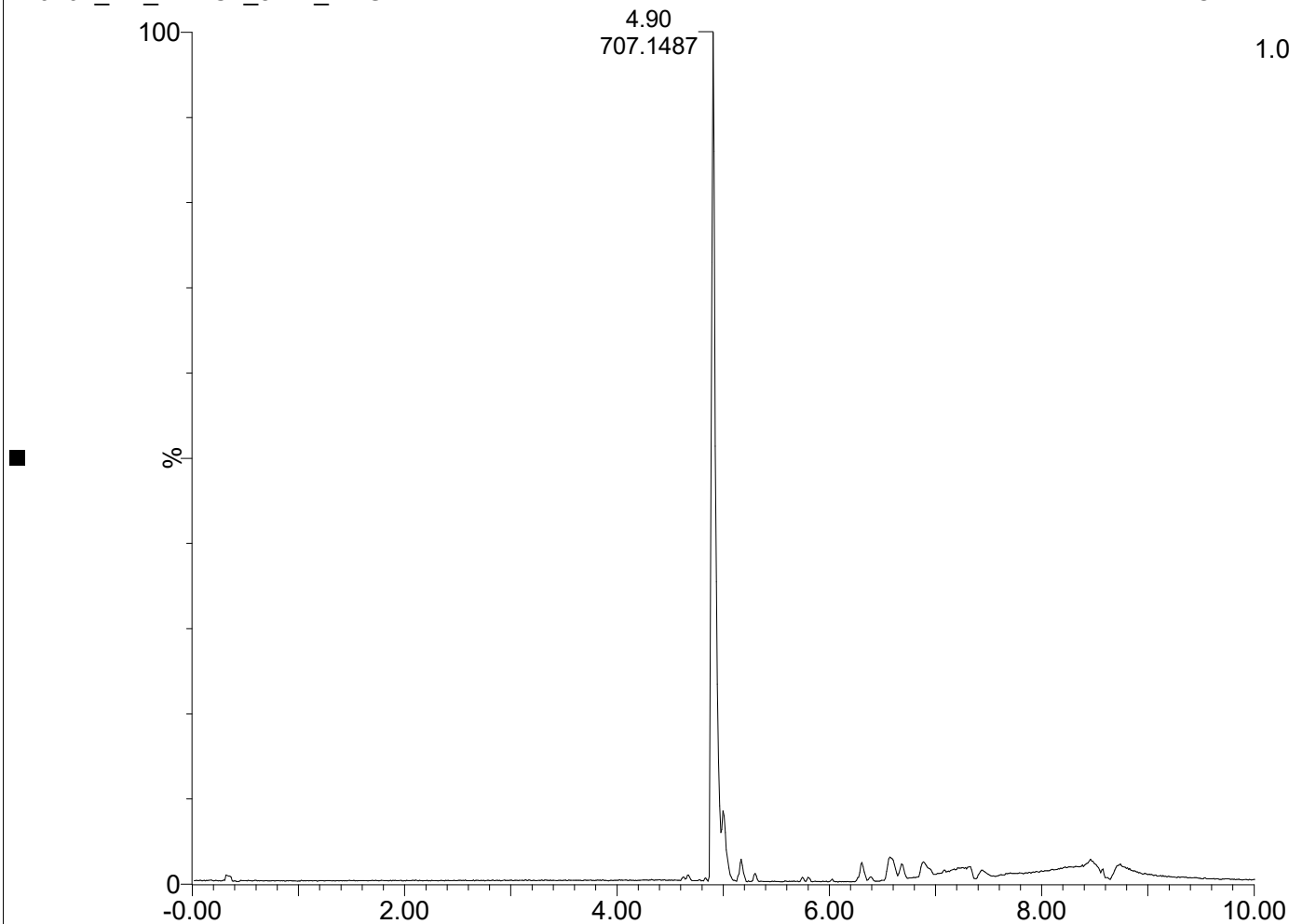


COMPOUND NO. S26 (METHOD A)

COL31

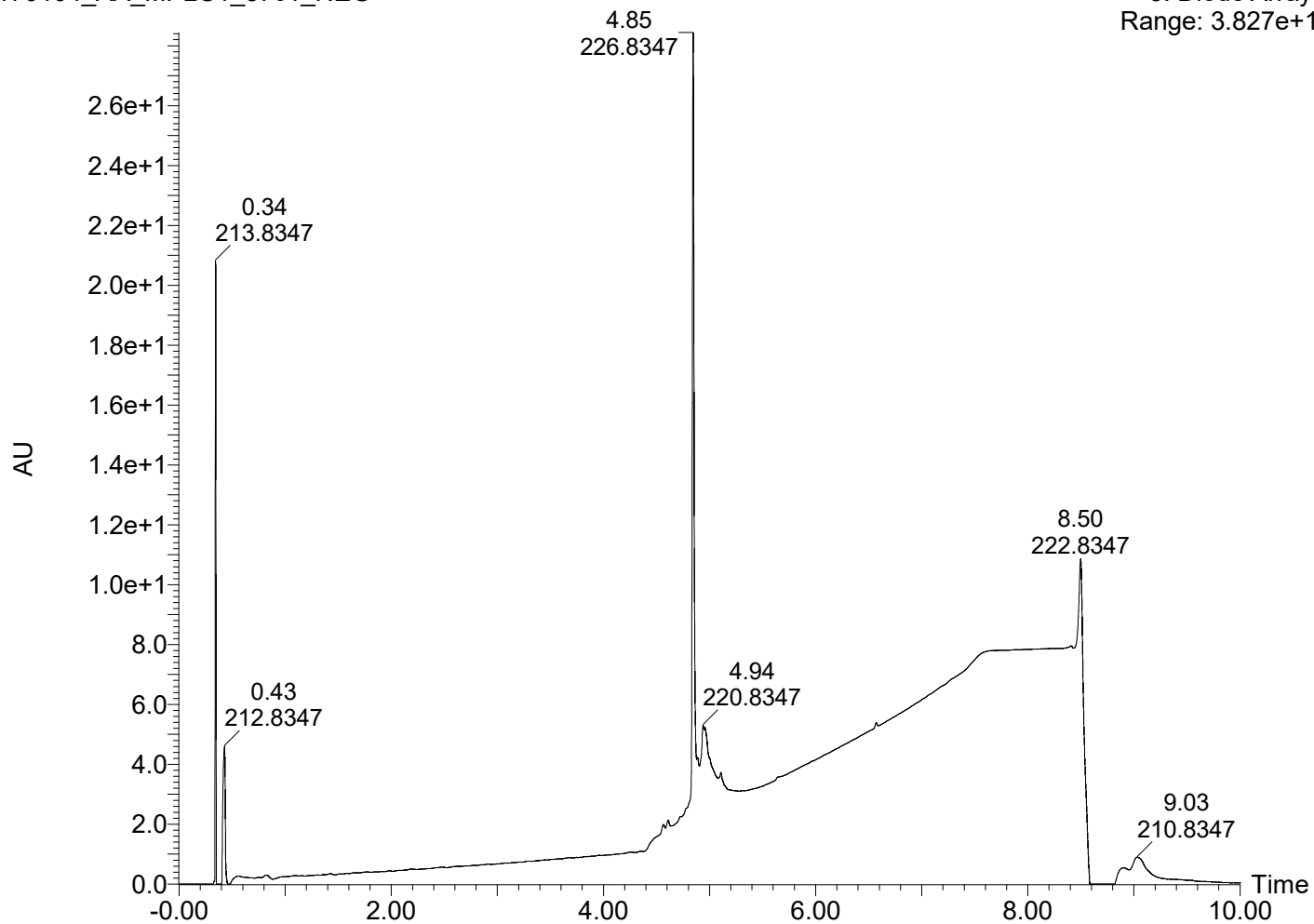
170104_AA_MPLC1_87c1_NEG

1: TOF MS ES-
BPI
1.06e5



170104_AA_MPLC1_87c1_NEG

3: Diode Array
Range: 3.827e+1



Single Mass Analysis

Tolerance = 15.0 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

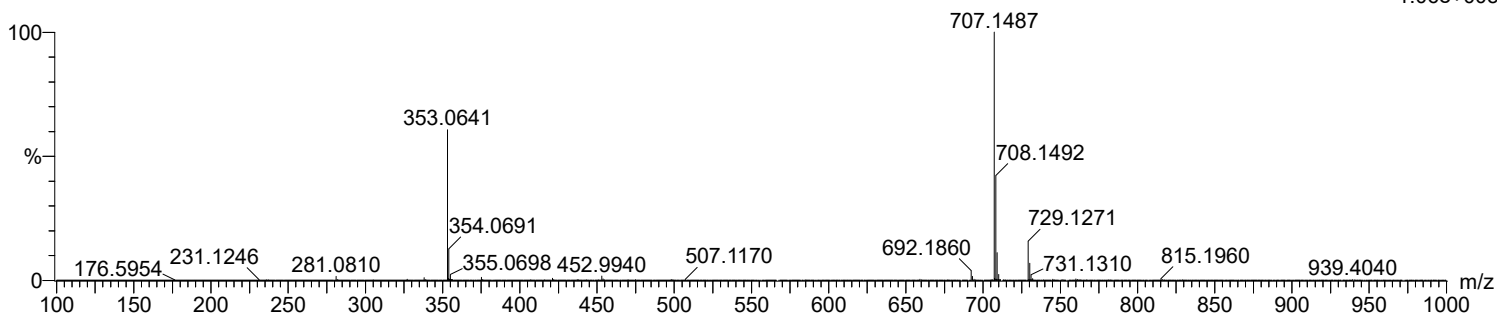
70 formula(e) evaluated with 2 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

COL31

170104_AA_MPLC1_87c1_NEG 422 (4.904)

1: TOF MS ES-
1.06e+005

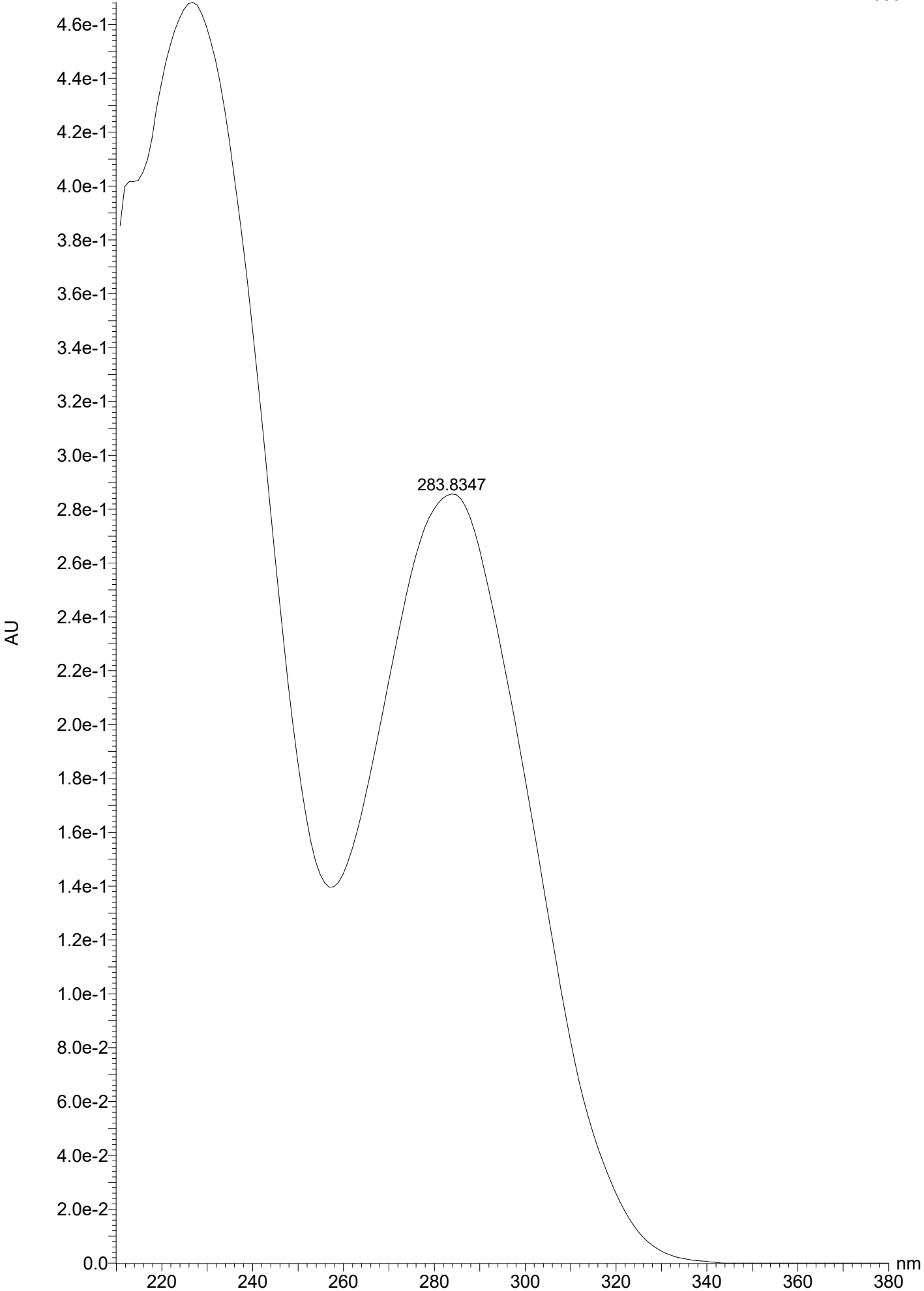
Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
353.0641	353.0661	-2.0	-5.7	13.5	360.2	0.000	100.00	C19 H13 O7
	353.0603	3.8	10.8	22.5	372.7	12.526	0.00	C26 H9 O2

COL31

170104_AA_MPLC1_87c1_NEG 5814 (4.844)

3: Diode Array
4.683e-1

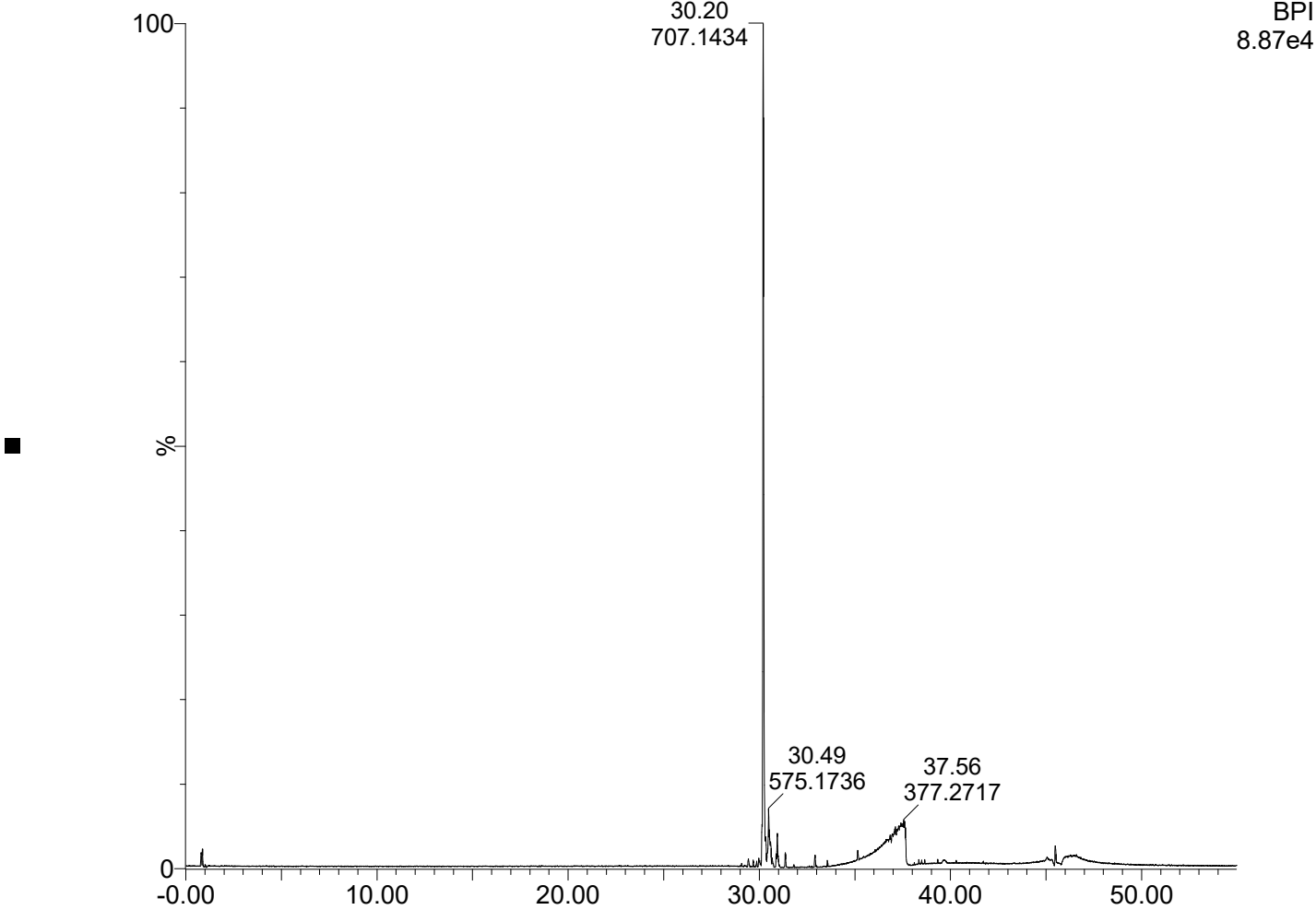


COMPOUND NO. S26 (METHOD B)

Col 32

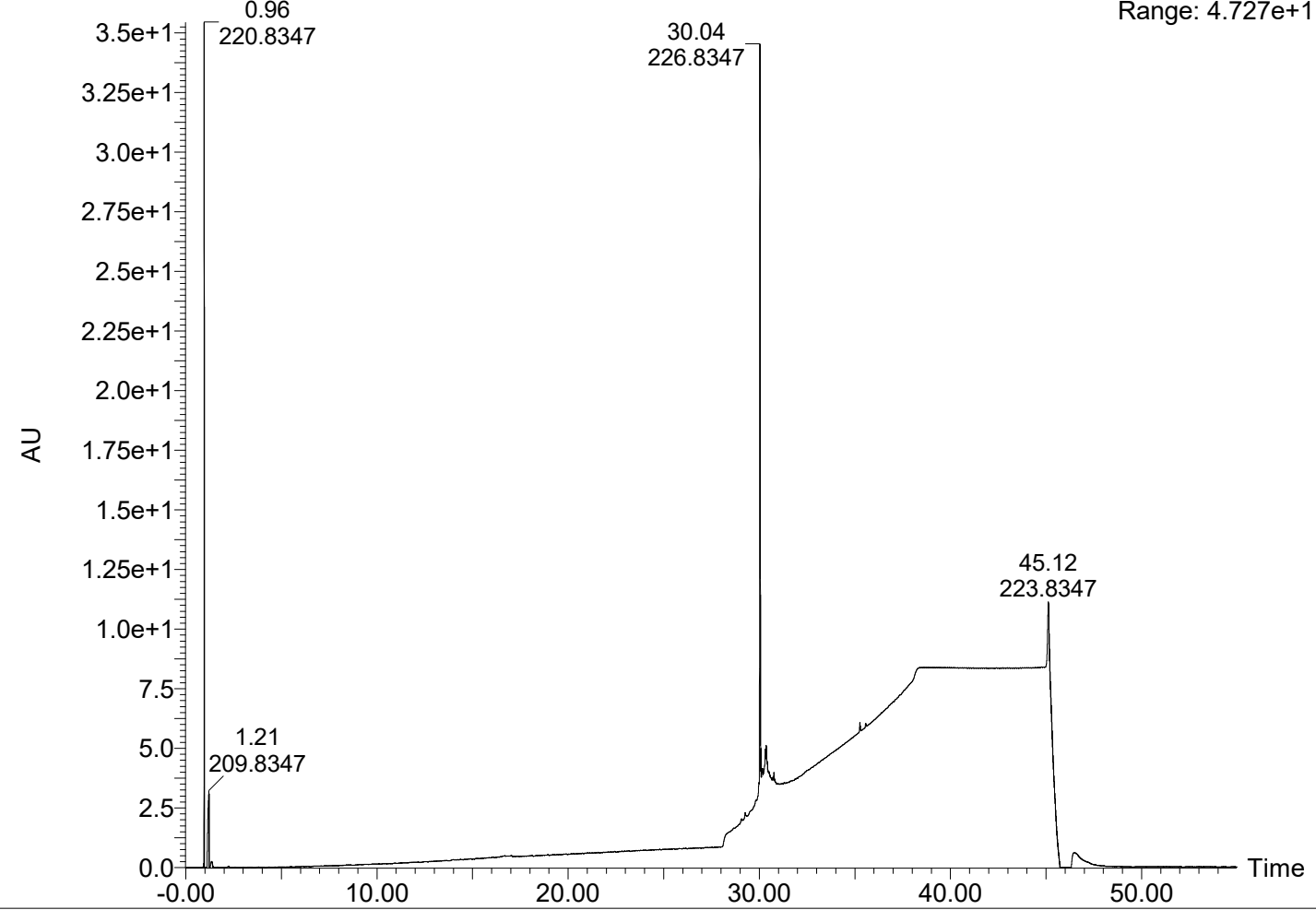
170125_AA_MPLC1_87c1_NEG

1: TOF MS ES-
BPI
8.87e4



170125_AA_MPLC1_87c1_NEG

3: Diode Array
Range: 4.727e+1



Single Mass Analysis

Tolerance = 15.0 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

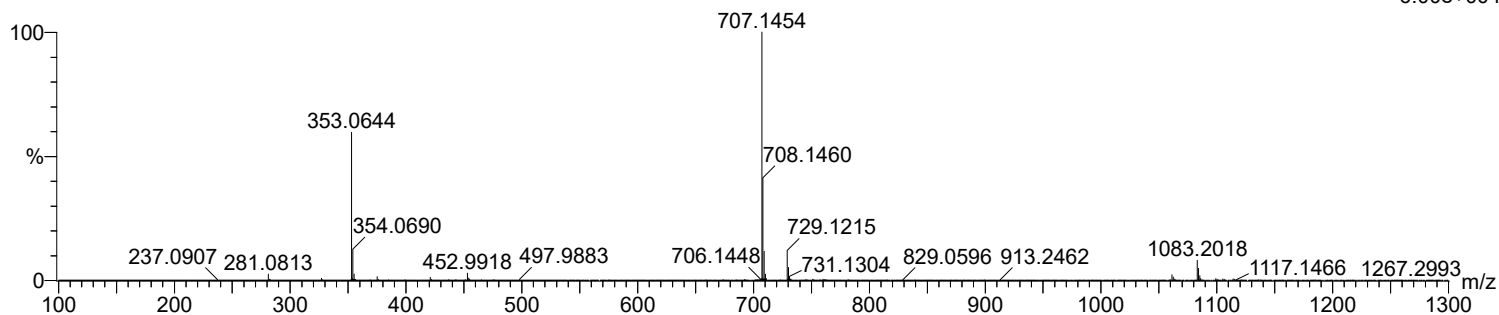
70 formula(e) evaluated with 2 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Col 32

170125_AA_MPLC1_87c1_NEG 2572 (30.226)

1: TOF MS ES-
6.00e+004

Minimum: -1.5
Maximum: 5.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
353.0644	353.0661	-1.7	-4.8	13.5	322.2	0.001	99.94	C19 H13 O7
	353.0603	4.1	11.6	22.5	329.6	7.430	0.06	C26 H9 O2

Col 32

170125_AA_MPLC1_87c1_NEG 36038 (30.036)

3: Diode Array
5.531e-1

