WEB350

Benjamin Weigel

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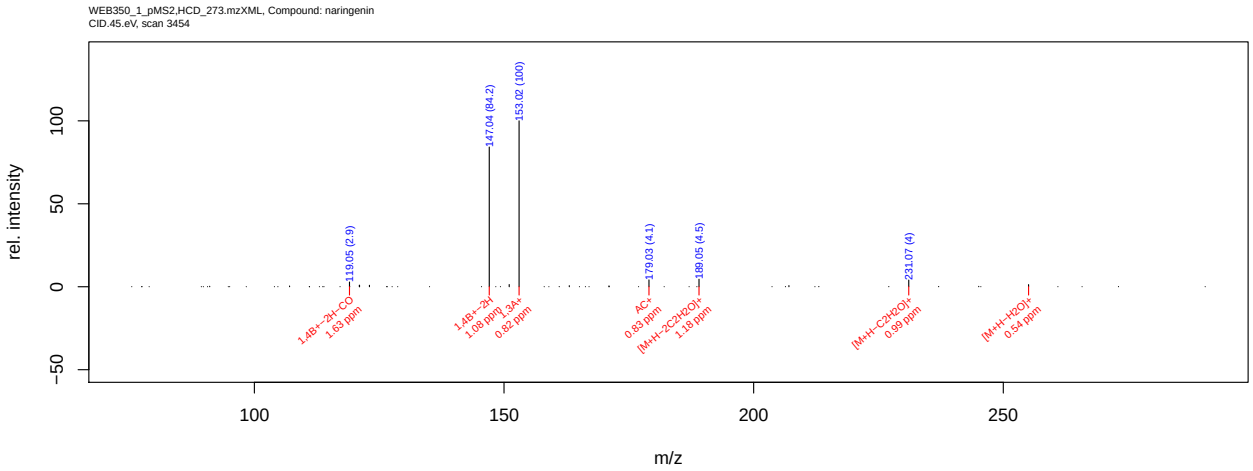
Contents

	substance	fragment	formula	MW	mz
1	naringenin	1,4B+-2H			147.04
2	naringenin	1,4B+-2H-2CO			91.05
3	naringenin	1,4B+-2H-CO			119.05
4	naringenin	AC+			179.03
5	naringenin	[M+H]+	C15H12O5	272.07	273.08
6	naringenin	[M+H-2C2H2O]+	C15H12O5	272.07	189.06

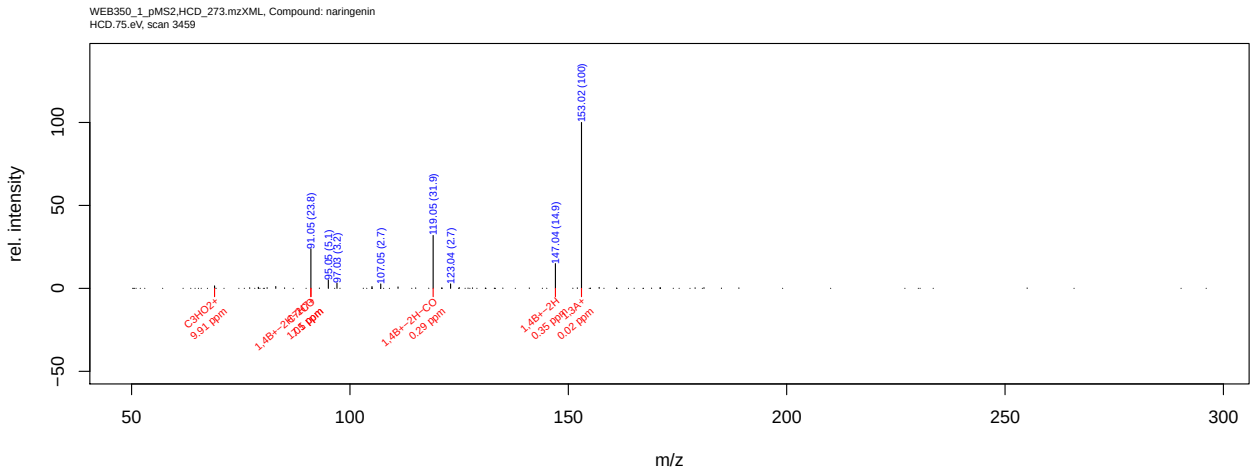
Automatic annotation of MS spectra

naringenin.CID.45eV



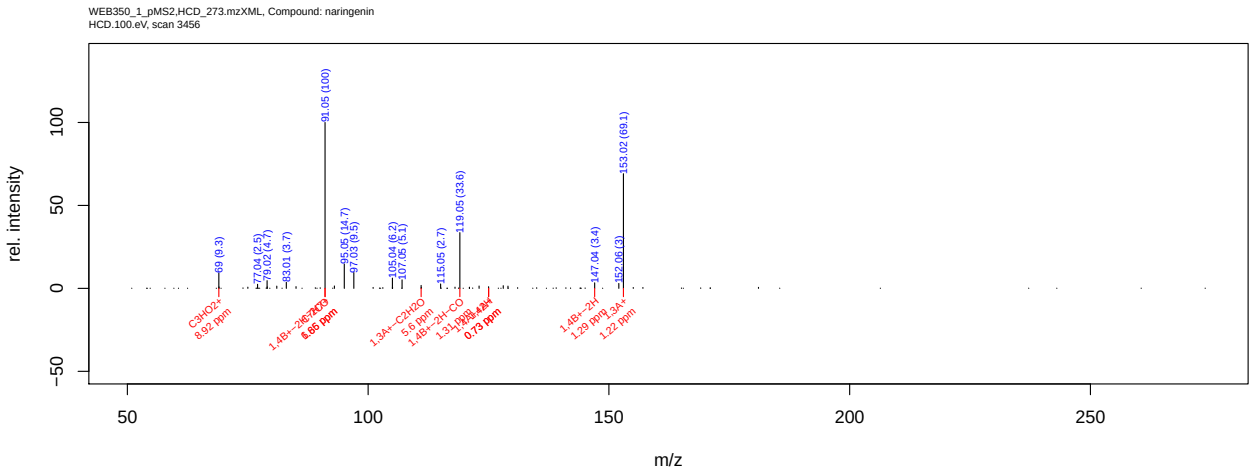
	mz	int	ppm	fragment
1	119.05	2.9	1.63	1,4B+-2H-CO
2	147.04	84.2	1.08	1,4B+-2H
3	153.02	100.0	0.82	1,3A+
4	179.03	4.1	0.83	AC+
5	189.05	4.5	1.18	[M+H-2C2H2O]+
6	231.07	4.0	0.99	[M+H-C2H2O]+
7	255.07	1.3	0.54	[M+H-H2O]+

naringenin.HCD.75eV



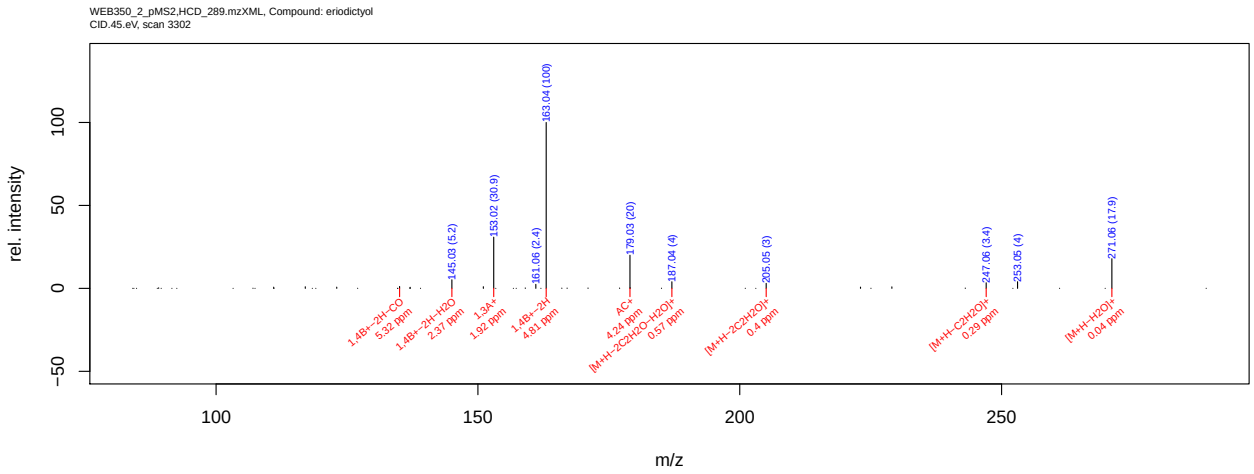
	mz	int	ppm	fragment
1	69.00	1.5	9.91	C3HO2+
2	91.05	23.8	1.01	1,4B+-2H-2CO
3	91.05	23.8	7.50	C7H7+
4	119.05	31.9	0.29	1,4B+-2H-CO
5	147.04	14.9	0.35	1,4B+-2H
6	153.02	100.0	0.02	1,3A+

naringenin.HCD.100eV



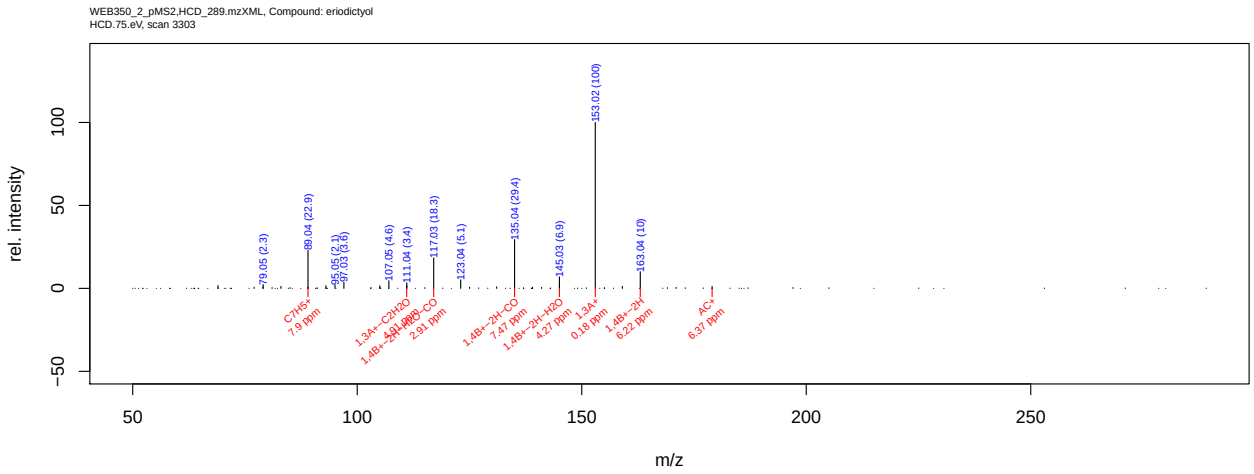
	mz	int	ppm	fragment
1	69.00	9.3	8.92	C3HO2+
2	91.05	100.0	1.85	1,4B+-2H-2CO
3	91.05	100.0	6.66	C7H7+
4	111.01	1.8	5.60	1,3A+-C2H2O
5	119.05	33.6	1.31	1,4B+-2H-CO
6	125.02	1.0	0.73	1,4A+
7	125.02	1.0	0.73	1,4A++2H
8	147.04	3.4	1.29	1,4B+-2H
9	153.02	69.1	1.22	1,3A+

eriodictyol.CID.45eV



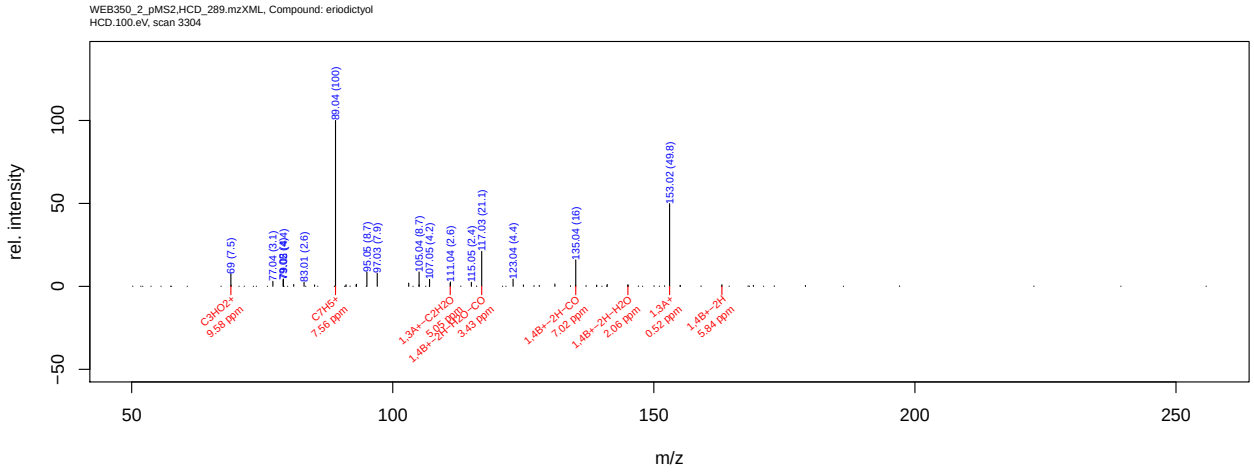
	mz	int	ppm	fragment
1	135.04	1.1	5.32	1,4B+-2H-CO
2	145.03	5.2	2.37	1,4B+-2H-H2O
3	153.02	30.9	1.92	1,3A+
4	163.04	100.0	4.81	1,4B+-2H
5	179.03	20.0	4.24	AC+
6	187.04	4.0	0.57	[M+H-2C2H2O-H2O]+
7	205.05	3.0	0.40	[M+H-2C2H2O]+
8	247.06	3.4	0.29	[M+H-C2H2O]+
9	271.06	17.9	0.04	[M+H-H2O]+

eriodictyol.HCD.75eV



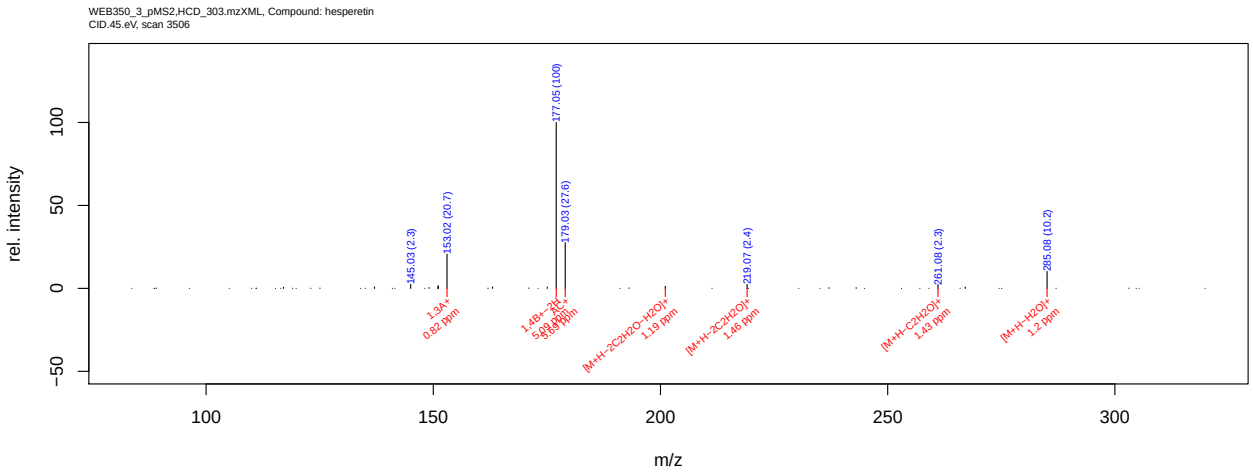
	mz	int	ppm	fragment
1	89.04	22.9	7.90	C7H5+
2	111.01	1.8	4.91	1,3A+-C2H2O
3	117.03	18.3	2.91	1,4B+-2H-H2O-CO
4	135.04	29.4	7.47	1,4B+-2H-CO
5	145.03	6.9	4.27	1,4B+-2H-H2O
6	153.02	100.0	0.18	1,3A+
7	163.04	10.0	6.22	1,4B+-2H
8	179.03	1.1	6.37	AC+

eriodictyol.HCD.100eV



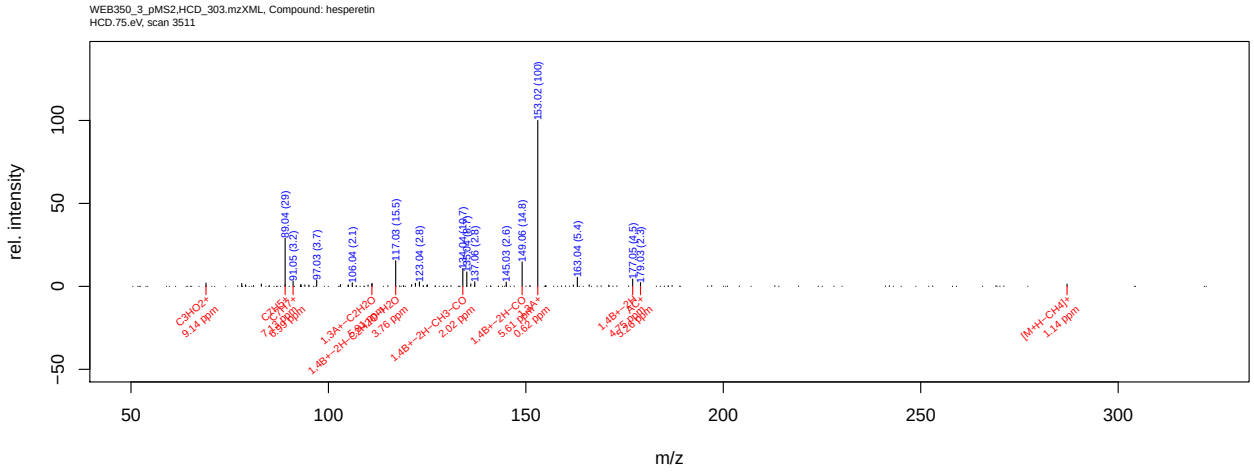
	mz	int	ppm	fragment
1	69.00	7.5	9.58	C3HO2+
2	89.04	100.0	7.56	C7H5+
3	111.01	1.9	5.05	1,3A+-C2H2O
4	117.03	21.1	3.43	1,4B+-2H-H2O-CO
5	135.04	16.0	7.02	1,4B+-2H-CO
6	145.03	1.0	2.06	1,4B+-2H-H2O
7	153.02	49.8	0.52	1,3A+
8	163.04	1.0	5.84	1,4B+-2H

hesperetin.CID.45eV



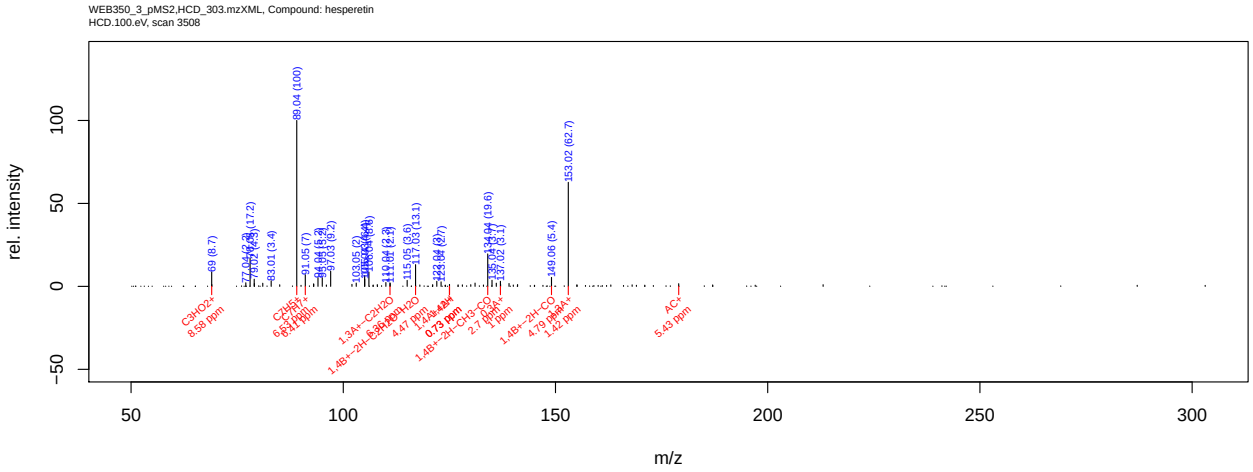
	mz	int	ppm	fragment
1	153.02	20.7	0.82	1,3A+
2	177.05	100.0	5.09	1,4B+-2H
3	179.03	27.6	5.69	AC+
4	201.05	1.3	1.19	[M+H-2C2H2O-H2O]+
5	219.07	2.4	1.46	[M+H-2C2H2O]+
6	261.08	2.3	1.43	[M+H-C2H2O]+
7	285.08	10.2	1.20	[M+H-H2O]+

hesperetin.HCD.75eV



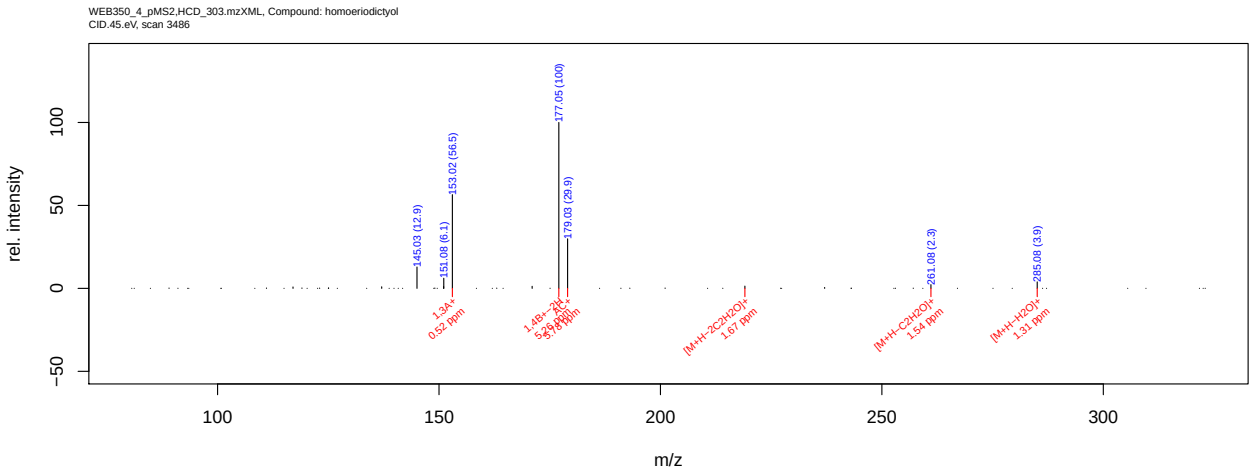
	mz	int	ppm	fragment
1	69.00	2.0	9.14	C3HO2+
2	89.04	29.0	7.13	C7H5+
3	91.05	3.2	6.99	C7H7+
4	111.01	1.4	5.81	1,3A+-C2H2O
5	117.03	15.5	3.76	1,4B+-2H-C2H2O-H2O
6	134.04	10.7	2.02	1,4B+-2H-CH3-CO
7	149.06	14.8	5.61	1,4B+-2H-CO
8	153.02	100.0	0.62	1,3A+
9	177.05	4.5	4.75	1,4B+-2H
10	179.03	2.3	5.26	AC+
11	287.06	1.4	1.14	[M+H-CH4]+

hesperetin.HCD.100eV



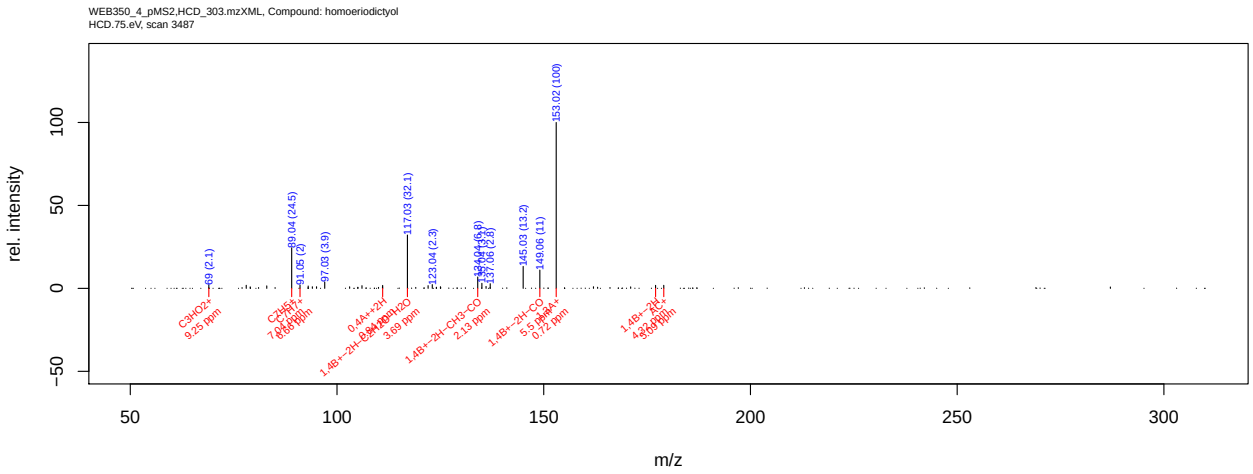
	mz	int	ppm	fragment
1	69.00	8.7	8.58	C3HO2+
2	89.04	100.0	6.53	C7H5+
3	91.05	7.0	6.41	C7H7+
4	111.01	2.1	6.36	1,3A+-C2H2O
5	117.03	13.1	4.47	1,4B+-2H-C2H2O-H2O
6	125.02	1.2	0.73	1,4A+
7	125.02	1.2	0.73	1,4A++2H
8	134.04	19.6	2.70	1,4B+-2H-CH3-CO
9	137.02	3.1	1.00	0,3A+
10	149.06	5.4	4.79	1,4B+-2H-CO
11	153.02	62.7	1.42	1,3A+
12	179.03	1.6	5.43	AC+

homoeriodictyol.CID.45eV



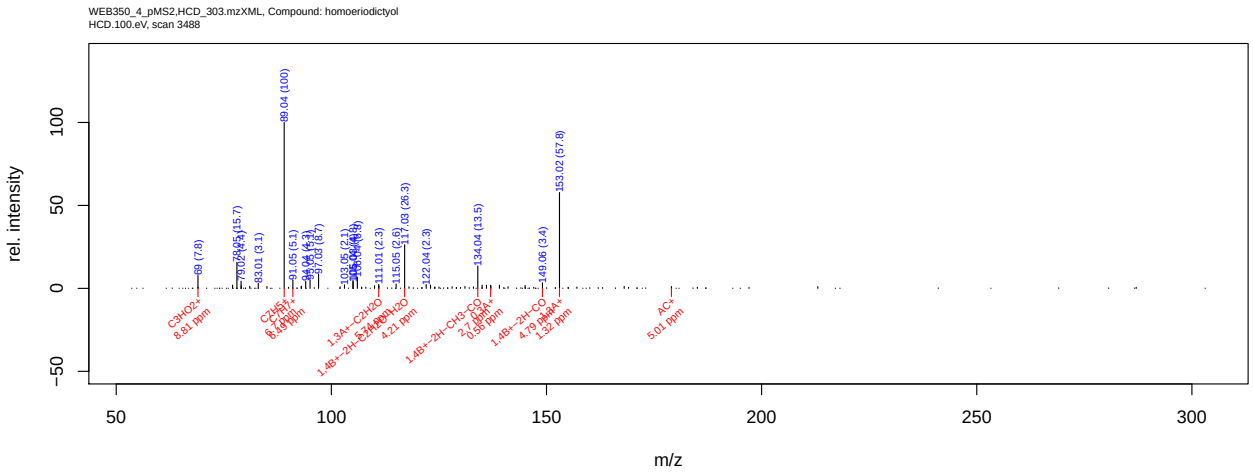
	mz	int	ppm	fragment
1	153.02	56.5	0.52	1,3A+
2	177.05	100.0	5.26	1,4B+-2H
3	179.03	29.9	5.78	AC+
4	219.07	1.4	1.67	[M+H-2C2H2O]+
5	261.08	2.3	1.54	[M+H-C2H2O]+
6	285.08	3.9	1.31	[M+H-H2O]+

homoeriodictyol.HCD.75eV



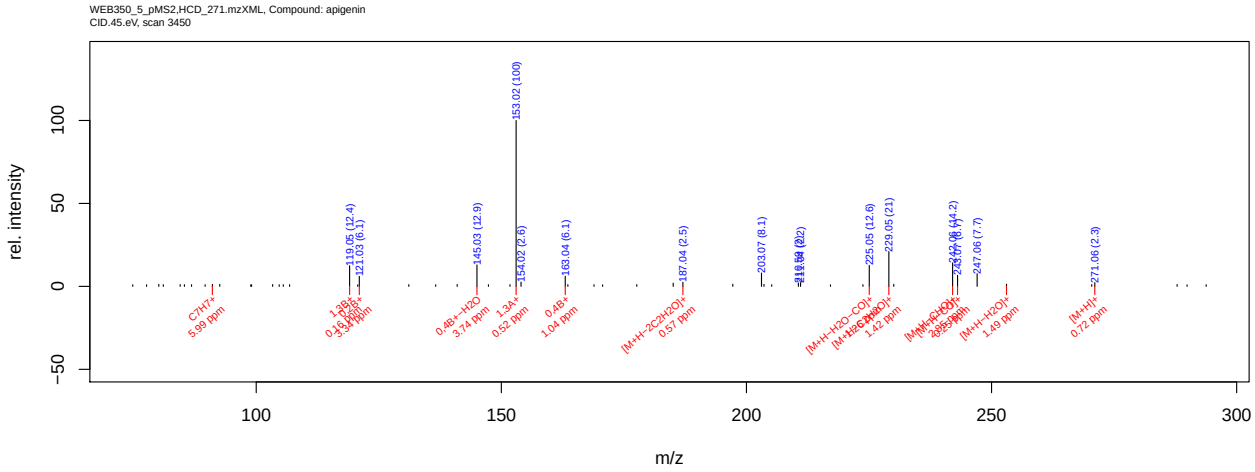
	mz	int	ppm	fragment
1	69.00	2.1	9.25	C3HO2+
2	89.04	24.5	7.04	C7H5+
3	91.05	2.0	6.66	C7H7+
4	111.04	1.8	0.84	0,4A++2H
5	117.03	32.1	3.69	1,4B+-2H-C2H2O-H2O
6	134.04	6.8	2.13	1,4B+-2H-CH3-CO
7	149.06	11.0	5.50	1,4B+-2H-CO
8	153.02	100.0	0.72	1,3A+
9	177.05	1.8	4.32	1,4B+-2H
10	179.03	1.8	5.09	AC+

homoeriodictyol.HCD.100eV



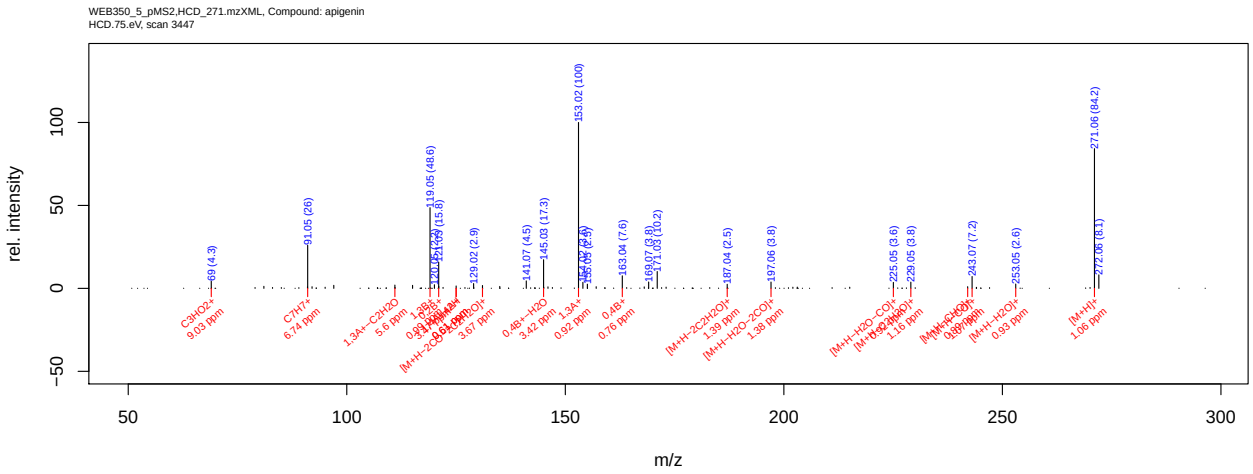
	mz	int	ppm	fragment
1	69.00	7.8	8.81	C3HO2+
2	89.04	100.0	6.70	C7H5+
3	91.05	5.1	6.49	C7H7+
4	111.01	2.3	5.74	1,3A+-C2H2O
5	117.03	26.3	4.21	1,4B+-2H-C2H2O-H2O
6	134.04	13.5	2.70	1,4B+-2H-CH3-CO
7	137.02	1.8	0.56	0,3A+
8	149.06	3.4	4.79	1,4B+-2H-CO
9	153.02	57.8	1.32	1,3A+
10	179.03	1.1	5.01	AC+

apigenin.CID.45eV



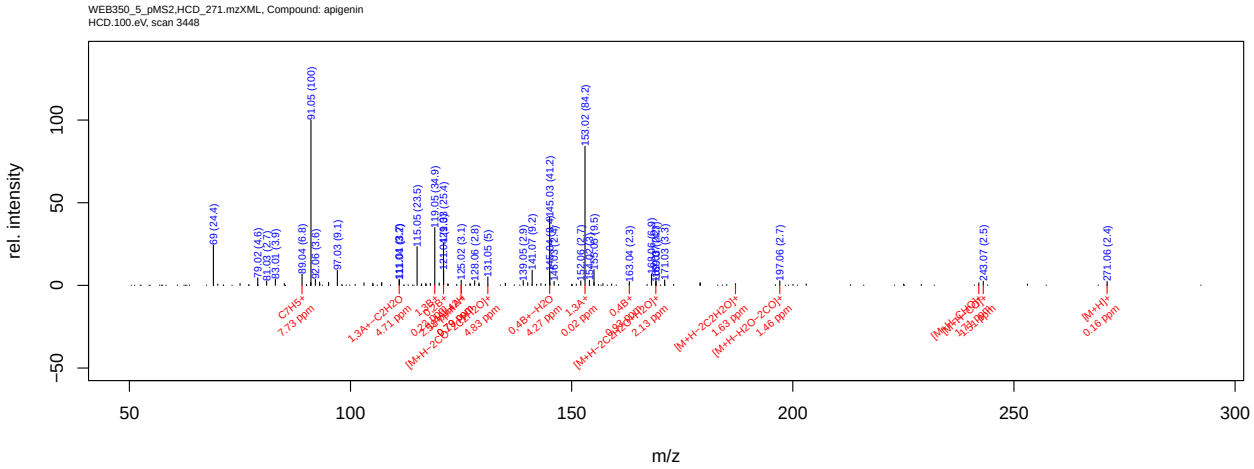
	mz	int	ppm	fragment
1	91.05	1.2	5.99	C7H7+
2	119.05	12.4	0.16	1,3B+
3	121.03	6.1	3.34	0,2B+
4	145.03	12.9	3.74	0,4B+-H2O
5	153.02	100.0	0.52	1,3A+
6	163.04	6.1	1.04	0,4B+
7	187.04	2.5	0.57	[M+H-2C2H2O]+
8	225.05	12.6	1.26	[M+H-H2O-CO]+
9	229.05	21.0	1.42	[M+H-C2H2O]+
10	242.06	14.2	2.85	[M+H-CHO]+
11	243.07	6.7	0.25	[M+H-CO]+
12	253.05	1.3	1.49	[M+H-H2O]+
13	271.06	2.3	0.72	[M+H]+

apigenin.HCD.75eV



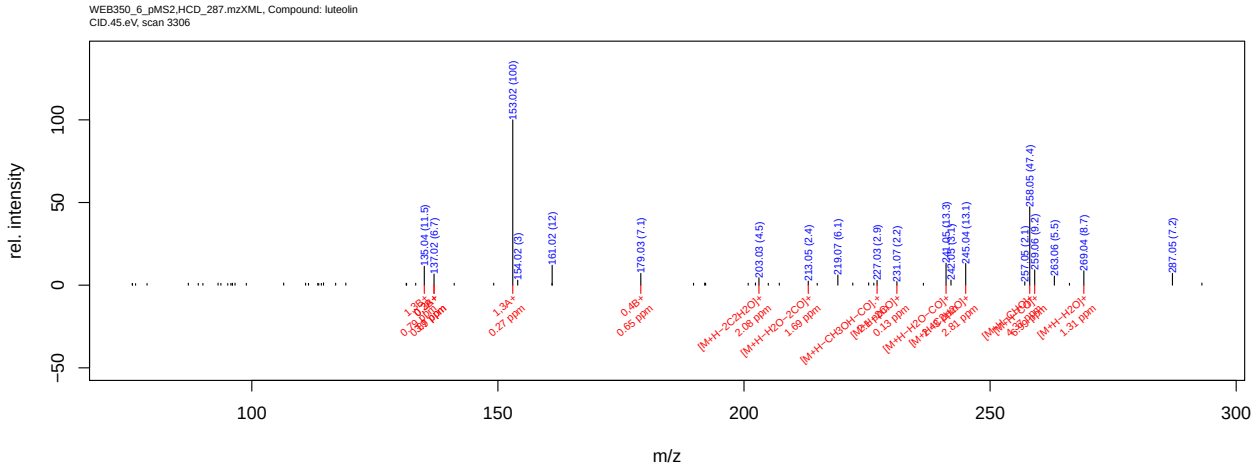
	mz	int	ppm	fragment
1	69.00	4.3	9.03	C3HO2+
2	91.05	26.0	6.74	C7H7+
3	111.01	2.0	5.60	1,3A+-C2H2O
4	119.05	48.6	0.99	1,3B+
5	121.03	15.8	3.47	0,2B+
6	125.02	1.5	0.61	1,4A+
7	125.02	1.5	0.61	1,4A++2H
8	131.05	1.7	3.67	[M+H-2CO-2C2H2O]+
9	145.03	17.3	3.42	0,4B+-H2O
10	153.02	100.0	0.92	1,3A+
11	163.04	7.6	0.76	0,4B+
12	187.04	2.5	1.39	[M+H-2C2H2O]+
13	197.06	3.8	1.38	[M+H-H2O-2CO]+
14	225.05	3.6	0.92	[M+H-H2O-CO]+
15	229.05	3.8	1.16	[M+H-C2H2O]+
16	242.06	1.0	0.89	[M+H-CHO]+
17	243.07	7.2	1.07	[M+H-CO]+
18	253.05	2.6	0.93	[M+H-H2O]+
19	271.06	84.2	1.06	[M+H]+

apigenin.HCD.100eV



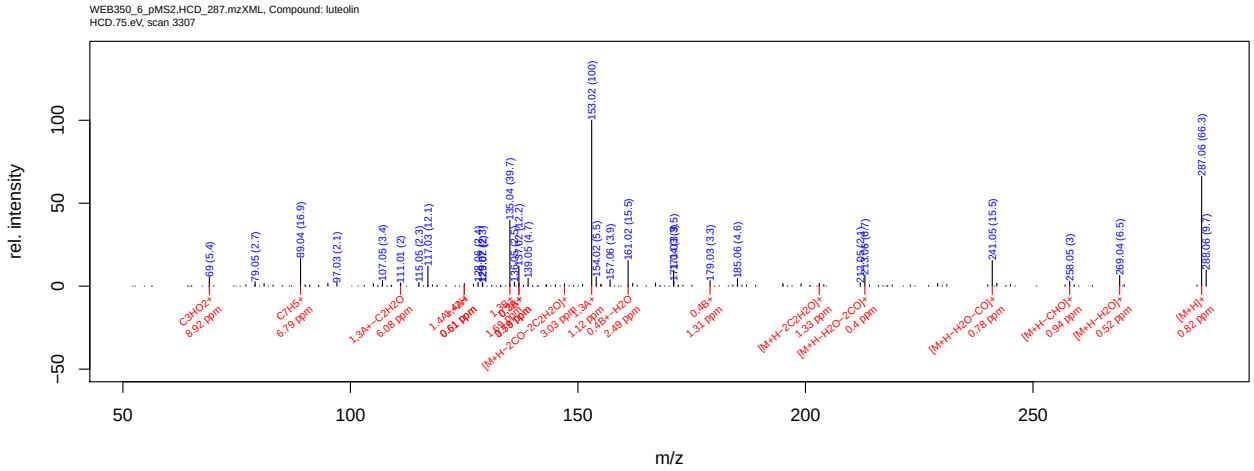
	mz	int	ppm	fragment
1	89.04	6.8	7.73	C7H5+
2	111.01	3.7	4.71	1,3A+-C2H2O
3	119.05	34.9	0.22	1,3B+
4	121.03	25.4	2.58	0,2B+
5	125.02	3.1	0.79	1,4A+
6	125.02	3.1	0.79	1,4A++2H
7	131.05	5.0	4.83	[M+H-2CO-2C2H2O]+
8	145.03	41.2	4.27	0,4B+-H2O
9	153.02	84.2	0.02	1,3A+
10	163.04	2.3	0.93	0,4B+
11	169.03	2.2	2.13	[M+H-2C2H2O-H2O]+
12	187.04	1.0	1.63	[M+H-2C2H2O]+
13	197.06	2.7	1.46	[M+H-H2O-2CO]+
14	242.06	1.5	1.71	[M+H-CHO]+
15	243.07	2.5	1.51	[M+H-CO]+
16	271.06	2.4	0.16	[M+H]+

luteolin.CID.45eV



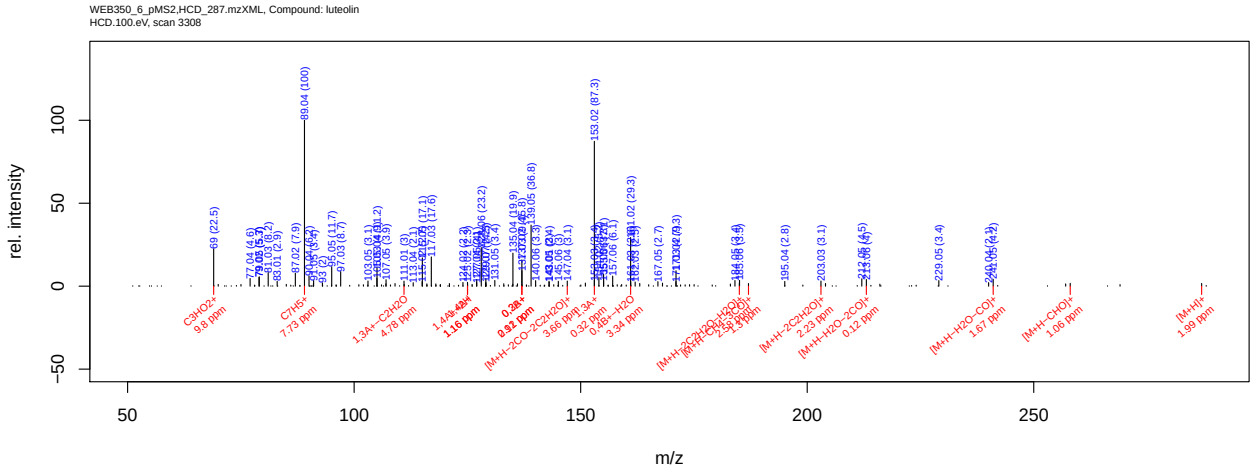
	mz	int	ppm	fragment
1	135.04	11.5	0.79	1,3B+
2	137.02	6.7	3.70	0,2B+
3	137.02	6.7	0.89	0,3A+
4	153.02	100.0	0.27	1,3A+
5	179.03	7.1	0.65	0,4B+
6	203.03	4.5	2.08	[M+H-2C2H2O]+
7	213.05	2.4	1.69	[M+H-H2O-2CO]+
8	227.03	2.9	2.10	[M+H-CH3OH-CO].+
9	231.07	2.2	0.13	[M+H-2CO]+
10	241.05	13.3	2.43	[M+H-H2O-CO]+
11	245.04	13.1	2.81	[M+H-C2H2O]+
12	258.05	47.4	4.37	[M+H-CHO]+
13	259.06	9.2	6.99	[M+H-CO]+
14	269.04	8.7	1.31	[M+H-H2O]+

luteolin.HCD.75eV



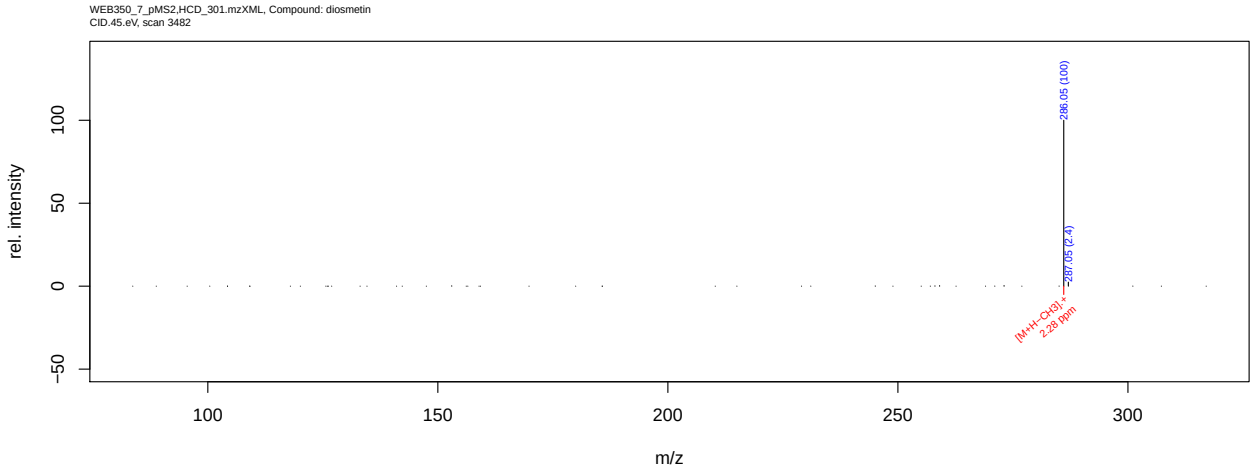
	mz	int	ppm	fragment
1	69.00	5.4	8.92	C3HO2+
2	89.04	16.9	6.79	C7H5+
3	111.01	2.0	6.08	1,3A+-C2H2O
4	125.02	1.7	0.61	1,4A+
5	125.02	1.7	0.61	1,4A++2H
6	135.04	39.7	1.69	1,3B+
7	137.02	12.2	3.59	0,2B+
8	137.02	12.2	0.78	0,3A+
9	147.04	1.5	3.03	[M+H-2CO-2C2H2O]+
10	153.02	100.0	1.12	1,3A+
11	161.02	15.5	2.49	0,4B+-H2O
12	179.03	3.3	1.31	0,4B+
13	203.03	1.7	1.33	[M+H-2C2H2O]+
14	213.06	6.7	0.40	[M+H-H2O-2CO]+
15	241.05	15.5	0.78	[M+H-H2O-CO]+
16	258.05	3.0	0.94	[M+H-CHO]+
17	269.04	6.5	0.52	[M+H-H2O]+
18	287.06	66.3	0.82	[M+H]+

luteolin.HCD.100eV



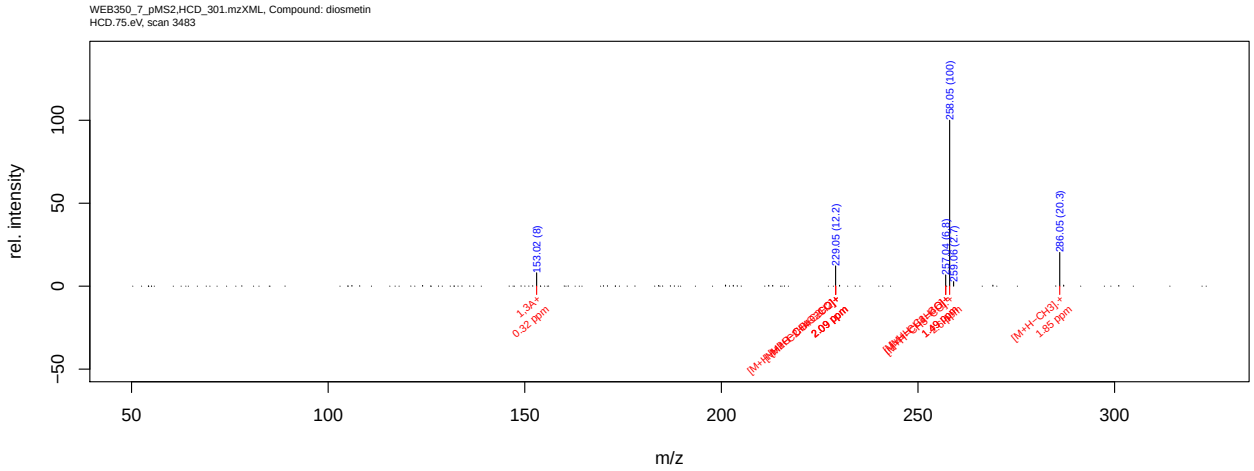
	mz	int	ppm	fragment
1	69.00	22.5	9.80	C3HO2+
2	89.04	100.0	7.73	C7H5+
3	111.01	3.0	4.78	1,3A+-C2H2O
4	125.02	2.3	1.16	1,4A+
5	125.02	2.3	1.16	1,4A++2H
6	137.02	15.8	2.92	0,2B+
7	137.02	15.8	0.11	0,3A+
8	147.04	3.1	3.66	[M+H-2CO-2C2H2O]+
9	153.02	87.3	0.32	1,3A+
10	161.02	29.3	3.34	0,4B+-H2O
11	185.02	1.9	2.58	[M+H-2C2H2O-H2O]+
12	187.04	1.6	1.30	[M+H-CH4-3CO]+
13	203.03	3.1	2.23	[M+H-2C2H2O]+
14	213.06	4.0	0.12	[M+H-H2O-2CO]+
15	241.05	4.2	1.67	[M+H-H2O-CO]+
16	258.05	1.7	1.06	[M+H-CHO]+
17	287.05	1.6	1.99	[M+H]+

diosmetin.CID.45eV



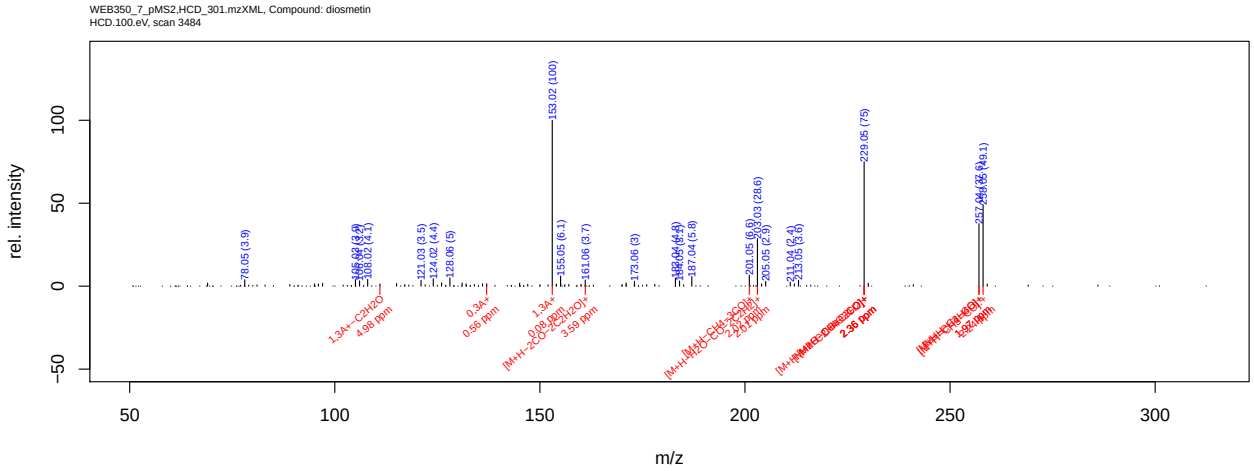
	mz	int	ppm	fragment
1	286.05	100.0	2.28	[M+H-CH3].+

diosmetin.HCD.75eV



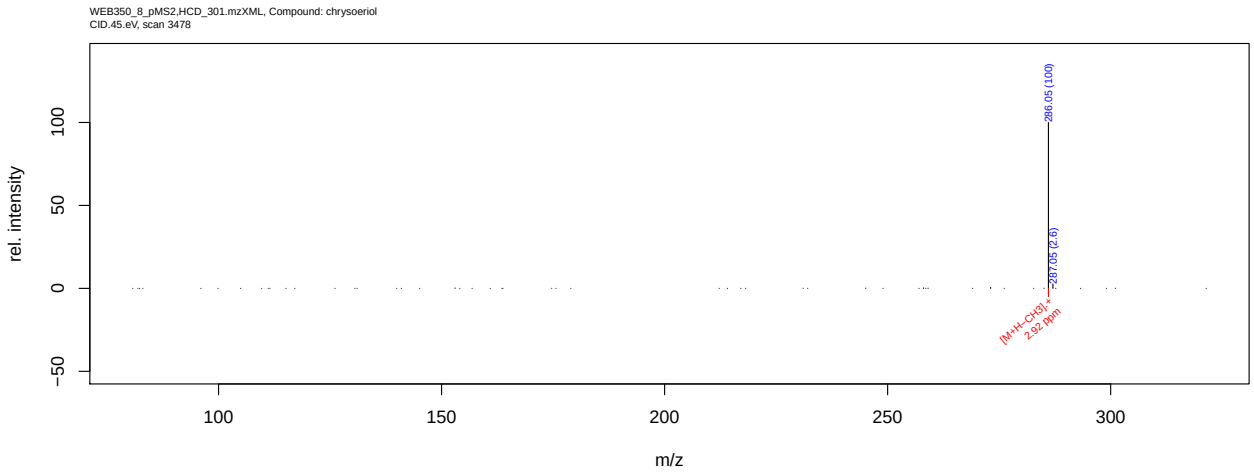
	mz	int	ppm	fragment
1	153.02	8.0	0.32	1,3A+
2	229.05	12.2	2.09	[M+h-C2H4O-CO]+
3	229.05	12.2	2.09	[M+H-CH4-2CO]+
4	229.05	12.2	2.09	[M+H-H2O-CO-C2H2]+
5	257.04	6.8	1.49	[M+H-C2H4O]+
6	257.04	6.8	1.49	[M+H-CH4-CO]+
7	258.05	100.0	2.60	[M+H-CH3-CO].+
8	286.05	20.3	1.85	[M+H-CH3].+

diosmetin.HCD.100eV



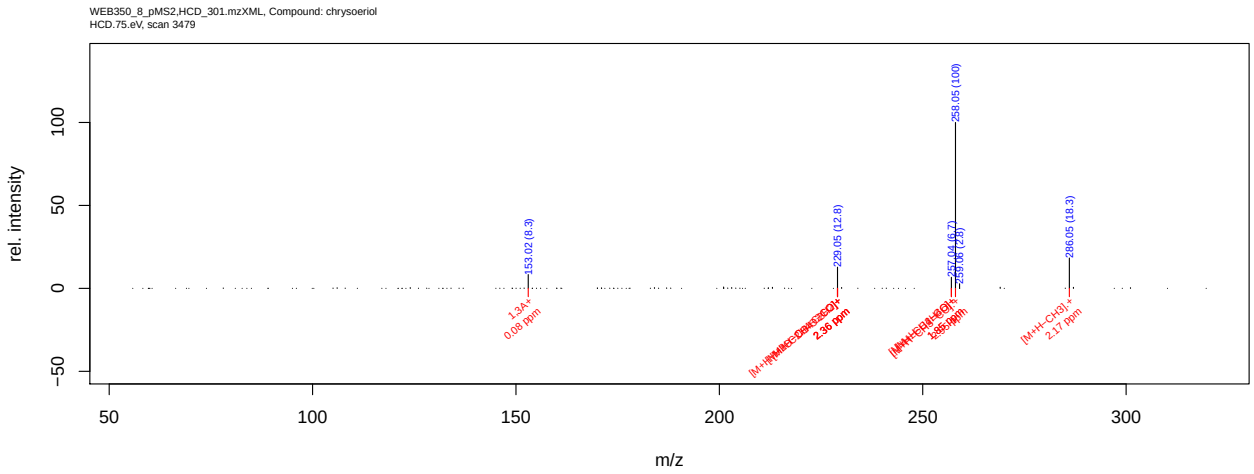
	mz	int	ppm	fragment
1	111.01	1.3	4.98	1,3A+-C2H2O
2	137.02	1.5	0.56	0,3A+
3	153.02	100.0	0.08	1,3A+
4	161.06	3.7	3.59	[M+H-2CO-2C2H2O]+
5	201.05	6.6	2.02	[M+H-CH4-3CO]+
6	203.03	28.6	2.01	[M+H-H2O-CO-2C2H2]+
7	229.05	75.0	2.36	[M+h-C2H4O-CO]+
8	229.05	75.0	2.36	[M+H-CH4-2CO]+
9	229.05	75.0	2.36	[M+H-H2O-CO-C2H2]+
10	257.04	37.6	1.97	[M+H-C2H4O]+
11	257.04	37.6	1.97	[M+H-CH4-CO]+
12	258.05	49.1	2.24	[M+H-CH3-CO].+

chrysoeriol.CID.45eV



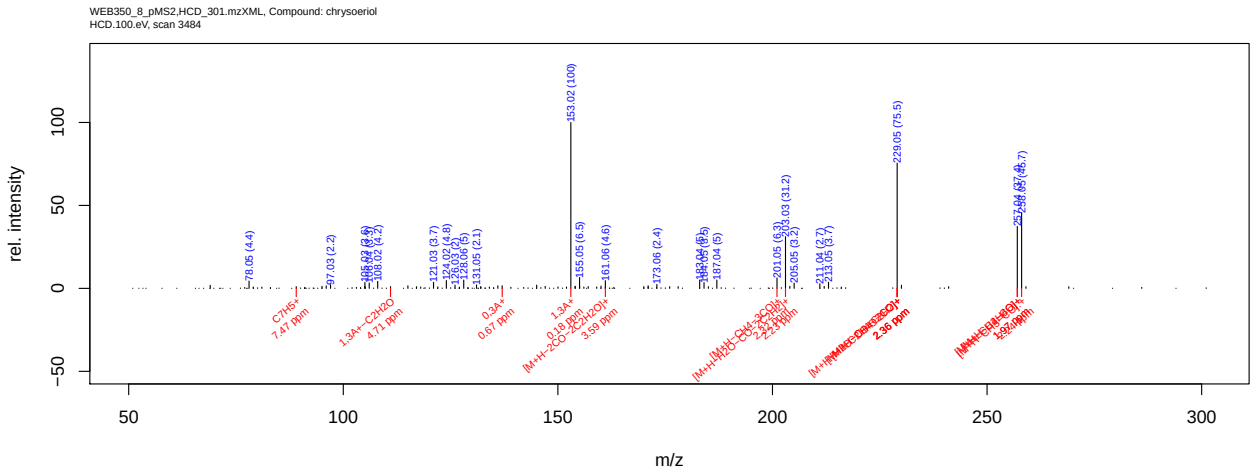
	mz	int	ppm	fragment
1	286.05	100.0	2.92	[M+H-CH3].+

chrysoeriol.HCD.75eV



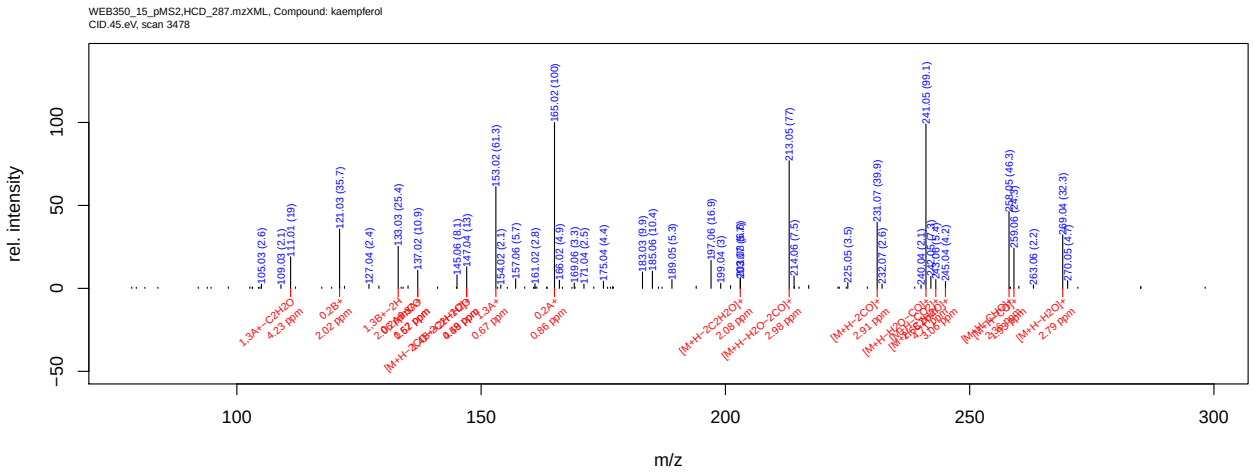
	mz	int	ppm	fragment
1	153.02	8.3	0.08	1,3A+
2	229.05	12.8	2.36	[M+h-C2H4O-CO]+
3	229.05	12.8	2.36	[M+H-CH4-2CO]+
4	229.05	12.8	2.36	[M+H-H2O-CO-C2H2]+
5	257.04	6.7	1.85	[M+H-C2H4O]+
6	257.04	6.7	1.85	[M+H-CH4-CO]+
7	258.05	100.0	2.95	[M+H-CH3-CO].+
8	286.05	18.3	2.17	[M+H-CH3].+

chrysoeriol.HCD.100eV



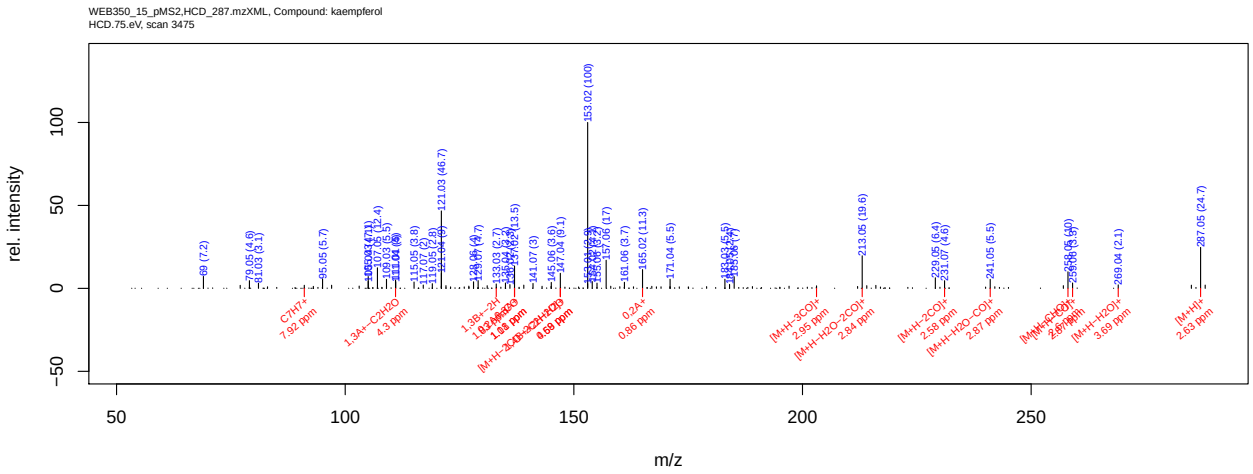
	mz	int	ppm	fragment
1	89.04	1.0	7.47	C7H5+
2	111.01	1.1	4.71	1,3A+-C2H2O
3	137.02	1.6	0.67	0,3A+
4	153.02	100.0	0.18	1,3A+
5	161.06	4.6	3.59	[M+H-2CO-2C2H2O]+
6	201.05	6.3	2.32	[M+H-CH4-3CO]+
7	203.03	31.2	2.23	[M+H-H2O-CO-2C2H2]+
8	229.05	75.5	2.36	[M+h-C2H4O-CO]+
9	229.05	75.5	2.36	[M+H-CH4-2CO]+
10	229.05	75.5	2.36	[M+H-H2O-CO-C2H2]+
11	257.04	37.4	1.97	[M+H-C2H4O]+
12	257.04	37.4	1.97	[M+H-CH4-CO]+
13	258.05	45.7	2.24	[M+H-CH3-CO].+

kaempferol.CID.45eV



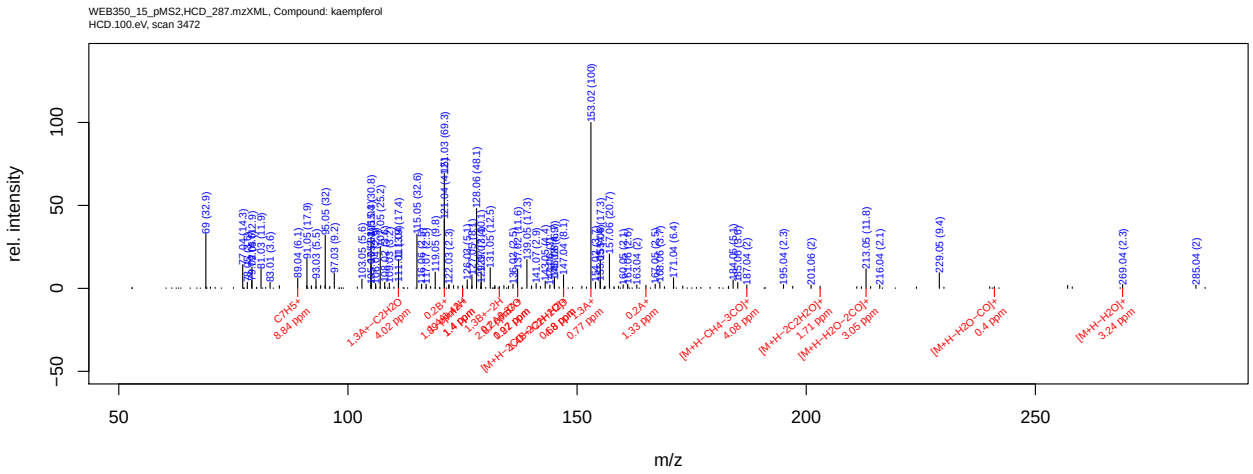
	mz	int	ppm	fragment
1	111.01	19.0	4.23	1,3A+-C2H2O
2	121.03	35.7	2.02	0,2B+
3	133.03	25.4	2.06	1,3B+-2H
4	137.02	10.9	1.52	0,2A+-CO
5	137.02	10.9	0.67	0,3A+
6	147.04	13.0	0.48	1,4B++2H-H2O
7	147.04	13.0	4.59	[M+H-2CO-2C2H2O]+
8	153.02	61.3	0.67	1,3A+
9	165.02	100.0	0.86	0,2A+
10	203.03	6.6	2.08	[M+H-2C2H2O]+
11	213.05	77.0	2.98	[M+H-H2O-2CO]+
12	231.07	39.9	2.91	[M+H-2CO]+
13	241.05	99.1	2.68	[M+H-H2O-CO]+
14	243.06	5.4	4.71	[M+H-CO2]+
15	245.04	4.2	3.06	[M+H-C2H2O]+
16	258.05	46.3	2.36	[M+H-CHO]+
17	259.06	24.3	1.93	[M+H-CO]+
18	269.04	32.3	2.79	[M+H-H2O]+

kaempferol.HCD.75eV



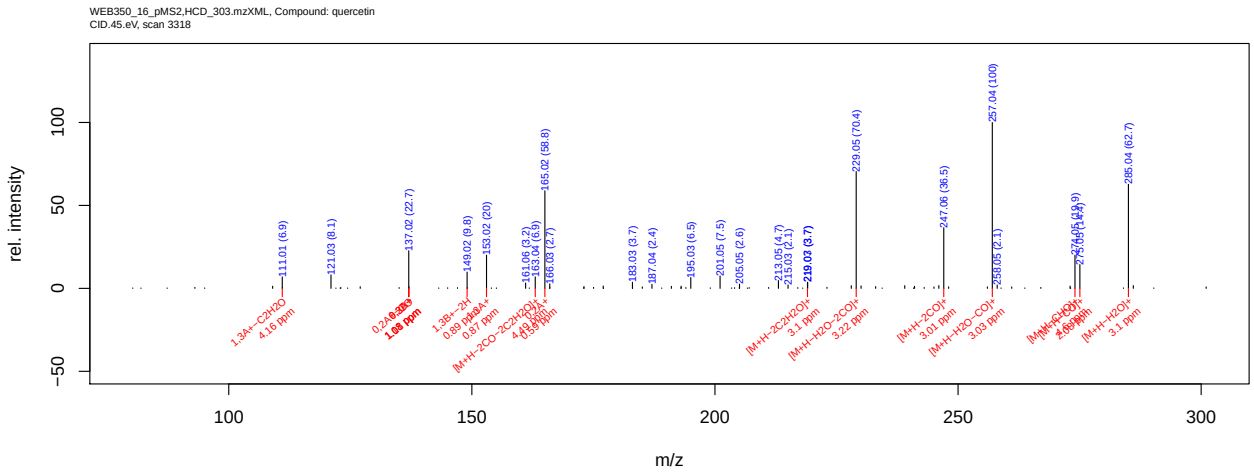
	mz	int	ppm	fragment
1	91.05	1.9	7.92	C7H7+
2	111.01	5.0	4.30	1,3A+-C2H2O
3	133.03	2.7	1.83	1,3B+-2H
4	137.02	13.5	1.08	0,2A+-CO
5	137.02	13.5	1.11	0,3A+
6	147.04	9.1	0.58	1,4B++2H-H2O
7	147.04	9.1	4.69	[M+H-2CO-2C2H2O]+
8	165.02	11.3	0.86	0,2A+
9	203.07	1.5	2.95	[M+H-3CO]+
10	213.05	19.6	2.84	[M+H-H2O-2CO]+
11	231.07	4.6	2.58	[M+H-2CO]+
12	241.05	5.5	2.87	[M+H-H2O-CO]+
13	258.05	10.0	2.60	[M+H-CHO]+
14	259.06	3.3	2.87	[M+H-CO]+
15	269.04	2.1	3.69	[M+H-H2O]+
16	287.05	24.7	2.63	[M+H]+

kaempferol.HCD.100eV



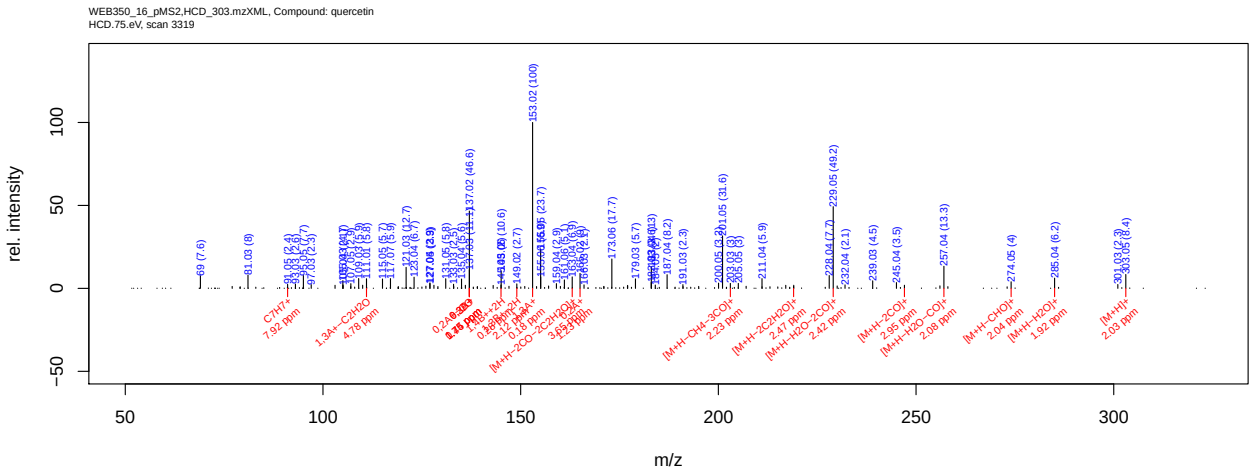
	mz	int	ppm	fragment
1	89.04	6.1	8.84	C7H5+
2	111.01	3.9	4.02	1,3A+-C2H2O
3	121.03	69.3	1.89	0,2B+
4	125.02	1.6	1.40	1,4A+
5	125.02	1.6	1.40	1,4A++2H
6	133.03	1.2	2.87	1,3B+-2H
7	137.02	11.6	0.97	0,2A+-CO
8	137.02	11.6	1.22	0,3A+
9	147.04	8.1	0.68	1,4B++2H-H2O
10	147.04	8.1	4.80	[M+H-2CO-2C2H2O]+
11	153.02	100.0	0.77	1,3A+
12	165.02	1.9	1.33	0,2A+
13	187.04	2.0	4.08	[M+H-CH4-3CO]+
14	203.03	1.3	1.71	[M+H-2C2H2O]+
15	213.05	11.8	3.05	[M+H-H2O-2CO]+
16	241.05	1.0	0.40	[M+H-H2O-CO]+
17	269.04	2.3	3.24	[M+H-H2O]+

quercetin.CID.45eV



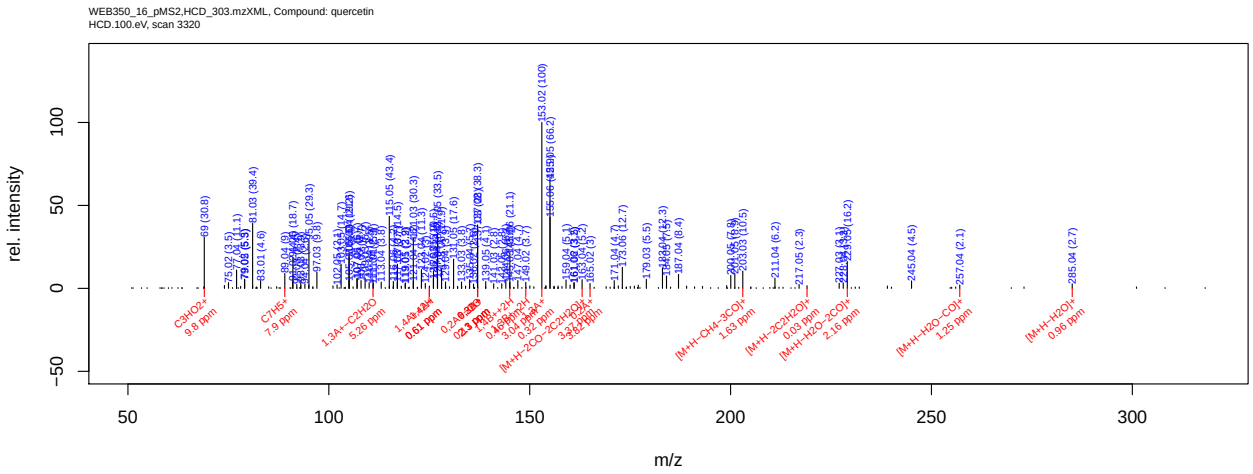
	mz	int	ppm	fragment
1	111.01	6.9	4.16	1,3A+-C2H2O
2	137.02	22.7	1.08	0,2A+-CO
3	137.02	22.7	1.08	0,2B+
4	137.02	22.7	1.11	0,3A+
5	149.02	9.8	0.89	1,3B+-2H
6	153.02	20.0	0.87	1,3A+
7	163.04	6.9	4.49	[M+H-2CO-2C2H2O]+
8	165.02	58.8	0.59	0,2A+
9	219.03	3.7	3.10	[M+H-2C2H2O]+
10	229.05	70.4	3.22	[M+H-H2O-2CO]+
11	247.06	36.5	3.01	[M+H-2CO]+
12	257.04	100.0	3.03	[M+H-H2O-CO]+
13	274.05	19.9	4.60	[M+H-CHO]+
14	275.05	14.4	2.08	[M+H-CO]+
15	285.04	62.7	3.10	[M+H-H2O]+

quercetin.HCD.75eV



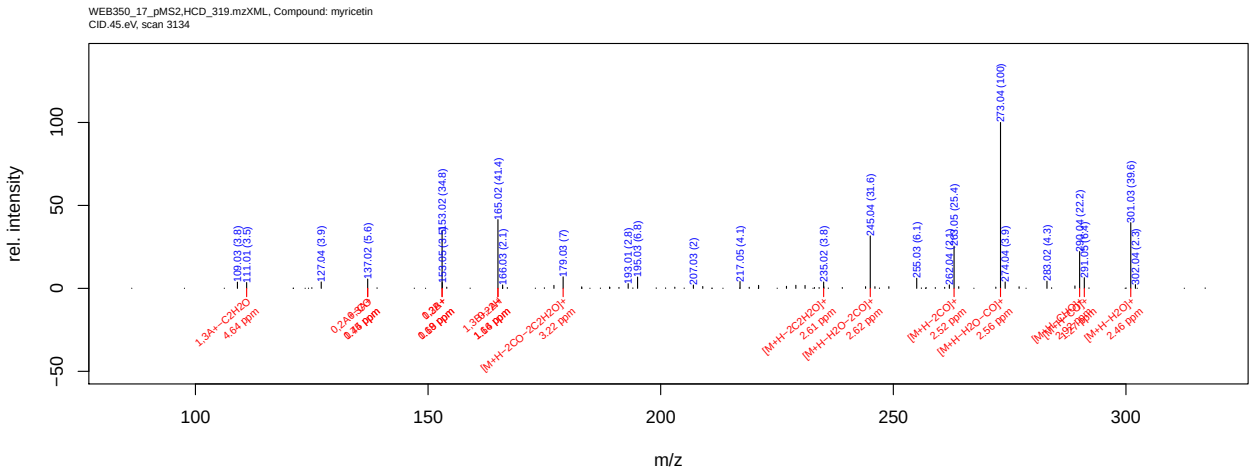
	mz	int	ppm	fragment
1	91.05	2.4	7.92	C7H7+
2	111.01	5.8	4.78	1,3A+-C2H2O
3	137.02	46.6	1.75	0,2A+-CO
4	137.02	46.6	1.75	0,2B+
5	137.02	46.6	0.44	0,3A+
6	145.03	2.0	0.28	1,4B++2H
7	149.02	2.7	2.12	1,3B+-2H
8	153.02	100.0	0.18	1,3A+
9	163.04	6.9	3.65	[M+H-2CO-2C2H2O]+
10	165.02	9.0	1.23	0,2A+
11	203.03	3.0	2.23	[M+H-CH4-3CO]+
12	219.03	1.1	2.47	[M+H-2C2H2O]+
13	229.05	49.2	2.42	[M+H-H2O-2CO]+
14	247.06	1.9	2.95	[M+H-2CO]+
15	257.04	13.3	2.08	[M+H-H2O-CO]+
16	274.05	4.0	2.04	[M+H-CHO]+
17	285.04	6.2	1.92	[M+H-H2O]+
18	303.05	8.4	2.03	[M+H]+

quercetin.HCD.100eV



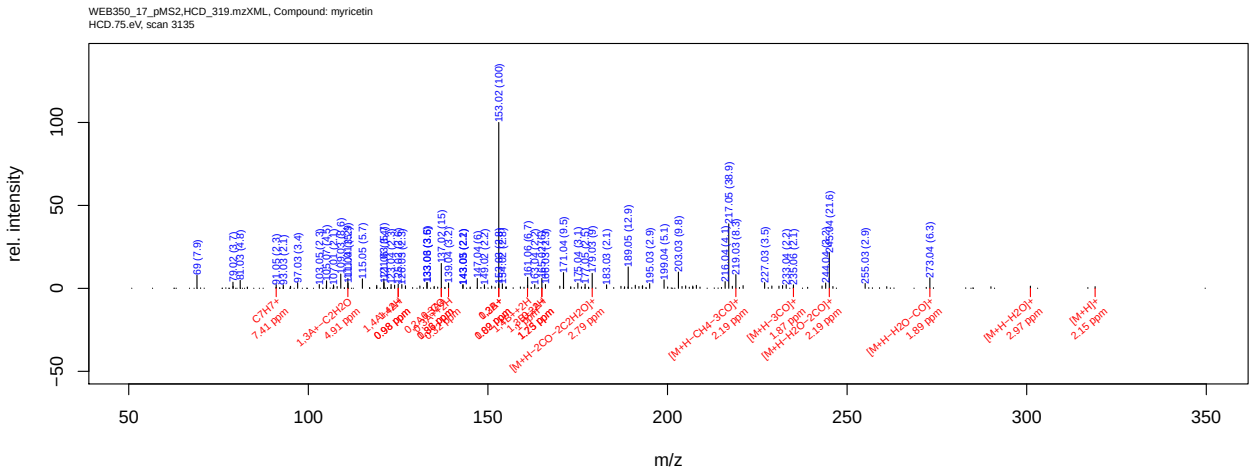
	mz	int	ppm	fragment
1	69.00	30.8	9.80	C3HO2+
2	89.04	9.0	7.90	C7H5+
3	111.01	5.1	5.26	1,3A+-C2H2O
4	125.02	1.4	0.61	1,4A+
5	125.02	1.4	0.61	1,4A++2H
6	137.02	38.3	2.30	0,2A+-CO
7	137.02	38.3	2.30	0,2B+
8	137.02	38.3	0.11	0,3A+
9	145.03	3.6	0.46	1,4B++2H
10	149.02	3.7	3.04	1,3B+-2H
11	153.02	100.0	0.32	1,3A+
12	163.04	5.2	3.37	[M+H-2CO-2C2H2O]+
13	165.02	3.0	3.82	0,2A+
14	203.03	10.5	1.63	[M+H-CH4-3CO]+
15	219.03	1.6	0.03	[M+H-2C2H2O]+
16	229.05	16.2	2.16	[M+H-H2O-2CO]+
17	257.04	2.1	1.25	[M+H-H2O-CO]+
18	285.04	2.7	0.96	[M+H-H2O]+

myricetin.CID.45eV



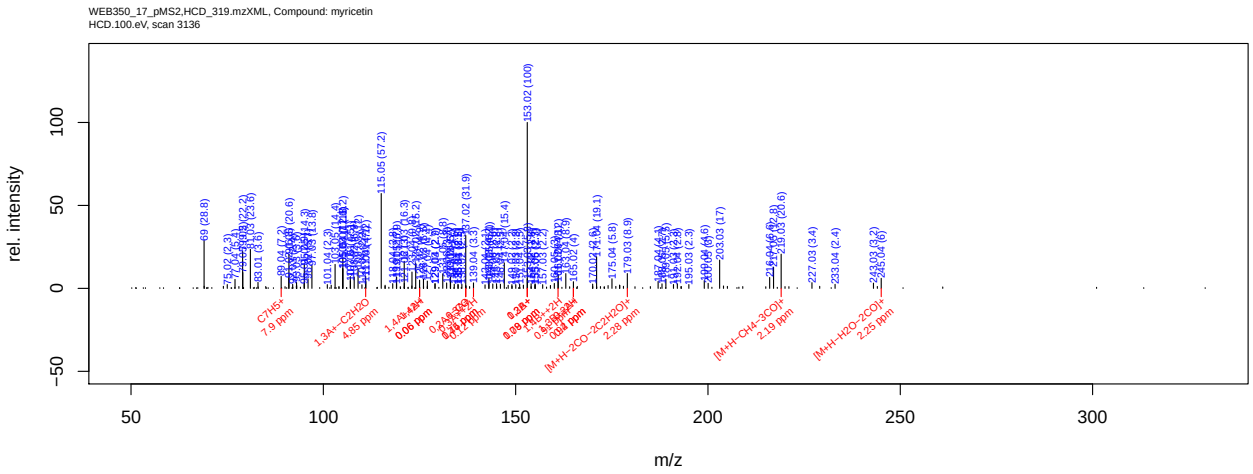
	mz	int	ppm	fragment
1	111.01	3.5	4.64	1,3A+-C2H2O
2	137.02	5.6	1.75	0,2A+-CO
3	137.02	5.6	0.44	0,3A+
4	153.02	34.8	1.69	0,2B+
5	153.02	34.8	0.18	1,3A+
6	165.02	41.4	1.14	0,2A+
7	165.02	41.4	1.66	1,3B+-2H
8	179.03	7.0	3.22	[M+H-2CO-2C2H2O]+
9	235.02	3.8	2.61	[M+H-2C2H2O]+
10	245.04	31.6	2.62	[M+H-H2O-2CO]+
11	263.05	25.4	2.52	[M+H-2CO]+
12	273.04	100.0	2.56	[M+H-H2O-CO]+
13	290.04	22.2	2.92	[M+H-CHO]+
14	291.05	6.4	1.27	[M+H-CO]+
15	301.03	39.6	2.46	[M+H-H2O]+

myricetin.HCD.75eV



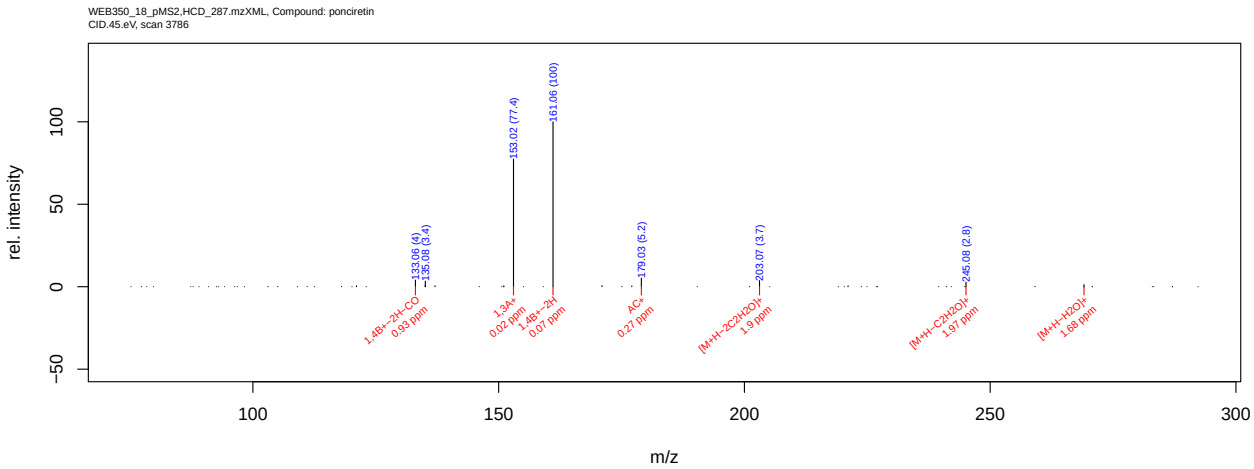
	mz	int	ppm	fragment
1	91.05	2.3	7.41	C7H7+
2	111.01	5.9	4.91	1,3A+-C2H2O
3	125.02	2.6	0.98	1,4A+
4	125.02	2.6	0.98	1,4A++2H
5	137.02	15.0	1.86	0,2A+-CO
6	137.02	15.0	0.33	0,3A+
7	139.04	3.2	0.32	0,3A++2H
8	153.02	100.0	1.89	0,2B+
9	153.02	100.0	0.02	1,3A+
10	161.02	1.9	1.00	1,4B++2H
11	165.02	6.0	1.23	0,2A+
12	165.02	6.0	1.75	1,3B+-2H
13	179.03	9.0	2.79	[M+H-2CO-2C2H2O]+
14	219.03	8.3	2.19	[M+H-CH4-3CO]+
15	235.06	2.1	1.87	[M+H-3CO]+
16	245.04	21.6	2.19	[M+H-H2O-2CO]+
17	273.04	6.3	1.89	[M+H-H2O-CO]+
18	301.03	1.4	2.97	[M+H-H2O]+
19	319.04	1.1	2.15	[M+H]+

myricetin.HCD.100eV



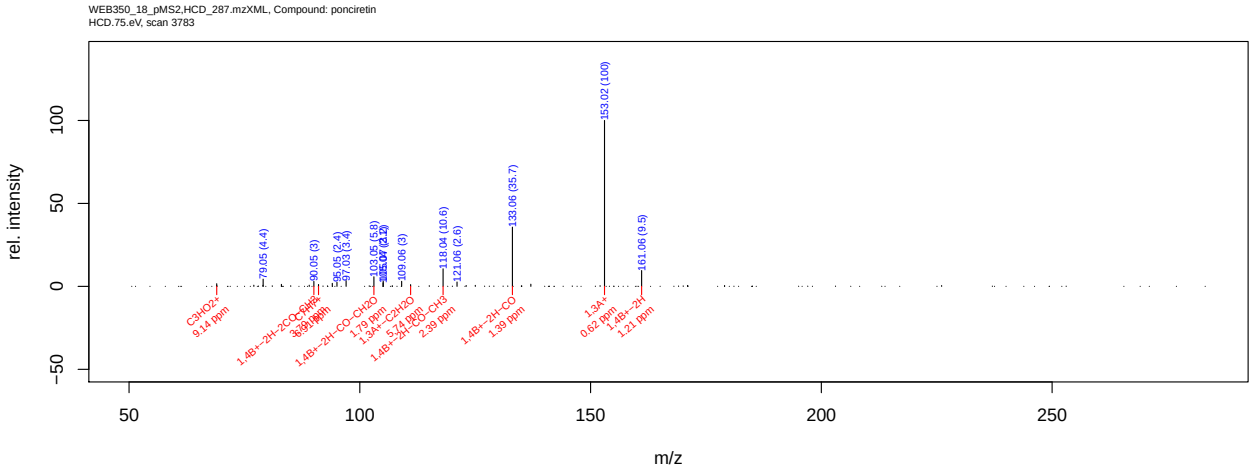
	mz	int	ppm	fragment
1	89.04	7.2	7.90	C7H5+
2	111.01	7.2	4.85	1,3A+-C2H2O
3	125.02	4.9	0.06	1,4A+
4	125.02	4.9	0.06	1,4A++2H
5	137.02	31.9	1.75	0,2A+-CO
6	137.02	31.9	0.44	0,3A+
7	139.04	3.3	0.12	0,3A++2H
8	153.02	100.0	1.79	0,2B+
9	153.02	100.0	0.08	1,3A+
10	161.02	4.1	0.91	1,4B++2H
11	165.02	4.0	0.40	0,2A+
12	165.02	4.0	0.92	1,3B+-2H
13	179.03	8.9	2.28	[M+H-2CO-2C2H2O]+
14	219.03	20.6	2.19	[M+H-CH4-3CO]+
15	245.04	6.0	2.25	[M+H-H2O-2CO]+

ponciretin.CID.45eV



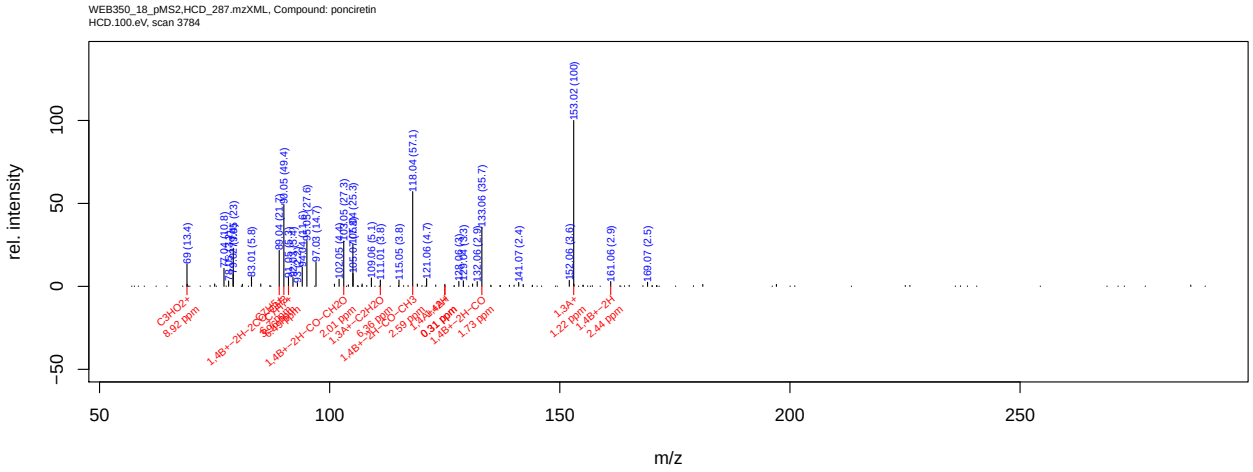
	mz	int	ppm	fragment
1	133.06	4.0	0.93	1,4B+-2H-CO
2	153.02	77.4	0.02	1,3A+
3	161.06	100.0	0.07	1,4B+-2H
4	179.03	5.2	0.27	AC+
5	203.07	3.7	1.90	[M+H-2C2H2O]+
6	245.08	2.8	1.97	[M+H-C2H2O]+
7	269.08	1.3	1.68	[M+H-H2O]+

ponciretin.HCD.75eV



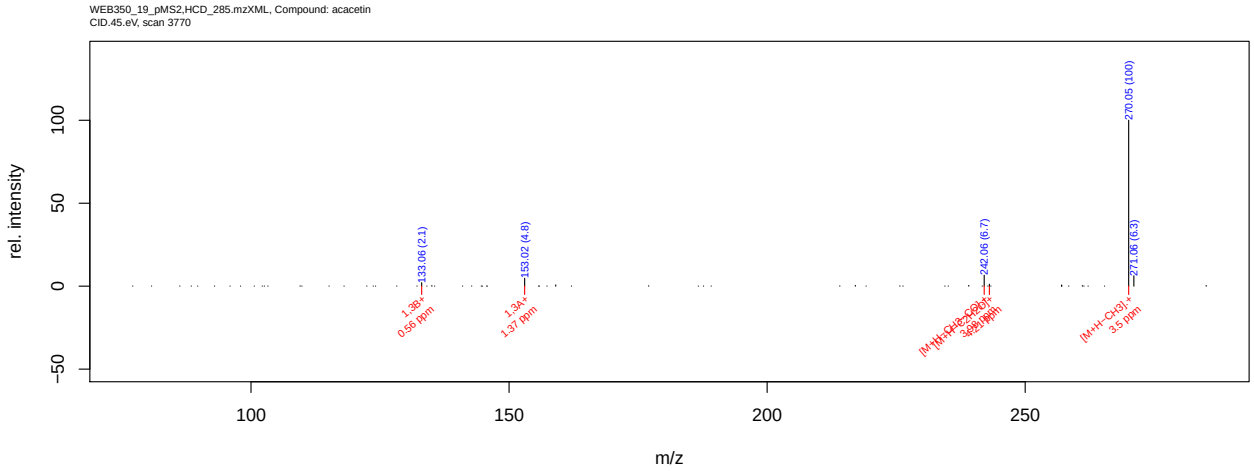
	mz	int	ppm	fragment
1	69.00	1.6	9.14	C3HO2+
2	90.05	3.0	3.79	1,4B+-2H-2CO-CH3
3	91.05	1.1	6.91	C7H7+
4	103.05	5.8	1.79	1,4B+-2H-CO-CH2O
5	111.01	1.1	5.74	1,3A+-C2H2O
6	118.04	10.6	2.39	1,4B+-2H-CO-CH3
7	133.06	35.7	1.39	1,4B+-2H-CO
8	153.02	100.0	0.62	1,3A+
9	161.06	9.5	1.21	1,4B+-2H

ponciretin.HCD.100eV



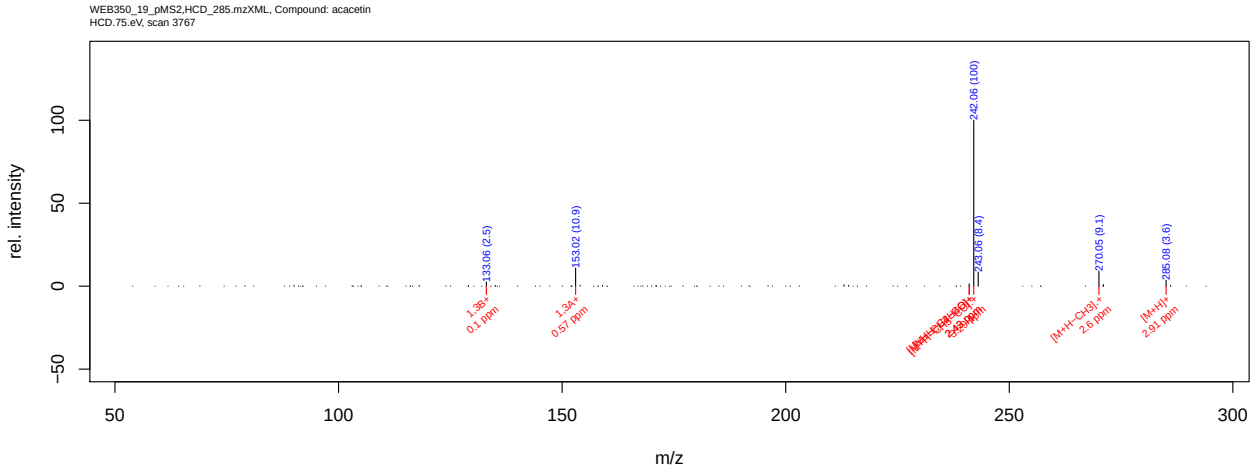
	mz	int	ppm	fragment
1	69.00	13.4	8.92	C3HO2+
2	89.04	21.7	6.70	C7H5+
3	90.05	49.4	3.96	1,4B+-2H-2CO-CH3
4	91.05	5.3	6.49	C7H7+
5	103.05	27.3	2.01	1,4B+-2H-CO-CH2O
6	111.01	3.8	6.36	1,3A+-C2H2O
7	118.04	57.1	2.59	1,4B+-2H-CO-CH3
8	125.02	1.3	0.31	1,4A+
9	125.02	1.3	0.31	1,4A++2H
10	133.06	35.7	1.73	1,4B+-2H-CO
11	153.02	100.0	1.22	1,3A+
12	161.06	2.9	2.44	1,4B+-2H

acacetin.CID.45eV



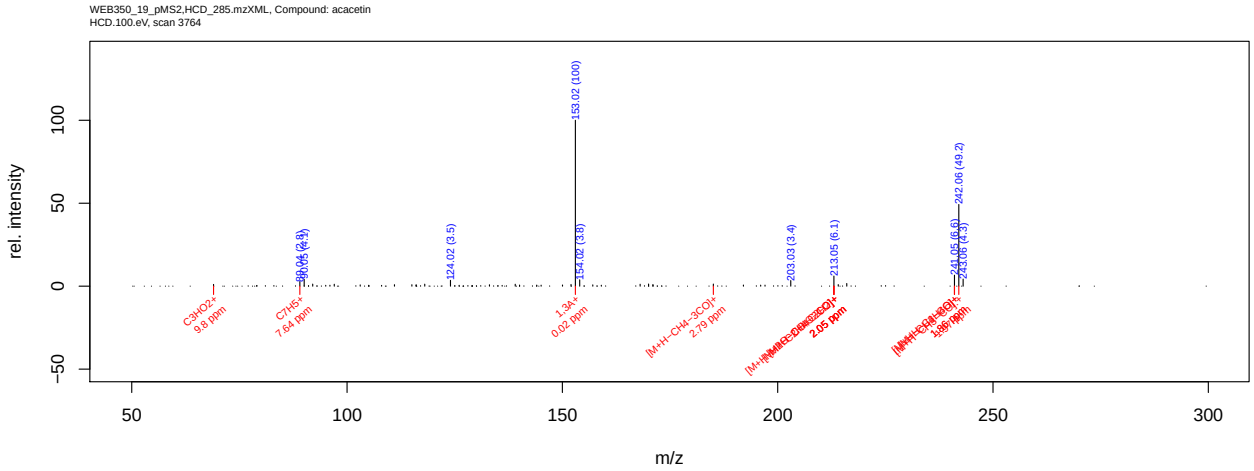
	mz	int	ppm	fragment
1	133.06	2.1	0.56	1,3B+
2	153.02	4.8	1.37	1,3A+
3	242.06	6.7	3.98	[M+H-CH3-CO].+
4	243.06	1.2	4.21	[M+H-C2H2O]+
5	270.05	100.0	3.50	[M+H-CH3].+

acacetin.HCD.75eV



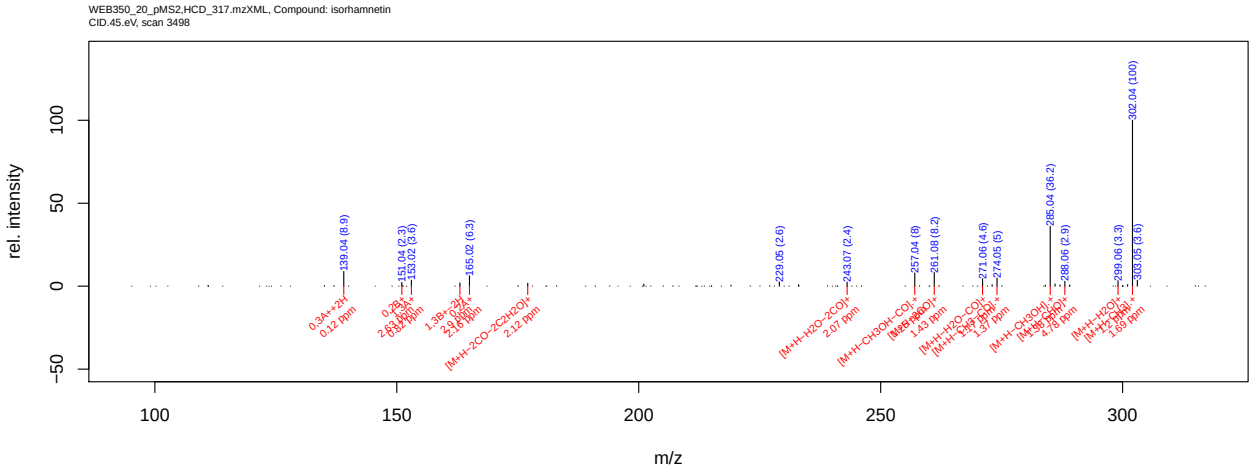
	mz	int	ppm	fragment
1	133.06	2.5	0.10	1,3B+
2	153.02	10.9	0.57	1,3A+
3	241.05	1.4	2.43	[M+H-C2H4O]+
4	241.05	1.4	2.43	[M+H-CH4-CO]+
5	242.06	100.0	3.29	[M+H-CH3-CO].+
6	270.05	9.1	2.60	[M+H-CH3].+
7	285.08	3.6	2.91	[M+H]+

acacetin.HCD.100eV



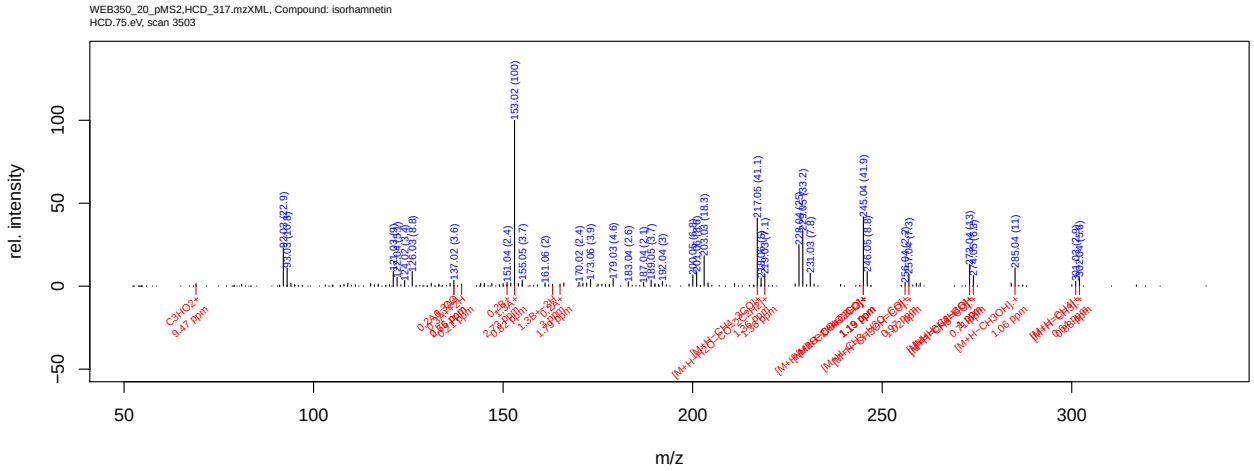
	mz	int	ppm	fragment
1	69.00	1.1	9.80	C3HO2+
2	89.04	2.8	7.64	C7H5+
3	153.02	100.0	0.02	1,3A+
4	185.06	1.3	2.79	[M+H-CH4-3CO]+
5	213.05	6.1	2.05	[M+h-C2H4O-CO]+
6	213.05	6.1	2.05	[M+H-CH4-2CO]+
7	213.05	6.1	2.05	[M+H-H2O-CO-C2H2]+
8	241.05	6.6	1.86	[M+H-C2H4O]+
9	241.05	6.6	1.86	[M+H-CH4-CO]+
10	242.06	49.2	1.97	[M+H-CH3-CO].+

isorhamnetin.CID.45eV



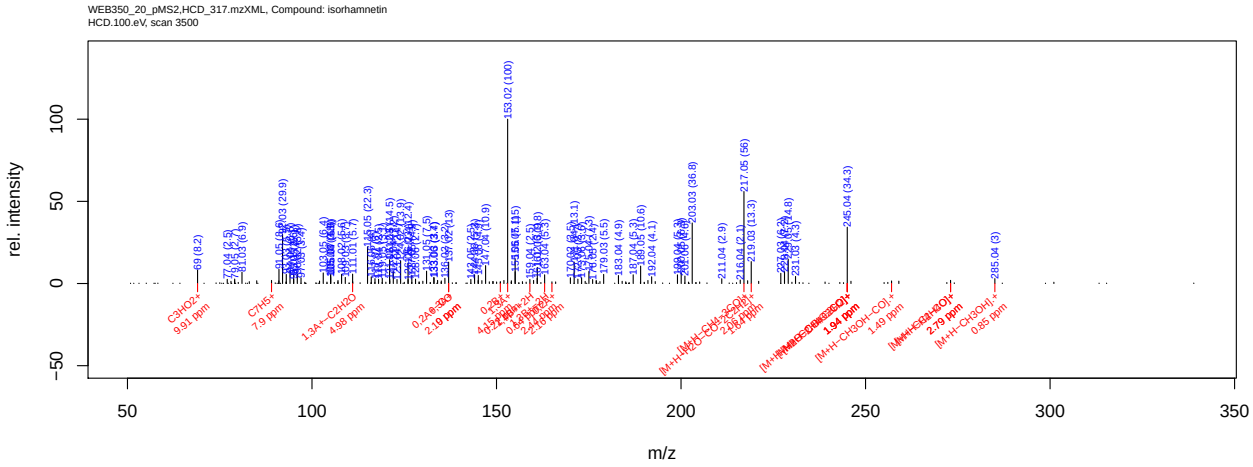
	mz	int	ppm	fragment
1	139.04	8.9	0.12	0,3A++2H
2	151.04	2.3	2.63	0,2B+
3	153.02	3.6	0.82	1,3A+
4	163.04	2.0	2.90	1,3B+-2H
5	165.02	6.3	2.16	0,2A+
6	177.05	1.8	2.12	[M+H-2CO-2C2H2O]+
7	243.07	2.4	2.07	[M+H-H2O-2CO]+
8	257.04	8.0	1.25	[M+H-CH3OH-CO].+
9	261.08	8.2	1.43	[M+H-2CO]+
10	271.06	4.6	1.17	[M+H-H2O-CO]+
11	274.05	5.0	1.37	[M+H-CH3-CO].+
12	285.04	36.2	1.38	[M+H-CH3OH].+
13	288.06	2.9	4.78	[M+H-CHO]+
14	299.06	3.3	1.20	[M+H-H2O]+
15	302.04	100.0	1.69	[M+H-CH3].+

isorhamnetin.HCD.75eV



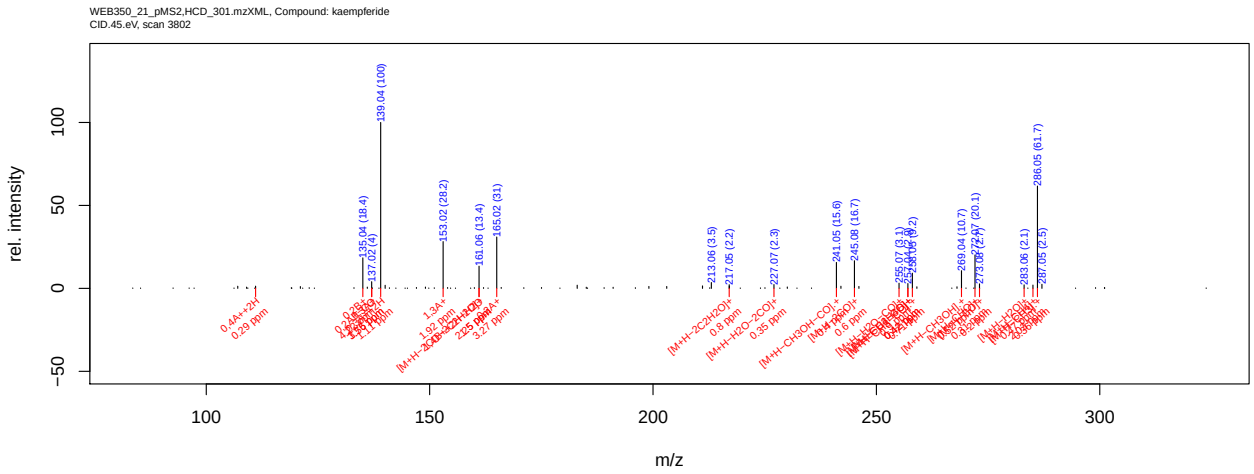
	mz	int	ppm	fragment
1	69.00	1.5	9.47	C3HO2+
2	137.02	3.6	2.75	0,2A+-CO
3	137.02	3.6	0.56	0,3A+
4	139.04	1.3	0.21	0,3A++2H
5	151.04	2.4	2.73	0,2B+
6	153.02	100.0	0.82	1,3A+
7	163.04	1.2	3.00	1,3B+-2H
8	165.02	1.3	1.79	0,2A+
9	217.05	41.1	1.36	[M+H-CH4-3CO]+
10	219.03	7.1	1.36	[M+H-H2O-CO-2C2H2]+
11	245.04	41.9	1.19	[M+h-C2H4O-CO]+
12	245.04	41.9	1.19	[M+H-CH4-2CO]+
13	245.04	41.9	1.19	[M+H-H2O-CO-C2H2]+
14	256.04	2.2	0.97	[M+H-CH3-H2O-CO]+
15	257.04	7.3	1.02	[M+H-CH3OH-CO].+
16	273.04	13.0	1.00	[M+H-C2H4O]+
17	273.04	13.0	1.00	[M+H-CH4-CO]+
18	274.05	6.3	0.71	[M+H-CH3-CO].+
19	285.04	11.0	1.06	[M+H-CH3OH].+
20	301.03	2.9	0.64	[M+H-CH4]+
21	302.04	5.6	0.88	[M+H-CH3].+

isorhamnetin.HCD.100eV



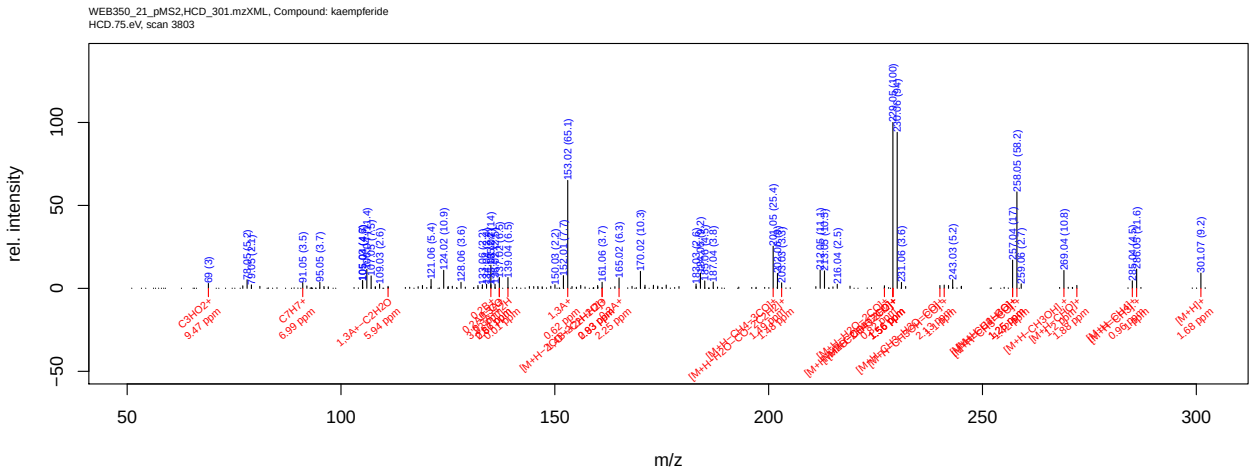
	mz	int	ppm	fragment
1	69.00	8.2	9.91	C3HO2+
2	89.04	1.9	7.90	C7H5+
3	111.01	5.7	4.98	1,3A+-C2H2O
4	137.02	13.0	2.19	0,2A+-CO
5	137.02	13.0	0.00	0,3A+
6	151.04	1.2	4.15	0,2B+
7	153.02	100.0	0.22	1,3A+
8	159.04	2.5	0.64	1,4B++2H
9	163.04	5.3	2.44	1,3B+-2H
10	165.02	1.0	2.16	0,2A+
11	217.05	56.0	2.06	[M+H-CH4-3CO]+
12	219.03	13.3	1.64	[M+H-H2O-CO-2C2H2]+
13	245.04	34.3	1.94	[M+h-C2H4O-CO]+
14	245.04	34.3	1.94	[M+H-CH4-2CO]+
15	245.04	34.3	1.94	[M+H-H2O-CO-C2H2]+
16	257.04	1.6	1.49	[M+H-CH3OH-CO].+
17	273.04	1.9	2.79	[M+H-C2H4O]+
18	273.04	1.9	2.79	[M+H-CH4-CO]+
19	285.04	3.0	0.85	[M+H-CH3OH].+

kaempferide.CID.45eV



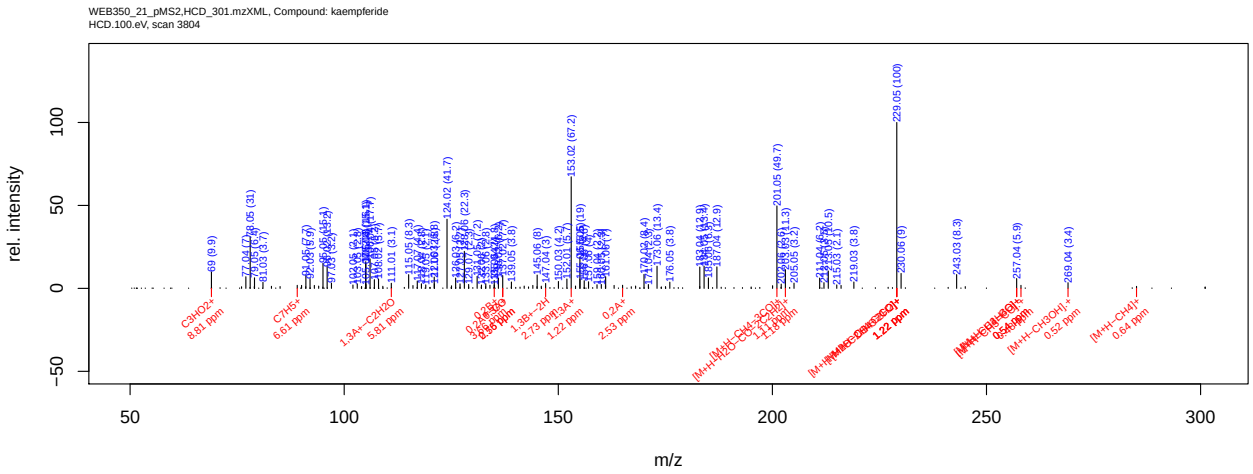
	mz	int	ppm	fragment
1	111.04	1.3	0.29	0,4A++2H
2	135.04	18.4	4.22	0,2B+
3	137.02	4.0	3.75	0,2A+-CO
4	137.02	4.0	1.56	0,3A+
5	139.04	100.0	1.11	0,3A++2H
6	153.02	28.2	1.92	1,3A+
7	161.06	13.4	2.25	1,4B++2H-H2O
8	161.06	13.4	1.50	[M+H-2CO-2C2H2O]+
9	165.02	31.0	3.27	0,2A+
10	217.05	2.2	0.80	[M+H-2C2H2O]+
11	227.07	2.3	0.35	[M+H-H2O-2CO]+
12	241.05	15.6	0.40	[M+H-CH3OH-CO].+
13	245.08	16.7	0.60	[M+H-2CO]+
14	255.07	3.1	0.90	[M+H-H2O-CO]+
15	257.04	2.9	0.42	[M+H-C2H4O]+
16	257.04	2.9	0.42	[M+H-CH4-CO]+
17	258.05	9.2	0.71	[M+H-CH3-CO].+
18	269.04	10.7	0.52	[M+H-CH3OH].+
19	272.07	20.1	0.31	[M+H-CHO]+
20	273.08	2.7	0.20	[M+H-CO]+
21	283.06	2.1	0.47	[M+H-H2O]+
22	285.04	2.0	2.03	[M+H-CH4]+
23	286.05	61.7	0.36	[M+H-CH3].+

kaempferide.HCD.75eV



	mz	int	ppm	fragment
1	69.00	3.0	9.47	C3HO2+
2	91.05	3.5	6.99	C7H7+
3	111.01	1.2	5.94	1,3A+-C2H2O
4	135.04	14.0	3.32	0,2B+
5	137.02	6.5	2.86	0,2A+-CO
6	137.02	6.5	0.67	0,3A+
7	139.04	6.5	0.01	0,3A++2H
8	153.02	65.1	0.62	1,3A+
9	161.06	3.7	0.93	1,4B++2H-H2O
10	161.06	3.7	2.83	[M+H-2CO-2C2H2O]+
11	165.02	6.3	2.25	0,2A+
12	201.05	25.4	1.49	[M+H-CH4-3CO]+
13	203.03	3.3	1.48	[M+H-H2O-CO-2C2H2]+
14	227.07	1.6	0.82	[M+H-H2O-2CO]+
15	229.05	100.0	1.56	[M+h-C2H4O-CO]+
16	229.05	100.0	1.56	[M+H-CH4-2CO]+
17	229.05	100.0	1.56	[M+H-H2O-CO-C2H2]+
18	240.04	1.8	2.13	[M+H-CH3-H2O-CO]+
19	241.05	2.0	1.10	[M+H-CH3OH-CO].+
20	257.04	17.0	1.25	[M+H-C2H4O]+
21	257.04	17.0	1.25	[M+H-CH4-CO]+
22	258.05	58.2	1.42	[M+H-CH3-CO].+
23	269.04	10.8	1.20	[M+H-CH3OH].+
24	272.07	1.8	1.88	[M+H-CHO]+
25	285.04	4.5	0.96	[M+H-CH4]+
26	286.05	11.6	1.00	[M+H-CH3].+
27	301.07	9.2	1.68	[M+H]+

kaempferide.HCD.100eV



	mz	int	ppm	fragment
1	69.00	9.9	8.81	C3HO2+
2	89.04	1.8	6.61	C7H5+
3	111.01	3.1	5.81	1,3A+-C2H2O
4	135.04	4.8	3.66	0,2B+
5	137.02	7.7	2.75	0,2A+-CO
6	137.02	7.7	0.56	0,3A+
7	147.04	3.0	2.73	1,3B+-2H
8	153.02	67.2	1.22	1,3A+
9	165.02	1.9	2.53	0,2A+
10	201.05	49.7	1.11	[M+H-CH4-3CO]+
11	203.03	11.3	1.18	[M+H-H2O-CO-2C2H2]+
12	229.05	100.0	1.22	[M+h-C2H4O-CO]+
13	229.05	100.0	1.22	[M+H-CH4-2CO]+
14	229.05	100.0	1.22	[M+H-H2O-CO-C2H2]+
15	257.04	5.9	0.54	[M+H-C2H4O]+
16	257.04	5.9	0.54	[M+H-CH4-CO]+
17	258.05	1.8	0.48	[M+H-CH3-CO].+
18	269.04	3.4	0.52	[M+H-CH3OH].+
19	285.04	1.2	0.64	[M+H-CH4]+