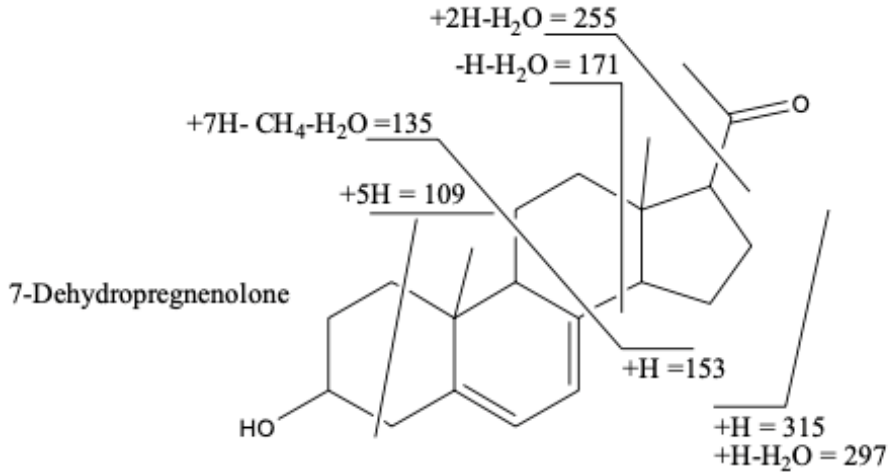
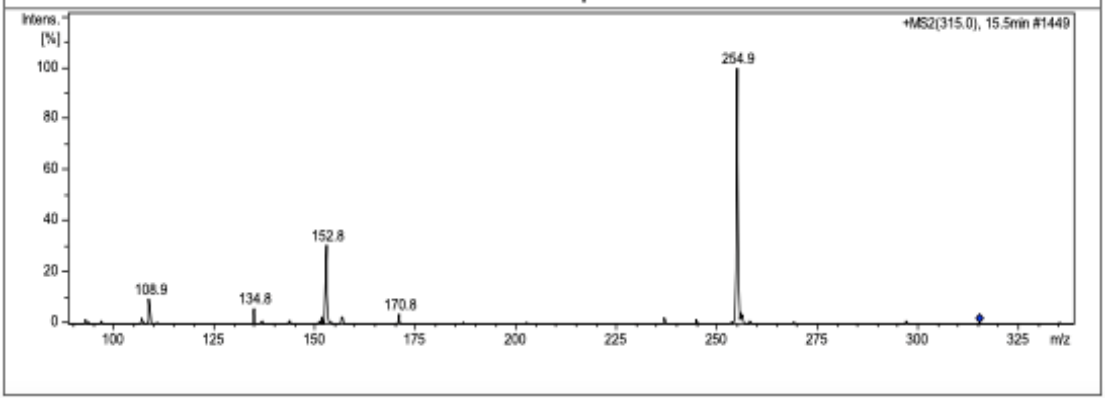
Supplementary Table S2. The product ion spectra of metabolites in the Table 1.

Spectrum Number	1	Detected Mass	315.2365
Adduct Formula	C 21 H 31 O 2		
Putative name	**NAME:** 7-Dehydropregnenolone		
Acc #	**Metlin:** x **HMDB:**HMDB13121 **KEGG:**x		

Interpretation

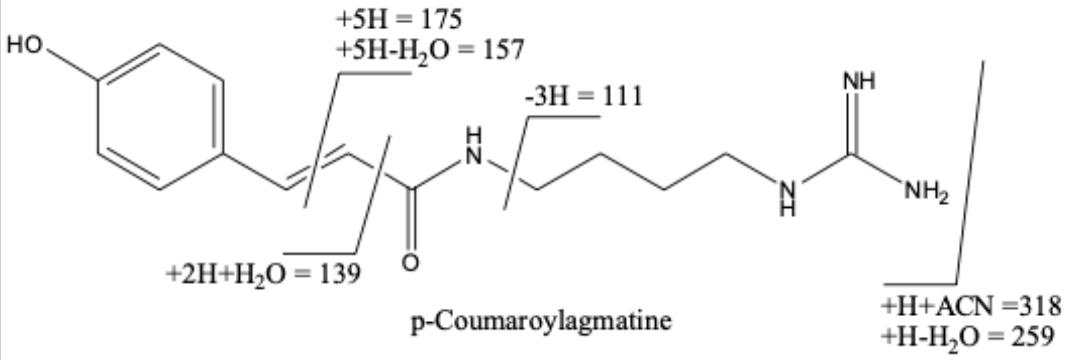


Product ion spectrum

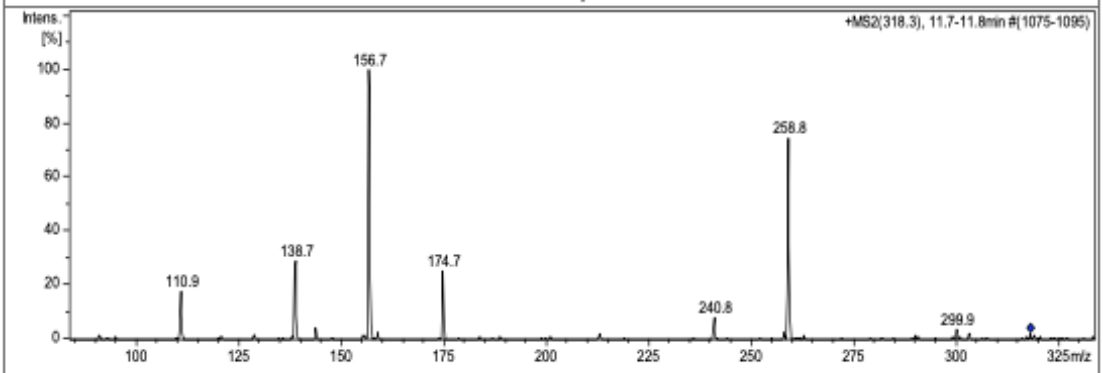


Spectrum Number	2	Detected Mass	318.1915
Adduct Formula	C 16 H 24 N 5 O 2		
Putative name	**NAME:** p-Coumaroylagmatine		
Acc #	**Metlin:** 66195 **HMDB:**x **KEGG:**C04498		

Interpretation

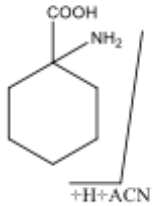


Product ion spectrum



Spectrum Number	3	Detected Mass	185.1286
Adduct Formula	C9H17N2O2		
Putative name	**NAME:** 1-Aminocyclohexanecarboxylic acid		
Acc #	**Metlin:** 6589 **HMDB:**HMDB02279 **KEGG:**x		

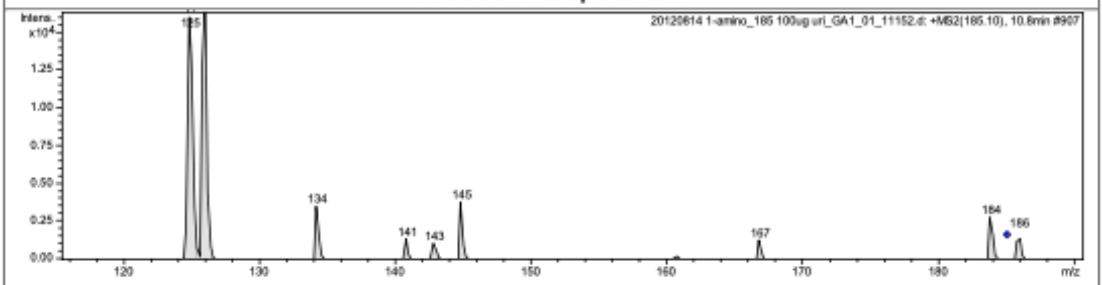
Interpretation



1-Aminocyclohexanecarboxylic acid

+H+ACN =185
+H+ACN-H_2O = 167
+2H =145
-NH_3 = 126
-H_2O = 125

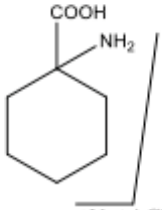
Product ion spectrum



Spectrum Number	4	Detected Mass	207.1107
Adduct Formula	C 9 H 16 N 2 Na O 2		
Putative name	**NAME:** 1-Aminocyclohexanecarboxylic acid		
Acc #	**Metlin:** 6589 **HMDB:**HMDB02279 **KEGG:**x		

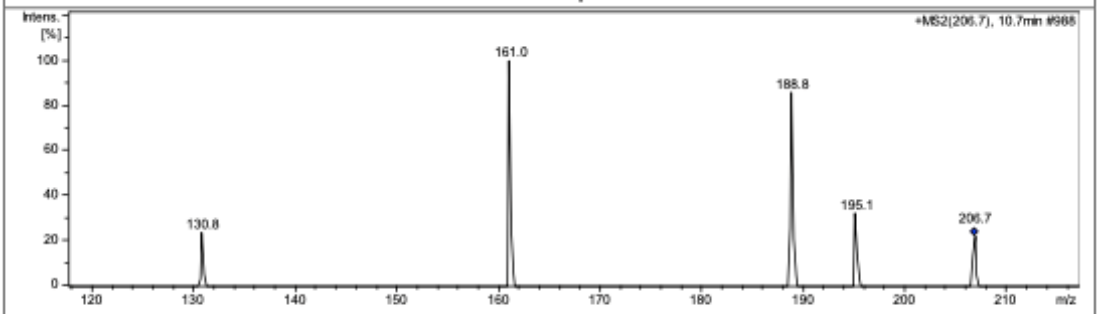
Interpretation

1-Aminocyclohexanecarboxylic acid



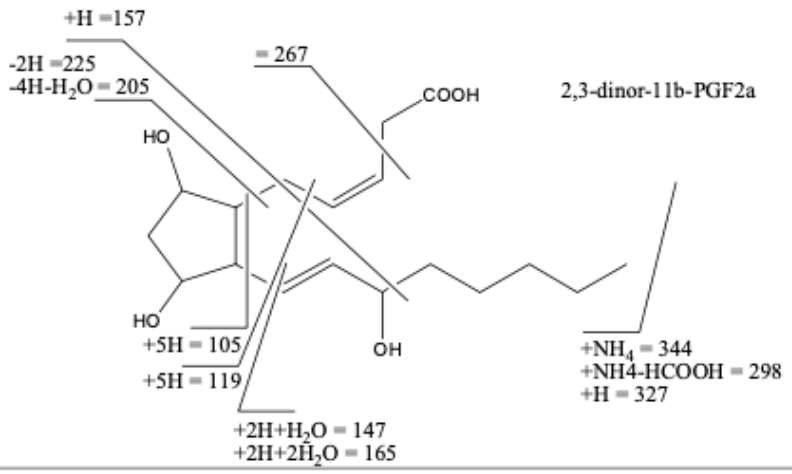
+Na+ACN =207
+Na+ACN-H_2O = 189
+Na+ACN-NH_3+5H =195
+NH_4 =161
+5H-NH_3 = 131

Product ion spectrum

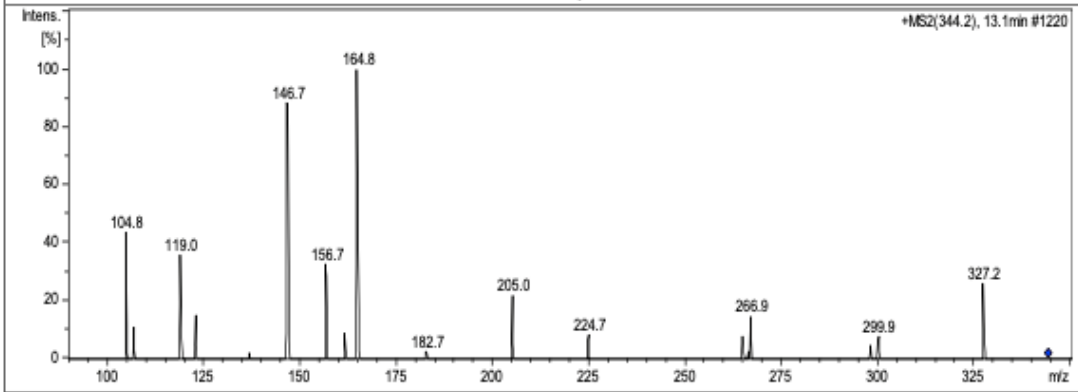


Spectrum Number	5	Detected Mass	344.2436
Adduct Formula	C 18 H 34 N O 5		
Putative name	**NAME:** 2,3-dinor-11b-PGF2α		
Acc #	**Metlin:** 36202 **HMDB:**x **KEGG:**C14794		

Interpretation

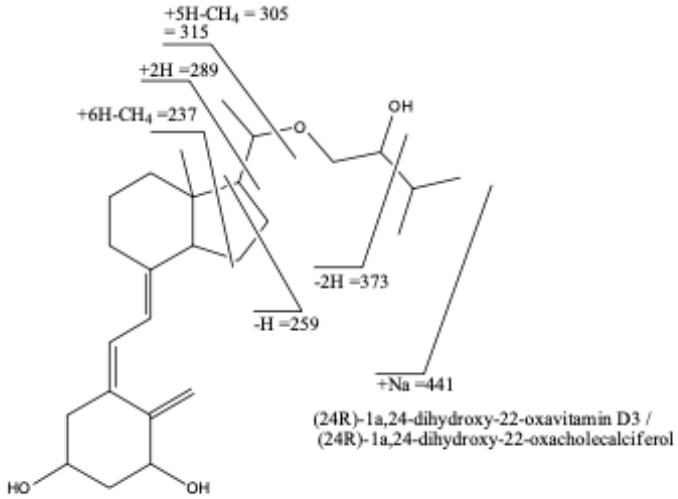


Product ion spectrum

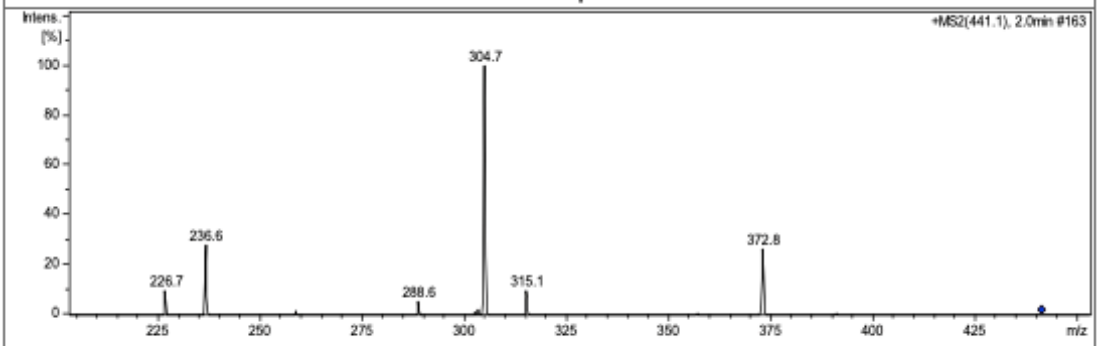


Spectrum Number	6	Detected Mass	441.2987
Adduct Formula	C 26 H 42 Na O 4		
Putative name	**NAME:** (24R)-1α,24-dihydroxy-22-oxacholecalciferol (24S)-1α,24-dihydroxy-22-oxacholecalciferol		
Acc #	**Metlin:** 41996 41998 **HMDB:**x **KEGG:**x		

Interpretation

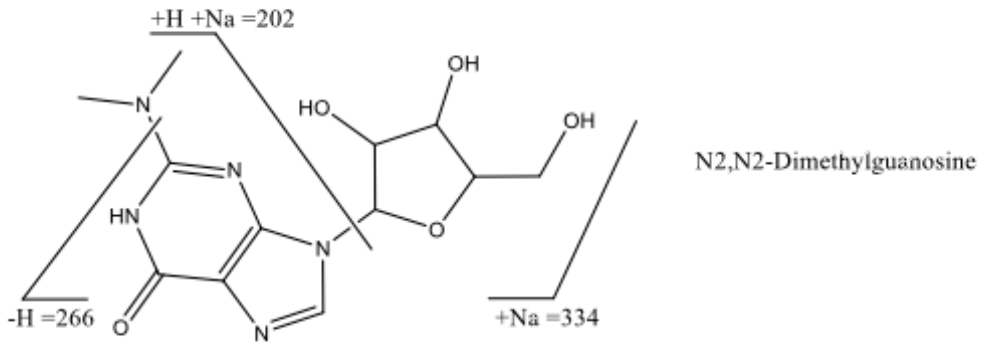


Product ion spectrum

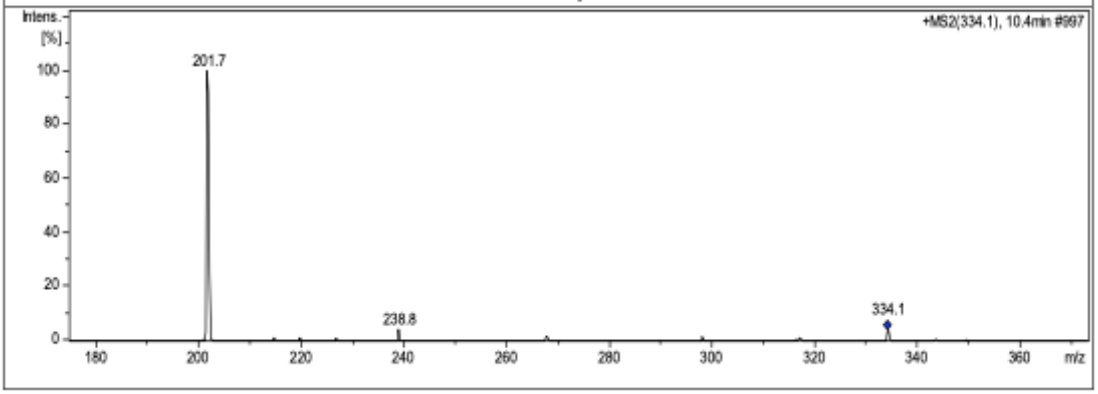


Spectrum Number	7	Detected Mass	334.1135
Adduct Formula	C 12 H 17 N 5 Na O 5		
Putative name	**NAME:** N2,N2-Dimethylguanosine		
Acc #	**Metlin:** 7086 **HMDB:**HMDB04824 **KEGG:**x		

Interpretation

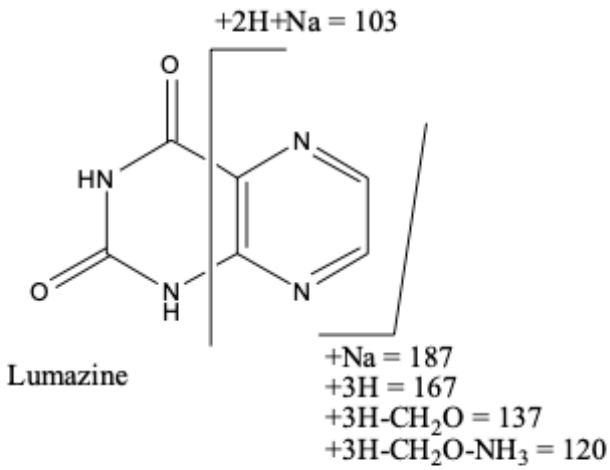


Product ion spectrum

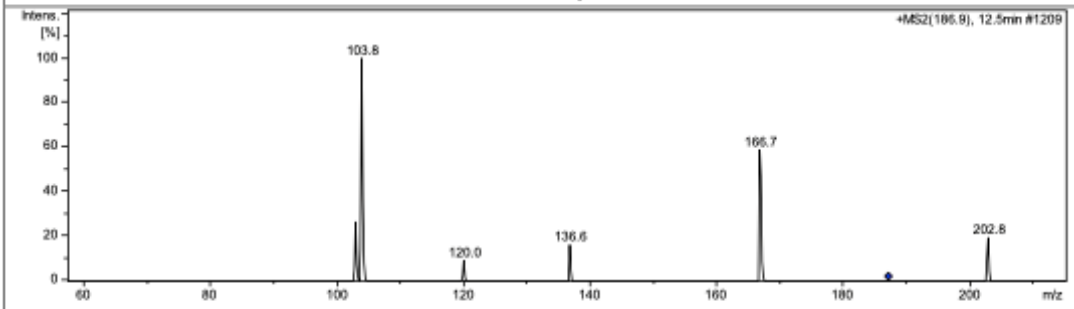


Spectrum Number	8	Detected Mass	187.0225
Adduct Formula	C 6 H 4 N 4 Na O 2		
Putative name	**NAME:** Lumazine		
Acc #	**Metlin:** 44770 **HMDB:**x **KEGG:**x		

Interpretation

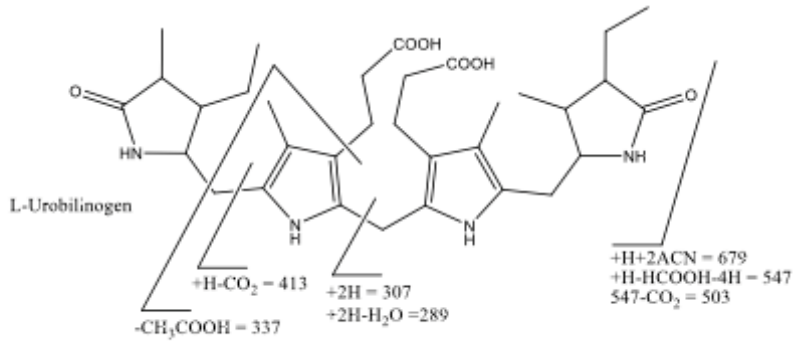


Product ion spectrum

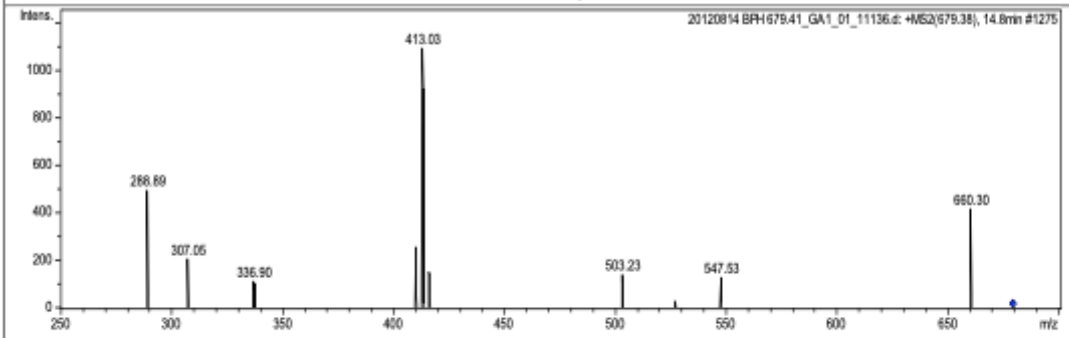


Spectrum Number	9	Detected Mass	679.4108
Adduct Formula	C 37 H 55 N 6 O 6		
Putative name	**NAME:** L-Urobilinogen		
Acc #	**Metlin:** x **HMDB:**HMDB04157 **KEGG:**x		

Interpretation

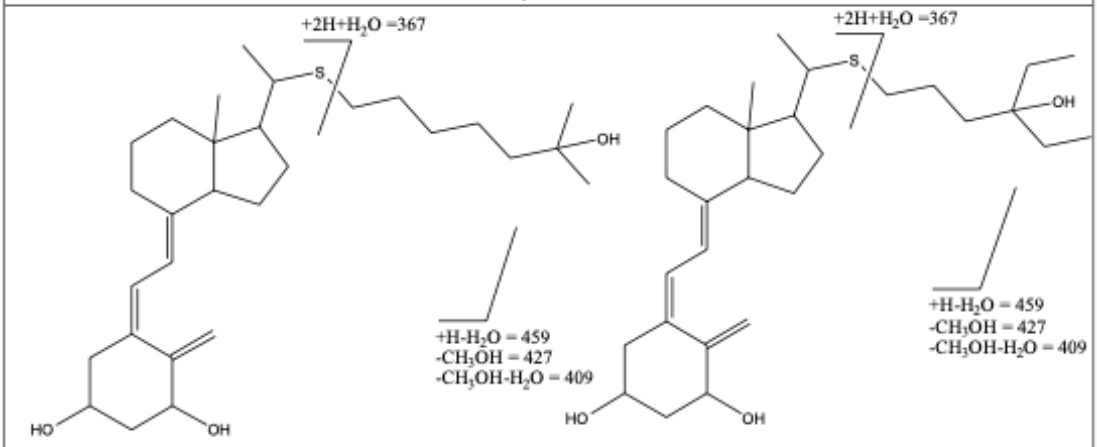


Product ion spectrum



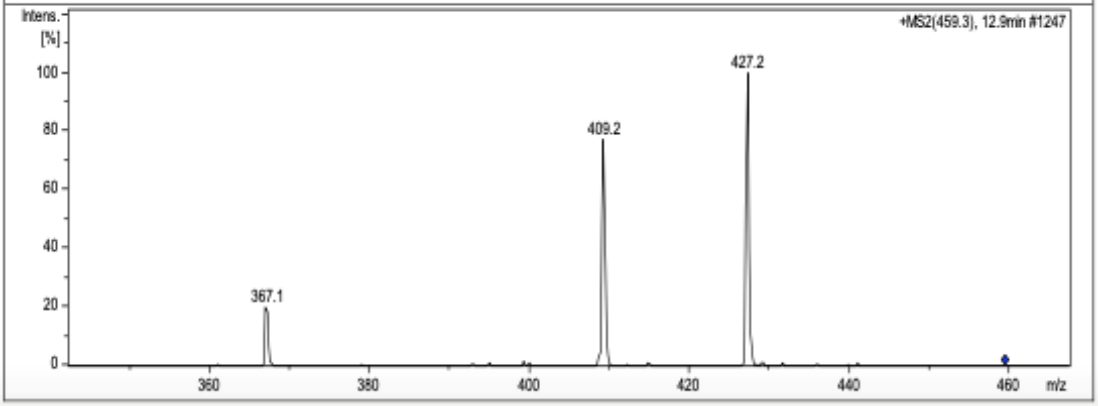
Spectrum Number	10	Detected Mass	459.3336
Adduct Formula	C 29 H 47 O 2 S		
Putative name	**NAME:** 1α,25-dihydroxy-24a-homo-26,27-dimethyl-22-thiavitamin D3 1α,25-dihydroxy-24a-homo-26,27-dimethyl-22-thiacholecalciferol 1α,25-dihydroxy-26,27-dimethyl-24a-homo-22-thia-20-epivitamin D3 1α,25-dihydroxy-26,27-dimethyl-24a-homo-22-thia-20-epicholecalcif		
Acc #	**Metlin:** 42352 42353 42354 42355 **HMDB:x** **KEGG:x**		

Interpretation



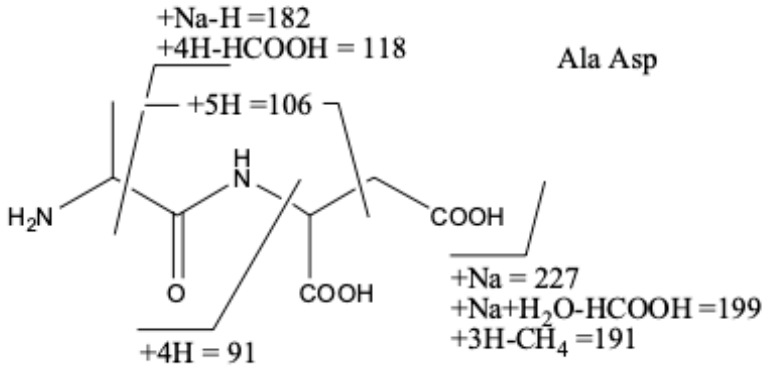
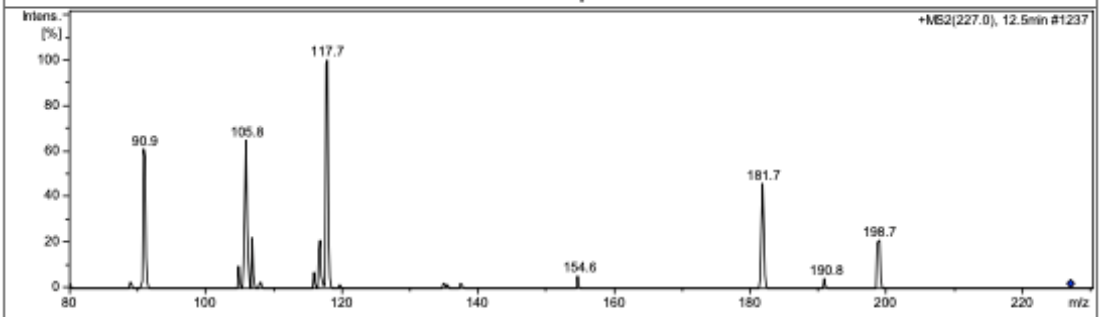
(5Z,7E)-(1S,3R)-26,27-dimethyl-24a-homo-9,10-seco-22-thia-5,7,10(19)-cholestatriene-1,3,25-triol
(5Z,7E)-(1S,3R)-24a,24b,24c-trihomo-9,10-seco-22-thia-5,7,10(19)-cholestatriene-1,3,25-triol

Product ion spectrum



Spectrum Number	11	Detected Mass	227.0599
Adduct Formula	C 7 H 12 N 2 Na O 5		
Putative name	**NAME:** Ala Asp		
Acc #	**Metlin:** 23907 **HMDB:**x **KEGG:**x		

Interpretation



Product ion spectrum