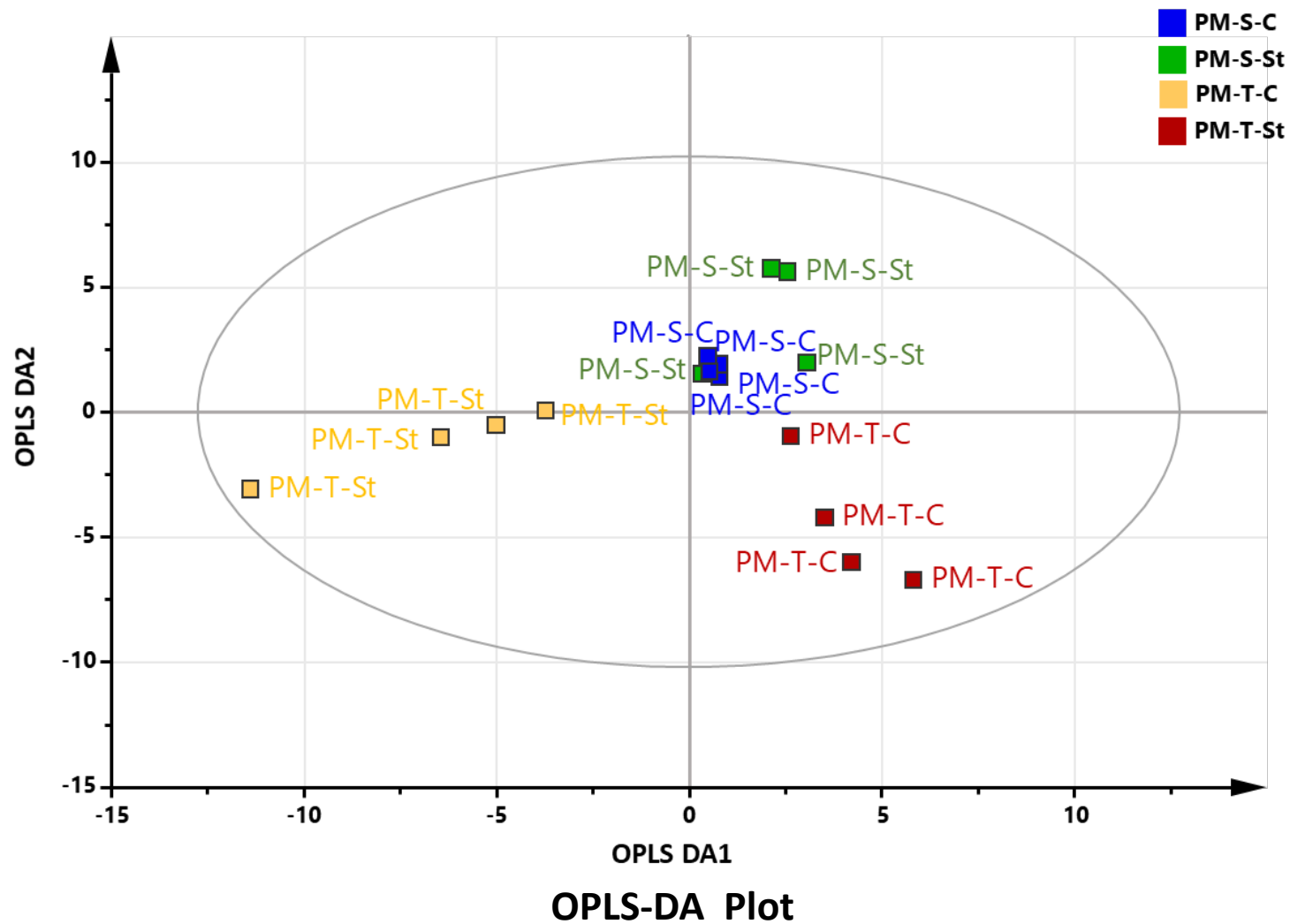


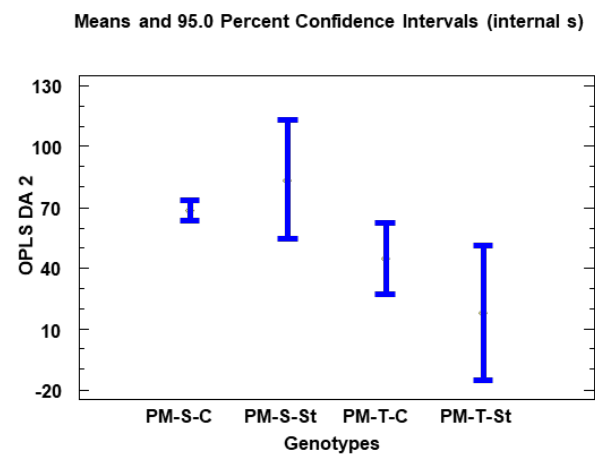
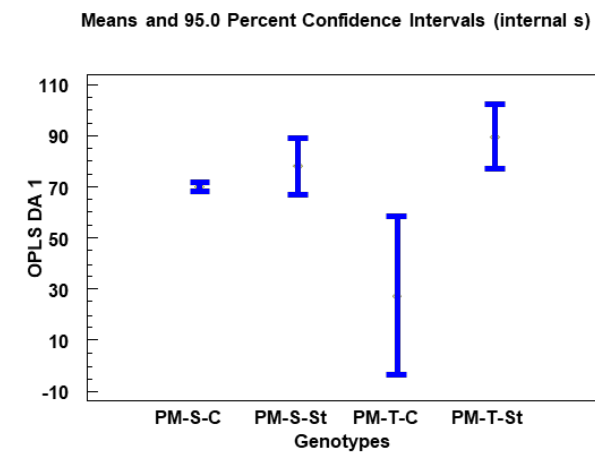


Fig. S1

(a)



(b)



OPLS-DA Loadings

Fig. S2

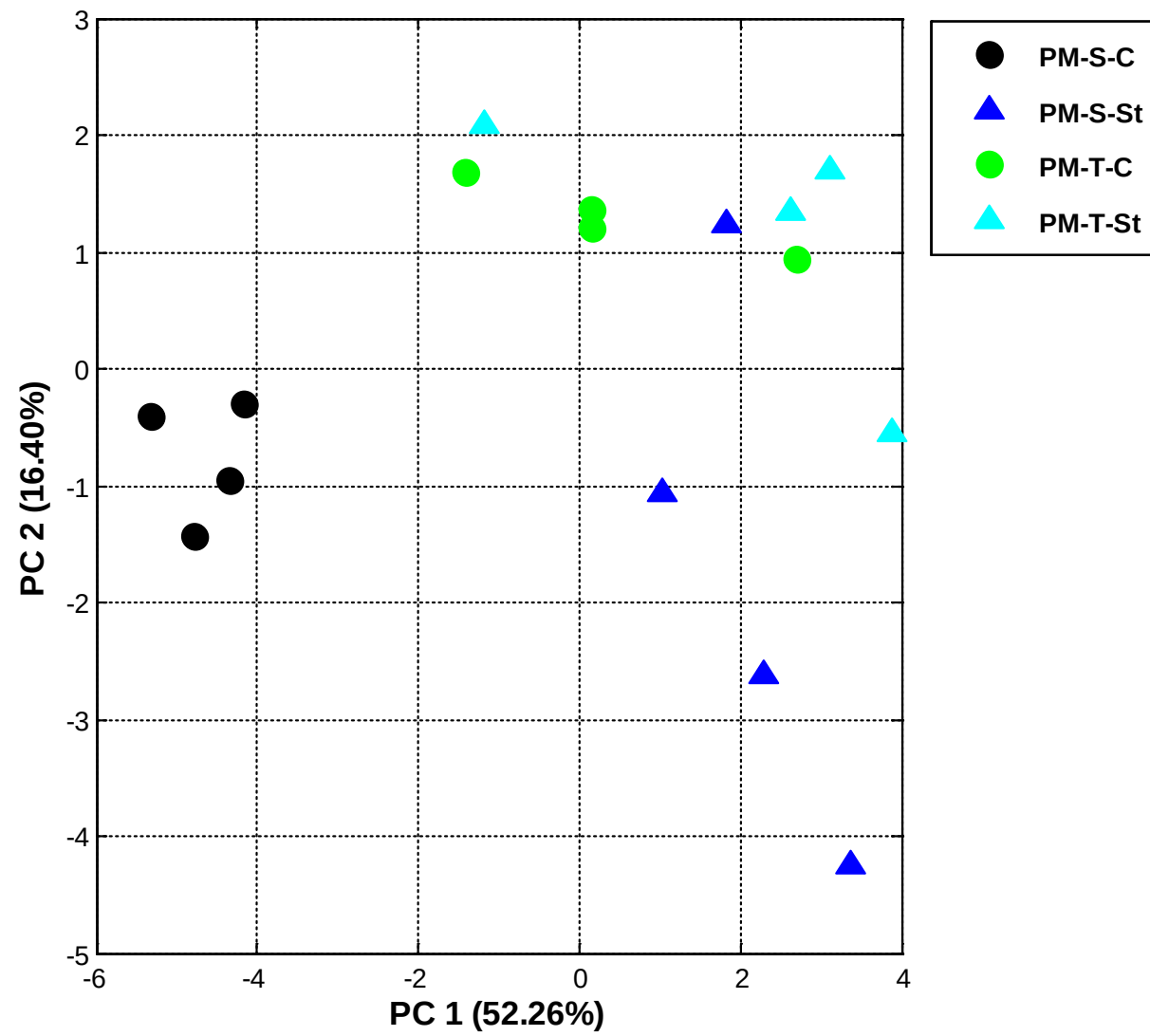
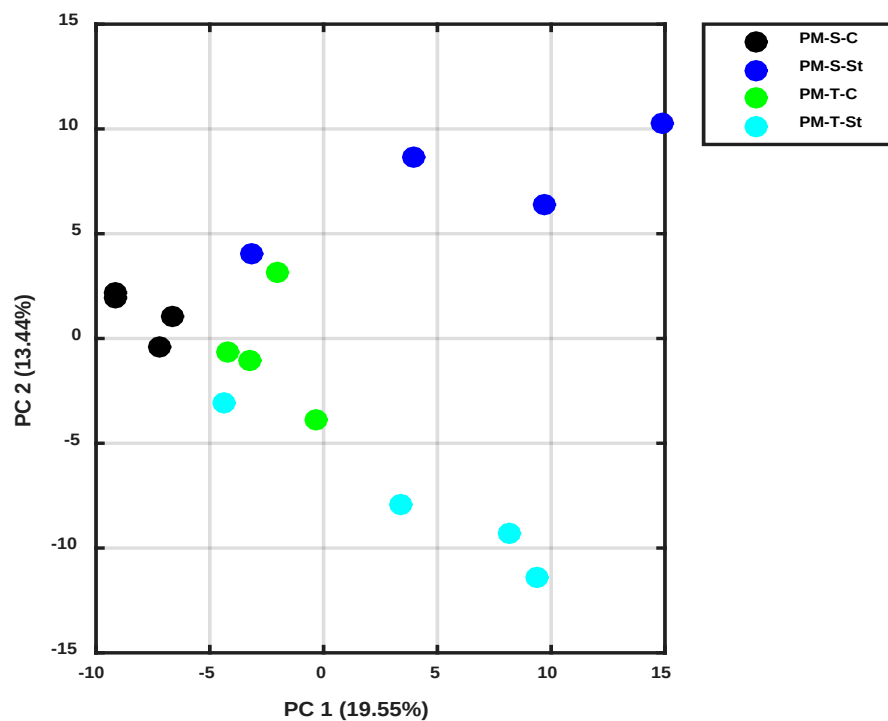


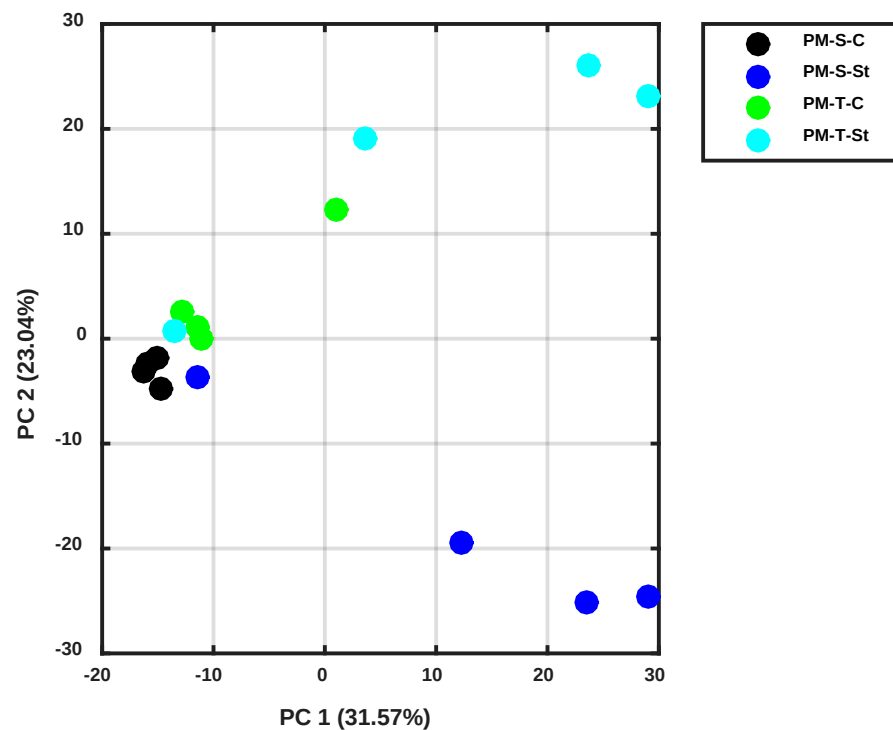
Fig. S3

(a)



Positive mode: Untargeted Analysis

(b)



Negative mode: Untargeted Analysis

Fig. S4

Compound 1	Formula	Ionspecies	m/z	RT [min]	Reference
Adenosine	C ₁₀ H ₁₃ N ₅ O ₄	[M+H] ⁺	268.105	3.33	https://www.mzcloud.org/DataViewer#Creferance297#T506#c#58583

sample_4 #330 RT: 3.25 AV: 1 NL: 4.88E4
F: ITMS + c ESI r d w Full ms2 267.96@cid35.00 [60.00-280.00]

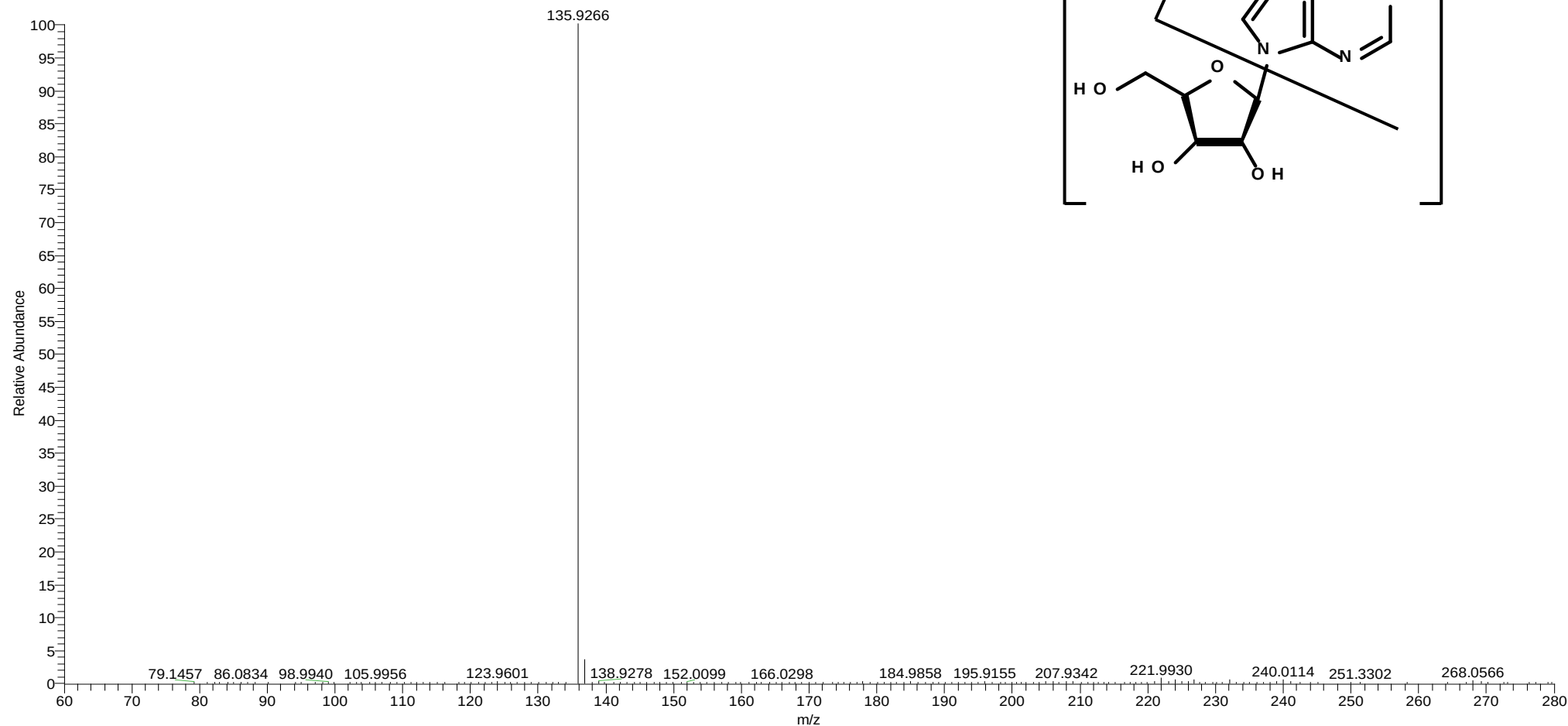
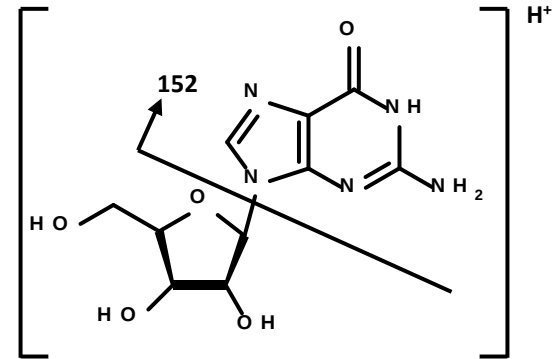
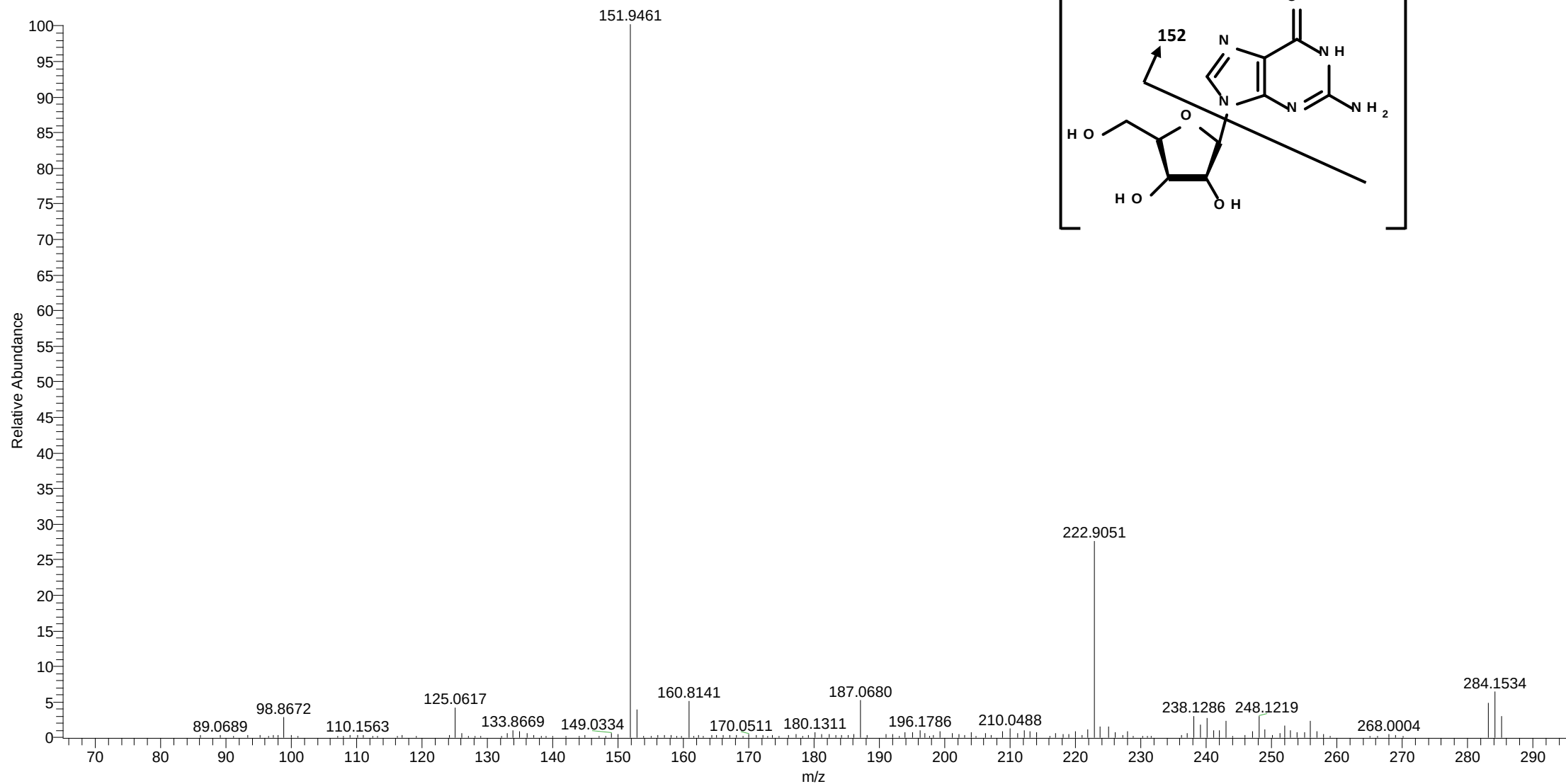


Fig. S5

Compound 2	Formula	Ionspecies	<i>m/z</i>	RT [min]	Reference
Guanosine	C ₁₀ H ₁₃ N ₅ O ₅	[M+H] ⁺	284.0989	3.62	http://www.massbank.jp/RecordDisplay.jsp?id=KO008966&dsn=Keio_Univ

sample_13 #359 RT: 3.57 AV: 1 NL: 2.20E3
F: ITMS + c ESI r d w Full ms2 284.10@cid35.00 [65.00-295.00]



Compound 3	Formula	Ionspecies	<i>m/z</i>	RT [min]	Reference
Riboflavin	C ₁₇ H ₂₀ N ₄ O ₆	[M+H] ⁺	377.1456	14.98	https://www.mzcloud.org/DataViewer#Reference590#T1080#c#141734

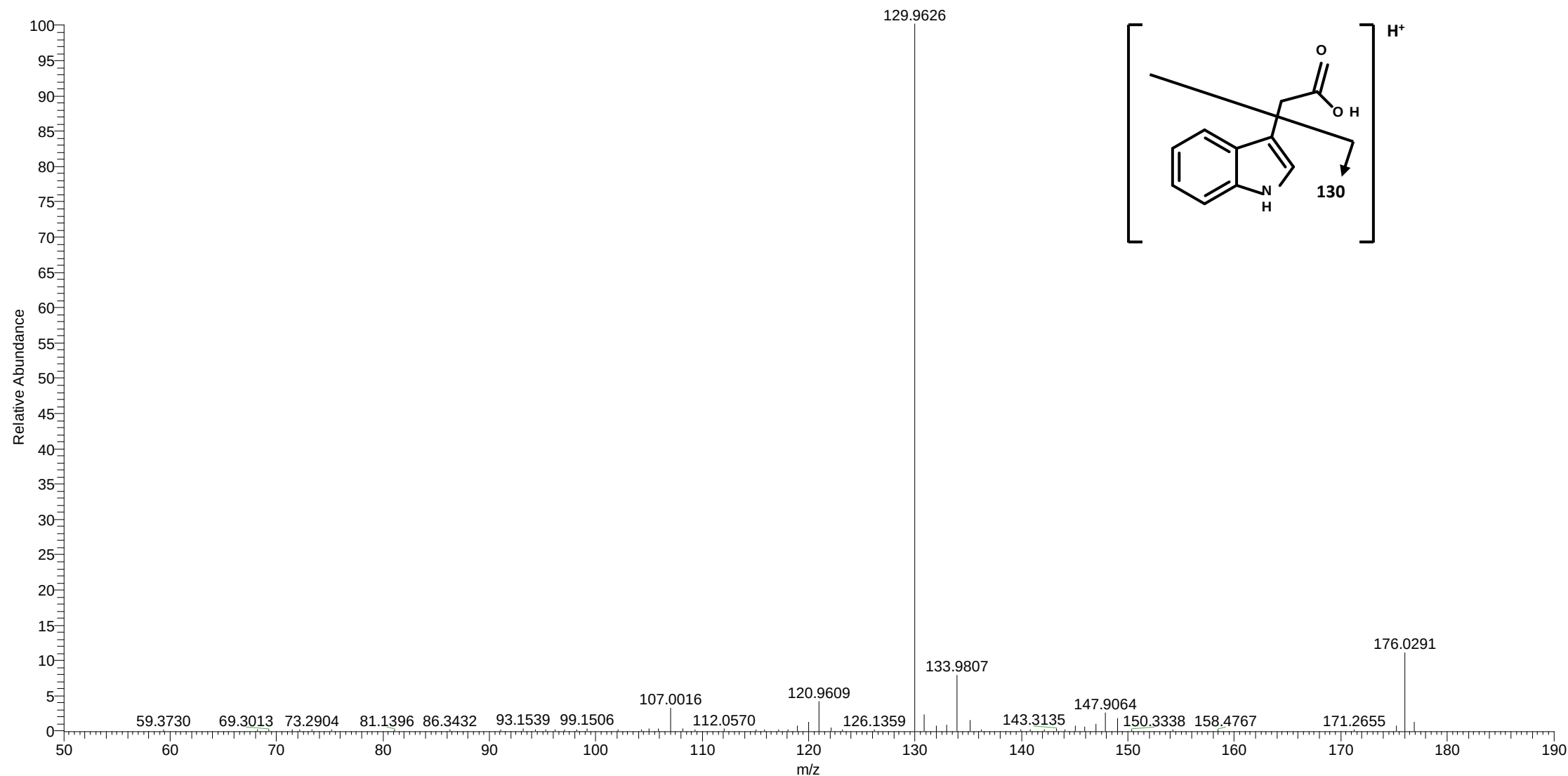
sample_4 #1483 RT: 14.99 AV: 1 NL: 5.94E5

F: ITMS + c ESI r d w Full ms2 377.14@cid35.00 [90.00-390.00]



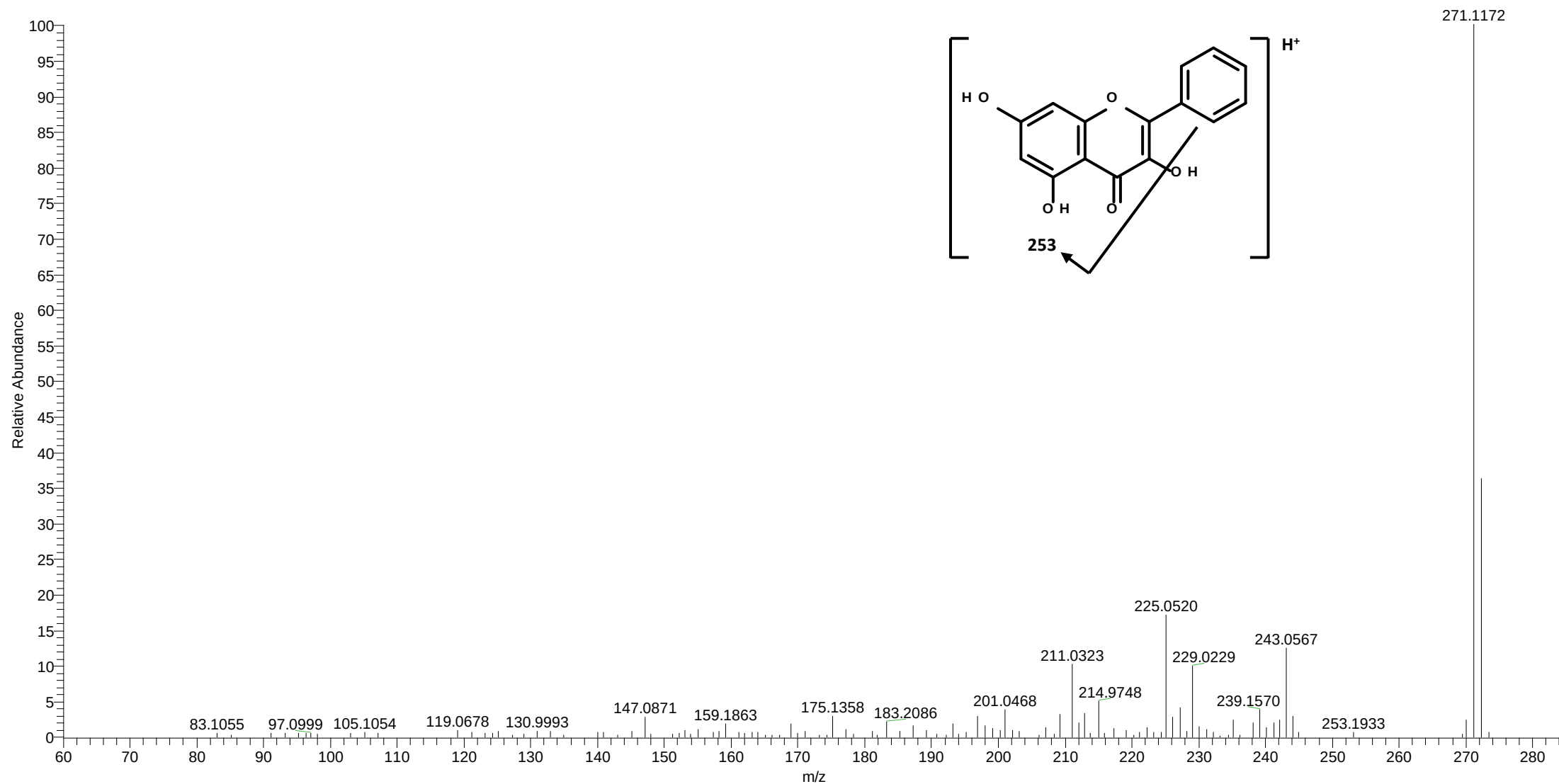
Compound 4	Formula	Ionspecies	<i>m/z</i>	RT [min]	Reference
Indoleacetic acid	C ₁₀ H ₉ NO ₂	[M+H] ⁺	176.0706	21.00	https://www.mzcloud.org/DataViewer#Creference445#T799#c#105167

sample_4 #2071 RT: 20.95 AV: 1 NL: 4.28E3
F: ITMS + c ESI r d w Full ms2 176.06@cid35.00 [50.00-190.00]



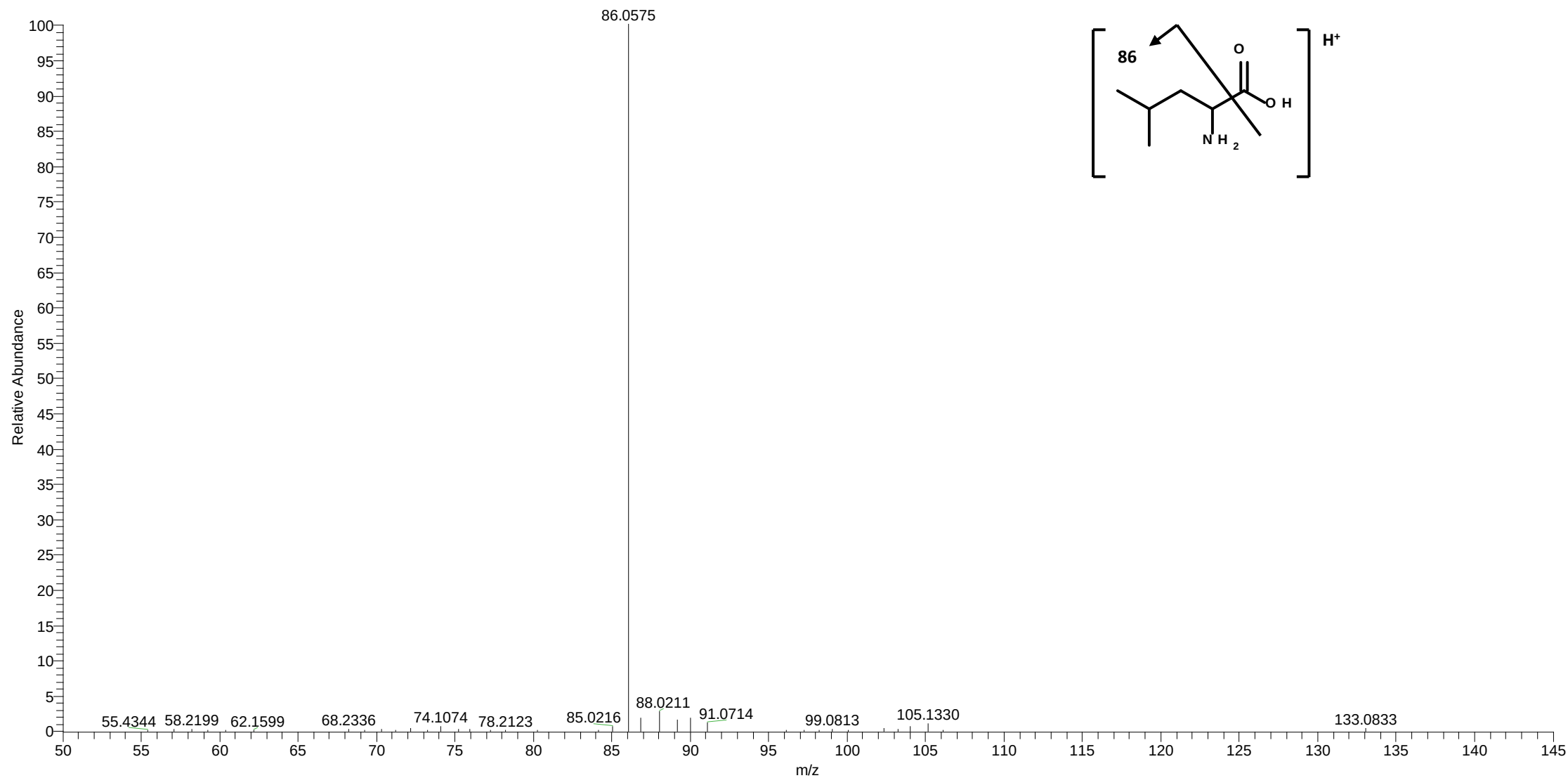
Compound 5	Formula	Ionspecies	<i>m/z</i>	RT [min]	Reference
Genistein/Galangin	C ₁₅ H ₁₀ O ₅	[M+H] ⁺	271.0601	26.39	https://www.mzcloud.org/DataViewer#Reference24#T57#c#11083

sample_16 #2911 RT: 30.01 AV: 1 NL: 7.93E2
F: ITMS + c ESI r d w Full ms2 271.06@cid35.00 [60.00-285.00]



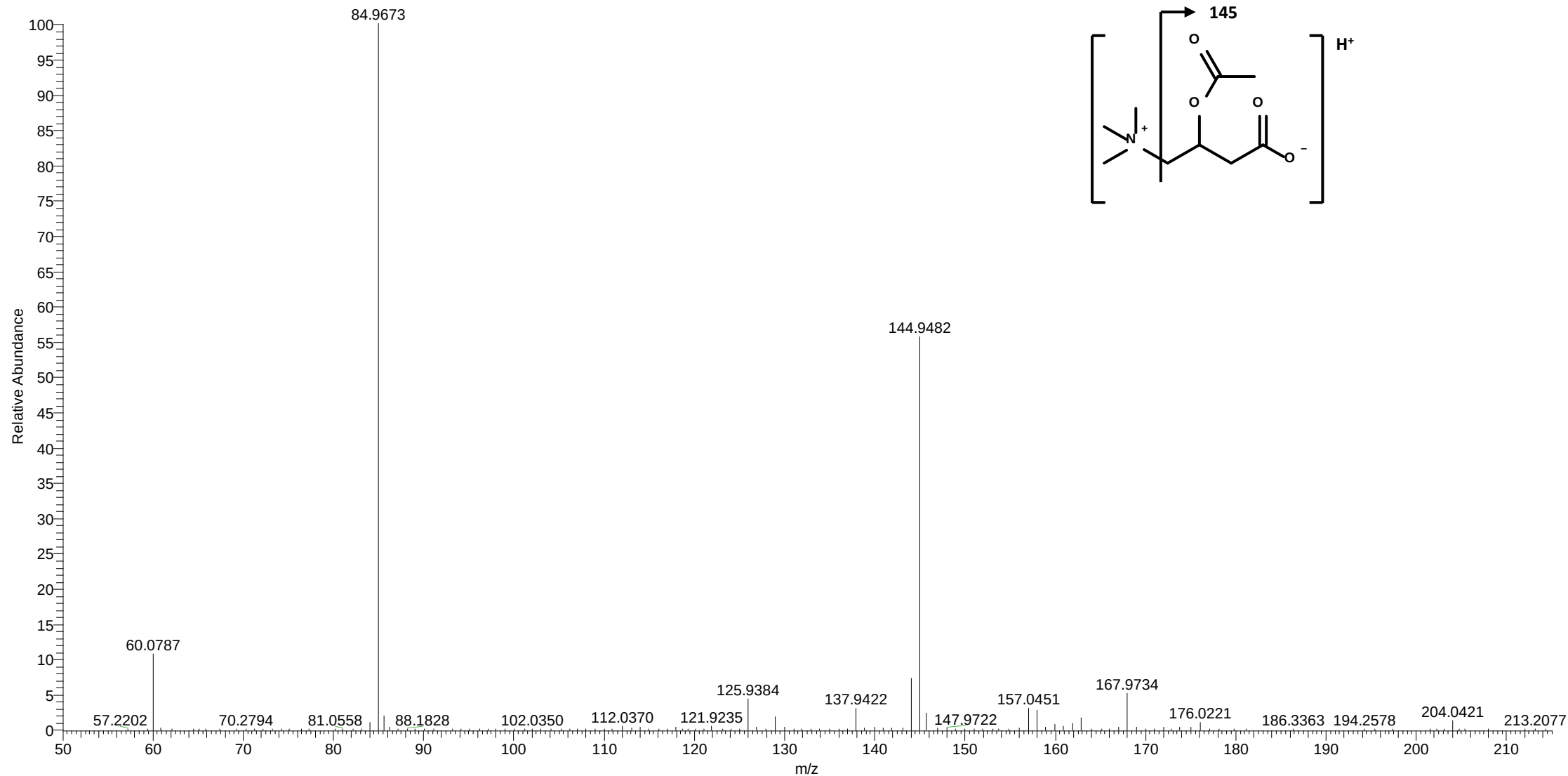
Compound 6	Formula	Ionspecies	<i>m/z</i>	RT [min]	Reference
Leucine/Isoleucine	C ₆ H ₁₃ NO ₂	[M+H] ⁺	132.1019	4.26	https://www.mzcloud.org/DataViewer#Creference6#T17#c#401581

sample_16 #366 RT: 3.73 AV: 1 NL: 4.71E3
F: ITMS + c ESI r d w Full ms2 132.10@cid35.00 [50.00-145.00]



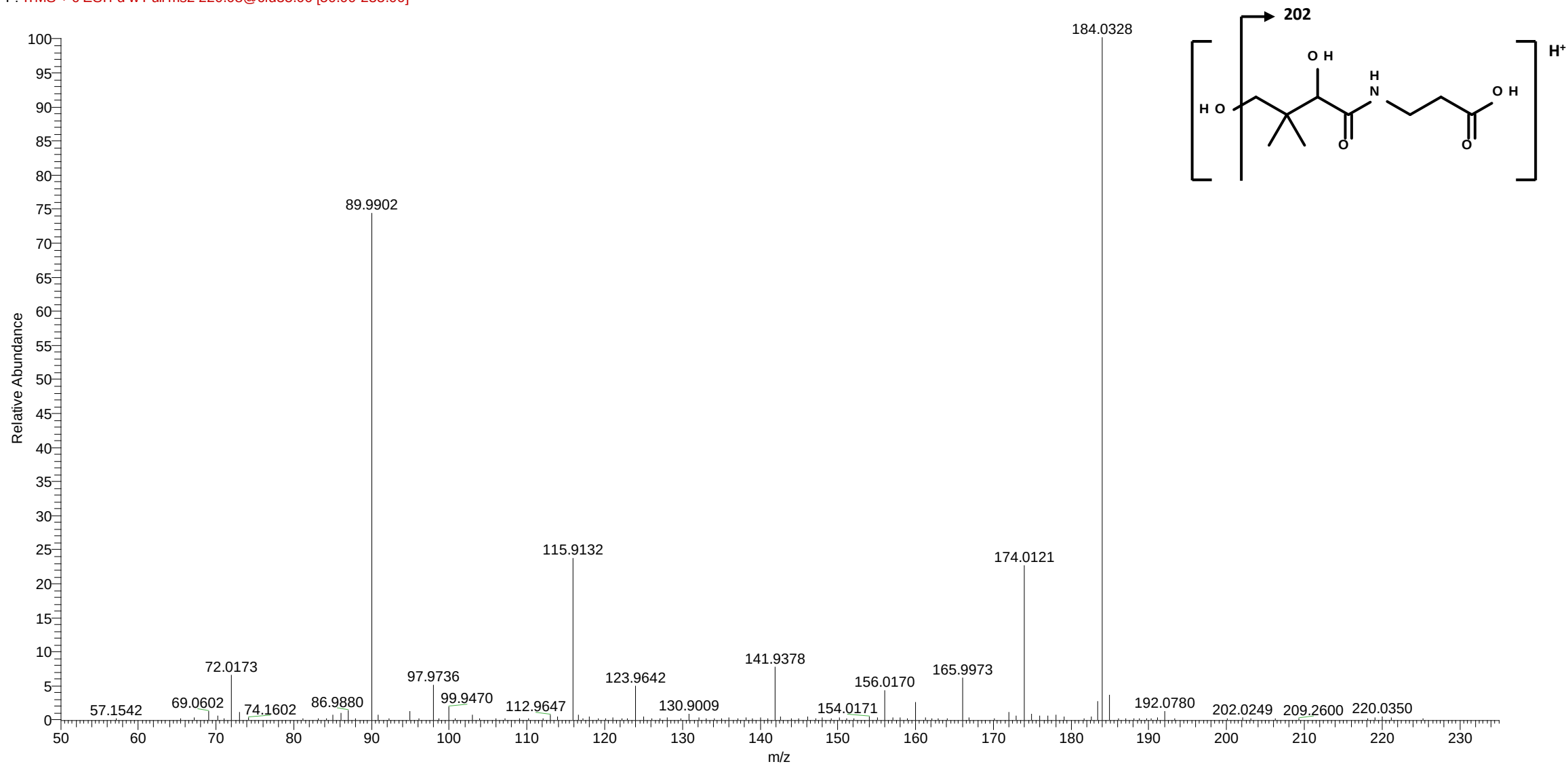
Compound 7	Formula	Ionspecies	<i>m/z</i>	RT [min]	Reference
Acetyl carnitine	C ₉ H ₁₇ NO ₄	[M+H] ⁺	204.123	2.80	https://www.mzcloud.org/DataViewer#Creference879#T1526#c#186875

sample_4 #275 RT: 2.72 AV: 1 NL: 4.41E4
F: ITMS + c ESI r d w Full ms2 204.14@cid35.00 [50.00-215.00]



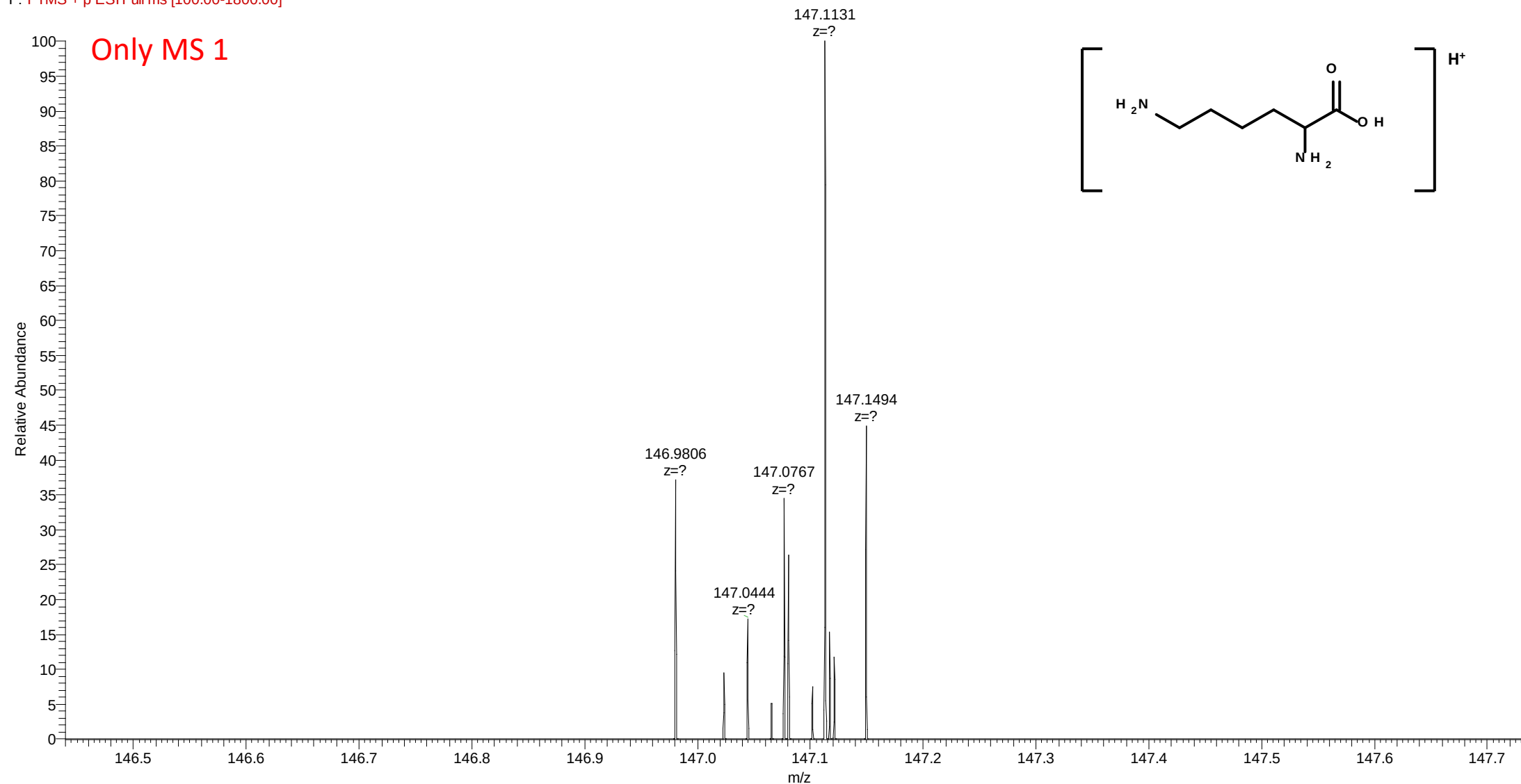
Compound 8	Formula	Ionspecies	m/z	RT [min]	Reference
Pantothenic acid	C ₉ H ₁₇ NO ₅	[M+H] ⁺	220.118	7.02	https://www.mzcloud.org/DataViewer#Reference536#T981#c#130088

sample_4 #747 RT: 7.49 AV: 1 NL: 1.86E4
F: ITMS + c ESI r d w Full ms2 220.08@cid35.00 [50.00-235.00]



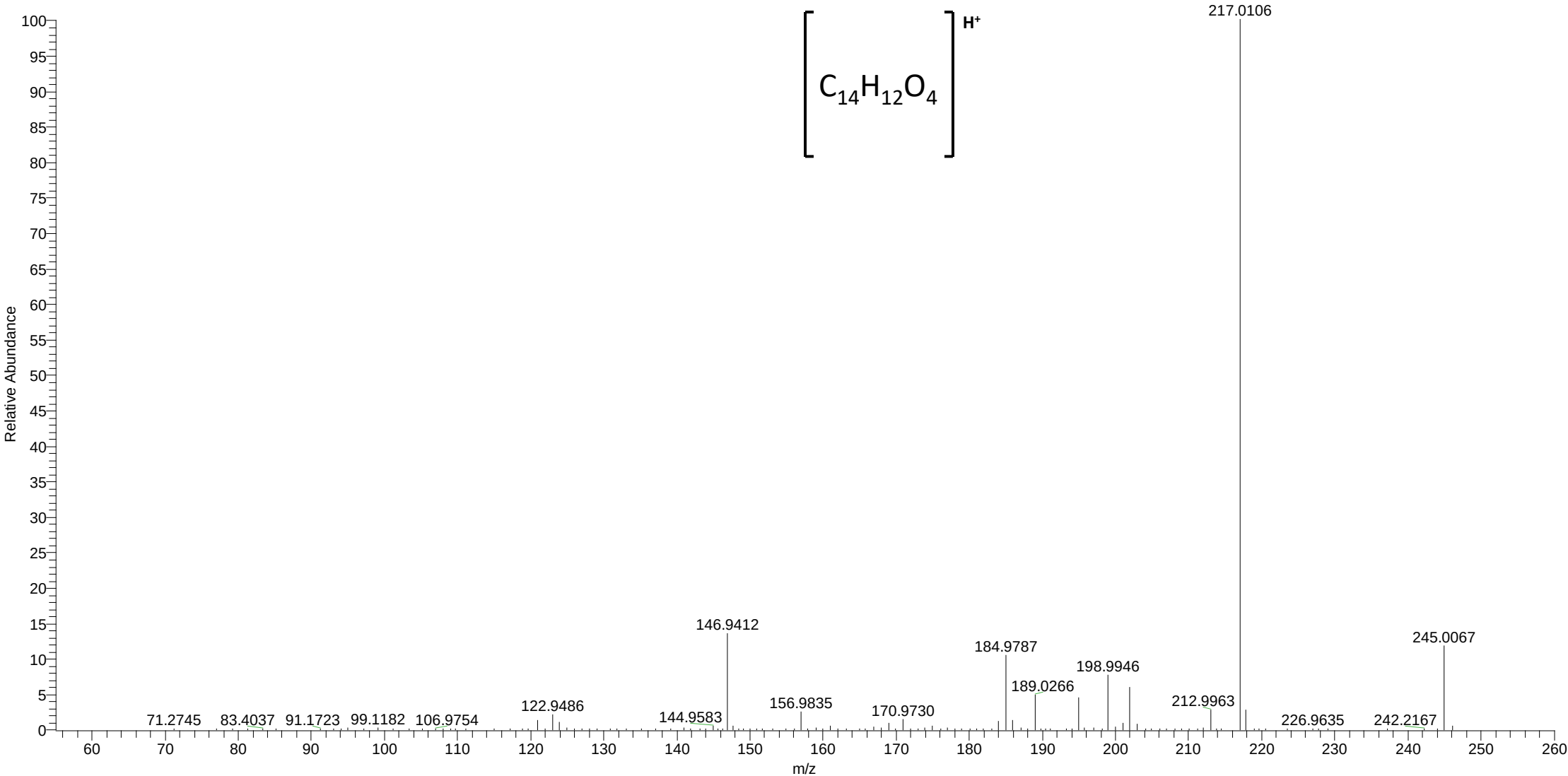
Compound 9	Formula	Ionspecies	<i>m/z</i>	RT [min]	Reference
Lysine	C ₆ H ₁₄ N ₂ O ₂	[M+H] ⁺	147.1128	4.26	Was not fragmented

sample_5 #429 RT: 4.26 AV: 1 NL: 5.89E3
F: FTMS + p ESI Full ms [100.00-1800.00]



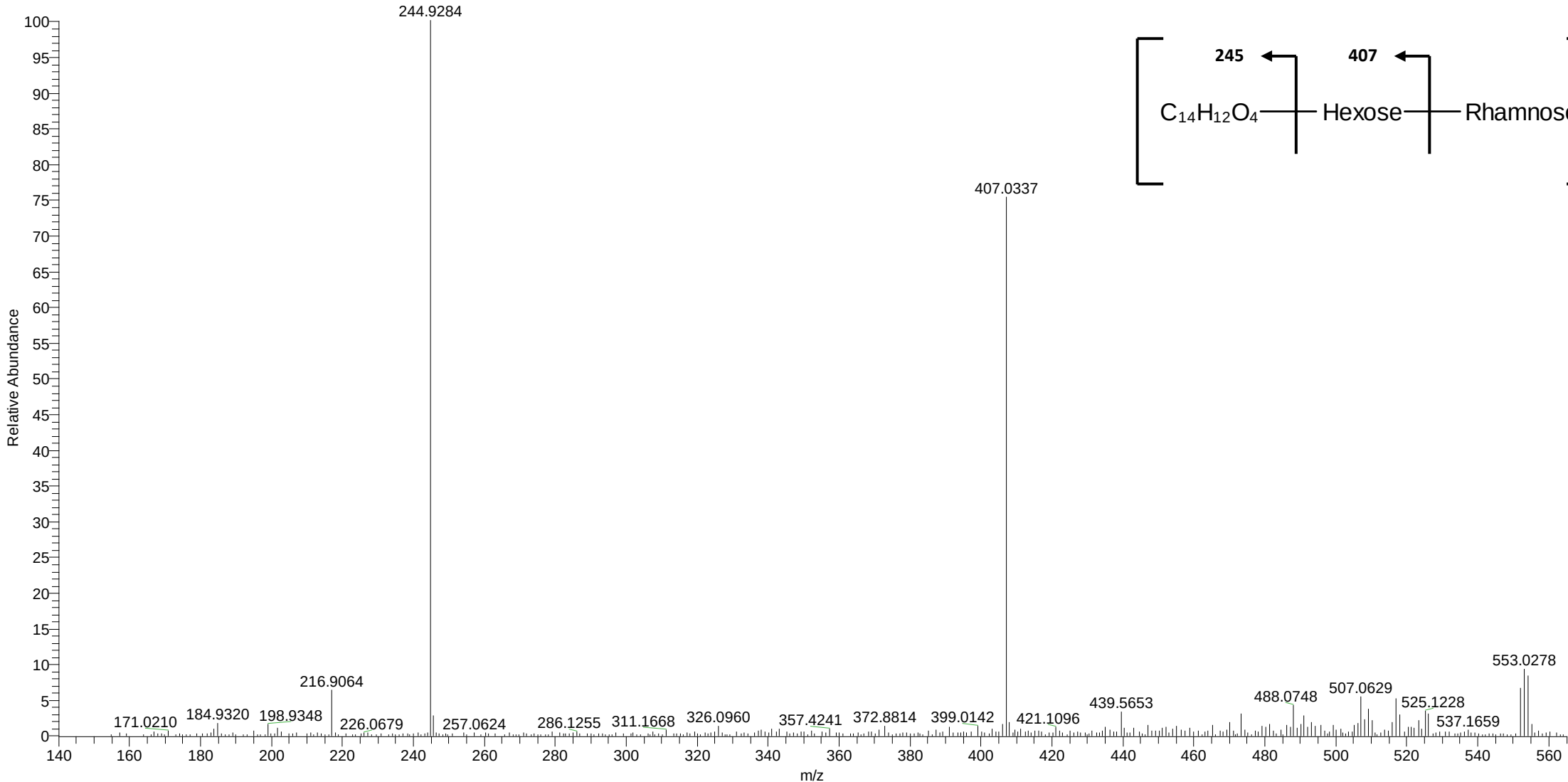
Compound 10	Formula	Ionspecies	<i>m/z</i>	RT [min]	Reference
Unknown1 putative phenolic	C ₁₄ H ₁₂ O ₄	[M+H] ⁺	245.0808	26.06	No reference available

sample_9 #2537 RT: 25.87 AV: 1 NL: 6.61E4
 F: ITMS + c ESI r d w Full ms2 245.08@cid35.00 [55.00-260.00]



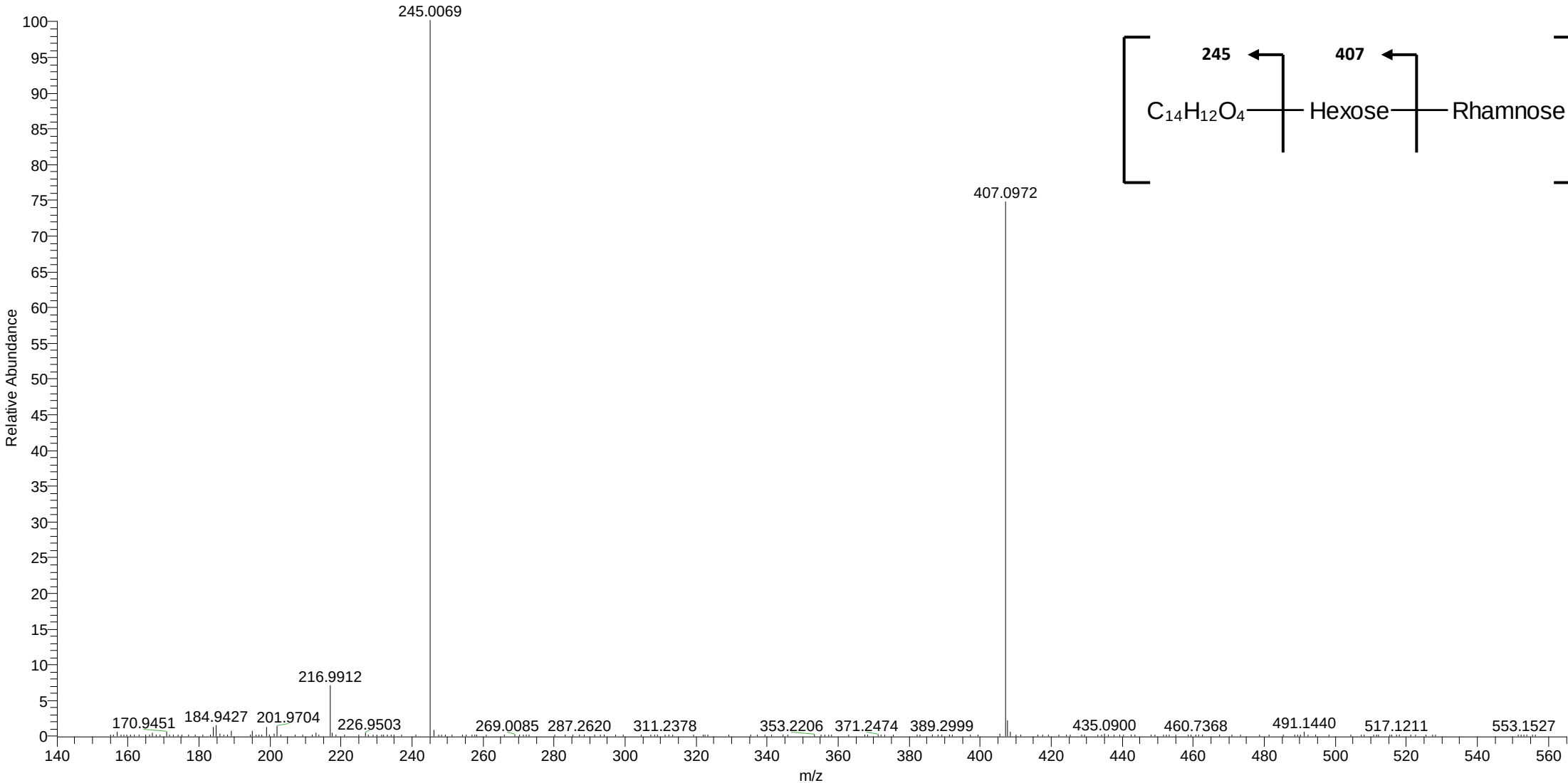
Compound 11	Formula	Ionspecies	<i>m/z</i>	RT [min]	Reference
Unknown2 putative phenolic hexosyl rhamnoside	C ₂₆ H ₃₂ O ₁₃	[M+H] ⁺	553.1916	19.90	No reference available

sample_4 #1951
RT: 19.75
AV: 1
NL: 3.17E3
F: ITMS + c ESI r d w Full ms2 553.19@cid35.00 [140.00-565.00]



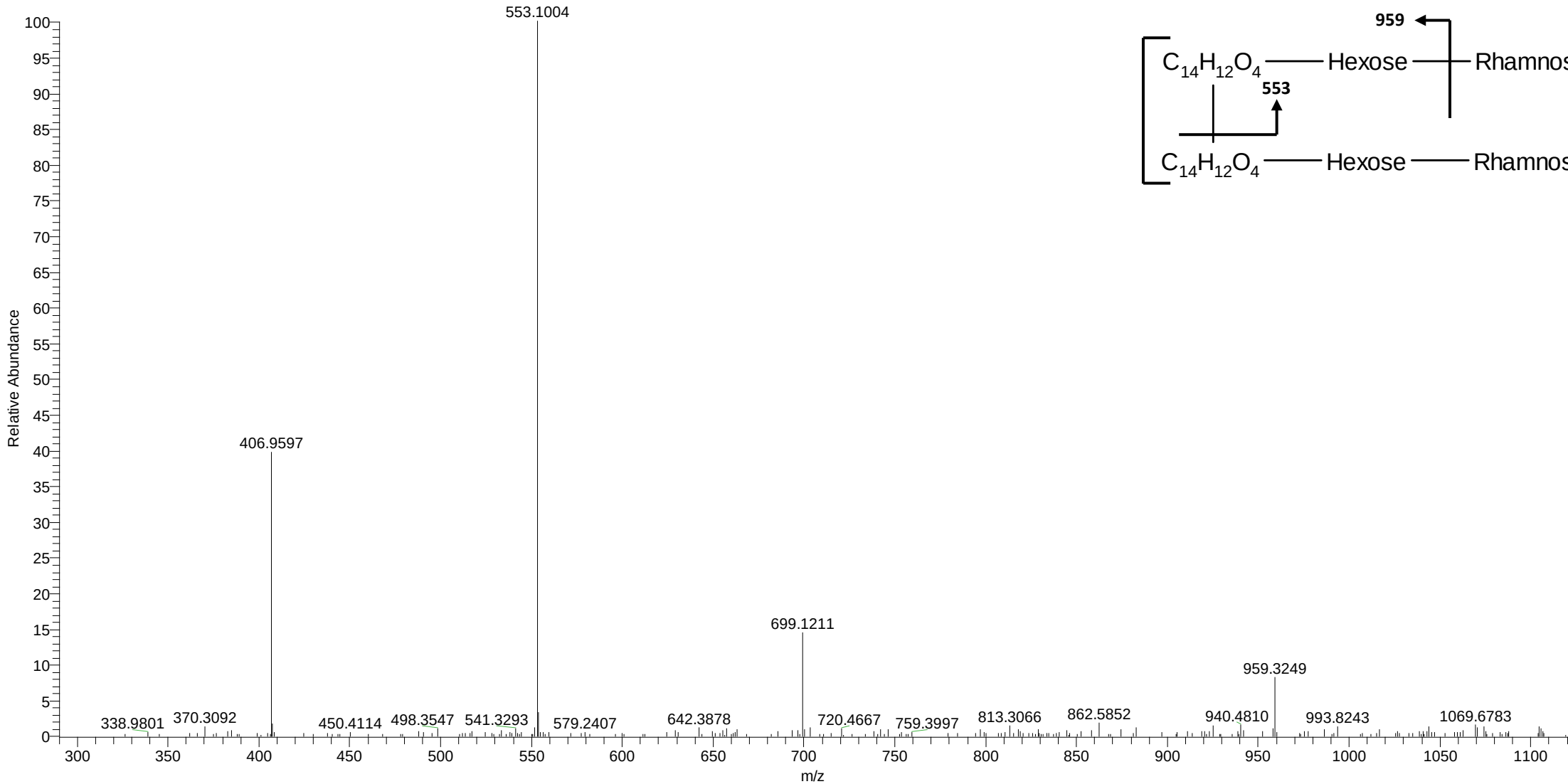
Compound 12	Formula	Ionspecies	<i>m/z</i>	RT [min]	Reference
Unknown3 putative phenolic hexosyl rhamnoside	C ₂₆ H ₃₂ O ₁₃	[M+H] ⁺	553.1916	19.22	No reference available

sample_4 #1890
 RT: 19.13
 AV: 1
 NL: 5.78E5
 F: ITMS + c ESI r d w Full ms2 553.19@cid35.00 [140.00-565.00]



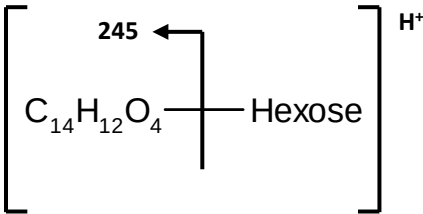
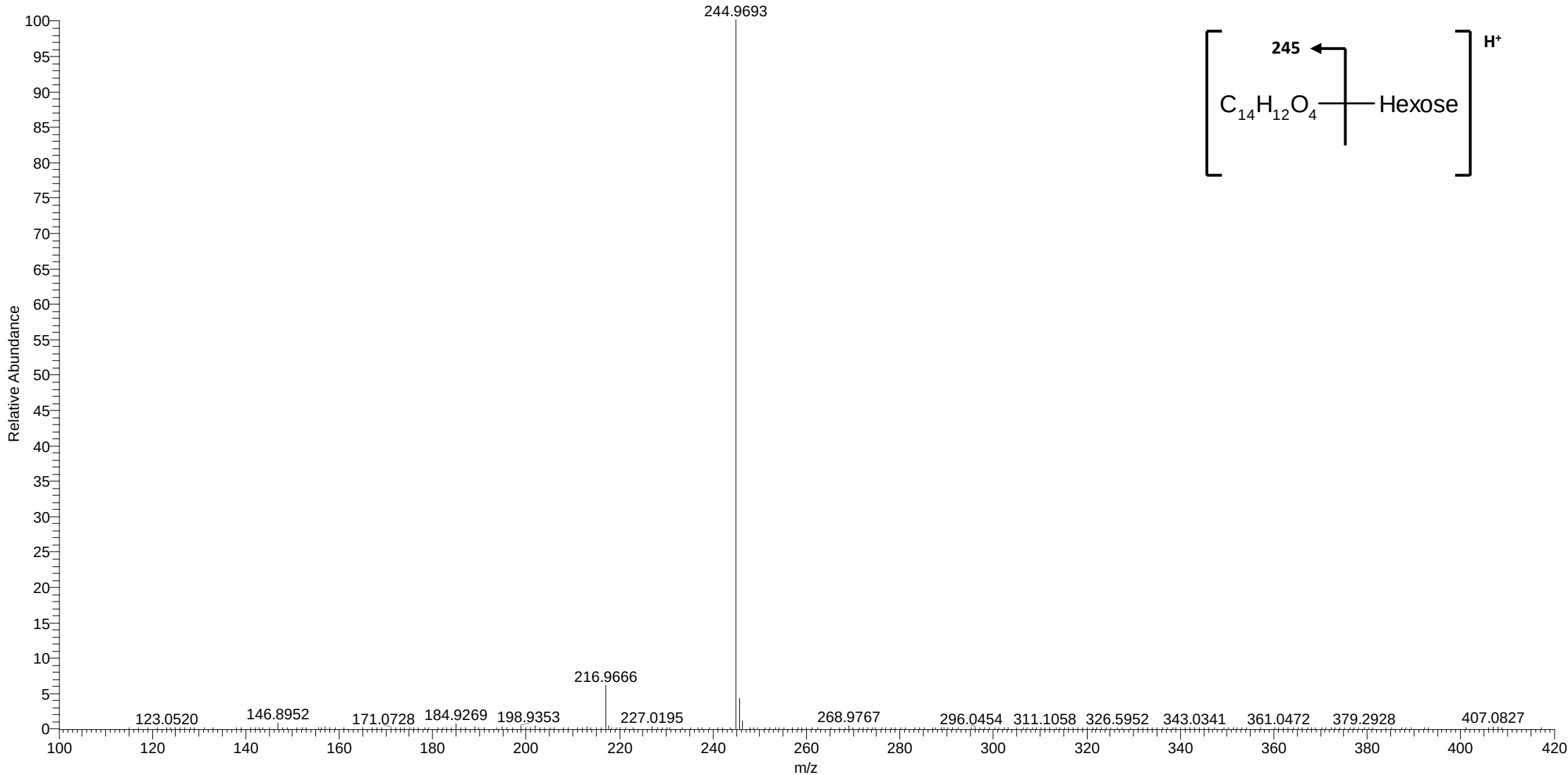
Compound 13	Formula	Ionspecies	m/z	RT [min]	Reference
Unknown4 putative phenolic hexosyl rhamnoside dimer	C ₅₂ H ₆₄ O ₂₆	[M+H] ⁺	1105.3759	19.22	No reference available

sample 4 #1891 RT: 19.13 AV: 1 NL: 2.14E3
 F: ITMS + c ESI r d w Full ms2 1105.38@cid35.00 [290.00-1120.00]



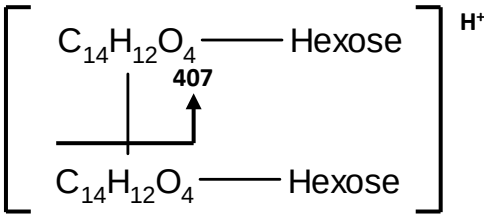
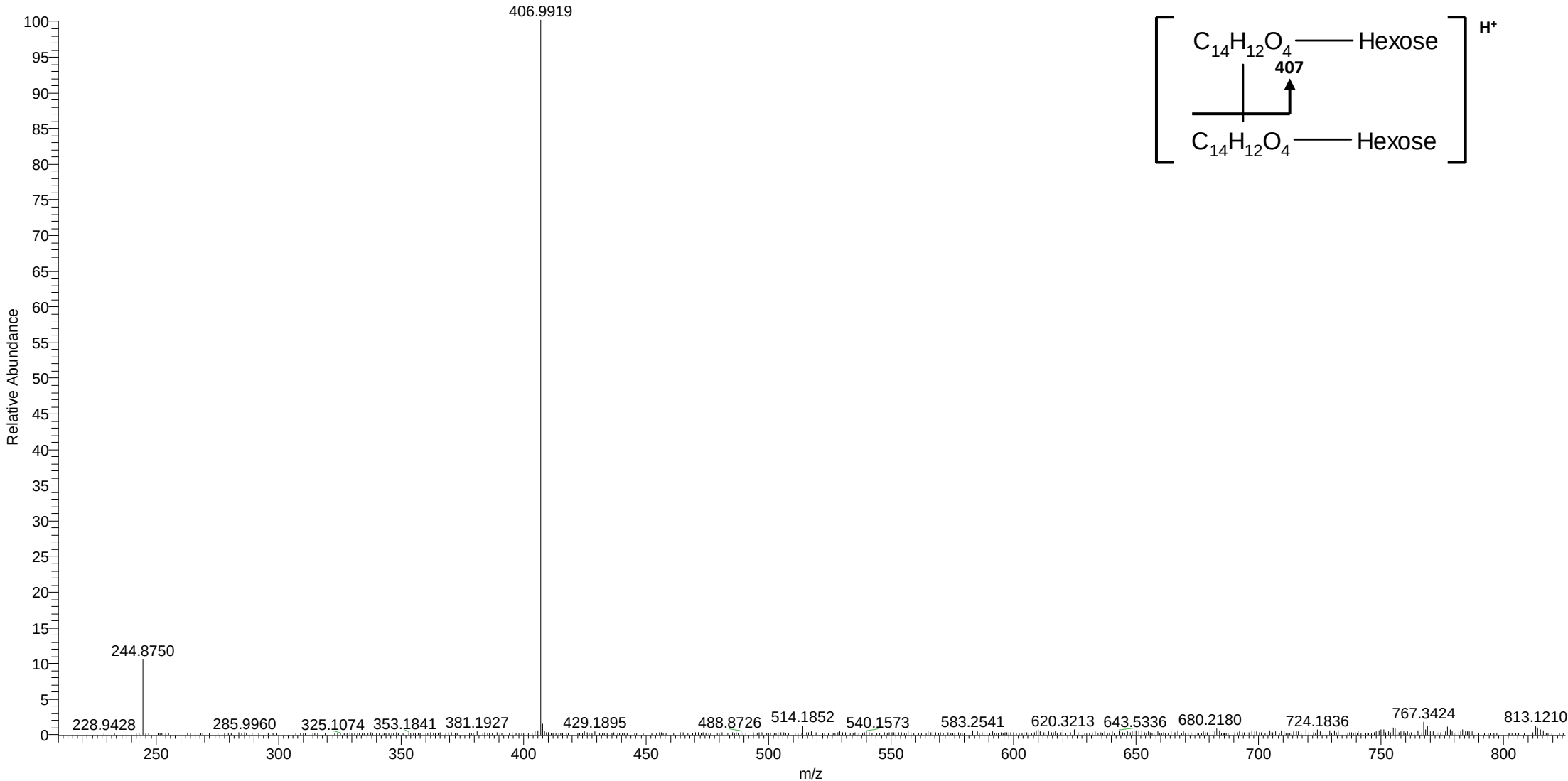
Compound 14	Formula	Ionspecies	<i>m/z</i>	RT [min]	Reference
Unknown5 putative phenolic hexoside	C ₂₀ H ₂₂ O ₉	[M+H] ⁺	407.1337	19.31	No reference available

sample_3 #1853 RT: 19.04 AV: 1 NL: 7.65E4
 F: ITMS + c ESI r d w Full ms2 407.13@cid35.00 [100.00-420.00]



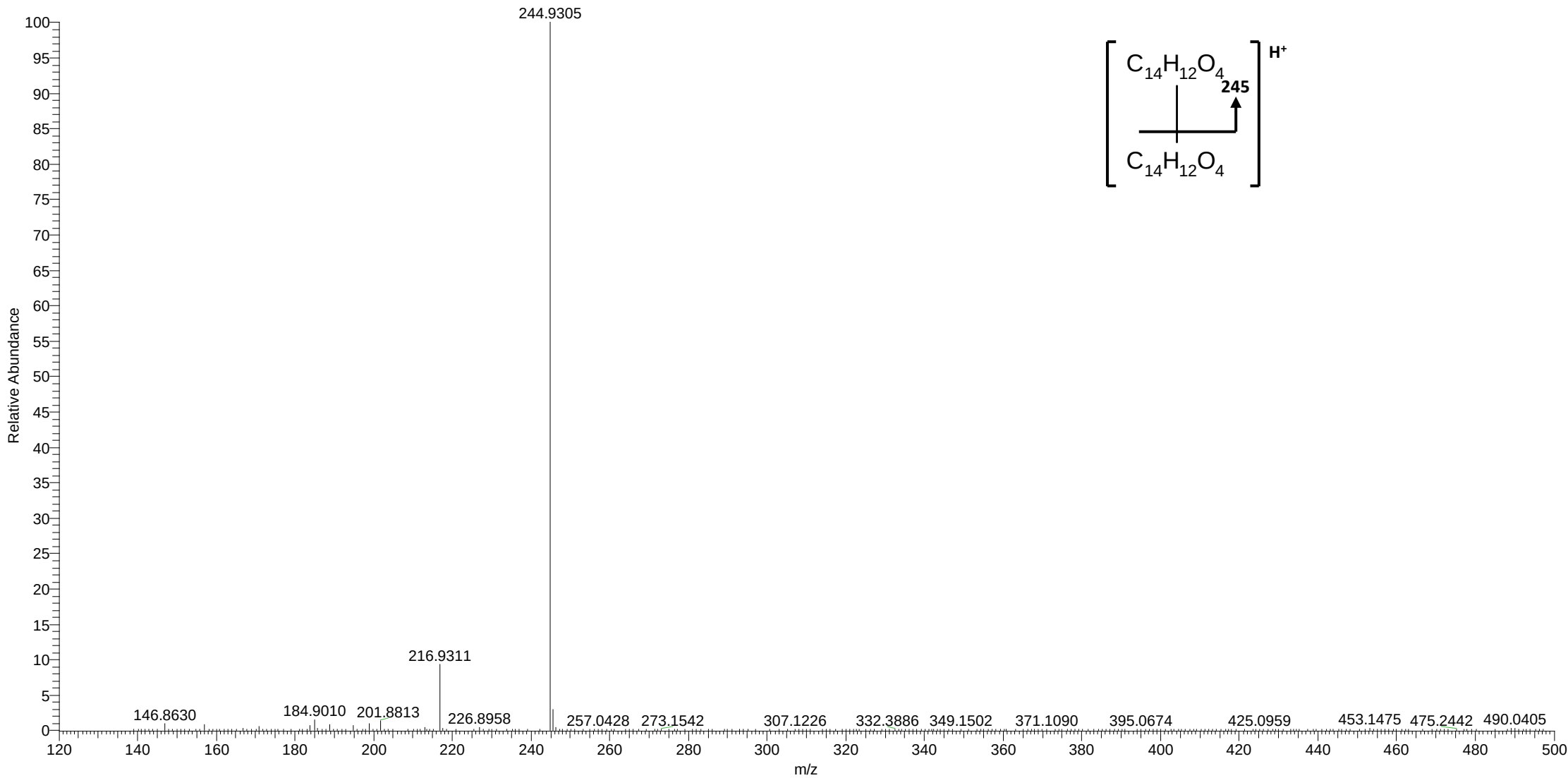
Compound 15	Formula	Ionspecies	m/z	RT [min]	Reference
Unknown6 putative phenolic hexoside dimer	C ₄₀ H ₄₄ O ₁₈	[M+H] ⁺	813.26	19.45	No reference available

sample_4 #1924
RT: 19.46
AV: 1
NL: 6.07E3
F: ITMS + c ESI r d w Full ms2 813.26@cid35.00 [210.00-825.00]



Compound 16	Formula	Ionspecies	<i>m/z</i>	RT [min]	Reference
Unknown7 putative phenolic dimer	C ₂₈ H ₂₄ O ₈	[M+H] ⁺	489.1544	25.45	No reference available

sample_4 #2517 RT: 25.56 AV: 1 NL: 1.07E5
 F: ITMS + c ESI r d w Full ms2 489.32@cid35.00 [120.00-500.00]



Compound 17	Formula	Ionspecies	<i>m/z</i>	RT [min]	Reference
Unknown8 putative phenolic dimer	C ₂₈ H ₂₄ O ₈	[M+H] ⁺	489.1544	26.23	No reference available

sample_4 #2583 RT: 26.24 AV: 1 NL: 2.13E2
 F: ITMS + c ESI r d w Full ms2 489.32@cid35.00 [120.00-500.00]

