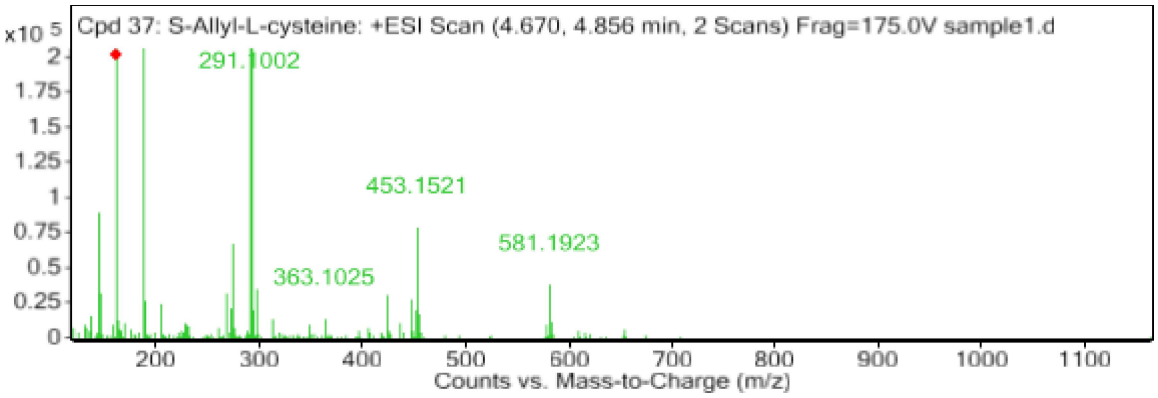
Fig. S1. *Showing HR-LCMS-MS zoomed spectrum showing the ionization peaks of organosulfur compounds detected in various extracts of garlic, with their chemical formula and structure*

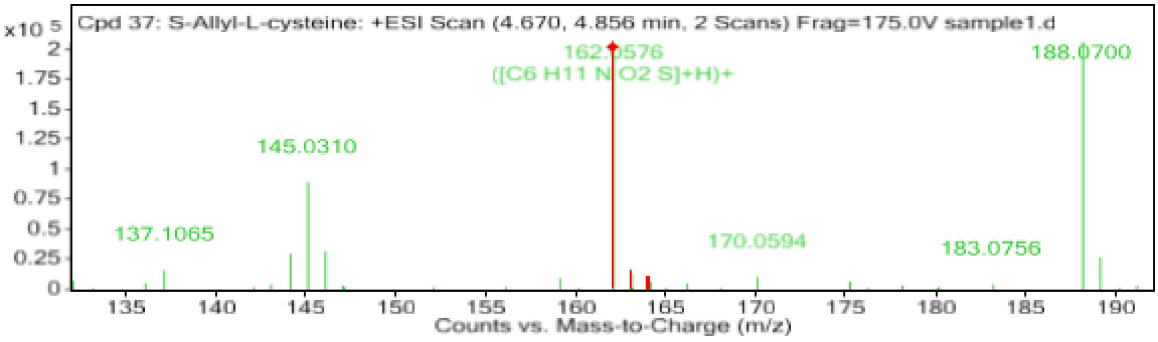
S-Allyl-L-cysteine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 37: S-Allyl-L-cysteine	**S-Allyl-L-cysteine**	162.0576	4.776	Auto MS/MS	161.0504

MS Spectrum



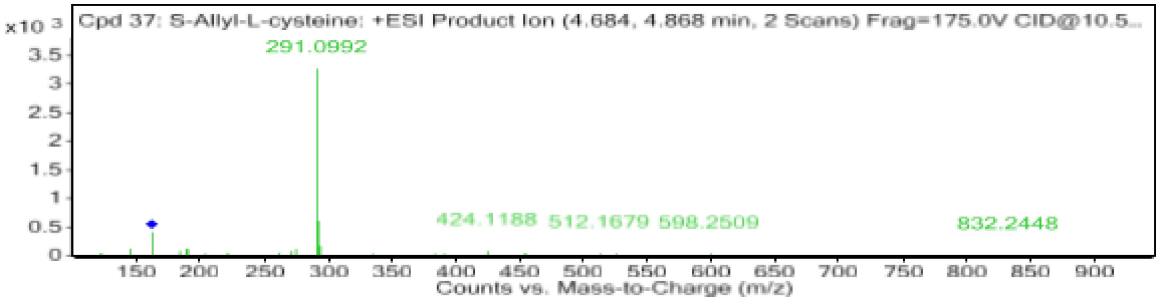
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.031			1	90169.55		
162.0576	162.0583	4.36	1	205944.42	C6 H11 N O2 S	(M+H)+
163.0611	163.061	-0.35	1	13979.36	C6 H11 N O2 S	(M+H)+
164.0549	164.0553	2.45	1	7853.33	C6 H11 N O2 S	(M+H)+
188.07			1	221843.31		
274.0736			1	68229.7		
291.1002			1	3544463.25		
292.1031			1	452477.53		
293.0989			1	163448.81		
453.1521			1	79904.23		

MSMS Spectrum



S-Allyl-L-cysteine (FG)

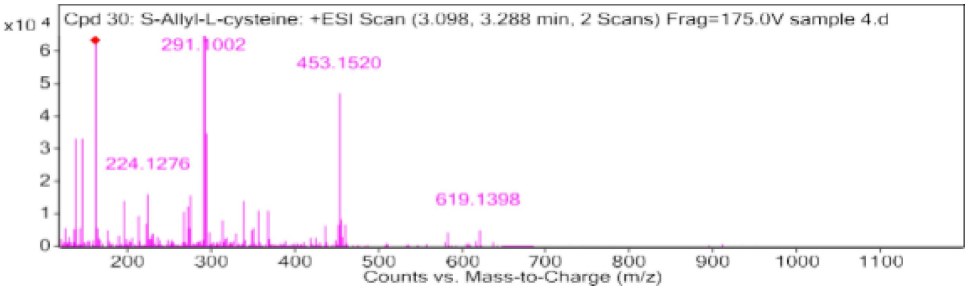
MS/MS Spectrum Peak List

m/z	*Calc m/z*	Diff (ppm)	z	Abund	Formula	Ion
145.0339				147.3		
162.0577	162.0583	4.02		434.48	C6 H11 N O2 S	(M+H)+
188.0707				146.06		
189.0753				130.47		
271.1306				99.55		
274.0724				142.69		
291.0992			1	3286.8		
292.1021			1	635.12		
293.1021			1	202.18		
424.1188				105.58		

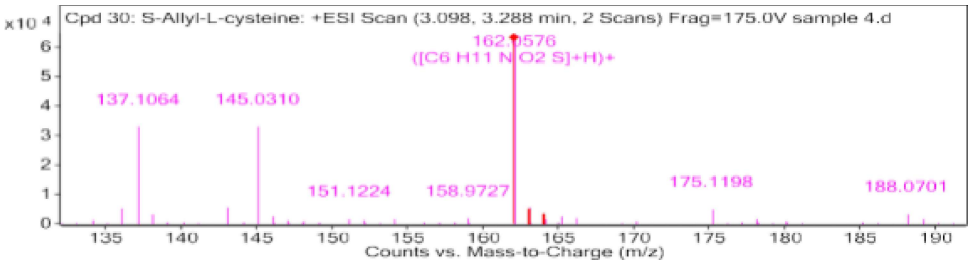
S-Allyl-L-cysteine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 30: S-Allyl-L-cysteine	**S-Allyl-L-cysteine**	162.0576	3.209	Auto MS/MS	161.0503

MS Spectrum



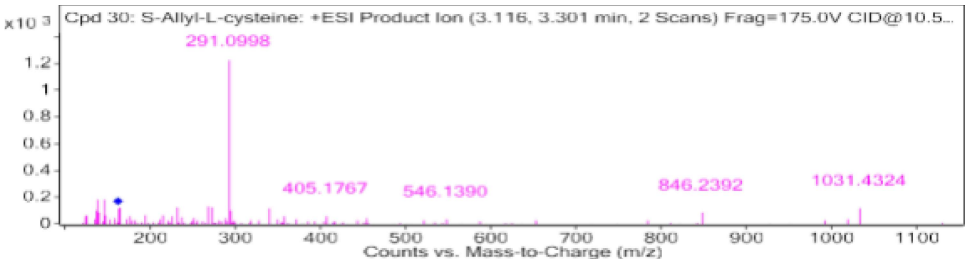
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
137.1064			1	33317.02		
145.031			1	33401.86		
162.0576	162.0583	4.61	1	64842.5	C6 H11 N O2 S	(M+H)+
163.0607	163.061	2.42	1	5879.19	C6 H11 N O2 S	(M+H)+
164.0539	164.0553	8.35	1	1964.54	C6 H11 N O2 S	(M+H)+
224.1276			1	16453.44		
291.1002			1	741278.75		
292.1032			1	98568.42		
293.0987			1	35200.95		
453.152			1	47506.56		

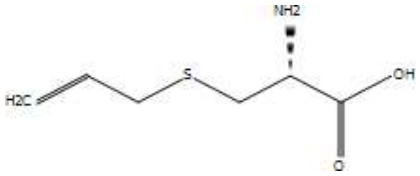
MSMS Spectrum



MS/~~MS Spectrum Peak List~~

m/z	z	Abund
137.1073		194.85
145.0299		191.62
164.0805		131.98
230.1383		130.34
267.1493		140.52
271.1282		129.51
291.0998	1	1232.84
292.1051	1	182.65
338.0691		126.53
1031.4324		127.64

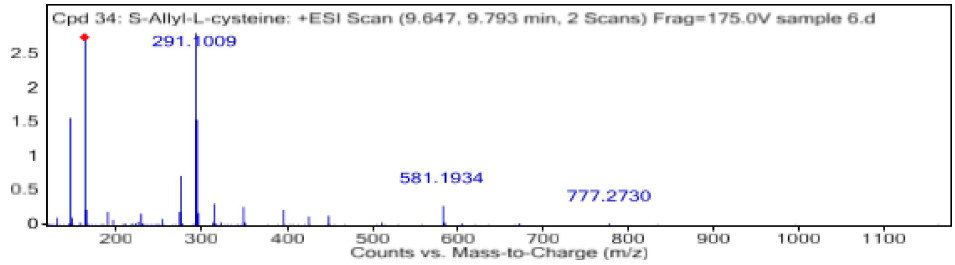
Compound Structure



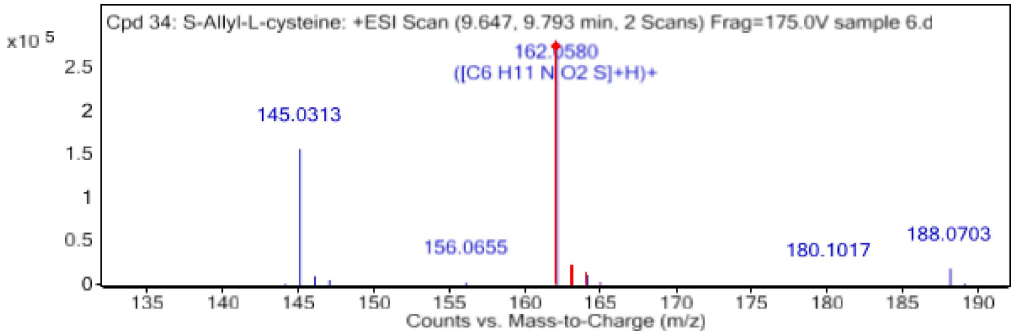
S-Allyl-L-cysteine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 34: S-Allyl-L-cysteine	**S-Allyl-L-cysteine**	162.058	9.732	Auto MS/MS	161.0507

MS Spectrum



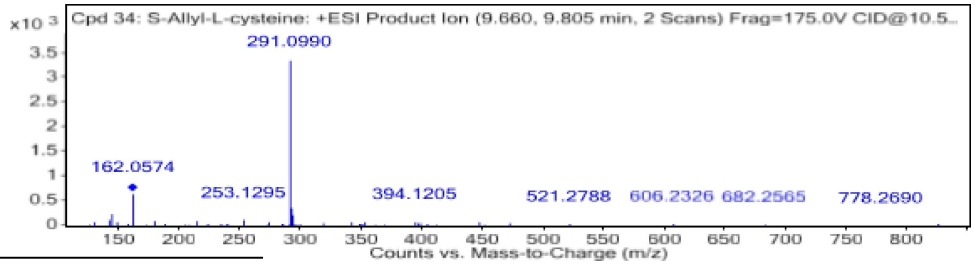
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.0313			1	156746.67		
162.058	162.0583	1.89	1	280173.31	C6 H11 N O2 S	(M+H)+
163.0611	163.061	-0.05	1	22810.6	C6 H11 N O2 S	(M+H)+
164.0546	164.0553	4.53	1	13317.54	C6 H11 N O2 S	(M+H)+
274.0741			1	72451.94		
291.1009			1	3340529		
292.1038			1	420003.25		
293.0996			1	154418.16		
313.0824			1	32242.06		
581.1934			1	29099.33		

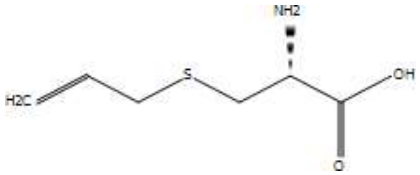
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
142.329		127.64
145.0298		245.21
162.0574		637.01
180.0739		94.28
215.0959		101.07
253.1295		114.96
291.099	1	3354.67
292.102	1	361.29
293.097	1	212.06
394.1205	1	87.08

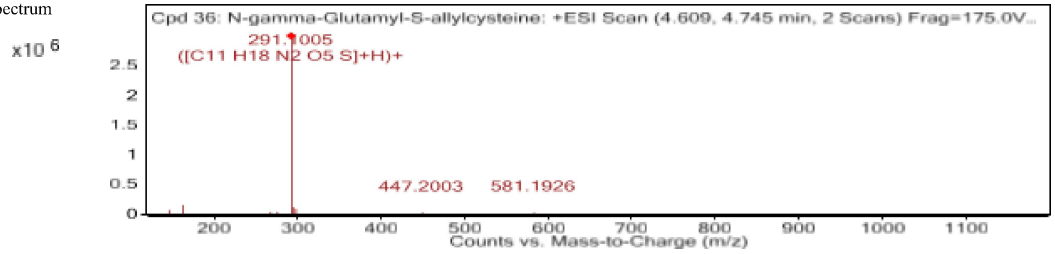
Compound Structure



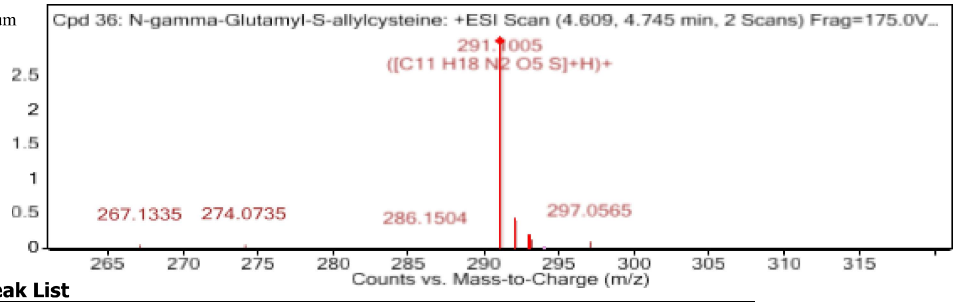
N-gamma-Glutamyl-S-allylcysteine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 36: N-gamma-Glutamyl-S-allylcysteine	**N-gamma-Glutamyl-S-allylcysteine**	291.1005	4.692	Auto MS/MS	290.0932

MS Spectrum



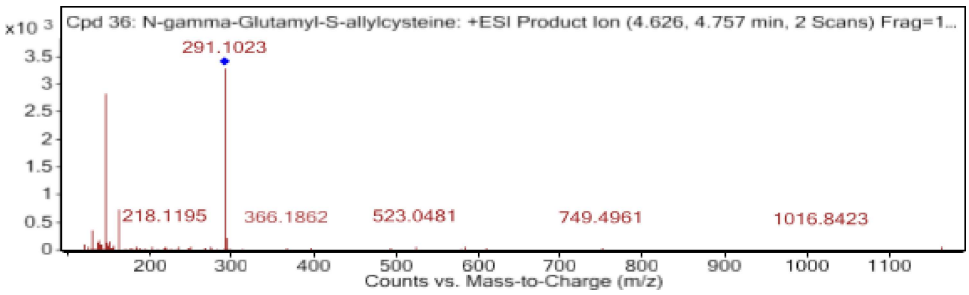
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.031			1	89004.83		
162.0577			1	177509.61		
267.1335			1	58555.16		
274.0735			1	68061.11		
291.1005	***291.1009***	1.56	1	3077709	C11 H18 N2 O5 S	(M+H)+
292.1033	***292.1038***	1.64	1	408536.53	C11 H18 N2 O5 S	(M+H)+
293.099	***293.0994***	1.39	1	149847.03	C11 H18 N2 O5 S	(M+H)+
297.0565			1	116861.4		
447.2003			1	47218.35		
581.1926			1	50753.96		

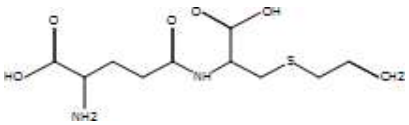
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0495	1	367.32
136.0607		160.26
137.1071		201.03
145.0317	1	2840.62
146.0309	1	197.69
150.9863		176.16
162.0582		751.18
291.1023	1	3303.67
292.1051	1	741.11
293.1019	1	237.28

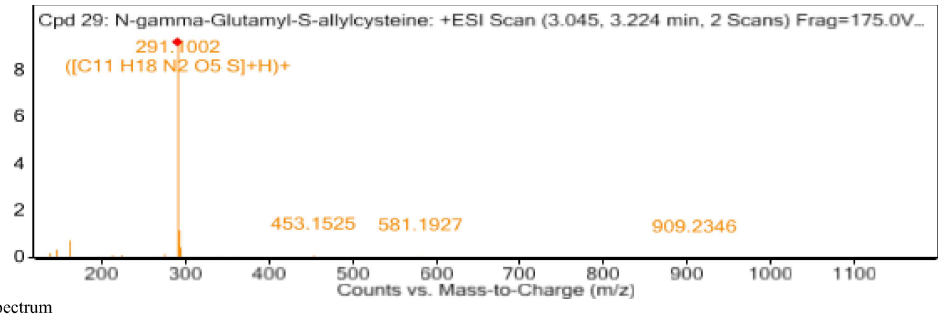
Compound Structure



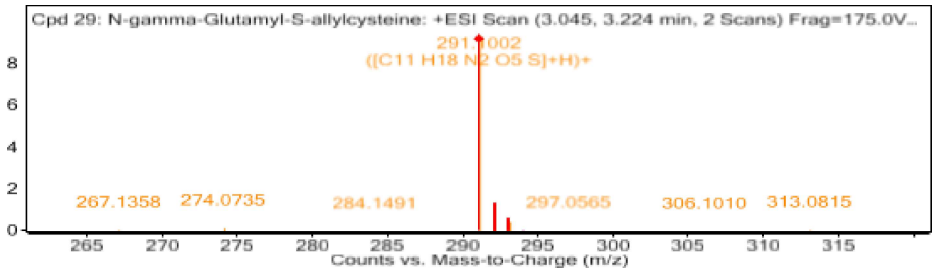
N-gamma-Glutamyl-S-allylcysteine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 29: N-gamma-Glutamyl-S-allylcysteine	**N-gamma-Glutamyl-S-allylcysteine**	291.1002	3.155	Auto MS/MS	290.093

MS Spectrum



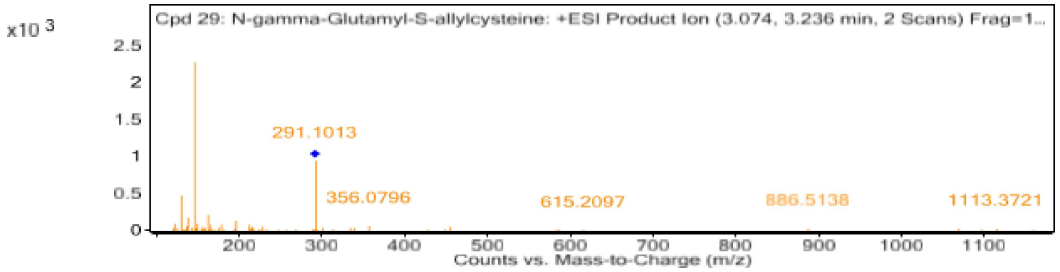
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
137.1064			1	26602.79		
145.0312			1	39058.05		
162.0576			1	79485.18		
213.1224			1	13399.62		
224.1275			1	16102.93		
274.0735			1	17122.51		
291.1002	291.1009	2.3	1	941710.94	C11 H18 N2 O5 S	(M+H)+
292.1032	292.1038	1.84	1	120510.58	C11 H18 N2 O5 S	(M+H)+
293.0991	293.0994	1.07	1	46902.65	C11 H18 N2 O5 S	(M+H)+
453.1525			1	13620.5		

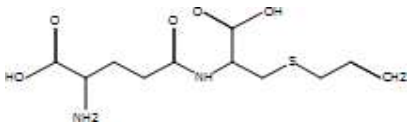
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
122.096		115.99
130.0502		493.89
137.1054		186.53
145.0311	1	2293.28
149.1058	1	116.57
162.0582		231.04
177.1012		98.2
195.1118	1	152.51
291.1013	2	960.5
292.1047	2	193.26

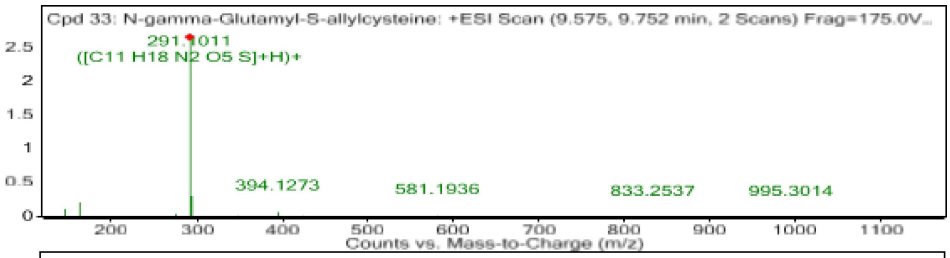
Compound Structure



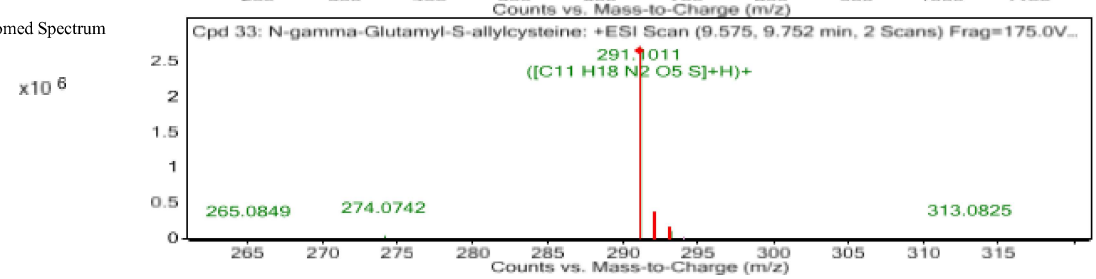
N-gamma-Glutamyl-S-allylcysteine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 33: N-gamma-Glutamyl-S-allylcysteine	**N-gamma-Glutamyl-S-allylcysteine**	291.1011	9.677	Auto MS/MS	290.0938

MS Spectrum



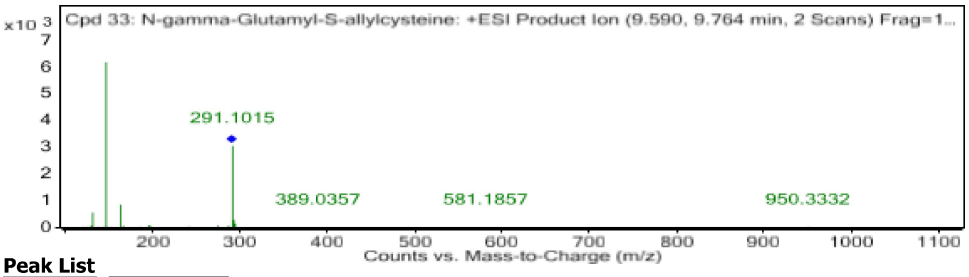
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.0314			1	130561.41		
162.0581			1	225254.39		
274.0742			1	57073.71		
291.1011	291.1009	-0.57	1	2711218.25	C11 H18 N2 O5 S	(M+H)+
292.1041	292.1038	-0.98	1	326837.31	C11 H18 N2 O5 S	(M+H)+
293.0999	293.0994	-1.66	1	124743.73	C11 H18 N2 O5 S	(M+H)+
347.0944			1	23873.44		
394.1273			1	84218.05		
424.12			1	29705.94		
581.1936			1	27569.21		

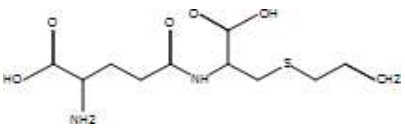
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0495	1	577.94
145.0311	1	6212.68
145.0778	2	115.16
146.0352	1	221.3
162.0569	1	910.32
165.1118		103.52
274.076		129.83
291.1015	1	3097.29
292.1019	1	346.74
293.0992	1	176.63

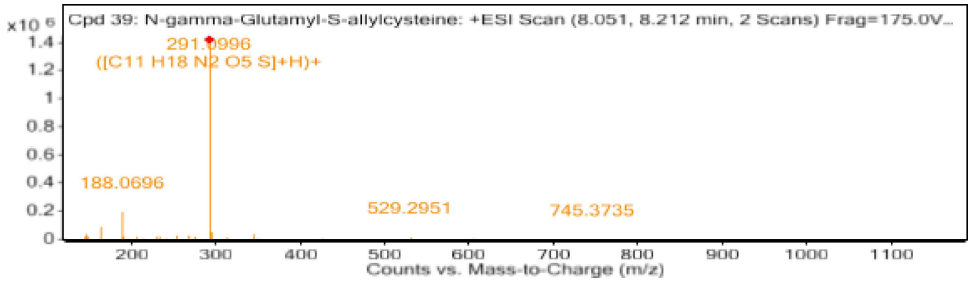
Compound Structure



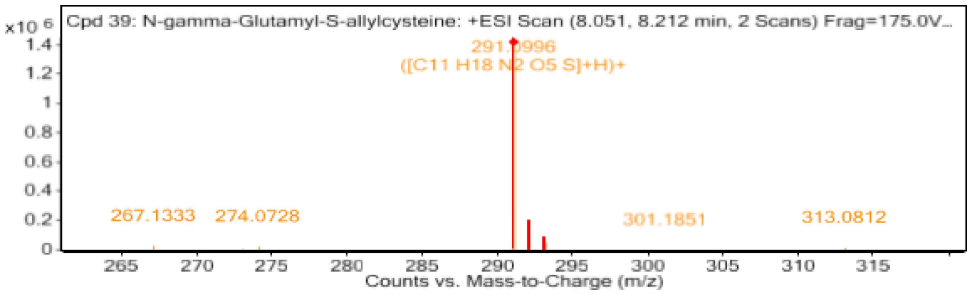
N-gamma-Glutamyl-S-allylcysteine (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 39: N-gamma-Glutamyl-S-allylcysteine	**N-gamma-Glutamyl-S-allylcysteine**	291.0996	8.144	Auto MS/MS	290.0923

MS Spectrum



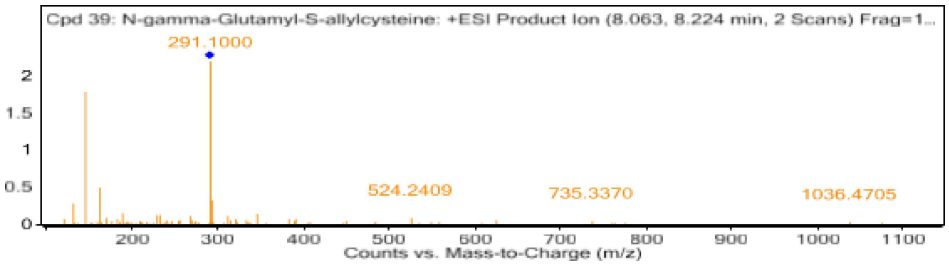
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.0309				47693.29		
162.0573			1	97595.69		
188.0696			1	199926.16		
231.1689				31704.39		
253.1218			1	35847.91		
267.1333			1	33763.1		
291.0996	291.1009	4.64	1	1450201	C11 H18 N2 O5 S	(M+H)+
292.1027	292.1038	3.83	1	169544.98	C11 H18 N2 O5 S	(M+H)+
293.0985	293.0994	3.28	1	62272.89	C11 H18 N2 O5 S	(M+H)+
344.1798			1	46014.84		

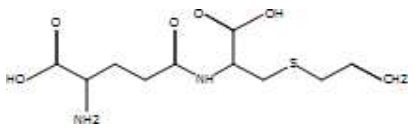
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.049		308.02
145.0302		1804.53
162.0566		520.57
188.0693		174.61
228.0672		149.05
231.168		149.39
267.1326		134.88
291.1	1	2214.18
292.0994	1	349.73
344.1777	1	158.51

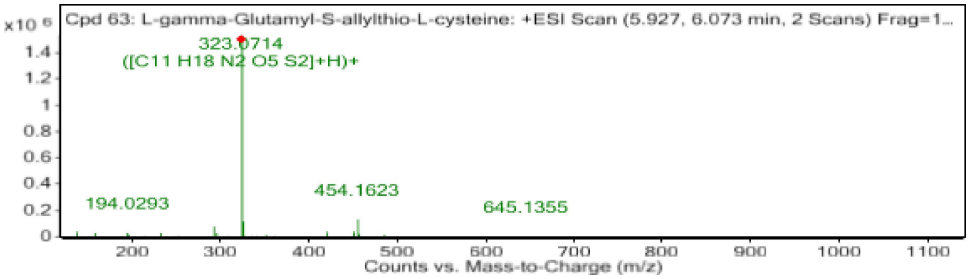
Compound Structure



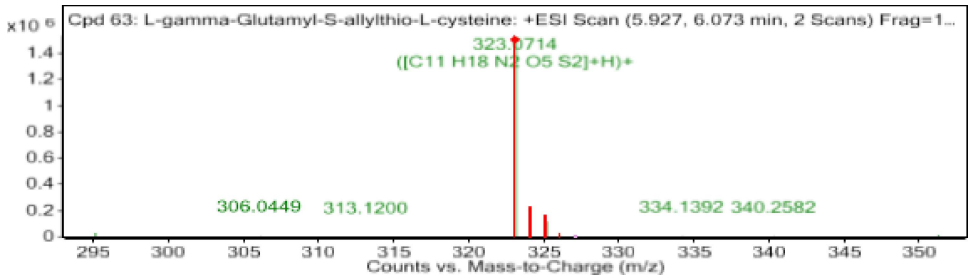
L-gamma-Glutamyl-S-allylthio- L-cysteine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 63: L-gamma-Glutamyl-S-allylthio-L-cysteine	**L-gamma-Glutamyl-S-allylthio-L-cysteine**	323.0714	6.013	Auto MS/MS	322.0642

MS Spectrum



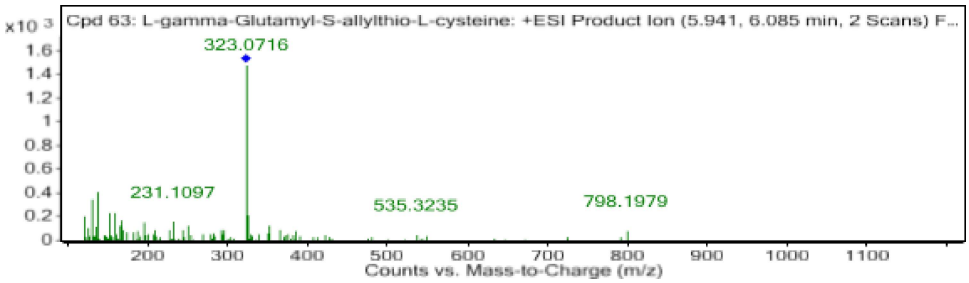
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
137.1064			1	45520.88		
291.0998			1	88783.43		
295.1274			1	41676.54		
323.0714	323.073	4.8	1	1534914	C11 H18 N2 O5 S2	(M+H)+
324.0745	324.0757	3.54	1	196654.98	C11 H18 N2 O5 S2	(M+H)+
325.0691	325.0704	4.04	1	122642.6	C11 H18 N2 O5 S2	(M+H)+
326.0719	326.0728	2.64	1	17167.48	C11 H18 N2 O5 S2	(M+H)+
419.146			1	51139.59		
450.134			1	44177.81		
454.1623			1	140253.98		

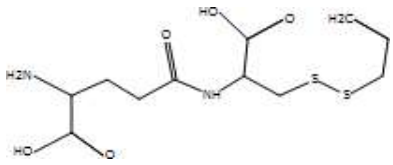
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0802		209.41
130.0493		357.24
137.1075		420.57
151.9823	1	239.36
158.0965	1	242.93
166.0847		175.67
194.0271		161.12
231.1097		164.39
323.0716	1	1482.5
324.072	1	225.76

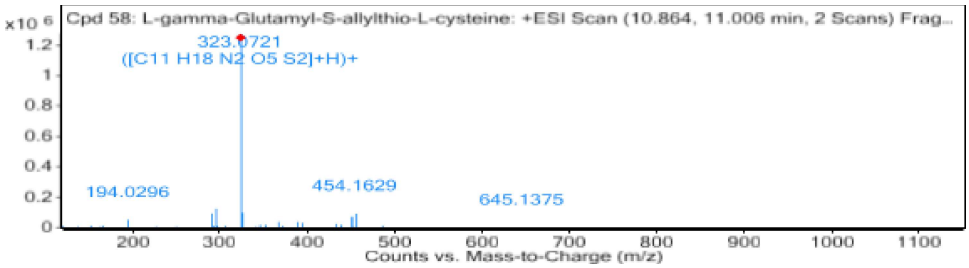
Compound Structure



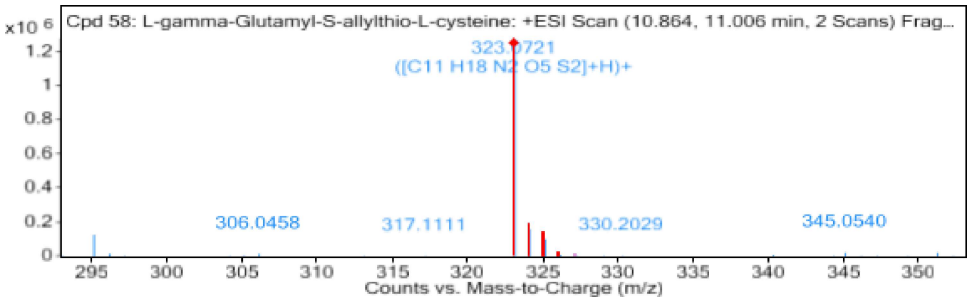
L-gamma-Glutamyl-S-allylthio- L-cysteine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 58: L-gamma-Glutamyl-S-allylthio-L-cysteine	**L-gamma-Glutamyl-S-allylthio-L-cysteine**	323.0721	10.948	Auto MS/MS	322.0649

MS Spectrum



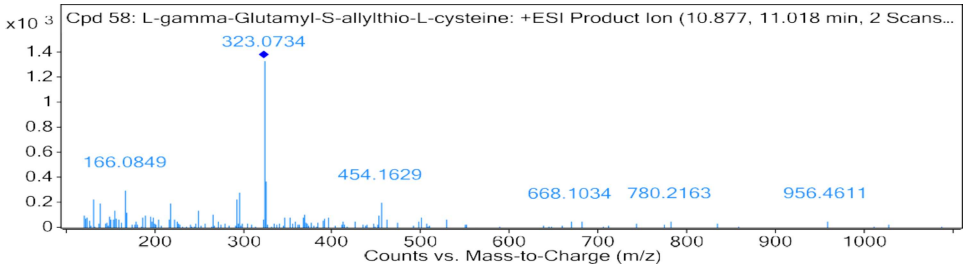
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
194.0296			1	56927.72		
291.1003			1	96230.69		
295.1281			1	132254.08		
323.0721	323.073	2.74	1	1276053.88	C11 H18 N2 O5 S2	(M+H)+
324.0752	324.0757	1.46	1	167495.05	C11 H18 N2 O5 S2	(M+H)+
325.0698	325.0704	1.98	1	108291.34	C11 H18 N2 O5 S2	(M+H)+
326.0722	326.0728	1.66	1	14264.46	C11 H18 N2 O5 S2	(M+H)+
367.1314			1	47555.96		
450.135			1	75850.48		
454.1629			1	99342.23		

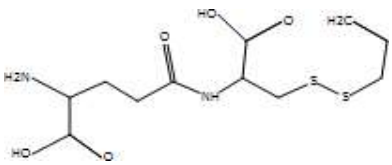
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0489		231.74
137.1056	1	198.01
154.0496		144.92
166.0849		305.42
217.081		198.95
291.0981	1	227.68
295.1274		284.48
323.0734	1	1334.37
325.0683	1	374.42
454.1629		205.59

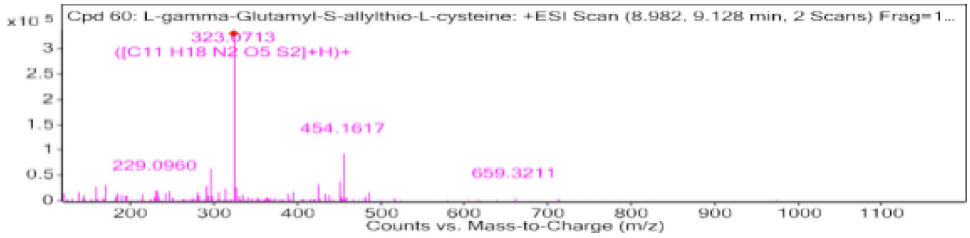
Compound Structure



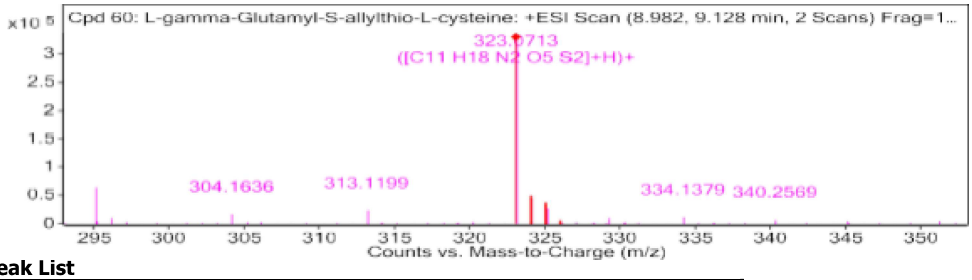
L-gamma-Glutamyl-S-allylthio- L-cysteine (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 60: L-gamma-Glutamyl-S-allylthio-L-cysteine	**L-gamma-Glutamyl-S-allylthio-L-cysteine**	323.0713	9.068	Auto MS/MS	322.0642

MS Spectrum



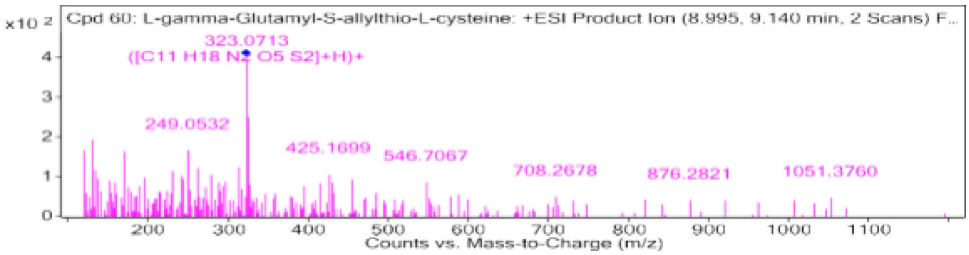
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
169.0751			1	32591.89		
291.0995			1	30678.06		
295.127			1	65258.38		
323.0713	323.073	5.09	1	336869	C11 H18 N2 O5 S2	(M+H)+
324.0745	324.0757	3.7	1	46546.63	C11 H18 N2 O5 S2	(M+H)+
325.0692	325.0704	3.87	1	30053.03	C11 H18 N2 O5 S2	(M+H)+
326.072	326.0728	2.26	1	3864.97	C11 H18 N2 O5 S2	(M+H)+
424.1689			1	34131.22		
450.1338			1	40546.44		
454.1617			1	96231.27		

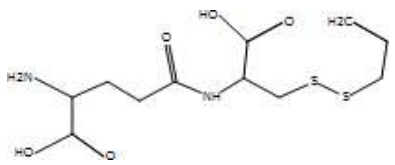
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	*Calc m/z*	Diff (ppm)	z	Abund	Formula	Ion
120.0112				168.23		
130.0502				194.52		
133.0654				119.95		
169.073				167.46		
229.0927				115.73		
249.0532				168.08		
261.1255				124		
313.1156				125.91		
323.0713	323.073	5.14		398.26	C11 H18 N2 O5 S2	(M+H)+
324.0716			1	252.7		

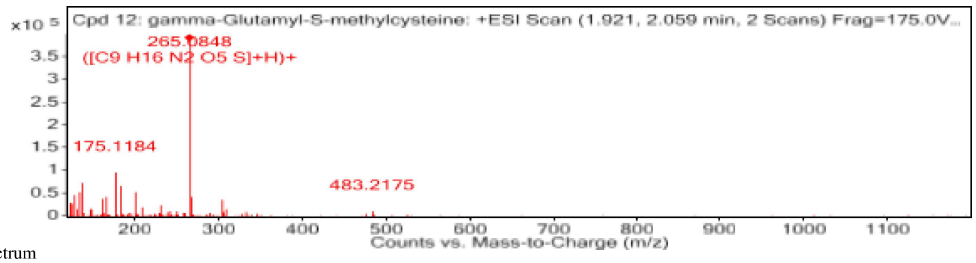
Compound Structure



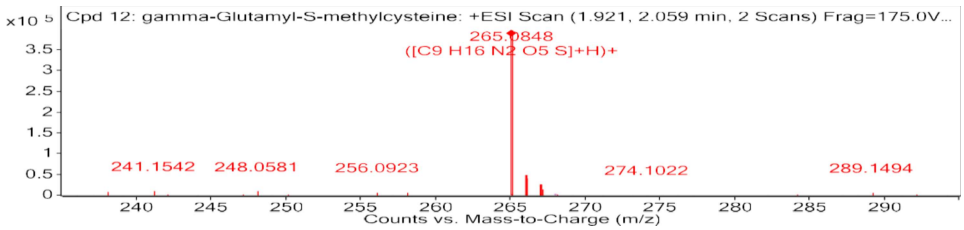
gamma-Glutamyl-S-methylcysteine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 12: gamma-Glutamyl-S-methylcysteine	**gamma-Glutamyl-S-methylcysteine**	265.0848	2.009	Auto MS/MS	264.0775

MS Spectrum



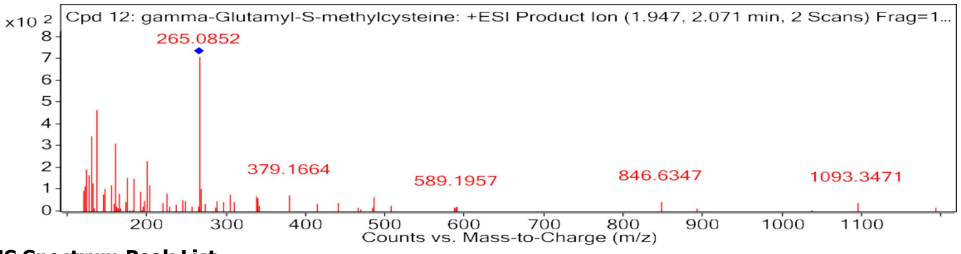
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
126.0659			1	47225.07		
132.1013			1	52733.97		
136.0753			1	73506.09		
175.1184			1	96916.63		
182.0441			1	49319.32		
182.0809			1	67134.96		
200.1023			1	53082.61		
265.0848	265.0853	1.94	1	399374.69	C9 H16 N2 O5 S	(M+H)+
266.0878	266.088	0.82	1	43000.82	C9 H16 N2 O5 S	(M+H)+
267.083	267.0835	1.65	1	16635.85	C9 H16 N2 O5 S	(M+H)+

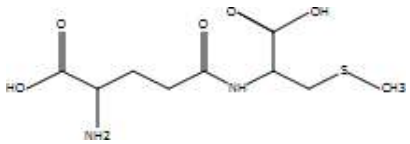
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
123.046		196.13
126.0661		169.12
130.0491		347.58
136.0428		180.29
136.0758	1	467.61
160.107	1	313.56
175.1179		159.08
200.1013		235.14
265.0852	1	711.53
266.0873	1	171.85

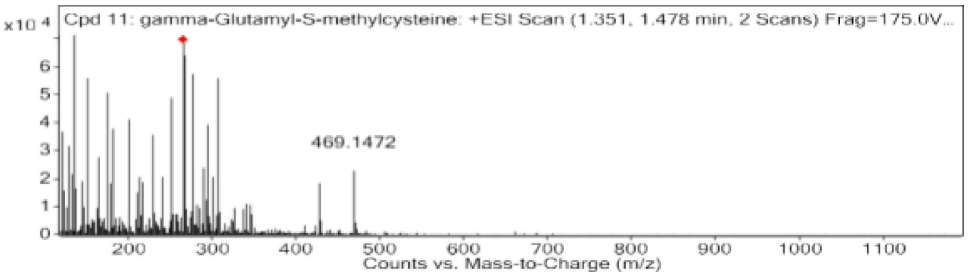
Compound Structure



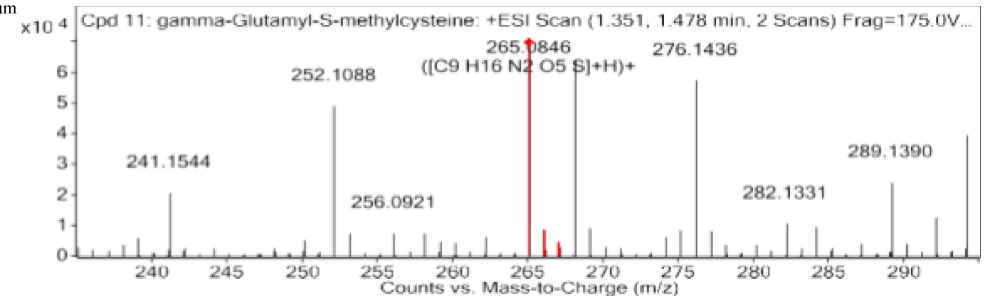
gamma-Glutamyl-S-methylcysteine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 11: gamma-Glutamyl-S-methylcysteine	**gamma-Glutamyl-S-methylcysteine**	265.0846	1.433	Auto MS/MS	264.0774

MS Spectrum



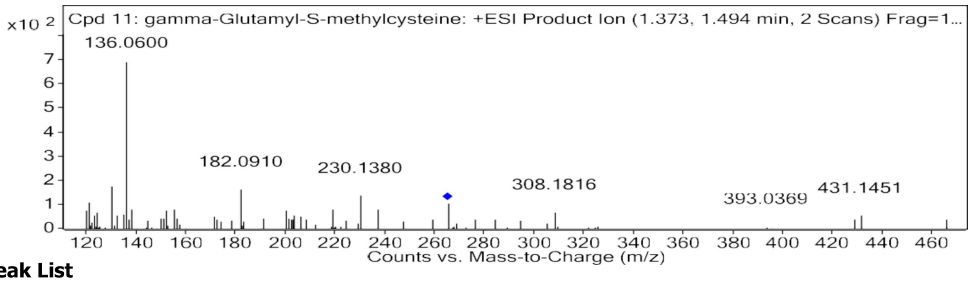
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
136.0613			1	107531.75		
152.056			1	56345.43		
175.1184				50932.82		
252.1088			1	49306.09		
265.0846	265.0853	2.64	1	71269.05	C9 H16 N2 O5 S	(M+H)+
266.0878	266.088	0.9	1	8865.53	C9 H16 N2 O5 S	(M+H)+
267.0844	267.0835	-3.43	1	3333.23	C9 H16 N2 O5 S	(M+H)+
268.1036			1	64451.67		
276.1436			1	57608.63		
307.0951			1	56077.53		

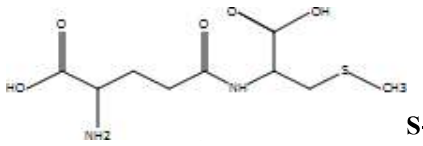
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
121		
0109		10.73
130.0488	1	178.3
136.0414	1	101.11
136.06	1	693.5
138.1019		82.63
182.091	1	165.42
219.0569		83.01
230.138		139.05
237.106		82.28
265.0857		106.84

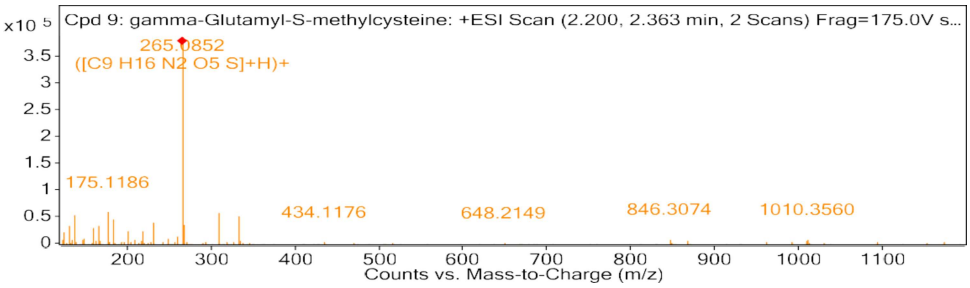
Compound Structure



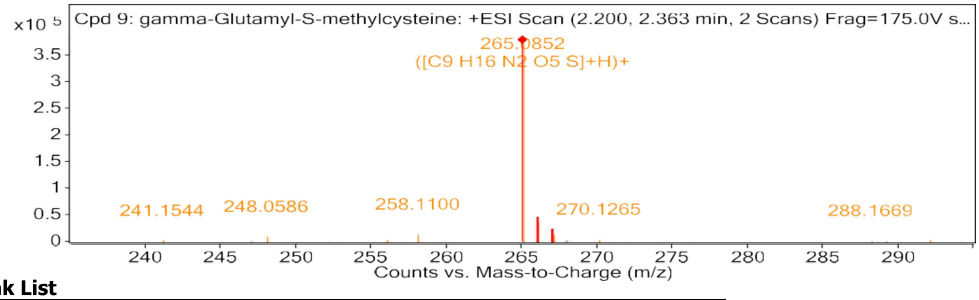
S-methylcysteine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 9: gamma-Glutamyl-S-methylcysteine	**gamma-Glutamyl-S-methylcysteine**	265.0852	2.302	Auto MS/MS	264.0779

MS Spectrum



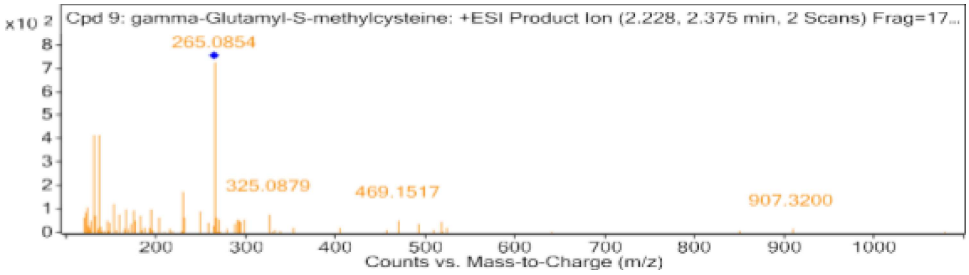
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
136.0426			1	54796.38		
136.0755			1	56957.34		
175.1186			1	61277.09		
182.0815			1	47530.69		
229.1547			1	41715.74		
265.0852	265.0853	0.33	1	388969.44	C9 H16 N2 O5 S	(M+H)+
266.0881	266.088	-0.19	1	38627.6	C9 H16 N2 O5 S	(M+H)+
267.0831	267.0835	1.32	1	16728.5	C9 H16 N2 O5 S	(M+H)+
307.0955			1	60721.82		
332.1336			1	54968.83		

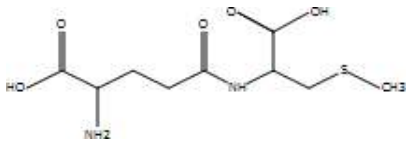
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
123.042		112.21
130.0498		419.65
136.0429	1	418.54
136.0754		212.03
152.0704		128.68
166.0535		105.23
175.1177		101.5
194.1182	1	103.99
229.1549	1	177.86
265.0854	2	729.82

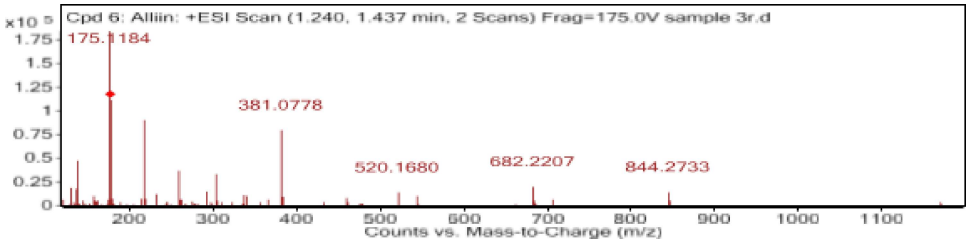
Compound Structure



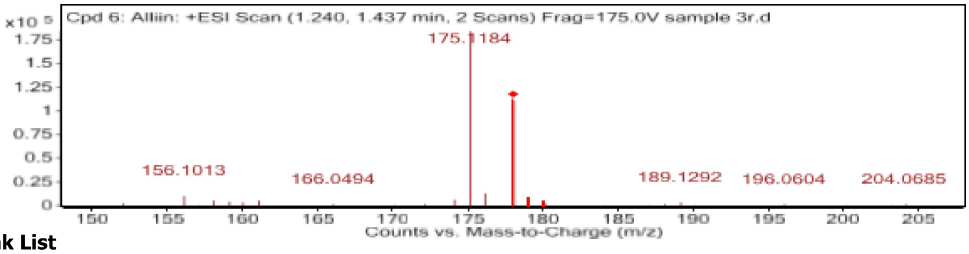
Alliin (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 6: Alliin	**Alliin**	178.0527	1.362	Auto MS/MS	177.0455

MS Spectrum



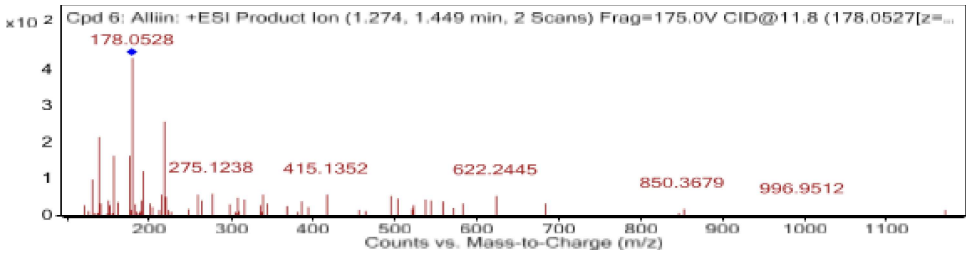
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
138.0541			1	48369.36		
175.1184			1	184746.16		
178.0527	178.0532	3.05	1	112149.73	C6 H11 N O3 S	(M+H)+
179.056	179.056	-0.37	1	8962.22	C6 H11 N O3 S	(M+H)+
180.0507	180.0505	-1.08	1	4054.74	C6 H11 N O3 S	(M+H)+
217.1291			1	91596.49		
258.1096			1	37657.23		
303.1654			1	33961.63		
381.0778			1	80892.51		
682.2207			1	21137.48		

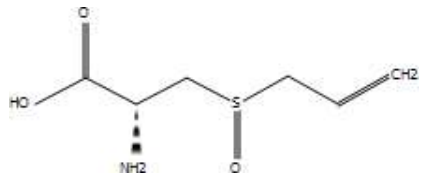
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0978		102.34
137.0129		217.72
138.055		96.78
156.0988		164.82
175.1178		166.85
178.0528		434.02
191.0897		125.67
217.1255	1	259.14
218.1	1	63.86
275.1238		61.8

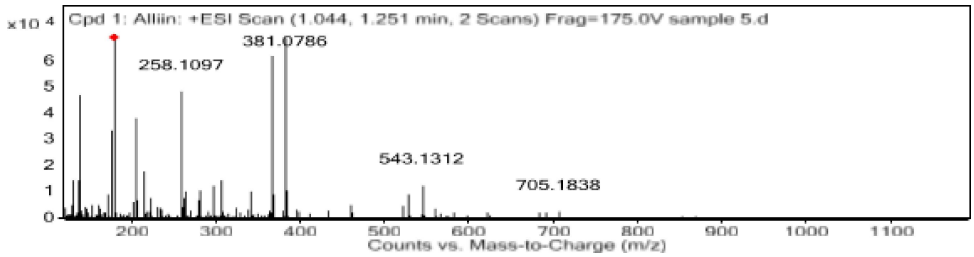
Compound Structure



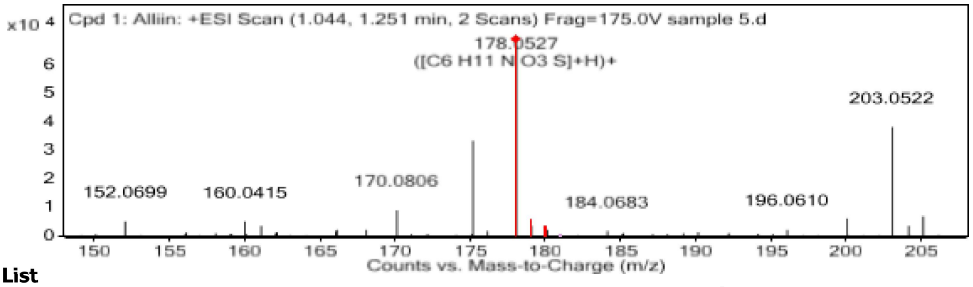
Alliin (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 1: Alliin	**Alliin**	178.0527	1.164	Auto MS/MS	177.0455

MS Spectrum



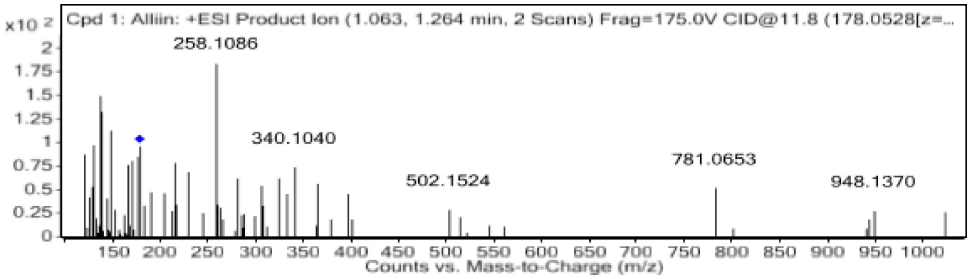
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
138.0542			1	47078.55		
175.1185			1	33854.94		
178.0527	178.0532	2.81	1	70488.39	C6 H11 N O3 S	(M+H)+
179.0556	179.056	1.95	1	3842.88	C6 H11 N O3 S	(M+H)+
180.0501	180.0505	2.01	1	2696.58	C6 H11 N O3 S	(M+H)+
203.0522			1	38534.14		
214.0705				18311.7		
258.1097			1	48701.36		
365.1046			1	62128.83		
381.0786			1	68902.71		

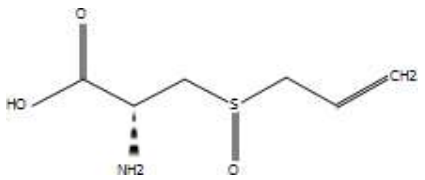
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0095		88.7
130.0497		98.54
136.0592		84.14
137.0152		149.67
138.0557	1	133.53
147.0759		114.11
170.0808		82.2
175.1219		86.19
178.0521		97.25
258.1086		184.91

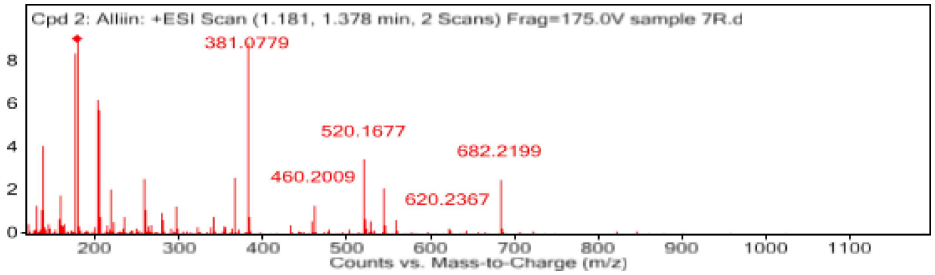
Compound Structure



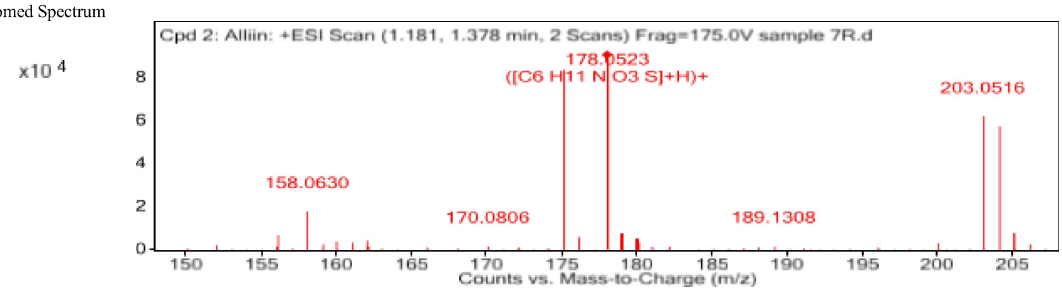
Alliin (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 2: Alliin	**Alliin**	178.0523	1.308	Auto MS/MS	177.045

MS Spectrum



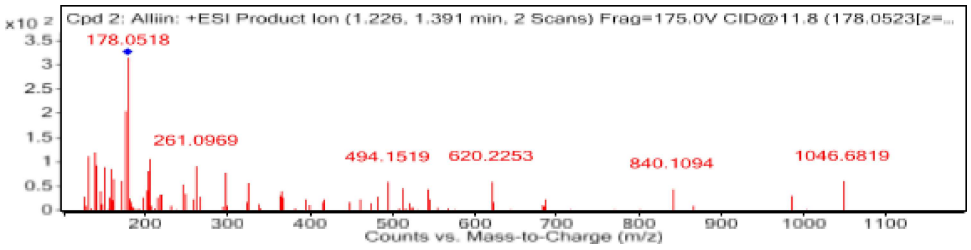
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
138.0542			1	40790.31		
175.1181			1	83683.05		
178.0523	178.0532	5.47	1	92496.82	C6 H11 N O3 S	(M+H)+
179.0558	179.056	0.74	1	7546.8	C6 H11 N O3 S	(M+H)+
180.0494	180.0505	5.96	1	3678.84	C6 H11 N O3 S	(M+H)+
203.0516				62409.69		
204.0681			1	57782.96		
365.1039			1	26335.82		
381.0779			1	88475.3		
520.1677			1	34663.2		

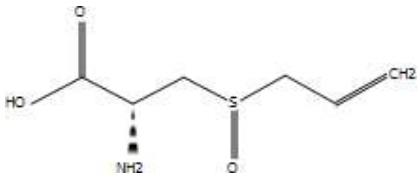
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0868		113.44
138.054		120.45
140.0704		94.22
149.0797		90.13
157.0143		86.55
175.1171		206
178.0518	2	315.9
203.0505		82.78
204.0656	1	107.89
261.0969		93.26

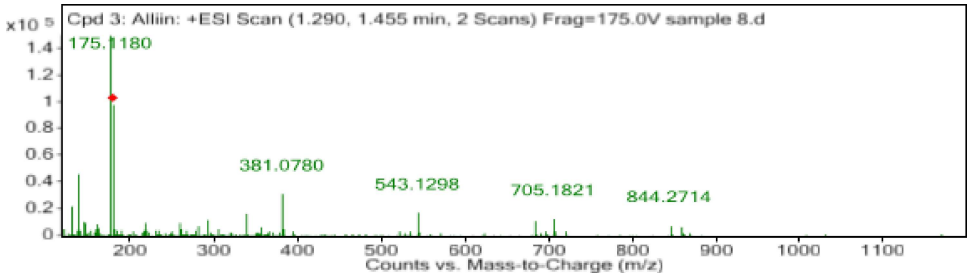
Compound Structure



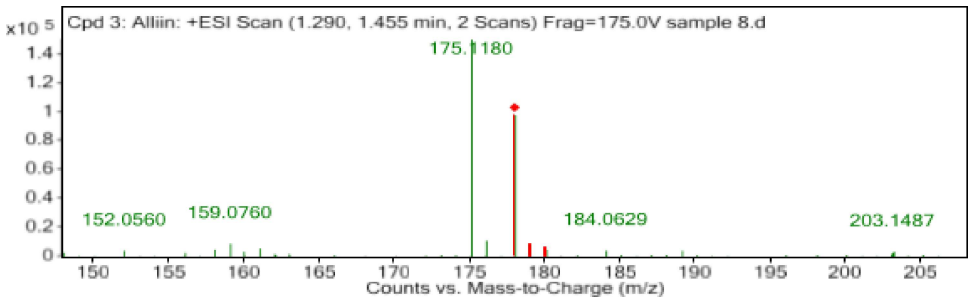
Alliin (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 3: Alliin	**Alliin**	178.0522	1.397	Auto MS/MS	177.045

MS Spectrum



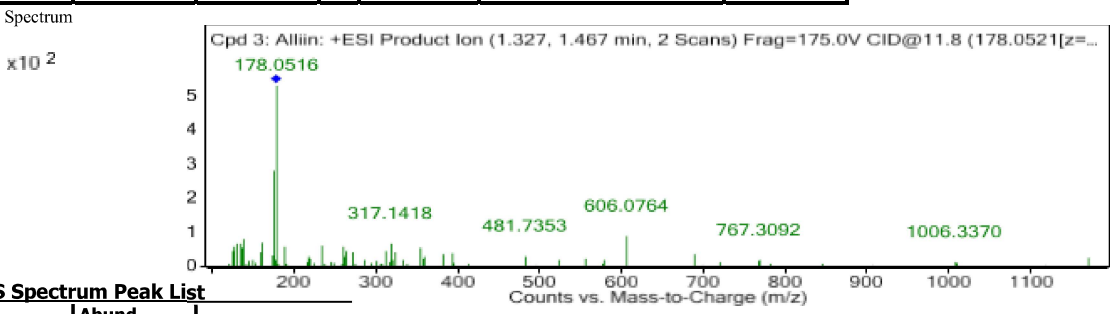
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
130.0858				22073.83		
138.0542			1	46570.95		
175.118			1	149861.72		
178.0522	178.0532	5.68	1	97806.94	C6 H11 N O3 S	(M+H)+
179.0557	179.056	1.27	1	7561.13	C6 H11 N O3 S	(M+H)+
180.0491	180.0505	7.69	1	5485.65	C6 H11 N O3 S	(M+H)+
337.1701			1	17182.36		
381.078			1	31510.08		
543.1298			1	17428.95		
705.1821			1	12909.02		

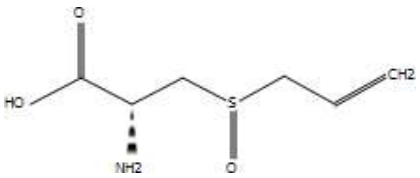
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	Abund
130.0851	68.57
135.0447	68.64
138.053	82.06
161.0242	71.87
175.1179	282.67
175.1438	61.6
178.0516	531.24
233.1086	63.07
317.1418	70.01
606.0764	91.8

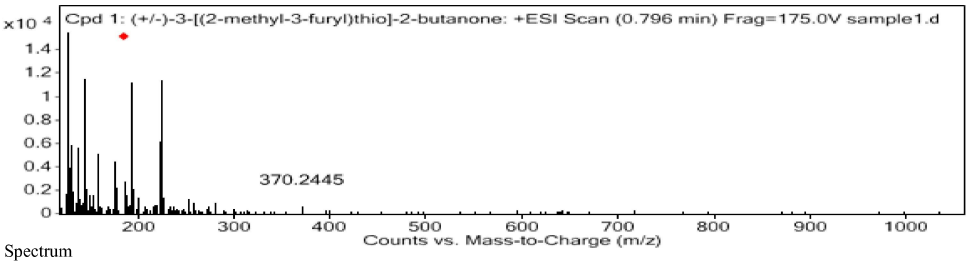
Compound Structure



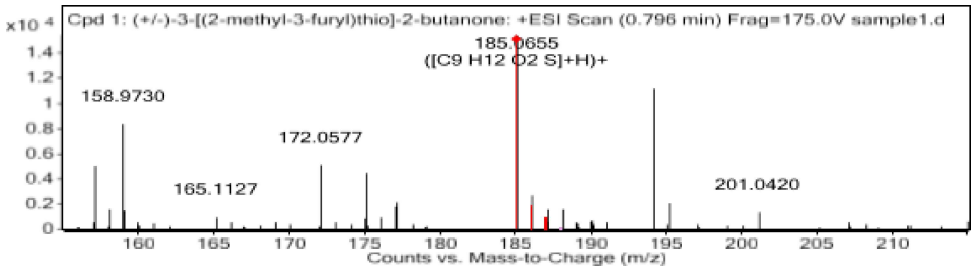
(+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 1: (+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone	**(+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone**	185.0655	0.814	Auto MS/MS	184.0582

MS Spectrum



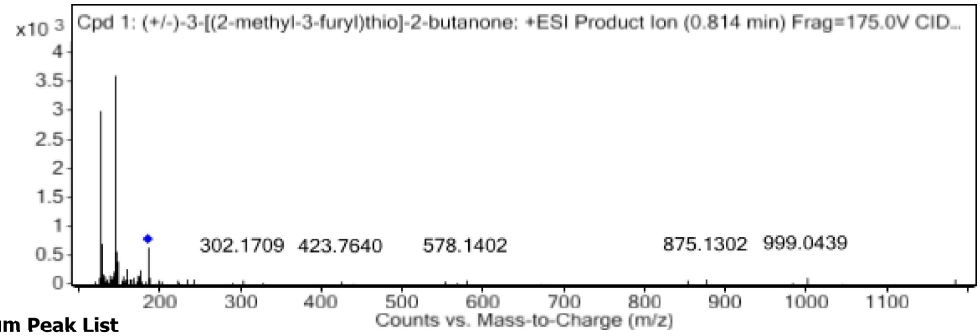
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
127.0234			1	17720.9		
143.0009			1	11529.46		
145.0343			1	11476.01		
158.973			1	8444.04		
185.0655	185.0631	-12.87	1	15463.82	C9 H12 O2 S	(M+H)+
186.0671	186.0662	-4.78	1	2768	C9 H12 O2 S	(M+H)+
187.0651	187.0605	-24.7	1	1705.72	C9 H12 O2 S	(M+H)+
194.1166			1	11218.56		
222.1115			1	6244.77		
224.1276			1	11499.64		

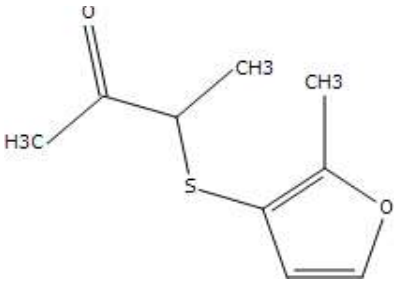
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
127.0227	1	2999.61
128.0247	1	720.2
129.0247	1	203.96
143.0019		237.69
145.0343	1	3621.28
146.0352	1	581.82
147.0299	1	417.45
159.052		273.37
175.0347		254.19
185.0639	1	653.01

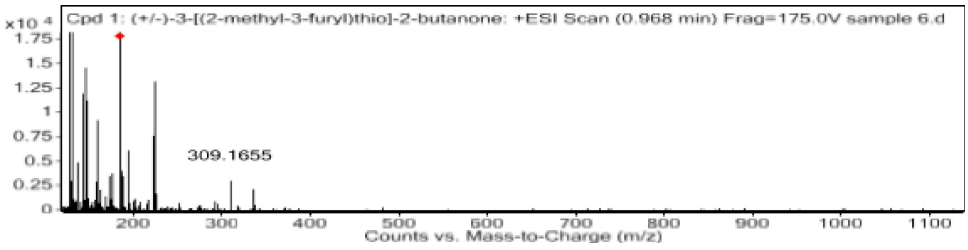
Compound Structure



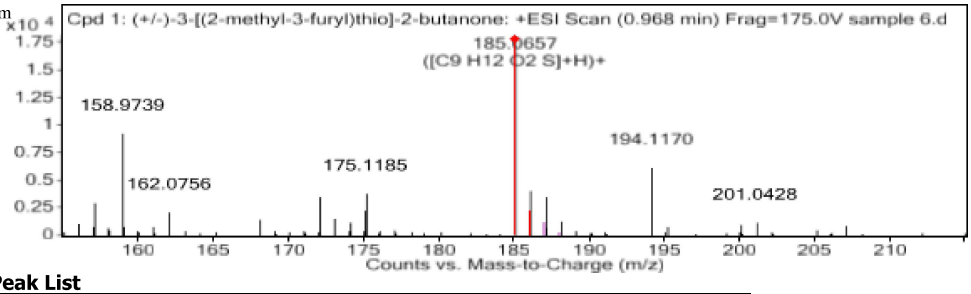
(+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 1: (+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone	**(+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone**	185.0657	0.986	Auto MS/MS	184.0581

MS Spectrum



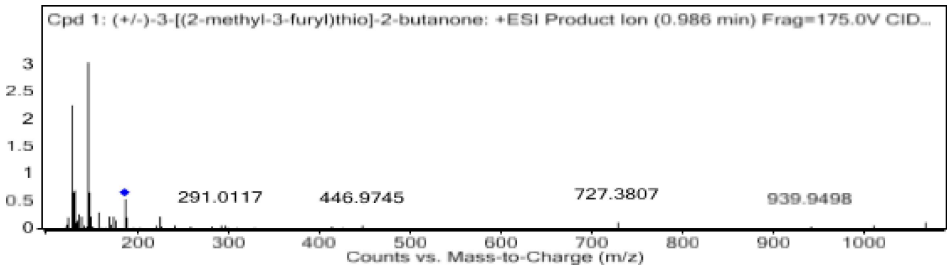
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
127.0239			1	21137.43		
130.086			1	21977.46		
143.0012			1	11997.19		
145.0342			1	14674.26		
147.1127			1	11270.98		
158.9739			1	9293.36		
185.0657	185.0631	-14.09	1	18192.18	C9 H12 O2 S	(M+H)+
186.0672	186.0662	-5.18	1	4106.31	C9 H12 O2 S	(M+H)+
222.1116			1	7680.2		
224.1282			1	13200.55		

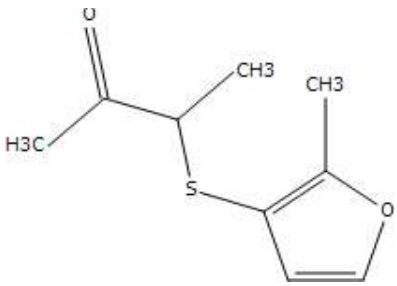
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
127.0233		2266.87
128.0235	1	680.88
130.0856		714.02
135.05		269.14
145.0347	1	3058.08
146.0361	1	673.52
147.0342	1	244.15
157.0706	1	304.73
168.0511		245.39
185.0663	1	551.39

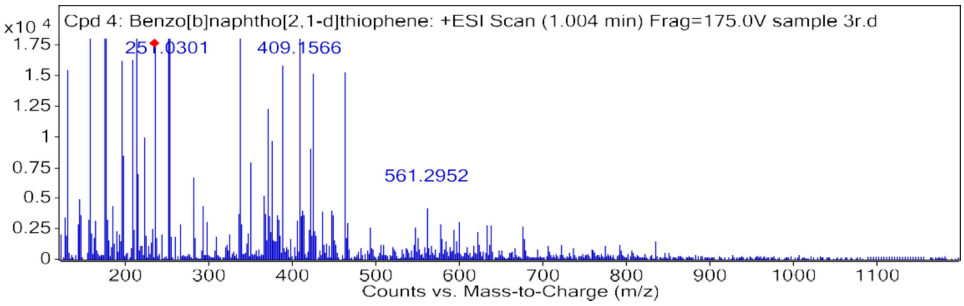
Compound Structure



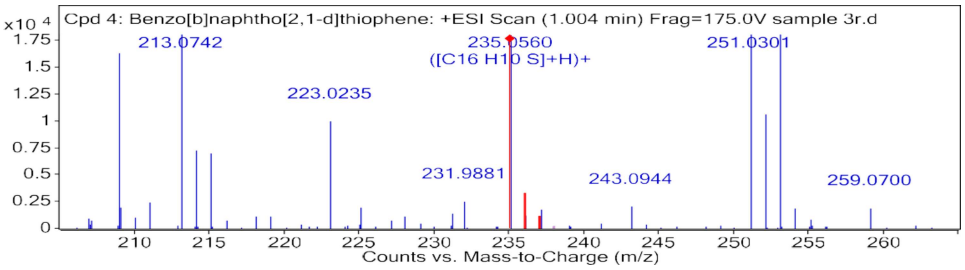
Benzo[b]naphtho[2,1-d]thiophene (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 4: Benzo[b]naphtho[2,1-	**Benzo[b]naphtho[2,1-d]thiophene**	235.056	1.022	Auto MS/MS	234.0486

MS Spectrum



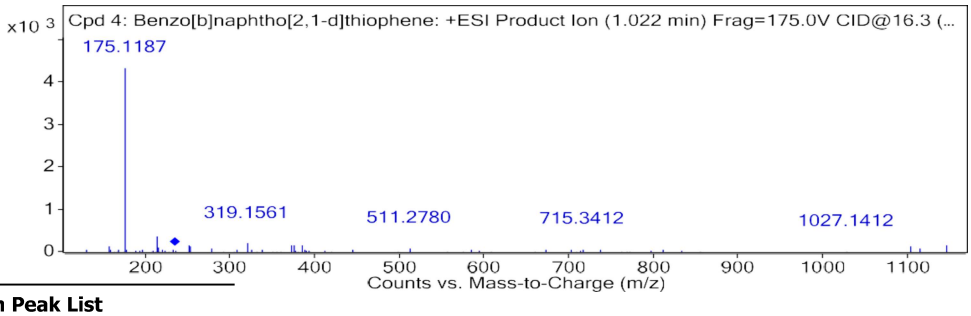
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
158.0916			1	20795.98		
175.1185			1	776474.31		
176.1211			1	55511.49		
213.0742			1	89967.17		
235.056	235.0576	6.63		18081.94	C16 H10 S	(M+H)+
236.0584	236.0608	10.03	1	1304.41	C16 H10 S	(M+H)+
237.0538	237.0561	9.9		1825.73	C16 H10 S	(M+H)+
251.0301			1	136350.56		
253.0282			1	21716.94		
409.1566			1	18662.01		

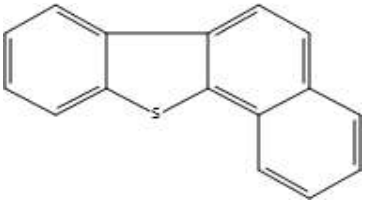
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
157.108		160.56
175.1187	1	4347.84
176.1225	1	1057.6
213.0728	1	393.1
251.0312		185.03
319.1561		221.83
371.1936		175.8
375.1253	1	183.08
384.0794		171.34
1144.156		190.74

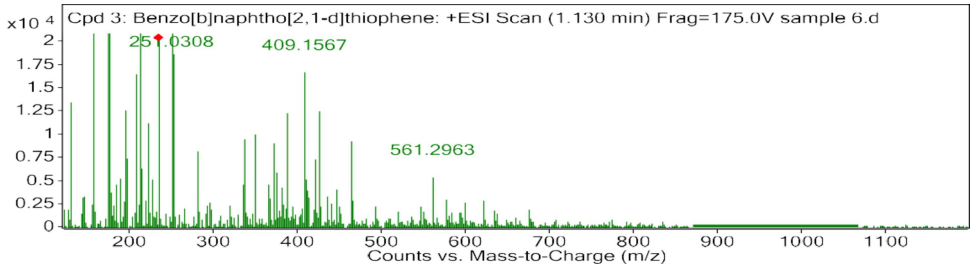
Compound Structure



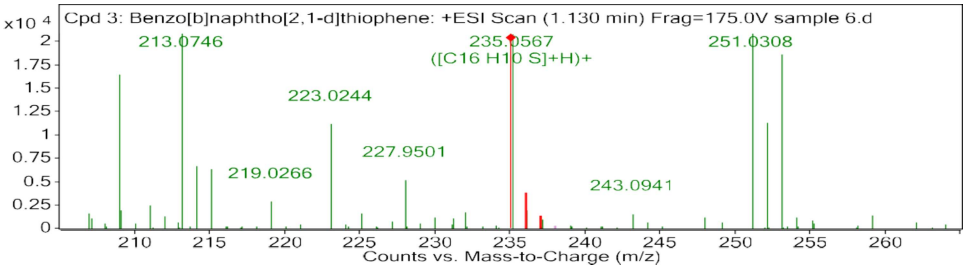
Benzo[b]naphtho[2,1-d]thiophene (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 3: Benzo[b]naphtho[2,1-	**Benzo[b]naphtho[2,1-d]thiophene**	235.0567	1.147	Auto MS/MS	234.0494

MS Spectrum



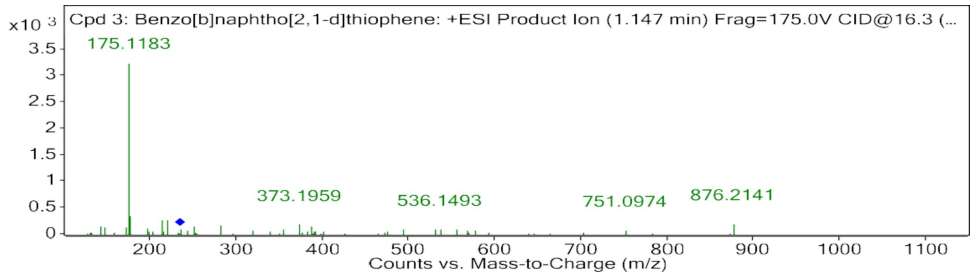
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
158.0919			1	21140.09		
175.1189			1	661189.88		
176.1218			1	42309.94		
213.0746			1	89787.43		
235.0567	235.0576	3.72	1	20911.65	C16 H10 S	(M+H)+
236.0595	236.0608	5.32	1	2073.97	C16 H10 S	(M+H)+
237.0551	237.0561	4.4	1	1117.16	C16 H10 S	(M+H)+
251.0308			1	130391.86		
253.0288			1	18705.04		
409.1567			1	16773.2		

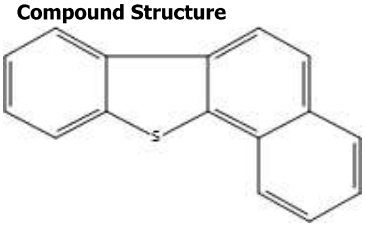
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
143.053		169.11
175.1183	1	3242.86
176.1226	1	368.85
213.0706		293.8
214.0769		193.01
219.0259		293.07
280.9801		186.55
373.1959		204.8
387.1844	1	184
876.2141		220.77

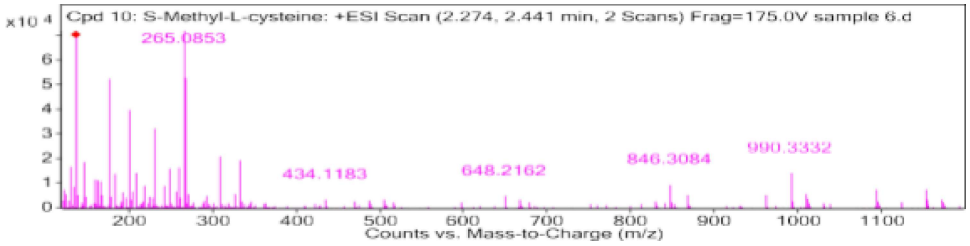
Compound Structure



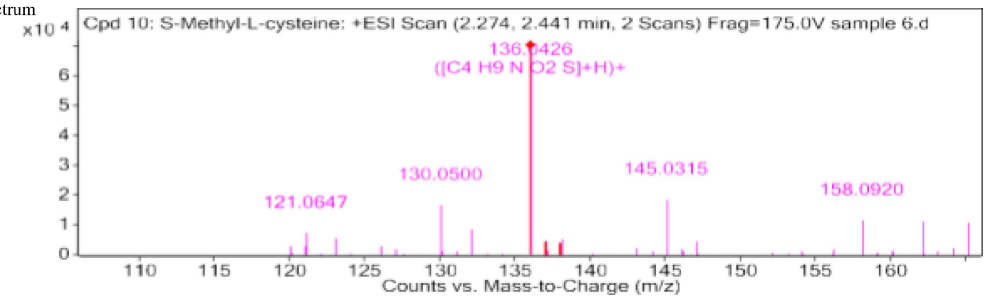
S-Methyl-L-cysteine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 10: S-Methyl-L-cysteine	**S-Methyl-L-cysteine**	136.0426	2.373	Auto MS/MS	135.0353

MS Spectrum



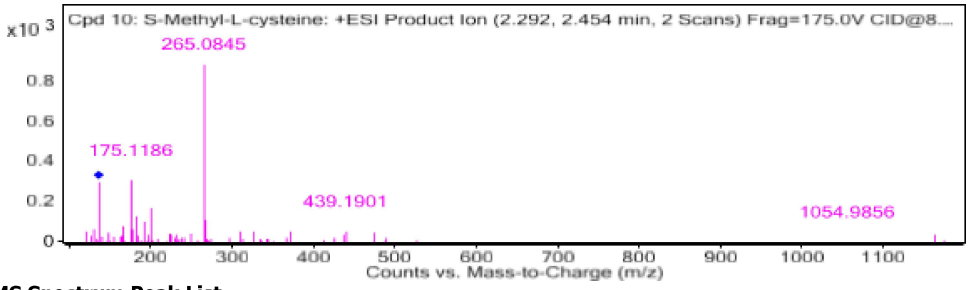
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
136.0426	136.0427	0.62	1	71843.34	C4 H9 N O2 S	(M+H)+
137.0455	137.0451	-2.87	1	5064.83	C4 H9 N O2 S	(M+H)+
138.0387	138.0394	5.32	1	3315.71	C4 H9 N O2 S	(M+H)+
175.1187			1	52567.63		
200.1026			1	39879.11		
229.1546			1	32632.66		
265.0853			1	500405.03		
266.0884			1	53050.69		
267.0831			1	23944.18		
307.0955			1	21147.36		

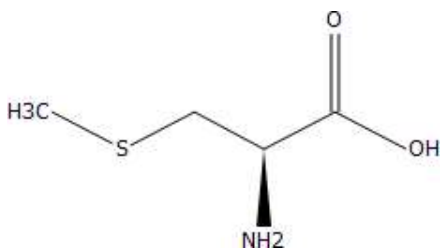
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0476		70.41
136.0413		301.69
165.0556		86.95
175.1186	1	312.37
176.147		66.83
182.0432		131.46
191.038		107.23
200.1005		174.33
265.0845	1	885.31
266.0872	1	118.56

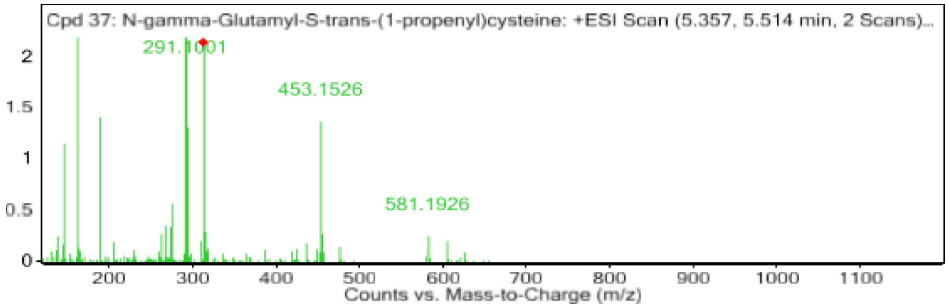
Compound Structure



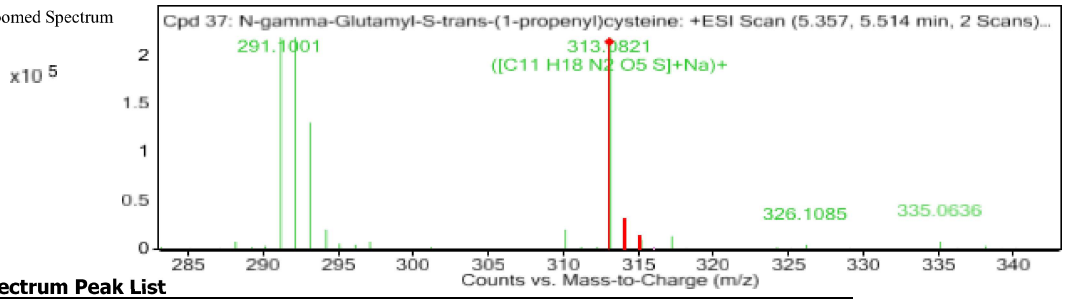
N-gamma-Glutamyl-S-trans-(1-propenyl)cysteine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 37: N-gamma-Glutamyl-S-trans-(1-propenyl)cysteine	**N-gamma-Glutamyl-S-trans-(1-propenyl)cysteine**	313.0821	5.449	Auto MS/MS	290.0929

MS Spectrum



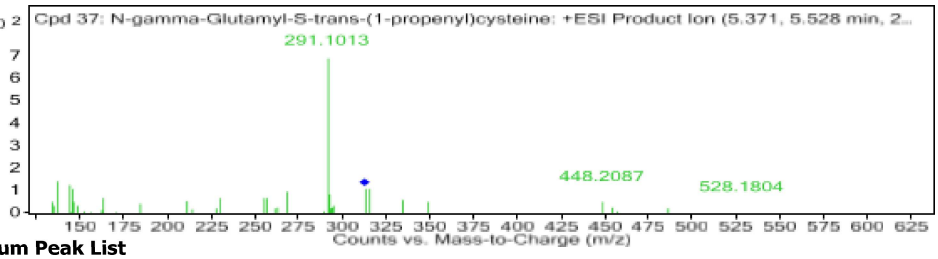
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.0309			1	115562.35		
162.0576			1	221428.28		
188.07			1	141602.84		
291.1001			1	2774021.5		
292.1032			1	350579.38		
293.0991			1	131943.56		
313.0821	313.0829	2.49	1	218694.34	C11 H18 N2 O5 S	(M+Na)+
314.0846	314.0857	3.48	1	30068.58	C11 H18 N2 O5 S	(M+Na)+
315.0816	315.0814	-0.74	1	10736.35	C11 H18 N2 O5 S	(M+Na)+
453.1526			1	137983.48		

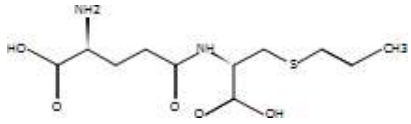
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
137.1048		143.88
144.0805		128.54
145.0302		111.47
163.0599		70.33
256.0885		71.7
268.0583		98.07
291.1013	1	693.38
292.1027	1	85.73
313.0841		112.5
315.1048		110.72

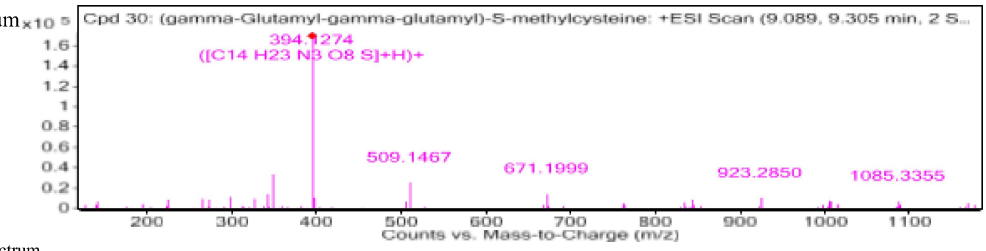
Compound Structure



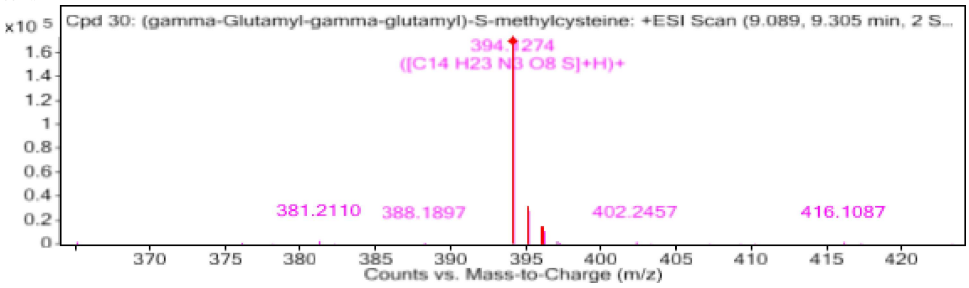
(gamma-Glutamyl-gamma-glutamyl)-S-methylcysteine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 30: (gamma-Glutamyl-gamma-glutamyl)-S-methylcysteine	**(gamma-Glutamyl-gamma-glutamyl)-S - methylcysteine**	394.1274	9.216	Auto MS/MS	393.1202

MS Spectrum



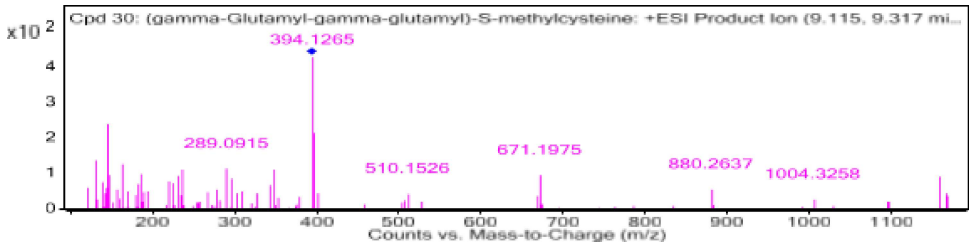
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
297.0566				12257.3		
325.1125			1	11156.29		
342.1389			1	15232.13		
347.0946			1	35012.07		
394.1274	394.1279	1.1	1	173406.3	C14 H23 N3 O8 S	(M+H)+
395.1302	395.1307	1.25	1	29010.7	C14 H23 N3 O8 S	(M+H)+
396.1285	396.1274	-2.76	1	11680.26	C14 H23 N3 O8 S	(M+H)+
509.1467			1	26447.94		
671.1999			1	15423.12		
923.285			2	11235.27		

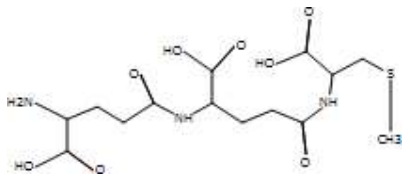
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0507		137.92
144.0103		148.74
144.0476		240.82
162.0569		127.12
234.0952		112.79
289.0915		114.45
347.0952		111.86
394.1265	1	427.84
395.1277	1	214.72
396.1218	1	103.9

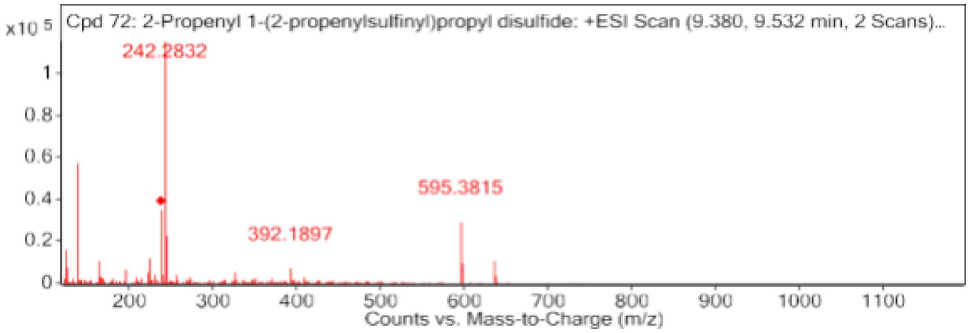
Compound Structure



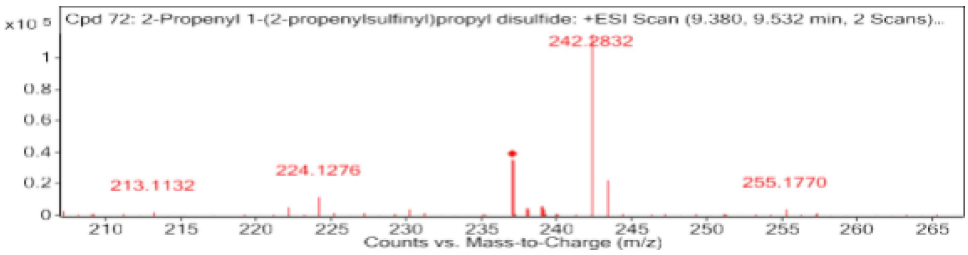
2-Propenyl 1-(2- propenylsulfinyl)propyl disulfide (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 72: 2-Propenyl 1-(2-propenylsulfinyl)propyl disulfide	**2-Propenyl 1-(2-propenylsulfinyl)propyl disulfide**	237.0425	9.471	Auto MS/MS	236.0353

MS Spectrum



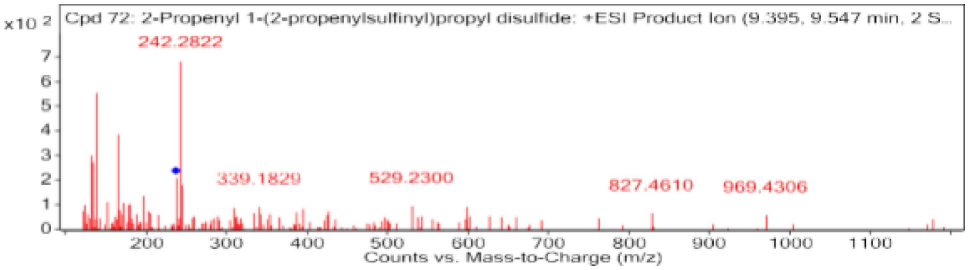
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
123.0809				16684.12		
137.1065			1	57633.64		
237.0425	237.0436	4.57	1	35600.72	C9 H16 O S3	(M+H)+
238.0452	238.0462	4.47	1	4226.95	C9 H16 O S3	(M+H)+
239.0386	239.04	5.72	1	4662.51	C9 H16 O S3	(M+H)+
240.0436	240.0425	-4.6	1	450.68	C9 H16 O S3	(M+H)+
241.039	241.0368	-9.03	1	360.64	C9 H16 O S3	(M+H)+
242.2832			1	115643.16		
243.2863			1	23421.23		
595.3815			1	29637.3		

MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
131.0508		303.83
132.0583		276.58
137.1053	1	557.61
151.1234		114.56
163.024		387.83
171.1004		109.99
196.0047		137.82
237.0423		213.75
242.2822	1	685.56
243.2869	1	185.02

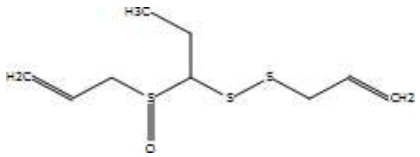
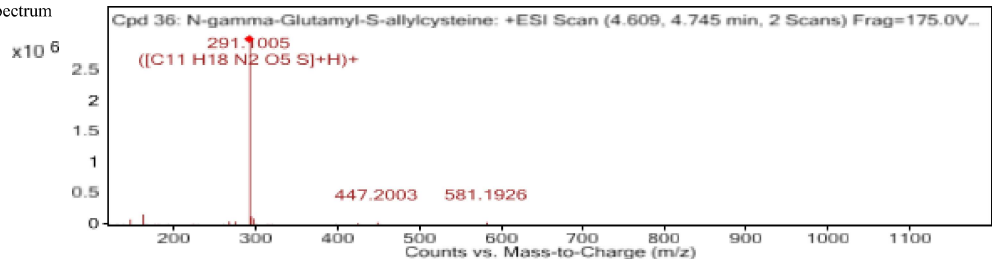


Fig. S2. *Showing HR-LCMS-MS zoomed spectrum showing the ionization peaks of amino acids detected in various extracts of garlic, with their chemical formula and structure*

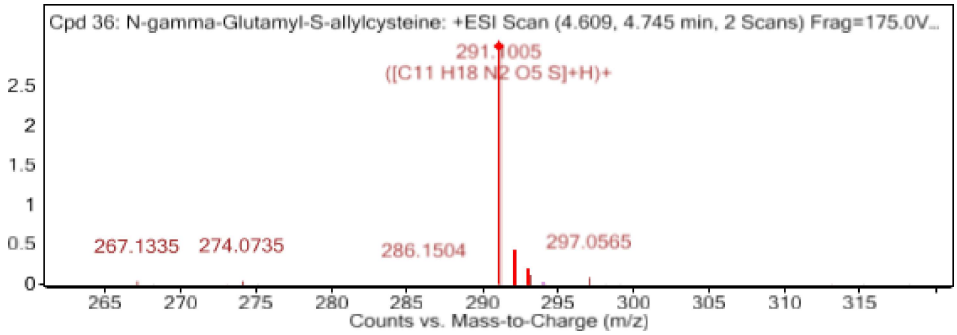
A1 N-gamma-Glutamyl-S-allylcysteine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 36: N-gamma-Glutamyl-S-allylcysteine	**N-gamma-Glutamyl-S-allylcysteine**	291.1005	4.692	Auto MS/MS	290.0932

MS Spectrum



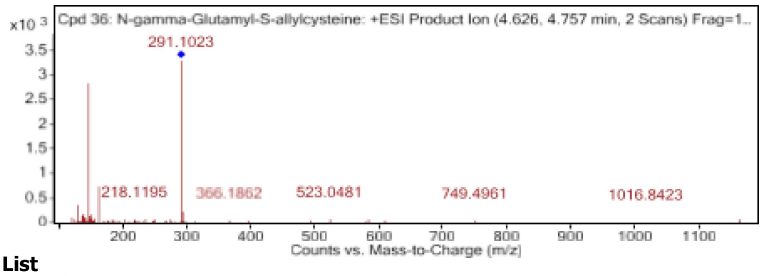
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.031			1	**89004.83**		
162.0577			1	**177509.61**		
267.1335			1	**58555.16**		
274.0735			1	**68061.11**		
291.1005	***291.1009***	**1.56**	1	**3077709**	**C11 H18 N2 O5 S**	**(M+H)+**
292.1033	***292.1038***	**1.64**	1	**408536.53**	**C11 H18 N2 O5 S**	**(M+H)+**
293.099	***293.0994***	**1.39**	1	**149847.03**	**C11 H18 N2 O5 S**	**(M+H)+**
297.0565			1	**116861.4**		
447.2003			1	**47218.35**		
581.1926			1	**50753.96**		

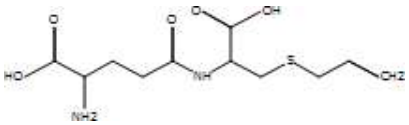
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0495	1	367.32
136.0607		160.26
137.1071		201.03
145.0317	1	2840.62
146.0309	1	197.69
150.9863		176.16
162.0582		751.18

Compound Structure



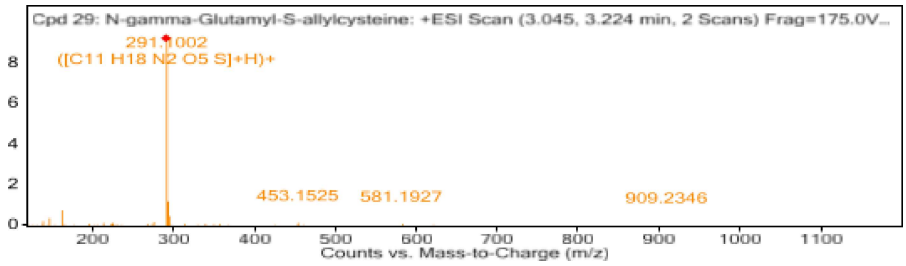
291.1023	1	3303.67
292.1051	1	741.11
293.1019	1	237.28

Compound Structure

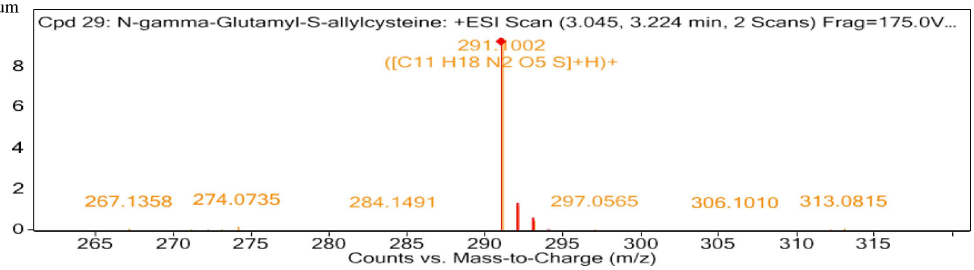
A1 N-gamma-Glutamyl-S-allylcysteine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 29: N-gamma-Glutamyl-S-allylcysteine	**N-gamma-Glutamyl-S-allylcysteine**	291.1002	3.155	Auto MS/MS	290.093

MS Spectrum



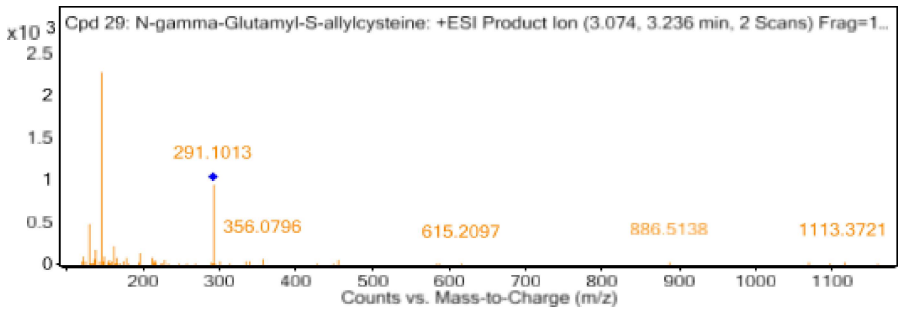
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
137.1064			1	26602.79		
145.0312			1	39058.05		
162.0576			1	79485.18		
213.1224			1	13399.62		
224.1275			1	16102.93		
274.0735			1	17122.51		
291.1002	291.1009	2.3	1	941710.94	C11 H18 N2 O5 S	(M+H)+
292.1032	292.1038	1.84	1	120510.58	C11 H18 N2 O5 S	(M+H)+
293.0991	293.0994	1.07	1	46902.65	C11 H18 N2 O5 S	(M+H)+
453.1525			1	13620.5		

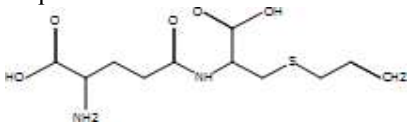
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
122.096		115.99
130.0502		493.89
137.1054		186.53
145.0311	1	2293.28
149.1058	1	116.57
162.0582		231.04
177.1012		98.2
195.1118	1	152.51
291.1013	2	960.5
292.1047	2	193.26

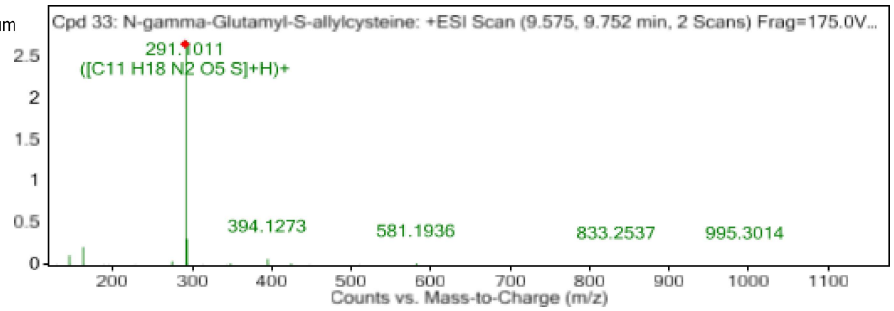
Compound Structure



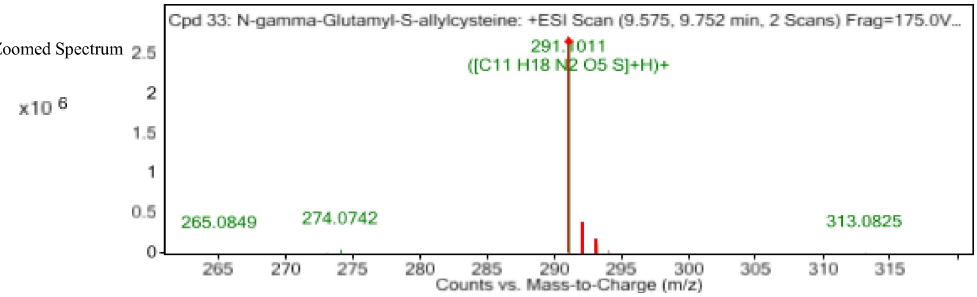
A1 N-gamma-Glutamyl-S-allylcysteine(HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 33: N-gamma-Glutamyl-S-allylcysteine	**N-gamma-Glutamyl-S-allylcysteine**	291.1011	9.677	Auto MS/MS	290.0938

MS Spectrum



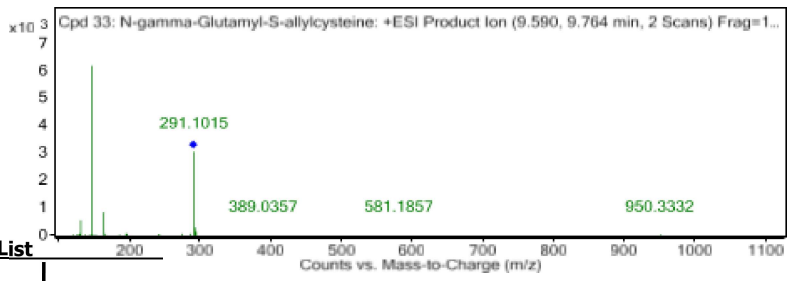
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.0314			1	130561.41		
162.0581			1	225254.39		
274.0742			1	57073.71		
291.1011	291.1009	-0.57	1	2711218.25	C11 H18 N2 O5 S	(M+H)+
292.1041	292.1038	-0.98	1	326837.31	C11 H18 N2 O5 S	(M+H)+
293.0999	293.0994	-1.66	1	124743.73	C11 H18 N2 O5 S	(M+H)+
347.0944			1	23873.44		
394.1273			1	84218.05		
424.12			1	29705.94		
581.1936			1	27569.21		

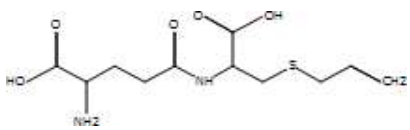
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0495	1	577.94
145.0311	1	6212.68
145.0778	2	115.16
146.0352	1	221.3
162.0569	1	910.32
165.1118		103.52
274.076		129.83
291.1015	1	3097.29
292.1019	1	346.74
293.0992	1	176.63

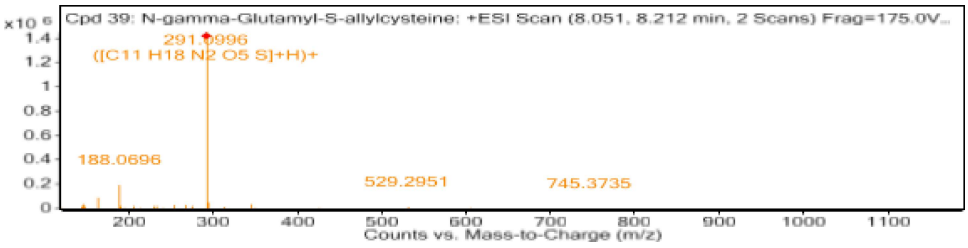
Compound Structure



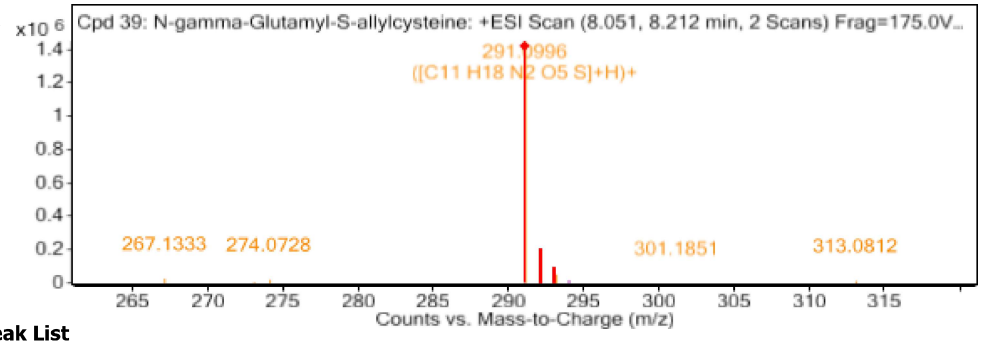
A1 N-gamma-Glutamyl-S-allylcysteine(AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 39: N-gamma-Glutamyl-S-allylcysteine	**N-gamma-Glutamyl-S-allylcysteine**	291.0996	8.144	Auto MS/MS	290.0923

MS Spectrum



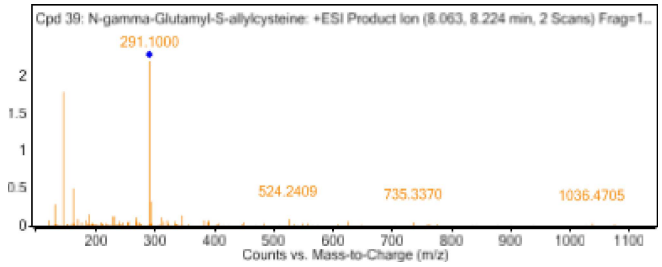
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.0309				47693.29		
162.0573			1	97595.69		
188.0696			1	199926.16		
231.1689				31704.39		
253.1218			1	35847.91		
267.1333			1	33763.1		
291.0996	291.1009	4.64	1	1450201	C11 H18 N2 O5 S	(M+H)+
292.1027	292.1038	3.83	1	169544.98	C11 H18 N2 O5 S	(M+H)+
293.0985	293.0994	3.28	1	62272.89	C11 H18 N2 O5 S	(M+H)+
344.1798			1	46014.84		

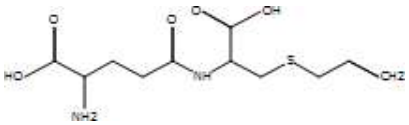
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.049		308.02
145.0302		1804.53
162.0566		520.57
188.0693		174.61
228.0672		149.05
231.168		149.39
267.1326		134.88
291.1	1	2214.18
292.0994	1	349.73
344.1777	1	158.51

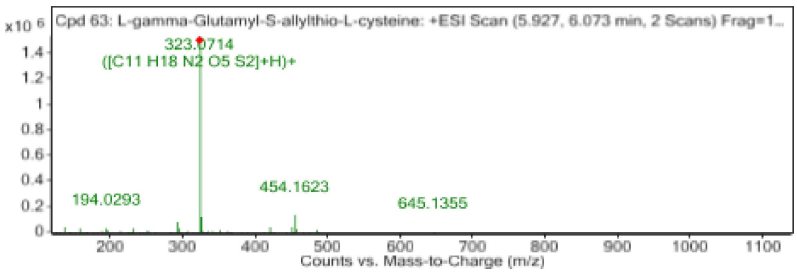
Compound Structure



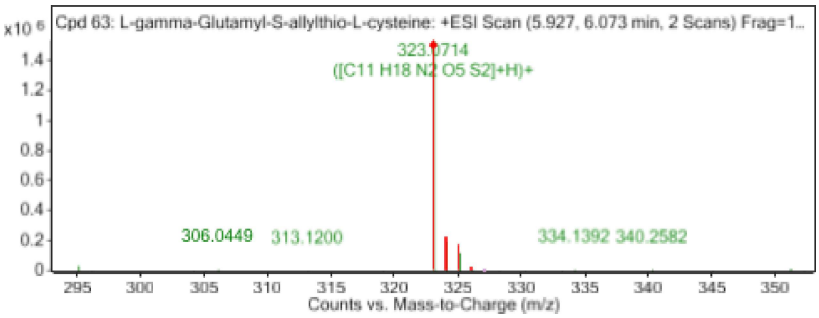
A2 L-gamma-Glutamyl-S-allylthio- L-cysteine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 63: L-gamma-Glutamyl-S-allylthio-L-cysteine	**L-gamma-Glutamyl-S-allylthio-L-cysteine**	323.0714	6.013	Auto MS/MS	322.0642

MS Spectrum



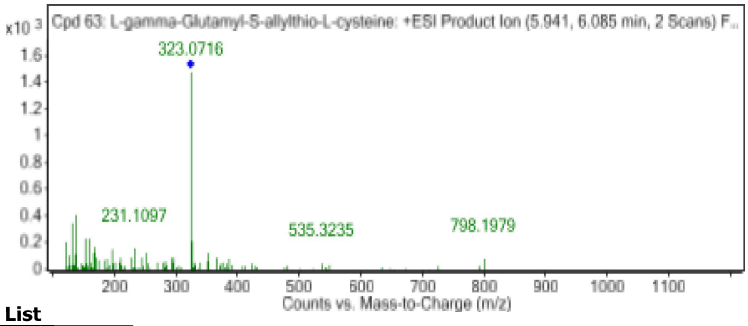
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
137.1064			1	45520.88		
291.0998			1	88783.43		
295.1274			1	41676.54		
323.0714	323.073	4.8	1	1534914	C11 H18 N2 O5 S2	(M+H)+
324.0745	324.0757	3.54	1	196654.98	C11 H18 N2 O5 S2	(M+H)+
325.0691	325.0704	4.04	1	122642.6	C11 H18 N2 O5 S2	(M+H)+
326.0719	326.0728	2.64	1	17167.48	C11 H18 N2 O5 S2	(M+H)+
419.146			1	51139.59		
450.134			1	44177.81		
454.1623			1	140253.98		

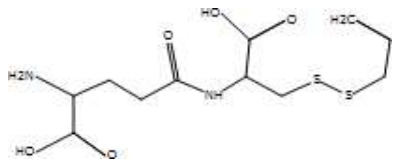
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0802		209.41
130.0493		357.24
137.1075		420.57
151.9823	1	239.36
158.0965	1	242.93
166.0847		175.67
194.0271		161.12
231.1097		164.39
323.0716	1	1482.5
324.072	1	225.76

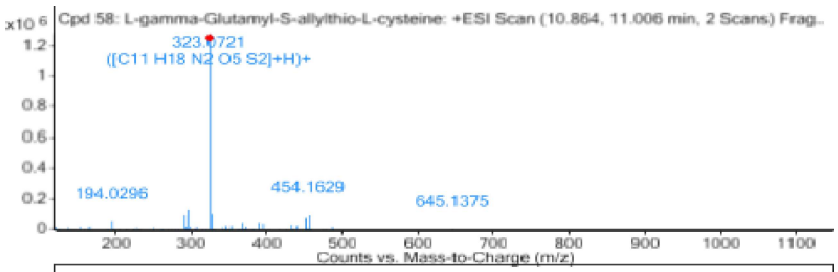
Compound Structure



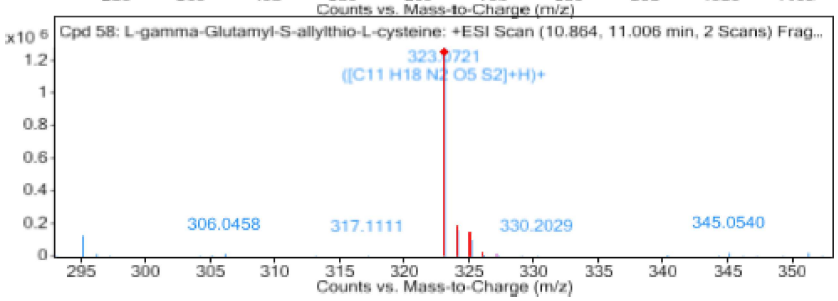
A2 L-gamma-Glutamyl-S-allylthio- L-cysteine (HG)

Compound Label		Name	*m/z*	RT	Algorithm
Cpd 58: L-gamma-Glutamyl-S-allylthio-L-cysteine		**L-gamma-Glutamyl-S-allylthio-L-cysteine**	323.0721	10.948	Auto MS/MS

MS Spectrum



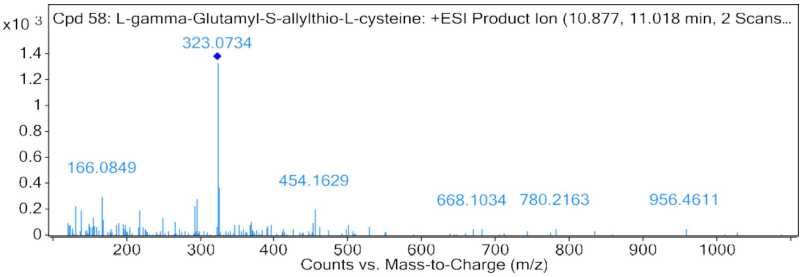
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
194.0296			1	56927.72		
291.1003			1	96230.69		
295.1281			1	132254.08		
323.0721	323.073	2.74	1	1276053.88	C11 H18 N2 O5 S2	(M+H)+
324.0752	324.0757	1.46	1	167495.05	C11 H18 N2 O5 S2	(M+H)+
325.0698	325.0704	1.98	1	108291.34	C11 H18 N2 O5 S2	(M+H)+
326.0722	326.0728	1.66	1	14264.46	C11 H18 N2 O5 S2	(M+H)+
367.1314			1	47555.96		
450.135			1	75850.48		
454.1629			1	99342.23		

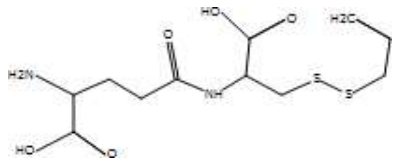
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0489		231.74
137.1056	1	198.01
154.0496		144.92
166.0849		305.42
217.081		198.95
291.0981	1	227.68
295.1274		284.48
323.0734	1	1334.37
325.0683	1	374.42
454.1629		205.59

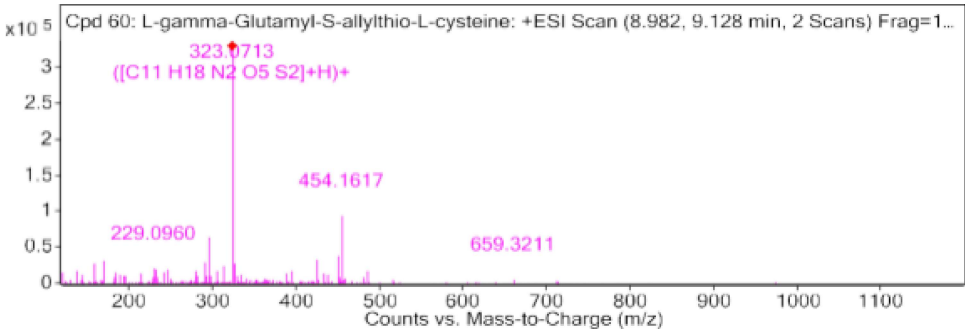
Compound Structure



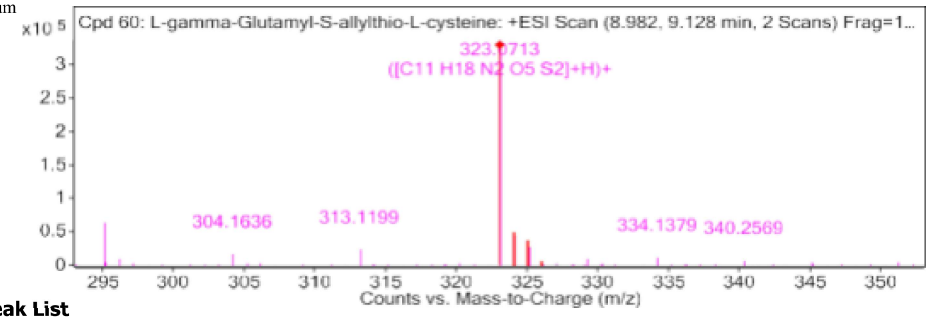
A2 L-gamma-Glutamyl-S-allylthio- L-cysteine (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 60: L-gamma-Glutamyl-S-allylthio-L-cysteine	**L-gamma-Glutamyl-S-allylthio-L-cysteine**	323.0713	9.068	Auto MS/MS	322.0642

MS Spectrum



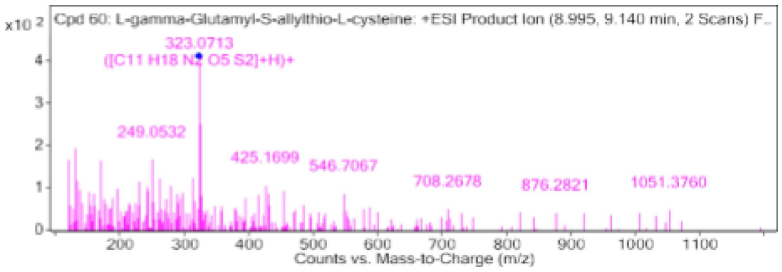
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
169.0751			1	32591.89		
291.0995			1	30678.06		
295.127			1	65258.38		
323.0713	323.073	5.09	1	336869	C11 H18 N2 O5 S2	(M+H)+
324.0745	324.0757	3.7	1	46546.63	C11 H18 N2 O5 S2	(M+H)+
325.0692	325.0704	3.87	1	30053.03	C11 H18 N2 O5 S2	(M+H)+
326.072	326.0728	2.26	1	3864.97	C11 H18 N2 O5 S2	(M+H)+
424.1689			1	34131.22		
450.1338			1	40546.44		
454.1617			1	96231.27		

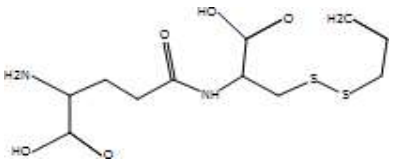
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	*Calc m/z*	Diff (ppm)	z	Abund	Formula	Ion
120.0112				168.23		
130.0502				194.52		
133.0654				119.95		
169.073				167.46		
229.0927				115.73		
249.0532				168.08		
261.1255				124		
313.1156				125.91		
323.0713	323.073	5.14		398.26	C11 H18 N2 O5 S2	(M+H)+
324.0716			1	252.7		

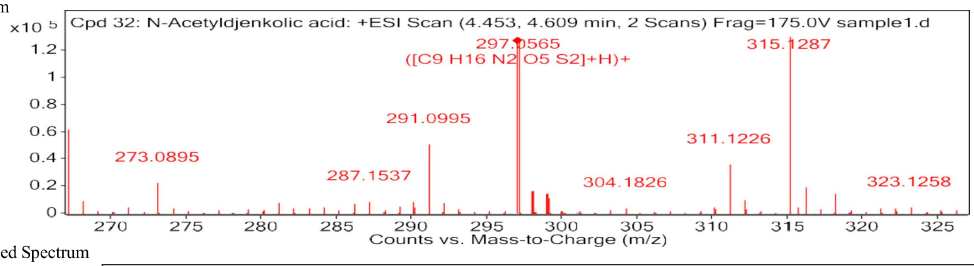
Compound Structure



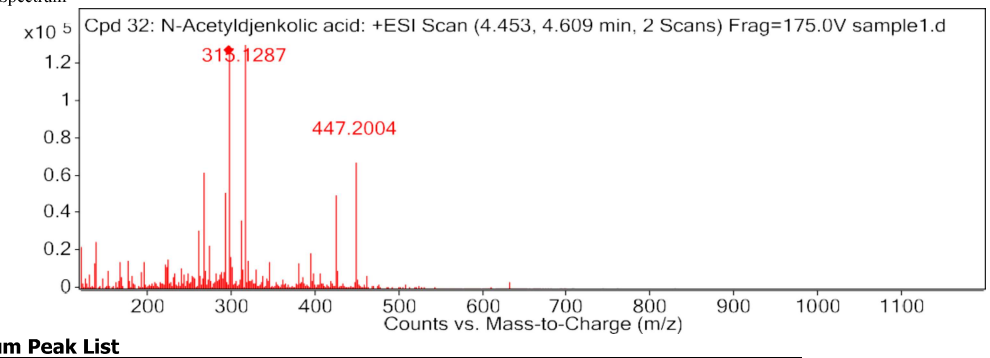
A3 N-Acetyldjenkolic acid (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 32: N-Acetyldjenkolic Acid	**N-Acetyldjenkolic acid**	297.0565	4.548	Auto MS/MS	296.0492

MS Spectrum



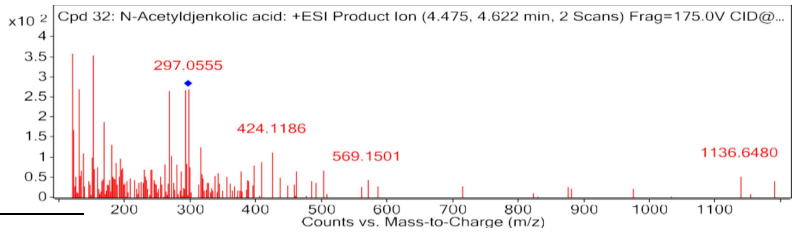
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
267.1332			1	62370.9		
291.0995			1	51390.94		
297.0565	297.0573	2.75	1	130102.69	C9 H16 N2 O5 S2	(M+H)+
298.0592	298.0599	2.22	1	17218.49	C9 H16 N2 O5 S2	(M+H)+
299.0531	299.0546	4.95	1	12015.77	C9 H16 N2 O5 S2	(M+H)+
300.0542	300.057	9.02	1	1371.34	C9 H16 N2 O5 S2	(M+H)+
311.1226			1	36971.21		
315.1287			1	137099.59		
424.1191			1	50461.09		
447.2004			1	67434.59		

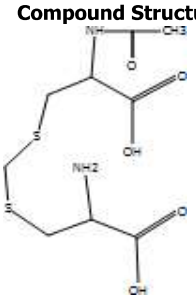
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0098		360.53
120.08		153.06
122.0074		169.92
130.0482		270.6
150.9869		356.53
168.0124		190.67
180.103	1	134.05
267.1335		267.1
291.1001		268.4
297.0555	1	270.96

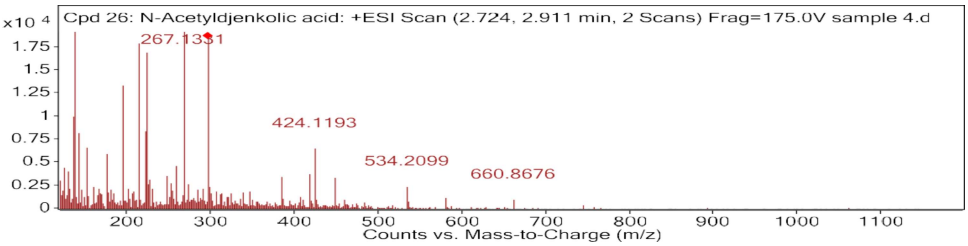
Compound Structure



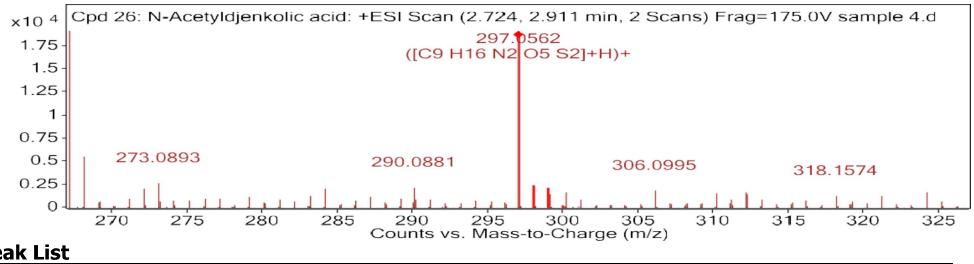
A3 N-Acetyldjenkolic acid (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 26: N-Acetyldjenkolic Acid	**N-Acetyldjenkolic acid**	297.0562	2.835	Auto MS/MS	296.049

MS Spectrum



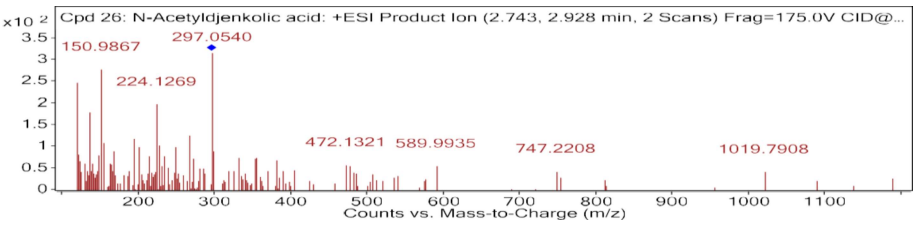
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
136.0618			1	10082.09		
137.1065			1	25710.88		
194.0296				13369.56		
213.1226			1	17948.91		
224.1274			1	16936.87		
267.1331			1	32673.57		
297.0562	297.0573	3.72	1	19130.82	C9 H16 N2 O5 S2	(M+H)+
298.0592	298.0599	2.4	1	2490.63	C9 H16 N2 O5 S2	(M+H)+
299.0537	299.0546	3.02	1	1528.91	C9 H16 N2 O5 S2	(M+H)+
300.0579	300.057	-3.22	1	273.4	C9 H16 N2 O5 S2	(M+H)+

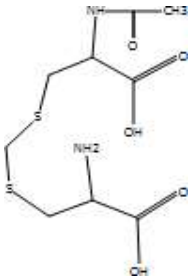
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	Abund
120.011	249.05
136.0595	181.07
150.9867	279.98
151.9814	111.36
155.0384	110.26
194.0315	119.56
224.1269	199.03
227.1723	104.37
266.6054	127.54
297.054	317.92

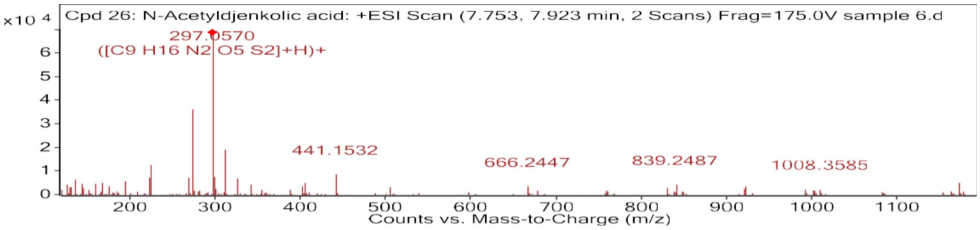
Compound Structure



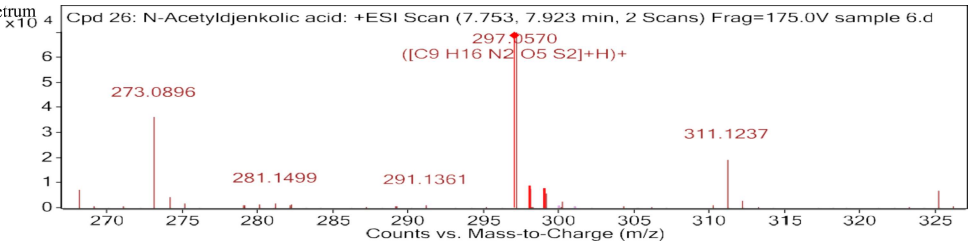
A3 N-Acetyldjenkolic acid (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 26: N-Acetyldjenkolic acid	**N-Acetyldjenkolic acid**	297.057	7.853	Auto MS/MS	296.0497

MS Spectrum



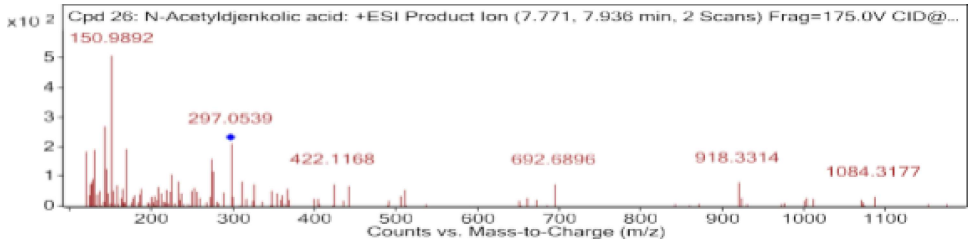
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
222.1117			1	7665.24		
224.1277			1	13179.99		
268.1038				7768.64		
273.0896			1	36375.35		
297.057	297.0573	1.16	1	70188.72	C9 H16 N2 O5 S2	(M+H)+
298.0602	298.0599	-0.99	1	7801.07	C9 H16 N2 O5 S2	(M+H)+
299.0535	299.0546	3.62	1	6226.46	C9 H16 N2 O5 S2	(M+H)+
311.1237			1	19680.85		
325.1118				7110.84		
441.1532			1	9008.66		

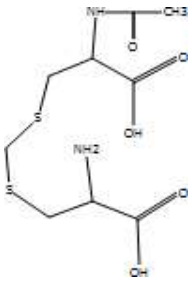
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0105		187.06
130.0475		193.12
143.0022		271.9
145.0345		128.56
150.9892	1	511.12
168.0149		197
224.1267		109.1
273.0891	1	161.2
275.0946	1	118.6
297.0539	1	213.31

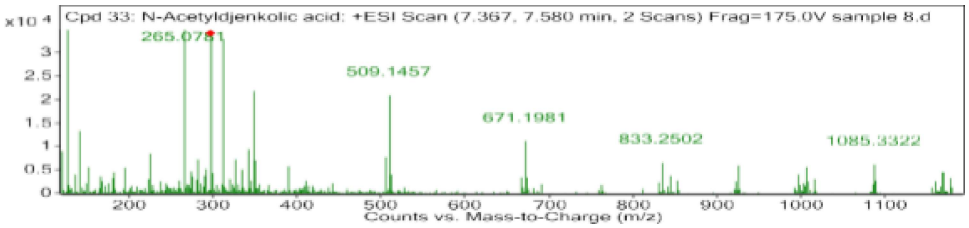
Compound Structure



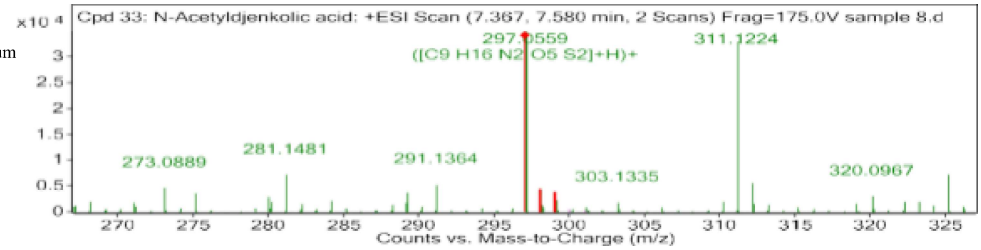
A3 N-Acetyldjenkolic acid (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 33: N-Acetyldjenkolic acid	**N-Acetyldjenkolic acid**	297.0559	7.493	Auto MS/MS	296.0487

MS Spectrum



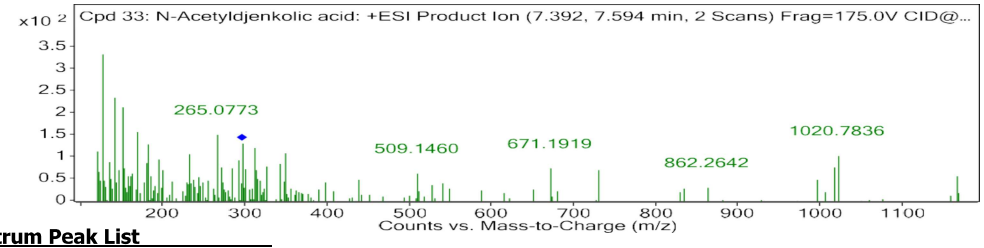
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
127.0494			1	36078.7		
140.0676				13515.19		
265.0781			1	79521.27		
297.0559	297.0573	4.72	1	34863.31	C9 H16 N2 O5 S2	(M+H)+
298.0583	298.0599	5.43	1	4413.09	C9 H16 N2 O5 S2	(M+H)+
299.0536	299.0546	3.11	1	2522.79	C9 H16 N2 O5 S2	(M+H)+
311.1224			1	33138.93		
347.0932			1	21900.08		
509.1457			1	21098.03		
671.1981			1	11282.17		

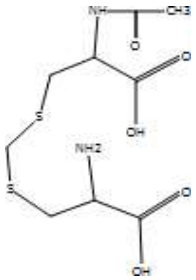
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0812		113.42
127.0486		335.59
140.0656		236.96
150.9869		214.34
168.0123		158.7
181.0949		131.28
181.1218		116.84
265.0773		152.51
297.0525	1	131.82
311.1208		121.81

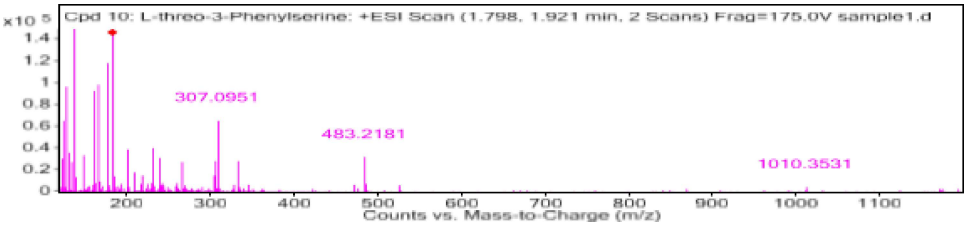
Compound Structure



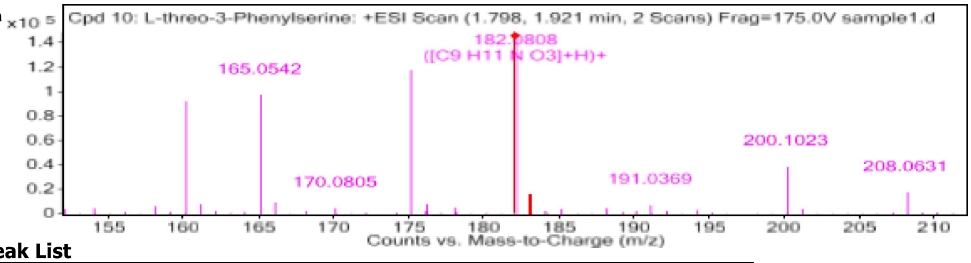
A4 L-threo-3-Phenylserine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 10: L-threo-3-Phenylserine	**L-threo-3-Phenylserine**	182.0808	1.877	Auto MS/MS	181.0735

MS Spectrum



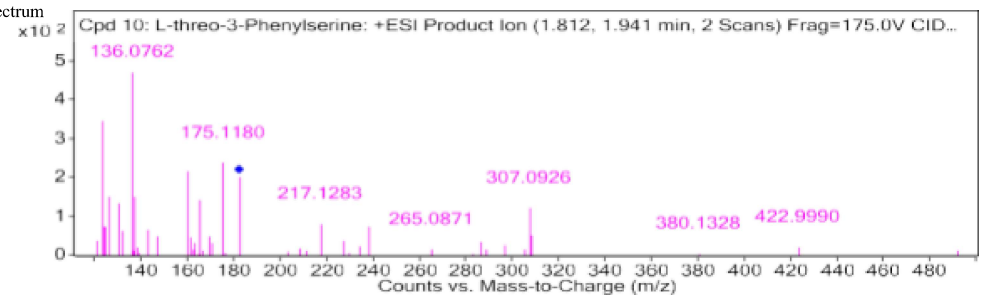
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
123.0434			1	64869.4		
126.0659			1	96804.41		
136.0754			1	165782.88		
160.1075			1	92691.31		
165.0542			1	97882.13		
175.1184			1	117772.3		
182.0441			1	52764.95		
182.0808	182.0812	2.02	1	148789.78	C9 H11 N O3	(M+H)+
183.0838	183.0843	2.77	1	14481.48	C9 H11 N O3	(M+H)+
307.0951			1	65549.48		

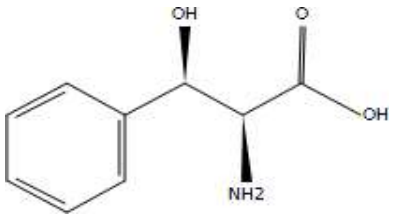
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
123.0434	1	347.27
126.0625		151.67
130.0495		134.05
136.0381		136.9
136.0762		471.91
137.0791		153.18
160.1063	1	216.78
165.0515		144.87
175.118	1	239.78
182.0838		203.76

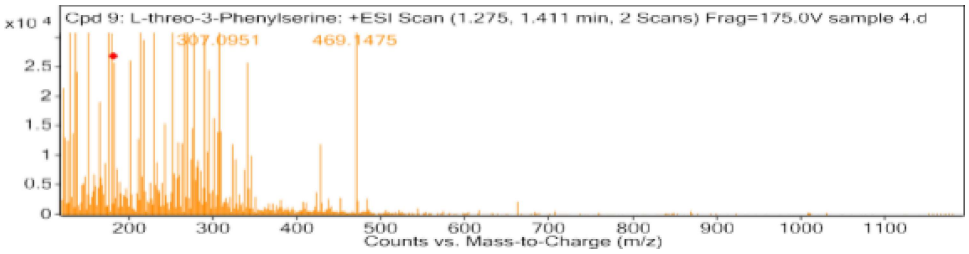
Compound Structure



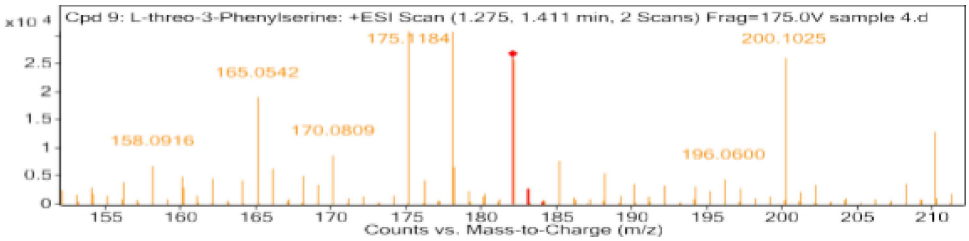
A4 L-threo-3-Phenylserine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 9: L-threo-3-Phenylserine	**L-threo-3-Phenylserine**	182.0811	1.382	Auto MS/MS	181.0732

MS Spectrum



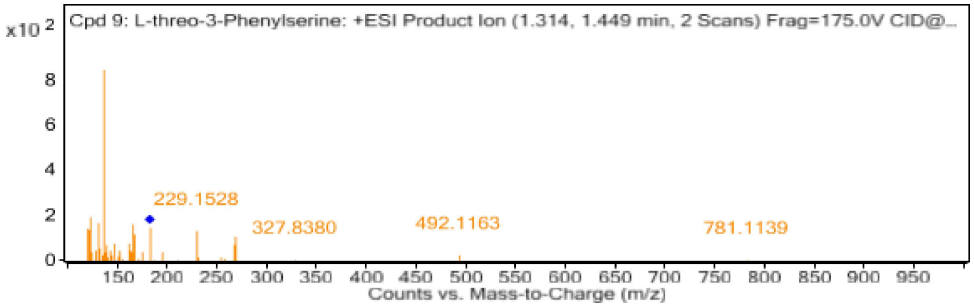
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
136.061			1	84476.3		
136.0729				47489.44		
175.1184			1	47398.39		
182.0811	182.0812	0.59		25826.34	C9 H11 N O3	(M+H)+
183.0838	183.0843	3.04	1	3051.22	C9 H11 N O3	(M+H)+
184.0701	184.0863	88.11	1	929.78	C9 H11 N O3	(M+H)+
214.0706			1	45683.59		
265.0846			1	63917.13		
276.1434			1	40785.05		
307.0951			1	93545.48		

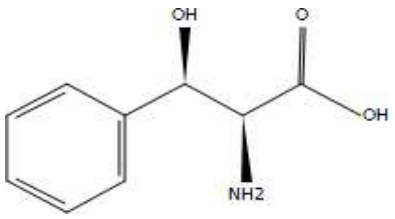
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0517		146.78
121.064		141.02
123.0457	1	200.54
130.0497	1	174.62
136.038		202.67
136.0753		851.1
165.0561		167.24
166.0574		120.01
182.1176		155.16
229.1528		136.61

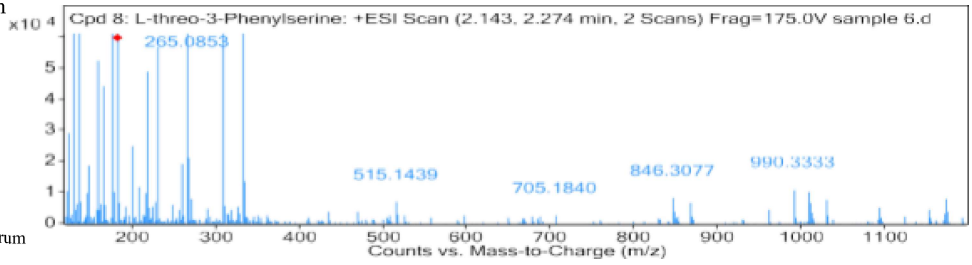
Compound Structure



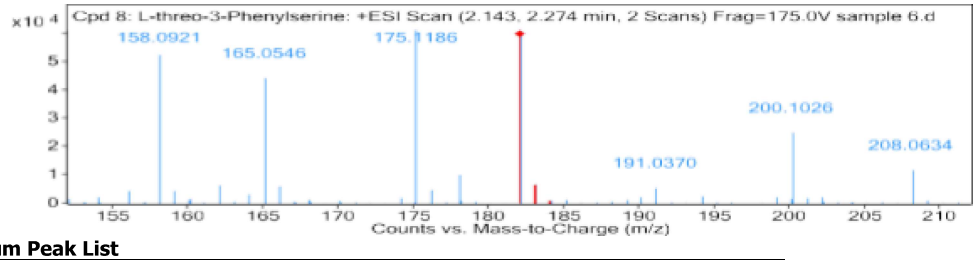
A4 L-threo-3-Phenylserine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 8: L-threo-3-Phenylserine	**L-threo-3-Phenylserine**	182.0811	2.233	Auto MS/MS	181.0739

MS Spectrum



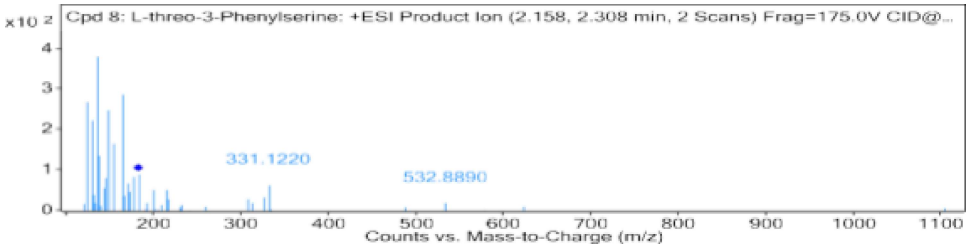
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
130.0499			1	67369.74		
136.0756			1	78697.79		
175.1186			1	79923.38		
182.0811	182.0812	0.26	1	60938.92	C9 H11 N O3	(M+H)+
183.0845	183.0843	-0.67	1	7056.16	C9 H11 N O3	(M+H)+
184.0867	184.0863	-1.97	1	758.72	C9 H11 N O3	(M+H)+
229.1546			1	56978.63		
265.0853			1	198058.25		
307.0956			1	114990.36		
332.1335			1	87246.07		

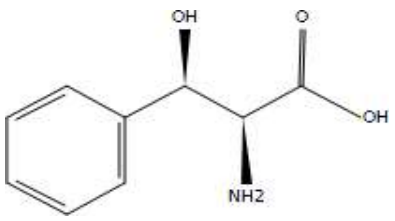
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
123.0436	1	269.61
130.0499		222.85
136.041		85.21
136.0755		381.62
137.0793		135.95
147.0431		247.86
154.05		166.6
165.0541	1	286.68
176.1236		83.6
182.0833	1	91.34

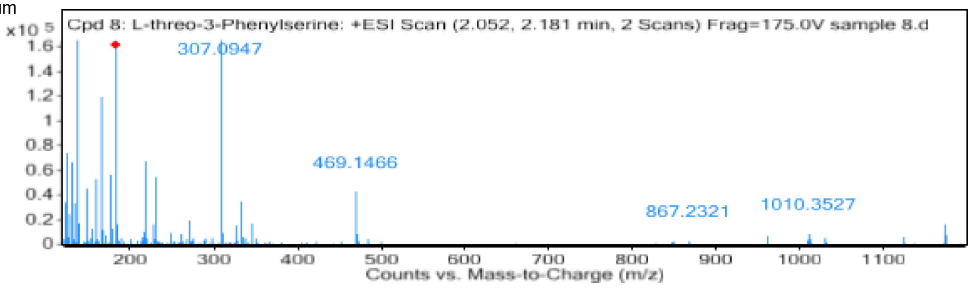
Compound Structure



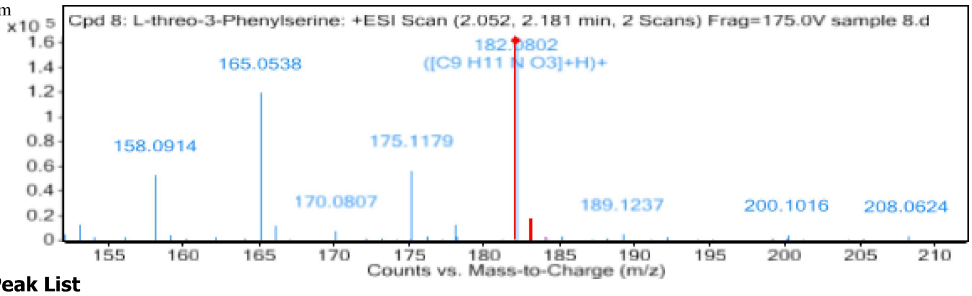
A4 L-threo-3-Phenylserine (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 8: L-threo-3-Phenylserine	**L-threo-3-Phenylserine**	182.0802	2.131	Auto MS/MS	181.0729

MS Spectrum



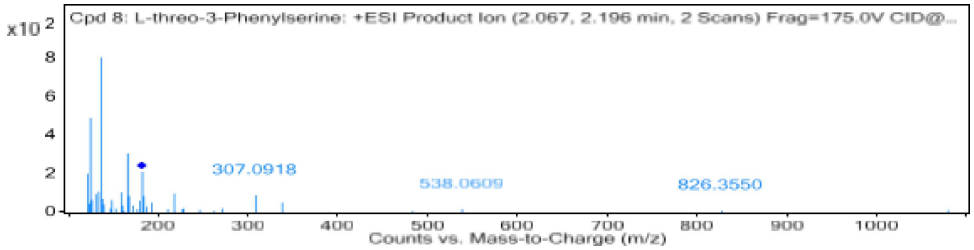
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
123.0436			1	75345.05		
130.0496			1	67060.05		
136.0752			1	226207.69		
165.0538			1	119975.66		
175.1179			1	57476.76		
182.0802	182.0812	5.19	1	165415.41	C9 H11 N O3	(M+H)+
183.0833	183.0843	5.61	1	16651.49	C9 H11 N O3	(M+H)+
217.081			1	67969.75		
229.1537			1	55714.66		
307.0947			1	226090.38		

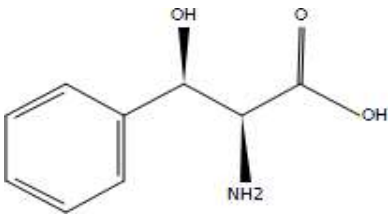
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	*Calc m/z*	Diff (ppm)	z	Abund	Formula	Ion
121.0643				204.25		
123.0441				491.71		
130.049				96.07		
132.1004				112.78		
136.0751			1	808.22		
158.0935				104.08		
165.0537			1	307.98		
182.0802	182.0812	5.57		211.9	C9 H11 N O3	(M+H)+
217.0832				101.88		
307.0918				90.84		

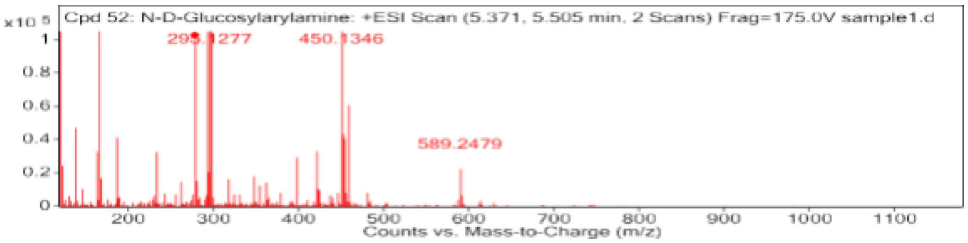
Compound Structure



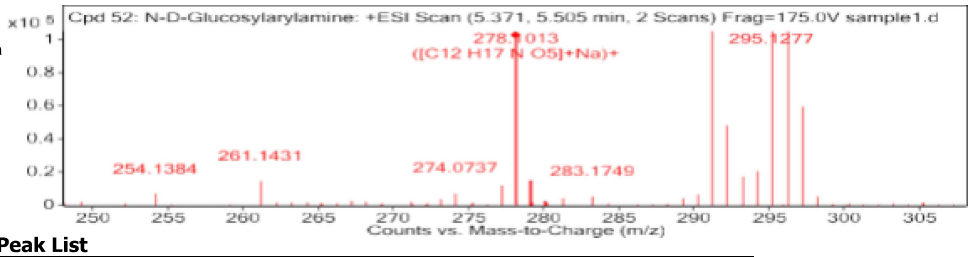
A5 N-D-Glucosylarylamine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 52: N-D-Glucosylarylamine	**N-D-Glucosylarylamine**	278.1013	5.456	Auto MS/MS	255.1121

MS Spectrum



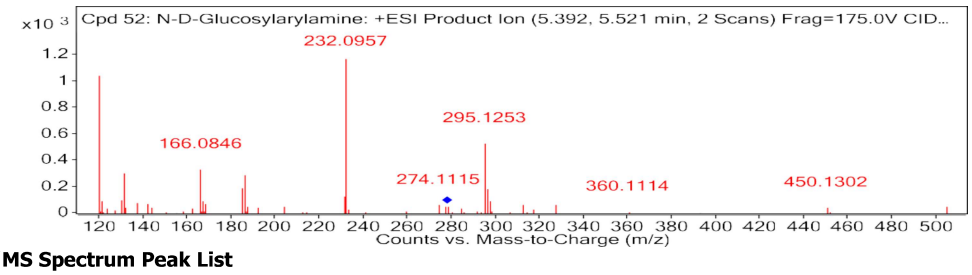
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
120.0803			1	241964.72		
166.0856			1	186332.92		
278.1013	278.0999	-5.04	1	104972.52	C12 H17 N O5	(M+Na)+
279.1047	279.1031	-5.46	1	15739.71	C12 H17 N O5	(M+Na)+
280.1089	280.1052	-13.35	1	2064.42	C12 H17 N O5	(M+Na)+
291.1002			1	356589.63		
295.1277			1	2972101		
296.1313			1	434145.88		
450.1346			1	217952		
457.1796			1	61340.83		

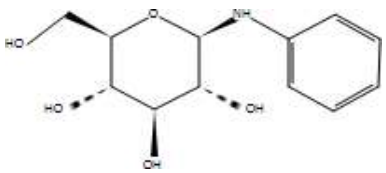
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	*z*	Abund
120.0806	1	244.12
130.049		108.07
131.0479		305.81
166.0846	1	338.62
185.1056		195.47
186.0893	1	291.95
231.1129		132.51
232.0957	1	1174.09
295.1253	1	535.16
296.1316	1	189.09

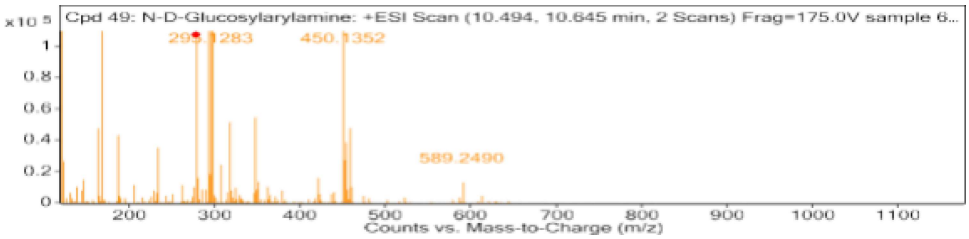
Compound Structure



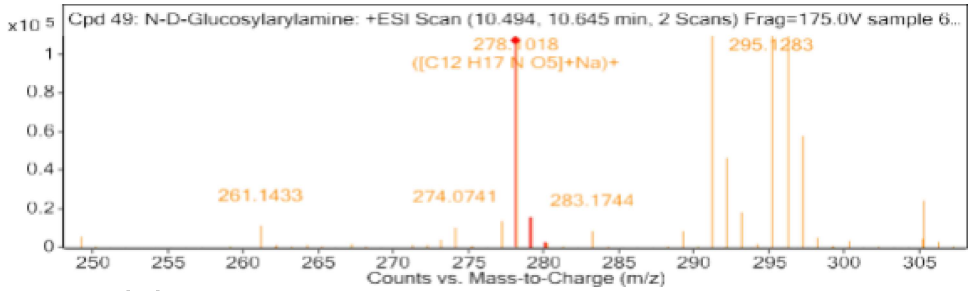
A5 N-D-Glucosylarylamine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 49: N-D-Glucosylarylamine	**N-D-Glucosylarylamine**	278.1018	10.584	Auto MS/MS	255.1126

MS Spectrum



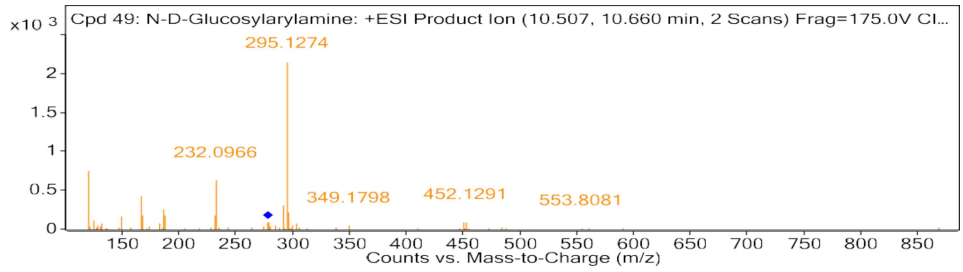
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
120.0806			1	252211.05		
166.0859			1	271266.81		
278.1018	278.0999	-6.78	1	109455.35	C12 H17 N O5	(M+Na)+
279.1053	279.1031	-7.86	1	16221.06	C12 H17 N O5	(M+Na)+
280.1072	280.1052	-7.15	1	2651.3	C12 H17 N O5	(M+Na)+
291.1008			1	349329.81		
295.1283			1	2690965.5		
296.132			1	399683.81		
297.134			1	58064.48		
450.1352			1	126761.76		

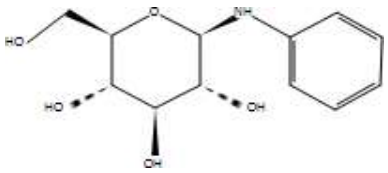
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0809	2	763.25
166.0859		441.37
167.0884		189.67
186.0912		272.85
187.0912		194.7
231.1107		192.75
232.0966		641.15
291.1005	1	322
295.1274	1	2154.8
296.1328	1	233.59

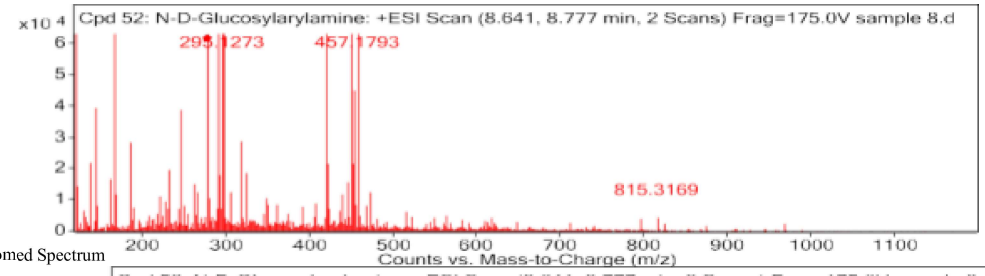
Compound Structure



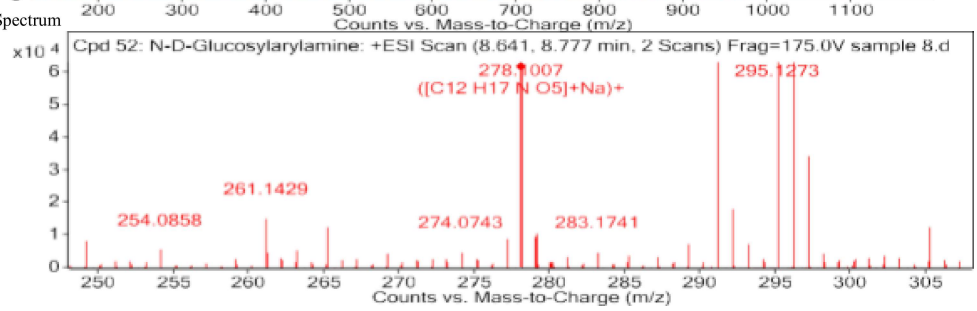
A5 N-D-Glucosylarylamine (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 52: N-D-Glucosylarylamine	**N-D-Glucosylarylamine**	278.1007	8.727	Auto MS/MS	255.1117

MS Spectrum



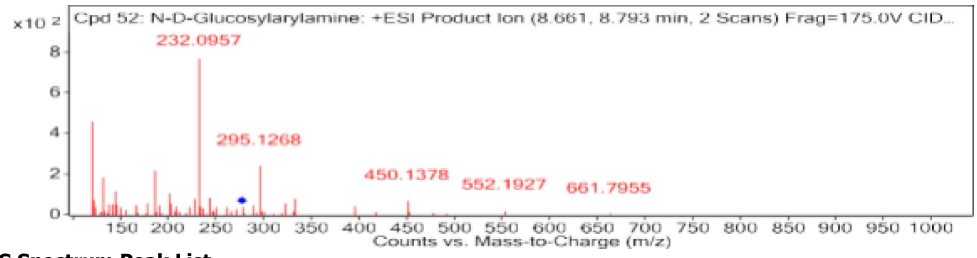
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
120.0805			1	142476.25		
166.0852			1	112785.24		
278.1007	278.0999	-3.05	1	63050.48	C12 H17 N O5	(M+Na)+
279.1053	279.1031	-7.77	1	10785.5	C12 H17 N O5	(M+Na)+
280.1069	280.1052	-6.28	1	1904.65	C12 H17 N O5	(M+Na)+
291.0996			1	134452.5		
295.1273			1	1457255.25		
296.1308			1	233042.19		
450.1342			1	96553.29		
457.1793			1	96961.87		

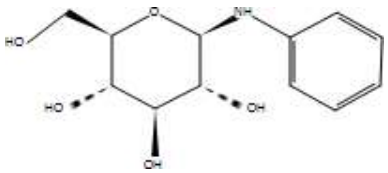
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0805	1	463.84
131.048		187.73
143.0854	1	119.58
185.1044		106.94
186.0897		223.08
201.1224		111.28
231.1106		139.92
232.0957	1	772.98
242.0914		88.48
295.1268	1	244.15

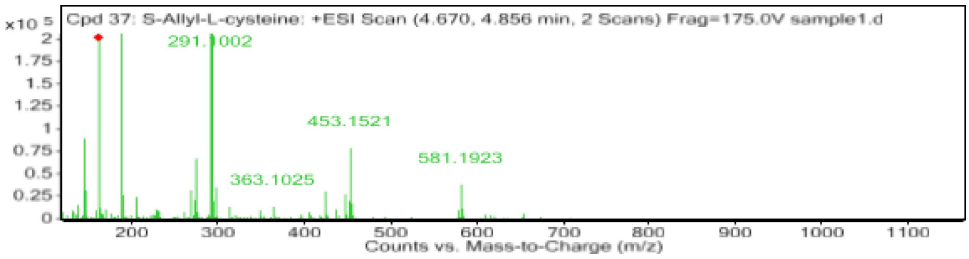
Compound Structure



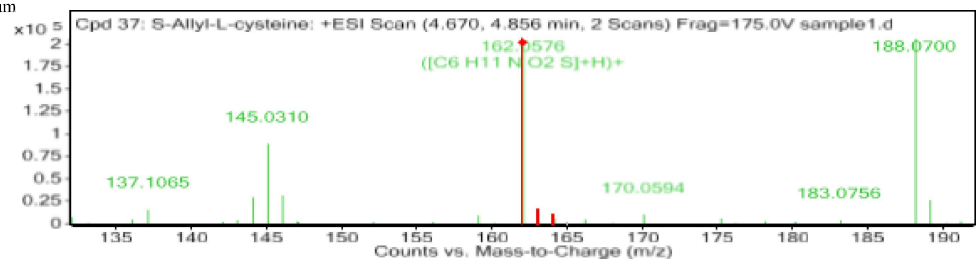
A6 S-Allyl-L-cysteine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 37: S-Allyl-L-cysteine	**S-Allyl-L-cysteine**	162.0576	4.776	Auto MS/MS	161.0504

MS Spectrum



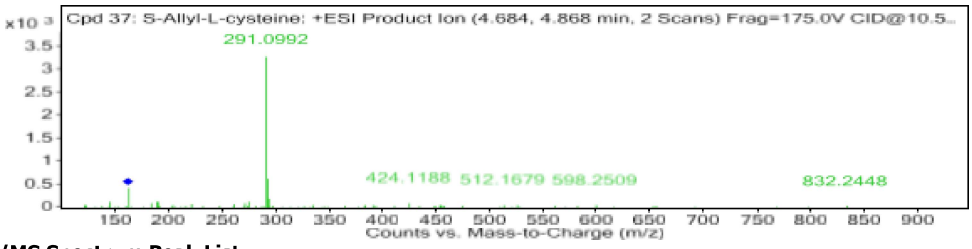
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.031			1	90169.55		
162.0576	162.0583	4.36	1	205944.42	C6 H11 N O2 S	(M+H)+
163.0611	163.061	-0.35	1	13979.36	C6 H11 N O2 S	(M+H)+
164.0549	164.0553	2.45	1	7853.33	C6 H11 N O2 S	(M+H)+
188.07			1	221843.31		
274.0736			1	68229.7		
291.1002			1	3544463.25		
292.1031			1	452477.53		
293.0989			1	163448.81		
453.1521			1	79904.23		

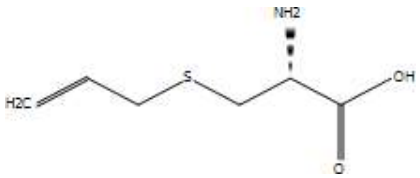
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	*Calc m/z*	Diff (ppm)	z	Abund	Formula	Ion
145.0339				147.3		
162.0577	162.0583	4.02		434.48	C6 H11 N O2 S	(M+H)+
188.0707				146.06		
189.0753				130.47		
271.1306				99.55		
274.0724				142.69		
291.0992			1	3286.8		
292.1021			1	635.12		
293.1021			1	202.18		
424.1188				105.58		

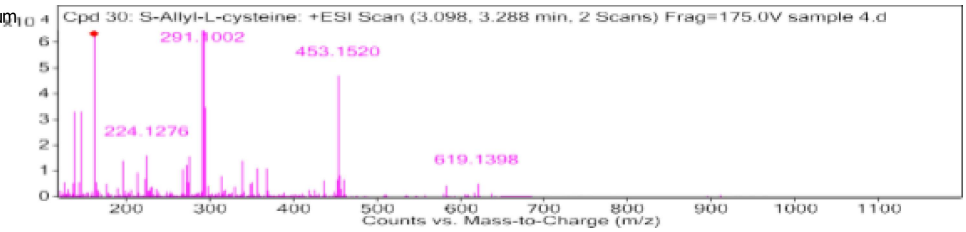
Compound Structure



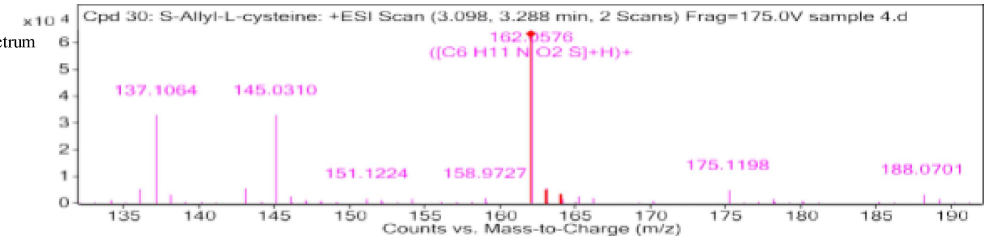
A6 S-Allyl-L-cysteine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 30: S-Allyl-L-cysteine	**S-Allyl-L-cysteine**	162.0576	3.209	Auto MS/MS	161.0503

MS Spectrum



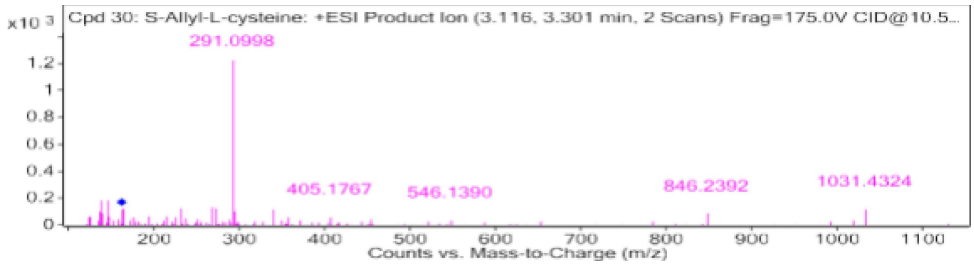
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
137.1064			1	33317.02		
145.031			1	33401.86		
162.0576	162.0583	4.61	1	64842.5	C6 H11 N O2 S	(M+H)+
163.0607	163.061	2.42	1	5879.19	C6 H11 N O2 S	(M+H)+
164.0539	164.0553	8.35	1	1964.54	C6 H11 N O2 S	(M+H)+
224.1276			1	16453.44		
291.1002			1	741278.75		
292.1032			1	98568.42		
293.0987			1	35200.95		
453.152			1	47506.56		

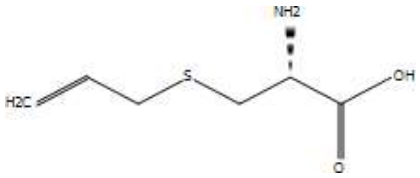
MSMS Spectrum



MS/~~MS Spectrum Peak List~~

m/z	z	Abund
137.1073		194.85
145.0299		191.62
164.0805		131.98
230.1383		130.34
267.1493		140.52
271.1282		129.51
291.0998	1	1232.84
292.1051	1	182.65
338.0691		126.53
1031.4324		127.64

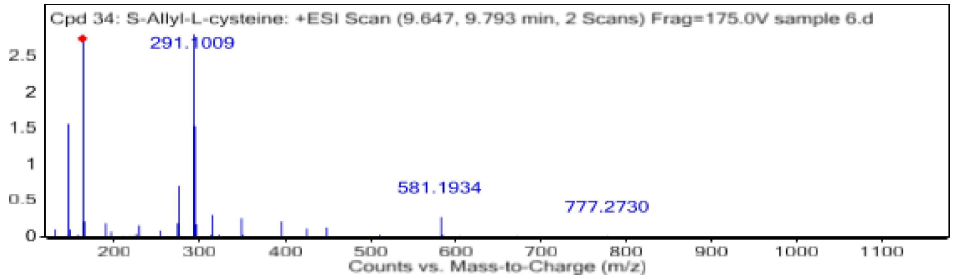
Compound Structure



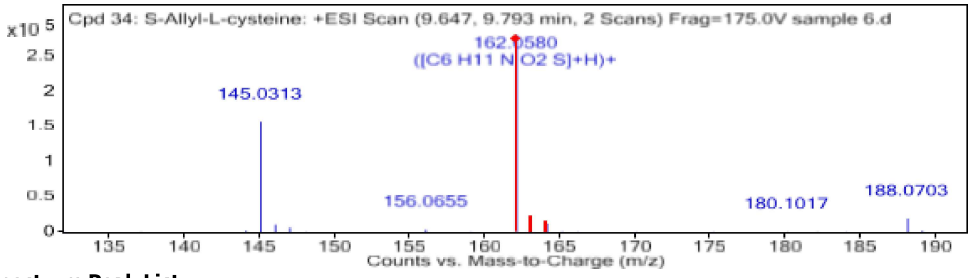
A6 S-Allyl-L-cysteine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 34: S-Allyl-L-cysteine	**S-Allyl-L-cysteine**	162.058	9.732	Auto MS/MS	161.0507

MS Spectrum



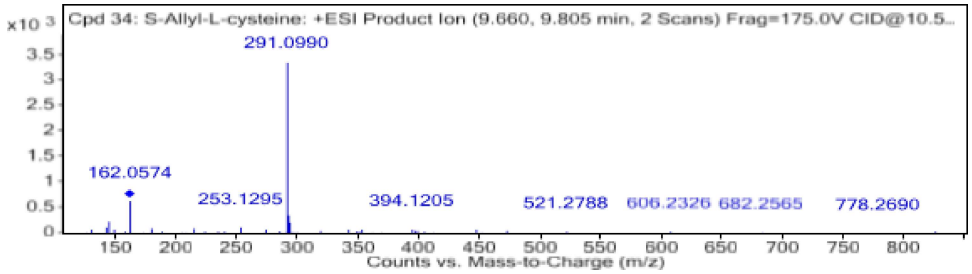
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.0313			1	156746.67		
162.058	162.0583	1.89	1	280173.31	C6 H11 N O2 S	(M+H)+
163.0611	163.061	-0.05	1	22810.6	C6 H11 N O2 S	(M+H)+
164.0546	164.0553	4.53	1	13317.54	C6 H11 N O2 S	(M+H)+
274.0741			1	72451.94		
291.1009			1	3340529		
292.1038			1	420003.25		
293.0996			1	154418.16		
313.0824			1	32242.06		
581.1934			1	29099.33		

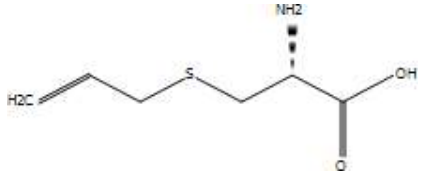
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
142.329		127.64
145.0298		245.21
162.0574		637.01
180.0739		94.28
215.0959		101.07
253.1295		114.96
291.099	1	3354.67
292.102	1	361.29
293.097	1	212.06
394.1205	1	87.08

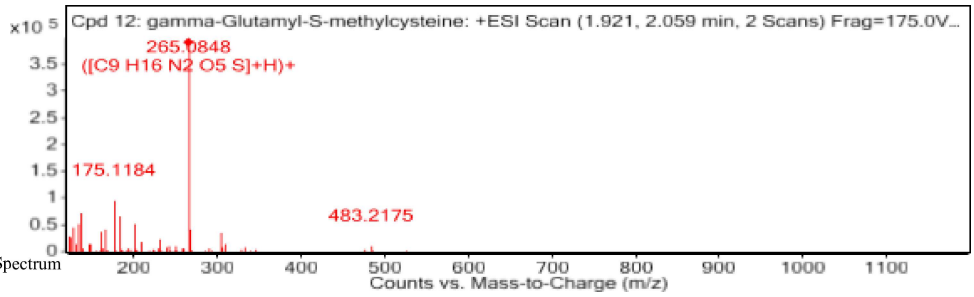
Compound Structure



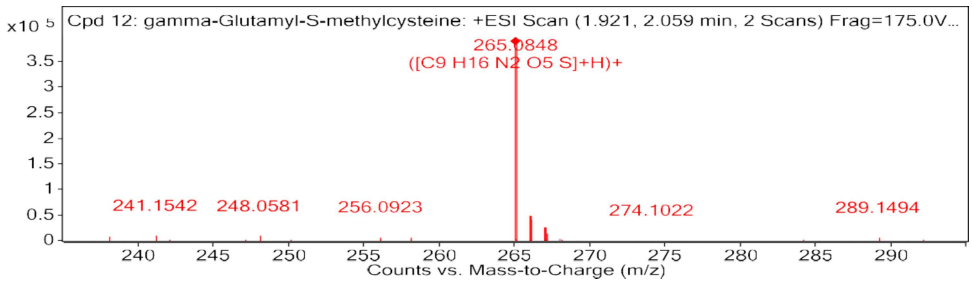
A7 gamma-Glutamyl-S-methylcysteine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 12: gamma-Glutamyl-S-methylcysteine	**gamma-Glutamyl-S-methylcysteine**	265.0848	2.009	Auto MS/MS	264.0775

MS Spectrum



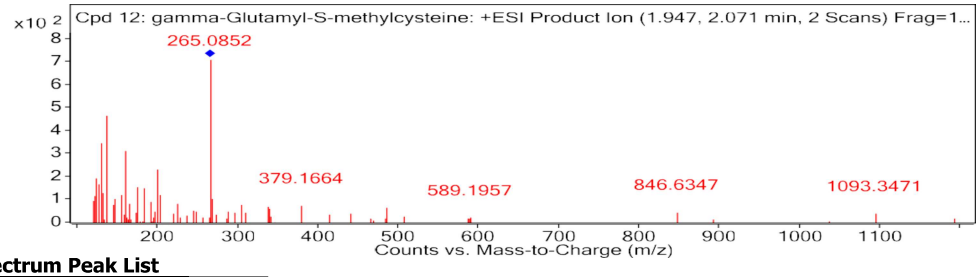
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
126.0659			1	47225.07		
132.1013			1	52733.97		
136.0753			1	73506.09		
175.1184			1	96916.63		
182.0441			1	49319.32		
182.0809			1	67134.96		
200.1023			1	53082.61		
265.0848	265.0853	1.94	1	399374.69	C9 H16 N2 O5 S	(M+H)+
266.0878	266.088	0.82	1	43000.82	C9 H16 N2 O5 S	(M+H)+
267.083	267.0835	1.65	1	16635.85	C9 H16 N2 O5 S	(M+H)+

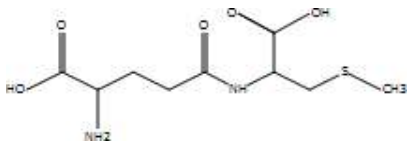
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
123.046		196.13
126.0661		169.12
130.0491		347.58
136.0428		180.29
136.0758	1	467.61
160.107	1	313.56
175.1179		159.08
200.1013		235.14
265.0852	1	711.53
266.0873	1	171.85

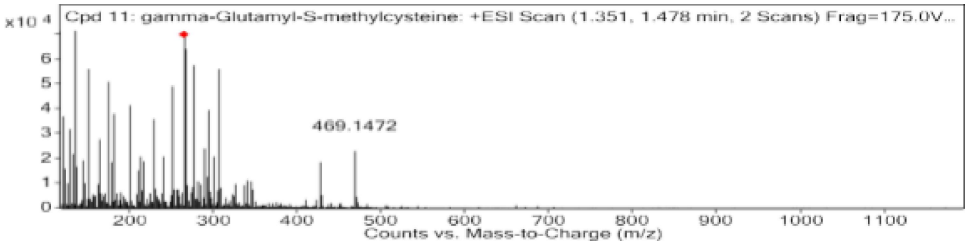
Compound Structure



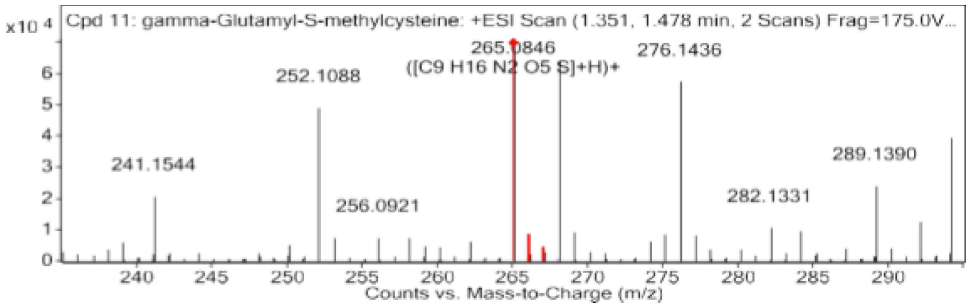
A7 gamma-Glutamyl-S-methylcysteine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 11: gamma-Glutamyl-S-methylcysteine	**gamma-Glutamyl-S-methylcysteine**	265.0846	1.433	Auto MS/MS	264.0774

MS Spectrum



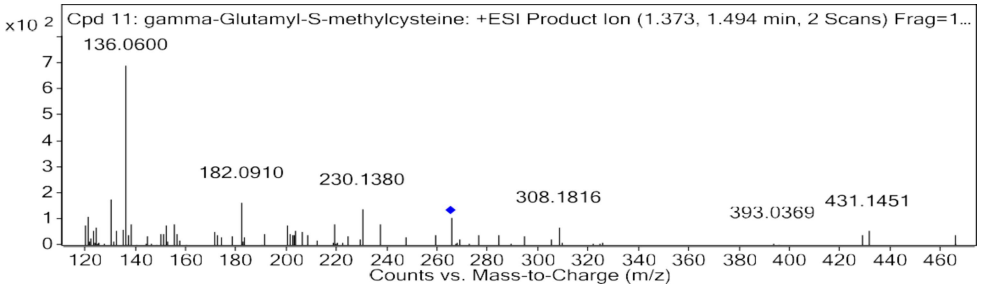
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
136.0613			1	107531.75		
152.056			1	56345.43		
175.1184				50932.82		
252.1088			1	49306.09		
265.0846	265.0853	2.64	1	71269.05	C9 H16 N2 O5 S	(M+H)+
266.0878	266.088	0.9	1	8865.53	C9 H16 N2 O5 S	(M+H)+
267.0844	267.0835	-3.43	1	3333.23	C9 H16 N2 O5 S	(M+H)+
268.1036			1	64451.67		
276.1436			1	57608.63		
307.0951			1	56077.53		

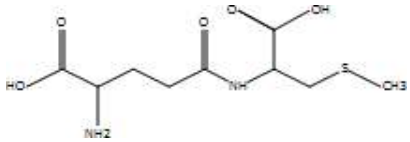
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
121		
.0109		10.73
130.0488	1	178.3
136.0414	1	101.11
136.06	1	693.5
138.1019		82.63
182.091	1	165.42
219.0569		83.01
230.138		139.05
237.106		82.28
265.0857		106.84

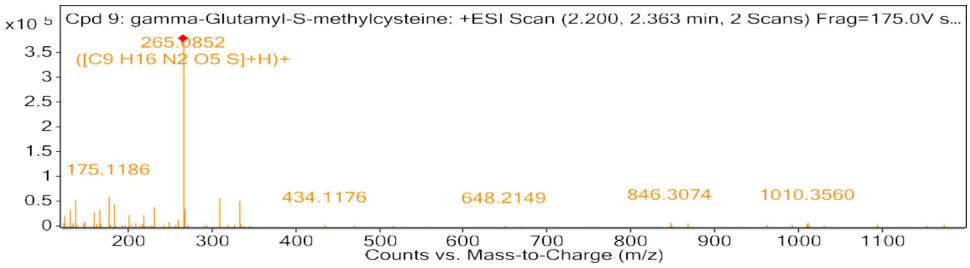
Compound Structure



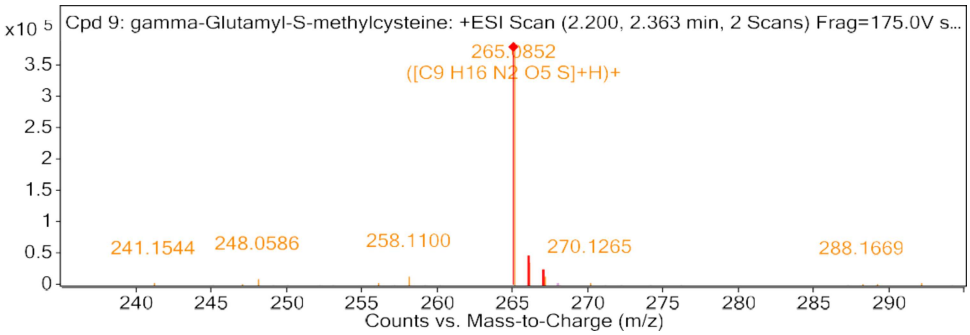
A7 gamma-Glutamyl-S-methylcysteine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 9: gamma-Glutamyl-S-methylcysteine	**gamma-Glutamyl-S-methylcysteine**	265.0852	2.302	Auto MS/MS	264.0779

MS Spectrum



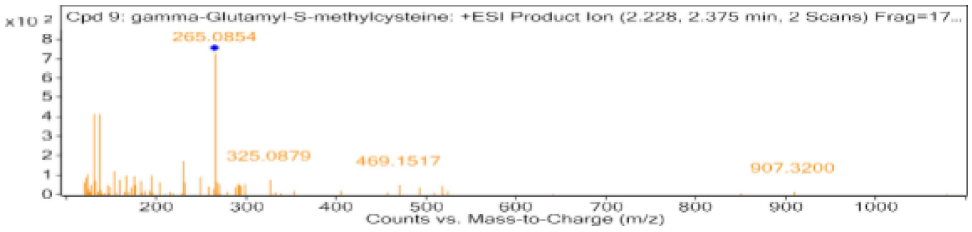
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
136.0426			1	54796.38		
136.0755			1	56957.34		
175.1186			1	61277.09		
182.0815			1	47530.69		
229.1547			1	41715.74		
265.0852	265.0853	0.33	1	388969.44	C9 H16 N2 O5 S	(M+H)+
266.0881	266.088	-0.19	1	38627.6	C9 H16 N2 O5 S	(M+H)+
267.0831	267.0835	1.32	1	16728.5	C9 H16 N2 O5 S	(M+H)+
307.0955			1	60721.82		
332.1336			1	54968.83		

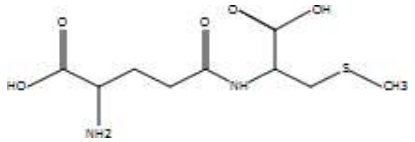
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
123.042		112.21
130.0498		419.65
136.0429	1	418.54
136.0754		212.03
152.0704		128.68
166.0535		105.23
175.1177		101.5
194.1182	1	103.99
229.1549	1	177.86
265.0854	2	729.82

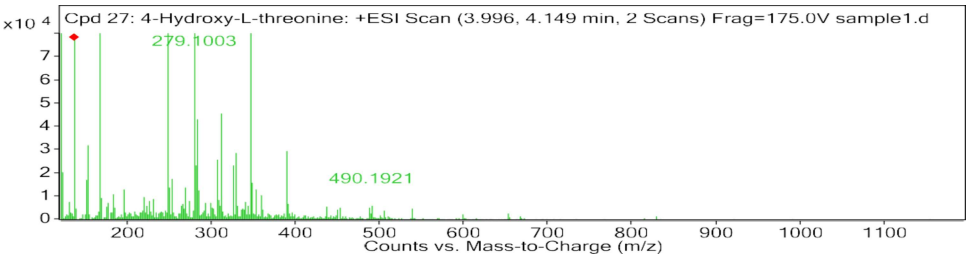
Compound Structure



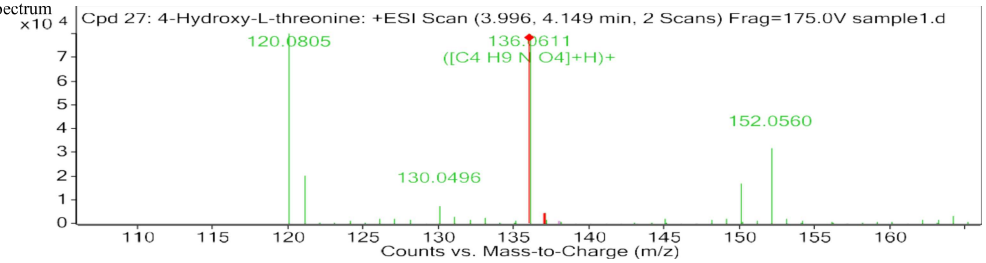
A8 4-Hydroxy-L-threonine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 27: 4-Hydroxy-L-threonine	**4-Hydroxy-L-threonine**	136.0611	4.086	Auto MS/MS	135.0538

MS Spectrum



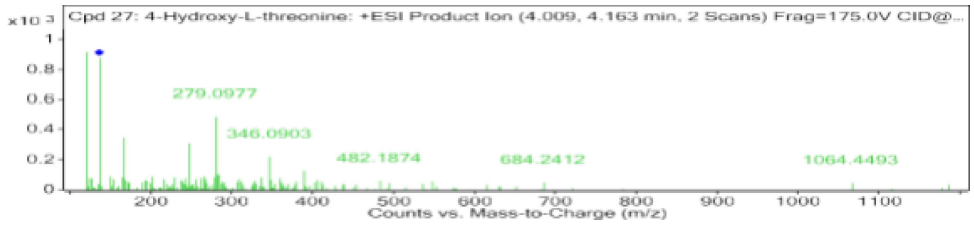
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
120.0805			1	215199.78		
136.0611	136.0604	-4.88	1	80087.27	C4 H9 N O4	(M+H)+
137.0642	137.0634	-5.38	1	4892.94	C4 H9 N O4	(M+H)+
152.056				32028.54		
166.0854			1	87830.53		
247.1283			1	119566.7		
279.1003			1	187339.91		
282.1184				43226.36		
310.1274			1	45967.52		
346.0901			1	113954.11		

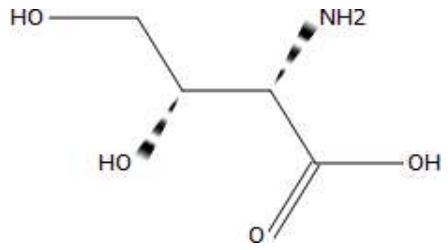
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0803		920.13
136.0601	1	878.89
137.1051		115
166.0858		354.7
247.1265		312.53
279.0977	1	492.33
280.1024	1	129.21
281.0944	1	108.99
346.0903	1	224.54
388.1853		132.9

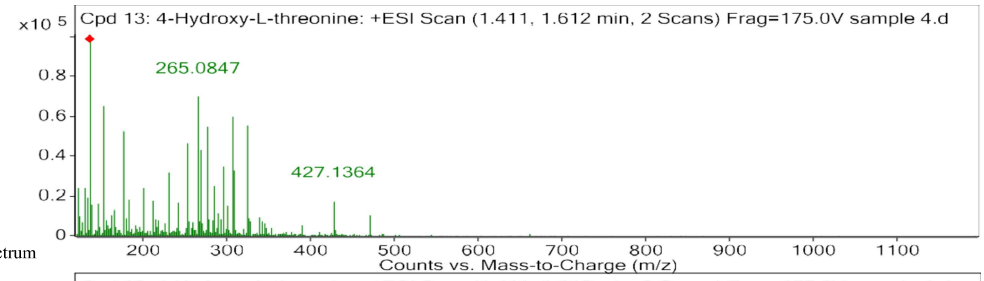
Compound Structure



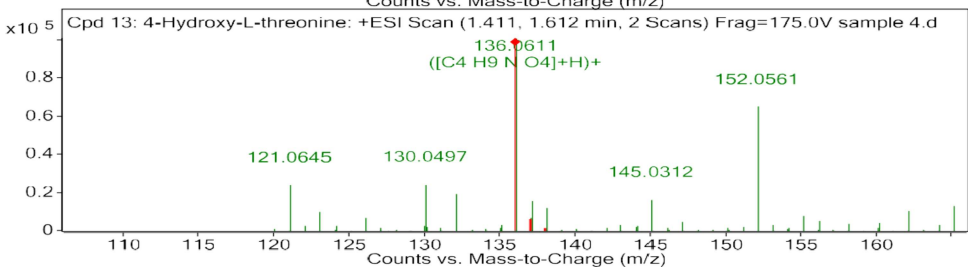
A8 4-Hydroxy-L-threonine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 13: 4-Hydroxy-L-threonine	**4-Hydroxy-L-threonine**	136.0611	1.528	Auto MS/MS	135.0525

MS Spectrum



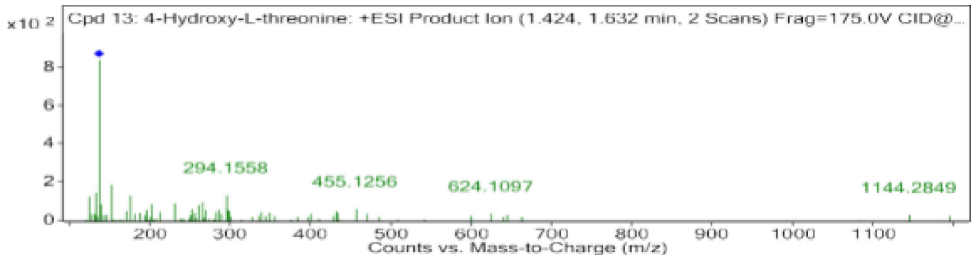
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
136.0611	136.0604	-4.56	1	100959.35	C4 H9 N O4	(M+H)+
137.0638	137.0634	-3.14	1	7247.97	C4 H9 N O4	(M+H)+
138.0542	138.0649	77.01	1	12412.25	C4 H9 N O4	(M+H)+
139.0549	139.0677	91.89	1	1112.59	C4 H9 N O4	(M+H)+
152.0561			1	65317.65		
175.1185			1	53039.3		
265.0847			1	70153.77		
276.1433			1	55147.97		
306.0996				60552.44		
324.1104			1	55555.56		

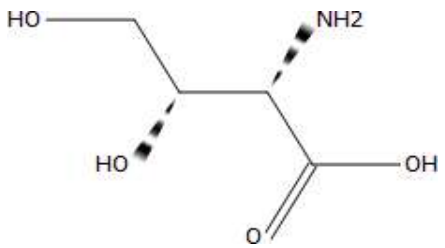
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
123.0428		132.13
132.1029		149.19
136.0622	1	840.75
138.0541	1	92.6
152.0546		190.37
175.119		136.28
202.1245		92.41
229.1533		93.15
265.0798	2	101.54
294.1558		137.94

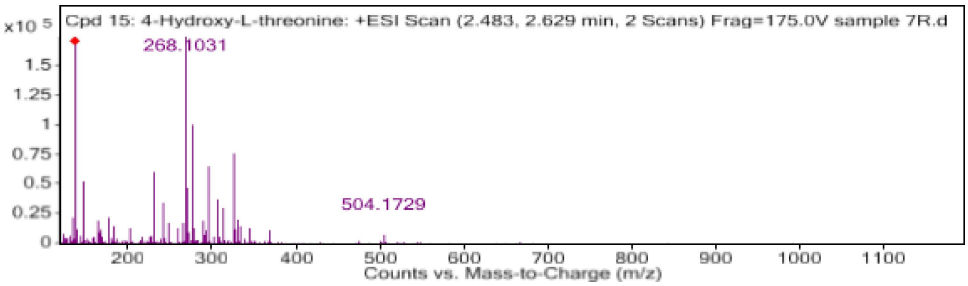
Compound Structure



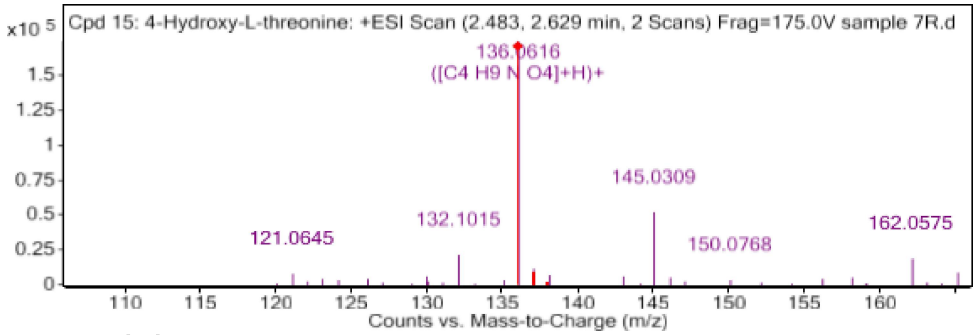
A8 4-Hydroxy-L-threonine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 15: 4-Hydroxy-L-threonine	**4-Hydroxy-L-threonine**	136.0616	2.57	Auto MS/MS	135.0538

MS Spectrum



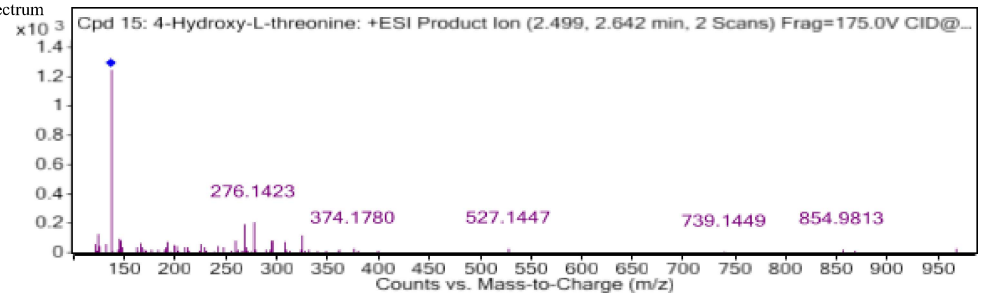
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
136.0616	136.0604	-8.36	1	174771.44	C4 H9 N O4	(M+H)+
137.0645	137.0634	-8.07	1	12551.13	C4 H9 N O4	(M+H)+
138.0543	138.0649	76.59	1	8025.36	C4 H9 N O4	(M+H)+
145.0309			1	53200.14		
229.1538			1	61142.94		
268.1031			1	370491.56		
269.106			1	47867.78		
276.143			1	100570.56		
294.1535			1	65569.69		
324.1099			1	76907.12		

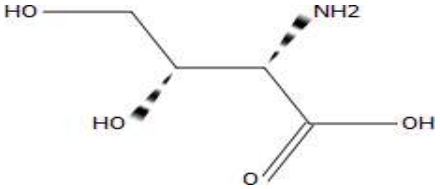
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
123.0553		133.13
136.0624	1	1252.1
137.0633	1	242.18
145.0298		105.76
258.1293		90.13
268.1026	1	204.79
276.1423	1	216.34
294.1513		89.25
295.155		90.28
324.1076		123.59

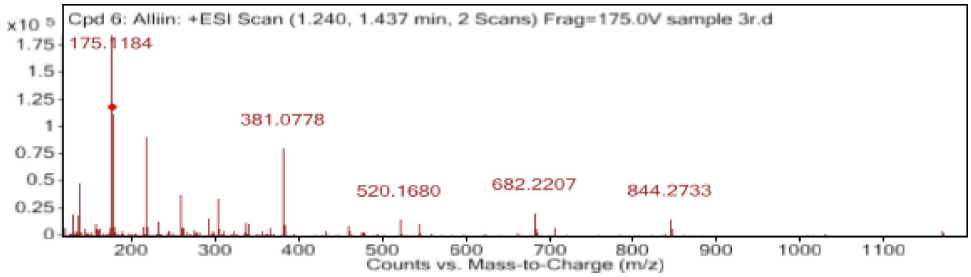
Compound Structure



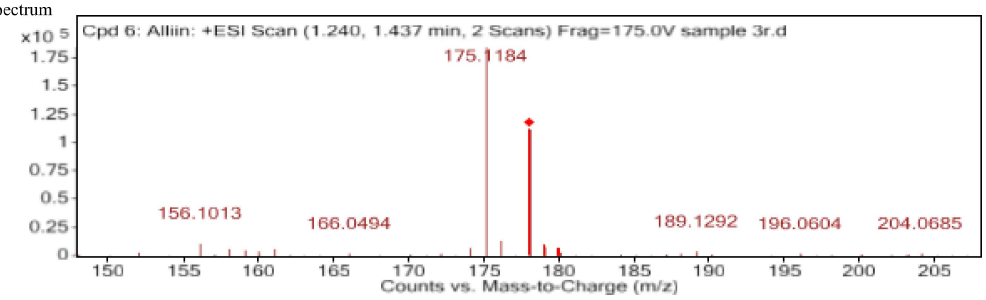
A9 Alliin (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 6: Alliin	**Alliin**	178.0527	1.362	Auto MS/MS	177.0455

MS Spectrum



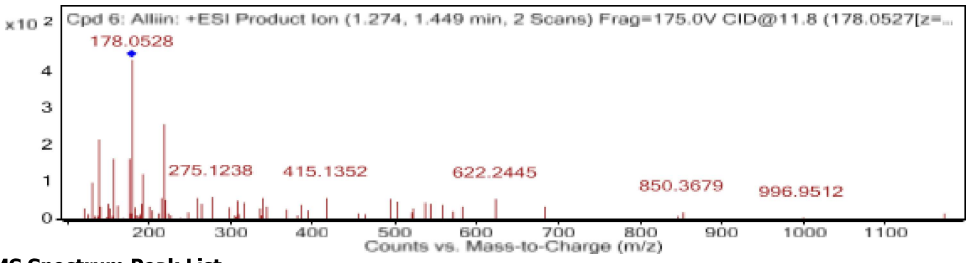
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
138.0541			1	48369.36		
175.1184			1	184746.16		
178.0527	178.0532	3.05	1	112149.73	C6 H11 N O3 S	(M+H)+
179.056	179.056	-0.37	1	8962.22	C6 H11 N O3 S	(M+H)+
180.0507	180.0505	-1.08	1	4054.74	C6 H11 N O3 S	(M+H)+
217.1291			1	91596.49		
258.1096			1	37657.23		
303.1654			1	33961.63		
381.0778			1	80892.51		
682.2207			1	21137.48		

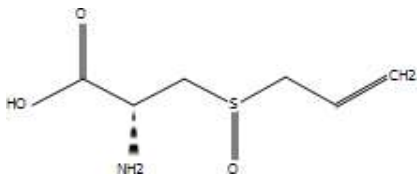
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0978		102.34
137.0129		217.72
138.055		96.78
156.0988		164.82
175.1178		166.85
178.0528		434.02
191.0897		125.67
217.1255	1	259.14
218.1	1	63.86
275.1238		61.8

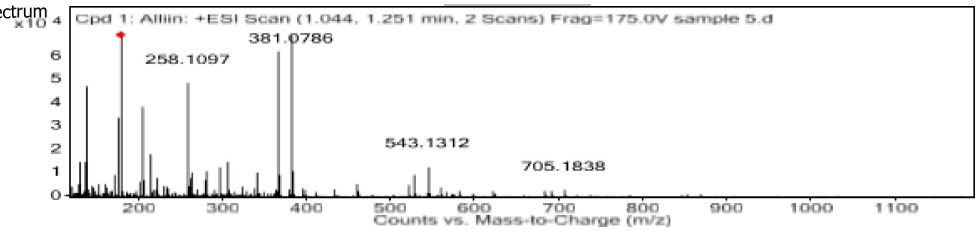
Compound Structure



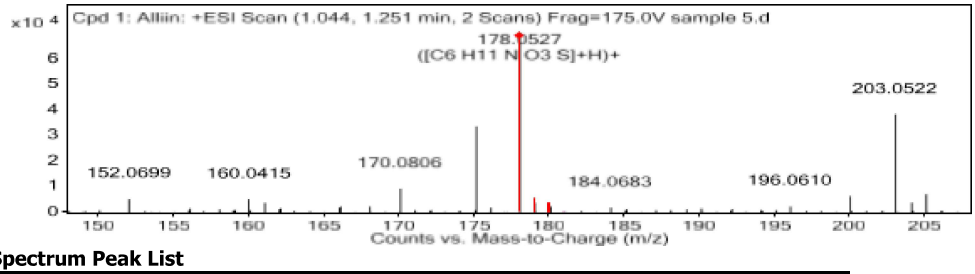
A9 Alliin (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 1: Alliin	**Alliin**	178.0527	1.164	Auto MS/MS	177.0455

MS Spectrum



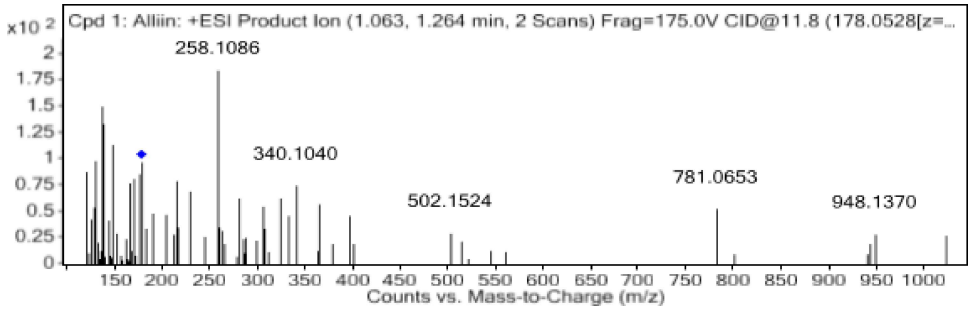
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
138.0542			1	47078.55		
175.1185			1	33854.94		
178.0527	178.0532	2.81	1	70488.39	C6 H11 N O3 S	(M+H)+
179.0556	179.056	1.95	1	3842.88	C6 H11 N O3 S	(M+H)+
180.0501	180.0505	2.01	1	2696.58	C6 H11 N O3 S	(M+H)+
203.0522			1	38534.14		
214.0705				18311.7		
258.1097			1	48701.36		
365.1046			1	62128.83		
381.0786			1	68902.71		

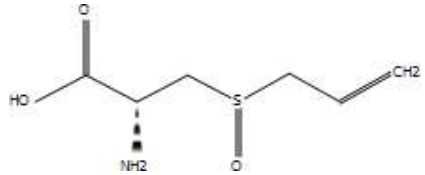
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0095		88.7
130.0497		98.54
136.0592		84.14
137.0152		149.67
138.0557	1	133.53
147.0759		114.11
170.0808		82.2
175.1219		86.19
178.0521		97.25
258.1086		184.91

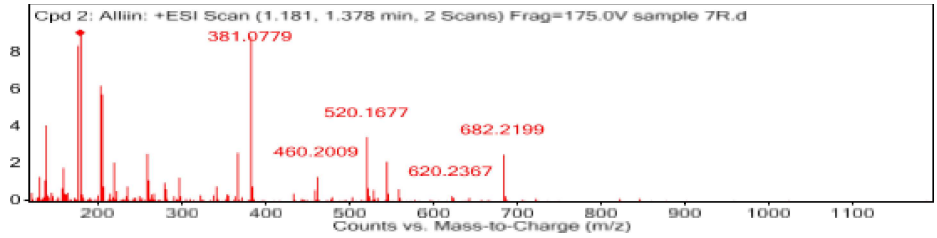
Compound Structure



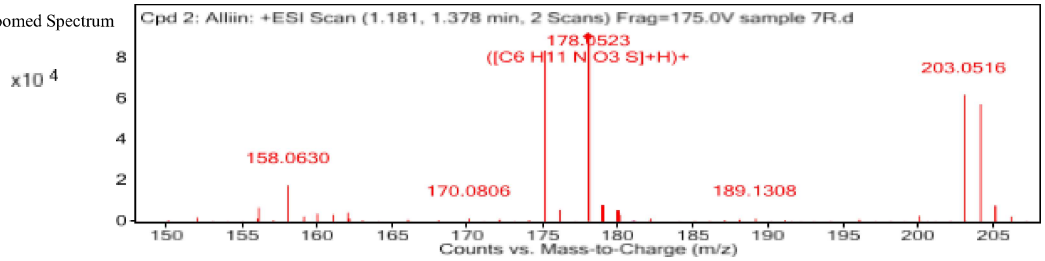
A9 Alliin (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 2: Alliin	**Alliin**	178.0523	1.308	Auto MS/MS	177.045

MS Spectrum



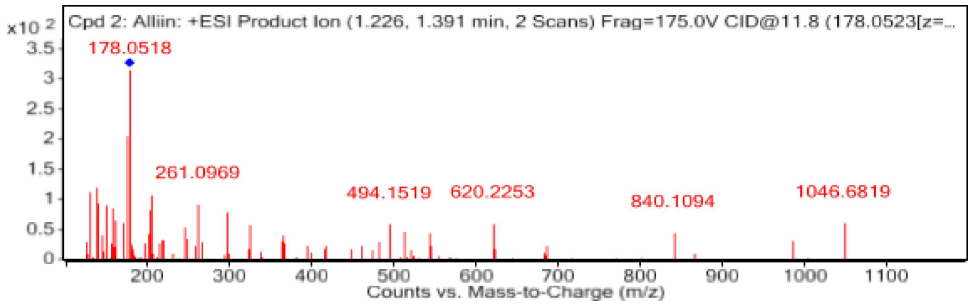
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
138.0542			1	40790.31		
175.1181			1	83683.05		
178.0523	178.0532	5.47	1	92496.82	C6 H11 N O3 S	(M+H)+
179.0558	179.056	0.74	1	7546.8	C6 H11 N O3 S	(M+H)+
180.0494	180.0505	5.96	1	3678.84	C6 H11 N O3 S	(M+H)+
203.0516				62409.69		
204.0681			1	57782.96		
365.1039			1	26335.82		
381.0779			1	88475.3		
520.1677			1	34663.2		

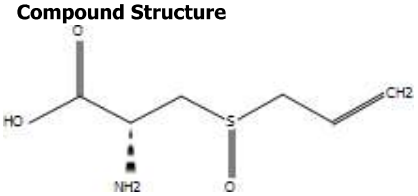
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0868		113.44
138.054		120.45
140.0704		94.22
149.0797		90.13
157.0143		86.55
175.1171		206
178.0518	2	315.9
203.0505		82.78
204.0656	1	107.89
261.0969		93.26

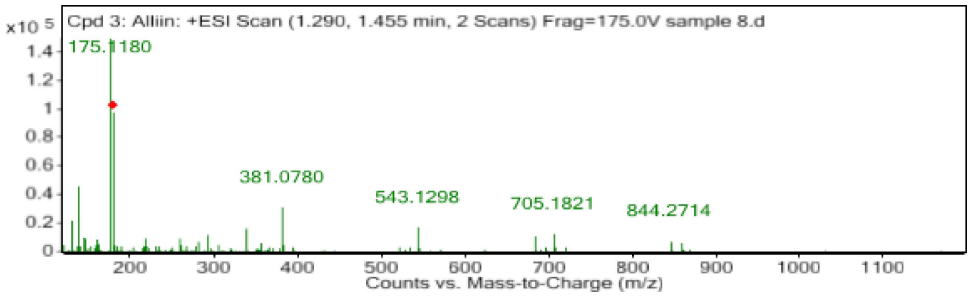
Compound Structure



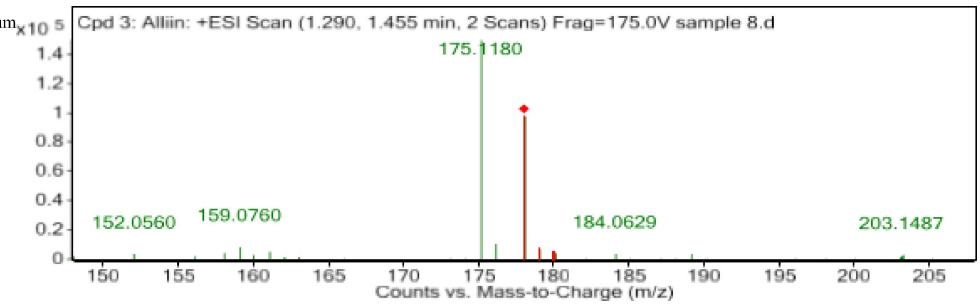
A9 Alliin (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 3: Alliin	**Alliin**	178.0522	1.397	Auto MS/MS	177.045

MS Spectrum



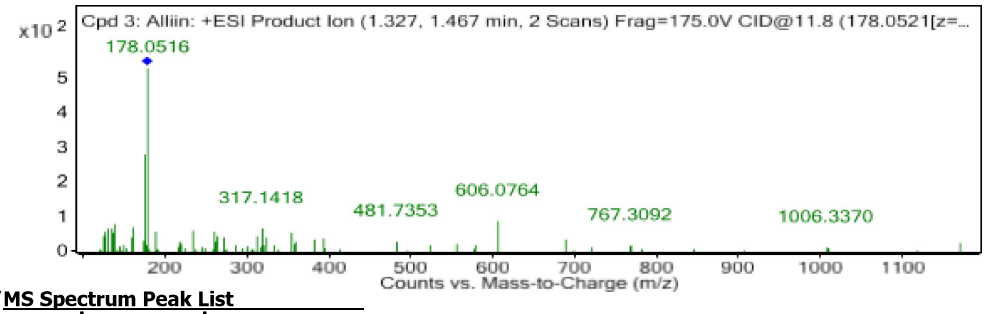
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
130.0858				22073.83		
138.0542			1	46570.95		
175.118			1	149861.72		
178.0522	178.0532	5.68	1	97806.94	C6 H11 N O3 S	(M+H)+
179.0557	179.056	1.27	1	7561.13	C6 H11 N O3 S	(M+H)+
180.0491	180.0505	7.69	1	5485.65	C6 H11 N O3 S	(M+H)+
337.1701			1	17182.36		
381.078			1	31510.08		
543.1298			1	17428.95		
705.1821			1	12909.02		

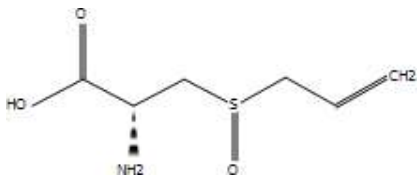
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	Abund
130.0851	68.57
135.0447	68.64
138.053	82.06
161.0242	71.87
175.1179	282.67
175.1438	61.6
178.0516	531.24
233.1086	63.07
317.1418	70.01
606.0764	91.8

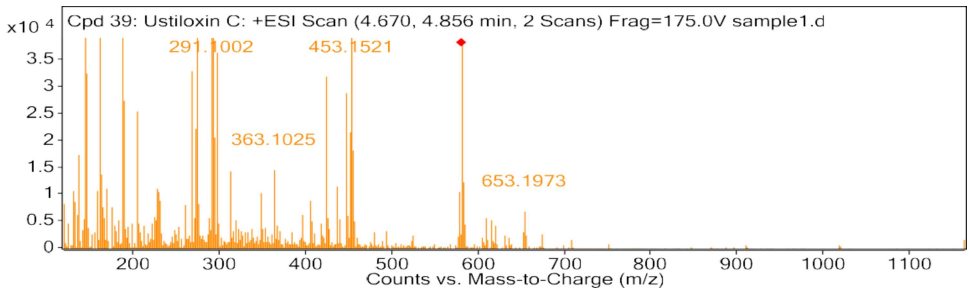
Compound Structure



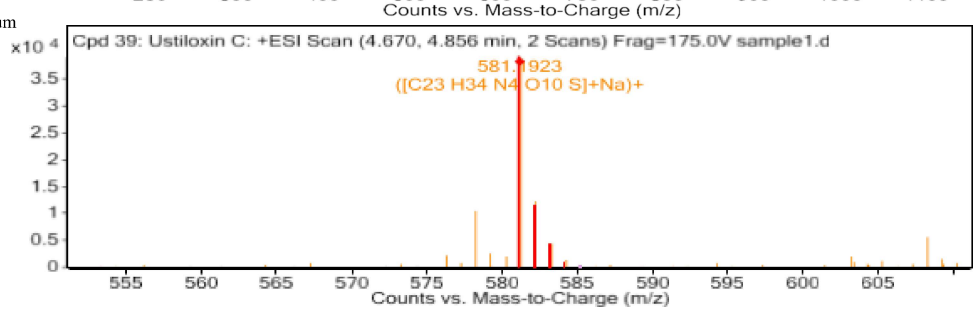
A10 Ustiloxin C (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 39: Ustiloxin C	**Ustiloxin C**	581.1923	4.797	Auto MS/MS	558.2027

MS Spectrum



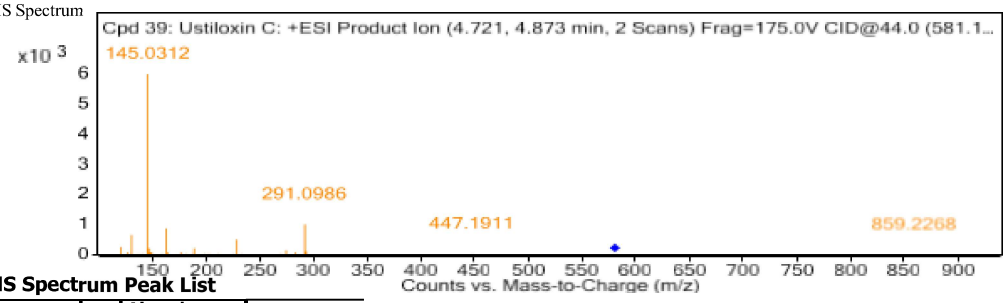
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.031			1	90169.55		
162.0576			1	205944.42		
188.07			1	221843.31		
291.1002			1	3544463.25		
292.1031			1	452477.53		
293.0989			1	163448.81		
581.1923	581.1888	-6	1	39077.64	C23 H34 N4 O10 S	(M+Na)+
582.1947	582.1917	-5.04	1	12427.27	C23 H34 N4 O10 S	(M+Na)+
583.1914	583.19	-2.42	1	4665.11	C23 H34 N4 O10 S	(M+Na)+
584.1922	584.1914	-1.32	1	1512.91	C23 H34 N4 O10 S	(M+Na)+

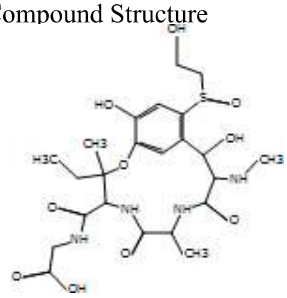
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0098		204.36
120.0784		280.78
130.0501		696.83
145.0312	1	6020.22
146.0309	1	254.04
162.0577	1	895.27
188.0686		245.11
228.0663		546.71
274.0728	1	187.27
291.0986	1	1055

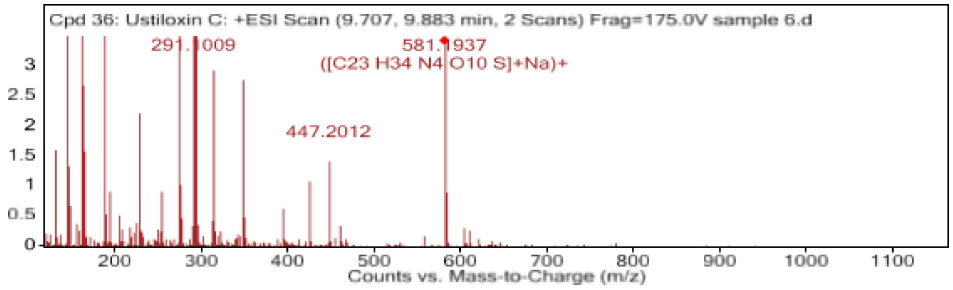
Compound Structure



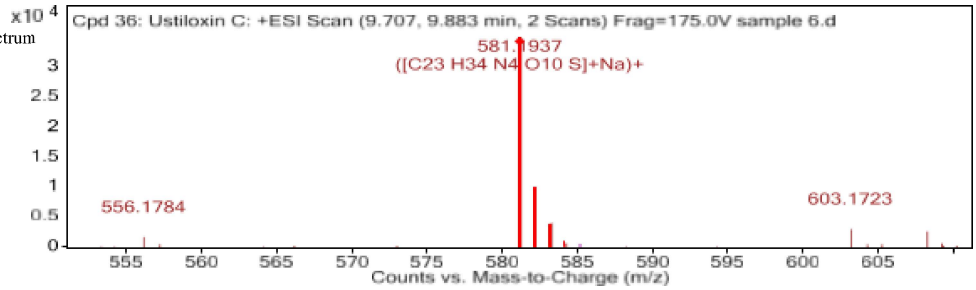
A10 Ustiloxin C (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 36: Ustiloxin C	**Ustiloxin C**	581.1937	9.81	Auto MS/MS	558.2042

MS Spectrum



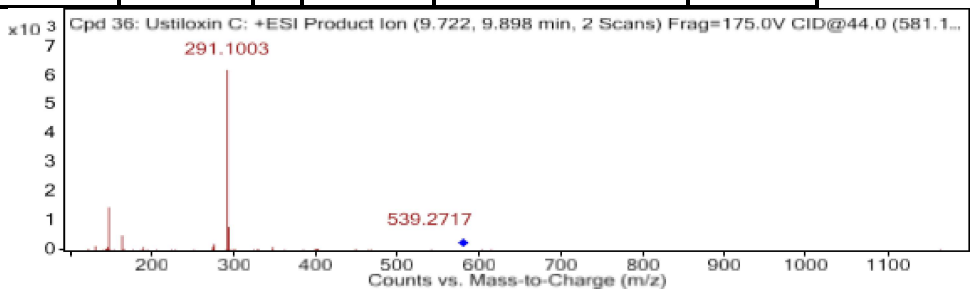
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.0313			1	194647.34		
162.058			1	348886.5		
274.0741			1	80796.06		
291.1009			1	4079262.5		
292.104			1	483934.03		
293.0995			1	191998.47		
581.1937	581.1888	-8.46	1	34871.62	C23 H34 N4 O10 S	(M+Na)+
582.1962	582.1917	-7.6	1	8942.41	C23 H34 N4 O10 S	(M+Na)+
583.193	583.19	-5.15	1	4162.5	C23 H34 N4 O10 S	(M+Na)+
584.1953	584.1914	-6.51	1	774.08	C23 H34 N4 O10 S	(M+Na)+

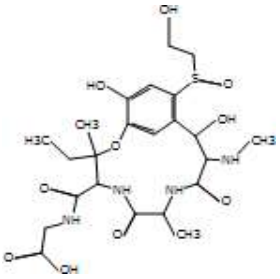
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0483		149.97
145.0316	1	1499.88
146.0333	1	108.24
162.0581	1	516.95
188.0686		114.11
273.0885		108.5
274.0731		222.89
291.1003	1	6211.34
292.1036	1	814.4
293.1003	1	513.44

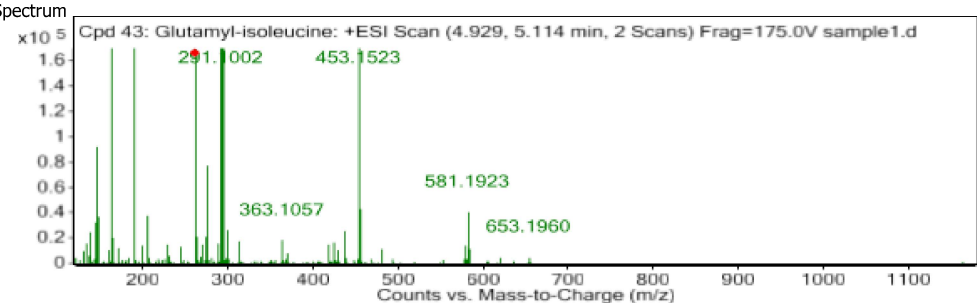
Compound Structure



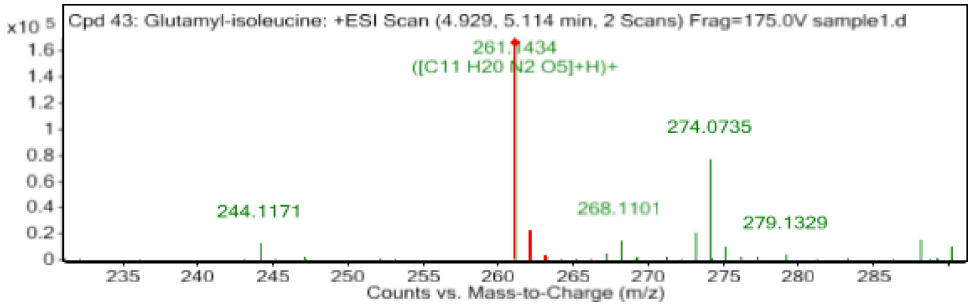
A11 Glutamyl-isoleucine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 43: Glutamyl-isoleucine	**Glutamyl-isoleucine**	261.1434	5.035	Auto MS/MS	260.1361

MS Spectrum



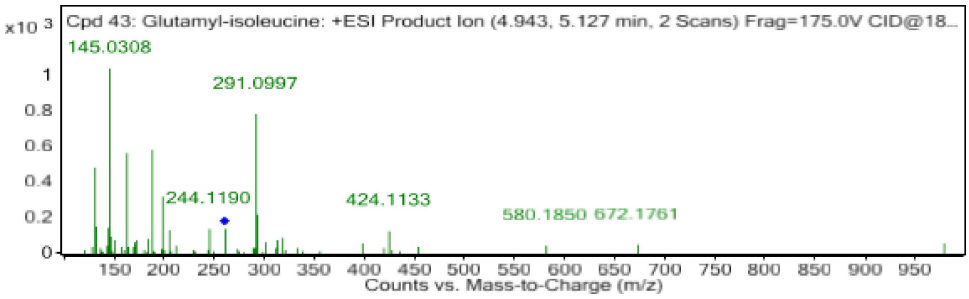
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.031			1	93003.86		
162.0577			1	278908.66		
188.0699			1	299744.59		
261.1434	261.1445	4.2	1	169964.28	C11 H20 N2 O5	(M+H)+
262.1467	262.1476	3.2	1	21515.25	C11 H20 N2 O5	(M+H)+
263.1472	263.1496	8.99	1	3457.29	C11 H20 N2 O5	(M+H)+
291.1002			1	3898072		
292.1032			1	489209.66		
293.099			1	184282.7		
453.1523			1	220005.77		

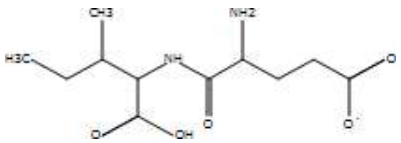
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0493		485.41
132.101		153.17
144.0776	2	148.25
145.0308		1042.65
162.0576		568.14
188.0704		586.29
198.1118	1	325.44
244.119	1	143.72
291.0997	1	788.01
292.1021	1	221.98

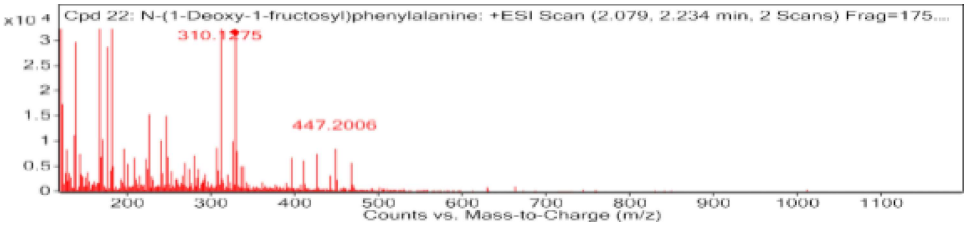
Compound Structure



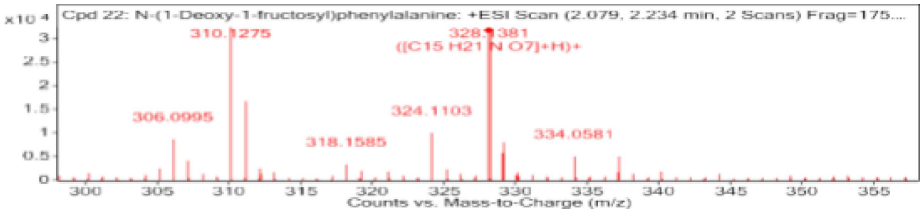
A12 N-(1-Deoxy-1-fructosyl)phenylalanine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 22: N-(1-Deoxy-1-fructosyl)phenylalanine	**N-(1-Deoxy-1-fructosyl)phenylalanin**	328.1381	2.181	Auto MS/MS	327.1307

MS Spectrum



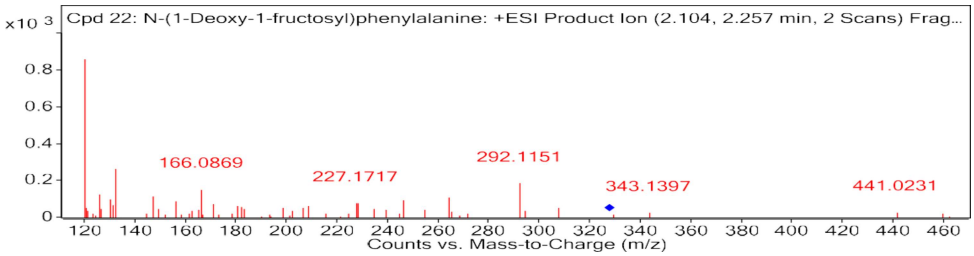
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
120.0804			1	173667.28		
121.0837			1	17525.91		
137.1065			1	29835.18		
166.0857			1	68360.03		
175.1183			1	28716.26		
181.0965			1	33424.63		
310.1275			1	37916.63		
328.1381	328.1391	2.9	1	32257.41	C15 H21 N O7	(M+H)+
329.1406	329.1424	5.36	1	6676.11	C15 H21 N O7	(M+H)+
330.1434	330.1444	3.18	1	915.19	C15 H21 N O7	(M+H)+

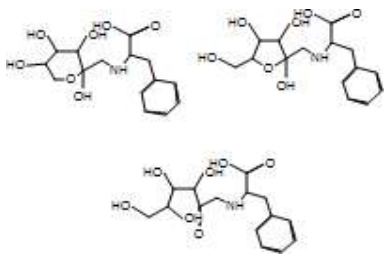
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0807	1	863.7
126.0534		126.56
130.0675		104.4
132.0801		266.8
147.0424		120.41
156.08		92.93
166.0869		156.88
246.1115		95.57
264.1257		113.56
292.1151		189.03

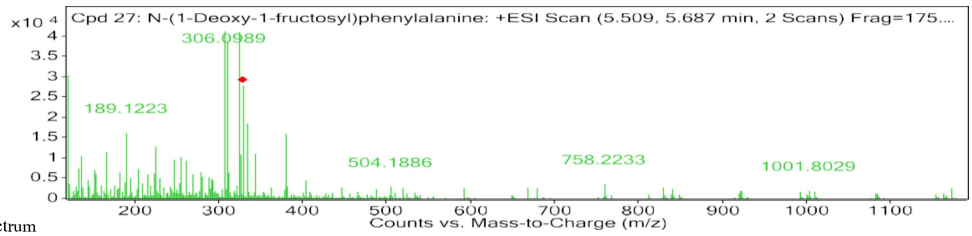
Compound Structure



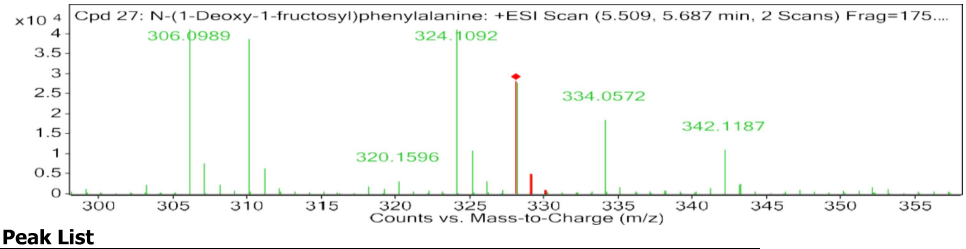
A12 N-(1-Deoxy-1-fructosyl)phenylalanine (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 27: N-(1-Deoxy-1-fructosyl)phenylalanine	**N-(1-Deoxy-1-fructosyl)phenylalanin**	328.1375	5.624	Auto MS/MS	327.1302

MS Spectrum



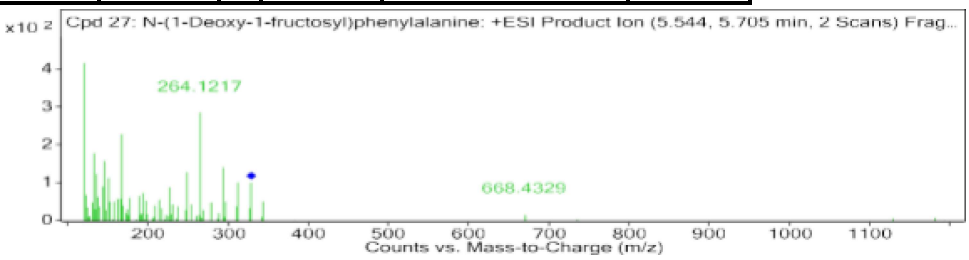
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
120.0806			1	30566.97		
189.1223				16444.9		
306.0989			1	44411.71		
310.1266			1	38852.2		
324.1092			1	41207.5		
328.1375	328.1391	4.91	1	28105.24	C15 H21 N O7	(M+H)+
329.1412	329.1424	3.57	1	5062.97	C15 H21 N O7	(M+H)+
330.1399	330.1444	13.77	1	801.11	C15 H21 N O7	(M+H)+
334.0572			1	18686.96		
379.2056			1	16209.46		

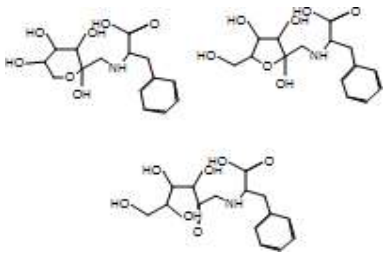
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0791		416.99
132.0799	1	178.63
134.0962		123.94
144.081		126.82
145.0327		158.79
150.1034		115.72
166.0858	1	228.79
247.0881		129.36
264.1217		285.78
292.1135		141.31

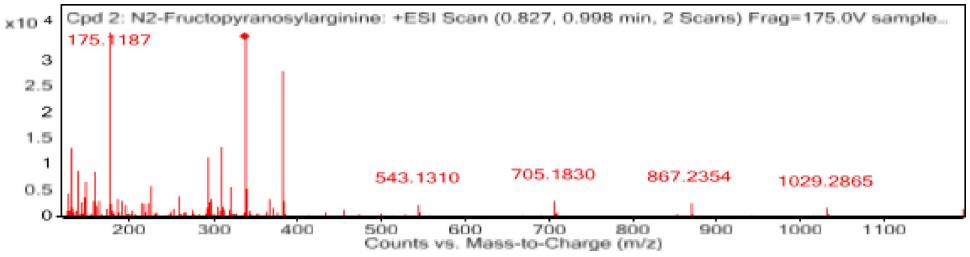
Compound Structure



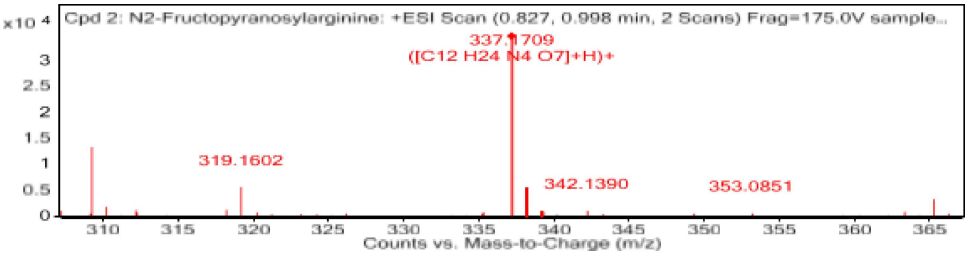
A13 N2-Fructopyranosylarginine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 2: N2-Fructopyranosylarginine	**N2-Fructopyranosylarginine**	337.1709	0.93	Auto MS/MS	336.1637

MS Spectrum



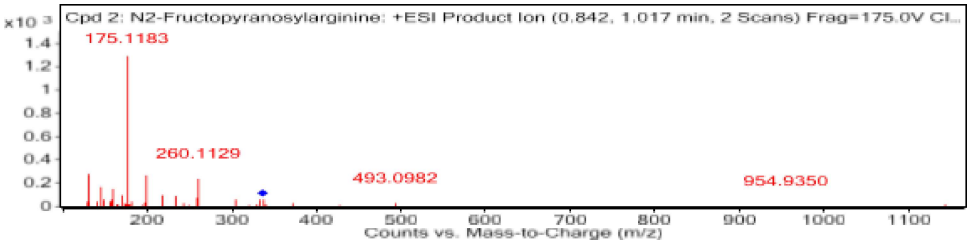
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
130.0867			1	13305.56		
137.1065			1	8914.91		
175.1187			1	335793.88		
176.1215			1	22865.08		
292.1974			1	11481.71		
309.1644			1	13444.44		
337.1709	337.1718	2.53	1	35440.18	C12 H24 N4 O7	(M+H)+
338.1743	338.1746	0.72	1	5455.07	C12 H24 N4 O7	(M+H)+
339.1763	339.1766	0.77	1	1071.11	C12 H24 N4 O7	(M+H)+
381.0783			1	28096.12		

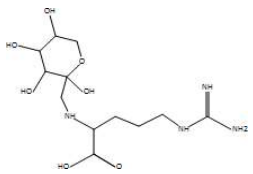
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0865		91.4
130.0984		287.12
145.0346		175.01
158.0916		163.85
169.1073		107.83
175.1183	1	1297.39
198.1135		277.35
217.1272		109.99
232.1166		98.02
260.1129		247.61

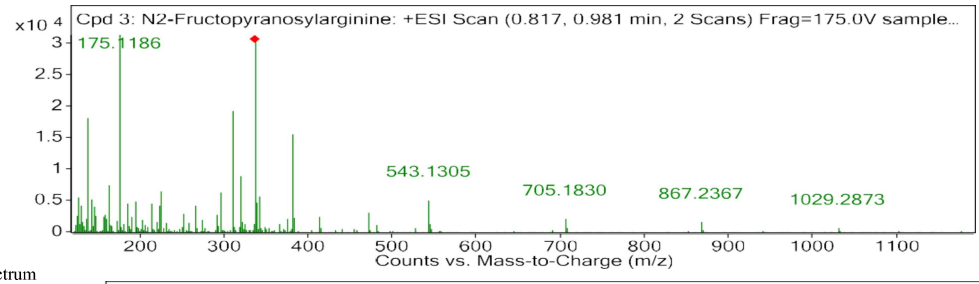
Compound Structure



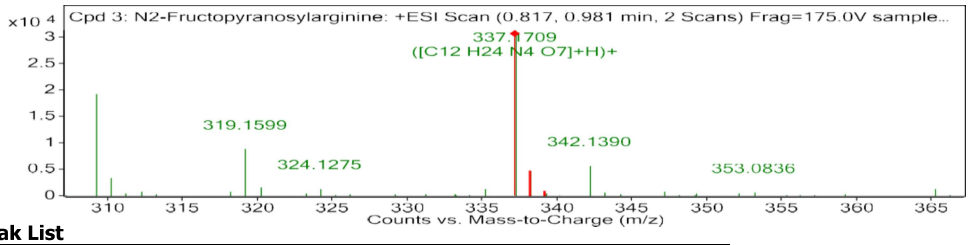
A13 N2-Fructopyranosylarginine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 3: N2-Fructopyranosylarginine	**N2-Fructopyranosylarginin**	337.1709	0.919	Auto MS/MS	336.1638

MS Spectrum



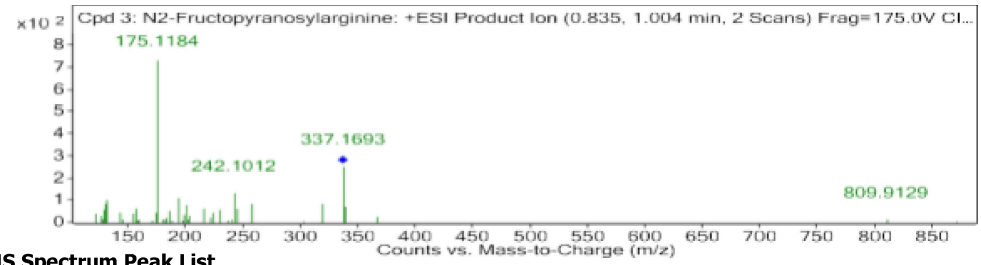
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
137.1068			1	18259.17		
162.0754				7619.16		
175.1186			1	118957.3		
176.1214			1	8965.21		
309.1649			1	19255.32		
319.1599			1	8967.17		
337.1709	337.1718	2.46	1	31214.16	C12 H24 N4 O7	(M+H)+
338.1743	338.1746	0.73	1	4873.57	C12 H24 N4 O7	(M+H)+
339.1765	339.1766	0.2	1	710.37	C12 H24 N4 O7	(M+H)+
381.0783			1	15542.62		

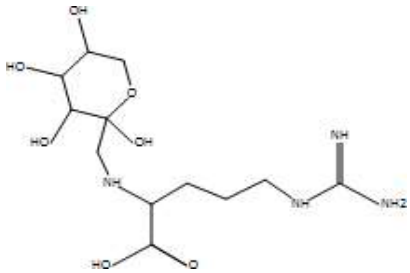
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	Abund
130.0972	90.1
131.0999	104.8
175.1184	735.93
194.0811	114.31
200.6369	85.09
242.1012	135.4
257.1602	86.65
319.1603	85.94
337.1693	256.47
338.2842	72.73

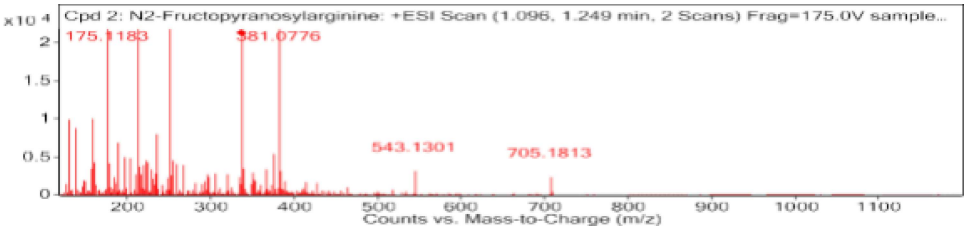
Compound Structure



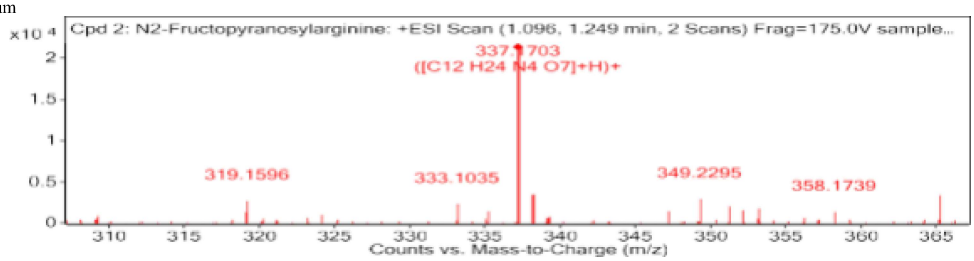
A13 N2-Fructopyranosylarginine (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 2: N2-Fructopyranosylarginine	**N2-Fructopyranosylarginin**	337.1703	1.19	Auto MS/MS	336.1631

MS Spectrum



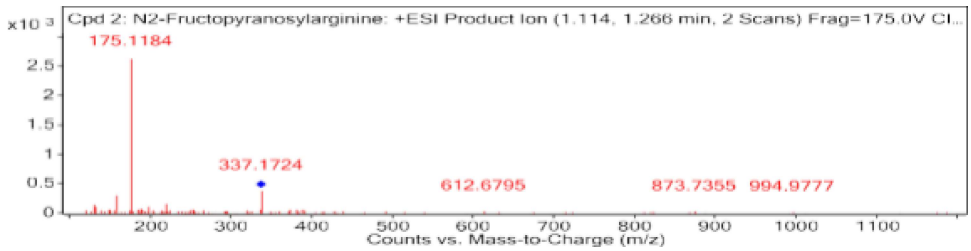
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
130.0955				9996.27		
158.0914				10070.77		
175.1183			1	347380.97		
176.1212			1	25260.14		
213.0737			1	27147		
251.0298			1	30610.21		
337.1703	337.1718	4.39	1	21812.52	C12 H24 N4 O7	(M+H)+
338.1736	338.1746	2.81	1	3556.83	C12 H24 N4 O7	(M+H)+
339.1744	339.1766	6.32	1	885.82	C12 H24 N4 O7	(M+H)+
381.0776			1	22561.54		

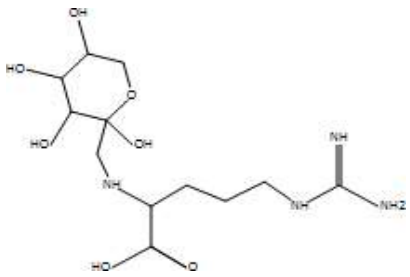
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0971		152.92
131.1284		120.85
158.0912		315.62
175.1184	1	2636.36
176.1236	1	161.5
187.1092		88.74
197.1001		88.25
198.116		129.68
219.0239		169.53
337.1724		395.35

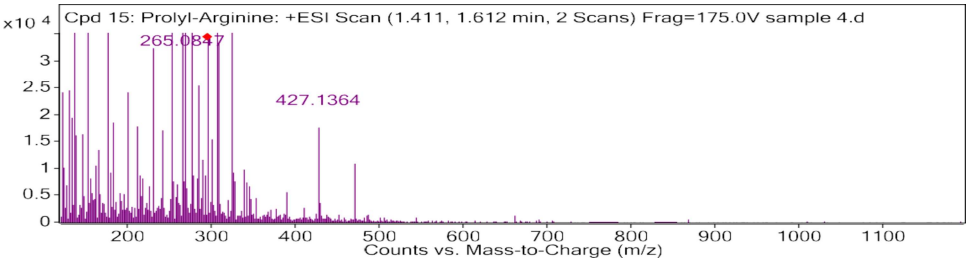
Compound Structure



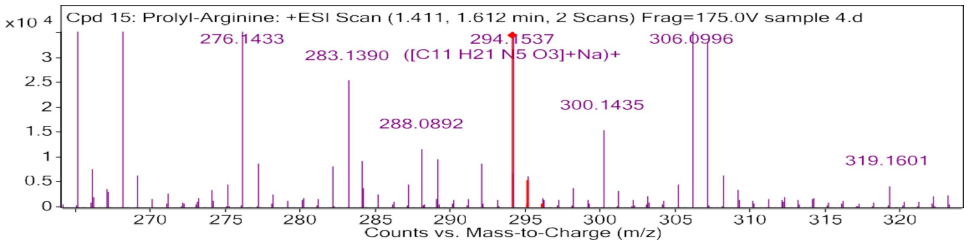
A14 Prolyl-Arginine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 15: Prolyl-Arginine	**Prolyl-Arginine**	294.1537	1.545	Auto MS/MS	271.1646

MS Spectrum



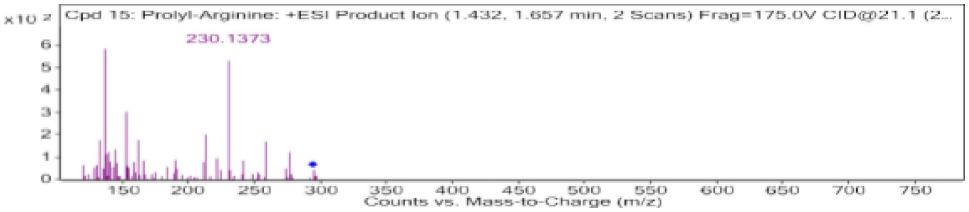
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
136.0611			1	100959.35		
152.0561			1	65317.65		
175.1185			1	53039.3		
265.0847			1	70153.77		
276.1433			1	55147.97		
294.1537	294.1537	-0.29	1	35176.39	C11 H21 N5 O3	(M+Na)+
295.1572	295.1563	-3.05	1	6282.32	C11 H21 N5 O3	(M+Na)+
296.1568	296.1584	5.43	1	1568.58	C11 H21 N5 O3	(M+Na)+
306.0996				60552.44		
324.1104			1	55555.56		

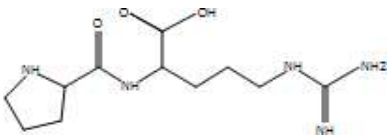
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
132		1
.1001 136	1	80.14 5
.0612		87.39
139.0859		127.77
144.1002		137.45
152.0563	1	306.93
161.0685	1	180.18
212.1279		203.27
230.1373	1	534.95
258.1335		173.76
276.1445		125.67

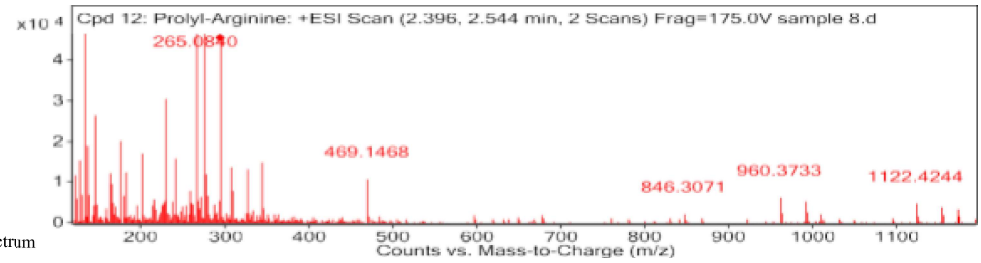
Compound Structure



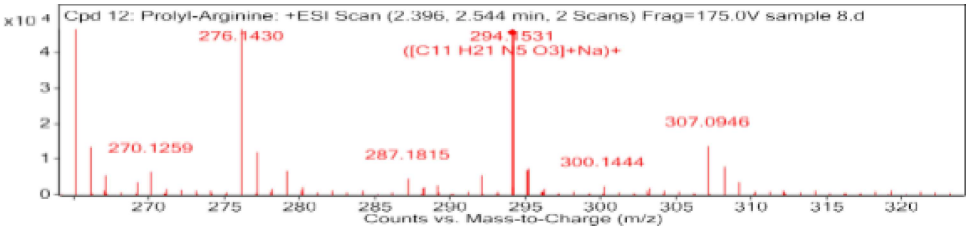
A14 Prolyl-Arginine (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 12: Prolyl-Arginine	**Prolyl-Arginine**	294.1531	2.49	Auto MS/MS	271.1641

MS Spectrum



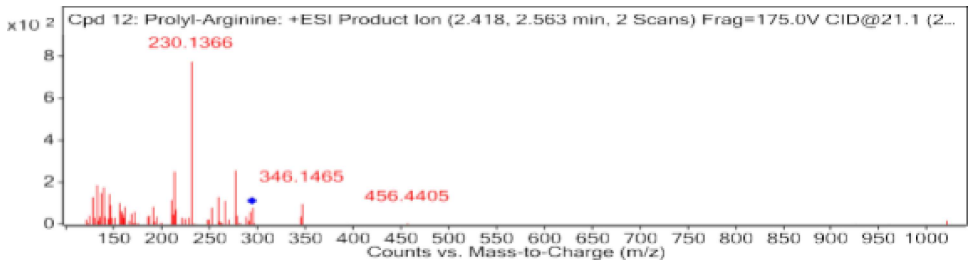
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
132.1016			1	47086.85		
136.0749				19177.95		
145.0311				26766.27		
175.1178				20466.67		
229.1539			1	30813.47		
265.084			1	128276.81		
276.143			1	76039.51		
294.1531	294.1537	1.89	1	46602.52	C11 H21 N5 O3	(M+Na)+
295.1574	295.1563	-4.04	1	7626.97	C11 H21 N5 O3	(M+Na)+
296.1581	296.1584	1.22	1	1876.8	C11 H21 N5 O3	(M+Na)+

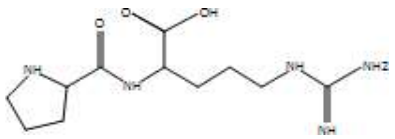
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
127.0381		133.52
132.1017		192.32
136.0758		152.26
138.0543		183.4
144.1018		148.22
210.1099		120.22
212.1277	1	254.92
230.1366		777.38
258.1321		133.03
276.1432		262.48

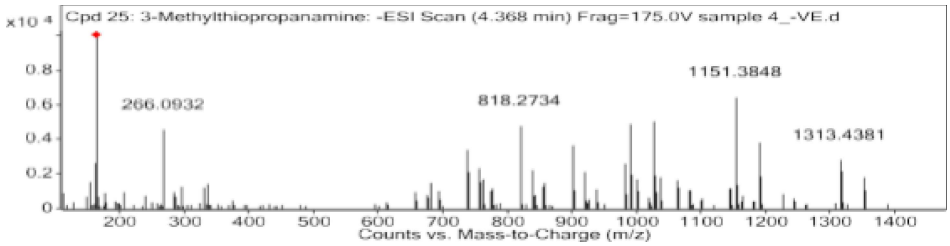
Compound Structure



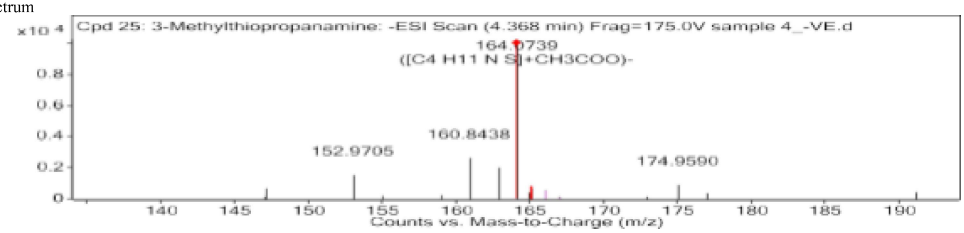
A15 3-Methylthiopropanamine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 25: 3-Methylthiopropanamine	**3-Methylthiopropanami**	164.0739	4.389	Auto MS/MS	105.06

MS Spectrum



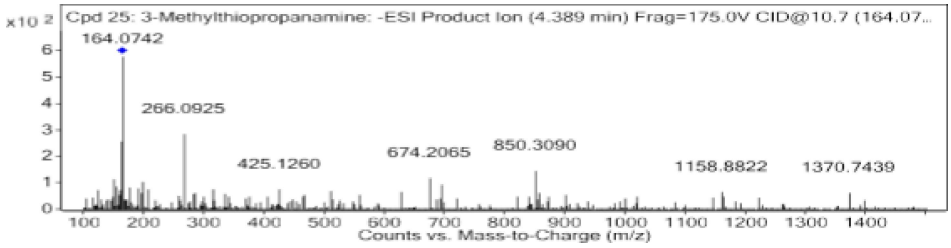
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
164.0739	164.0751	7.41	1	10267.79	C4 H11 N S	(M+CH3COO)-
165.0764	165.0778	8.57	1	759.23	C4 H11 N S	(M+CH3COO)-
266.0932				4584.08		
818.2734			2	4825.35		
818.7729			2	3954.61		
899.2991			2	3719.28		
989.3312			1	4899.81		
1025.3067			1	5091.43		
1151.3848			1	6481.79		
1187.3611			1	3881.65		

MSMS Spectrum



MS/MS Spectrum Peak List

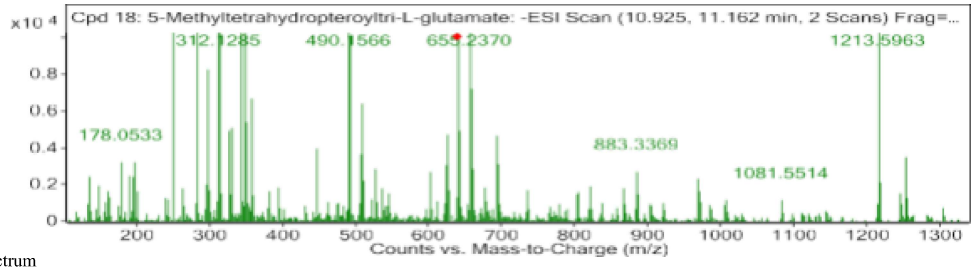
m/z	Abund
150.0426	116.26
152.9703	91
162.8416	261.33
164.0742	580.6
174.9579	86.16
197.8088	108.43
266.0925	287.23
674.2065	121.77
692.6907	95.88
850.309	149.14

Compound Structure

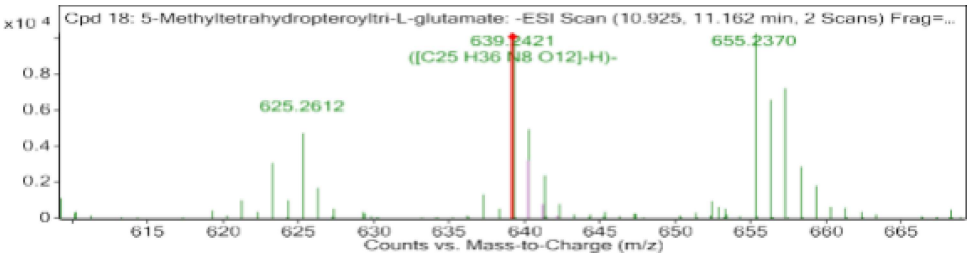
A16 5-Methyltetrahydropteroyltri-L-glutamate (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 18: 5-Methyltetrahydropteroyltri-L-glutamate	**5-Methyltetrahydropteroyltri-L-glutamate**	639.2421	11.075	Auto MS/MS	640.2494

MS Spectrum



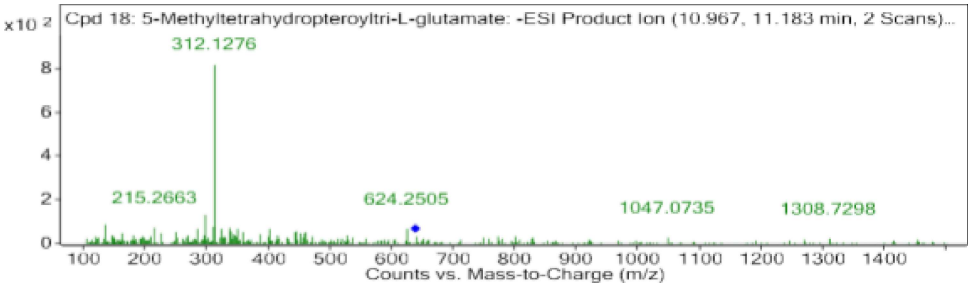
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
248.9765				26482.55		
282.1171			1	19124.74		
312.1285			1	624925.38		
313.1316			1	116432.61		
314.1345			1	13102.25		
342.1387			1	13028.94		
348.1056			1	14676.35		
490.1566			1	34007.99		
639.2421	639.238	-6.48	1	10290.14	C25 H36 N8 O12	(M-H)-
655.237			1	17718.54		

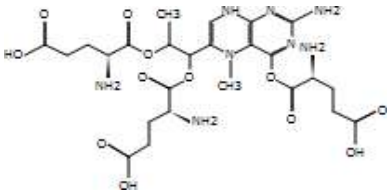
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
135.0457		93.4
215.2663		77.47
283.099		75.81
296.1069	1	138.53
310.1164		84.59
311.0796		83.98
312.1276	1	820.47
313.1295	1	145.65
336.0945		76.56
400.1375		74.29

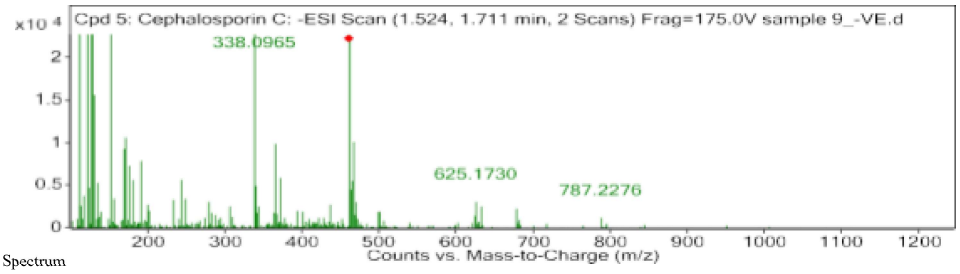
Compound Structure



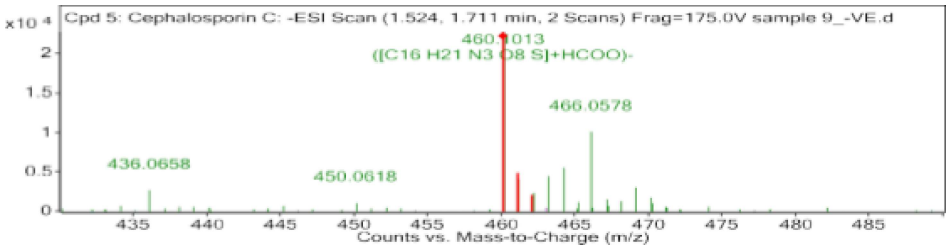
A17 Cephalosporin C (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 5: Cephalosporin C	**Cephalosporin C**	460.1013	1.635	Auto MS/MS	415.1032

MS Spectrum



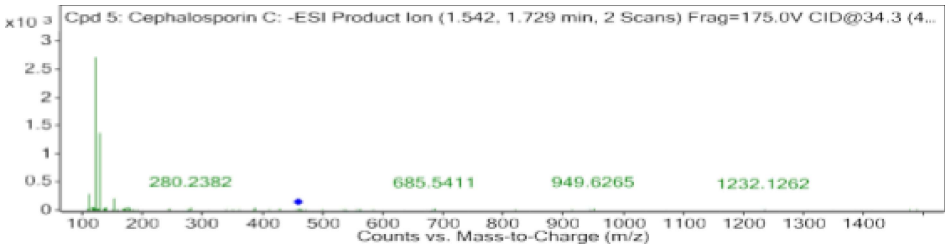
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
110.9599				35154.38		
120.9982			1	105266.95		
126.9549			1	195025.08		
128.0369			1	70212.84		
128.9509			1	15636.55		
151.028			1	27925.24		
338.0965			1	37230.31		
460.1013	460.1031	4.03	1	22716.81	C16 H21 N3 O8 S	(M+HCOO)-
461.1041	461.1061	4.28	1	4181.21	C16 H21 N3 O8 S	(M+HCOO)-
462.1032	462.1034	0.33	1	2458.08	C16 H21 N3 O8 S	(M+HCOO)-

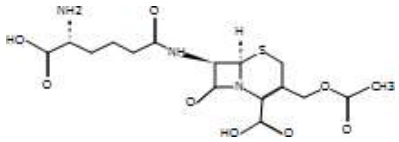
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
110.96		302.99
114.0579		89.12
120.9978	1	2731.92
126.9547	1	1384.61
127.9556	1	77.13
128.037		516.93
128.9489	1	81.05
138.0212		71.38
151.0269	1	230.42
176.0409		84.24

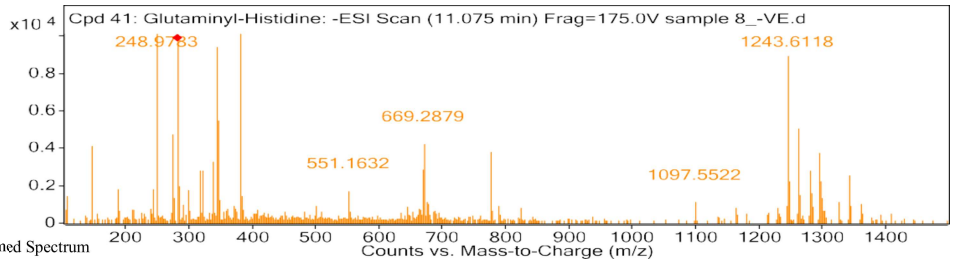
Compound Structure



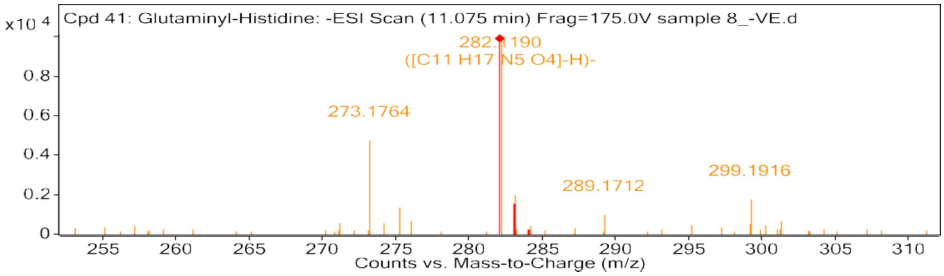
A18 Glutaminyl-Histidine (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 41: Glutaminyl-Histidine	**Glutaminyl-Histidine**	282.119	11.096	Auto MS/MS	283.1265

MS Spectrum



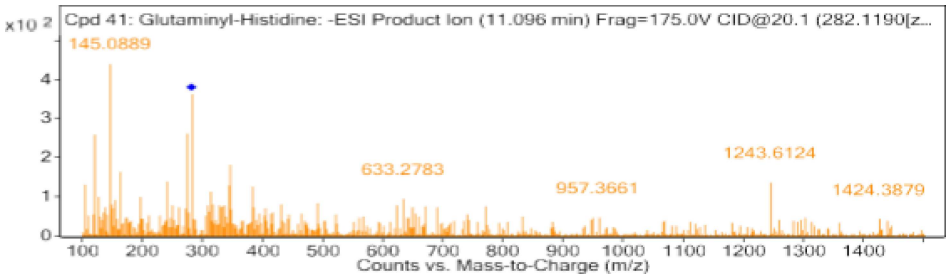
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
248.9783				22768.76		
273.1764				4785.35		
282.119	282.1208	6.14	1	10130.08	C11 H17 N5 O4	(M-H)-
283.122	283.1234	4.95	1	2010.8	C11 H17 N5 O4	(M-H)-
284.1265	284.1255	-3.45	1	492.36	C11 H17 N5 O4	(M-H)-
343.219			1	9443.93		
345.2345			1	5511.52		
381.1193			1	10167.35		
1243.6118			1	8969.41		
1259.6074			1	5115.71		

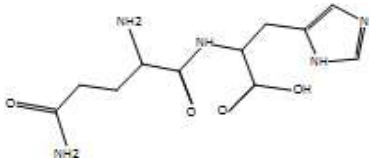
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
104.986		135.3
119.0527		262.88
145.0889		442.5
162.0594		167.02
241.1156		141.82
273.177		263.52
282.114	1	363.96
343.2191		132.33
345.2341	1	185.29
1243.6124		141.01

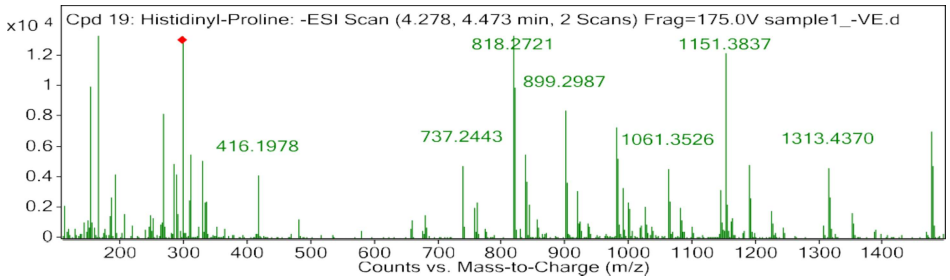
Compound Structure



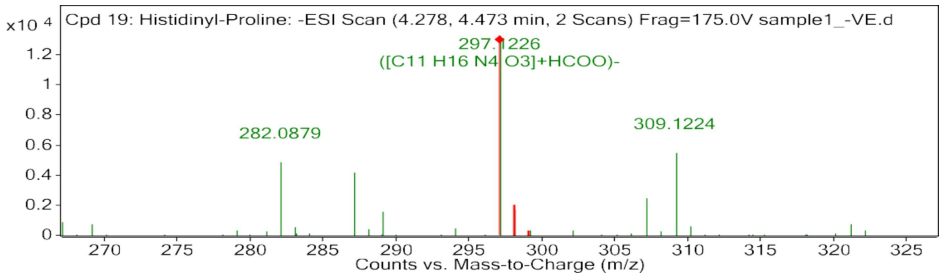
A19 Histidinyl-Proline (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 19: Histidinyl-Proline	**Histidinyl-Proline**	297.1226	4.399	Auto MS/MS	252.1244

MS Spectrum



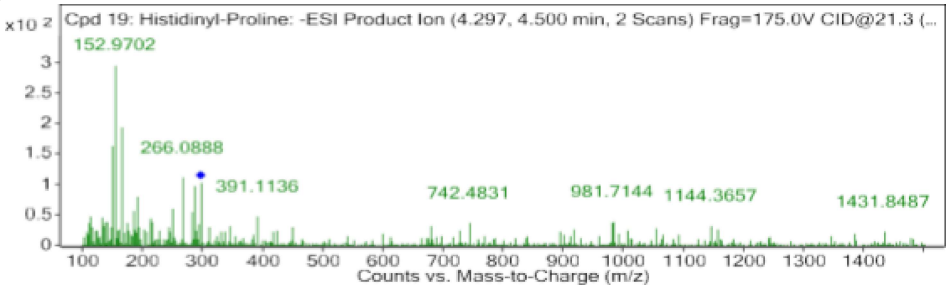
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
152.9702				10006.86		
164.0733			1	18290.73		
266.0928				8209.76		
297.1226	297.1204	-7.32	1	13313.15	C11 H16 N4 O3	(M+HCOO)-
298.1258	298.1232	-8.7	1	1757.22	C11 H16 N4 O3	(M+HCOO)-
299.1262	299.1253	-2.81	1	436.04	C11 H16 N4 O3	(M+HCOO)-
818.2721			2	13944.82		
818.7731			2	9981.27		
899.2987			2	8442.08		
1151.3837			1	12210.8		

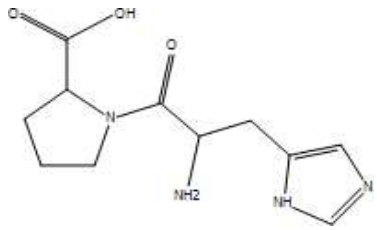
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
150.0438		165.49
152.9702		296.88
164.0715		195.54
185.0493		58.91
191.0229		80.87
249.0936		61.39
266.0888		112.76
282.0888		57.24
287.0911		99.4
297.1229	1	104.09

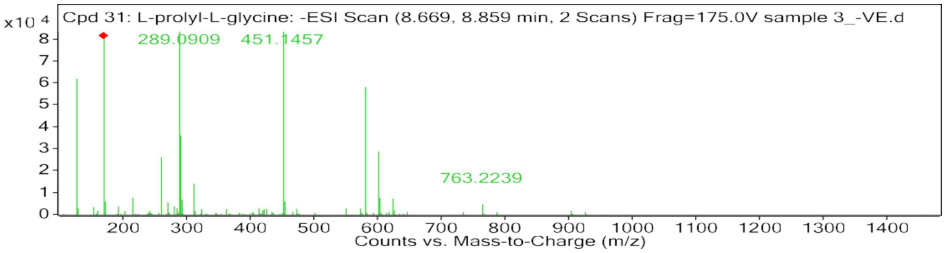
Compound Structure



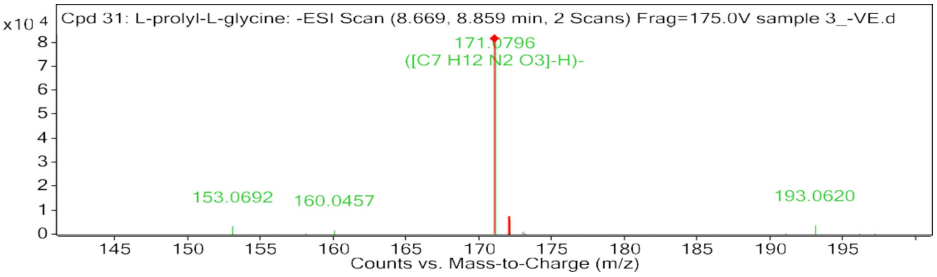
A20 L-prolyl-L-glycine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 31: L-prolyl-L-glycine	**L-prolyl-L-glycine**	171.0796	8.783	Auto MS/MS	172.0869

MS Spectrum



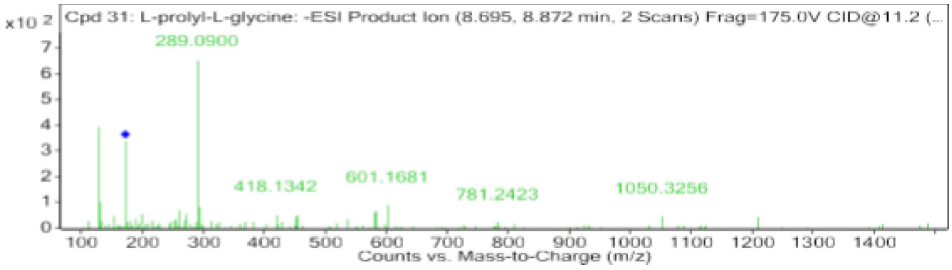
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
128.0368			1	62146.52		
171.0796	171.0775	-12.26	1	83232.37	C7 H12 N2 O3	(M-H)-
172.0829	172.0804	-14.83	1	6347.28	C7 H12 N2 O3	(M-H)-
259.1334			1	26450.56		
289.0909			1	275799.53		
290.0938			1	36403.9		
451.1457			1	101672.59		
452.1488			1	17946		
579.1883			1	58386.49		
601.1703			1	29184.86		

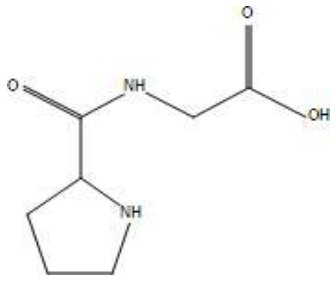
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
127.0886		3.43
128.0363	1	93.48
129.0396	1	03.9
130.0833		9.51
171.0791		39.8
259.1309		4.18
289.09	2 1	54.5
290.0943	1	32.36
291.0894	1	6.79
601.1681		2.59

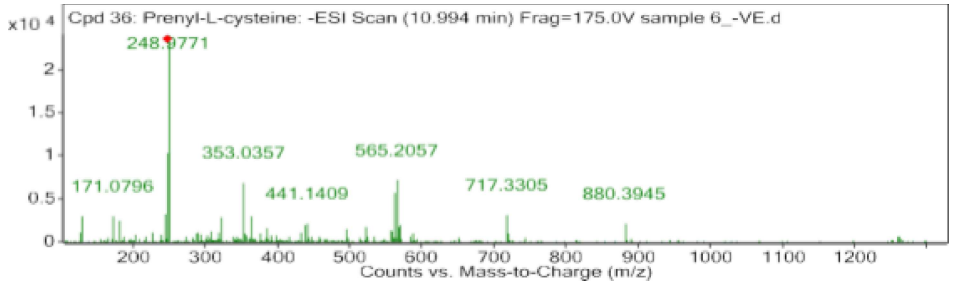
Compound Structure



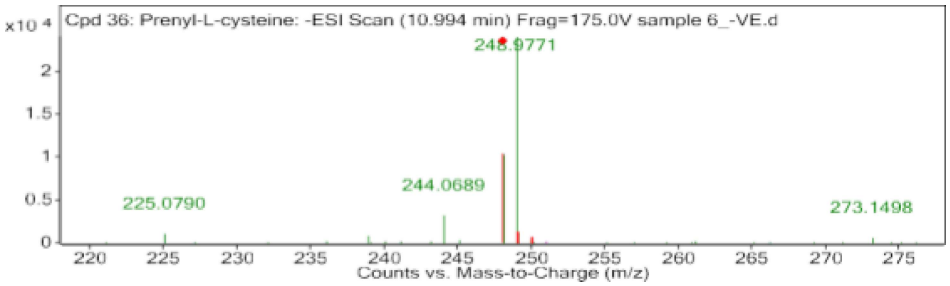
A21 Prenyl-L-cysteine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 36: Prenyl-L-cysteine	**Prenyl-L-cysteine**	248.0962	11.015	Auto MS/MS	189.0825

MS Spectrum



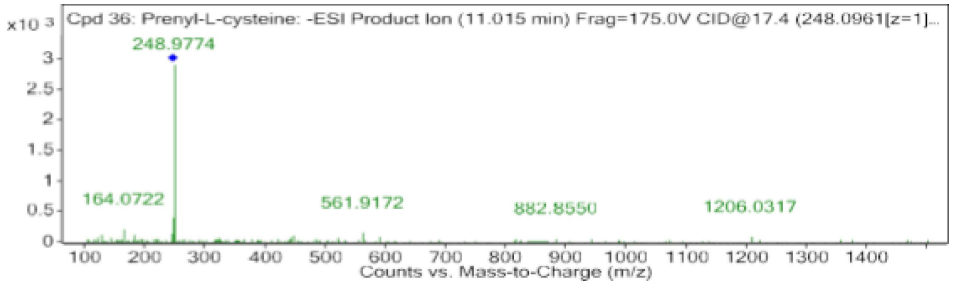
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
171.0796				3101.78		
244.0689				3397.28		
248.0962	248.0962	0.1	1	10387.13	C8 H15 N O2 S	(M+CH3COO)-
248.9771			1	24035.35		
249.0994	249.0992	-1.07	1	1406.31	C8 H15 N O2 S	(M+CH3COO)-
250.1012	250.0943	-27.53	1	210.16	C8 H15 N O2 S	(M+CH3COO)-
353.0357			1	6986.42		
561.1769			1	5806.57		
565.2057			1	7258.77		
717.3305			1	3248.47		

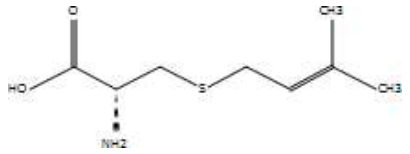
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
128.0364		130.99
164.0722		233.22
181.0909		131.26
244.0686		160.77
248.0974	1	415.64
248.9774	1	2915.61
249.9774	1	113.45
446.2378		122.22
561.9172		173.14
1206.0317		108.06

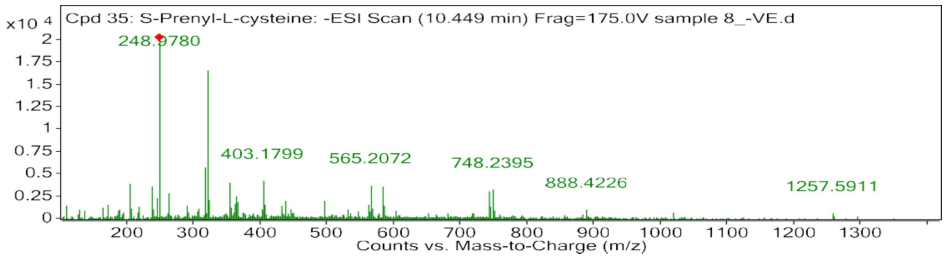
Compound Structure



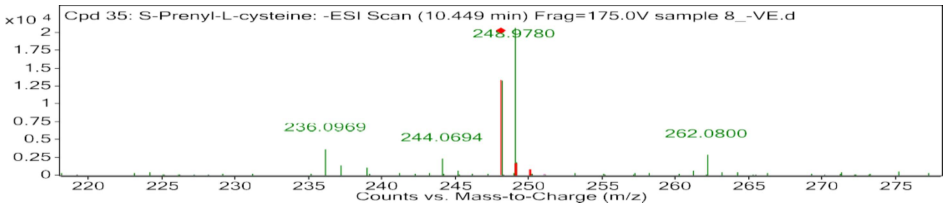
A22 S-Prenyl-L-cysteine (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 35: S-Prenyl-L-cysteine	**S-Prenyl-L-cysteine**	248.0974	10.468	Auto MS/MS	189.0837

MS Spectrum



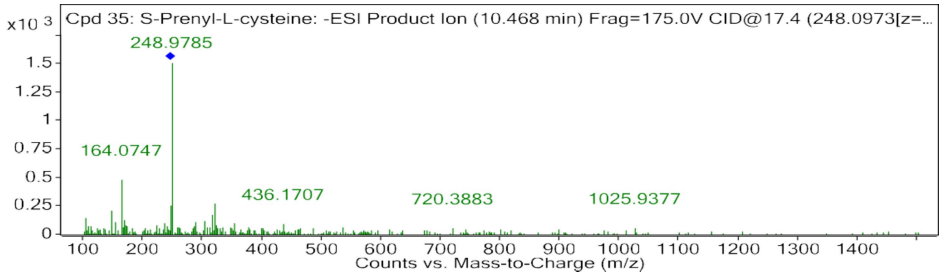
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
204.0693				4041.25		
248.0974	248.0962	-4.64	1	13372.06	C8 H15 N O2 S	(M+CH3COO)-
248.978				20734.38		
249.1001	249.0992	-3.51	1	1949.01	C8 H15 N O2 S	(M+CH3COO)-
250.1084	250.0943	-56.29	1	341.03	C8 H15 N O2 S	(M+CH3COO)-
317.1598			1	5895.58		
321.0707			1	16723.44		
353.1369			1	4194.06		
403.1799			1	4372.42		
565.2072			1	3871.27		

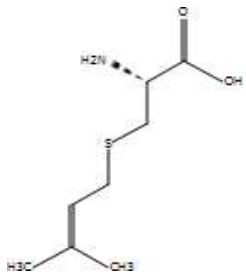
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
103.0565		155.81
147.047	1	220.03
164.0747	1	491.03
169.064		140.13
248.0962		263.3
248.9785	1	1513.02
289.1272		114.13
303.1001		122.91
317.1607		180.29
321.0689		283.76

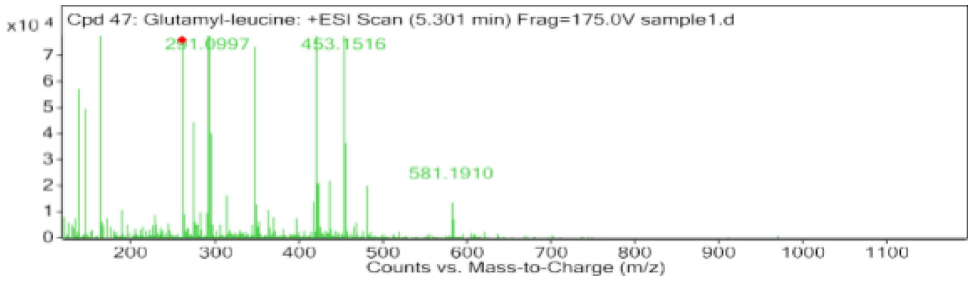
Compound Structure



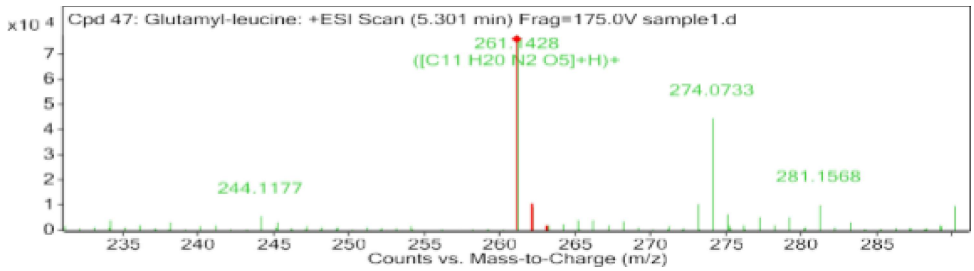
A23 Glutamyl-leucine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 47: Glutamyl-leucine	**Glutamyl-leucine**	261.1428	5.315	Auto MS/MS	260.1356

MS Spectrum



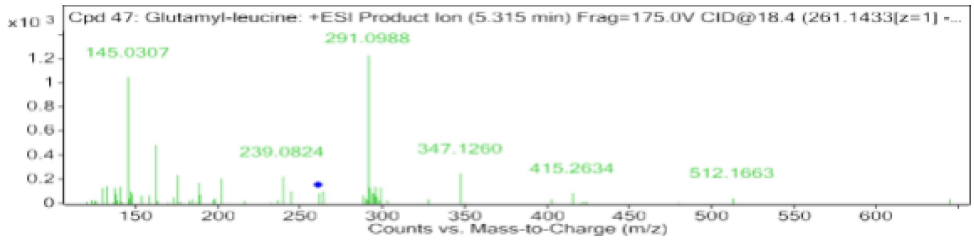
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
162.0574			1	189186.84		
261.1428	261.1445	6.36	1	77388.96	C11 H20 N2 O5	(M+H)+
262.1467	262.1476	3.28	1	9726.3	C11 H20 N2 O5	(M+H)+
263.1466	263.1496	11.15	1	2476.52	C11 H20 N2 O5	(M+H)+
291.0997			1	2231518.25		
292.1027			1	290159.75		
293.1023			1	105632.01		
347.1255			1	73248.99		
420.1417			1	121764.27		
453.1516			1	180334.41		

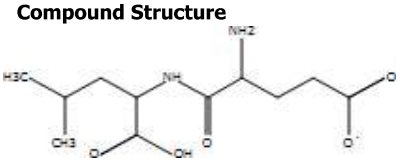
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
132.1015		157.41
145.0307		1052.37
162.0568		490.41
175.1178		240.83
188.0684		174.61
202.1332		211.45
239.0824		229.15
291.0988	1	1230.89
295.1585		148.4
347.126		255.23

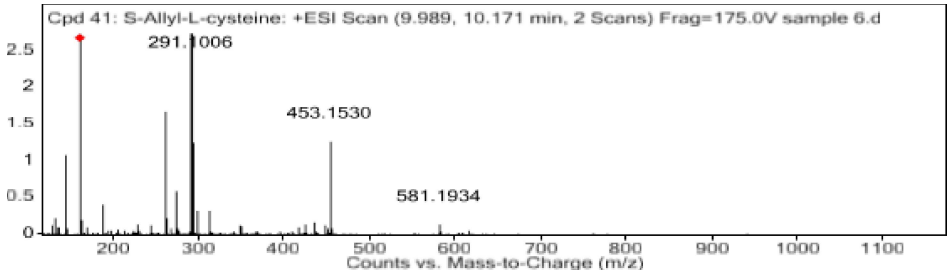
Compound Structure



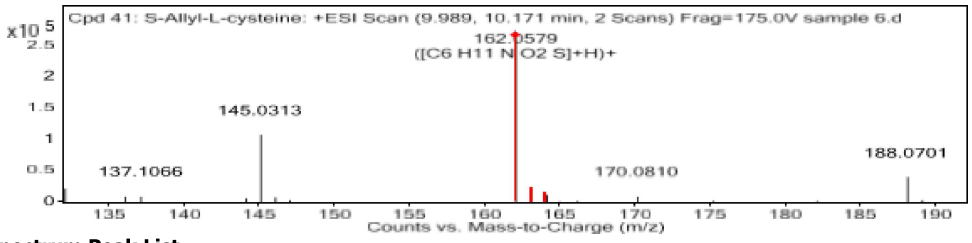
A23 Glutamyl-leucine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 41: S-Allyl-L-cysteine	**S-Allyl-L-cysteine**	162.0579	10.093	Auto MS/MS	161.0507

MS Spectrum



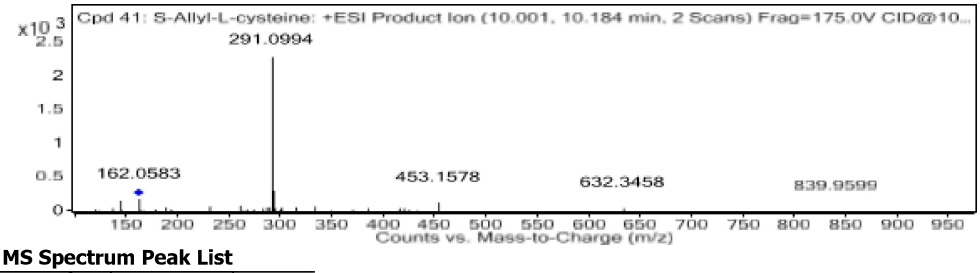
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.0313			1	107694		
162.0579	162.0583	2.43	1	271859.31	C6 H11 N O2 S	(M+H)+
163.061	163.061	0.14	1	20089.64	C6 H11 N O2 S	(M+H)+
164.0547	164.0553	3.54	1	12175.26	C6 H11 N O2 S	(M+H)+
261.1441			1	166161.09		
274.0743			1	58878.62		
291.1006			1	2628658.5		
292.1037			1	333243.44		
293.0996			1	125234.59		
453.153			1	126693.32		

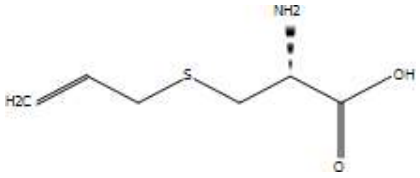
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
145.0307		60.14
162.0583		187.79
231.1202		78
261.1414	1	101.3
286.1415		73.88
291.0994	1	2284.01
292.1048	1	261.59
293.0952	1	316.84
333.1155		75.36
453.1578		138.66

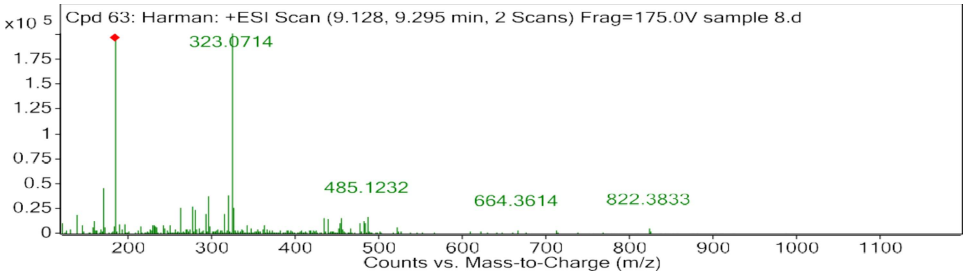
Compound Structure



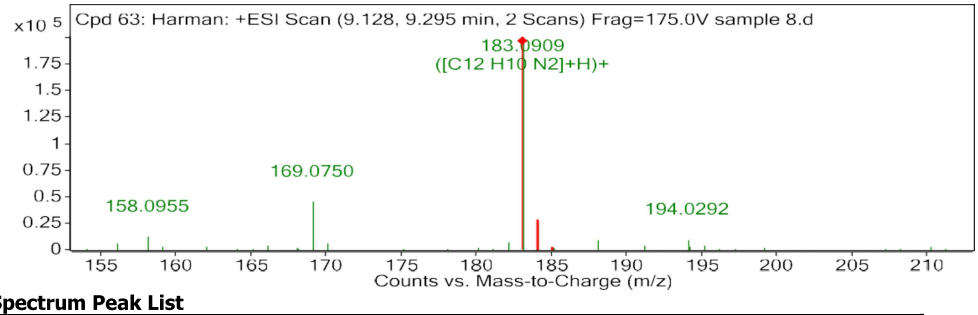
A24 Harman (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 63: Harman	**Harman**	183.0909	9.234	Auto MS/MS	182.0836

MS Spectrum



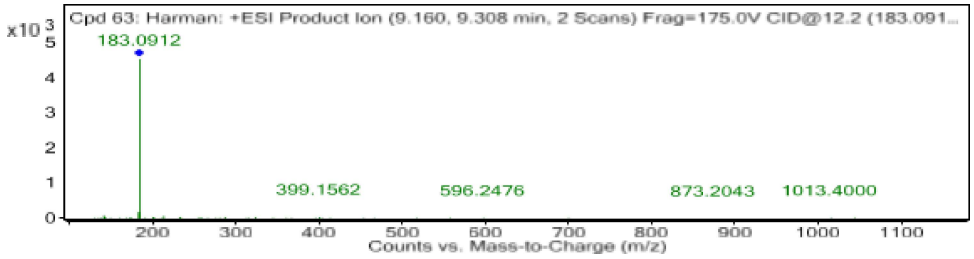
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
169.075			1	46196.53		
183.0909	183.0917	4.33	1	201239.91	C12 H10 N2	(M+H)+
184.0939	184.0947	4.49	1	27797.65	C12 H10 N2	(M+H)+
185.0993	185.0977	-8.2	1	2701.8	C12 H10 N2	(M+H)+
275.1578			1	28397.69		
295.1271			1	38732.24		
318.1793			1	39469.13		
323.0714			1	303465.41		
324.0746			1	42248.23		
325.0692			1	27202.14		

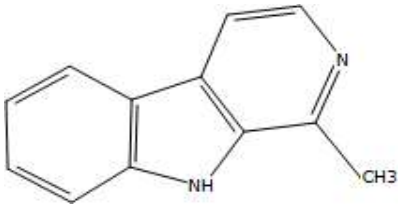
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
140.0481		131.13
182.0817		218.21
183.0912	1	4566.38
184.0926	1	396.06
213.1041		97.9
231.1193		85.57
258.1312		94.64
286.0895		83.85
323.073		80.93
399.1562		88.17

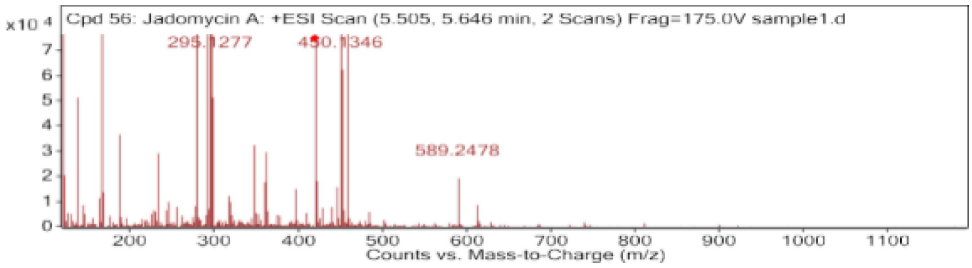
Compound Structure



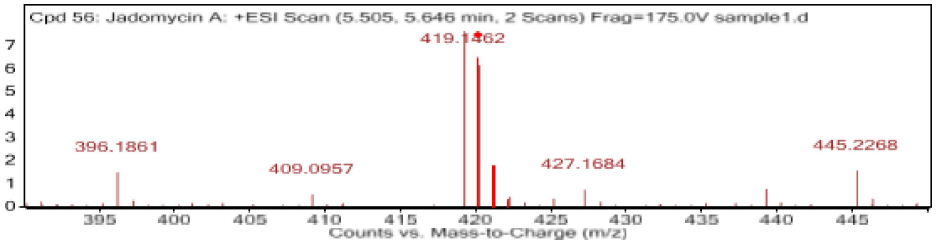
A25 Jadomycin A (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 56: Jadomycin A	**Jadomycin A**	420.1437	5.6	Auto MS/MS	419.137

MS Spectrum



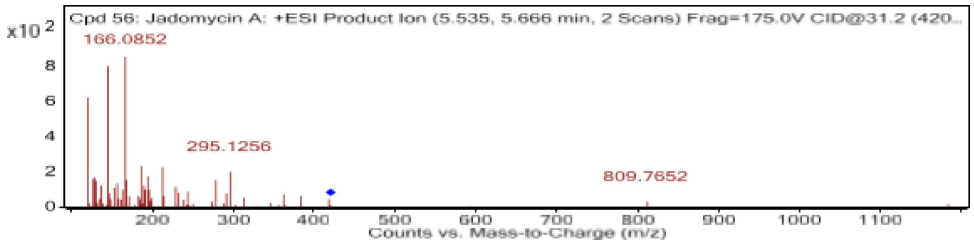
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
120.0803			1	203784.31		
166.0856			1	156699.7		
278.1012			1	92125.84		
291.0998			1	135237.5		
295.1277			1	2503168.25		
296.1313			1	361339.22		
420.1437	420.1442	1.21	1	61881.98	C24 H21 N O6	(M+H)+
421.1497	421.1475	-5.26	1	18551.22	C24 H21 N O6	(M+H)+
422.1495	422.1501	1.56	1	4910.91	C24 H21 N O6	(M+H)+
450.1346			1	301715.97		

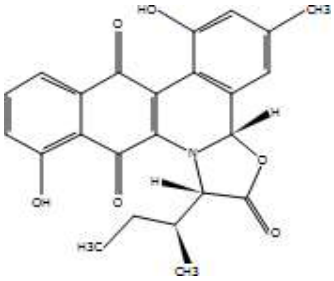
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.08		626.55
127.0216		164.17
128.07	1	175.87
145.0317	1	801.92
166.0852	1	855.68
167.0907	1	159.99
186.0916	1	236.5
194.0809		178.01
212.0919		232.71
295.1256	1	204.79

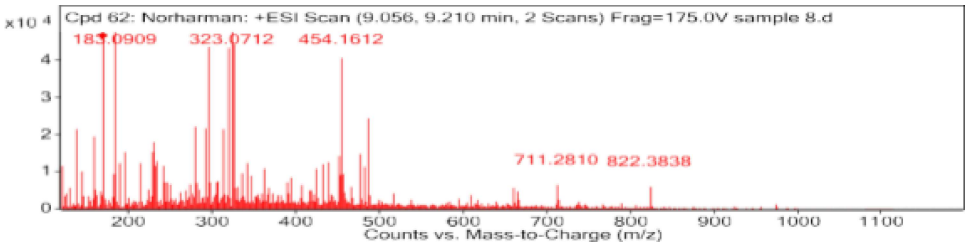
Compound Structure



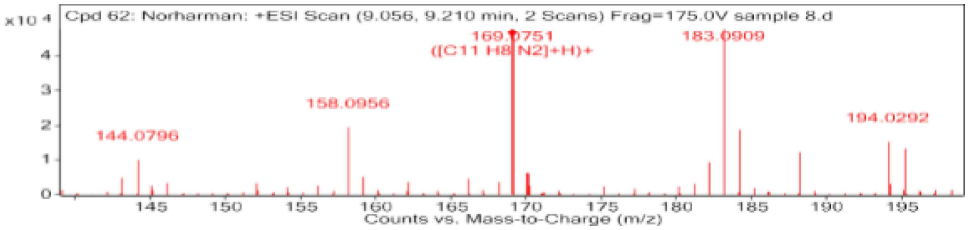
A26 Norharman (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 62: Norharman	**Norharman**	169.0751	9.152	Auto MS/MS	168.0679

MS Spectrum



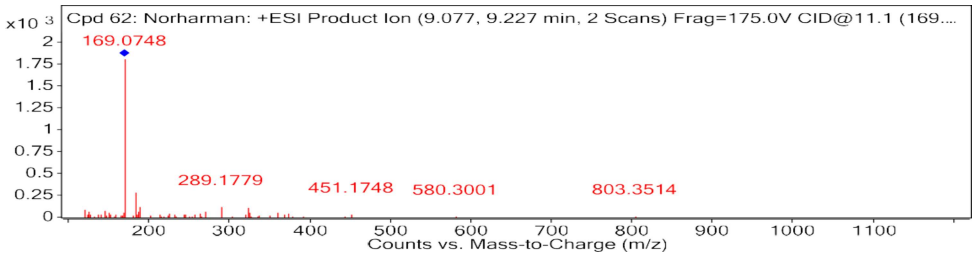
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
169.0751	169.076	5.5	1	47751.36	C11 H8 N2	(M+H)+
170.0778	170.079	7.29	1	6062.47	C11 H8 N2	(M+H)+
171.0882	171.082	-36.34	1	996.39	C11 H8 N2	(M+H)+
183.0909			1	151160.28		
295.1269			1	43791.02		
318.1795			1	43669.34		
323.0712			1	47500		
324.074			1	65466.64		
325.0689			1	44607.31		
454.1612			1	40764		

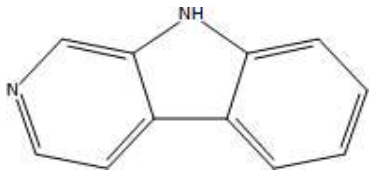
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0794		96.85
144.0813		83.44
169.0748	1	1812.88
170.0573		80.85
170.0763	1	132.36
183.0907	1	292.59
188.0703		130.04
270.1247		76.5
289.1779		128.78
323.0696		123.55

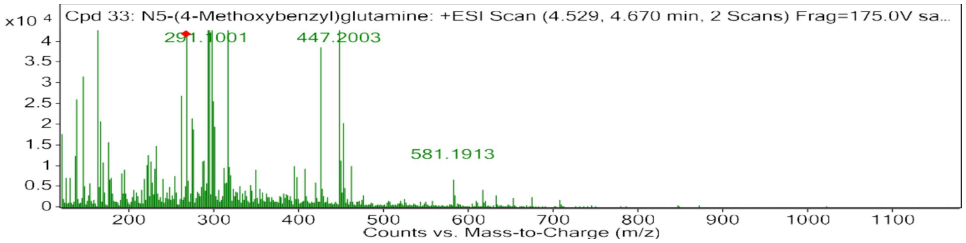
Compound Structure



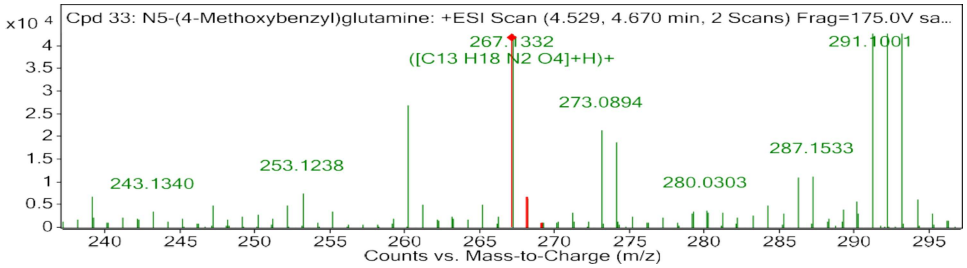
A27 N5-(4-Methoxybenzyl)glutamine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 33: N5-(4-Methoxybenzyl)glutamine	**N5-(4-Methoxybenzyl)glutam**	267.1332	4.622	Auto MS/MS	266.1261

MS Spectrum



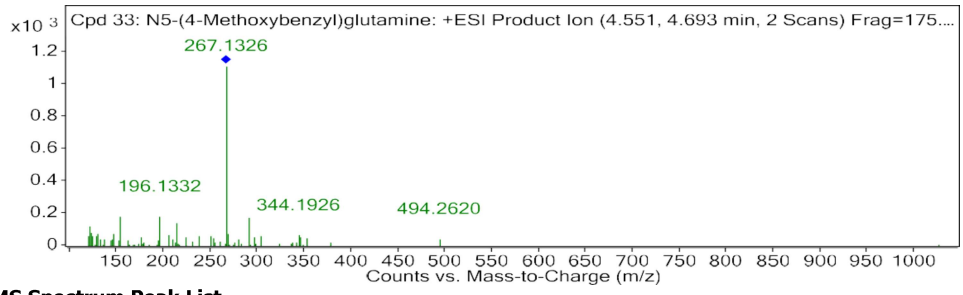
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
162.0576			1	63352.87		
267.1332	267.1339	2.73	1	42795.76	C13 H18 N2 O4	(M+H)+
268.1377	268.137	-2.59	1	6513.75	C13 H18 N2 O4	(M+H)+
269.1378	269.1393	5.64	1	1083.54	C13 H18 N2 O4	(M+H)+
291.1001			1	1076436.25		
292.1031			1	137160.5		
293.0993			1	49768.42		
297.0566			1	216997.25		
315.1287			1	60300.25		
447.2003			1	49132.85		

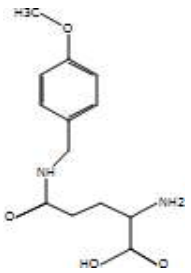
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
121.0624		129.91
123.07		86.91
130.049		81.18
146.1184	1	81.96
154.0851		184
196.1332		188.99
214.1421	1	144.43
267.1326	1	1117.76
268.1318	1	82.47
291.0982		180.68

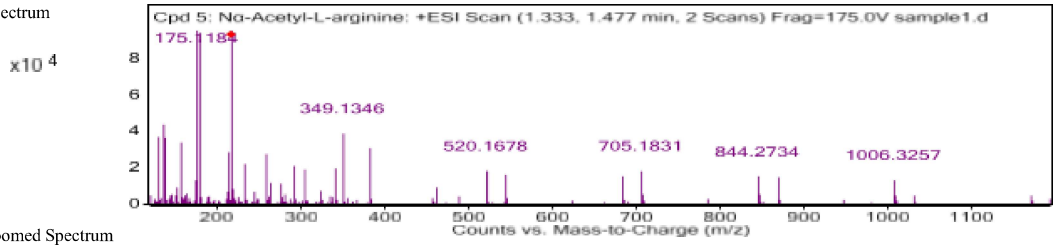
Compound Structure



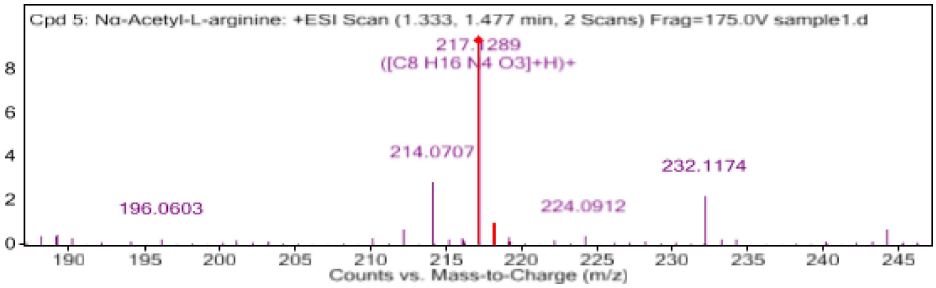
A28 Nα-Acetyl-L-arginine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 5: Nα-Acetyl-L-arginine:	Nα-Acetyl-L-arginine	217.1289	1.419	Auto MS/MS	216.1217

MS Spectrum



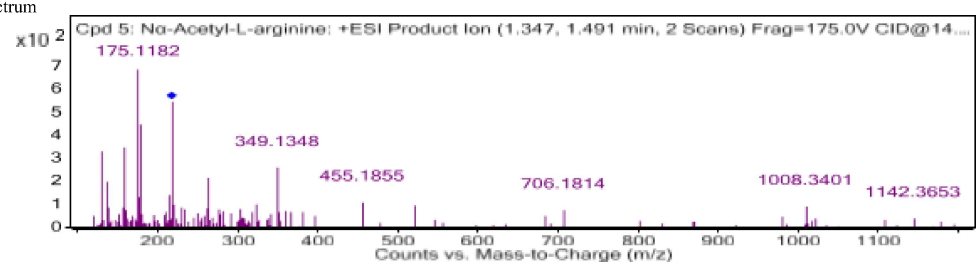
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
130.0862				37272.21		
136.0611			1	44262.56		
138.0543			1	36773.9		
156.1014			1	34397.51		
175.1184			1	128435.78		
178.0526			1	90589.38		
217.1289	217.1295	2.82	1	95055.12	C8 H16 N4 O3	(M+H)+
218.1318	218.132	1.01	1	8928.31	C8 H16 N4 O3	(M+H)+
219.1334	219.1341	3.23	1	2169.19	C8 H16 N4 O3	(M+H)+
349.1346			1	39178.25		

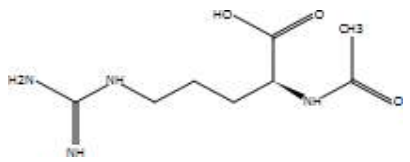
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0485		186.59
130.0876		332.82
136.0607		203.21
158.0882	1	351.46
175.1182	1	689.08
178.0531		447.84
214.0708		143.82
217.128	1	549.01
262.1272		220.17
349.1348	1	262.56

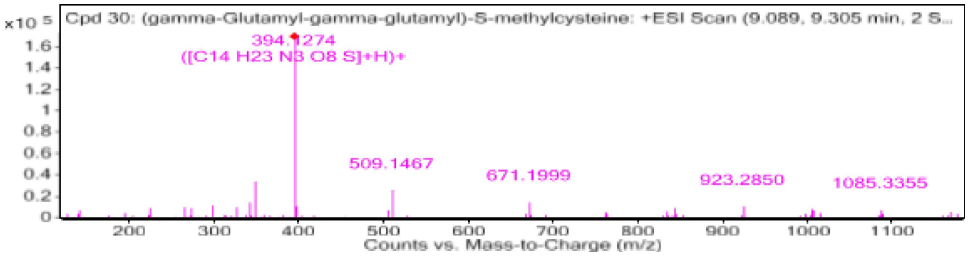
Compound Structure



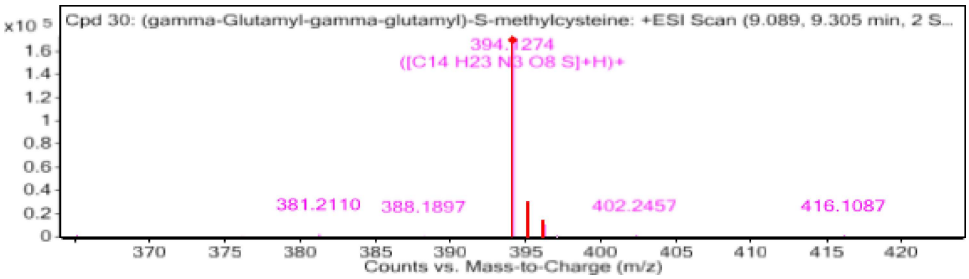
A29 (gamma-Glutamyl-gamma-glutamyl)-S-methylcysteine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 30: (gamma-Glutamyl-gamma-glutamyl)-S-methylcysteine	**(gamma-Glutamyl-gamma-glutamyl)-S - methylcysteine**	394.1274	9.216	Auto MS/MS	393.1202

MS Spectrum



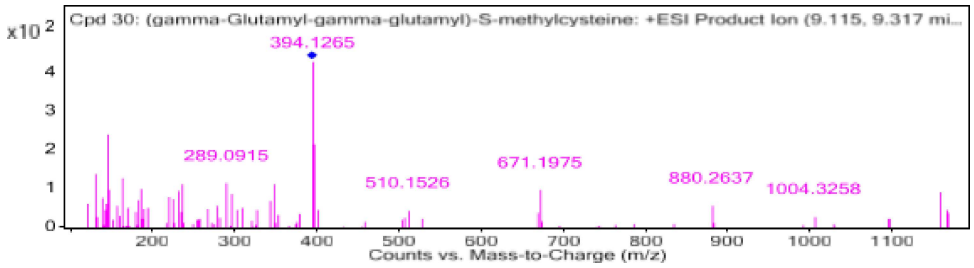
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
297.0566				12257.3		
325.1125			1	11156.29		
342.1389			1	15232.13		
347.0946			1	35012.07		
394.1274	394.1279	1.1	1	173406.3	C14 H23 N3 O8 S	(M+H)+
395.1302	395.1307	1.25	1	29010.7	C14 H23 N3 O8 S	(M+H)+
396.1285	396.1274	-2.76	1	11680.26	C14 H23 N3 O8 S	(M+H)+
509.1467			1	26447.94		
671.1999			1	15423.12		
923.285			2	11235.27		

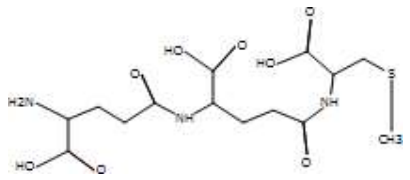
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0507		137.92
144.0103		148.74
144.0476		240.82
162.0569		127.12
234.0952		112.79
289.0915		114.45
347.0952		111.86
394.1265	1	427.84
395.1277	1	214.72
396.1218	1	103.9

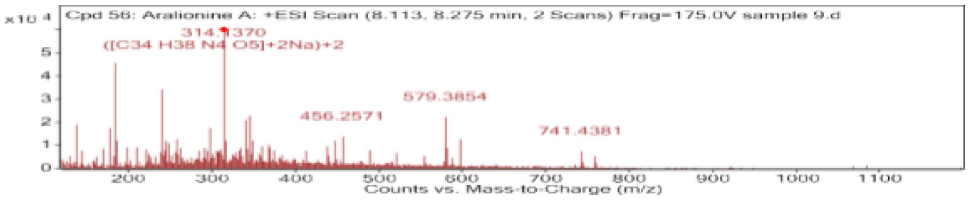
Compound Structure



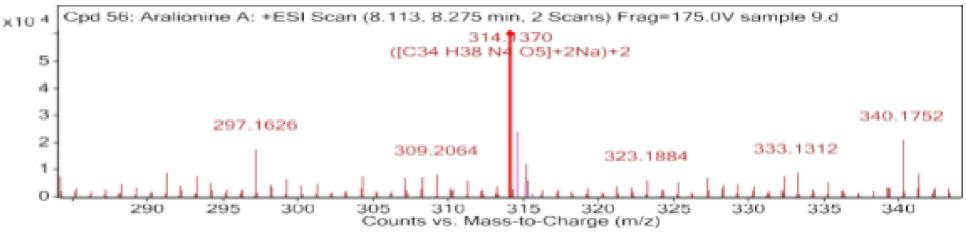
A30 Aralionine A (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 56: Aralionine A	**Aralionine A**	314.137	8.228	Auto MS/MS	582.2955

MS Spectrum



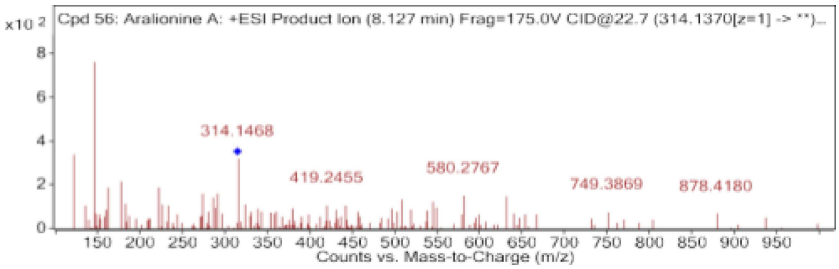
MS Zoomed Spectrum

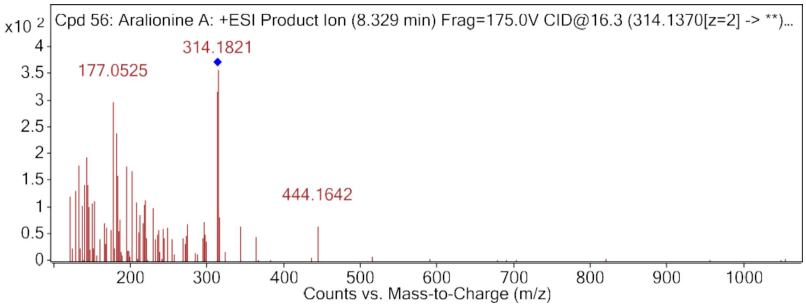


MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
137.1065				19207.9		
178.1217				17733.23		
183.0907			1	45924.55		
240.2051			1	34619.22		
297.1626				17853.98		
314.137	314.1313	-18.07	1	61421.18	C34 H38 N4 O5	(M+2Na)+2
340.1752			1	21197.34		
344.1477			1	23057.29		
456.2571				14069.17		
579.3854			1	22496.02		

MSMS Spectrum

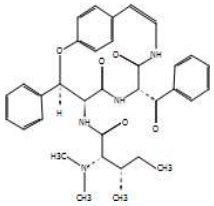




MS/MS Spectrum Peak List

m/z	z	Abund
121.0639		343.31
145.028		765.29
161.0964		190.83
176.0719		219.13
177.0553		201.26
221.0737		193.03
273.1863		165.68
290.0963		162.73
314.1468		323.65
580.2767		154.42
132.0784		181.45
142.0634		194.71
177.0525	1	298.63
182.08		241.32
195.0911		178.37
201.0947		170.03
312.193		177.36
313.1876		318.6
314.1245		183.33
314.1821	2	360.3

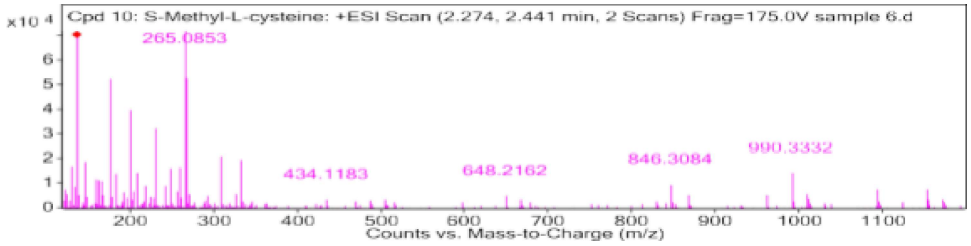
Compound Structure



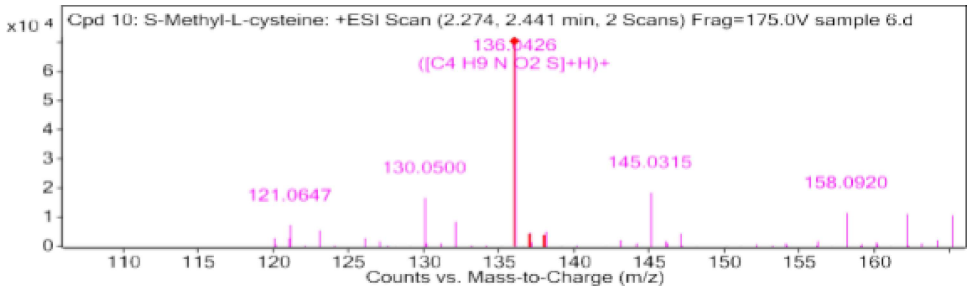
A31 S-Methyl-L-cysteine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 10: S-Methyl-L-cysteine	**S-Methyl-L-cysteine**	136.0426	2.373	Auto MS/MS	135.0353

MS Spectrum



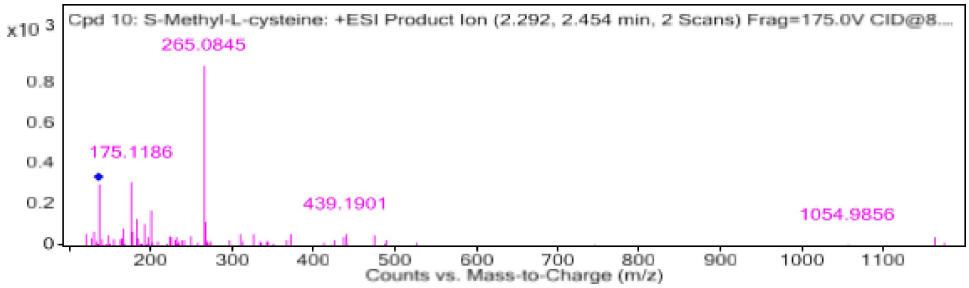
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
136.0426	136.0427	0.62	1	71843.34	C4 H9 N O2 S	(M+H)+
137.0455	137.0451	-2.87	1	5064.83	C4 H9 N O2 S	(M+H)+
138.0387	138.0394	5.32	1	3315.71	C4 H9 N O2 S	(M+H)+
175.1187			1	52567.63		
200.1026			1	39879.11		
229.1546			1	32632.66		
265.0853			1	500405.03		
266.0884			1	53050.69		
267.0831			1	23944.18		
307.0955			1	21147.36		

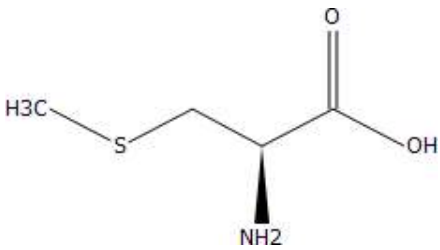
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0476		70.41
136.0413		301.69
165.0556		86.95
175.1186	1	312.37
176.147		66.83
182.0432		131.46
191.038		107.23
200.1005		174.33
265.0845	1	885.31
266.0872	1	118.56

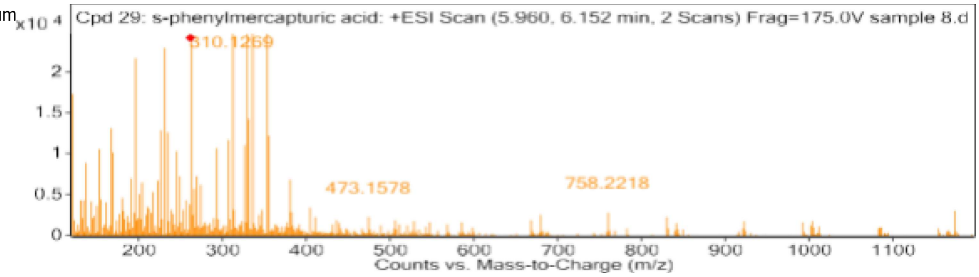
Compound Structure



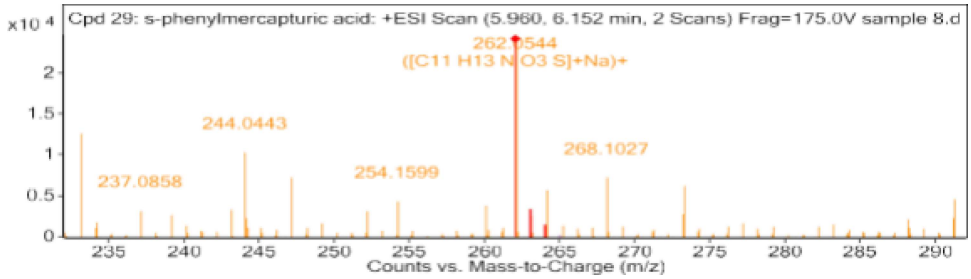
A32 s-phenylmercapturic acid (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 29: s-phenylmercapturic acid	**s-phenylmercapturic acid**	262.0544	6.076	Auto MS/MS	239.0653

MS Spectrum



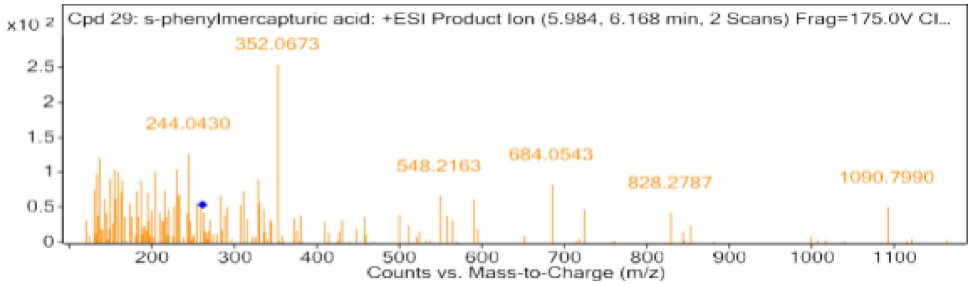
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
194.0293			1	21745.26		
229.1173			1	23108.23		
262.0544	262.0508	-13.45	1	24707.04	C11 H13 N O3 S	(M+Na)+
263.0578	263.0538	-15.3	1	2708.93	C11 H13 N O3 S	(M+Na)+
264.0586	264.0489	-36.8	1	464.59	C11 H13 N O3 S	(M+Na)+
310.1269			1	120197.67		
311.1304			1	21588.37		
328.1374			1	91305.91		
334.0576			1	25260.61		
352.068			1	85860.88		

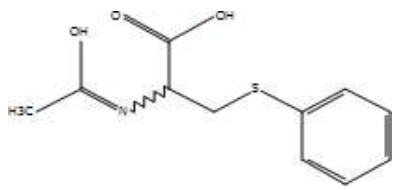
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	Abund
132.1007	99.77
136.0618	121.65
148.0252	92.7
153.1287	105.5
158.0903	101.46
204.0822	102.68
229.1534	104.51
244.043	128.6
328.1383	91.35
352.0673	255.28

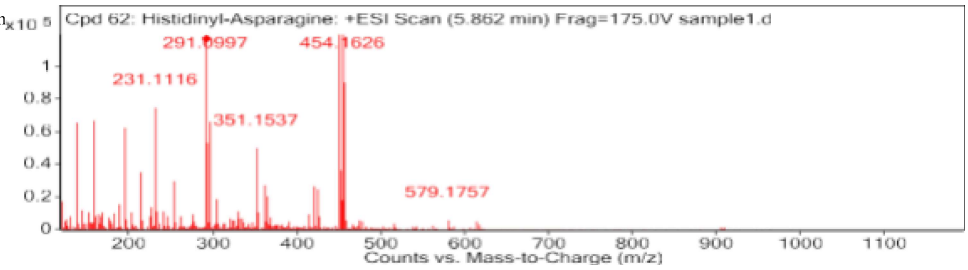
Compound Structure



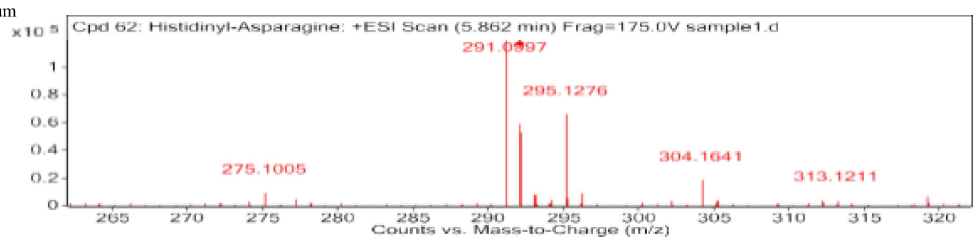
A33 Histidinyl-Asparagine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 62: Histidinyl-Asparagine	**Histidinyl-Asparagine**	292.1022	5.892	Auto MS/MS	269.112

MS Spectrum



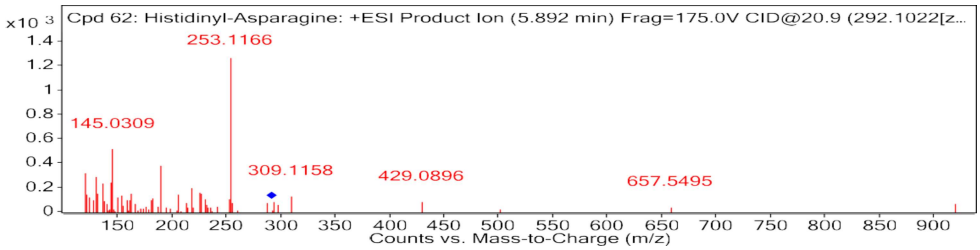
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
158.0957			1	67601.48		
231.1116			1	75548.2		
291.0997				119795.15		
292.1022	292.1016	-1.95	1	53881.93	C10 H15 N5 O4	(M+Na)+
293.1021	293.1041	6.88	1	8801	C10 H15 N5 O4	(M+Na)+
294.0987	294.1062	25.67	1	5149.09	C10 H15 N5 O4	(M+Na)+
295.1276			1	66586.61		
450.1342			1	181590.48		
454.1626			1	391491.97		
455.1652			1	90502.5		

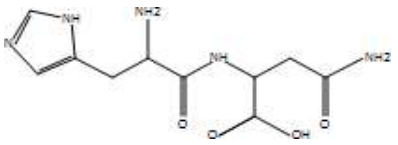
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
120.0792		323.9
130.0493		296.79
136.0596		246.13
143.0575		248.11
145.0309	1	524.45
162.0567		163.1
189.1022		384.84
218.1301		205.31
225.1283		170.69
253.1166		1273.94

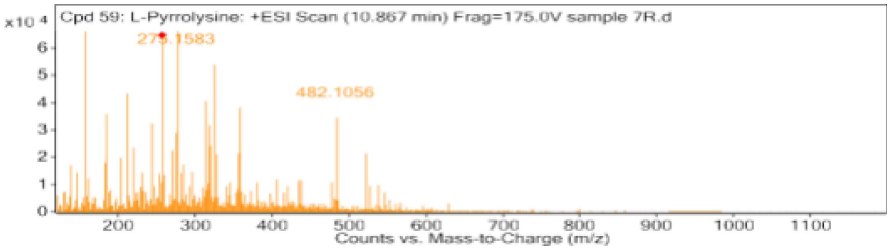
Compound Structure



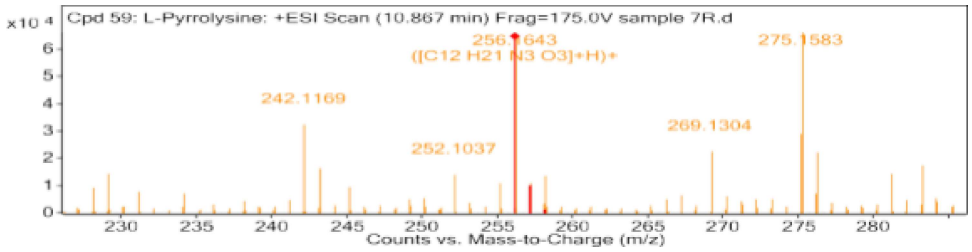
A34 L-Pyrrolysine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 59: L-Pyrrolysine	**L-Pyrrolysine**	256.1643	10.883	Auto MS/MS	255.157

MS Spectrum



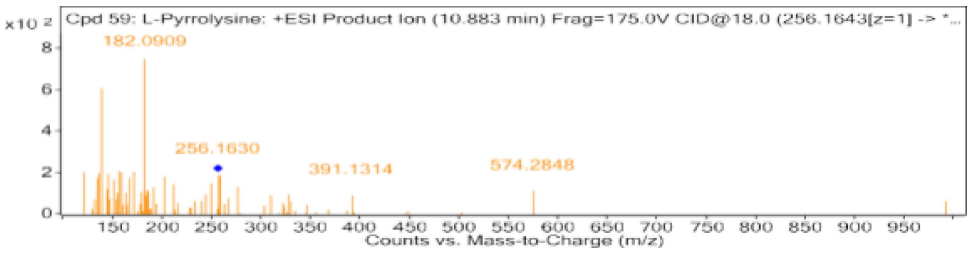
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
156.0797			1	76048.52		
183.0911			1	36273.1		
211.1426			1	43660.31		
256.1643	256.1656	4.92	1	66131.53	C12 H21 N3 O3	(M+H)+
257.1679	257.1685	2.32	1	11156.89	C12 H21 N3 O3	(M+H)+
258.1668	258.1708	15.41	1	2748.15	C12 H21 N3 O3	(M+H)+
275.1583			1	158921.02		
313.1201			1	40848.38		
323.0708			1	54243.69		
357.1282			1	38471.88		

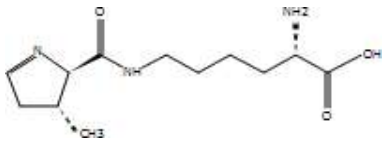
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
121.0732		206.94
136.0589		202.4
138.1021		614.18
145.0322		197.25
156.0786		211.53
159.09		208.24
170.0581		206.85
182.0909	1	753.75
256.163		195.77
258.13		191.25

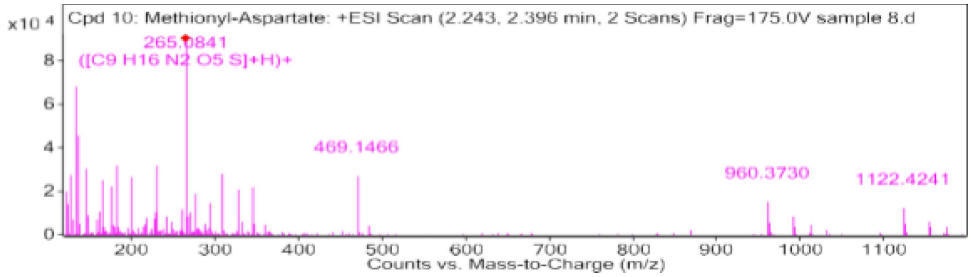
Compound Structure



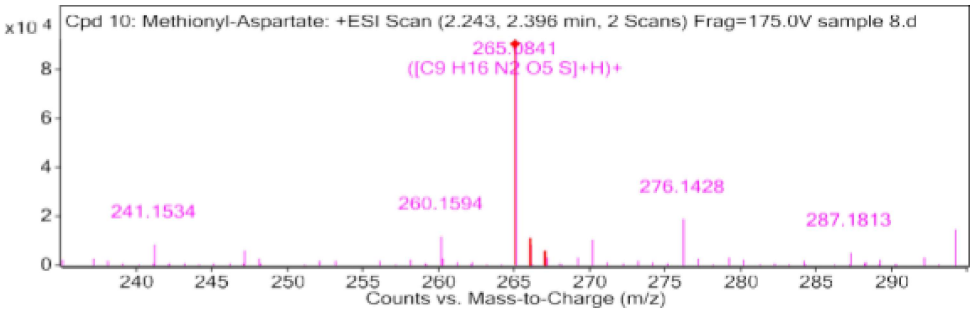
A35 Methionyl-Aspartate (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 10: Methionyl-Aspartate	**Methionyl-Aspartate**	265.0841	2.334	Auto MS/MS	264.0769

MS Spectrum



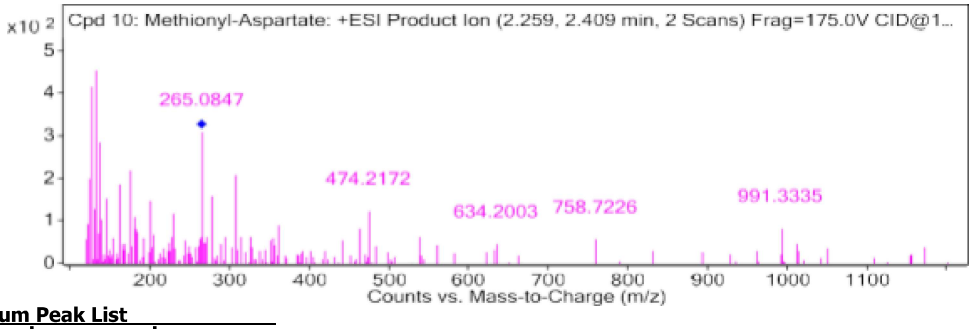
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
126.0657				27995.04		
132.1015			1	68527.27		
136.0752			1	46160.56		
145.031				30733.92		
182.0805			1	32547.15		
229.1537			1	32489.11		
265.0841	265.0853	4.51	1	92352.36	C9 H16 N2 O5 S	(M+H)+
266.0876	266.088	1.56	1	9179.05	C9 H16 N2 O5 S	(M+H)+
267.0823	267.0835	4.45	1	3859.59	C9 H16 N2 O5 S	(M+H)+
307.0948			1	28492.07		

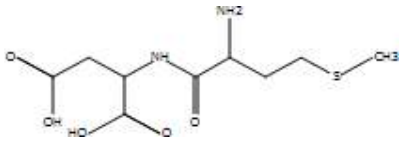
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
123.0433		202.86
126.0649		416.17
132.1007		456
136.0424		285.42
136.0744		237.58
162.0582		187.48
175.1197	1	221.87
265.0847	1	311.32
276.1435		159.5
307.0923		208.77

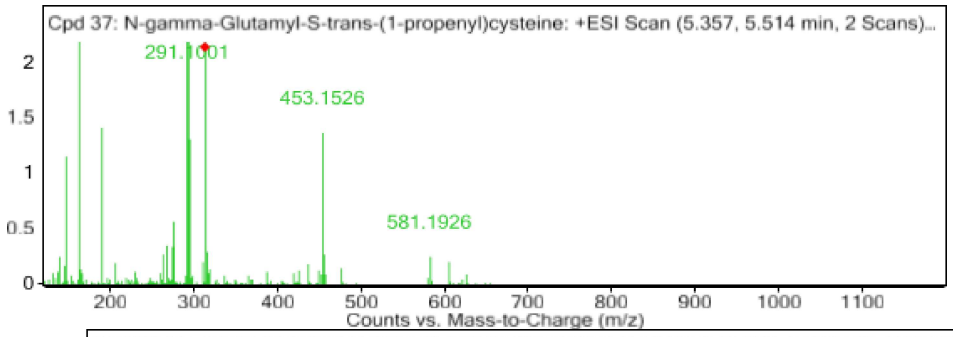
Compound Structure



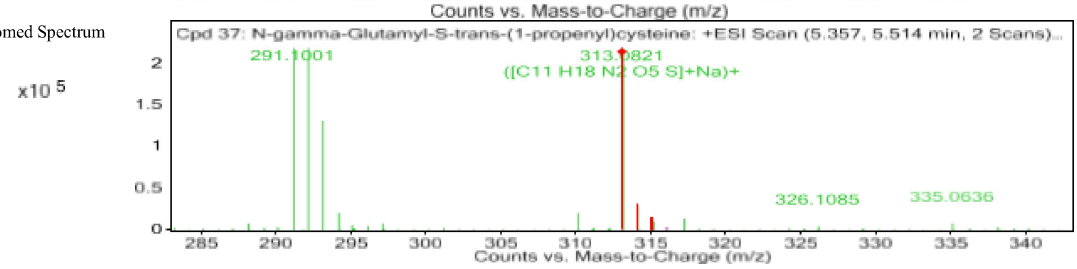
A36 N-gamma-Glutamyl-S-trans-(1-propenyl)cysteine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 37: N-gamma-Glutamyl-S-trans-(1-propenyl)cysteine	**N-gamma-Glutamyl-S-trans-(1-propenyl)cysteine**	313.0821	5.449	Auto MS/MS	290.0929

MS Spectrum



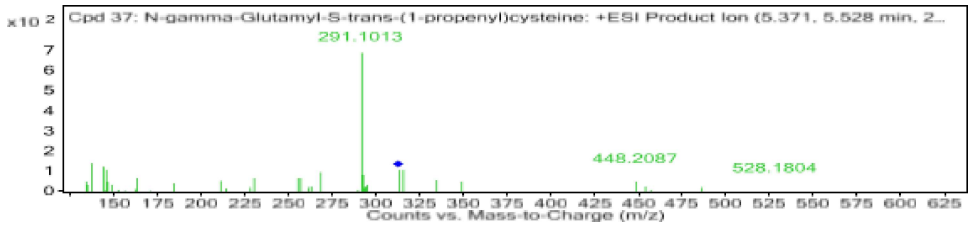
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
145.0309			1	115562.35		
162.0576			1	221428.28		
188.07			1	141602.84		
291.1001			1	2774021.5		
292.1032			1	350579.38		
293.0991			1	131943.56		
313.0821	313.0829	2.49	1	218694.34	C11 H18 N2 O5 S	(M+Na)+
314.0846	314.0857	3.48	1	30068.58	C11 H18 N2 O5 S	(M+Na)+
315.0816	315.0814	-0.74	1	10736.35	C11 H18 N2 O5 S	(M+Na)+
453.1526			1	137983.48		

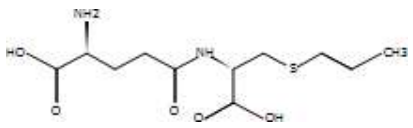
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
137.1048		143.88
144.0805		128.54
145.0302		111.47
163.0599		70.33
m/z	z	Abund
256.0885		71.7
268.0583		98.07
291.1013	1	693.38
292.1027	1	85.73
313.0841		112.5
315.1048		110.72

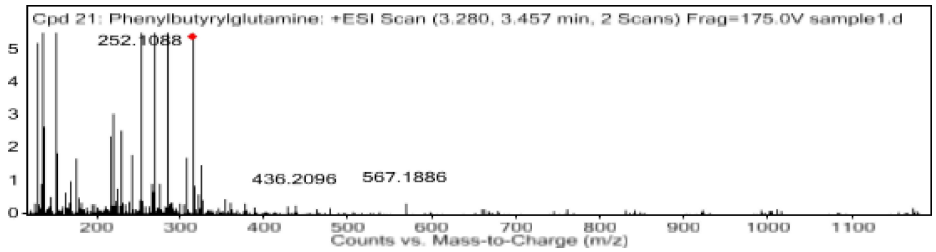
Compound Structure



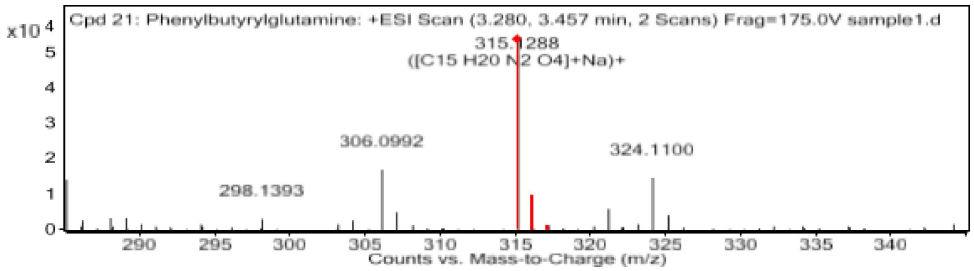
A37 Phenylbutyrylglutamine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 21: Phenylbutyrylglutamine	**Phenylbutyrylglutamine**	315.1288	3.389	Auto MS/MS	292.1396

MS Spectrum



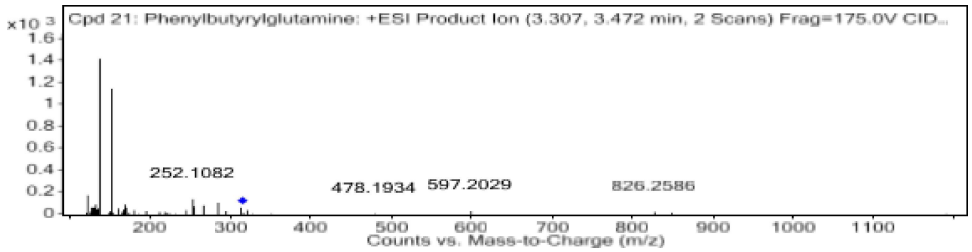
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
130.0496			1	52008.57		
136.0613			1	412011.06		
152.0561			1	314865		
252.1088			1	310747.63		
253.1118			1	36117.62		
268.1036			1	85375.22		
284.098			1	84880.88		
315.1288	315.1315	8.54	1	54978.9	C15 H20 N2 O4	(M+Na)+
316.132	316.1347	8.54	1	8706.13	C15 H20 N2 O4	(M+Na)+
317.1354	317.137	5.14	1	1610.62	C15 H20 N2 O4	(M+Na)+

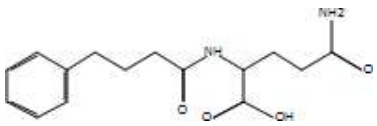
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
122.097		177.51
131.0845		89.52
132.1001		88.17
136.0607	1	1422.92
137.064	1	144
152.0558		1150.11
168.1023		91.43
252.1082	1	143.73
265.0854		81.39
284.0949		109.88

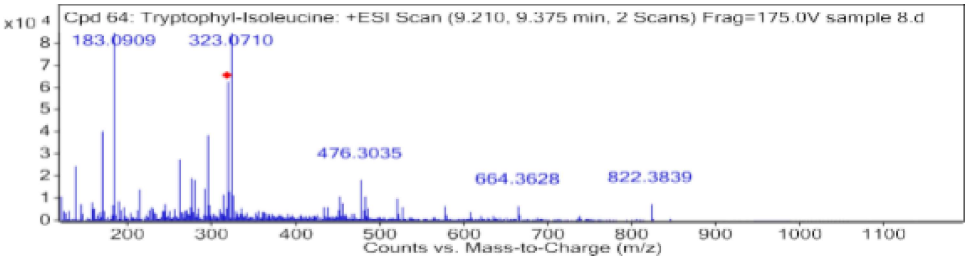
Compound Structure



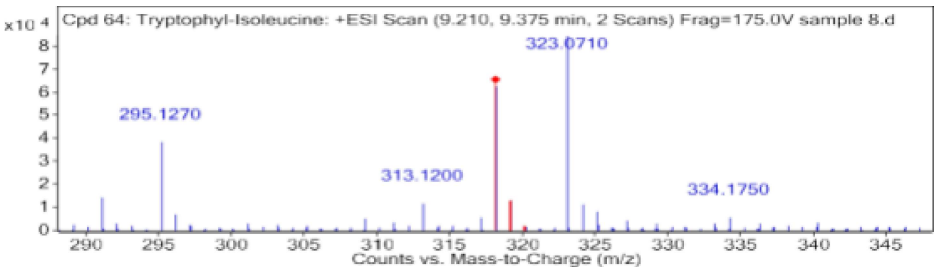
A38 Tryptophyl-Isoleucine (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 64: Tryptophyl-Isoleucine	**Tryptophyl-Isoleucine**	318.1793	9.307	Auto MS/MS	317.1719

MS Spectrum



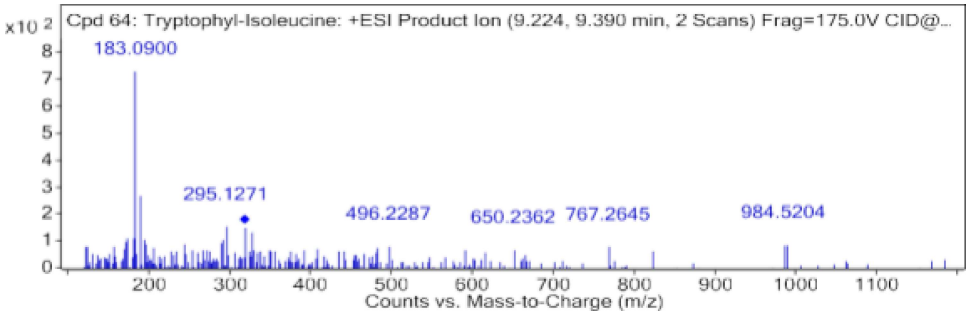
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
137.1063				24786.64		
169.0751			1	40805.45		
183.0909			1	313988.5		
184.0937			1	41638.14		
261.158			1	28082.12		
295.127			1	38745.98		
318.1793	318.1812	5.89	1	62773.76	C17 H23 N3 O3	(M+H)+
319.1817	319.1843	8.07	1	13382.27	C17 H23 N3 O3	(M+H)+
320.1834	320.1868	10.76	1	2181.54	C17 H23 N3 O3	(M+H)+
323.071			1	84714.76		

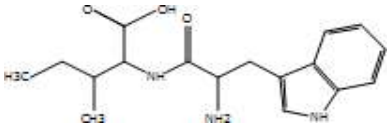
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
172.1301		114.56
180.0643		114.77
183.09	1	732.54
188.071		271.76
193.0958		109.9
291.0993		107.54
295.1271		156.21
318.0925		105.51
318.1779		152.75
327.1379		136.76

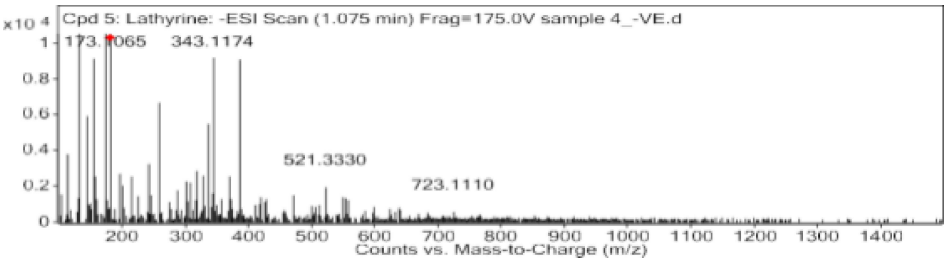
Compound Structure



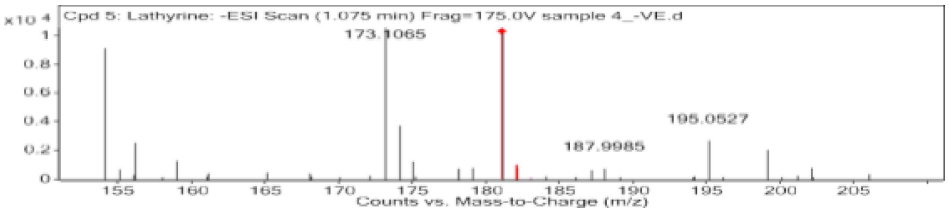
A39 Lathyrine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 5: Lathyrine	**Lathyrine**	181.0733	1.095	Auto MS/MS	182.0807

MS Spectrum



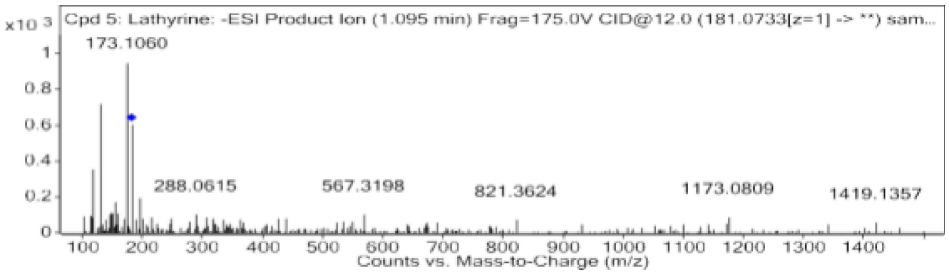
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
131.0479			1	15890.77		
131.084			1	31393.83		
145.0997				5945.97		
154.0635			1	9155.24		
173.1065			1	54241.02		
181.0733	181.0731	-1.05	1	10522.45	C7 H10 N4 O2	(M-H)-
182.0772	182.0755	-9.53	1	858.01	C7 H10 N4 O2	(M-H)-
257.0688			1	6727.76		
343.1174			1	9199.93		
385.1762			1	9100.6		

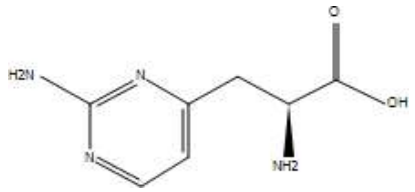
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
118.0534		357.54
131.0478		724.25
131.0839		523.1
148.0619		118.59
150.0261		114.67
154.0649		175.7
173.106	1	952.28
174.1106	1	129.42
181.0738	1	609.97
195.0539		198.66

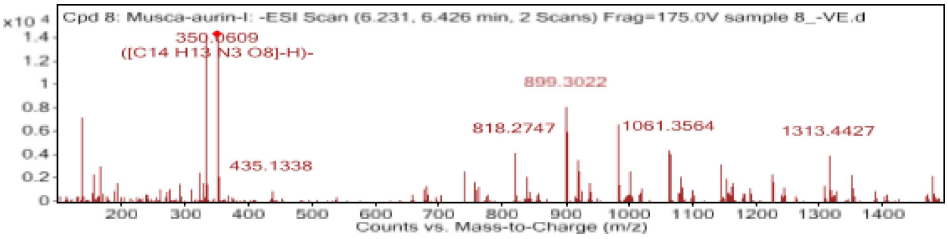
Compound Structure



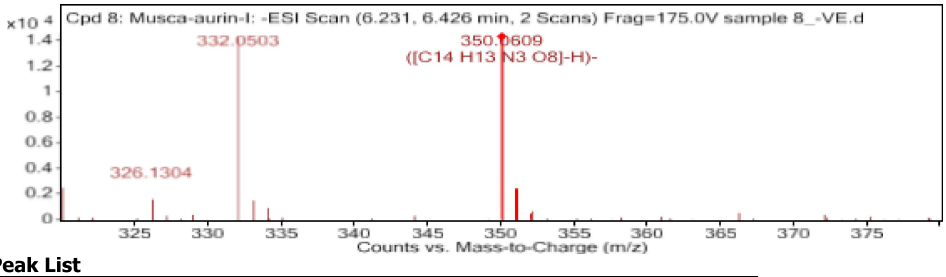
A40 Musca-aurin-I (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 8: Musca-aurin-I	**Musca-aurin-I**	350.0609	6.348	Auto MS/MS	351.0679

MS Spectrum



MS Zoomed Spectrum



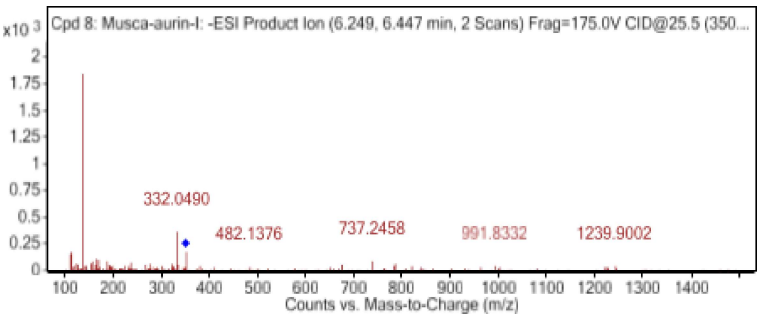
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	I	n
136.0424				7231.41			
332.0503			1	14327.47			
350.0609	350.063	5.92	1	14605.03	C14 H13 N3 O8	(	M-H)-
351.0638	351.066	6.26	1	2175.14	C14 H13 N3 O8	(	M-H)-
352.0606	352.068	21.02	1	762	C14 H13 N3 O8		(M-H)-
899.3022			2	8167.48			
899.8046			2	6012.29			
980.329			2	6645.88			
980.8312			2	4977.77			
1061.3564			2	4421.62			

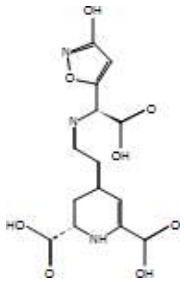
MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
111.0116		161.76
112.0415		185.78
136.0421	1	1851.92
137.0439	1	121.37
154.9865		97.8
164.073		125.6
168.0142		107.8
332.0490		373.88
350.0597		192
737.2458		98.31



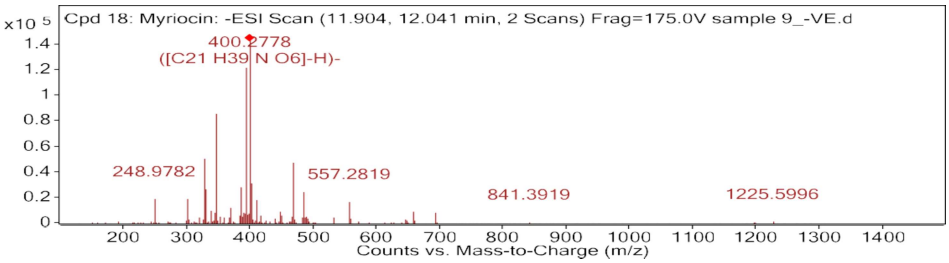
Compound Structure



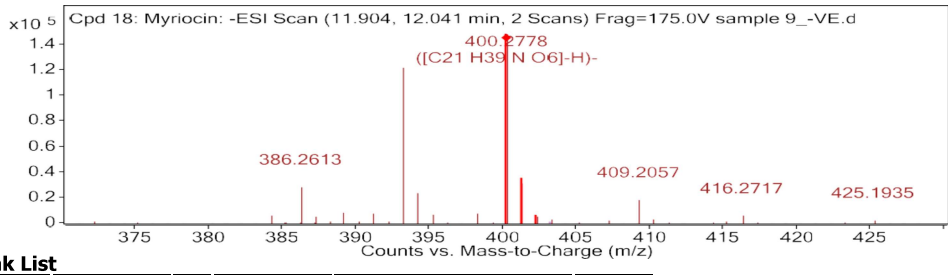
A41 Myriocin (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 18: Myriocin	**Myriocin**	400.2778	11.985	Auto MS/MS	401.2851

MS Spectrum



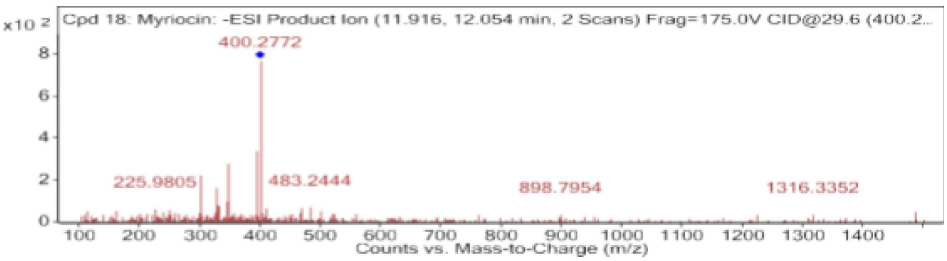
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
327.2237			1	50992.14		
329.2386			1	27642.6		
345.2347			1	86744.67		
386.2613			1	29242.96		
393.2024			1	122783.27		
400.2778	400.2705	-18.36	1	148468.16	C21 H39 N O6	(M-H)-
401.2806	401.2738	-17.02	1	31897.45	C21 H39 N O6	(M-H)-
402.2875	402.2763	-27.72	1	6020.07	C21 H39 N O6	(M-H)-
467.2399			1	48072.08		
483.2437			1	25294.65		

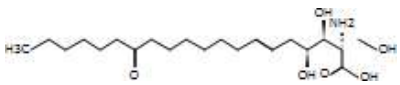
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
301.	1	2068 24.66
327.	1	2226 65.4
329.		2382 3.75
330.		2396 8.41
344.		2495 03.54
345.	1	2331 80.6
346.	1	2393 8.09
393.	1	2017 39.31
400.	1	2772 70.39
401.	1	2763 80.61

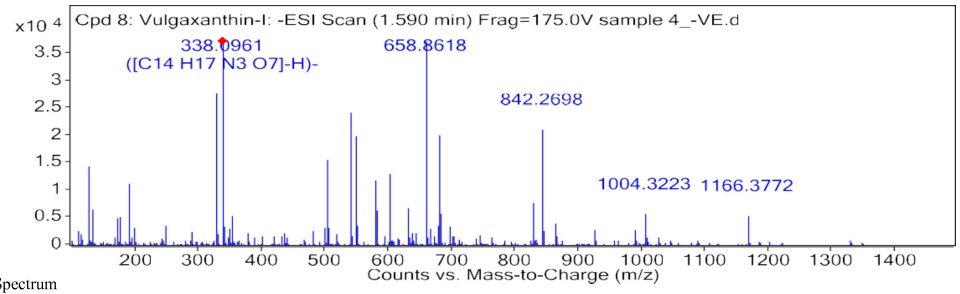
Compound Structure



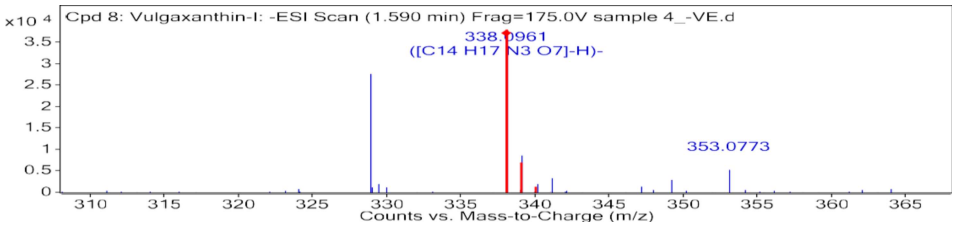
A42 Vulgaxanthin-I (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 8: Vulgaxanthin-I	**Vulgaxanthin-I**	338.0961	1.606	Auto MS/MS	339.1034

MS Spectrum



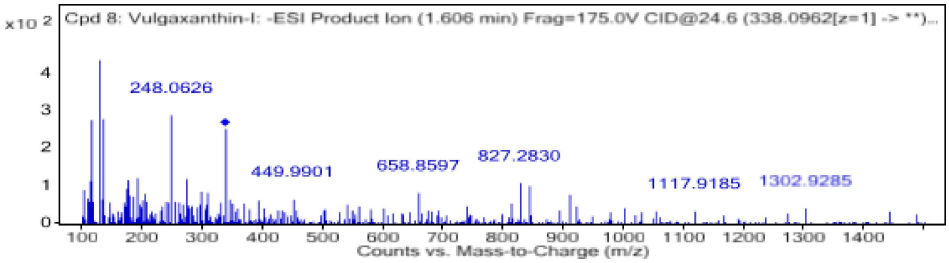
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
328.928			2	27897.27		
338.0961	338.0994	9.8	1	38033.2	C14 H17 N3 O7	(M-H)-
339.0997	339.1024	7.92	1	8903.26	C14 H17 N3 O7	(M-H)-
340.0987	340.1044	16.75	1	2060.19	C14 H17 N3 O7	(M-H)-
503.1678			1	15683.9		
539.1452			1	24349.26		
549.1738			1	19916.54		
658.8618			1	37313.13		
680.2155			1	20204.58		
842.2698			1	21236.89		

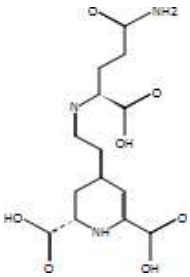
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
113.049		115.69
114.0585	1	276.82
126.9542		436.68
135.0003		278.58
176.0415		116.65
191.0224		123.04
248.0626		290.03
274.013		121.27
338.0972		251.81
827.283		108.86

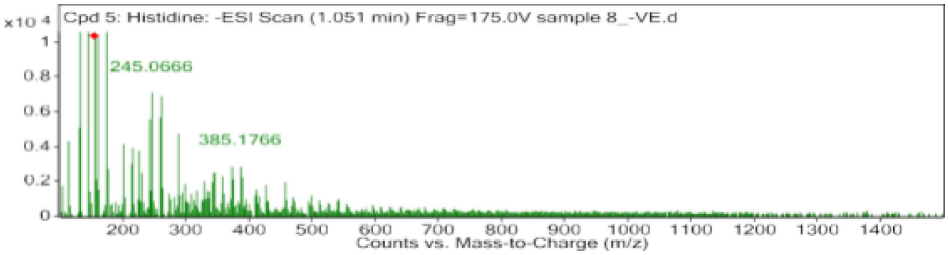
Compound Structure



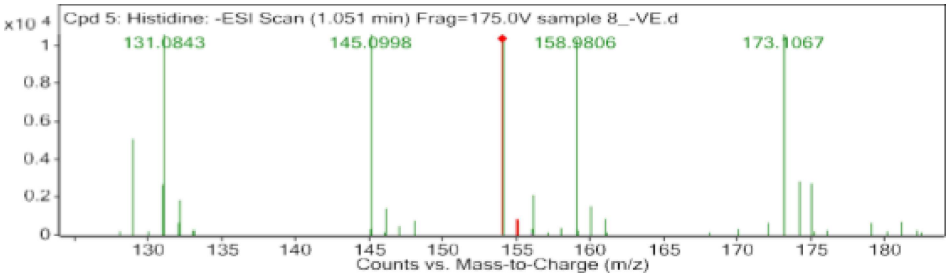
A43 Histidine (AG)

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 5: Histidine	Histidine	154.0638	1.071	Auto MS/MS	155.0712

MS Spectrum



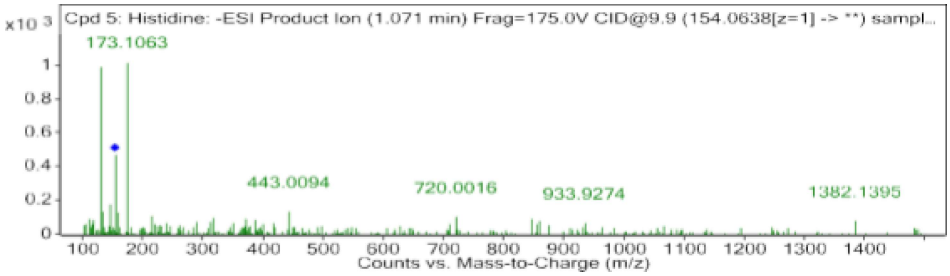
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
131.0843			1	45367.01		
145.0998			1	21084.69		
154.0638	154.0622	-10.54	1	10581.09	C6 H9 N3 O2	(M-H)-
155.0672	155.0647	-16.04	1	820.5	C6 H9 N3 O2	(M-H)-
158.9806			1	10336.71		
173.1067			1	41833		
241.0941				5620.29		
245.0666			1	7120.92		
257.0696				5719.35		
259.0815			1	6906.41		

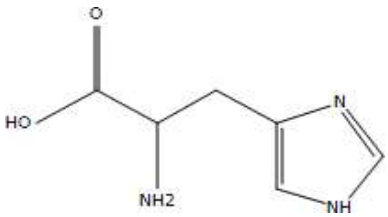
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
131.0841	1	95.45
132.0826		38.41
145.0989		82.08
154.0639	1	474
158.9807		32.32
173.1063		10
215.0155		18.65
316.0336		14.51
443.0094		01.95
720.0016		41.64
		09.23

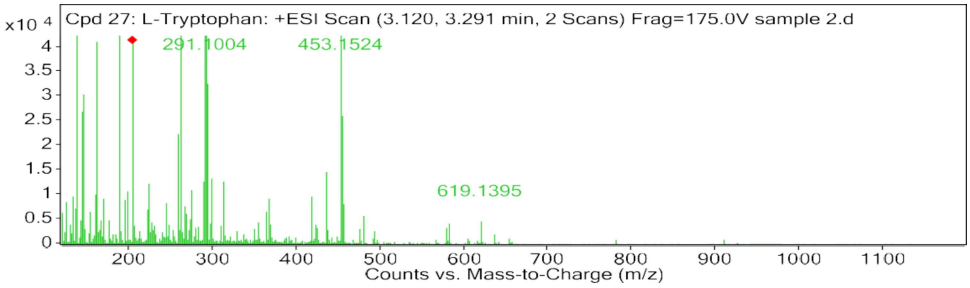
Compound Structure



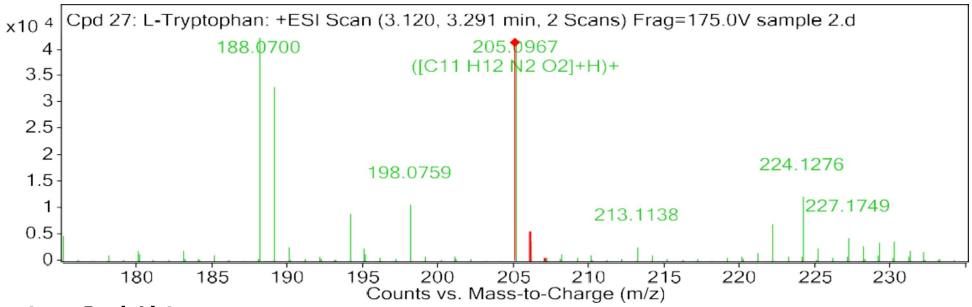
A44 L-Tryptophan (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 27: L-Tryptophan	**L-Tryptophan**	205.0967	3.227	Auto MS/MS	204.0896

MS Spectrum



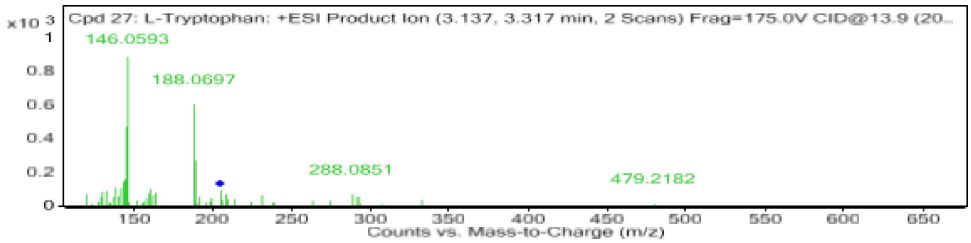
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
137.1066			1	50422.42		
162.0576			1	41249.58		
188.07			1	254621.02		
205.0967	205.0972	2.39	1	42300.05	C11 H12 N2 O2	(M+H)+
206.1006	206.1002	-1.87	1	3933.27	C11 H12 N2 O2	(M+H)+
207.1075	207.1026	-23.82	1	814.5	C11 H12 N2 O2	(M+H)+
261.1437			1	93496.28		
291.1004			1	656632.5		
292.1031			1	83238.99		
453.1524			1	133928.38		

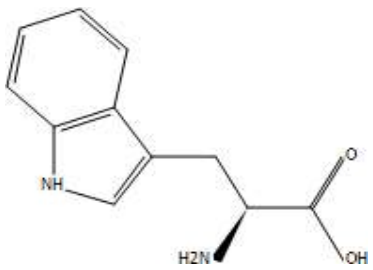
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
138.11		118.15
142.0629		110.5
143.0733		148.31
144.0802	1	165.32
145.0307		477.46
146.0593		893.7
160.0733		106.04
188.0697		608.22
189.0718		276.33
205.0947		101.99

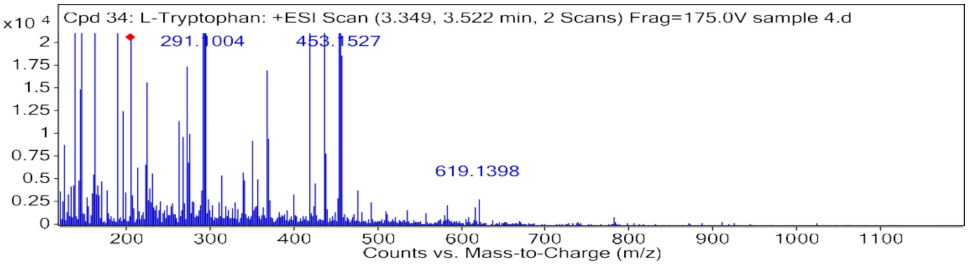
Compound Structure



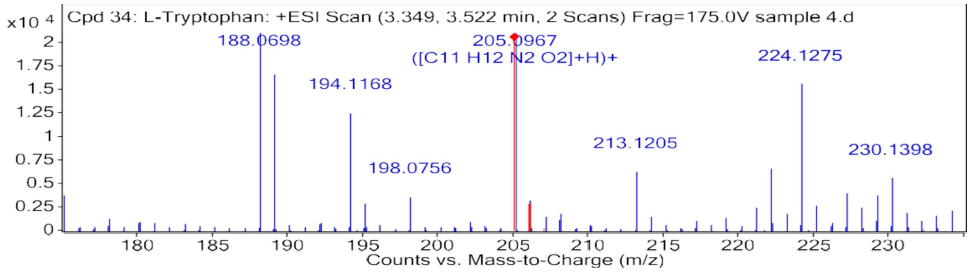
A44 L-Tryptophan (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 34: L-Tryptophan	**L-Tryptophan**	205.0967	3.46	Auto MS/MS	204.0895

MS Spectrum



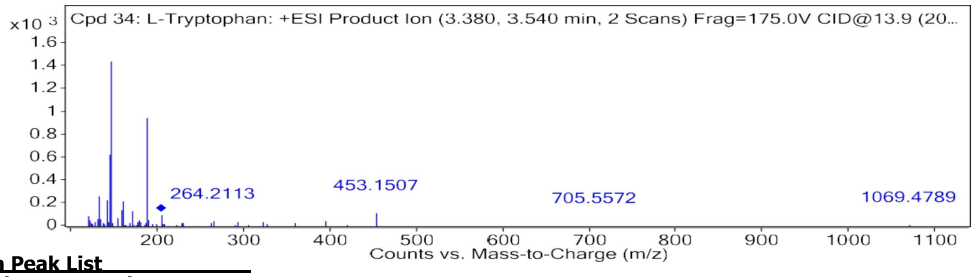
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
137.1066			1	52760.13		
162.0575			1	41062.46		
188.0698			1	127204.59		
205.0967	205.0972	2.38	1	21126.18	C11 H12 N2 O2	(M+H)+
206.1003	206.1002	-0.39	1	3339.46	C11 H12 N2 O2	(M+H)+
291.1004			1	459648.44		
292.1032			1	61383.21		
435.142			1	34865.59		
453.1527			1	300201.91		
454.1554			1	59104.86		

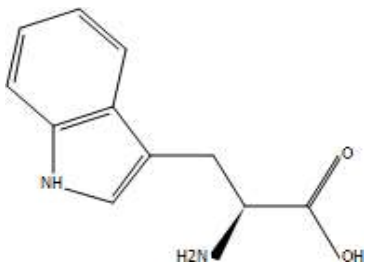
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
132.0801	1	270.58
142.063	1	235.41
144.0796	1	635.26
145.0302		142.33
146.0597	1	1447.82
159.0907		147.06
160.0983		225.3
170.0622		136.31
188.0693	1	955.11
453.1507		122.3

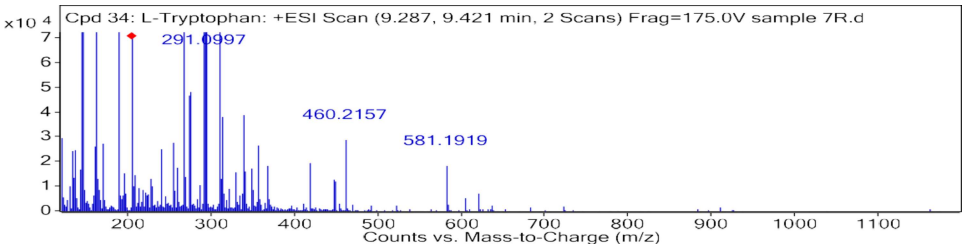
Compound Structure



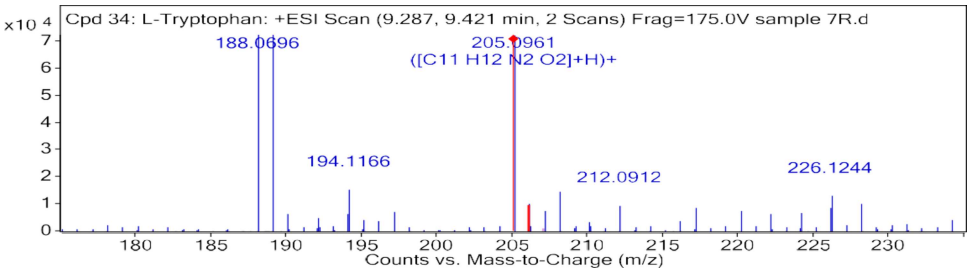
A44 L-Tryptophan (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 34: L-Tryptophan	**L-Tryptophan**	205.0961	9.386	Auto MS/MS	204.0889

MS Spectrum



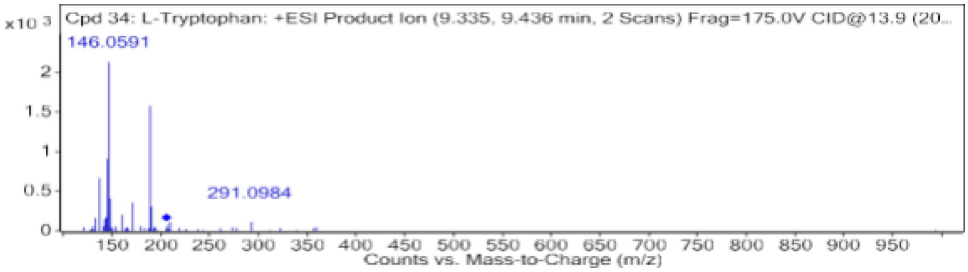
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
146.0593			1	91433.18		
162.0574			1	171418.3		
188.0696			1	638657.13		
205.0961	205.0972	5.37	1	72223.84	C11 H12 N2 O2	(M+H)+
206.1001	206.1002	0.46	1	10422.76	C11 H12 N2 O2	(M+H)+
267.1327			1	86152.41		
291.0997			1	2591159.5		
292.1028			1	301258.22		
293.0982			1	120550.61		
310.1133			1	94870.61		

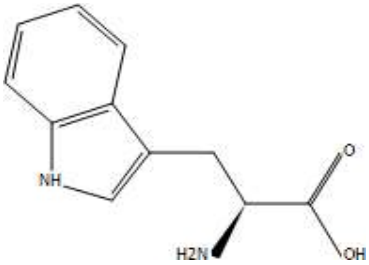
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
136.0603		677
144.0795	1	924.06
145.0299		460.12
145.0809	1	259.08
146.0591	1	2144.17
147.0629	1	419.87
159.0899		223.41
170.06		376.13
188.0692	1	1584.72
189.0721	1	325.29

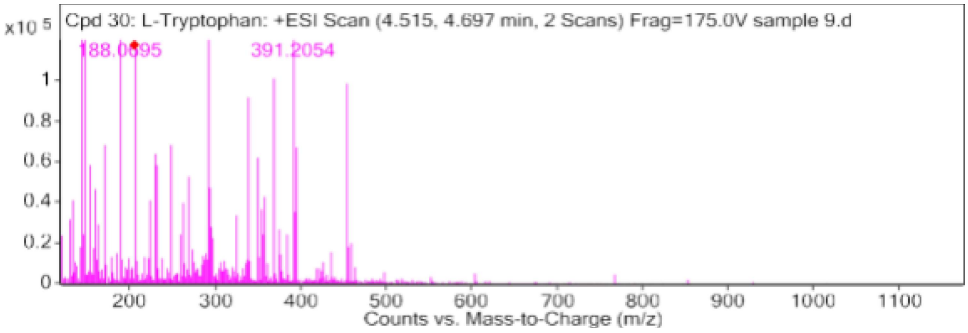
Compound Structure



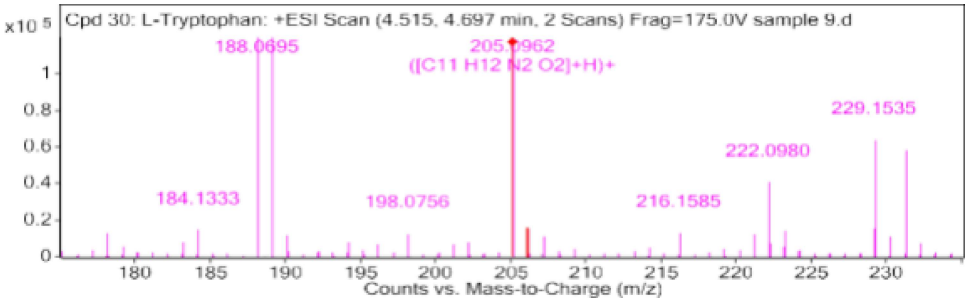
A44 L-Tryptophan (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 30: L-Tryptophan	**L-Tryptophan**	205.0962	4.621	Auto MS/MS	204.089

MS Spectrum



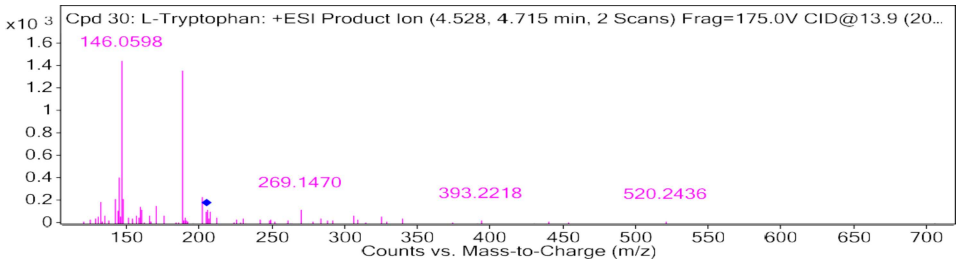
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
144.08			1	210359.22		
146.0594			1	165333.63		
188.0695			1	1092313.38		
189.073			1	136031.59		
205.0962	205.0972	4.79	1	119920.16	C11 H12 N2 O2	(M+H)+
206.0998	206.1002	1.81	1	15364.9	C11 H12 N2 O2	(M+H)+
291.0998			1	369155.94		
367.1482			1	101539.39		
391.2054			1	167993.61		
453.1515			1	98907.63		

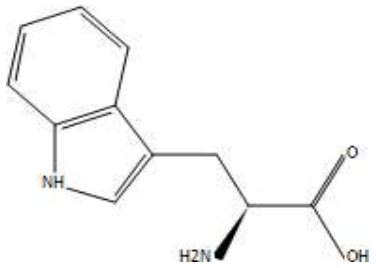
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	*Calc m/z*	Diff (ppm)	z	Abund	Formula	Ion
132.081				200.6		
142.0649				229.53		
144.0809			1	417.45		
146.0598			1	1455.7		
147.0637			1	228.6		
159.0902				156.22		
170.0578				163.87		
188.0701			1	1366.47		
201.0997				240.17		
205.0962	205.0972	4.65		132.33	C11 H12 N2 O2	(M+H)+

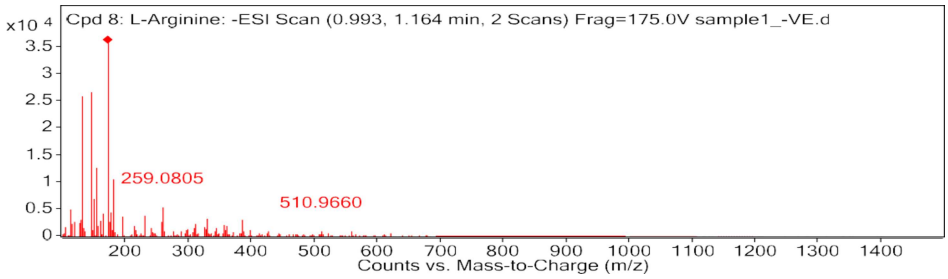
Compound Structure



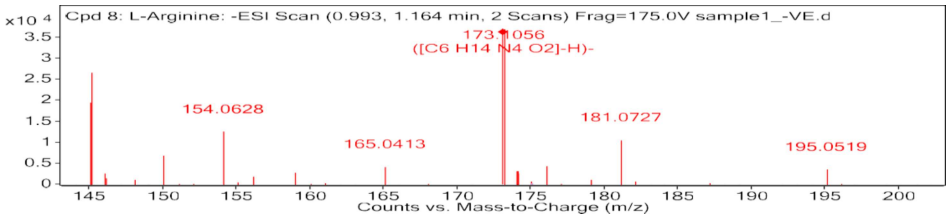
A45 L-Arginine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 8: L-Arginine	**L-Arginine**	173.1056	1.094	Auto MS/MS	174.1129

MS Spectrum



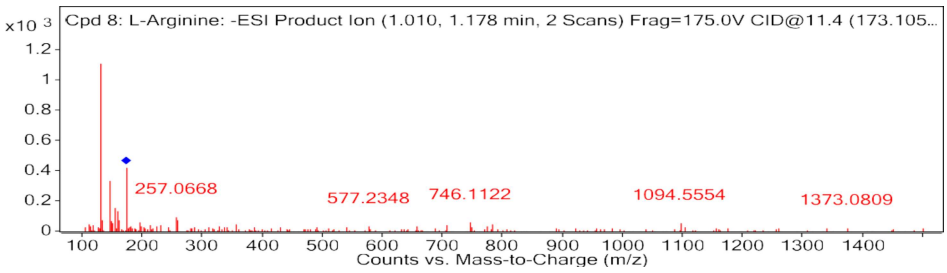
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
131.0472			1	17725.96		
131.0835			1	26077.28		
145.0626			1	19744.25		
145.0989			1	26819.89		
150.0235				6985.04		
154.0628			1	12794.74		
173.1056	173.1044	-6.81	1	37088.89	C6 H14 N4 O2	(M-H)-
174.1081	174.1067	-7.87	1	2885.36	C6 H14 N4 O2	(M-H)-
181.0727			1	10751.24		
259.0805			1	5547.41		

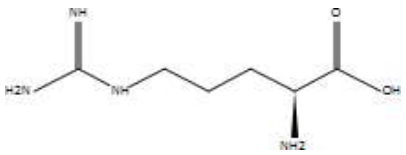
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
131.0464		200.6
131.0837	1	1117.07
132.0866	1	81.84
145.0612		130.59
145.0989	1	341.03
146.047		86.71
154.0623		158.51
158.9797		140.24
173.1058	1	429.56
257.0668		101.25

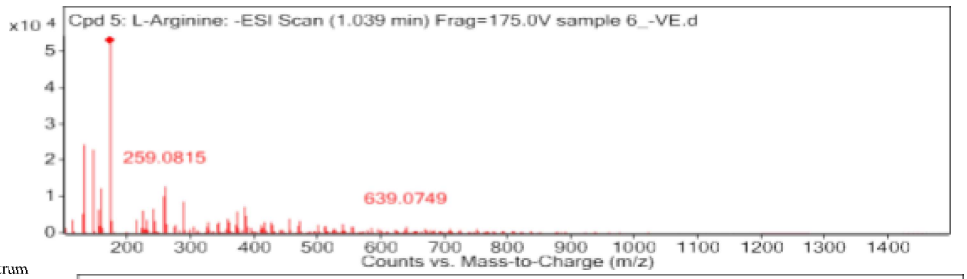
Compound Structure



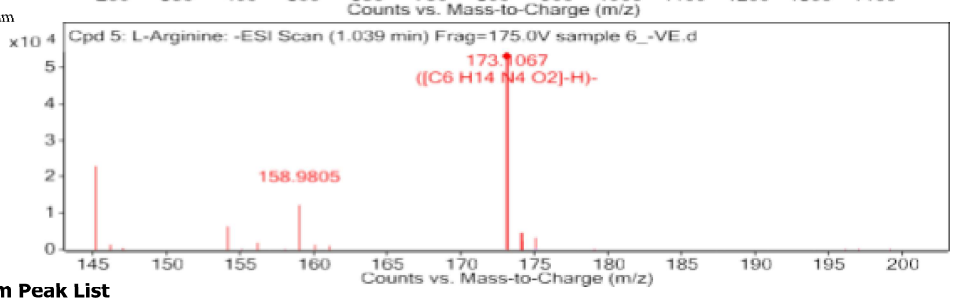
A45 L-Arginine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 5: L-Arginine	**L-Arginine**	173.1067	1.054	Auto MS/MS	174.114

MS Spectrum



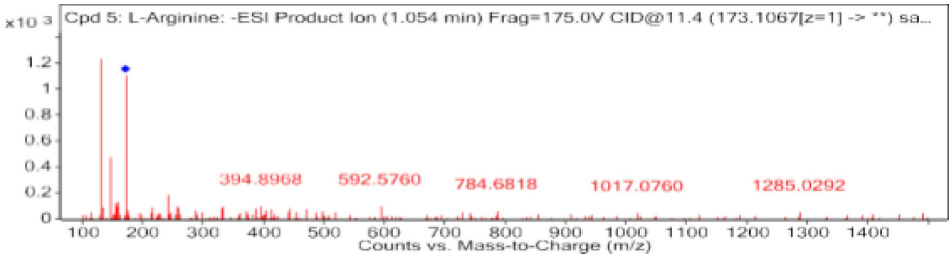
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
131.0842			1	24699.2		
145.0996			1	23278.64		
158.9805			1	12492.91		
173.1067	173.1044	-13.04	1	54258	C6 H14 N4 O2	(M-H)-
174.1097	174.1067	-17.44	1	2731.19	C6 H14 N4 O2	(M-H)-
241.0918				6927.34		
257.0684				10389.05		
259.0815			1	13203.65		
287.0888			1	9076.41		
385.1762			1	7582.11		

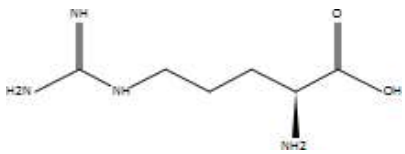
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
131.0846	1	1240.5
145.1003	1	479.04
154.0635		134.18
156.0782		105.13
158.9803		137.32
173.1072		1115.93
241.0952	1	190.68
257.0682	1	106.93
394.8968		102.53
592.576		103.09

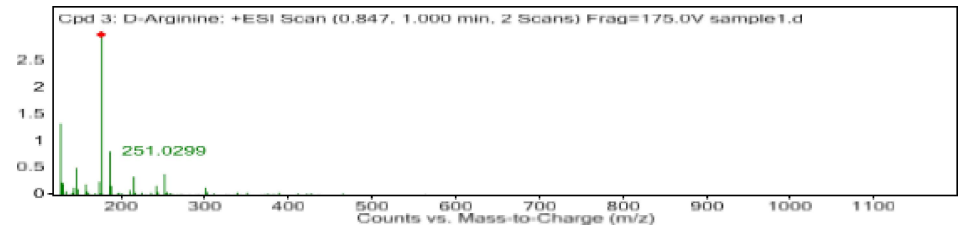
Compound Structure



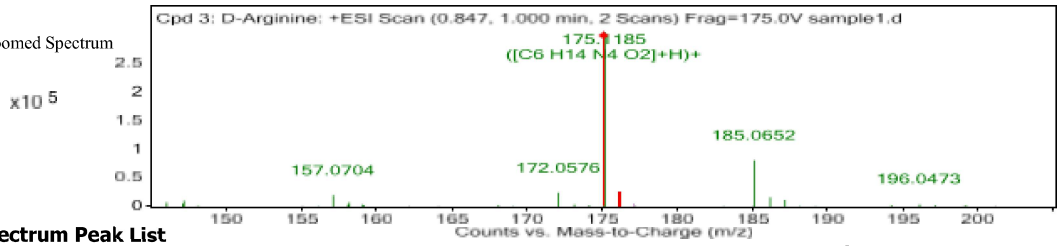
A46 D-Arginine (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 3: D-Arginine	**D-Arginine**	175.1185	0.946	Auto MS/MS	174.1113

MS Spectrum



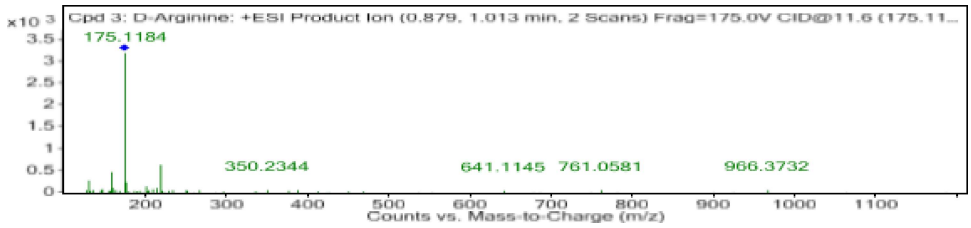
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
127.0234			1	134542.78		
128.0248			1	23692.6		
129.0212			1	22362.37		
145.0341			1	50830.11		
172.0576			1	24668.57		
175.1185	175.119	2.38	1	305963.31	C6 H14 N4 O2	(M+H)+
176.1214	176.1213	-0.94	1	21880.29	C6 H14 N4 O2	(M+H)+
185.0652			1	81831.7		
213.074			1	35301.29		
251.0299			1	39080.08		

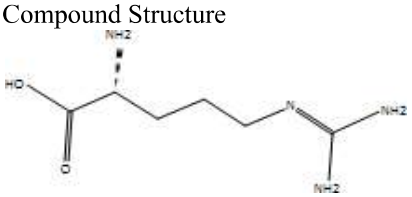
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0971		295.99
147.0315	1	97.23
158.0913	1	476.58
159.0945	1	113.33
175.1184	1	3193.63
176.1207	1	251.18
200.9716		153.14
208.9709		87.72
213.0716		120.4
218.9827	1	655.59

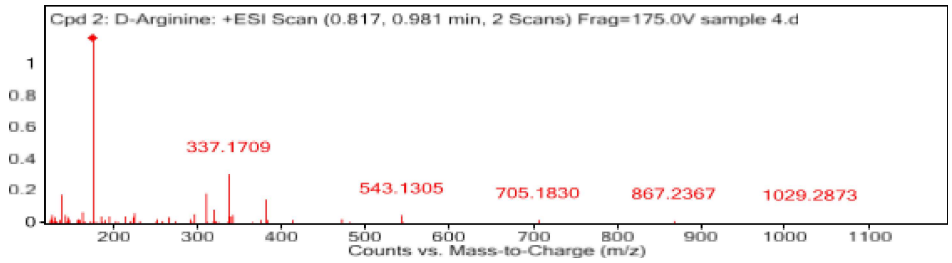
Compound Structure



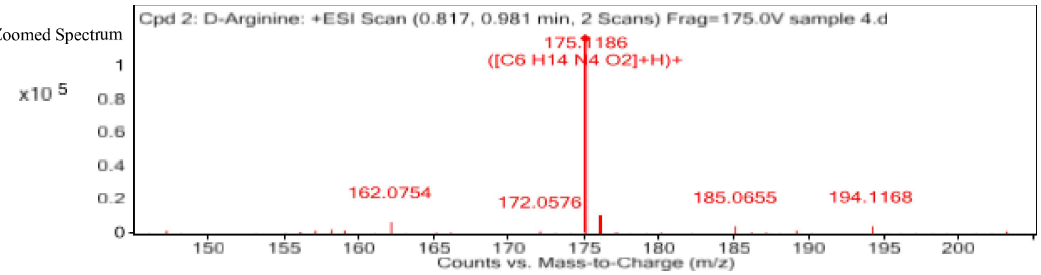
A46 D-Arginine (DG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 2: D-Arginine	**D-Arginine**	175.1186	0.913	Auto MS/MS	174.1113

MS Spectrum



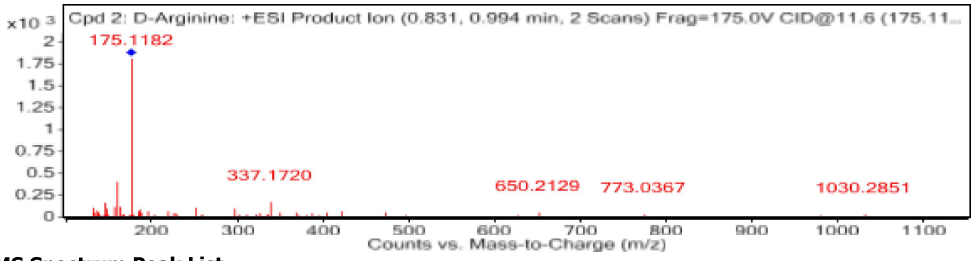
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
137.1068			1	18259.17		
162.0754				7619.16		
175.1186	175.119	2.28	1	118957.3	C6 H14 N4 O2	(M+H)+
176.1214	176.1213	-0.58	1	8965.21	C6 H14 N4 O2	(M+H)+
224.1272			1	6523.39		
296.0654				6363.41		
309.1649			1	19255.32		
319.1599			1	8967.17		
337.1709			1	31214.16		
381.0783			1	15542.62		

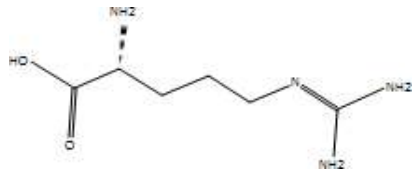
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0955		124.75
145.0344		173.49
156.0401		131.05
158.0893		415.51
162.0743		125.74
175.1182	1	1817.38
176.1202	1	150.88
250.1696		120.17
295.1473		107.33
337.172	1	182.57

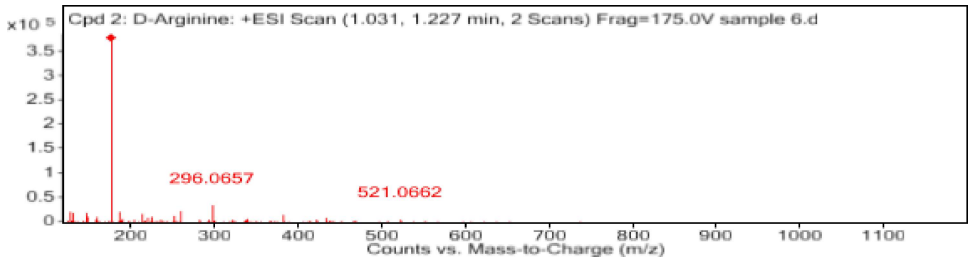
Compound Structure



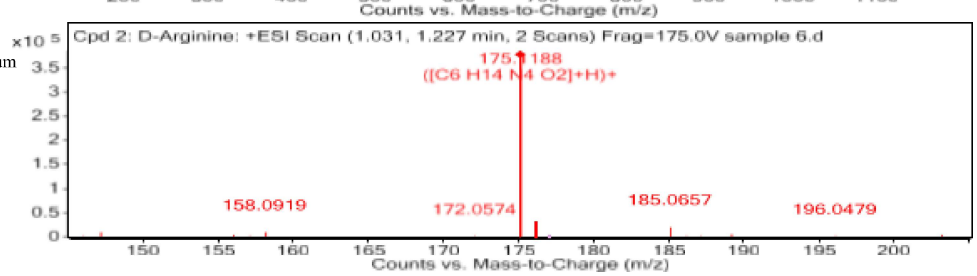
A46 D-Arginine (HG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 2: D-Arginine	**D-Arginine**	175.1188	1.141	Auto MS/MS	174.1116

MS Spectrum



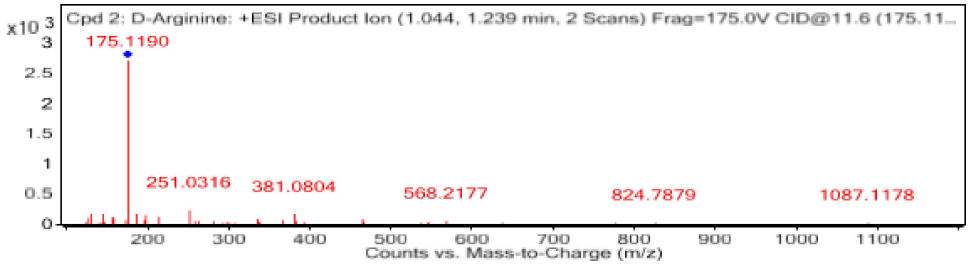
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
127.0237			1	20997.25		
130.0862			1	19371.83		
145.0344			1	20506.11		
175.1188	175.119	0.62	1	384877.69	C6 H14 N4 O2	(M+H)+
176.1218	176.1213	-3.34	1	28176.55	C6 H14 N4 O2	(M+H)+
185.0657			1	22628.17		
213.0745			1	17270.04		
258.1101			1	24257.74		
296.0657			1	34923		
381.0788			1	15170.67		

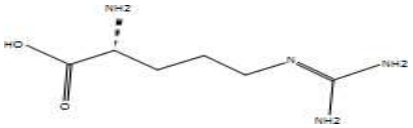
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	*Calc m/z*	Diff (ppm)	z	Abund	Formula	Ion
130.0947				203.89		
145.0342			1	194.51		
156.0407				139.56		
175.119			1	2730.6		
176.1218	176.1213	-3.16	1	148.68	C6 H14 N4 O2	(M+H)+
185.0635				202.78		
197.0985				175.37		
213.0734				149.97		
251.0316			1	261.05		
381.0804				191.28		

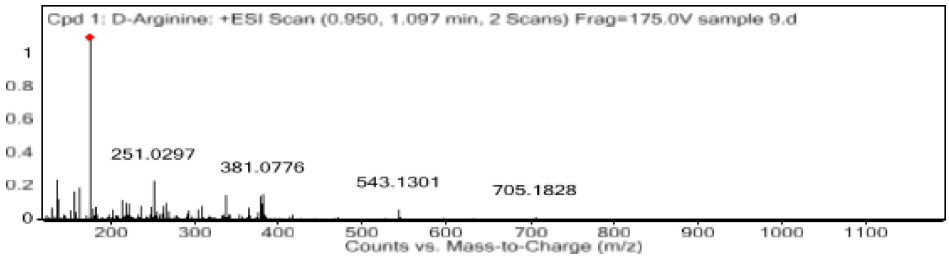
Compound Structure



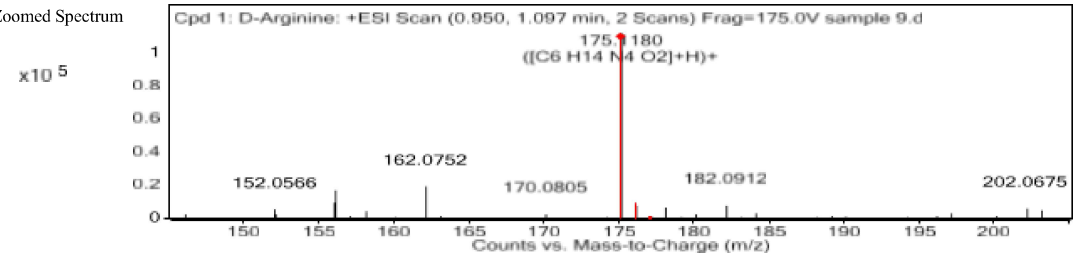
A46 D-Arginine (AG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 1: D-Arginine	**D-Arginine**	175.118	1.037	Auto MS/MS	174.1108

MS Spectrum



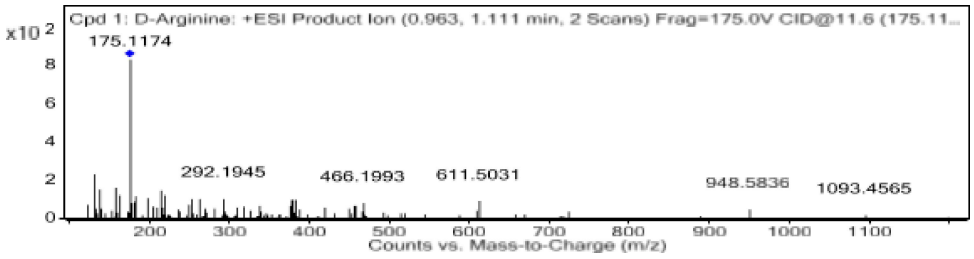
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
136.0613			1	24464.57		
156.1009				17148.16		
162.0752				19462.32		
175.118	175.119	5.27	1	112442	C6 H14 N4 O2	(M+H)+
176.1211	176.1213	0.94	1	8111.91	C6 H14 N4 O2	(M+H)+
177.1229	177.1233	1.99	1	1185.95	C6 H14 N4 O2	(M+H)+
251.0297				23554.62		
337.1703			1	14989.29		
378.0606			1	14263.67		
381.0776			1	15539.78		

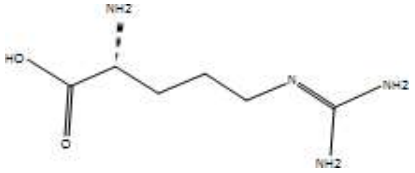
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
130.0967		236.39
136.0591		154.67
156.0733		121.94
156.101	1	165.79
162.0731		125.59
175.1174	1	833.16
181.9481		110.77
181.9769		120.37
213.0717		147.35
218.1369		126.8

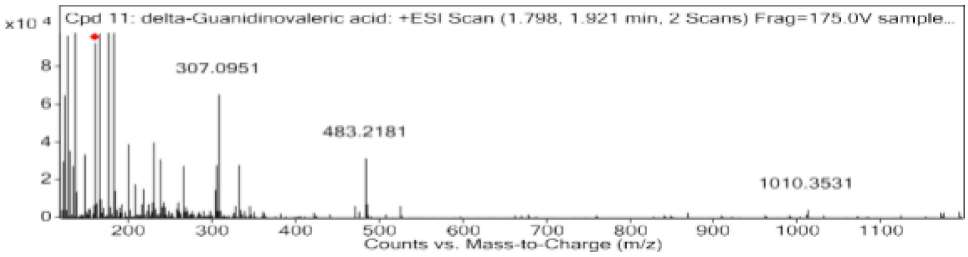
Compound Structure

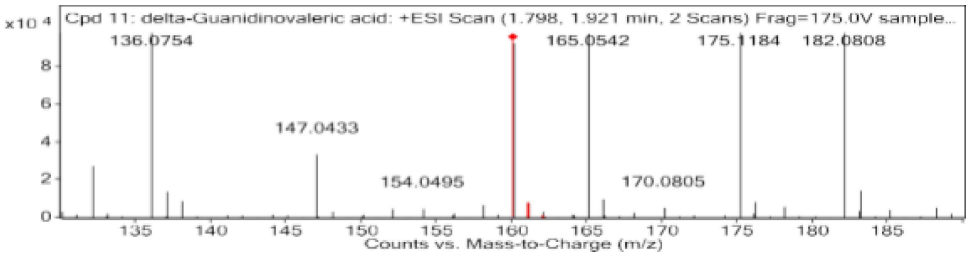


A47 delta-Guanidinovaleric acid (FG)

Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 11: delta-Guanidinovaleric acid	**delta-Guanidinovaleric acid**	160.1075	1.88	Auto MS/MS	159.1003

MS Spectrum



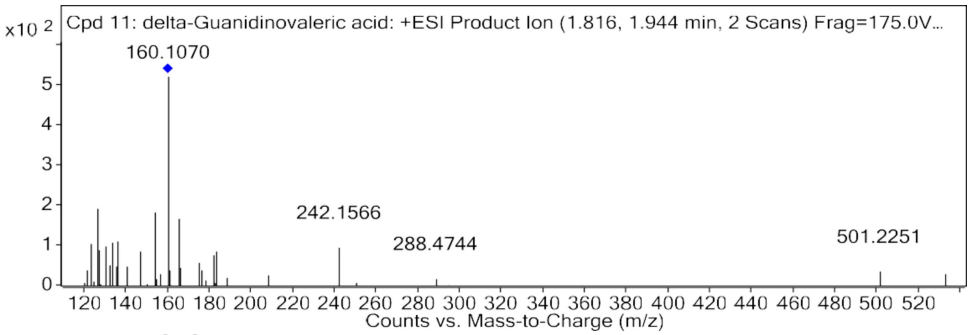


MS Zoomed Spectrum

MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
123.0434			1	64869.4		
126.0659			1	96804.41		
136.0754			1	165782.88		
160.1075	160.1081	3.28	1	92691.31	C6 H13 N3 O2	(M+H)+
161.1103	161.1106	2.05	1	8091.29	C6 H13 N3 O2	(M+H)+
162.1123	162.1126	1.71	1	1032.5	C6 H13 N3 O2	(M+H)+
165.0542			1	97882.13		
175.1184			1	117772.3		
182.0808			1	148789.78		
307.0951			1	65549.48		

MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
123.0449		107.74
126.0662		193.5
127.0372		91.09
130.0463		100.41
133.1026		109.26
136.074		113.58
154.0494		185.52
160.107	1	523.93
165.0564		170.44
242.1566		96.88

Compound Structure