

# Determination of Major, Minor and Chiral Components as Quality and Authenticity Markers of *Rosa damascena* Oil by GC-FID

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## Validation Data

Table S1: Resolution (Rs), recovery excess (RE) in % for authentic rose oil (RO) samples originating from Bulgaria (BG), Morocco (MA) and Turkey (TR) as well as lavender, rosemary, lemon and caraway oil. The RE is presented as the mean value with standard deviation. The number of repeated measurements are given with n. Samples were analysed on a DB-wax column.

Analyte	Rs	RE Authentic RO [%] (n=5)		RE RO <sub>BG</sub> [%] (n=3)	RE RO <sub>MA</sub> [%] (n=3)	RE RO <sub>TR</sub> [%] (n=3)	RE RO <sub>real</sub> [%] (n=3)	RE Lavender [%] (n=2)	RE Rosemary [%] (n=2)	RE Lemon [%] (n=2)	RE Caraway [%] (n=2)
		QC <sub>high</sub>	QC <sub>low</sub>								
<b>α-pinene</b>	16.1	104,5 ± 9.8	110,0 ± 3.2	94,6 ± 2.0	99,5 ± 7.3	87,8 ± 2.2	92,5 ± 1.2	99,0 ± 2.7	111,3 ± 4.7	98,6 ± 1.5	101,7 ± 3.1
<b>Camphene</b>	12.3	107,1 ± 8.4	107,3 ± 12.9	104,4 ± 4.4	111,2 ± 3.3	101,3 ± 3.5	109,3 ± 4.5	104,3 ± 2.3	133,3 ± 9.4	119,2 ± 4.8	110,9 ± 0.0
<b>(-)-β-pinene</b>	22.7	107,2 ± 11.7	119,9 ± 3.9	95,3 ± 3.0	99,1 ± 9.5	86,5 ± 3.5	91,2 ± 3.0	90,6 ± 7.5	142,0 ± 14.6	133,3 ± 11.5	103,0 ± 3.5
<b>α-terpinene</b>	6.0	106,5 ± 15.7	88,3 ± 10.3	91,9 ± 1.7	98,3 ± 9.2	86,6 ± 3.1	89,9 ± 2.6	95,7 ± 1.6	105,6 ± 4.5	101,6 ± 1.7	105,0 ± 5.7
<b>limonene</b>	28.3	104,7 ± 13.6	84,2 ± 5.9	89,6 ± 1.7	99,5 ± 10.7	82,6 ± 4.0	90,2 ± 1.5	91,6 ± 2.3	126,6 ± 13.0	259,3 ± 10.8	568,4 ± 131.2
<b>p-cymene</b>	34.1	104,6 ± 12.9	114,0 ± 6.1	94,3 ± 2.8	98,1 ± 9.9	90,2 ± 1.5	88,1 ± 1.6	104,4 ± 4.0	116,2 ± 8.1	97,6 ± 0.5	107,9 ± 5.3
<b>(+/-)-rose oxide</b>	17.6	103,7 ± 16.7	114,6 ± 5.6	90,7 ± 1.9	85,7 ± 2.7	80,0 ± 1.8	84,2 ± 3.0	96,0 ± 2.4	101,9 ± 4.4	92,7 ± 0.4	103,4 ± 5.5
<b>cis-3-hexen-1-ol</b>	85.8	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
<b>linalool</b>	11.3	104,1 ± 16.8	99,4 ± 8.6	85,9 ± 3.0	94,1 ± 6.7	83,2 ± 2.2	84,8 ± 3.4	93,8 ± 6.8	104,5 ± 6.0	93,0 ± 1.2	103,9 ± 5.5
<b>β-caryophyllene</b>	16.8	95,5 ± 16.2	97,2 ± 15.9	80,5 ± 1.2	85,3 ± 7.5	100,2 ± 2.0	82,5 ± 6.9	73,3 ± 2.1	123,0 ± 26.2	85,5 ± 1.7	104,2 ± 5.1
<b>β-damascenone</b>	6.3	94,6 ± 16.6	103,5 ± 3.7	87,5 ± 7.8	85,1 ± 5.7	87,5 ± 1.7	85,7 ± 4.6	92,8 ± 0.8	105,5 ± 14.2	99,2 ± 8.4	111,9 ± 6.6
<b>citronellyl acetate</b>	4.0	96,7 ± 13.6	116,5 ± 14.5	81,9 ± 0.9	92,2 ± 5.6	82,8 ± 1.2	83,6 ± 3.7	95,9 ± 0.3	110,2 ± 10.9	101,8 ± 8.9	111,8 ± 8.5
<b>citral</b>	14.2	102,6 ± 16.5	119,2 ± 9.3	86,1 ± 7.4	85,1 ± 8.3	87,7 ± 1.5	83,1 ± 9.0	91,2 ± 2.3	108,6 ± 9.3	112,7 ± 4.7	107,6 ± 7.4
<b>neryl acetate</b>	8.5	93,2 ± 14.5	115,5 ± 13.5	85,0 ± 1.8	92,8 ± 8.0	81,4 ± 0.5	84,3 ± 6.7	92,6 ± 0.1	105,2 ± 7.7	105,1 ± 0.6	750,9 ± 161.1
<b>geranyl acetate</b>	4.8	106,9 ± 12.1	103,2 ± 11.8	81,7 ± 2.7	81,1 ± 4.5	93,5 ± 1.8	84,8 ± 8.6	115,6 ± 0.8	92,9 ± 3.4	82,4 ± 8.8	90,6 ± 5.0
<b>citronellol</b>	10.6	110,2 ± 9.5	82,6 ± 18.8	109,6 ± 3.6	88,8 ± 5.5	87,0 ± 2.6	113,3 ± 10.2	92,9 ± 0.8	98,5 ± 6.4	87,9 ± 0.0	101,9 ± 6.4
<b>nerol</b>	2.4	93,9 ± 17.7	104,3 ± 10.0	104,1 ± 3.2	92,7 ± 4.9	92,8 ± 1.6	88,1 ± 6.5	95,3 ± 0.4	96,8 ± 6.3	93,1 ± 6.7	100,2 ± 6.2
<b>phenylethanol</b>	13.0	103,6 ± 17.4	119,1 ± 9.3	101,4 ± 4.2	98,6 ± 5.1	85,0 ± 1.0	95,5 ± 4.4	105,5 ± 0.4	109,7 ± 6.1	101,2 ± 2.4	109,0 ± 5.2
<b>geraniol</b>	44.0	93,9 ± 16.3	110,7 ± 11.0	103,2 ± 3.2	83,9 ± 4.8	87,3 ± 1.4	82,3 ± 7.1	89,5 ± 1.2	94,6 ± 6.7	84,1 ± 0.1	98,5 ± 6.4
<b>methyleugenol</b>	38.6	91,8 ± 18.0	90,8 ± 10.1	81,9 ± 1.8	83,0 ± 5.5	82,0 ± 2.9	85,3 ± 11.4	90,5 ± 0.4	97,6 ± 7.3	83,7 ± 1.0	104,5 ± 5.9
<b>eugenol</b>	47.6	110,5 ± 11.1	100,8 ± 14.7	104,7 ± 1.3	92,4 ± 3.2	96,7 ± 1.1	99,9 ± 4.5	95,4 ± 0.6	107,9 ± 14.2	93,9 ± 0.7	115,1 ± 8.8
<b>farnesol</b>	0	87,5 ± 30.1	96,0 ± 17.8	97,6 ± 4.7	89,5 ± 15.7	116,3 ± 15.7	88,1 ± 9.8	99,1 ± 2.8	110,9 ± 12.2	101,6 ± 7.1	125,3 ± 10.9

Table S2: Resolution (Rs), recovery excess (RE) in % for authentic rose oil (RO) samples originating from Bulgaria (BG), Morocco (MA) and Turkey (TR) as well as lavender, rosemary, lemon and caraway oil. The RE is presented as the mean value with standard deviation. The number of repeated measurements are given with n. Samples were analysed on a chiral column.

Analyte	Rs	RE Authentic RO [%] (n=5)		RE RO <sub>BG</sub> [%] (n=3)	RE RO <sub>MA</sub> [%] (n=3)	RE RO <sub>TR</sub> [%] (n=3)	RE RO <sub>real</sub> [%] (n=3)	RE Lavender [%] (n=3)	RE Rosemary [%] (n=3)	RE Lemon [%] (n=3)	RE Caraway [%] (n=3)
		QC <sub>high</sub>	QC <sub>low</sub>								
(+)- $\alpha$ -pinene	2.4	91,2 $\pm$ 0.9	88,0 $\pm$ 0.8	87,7 $\pm$ 0.2	92,2 $\pm$ 0.8	89,3 $\pm$ 0.5	92,4 $\pm$ 4.1	94,4 $\pm$ 8.4	96,5 $\pm$ 3.3	90,7 $\pm$ 0.9	87,8 $\pm$ 2.9
(+/-)-camphene	5.9	100,2 $\pm$ 1.6	118,3 $\pm$ 3.2	104,7 $\pm$ 1.4	109,2 $\pm$ 1.5	104,3 $\pm$ 2.2	111,6 $\pm$ 1.3	116,0 $\pm$ 6.5	116,3 $\pm$ 5.8	117,3 $\pm$ 4.8	100,4 $\pm$ 1.9
(+/-)-camphene	12.0	91,7 $\pm$ 6.3	107,3 $\pm$ 3.5	92,0 $\pm$ 4.3	98,0 $\pm$ 1.0	91,9 $\pm$ 1.5	95,3 $\pm$ 4.3	104,6 $\pm$ 12.4	98,7 $\pm$ 12.4	94,3 $\pm$ 4.5	87,1 $\pm$ 5.5
(-)- $\beta$ -pinene	28.6	91,1 $\pm$ 1.8	105,3 $\pm$ 10.5	91,6 $\pm$ 1.1	96,6 $\pm$ 0.8	93,4 $\pm$ 0.4	95,6 $\pm$ 4.7	100,3 $\pm$ 9.6	105,4 $\pm$ 11.4	83,5 $\pm$ 18.0	89,0 $\pm$ 3.3
cis-3-hexen-1-ol	8.3	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
$\alpha$ -terpinene	7.9	91,9 $\pm$ 1.5	100,8 $\pm$ 2.6	91,9 $\pm$ 4.2	92,5 $\pm$ 4.6	89,6 $\pm$ 1.5	94,8 $\pm$ 3.0	93,9 $\pm$ 6.2	99,2 $\pm$ 12.8	95,6 $\pm$ 7.7	90,8 $\pm$ 3.4
limonene	1.2	99,7 $\pm$ 4.8	119,8 $\pm$ 2.9	88,5 $\pm$ 1.9	101,5 $\pm$ 7.5	91,1 $\pm$ 2.4	97,2 $\pm$ 4.9	98,1 $\pm$ 4.6	108,2 $\pm$ 24.3	54,6 $\pm$ 101.9	229,5 $\pm$ 102.2
p-cymene	30.6	97,2 $\pm$ 3.9	116,1 $\pm$ 1.9	89,8 $\pm$ 1.3	89,7 $\pm$ 3.0	90,6 $\pm$ 0.9	88,8 $\pm$ 1.8	86,1 $\pm$ 18.8	87,7 $\pm$ 13.3	36,7 $\pm$ 7.4	252,1 $\pm$ 420.3
(+)-rose oxide	1.5	96,4 $\pm$ 2.0	106,5 $\pm$ 5.9	88,7 $\pm$ 0.7	96,7 $\pm$ 1.4	91,5 $\pm$ 0.1	96,6 $\pm$ 4.7	93,6 $\pm$ 6.2	103,0 $\pm$ 3.1	92,0 $\pm$ 4.0	107,7 $\pm$ 6.0
(-)-rose oxide	27.1	98,7 $\pm$ 1.6	112,6 $\pm$ 5.1	91,4 $\pm$ 1.2	96,5 $\pm$ 2.1	93,6 $\pm$ 0.3	97,4 $\pm$ 3.7	93,6 $\pm$ 1.8	96,9 $\pm$ 1.8	94,1 $\pm$ 4.3	95,5 $\pm$ 3.6
(+/-)-linalool	6.7	95,1 $\pm$ 1.5	87,5 $\pm$ 3.9	86,5 $\pm$ 1.5	91,3 $\pm$ 1.2	88,4 $\pm$ 1.7	93,7 $\pm$ 7.5	128,5 $\pm$ 88.5	97,4 $\pm$ 2.6	94,4 $\pm$ 3.1	89,9 $\pm$ 3.7
(+/-)-linalool	58.4	95,3 $\pm$ 1.3	110,4 $\pm$ 3.1	86,6 $\pm$ 1.4	92,3 $\pm$ 0.8	89,1 $\pm$ 1.4	94,8 $\pm$ 6.7	90,4 $\pm$ 3.8	94,7 $\pm$ 1.7	89,0 $\pm$ 1.7	94,7 $\pm$ 4.2
phenylethanol	6.7	91,7 $\pm$ 1.8	92,0 $\pm$ 1.5	88,8 $\pm$ 0.8	89,9 $\pm$ 3.1	87,9 $\pm$ 3.1	92,2 $\pm$ 4.0	82,8 $\pm$ 3.4	90,5 $\pm$ 0.6	91,1 $\pm$ 2.6	85,5 $\pm$ 3.6
cis/trans-citral	9.0	107,8 $\pm$ 2.3	117,7 $\pm$ 7.1	93,0 $\pm$ 2.8	98,4 $\pm$ 6.1	86,2 $\pm$ 5.8	96,3 $\pm$ 8.7	81,0 $\pm$ 2.2	91,3 $\pm$ 5.0	89,5 $\pm$ 7.2	104,0 $\pm$ 13.7
(+/-)-citronellol	0.9	103,7 $\pm$ 3.7	107,4 $\pm$ 2.6	106,1 $\pm$ 5.3	117,6 $\pm$ 10.7	106,5 $\pm$ 7.4	95,9 $\pm$ 10.6	103,8 $\pm$ 3.6	97,6 $\pm$ 3.4	100,2 $\pm$ 3.2	99,5 $\pm$ 5.8
(+/-)-citronellol	2.2	103,0 $\pm$ 2.7	118,6 $\pm$ 13.0	90,5 $\pm$ 4.9	104,6 $\pm$ 9.4	99,1 $\pm$ 9.1	84,8 $\pm$ 9.1	101,1 $\pm$ 4.3	103,5 $\pm$ 2.9	99,5 $\pm$ 2.4	95,3 $\pm$ 3.2
nerol	7.7	94,5 $\pm$ 1.5	103,0 $\pm$ 5.3	89,9 $\pm$ 2.2	94,2 $\pm$ 4.4	101,0 $\pm$ 2.5	98,7 $\pm$ 12.8	92,5 $\pm$ 3.2	96,9 $\pm$ 2.2	94,3 $\pm$ 2.8	111,3 $\pm$ 35.4

<b>cis/trans-citral</b>	7.3	103,2 ± 3.2	117,0 ± 2.2	99,7 ± 3.7	104,8 ± 7.9	97,7 ± 3.7	104,2 ± 8.2	98,5 ± 8.1	96,8 ± 3.8	95,4 ± 8.5	96,1 ± 8.0
<b>geraniol</b>	5.9	94,5 ± 1.5	112,2 ± 4.7	87,5 ± 3.4	93,9 ± 1.6	98,3 ± 1.4	99,1 ± 9.6	92,4 ± 4.1	92,6 ± 2.1	90,2 ± 2.7	88,4 ± 4.3
<b>(+/-)-citronellyl acetate</b>	0.8	107,0 ± 5.7	110,8 ± 4.7	89,0 ± 3.7	110,7 ± 11.0	85,4 ± 4.4	88,6 ± 17.8	103,7 ± 8.9	103,2 ± 3.9	98,8 ± 4.6	116,4 ± 19.8
<b>(+/-)-citronellyl acetate</b>	4.1	109,0 ± 2.5	117,6 ± 3.0	91,6 ± 2.3	101,9 ± 8.9	94,5 ± 4.2	100,7 ± 8.5	89,6 ± 9.3	107,4 ± 3.5	97,9 ± 13.6	89,8 ± 11.5
<b>neryl acetate</b>	6.5	95,3 ± 2.0	108,2 ± 1.5	92,4 ± 3.1	97,4 ± 1.7	89,7 ± 2.6	90,8 ± 11.1	92,8 ± 9.6	94,0 ± 1.7	92,9 ± 3.7	88,5 ± 6.5
<b>(cis/trans)-β-damascenone</b>	8.4	97,6 ± 2.2	86,3 ± 0.0	99,4 ± 3.2	105,7 ± 11.5	85,0 ± 6.9	94,8 ± 11.7	86,7 ± 6.0	100,4 ± 9.0	89,2 ± 12.2	85,6 ± 0.6
<b>geranyl acetate</b>	0.7	93,3 ± 8.7	109,6 ± 4.7	81,7 ± 3.9	80,2 ± 1.4	81,2 ± 3.2	87,6 ± 10.6	91,2 ± 4.0	84,8 ± 3.1	103,1 ± 18.4	103,7 ± 2.3
<b>β-caryophyllene</b>	1.9	101,0 ± 11.8	110,3 ± 3.3	93,5 ± 0.6	92,4 ± 3.6	88,4 ± 2.7	93,6 ± 3.3	95,0 ± 9.1	109,5 ± 9.9	113,9 ± 15.2	99,1 ± 1.8
<b>(cis/trans)-β-damascenone</b>	4.0	96,9 ± 3.0	119,4 ± 3.5	91,7 ± 4.4	92,1 ± 5.2	89,8 ± 5.1	86,7 ± 6.7	90,7 ± 5.8	90,4 ± 2.3	93,2 ± 10.2	88,6 ± 10.2
<b>β-damascone</b>	7.6	95,9 ± 2.3	96,9 ± 3.0	93,5 ± 3.3	97,9 ± 1.4	92,6 ± 2.8	93,1 ± 4.7	92,7 ± 4.0	94,1 ± 2.3	94,4 ± 4.2	90,5 ± 3.4
<b>eugenol</b>	11.6	97,3 ± 2.3	85,5 ± 13.2	91,5 ± 4.8	95,9 ± 1.7	102,8 ± 2.7	108,9 ± 9.6	91,9 ± 3.6	96,9 ± 2.7	94,5 ± 4.2	91,2 ± 3.3
<b>methyleugenol</b>	76.1	95,2 ± 1.8	83,8 ± 12.6	91,0 ± 4.1	98,4 ± 1.1	101,6 ± 3.7	102,7 ± 9.9	94,7 ± 3.3	99,3 ± 2.5	96,1 ± 4.4	93,4 ± 4.0
<b>farnesol</b>	0	95,8 ± 1.6	108,1 ± 10.1	97,4 ± 20.8	120,0 ± 4.9	113,9 ± 8.5	118,3 ± 19.8	102,8 ± 17.8	117,6 ± 7.1	114,5 ± 6.2	114,7 ± 4.9

Table S3: Results for robustness testing on the DB-wax column.

	Analyte	$\alpha$ -pinene	Camphene	(-)- $\beta$ -pinene	$\alpha$ -terpinene	limonene	p-cymene	(+/-)-rose oxide	cis-3-hexen-1-ol	linalool	$\beta$ -caryophyllene	$\beta$ -damascenone
Standard method	RT [min]	4.25	5.36	6.84	10.98	12.43	18.28	22.52	24.03	29.00	29.83	31.17
	R <sub>s</sub>	16.1	12.3	22.7	6.0	28.3	34.1	17.6	85.8	11.3	16.8	6.3
FID temp. 275 °C	Fold change	1,02	1,03	1,01	1,03	1,01	1,01	1,04	1,00	1,04	1,04	1,18
FID temp. 225 °C	Fold change	0,95	0,96	0,95	0,94	0,96	0,93	0,92	1,00	0,92	0,88	0,87
Inlet temp. 240 °C	Fold change	1,05	1,05	1,06	1,06	1,07	1,05	1,06	1,00	1,07	1,09	1,08
Inlet temp. 220 °C	Fold change	0,94	0,96	0,93	0,93	0,93	0,92	0,91	1,00	0,92	0,89	0,88

Split ratio 1:100	Fold change	1,07	1,06	1,08	1,07	1,09	1,08	1,11	1,00	1,10	1,13	1,10
Split ratio 1:25	Fold change	1,10	1,11	1,10	1,18	1,14	1,12	1,14	1,00	1,13	1,16	1,15
Flow 2.5 ml/min	RT [min]	3.67	4.65	5.90	9.43	10.67	16.78	21.54	23.20	28.27	28.99	30.45
	R <sub>s</sub>	12.2	12.9	27.2	7.2	35.3	35.1	17.5	68.8	8.4	14.4	5.0
Flow 1.5 ml/min	RT [min]	5.16	6.54	8.31	13.31	15.07	19.93	23.74	25.12	29.93	30.86	32.11
	R <sub>s</sub>	11.6	13.1	34.7	8.7	27.3	35.7	18.4	73.2	11.8	15.4	6.5
Temperature ramp 7.5 °C/min	RT [min]	4.24	5.37	6.82	10.91	12.35	17.82	21.04	22.12	25.56	26.26	27.09
	R <sub>s</sub>	12.3	11.9	22.3	6.7	33.4	35.3	14.8	70.0	14.2	16.9	7.1
Temperature ramp 2.5 °C/min	RT [min]	4.24	5.37	6.82	10.92	12.36	18.87	25.39	28.13	37.31	38.24	41.33
	R <sub>s</sub>	13.3	12.2	26.9	7.7	48.0	27.1	15.2	70.3	8.4	23.7	7.4

	Analyte	citronellyl acetate	citral	neryl acetate	geranyl acetate	citronellol	nerol	phenylethanol	geraniol	methyleugenol	eugenol	farnesol
Standard method	RT [min]	31.70	32.00	33.17	33.86	34.17	34.87	35.00	35.89	39.10	41.92	45.38
	R <sub>s</sub>	4.0	14.2	8.5	4.8	10.6	2.4	13.0	44.0	38.6	47.6	NA
FID temp. 275 °C	Fold change	1,08	1,10	1,06	1,04	1,05	1,05	1,05	1,05	1,04	1,20	1,06
FID temp. 225 °C	Fold change	0,88	0,89	0,89	0,88	0,90	0,92	0,91	0,91	0,89	0,84	0,85
Inlet temp. 240 °C	Fold change	1,02	1,08	1,07	1,07	1,10	1,09	1,10	1,08	1,04	1,06	1,02
Inlet temp. 220 °C	Fold change	0,95	0,89	0,87	0,88	0,92	0,94	0,90	0,88	0,85	0,88	0,95

Split ratio 1:100	Fold change	1,07	0,94	1,11	1,07	1,17	1,16	1,17	1,13	1,13	1,19	1,14
Split ratio 1:1:25	Fold change	1,13	1,20	1,14	1,14	1,13	1,17	1,17	1,14	1,16	1,10	1,16
Flow 2.5 ml/min	RT [min]	30.96	31.25	32.44	33.13	33.47	34.16	34.30	35.19	38.37	41.17	44.65
	R <sub>s</sub>	2.9	11.7	6.8	4.5	10.9	1.6	10.0	37.0	28.5	43.2	NA
Flow 1.5 ml/min	RT [min]	32.64	33.00	34.11	34.79	35.08	35.80	35.99	36.81	40.04	42.88	46.31
	R <sub>s</sub>	4.4	13.6	8.4	4.1	11.8	2.7	10.8	42.3	37.2	45.0	NA
Temperature ramp 7.5 °C/min	RT [min]	27.44	27.72	28.45	28.91	29.10	29.60	29.74	30.77	32.47	34.41	36.68
	R <sub>s</sub>	5.7	11.0	7.0	3.4	11.3	2.5	9.6	44.8	39.5	46.2	NA
Temperature ramp 2.5 °C/min	RT [min]	42.29	42.75	45.11	46.47	47.22	48.47	48.67	50.54	56.63	62.00	69.07



	$R_s$	3.5	16.6	9.6	5.3	8.8	1.4	13.1	64.2	37.7	54.5	NA
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Table S4: Results for robustness testing on the chiral column.

	Analyte	$\alpha$ -pinene	camphene	camphene	(-)- $\beta$ -pinene	cis-3-hexen-1-ol	$\alpha$ -terpinene	limonene	p-cymene	(+)-rose oxide	(-)-rose oxide	linalool	linalool	phenylethanol	cis/trans-citral	citronellol
Standard method	RT [min]	9.58	9.77	10.27	11.49	15.21	16.26	17.06	17.16	20.28	20.43	23.18	23.87	29.82	30.66	31.95
	R <sub>s</sub>	2.4	5.9	12.0	28.6	8.3	7.9	1.2	30.6	1.5	27.1	6.7	58.4	6.7	9.0	0.9
FID temp 280 °C	Fold change	1,06	1,10	1,07	1,07	1,00	1,07	1,09	1,05	1,10	1,10	1,14	1,13	1,09	1,13	1,07
FID temp 240 °C	Fold change	1,03	1,02	1,05	1,04	1,00	1,04	1,07	0,98	1,09	1,07	1,08	1,07	1,04	1,06	1,08
Inlet temp. 260 °C	Fold change	1,02	1,07	1,02	1,02	1,00	1,04	1,02	1,07	1,06	1,07	1,05	1,05	1,03	1,05	0,99
Inlet temp 220 °C	Fold change	0,94	0,93	0,94	0,92	1,00	0,86	0,91	0,93	0,91	0,89	0,95	0,95	0,92	0,91	0,91
Split flow 200 ml/min	Fold change	1,07	1,08	1,07	1,08	1,00	1,09	1,09	1,10	1,14	1,14	1,14	1,14	1,09	1,17	1,09
Split flow 80 ml/min	Fold change	0,98	1,00	0,98	0,98	1,00	0,95	1,00	0,94	0,98	0,97	1,01	1,01	0,99	1,00	1,01
Constant flow 120 kPa	RT [min]	8.51	8.67	9.17	10.29	13.99	14.90	15.67	15.75	18.74	18.89	21.71	22.41	28.35	28.99	30.35

	R <sub>s</sub>	1.4	4.5	10.0	27.1	6.7	5.6	0.6	24.0	1.4	22.6	5.6	43.8	41.6	11.8	0.9
Flow const. Pressure 80 kPa	RT [min]	11.05	11.30	11.83	13.13	16.82	18.09	18.89	19.02	22.28	22.43	25.07	25.74	31.67	32.79	33.98
	R <sub>s</sub>	2.3	4.8	11.8	30.03	8.6	6.5	1.3	26.7	1.2	19.5	4.9	43.7	8.3	8.8	0.7
Temperature ramp 4 °C/min	RT [min]	8.09	8.28	8.59	9.38	11.20	12.12	12.57	12.66	14.49	14.57	15.78	16.09	19.04	19.19	20.40
	R <sub>s</sub>	2.6	4.2	10.7	19.2	9.7	5.5	1.1	27.7	1.2	17.8	4.6	45.8	1.6	10.6	0.7
Temperature ramp 1 °C/min	RT [min]	10.90	11.06	11.81	13.51	20.12	21.17	22.52	22.52	27.66	27.92	33.71	35.16	46.87	49.46	50.26
	R <sub>s</sub>	1.3	6.1	11.9	31.5	5.0	7.1	24.1	24.1	1.4	30.5	6.4	51.6	12.7	4.4	1.2
	Analyte	citronellol	nerol	cis/trans- citral	geraniol	citronellyl acetate	citronellyl acetate	neryl acetate	(cis/trans)- β- damasceno ne	geran yl acetat e	β- caryophyll ene	(cis/trans)- β- damascen one	β- damascon e	eugenol	methyleug enol	farnesol
Standard method	RT [min]	32.06	32.35	33.26	34.30	35.16	35.27	35.87	36.70	37.78	37.87	38.11	38.64	39.61	41.11	58.67
	R <sub>s</sub>	2.2	7.7	7.3	5.9	0.8	4.1	6.5	8.4	0.7	1.9	4.0	7.6	11.6	76.1	-
FID temp 280 °C	RT [min]	32.06	32.35	33.26	34.30	35.16	35.27	35.87	36.70	37.78	37.87	38.11	38.64	39.61	41.11	58.67
	Fold change	1,02	1,11	1,11	1,13	1,16	1,12	1,13	1,13	1,05	1,03	1,16	1,14	1,14	1,12	1,15
FID temp 240 °C	RT [min]	32.06	32.35	33.26	34.30	35.16	35.27	35.87	36.70	37.78	37.87	38.11	38.64	39.61	41.11	58.67

	Fold change	1,04	1,06	1,06	1,07	1,14	1,09	1,07	1,09	1,01	0,96	1,10	1,09	1,15	1,12	1,08
Inlet temp - 260 °C	RT [min]	32.06	32.35	33.26	34.30	35.16	35.27	35.87	36.70	37.78	37.87	38.11	38.64	39.61	41.11	58.67
	Fold change	0,97	1,05	1,04	1,05	1,19	1,20	1,05	1,09	0,98	1,01	1,06	1,03	1,08	1,08	1,04
Inlet Temp - 220 °C	RT [min]	32.06	32.35	33.26	34.30	35.16	35.27	35.87	36.70	37.78	37.87	38.11	38.64	39.61	41.11	58.67
	Fold change	0,89	0,91	0,90	0,90	0,94	0,91	0,89	0,89	0,89	0,87	0,91	0,88	0,89	0,90	0,84
Spilt flow 200 ml/min	Fold change	1,05	1,13	1,13	1,16	1,29	1,28	1,13	1,14	1,17	1,18	1,17	1,16	1,19	1,17	1,31
Spilt flow 80 ml/min	Fold change	1,00	0,92	0,98	1,01	1,06	1,03	0,97	0,96	1,04	1,03	1,00	0,98	1,03	1,00	0,99
Constant flow 120 kPa	RT [min]	30.47	30.75	31.55	32.69	33.38	33.51	34.06	34.76	35.97	35.97	36.35	36.70	37.79	39.28	56.67
	R <sub>s</sub>	1.9	6.2	7.7	4.8	1.0	4.3	5.4	7.3	2.4	NA	2.3	7.5	11.2	123.6	NA
Flow const. Pressure	RT [min]	34.07	34.36	35.41	36.34	37.40	37.50	38.15	39.16	40.05	40.34	40.34	41.10	41.93	43.45	61.16

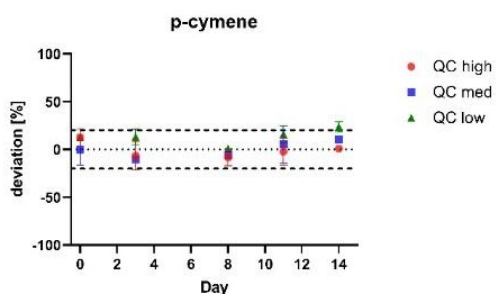
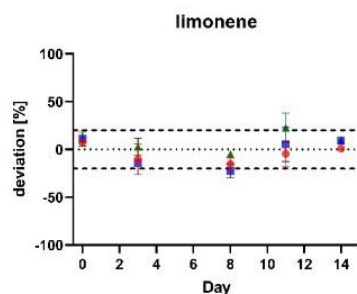
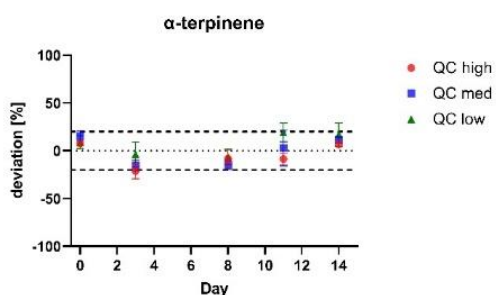
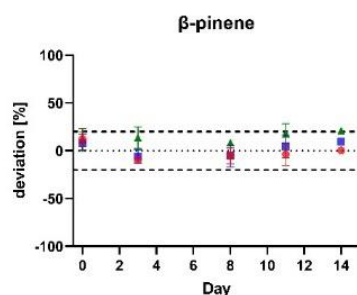
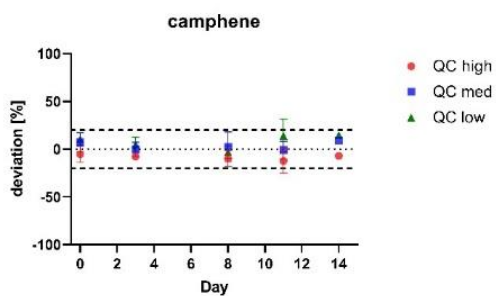
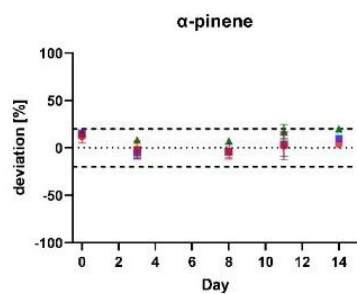
	R <sub>s</sub>	2.1	7.4	6.5	7.4	0.7	4.6	7.1	6.3	1.9	5.0	NA	5.4	10.0	130.6	NA
Temperature ramp 4 °C/min	RT [min]	20.45	20.6	21.27	21.61	22.38	22.38	22.82	23.53	23.76	23.85	24.14	24.50	24.75	25.54	34.12
	R <sub>s</sub>	2.0	8.2	4.2	7.6	3.6	3.6	6.3	2.5	1.1	3.6	4.4	2.7	9.3	68.9	NA
Temperature ramp 1 °C/min	RT [min]	50.52	51.08	52.03	54.83	55.23	55.54	56.36	57.08	59.49	60.26	60.92	61.17	63.68	66.56	100.56
	R <sub>s</sub>	2.3	3.9	11.5	1.6	1.3	3.4	3.1	10.3	3.3	2.8	1.1	9.0	11.4	120.1	NA

Table S5: concentration determination of 10 authentic rose oils after analysis on a DB-wax column. Bold numbers are concentrations slightly out of the calibration range.

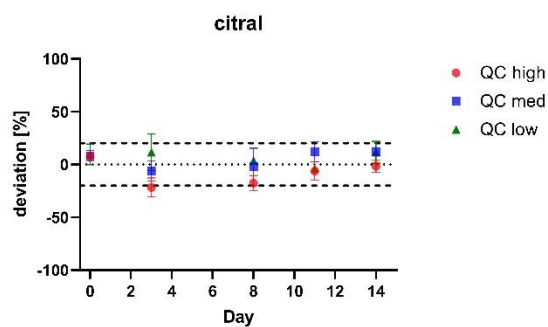
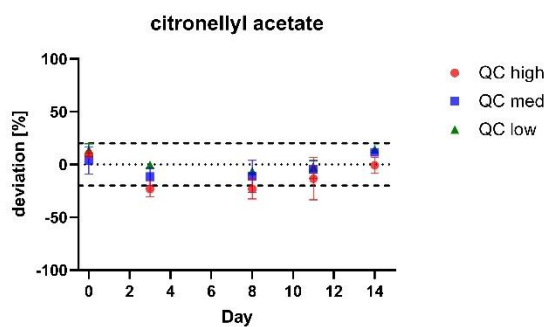
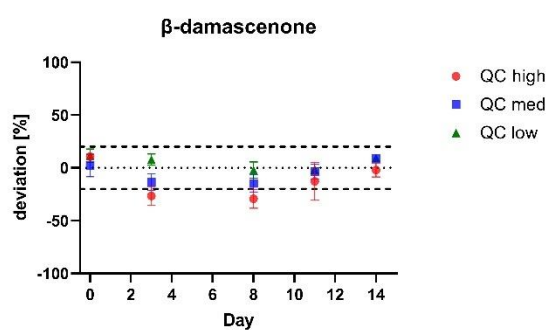
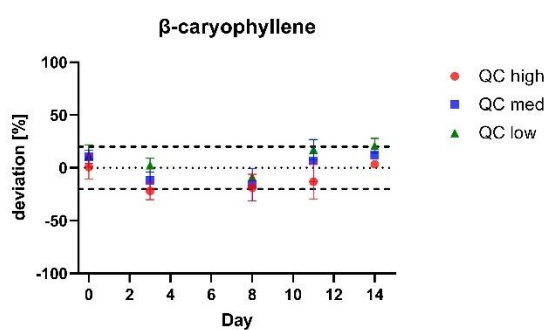
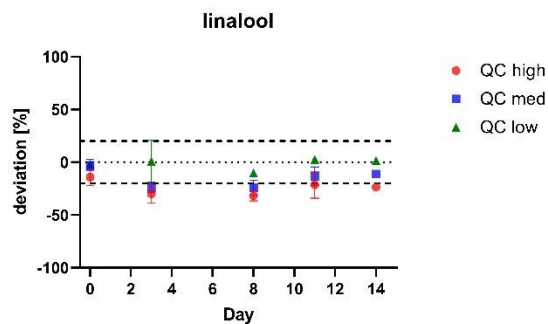
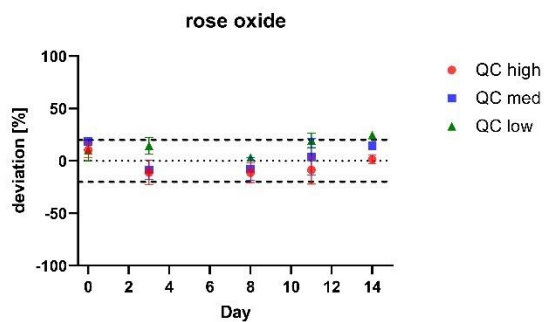
Species	<i>R.</i> <i>damascena</i>	<i>P.</i> <i>graveolens</i>	<i>P.</i> <i>graveolens</i>	<i>R.</i> <i>damascena</i>	<i>R.</i> <i>damascena</i>	<i>R.</i> <i>damascena</i>	<i>R.</i> <i>damascena</i>	<i>R.</i> <i>damascena</i>	<i>R.</i> <i>damascena</i>	<i>R.</i> <i>damascena</i>
Quality	pure	pure	pure	10%	pure	pure	pure	pure	pure	10%
Origin	Bulgaria	NA	NA	Morocco	Turkey	Bulgaria	Bulgaria	Turkey	Turkey	Bulgaria
analyte	conc [mg/ml]	conc [mg/ml]	conc [mg/ml]	conc [mg/ml]	conc [mg/ml]	conc [mg/ml]	conc [mg/ml]	conc [mg/ml]	conc [mg/ml]	conc [mg/ml]
$\alpha$ -pinene	1.62 $\pm$ 0.00	1.99 $\pm$ 0.02	3.24 $\pm$ 0.02	0.51 $\pm$ 0.01	5.11 $\pm$ 0.01	6.24 $\pm$ 0.04	2.94 $\pm$ 0.01	3.60 $\pm$ 0.02	14.24 $\pm$ 0.05	0.58 $\pm$ 0.03
camphene	0.03 $\pm$ 0.00	0.04 $\pm$ 0.00	0.05 $\pm$ 0.00	n.d.	0.04 $\pm$ 0.00	0.05 $\pm$ 0.00	0.04 $\pm$ 0.00	0.04 $\pm$ 0.00	0.05 $\pm$ 0.00	0.03 $\pm$ 0.00
$\beta$ -pinene	0.41 $\pm$ 0.00	0.04 $\pm$ 0.00	0.06 $\pm$ 0.00	0.16 $\pm$ 0.00	2.05 $\pm$ 0.08	2.19 $\pm$ 0.01	0.70 $\pm$ 0.00	1.45 $\pm$ 0.03	2.78 $\pm$ 0.08	0.16 $\pm$ 0.01
$\alpha$ -terpinene	0.02 $\pm$ 0.00	0.04 $\pm$ 0.00	0.07 $\pm$ 0.00	n.d.	0.05 $\pm$ 0.00	0.14 $\pm$ 0.00	0.03 $\pm$ 0.00	0.12 $\pm$ 0.00	0.21 $\pm$ 0.02	0.02 $\pm$ 0.00
limonene	0.12 $\pm$ 0.00	1.46 $\pm$ 0.05	1.99 $\pm$ 0.09	0.25 $\pm$ 0.01	0.28 $\pm$ 0.00	0.33 $\pm$ 0.00	0.23 $\pm$ 0.00	0.25 $\pm$ 0.00	0.40 $\pm$ 0.00	0.23 $\pm$ 0.91
p-cymene	0.21 $\pm$ 0.00	0.42 $\pm$ 0.01	<b>1.06 <math>\pm</math> 0.01</b>	0.09 $\pm$ 0.00	0.55 $\pm$ 0.01	0.25 $\pm$ 0.00	0.49 $\pm$ 0.00	0.38 $\pm$ 0.00	0.67 $\pm$ 0.00	0.03 $\pm$ 0.00
(+/-)-rose oxide	6.18 $\pm$ 0.03	16.12 $\pm$ 0.20	18.46 $\pm$ 0.14	0.26 $\pm$ 0.00	<b>2.67 <math>\pm</math> 0.07</b>	1.75 $\pm$ 0.04	2.83 $\pm$ 0.05	4.92 $\pm$ 0.00	2.12 $\pm$ 0.02	0.20 $\pm$ 0.01
linalool	14.79 $\pm$ 0.09	63.94 $\pm$ 0.34	69.88 $\pm$ 0.16	1.84 $\pm$ 0.04	8.85 $\pm$ 0.08	14.27 $\pm$ 0.19	17.79 $\pm$ 0.09	6.78 $\pm$ 0.05	10.51 $\pm$ 0.11	1.19 $\pm$ 0.04
$\beta$ -caryophyllene	12.42 $\pm$ 0.32	11.12 $\pm$ 0.10	13.11 $\pm$ 0.09	0.63 $\pm$ 0.02	8.90 $\pm$ 0.31	8.22 $\pm$ 0.14	5.74 $\pm$ 0.08	10.13 $\pm$ 0.30	8.62 $\pm$ 0.90	0.32 $\pm$ 0.02
$\beta$ -damascenone	1.51 $\pm$ 0.22	6.45 $\pm$ 0.25	6.86 $\pm$ 0.10	0.37 $\pm$ 0.05	2.41 $\pm$ 0.08	1.81 $\pm$ 0.14	1.69 $\pm$ 0.08	2.12 $\pm$ 0.16	2.08 $\pm$ 0.01	0.31 $\pm$ 0.01
citronellyl acetate	9.89 $\pm$ 0.17	8.27 $\pm$ 0.07	9.34 $\pm$ 0.31	0.53 $\pm$ 0.01	9.90 $\pm$ 0.17	4.42 $\pm$ 0.07	5.21 $\pm$ 0.19	9.57 $\pm$ 0.11	9.88 $\pm$ 0.32	0.25 $\pm$ 0.01
citral	11.81 $\pm$ 0.23	9.19 $\pm$ 0.06	10.66 $\pm$ 0.06	0.76 $\pm$ 0.08	5.68 $\pm$ 0.12	12.89 $\pm$ 0.22	13.07 $\pm$ 0.02	6.93 $\pm$ 0.14	7.92 $\pm$ 0.30	0.98 $\pm$ 0.04
neryl acetate	15.27 $\pm$ 0.24	12.74 $\pm$ 0.13	13.36 $\pm$ 0.08	0.49 $\pm$ 0.01	7.47 $\pm$ 0.12	9.52 $\pm$ 0.16	10.11 $\pm$ 0.07	6.53 $\pm$ 0.08	7.73 $\pm$ 0.24	0.65 $\pm$ 0.02
geranyl acetate	28.54 $\pm$ 0.65	7.23 $\pm$ 0.06	7.90 $\pm$ 0.06	1.04 $\pm$ 0.03	15.74 $\pm$ 0.27	15.79 $\pm$ 0.26	11.82 $\pm$ 0.09	20.84 $\pm$ 0.15	27.20 $\pm$ 0.16	0.87 $\pm$ 0.04
citronellol	503.42 $\pm$ 8.22	479.94 $\pm$ 3.50	496.13 $\pm$ 2.97	55.38 $\pm$ 1.40	433.24 $\pm$ 5.56	300.10 $\pm$ 4.18	297.12 $\pm$ 2.21	419.55 $\pm$ 4.16	378.10 $\pm$ 2.23	33.81 $\pm$ 1.49
nerol	204.05 $\pm$ 3.53	4.39 $\pm$ 0.18	4.11 $\pm$ 0.10	14.28 $\pm$ 0.20	101.25 $\pm$ 1.29	124.17 $\pm$ 1.69	107.74 $\pm$ 1.00	86.26 $\pm$ 0.84	111.13 $\pm$ 0.64	10.65 $\pm$ 0.23
phenylethanol	0.97 $\pm$ 0.02	0.19 $\pm$ 0.01	0.18 $\pm$ 0.01	0.22 $\pm$ 0.01	<b>2.12 <math>\pm</math> 0.06</b>	0.93 $\pm$ 0.05	1.11 $\pm$ 0.31	4.11 $\pm$ 0.05	4.40 $\pm$ 0.04	0.12 $\pm$ 0.00
geraniol	499.85 $\pm$ 9.12	221.04 $\pm$ 1.78	209.02 $\pm$ 1.00	29.52 $\pm$ 0.55	220.03 $\pm$ 2.75	300.28 $\pm$ 4.29	210.33 $\pm$ 1.57	199.17 $\pm$ 2.21	270.95 $\pm$ 2.09	23.73 $\pm$ 0.50
methyleugenol	28.25 $\pm$ 0.69	8.14 $\pm$ 0.75	6.27 $\pm$ 0.06	4.16 $\pm$ 0.07	32.84 $\pm$ 0.38	8.97 $\pm$ 0.17	29.63 $\pm$ 0.29	34.61 $\pm$ 0.61	35.98 $\pm$ 0.55	0.50 $\pm$ 0.02
eugenol	21.93 $\pm$ 0.72	3.39 $\pm$ 0.07	3.02 $\pm$ 0.04	3.19 $\pm$ 0.06	15.32 $\pm$ 0.45	12.25 $\pm$ 0.34	8.00 $\pm$ 0.11	13.31 $\pm$ 0.12	22.19 $\pm$ 1.47	0.73 $\pm$ 0.01
farnesol	<b>81.18 <math>\pm</math> 5.82</b>	2.95 $\pm$ 0.27	0.49 $\pm$ 0.07	3.73 $\pm$ 0.19	23.16 $\pm$ 0.57	30.92 $\pm$ 0.57	<b>40.26 <math>\pm</math> 0.47</b>	23.53 $\pm$ 0.52	29.20 $\pm$ 1.25	3.21 $\pm$ 0.15

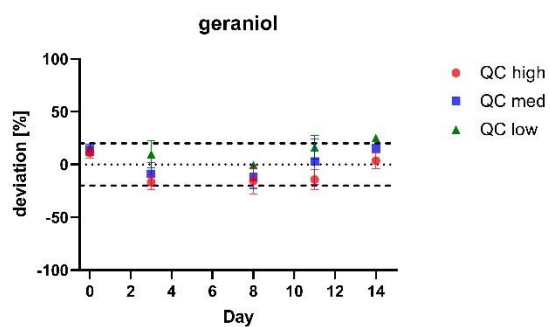
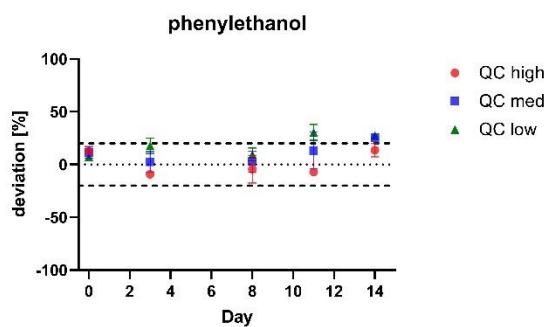
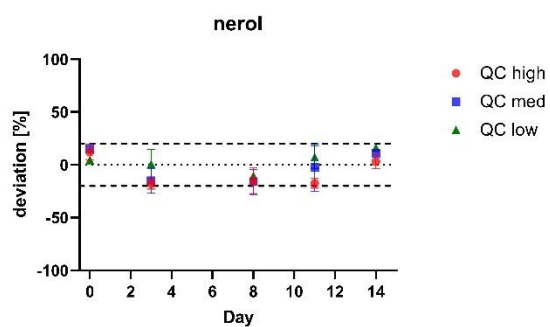
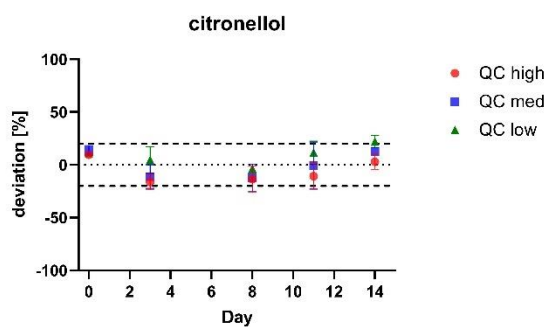
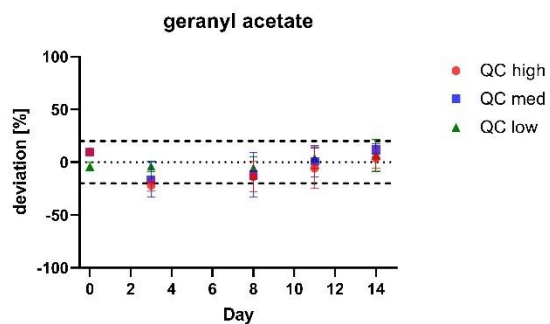
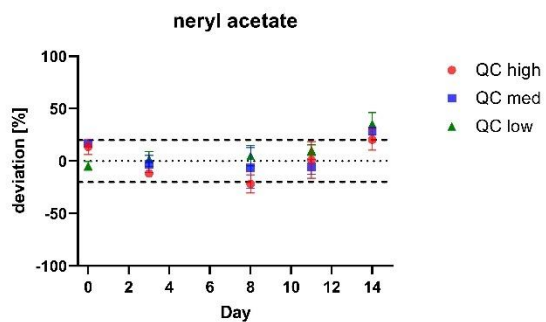
Table S6: Concentration determination of 10 authentic rose oils after chiral analysis. Bold numbers are concentrations slightly out of the calibration range. EE and DE for stereoisomers is given.

[illegible]









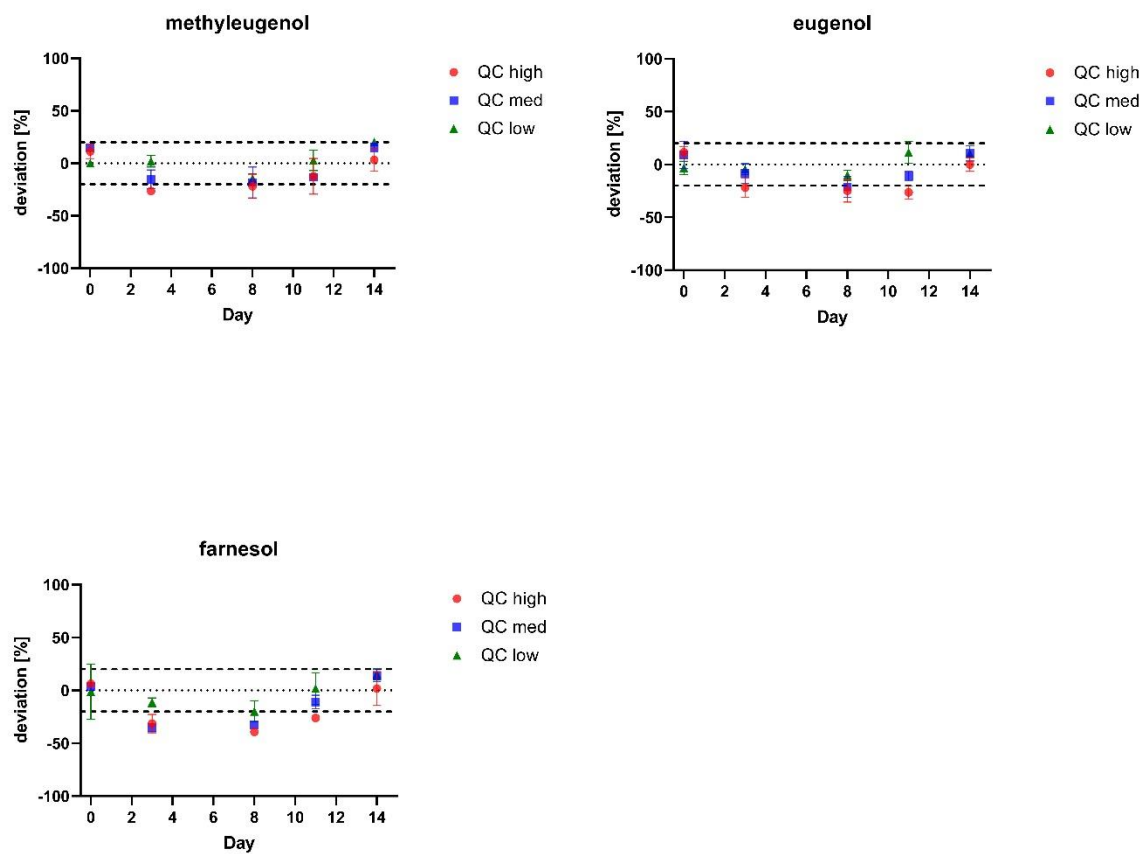
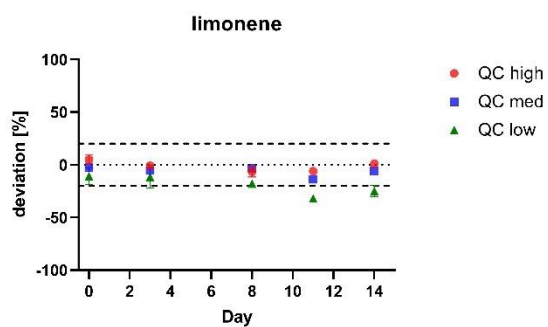
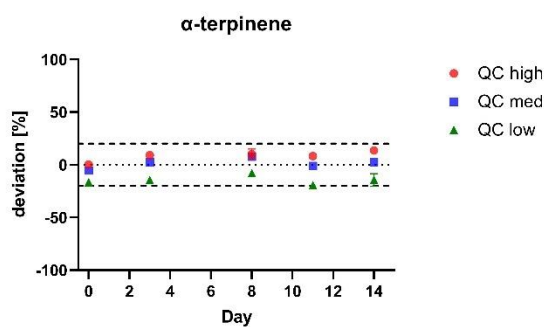
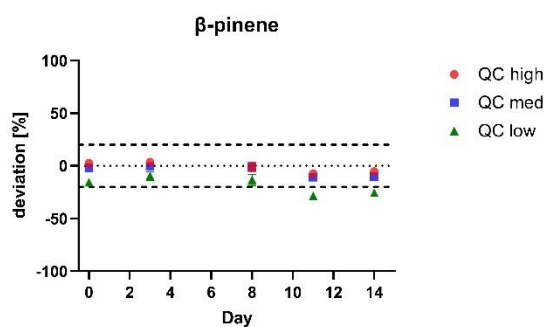
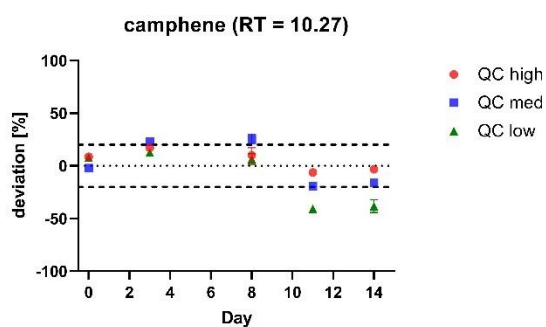
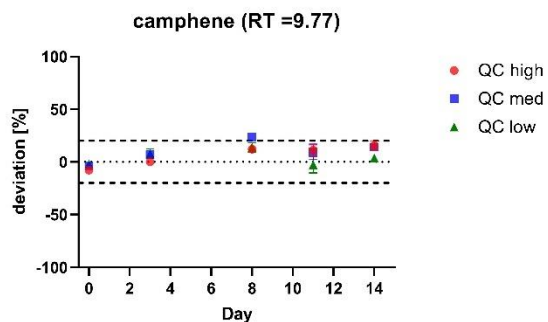
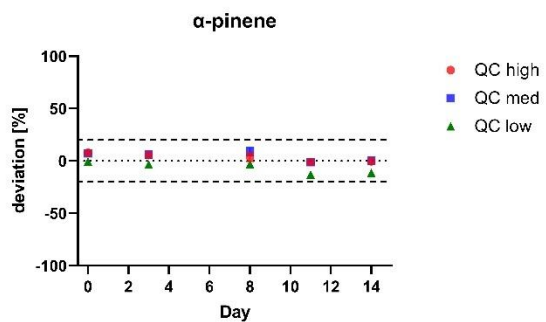
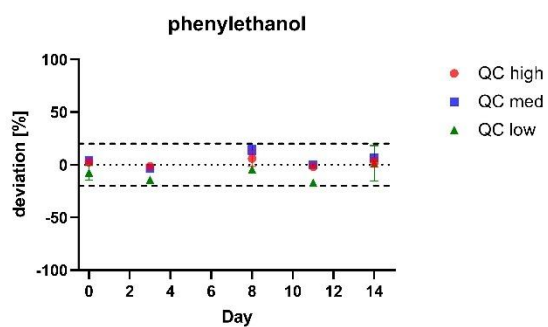
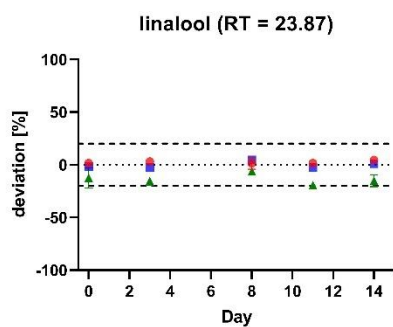
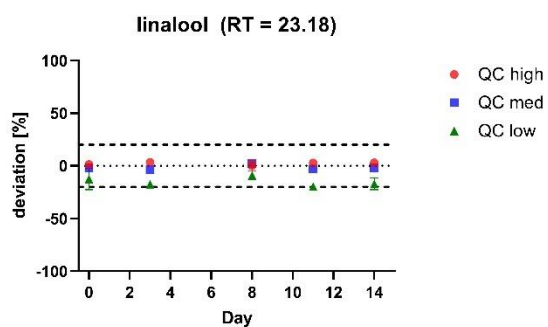
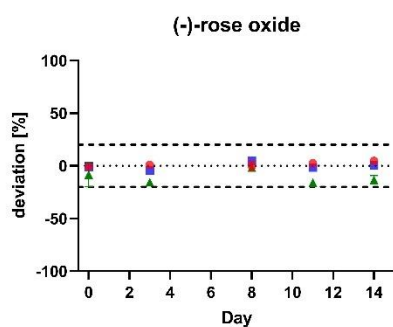
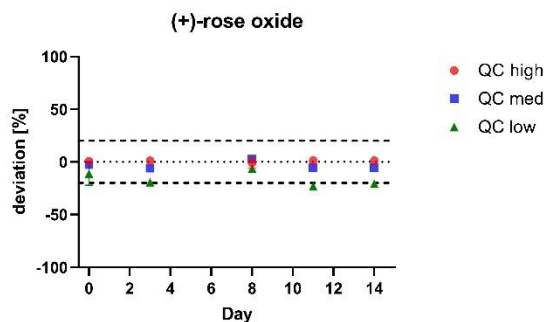
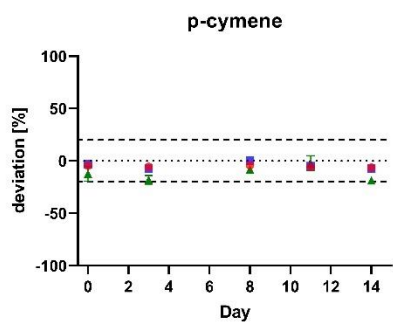
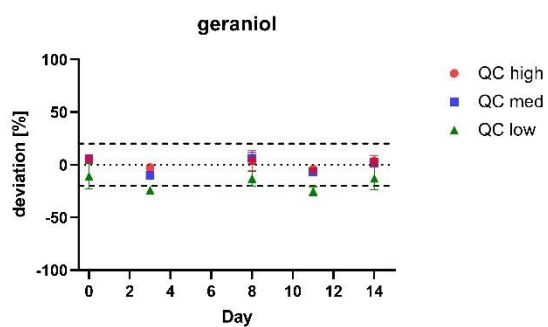
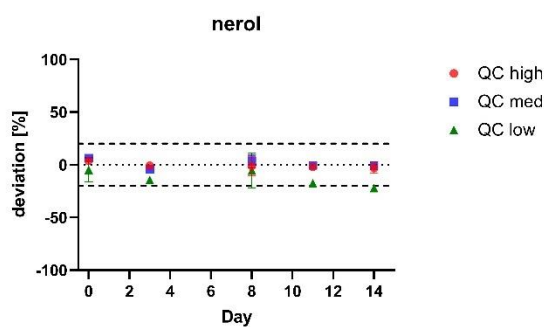
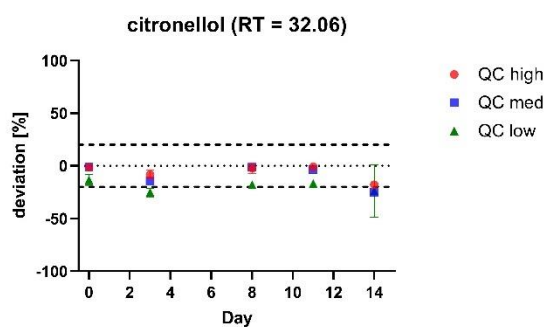
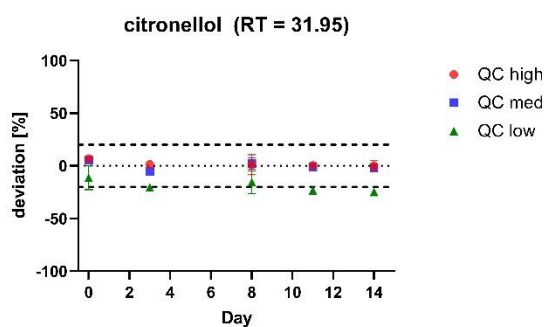
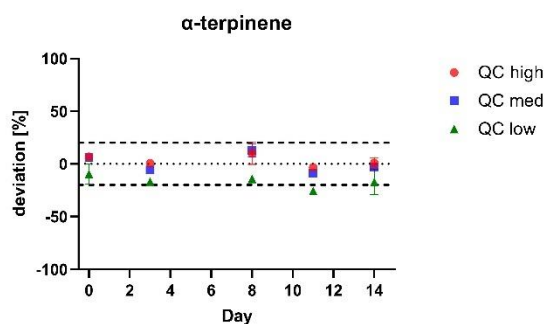
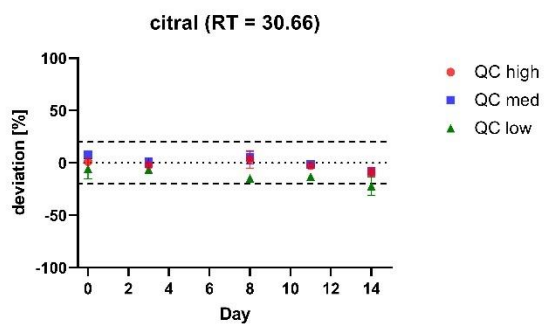
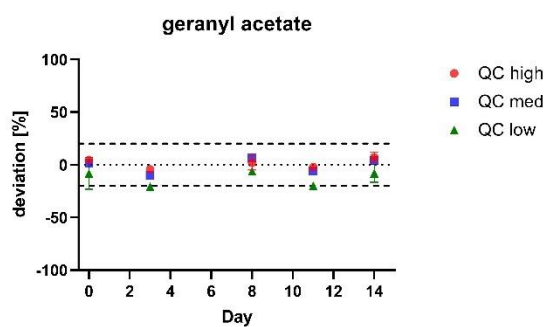
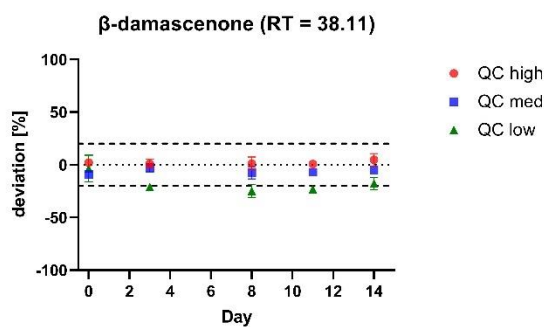
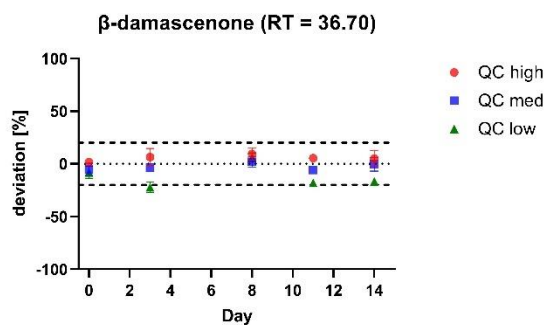
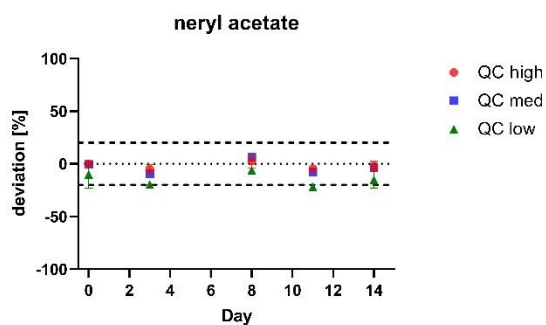
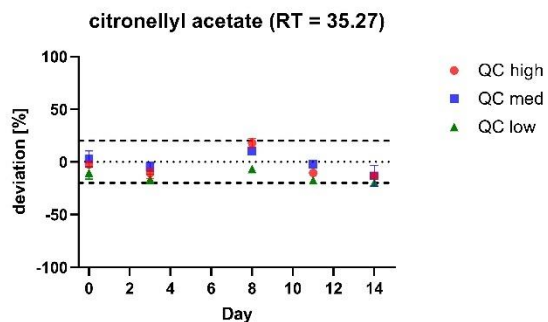
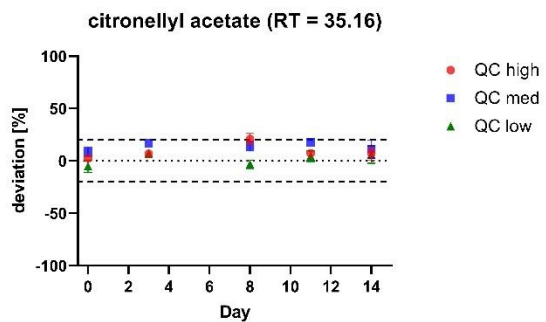


Figure S1: QC stability for samples analysed on the DB Wax column. Thick stippled lines indicate a 20% deviation from measured to calculated value. Validation took place on 5 days during a course of 2 weeks.









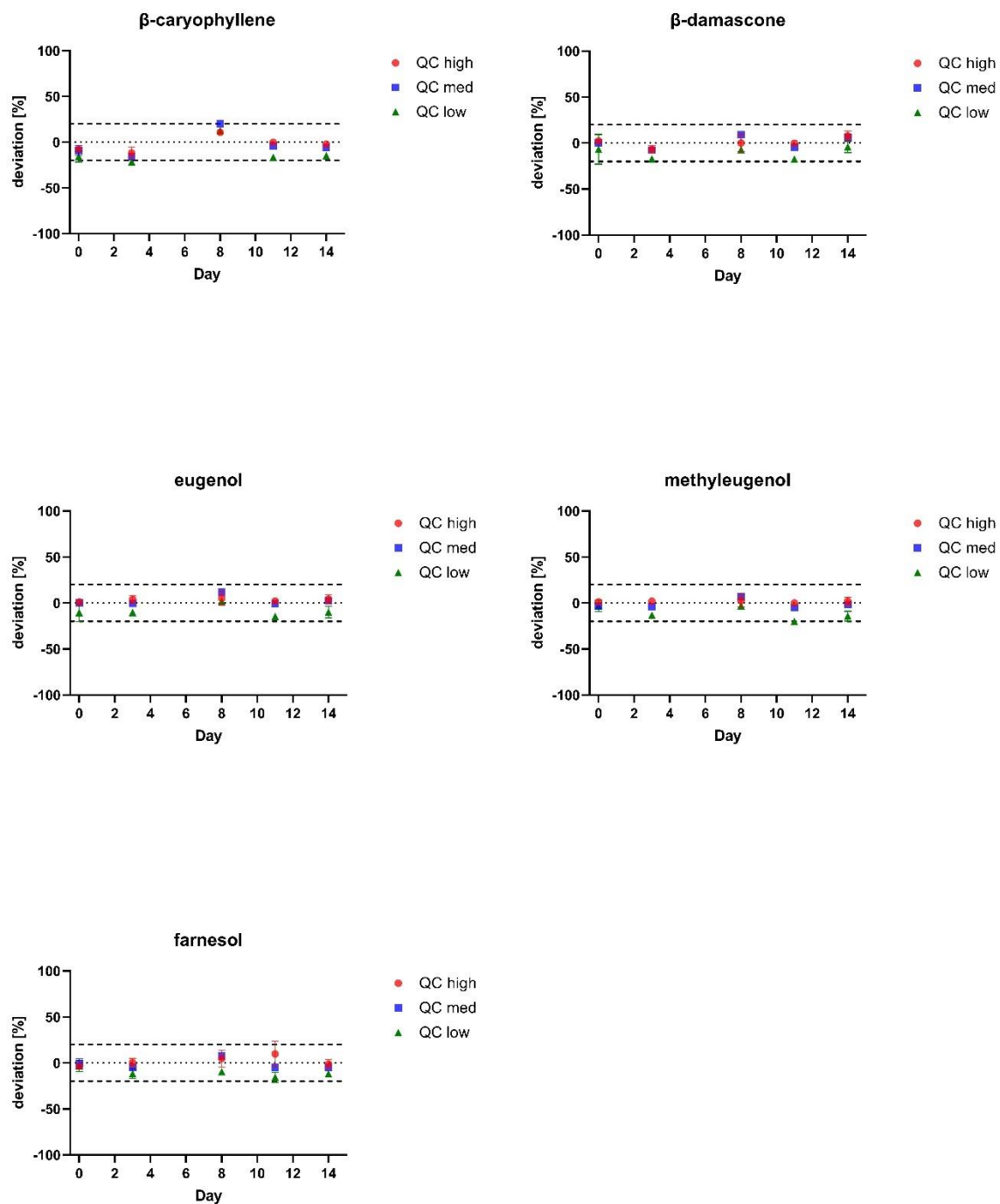


Figure S2: QC stability for samples analysed on the chiral column. Thick stippled lines indicate a 20% deviation from measured to calculated value. Validation took place on 5 days during a course of 2 weeks.



## Matlab-Code

%% Script used for the chromatographic peak integration from data collected using ChromCard. Data can be downloaded as a txt-file (export data as ASCII).  
%% Retention times for peaks have to be selected beforehand and imported as a txt-file to the script.

```
peak_width          = 0.1; %% Select desired peak width. As a default 0.1 can be
selected
peak_width_half     = peak_width/2;
retention_times     = readmatrix("Retention_times.txt"); %%import retention times
as a column in form of a txt file
peak_bounds_start   = abs(retention_times - peak_width_half);
peak_bounds_end     = abs(retention_times + peak_width_half);
peak_bounds         = zeros(1, length(retention_times)*2);
npeaks              = length(peak_bounds)/2;

for i=1:npeaks

    peak_bounds(2*i-1) = peak_bounds_start(i);
    peak_bounds(2*i)   = peak_bounds_end(i);

end

idx_peak_bounds = zeros(1, length(peak_bounds)); % zero vector with number of Peak
bounds
peaks           = zeros(1, npeaks); % zero vector with amount of peaks -> used to
store area under the curve

% upload data as .txt file

Chrom_Data      = readmatrix("myData.txt"); %Import ChromCard Data as txt file
time            = Chrom_Data(:,1); % extract time as vector in minutes
uV              = Chrom_Data(:, end); % extract uV as vector
noiseThresh     = 1340; % read from chromatogram where the noise is about
Ts              = time(2)-time(1); % sampling interval (in what amount of time
is a data point constructed in [min])

noise           = uV;
noise(noise > noiseThresh) = NaN; % NaN=not a number, defines value not as zero
but not defined yet, defines noise as all values below the noise

% Moving Average for noise filtering
T_window       = 1; % min ... width over which the moving average is taken
nSamples       = T_window / Ts; % amounts of data points that are collected over a
minute
noise_avg      = movmean(noise, nSamples, 'omitnan'); % movmean -> returns mean
values over an array -> sliding window. Noise (is uV below threshold), nSamples is
data points for a certain time frame and omitnan a function which jumps over NaN
values

% Determine Peak Index and Integration

for i=1:npeaks
```

```

        timeDiffStart      = abs(time - peak_bounds(2*i - 1)); % find minimum
difference between peak bounds and time
        timeDiffMinStart   = min(timeDiffStart);
        idxPkStart         = find(timeDiffStart == timeDiffMinStart); % find index of
minimum (equal to index of startpeak)
        timeDiffEnd        = abs(time - peak_bounds(2*i));
        timeDiffMinEnd     = min(timeDiffEnd);
        idxPkEnd           = find(timeDiffEnd == timeDiffMinEnd);
        idx_peak_bounds(2*i-1) = idxPkStart;
        idx_peak_bounds(2*i)   = idxPkEnd;
        peaks(i)              = trapz(time(idxPkStart:idxPkEnd,1),
uV(idxPkStart:idxPkEnd,1) - noise_avg(idxPkStart))*60; % Integration + Offset
correction, Unit is s*uV

        meep = noise_avg(idxPkStart);
        if (isscalar(meep) && isfinite(meep))
            % Plot area of peaks
            plot(time,uV)
            xlabel('time [min]');
            ylabel('uV');
            legend('Data');
            hold on;
        %
            area(time(idxPkStart:idxPkEnd,1),uV(idxPkStart:idxPkEnd,1),
noise_avg(idxPkStart))

            area(time(idxPkStart:idxPkEnd,1),uV(idxPkStart:idxPkEnd,1), meep)

            colororder('red')
        end
    end

area = transpose(peaks);
area_RT = [retention_times(:), area(:)];

filename = 'myData.xlsx' %write data output from integration as an excel file
xlswrite(filename, area_RT)

clear all

```

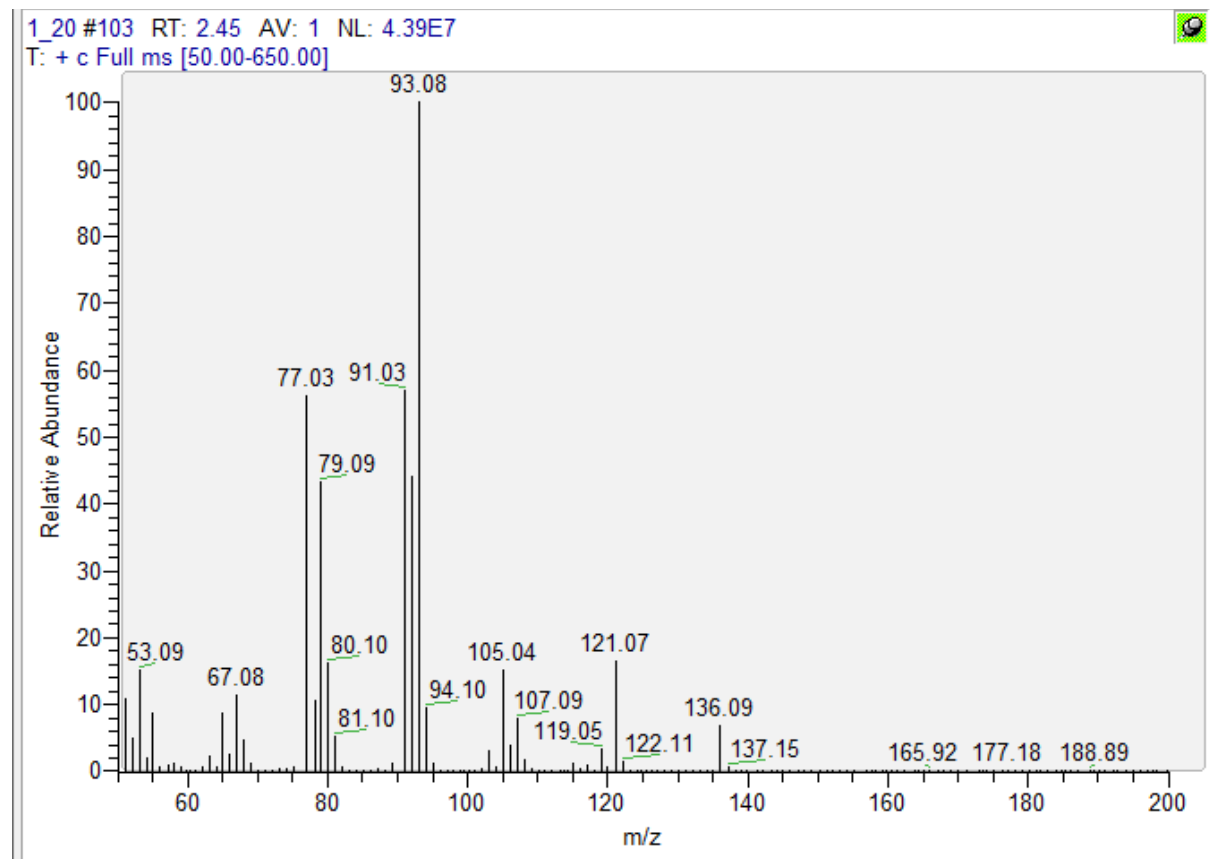
## MS-spectra:

Table 1: detailed information about the samples analysed using GC-MS.

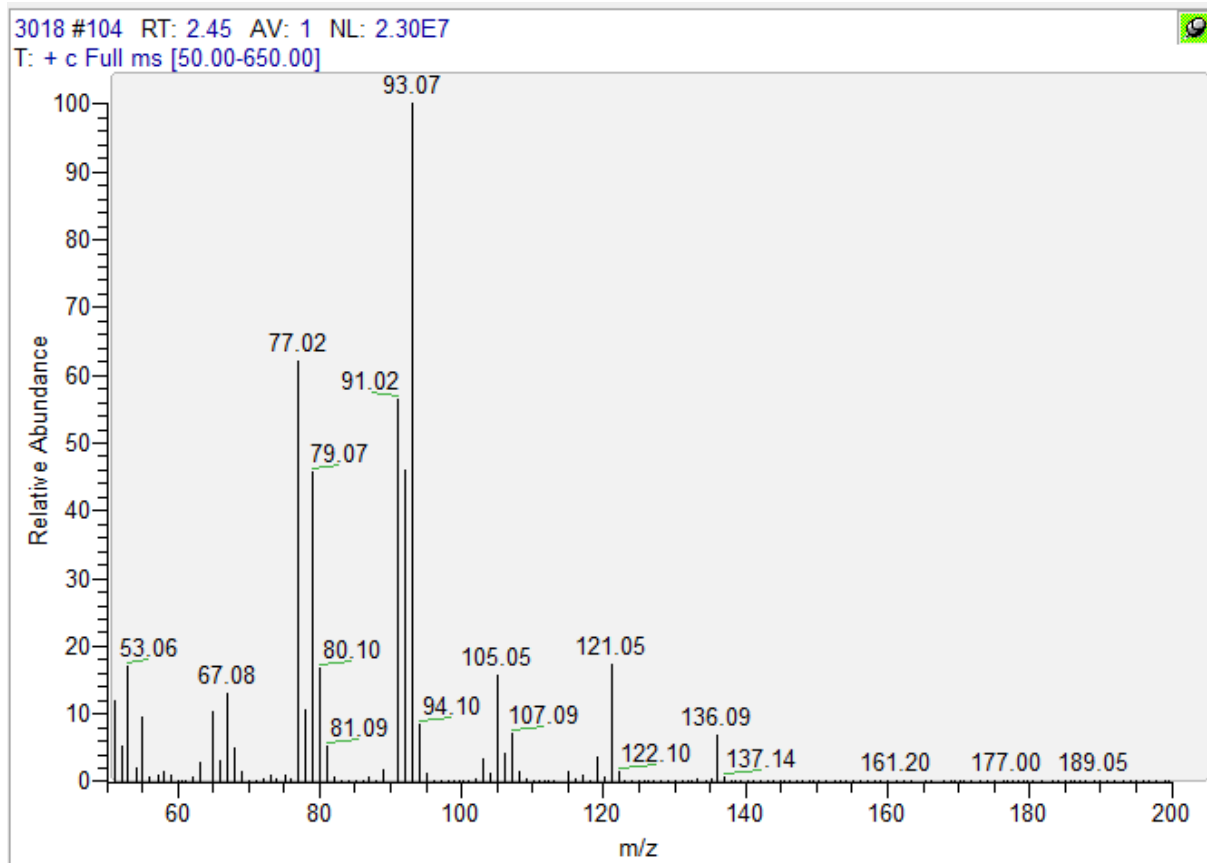
Number	3018	3057	3058	3053	3021	3072	3073
species	<i>R. damascena</i>	<i>P. graveolens</i>	<i>P. graveolens</i>	<i>R. damascena</i>	<i>R. damascena</i>	<i>R. damascena</i>	<i>R. damascena</i>
quality	pure	pure	pure	10%	pure	pure	pure
origin	Bulgaria	NA	NA	Morocco	Turkey	Bulgaria	Bulgaria

Alpha pinene

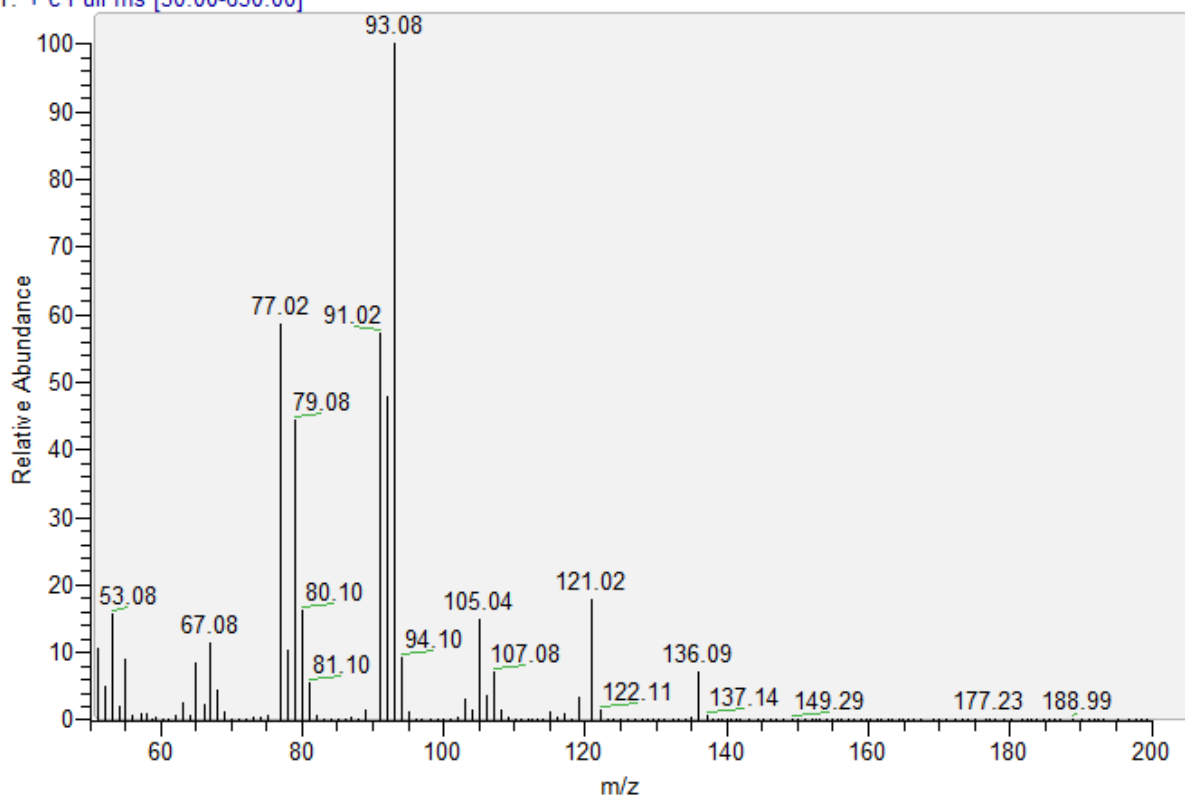
Reference:



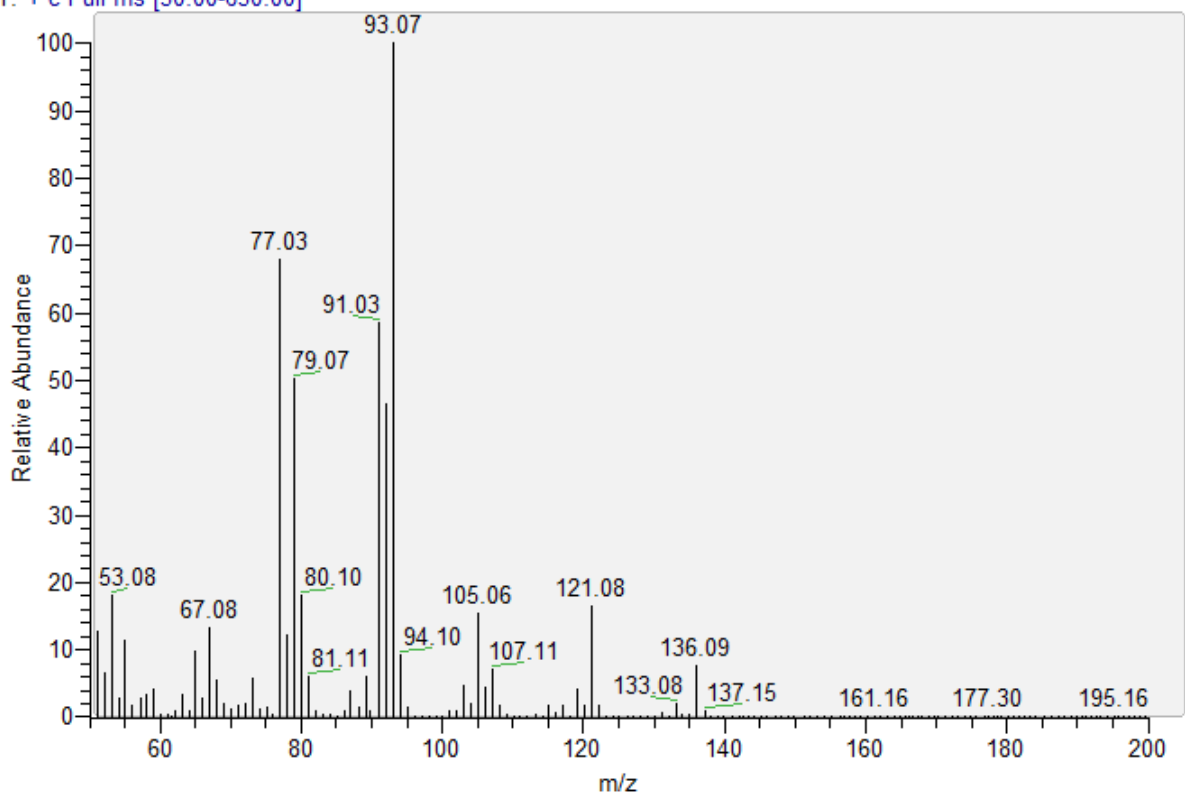
Samples:



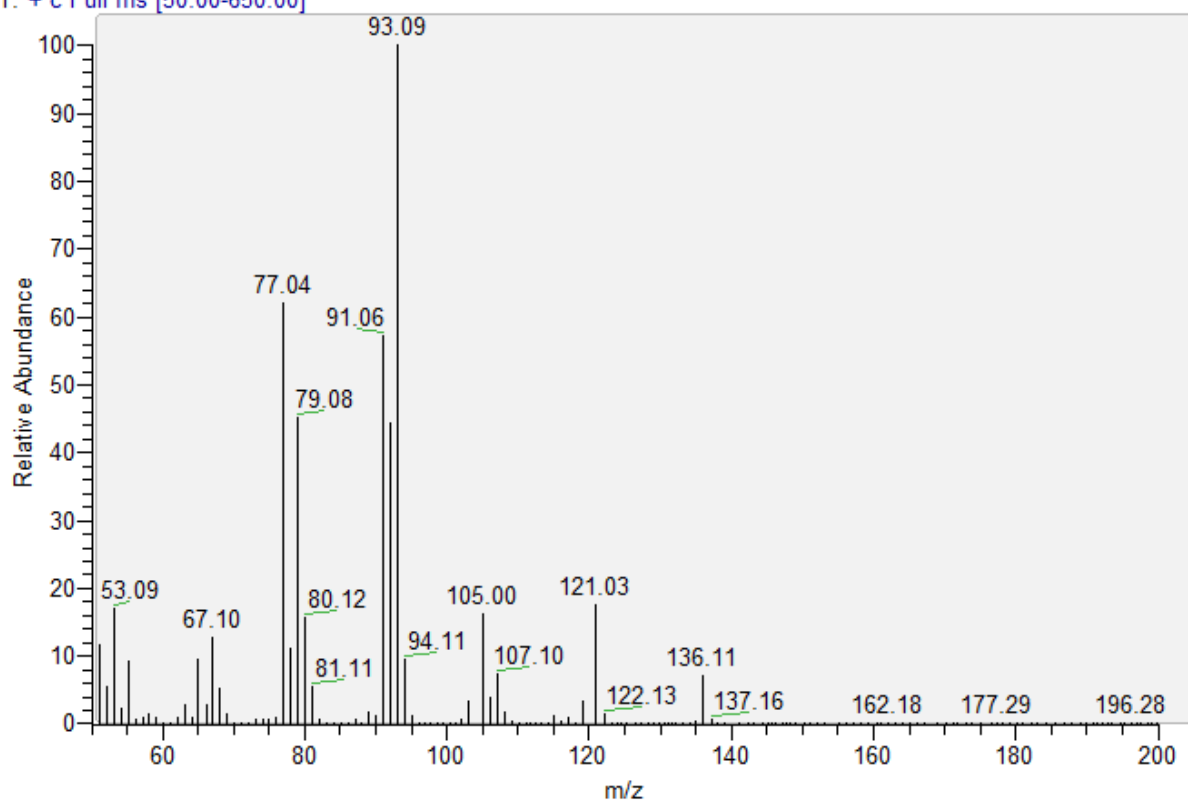
3021 #104 RT: 2.46 AV: 1 NL: 7.16E7  
T: + c Full ms [50.00-650.00]



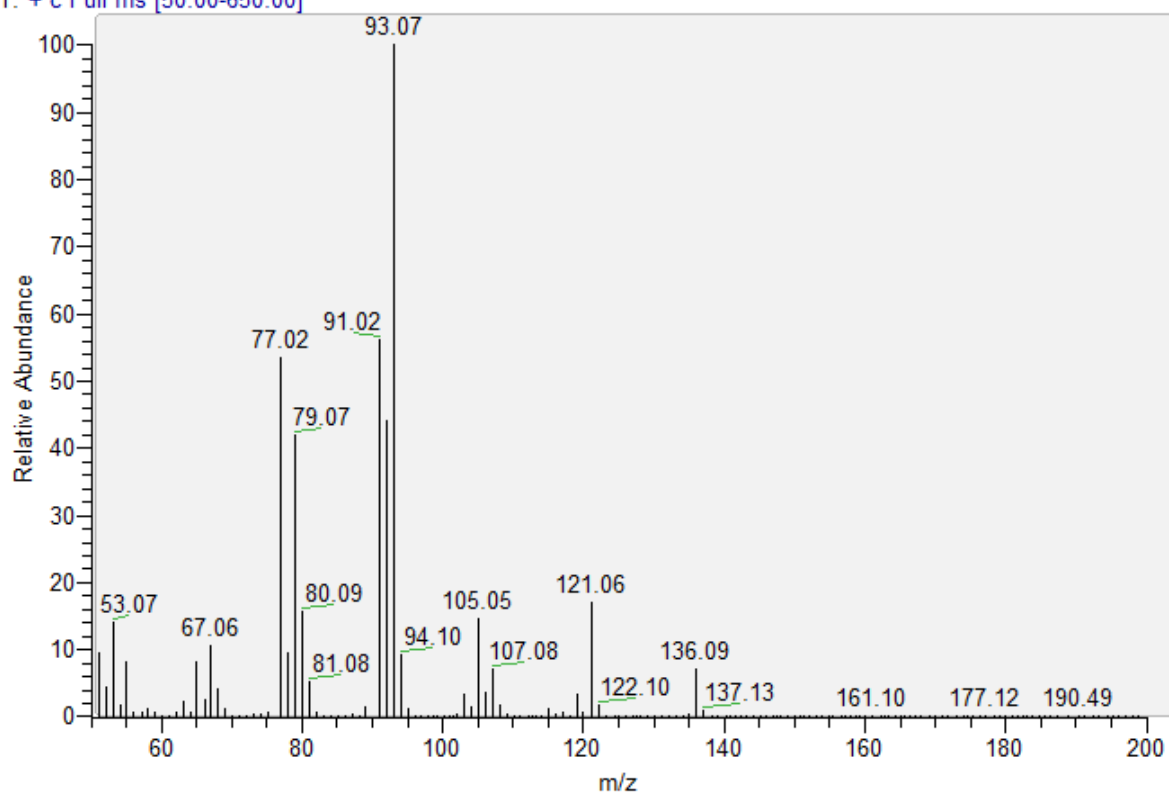
3053 #103-104 RT: 2.44-2.46 AV: 2 NL: 2.51E6  
T: + c Full ms [50.00-650.00]



3057 #105 RT: 2.45 AV: 1 NL: 1.82E7  
T: + c Full ms [50.00-650.00]

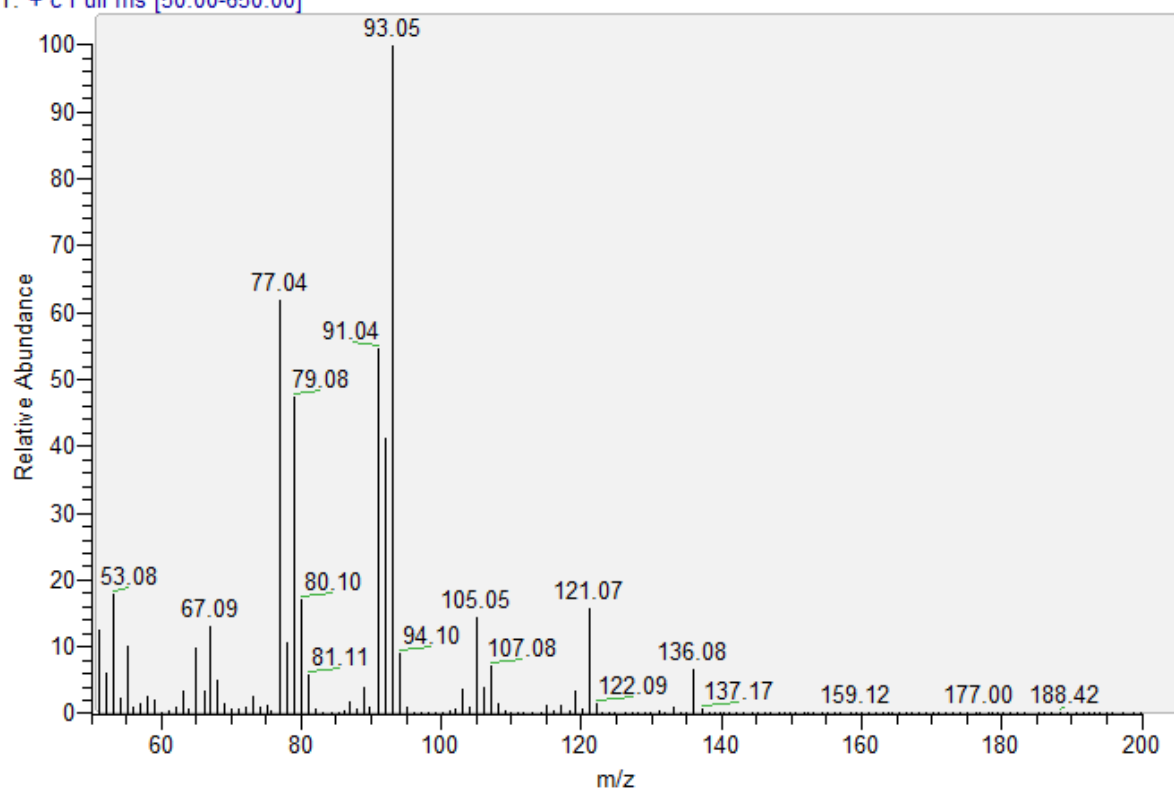


3058 #102 RT: 2.44 AV: 1 NL: 4.80E7  
T: + c Full ms [50.00-650.00]

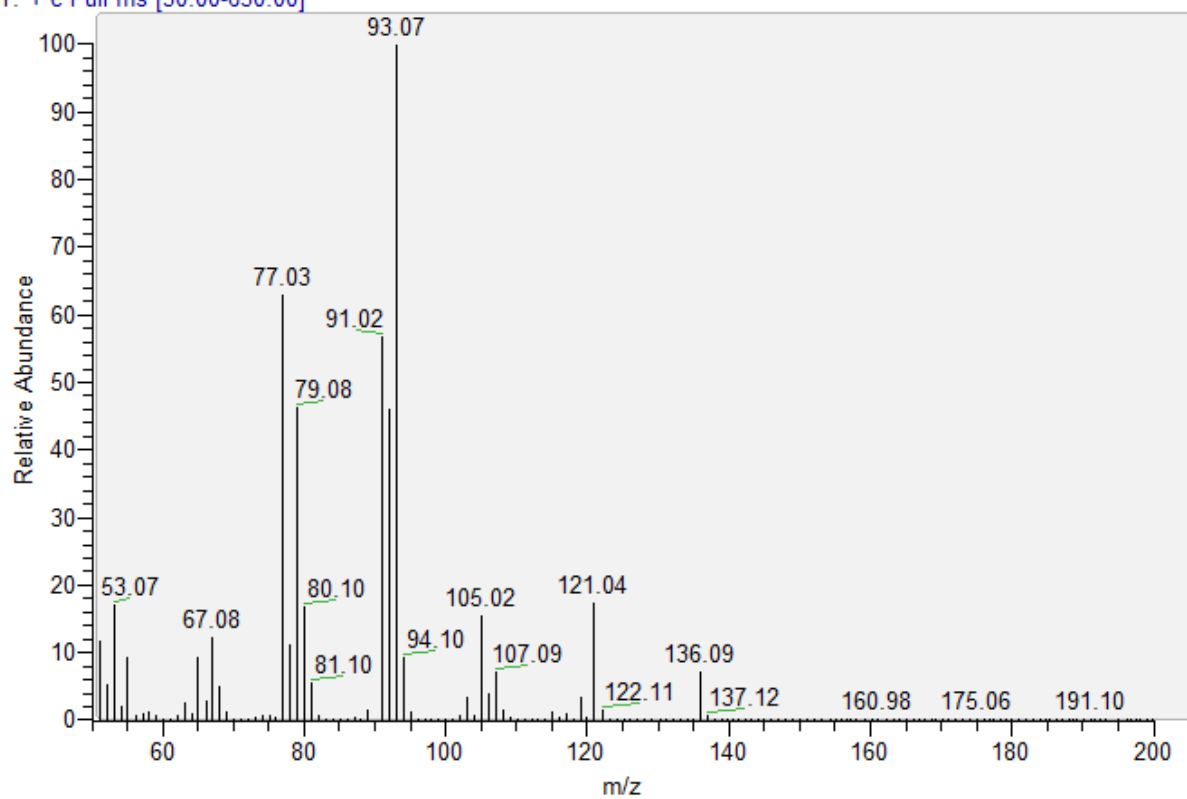




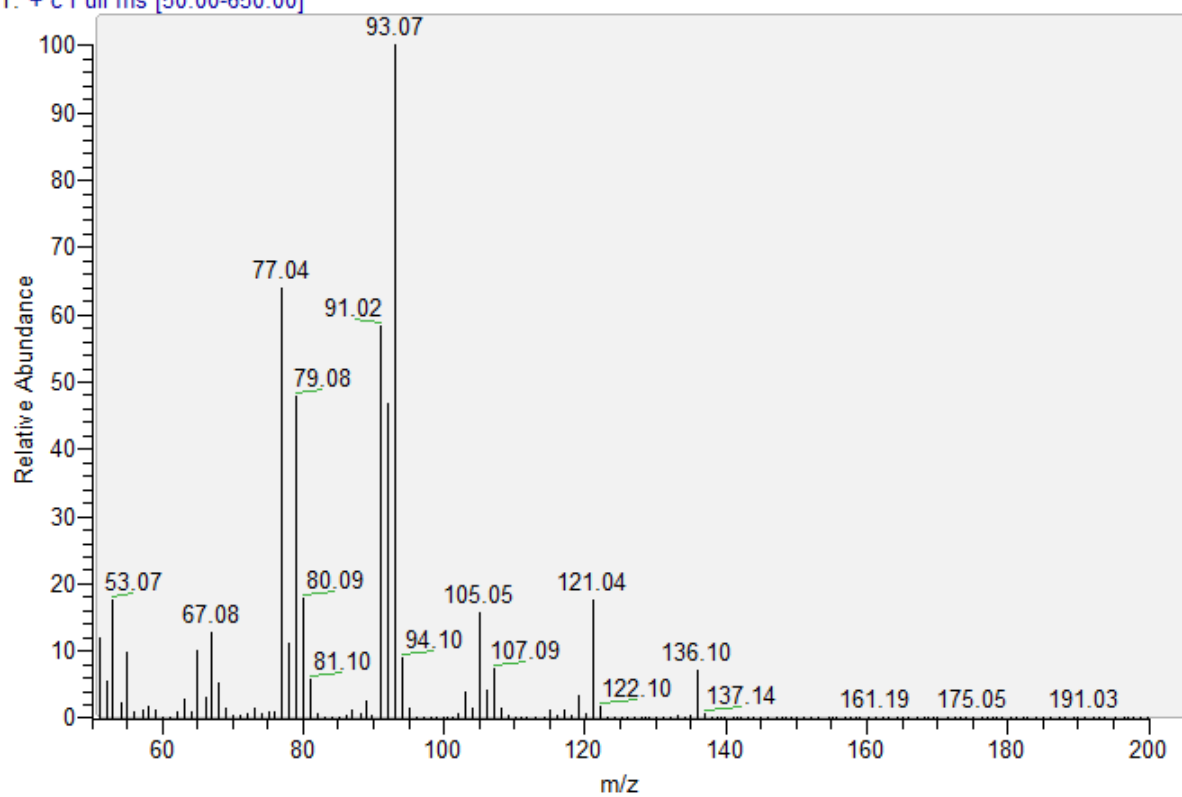
3070 #104 RT: 2.46 AV: 1 NL: 5.34E6  
T: + c Full ms [50.00-650.00]



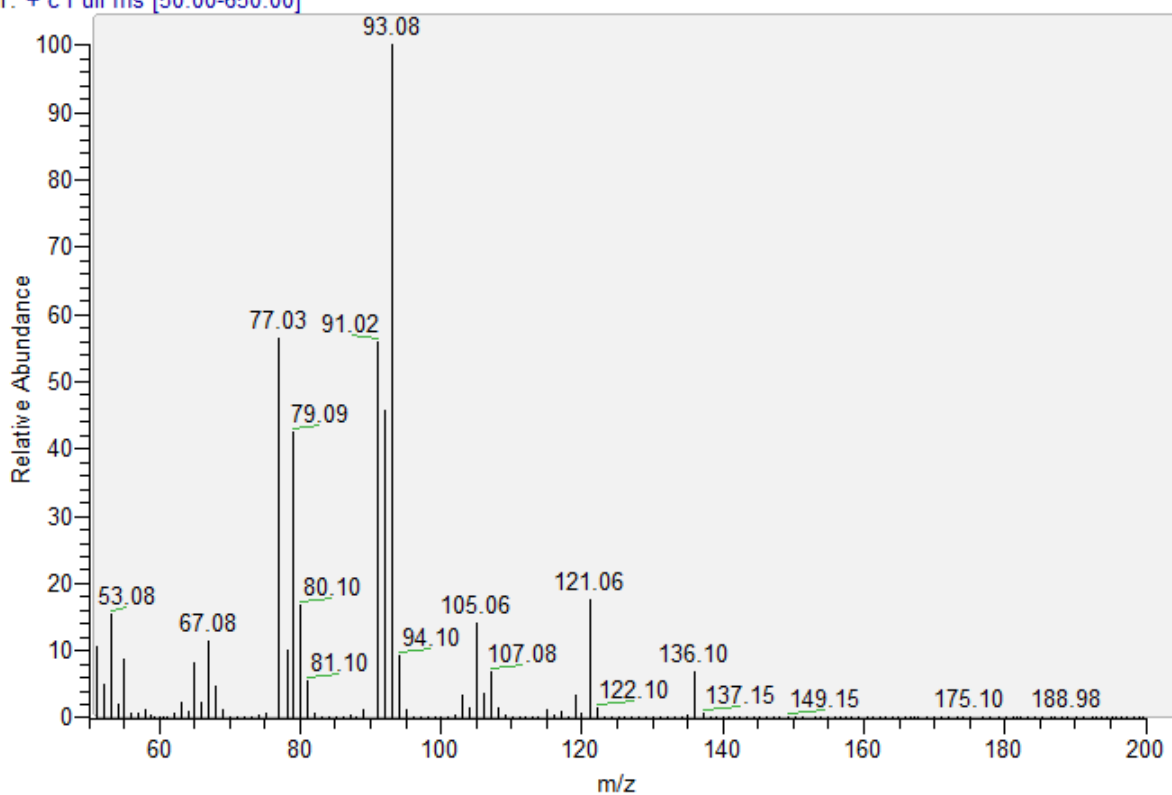
3072 #103-104 RT: 2.45-2.47 AV: 2 NL: 3.90E7  
T: + c Full ms [50.00-650.00]



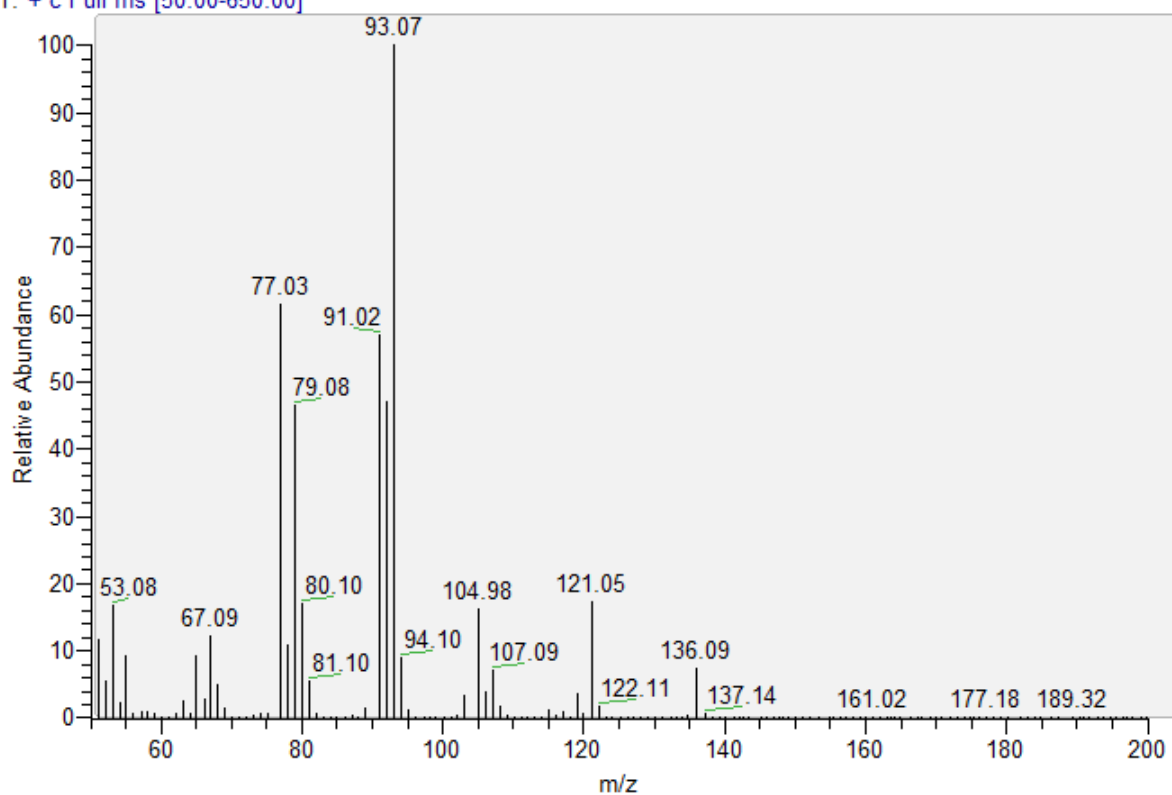
3073 #102-103 RT: 2.43-2.45 AV: 2 NL: 1.20E7  
T: + c Full ms [50.00-650.00]



3074 #104 RT: 2.46 AV: 1 NL: 8.46E7  
T: + c Full ms [50.00-650.00]



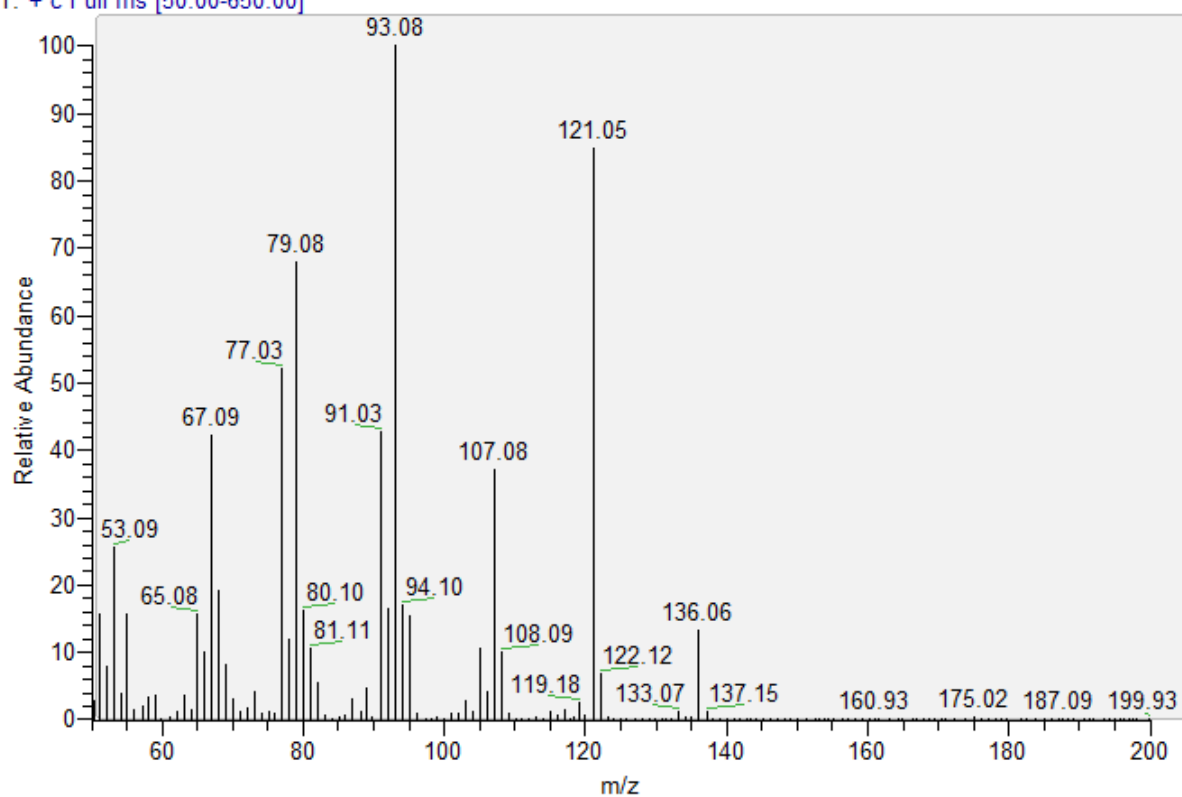
3075 #103 RT: 2.46 AV: 1 NL: 3.50E7  
T: + c Full ms [50.00-650.00]



Camphene

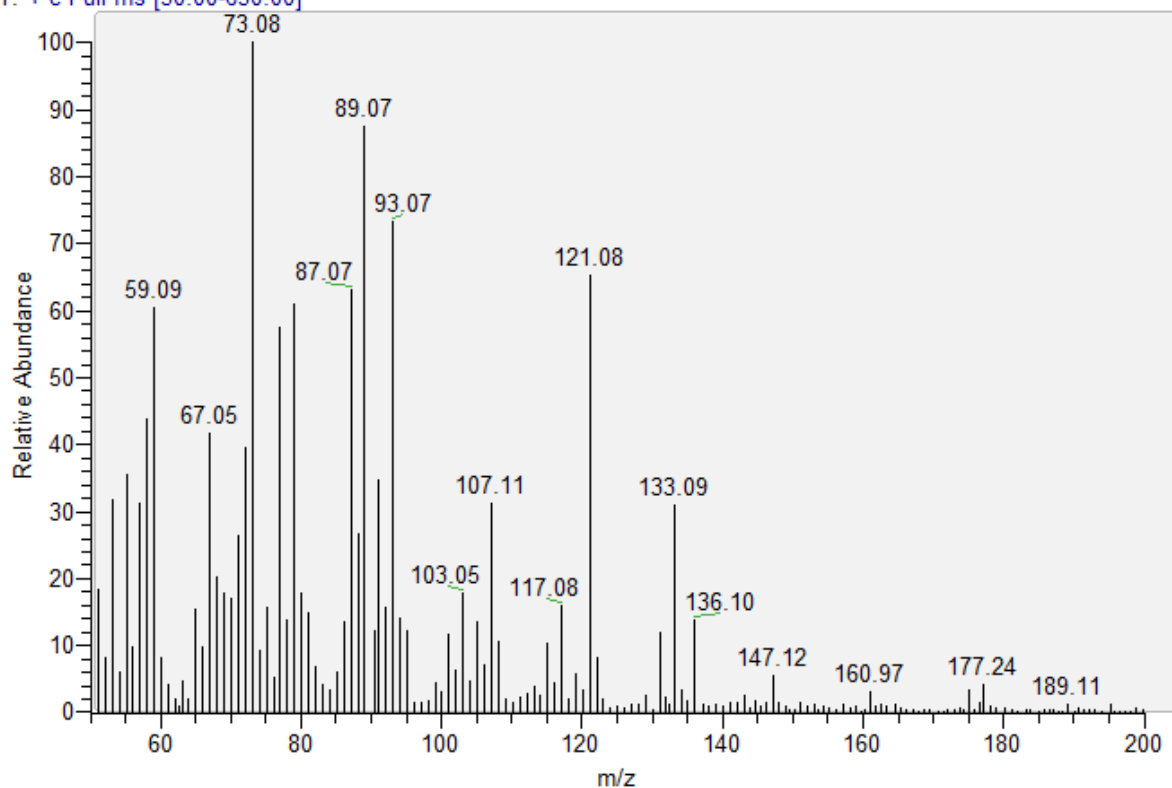
Reference

1\_20 #128 RT: 3.05 AV: 1 NL: 2.87E6  
T: + c Full ms [50.00-650.00]

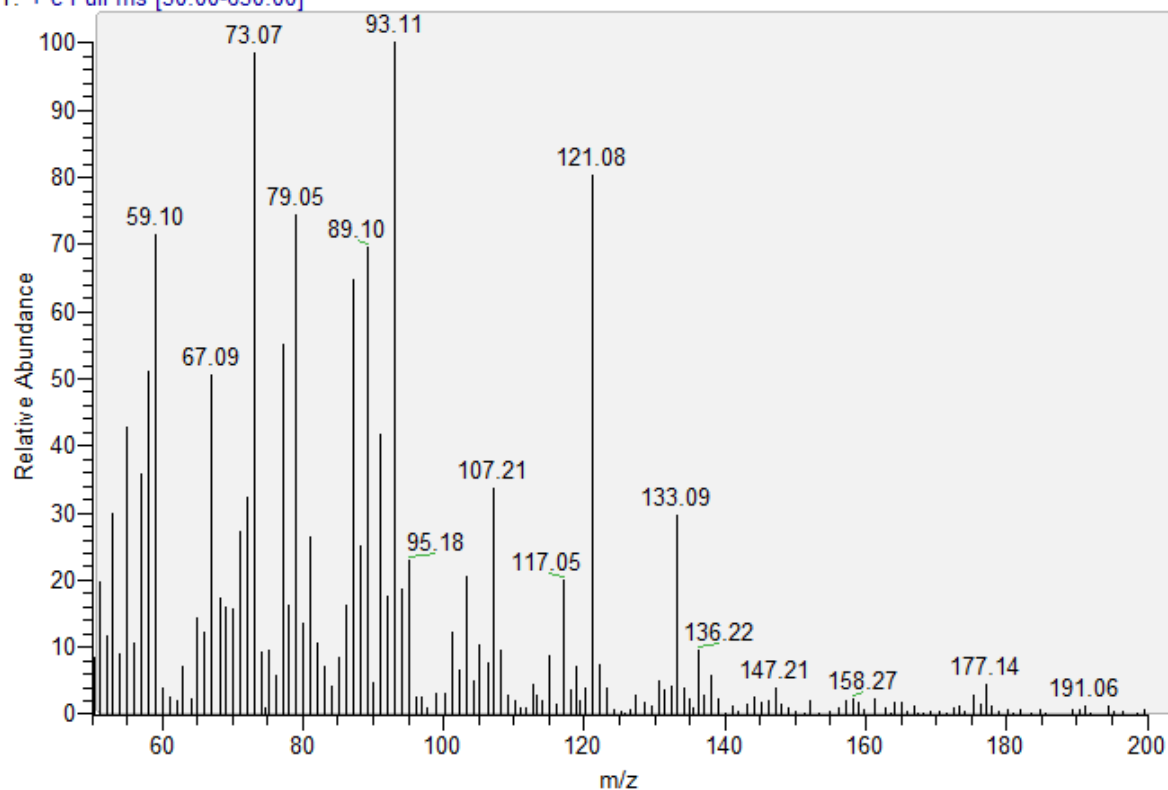


Samples:

3021 #128-129 RT: 3.03-3.06 AV: 2 NL: 1.54E5  
T: + c Full ms [50.00-650.00]

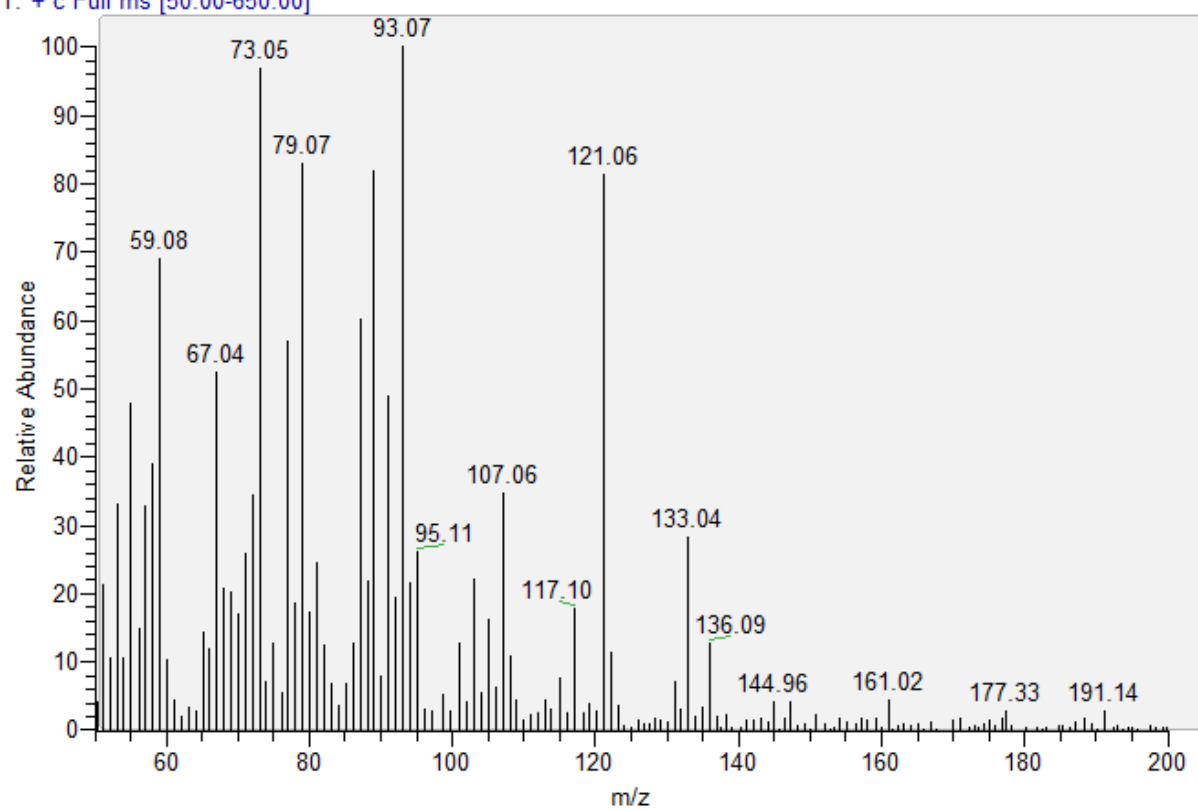


3057 #130 RT: 3.04 AV: 1 NL: 1.00E5  
T: + c Full ms [50.00-650.00]

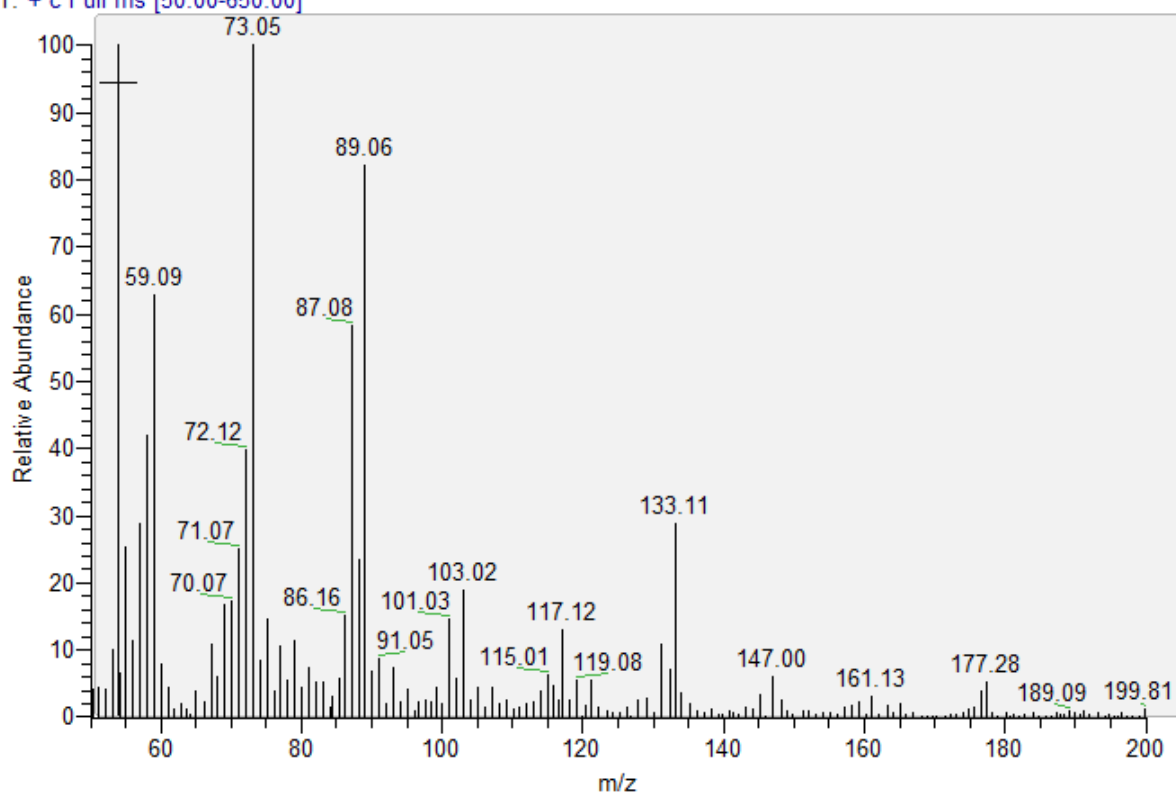




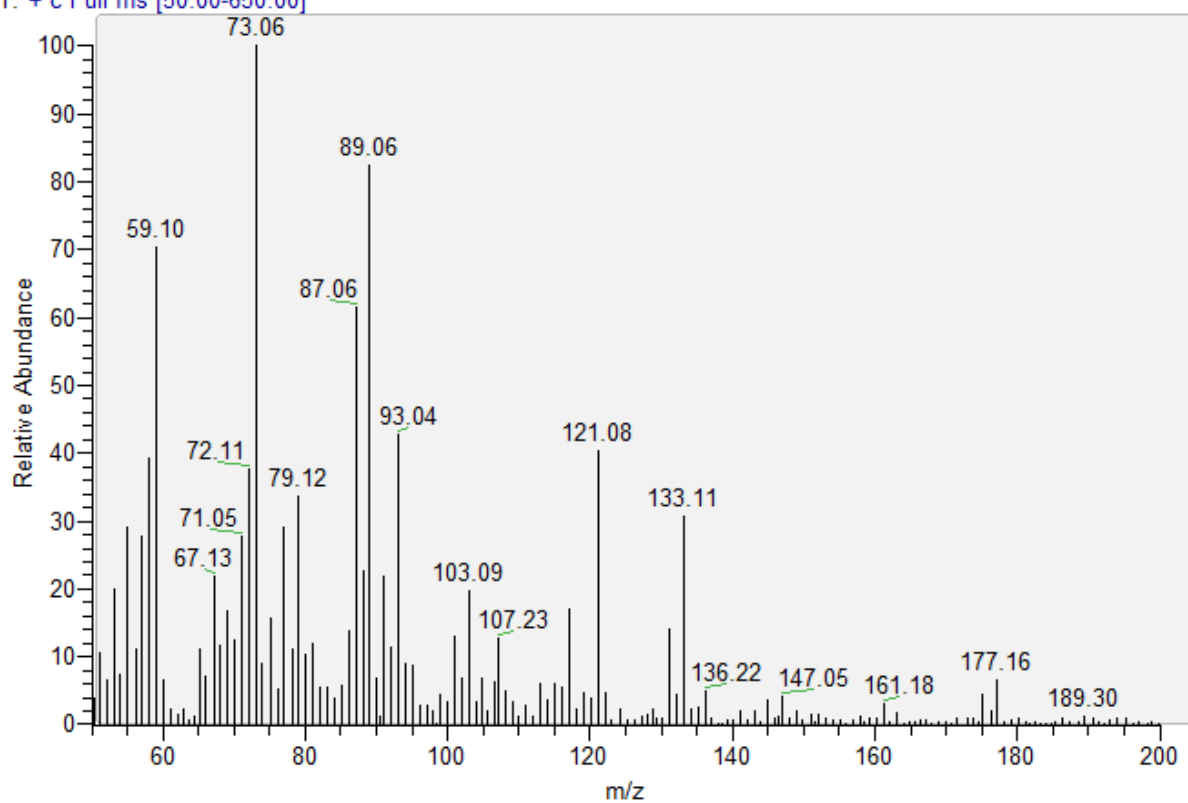
3058 #127 RT: 3.03 AV: 1 NL: 1.64E5  
T: + c Full ms [50.00-650.00]



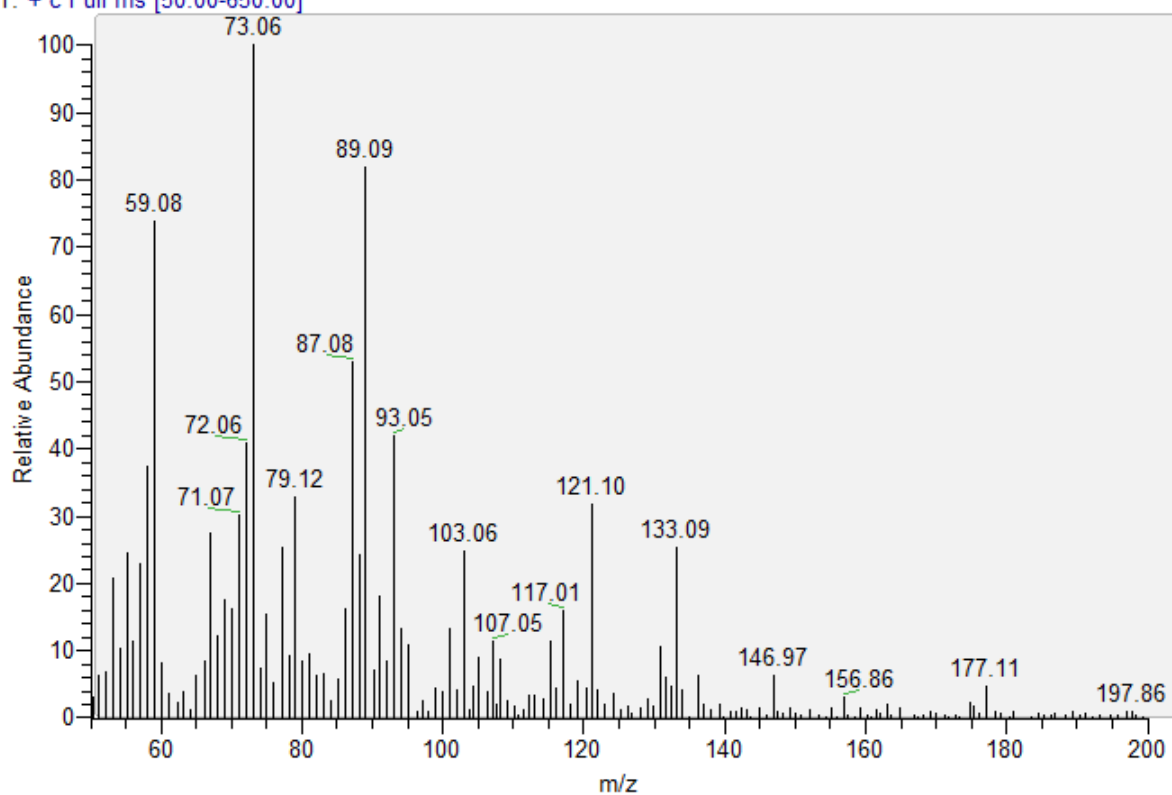
3053 #127-128 RT: 3.01-3.03 AV: 2 NL: 1.45E5  
T: + c Full ms [50.00-650.00]



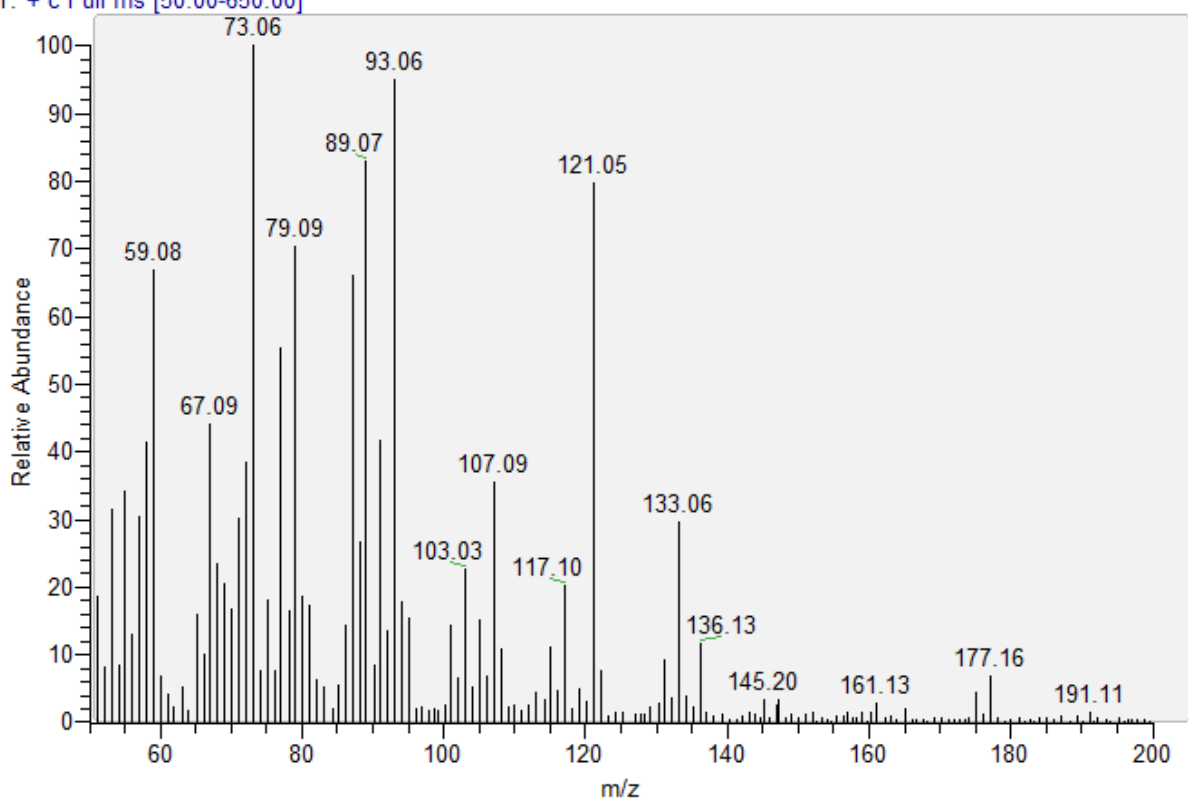
3075 #127-128 RT: 3.03-3.05 AV: 2 NL: 1.40E5  
T: + c Full ms [50.00-650.00]



3018 #129 RT: 3.04 AV: 1 NL: 1.44E5  
T: + c Full ms [50.00-650.00]



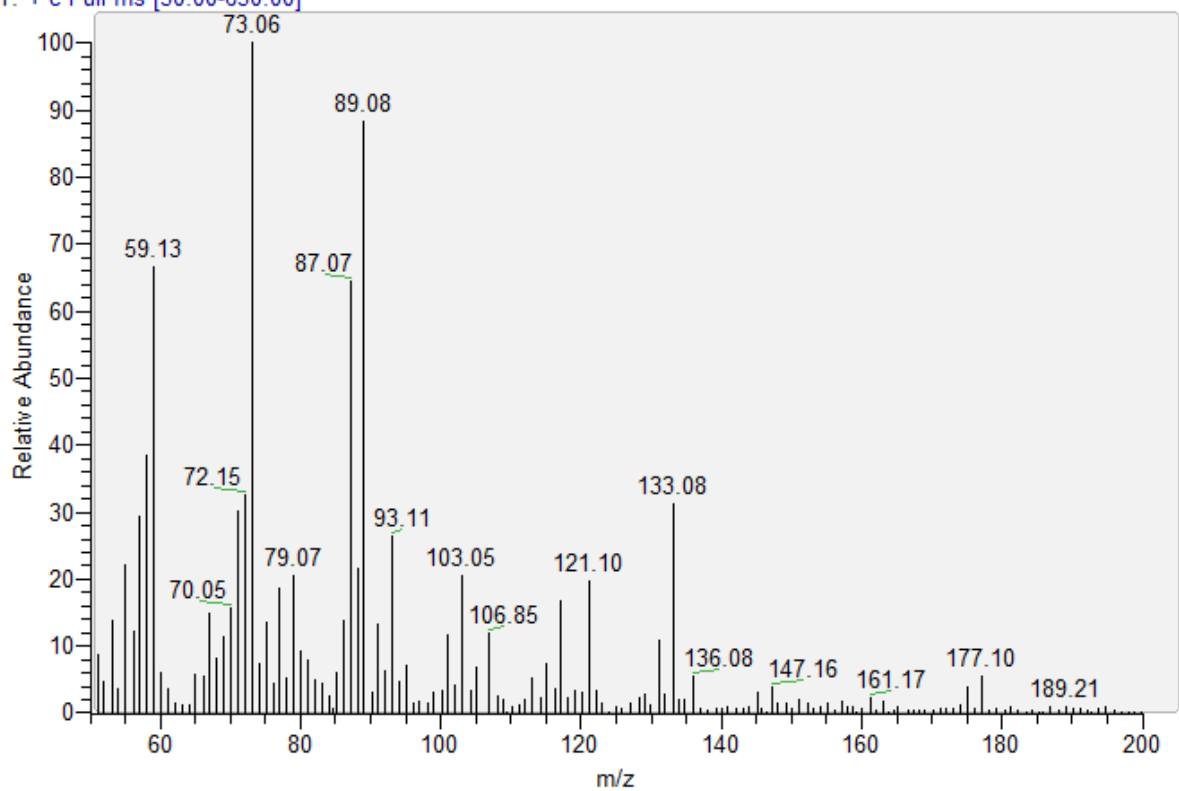
3074 #128-129 RT: 3.04-3.06 AV: 2 NL: 1.48E5  
T: + c Full ms [50.00-650.00]



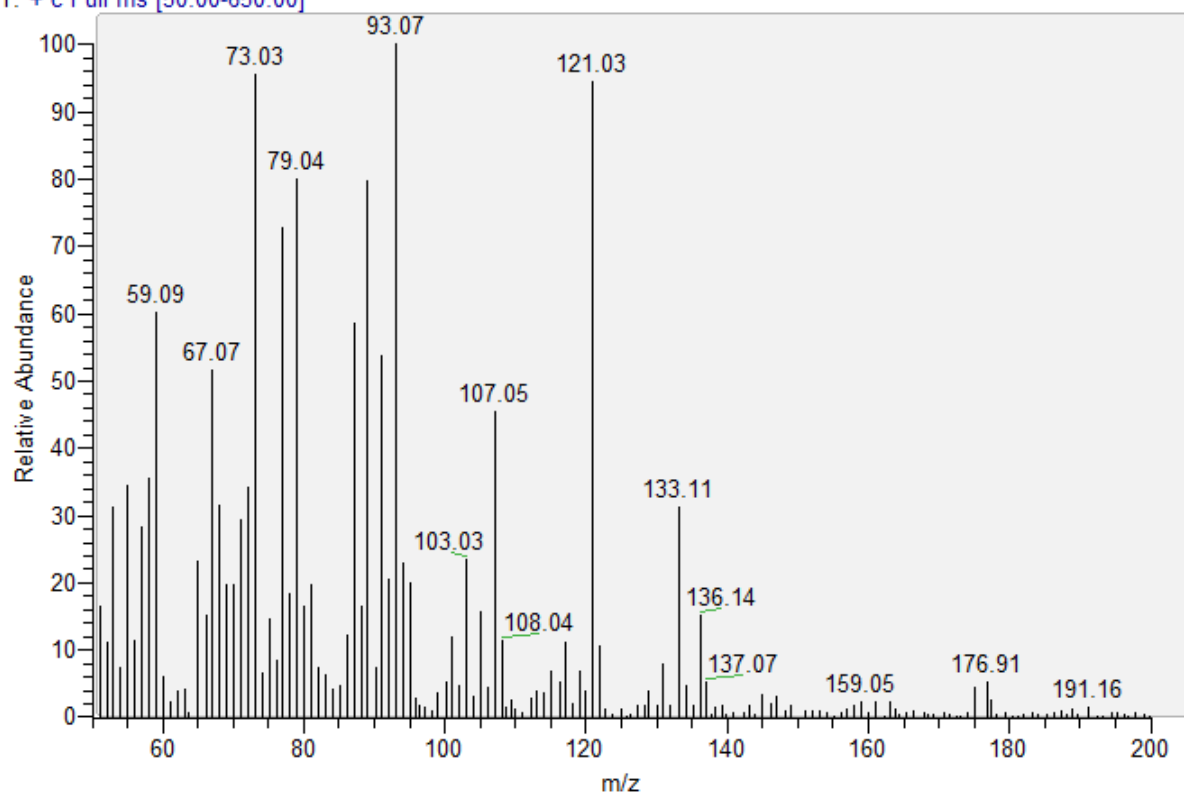
3073 #127-128 RT: 3.02-3.04 AV: 2 NL: 1.70E5



T: + c Full ms [50.00-650.00]

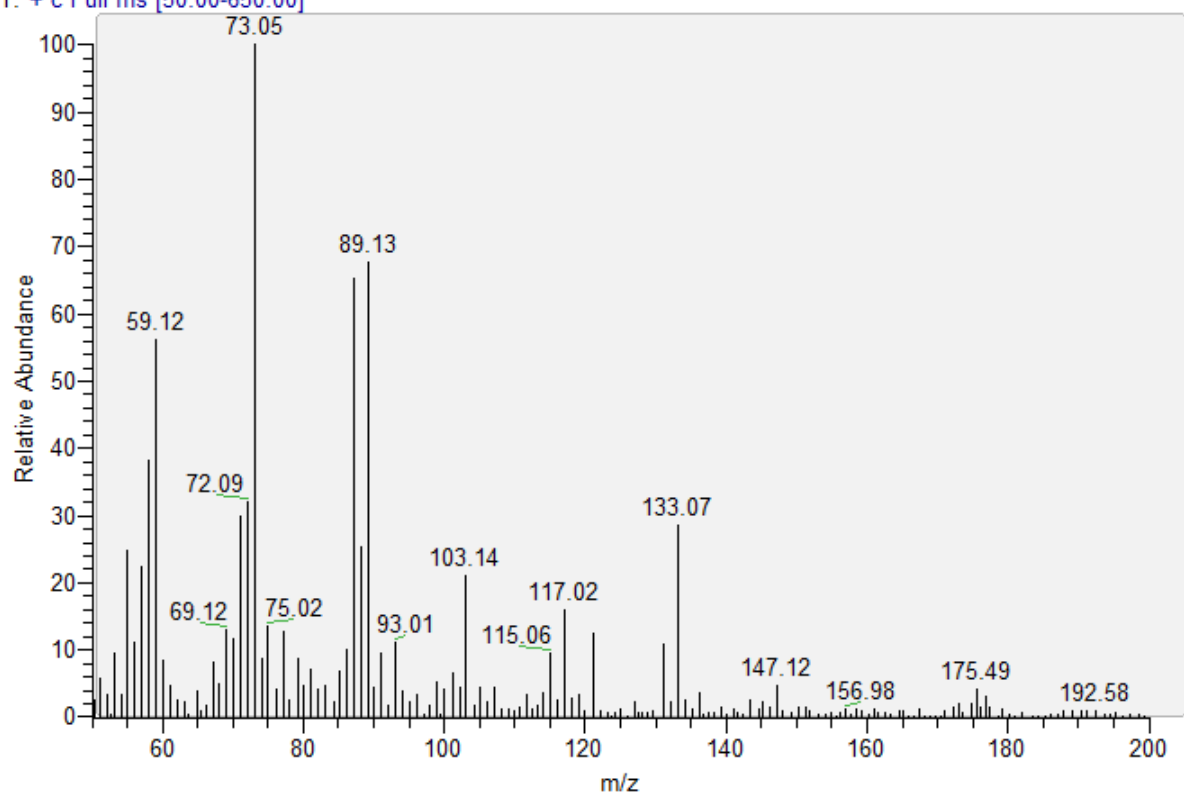


3072 #128 RT: 3.04 AV: 1 NL: 1.57E5  
T: + c Full ms [50.00-650.00]



3070 #129 RT: 3.04 AV: 1 NL: 1.47E5

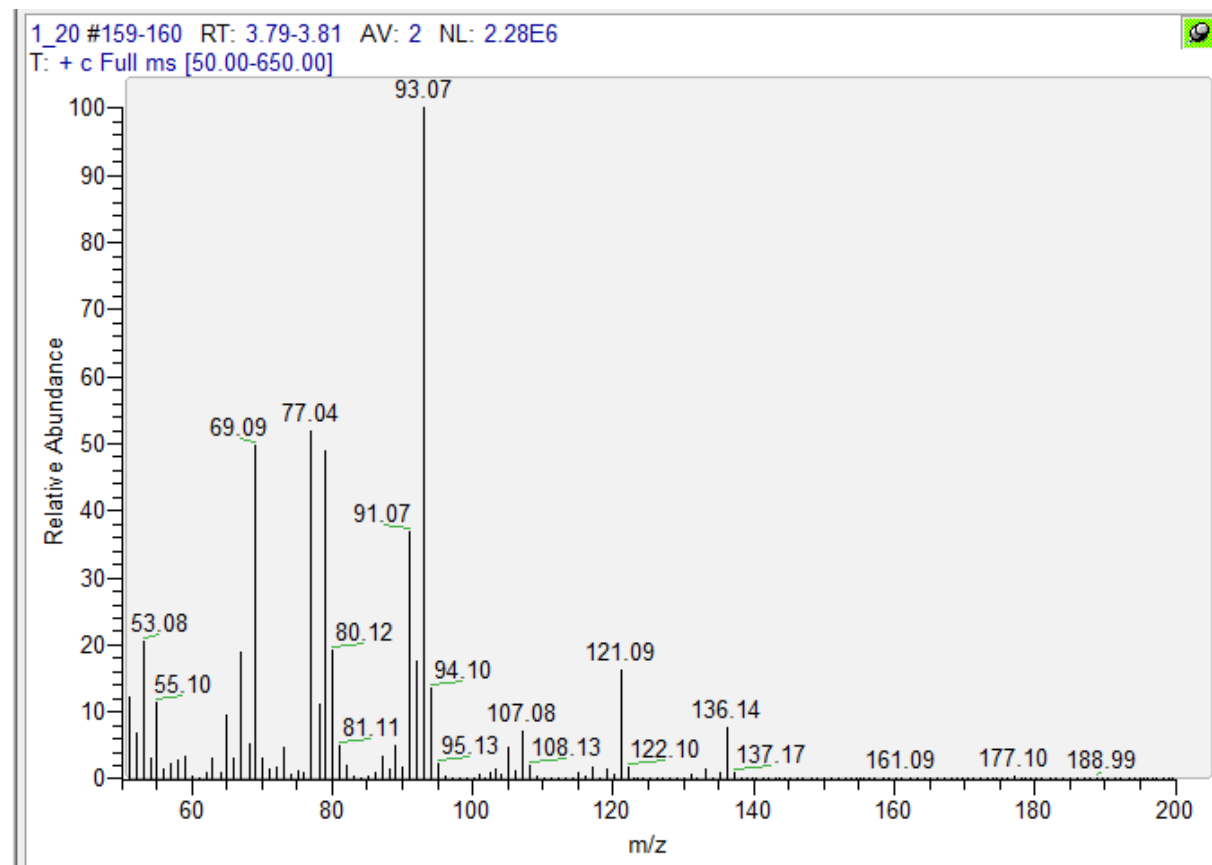
T: + c Full ms [50.00-650.00]





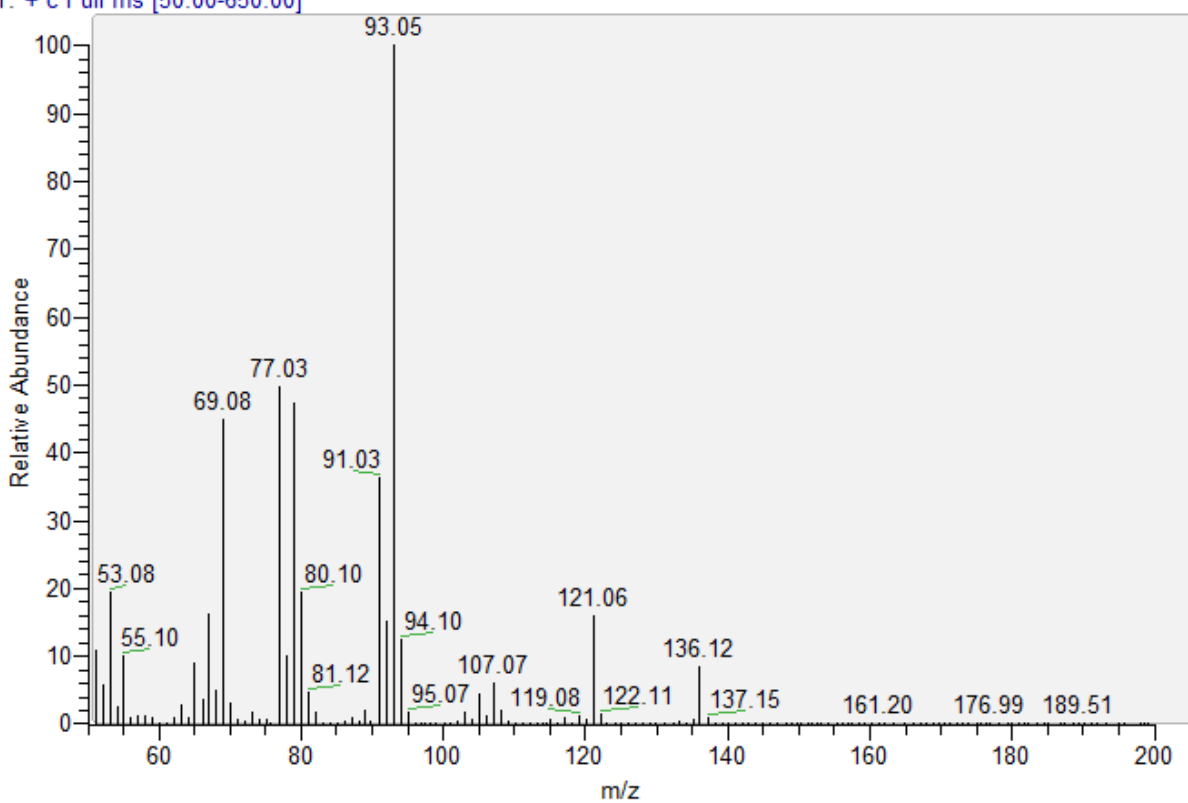
Beta Pinene:

Reference:

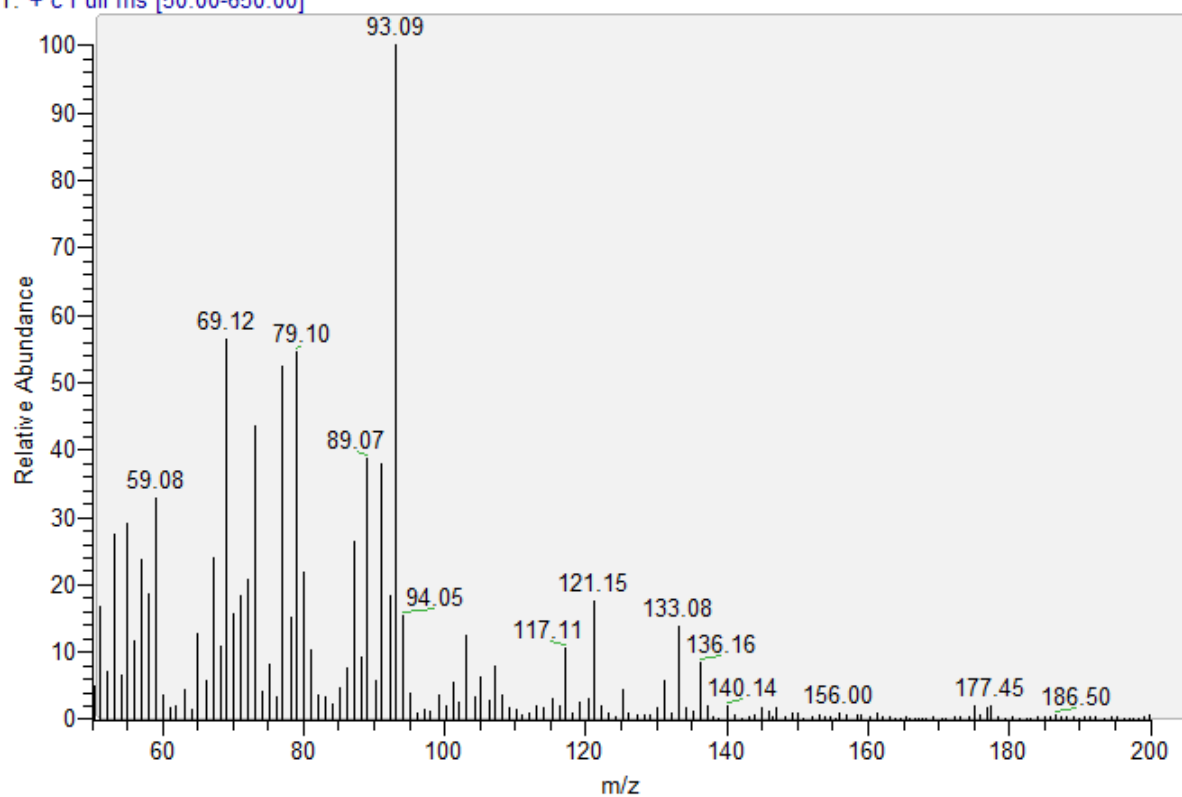


Samples:

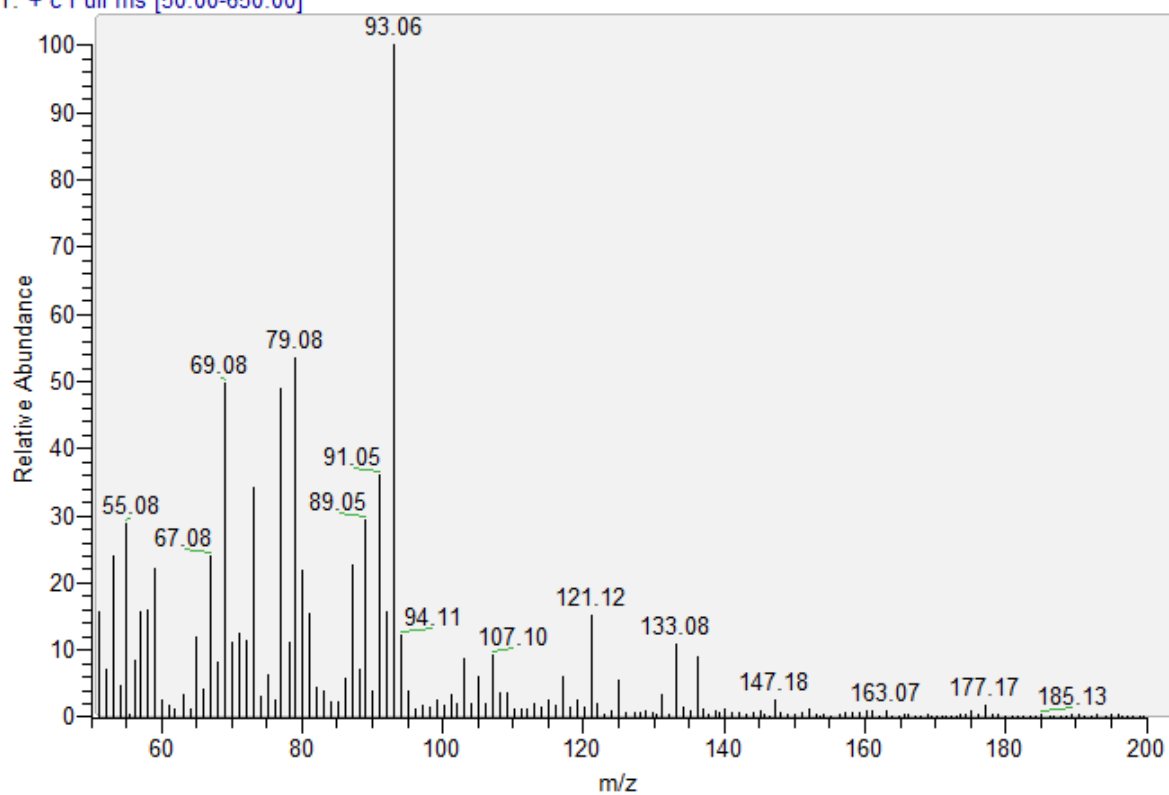
3021 #160 RT: 3.79 AV: 1 NL: 1.05E7  
T: + c Full ms [50.00-650.00]



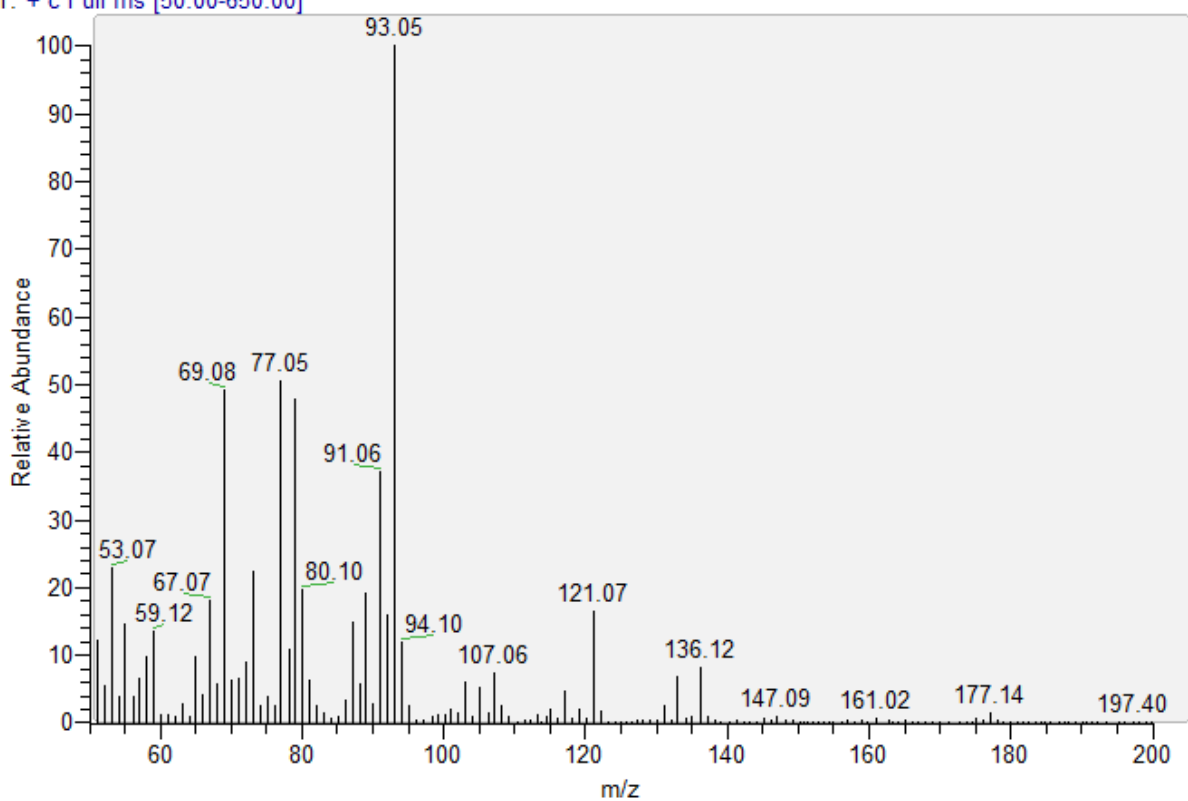
3057 #161-162 RT: 3.77-3.80 AV: 2 NL: 1.88E5  
T: + c Full ms [50.00-650.00]



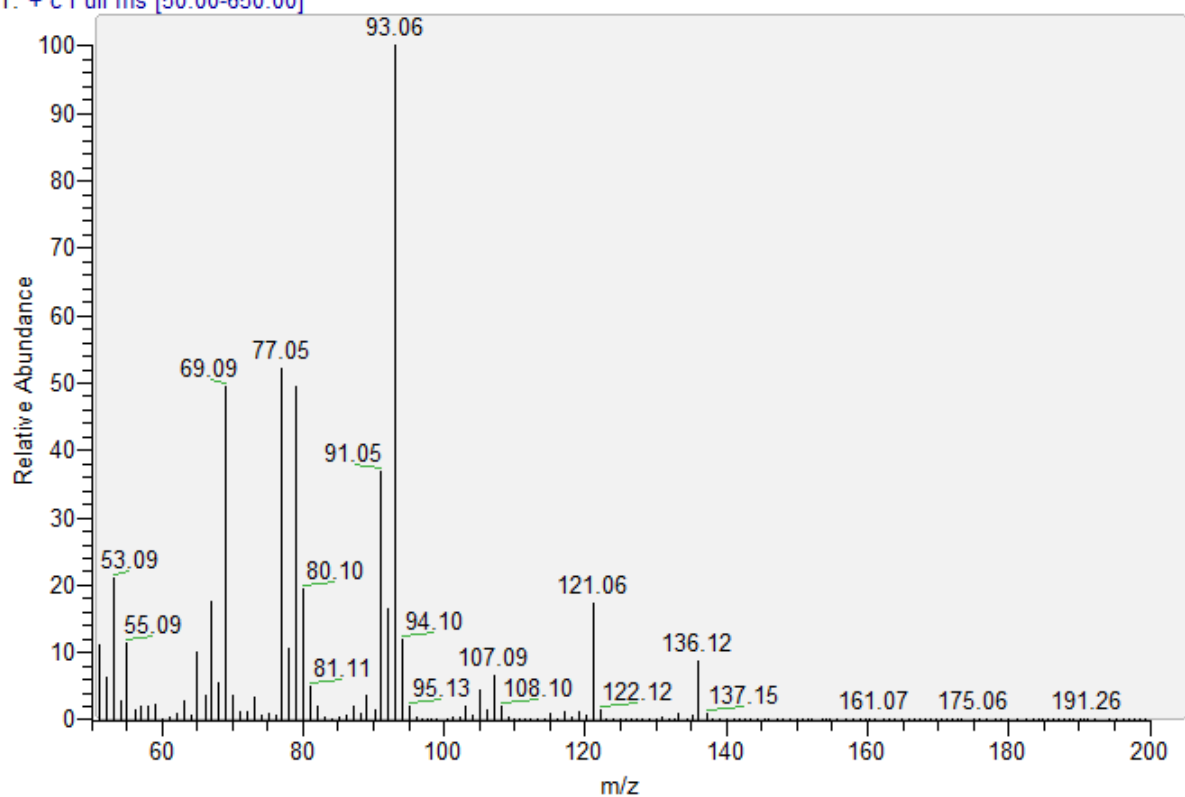
3058 #158-159 RT: 3.77-3.80 AV: 2 NL: 4.17E5  
T: + c Full ms [50.00-650.00]



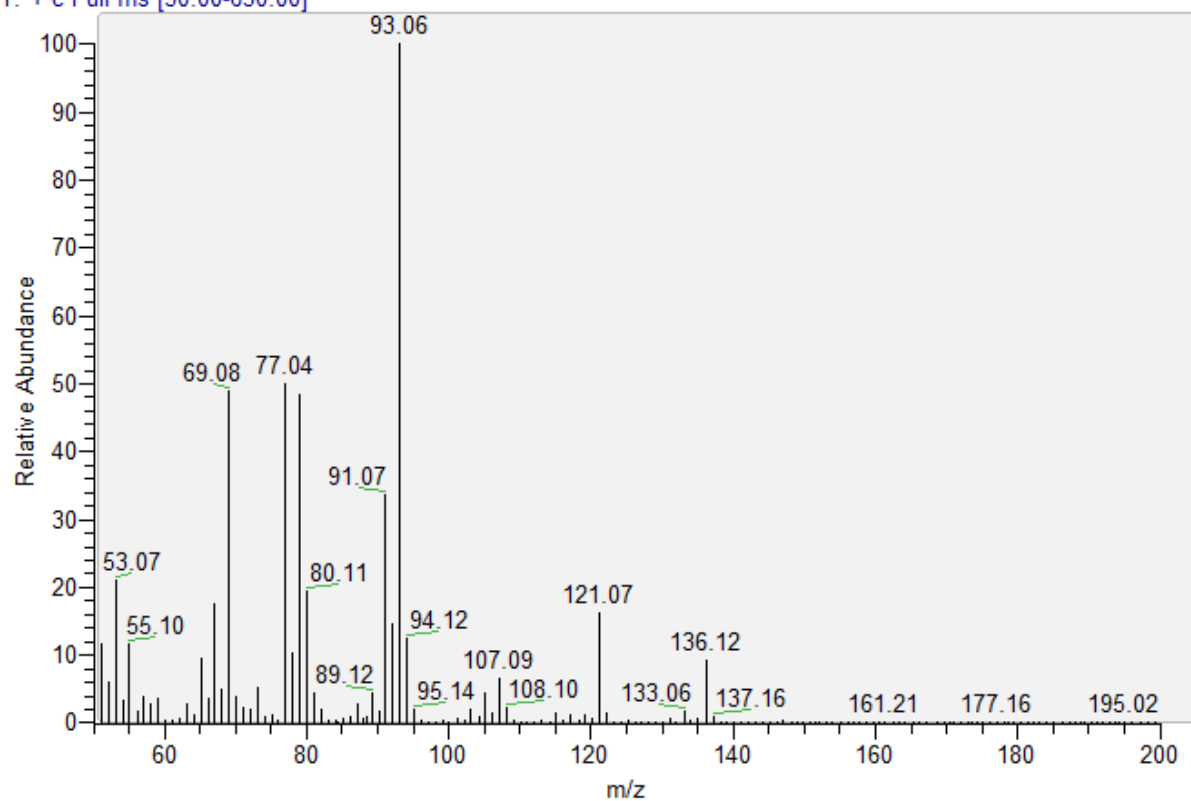
3053 #159-161 RT: 3.77-3.82 AV: 3 NL: 6.00E5  
T: + c Full ms [50.00-650.00]



3075 #159-160 RT: 3.78-3.81 AV: 2 NL: 4.18E6  
T: + c Full ms [50.00-650.00]

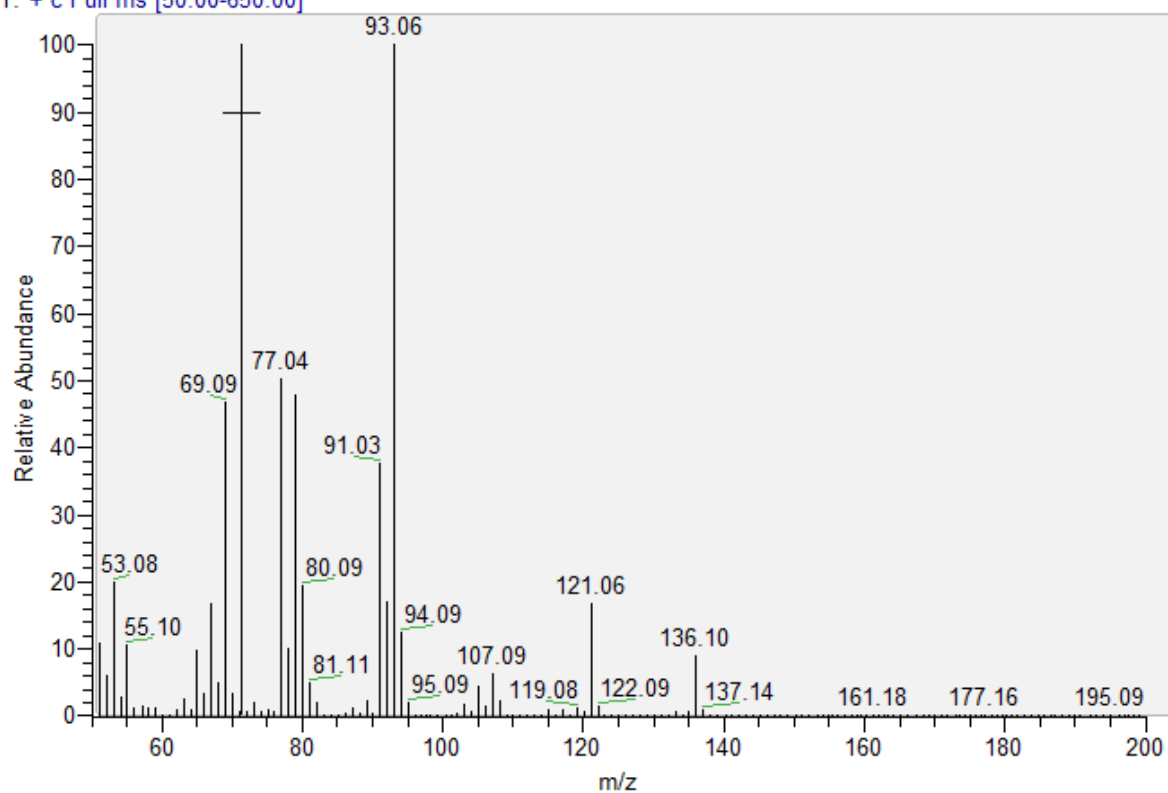


3018 #160-161 RT: 3.78-3.80 AV: 2 NL: 2.63E6  
T: + c Full ms [50.00-650.00]

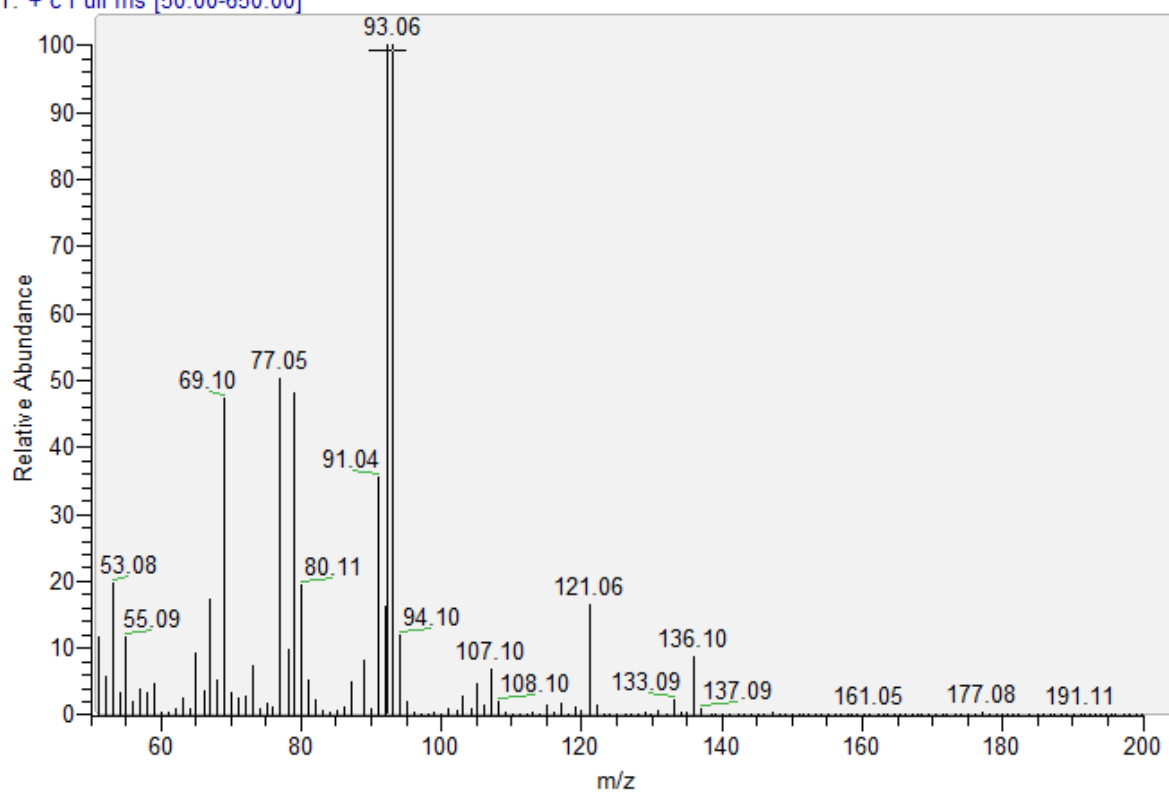




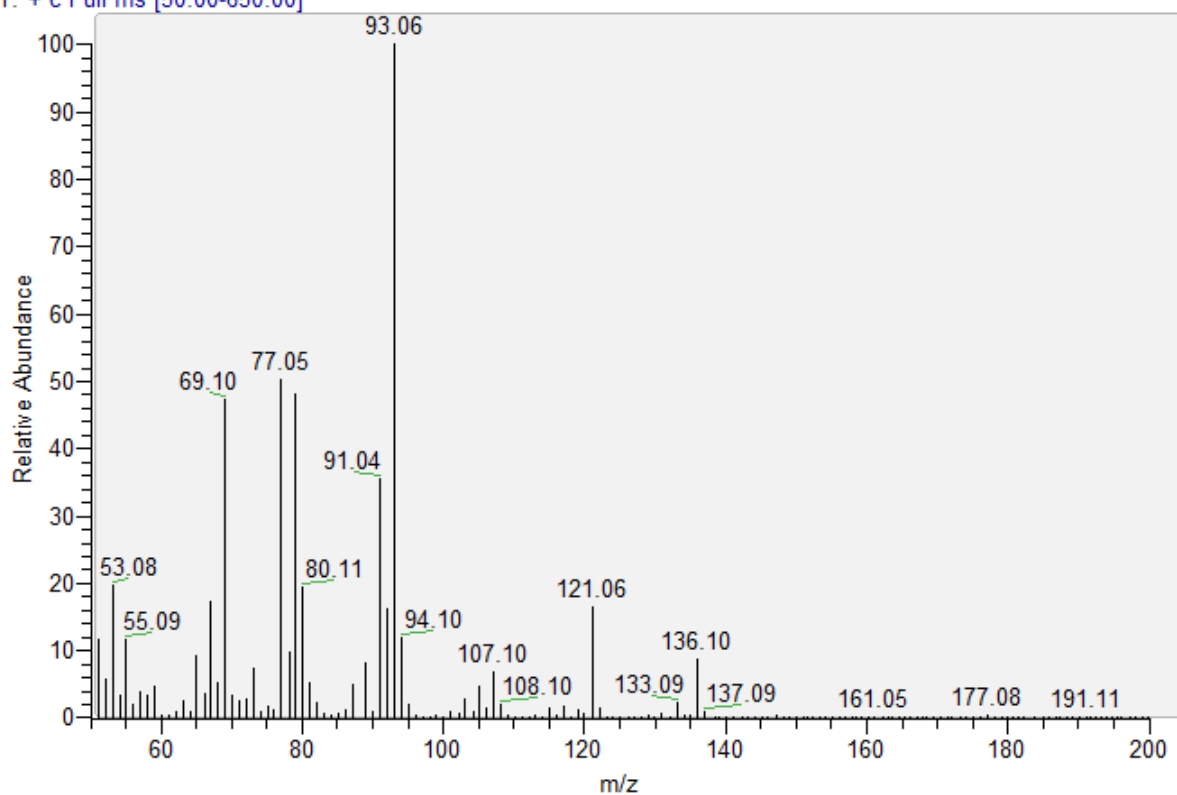
3074 #160-161 RT: 3.79-3.81 AV: 2 NL: 8.36E6  
T: + c Full ms [50.00-650.00]



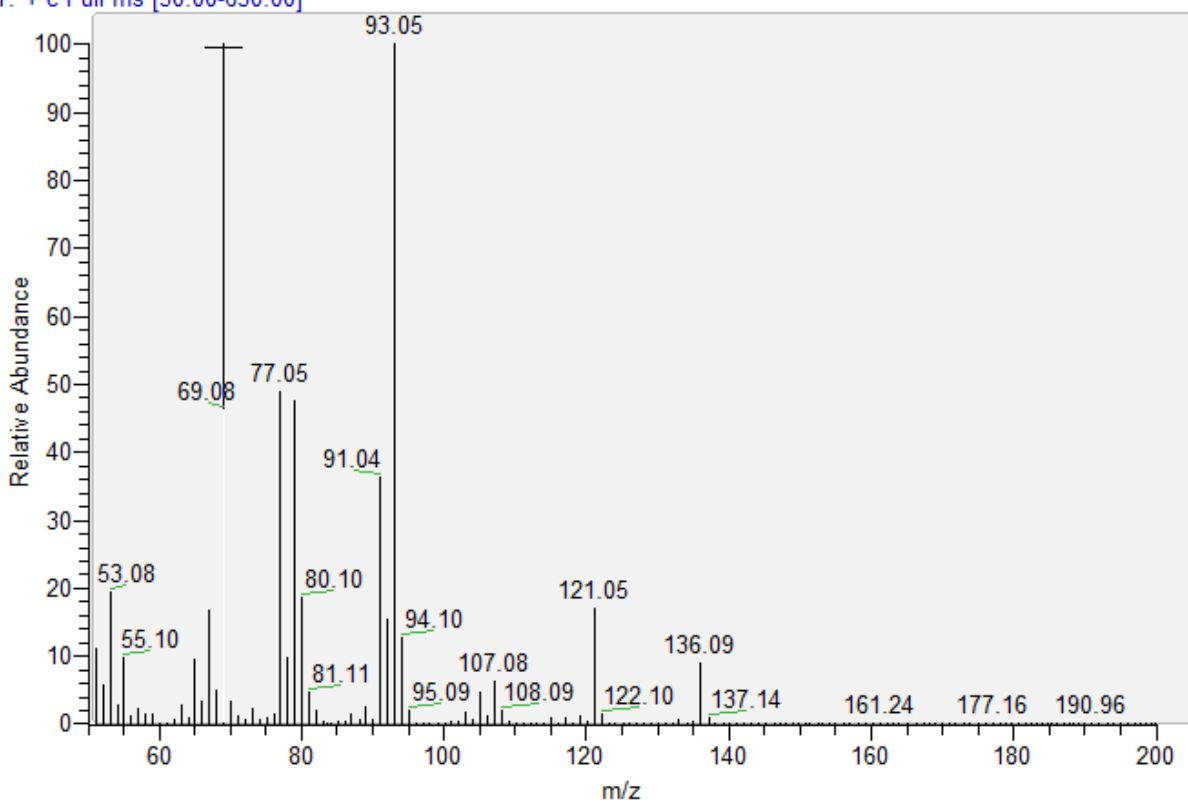
3073 #159-160 RT: 3.78-3.81 AV: 2 NL: 2.26E6  
T: + c Full ms [50.00-650.00]



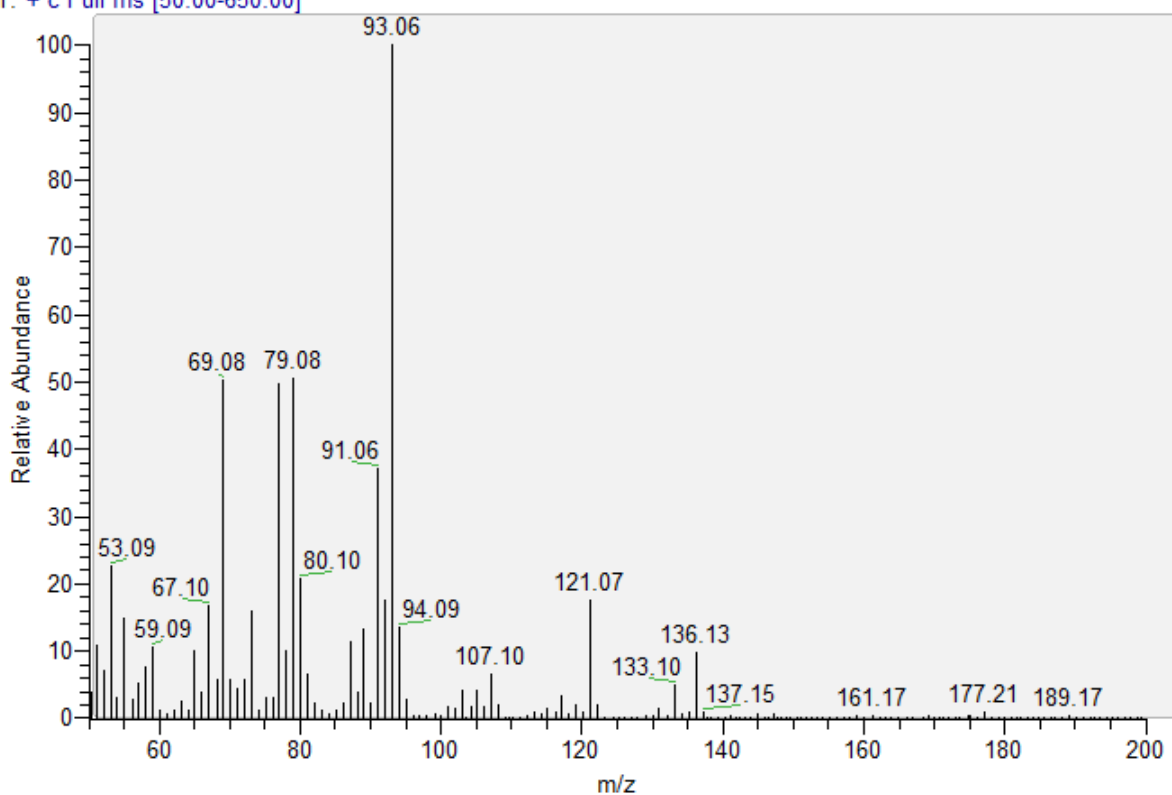
3073 #159-160 RT: 3.78-3.81 AV: 2 NL: 2.26E6  
T: + c Full ms [50.00-650.00]



3072 #159-160 RT: 3.78-3.80 AV: 2 NL: 6.90E6  
T: + c Full ms [50.00-650.00]

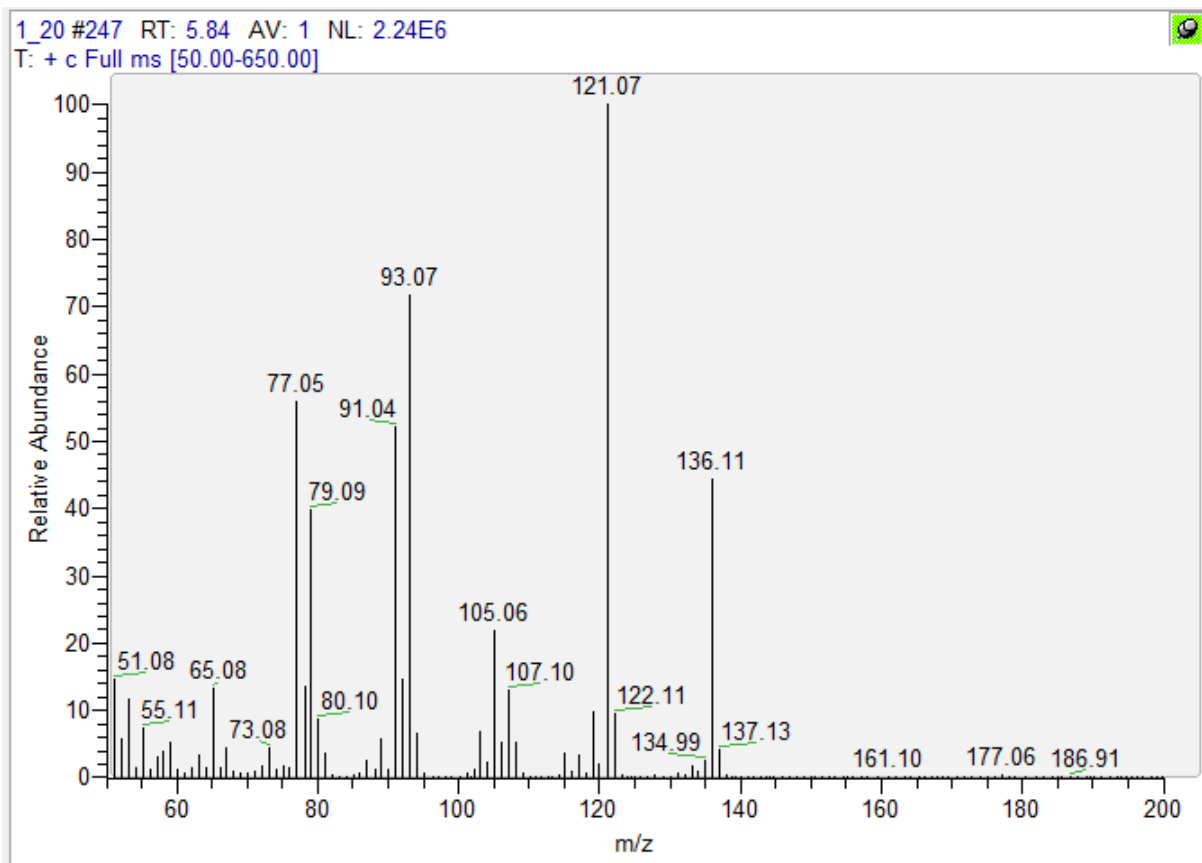


3070 #160-161 RT: 3.78-3.80 AV: 2 NL: 7.94E5  
T: + c Full ms [50.00-650.00]



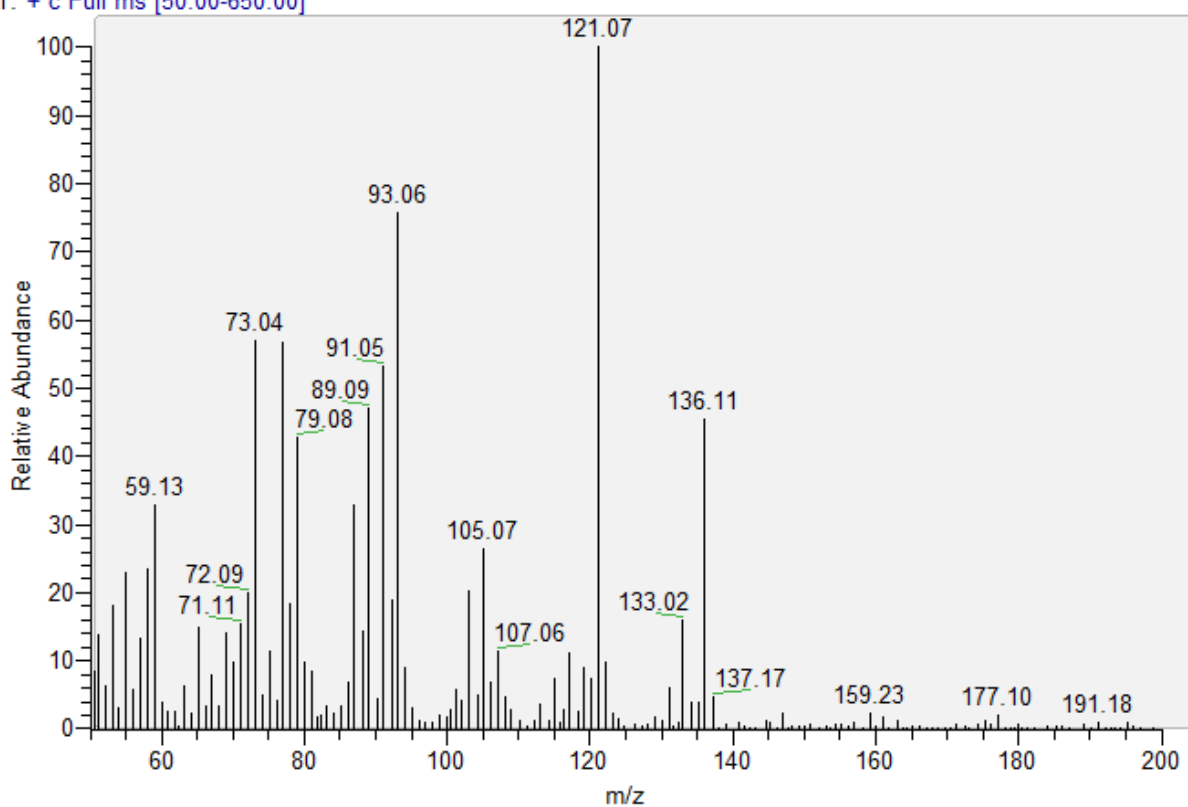
# Alpha Terpinene

Reference:



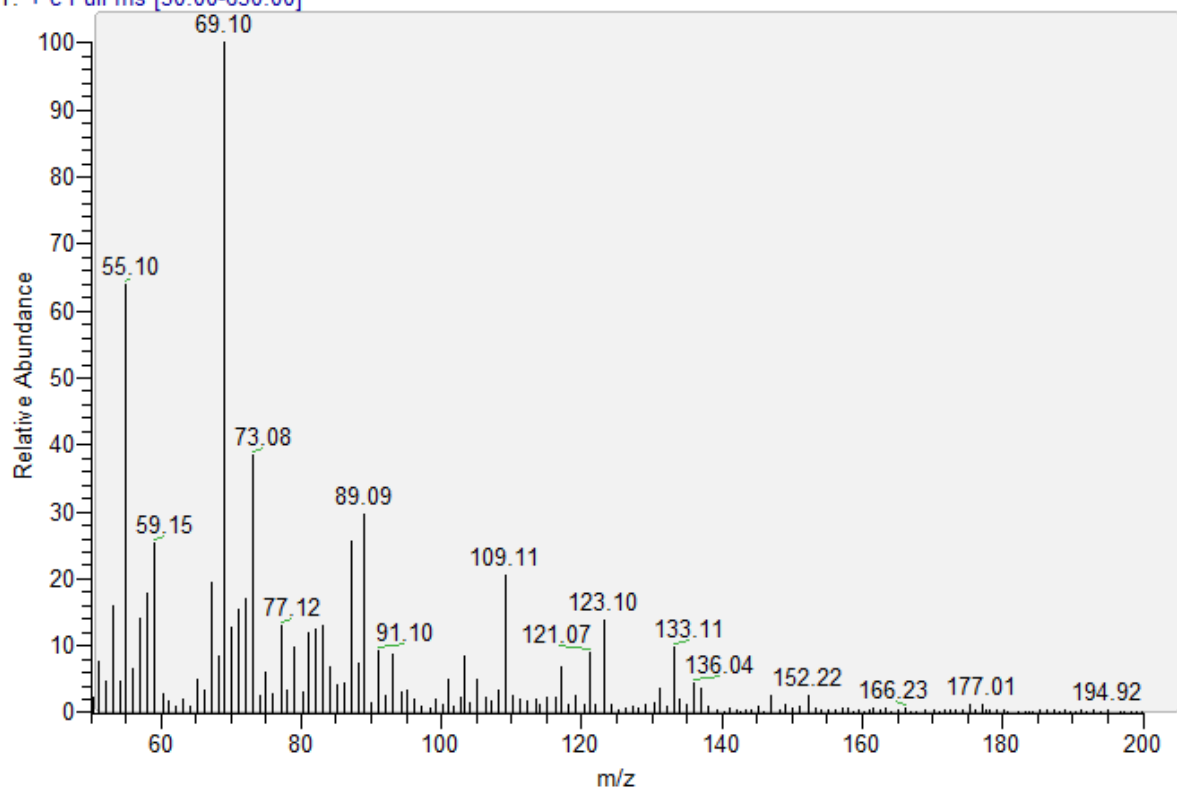
Samples:

3021 #246 RT: 5.83 AV: 1 NL: 2.27E5  
T: + c Full ms [50.00-650.00]

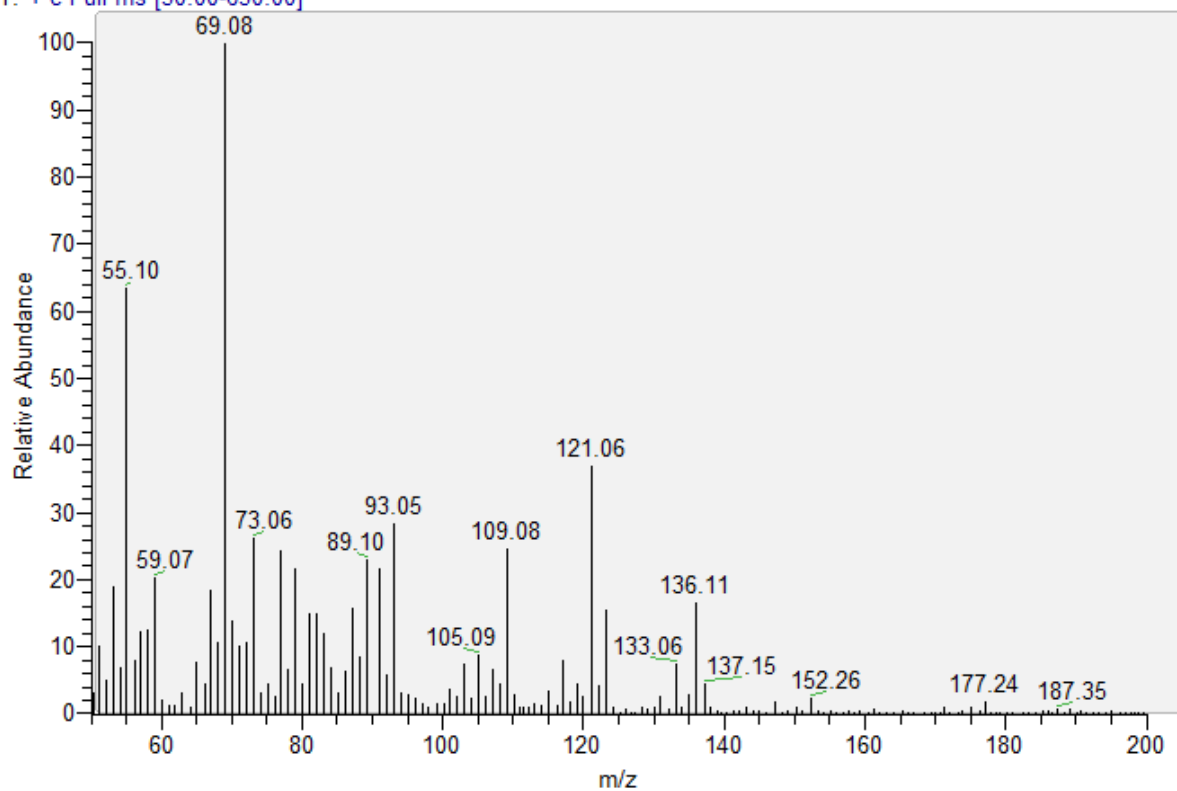




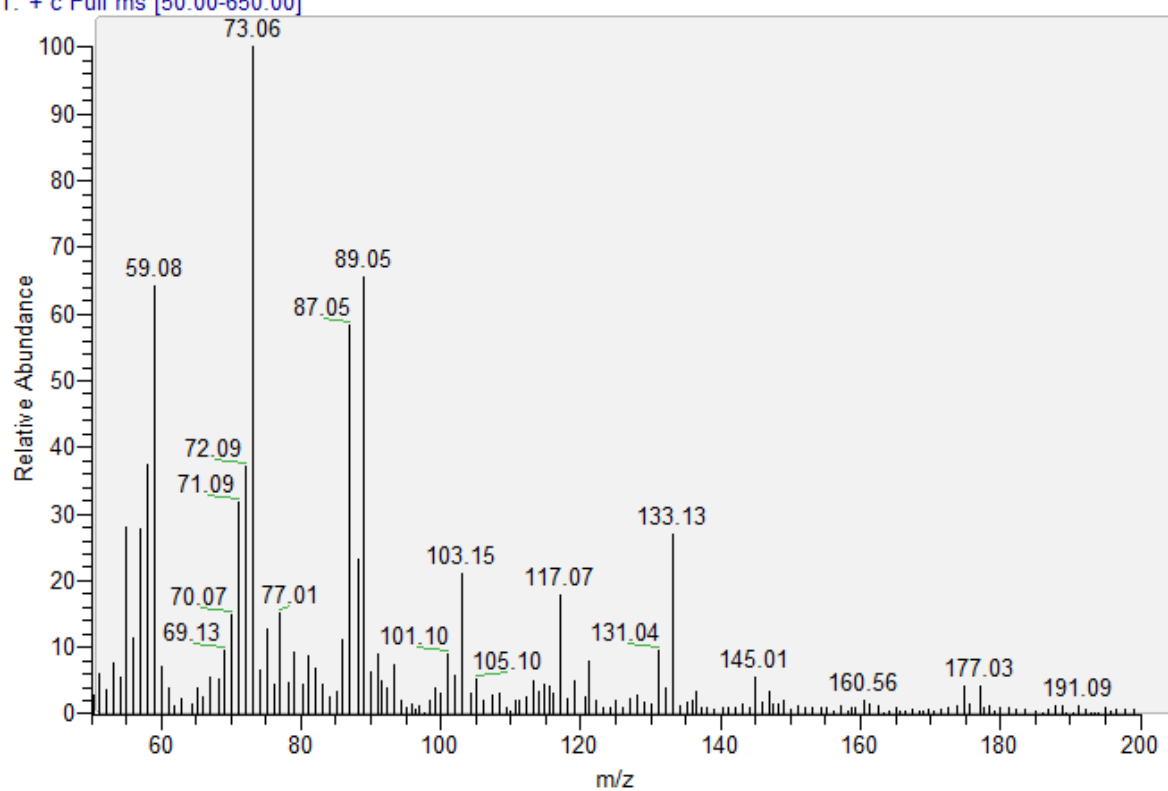
3057 #247-248 RT: 5.81-5.83 AV: 2 NL: 1.79E5  
T: + c Full ms [50.00-650.00]



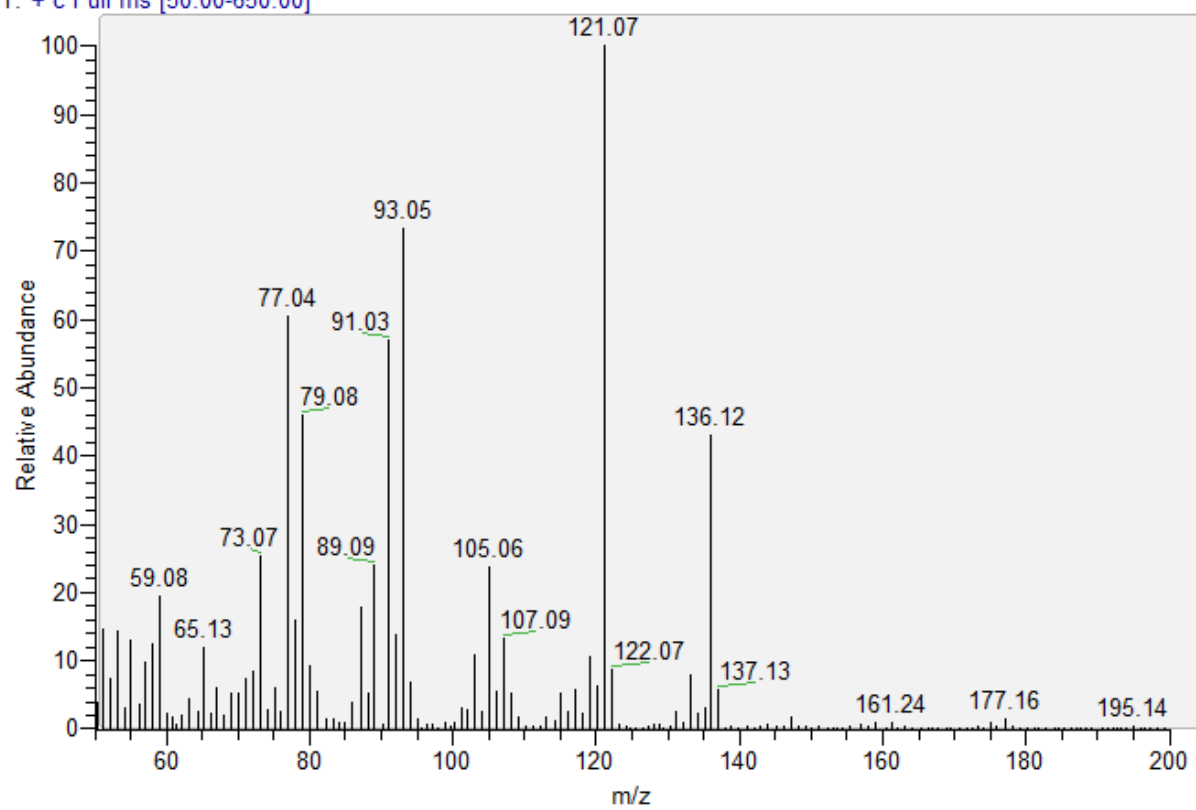
3058 #244 RT: 5.82 AV: 1 NL: 3.80E5  
T: + c Full ms [50.00-650.00]



3053 #245-246 RT: 5.82-5.84 AV: 2 NL: 1.15E5  
T: + c Full ms [50.00-650.00]

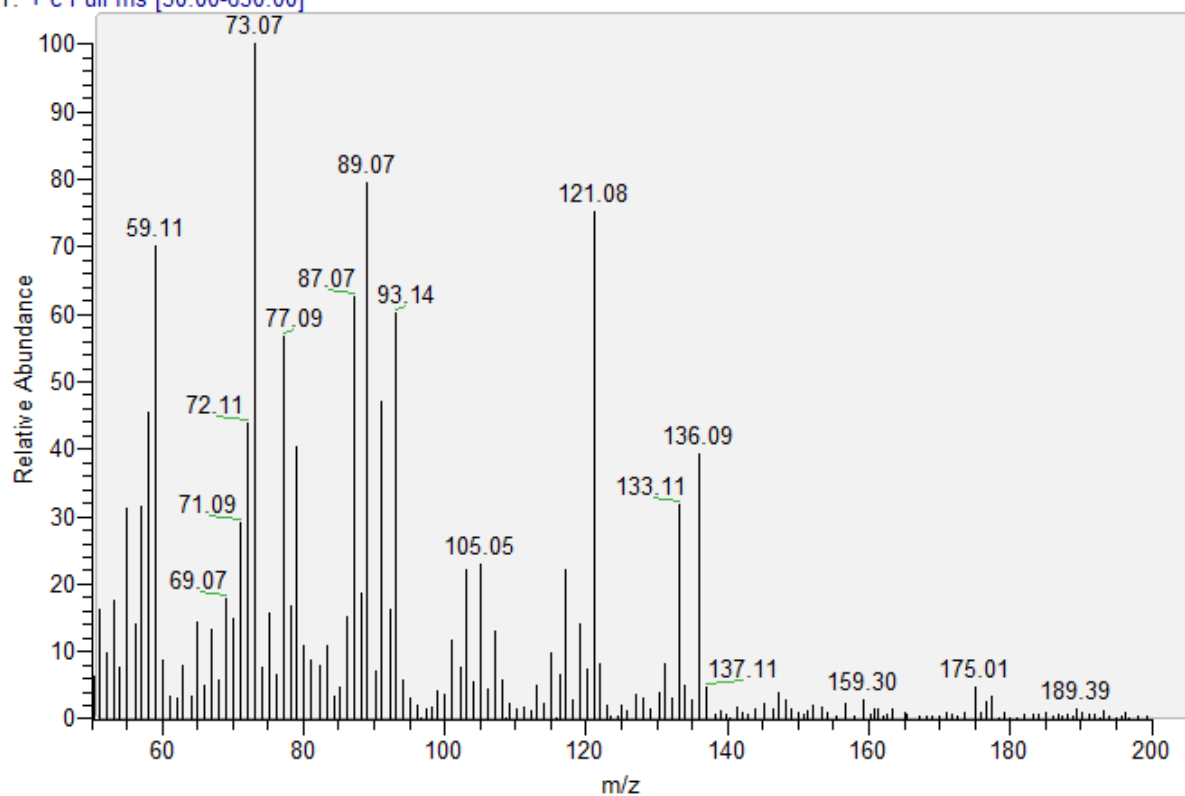


3075 #245-246 RT: 5.83-5.85 AV: 2 NL: 4.08E5  
T: + c Full ms [50.00-650.00]

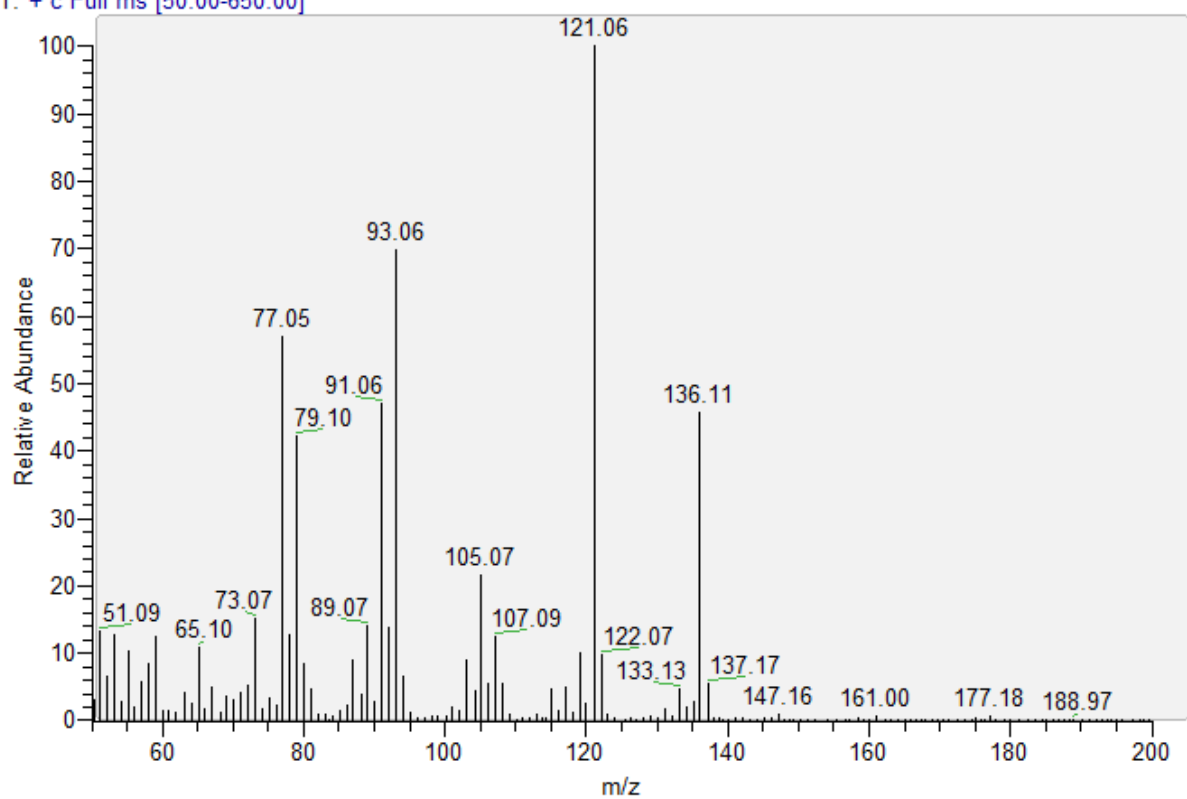


3018 #246-247 RT: 5.82-5.84 AV: 2 NL: 1.02E5

T: + c Full ms [50.00-650.00]



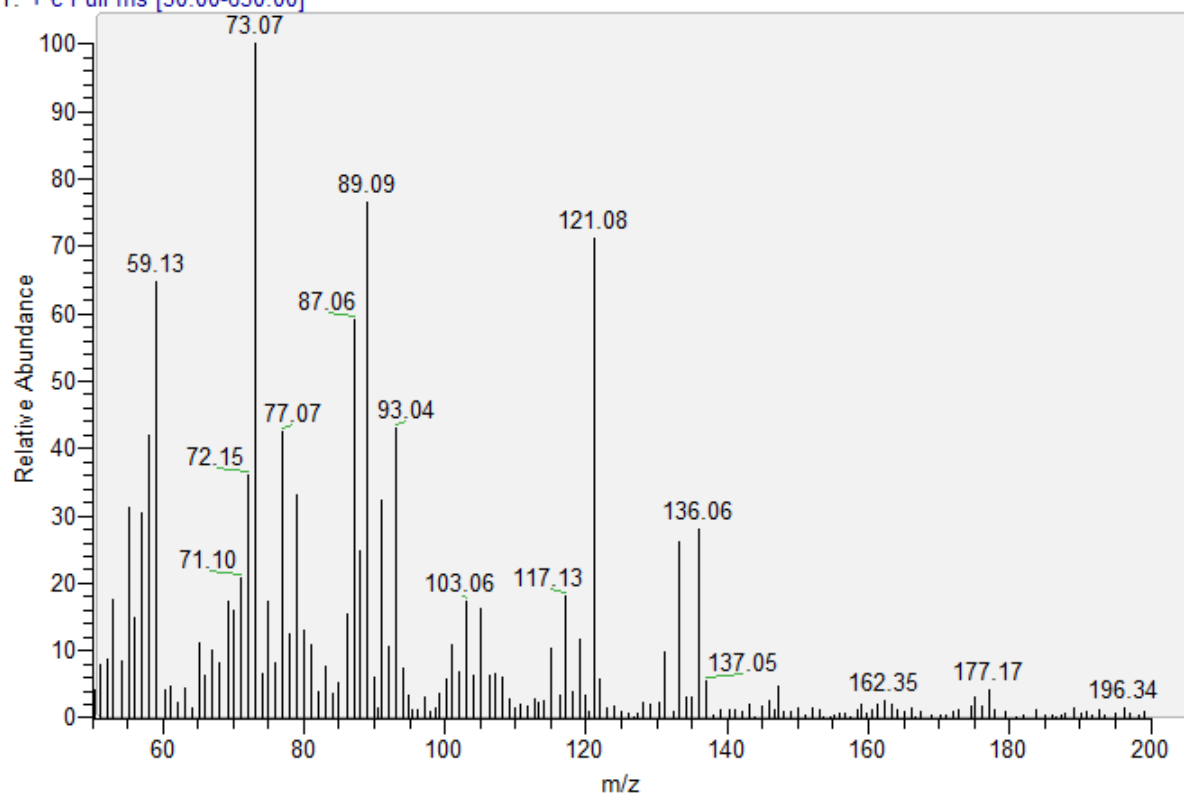
3074 #246-247 RT: 5.83-5.85 AV: 2 NL: 7.56E5  
T: + c Full ms [50.00-650.00]



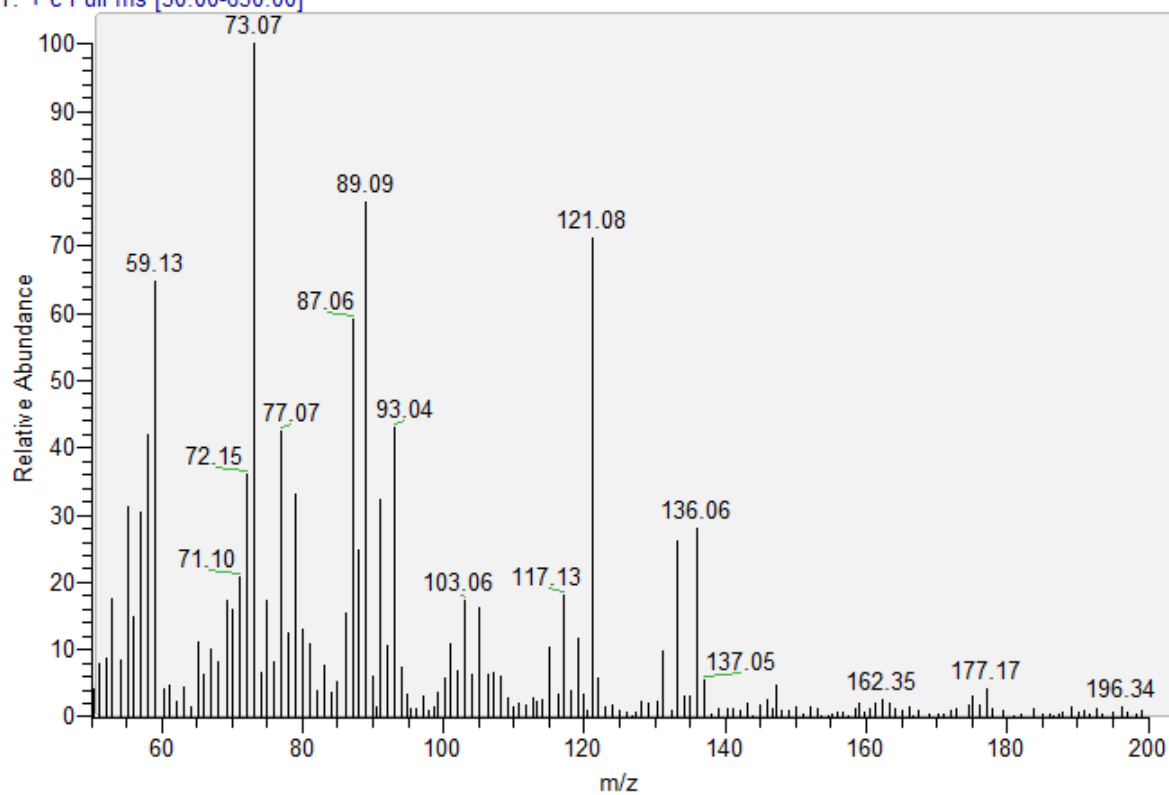
3073 #245 RT: 5.83 AV: 1 NL: 1.23E5



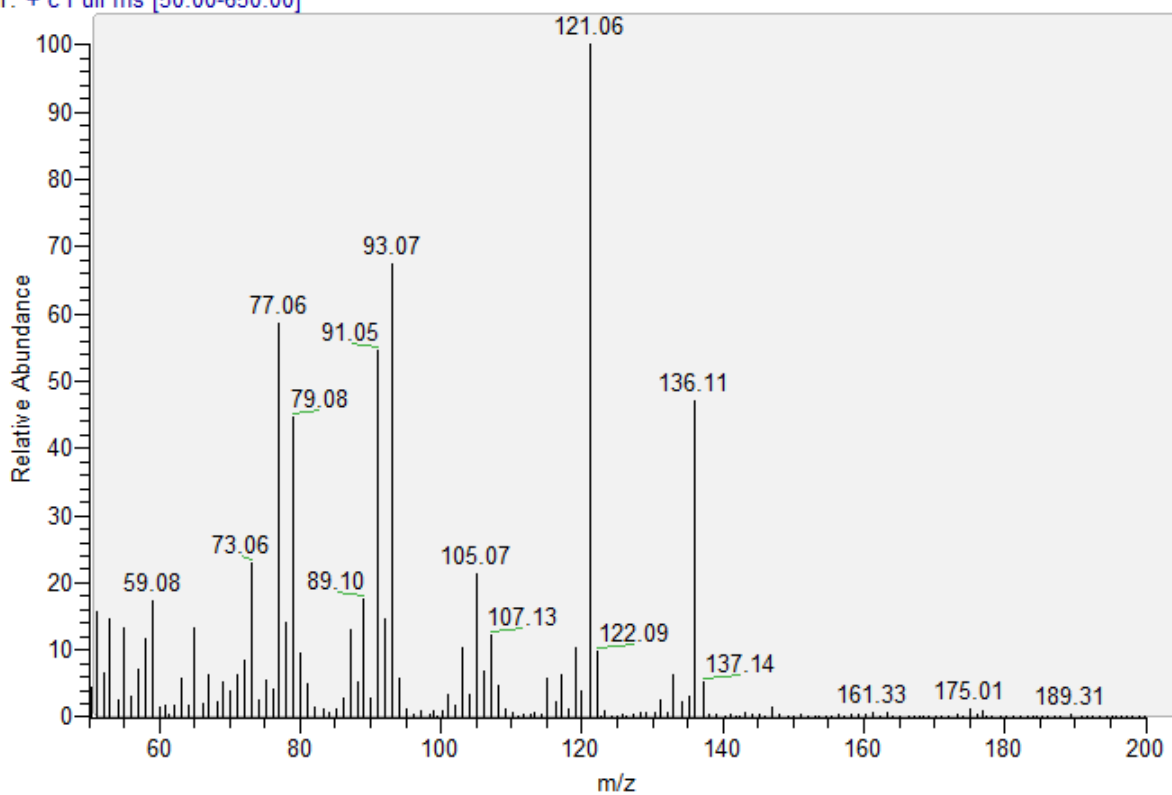
T: + c Full ms [50.00-650.00]



3073 #245 RT: 5.83 AV: 1 NL: 1.23E5  
T: + c Full ms [50.00-650.00]

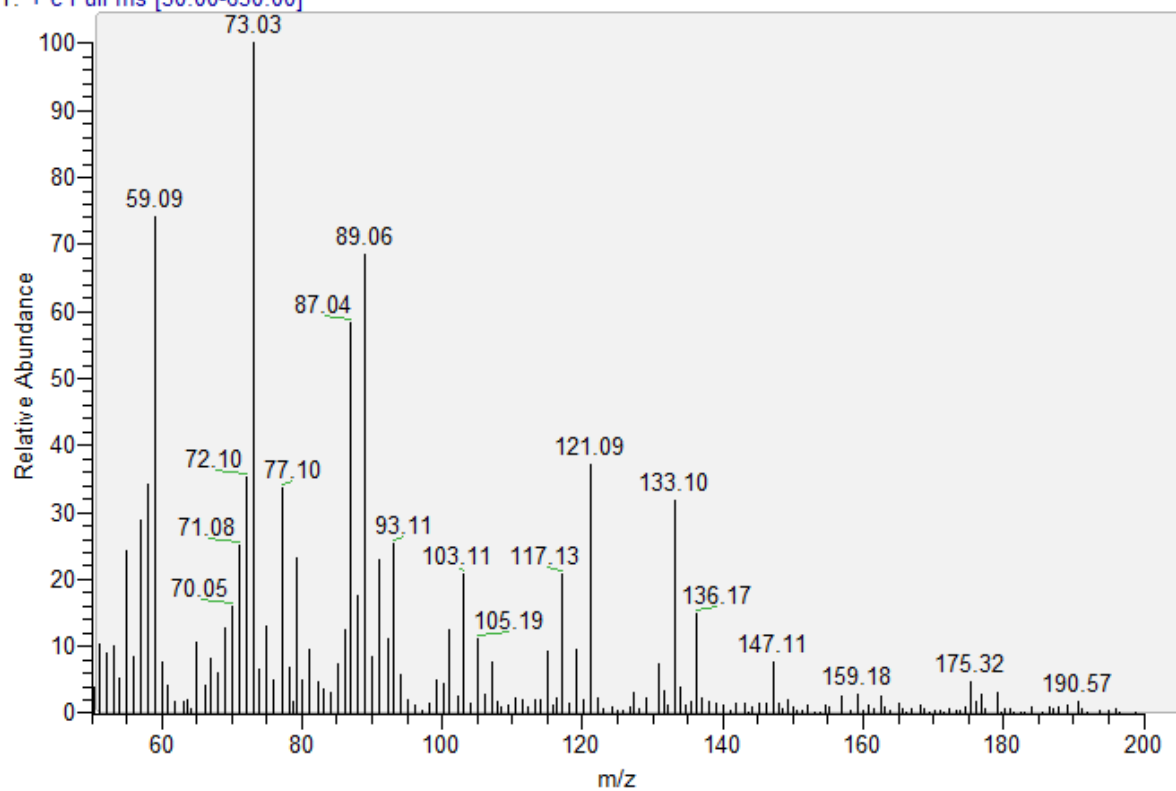


3072 #245-246 RT: 5.83-5.85 AV: 2 NL: 5.15E5  
T: + c Full ms [50.00-650.00]



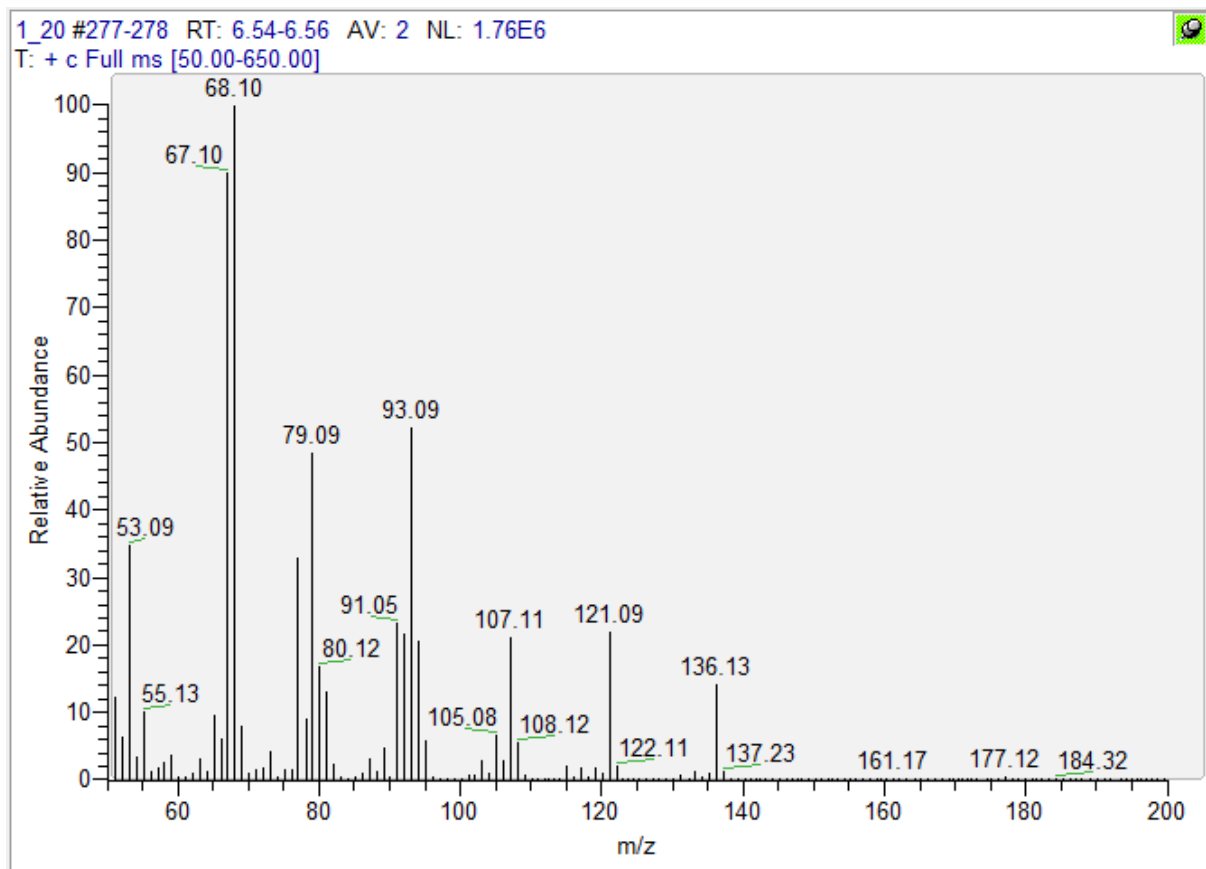


3070 #246 RT: 5.83 AV: 1 NL: 1.17E5  
T: + c Full ms [50.00-650.00]



Limonene

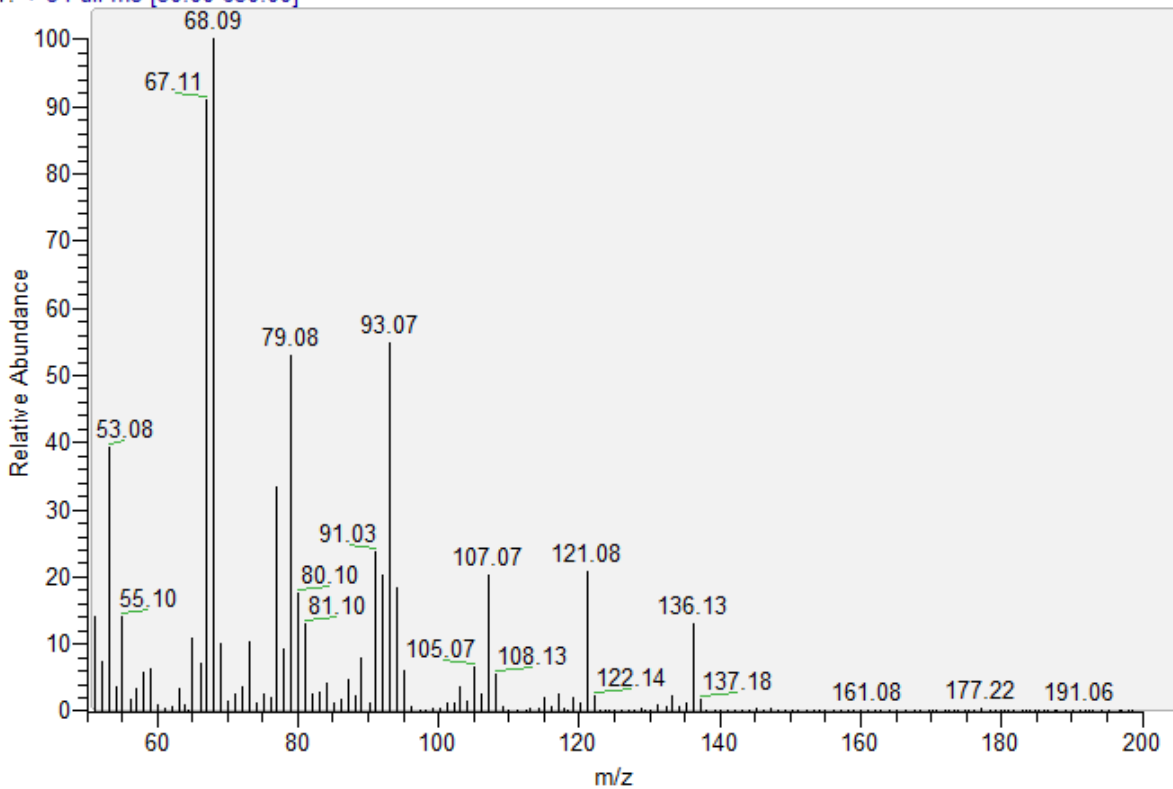
Reference:



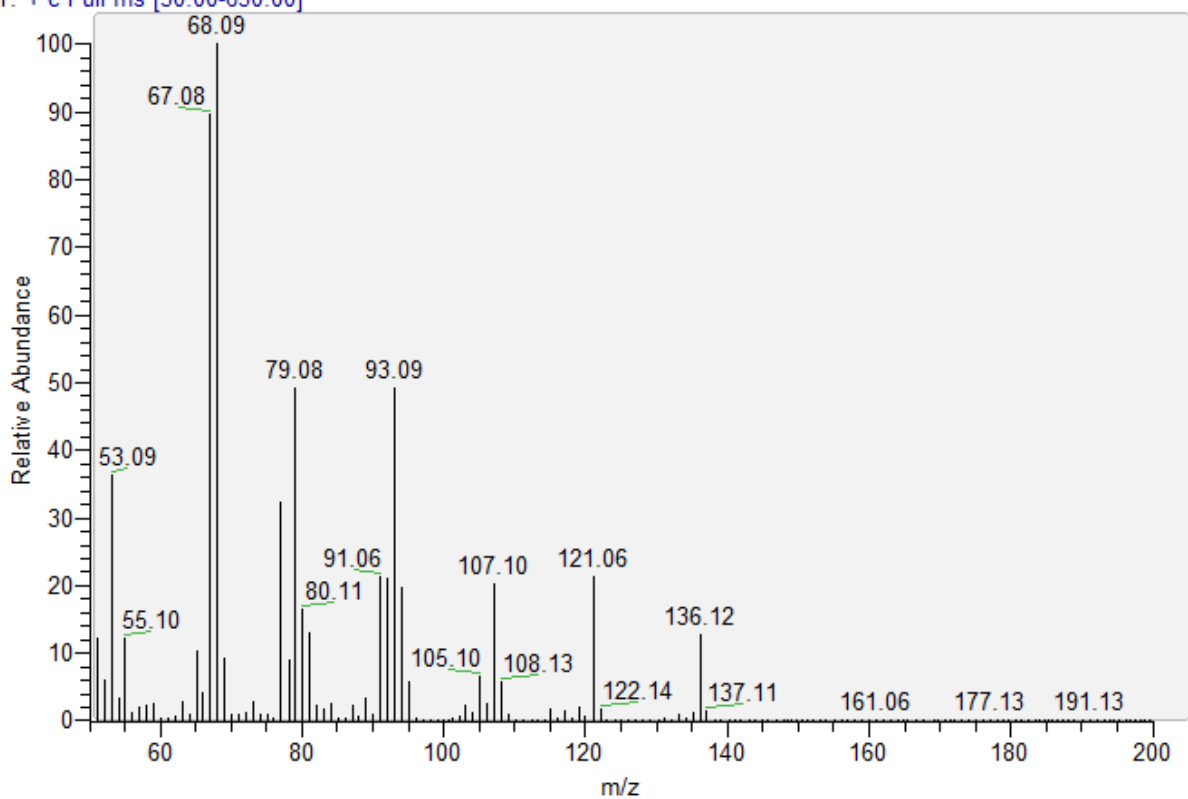
Samples:

3021 #276-277 RT: 6.55-6.57 AV: 2 NL: 1.12E6

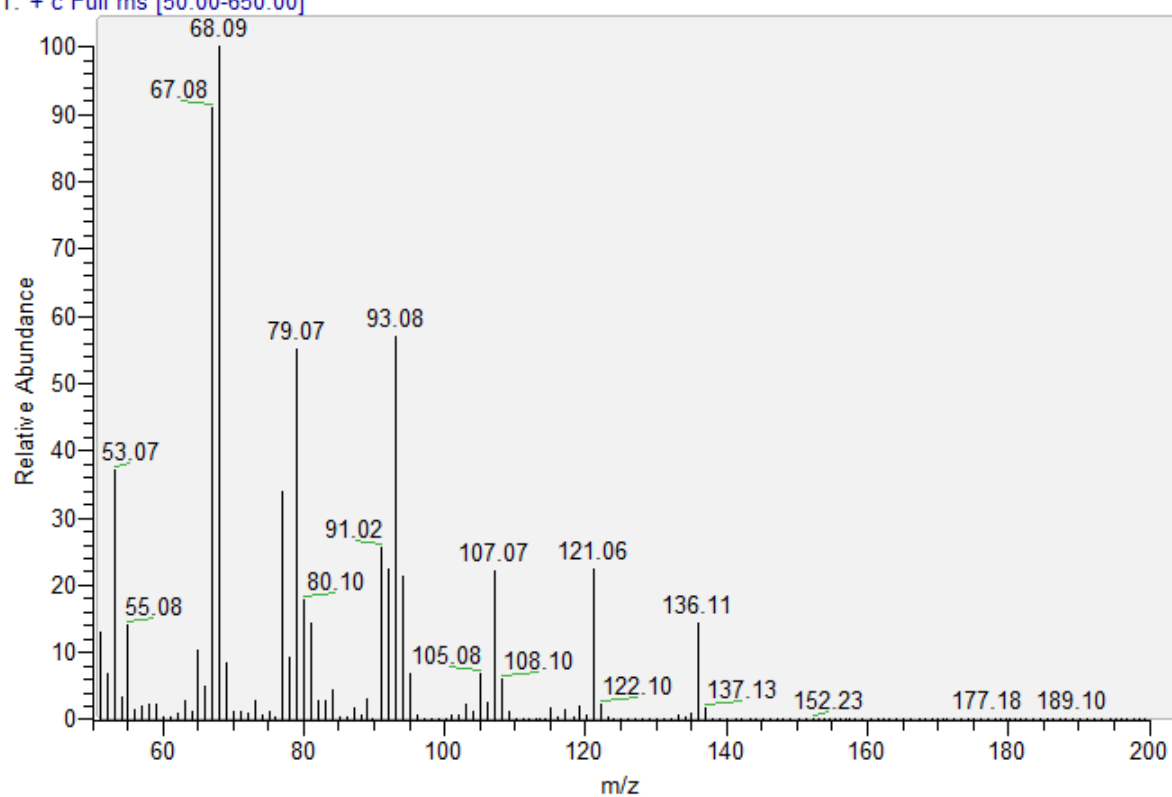
T: + c Full ms [50.00-650.00]



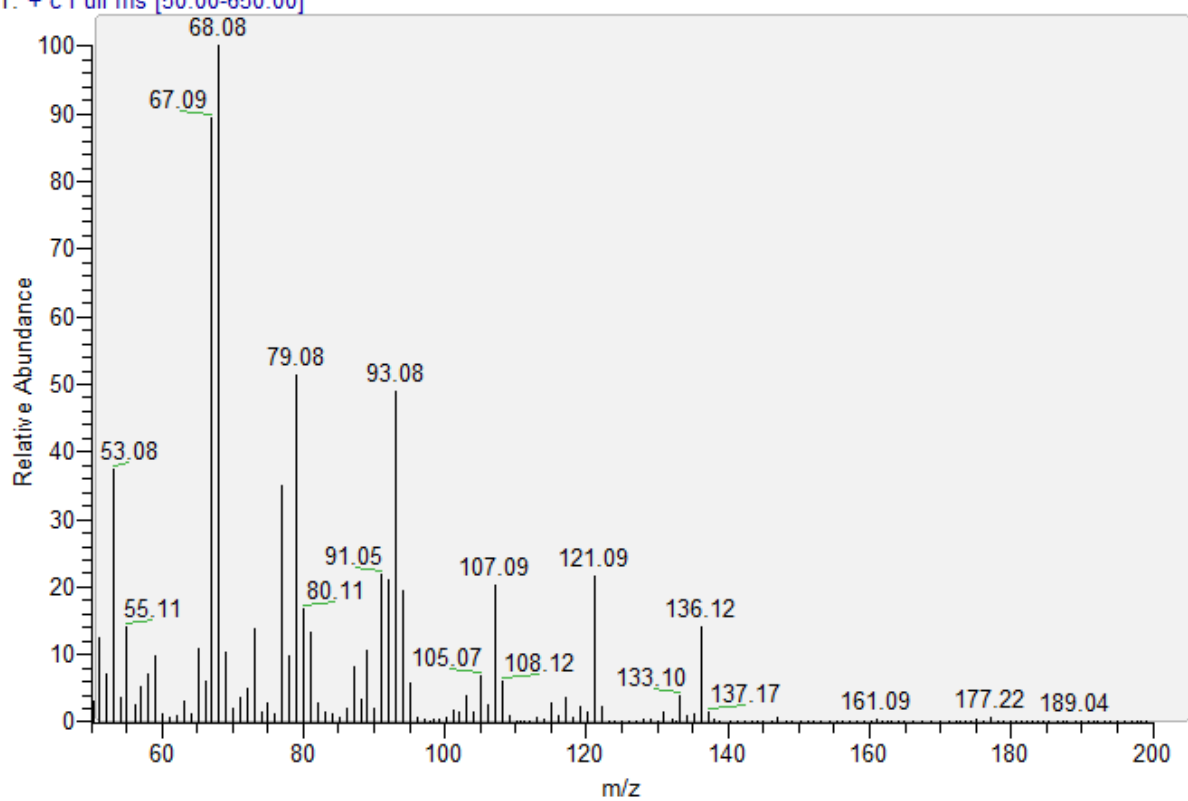
3057 #278-279 RT: 6.54-6.57 AV: 2 NL: 2.36E6  
T: + c Full ms [50.00-650.00]



3058 #274-276 RT: 6.53-6.58 AV: 3 NL: 3.86E6  
T: + c Full ms [50.00-650.00]



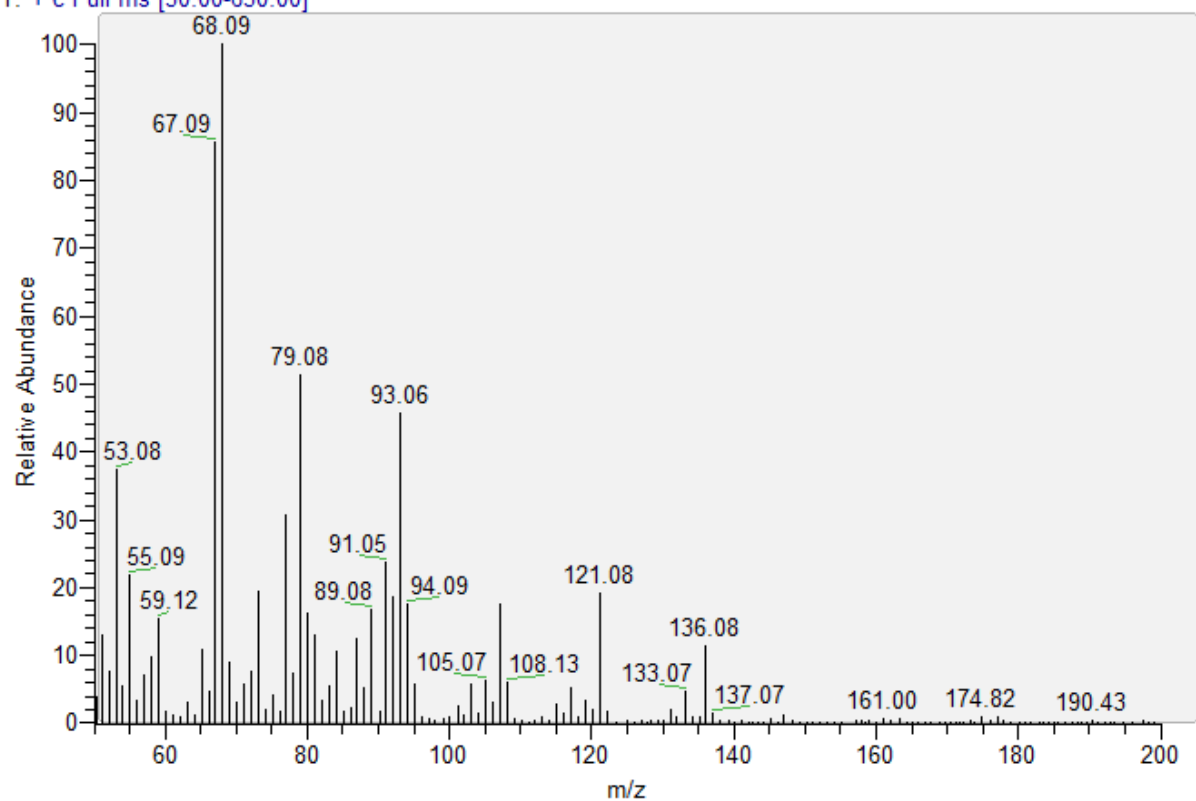
3053 #275-277 RT: 6.53-6.58 AV: 3 NL: 7.05E5  
T: + c Full ms [50.00-650.00]



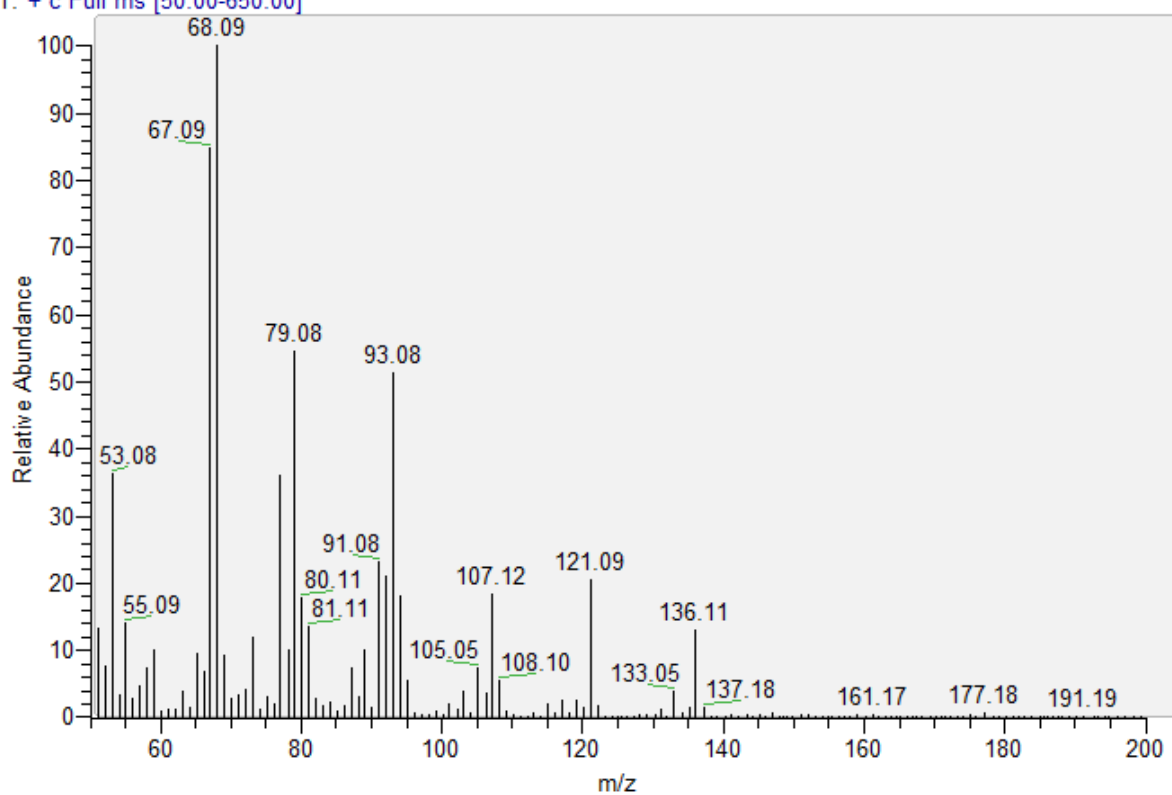
3018 #277-278 RT: 6.55-6.58 AV: 2 NL: 4.80E5



T: + c Full ms [50.00-650.00]

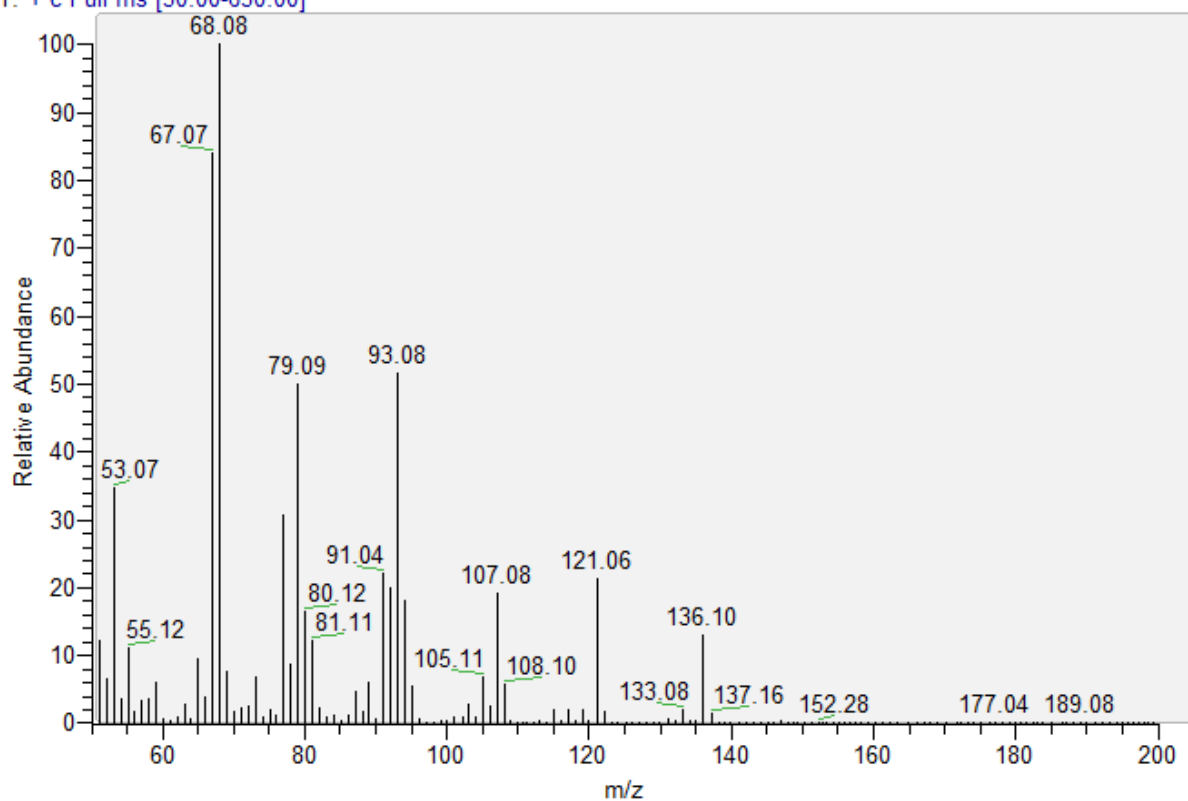


3075 #275-276 RT: 6.54-6.56 AV: 2 NL: 7.69E5  
T: + c Full ms [50.00-650.00]

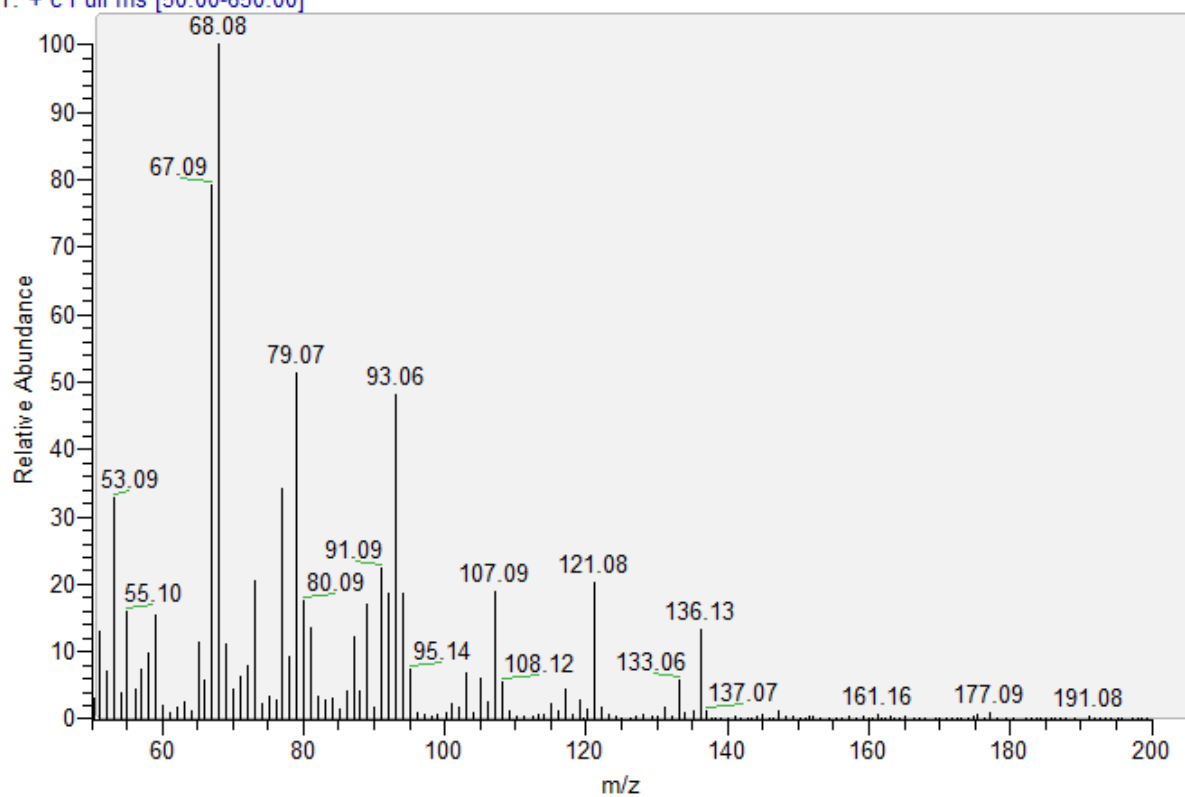




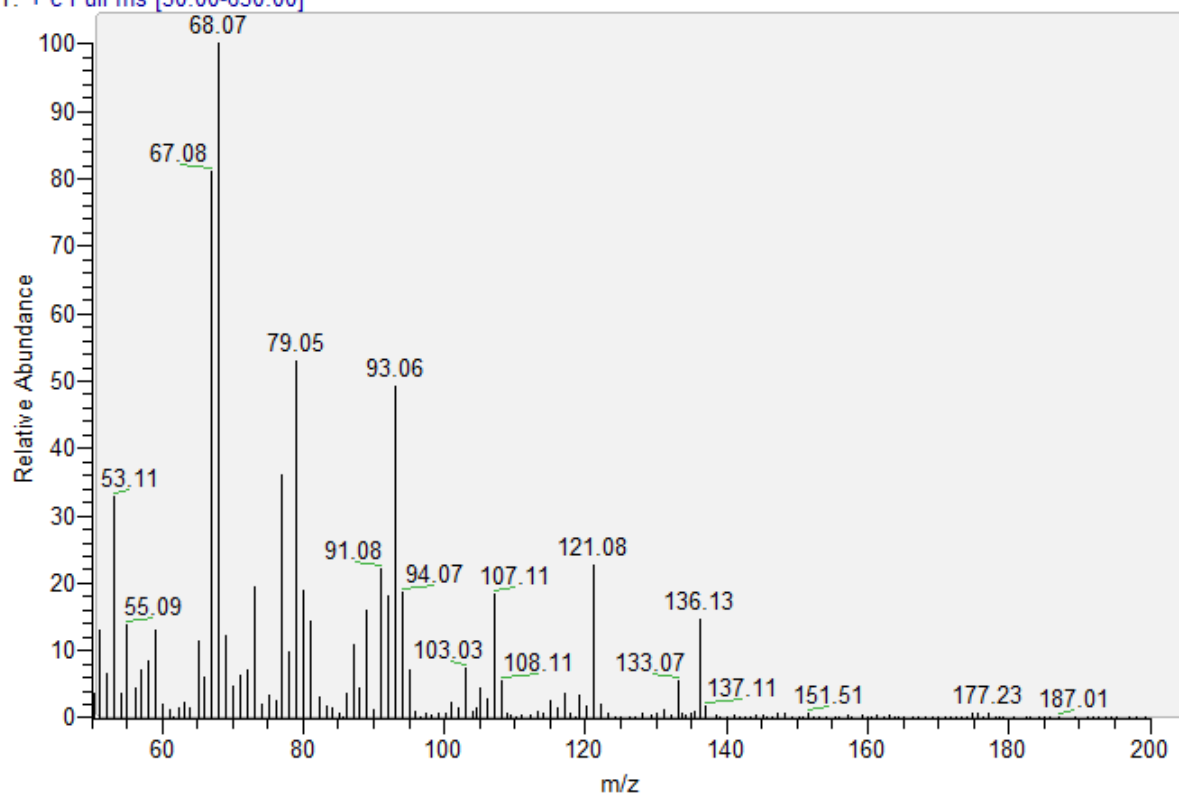
3074 #276-277 RT: 6.54-6.56 AV: 2 NL: 1.40E6  
T: + c Full ms [50.00-650.00]



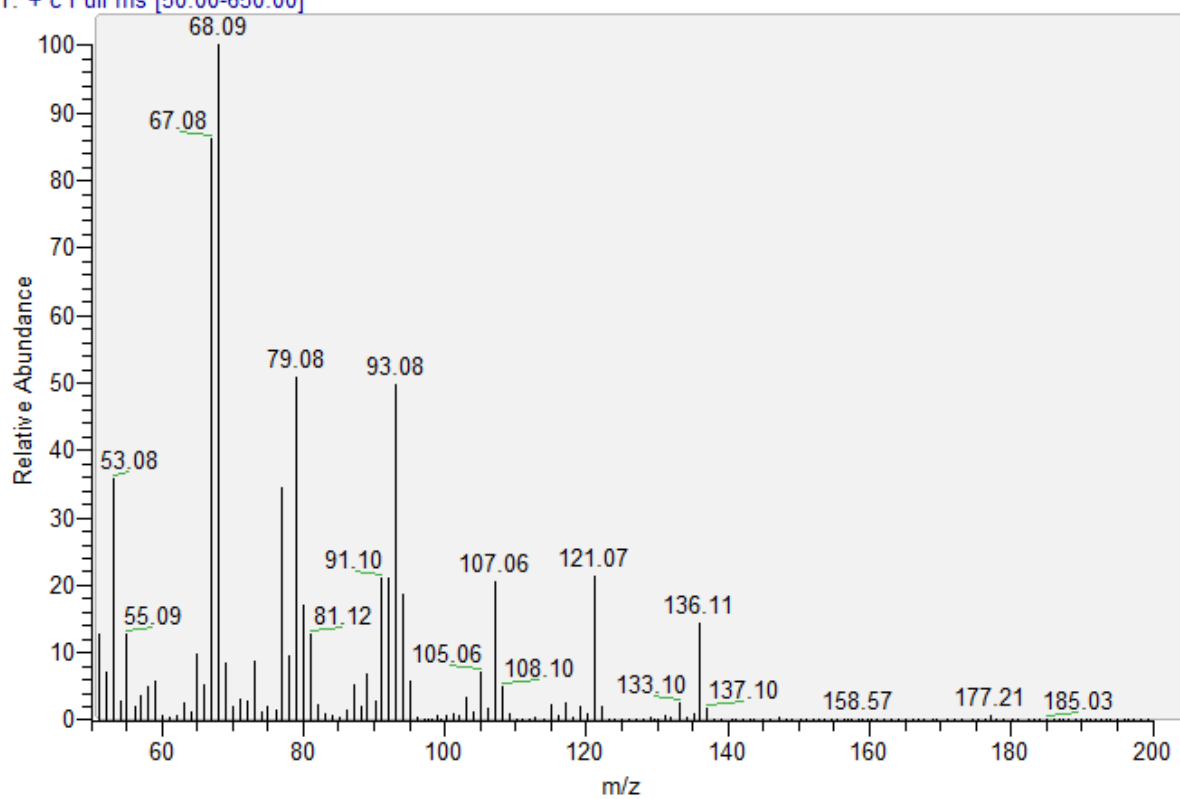
3073 #275-276 RT: 6.54-6.57 AV: 2 NL: 5.12E5  
T: + c Full ms [50.00-650.00]



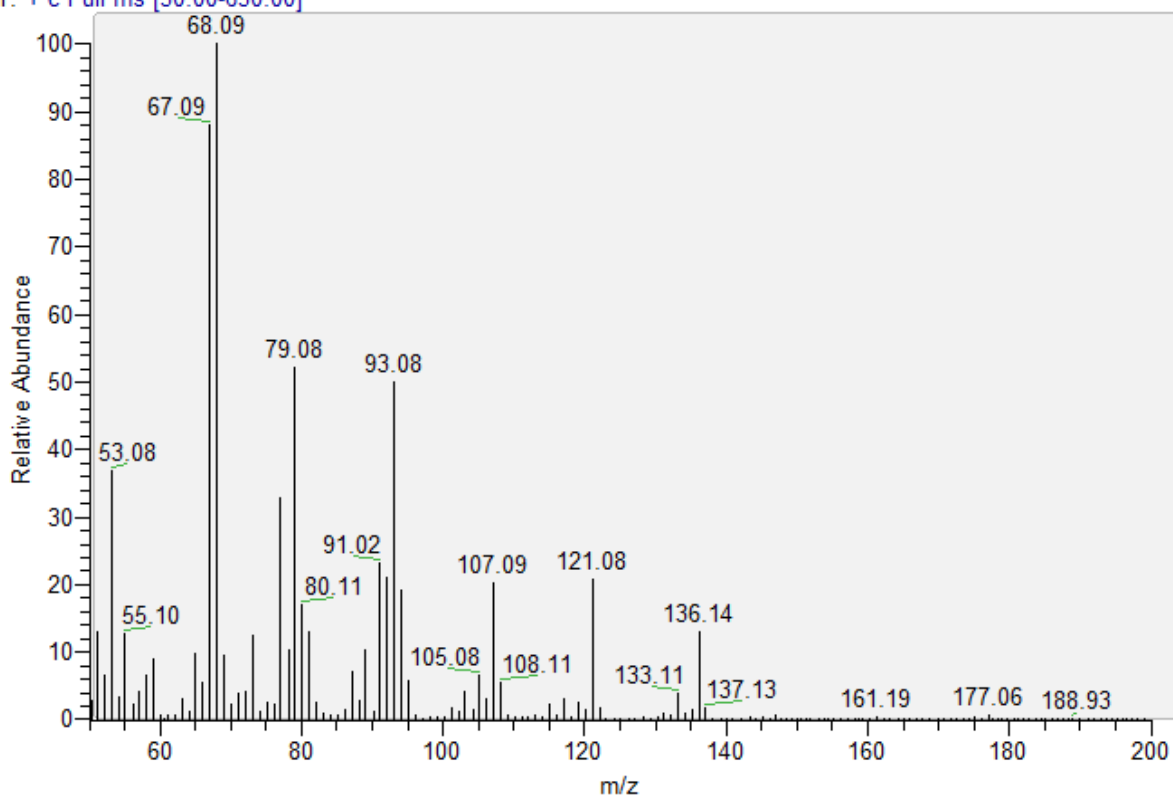
3073 #275 RT: 6.54 AV: 1 NL: 5.83E5  
T: + c Full ms [50.00-650.00]



3072 #275-276 RT: 6.54-6.57 AV: 2 NL: 1.13E6  
T: + c Full ms [50.00-650.00]

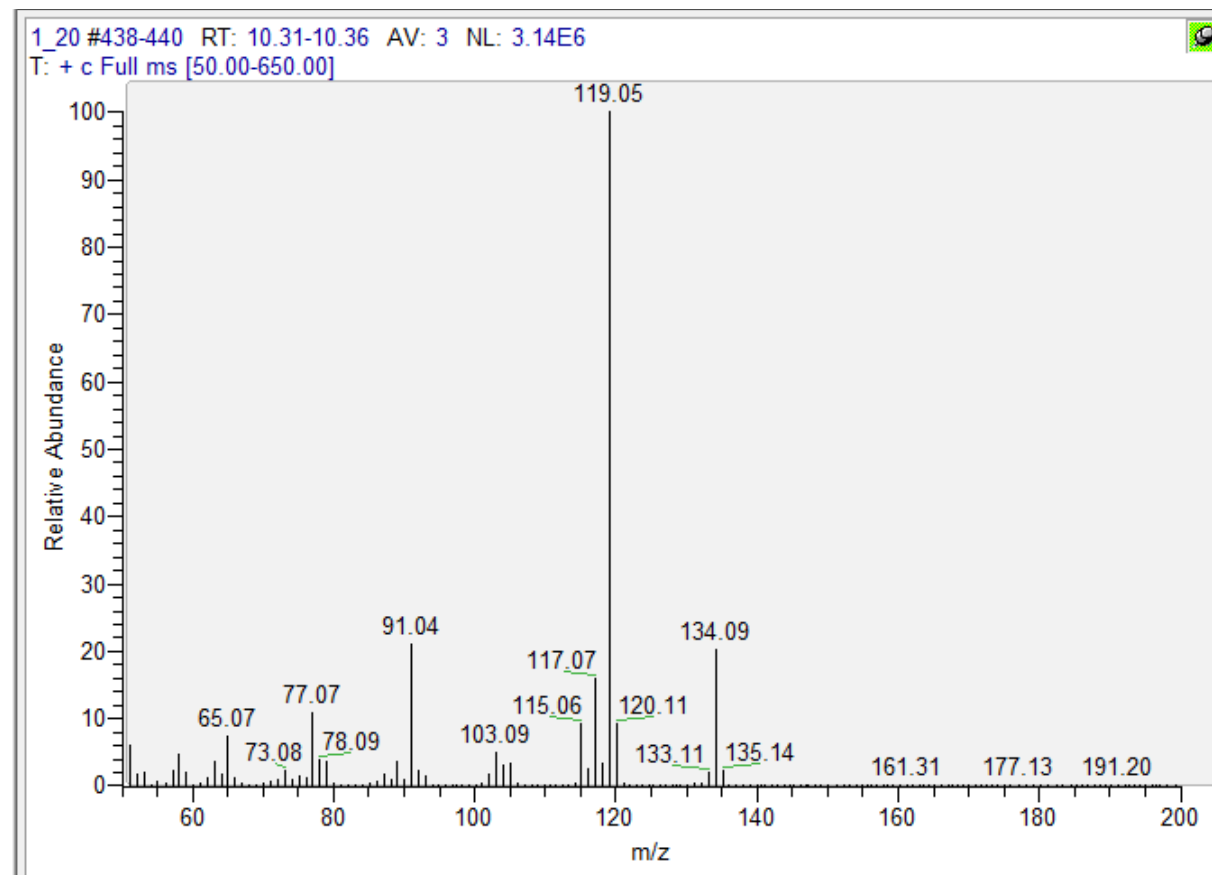


3070 #275-277 RT: 6.52-6.57 AV: 3 NL: 7.50E5  
T: + c Full ms [50.00-650.00]



p-cymene

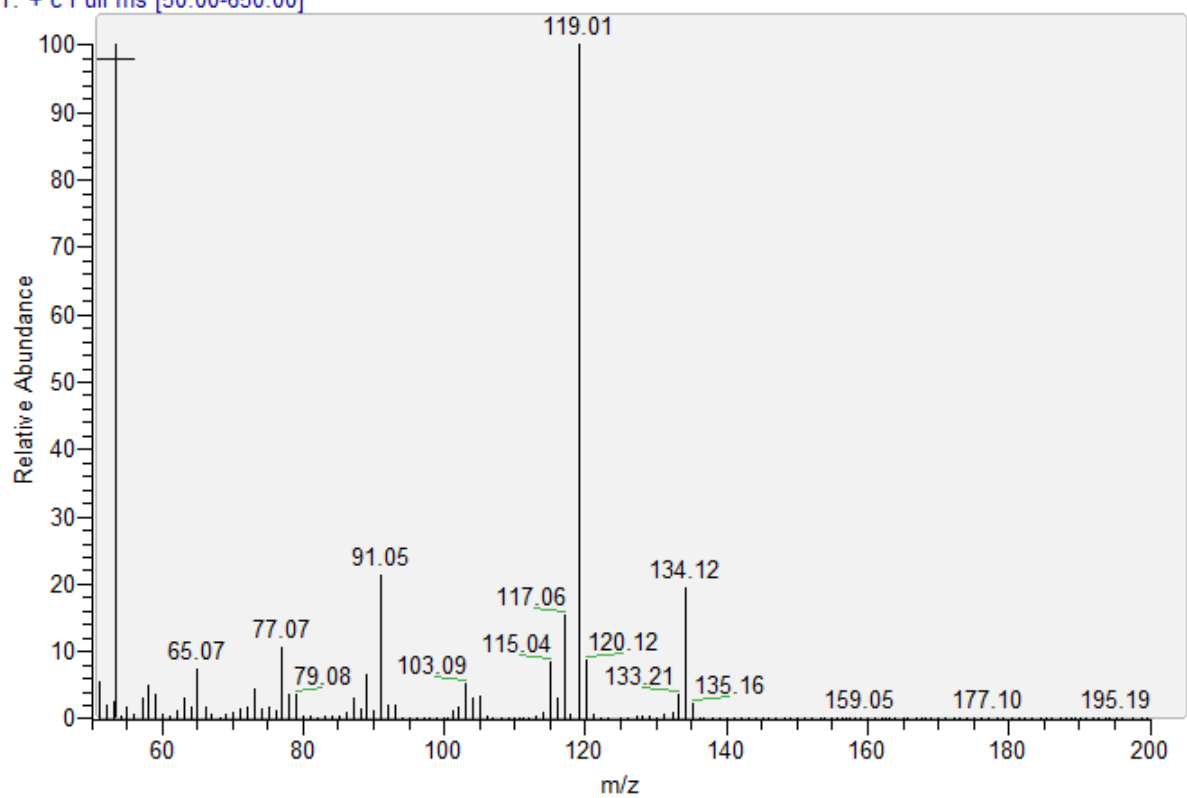
Reference:



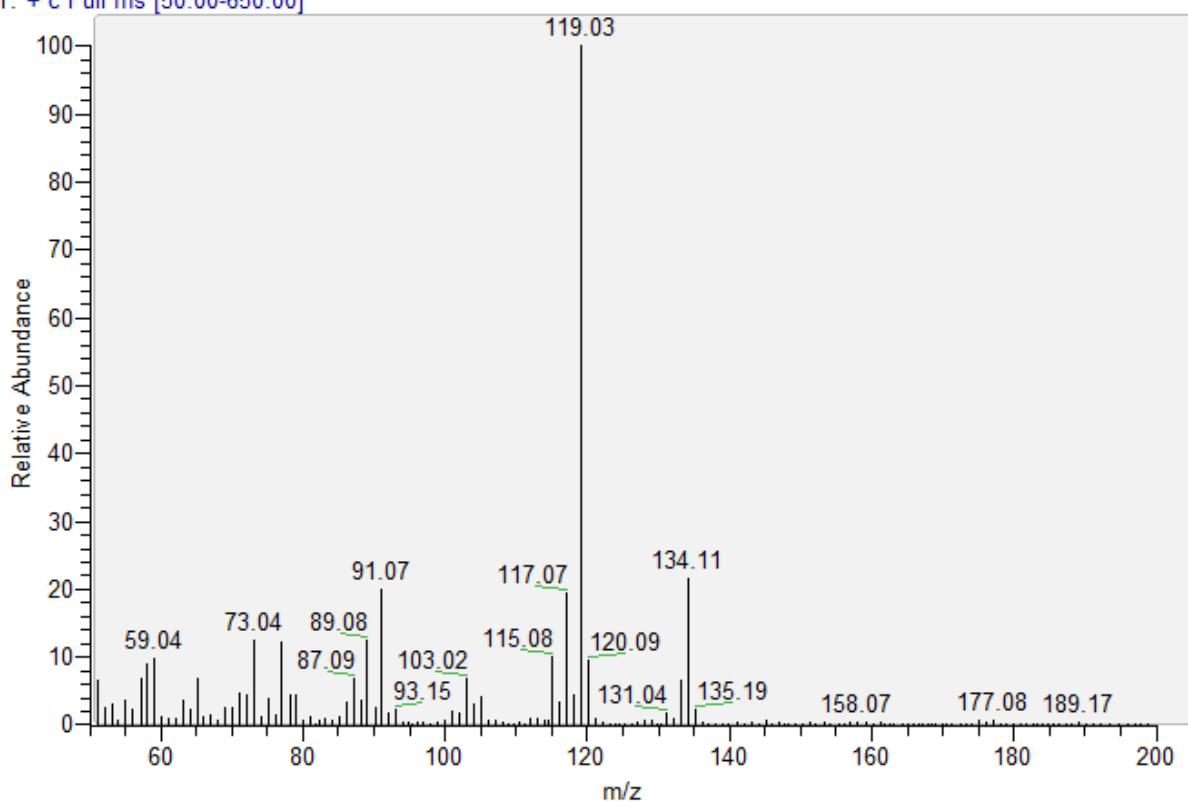
## Samples

3018 #436-437 RT: 10.32-10.35 AV: 2 NL: 1.54E6

T: + c Full ms [50.00-650.00]

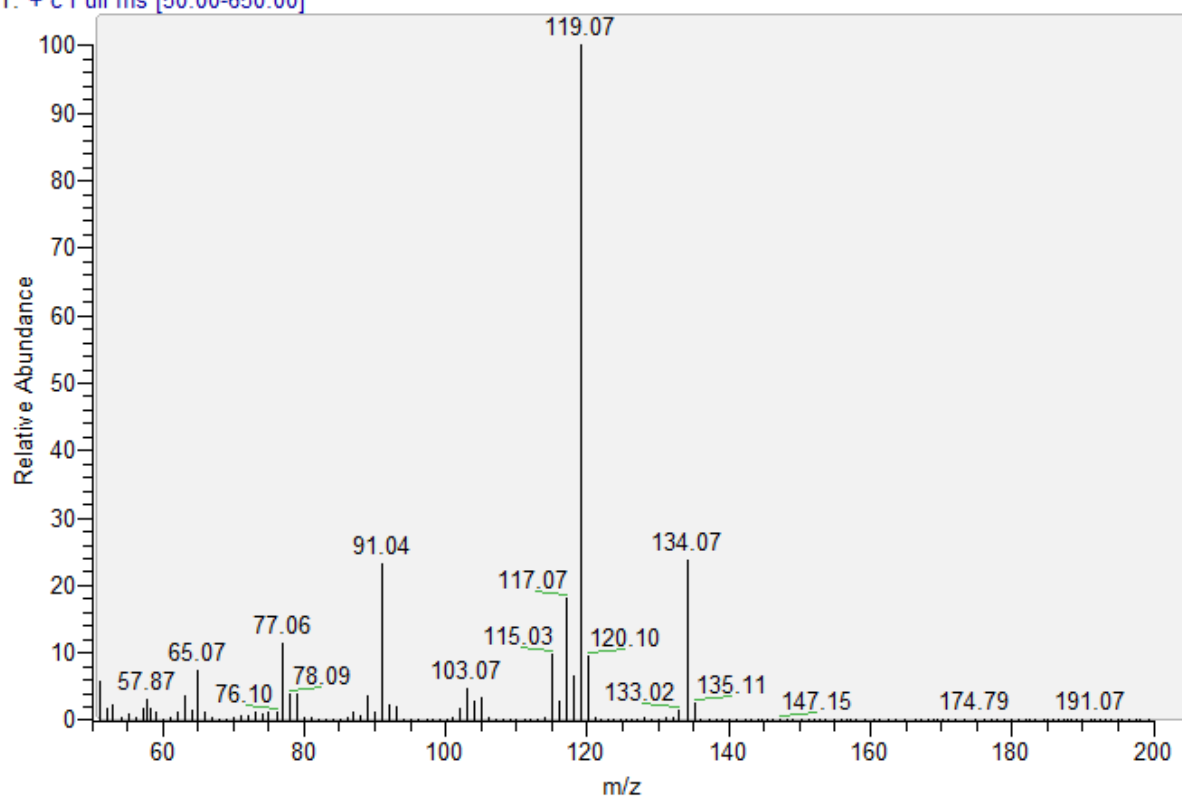


3053 #434-435 RT: 10.31-10.34 AV: 2 NL: 4.93E5  
T: + c Full ms [50.00-650.00]

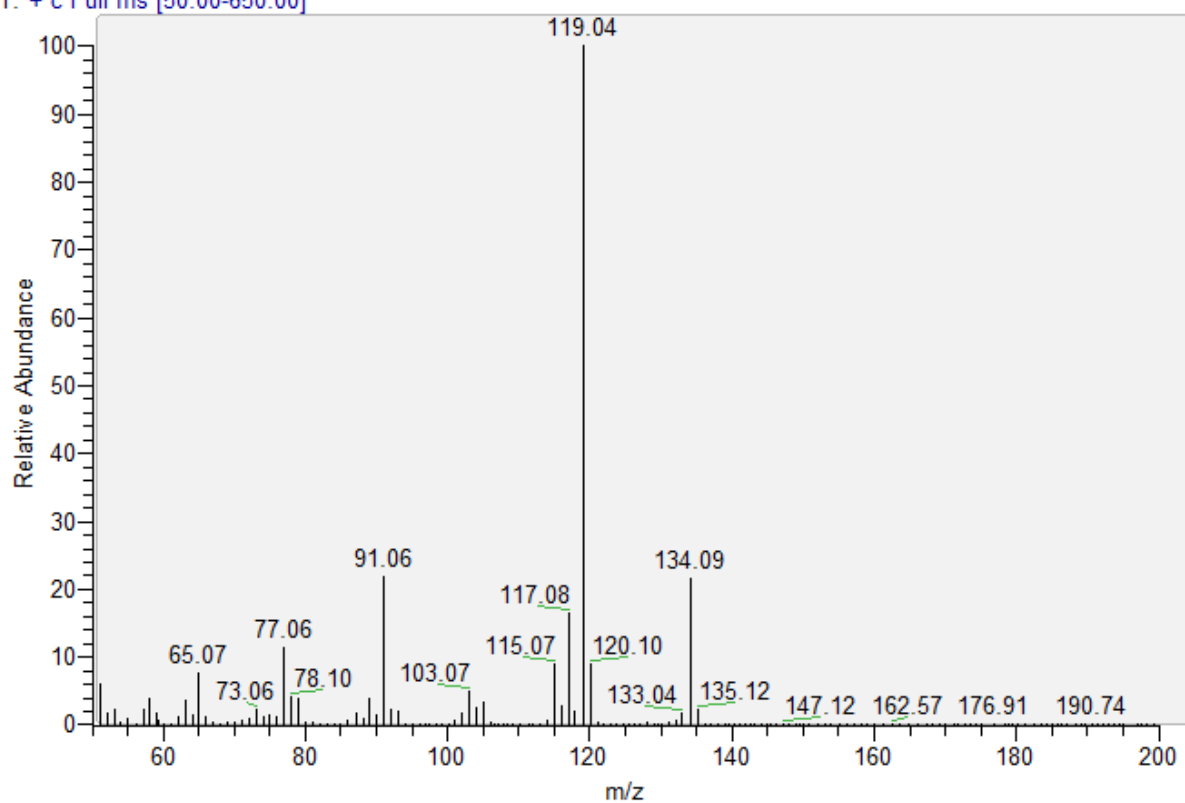




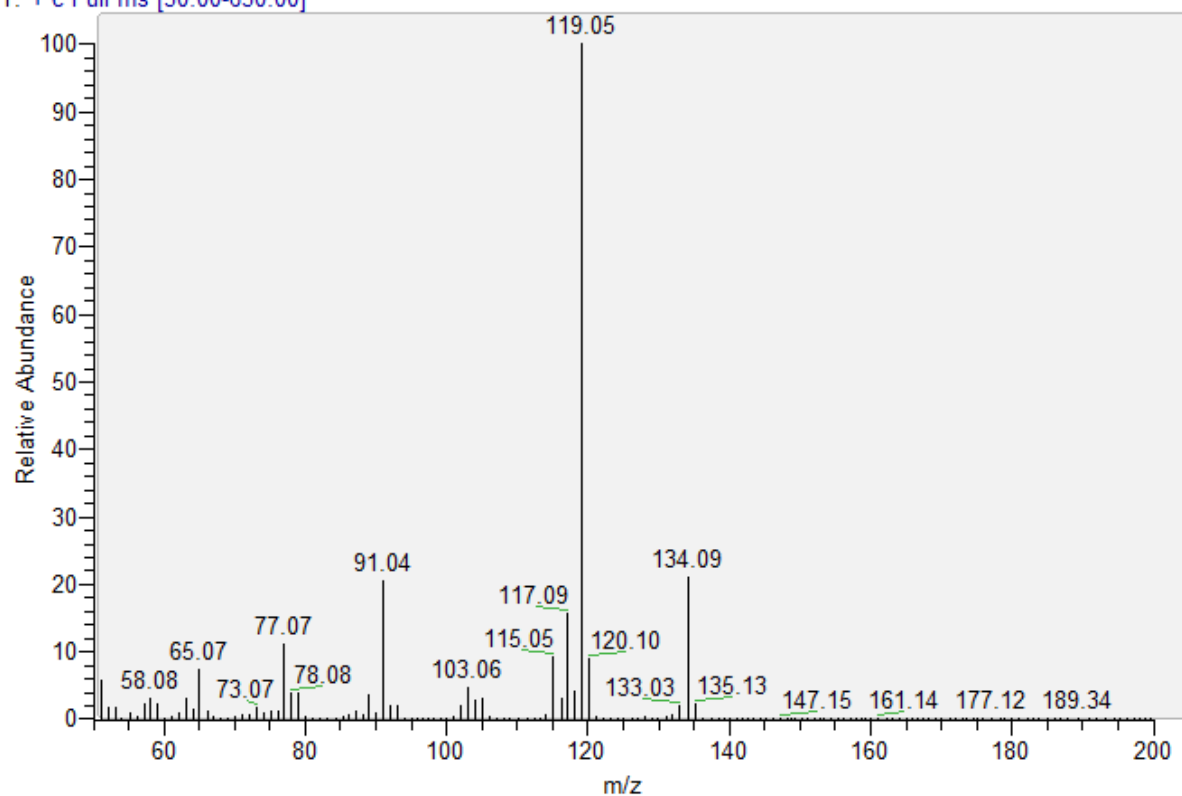
3058 #433-434 RT: 10.32-10.34 AV: 2 NL: 6.30E6  
T: + c Full ms [50.00-650.00]



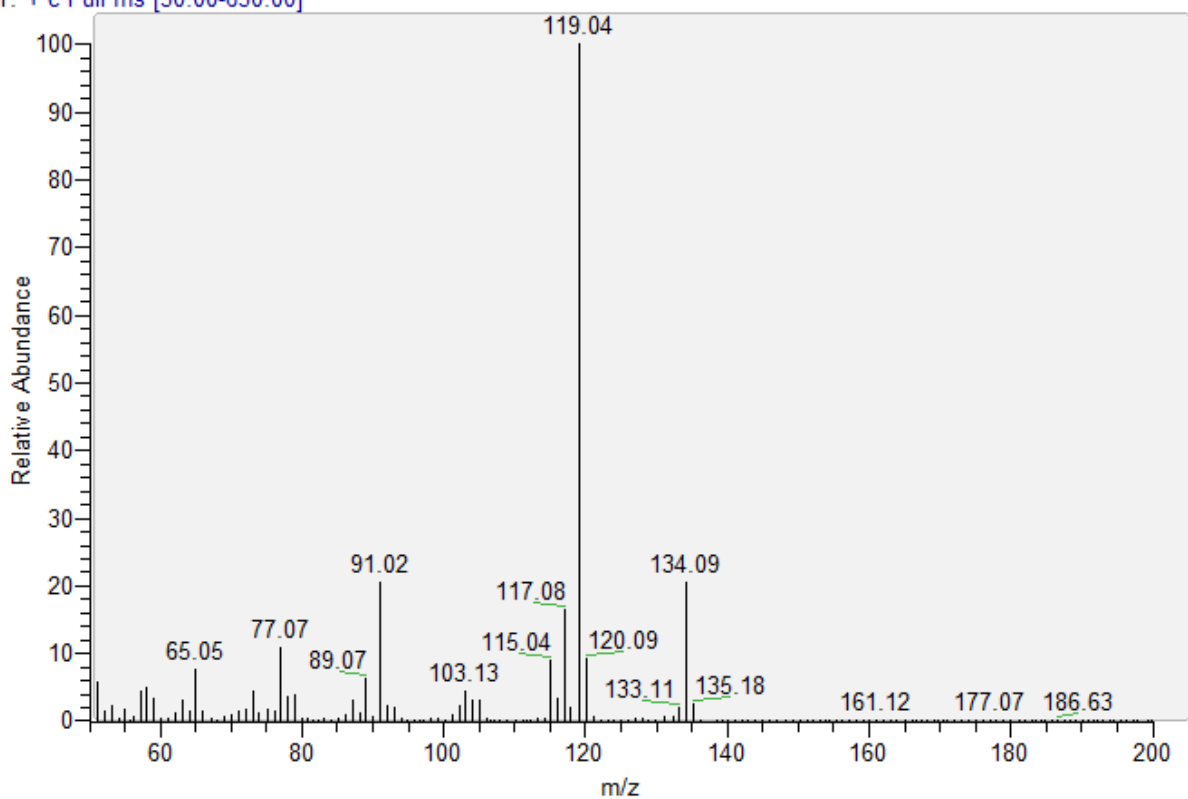
3057 #437-438 RT: 10.32-10.34 AV: 2 NL: 3.05E6  
T: + c Full ms [50.00-650.00]



3021 #435-436 RT: 10.33-10.35 AV: 2 NL: 4.11E6  
T: + c Full ms [50.00-650.00]



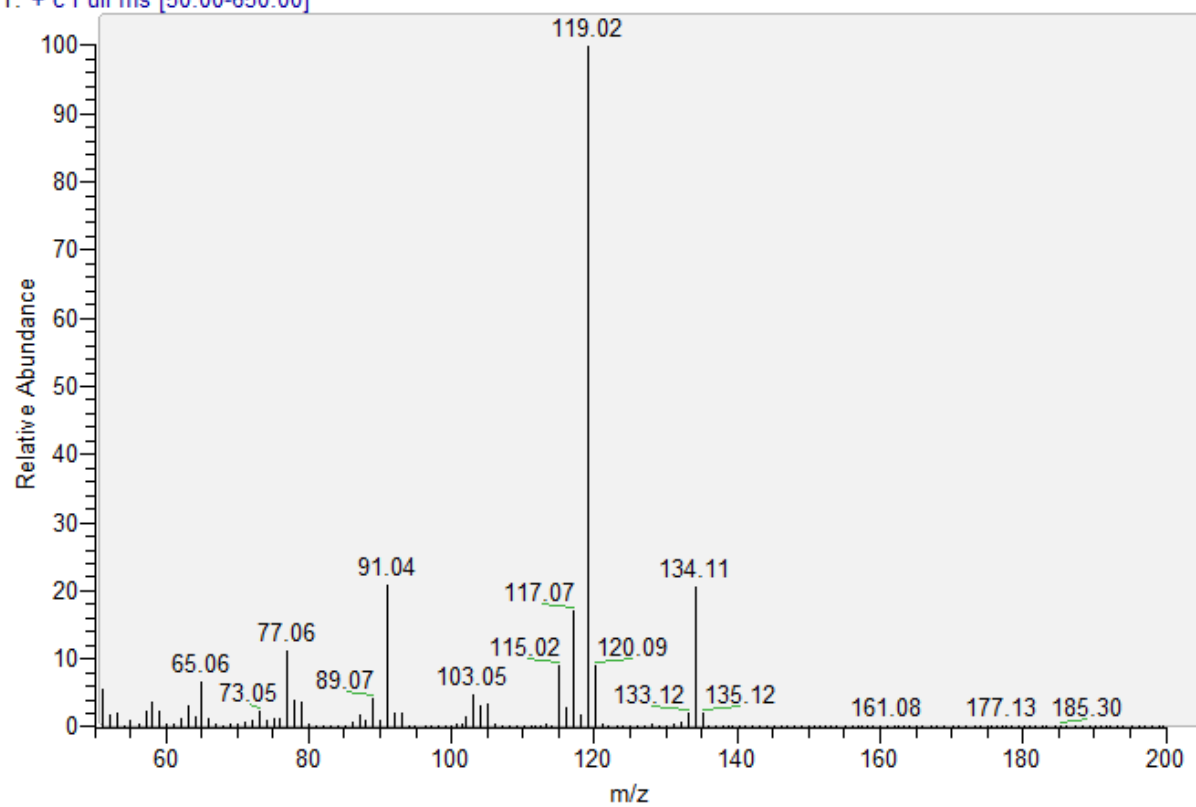
3075 #434-435 RT: 10.33-10.35 AV: 2 NL: 1.57E6  
T: + c Full ms [50.00-650.00]



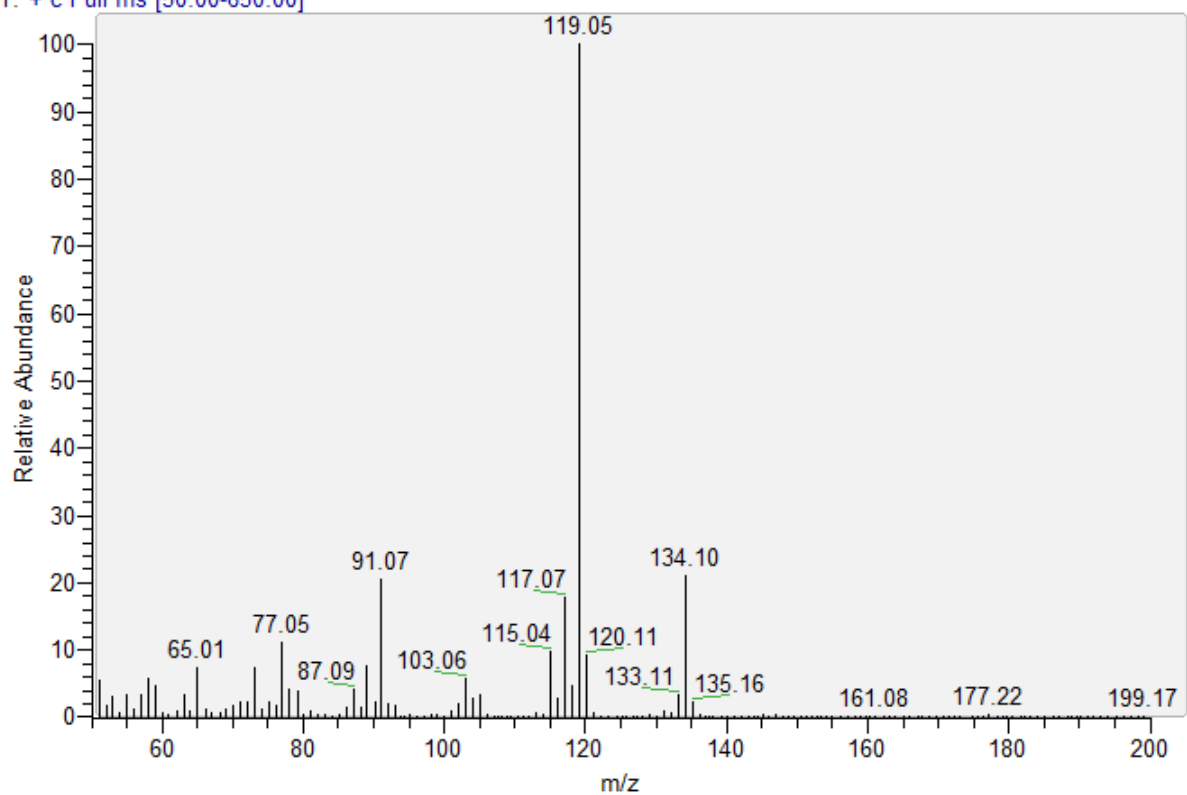
3074 #435-437 RT: 10.32-10.37 AV: 3 NL: 3.34E6



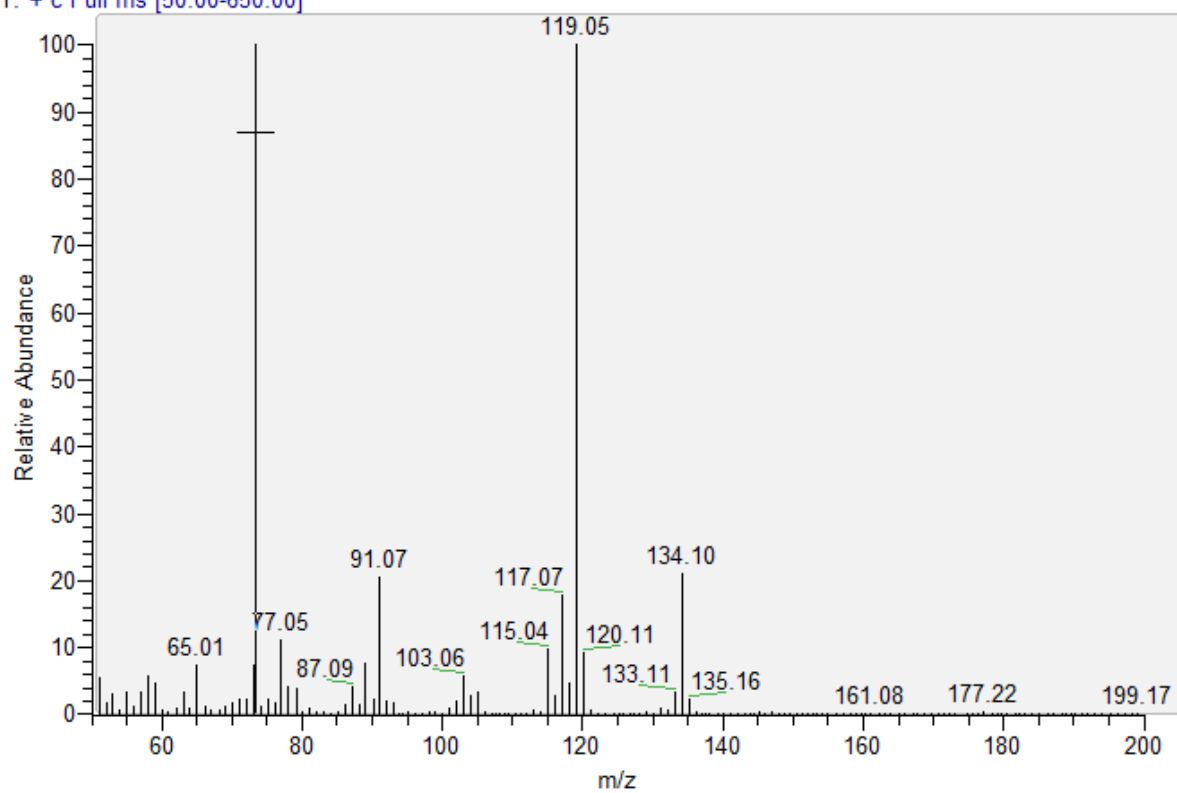
T: + c Full ms [50.00-650.00]



3073 #433-434 RT: 10.31-10.33 AV: 2 NL: 1.09E6  
T: + c Full ms [50.00-650.00]



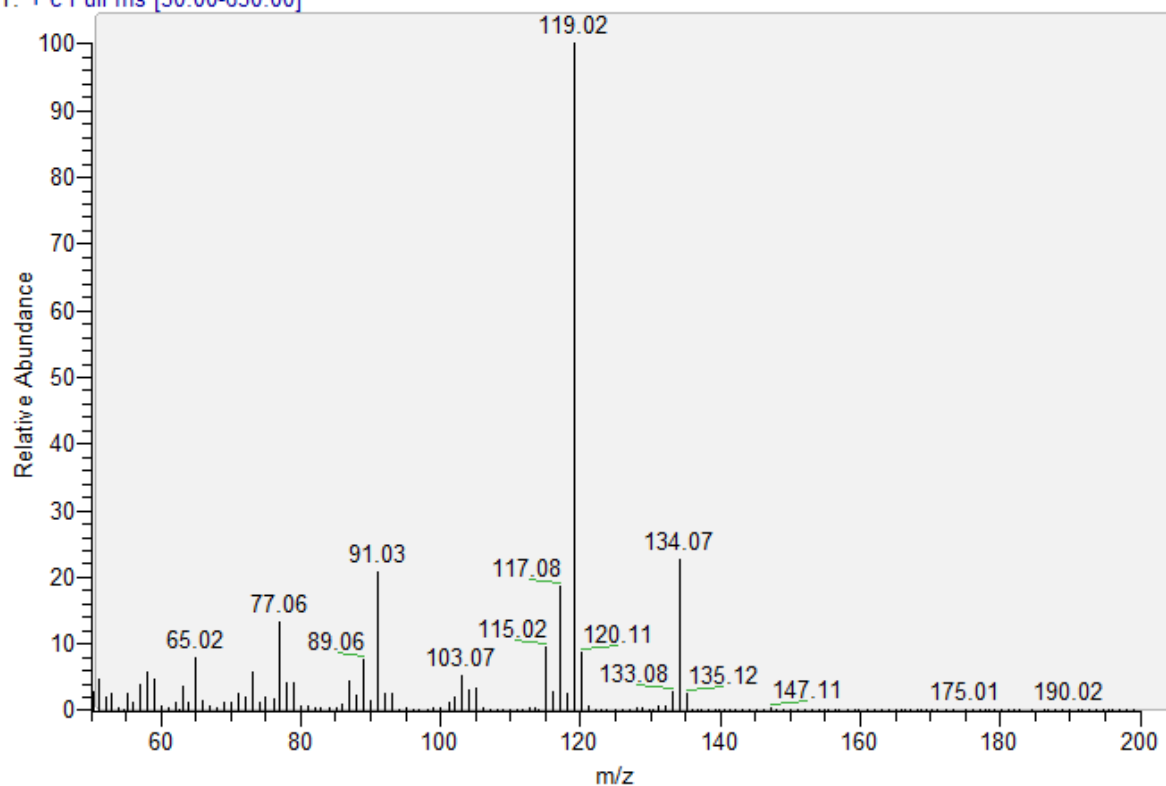
3073 #433-434 RT: 10.31-10.33 AV: 2 NL: 1.09E6  
T: + c Full ms [50.00-650.00]



3072 #434-435 RT: 10.33-10.35 AV: 2 NL: 1.26E6



T: + c Full ms [50.00-650.00]

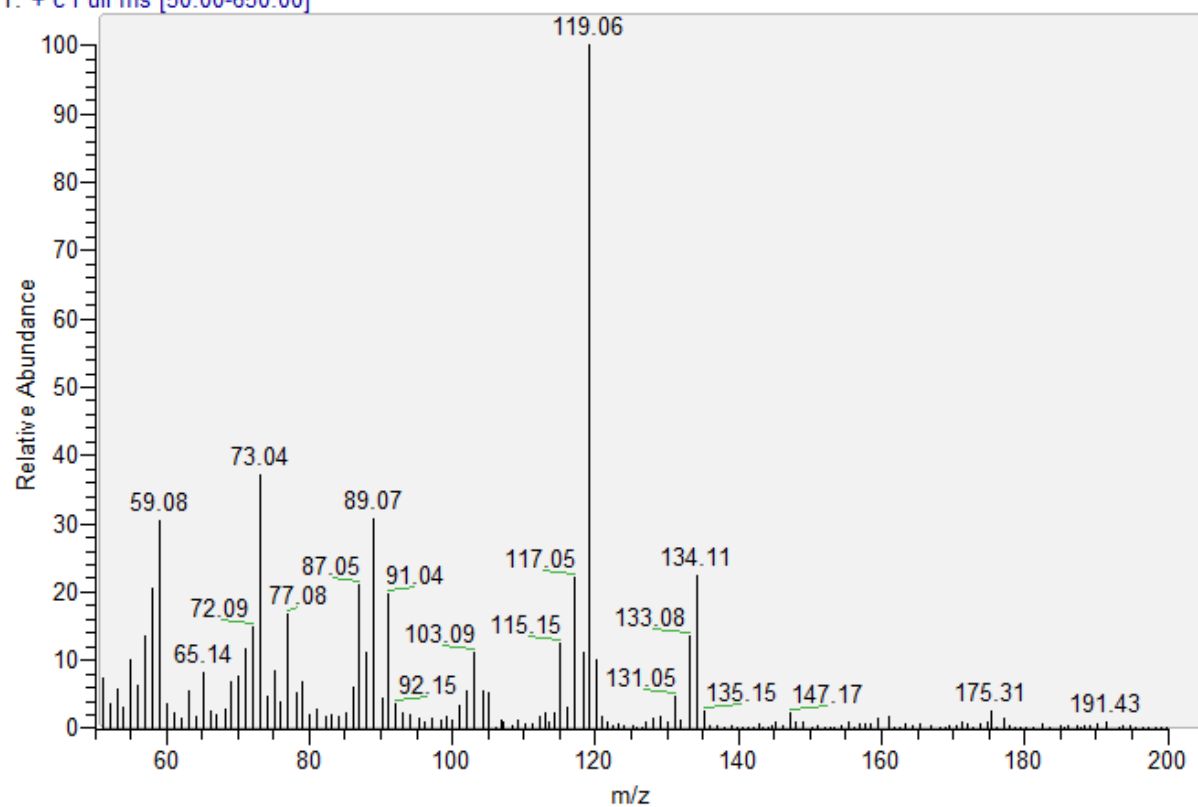




3070 #436-437 RT: 10.33-10.35 AV: 2 NL: 1.75E5

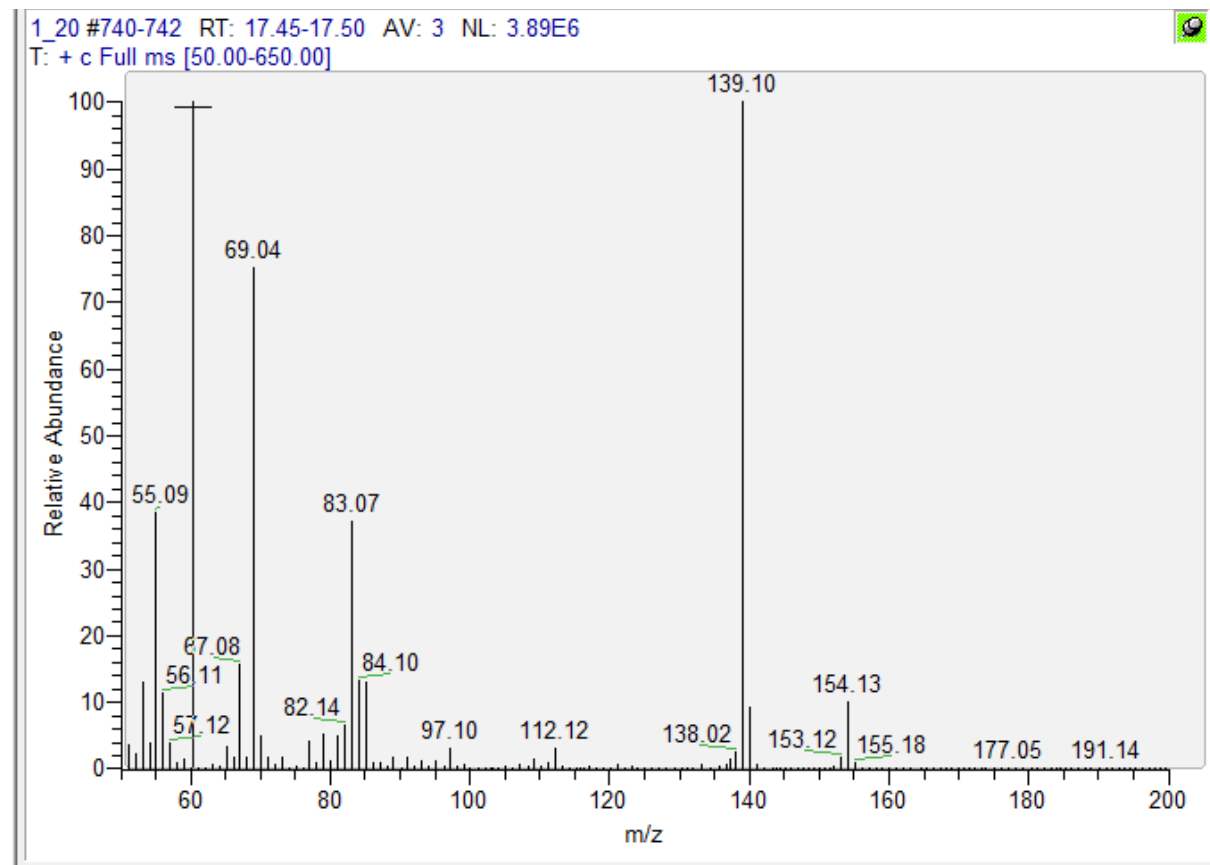


T: + c Full ms [50.00-650.00]



Rose oxide

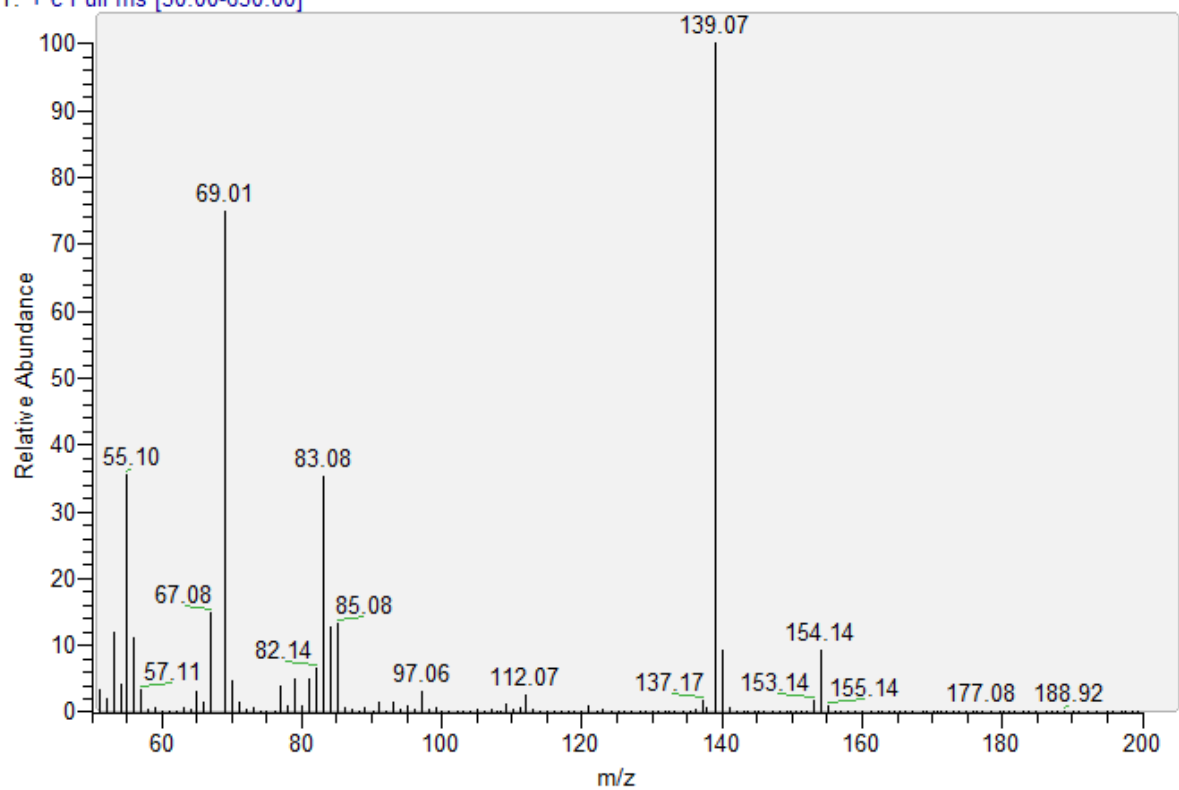
Reference:



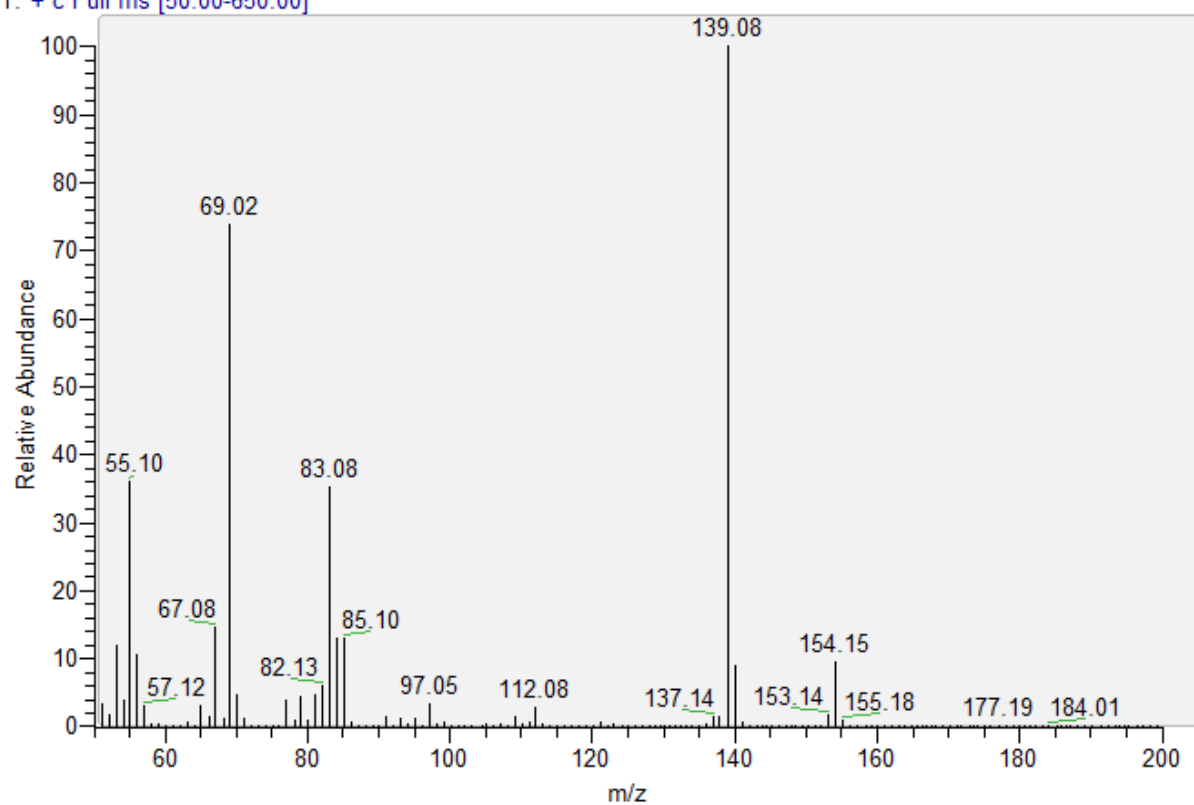
Samples:

3021 #737-738 RT: 17.49-17.52 AV: 2 NL: 1.13E7

T: + c Full ms [50.00-650.00]



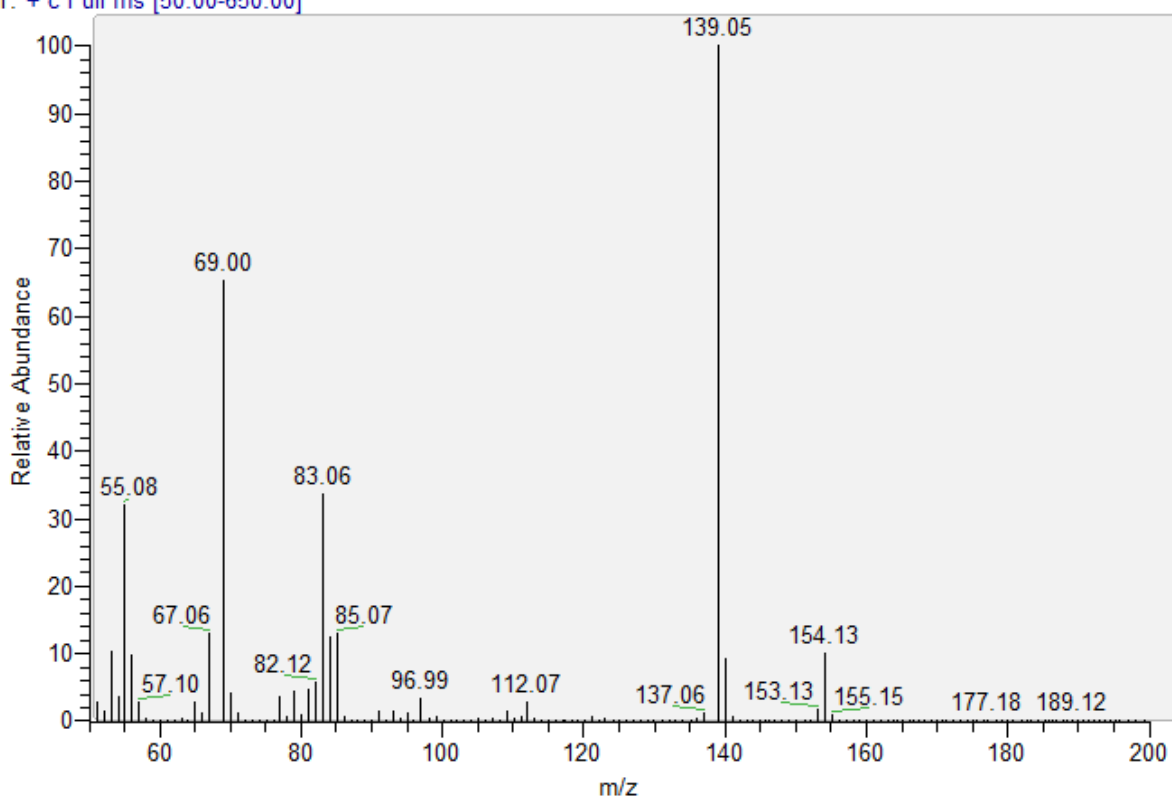
3057 #740-742 RT: 17.50-17.54 AV: 3 NL: 2.69E7  
T: + c Full ms [50.00-650.00]



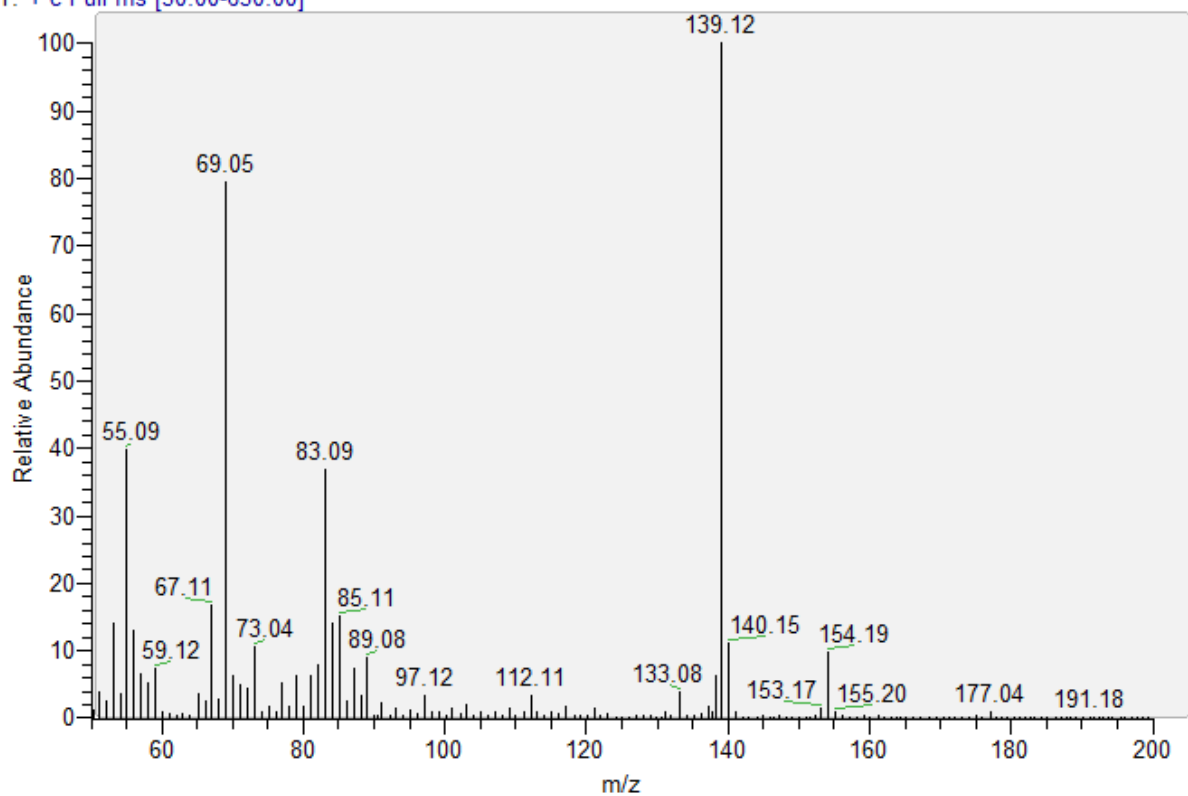
3058 #735-737 RT: 17.52-17.57 AV: 3 NL: 5.30E7



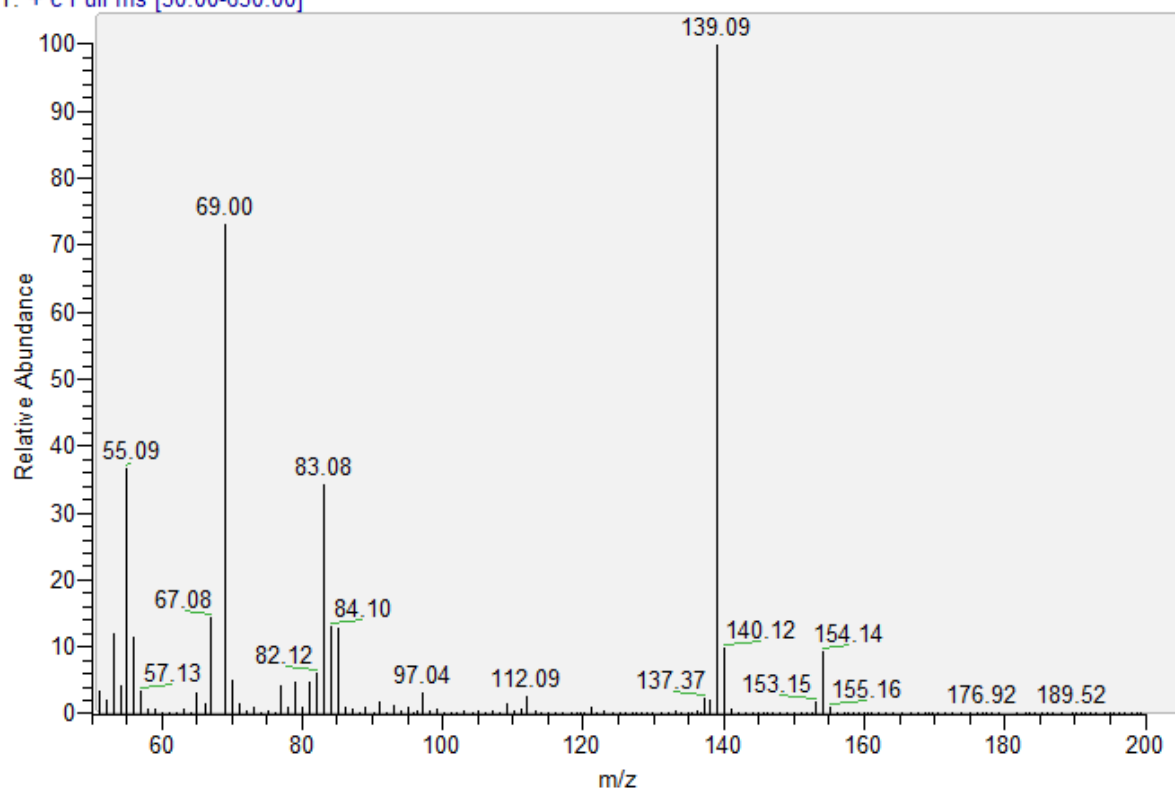
T: + c Full ms [50.00-650.00]



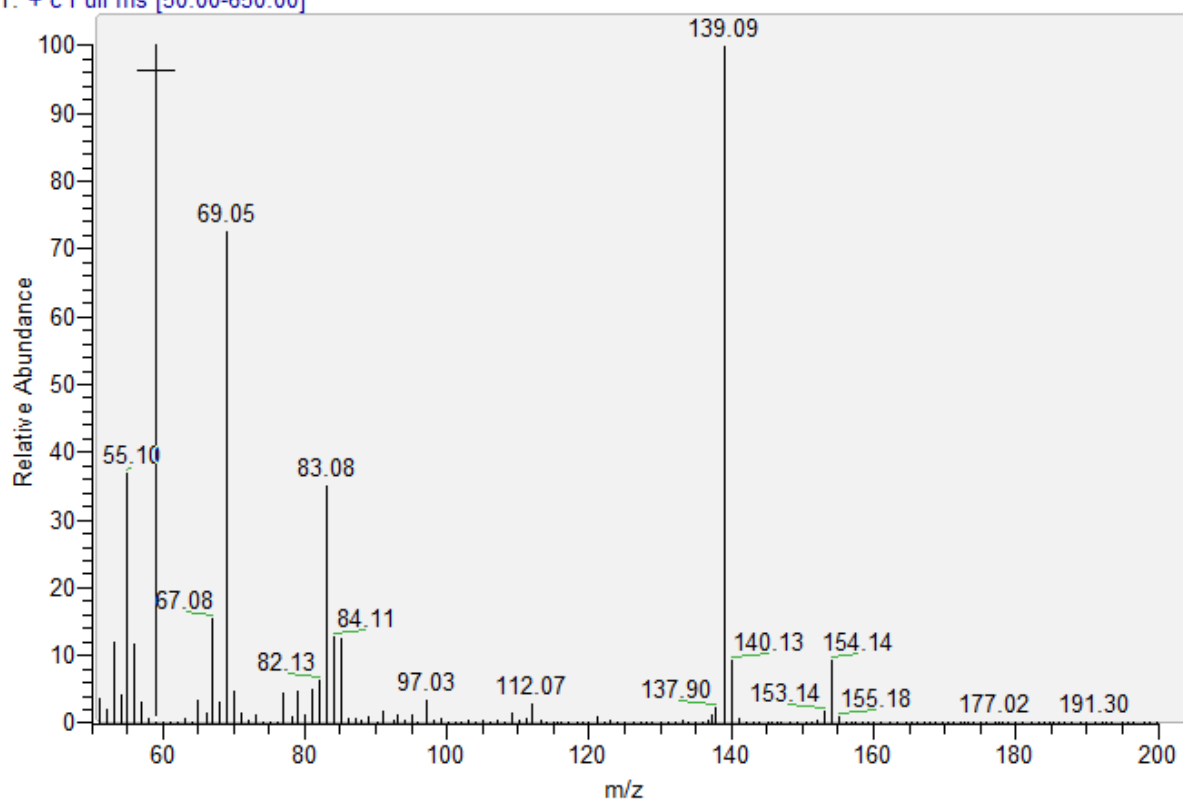
3053 #734-736 RT: 17.45-17.50 AV: 3 NL: 6.05E5  
T: + c Full ms [50.00-650.00]



3018 #739-740 RT: 17.48-17.50 AV: 2 NL: 7.86E6  
T: + c Full ms [50.00-650.00]

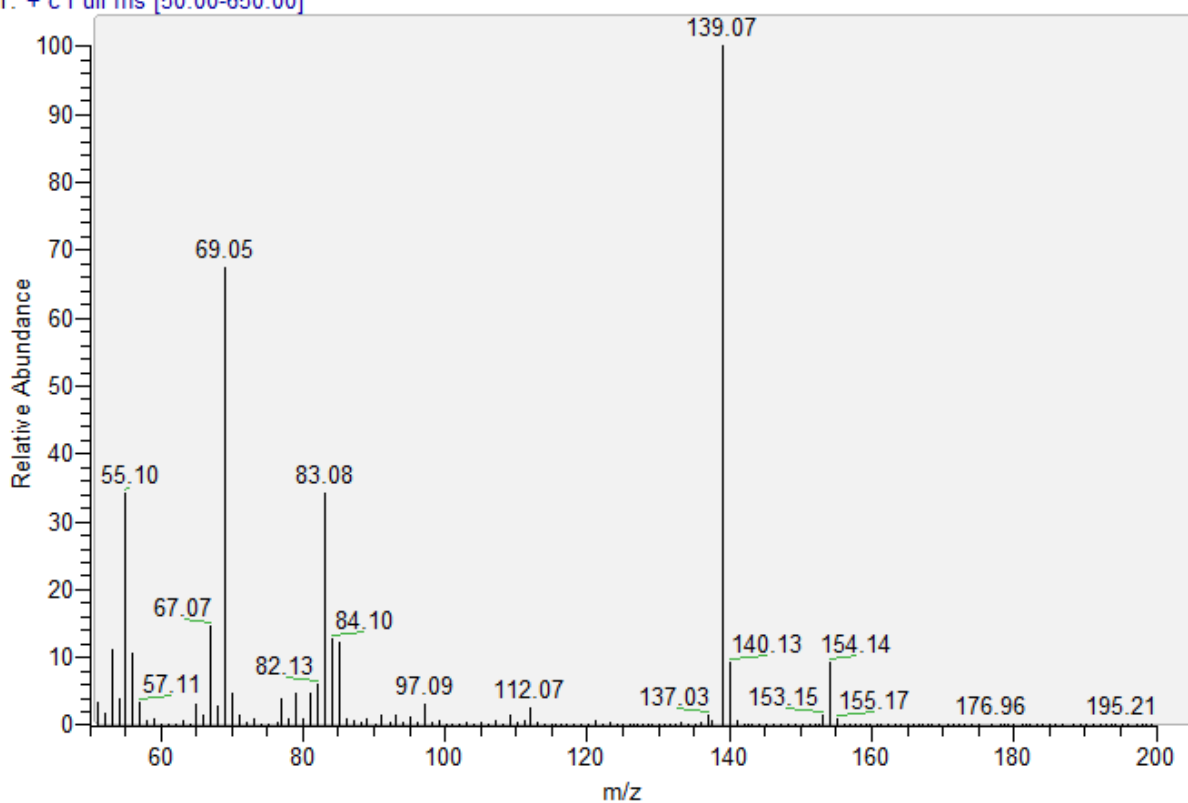


3075 #735-736 RT: 17.49-17.52 AV: 2 NL: 6.79E6  
T: + c Full ms [50.00-650.00]

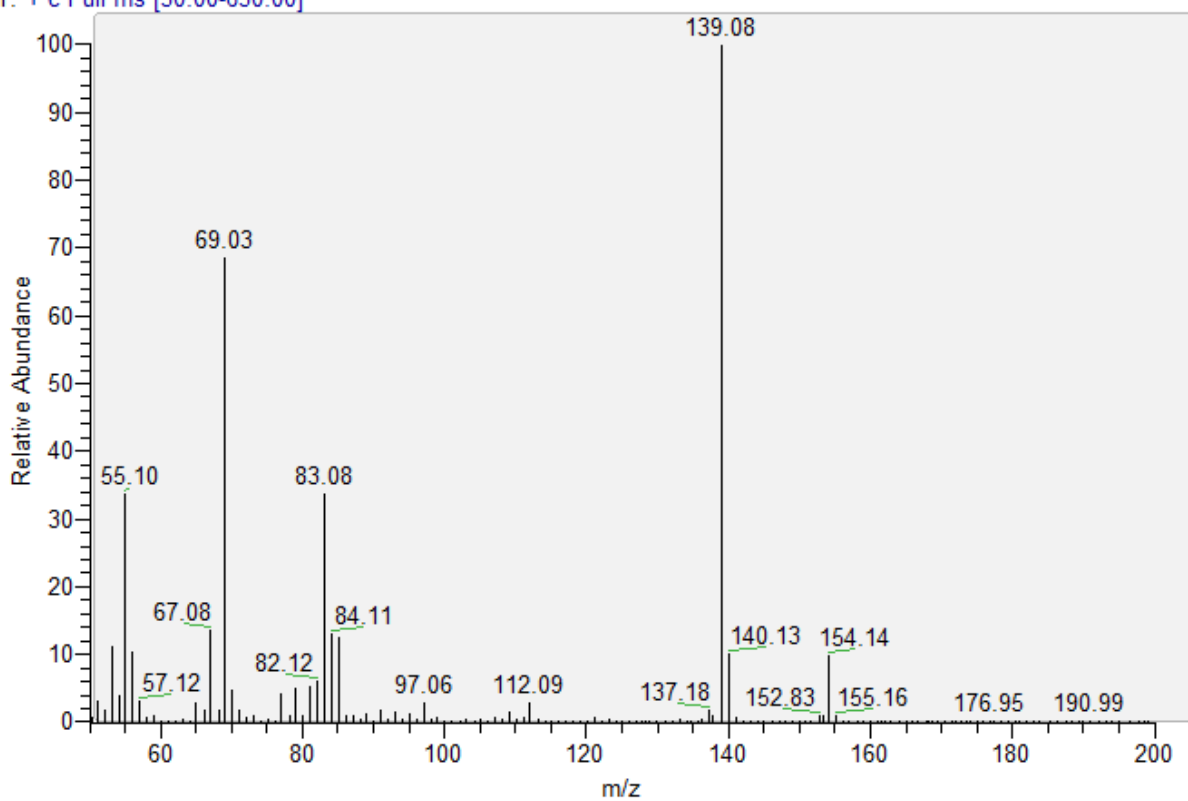




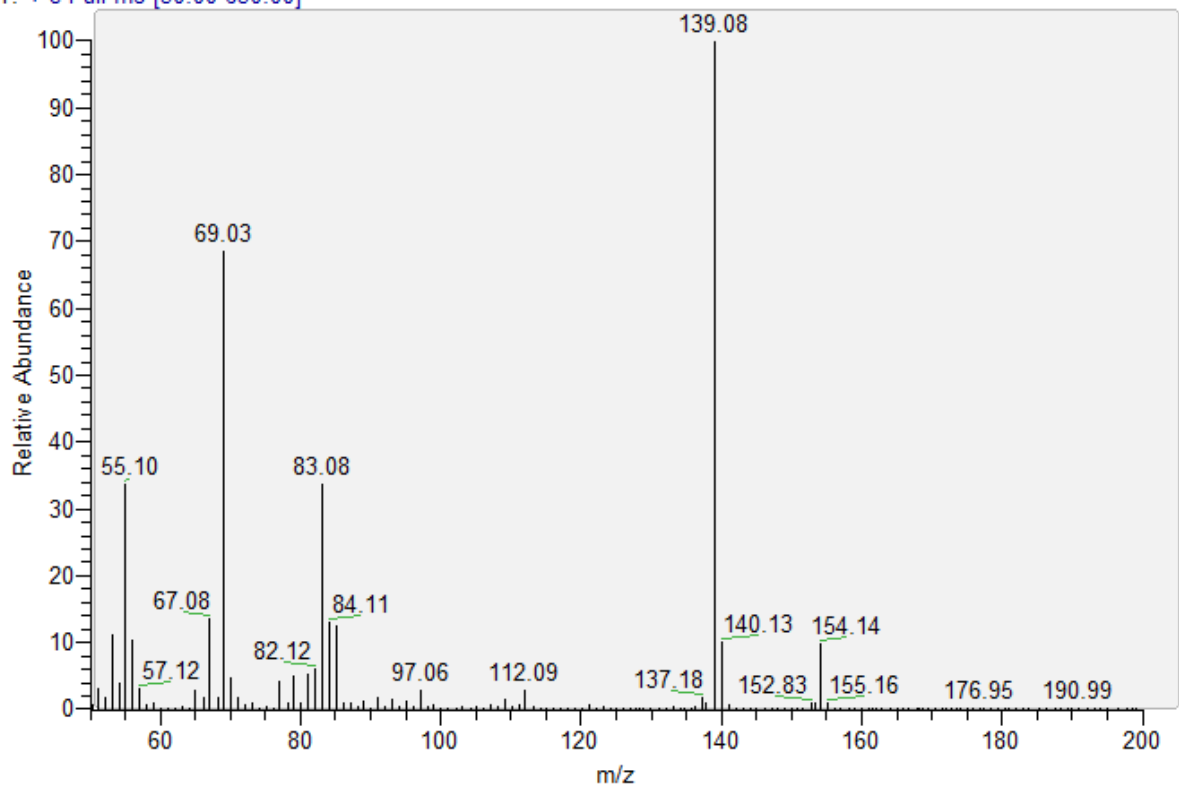
3074 #737-738 RT: 17.48-17.51 AV: 2 NL: 6.74E6  
T: + c Full ms [50.00-650.00]



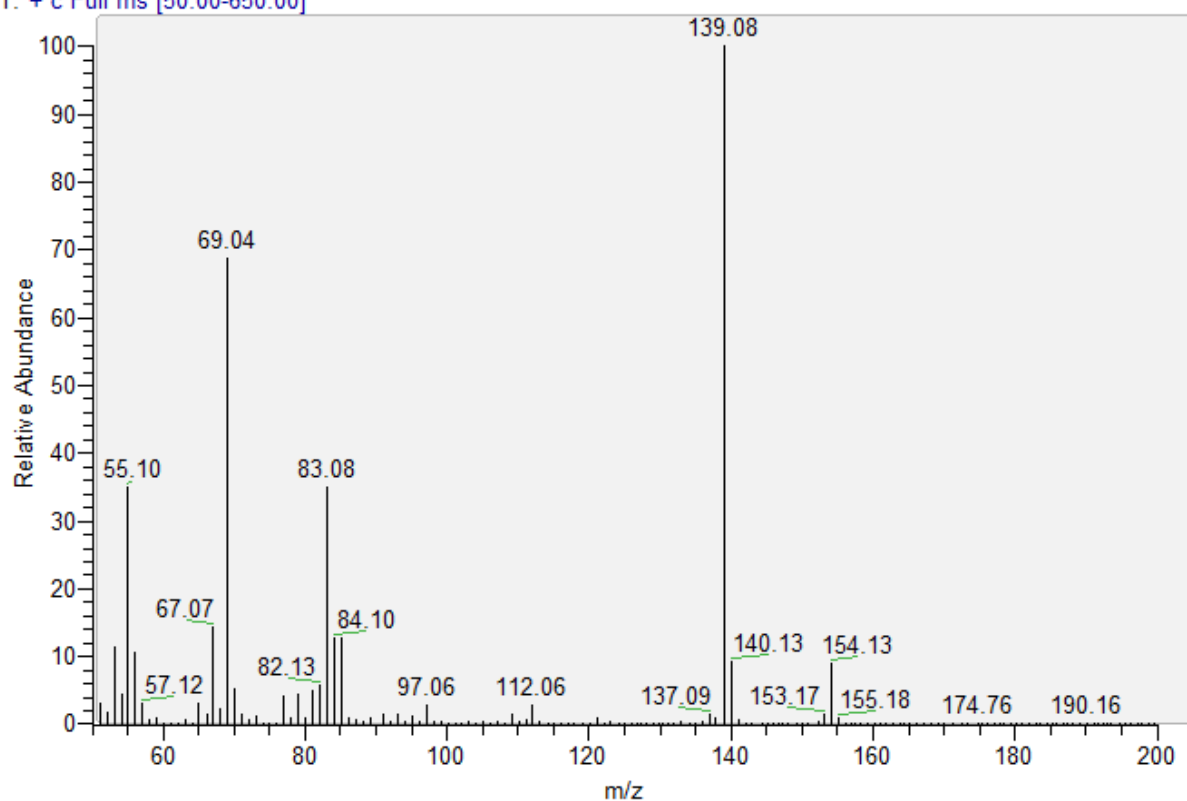
3073 #733-734 RT: 17.46-17.48 AV: 2 NL: 5.85E6  
T: + c Full ms [50.00-650.00]



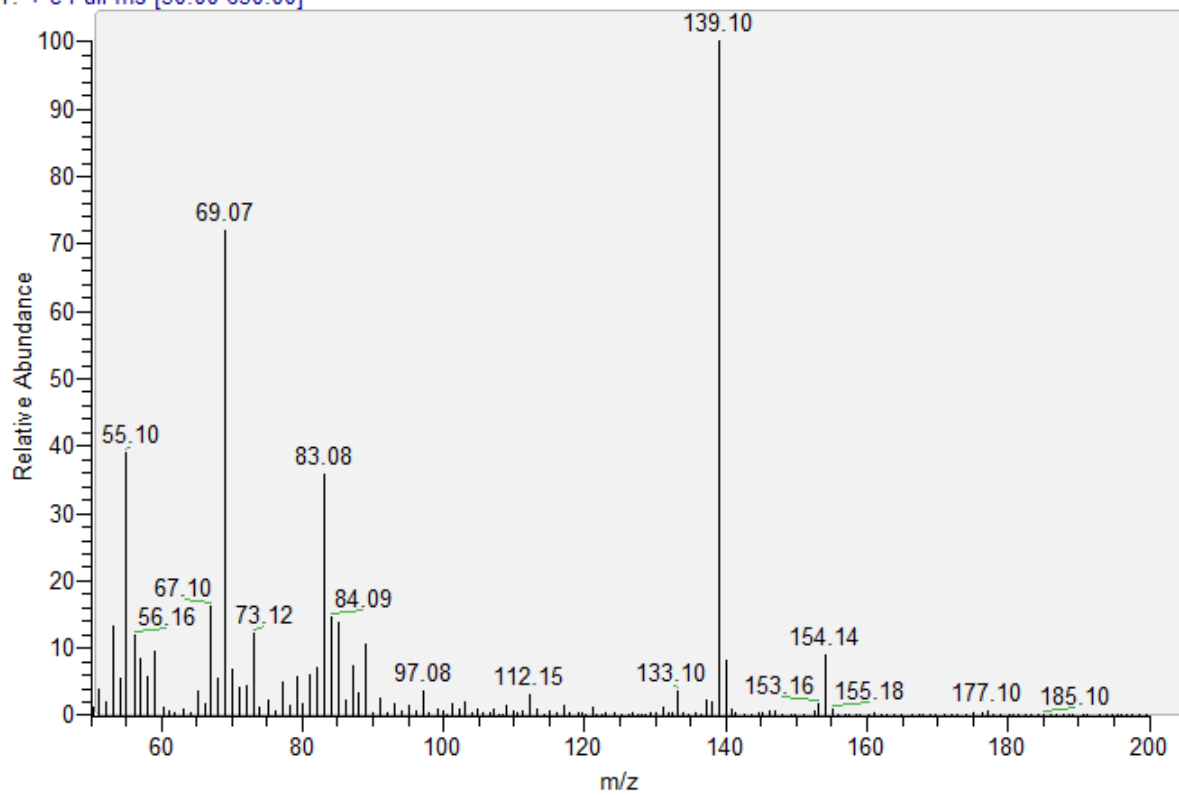
3073 #733-734 RT: 17.46-17.48 AV: 2 NL: 5.85E6  
T: + c Full ms [50.00-650.00]



3072 #734-735 RT: 17.47-17.49 AV: 2 NL: 6.09E6  
T: + c Full ms [50.00-650.00]



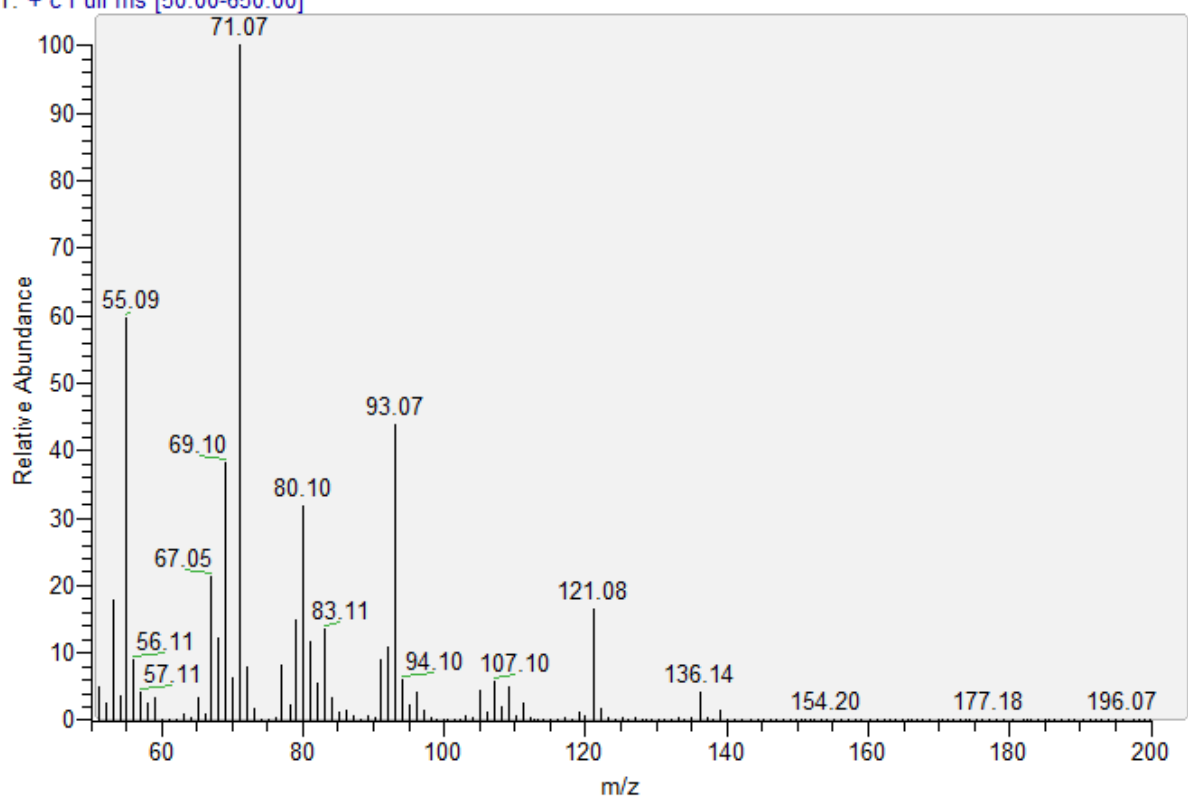
3070 #736-737 RT: 17.46-17.49 AV: 2 NL: 4.87E5  
T: + c Full ms [50.00-650.00]



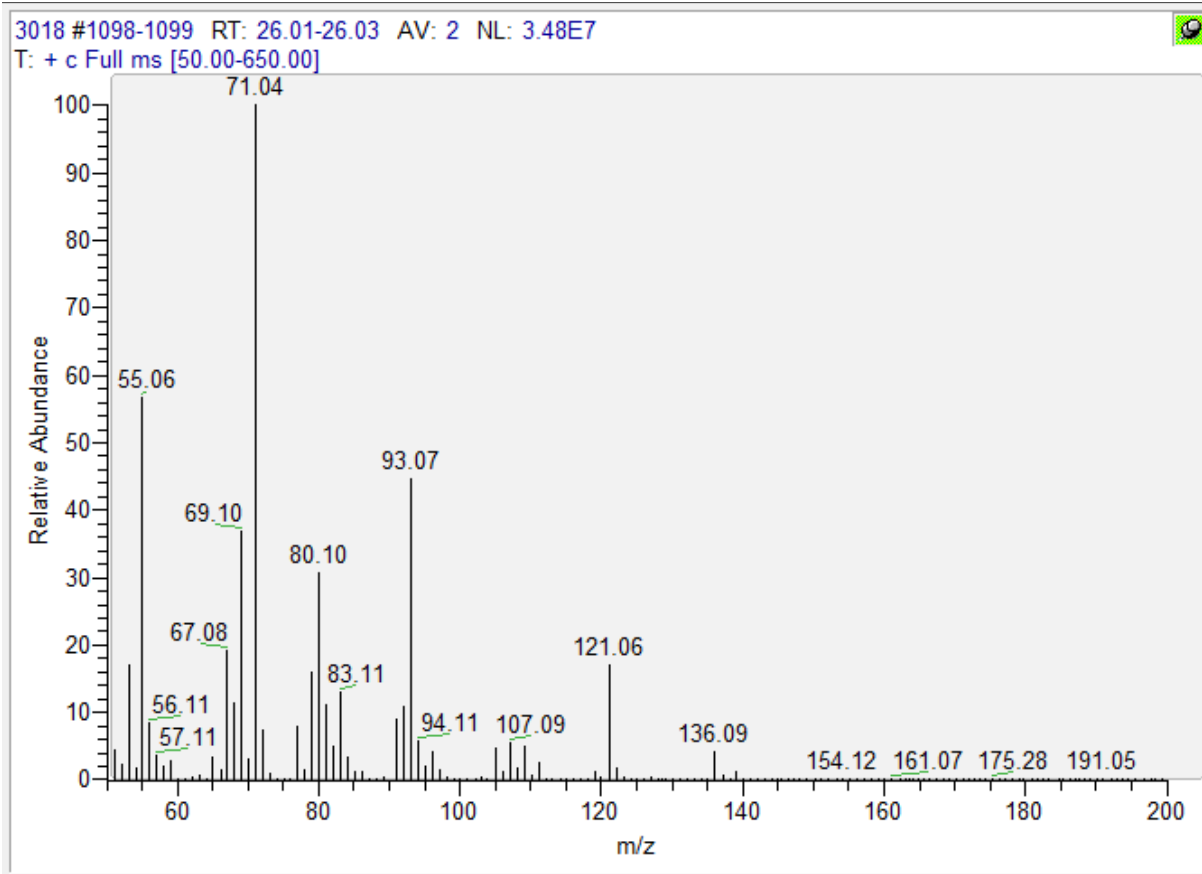
Linalool

Reference

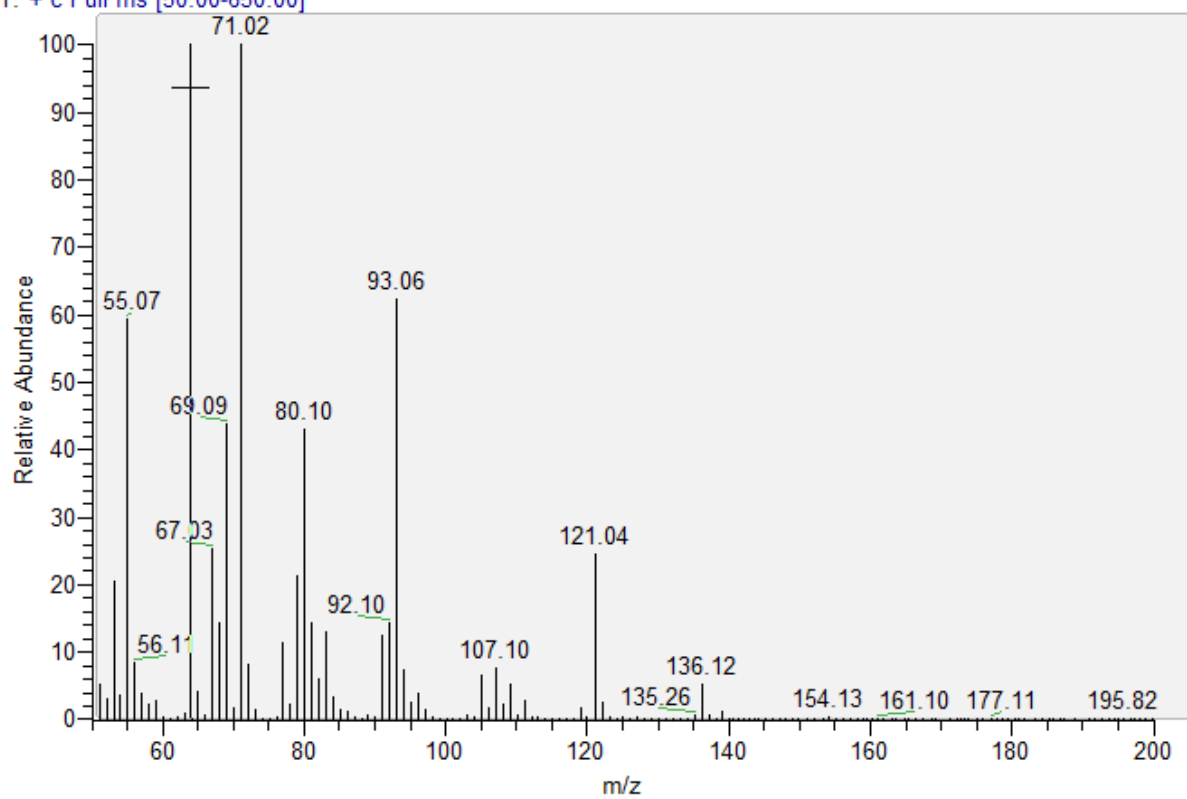
1\_20 #1099-1100 RT: 25.99-26.02 AV: 2 NL: 4.54E6  
T: + c Full ms [50.00-650.00]



Samples:

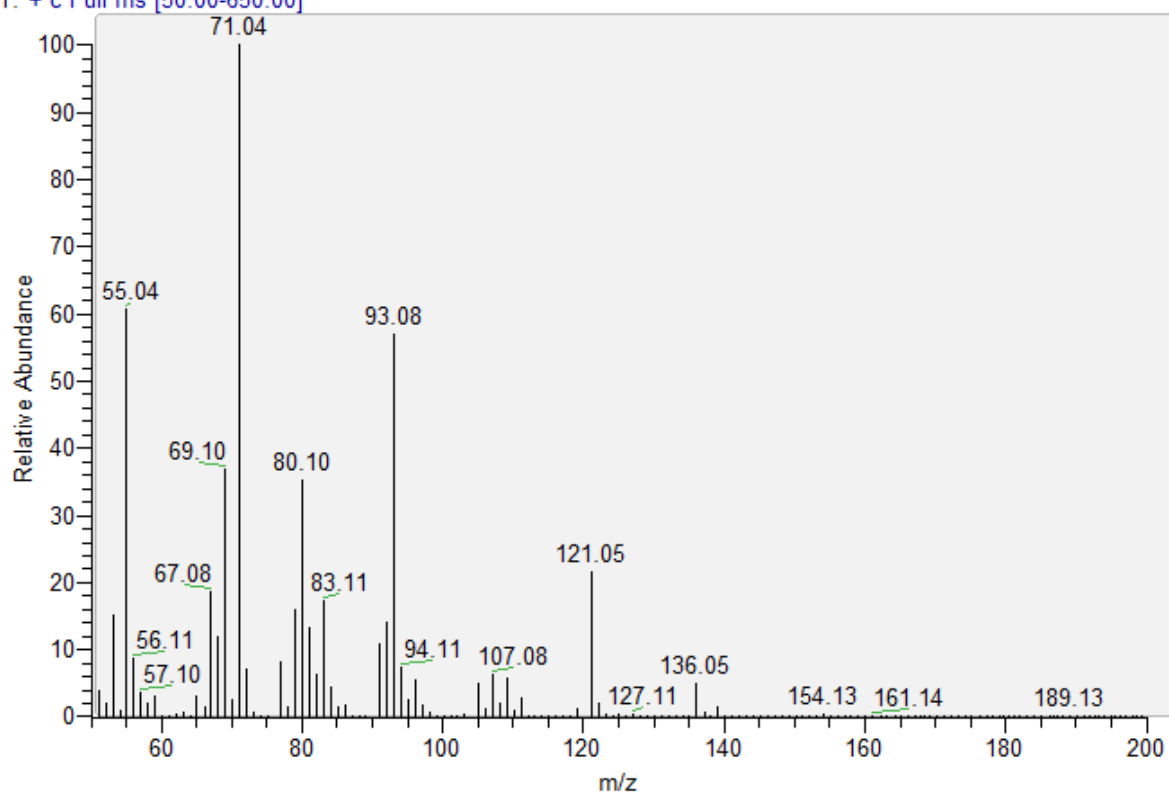


3053 #1093-1094 RT: 25.99-26.01 AV: 2 NL: 7.62E6  
T: + c Full ms [50.00-650.00]

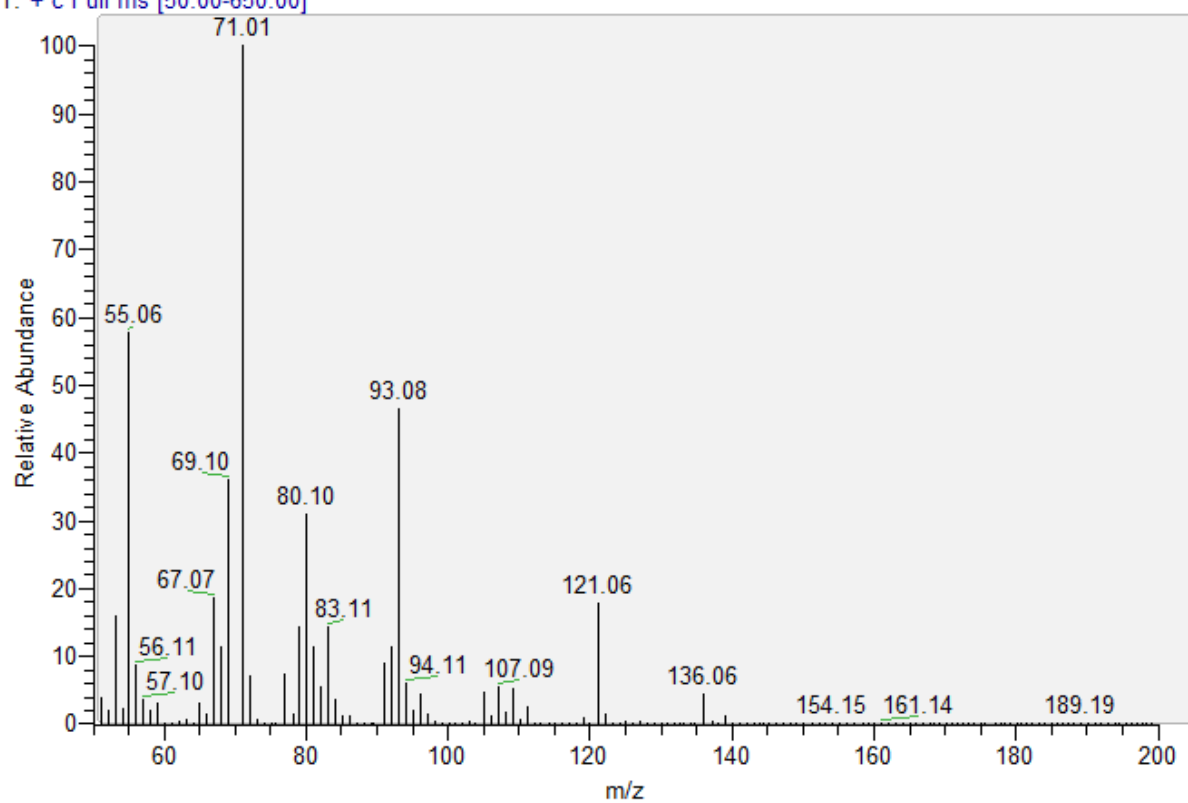




3058 #1094-1096 RT: 26.08-26.13 AV: 3 NL: 2.10E8  
T: + c Full ms [50.00-650.00]



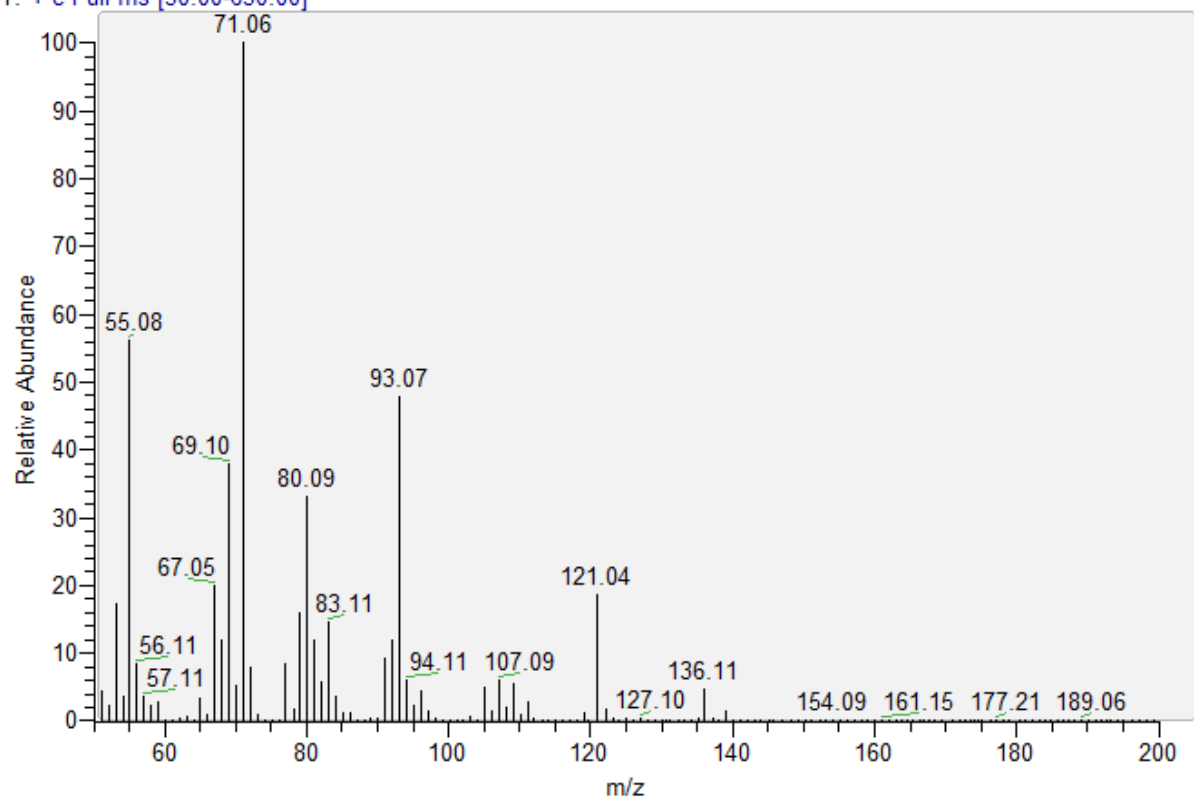
3057 #1099-1101 RT: 26.03-26.07 AV: 3 NL: 1.41E8  
T: + c Full ms [50.00-650.00]



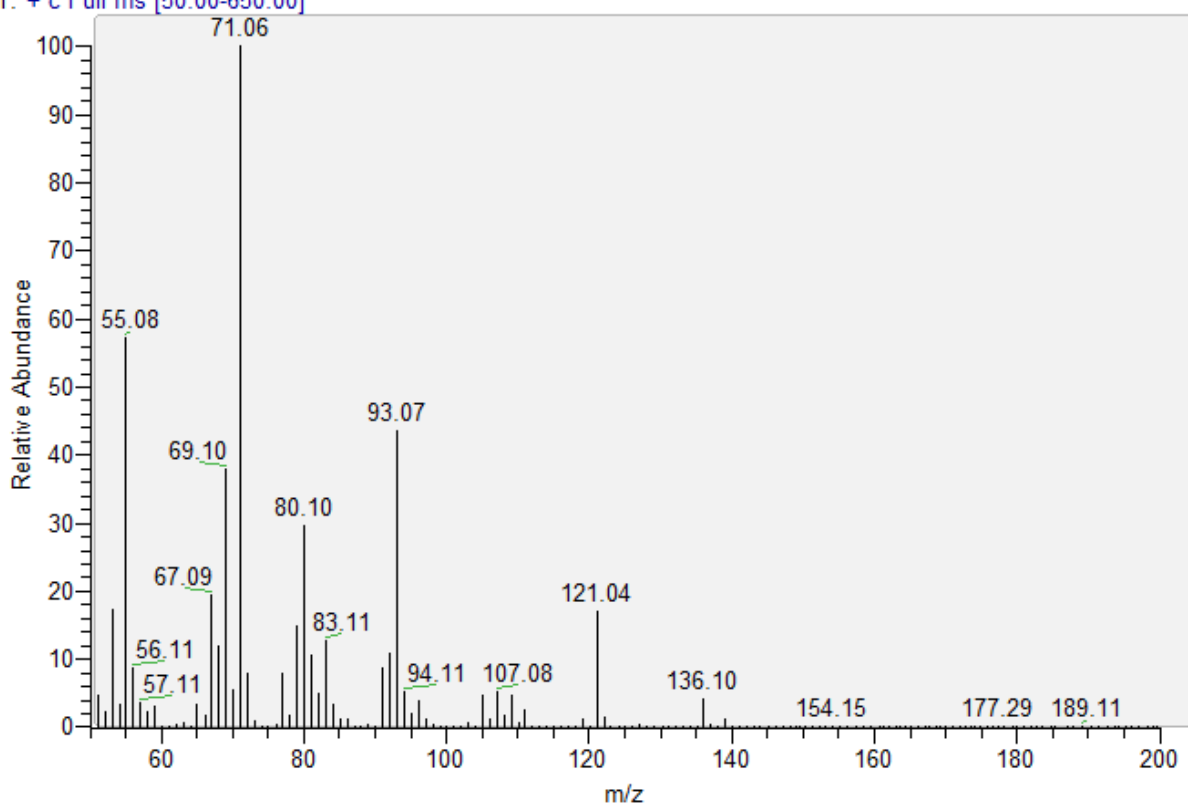
3021 #1094-1095 RT: 26.00-26.03 AV: 2 NL: 3.55E7



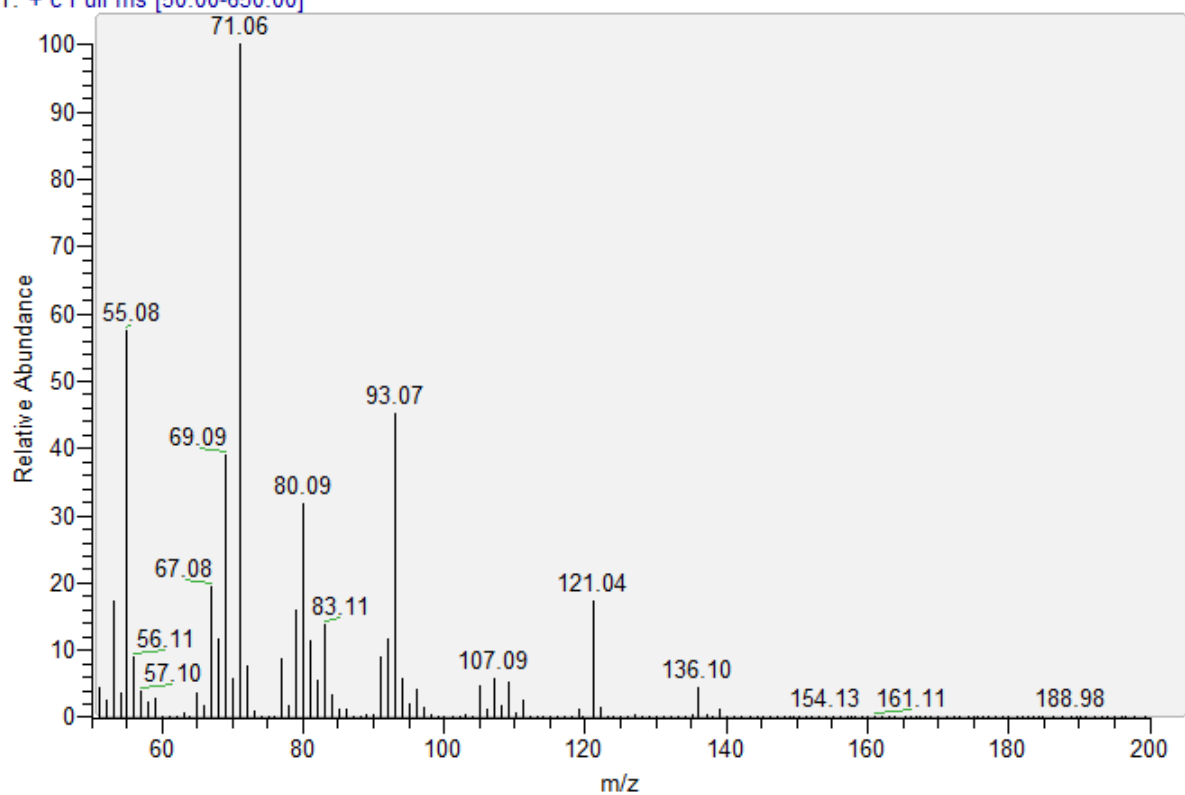
T: + c Full ms [50.00-650.00]



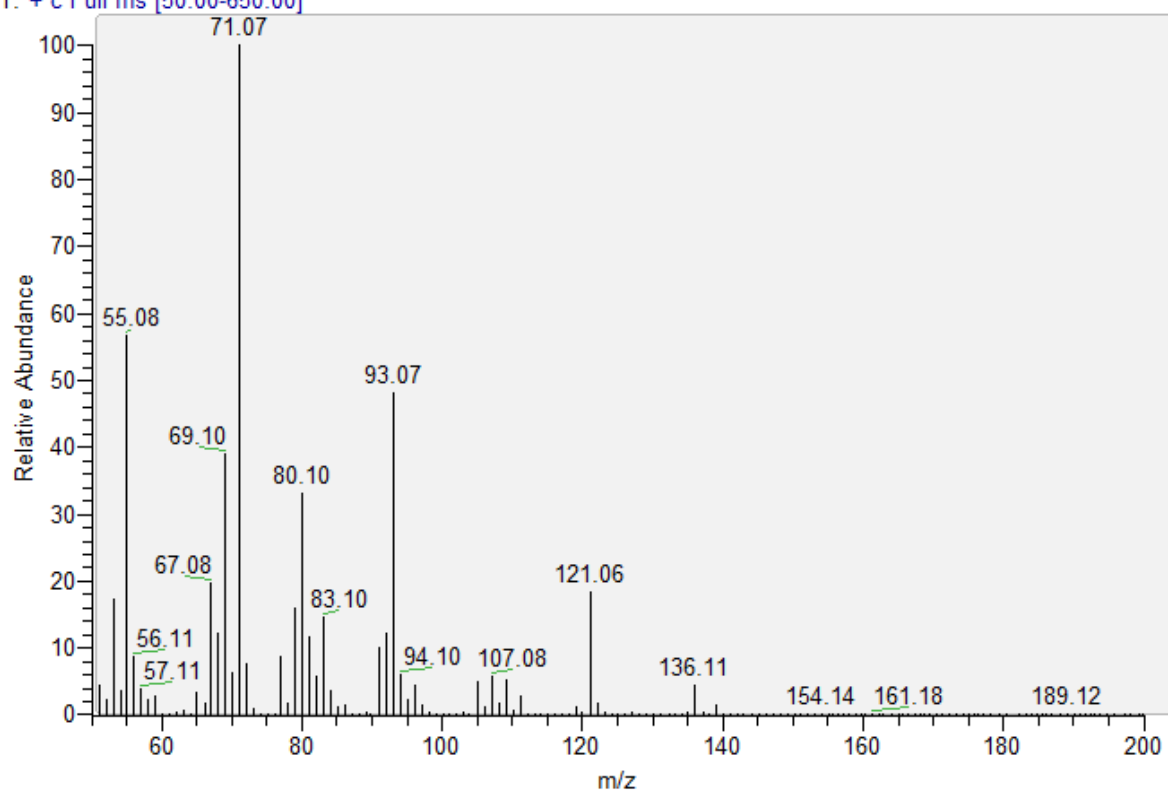
3075 #1093-1094 RT: 26.01-26.04 AV: 2 NL: 1.67E7  
T: + c Full ms [50.00-650.00]



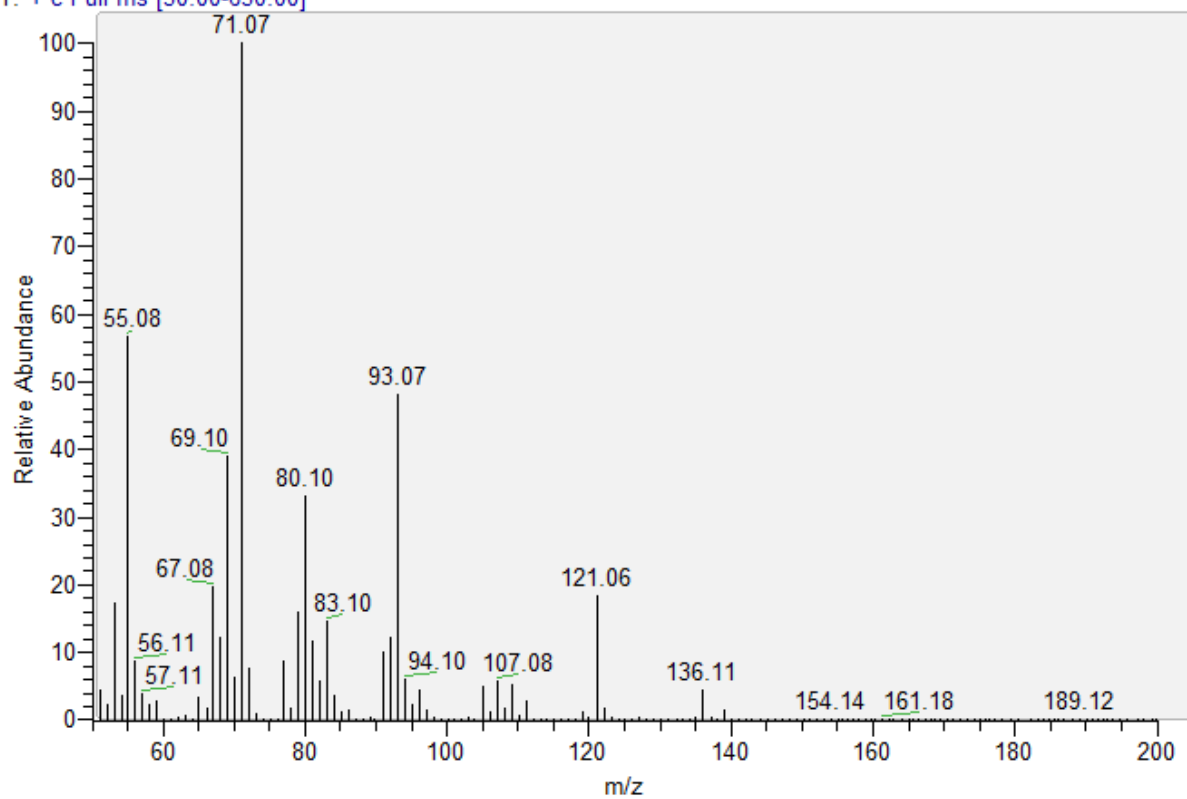
3074 #1095-1096 RT: 26.01-26.04 AV: 2 NL: 2.81E7  
T: + c Full ms [50.00-650.00]



3073 #1094-1095 RT: 26.02-26.04 AV: 2 NL: 3.99E7  
T: + c Full ms [50.00-650.00]



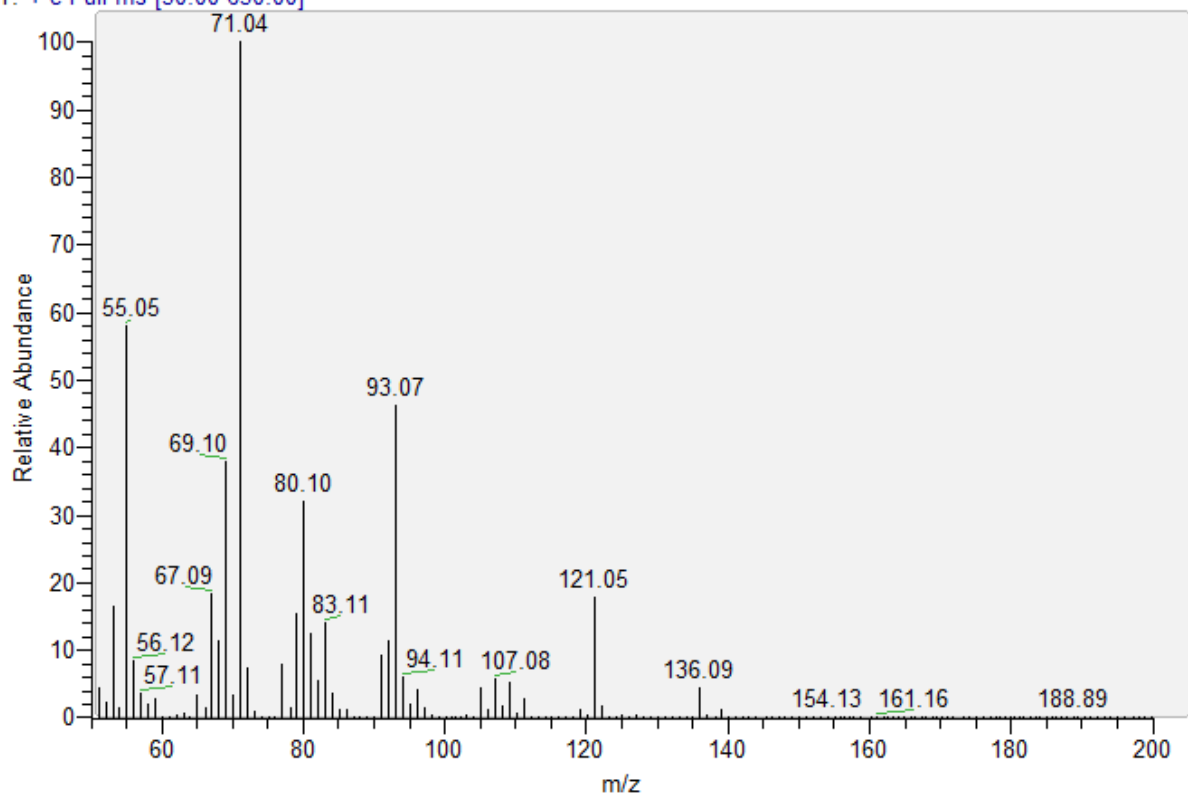
3073 #1094-1095 RT: 26.02-26.04 AV: 2 NL: 3.99E7  
T: + c Full ms [50.00-650.00]



3072 #1093-1094 RT: 26.02-26.04 AV: 2 NL: 5.89E7



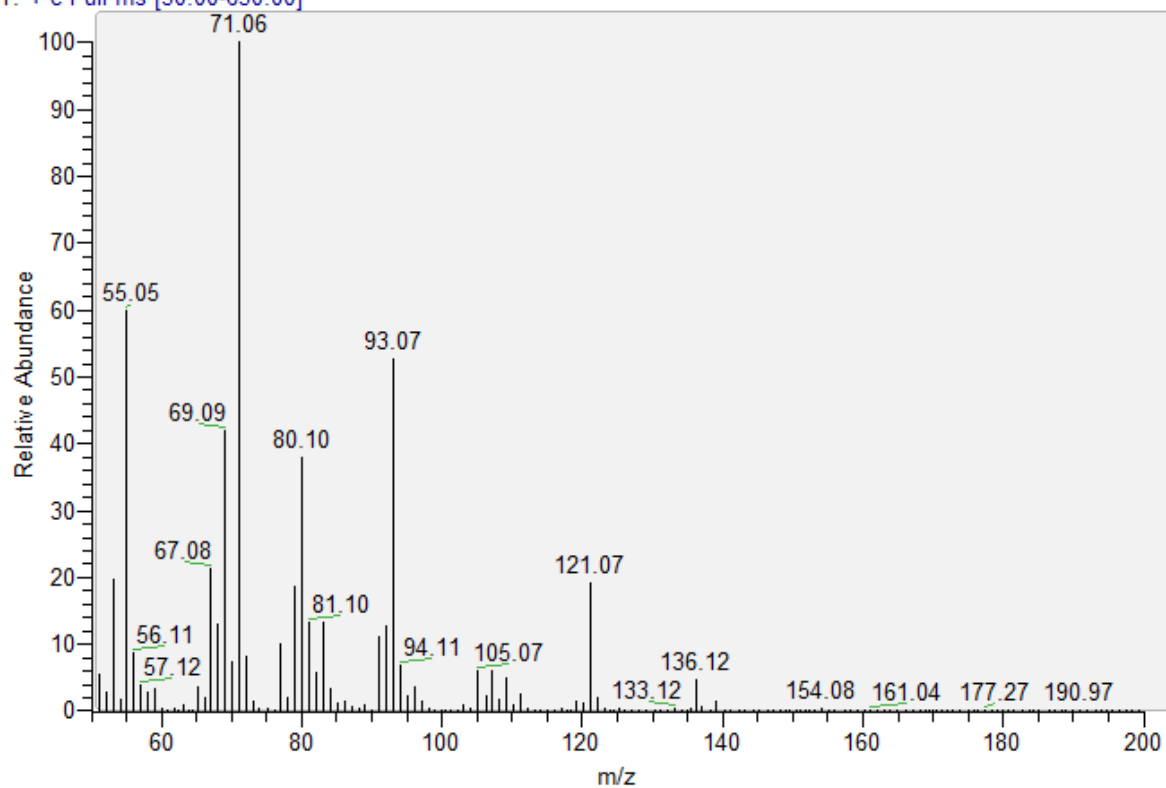
T: + c Full ms [50.00-650.00]





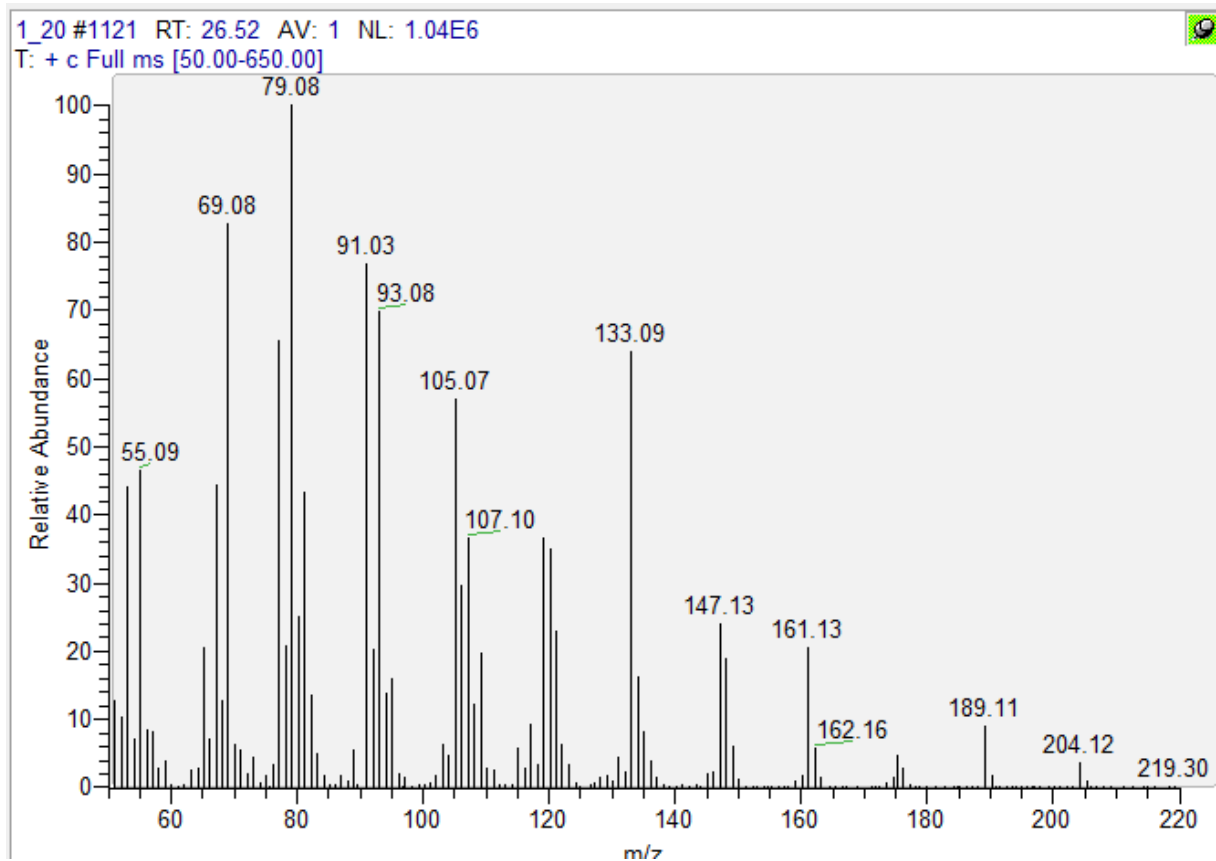
3070 #1094-1095 RT: 25.99-26.01 AV: 2 NL: 5.08E6

T: + c Full ms [50.00-650.00]



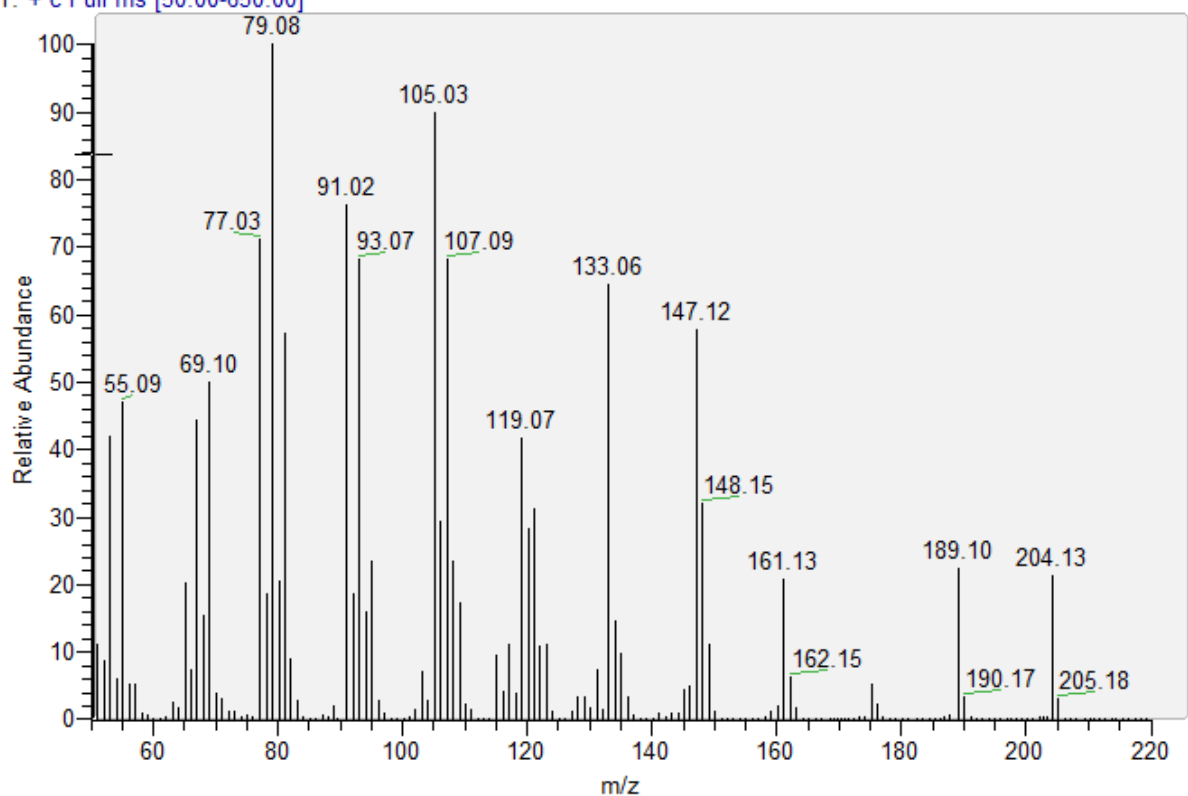
# Beta Caryophyllene

Reference:

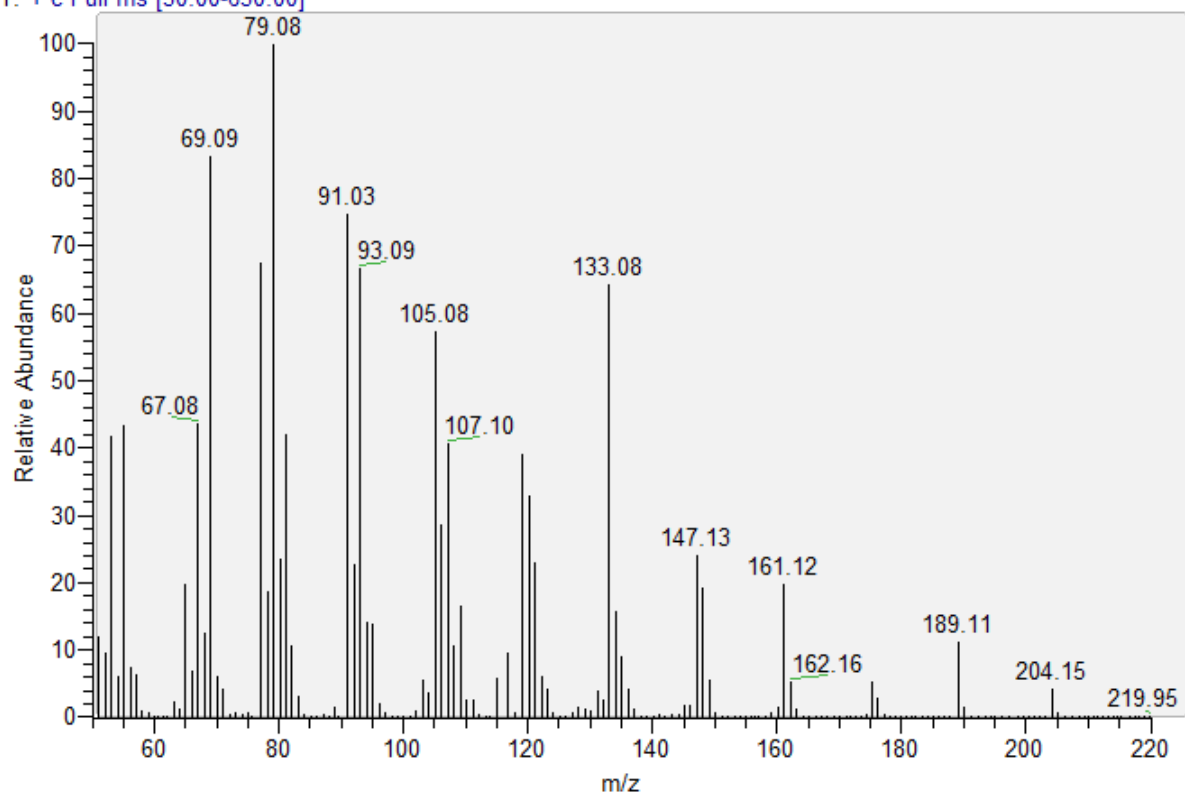


Samples:

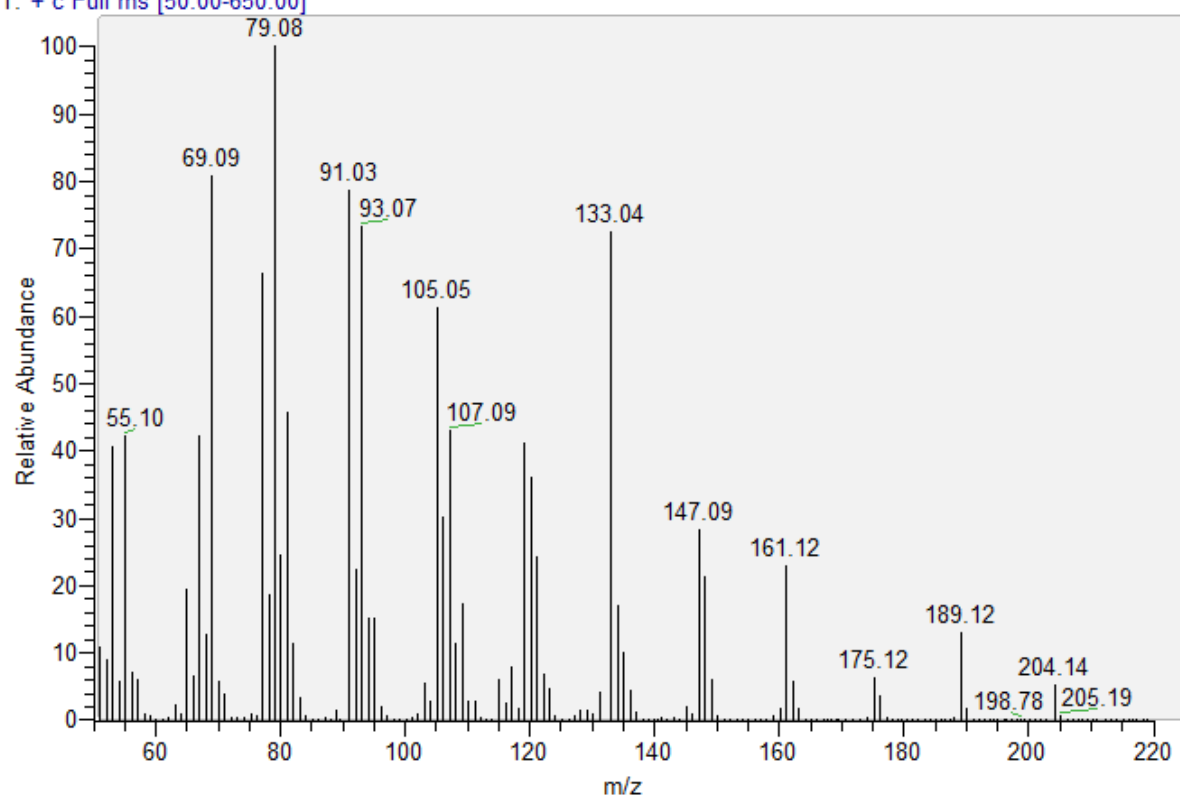
3021 #1117-1118 RT: 26.55-26.57 AV: 2 NL: 1.27E7  
T: + c Full ms [50.00-650.00]



3057 #1121-1122 RT: 26.55-26.58 AV: 2 NL: 1.37E7  
T: + c Full ms [50.00-650.00]



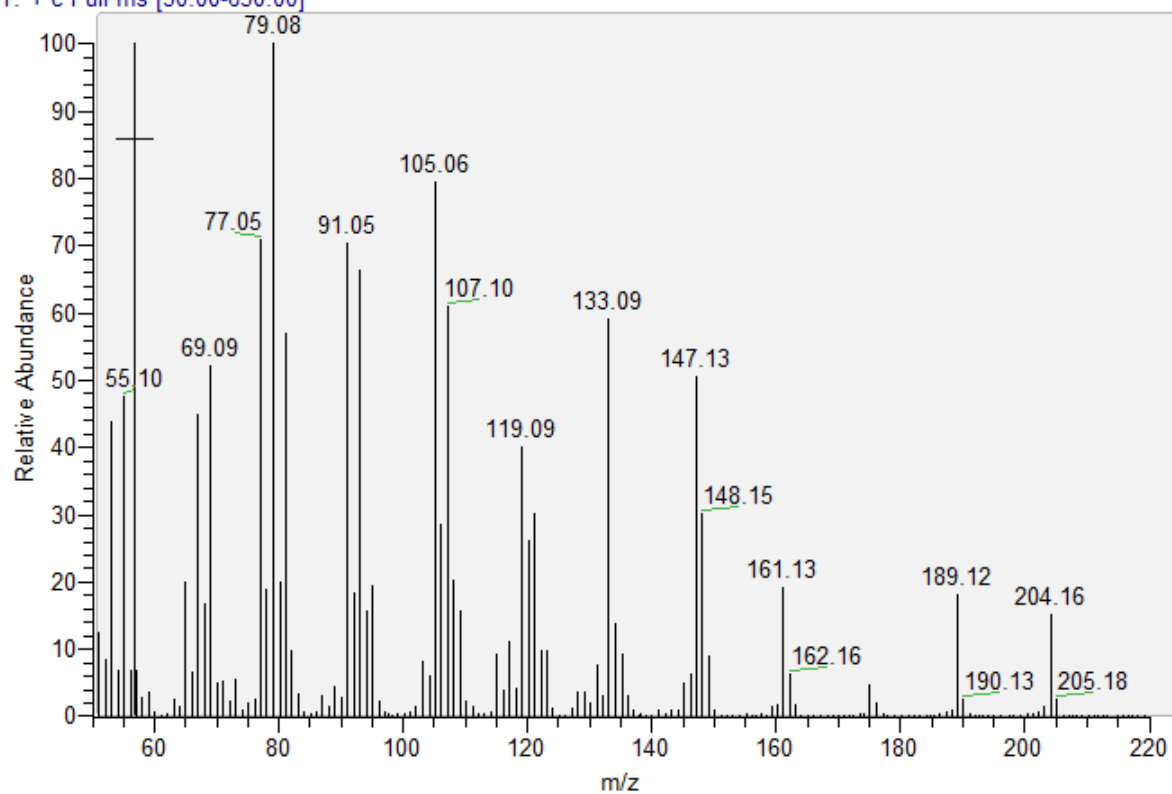
3058 #1116-1118 RT: 26.61-26.66 AV: 3 NL: 1.89E7  
T: + c Full ms [50.00-650.00]



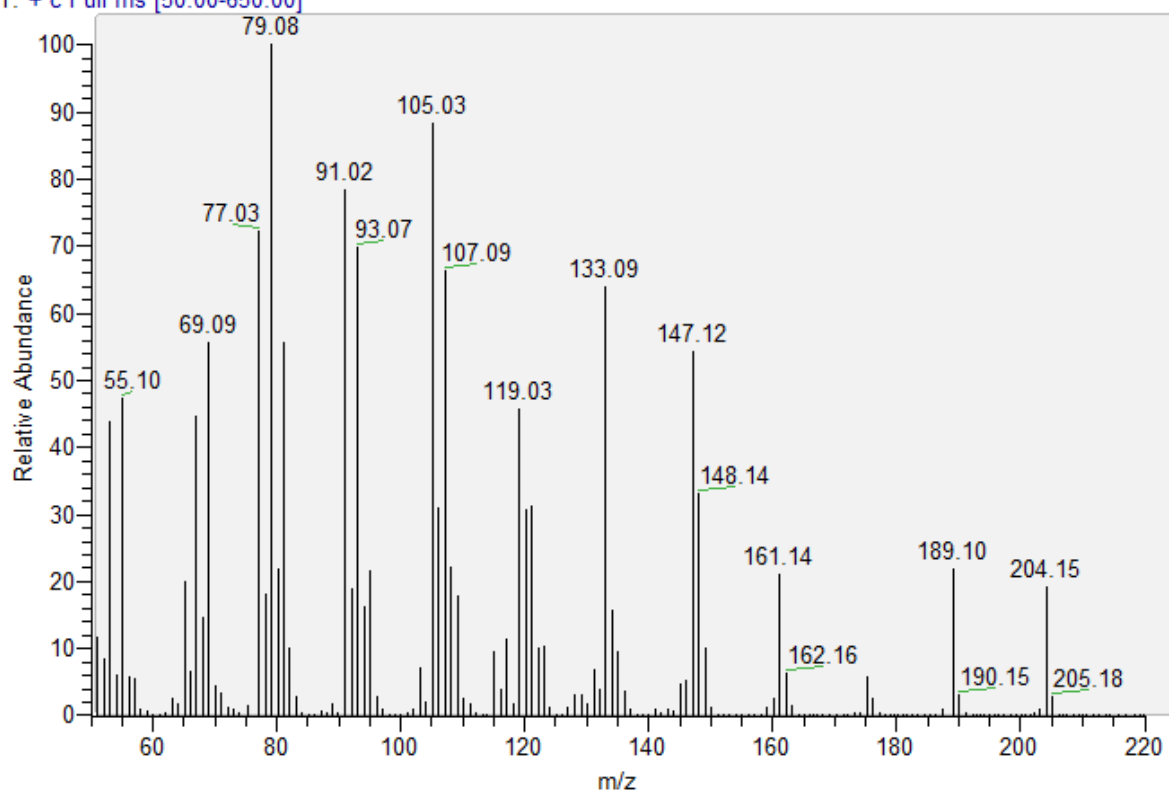
3053 #1115-1117 RT: 26.51-26.56 AV: 3 NL: 9.78E5



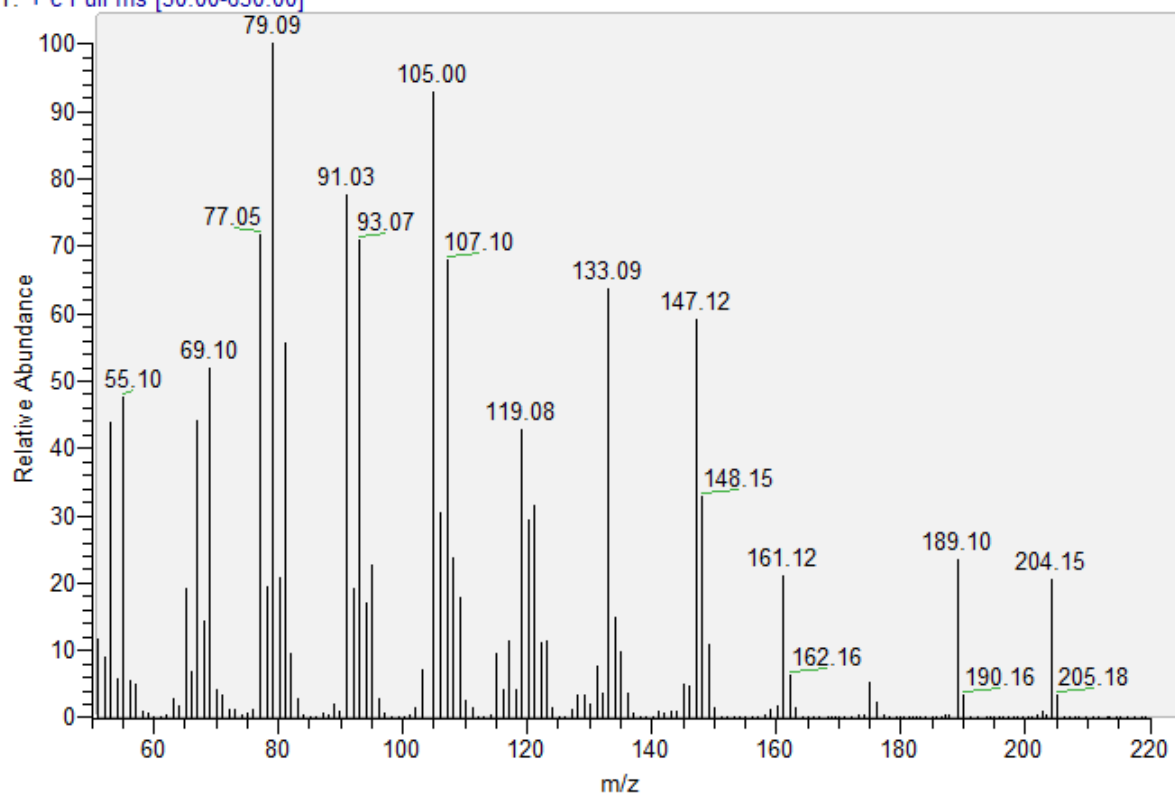
T: + c Full ms [50.00-650.00]



3018 #1120-1121 RT: 26.53-26.56 AV: 2 NL: 1.03E7  
T: + c Full ms [50.00-650.00]

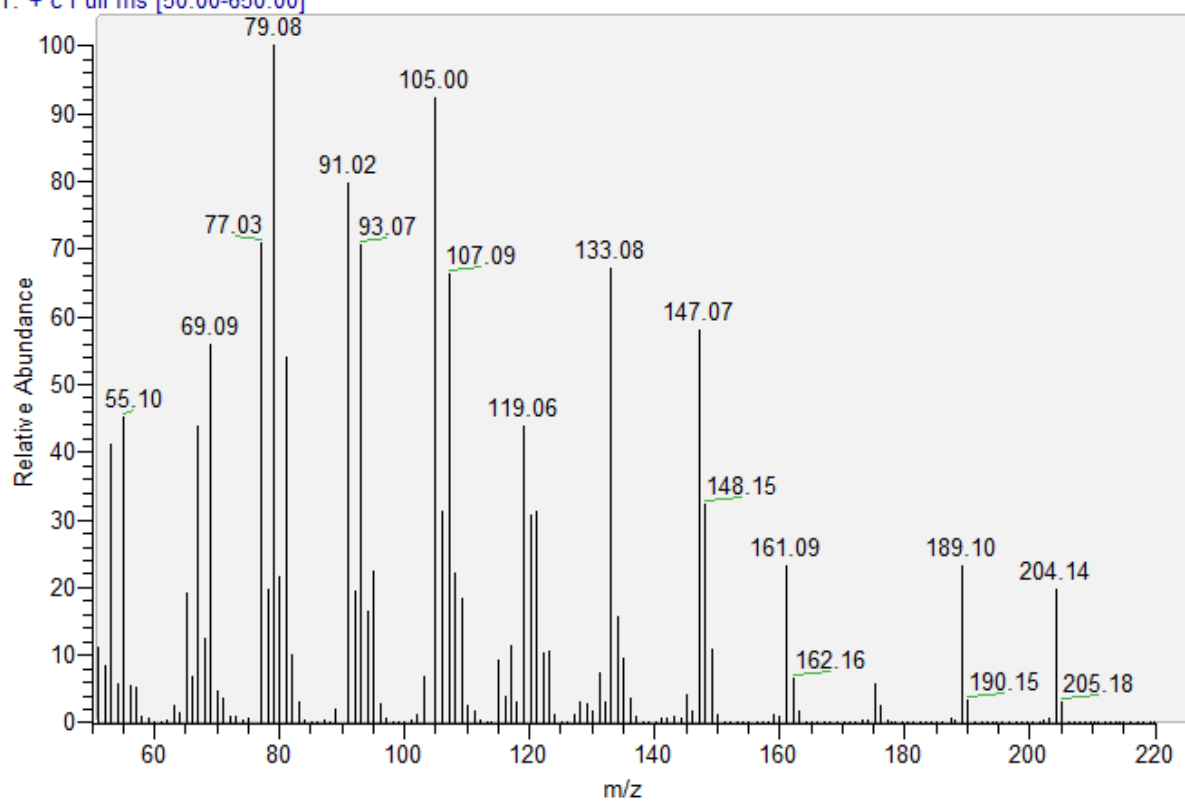


3075 #1115-1116 RT: 26.54-26.56 AV: 2 NL: 1.15E7  
T: + c Full ms [50.00-650.00]

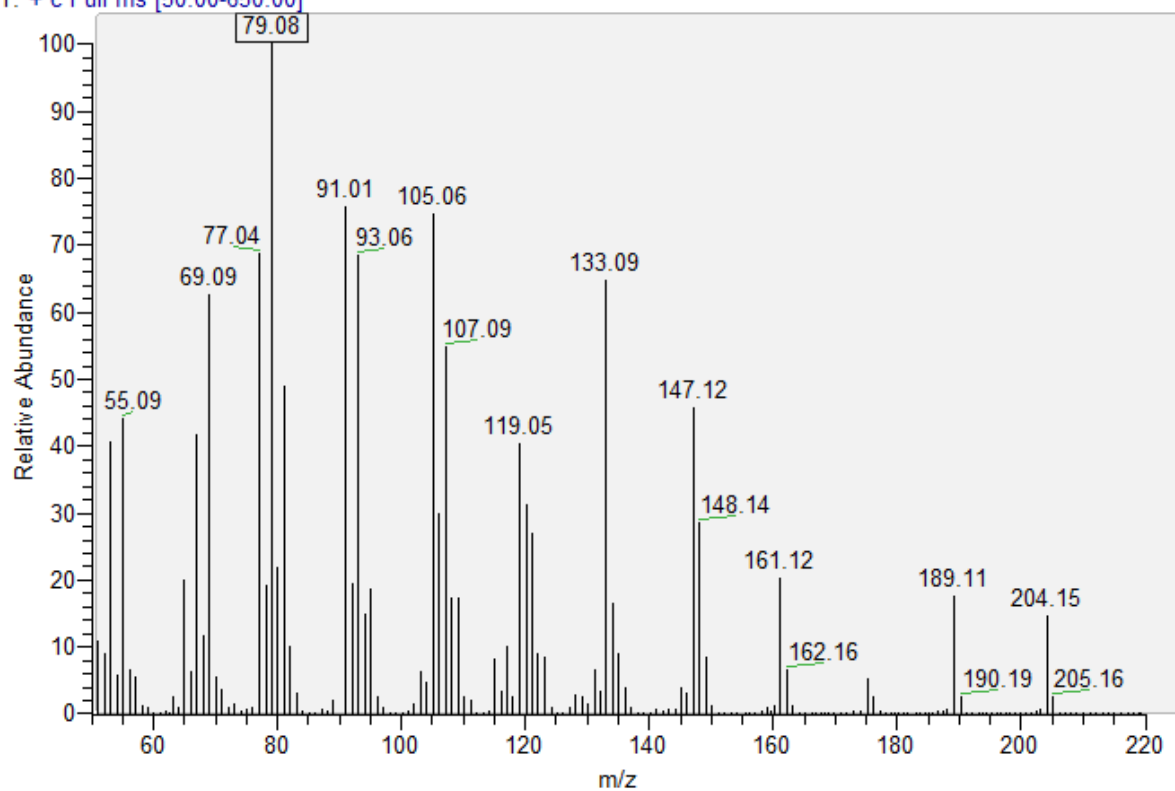




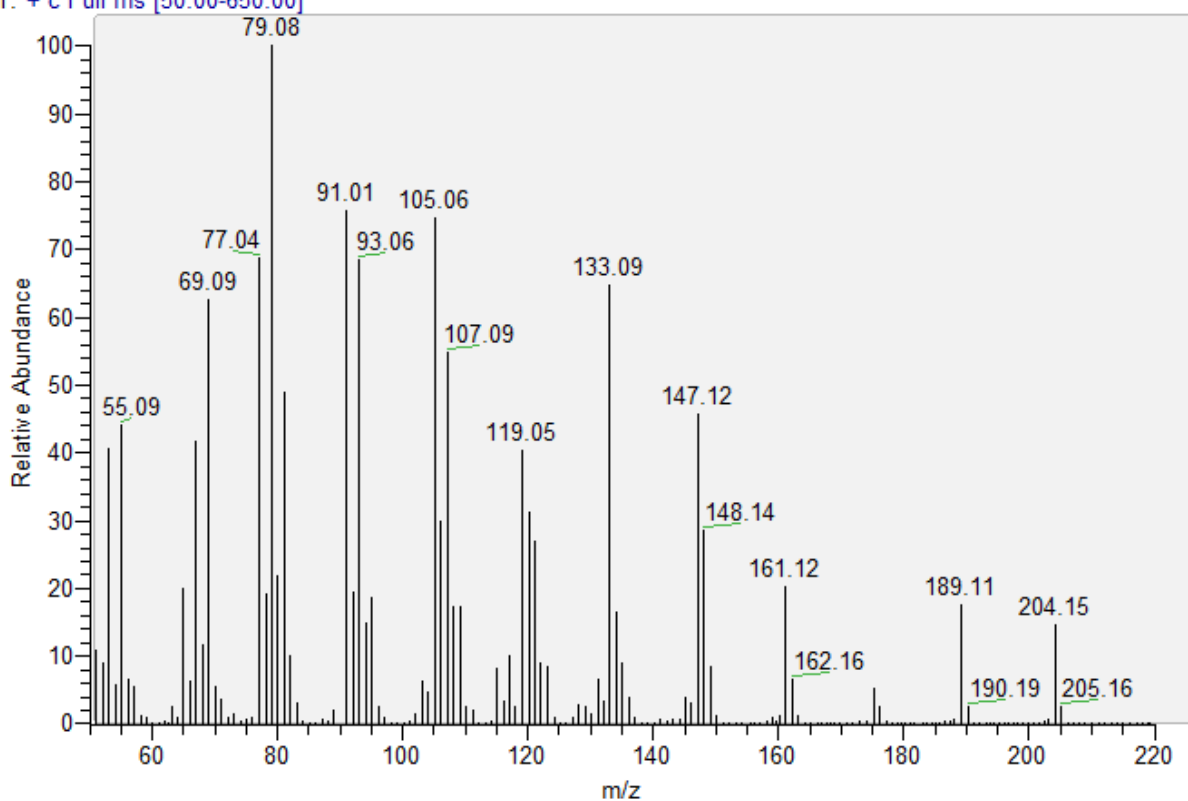
3074 #1117-1118 RT: 26.54-26.56 AV: 2 NL: 1.71E7  
T: + c Full ms [50.00-650.00]



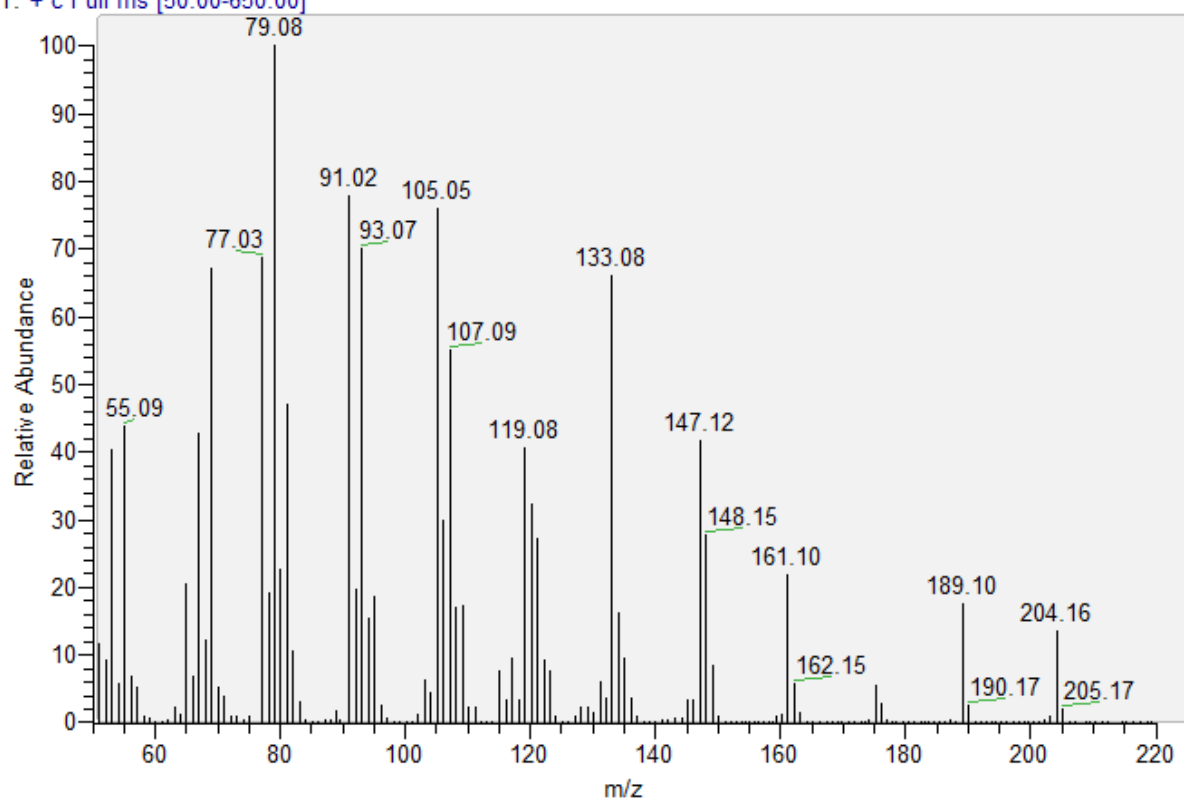
3073 #1115-1116 RT: 26.52-26.54 AV: 2 NL: 5.80E6  
T: + c Full ms [50.00-650.00]



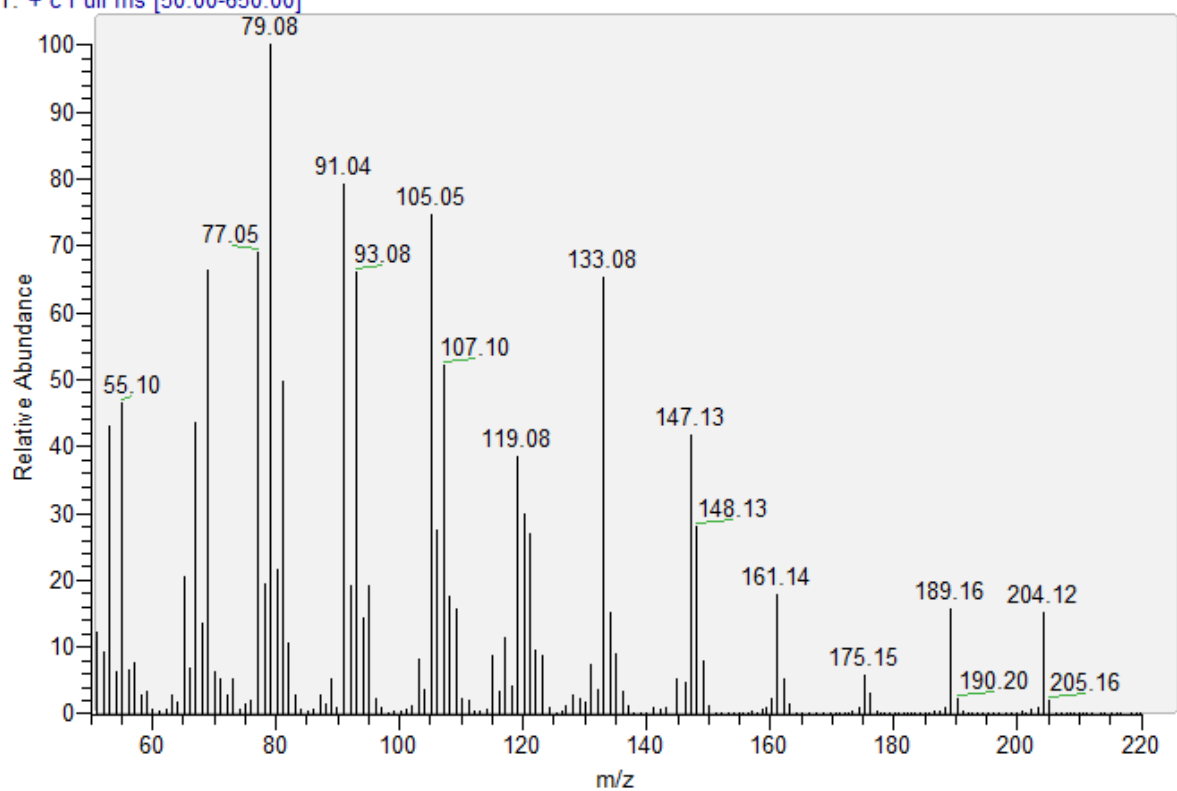
3073 #1115-1116 RT: 26.52-26.54 AV: 2 NL: 5.80E6  
T: + c Full ms [50.00-650.00]



3072 #1115 RT: 26.54 AV: 1 NL: 1.09E7  
T: + c Full ms [50.00-650.00]

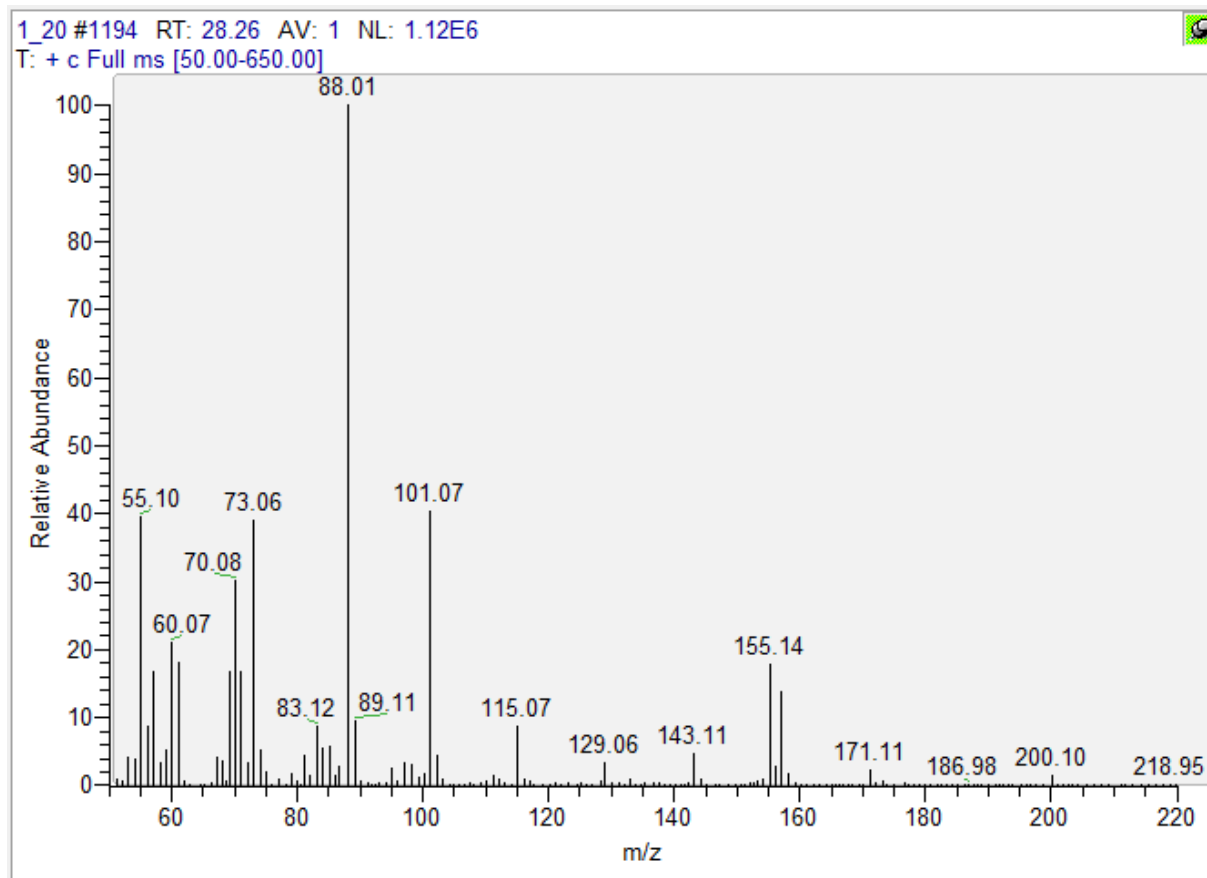


3070 #1116-1117 RT: 26.52-26.54 AV: 2 NL: 9.15E5  
T: + c Full ms [50.00-650.00]



Beta damascenone:

Reference:

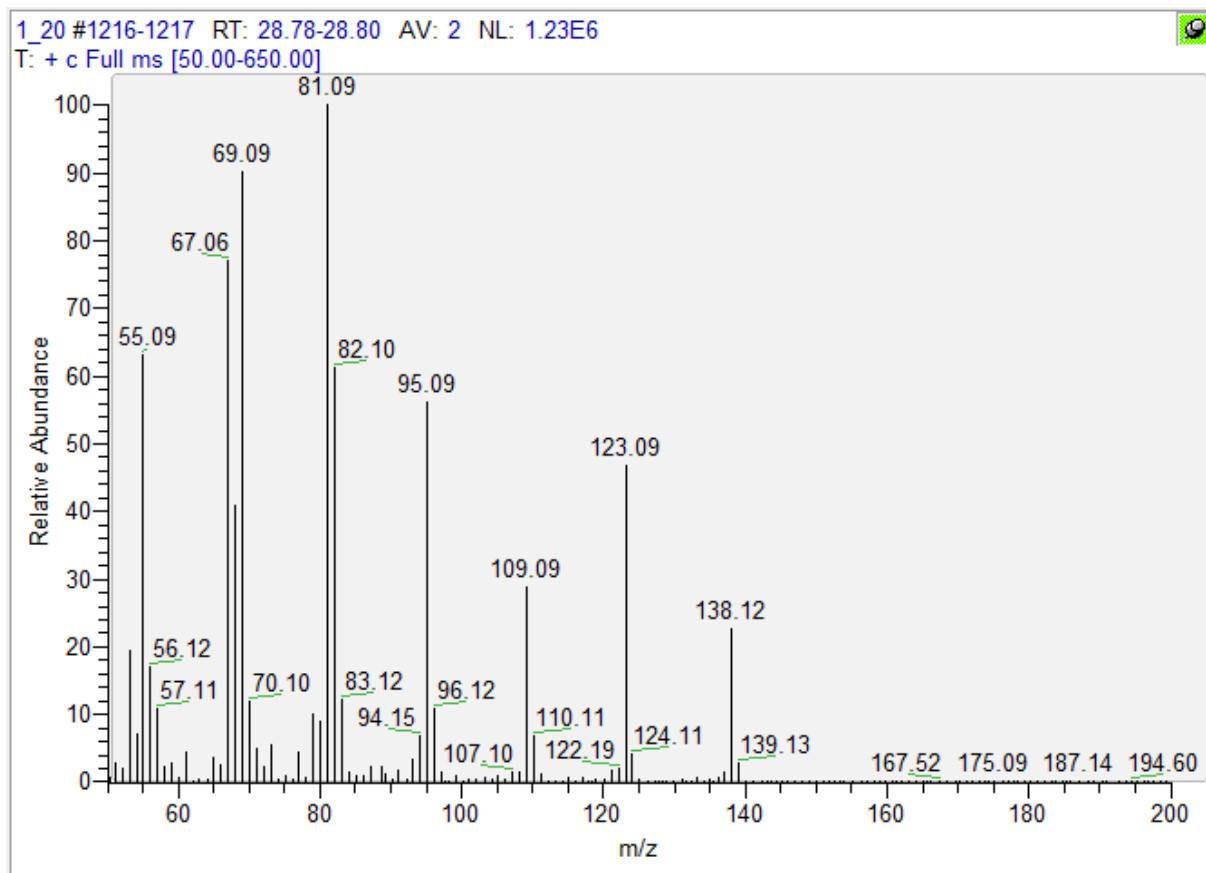


Samples:

Not detected in any samples.

Citronellyl acetate

Reference

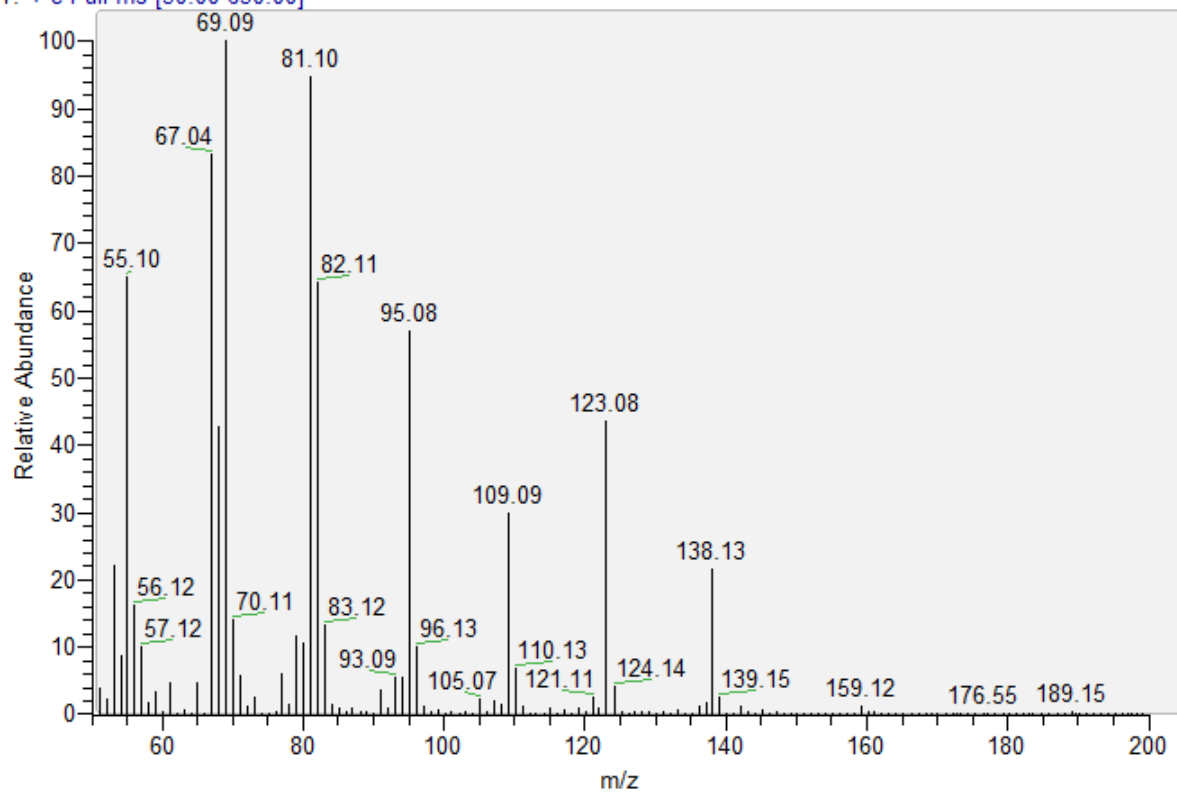


Samples:

3057 #1215-1217 RT: 28.79-28.84 AV: 3 NL: 8.81E6

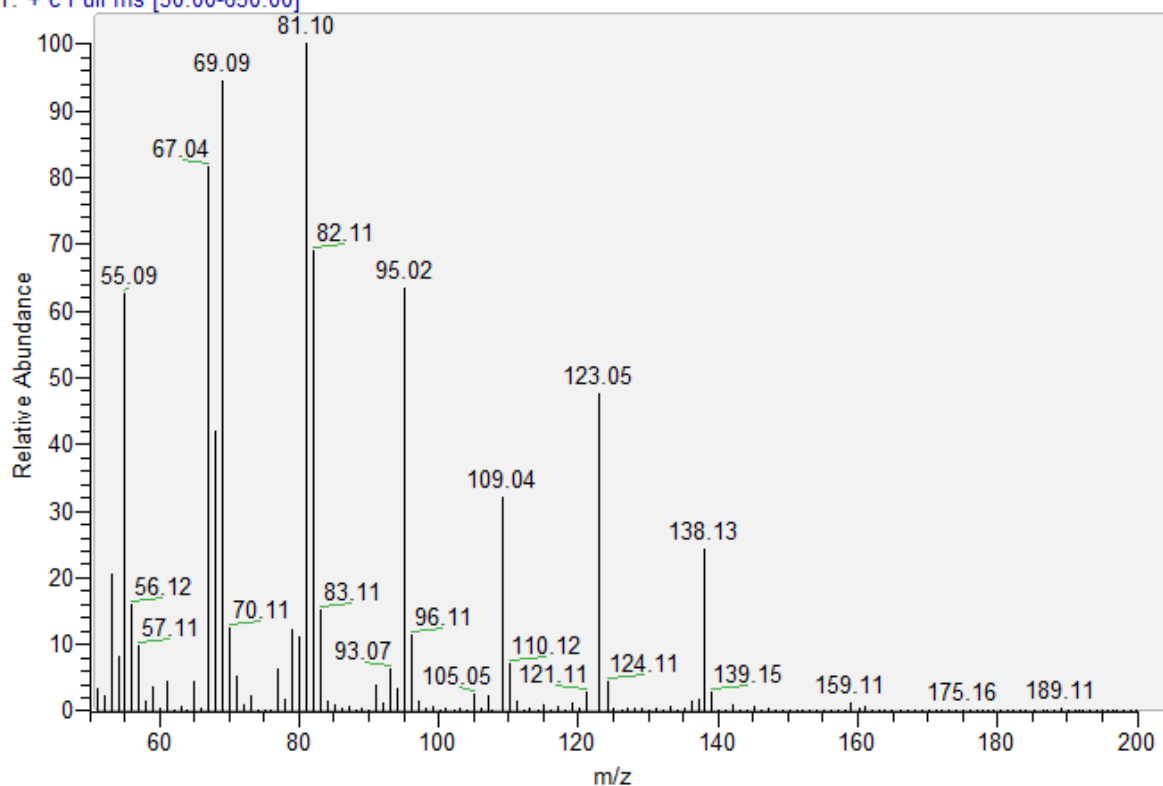


T: + c Full ms [50.00-650.00]

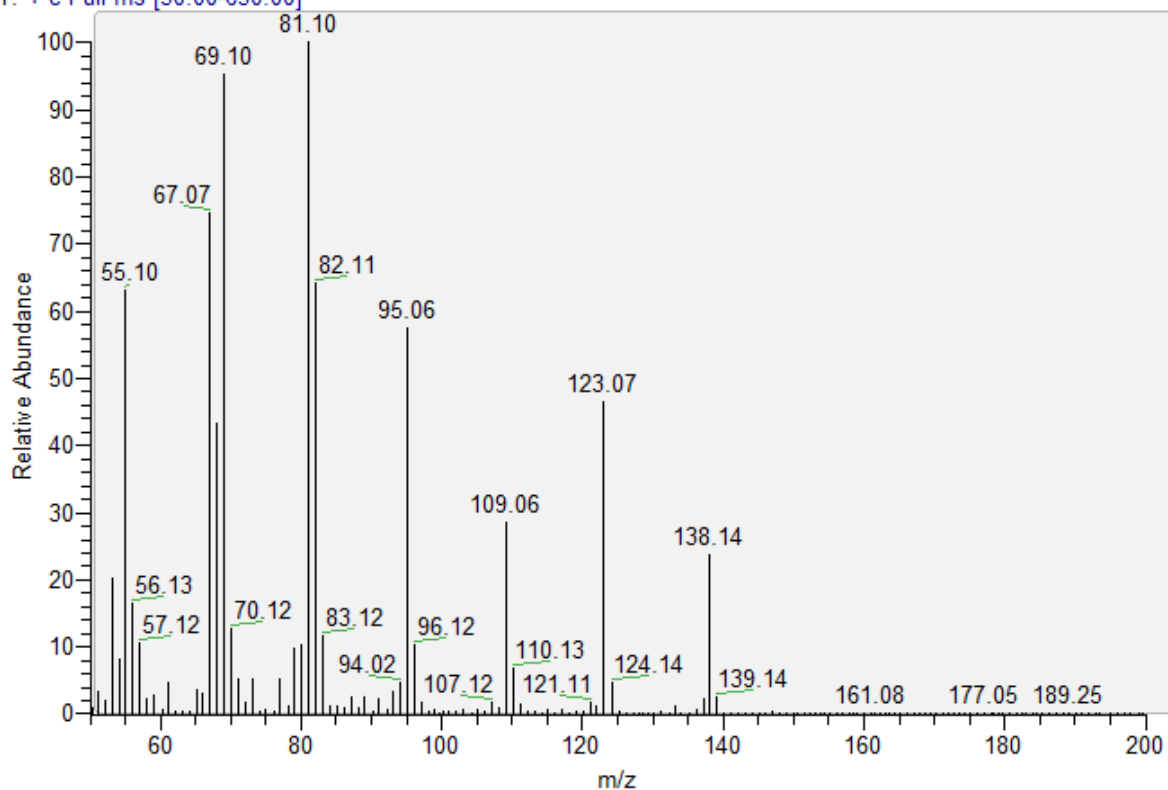




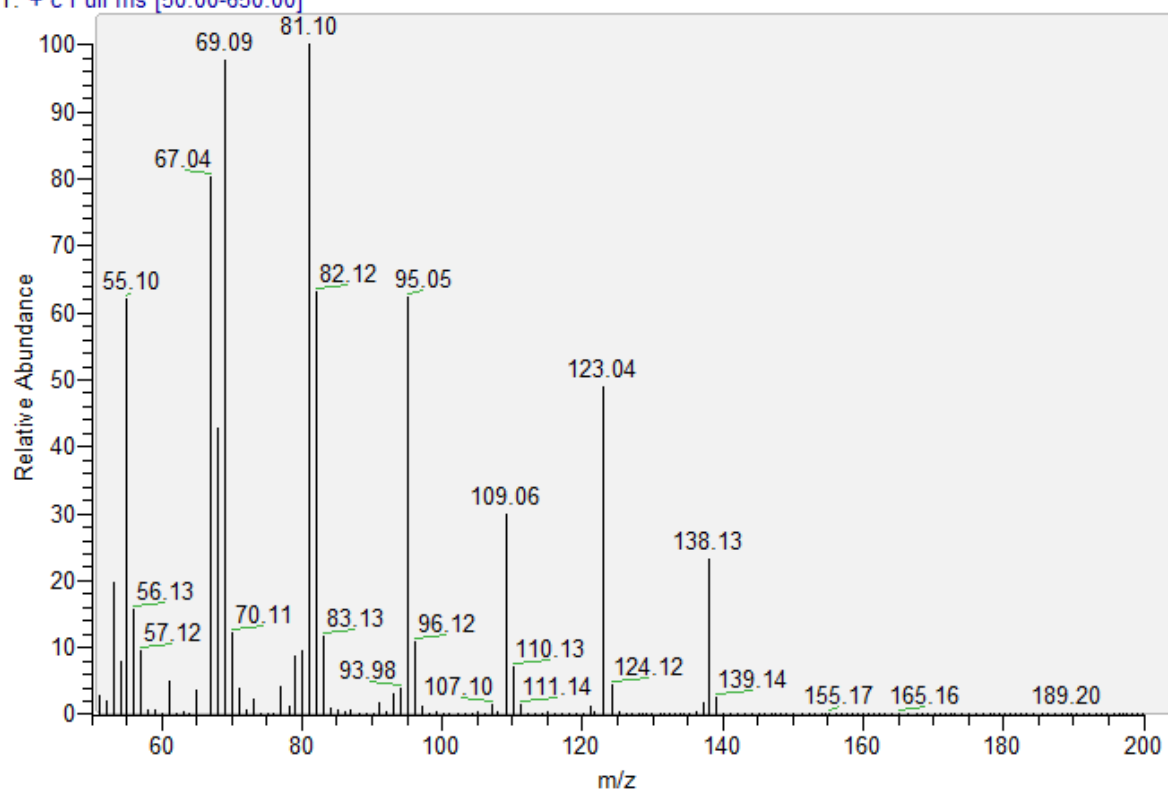
3058 #1209-1211 RT: 28.83-28.88 AV: 3 NL: 1.74E7  
T: + c Full ms [50.00-650.00]



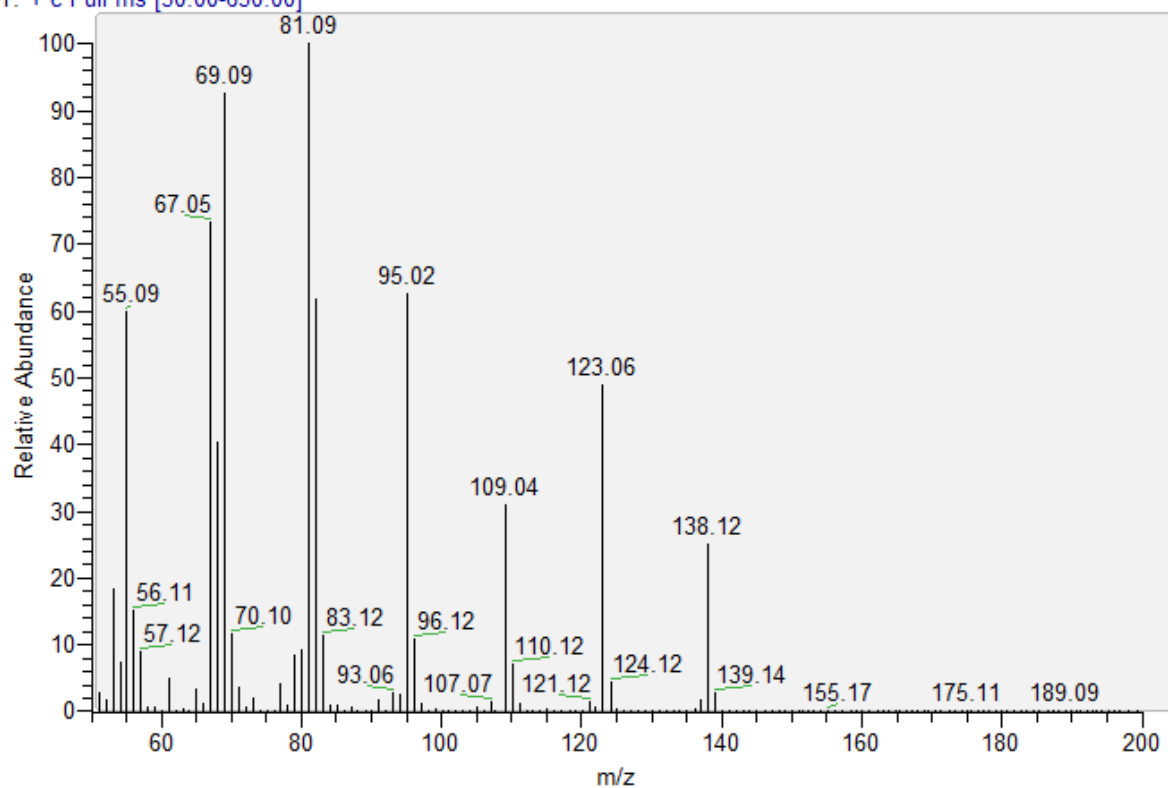
3053 #1210-1212 RT: 28.78-28.83 AV: 3 NL: 1.21E6  
T: + c Full ms [50.00-650.00]



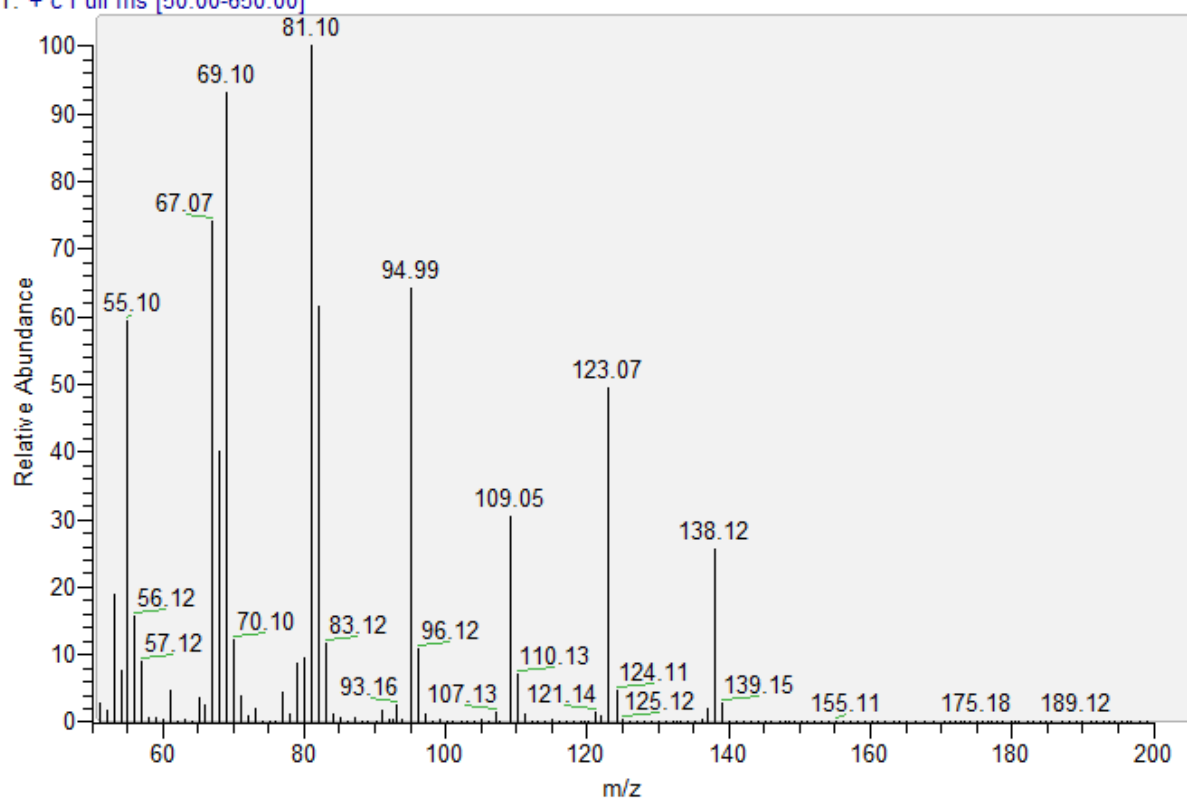
3018 #1216-1217 RT: 28.82-28.84 AV: 2 NL: 1.39E7  
T: + c Full ms [50.00-650.00]



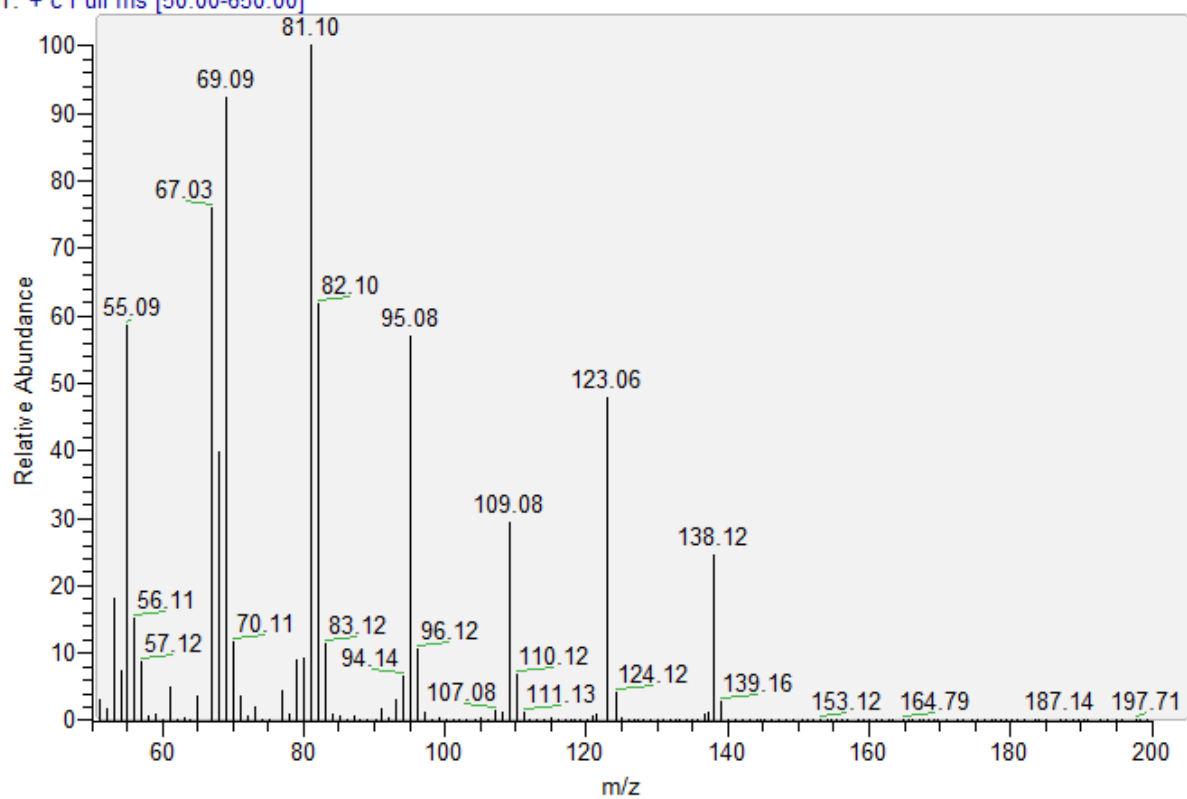
3021 #1212-1213 RT: 28.82-28.84 AV: 2 NL: 2.71E7  
T: + c Full ms [50.00-650.00]



3075 #1210-1211 RT: 28.80-28.83 AV: 2 NL: 1.76E7  
T: + c Full ms [50.00-650.00]

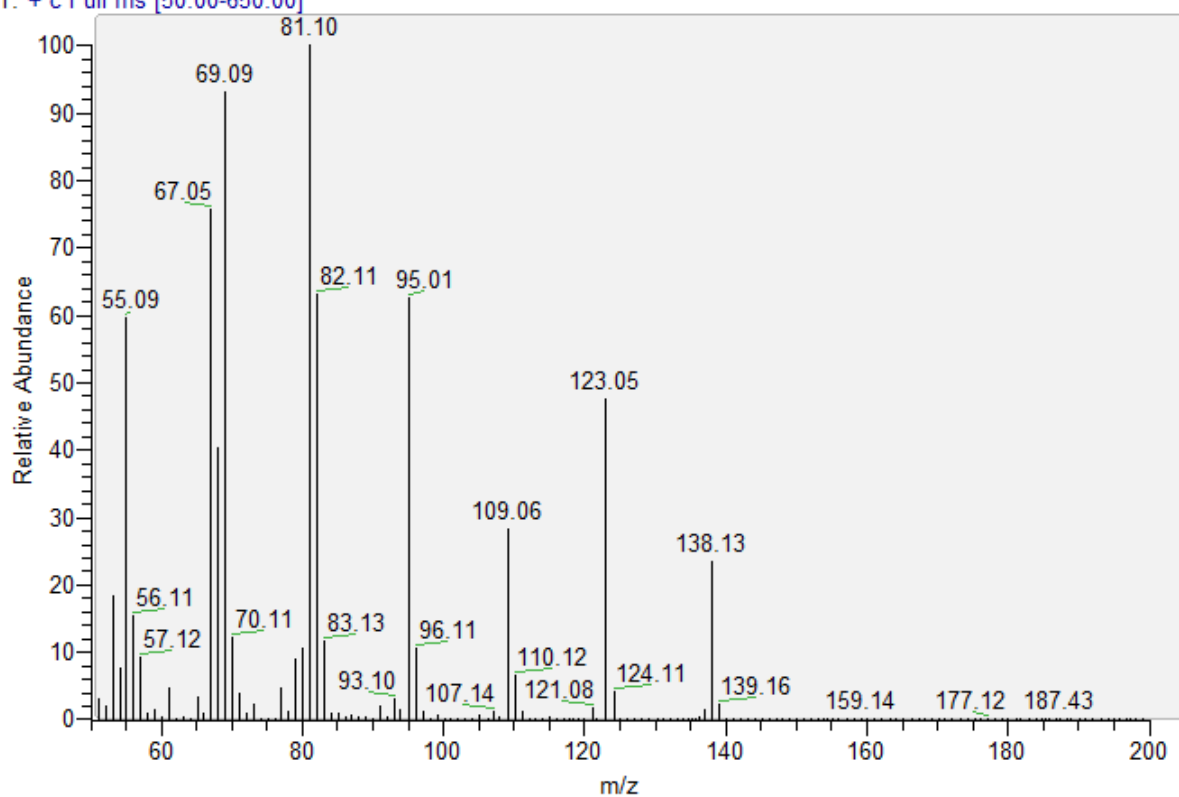


3074 #1213 RT: 28.83 AV: 1 NL: 2.32E7  
T: + c Full ms [50.00-650.00]

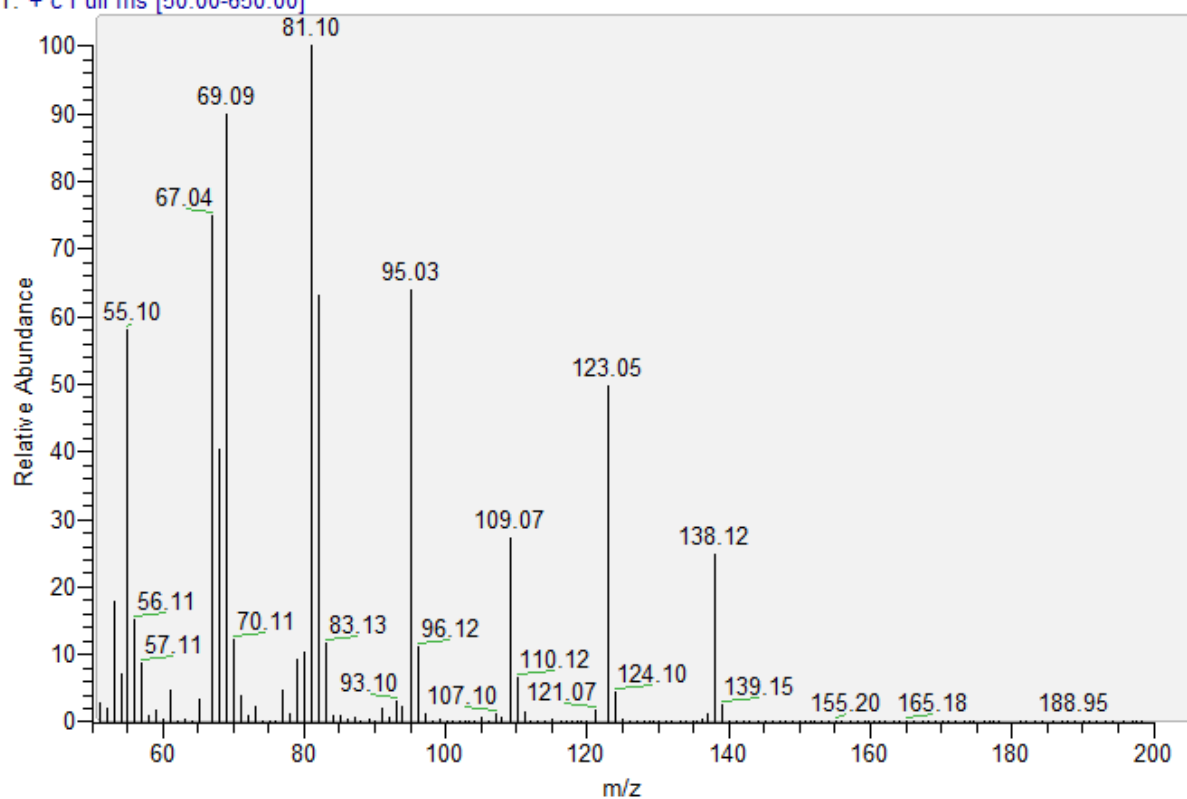


3073 #1211-1212 RT: 28.81-28.84 AV: 2 NL: 7.97E6

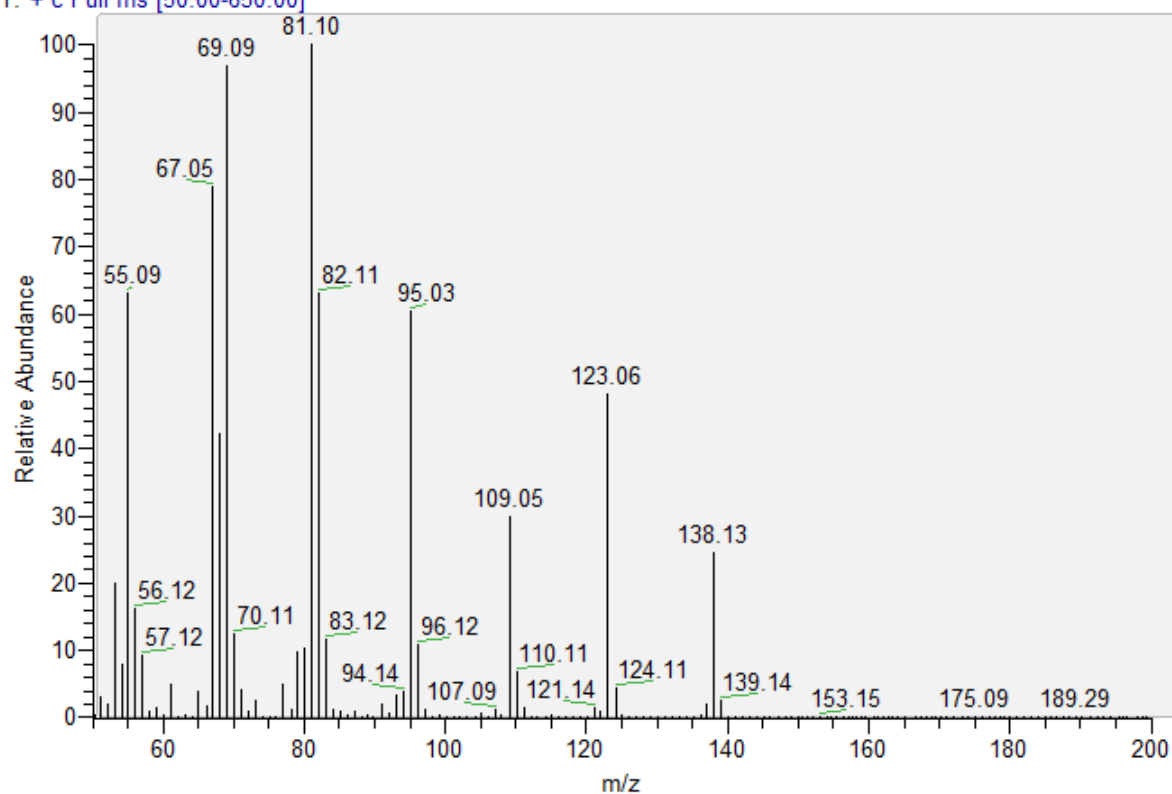
T: + c Full ms [50.00-650.00]



3073 #1211 RT: 28.81 AV: 1 NL: 9.51E6  
T: + c Full ms [50.00-650.00]

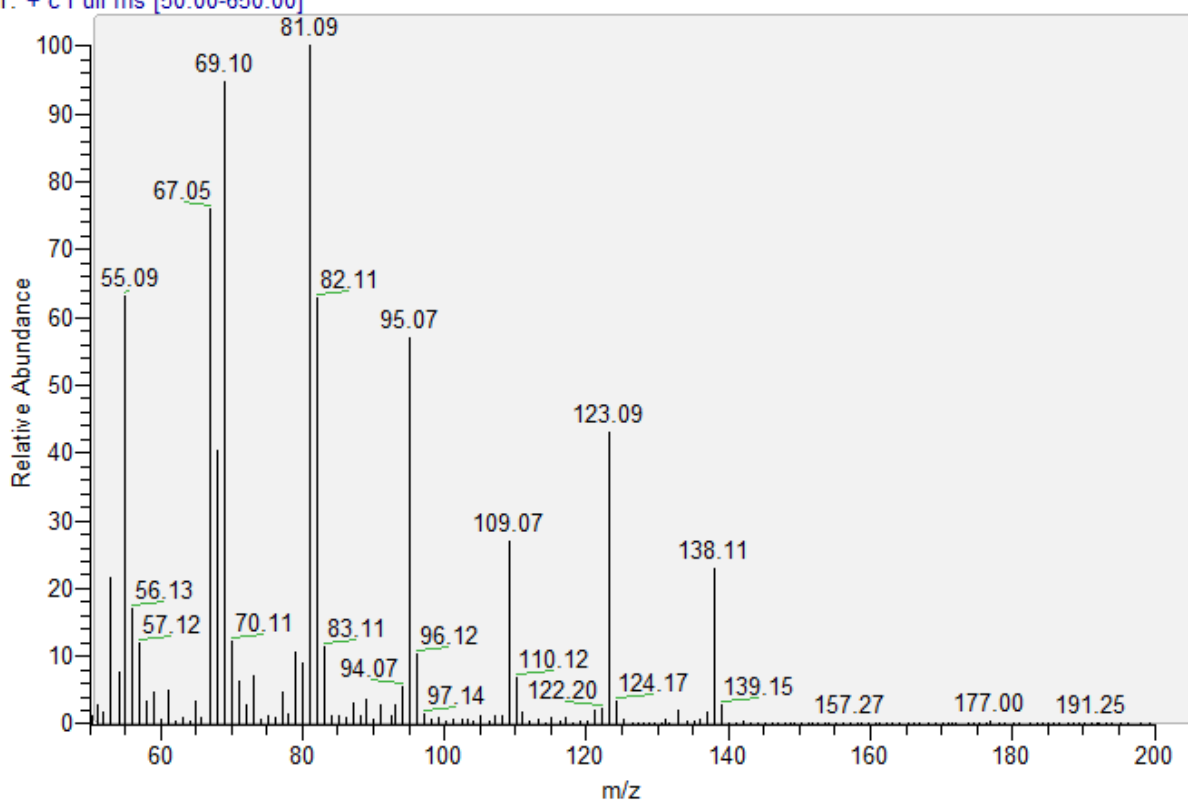


3072 #1210-1211 RT: 28.81-28.84 AV: 2 NL: 8.58E6  
T: + c Full ms [50.00-650.00]





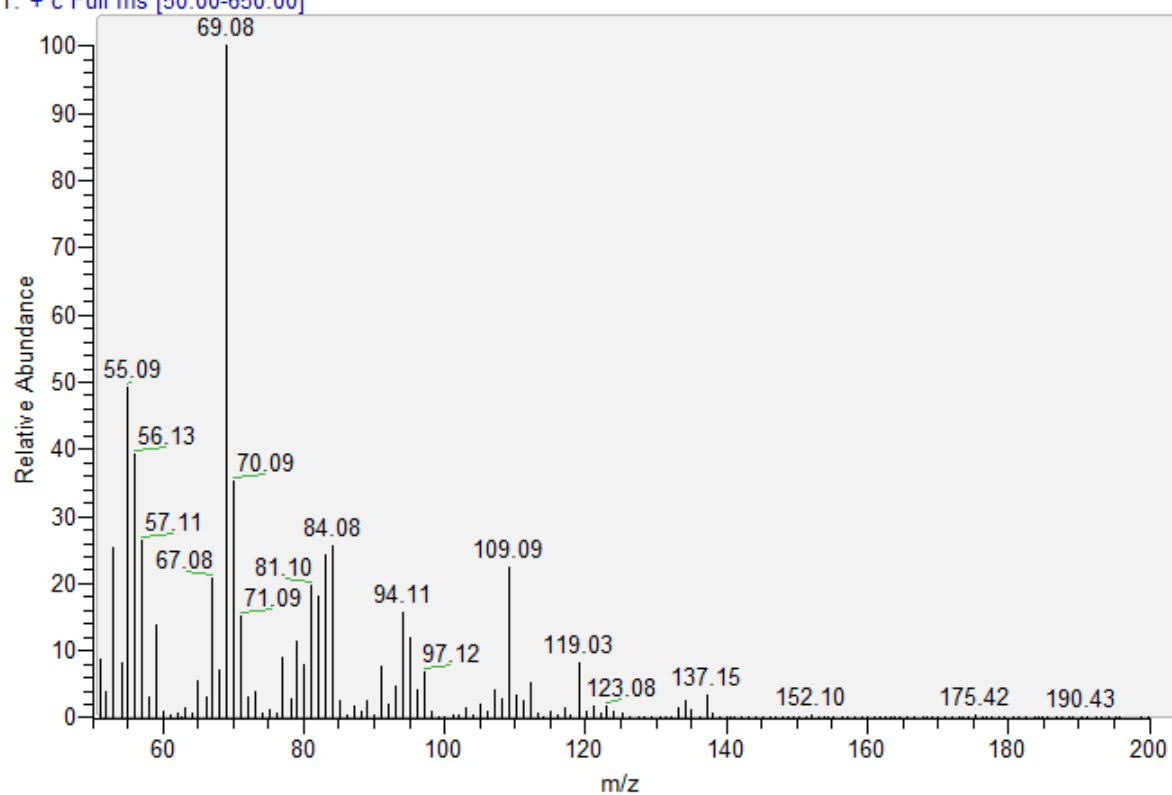
3070 #1212-1213 RT: 28.79-28.82 AV: 2 NL: 8.26E5  
T: + c Full ms [50.00-650.00]



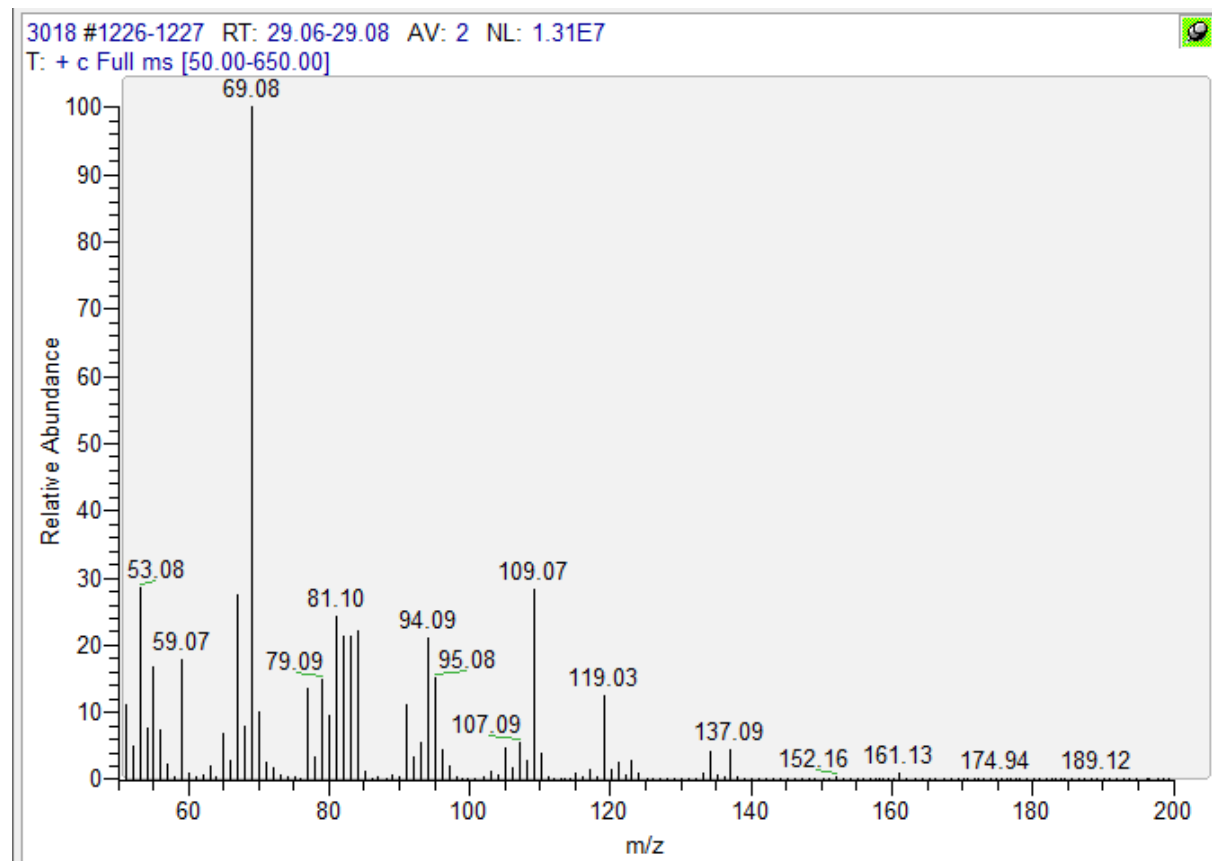
Citral

Reference

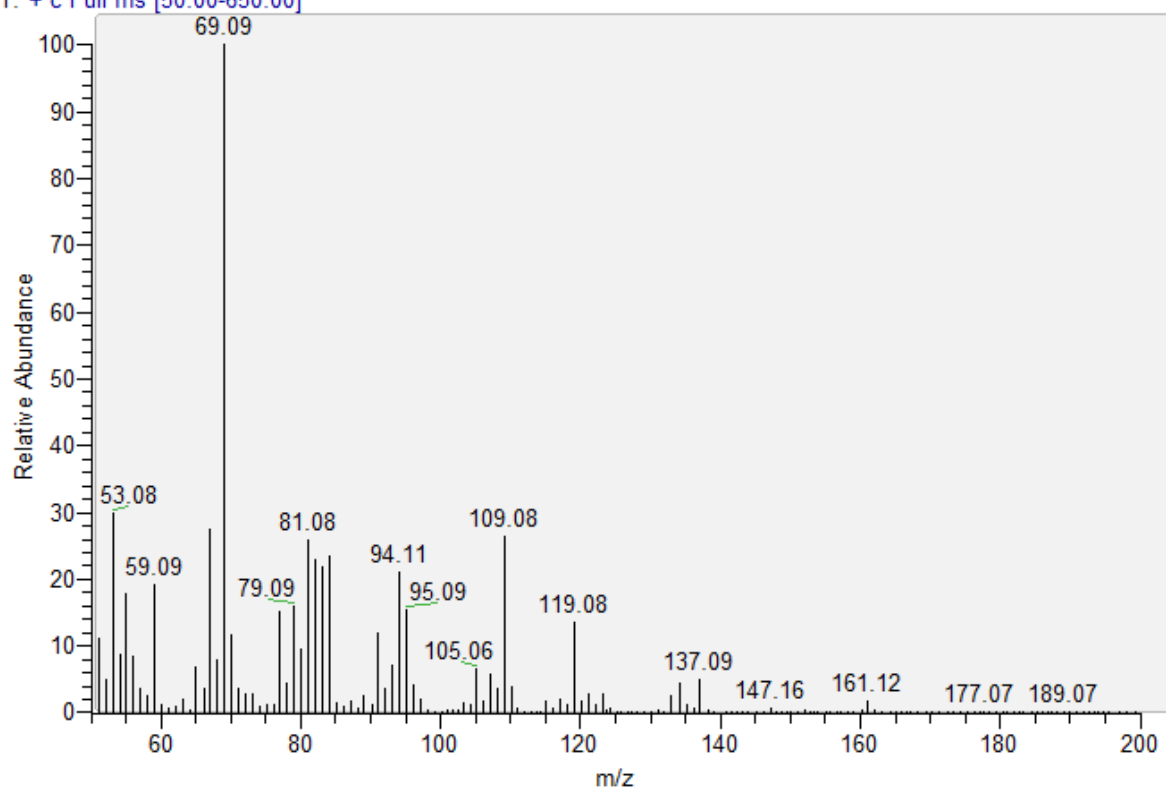
1\_20 #1227 RT: 29.04 AV: 1 NL: 1.23E6  
T: + c Full ms [50.00-650.00]



## Samples



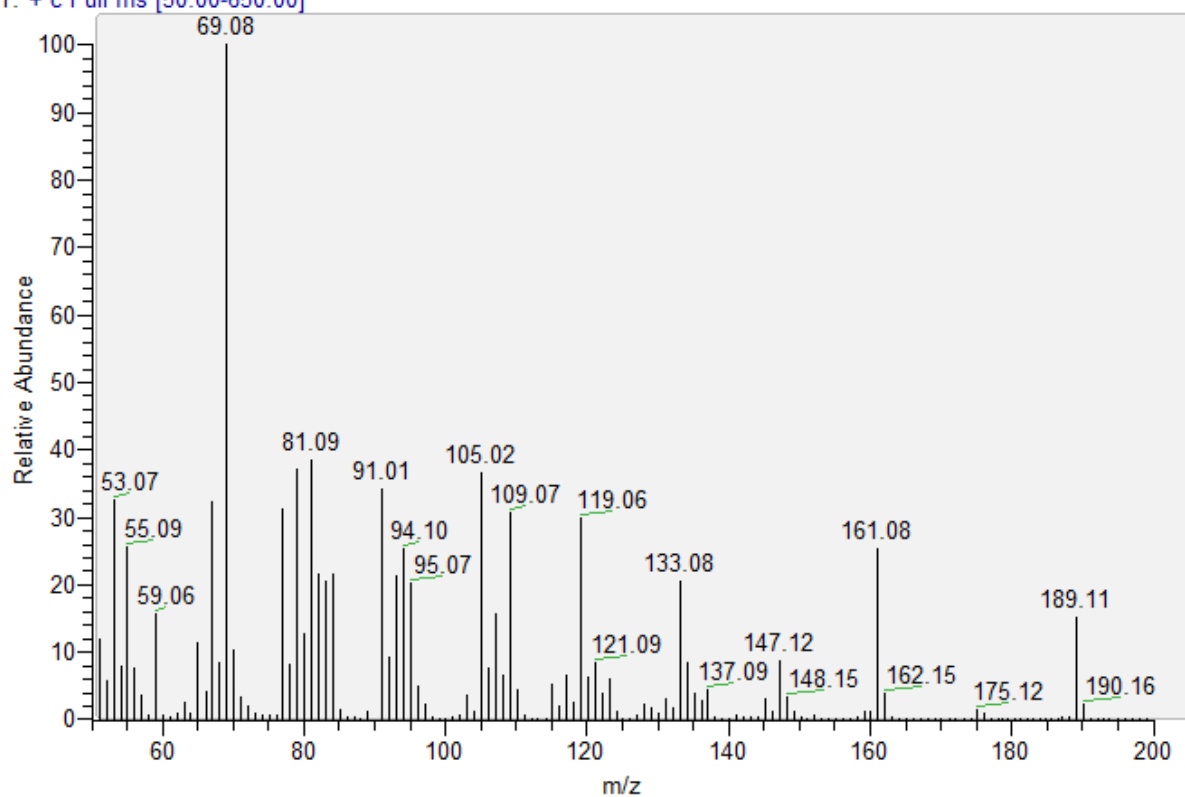
3053 #1221-1222 RT: 29.04-29.06 AV: 2 NL: 1.33E6  
T: + c Full ms [50.00-650.00]



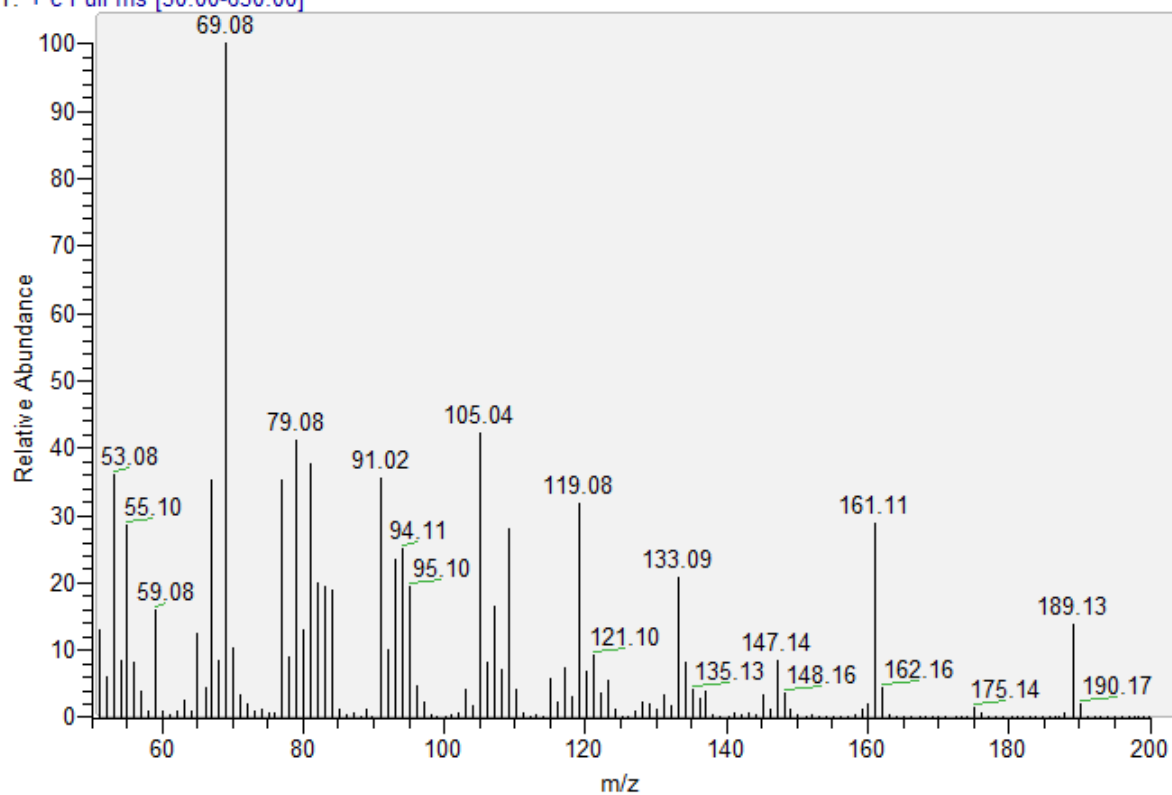
3058 #1220-1222 RT: 29.09-29.14 AV: 3 NL: 1.95E7



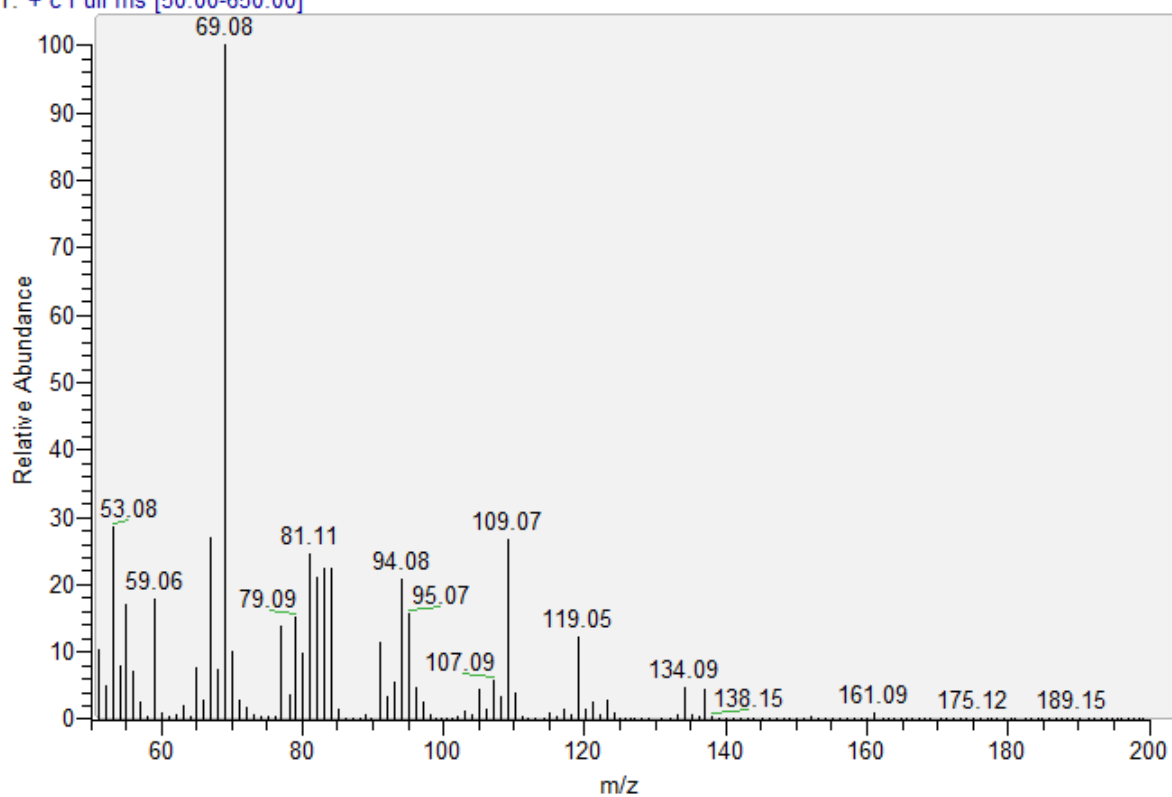
T: + c Full ms [50.00-650.00]



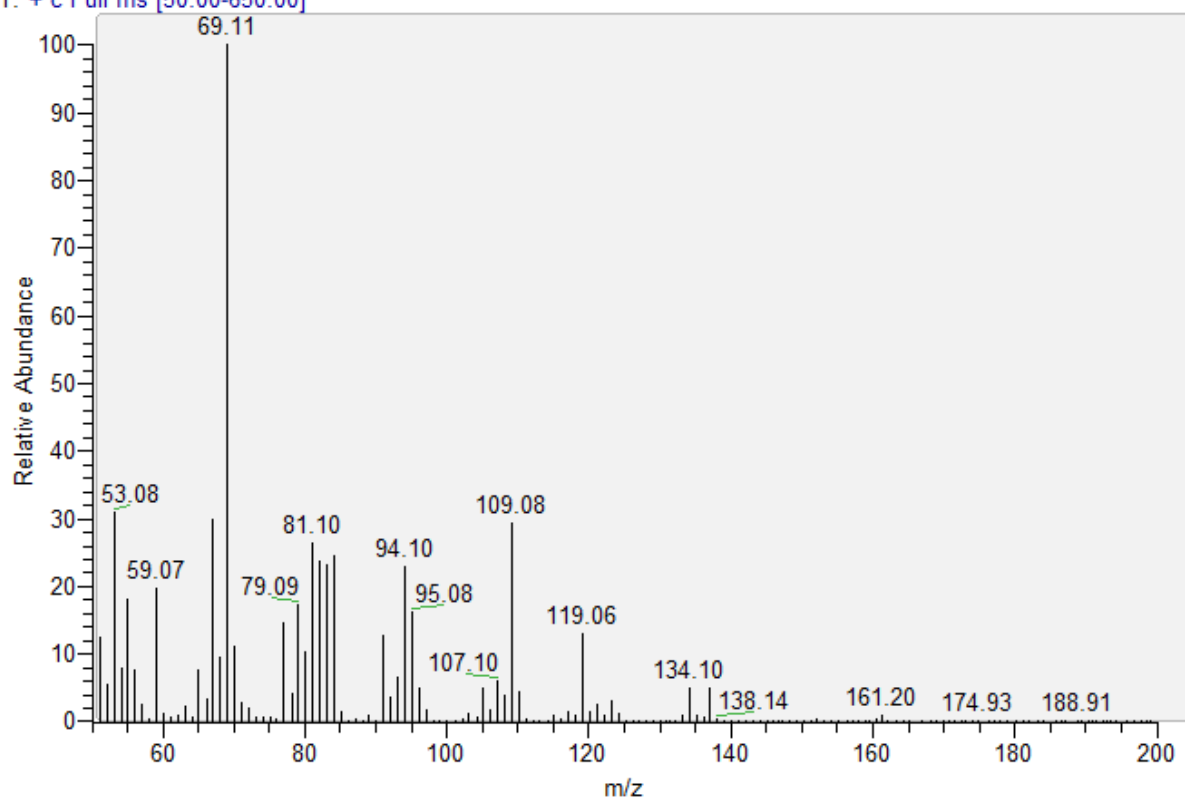
3057 #1226-1228 RT: 29.05-29.10 AV: 3 NL: 1.06E7  
T: + c Full ms [50.00-650.00]



3021 #1222-1223 RT: 29.06-29.08 AV: 2 NL: 1.16E7  
T: + c Full ms [50.00-650.00]

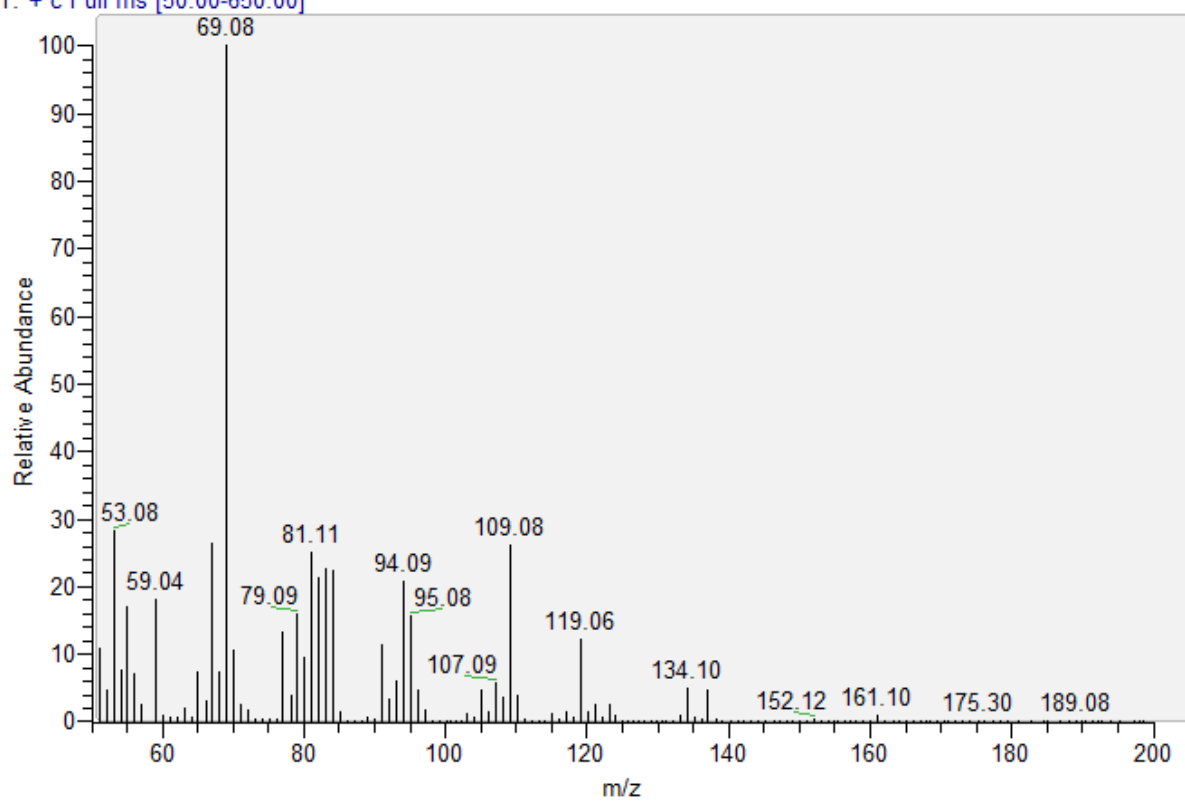


3075 #1221 RT: 29.07 AV: 1 NL: 1.11E7  
T: + c Full ms [50.00-650.00]

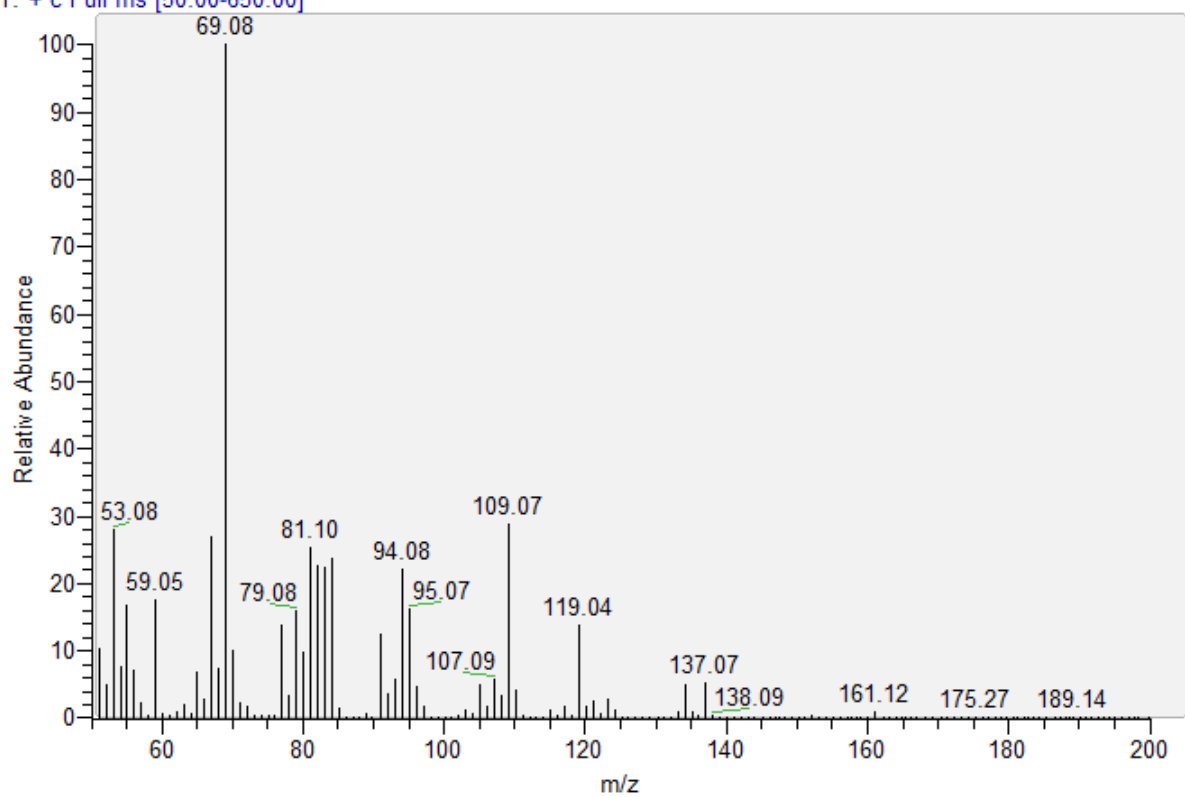




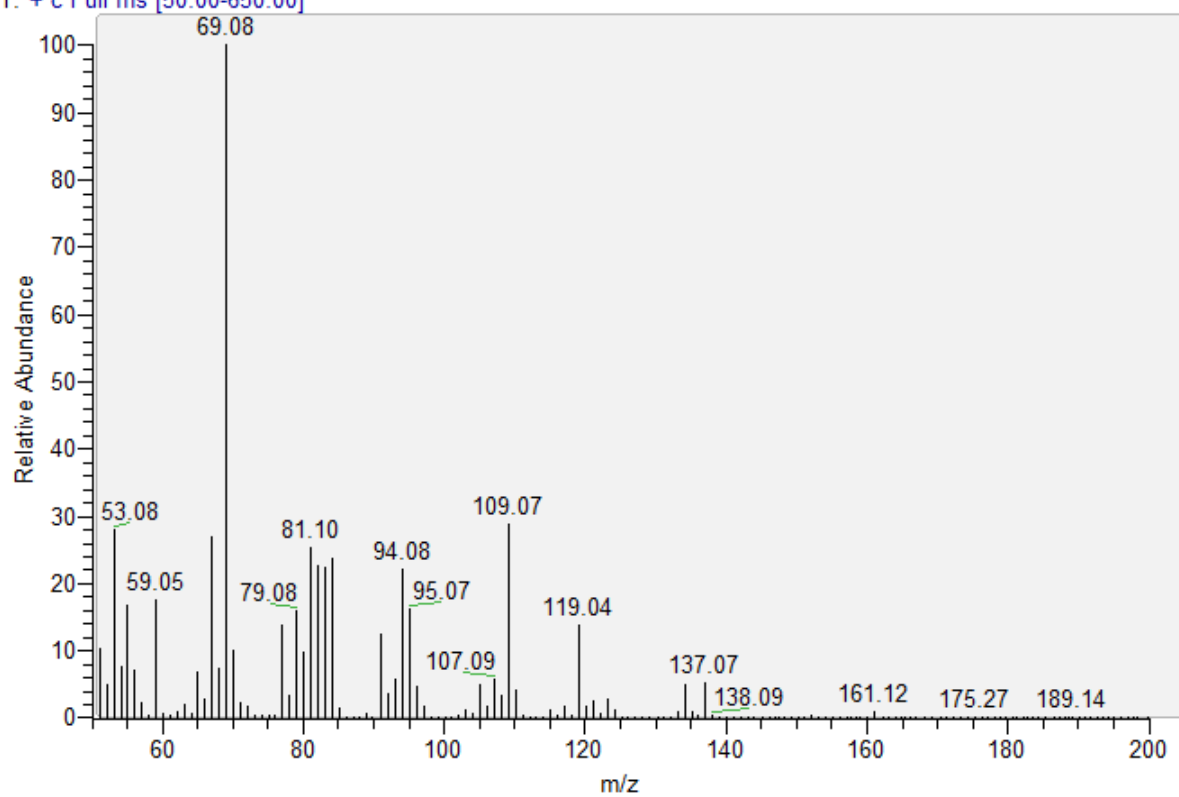
3074 #1223 RT: 29.07 AV: 1 NL: 1.28E7  
T: + c Full ms [50.00-650.00]



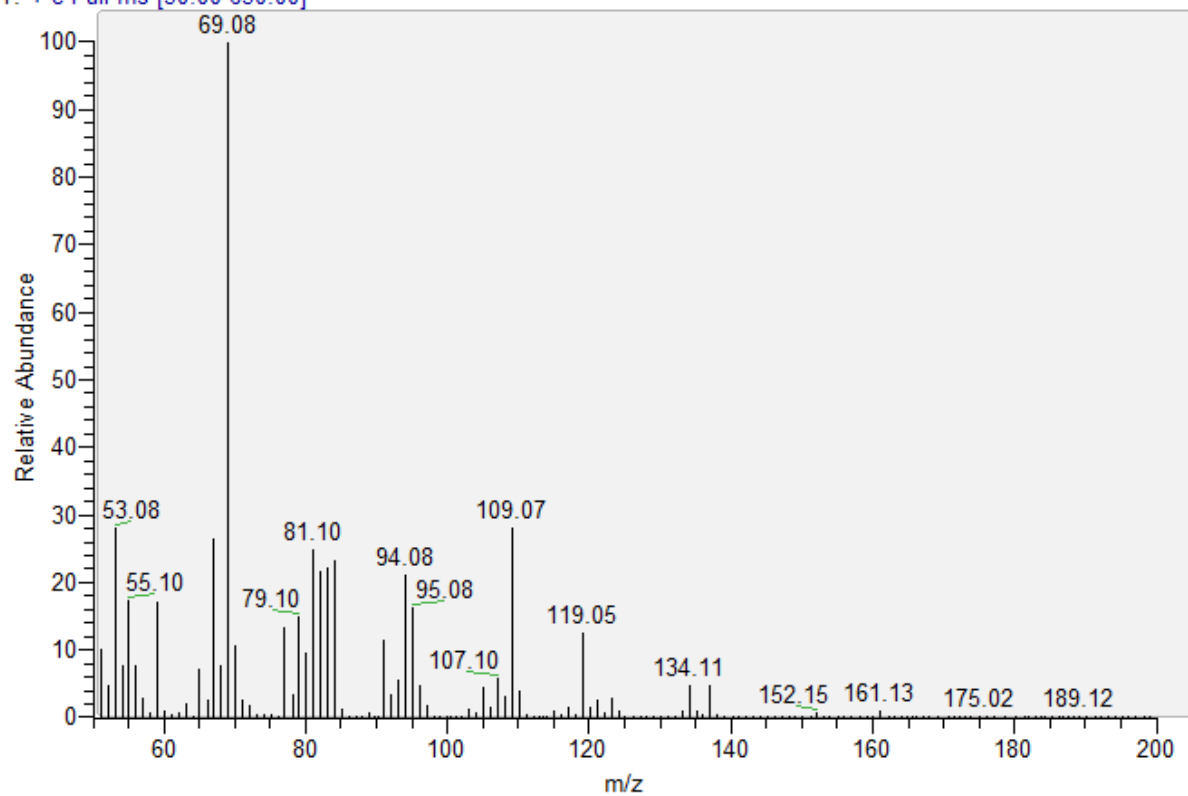
3073 #1221-1222 RT: 29.05-29.07 AV: 2 NL: 1.59E7  
T: + c Full ms [50.00-650.00]



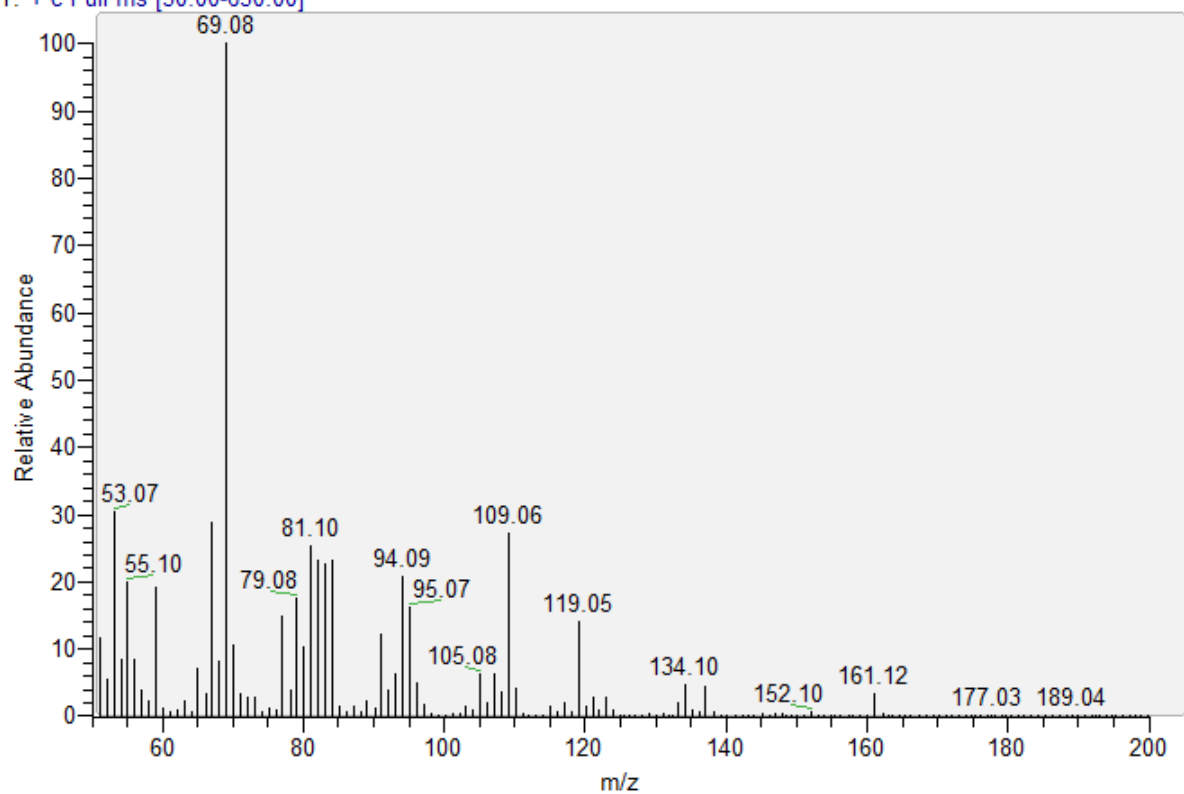
3073 #1221-1222 RT: 29.05-29.07 AV: 2 NL: 1.59E7  
T: + c Full ms [50.00-650.00]



3072 #1220-1221 RT: 29.05-29.08 AV: 2 NL: 2.06E7  
T: + c Full ms [50.00-650.00]



3070 #1222-1224 RT: 29.03-29.08 AV: 3 NL: 1.60E6  
T: + c Full ms [50.00-650.00]

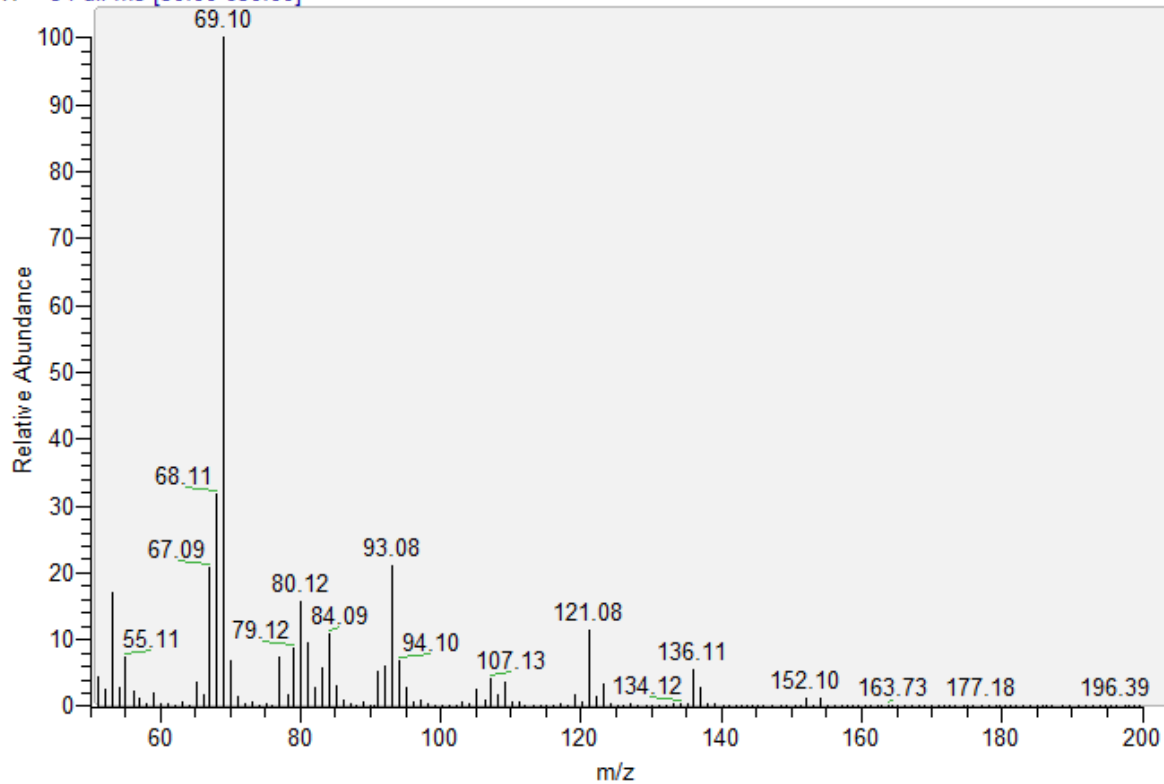


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Reference

1\_20 #1280-1281 RT: 30.31-30.33 AV: 2 NL: 5.02E6

T: + c Full ms [50.00-650.00]

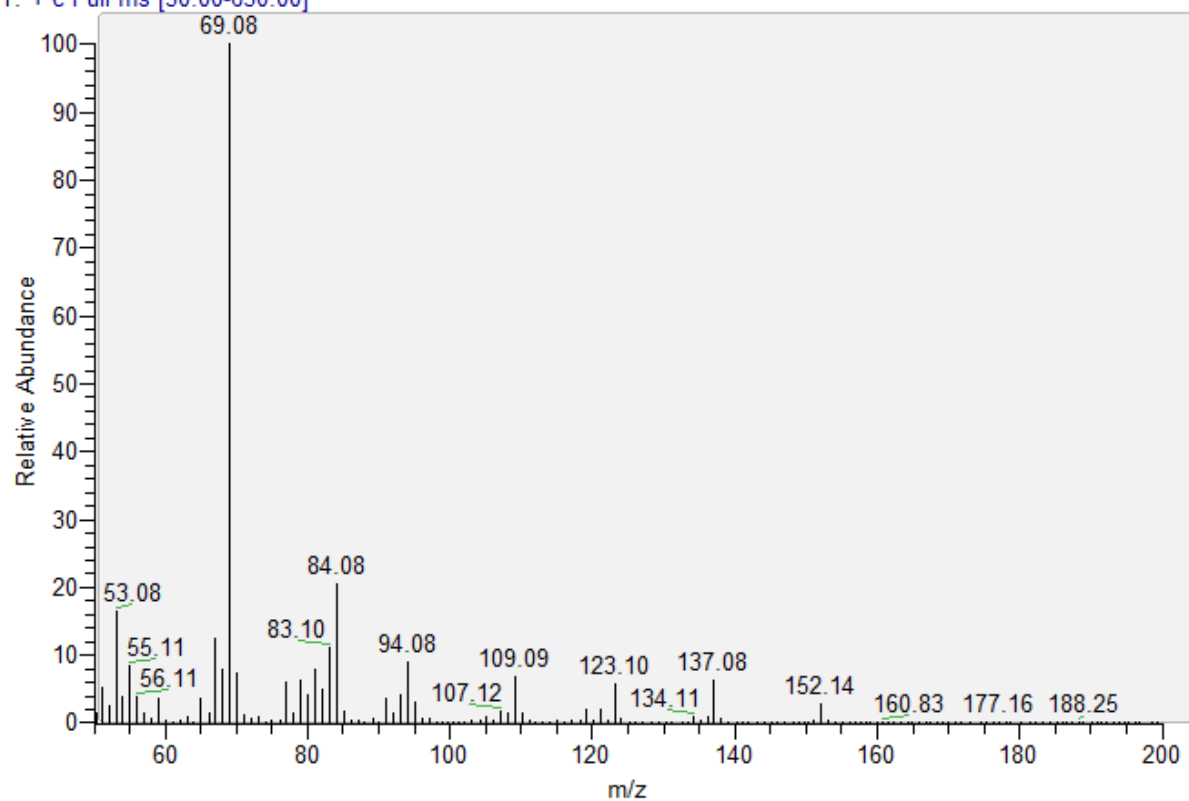


Samples

3053 #1274-1275 RT: 30.30-30.33 AV: 2 NL: 4.59E6

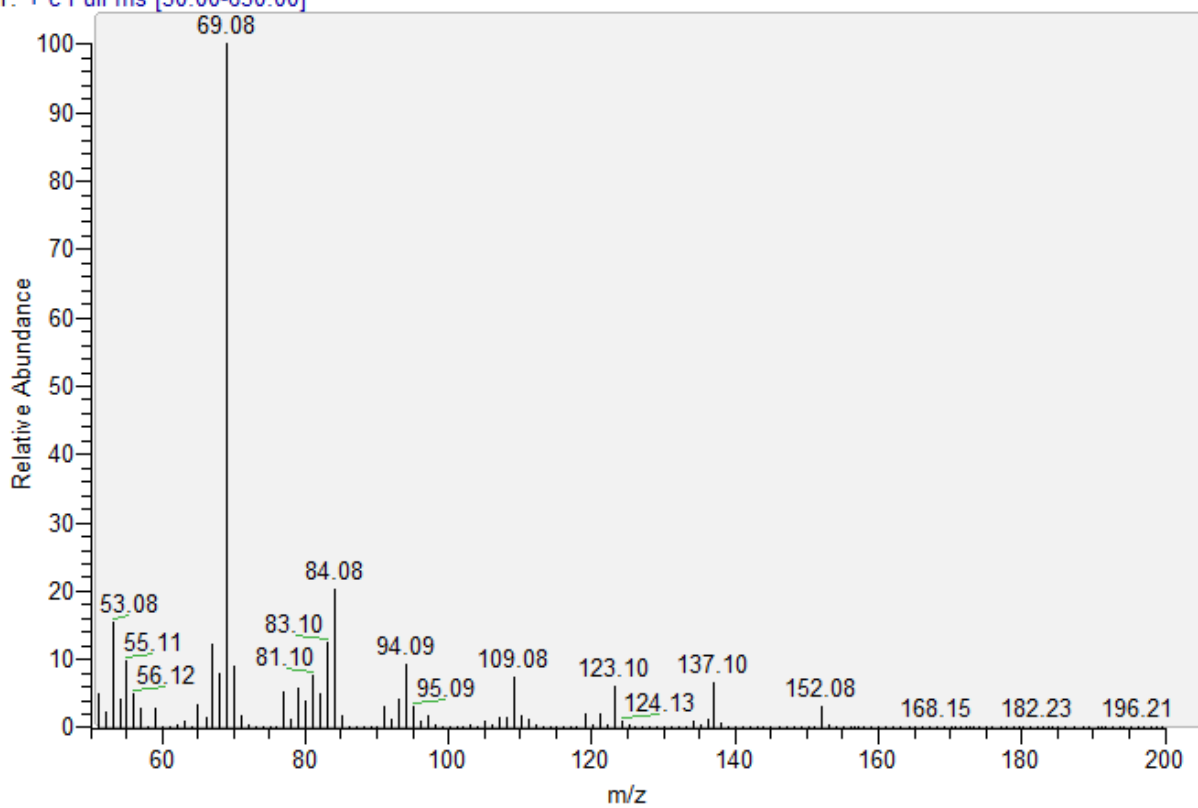


T: + c Full ms [50.00-650.00]

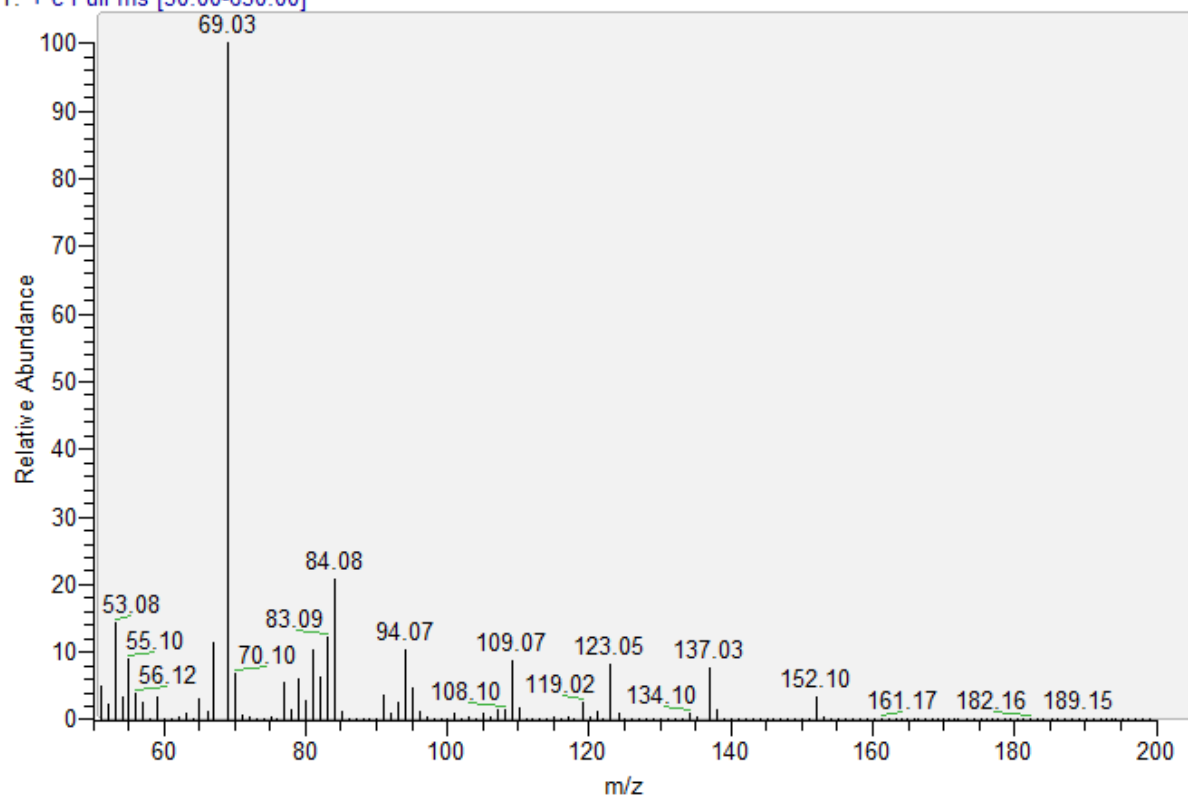




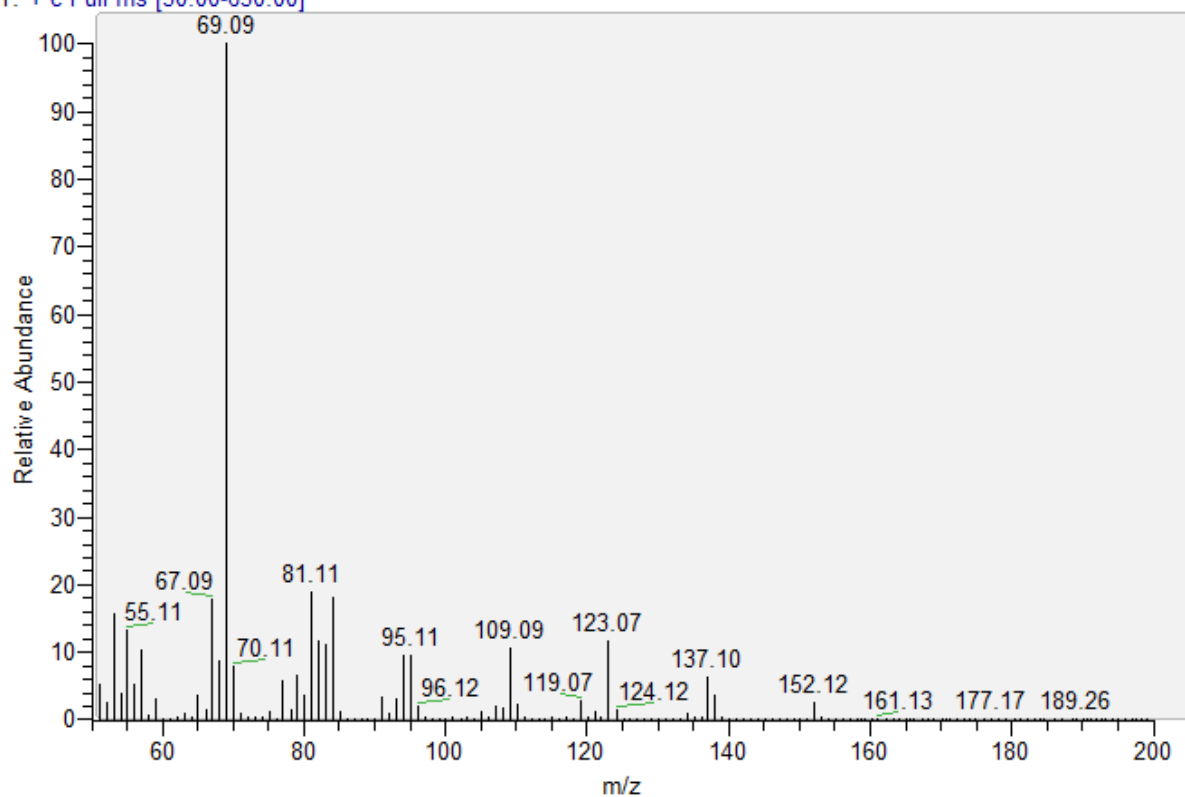
3018 #1279-1280 RT: 30.32-30.35 AV: 2 NL: 7.85E7  
T: + c Full ms [50.00-650.00]



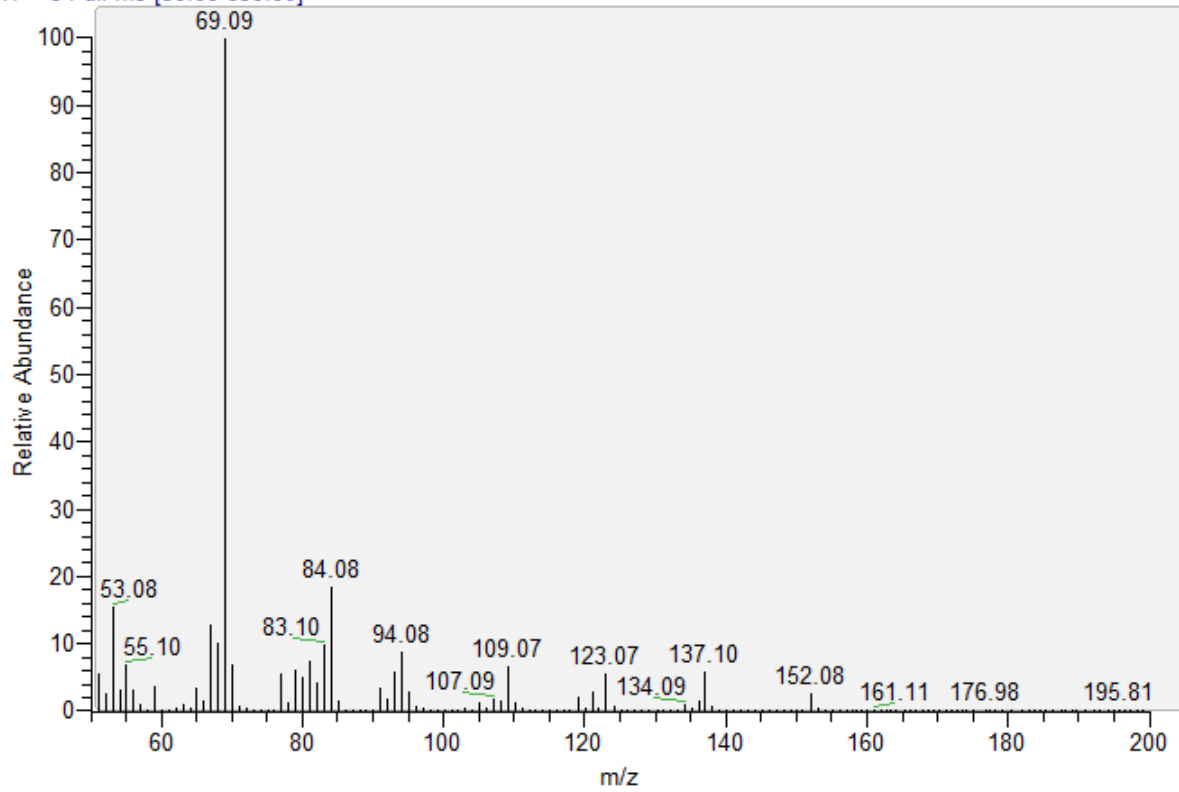
3058 #1273-1274 RT: 30.36-30.38 AV: 2 NL: 8.97E7  
T: + c Full ms [50.00-650.00]



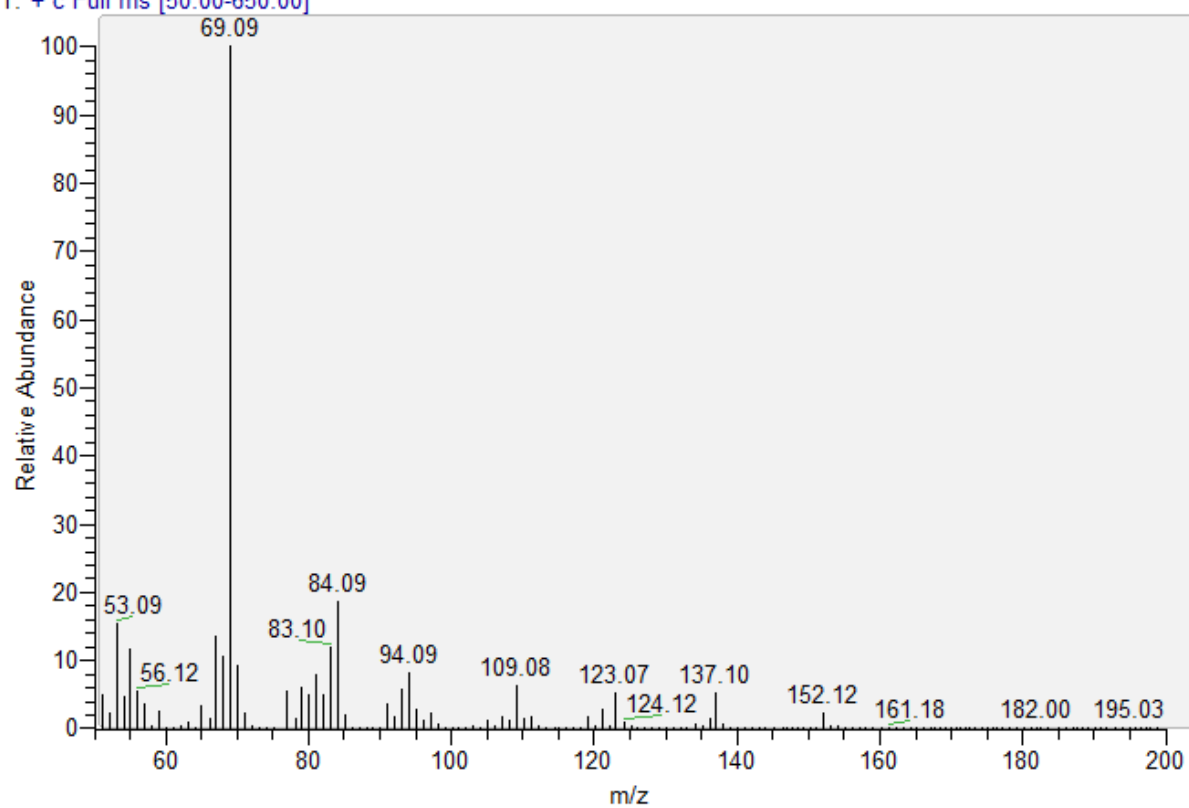
3057 #1279-1281 RT: 30.32-30.36 AV: 3 NL: 3.68E7  
T: + c Full ms [50.00-650.00]



3021 #1276-1277 RT: 30.34-30.37 AV: 2 NL: 6.39E7  
T: + c Full ms [50.00-650.00]



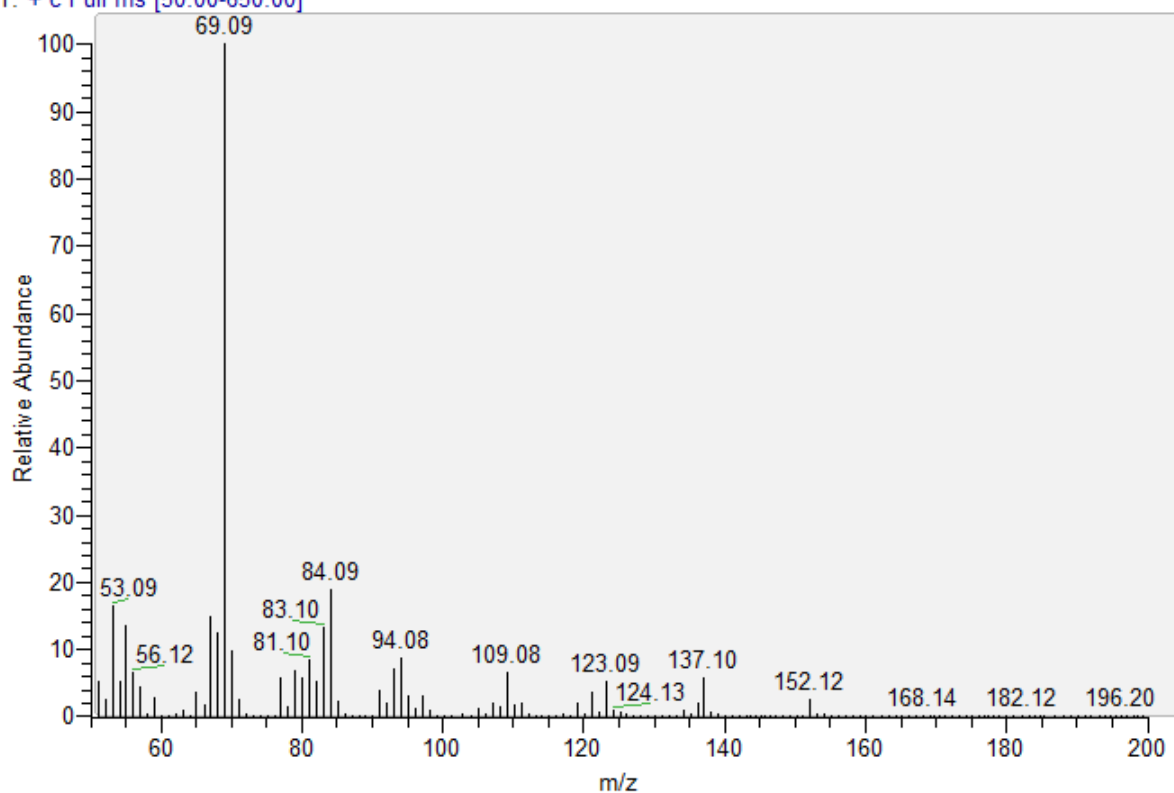
3075 #1274-1275 RT: 30.33-30.35 AV: 2 NL: 4.04E7  
T: + c Full ms [50.00-650.00]



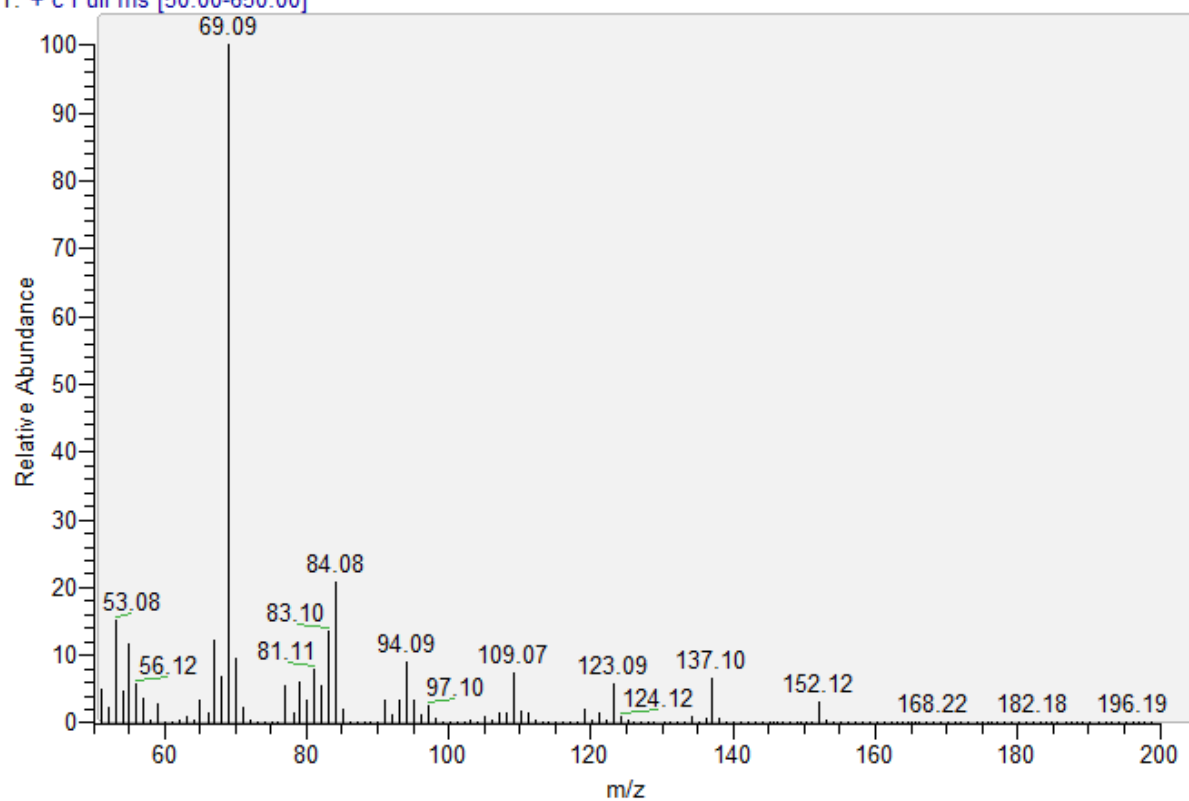
3074 #1276-1277 RT: 30.33-30.36 AV: 2 NL: 4.07E7



T: + c Full ms [50.00-650.00]



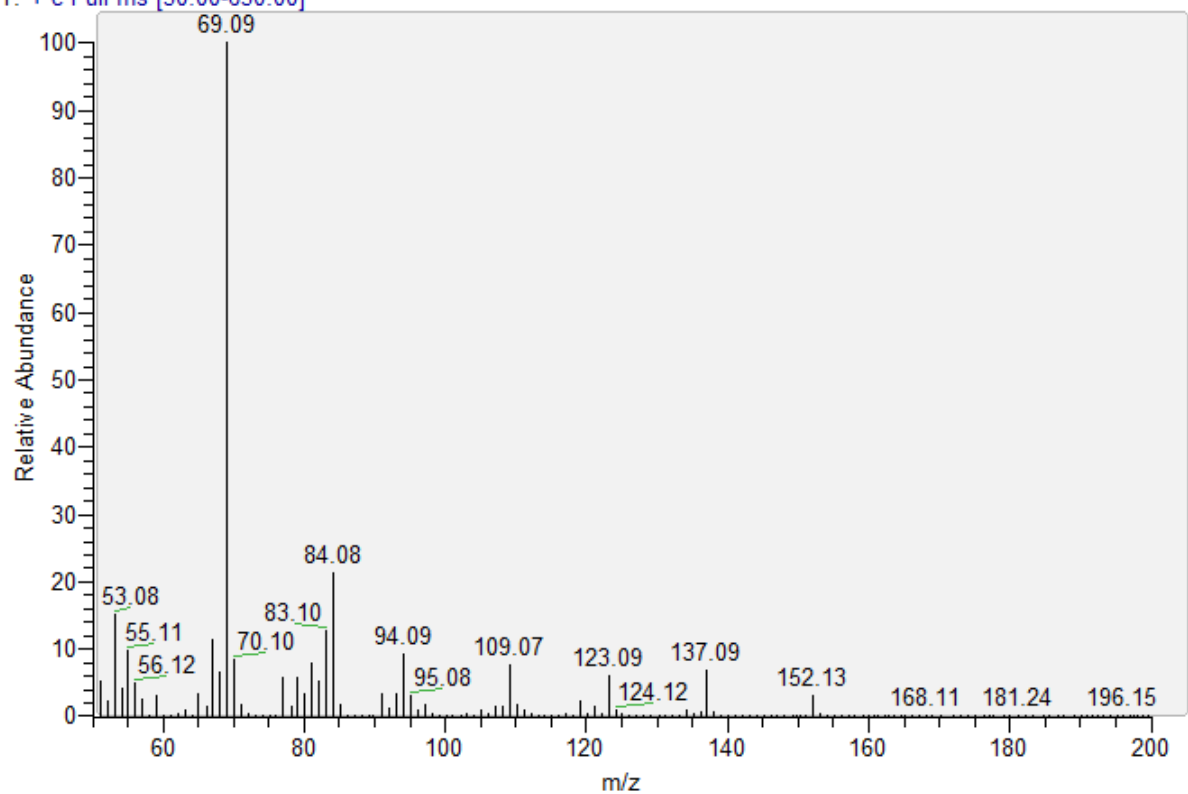
3073 #1274-1276 RT: 30.32-30.36 AV: 3 NL: 4.24E7  
T: + c Full ms [50.00-650.00]



3073 #1275 RT: 30.34 AV: 1 NL: 6.60E7

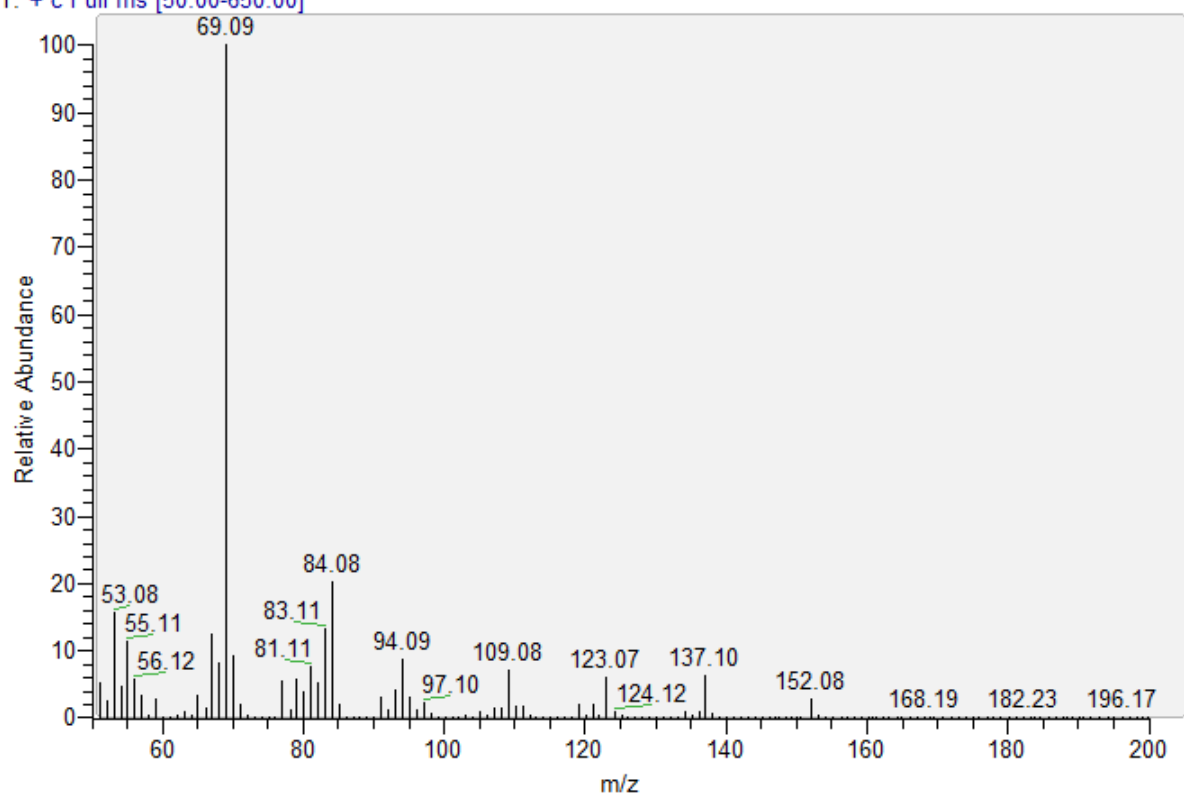


T: + c Full ms [50.00-650.00]

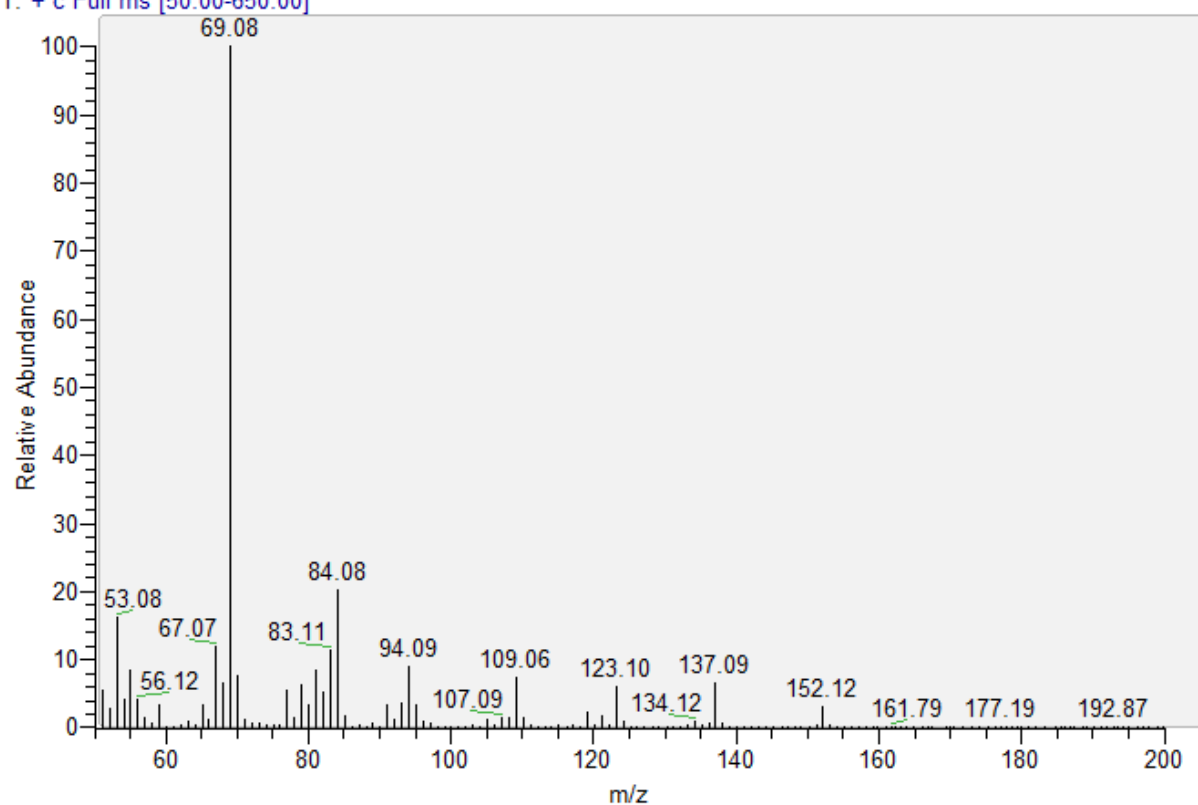




3072 #1273-1275 RT: 30.32-30.36 AV: 3 NL: 5.52E7  
T: + c Full ms [50.00-650.00]

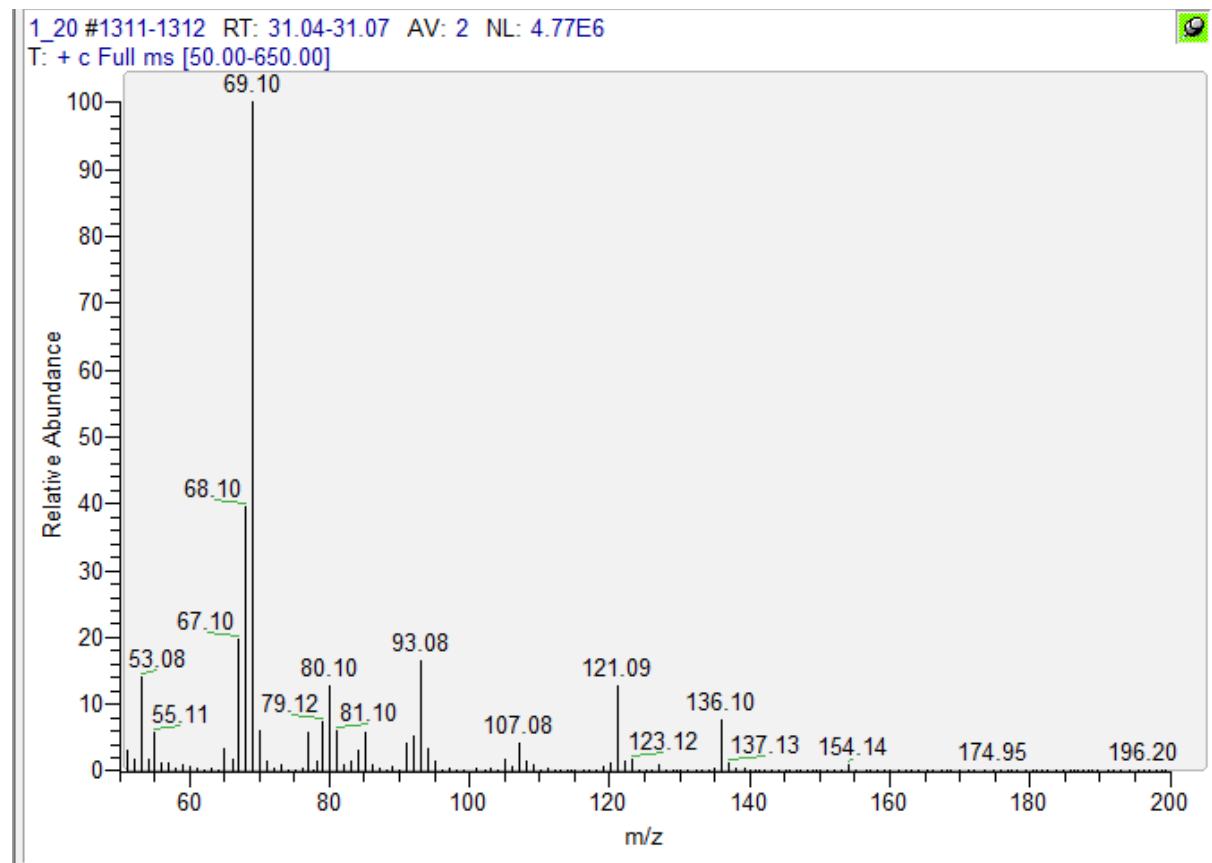


3070 #1275-1276 RT: 30.30-30.32 AV: 2 NL: 5.80E6  
T: + c Full ms [50.00-650.00]



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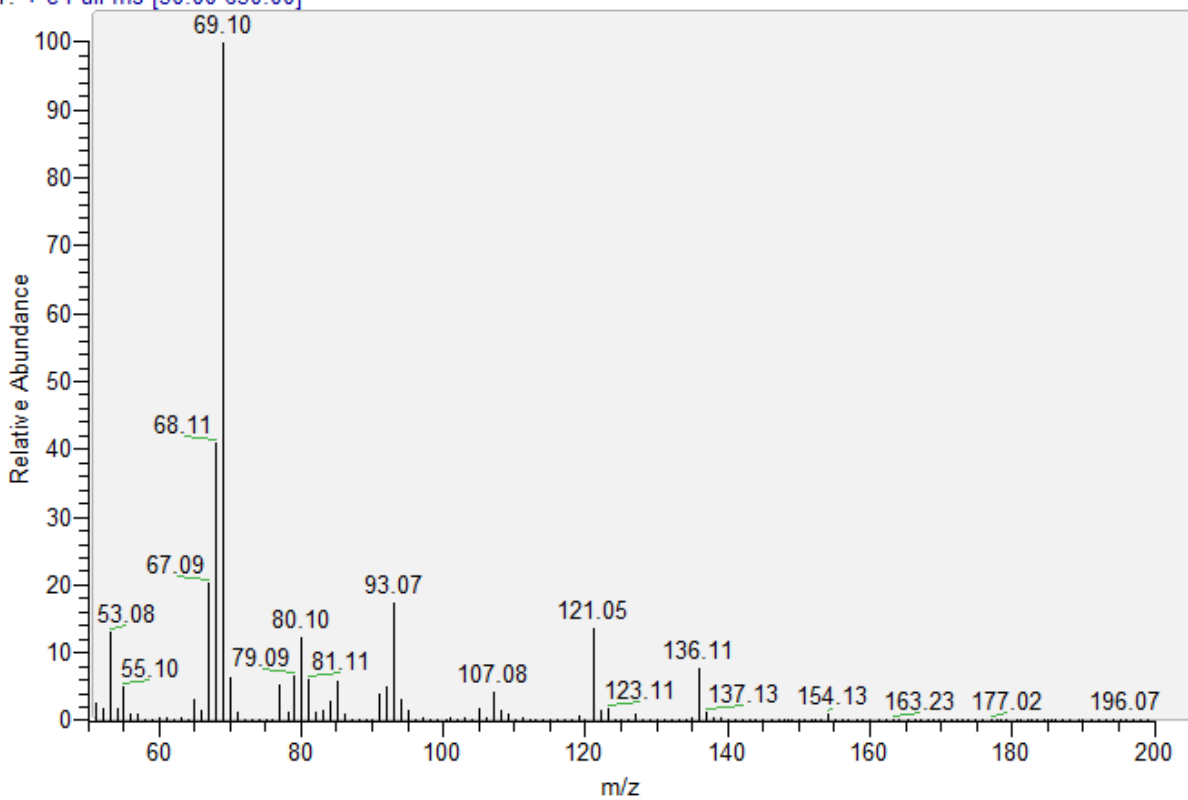


Samples:

3018 #1311-1312 RT: 31.09-31.11 AV: 2 NL: 9.01E7



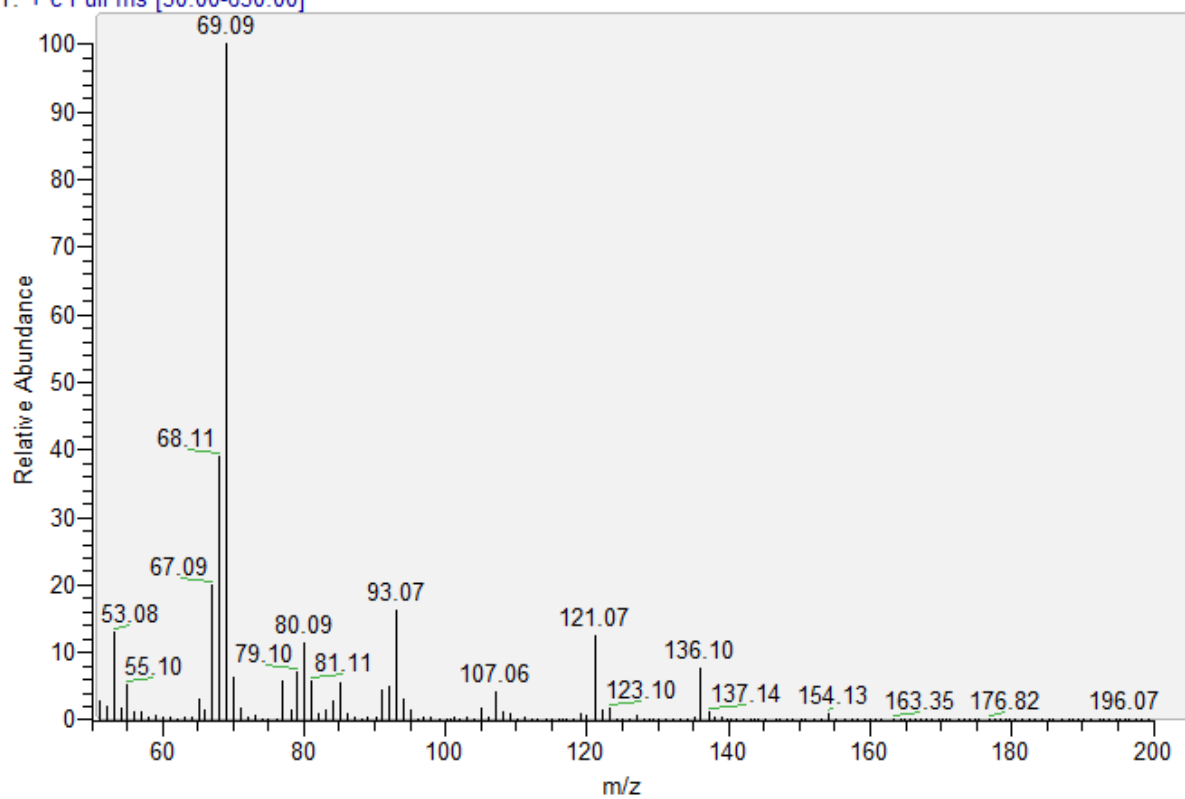
T: + c Full ms [50.00-650.00]



3053 #1305-1306 RT: 31.04-31.07 AV: 2 NL: 7.75E6



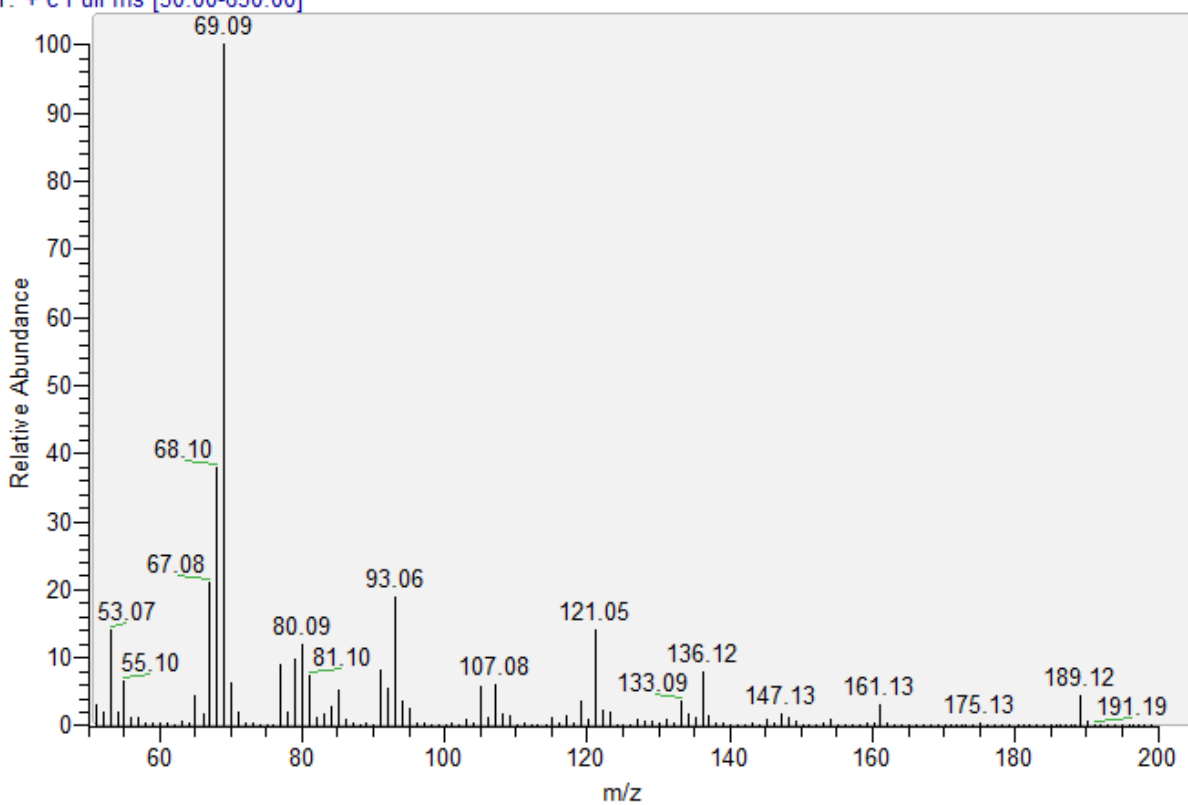
T: + c Full ms [50.00-650.00]



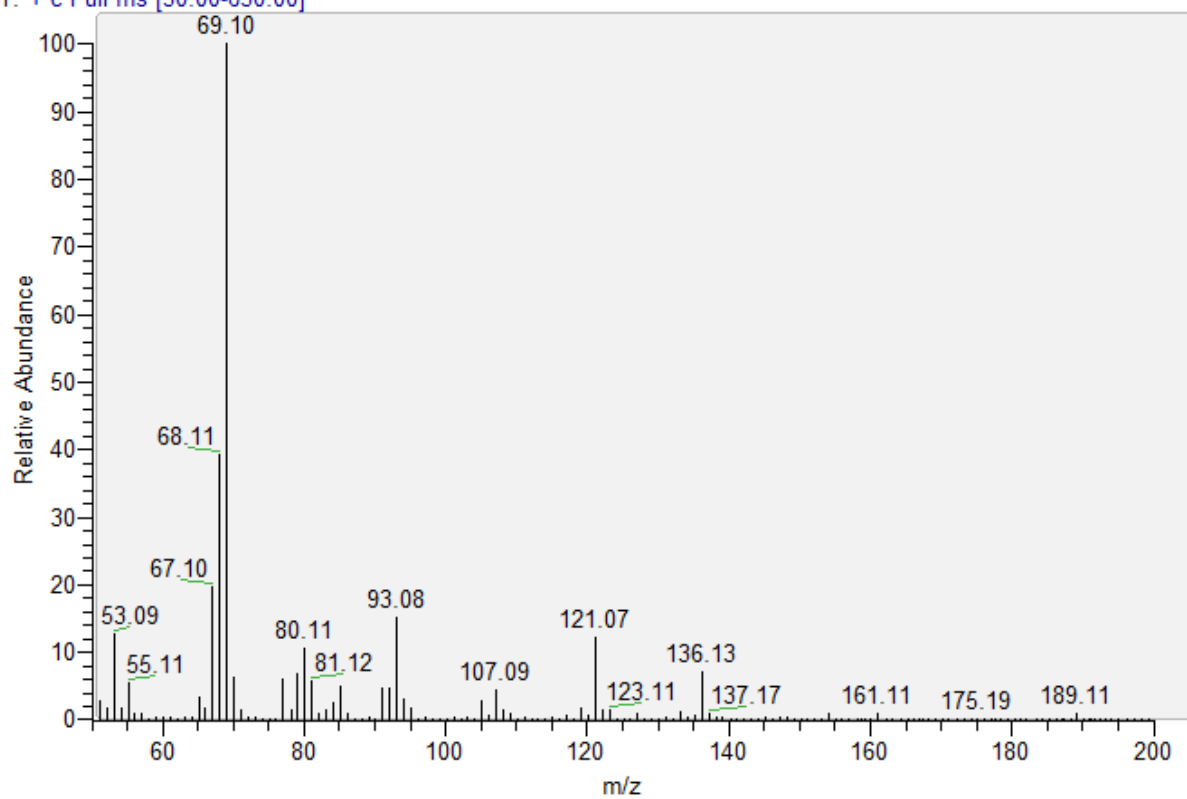
3058 #1303-1305 RT: 31.07-31.12 AV: 3 NL: 2.68E7



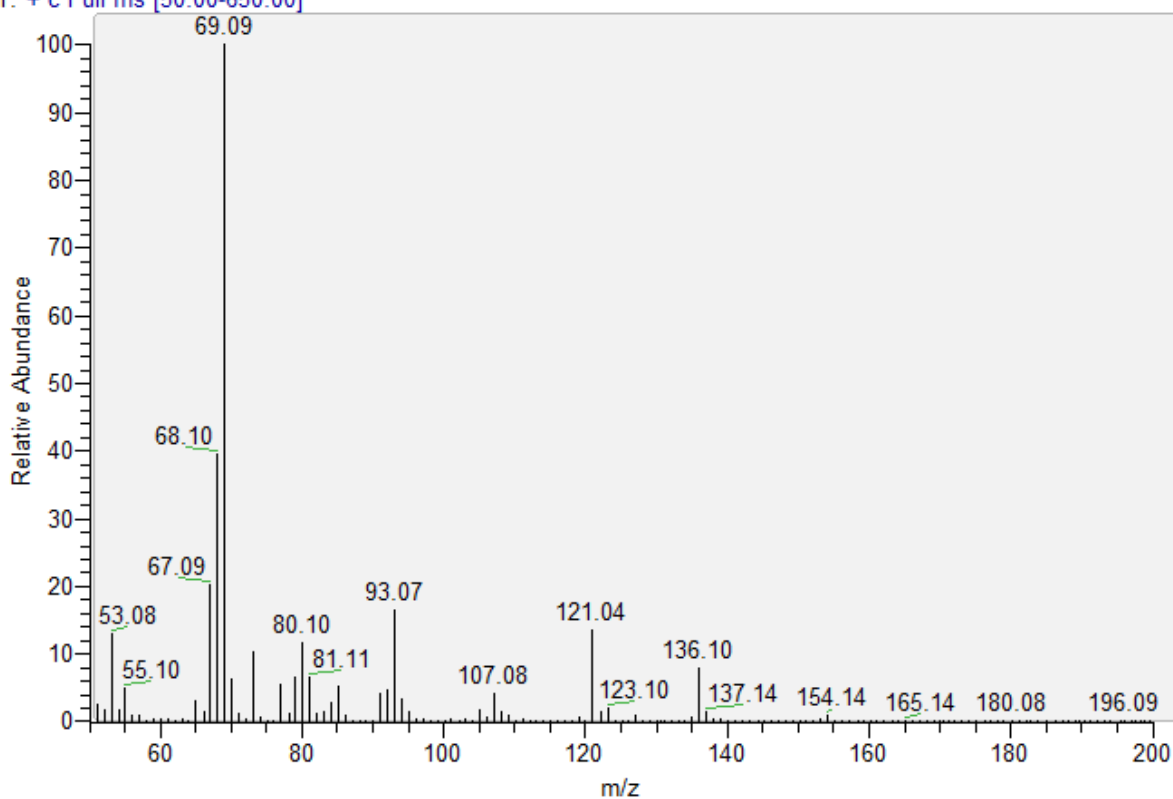
T: + c Full ms [50.00-650.00]



3057 #1310-1311 RT: 31.05-31.08 AV: 2 NL: 1.79E7  
T: + c Full ms [50.00-650.00]



3021 #1307-1309 RT: 31.08-31.13 AV: 3 NL: 7.44E7  
T: + c Full ms [50.00-650.00]

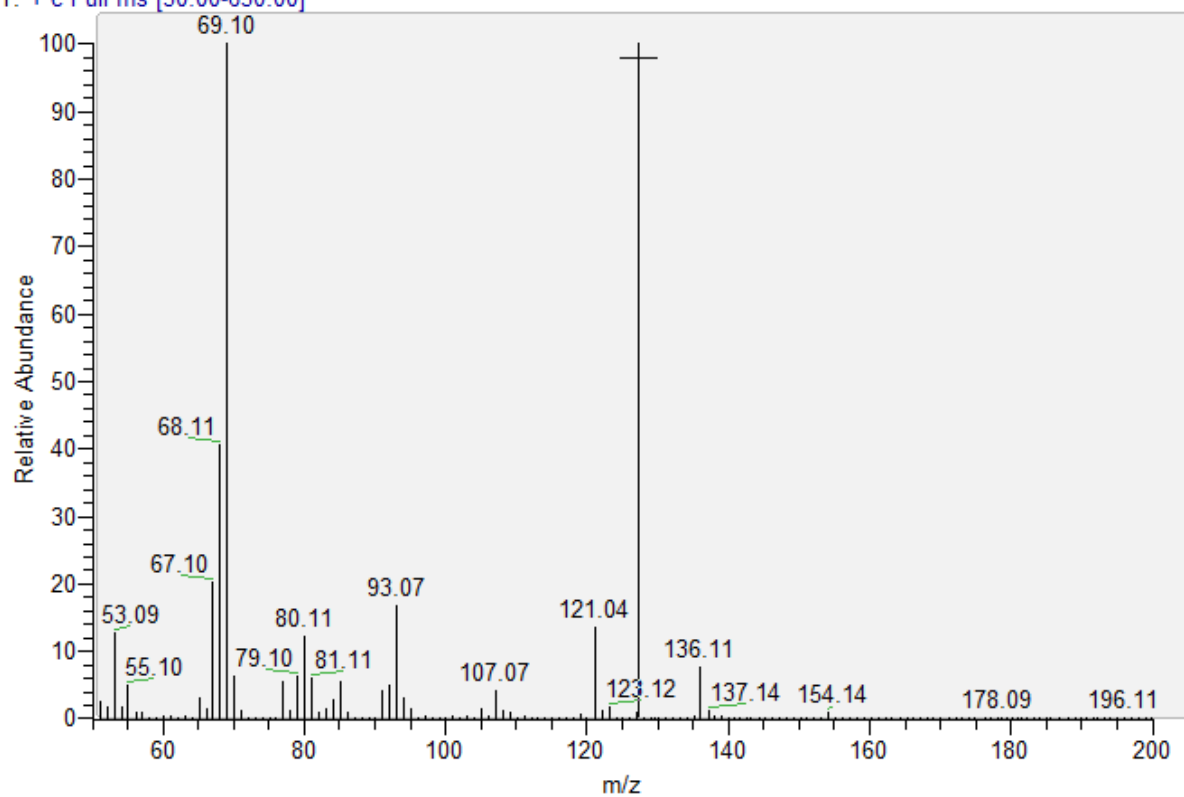




3075 #1306-1307 RT: 31.09-31.12 AV: 2 NL: 7.96E7



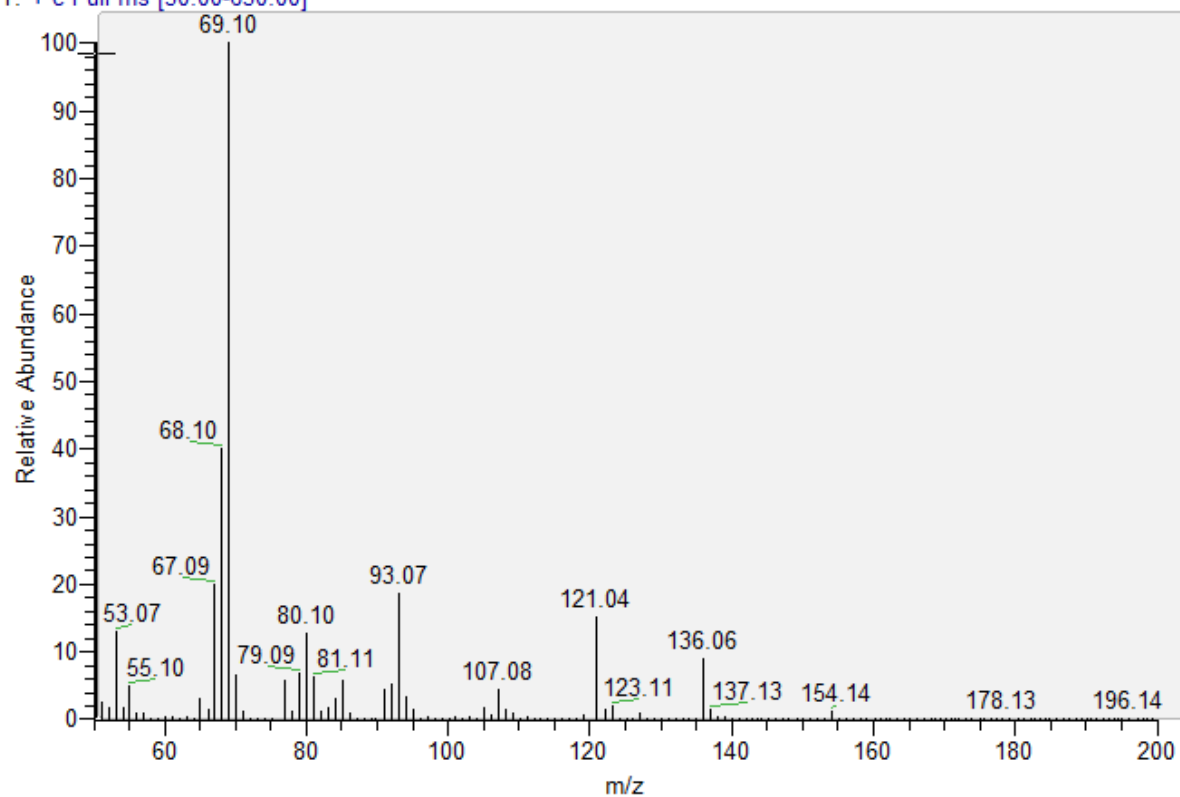
T: + c Full ms [50.00-650.00]



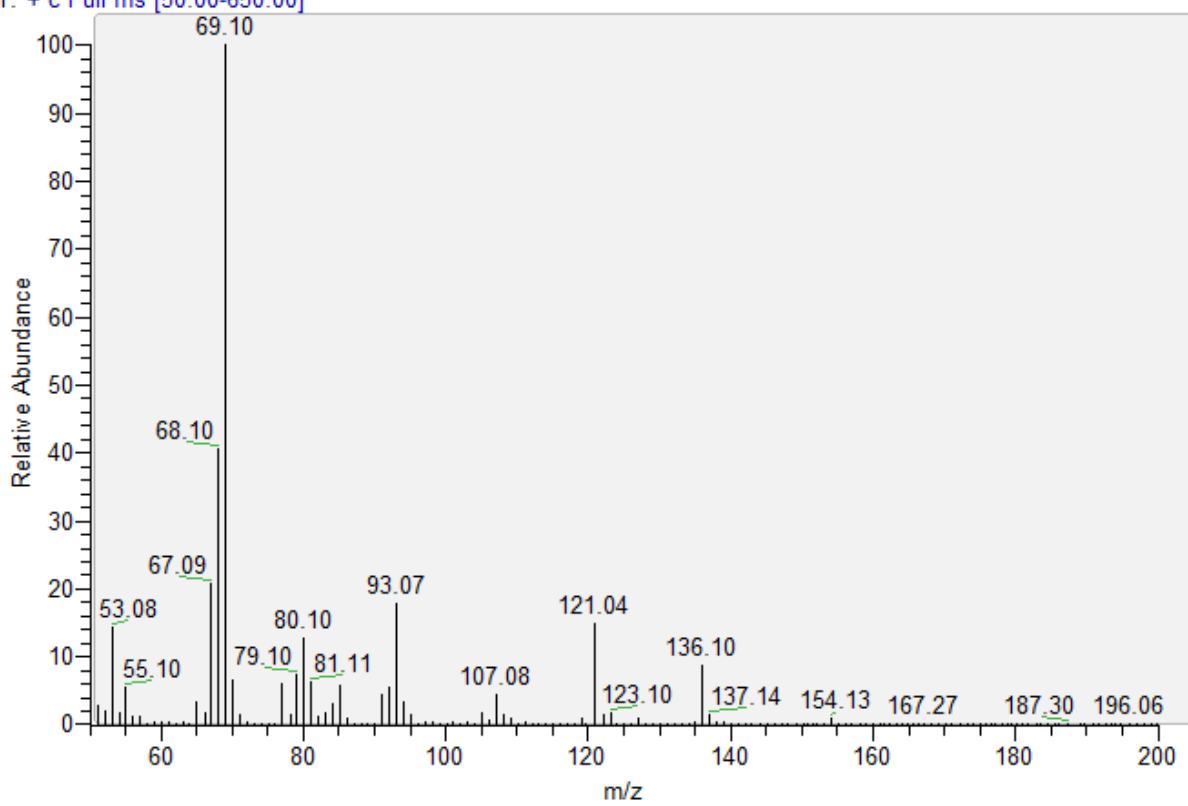
3074 #1307-1308 RT: 31.07-31.10 AV: 2 NL: 9.26E7



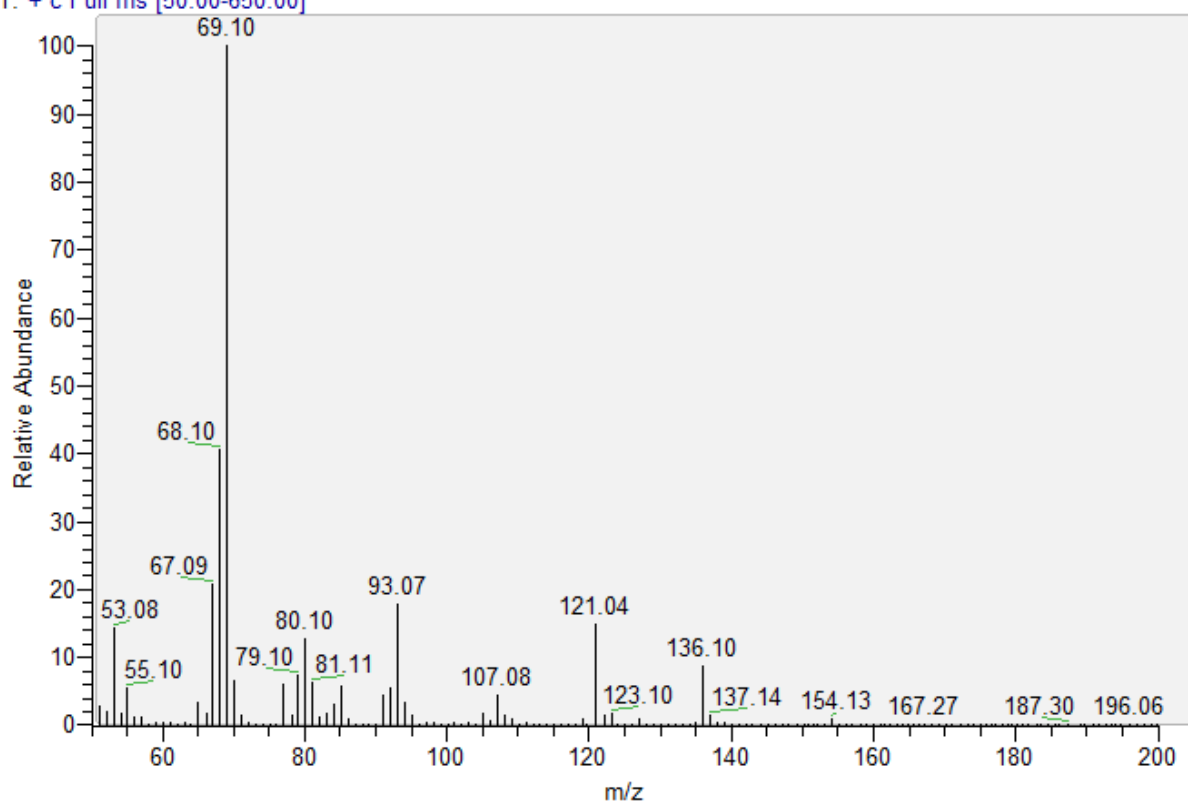
T: + c Full ms [50.00-650.00]



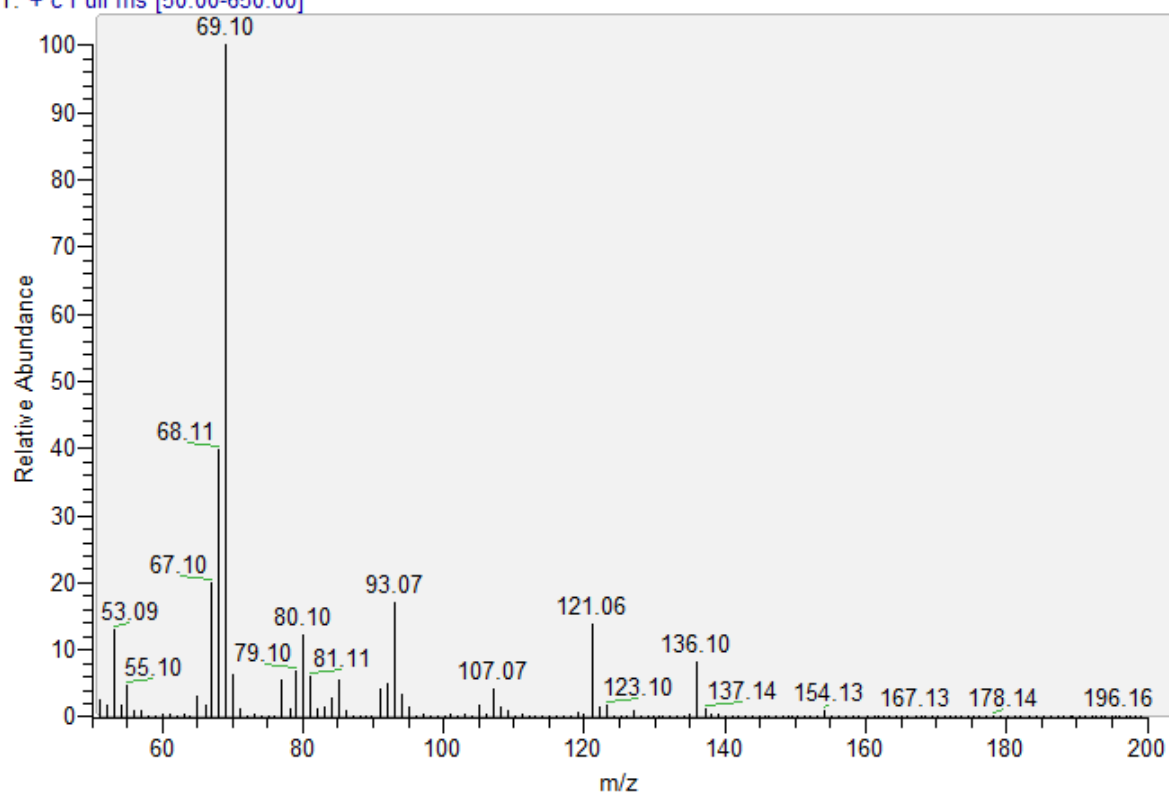
3073 #1305-1306 RT: 31.06-31.08 AV: 2 NL: 3.40E7  
T: + c Full ms [50.00-650.00]



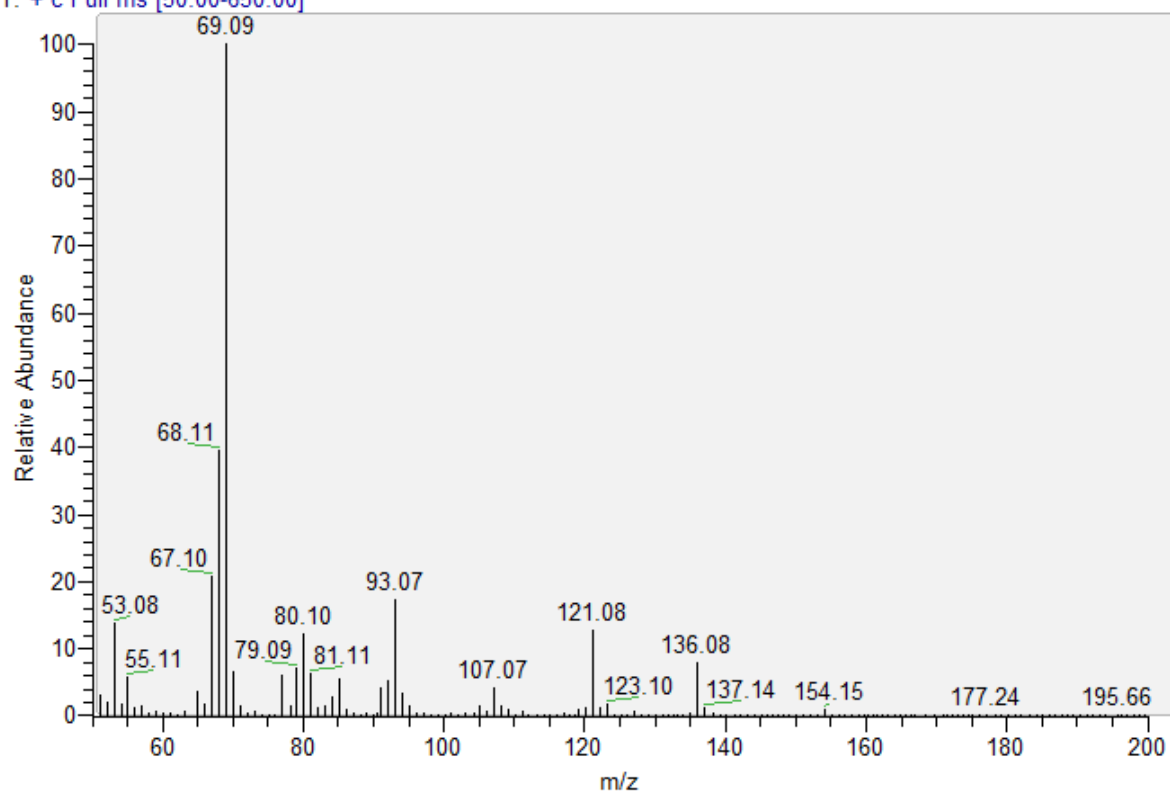
3073 #1305-1306 RT: 31.06-31.08 AV: 2 NL: 3.40E7  
T: + c Full ms [50.00-650.00]



3072 #1305-1306 RT: 31.08-31.10 AV: 2 NL: 6.44E7  
T: + c Full ms [50.00-650.00]

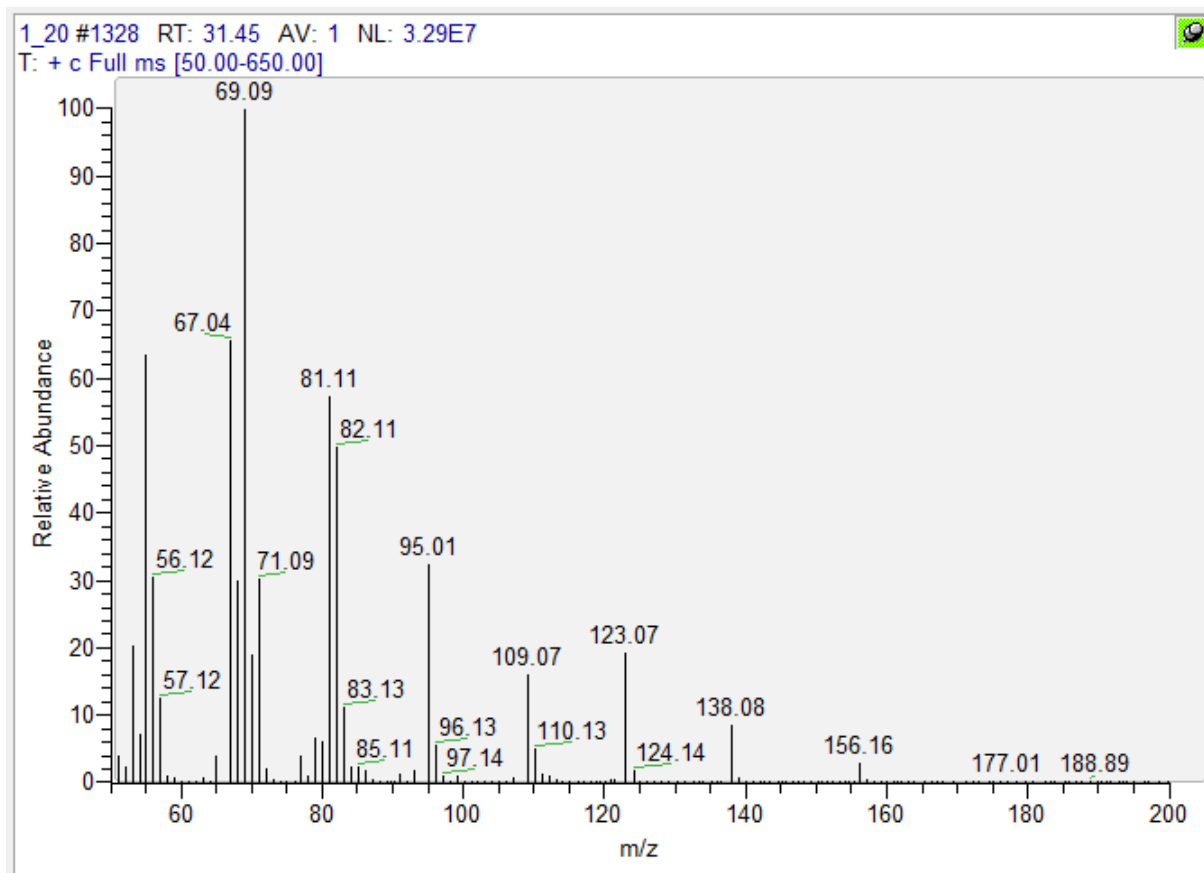


3070 #1306-1307 RT: 31.04-31.06 AV: 2 NL: 6.28E6  
T: + c Full ms [50.00-650.00]



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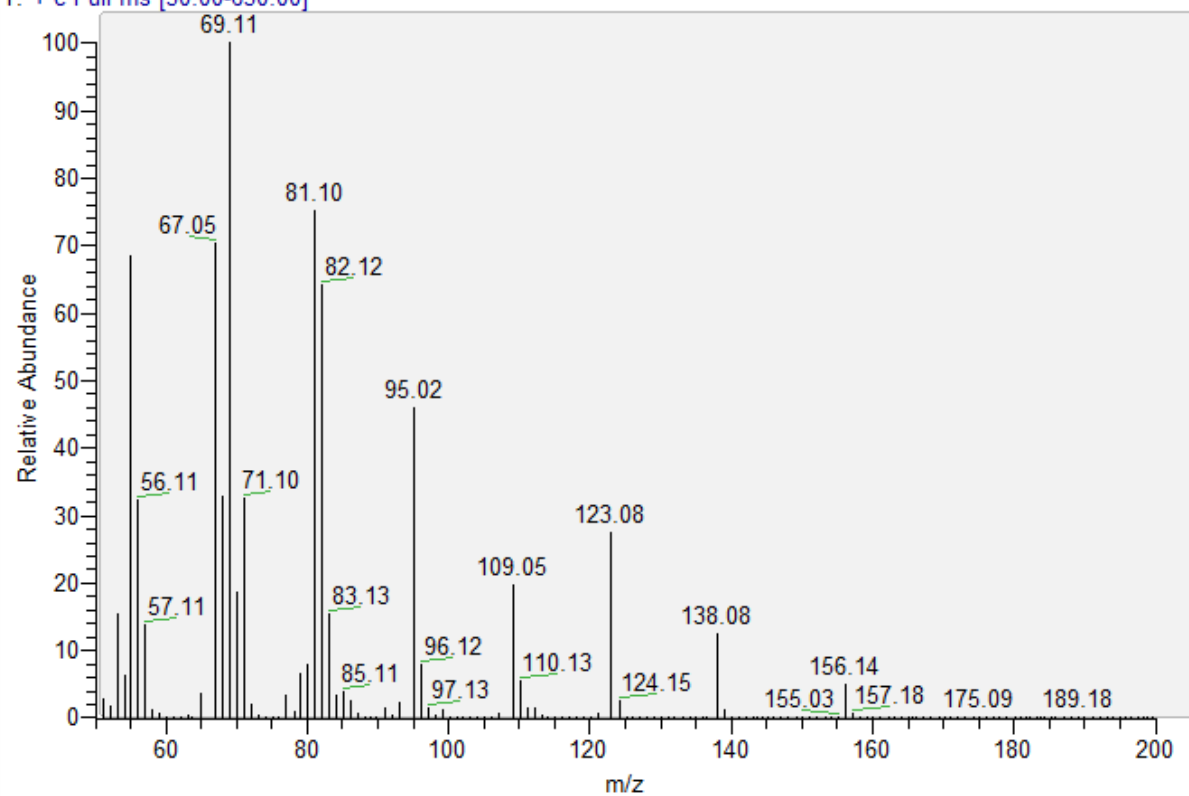
Reference:



Samples:

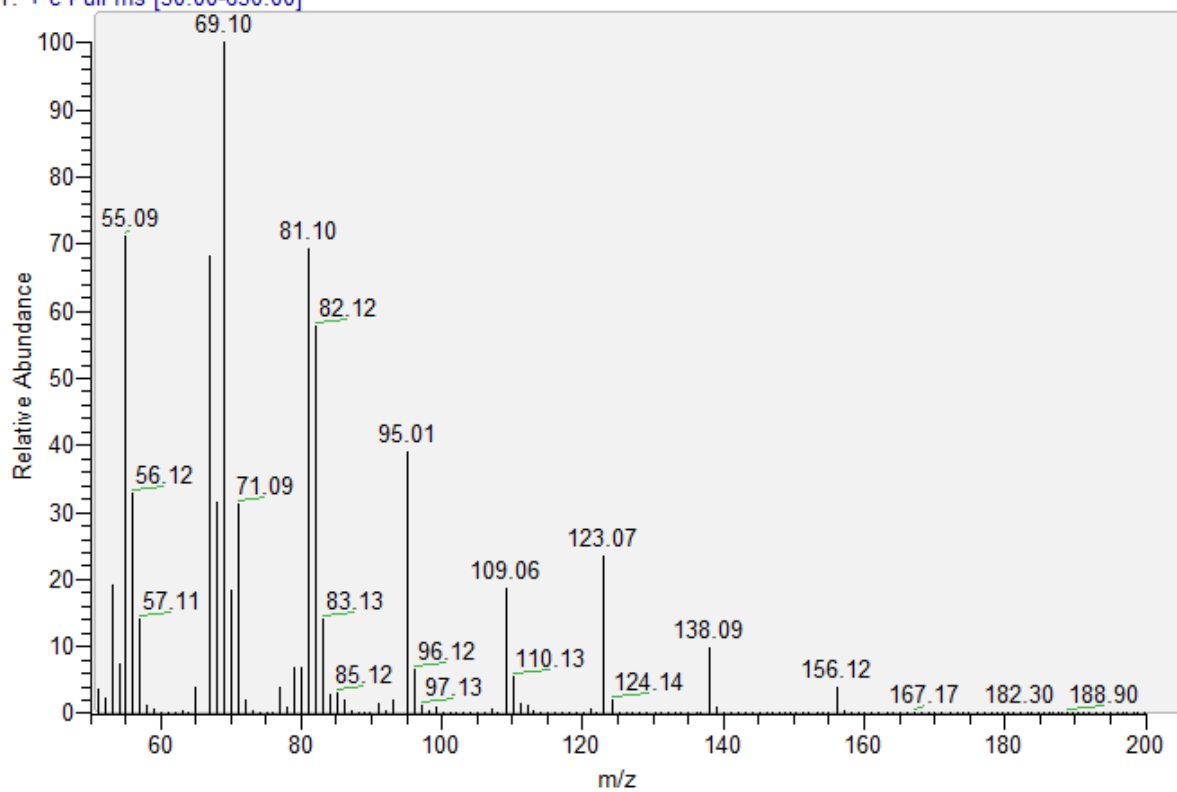
3018 #1331-1333 RT: 31.56-31.61 AV: 3 NL: 2.74E8

T: + c Full ms [50.00-650.00]

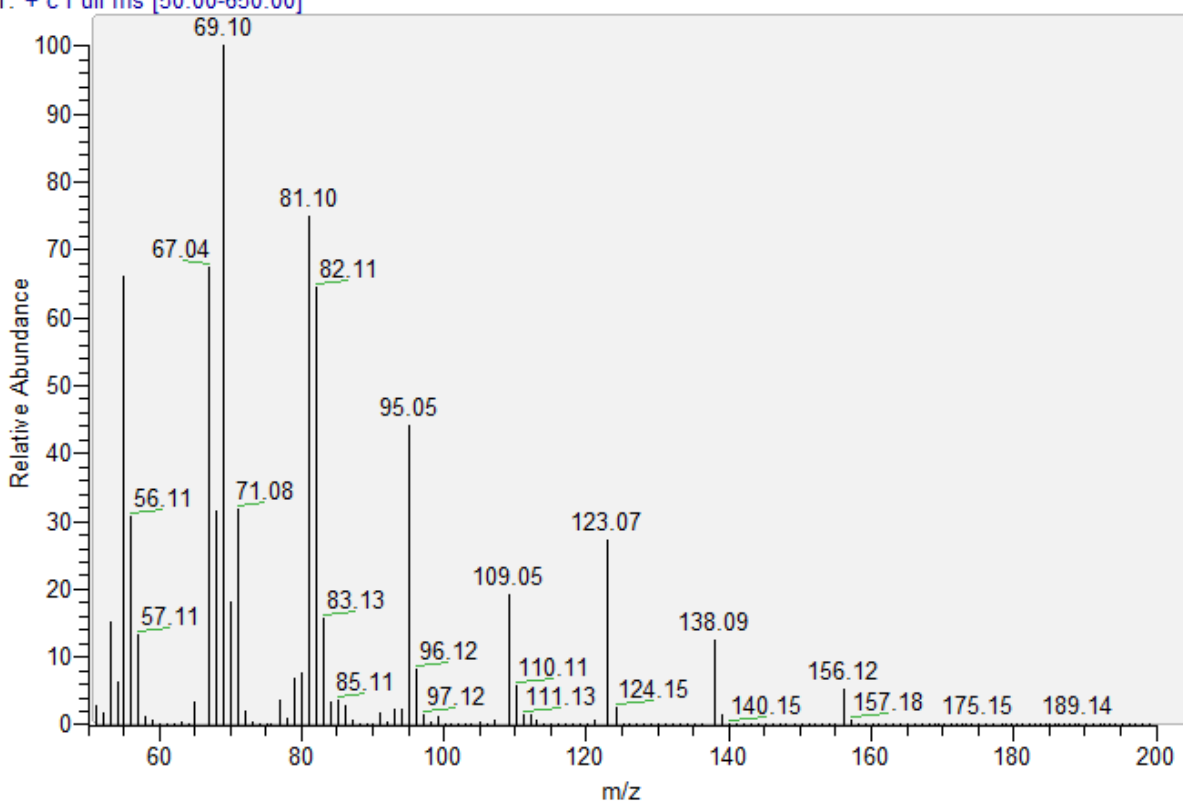




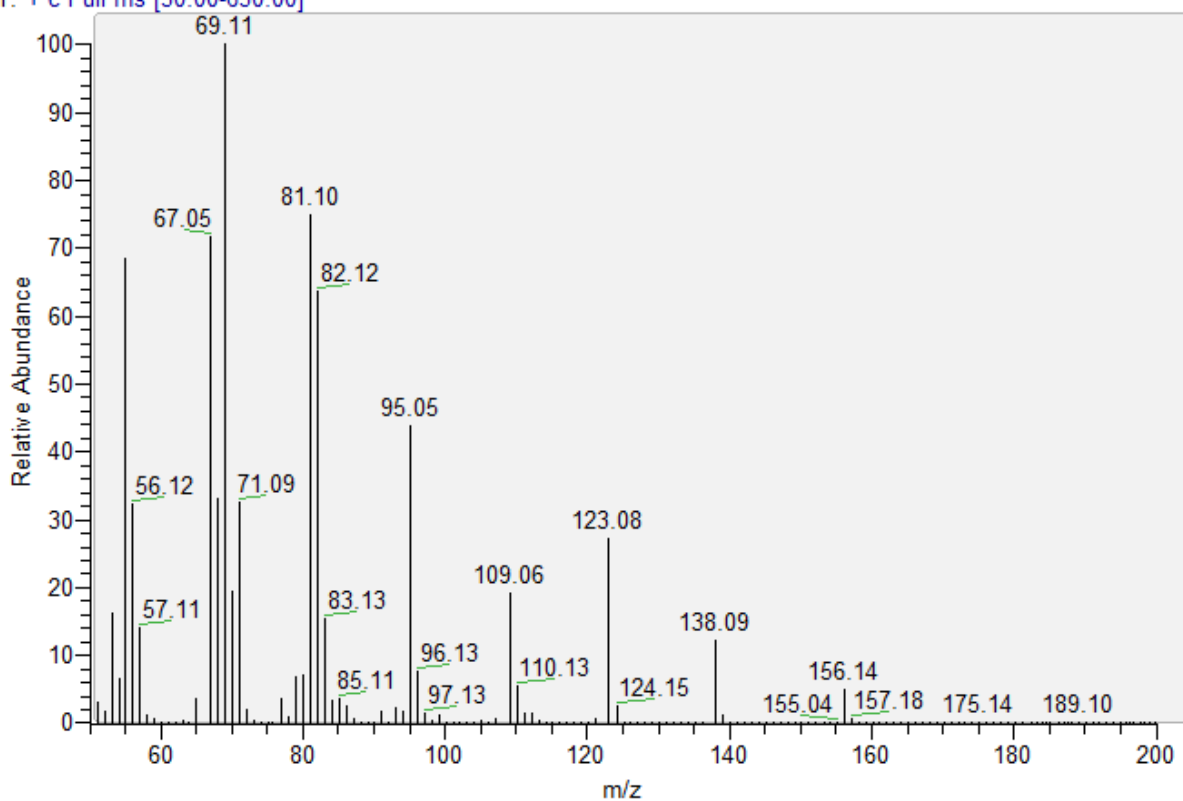
3053 #1323-1325 RT: 31.47-31.52 AV: 3 NL: 1.21E8  
T: + c Full ms [50.00-650.00]



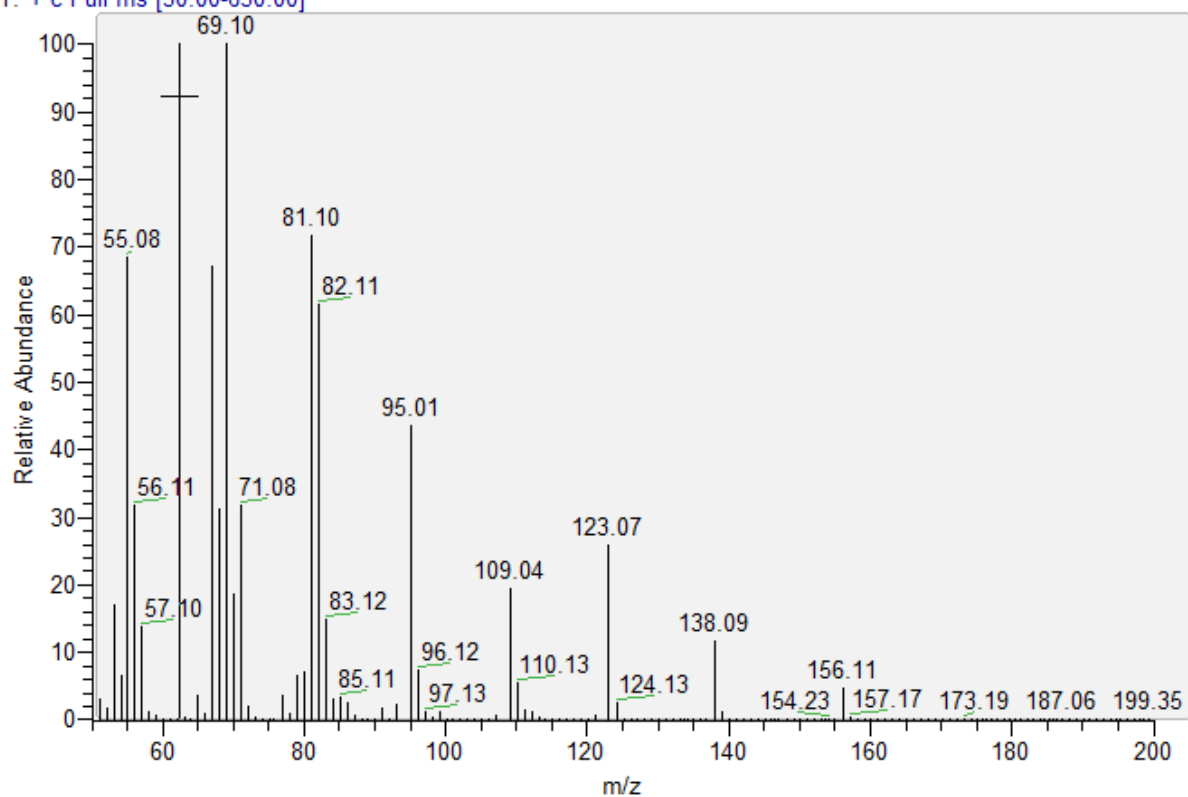
3058 #1324-1326 RT: 31.57-31.62 AV: 3 NL: 2.85E8  
T: + c Full ms [50.00-650.00]



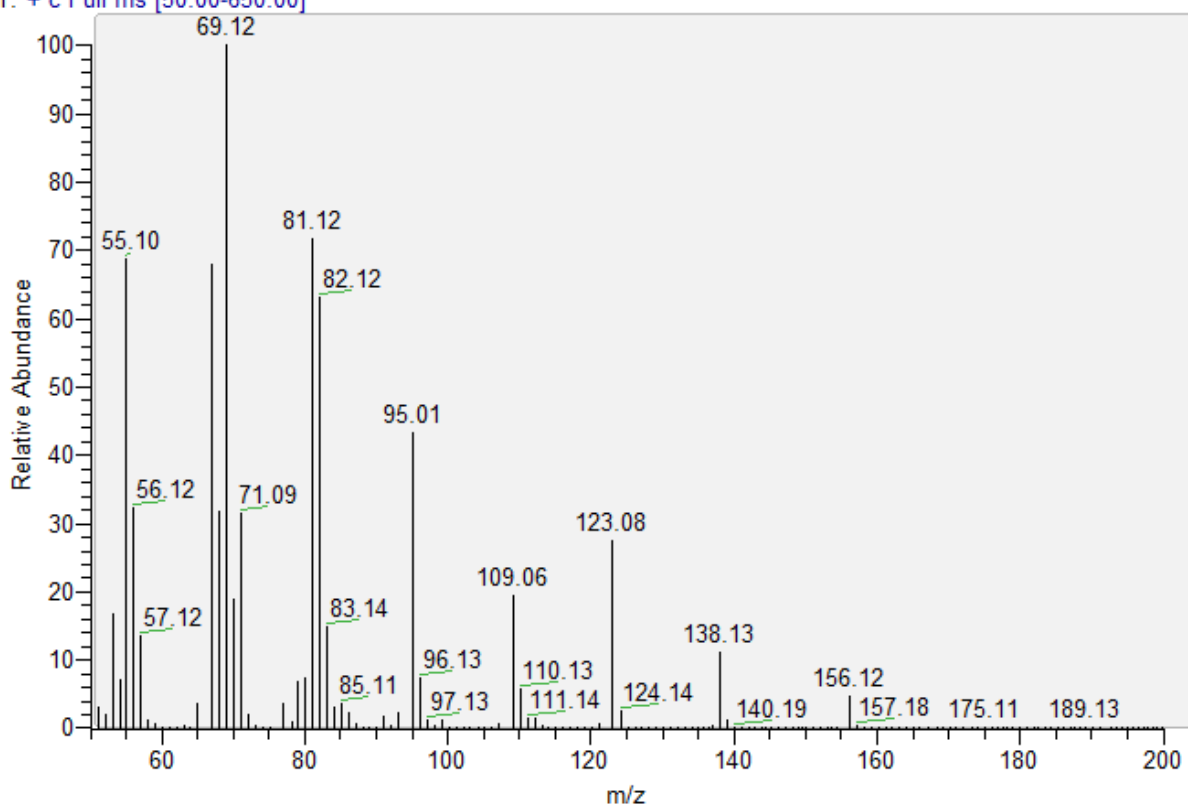
3057 #1330-1333 RT: 31.53-31.60 AV: 4 NL: 2.72E8  
T: + c Full ms [50.00-650.00]



3021 #1325-1328 RT: 31.51-31.58 AV: 4 NL: 2.33E8  
T: + c Full ms [50.00-650.00]



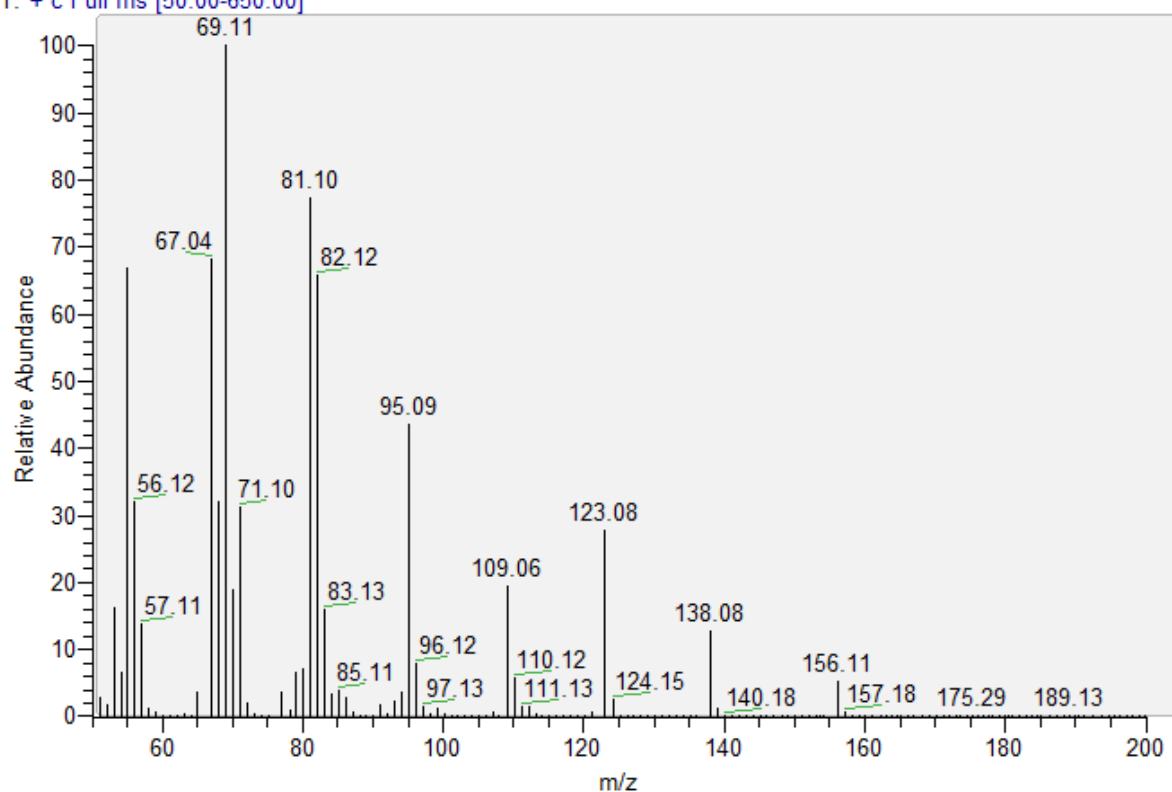
3075 #1325 RT: 31.54 AV: 1 NL: 2.05E8  
T: + c Full ms [50.00-650.00]



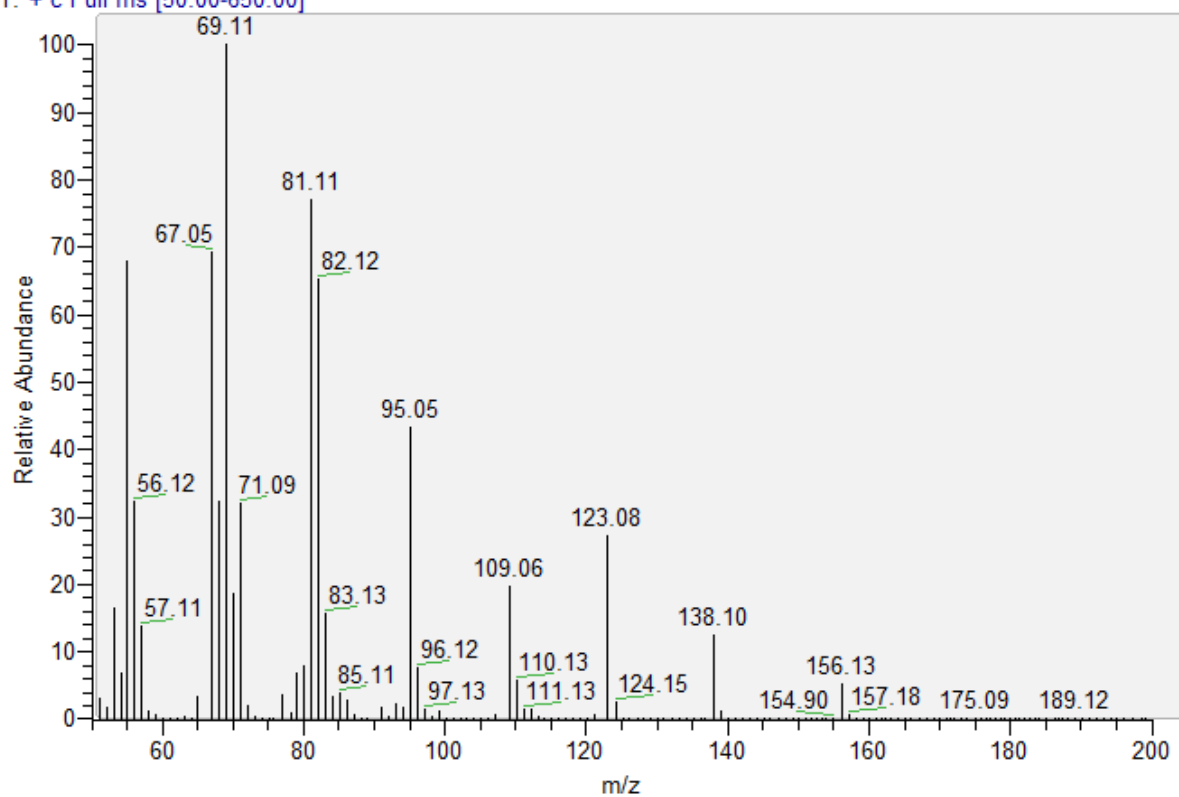
3074 #1328-1329 RT: 31.58-31.60 AV: 2 NL: 2.64E8



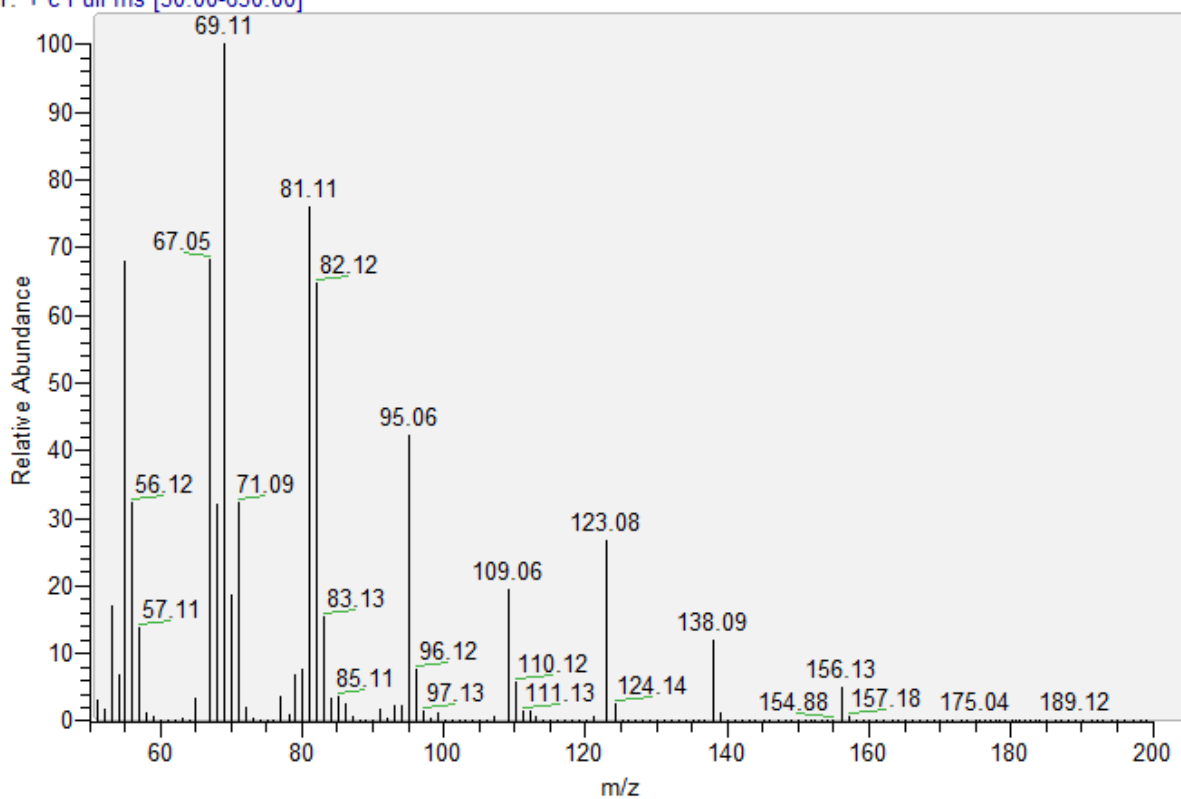
T: + c Full ms [50.00-650.00]



3073 #1326-1327 RT: 31.56-31.58 AV: 2 NL: 2.29E8  
T: + c Full ms [50.00-650.00]

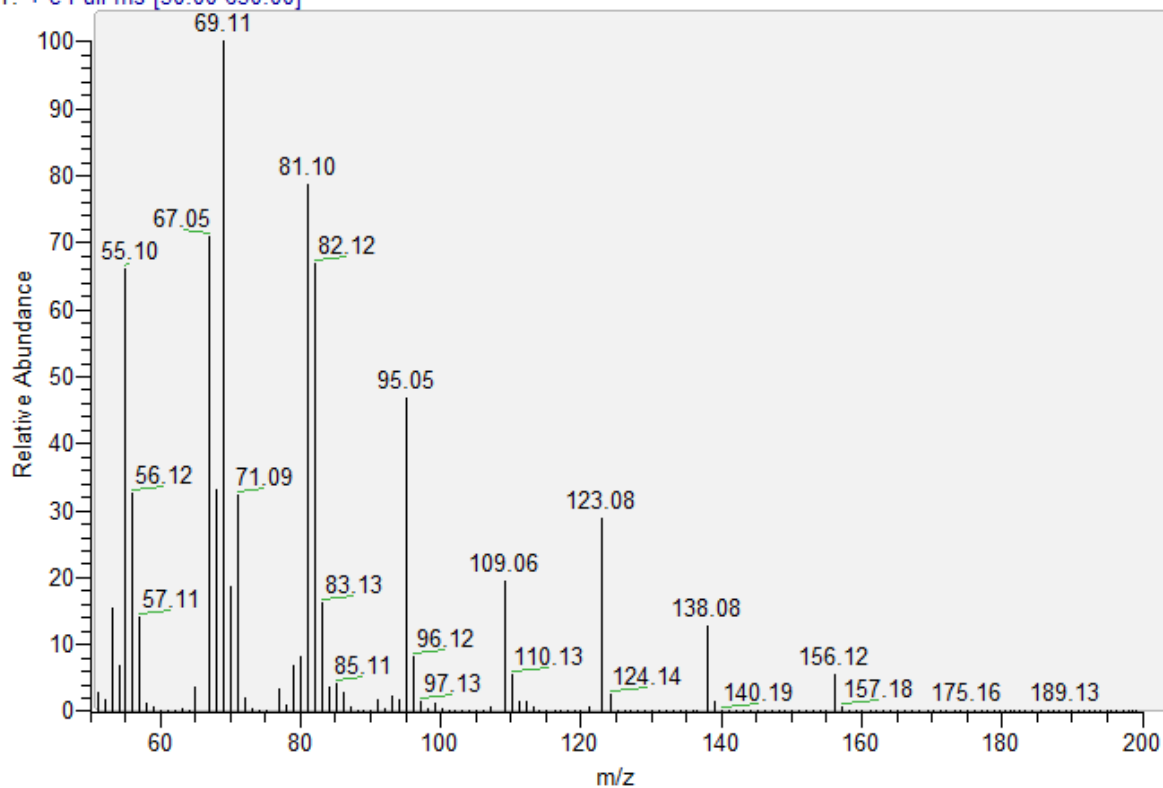


3073 #1325-1327 RT: 31.53-31.58 AV: 3 NL: 2.14E8  
T: + c Full ms [50.00-650.00]

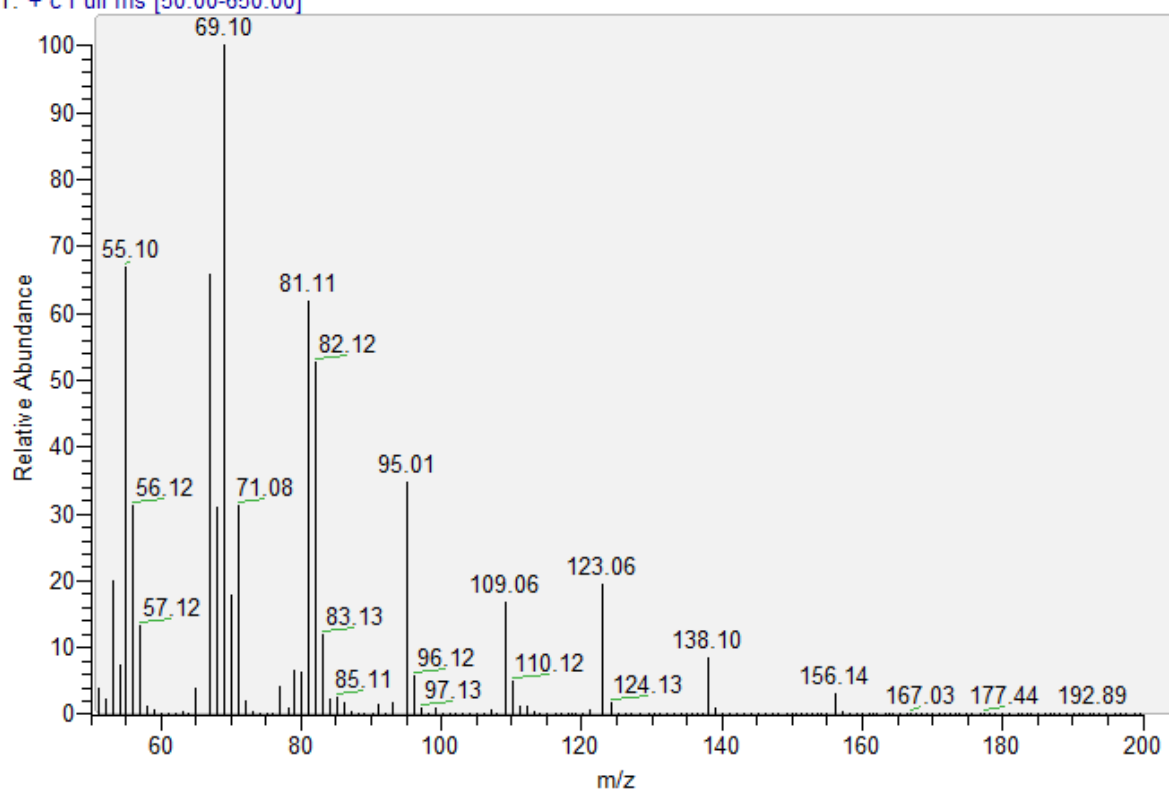




3072 #1326-1329 RT: 31.58-31.65 AV: 4 NL: 2.71E8  
T: + c Full ms [50.00-650.00]

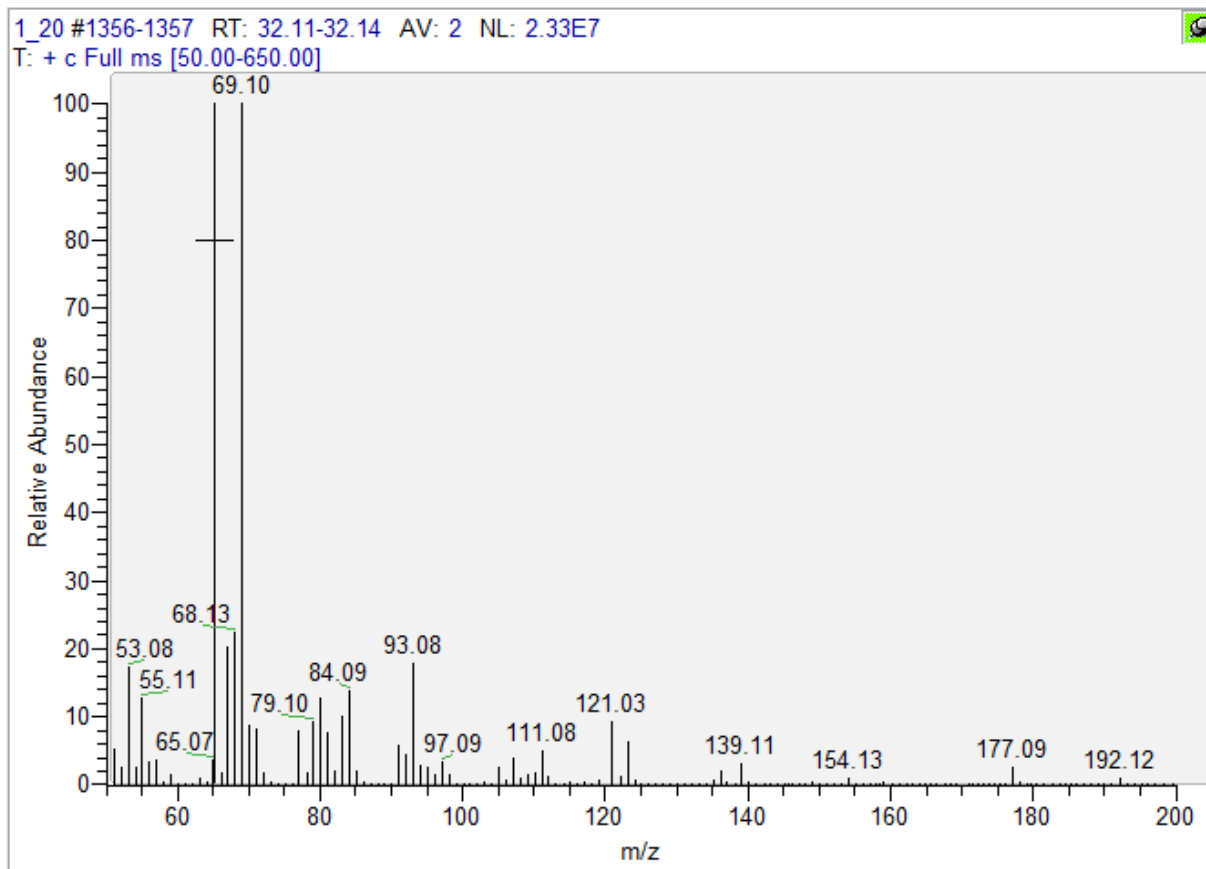


3070 #1324-1325 RT: 31.46-31.49 AV: 2 NL: 7.33E7  
T: + c Full ms [50.00-650.00]



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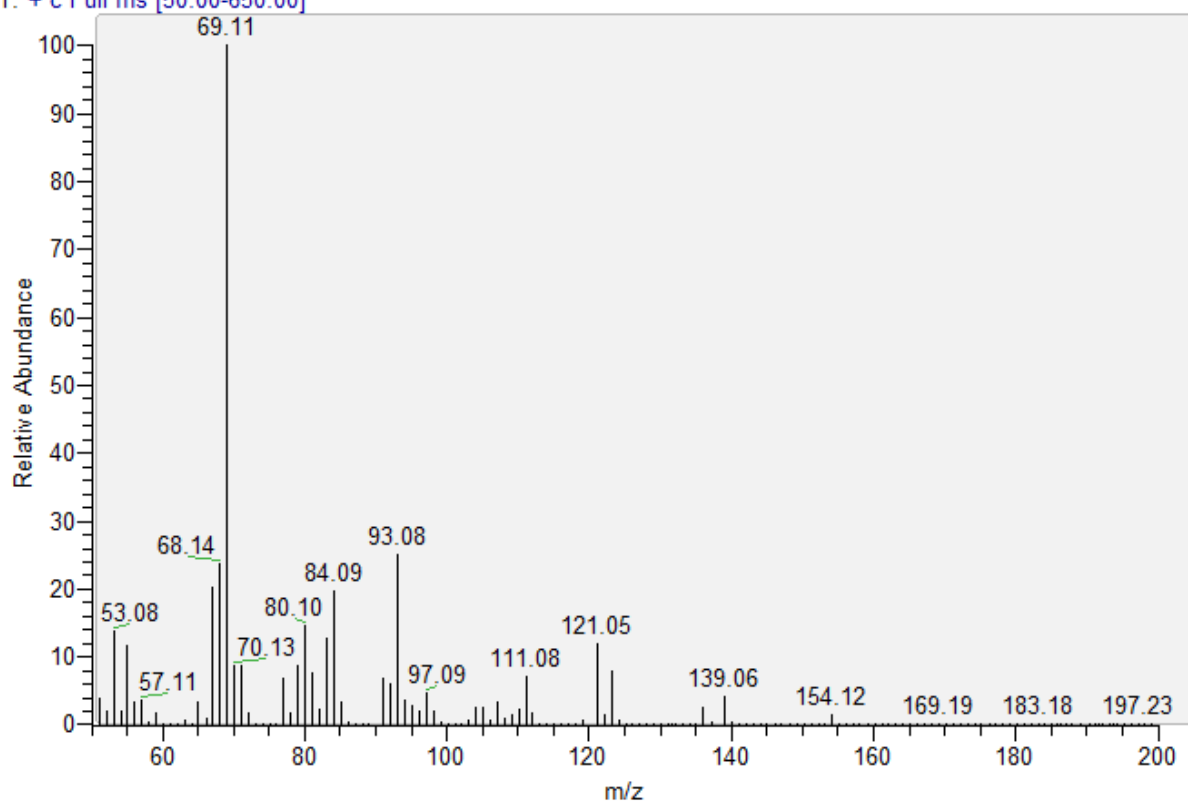
Reference:



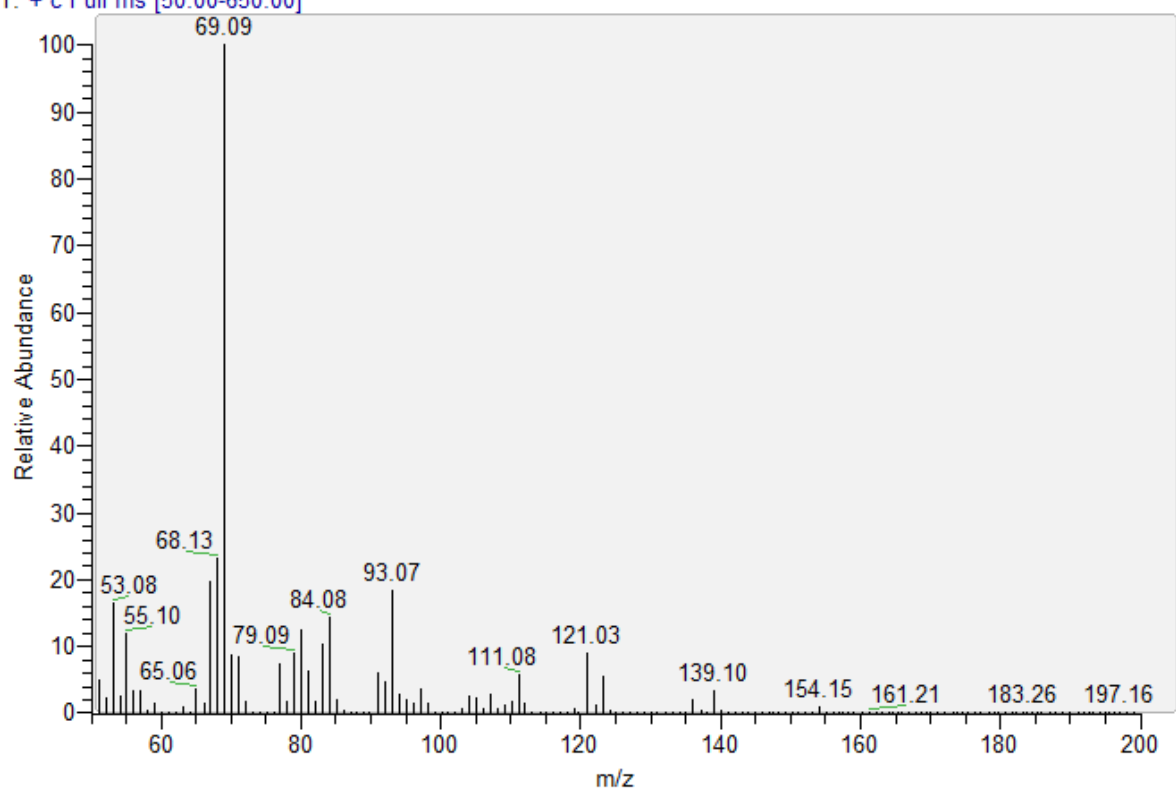
Samples:

3018 #1358-1360 RT: 32.21-32.26 AV: 3 NL: 3.51E8

T: + c Full ms [50.00-650.00]



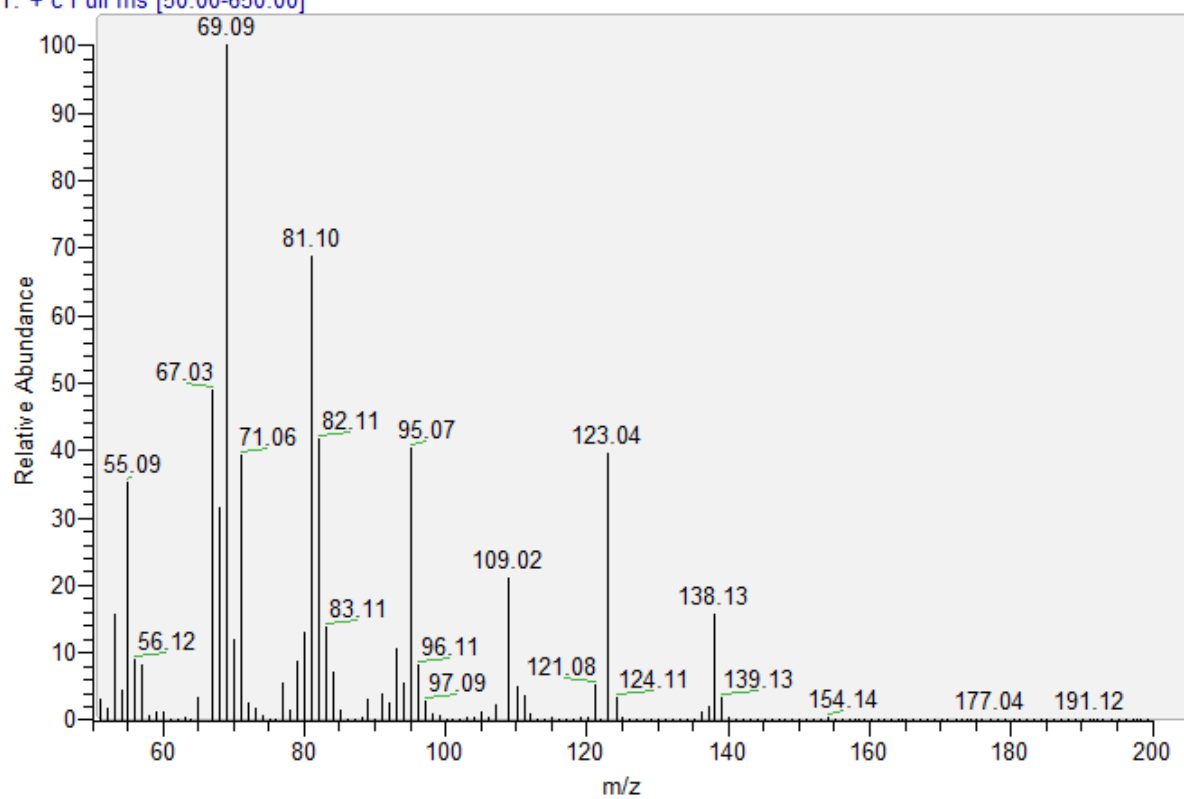
3053 #1351-1352 RT: 32.14-32.17 AV: 2 NL: 7.77E7  
T: + c Full ms [50.00-650.00]



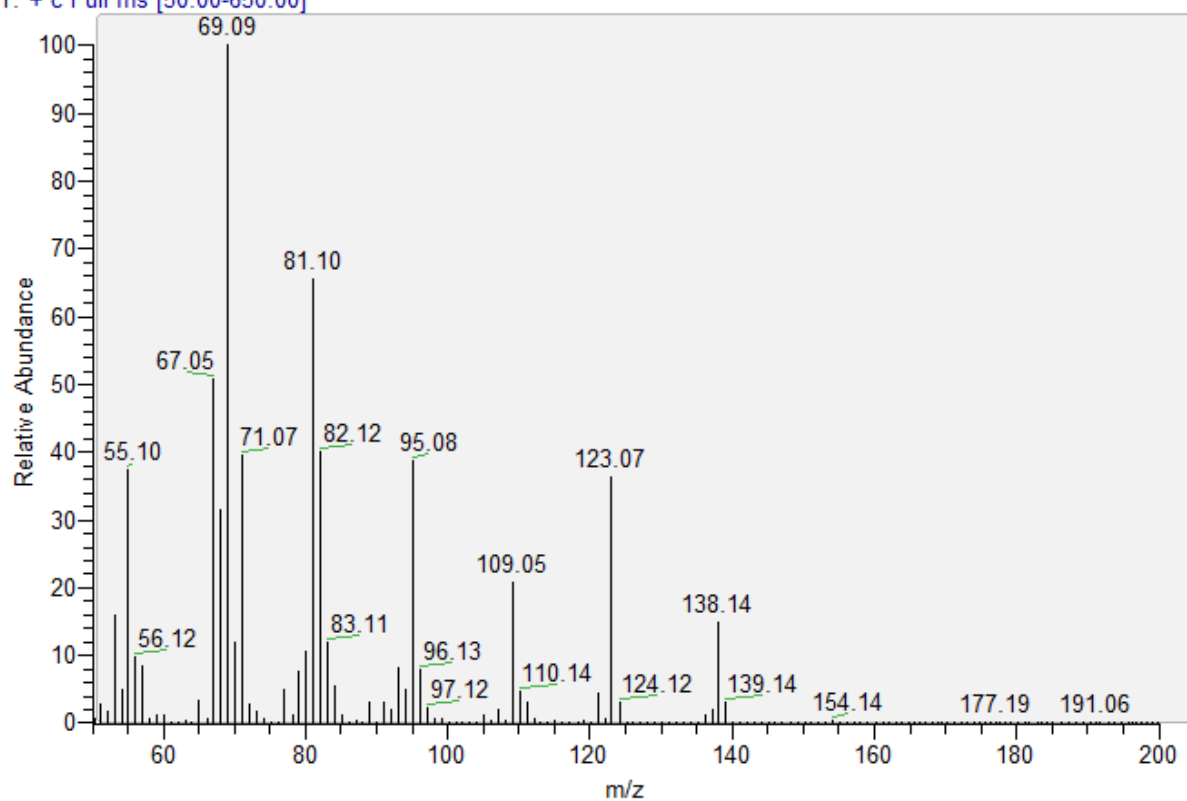
3058 #1349-1351 RT: 32.17-32.22 AV: 3 NL: 4.52E7



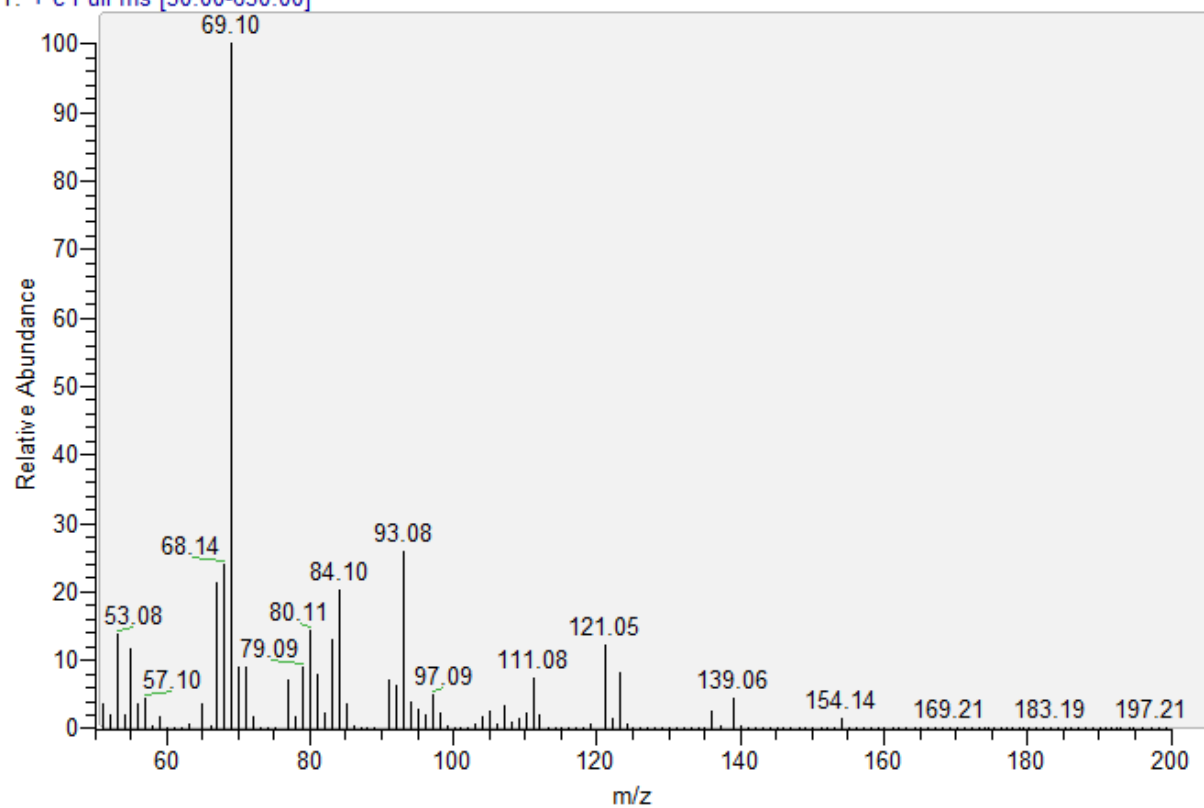
T: + c Full ms [50.00-650.00]



3057 #1354-1356 RT: 32.10-32.15 AV: 3 NL: 1.96E7  
T: + c Full ms [50.00-650.00]

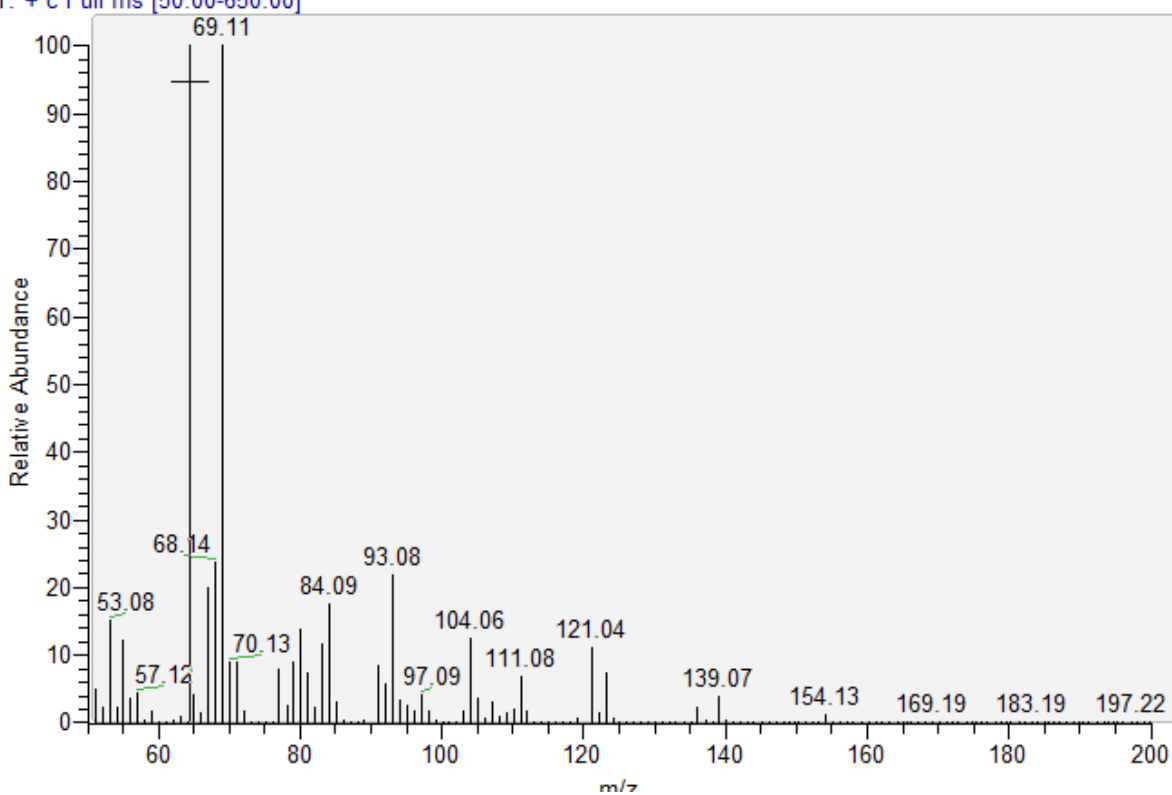


3021 #1356-1358 RT: 32.25-32.30 AV: 3 NL: 3.79E8  
T: + c Full ms [50.00-650.00]





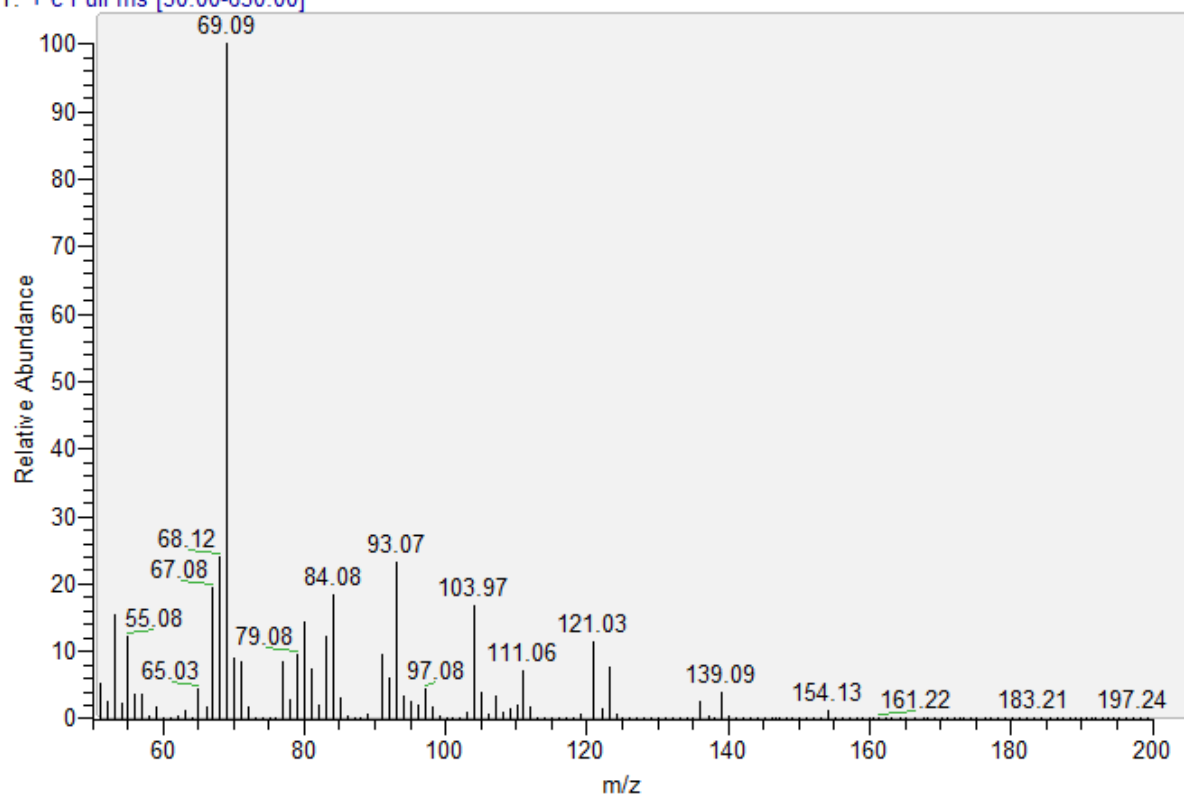
3075 #1351-1354 RT: 32.17-32.24 AV: 4 NL: 2.04E8  
T: + c Full ms [50.00-650.00]



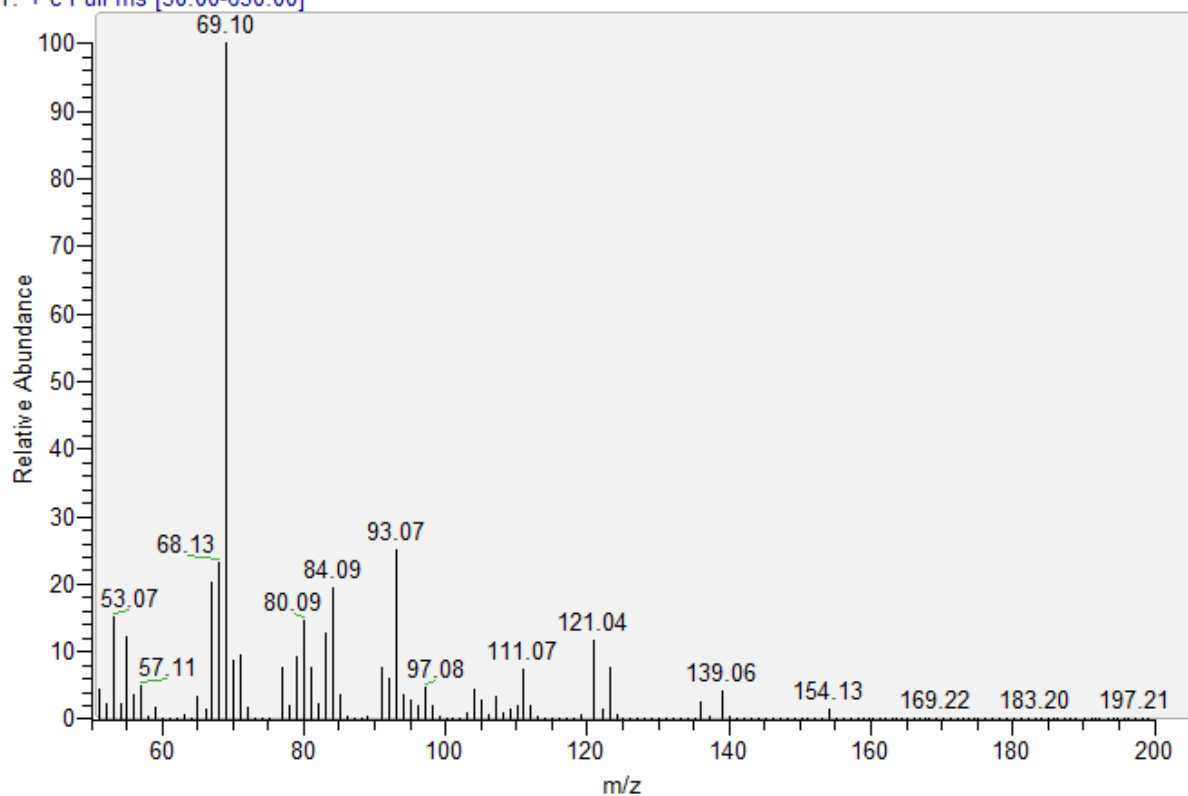
3074 #1354-1355 RT: 32.20-32.22 AV: 2 NL: 2.65E8



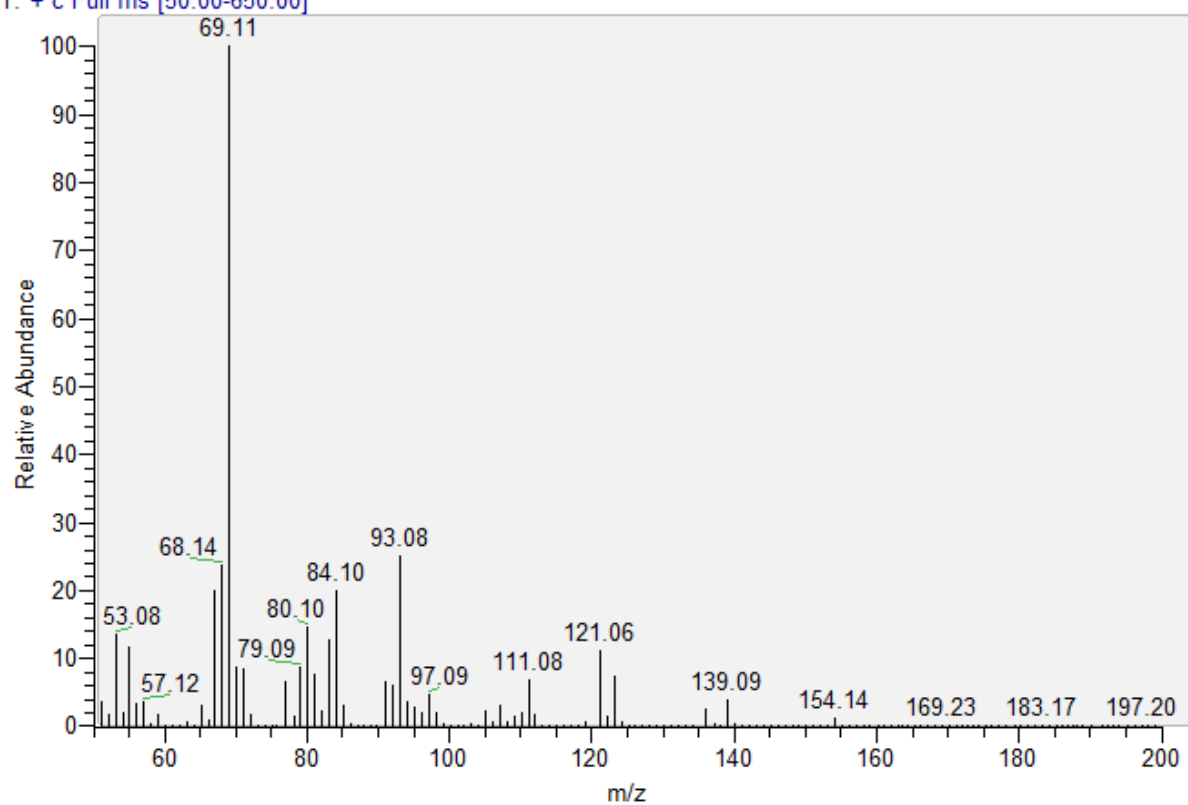
T: + c Full ms [50.00-650.00]



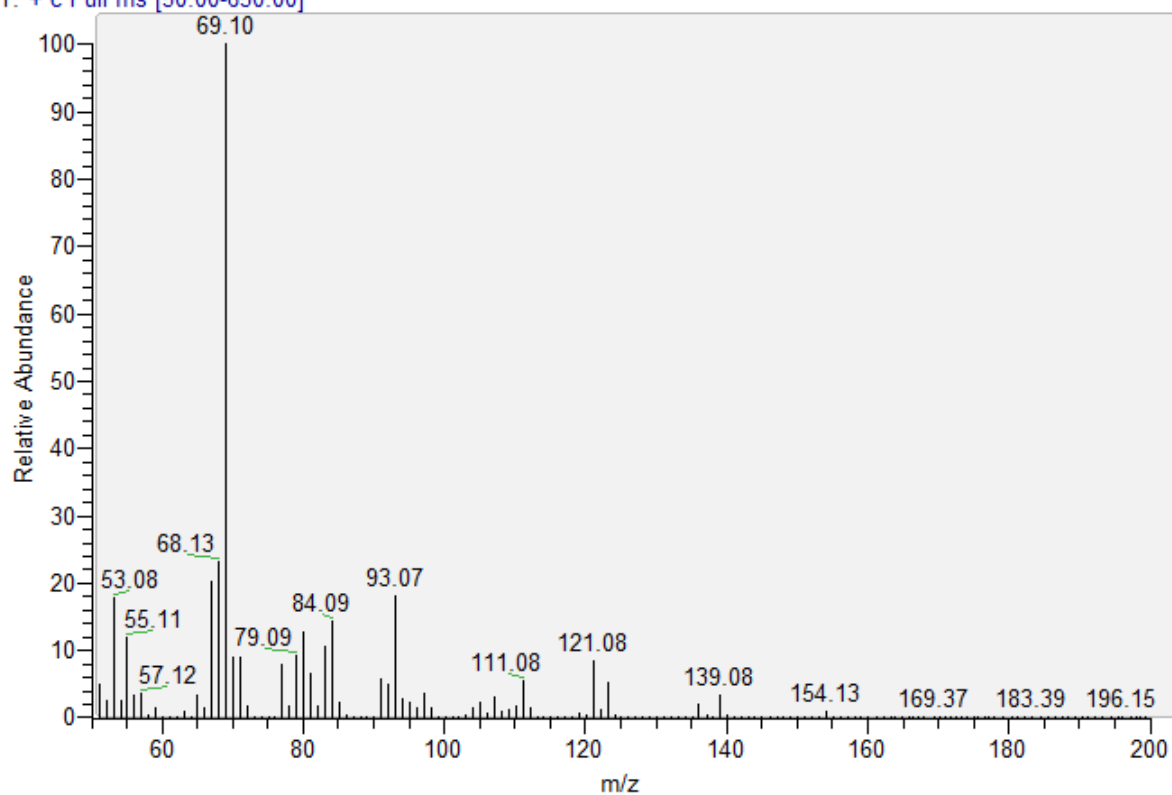
3073 #1353-1354 RT: 32.20-32.23 AV: 2 NL: 2.95E8  
T: + c Full ms [50.00-650.00]



3072 #1354-1356 RT: 32.25-32.29 AV: 3 NL: 3.85E8  
T: + c Full ms [50.00-650.00]

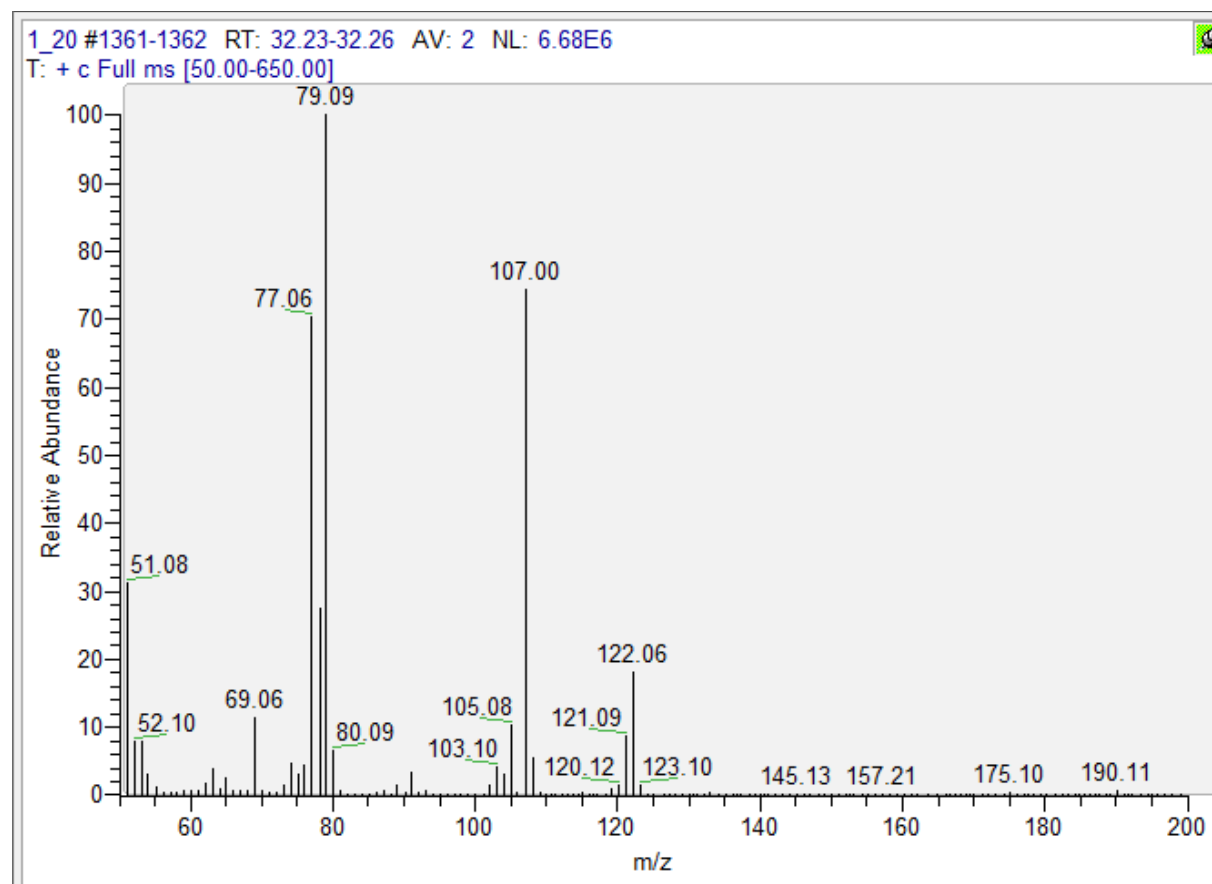


3070 #1351-1353 RT: 32.11-32.16 AV: 3 NL: 4.13E7  
T: + c Full ms [50.00-650.00]



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Reference

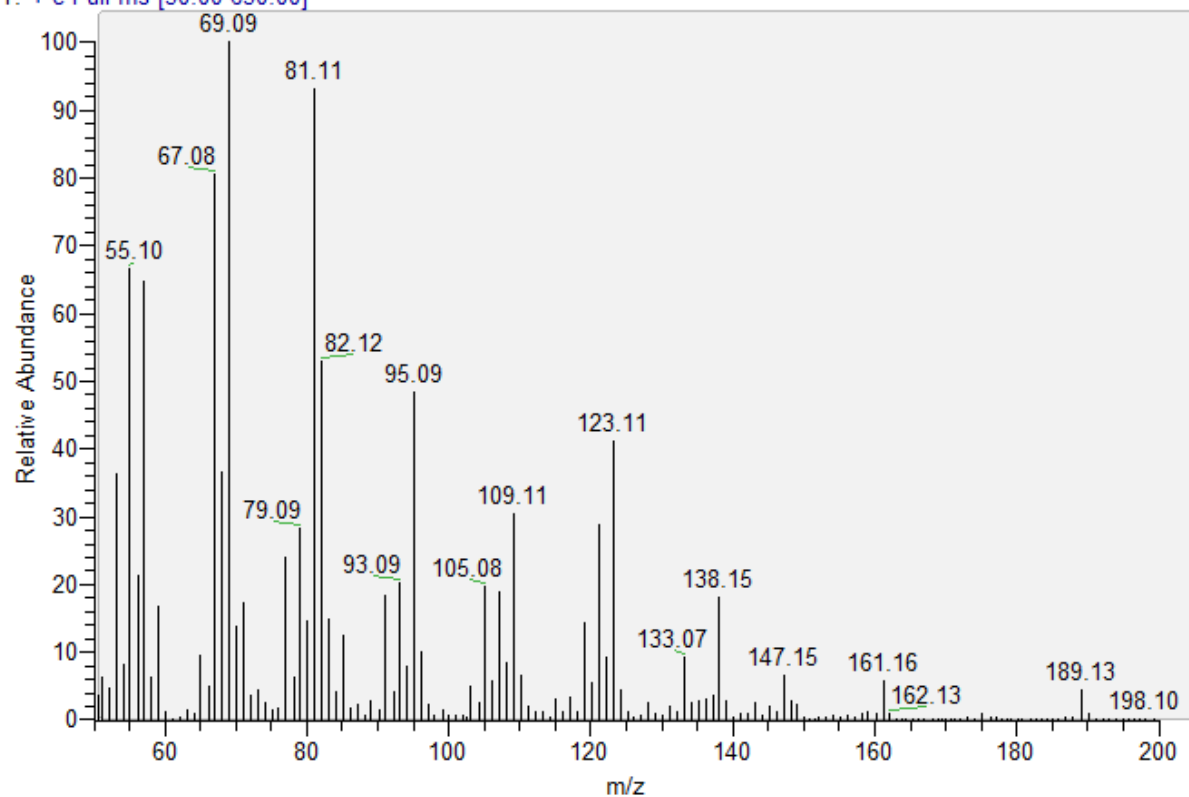


## Samples

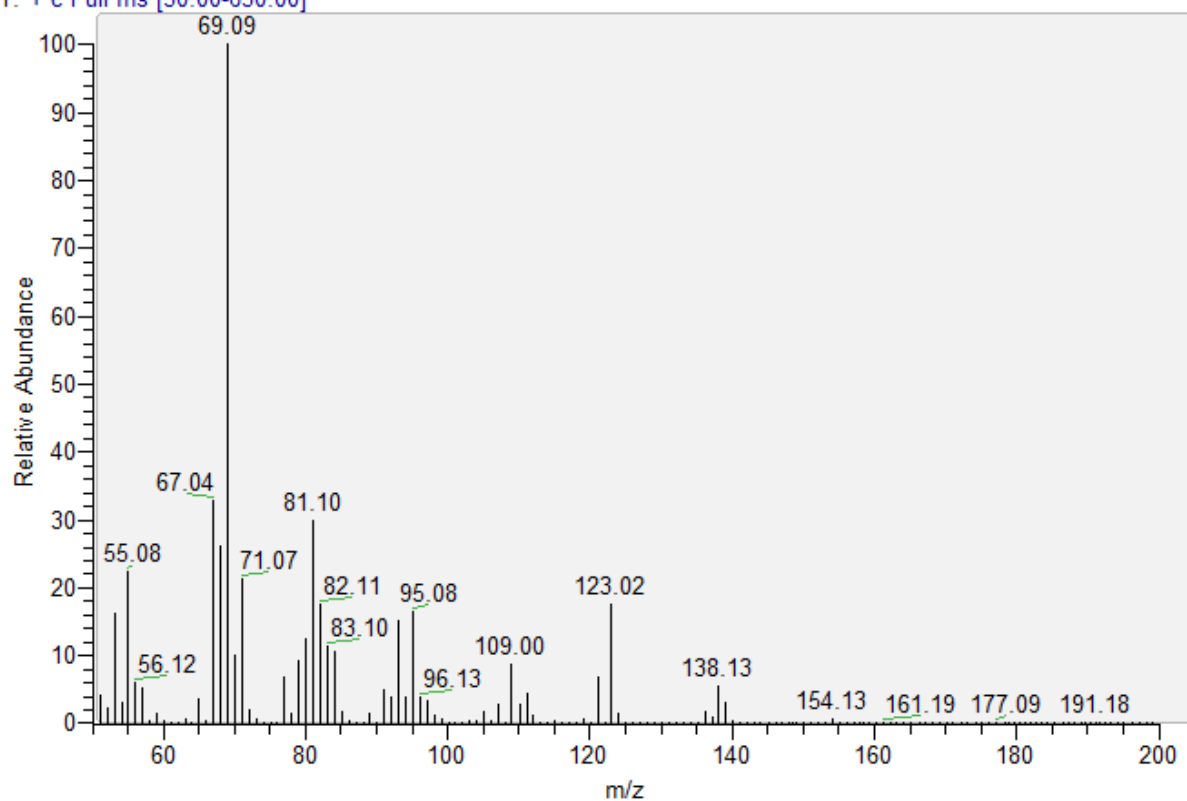
3057 #1361-1362 RT: 32.27-32.29 AV: 2 NL: 1.16E6



T: + c Full ms [50.00-650.00]

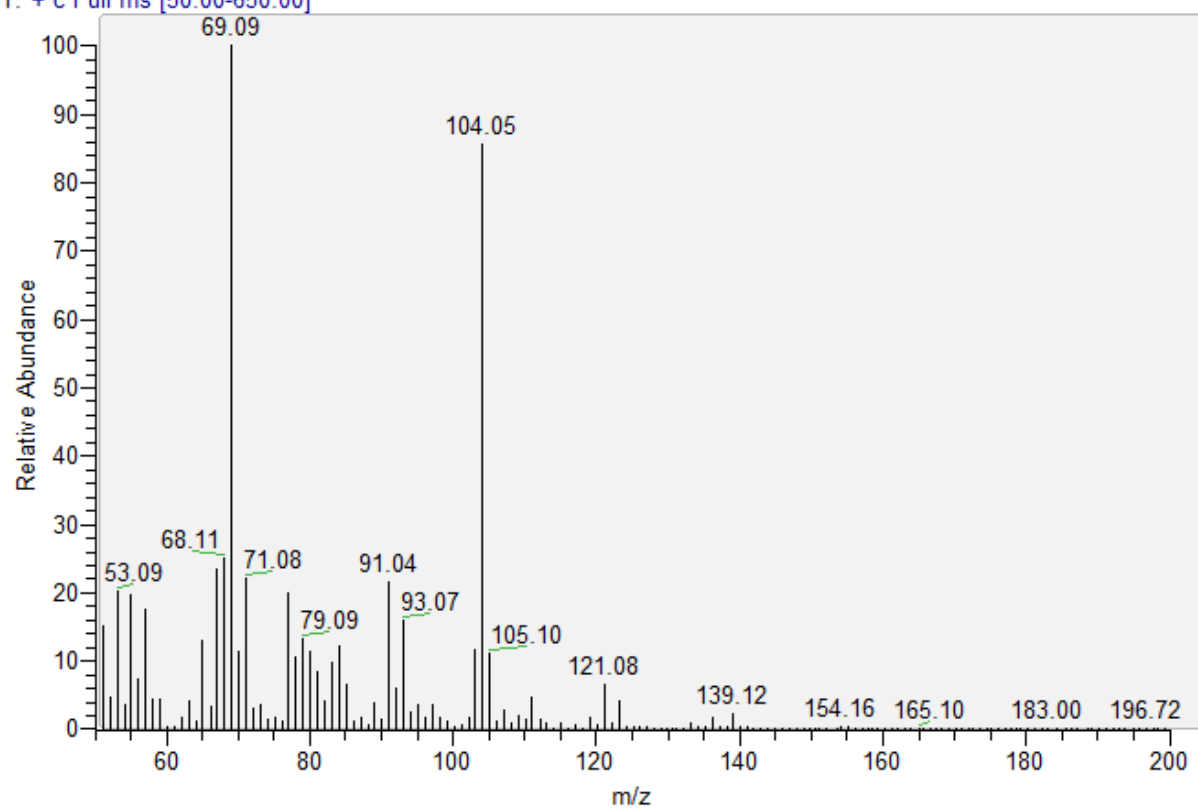


3058 #1351-1352 RT: 32.22-32.24 AV: 2 NL: 4.46E7  
T: + c Full ms [50.00-650.00]

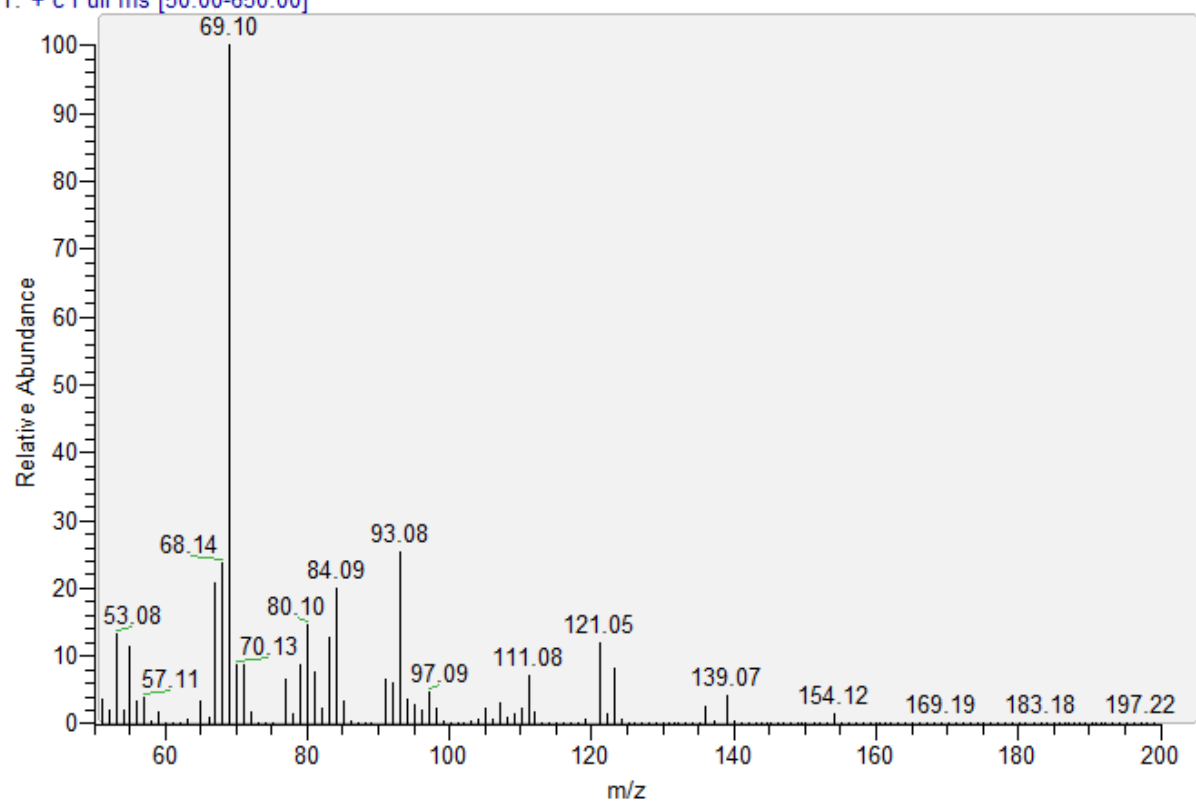




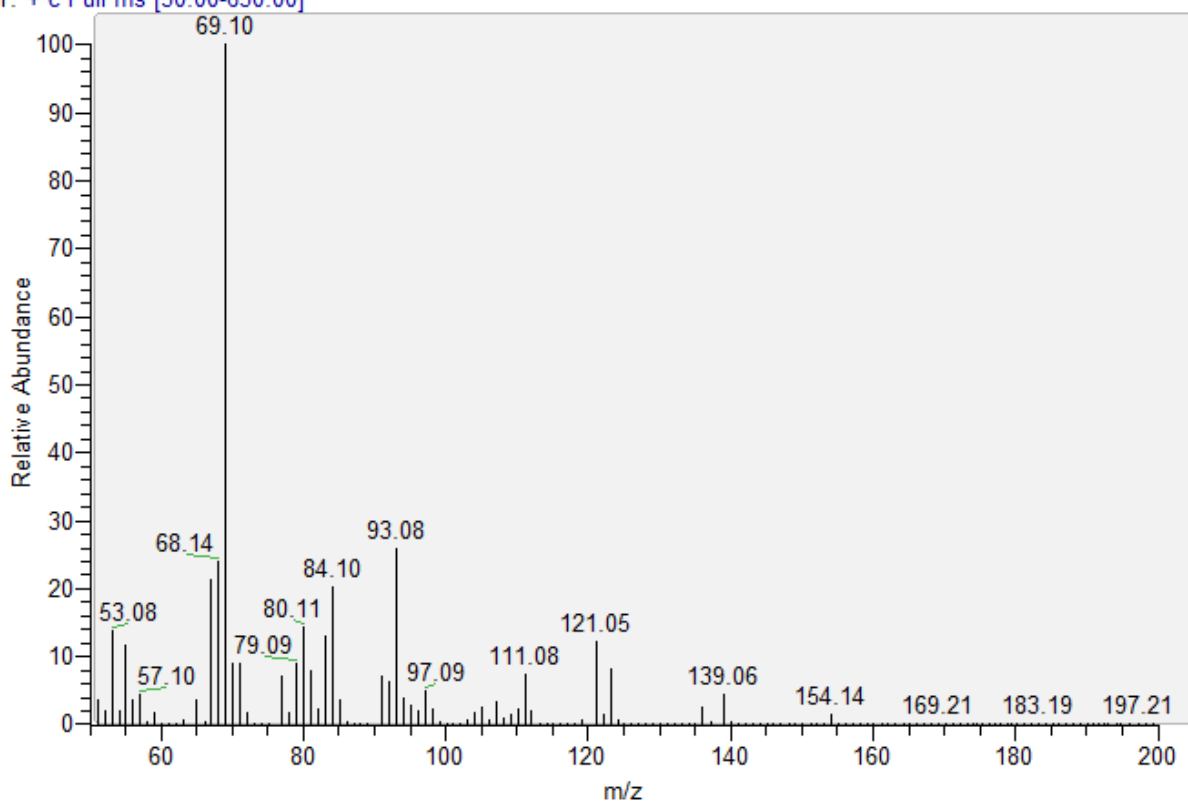
3053 #1353-1355 RT: 32.19-32.24 AV: 3 NL: 1.52E6  
T: + c Full ms [50.00-650.00]



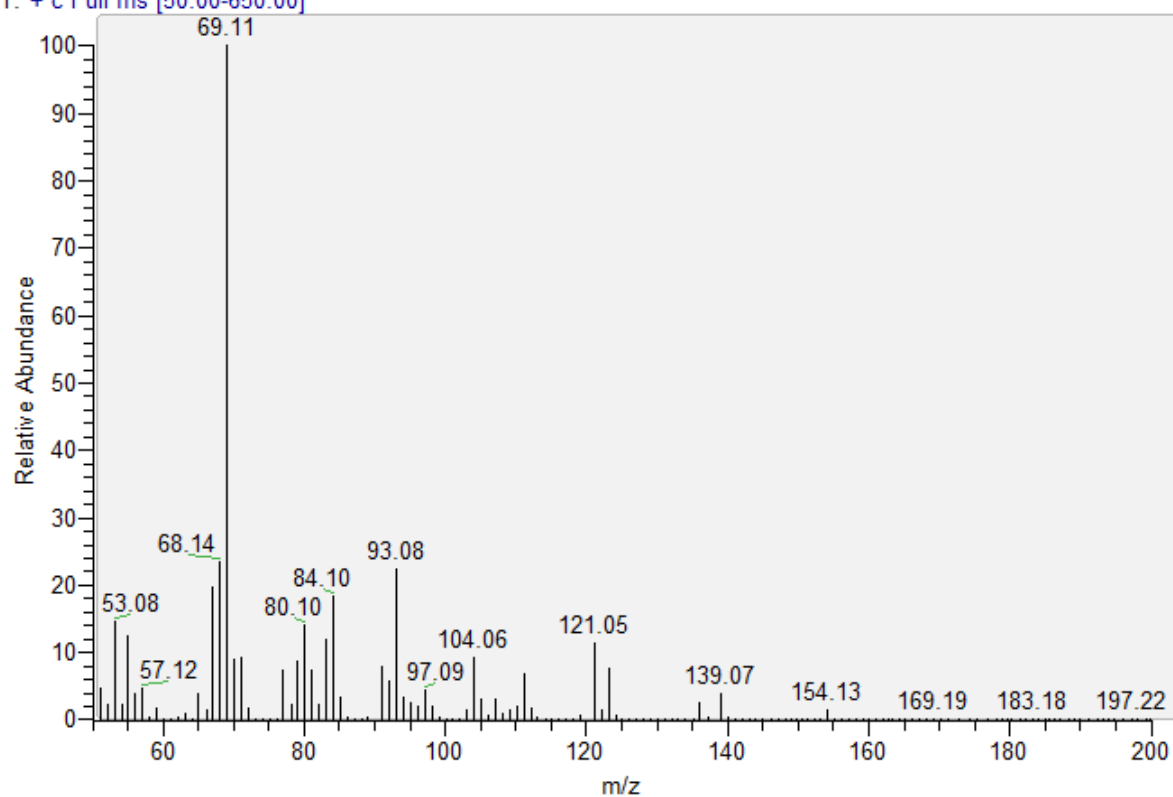
3018 #1359-1360 RT: 32.23-32.26 AV: 2 NL: 3.98E8  
T: + c Full ms [50.00-650.00]



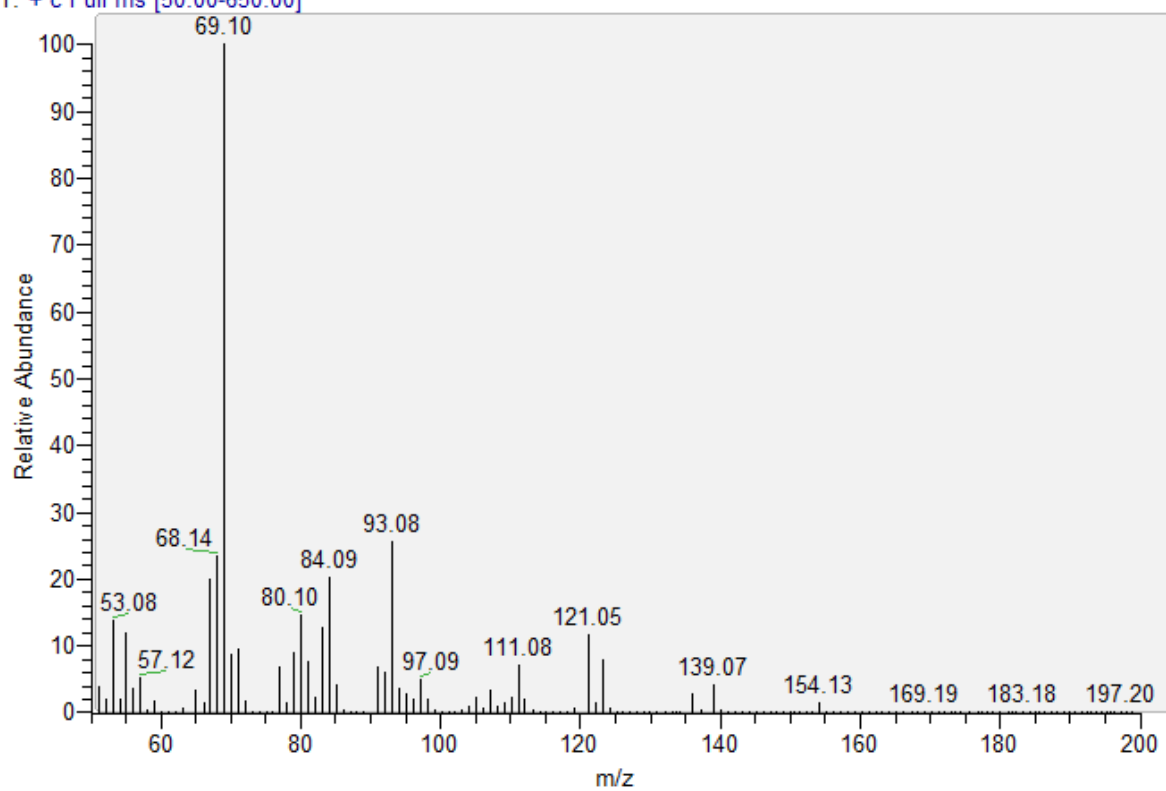
3021 #1356-1358 RT: 32.25-32.30 AV: 3 NL: 3.79E8  
T: + c Full ms [50.00-650.00]



3075 #1353-1354 RT: 32.21-32.24 AV: 2 NL: 2.88E8  
T: + c Full ms [50.00-650.00]



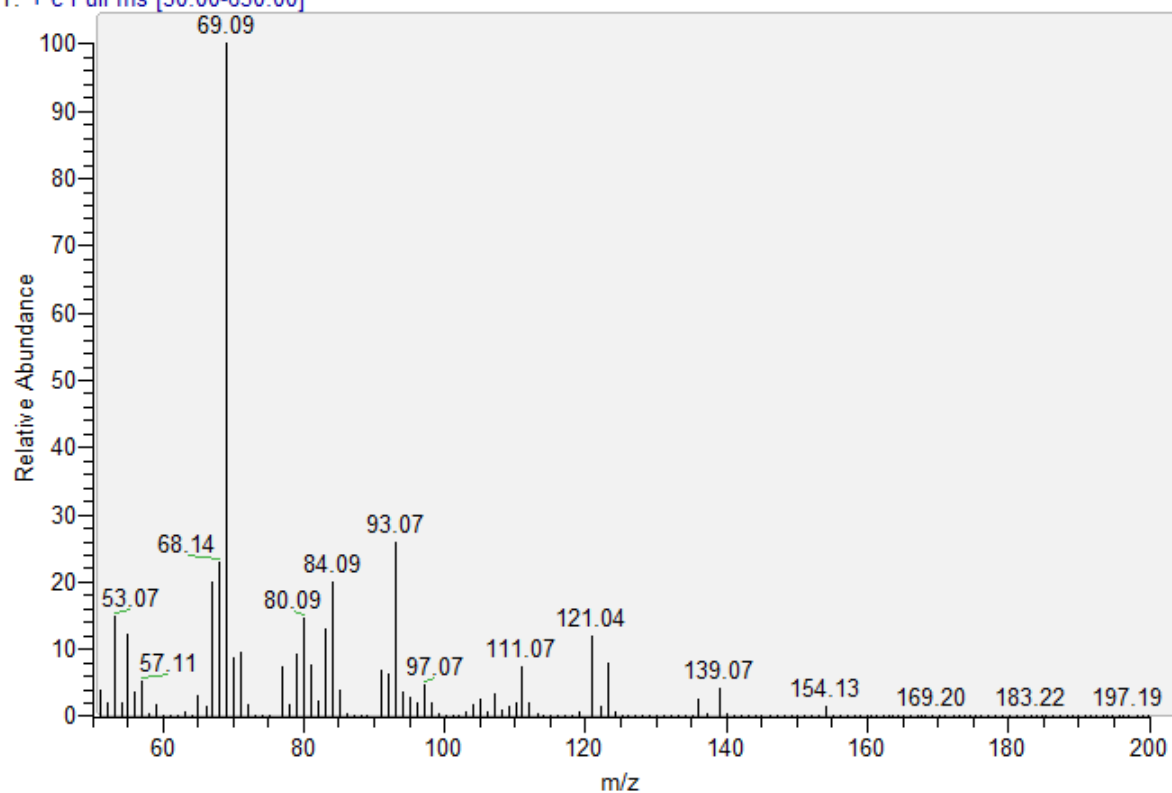
3074 #1356 RT: 32.24 AV: 1 NL: 3.65E8  
T: + c Full ms [50.00-650.00]



3073 #1354 RT: 32.23 AV: 1 NL: 3.36E8



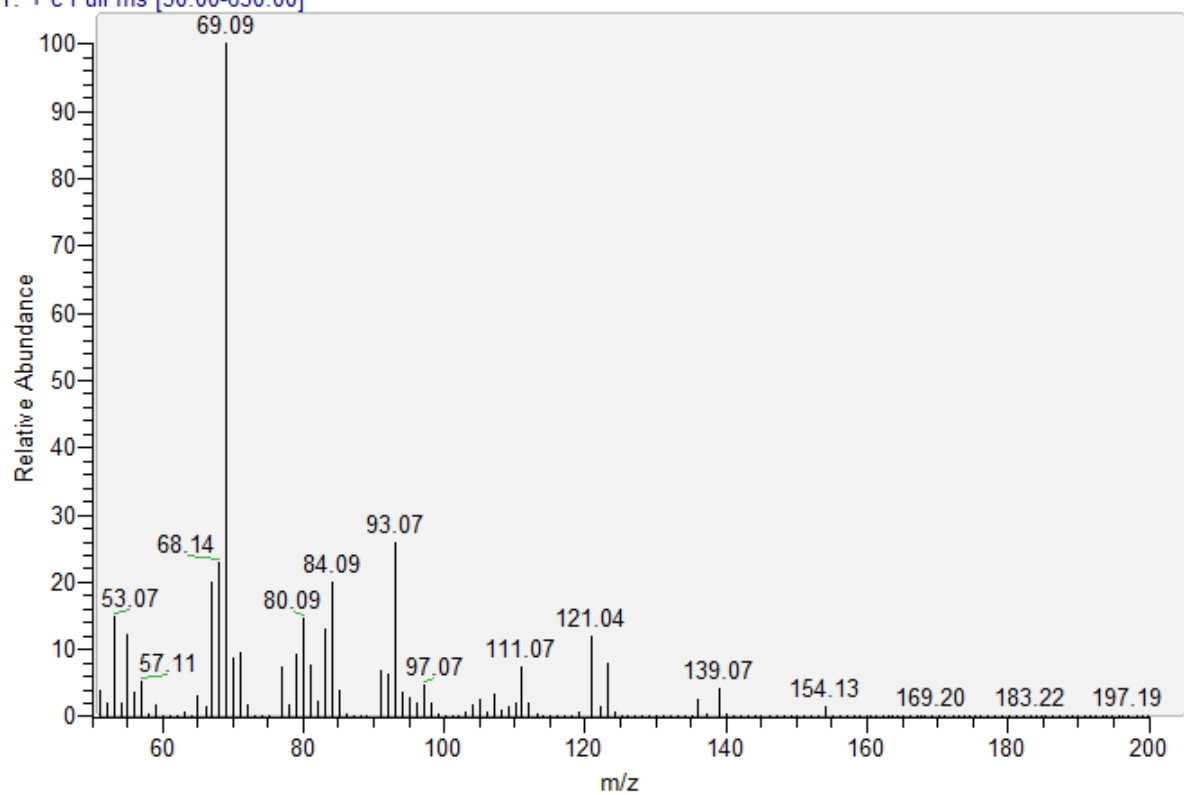
T: + c Full ms [50.00-650.00]



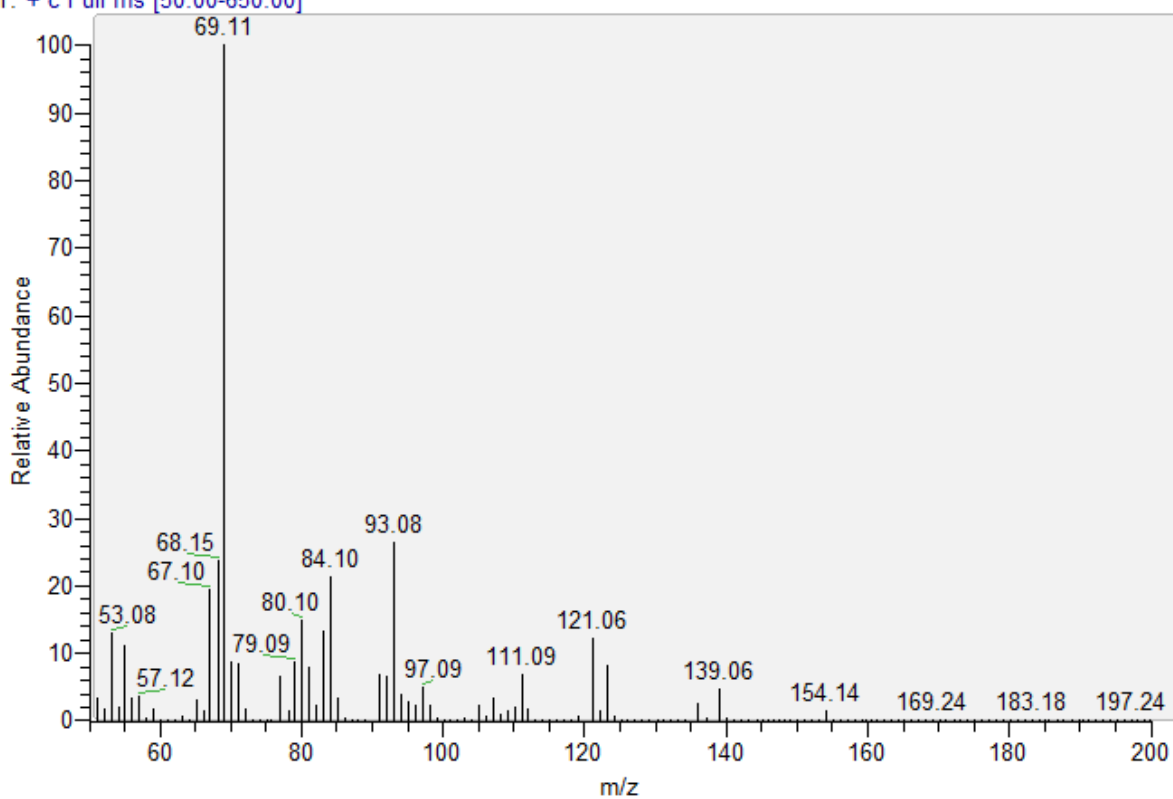
3073 #1354 RT: 32.23 AV: 1 NL: 3.36E8



T: + c Full ms [50.00-650.00]



3072 #1355 RT: 32.27 AV: 1 NL: 4.20E8  
T: + c Full ms [50.00-650.00]

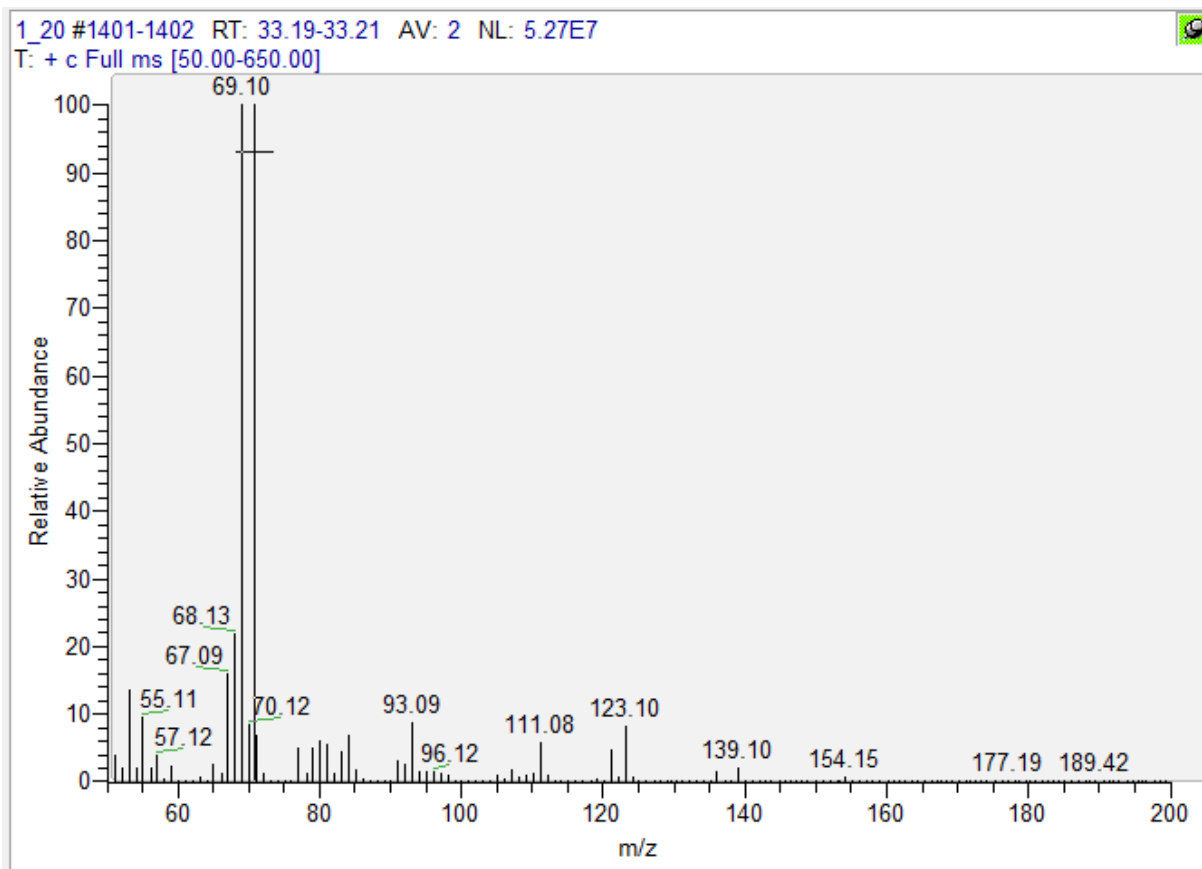


In 3070: ND

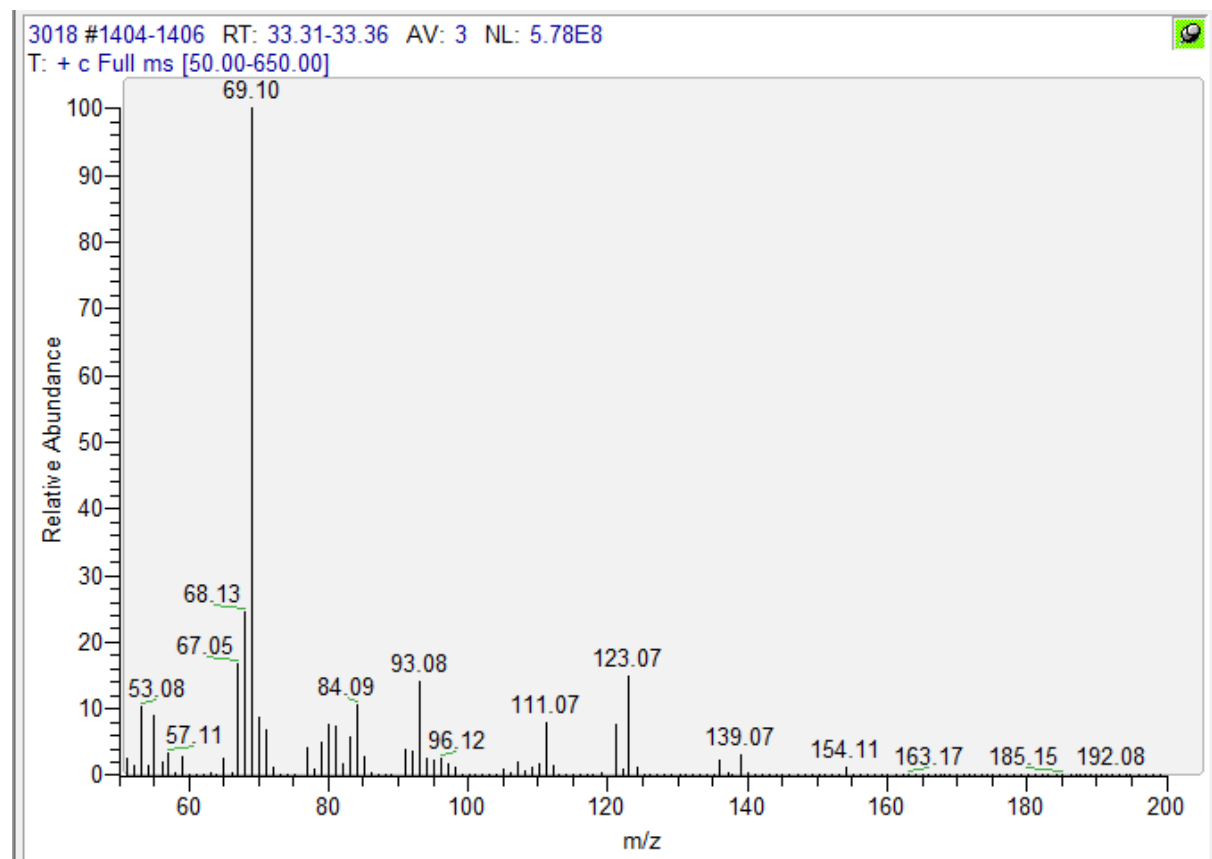


Geraniol:

Reference:



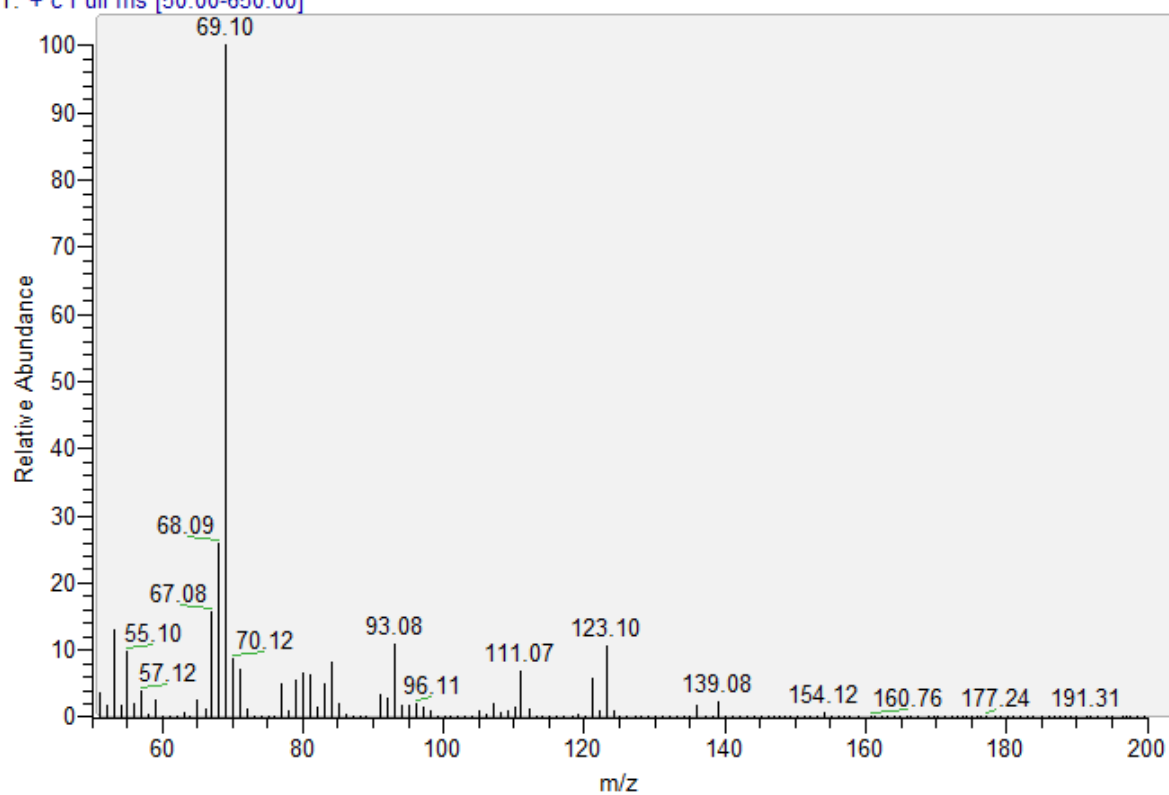
Samples:



3053 #1396-1397 RT: 33.22-33.24 AV: 2 NL: 1.87E8



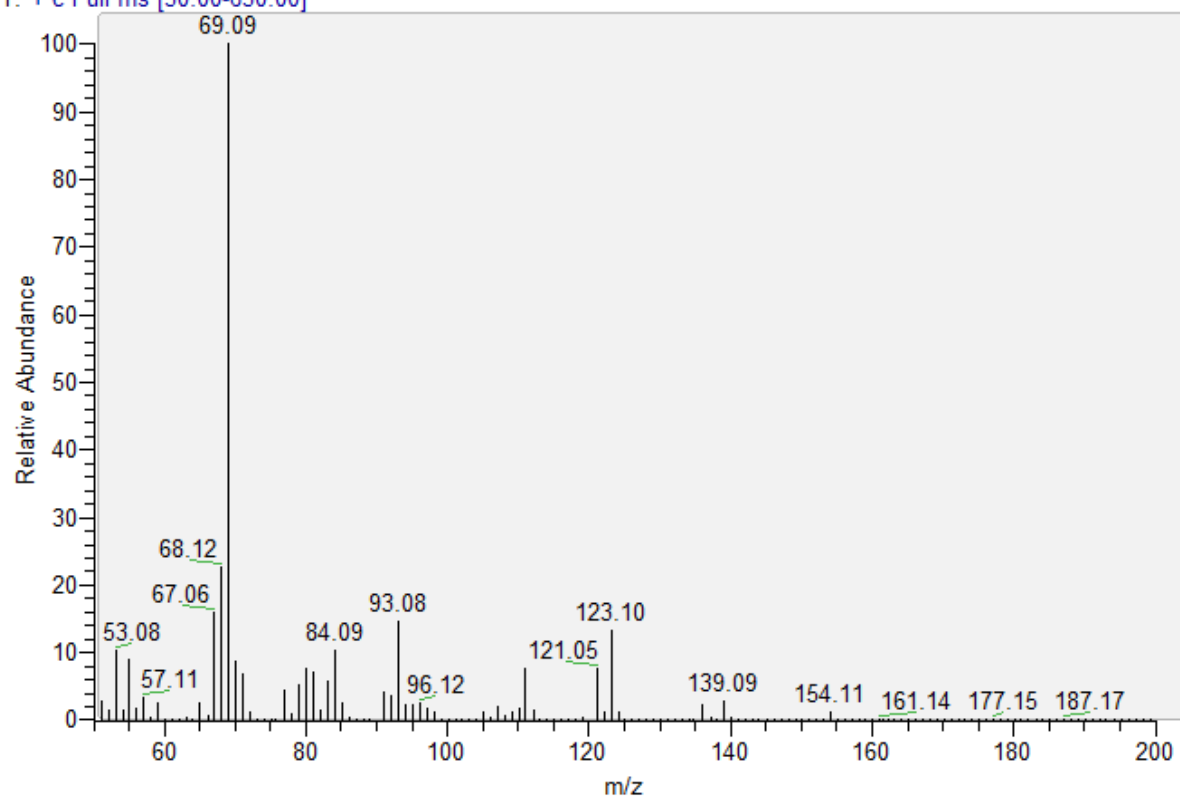
T: + c Full ms [50.00-650.00]



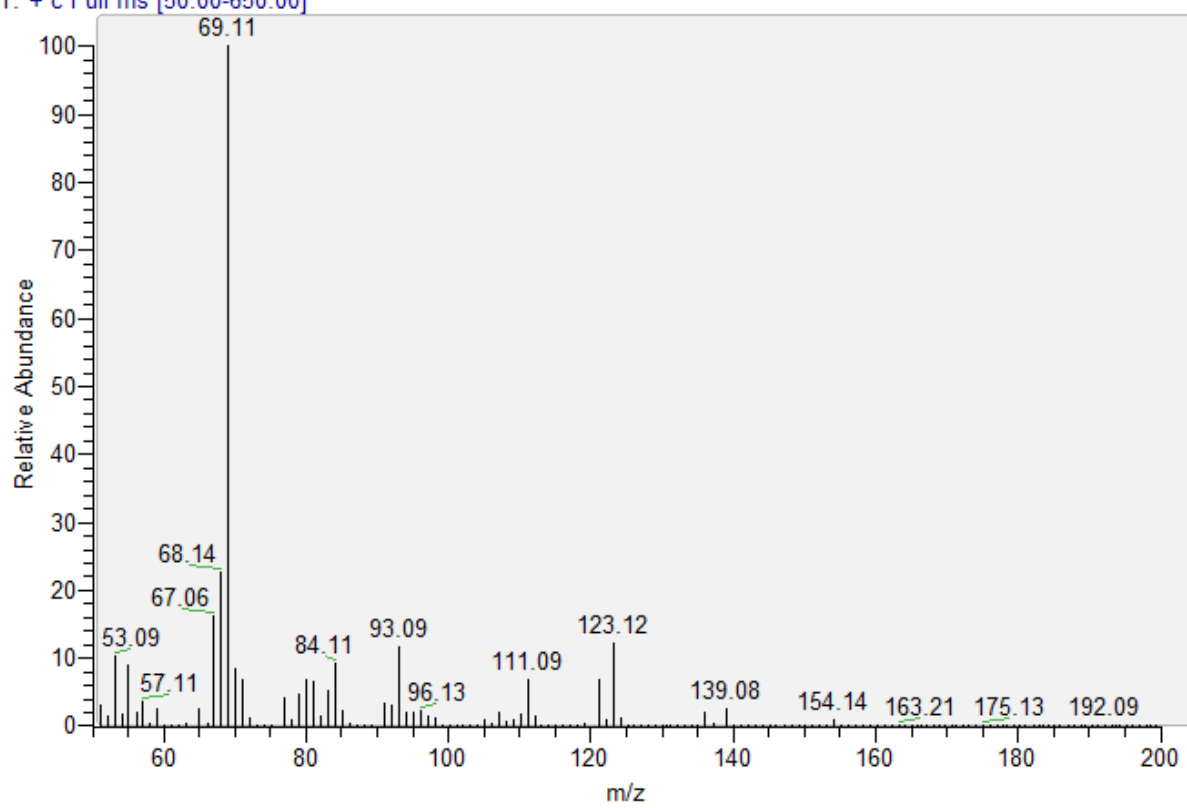
3058 #1396-1399 RT: 33.29-33.37 AV: 4 NL: 5.34E8



T: + c Full ms [50.00-650.00]



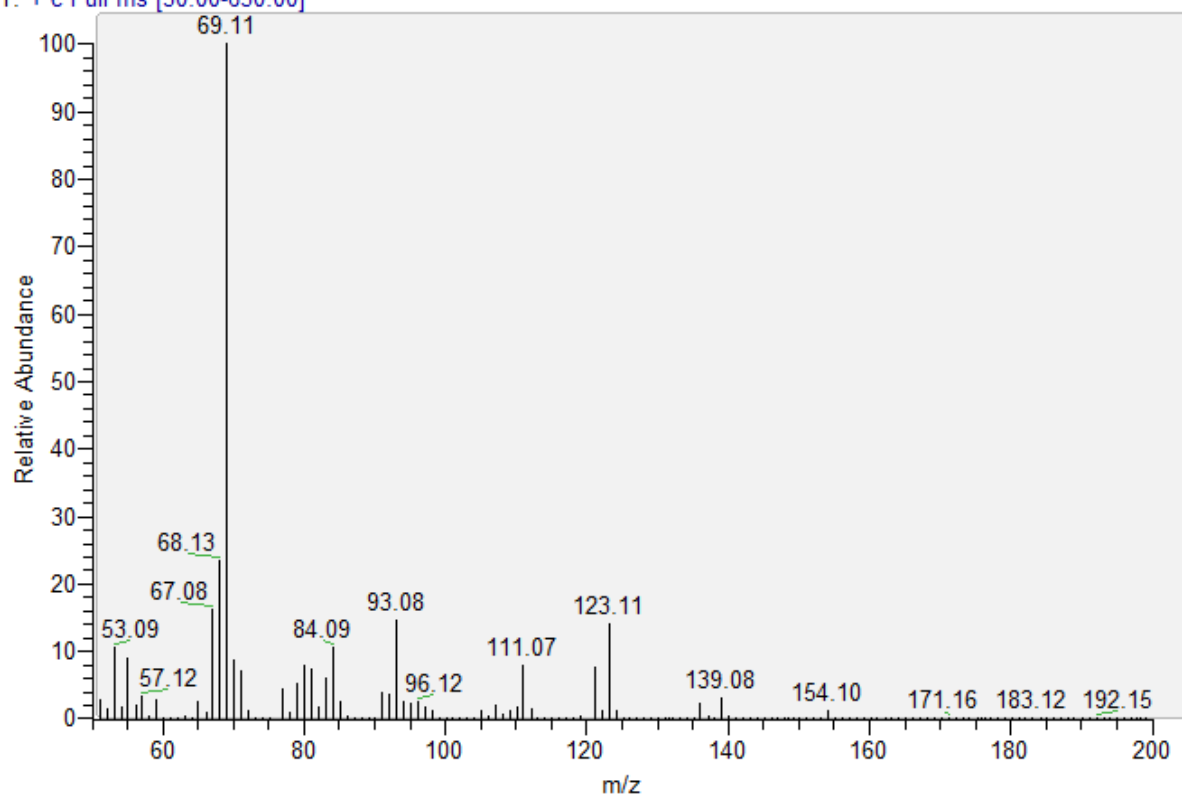
3057 #1403-1404 RT: 33.27-33.29 AV: 2 NL: 4.75E8  
T: + c Full ms [50.00-650.00]



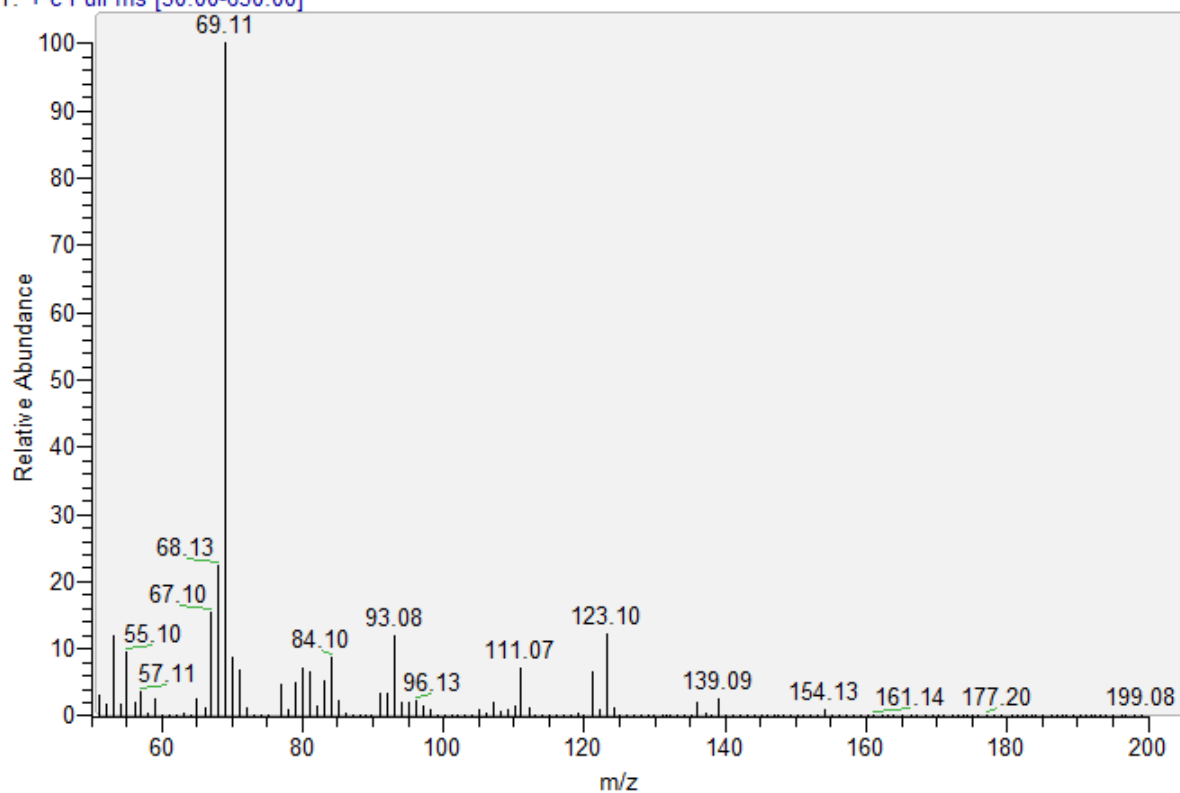
3021 #1400-1403 RT: 33.30-33.37 AV: 4 NL: 5.12E8



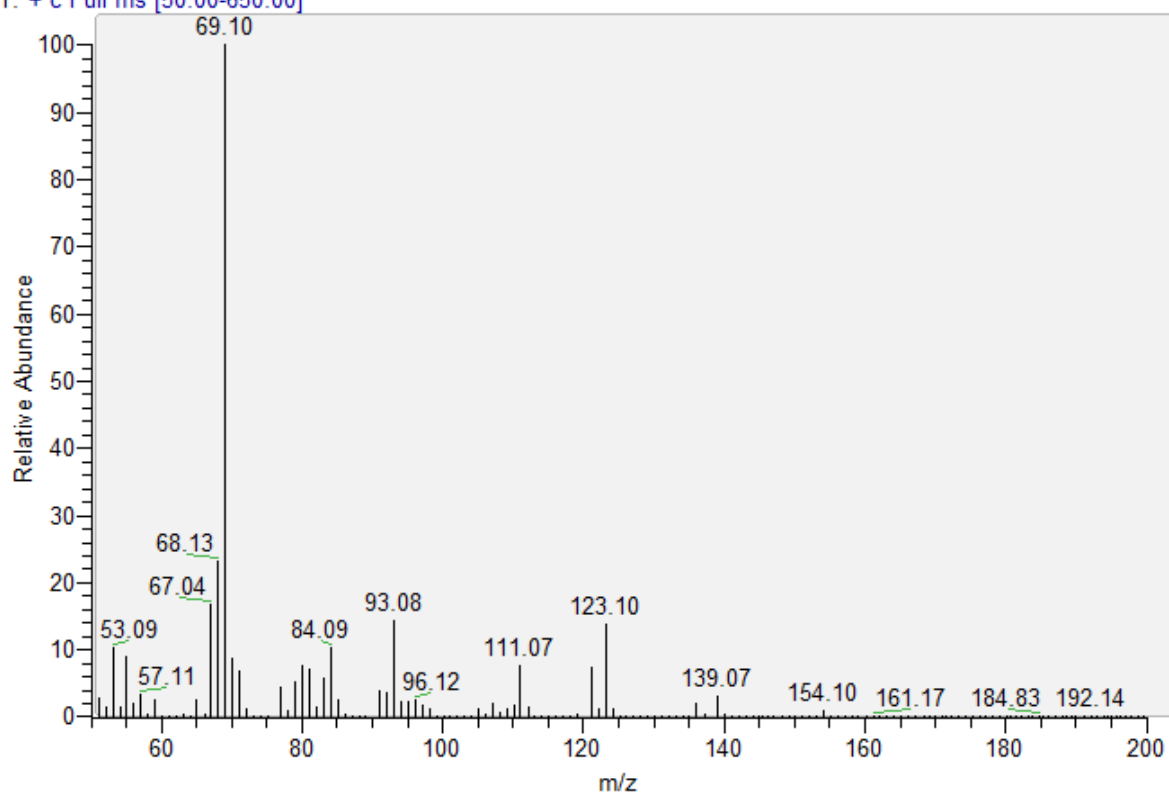
T: + c Full ms [50.00-650.00]



3075 #1396-1398 RT: 33.24-33.29 AV: 3 NL: 3.22E8  
T: + c Full ms [50.00-650.00]

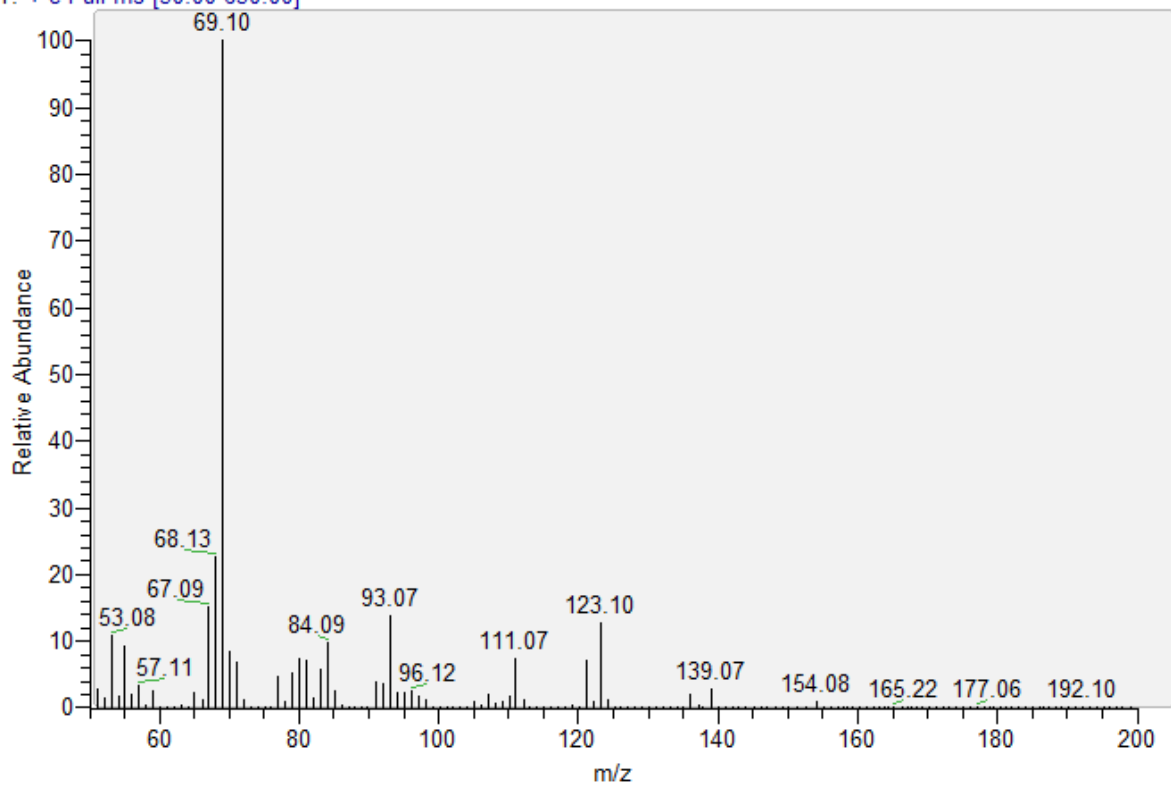


3074 #1400-1402 RT: 33.29-33.34 AV: 3 NL: 5.12E8  
T: + c Full ms [50.00-650.00]

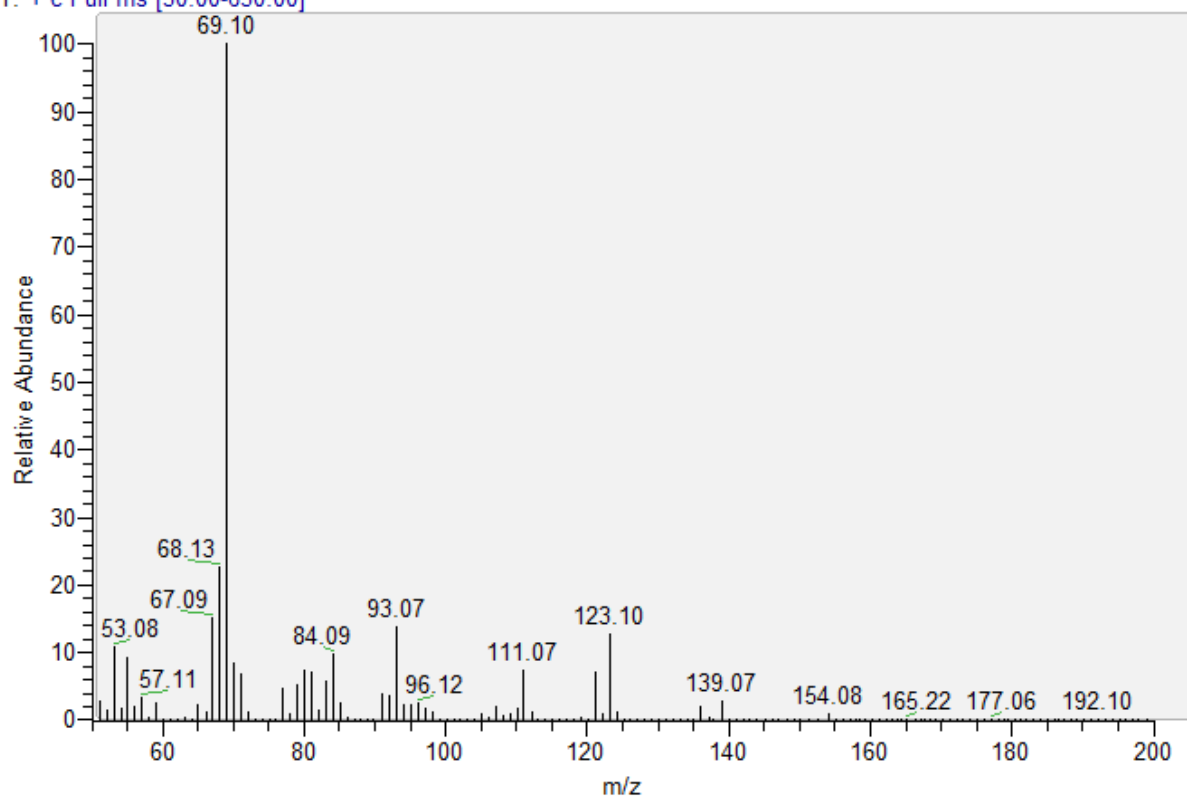




3073 #1398-1400 RT: 33.27-33.32 AV: 3 NL: 4.79E8  
T: + c Full ms [50.00-650.00]



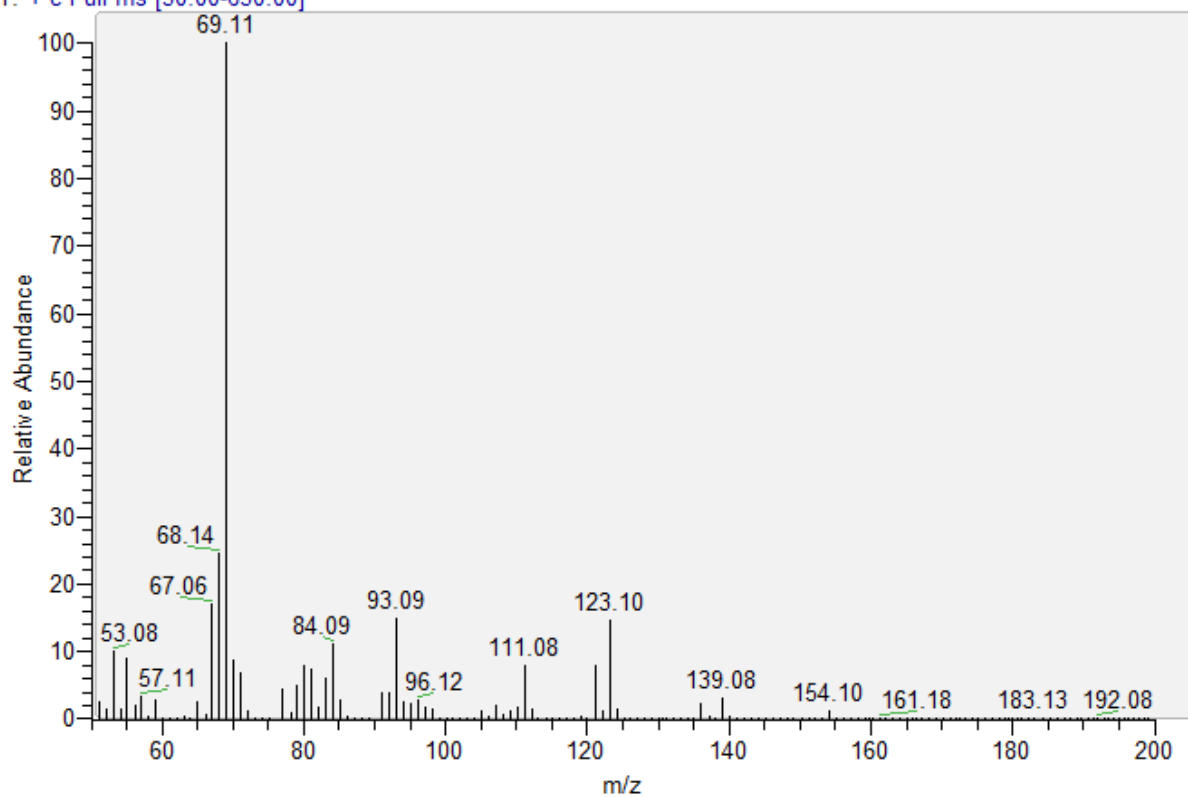
3073 #1398-1400 RT: 33.27-33.32 AV: 3 NL: 4.79E8  
T: + c Full ms [50.00-650.00]



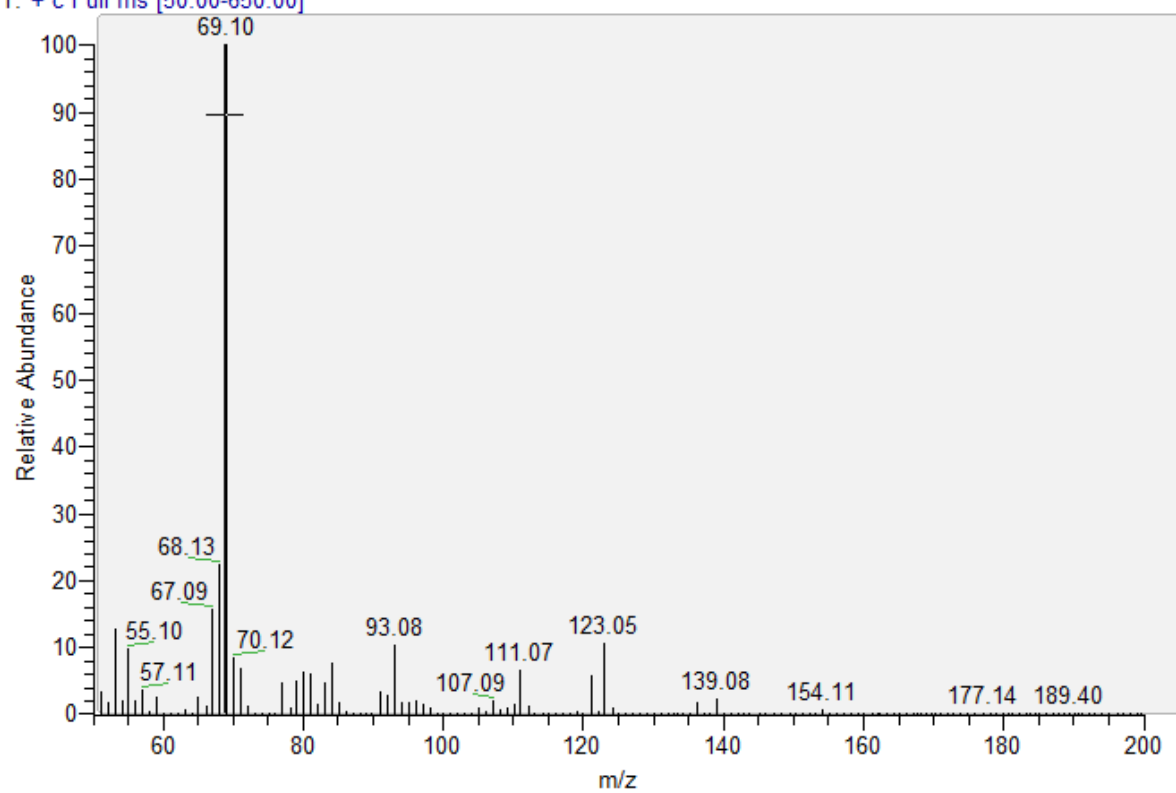
3072 #1398-1402 RT: 33.30-33.39 AV: 5 NL: 5.58E8



T: + c Full ms [50.00-650.00]

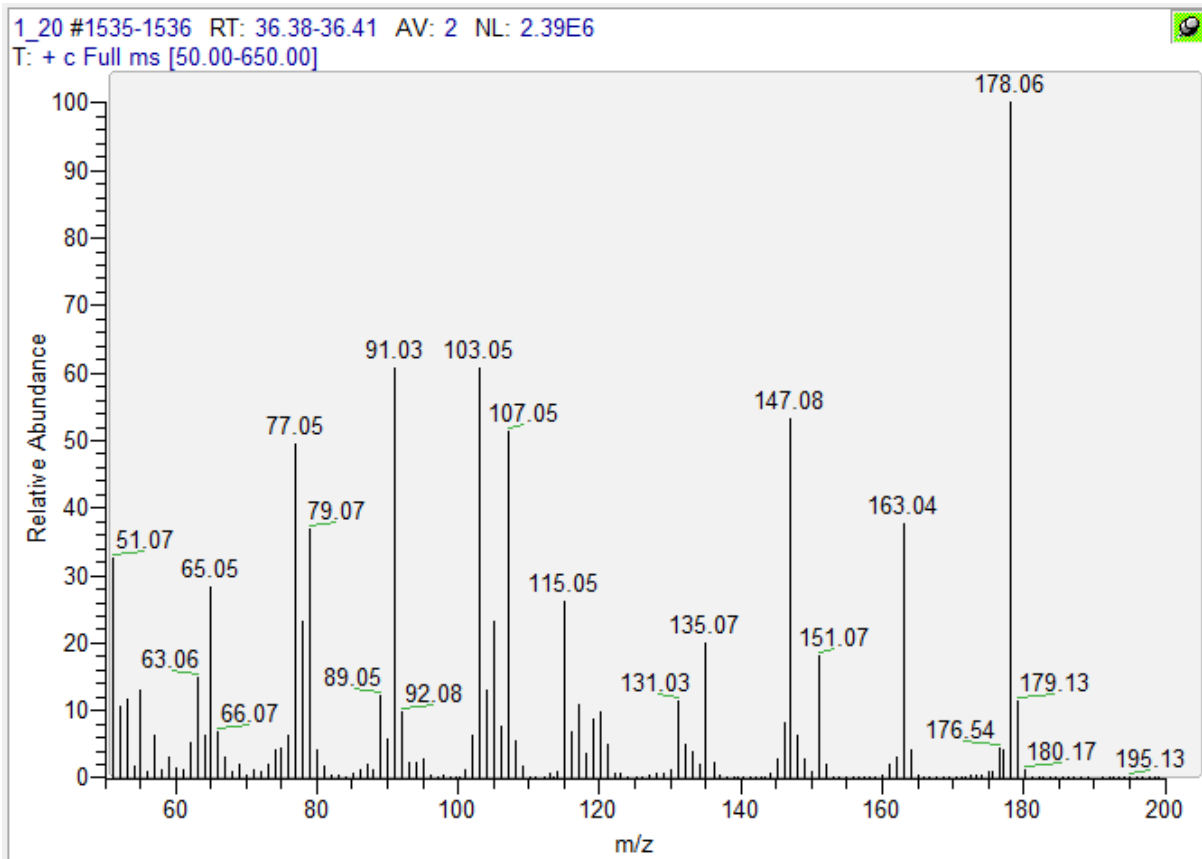


3070 #1397-1398 RT: 33.20-33.23 AV: 2 NL: 1.56E8  
T: + c Full ms [50.00-650.00]

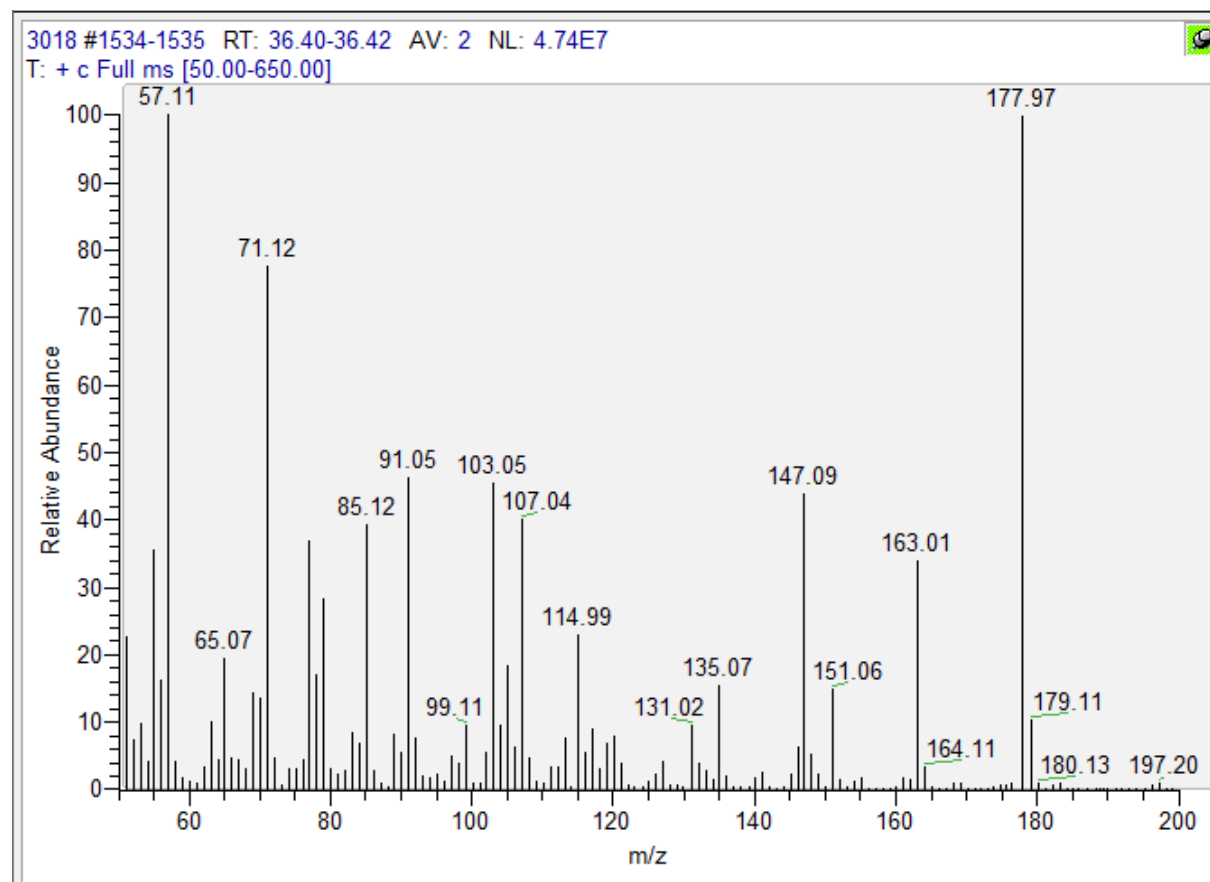


Methyleugenol

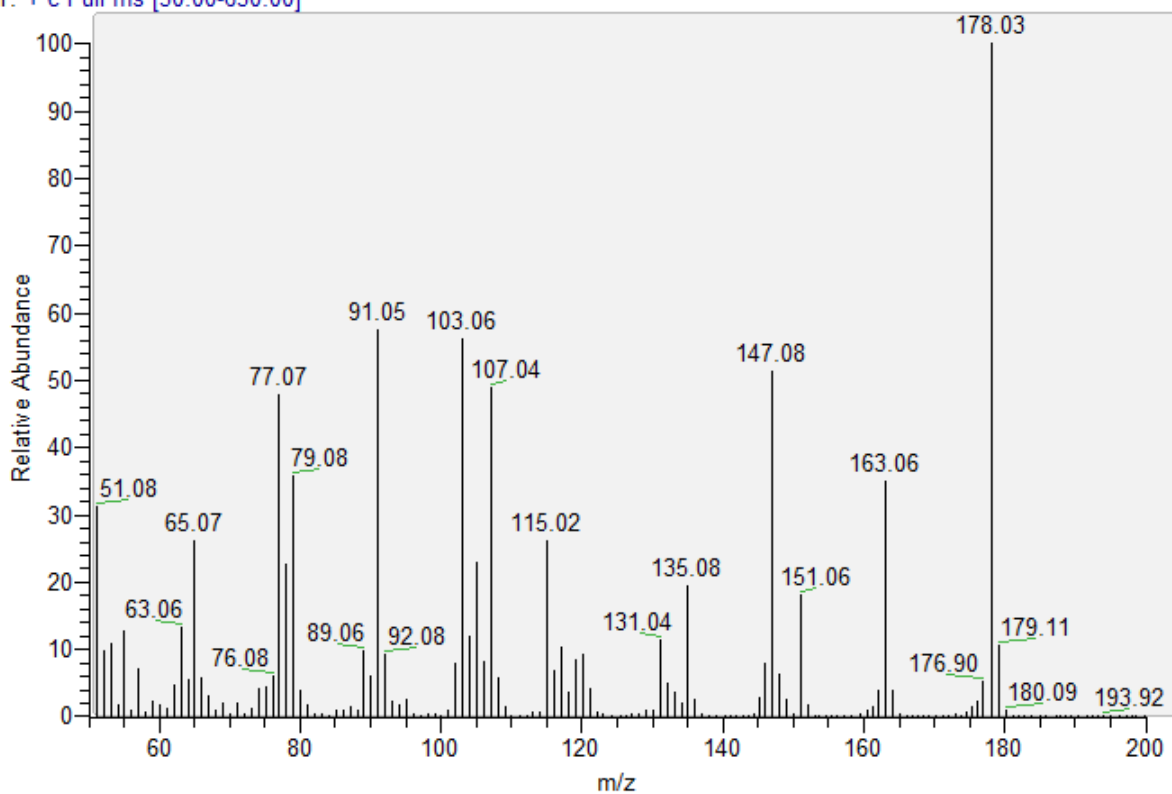
Reference:



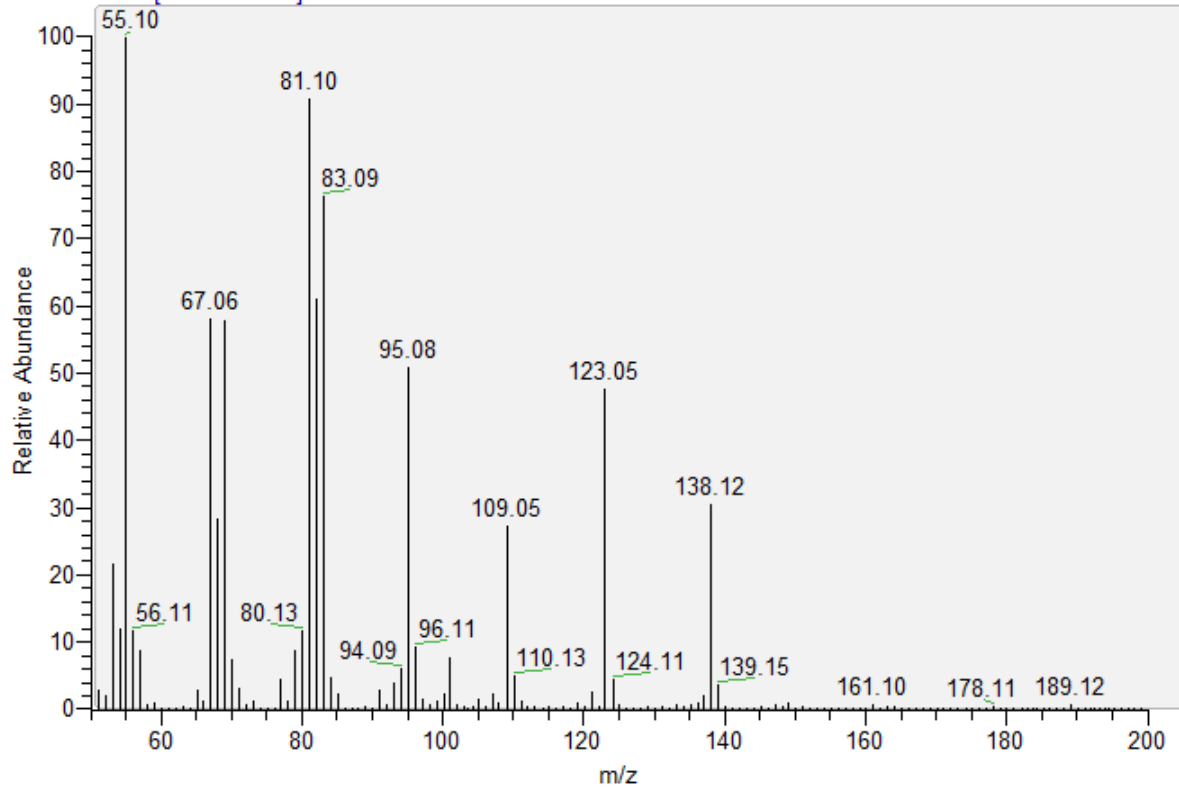
Samples:"



3053 #1529-1530 RT: 36.38-36.41 AV: 2 NL: 6.88E6  
T: + c Full ms [50.00-650.00]

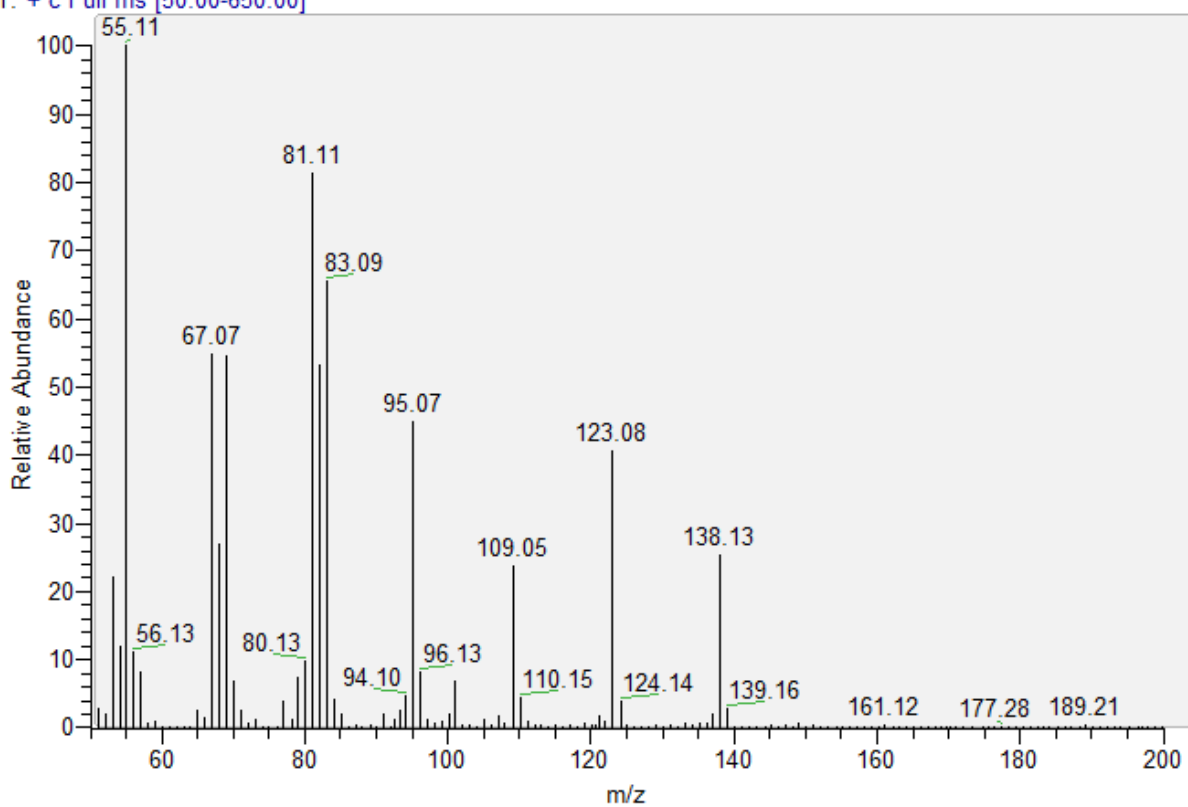


3058 #1524-1526 RT: 36.35-36.40 AV: 3 NL: 1.20E7  
T: + c Full ms [50.00-650.00]

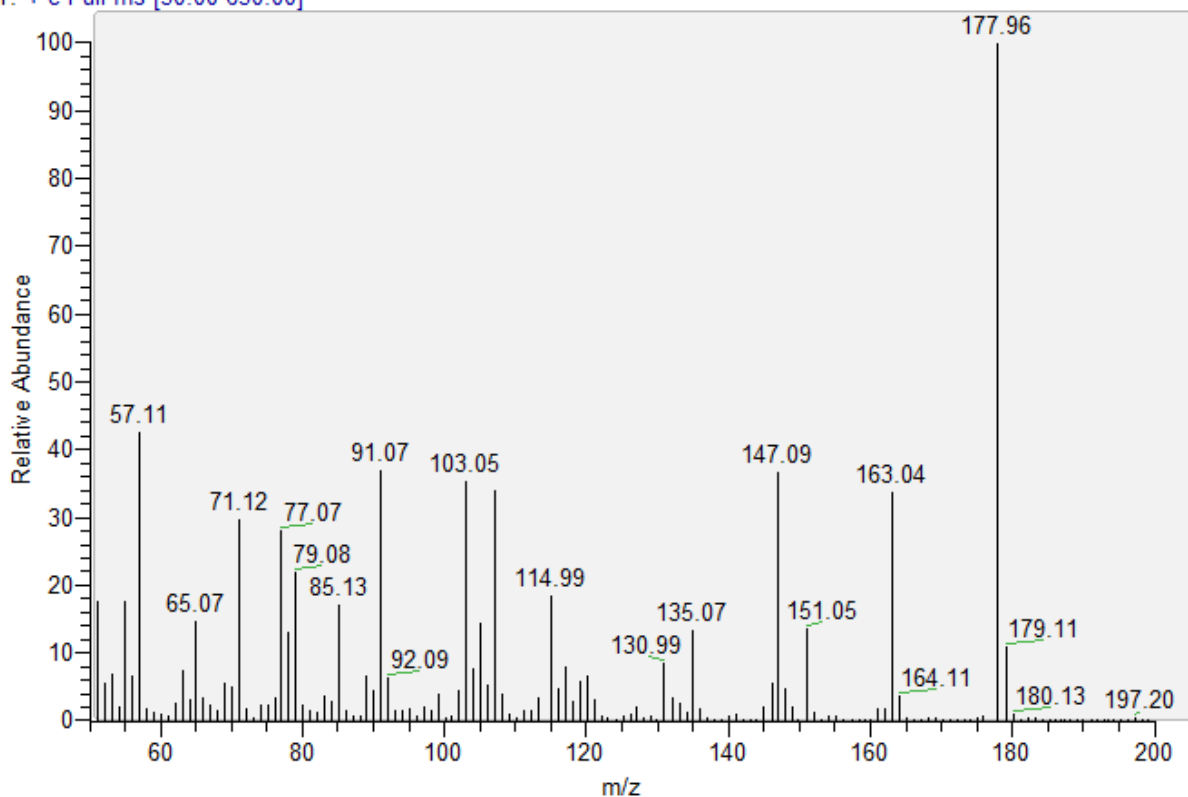




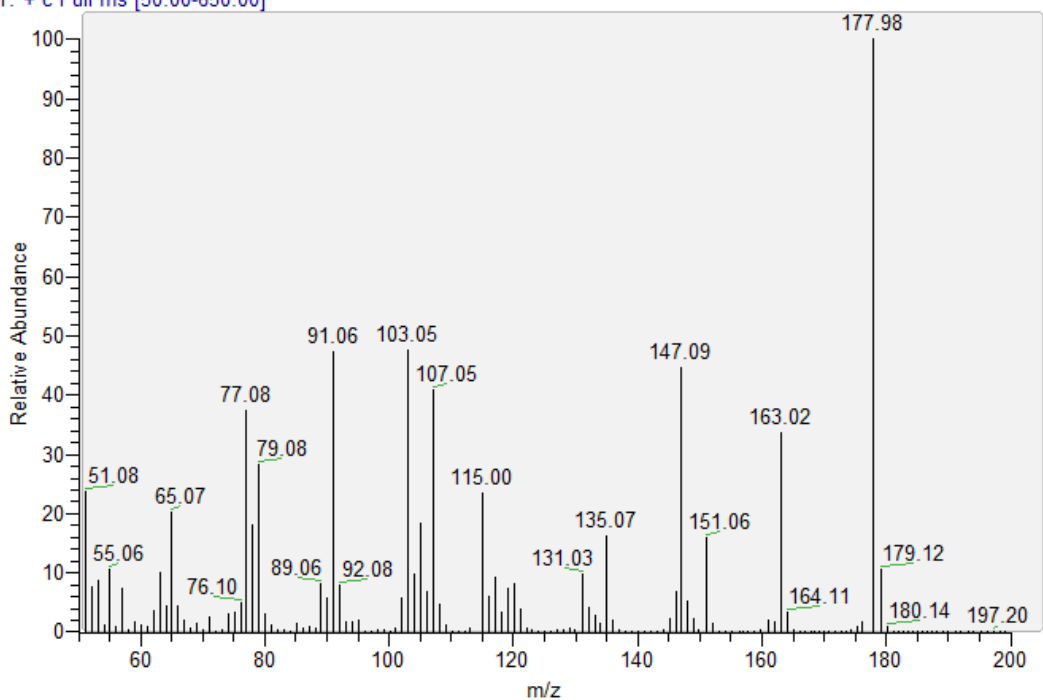
3057 #1532-1533 RT: 36.34-36.36 AV: 2 NL: 7.53E6  
T: + c Full ms [50.00-650.00]



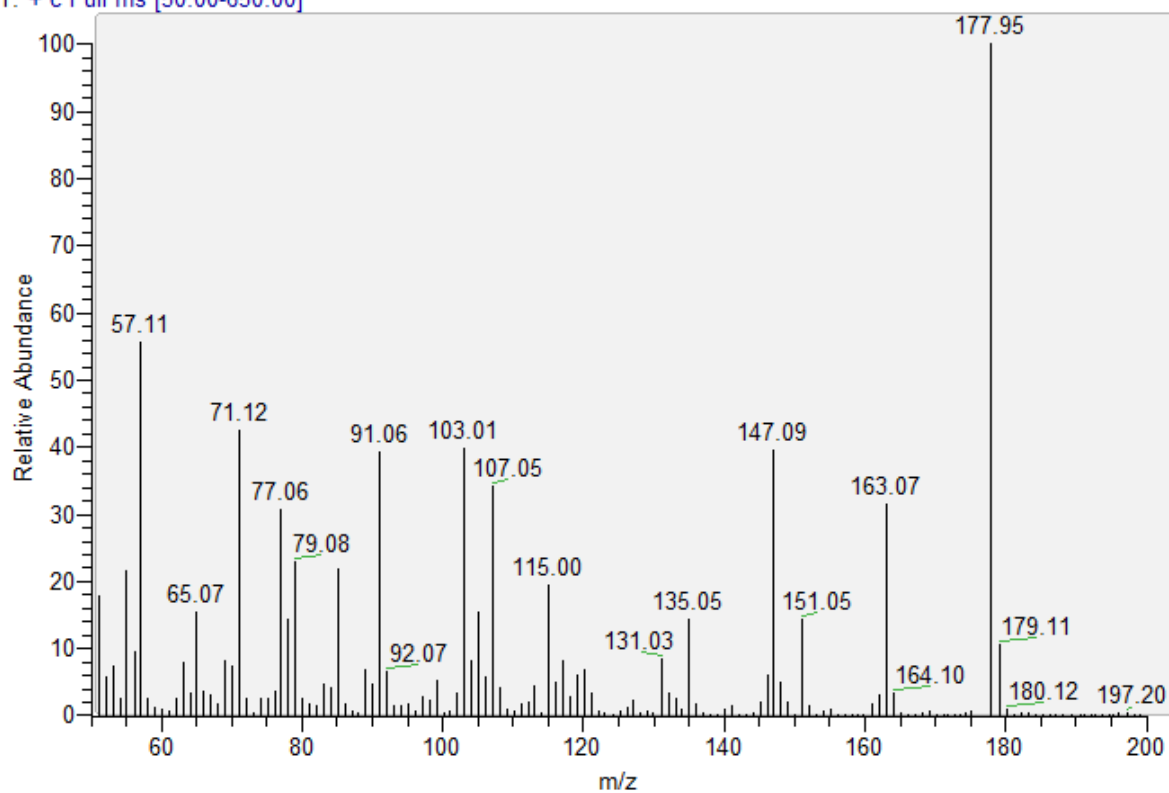
3021 #1531-1532 RT: 36.42-36.44 AV: 2 NL: 1.17E8  
T: + c Full ms [50.00-650.00]



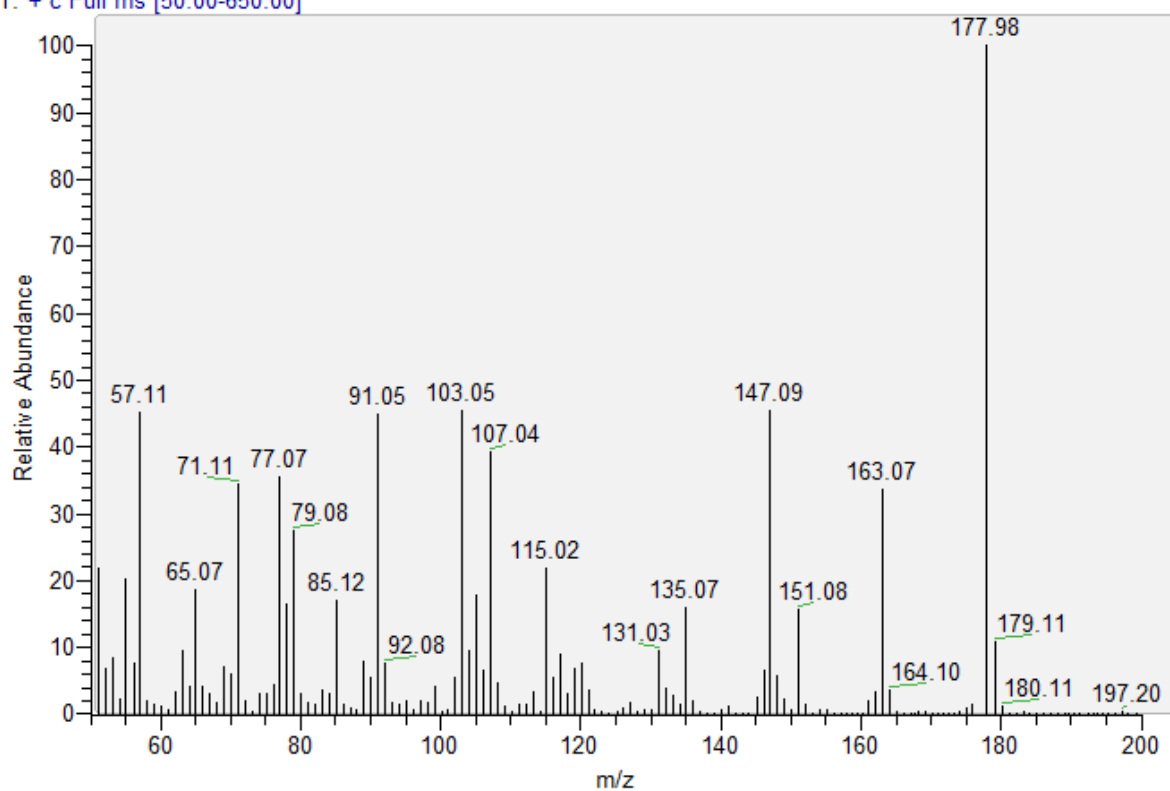
3075 #1529-1530 RT: 36.41-36.44 AV: 2 NL: 7.16E7  
T: + c Full ms [50.00-650.00]



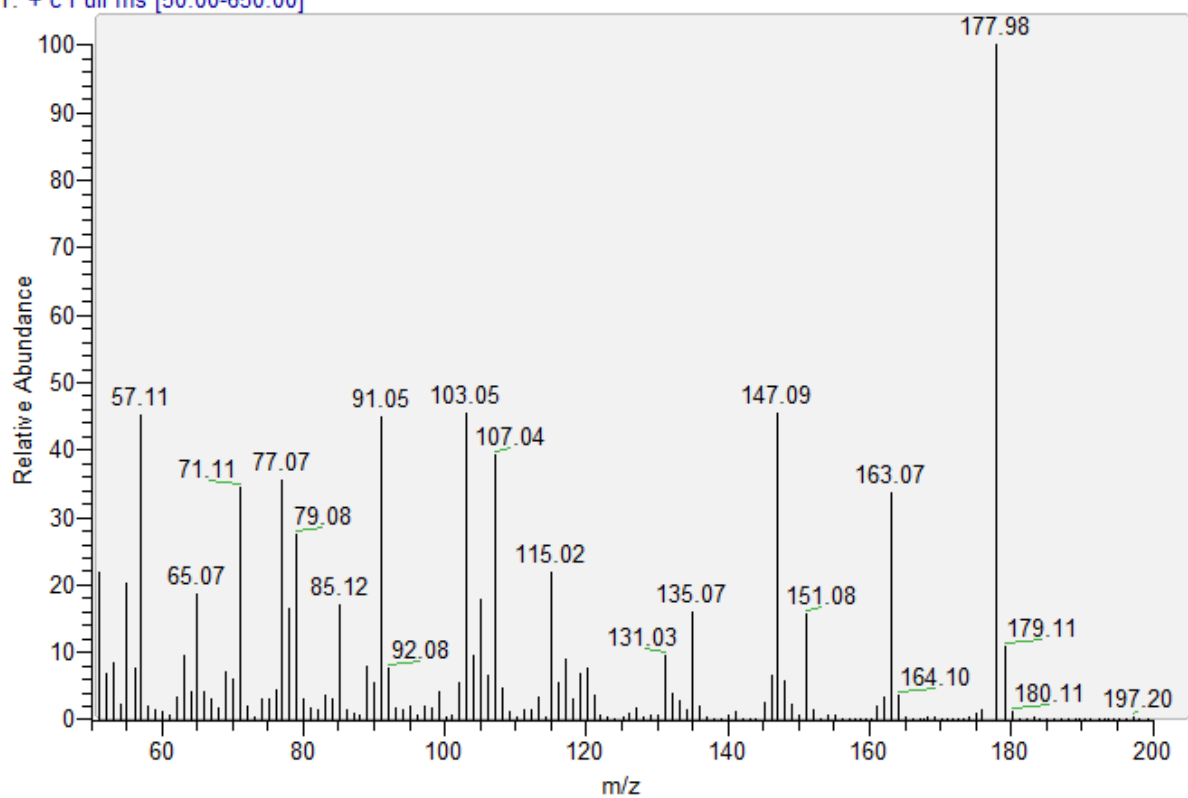
3074 #1530-1531 RT: 36.40-36.42 AV: 2 NL: 6.84E7  
T: + c Full ms [50.00-650.00]



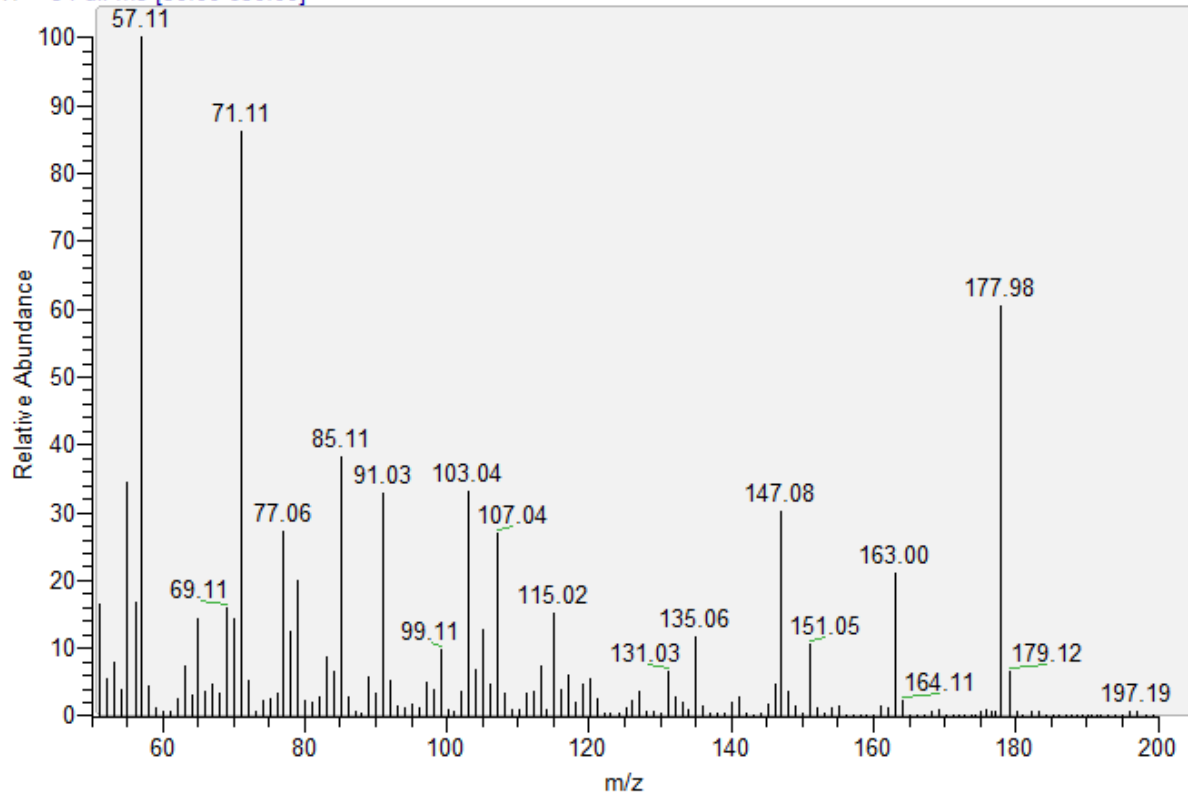
3073 #1529-1530 RT: 36.39-36.42 AV: 2 NL: 4.70E7  
T: + c Full ms [50.00-650.00]



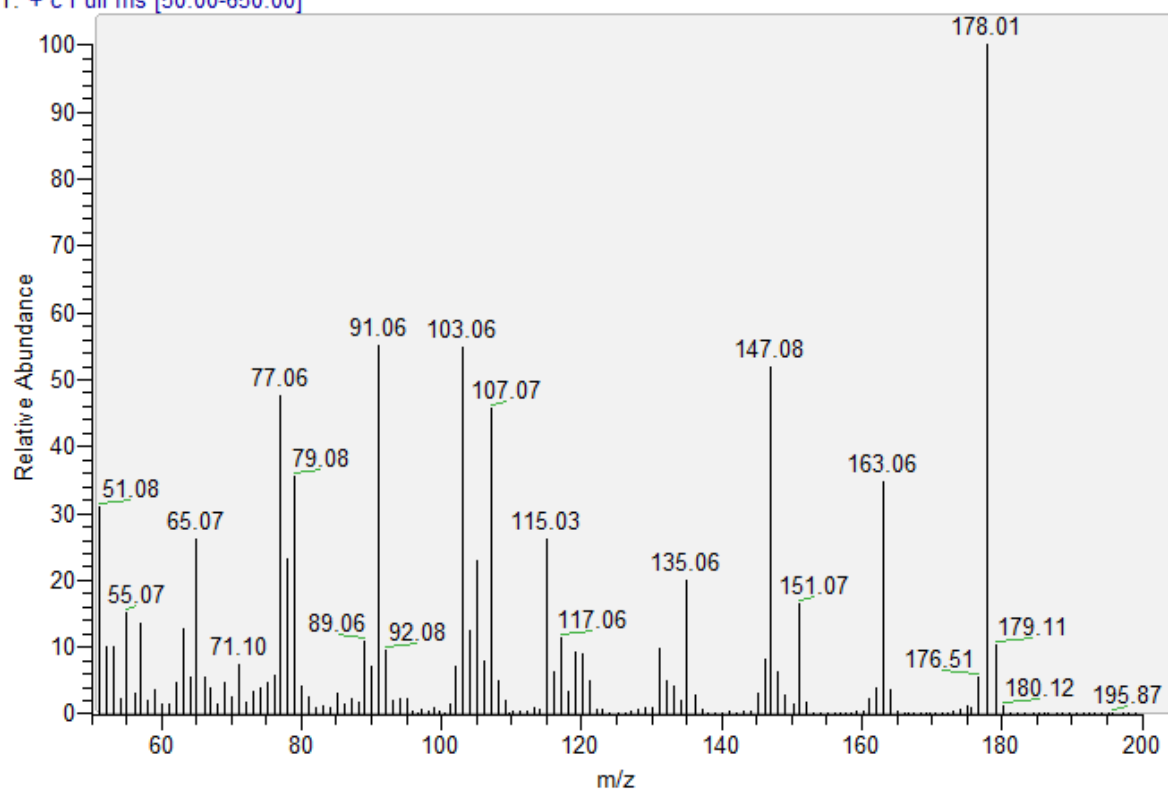
3073 #1529-1530 RT: 36.39-36.42 AV: 2 NL: 4.70E7  
T: + c Full ms [50.00-650.00]



3072 #1527-1529 RT: 36.37-36.42 AV: 3 NL: 2.19E7  
T: + c Full ms [50.00-650.00]

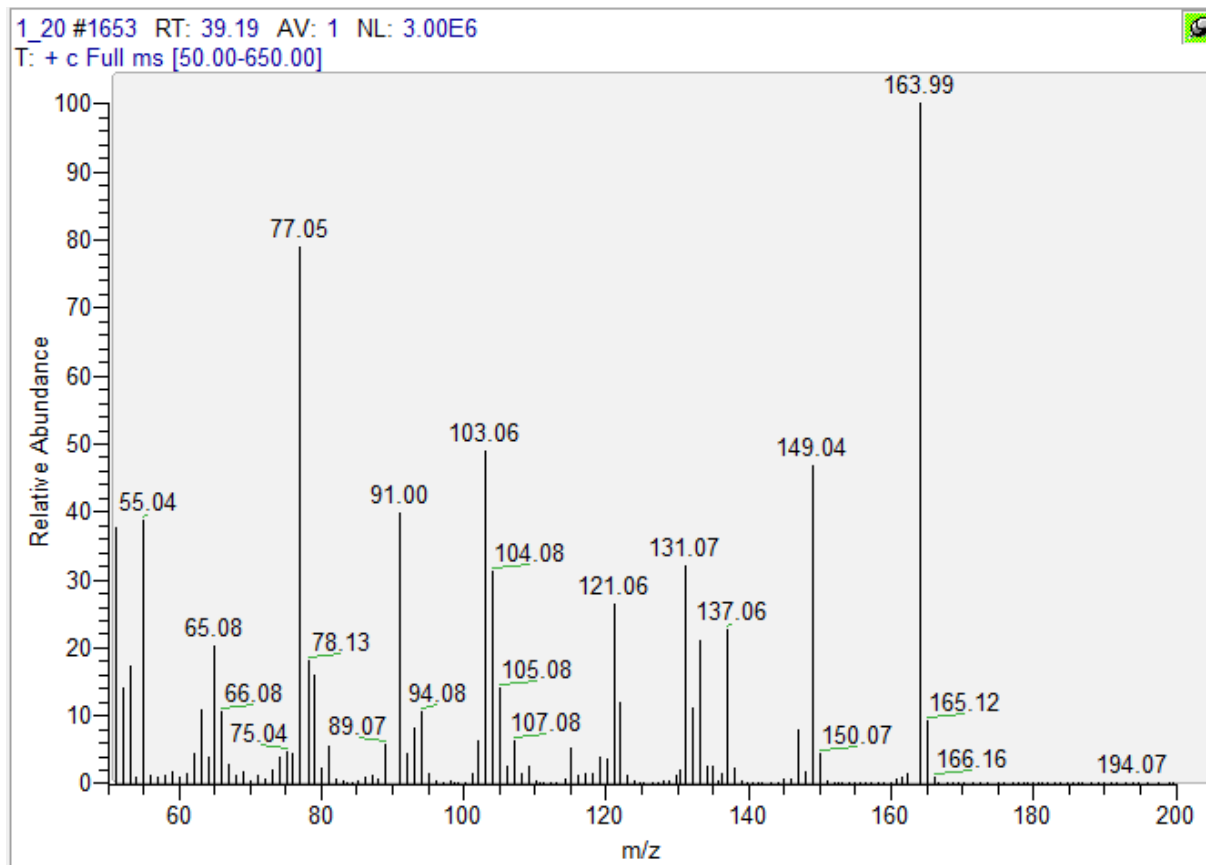


3070 #1530-1531 RT: 36.37-36.40 AV: 2 NL: 1.42E6  
T: + c Full ms [50.00-650.00]



Eugenol

Reference:

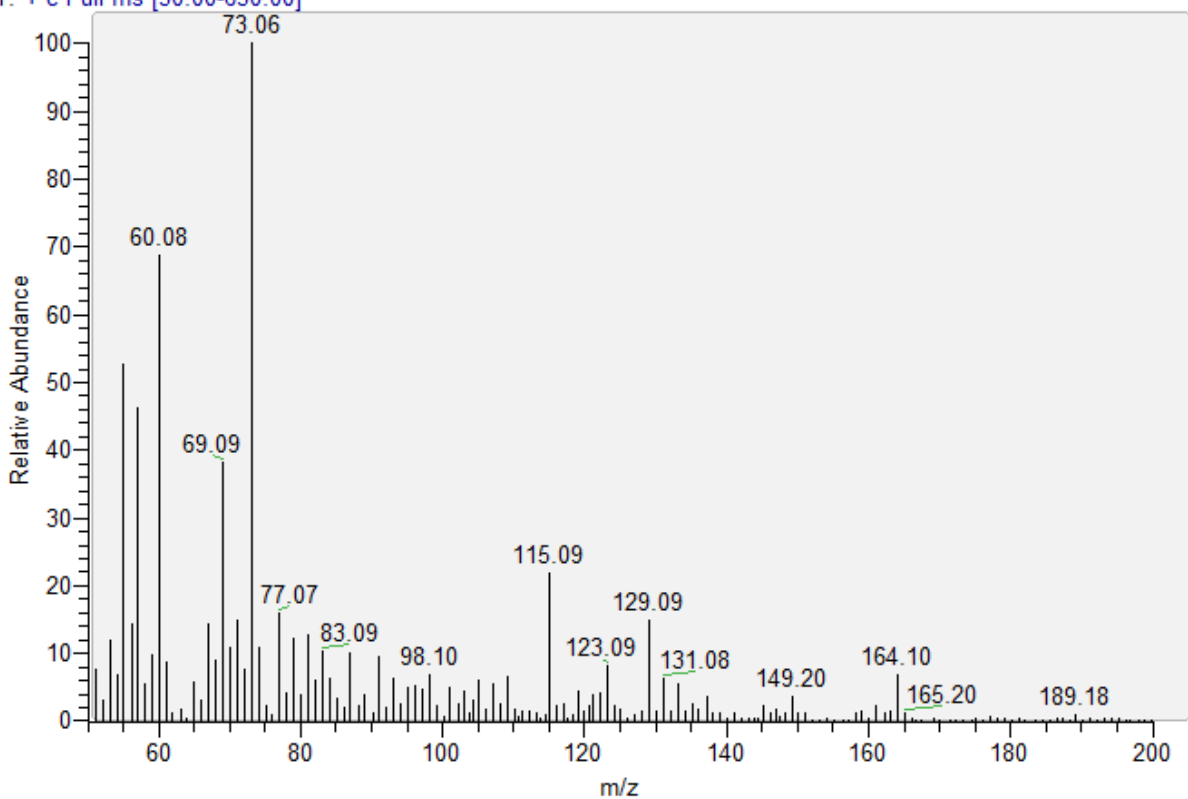




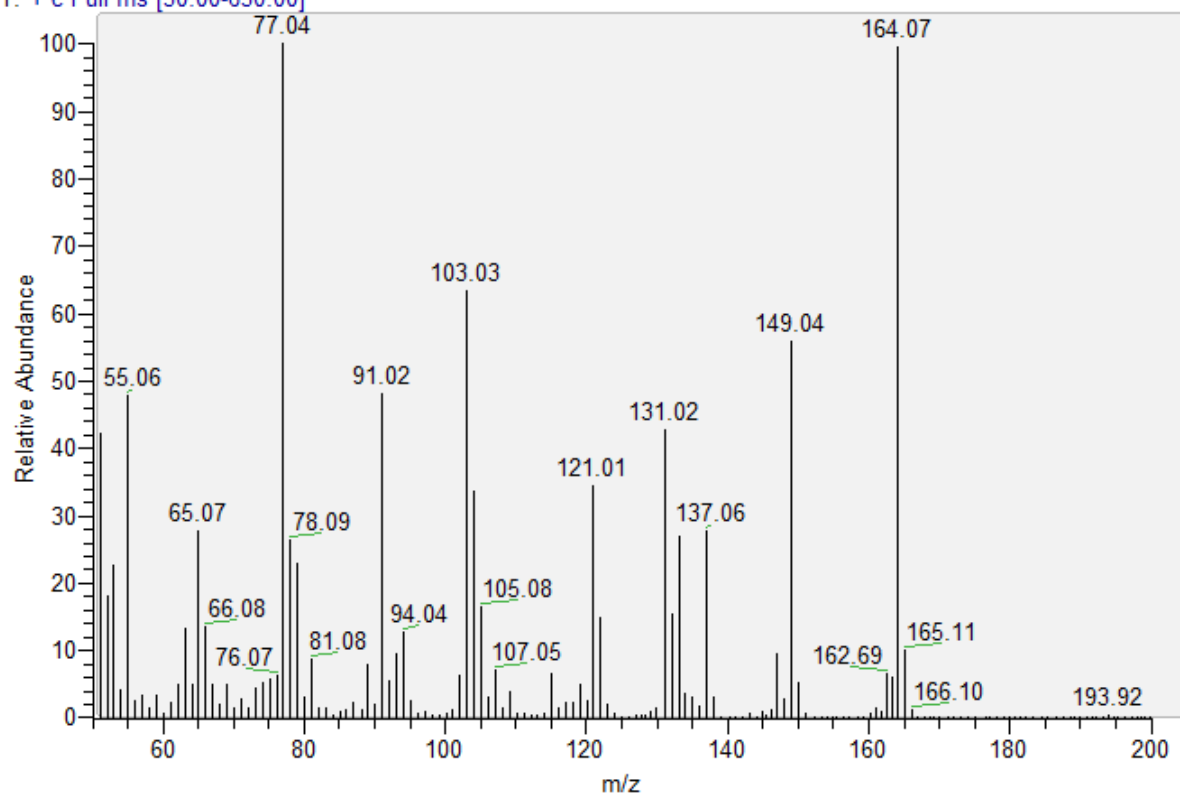
Samples:

3021 #1656 RT: 39.40 AV: 1 NL: 9.07E5

T: + c Full ms [50.00-650.00]

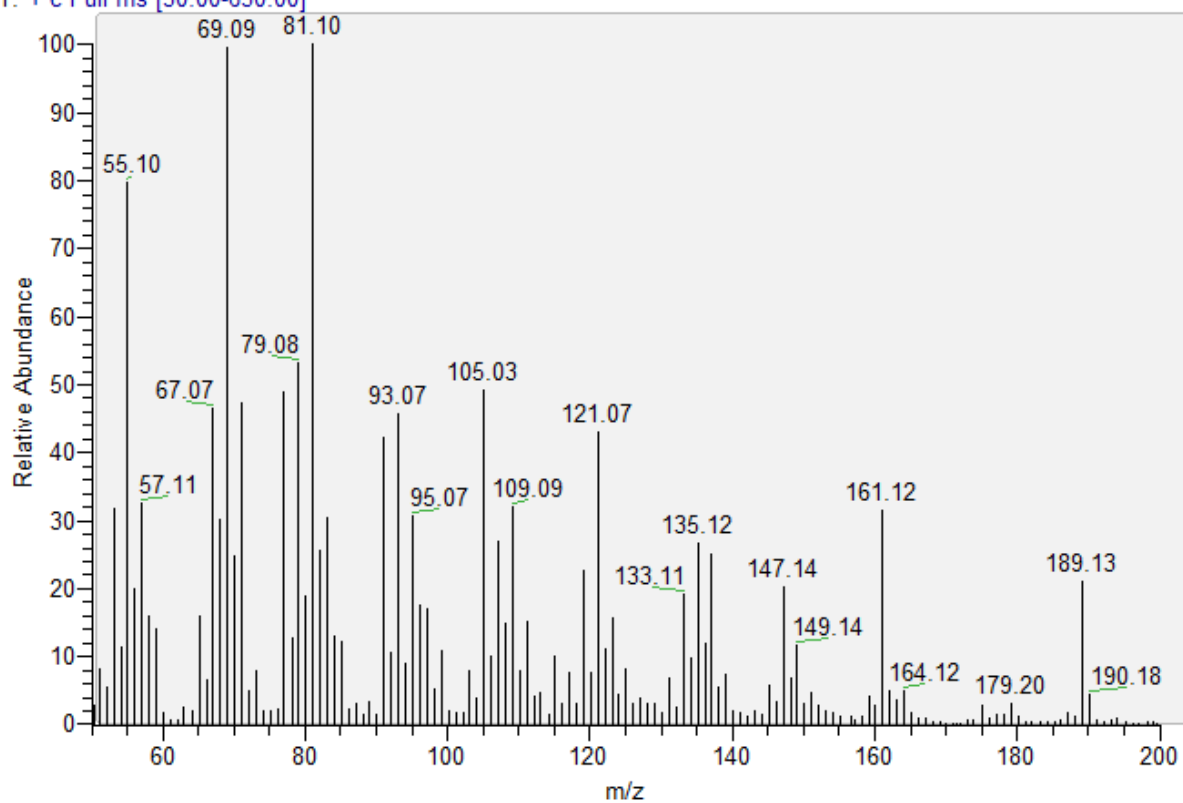


3053 #1647-1648 RT: 39.19-39.22 AV: 2 NL: 1.43E6  
T: + c Full ms [50.00-650.00]

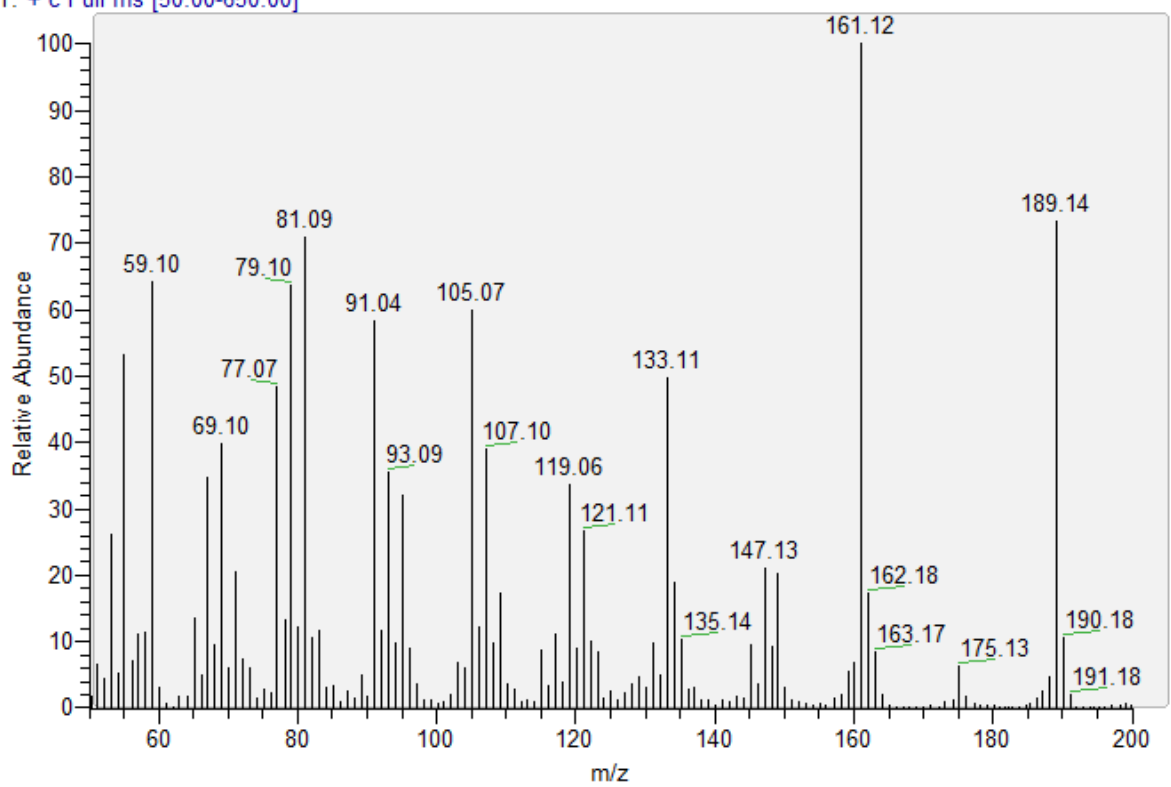


3058 #1644-1645 RT: 39.21-39.24 AV: 2 NL: 1.02E6

T: + c Full ms [50.00-650.00]



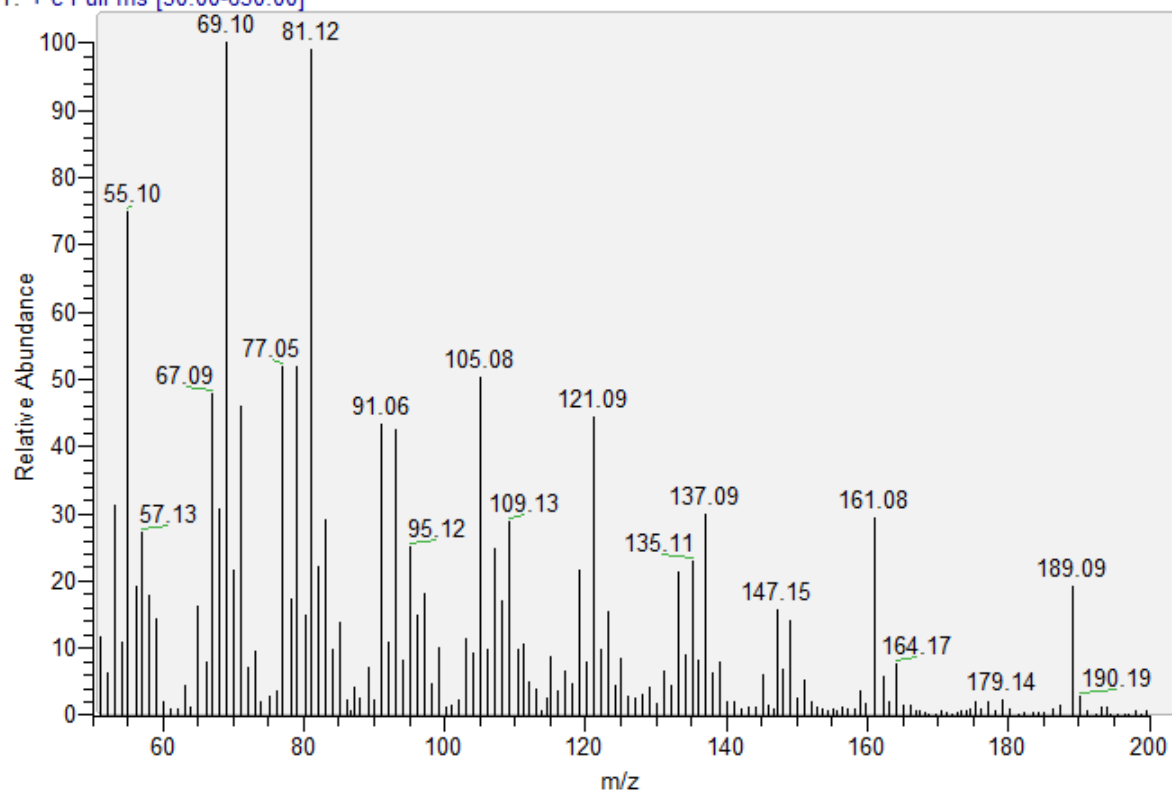
3057 #1655-1657 RT: 39.27-39.32 AV: 3 NL: 8.94E5  
T: + c Full ms [50.00-650.00]



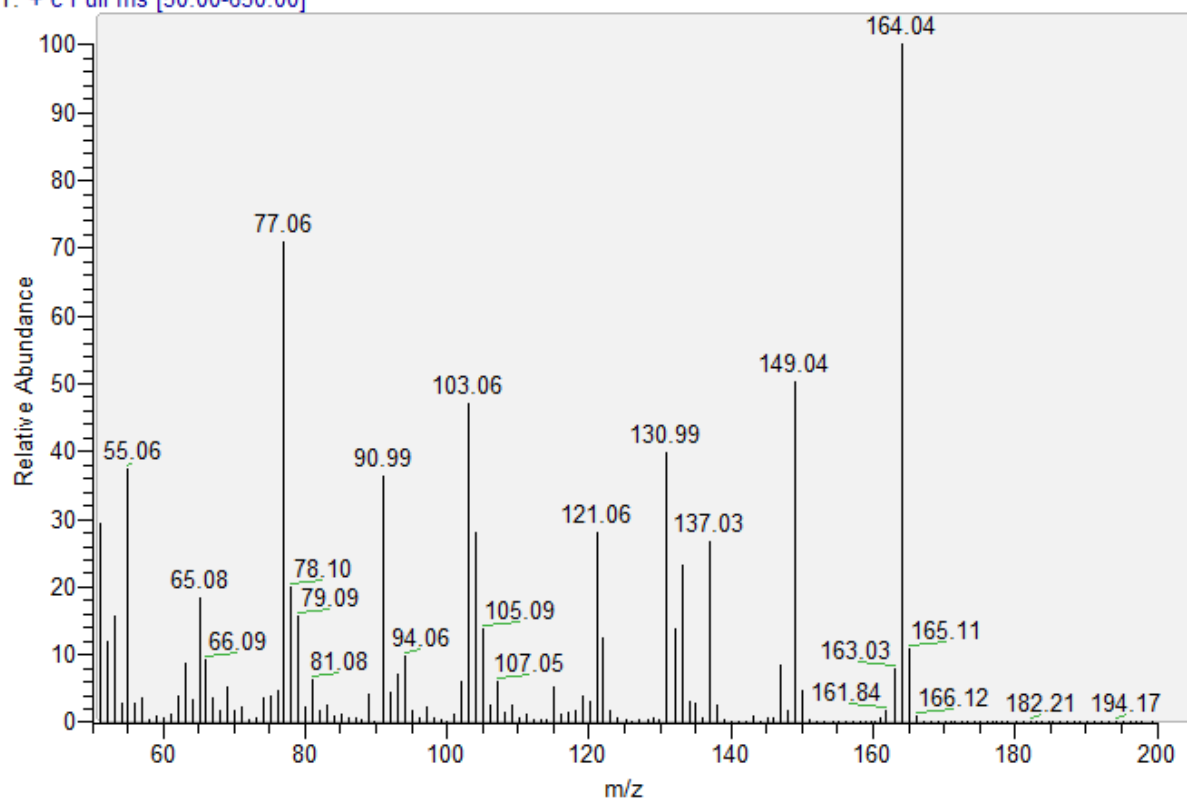
3057 #1652 RT: 39.20 AV: 1 NL: 4.50E5



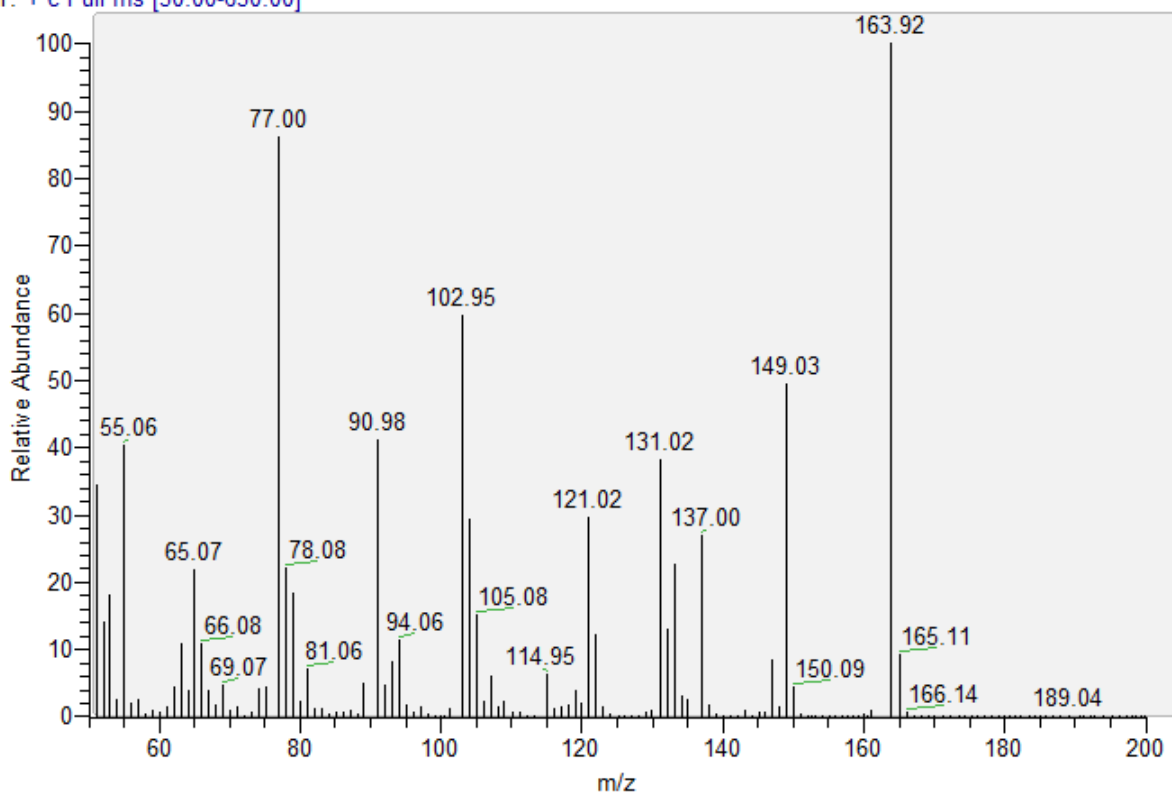
T: + c Full ms [50.00-650.00]



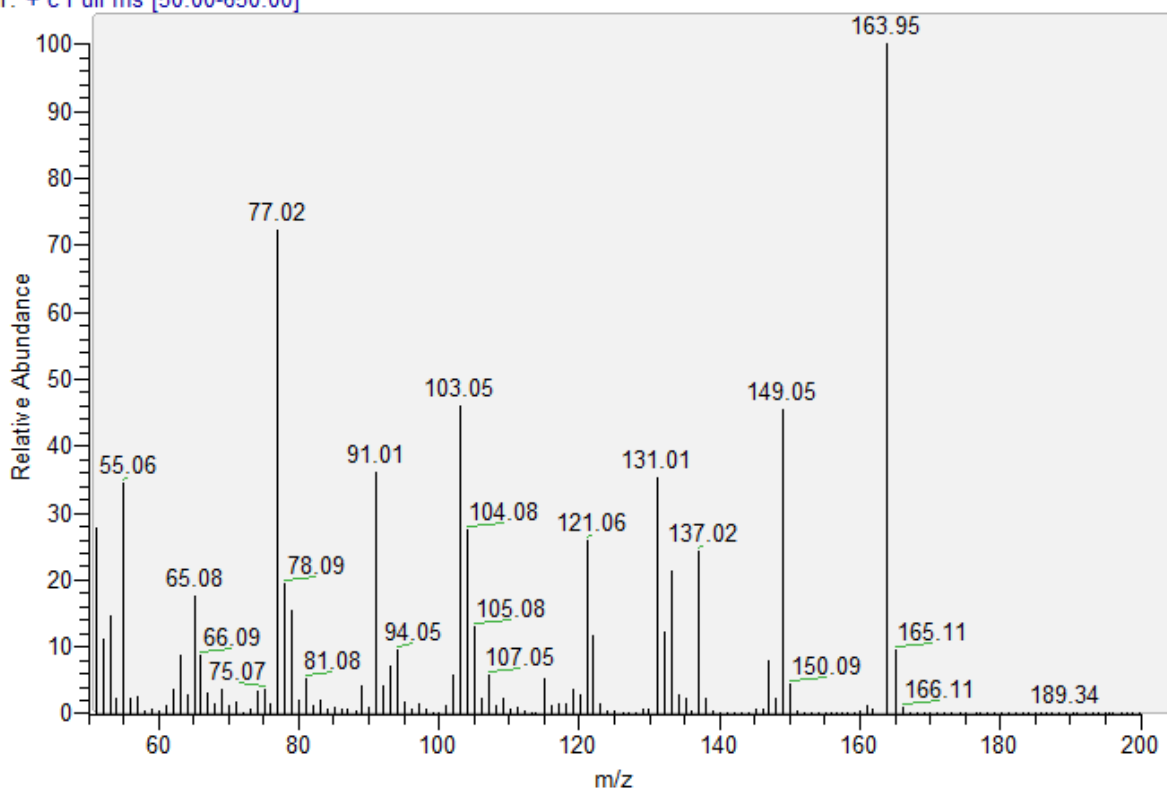
3021 #1647-1648 RT: 39.18-39.20 AV: 2 NL: 3.85E7  
T: + c Full ms [50.00-650.00]



3075 #1646 RT: 39.20 AV: 1 NL: 3.11E7  
T: + c Full ms [50.00-650.00]

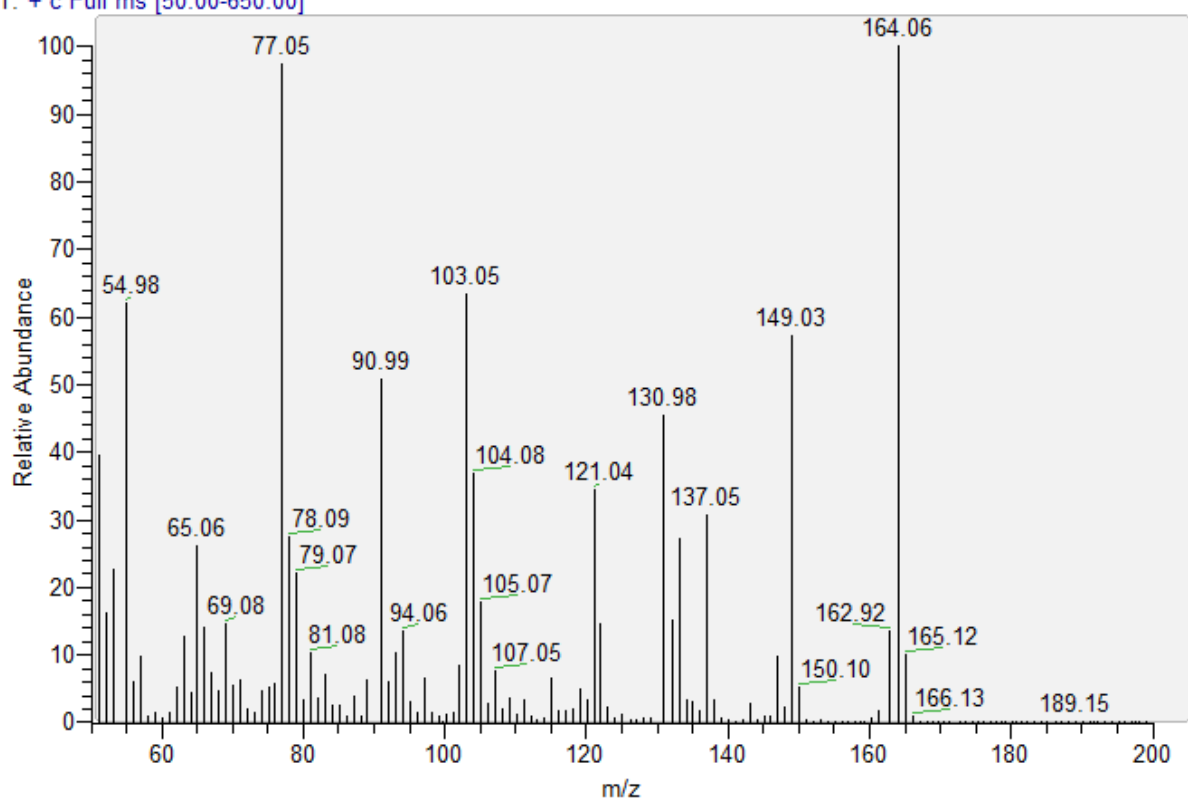


3074 #1647-1648 RT: 39.19-39.21 AV: 2 NL: 4.03E7  
T: + c Full ms [50.00-650.00]

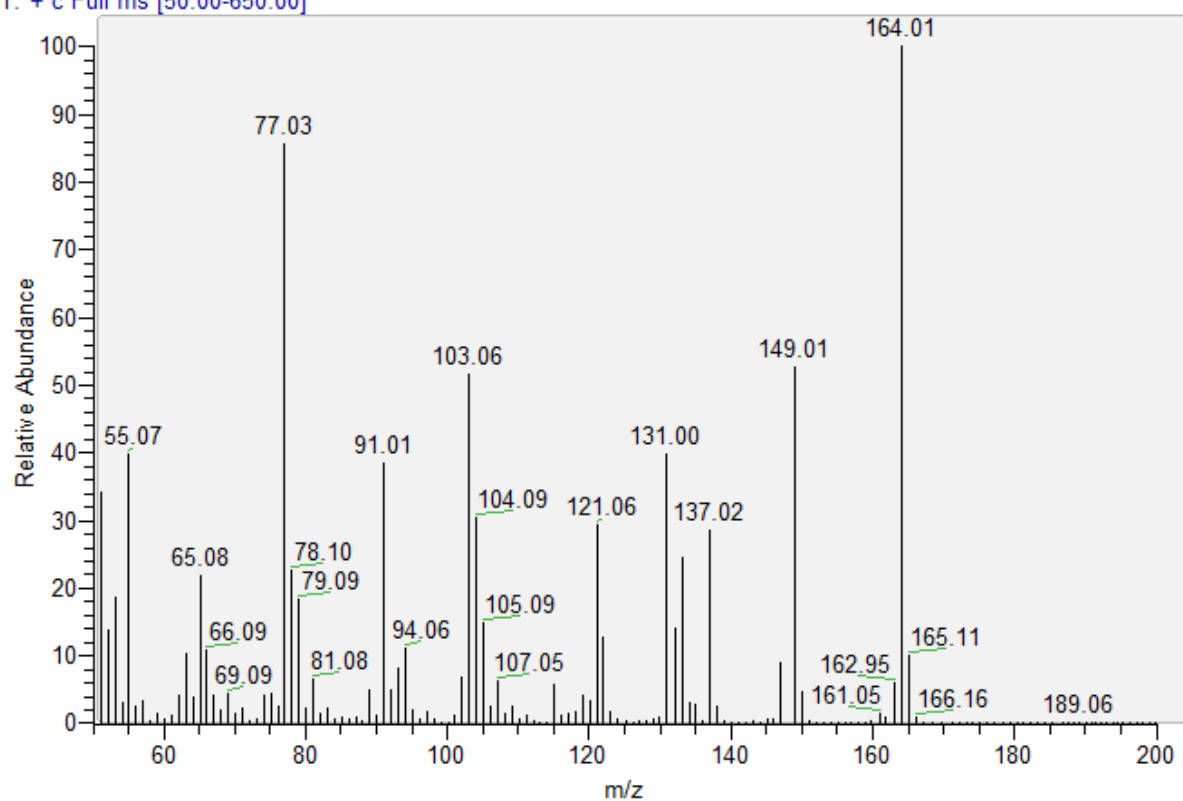




3073 #1647 RT: 39.20 AV: 1 NL: 8.39E6  
T: + c Full ms [50.00-650.00]



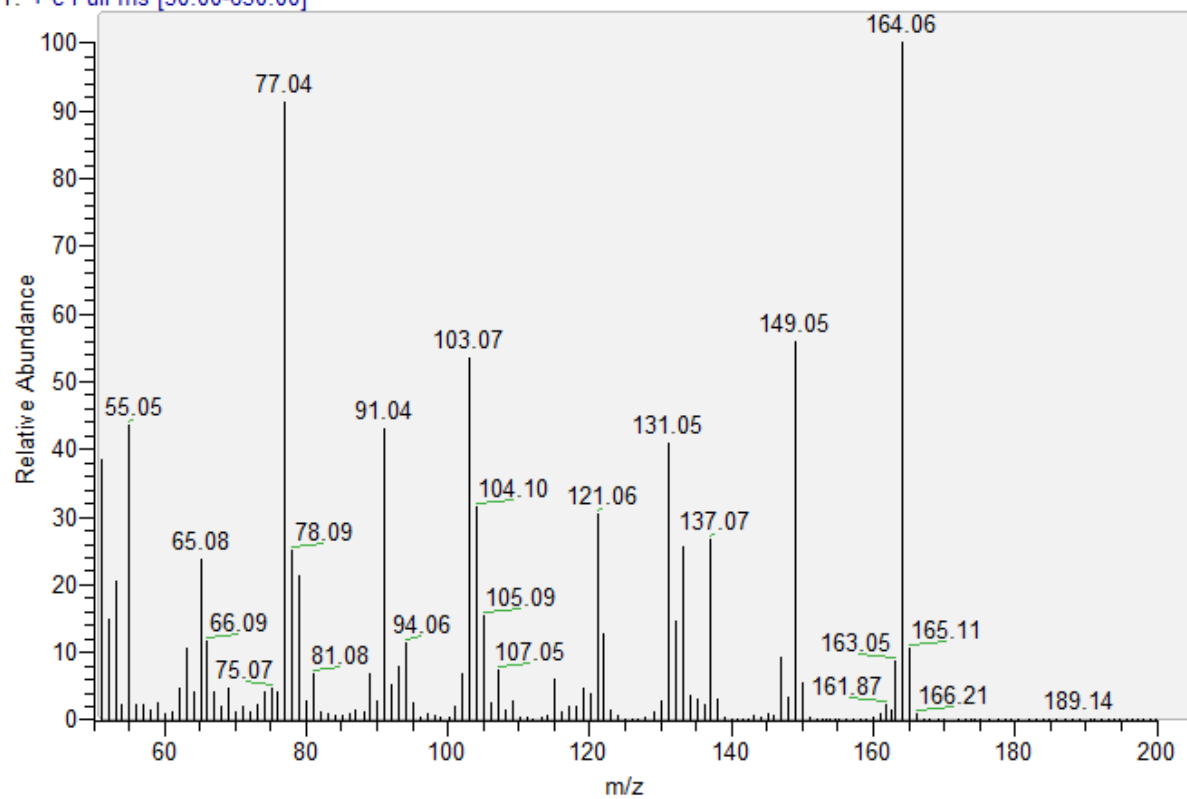
3072 #1645-1646 RT: 39.19-39.21 AV: 2 NL: 2.46E7  
T: + c Full ms [50.00-650.00]



3070 #1648 RT: 39.19 AV: 1 NL: 2.19E6

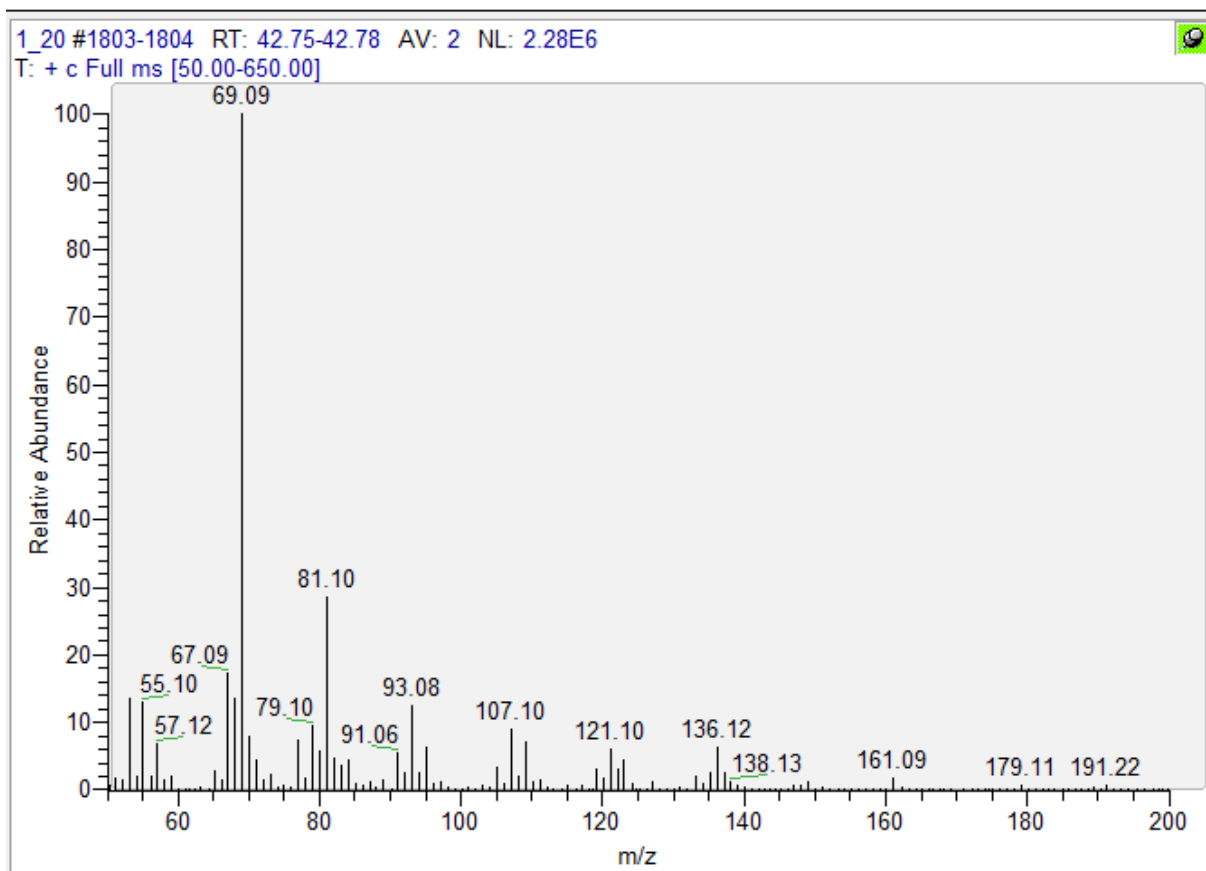


T: + c Full ms [50.00-650.00]



Farnesol

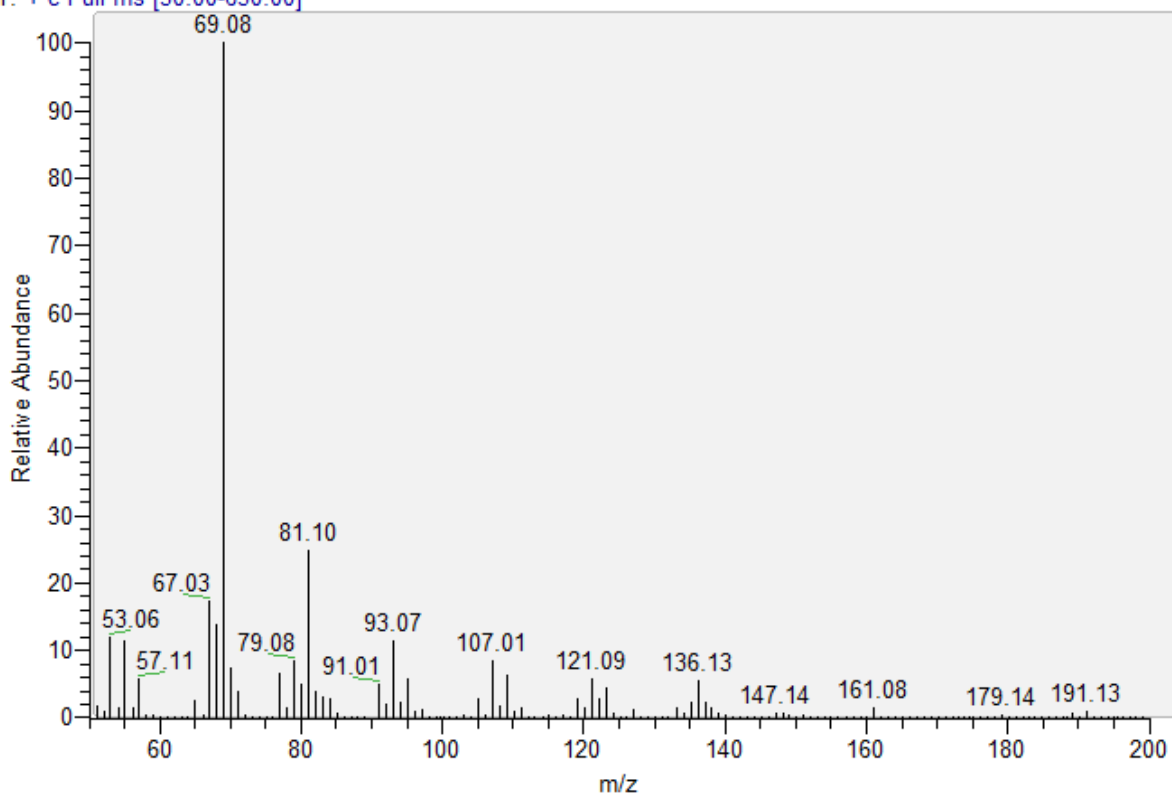
Reference:



Samples:

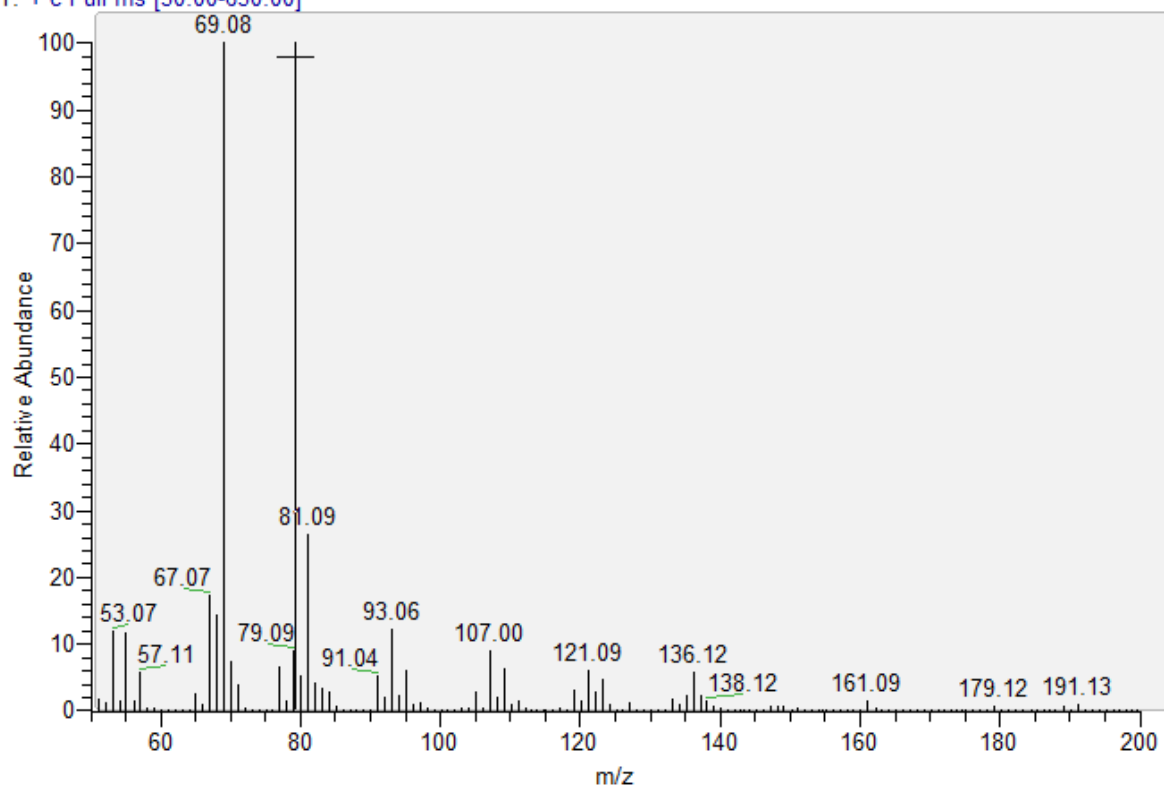
3075 #1796-1797 RT: 42.78-42.81 AV: 2 NL: 5.68E7

T: + c Full ms [50.00-650.00]

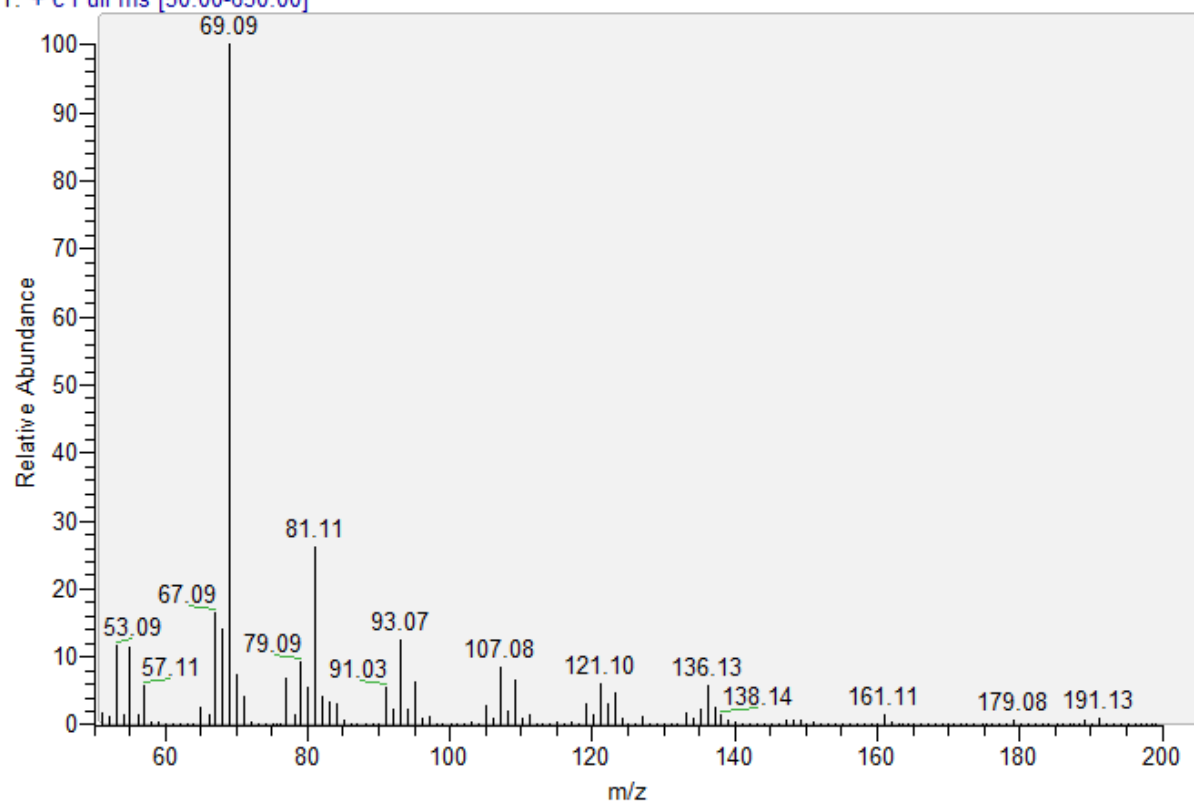


3074 #1798-1799 RT: 42.78-42.81 AV: 2 NL: 6.22E7

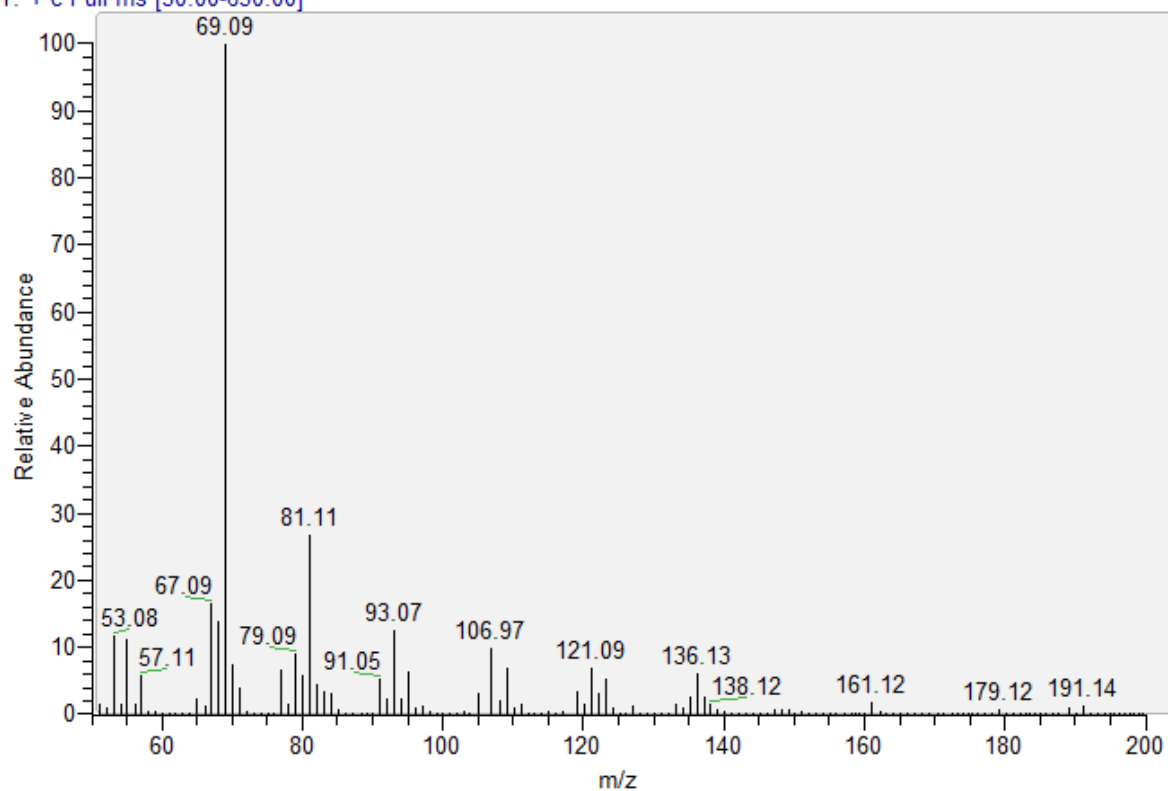
T: + c Full ms [50.00-650.00]



3073 #1797-1798 RT: 42.78-42.80 AV: 2 NL: 7.42E7  
T: + c Full ms [50.00-650.00]

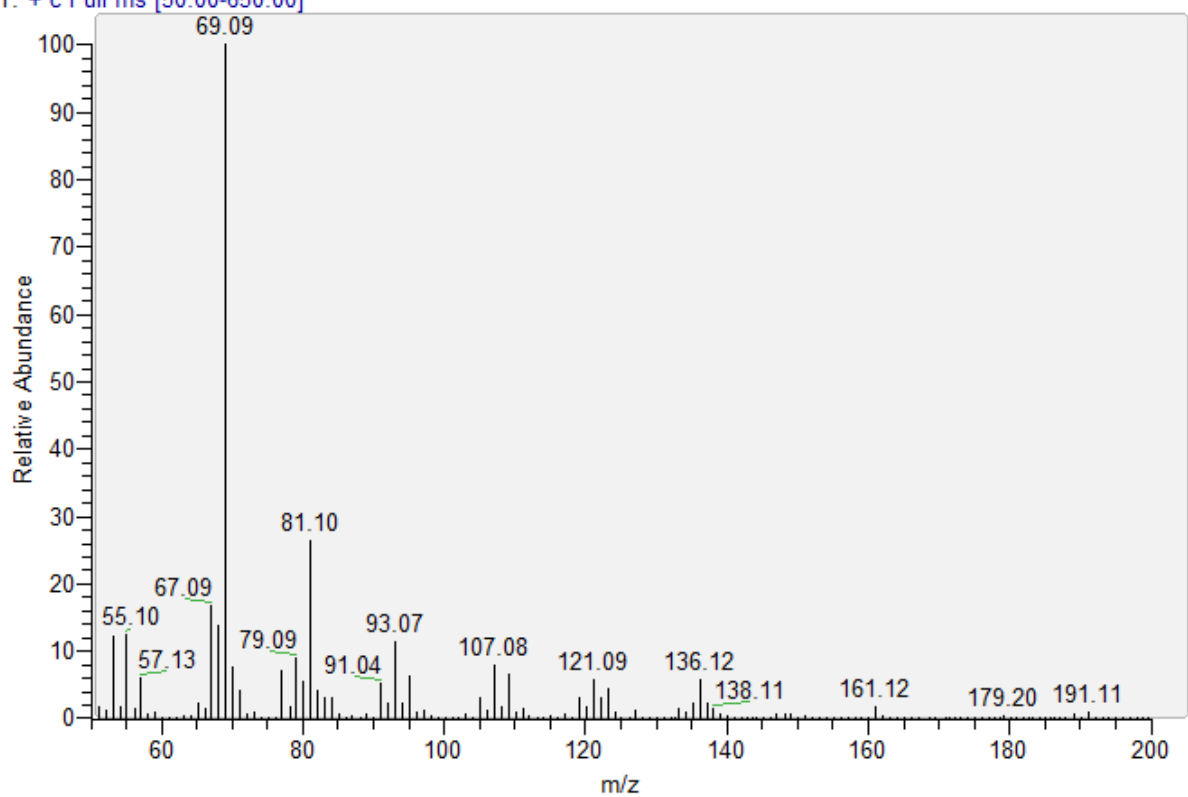


3072 #1796 RT: 42.79 AV: 1 NL: 1.18E8  
T: + c Full ms [50.00-650.00]

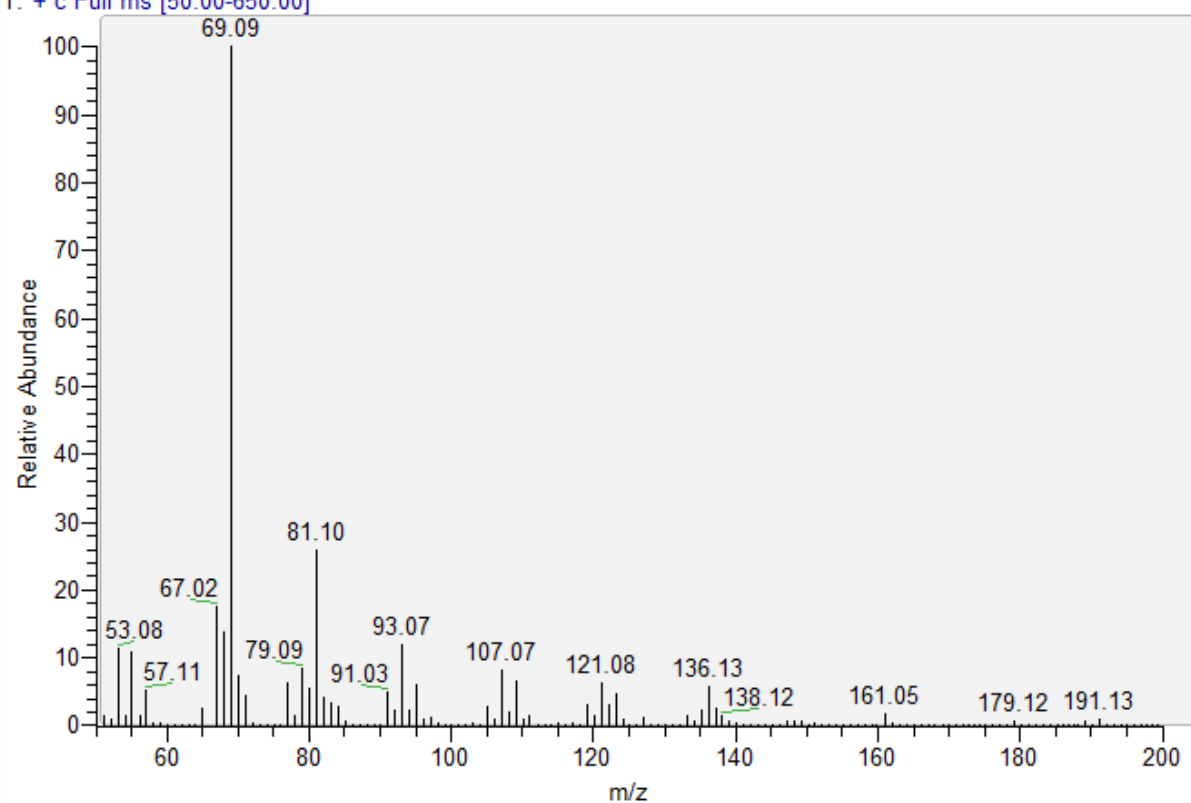




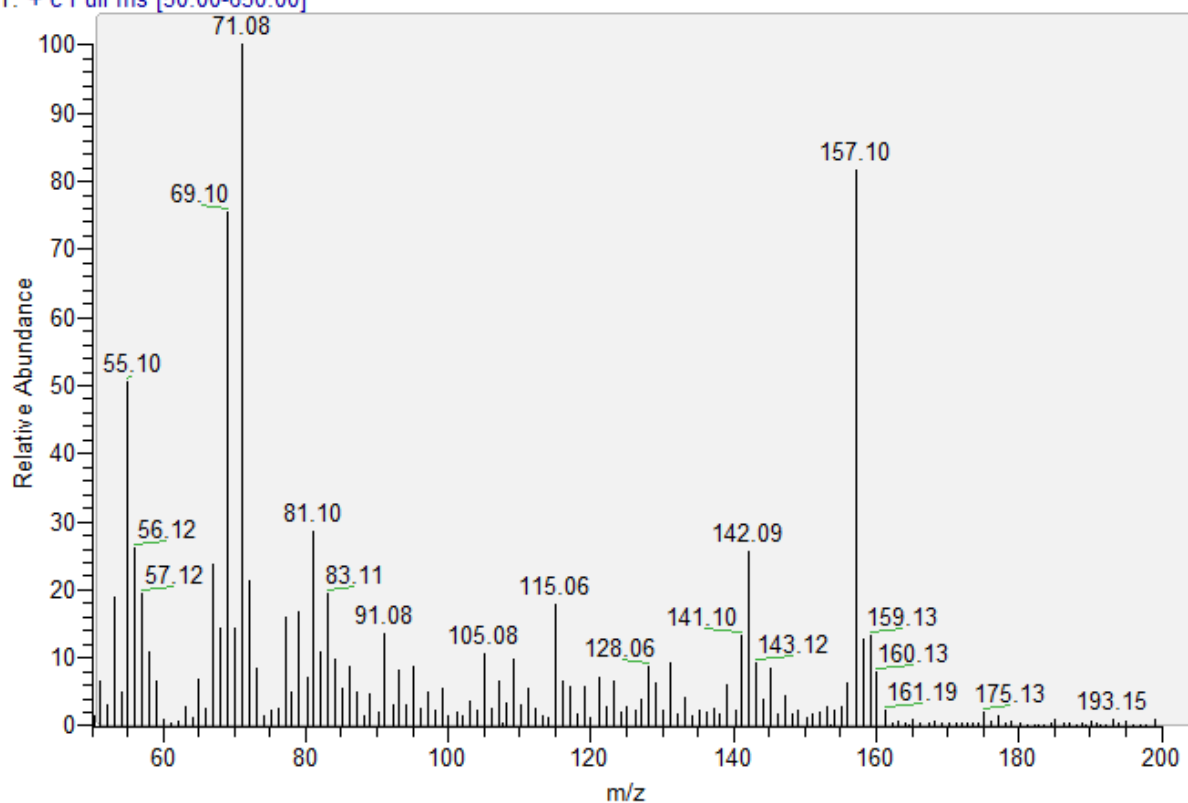
3070 #1798-1799 RT: 42.76-42.78 AV: 2 NL: 7.29E6  
T: + c Full ms [50.00-650.00]



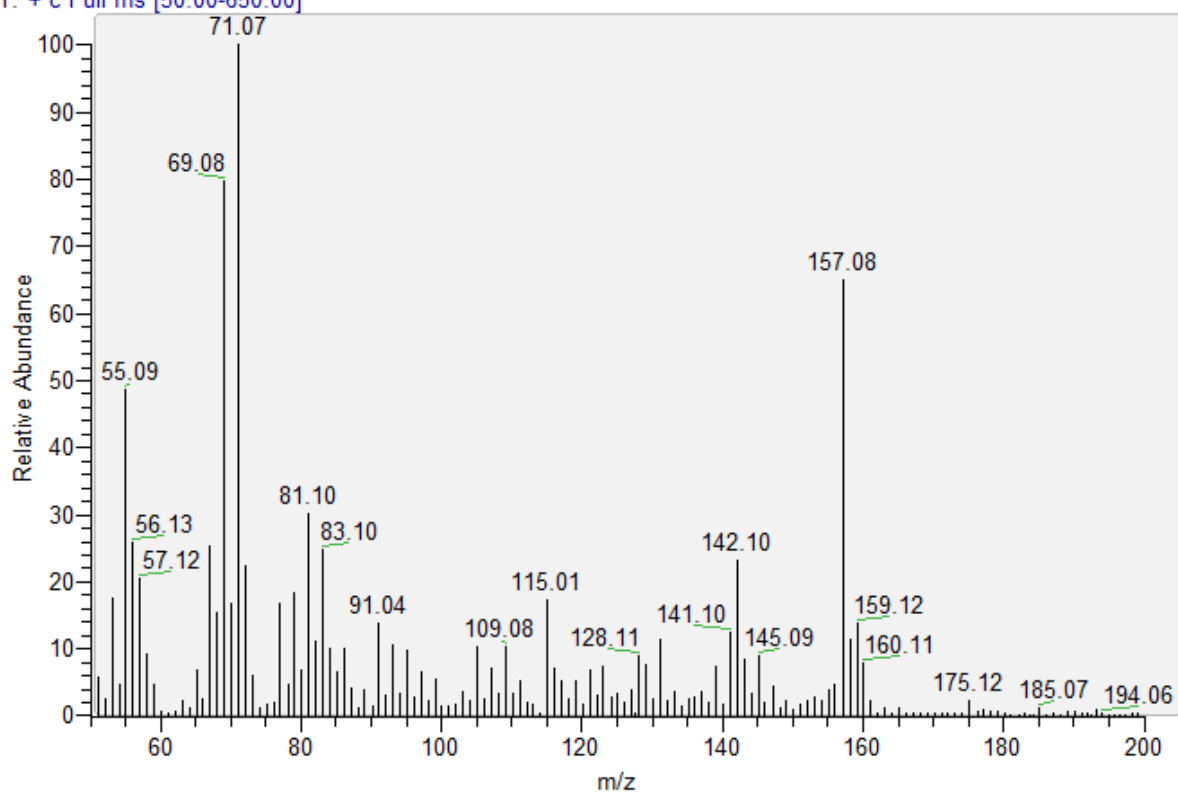
3021 #1798-1799 RT: 42.78-42.80 AV: 2 NL: 1.03E8  
T: + c Full ms [50.00-650.00]



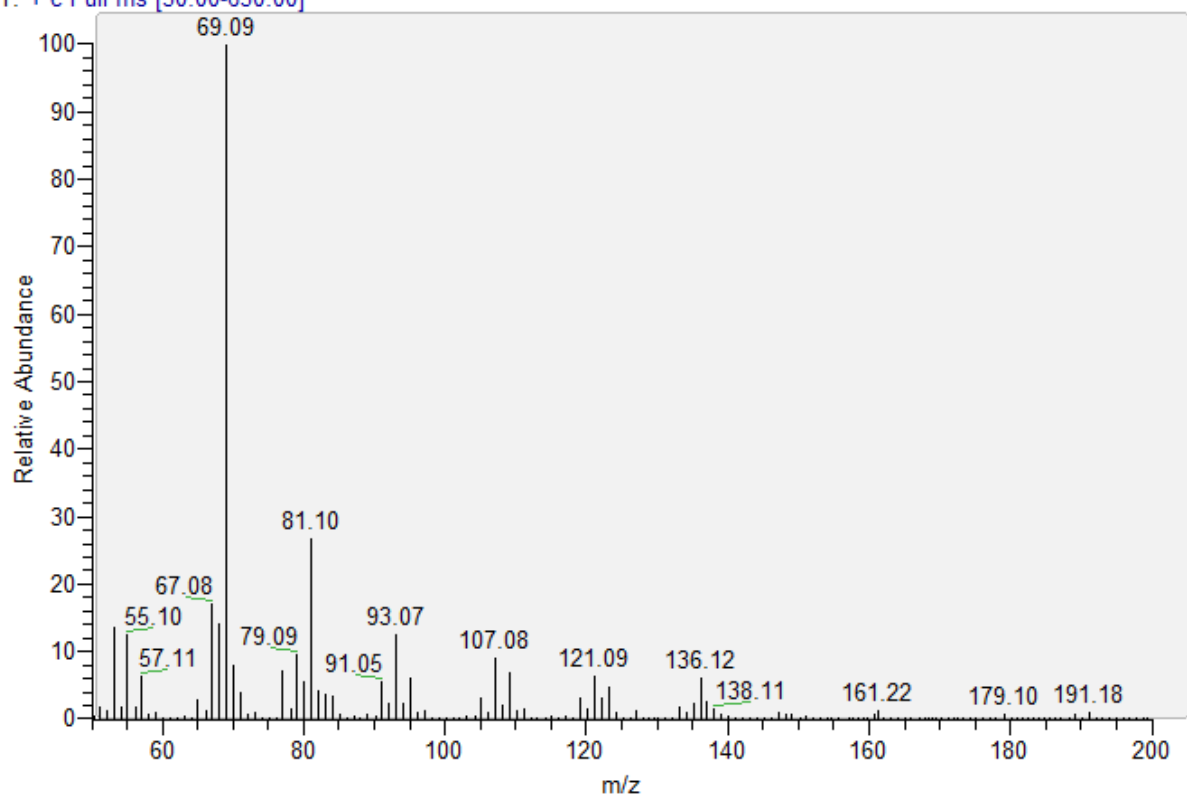
3057 #1802-1803 RT: 42.77-42.80 AV: 2 NL: 7.72E5  
T: + c Full ms [50.00-650.00]



3058 #1794-1795 RT: 42.79-42.81 AV: 2 NL: 1.94E6  
T: + c Full ms [50.00-650.00]



3053 #1796-1797 RT: 42.75-42.77 AV: 2 NL: 7.47E6  
T: + c Full ms [50.00-650.00]



3018 #1802 RT: 42.79 AV: 1 NL: 1.43E8  
T: + c Full ms [50.00-650.00]

