WEB350

Benjamin Weigel

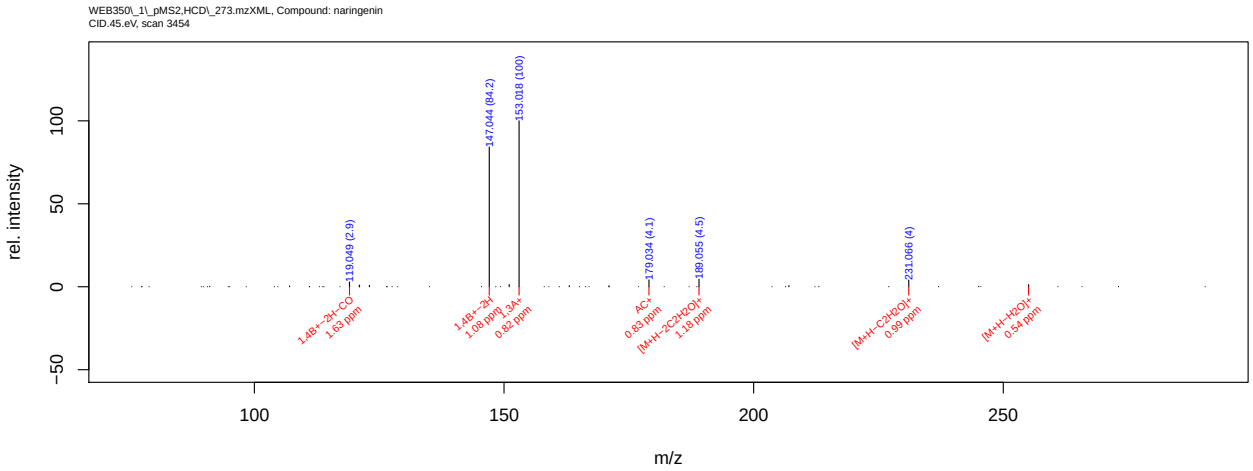
10/01/2015

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

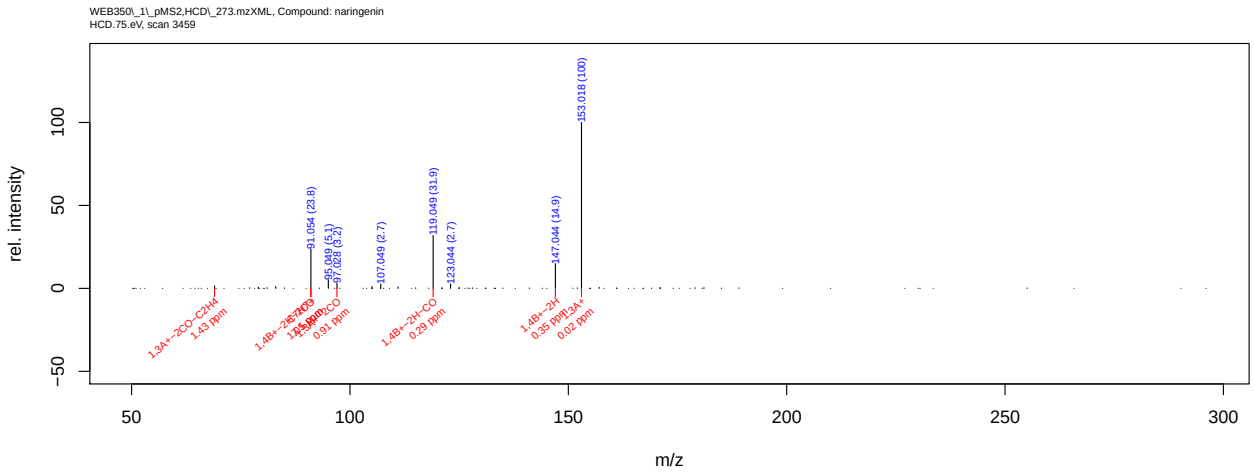
Automatic annotation of MS spectra

naringenin.CID.45eV



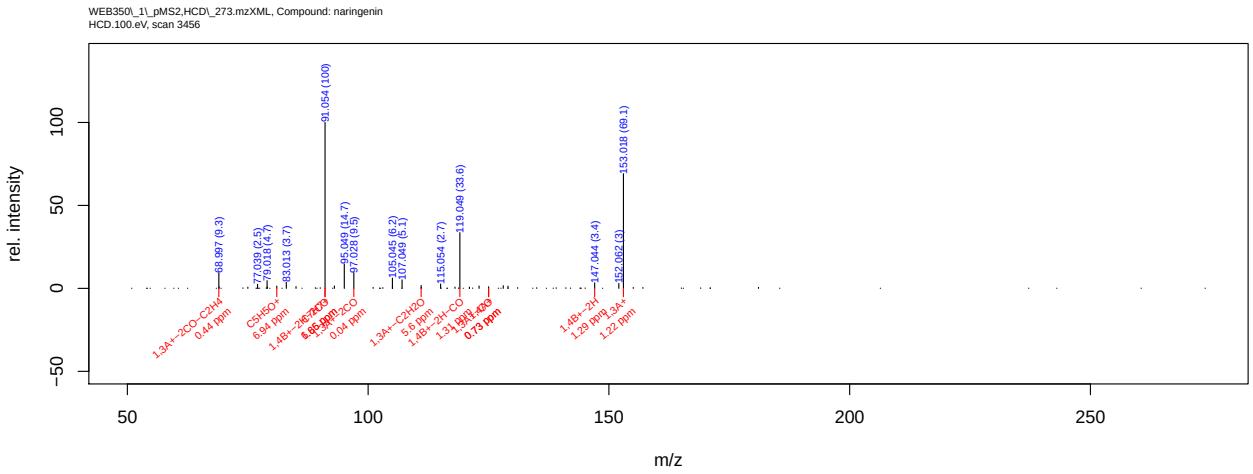
	mz	int	ppm	fragment
1	119.05	2.9	1.63	1,4B+-2H-CO
2	147.04	84.2	1.08	1,4B+-2H
3	153.02	100.0	0.82	1,3A+
4	179.03	4.1	0.83	AC+
5	189.05	4.5	1.18	[M+H-2C2H2O]+
6	231.07	4.0	0.99	[M+H-C2H2O]+
7	255.07	1.3	0.54	[M+H-H2O]+

naringenin.HCD.75eV



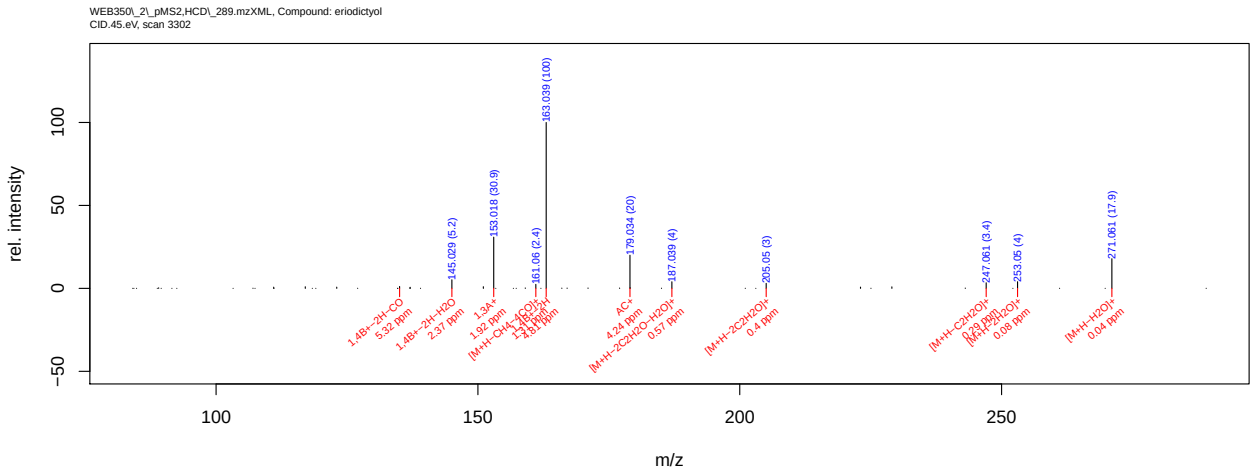
	mz	int	ppm	fragment
1	69.00	1.5	1.43	1,3A+-2CO-C2H4
2	91.05	23.8	1.01	1,4B+-2H-2CO
3	91.05	23.8	7.50	C7H7+
4	97.03	3.2	0.91	1,3A+-2CO
5	119.05	31.9	0.29	1,4B+-2H-CO
6	147.04	14.9	0.35	1,4B+-2H
7	153.02	100.0	0.02	1,3A+

naringenin.HCD.100eV



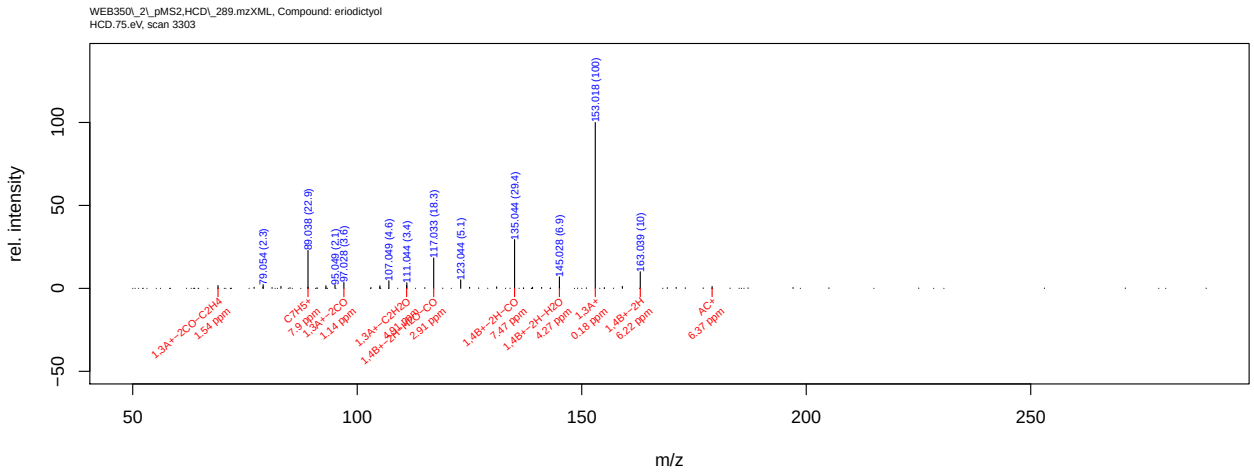
	mz	int	ppm	fragment
1	69.00	9.3	0.44	1,3A+-2CO-C2H4
2	81.03	1.4	6.94	C5H5O+
3	91.05	100.0	1.85	1,4B+-2H-2CO
4	91.05	100.0	6.66	C7H7+
5	97.03	9.5	0.04	1,3A+-2CO
6	111.01	1.8	5.60	1,3A+-C2H2O
7	119.05	33.6	1.31	1,4B+-2H-CO
8	125.02	1.0	0.73	1,3A+-CO
9	125.02	1.0	0.73	1,4A+
10	147.04	3.4	1.29	1,4B+-2H
11	153.02	69.1	1.22	1,3A+

eriodictyol.CID.45eV



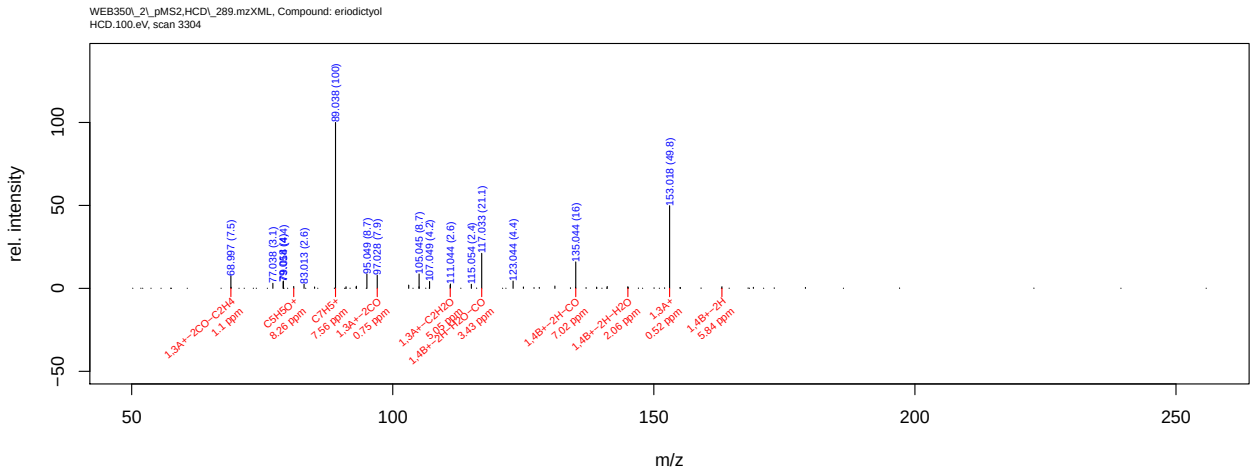
	mz	int	ppm	fragment
1	135.04	1.1	5.32	1,4B+-2H-CO
2	145.03	5.2	2.37	1,4B+-2H-H2O
3	153.02	30.9	1.92	1,3A+
4	161.06	2.4	1.31	[M+H-CH4-4CO]+
5	163.04	100.0	4.81	1,4B+-2H
6	179.03	20.0	4.24	AC+
7	187.04	4.0	0.57	[M+H-2C2H2O-H2O]+
8	205.05	3.0	0.40	[M+H-2C2H2O]+
9	247.06	3.4	0.29	[M+H-C2H2O]+
10	253.05	4.0	0.08	[M+H-2H2O]+
11	271.06	17.9	0.04	[M+H-H2O]+

eriodictyol.HCD.75eV



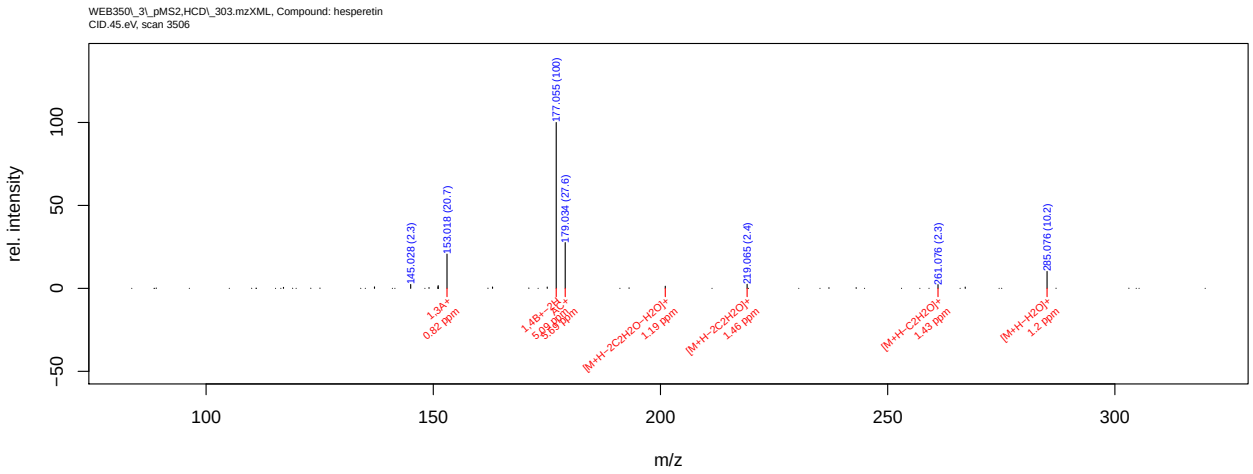
	mz	int	ppm	fragment
1	69.00	1.7	1.54	1,3A+-2CO-C2H4
2	89.04	22.9	7.90	C7H5+
3	97.03	3.6	1.14	1,3A+-2CO
4	111.01	1.8	4.91	1,3A+-C2H2O
5	117.03	18.3	2.91	1,4B+-2H-H2O-CO
6	135.04	29.4	7.47	1,4B+-2H-CO
7	145.03	6.9	4.27	1,4B+-2H-H2O
8	153.02	100.0	0.18	1,3A+
9	163.04	10.0	6.22	1,4B+-2H
10	179.03	1.1	6.37	AC+

eriodictyol.HCD.100eV



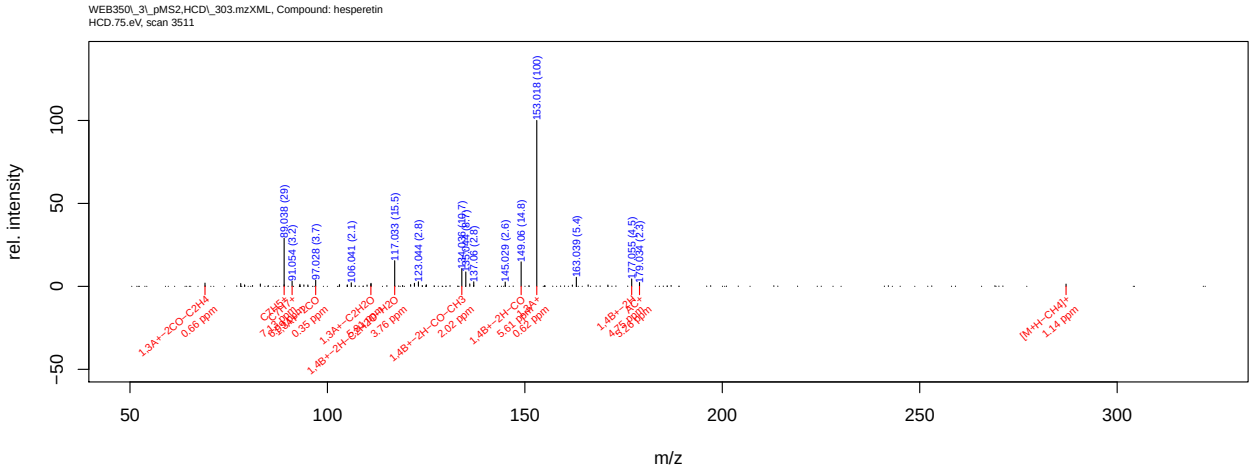
	mz	int	ppm	fragment
1	69.00	7.5	1.10	1,3A+-2CO-C2H4
2	81.03	1.2	8.26	C5H5O+
3	89.04	100.0	7.56	C7H5+
4	97.03	7.9	0.75	1,3A+-2CO
5	111.01	1.9	5.05	1,3A+-C2H2O
6	117.03	21.1	3.43	1,4B+-2H-H2O-CO
7	135.04	16.0	7.02	1,4B+-2H-CO
8	145.03	1.0	2.06	1,4B+-2H-H2O
9	153.02	49.8	0.52	1,3A+
10	163.04	1.0	5.84	1,4B+-2H

hesperetin.CID.45eV



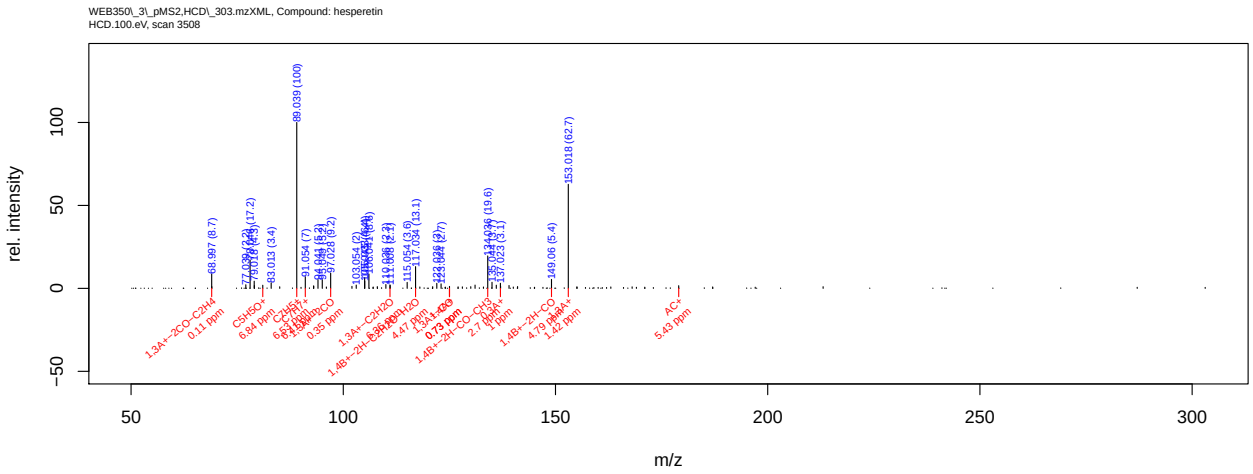
	mz	int	ppm	fragment
1	153.02	20.7	0.82	1,3A+
2	177.05	100.0	5.09	1,4B+-2H
3	179.03	27.6	5.69	AC+
4	201.05	1.3	1.19	[M+H-2C2H2O-H2O]+
5	219.07	2.4	1.46	[M+H-2C2H2O]+
6	261.08	2.3	1.43	[M+H-C2H2O]+
7	285.08	10.2	1.20	[M+H-H2O]+

hesperetin.HCD.75eV



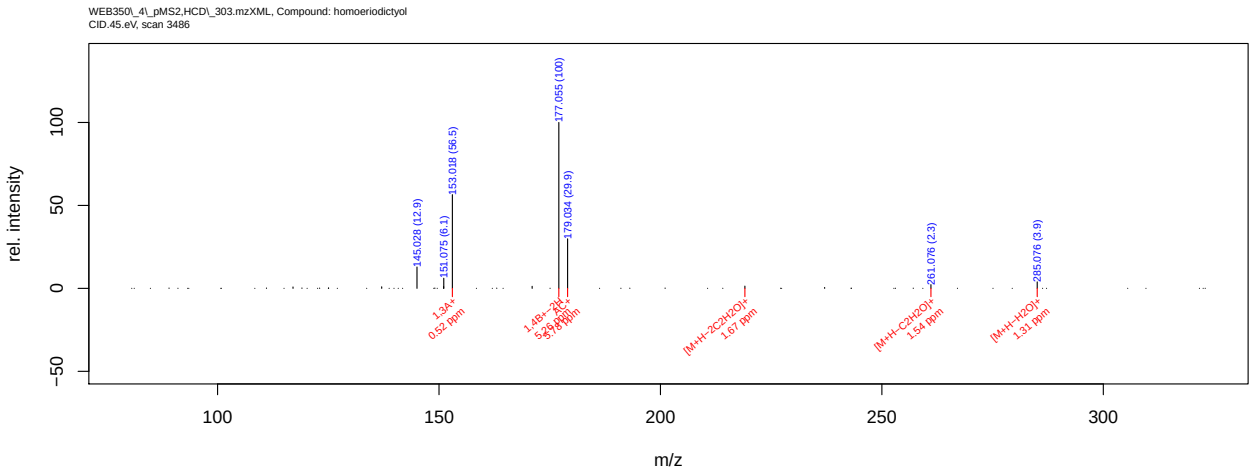
	mz	int	ppm	fragment
1	69.00	2.0	0.66	1,3A+-2CO-C2H4
2	89.04	29.0	7.13	C7H5+
3	91.05	3.2	6.99	C7H7+
4	97.03	3.7	0.35	1,3A+-2CO
5	111.01	1.4	5.81	1,3A+-C2H2O
6	117.03	15.5	3.76	1,4B+-2H-C2H2O-H2O
7	134.04	10.7	2.02	1,4B+-2H-CO-CH3
8	149.06	14.8	5.61	1,4B+-2H-CO
9	153.02	100.0	0.62	1,3A+
10	177.05	4.5	4.75	1,4B+-2H
11	179.03	2.3	5.26	AC+
12	287.06	1.4	1.14	[M+H-CH4]+

hesperetin.HCD.100eV



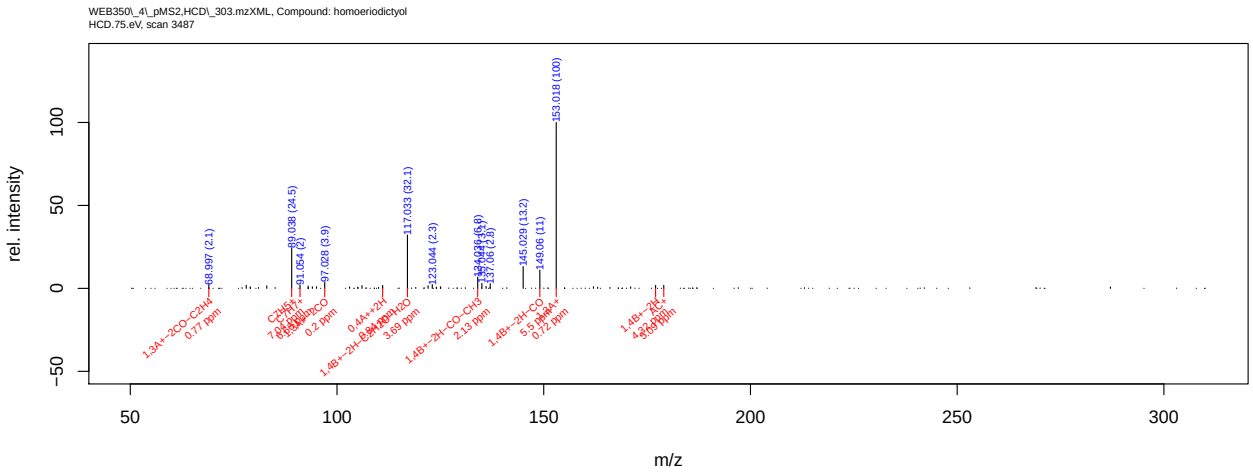
	mz	int	ppm	fragment
1	69.00	8.7	0.11	1,3A+-2CO-C2H4
2	81.03	1.9	6.84	C5H5O+
3	89.04	100.0	6.53	C7H5+
4	91.05	7.0	6.41	C7H7+
5	97.03	9.2	0.35	1,3A+-2CO
6	111.01	2.1	6.36	1,3A+-C2H2O
7	117.03	13.1	4.47	1,4B+-2H-C2H2O-H2O
8	125.02	1.2	0.73	1,3A+-CO
9	125.02	1.2	0.73	1,4A+
10	134.04	19.6	2.70	1,4B+-2H-CO-CH3
11	137.02	3.1	1.00	0,3A+
12	149.06	5.4	4.79	1,4B+-2H-CO
13	153.02	62.7	1.42	1,3A+
14	179.03	1.6	5.43	AC+

homoeriodictyol.CID.45eV



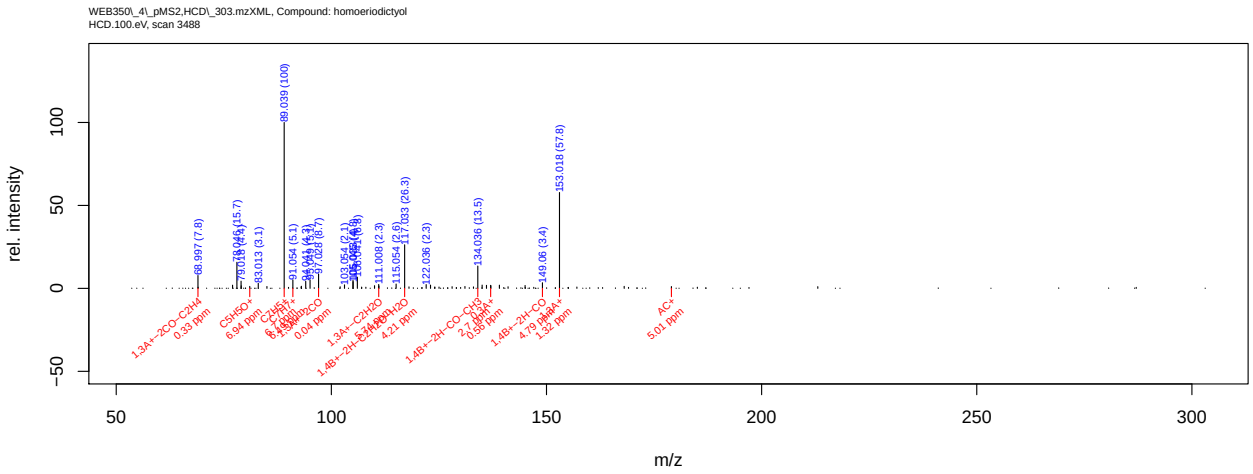
	mz	int	ppm	fragment
1	153.02	56.5	0.52	1,3A+
2	177.05	100.0	5.26	1,4B+-2H
3	179.03	29.9	5.78	AC+
4	219.07	1.4	1.67	[M+H-2C2H2O]+
5	261.08	2.3	1.54	[M+H-C2H2O]+
6	285.08	3.9	1.31	[M+H-H2O]+

homoeriodictyol.HCD.75eV



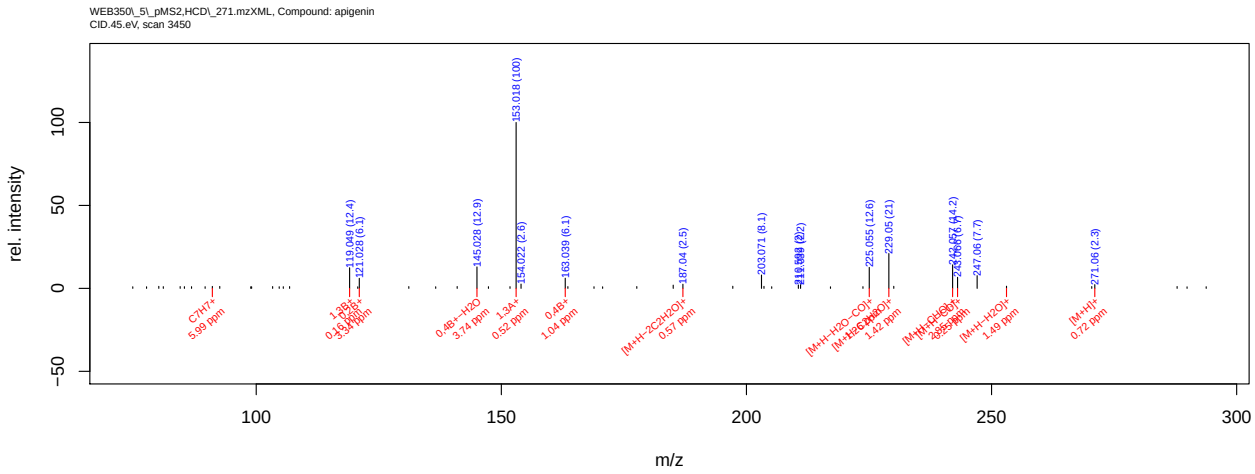
	mz	int	ppm	fragment
1	69.00	2.1	0.77	1,3A+-2CO-C2H4
2	89.04	24.5	7.04	C7H5+
3	91.05	2.0	6.66	C7H7+
4	97.03	3.9	0.20	1,3A+-2CO
5	111.04	1.8	0.84	0,4A++2H
6	117.03	32.1	3.69	1,4B+-2H-C2H2O-H2O
7	134.04	6.8	2.13	1,4B+-2H-CO-CH3
8	149.06	11.0	5.50	1,4B+-2H-CO
9	153.02	100.0	0.72	1,3A+
10	177.05	1.8	4.32	1,4B+-2H
11	179.03	1.8	5.09	AC+

homoeriodictyol.HCD.100eV



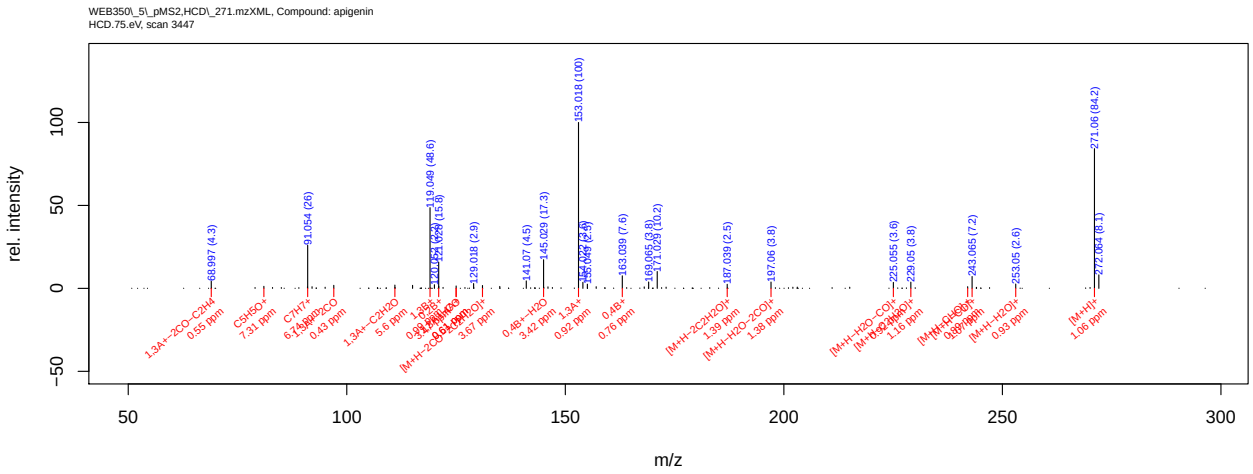
	mz	int	ppm	fragment
1	69.00	7.8	0.33	1,3A+-2CO-C2H4
2	81.03	1.2	6.94	C5H5O+
3	89.04	100.0	6.70	C7H5+
4	91.05	5.1	6.49	C7H7+
5	97.03	8.7	0.04	1,3A+-2CO
6	111.01	2.3	5.74	1,3A+-C2H2O
7	117.03	26.3	4.21	1,4B+-2H-C2H2O-H2O
8	134.04	13.5	2.70	1,4B+-2H-CO-CH3
9	137.02	1.8	0.56	0,3A+
10	149.06	3.4	4.79	1,4B+-2H-CO
11	153.02	57.8	1.32	1,3A+
12	179.03	1.1	5.01	AC+

apigenin.CID.45eV



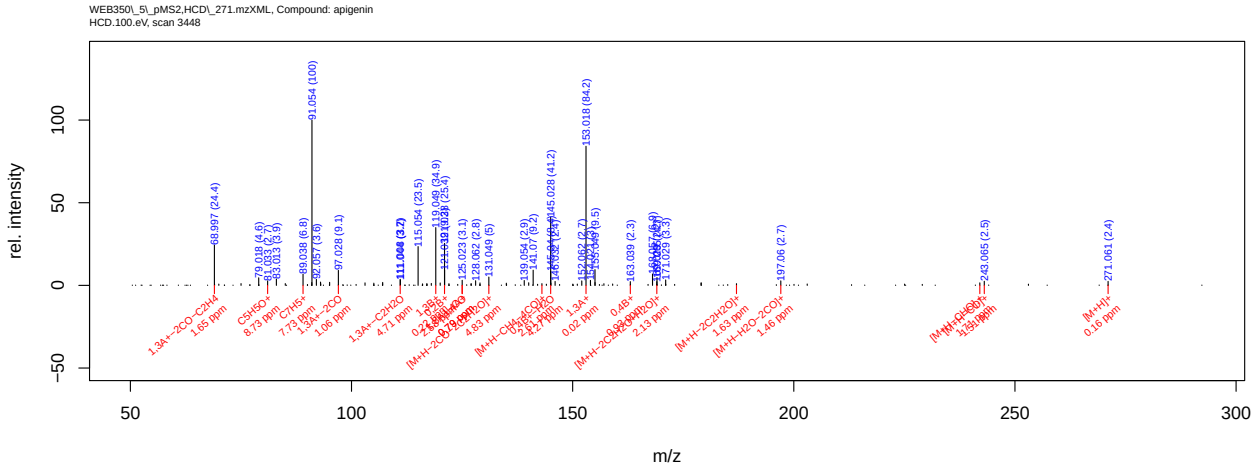
	mz	int	ppm	fragment
1	91.05	1.2	5.99	C7H7+
2	119.05	12.4	0.16	1,3B+
3	121.03	6.1	3.34	0,2B+
4	145.03	12.9	3.74	0,4B+-H2O
5	153.02	100.0	0.52	1,3A+
6	163.04	6.1	1.04	0,4B+
7	187.04	2.5	0.57	[M+H-2C2H2O]+
8	225.05	12.6	1.26	[M+H-H2O-CO]+
9	229.05	21.0	1.42	[M+H-C2H2O]+
10	242.06	14.2	2.85	[M+H-CHO].+
11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



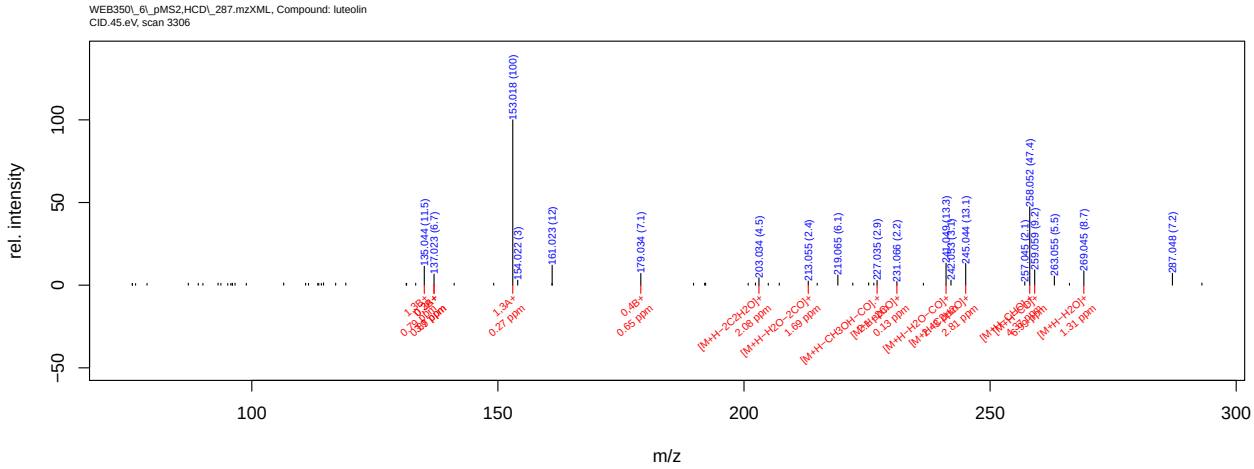
	mz	int	ppm	fragment
1	69.00	4.3	0.55	1,3A+-2CO-C2H4
2	81.03	1.2	7.31	C5H5O+
3	91.05	26.0	6.74	C7H7+
4	97.03	1.8	0.43	1,3A+-2CO
5	111.01	2.0	5.60	1,3A+-C2H2O
6	119.05	48.6	0.99	1,3B+
7	121.03	15.8	3.47	0,2B+
8	125.02	1.5	0.61	1,3A+-CO
9	125.02	1.5	0.61	1,4A+
10	131.05	1.7	3.67	[M+H-2CO-2C2H2O]+
11	145.03	17.3	3.42	0,4B+-H2O
12	153.02	100.0	0.92	1,3A+
13	163.04	7.6	0.76	0,4B+
14	187.04	2.5	1.39	[M+H-2C2H2O]+
15	197.06	3.8	1.38	[M+H-H2O-2CO]+
16	225.05	3.6	0.92	[M+H-H2O-CO]+
17	229.05	3.8	1.16	[M+H-C2H2O]+
18	242.06	1.0	0.89	[M+H-CHO].+
19	243.07	7.2	1.07	[M+H-CO]+
20	253.05	2.6	0.93	[M+H-H2O]+
21	271.06	84.2	1.06	[M+H]+

apigenin.HCD.100eV



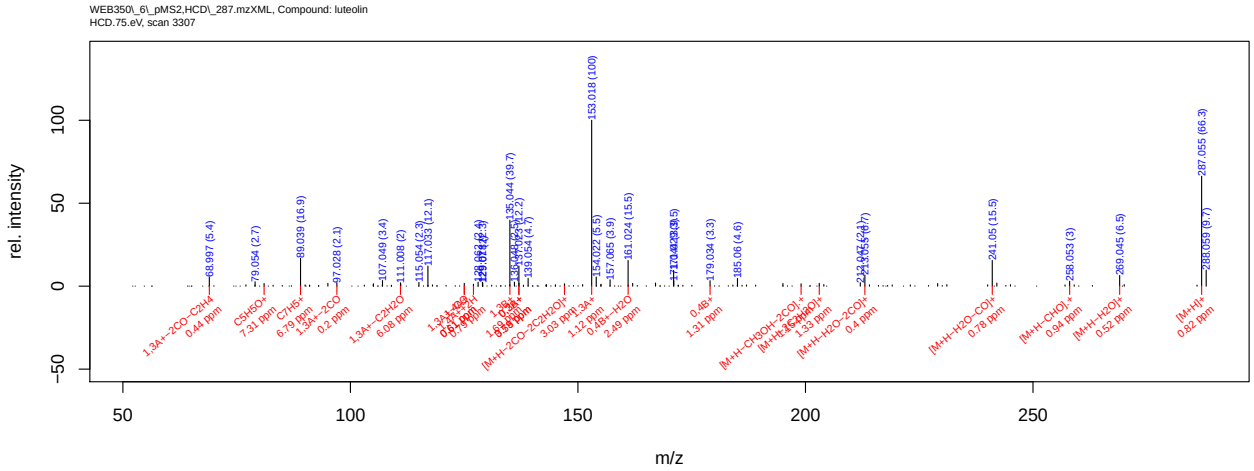
	mz	int	ppm	fragment
1	69.00	24.4	1.65	1,3A+-2CO-C2H4
2	81.03	2.7	8.73	C5H5O+
3	89.04	6.8	7.73	C7H5+
4	97.03	9.1	1.06	1,3A+-2CO
5	111.01	3.7	4.71	1,3A+-C2H2O
6	119.05	34.9	0.22	1,3B+
7	121.03	25.4	2.58	0,2B+
8	125.02	3.1	0.79	1,3A+-CO
9	125.02	3.1	0.79	1,4A+
10	131.05	5.0	4.83	[M+H-2CO-2C2H2O]+
11	143.05	1.1	2.61	[M+H-CH4-4CO]+
12	145.03	41.2	4.27	0,4B+-H2O
13	153.02	84.2	0.02	1,3A+
14	163.04	2.3	0.93	0,4B+
15	169.03	2.2	2.13	[M+H-2C2H2O-H2O]+
16	187.04	1.0	1.63	[M+H-2C2H2O]+
17	197.06	2.7	1.46	[M+H-H2O-2CO]+
18	242.06	1.5	1.71	[M+H-CHO].+
19	243.07	2.5	1.51	[M+H-CO]+
20	271.06	2.4	0.16	[M+H]+

luteolin.CID.45eV



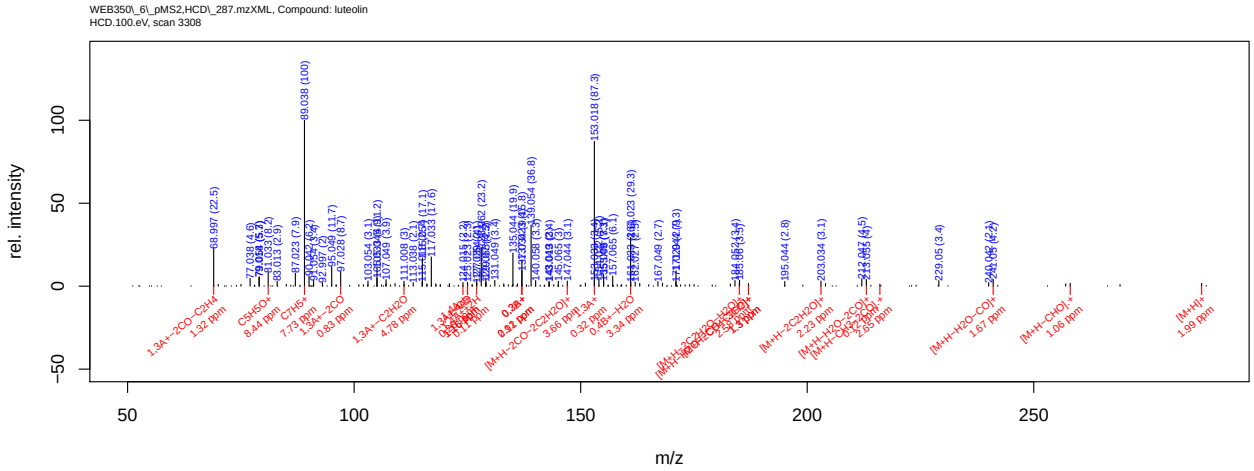
	mz	int	ppm	fragment
1	135.04	11.5	0.79	1,3B+
2	137.02	6.7	3.70	0,2B+
3	137.02	6.7	0.89	0,3A+
4	153.02	100.0	0.27	1,3A+
5	179.03	7.1	0.65	0,4B+
6	203.03	4.5	2.08	[M+H-2C2H2O]+
7	213.05	2.4	1.69	[M+H-H2O-2CO]+
8	227.03	2.9	2.10	[M+H-CH3OH-CO].+
9	231.07	2.2	0.13	[M+H-2CO]+
10	241.05	13.3	2.43	[M+H-H2O-CO]+
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



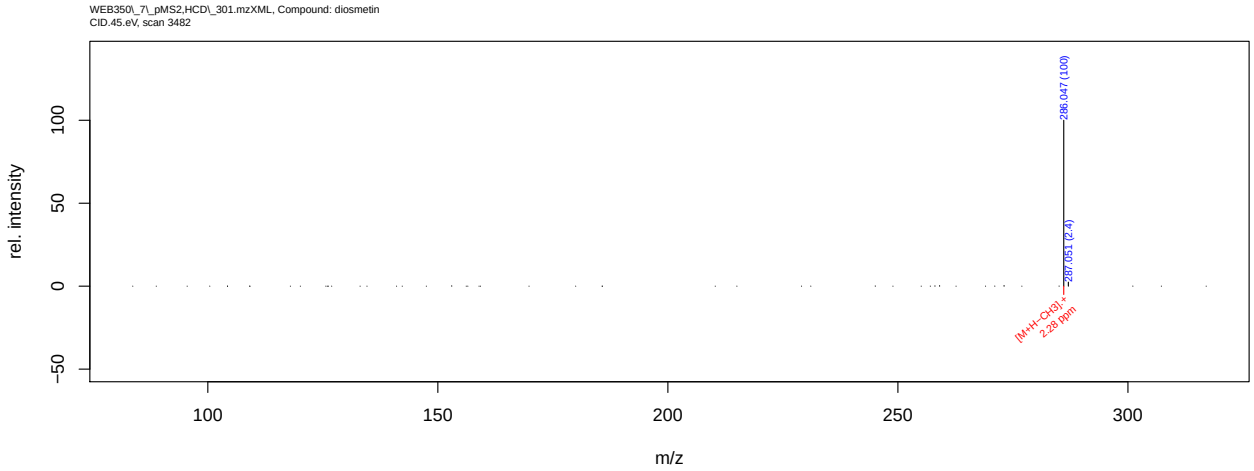
	mz	int	ppm	fragment
1	69.00	5.4	0.44	1,3A+-2CO-C2H4
2	81.03	1.6	7.31	C5H5O+
3	89.04	16.9	6.79	C7H5+
4	97.03	2.1	0.20	1,3A+-2CO
5	111.01	2.0	6.08	1,3A+-C2H2O
6	125.02	1.7	0.61	1,3A+-CO
7	125.02	1.7	0.61	1,4A+
8	127.04	1.2	0.79	1,4A++2H
9	135.04	39.7	1.69	1,3B+
10	137.02	12.2	3.59	0,2B+
11	137.02	12.2	0.78	0,3A+
12	147.04	1.5	3.03	[M+H-2CO-2C2H2O]+
13	153.02	100.0	1.12	1,3A+
14	161.02	15.5	2.49	0,4B+-H2O
15	179.03	3.3	1.31	0,4B+
16	199.04	1.4	1.15	[M+H-CH3OH-2CO].+
17	203.03	1.7	1.33	[M+H-2C2H2O]+
18	213.06	6.7	0.40	[M+H-H2O-2CO]+
19	241.05	15.5	0.78	[M+H-H2O-CO]+
20	258.05	3.0	0.94	[M+H-CHO].+
21	269.04	6.5	0.52	[M+H-H2O]+
22	287.06	66.3	0.82	[M+H]+

luteolin.HCD.100eV



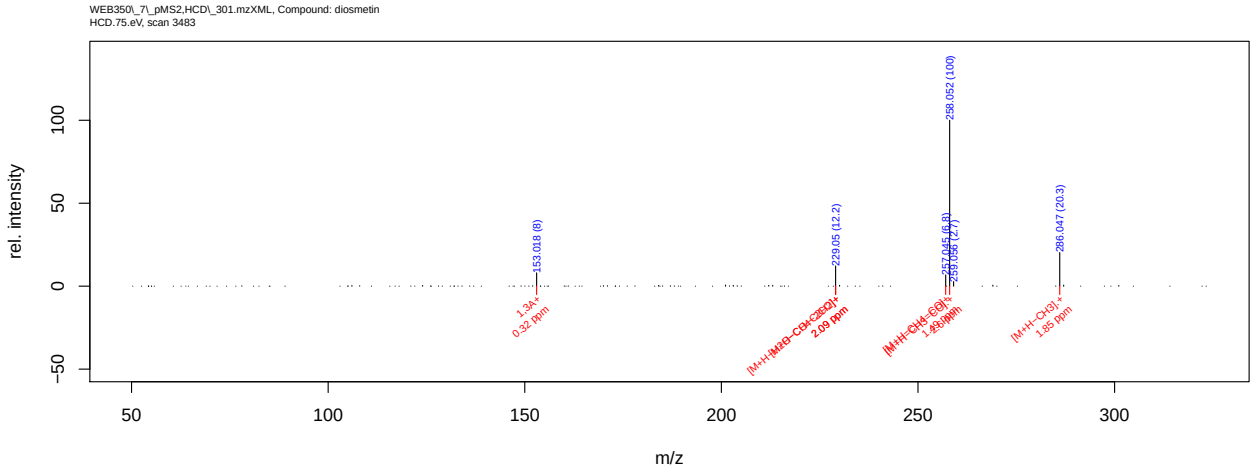
	mz	int	ppm	fragment
1	69.00	22.5	1.32	1,3A+-2CO-C2H4
2	81.03	8.2	8.44	C5H5O+
3	89.04	100.0	7.73	C7H5+
4	97.03	8.7	0.83	1,3A+-2CO
5	111.01	3.0	4.78	1,3A+-C2H2O
6	124.02	2.2	0.28	1,4A.+
7	125.02	2.3	1.16	1,3A+-CO
8	125.02	2.3	1.16	1,4A+
9	127.04	2.1	0.11	1,4A++2H
10	137.02	15.8	2.92	0,2B+
11	137.02	15.8	0.11	0,3A+
12	147.04	3.1	3.66	[M+H-2CO-2C2H2O]+
13	153.02	87.3	0.32	1,3A+
14	161.02	29.3	3.34	0,4B+-H2O
15	185.02	1.9	2.58	[M+H-2C2H2O-H2O]+
16	187.04	1.6	1.30	[M+H-CH4-3CO]+
17	187.04	1.6	1.30	[M+H-H2O-2CO-C2H2]+
18	203.03	3.1	2.23	[M+H-2C2H2O]+
19	213.06	4.0	0.12	[M+H-H2O-2CO]+
20	216.04	1.2	2.65	[M+H-CH3-2CO].+
21	241.05	4.2	1.67	[M+H-H2O-CO]+
22	258.05	1.7	1.06	[M+H-CHO].+
23	287.05	1.6	1.99	[M+H]+

diosmetin.CID.45eV



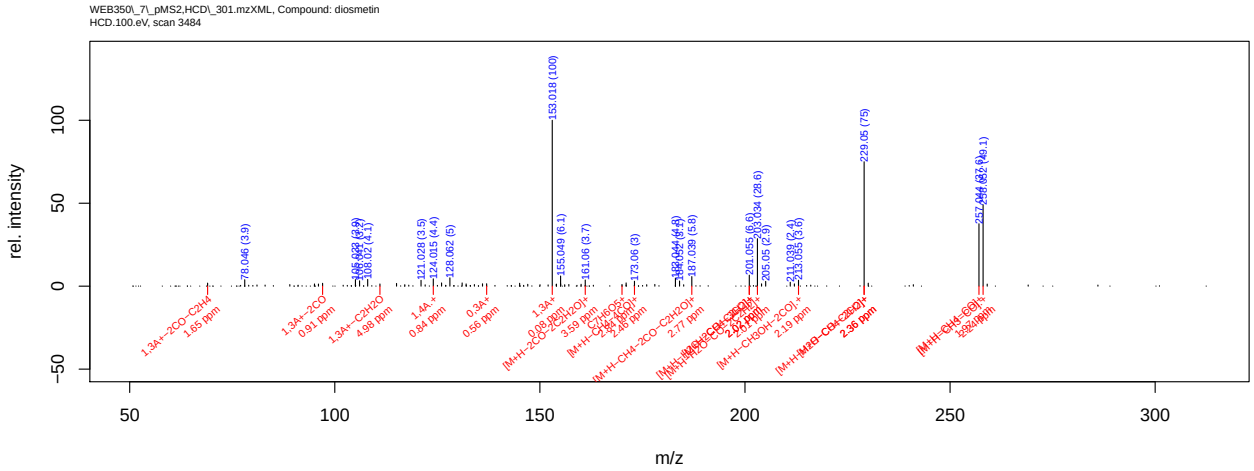
	mz	int	ppm	fragment
1	286.05	100.0	2.28	[M+H-CH3].+

diosmetin.HCD.75eV



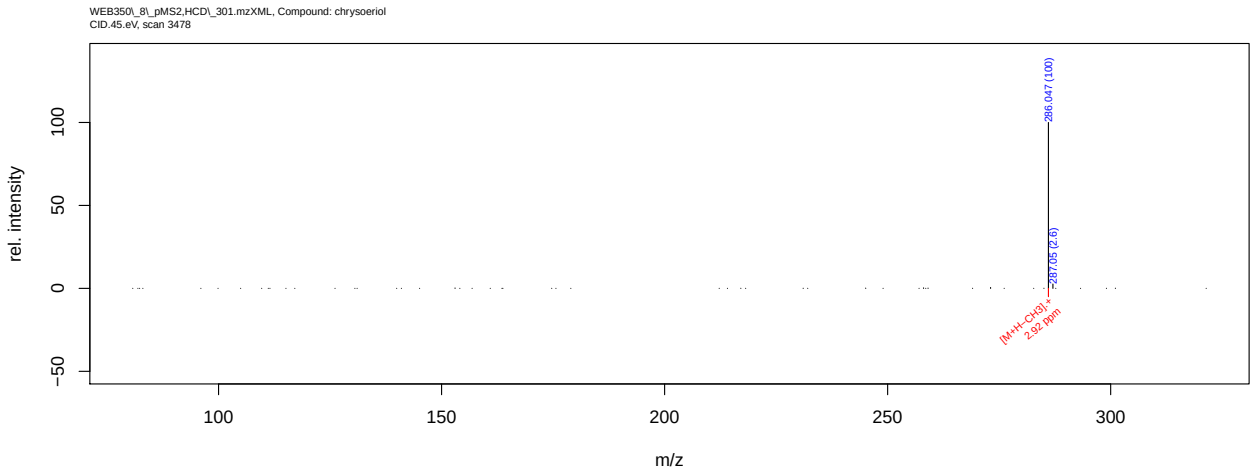
	mz	int	ppm	fragment
1	153.02	8.0	0.32	1,3A+
2	229.05	12.2	2.09	[M+H-CH4-2CO]+
3	229.05	12.2	2.09	[M+H-H2O-CO-C2H2]+
4	257.04	6.8	1.49	[M+H-CH4-CO]+
5	258.05	100.0	2.60	[M+H-CH3-CO].+
6	286.05	20.3	1.85	[M+H-CH3].+

diosmetin.HCD.100eV



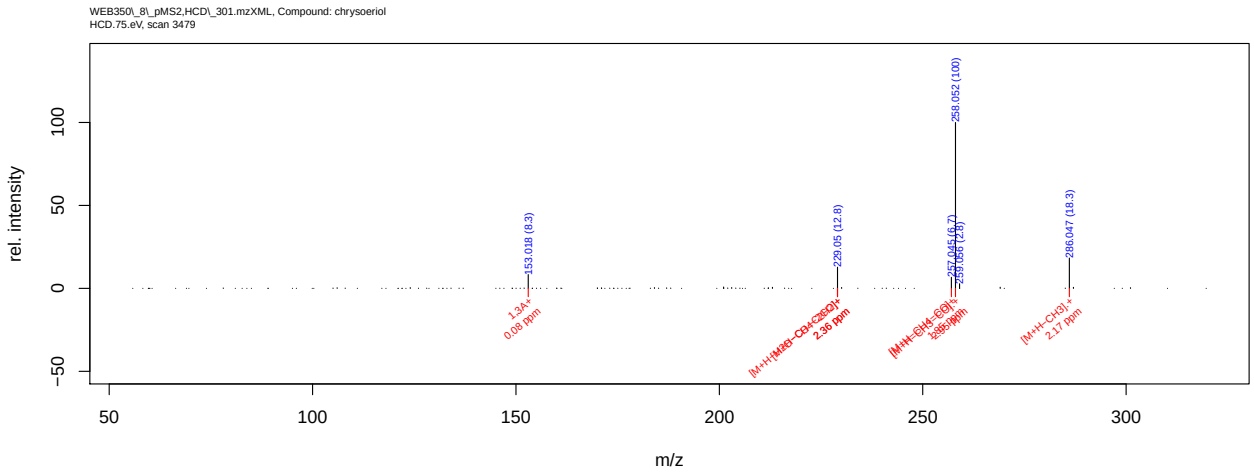
	mz	int	ppm	fragment
1	69.00	1.8	1.65	1,3A+-2CO-C2H4
2	97.03	1.7	0.91	1,3A+-2CO
3	111.01	1.3	4.98	1,3A+-C2H2O
4	124.02	4.4	0.84	1,4A.+
5	137.02	1.5	0.56	0,3A+
6	153.02	100.0	0.08	1,3A+
7	161.06	3.7	3.59	[M+H-2CO-2C2H2O]+
8	170.02	1.1	2.84	C7H6O5+
9	173.06	3.0	2.46	[M+H-CH4-4CO]+
10	187.04	5.8	2.77	[M+H-CH4-2CO-C2H2O]+
11	201.05	6.6	2.02	[M+H-CH4-3CO]+
12	201.05	6.6	2.02	[M+H-H2O-2CO-C2H2]+
13	203.03	28.6	2.01	[M+H-H2O-CO-2C2H2]+
14	213.05	3.6	2.19	[M+H-CH3OH-2CO].+
15	229.05	75.0	2.36	[M+H-CH4-2CO]+
16	229.05	75.0	2.36	[M+H-H2O-CO-C2H2]+
17	257.04	37.6	1.97	[M+H-CH4-CO]+
18	258.05	49.1	2.24	[M+H-CH3-CO].+

chrysoeriol.CID.45eV



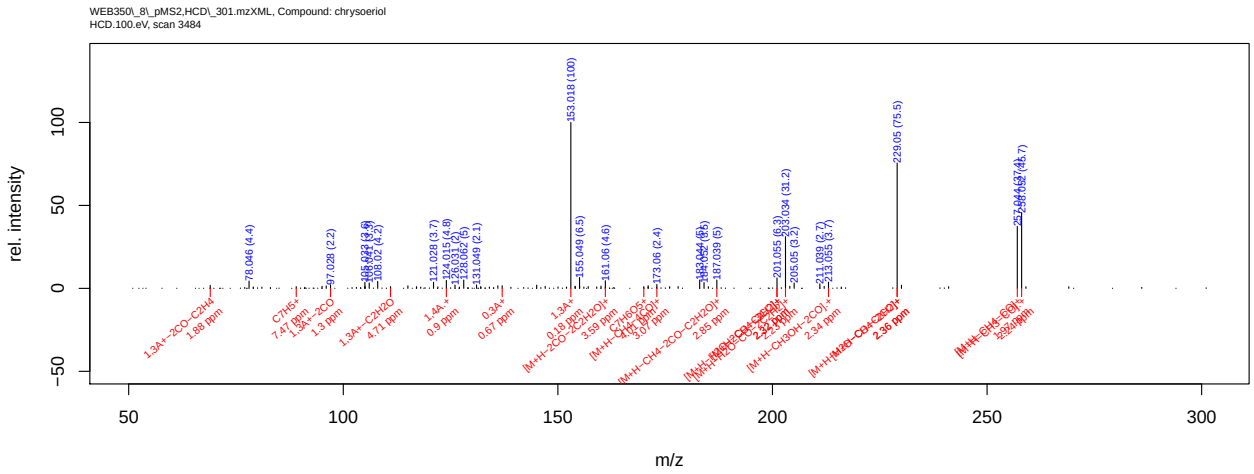
	mz	int	ppm	fragment
1	286.05	100.0	2.92	[M+H-CH3].+

chrysoeriol.HCD.75eV



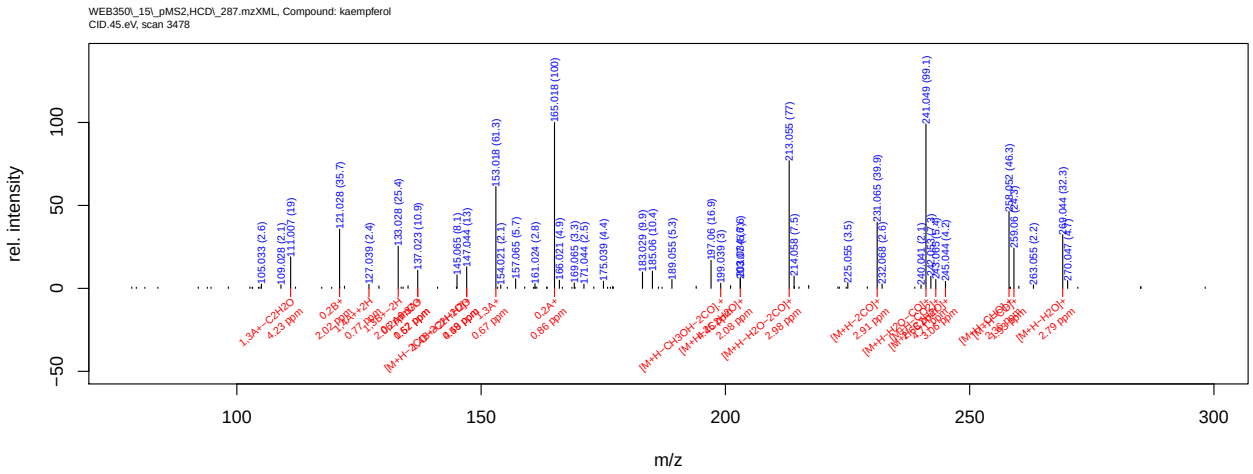
	mz	int	ppm	fragment
1	153.02	8.3	0.08	1,3A+
2	229.05	12.8	2.36	[M+H-CH4-2CO]+
3	229.05	12.8	2.36	[M+H-H2O-CO-C2H2]+
4	257.04	6.7	1.85	[M+H-CH4-CO]+
5	258.05	100.0	2.95	[M+H-CH3-CO].+
6	286.05	18.3	2.17	[M+H-CH3].+

chrysoeriol.HCD.100eV



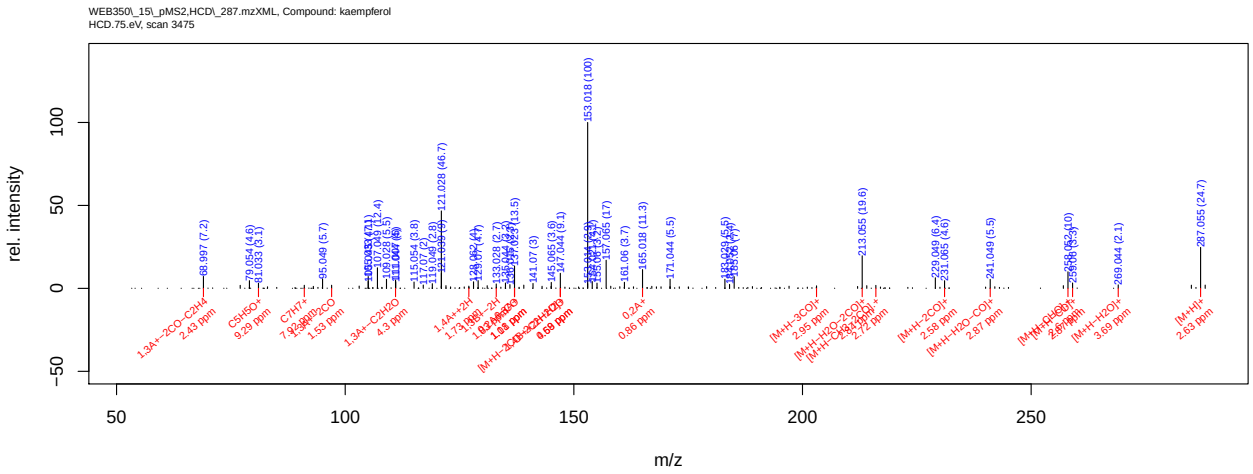
	mz	int	ppm	fragment
1	69.00	1.9	1.88	1,3A+-2CO-C2H4
2	89.04	1.0	7.47	C7H5+
3	97.03	2.2	1.30	1,3A+-2CO
4	111.01	1.1	4.71	1,3A+-C2H2O
5	124.02	4.8	0.90	1,4A.+
6	137.02	1.6	0.67	0,3A+
7	153.02	100.0	0.18	1,3A+
8	161.06	4.6	3.59	[M+H-2CO-2C2H2O]+
9	170.02	1.1	4.01	C7H6O5+
10	173.06	2.4	3.07	[M+H-CH4-4CO]+
11	187.04	5.0	2.85	[M+H-CH4-2CO-C2H2O]+
12	201.05	6.3	2.32	[M+H-CH4-3CO]+
13	201.05	6.3	2.32	[M+H-H2O-2CO-C2H2]+
14	203.03	31.2	2.23	[M+H-H2O-CO-2C2H2]+
15	213.05	3.7	2.34	[M+H-CH3OH-2CO].+
16	229.05	75.5	2.36	[M+H-CH4-2CO]+
17	229.05	75.5	2.36	[M+H-H2O-CO-C2H2]+
18	257.04	37.4	1.97	[M+H-CH4-CO]+
19	258.05	45.7	2.24	[M+H-CH3-CO].+

kaempferol.CID.45eV



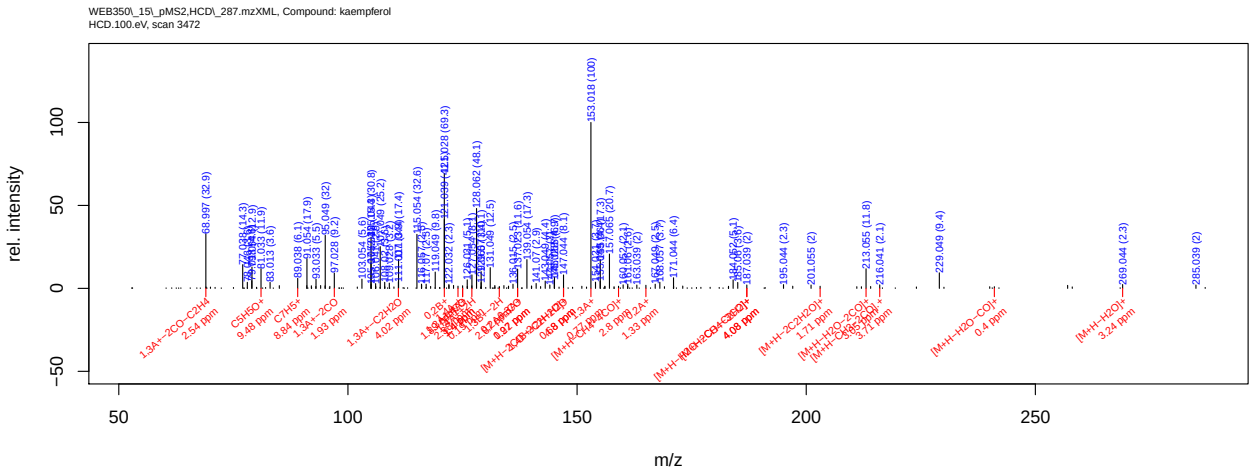
	mz	int	ppm	fragment
1	111.01	19.0	4.23	1,3A+-C2H2O
2	121.03	35.7	2.02	0,2B+
3	127.04	2.4	0.77	1,4A++2H
4	133.03	25.4	2.06	1,3B+-2H
5	137.02	10.9	1.52	0,2A+-CO
6	137.02	10.9	0.67	0,3A+
7	147.04	13.0	0.48	1,4B++2H-H2O
8	147.04	13.0	4.59	[M+H-2CO-2C2H2O]+
9	153.02	61.3	0.67	1,3A+
10	165.02	100.0	0.86	0,2A+
11	199.04	3.0	4.45	[M+H-CH3OH-2CO].+
12	203.03	6.6	2.08	[M+H-2C2H2O]+
13	213.05	77.0	2.98	[M+H-H2O-2CO]+
14	231.07	39.9	2.91	[M+H-2CO]+
15	241.05	99.1	2.68	[M+H-H2O-CO]+
16	243.06	5.4	4.71	[M+H-CO2]+
17	245.04	4.2	3.06	[M+H-C2H2O]+
18	258.05	46.3	2.36	[M+H-CHO].+
19	259.06	24.3	1.93	[M+H-CO]+
20	269.04	32.3	2.79	[M+H-H2O]+

kaempferol.HCD.75eV



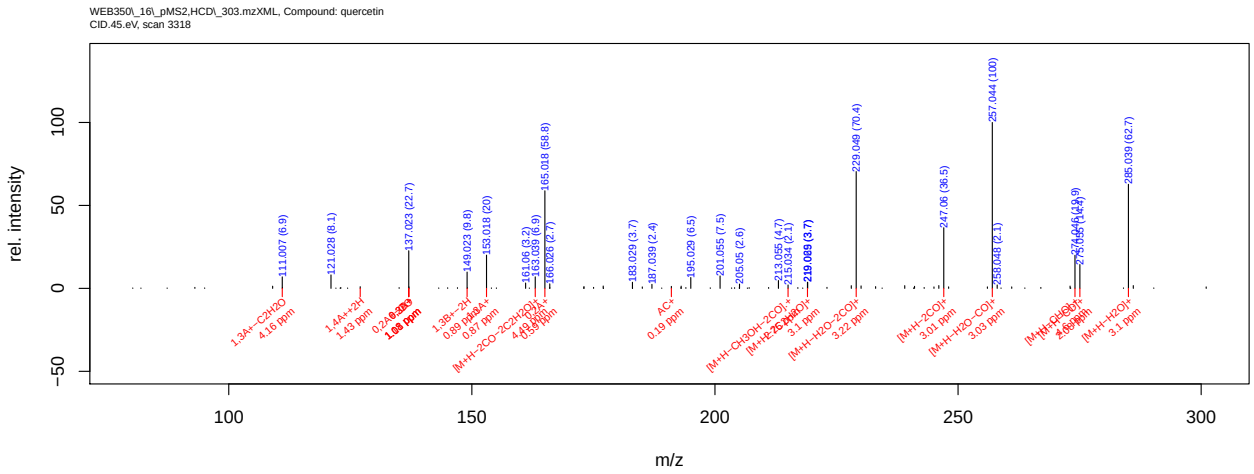
	mz	int	ppm	fragment
1	69.00	7.2	2.43	1,3A+-2CO-C2H4
2	81.03	3.1	9.29	C5H5O+
3	91.05	1.9	7.92	C7H7+
4	97.03	1.9	1.53	1,3A+-2CO
5	111.01	5.0	4.30	1,3A+-C2H2O
6	127.04	1.4	1.73	1,4A++2H
7	133.03	2.7	1.83	1,3B+-2H
8	137.02	13.5	1.08	0,2A+-CO
9	137.02	13.5	1.11	0,3A+
10	147.04	9.1	0.58	1,4B++2H-H2O
11	147.04	9.1	4.69	[M+H-2CO-2C2H2O]+
12	165.02	11.3	0.86	0,2A+
13	203.07	1.5	2.95	[M+H-3CO]+
14	213.05	19.6	2.84	[M+H-H2O-2CO]+
15	216.04	1.8	2.72	[M+H-CH3-2CO].+
16	231.07	4.6	2.58	[M+H-2CO]+
17	241.05	5.5	2.87	[M+H-H2O-CO]+
18	258.05	10.0	2.60	[M+H-CHO].+
19	259.06	3.3	2.87	[M+H-CO]+
20	269.04	2.1	3.69	[M+H-H2O]+
21	287.05	24.7	2.63	[M+H]+

kaempferol.HCD.100eV



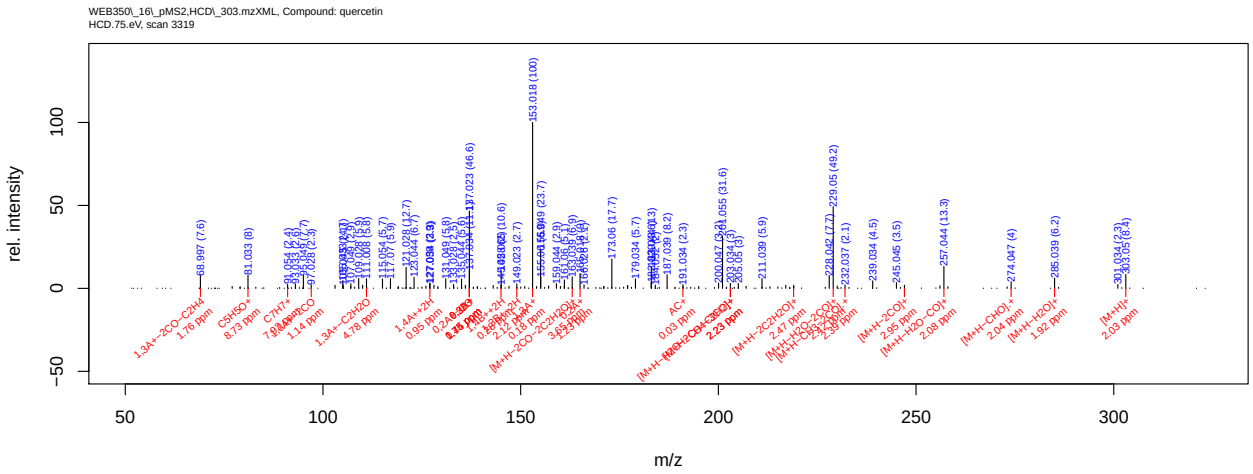
	mz	int	ppm	fragment
1	69.00	32.9	2.54	1,3A+-2CO-C2H4
2	81.03	11.9	9.48	C5H5O+
3	89.04	6.1	8.84	C7H5+
4	97.03	9.2	1.93	1,3A+-2CO
5	111.01	3.9	4.02	1,3A+-C2H2O
6	121.03	69.3	1.89	0,2B+
7	124.02	1.3	2.38	1,4A.+
8	125.02	1.6	1.40	1,3A+-CO
9	125.02	1.6	1.40	1,4A+
10	127.04	1.6	0.19	1,4A++2H
11	133.03	1.2	2.87	1,3B+-2H
12	137.02	11.6	0.97	0,2A+-CO
13	137.02	11.6	1.22	0,3A+
14	147.04	8.1	0.68	1,4B++2H-H2O
15	147.04	8.1	4.80	[M+H-2CO-2C2H2O]+
16	153.02	100.0	0.77	1,3A+
17	159.04	1.3	2.80	[M+H-CH4-4CO]+
18	165.02	1.9	1.33	0,2A+
19	187.04	2.0	4.08	[M+H-CH4-3CO]+
20	187.04	2.0	4.08	[M+H-H2O-2CO-C2H2]+
21	203.03	1.3	1.71	[M+H-2C2H2O]+
22	213.05	11.8	3.05	[M+H-H2O-2CO]+
23	216.04	2.1	3.71	[M+H-CH3-2CO].+
24	241.05	1.0	0.40	[M+H-H2O-CO]+
25	269.04	2.3	3.24	[M+H-H2O]+

quercetin.CID.45eV



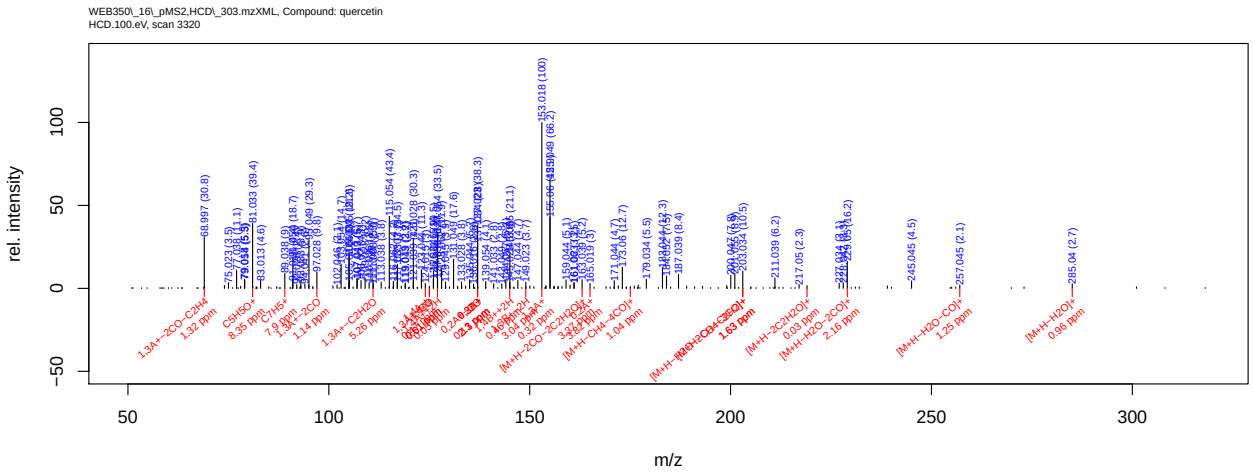
	mz	int	ppm	fragment
1	111.01	6.9	4.16	1,3A+-C2H2O
2	127.04	1.0	1.43	1,4A++2H
3	137.02	22.7	1.08	0,2A+-CO
4	137.02	22.7	1.08	0,2B+
5	137.02	22.7	1.11	0,3A+
6	149.02	9.8	0.89	1,3B+-2H
7	153.02	20.0	0.87	1,3A+
8	163.04	6.9	4.49	[M+H-2CO-2C2H2O]+
9	165.02	58.8	0.59	0,2A+
10	191.03	1.2	0.19	AC+
11	215.03	2.1	2.75	[M+H-CH3OH-2CO].+
12	219.03	3.7	3.10	[M+H-2C2H2O]+
13	229.05	70.4	3.22	[M+H-H2O-2CO]+
14	247.06	36.5	3.01	[M+H-2CO]+
15	257.04	100.0	3.03	[M+H-H2O-CO]+
16	274.05	19.9	4.60	[M+H-CHO].+
17	275.05	14.4	2.08	[M+H-CO]+
18	285.04	62.7	3.10	[M+H-H2O]+

quercetin.HCD.75eV



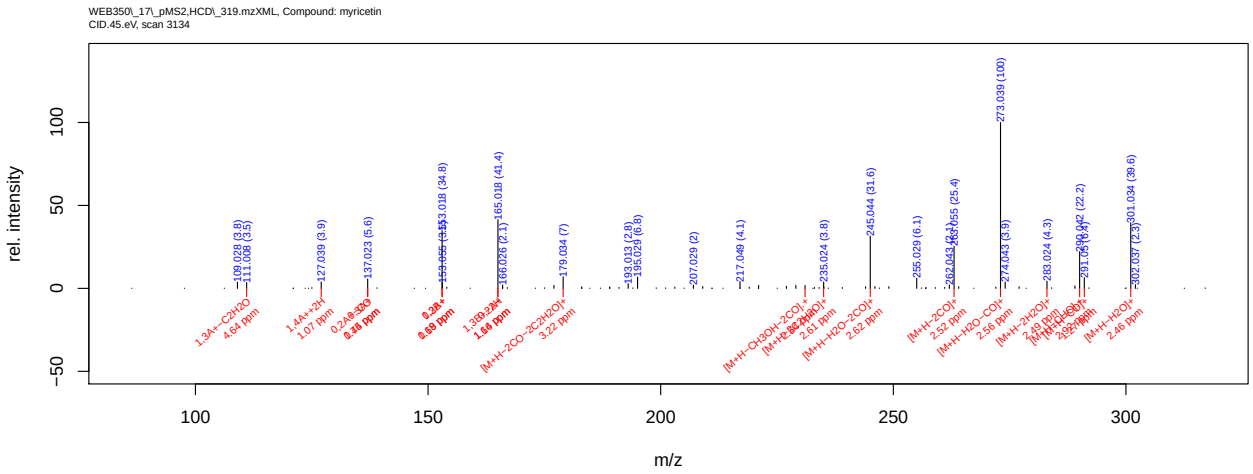
	mz	int	ppm	fragment
1	69.00	7.6	1.76	1,3A+-2CO-C2H4
2	81.03	8.0	8.73	C5H5O+
3	91.05	2.4	7.92	C7H7+
4	97.03	2.3	1.14	1,3A+-2CO
5	111.01	5.8	4.78	1,3A+-C2H2O
6	127.04	2.9	0.95	1,4A++2H
7	137.02	46.6	1.75	0,2A+-CO
8	137.02	46.6	1.75	0,2B+
9	137.02	46.6	0.44	0,3A+
10	145.03	2.0	0.28	1,4B++2H
11	149.02	2.7	2.12	1,3B+-2H
12	153.02	100.0	0.18	1,3A+
13	163.04	6.9	3.65	[M+H-2CO-2C2H2O]+
14	165.02	9.0	1.23	0,2A+
15	191.03	2.3	0.03	AC+
16	203.03	3.0	2.23	[M+H-CH4-3CO]+
17	203.03	3.0	2.23	[M+H-H2O-2CO-C2H2]+
18	219.03	1.1	2.47	[M+H-2C2H2O]+
19	229.05	49.2	2.42	[M+H-H2O-2CO]+
20	232.04	2.1	2.39	[M+H-CH3-2CO].+
21	247.06	1.9	2.95	[M+H-2CO]+
22	257.04	13.3	2.08	[M+H-H2O-CO]+
23	274.05	4.0	2.04	[M+H-CHO].+
24	285.04	6.2	1.92	[M+H-H2O]+
25	303.05	8.4	2.03	[M+H]+

quercetin.HCD.100eV



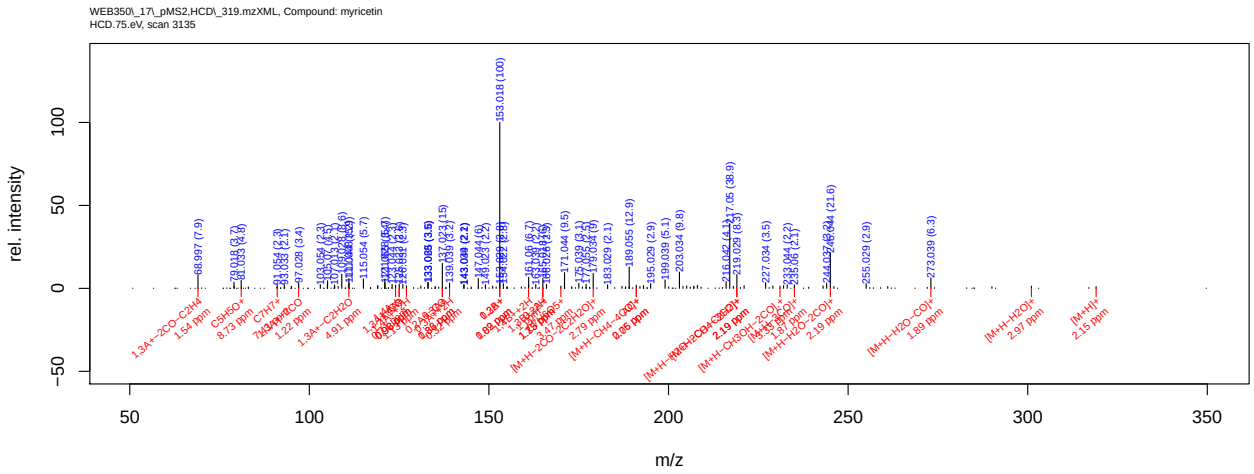
	mz	int	ppm	fragment
1	69.00	30.8	1.32	1,3A+-2CO-C2H4
2	81.03	39.4	8.35	C5H5O+
3	89.04	9.0	7.90	C7H5+
4	97.03	9.8	1.14	1,3A+-2CO
5	111.01	5.1	5.26	1,3A+-C2H2O
6	124.02	3.0	0.47	1,4A.+
7	125.02	1.4	0.61	1,3A+-CO
8	125.02	1.4	0.61	1,4A+
9	127.04	6.4	0.05	1,4A++2H
10	137.02	38.3	2.30	0,2A+-CO
11	137.02	38.3	2.30	0,2B+
12	137.02	38.3	0.11	0,3A+
13	145.03	3.6	0.46	1,4B++2H
14	149.02	3.7	3.04	1,3B+-2H
15	153.02	100.0	0.32	1,3A+
16	163.04	5.2	3.37	[M+H-2CO-2C2H2O]+
17	165.02	3.0	3.82	0,2A+
18	175.04	1.2	1.04	[M+H-CH4-4CO]+
19	203.03	10.5	1.63	[M+H-CH4-3CO]+
20	203.03	10.5	1.63	[M+H-H2O-2CO-C2H2]+
21	219.03	1.6	0.03	[M+H-2C2H2O]+
22	229.05	16.2	2.16	[M+H-H2O-2CO]+
23	257.04	2.1	1.25	[M+H-H2O-CO]+
24	285.04	2.7	0.96	[M+H-H2O]+

myricetin.CID.45eV



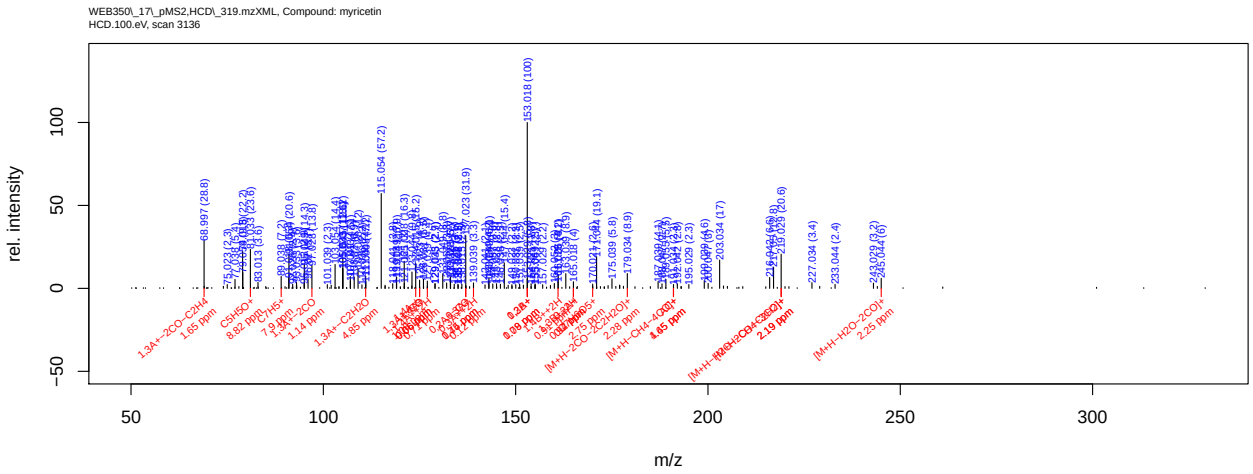
	mz	int	ppm	fragment
1	111.01	3.5	4.64	1,3A+-C2H2O
2	127.04	3.9	1.07	1,4A++2H
3	137.02	5.6	1.75	0,2A+-CO
4	137.02	5.6	0.44	0,3A+
5	153.02	34.8	1.69	0,2B+
6	153.02	34.8	0.18	1,3A+
7	165.02	41.4	1.14	0,2A+
8	165.02	41.4	1.66	1,3B+-2H
9	179.03	7.0	3.22	[M+H-2CO-2C2H2O]+
10	231.03	1.8	2.54	[M+H-CH3OH-2CO].+
11	235.02	3.8	2.61	[M+H-2C2H2O]+
12	245.04	31.6	2.62	[M+H-H2O-2CO]+
13	263.05	25.4	2.52	[M+H-2CO]+
14	273.04	100.0	2.56	[M+H-H2O-CO]+
15	283.02	4.3	2.49	[M+H-2H2O]+
16	290.04	22.2	2.92	[M+H-CHO].+
17	291.05	6.4	1.27	[M+H-CO]+
18	301.03	39.6	2.46	[M+H-H2O]+

myricetin.HCD.75eV



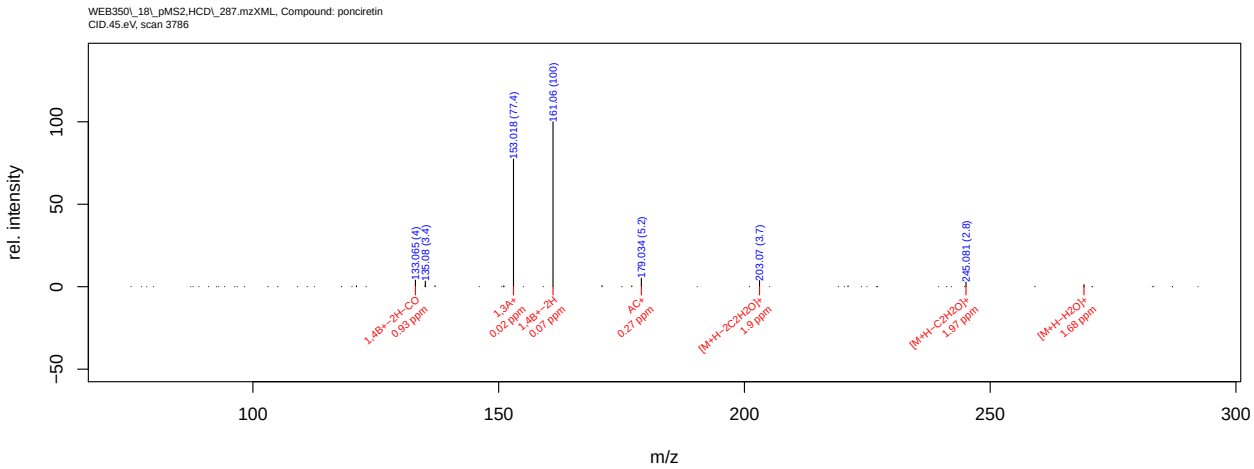
	mz	int	ppm	fragment
1	69.00	7.9	1.54	1,3A+-2CO-C2H4
2	81.03	4.8	8.73	C5H5O+
3	91.05	2.3	7.41	C7H7+
4	97.03	3.4	1.22	1,3A+-2CO
5	111.01	5.9	4.91	1,3A+-C2H2O
6	124.02	2.0	0.71	1,4A.+
7	125.02	2.6	0.98	1,3A+-CO
8	125.02	2.6	0.98	1,4A+
9	127.04	1.6	1.13	1,4A++2H
10	137.02	15.0	1.86	0,2A+-CO
11	137.02	15.0	0.33	0,3A+
12	139.04	3.2	0.32	0,3A++2H
13	153.02	100.0	1.89	0,2B+
14	153.02	100.0	0.02	1,3A+
15	161.02	1.9	1.00	1,4B++2H
16	165.02	6.0	1.23	0,2A+
17	165.02	6.0	1.75	1,3B+-2H
18	170.02	1.4	3.47	C7H6O5+
19	179.03	9.0	2.79	[M+H-2CO-2C2H2O]+
20	191.03	1.9	0.75	AC+
21	191.03	1.9	2.06	[M+H-CH4-4CO]+
22	219.03	8.3	2.19	[M+H-CH4-3CO]+
23	219.03	8.3	2.19	[M+H-H2O-2CO-C2H2]+
24	231.03	1.4	3.33	[M+H-CH3OH-2CO].+
25	235.06	2.1	1.87	[M+H-3CO]+
26	245.04	21.6	2.19	[M+H-H2O-2CO]+
27	273.04	6.3	1.89	[M+H-H2O-CO]+
28	301.03	1.4	2.97	[M+H-H2O]+
29	319.04	1.1	2.15	[M+H]+

myricetin.HCD.100eV



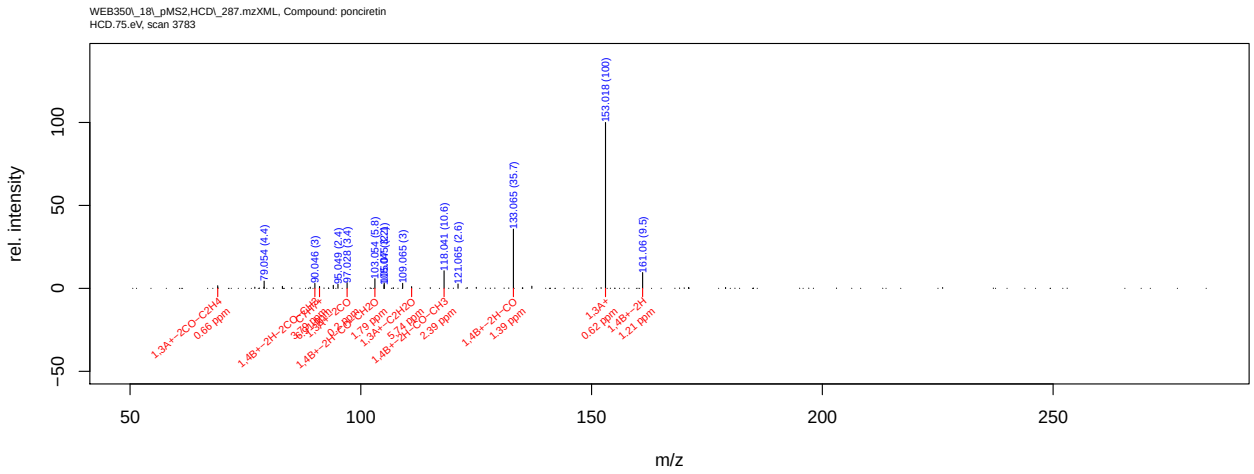
	mz	int	ppm	fragment
1	69.00	28.8	1.65	1,3A+-2CO-C2H4
2	81.03	23.6	8.82	C5H5O+
3	89.04	7.2	7.90	C7H5+
4	97.03	13.8	1.14	1,3A+-2CO
5	111.01	7.2	4.85	1,3A+-C2H2O
6	124.02	15.2	1.08	1,4A.+
7	125.02	4.9	0.06	1,3A+-CO
8	125.02	4.9	0.06	1,4A+
9	127.04	4.4	0.71	1,4A++2H
10	137.02	31.9	1.75	0,2A+-CO
11	137.02	31.9	0.44	0,3A+
12	139.04	3.3	0.12	0,3A++2H
13	153.02	100.0	1.79	0,2B+
14	153.02	100.0	0.08	1,3A+
15	161.02	4.1	0.91	1,4B++2H
16	165.02	4.0	0.40	0,2A+
17	165.02	4.0	0.92	1,3B+-2H
18	170.02	2.6	2.75	C7H6O5+
19	179.03	8.9	2.28	[M+H-2CO-2C2H2O]+
20	191.03	2.3	1.65	AC+
21	191.03	2.3	4.45	[M+H-CH4-4CO]+
22	219.03	20.6	2.19	[M+H-CH4-3CO]+
23	219.03	20.6	2.19	[M+H-H2O-2CO-C2H2]+
24	245.04	6.0	2.25	[M+H-H2O-2CO]+

ponciretin.CID.45eV



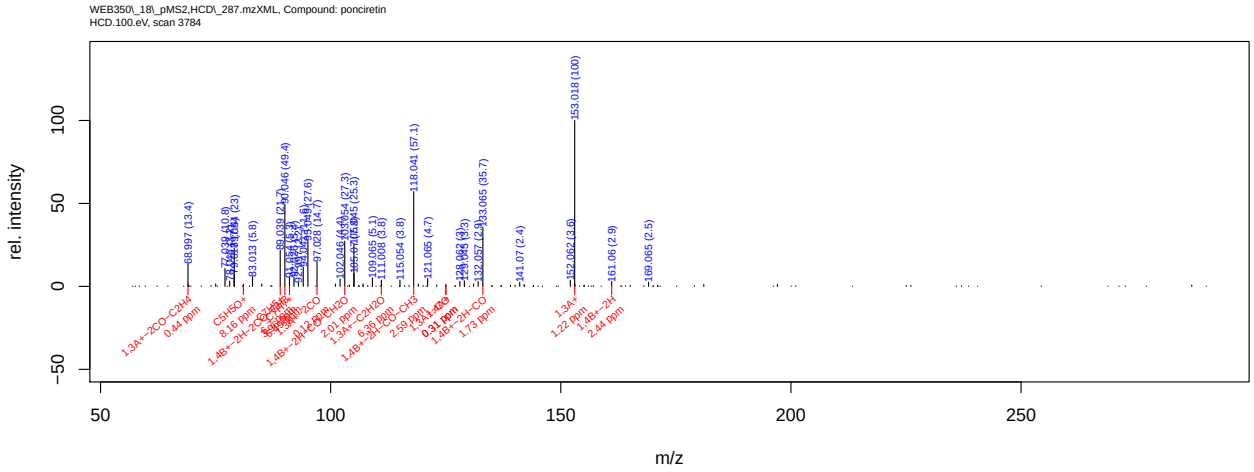
	mz	int	ppm	fragment
1	133.06	4.0	0.93	1,4B+-2H-CO
2	153.02	77.4	0.02	1,3A+
3	161.06	100.0	0.07	1,4B+-2H
4	179.03	5.2	0.27	AC+
5	203.07	3.7	1.90	[M+H-2C2H2O]+
6	245.08	2.8	1.97	[M+H-C2H2O]+
7	269.08	1.3	1.68	[M+H-H2O]+

ponciretin.HCD.75eV



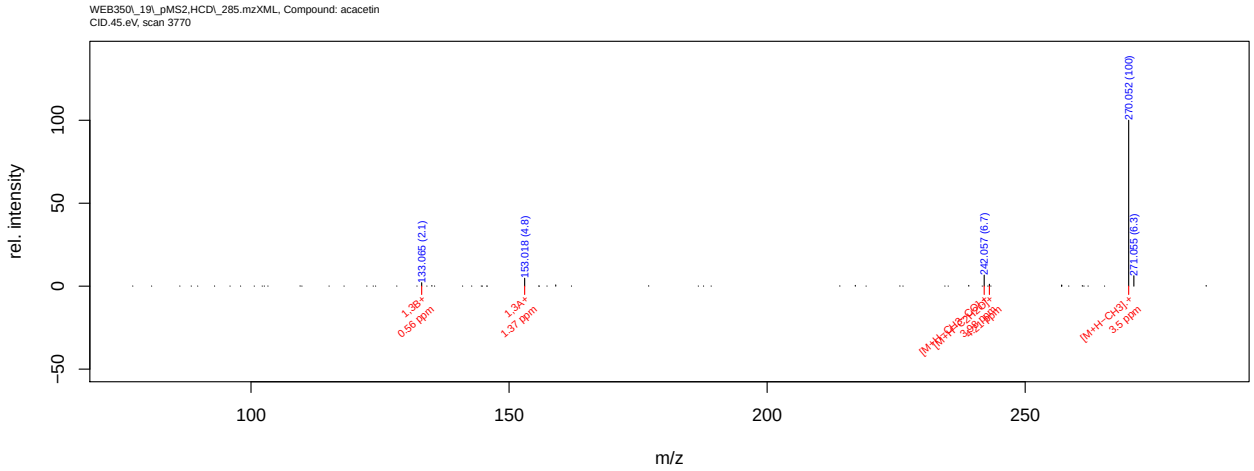
	mz	int	ppm	fragment
1	69.00	1.6	0.66	1,3A+-2CO-C2H4
2	90.05	3.0	3.79	1,4B+-2H-2CO-CH3
3	91.05	1.1	6.91	C7H7+
4	97.03	3.4	0.20	1,3A+-2CO
5	103.05	5.8	1.79	1,4B+-2H-CO-CH2O
6	111.01	1.1	5.74	1,3A+-C2H2O
7	118.04	10.6	2.39	1,4B+-2H-CO-CH3
8	133.06	35.7	1.39	1,4B+-2H-CO
9	153.02	100.0	0.62	1,3A+
10	161.06	9.5	1.21	1,4B+-2H

ponciretin.HCD.100eV



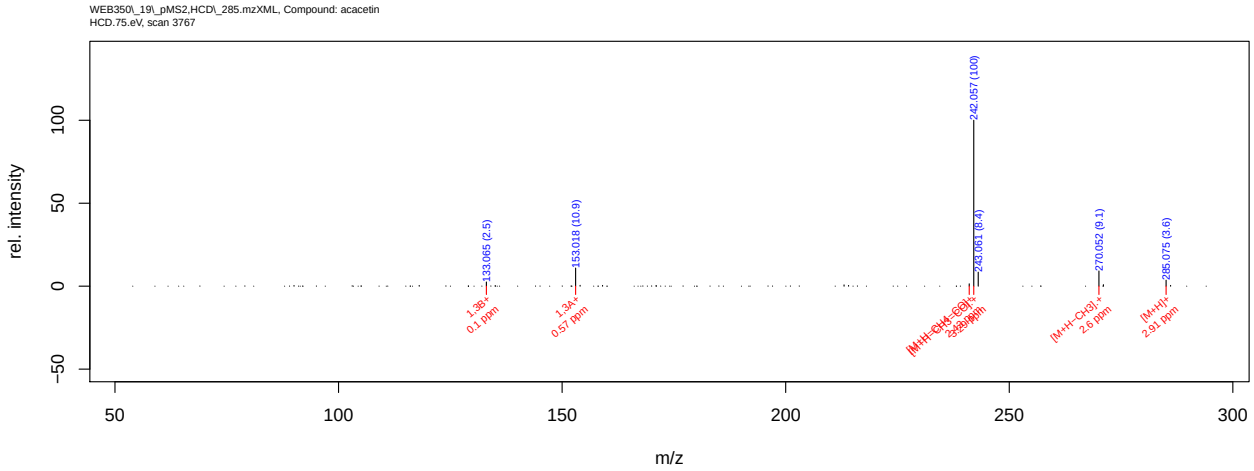
	mz	int	ppm	fragment
1	69.00	13.4	0.44	1,3A+-2CO-C2H4
2	81.03	1.3	8.16	C5H5O+
3	89.04	21.7	6.70	C7H5+
4	90.05	49.4	3.96	1,4B+-2H-2CO-CH3
5	91.05	5.3	6.49	C7H7+
6	97.03	14.7	0.12	1,3A+-2CO
7	103.05	27.3	2.01	1,4B+-2H-CO-CH2O
8	111.01	3.8	6.36	1,3A+-C2H2O
9	118.04	57.1	2.59	1,4B+-2H-CO-CH3
10	125.02	1.3	0.31	1,3A+-CO
11	125.02	1.3	0.31	1,4A+
12	133.06	35.7	1.73	1,4B+-2H-CO
13	153.02	100.0	1.22	1,3A+
14	161.06	2.9	2.44	1,4B+-2H

acacetin.CID.45eV



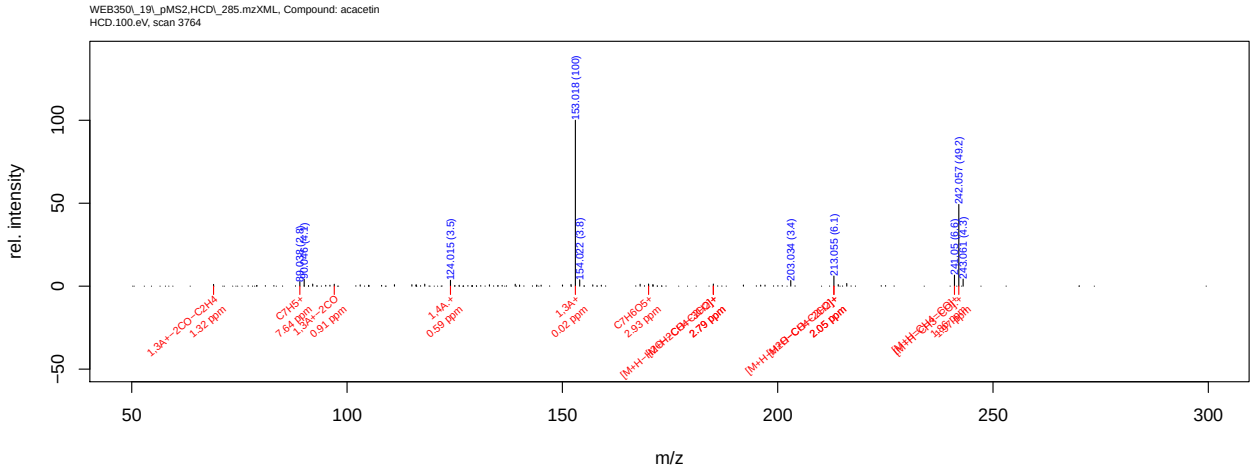
	mz	int	ppm	fragment
1	133.06	2.1	0.56	1,3B+
2	153.02	4.8	1.37	1,3A+
3	242.06	6.7	3.98	[M+H-CH3-CO].+
4	243.06	1.2	4.21	[M+H-C2H2O]+
5	270.05	100.0	3.50	[M+H-CH3].+

acacetin.HCD.75eV



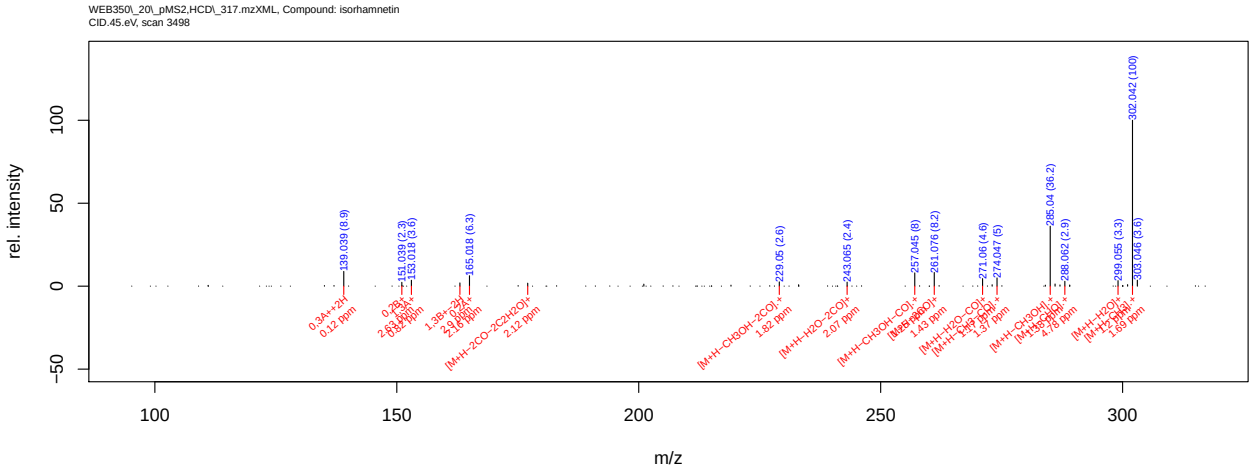
	mz	int	ppm	fragment
1	133.06	2.5	0.10	1,3B+
2	153.02	10.9	0.57	1,3A+
3	241.05	1.4	2.43	[M+H-CH4-CO]+
4	242.06	100.0	3.29	[M+H-CH3-CO].+
5	270.05	9.1	2.60	[M+H-CH3].+
6	285.08	3.6	2.91	[M+H]+

acacetin.HCD.100eV



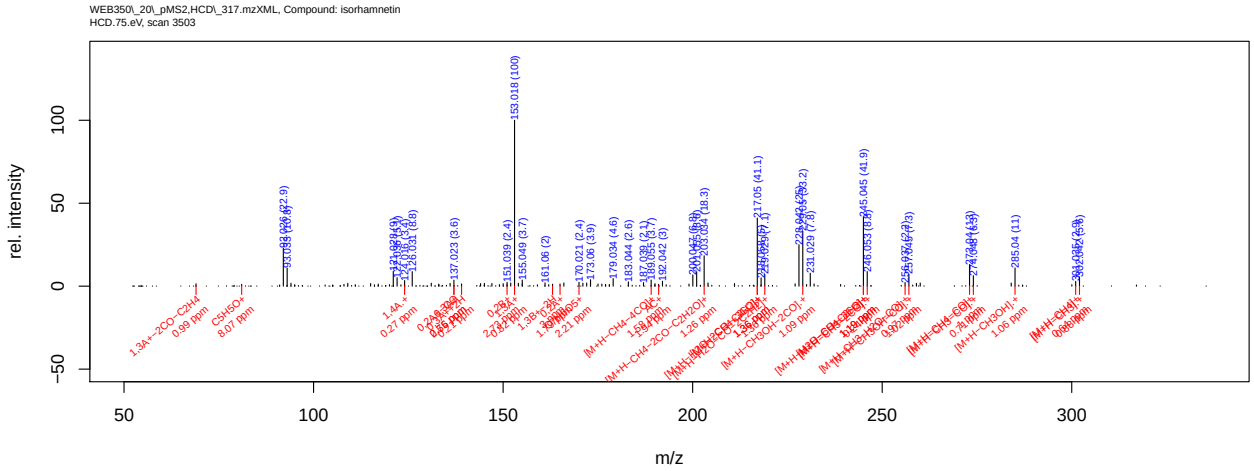
	mz	int	ppm	fragment
1	69.00	1.1	1.32	1,3A+-2CO-C2H4
2	89.04	2.8	7.64	C7H5+
3	97.03	1.2	0.91	1,3A+-2CO
4	124.02	3.5	0.59	1,4A.+
5	153.02	100.0	0.02	1,3A+
6	170.02	1.3	2.93	C7H6O5+
7	185.06	1.3	2.79	[M+H-CH4-3CO]+
8	185.06	1.3	2.79	[M+H-H2O-2CO-C2H2]+
9	213.05	6.1	2.05	[M+H-CH4-2CO]+
10	213.05	6.1	2.05	[M+H-H2O-CO-C2H2]+
11	241.05	6.6	1.86	[M+H-CH4-CO]+
12	242.06	49.2	1.97	[M+H-CH3-CO].+

isorhamnetin.CID.45eV



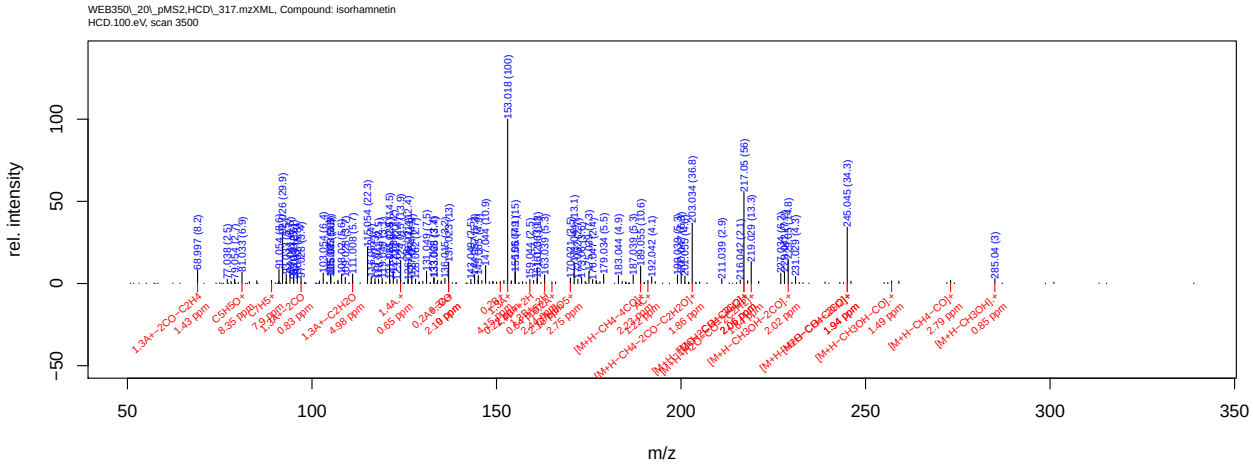
	mz	int	ppm	fragment
1	139.04	8.9	0.12	0,3A++2H
2	151.04	2.3	2.63	0,2B+
3	153.02	3.6	0.82	1,3A+
4	163.04	2.0	2.90	1,3B+-2H
5	165.02	6.3	2.16	0,2A+
6	177.05	1.8	2.12	[M+H-2CO-2C2H2O]+
7	229.05	2.6	1.82	[M+H-CH3OH-2CO].+
8	243.07	2.4	2.07	[M+H-H2O-2CO]+
9	257.04	8.0	1.25	[M+H-CH3OH-CO].+
10	261.08	8.2	1.43	[M+H-2CO]+
11	271.06	4.6	1.17	[M+H-H2O-CO]+
12	274.05	5.0	1.37	[M+H-CH3-CO].+
13	285.04	36.2	1.38	[M+H-CH3OH].+
14	288.06	2.9	4.78	[M+H-CHO].+
15	299.06	3.3	1.20	[M+H-H2O]+
16	302.04	100.0	1.69	[M+H-CH3].+

isorhamnetin.HCD.75eV



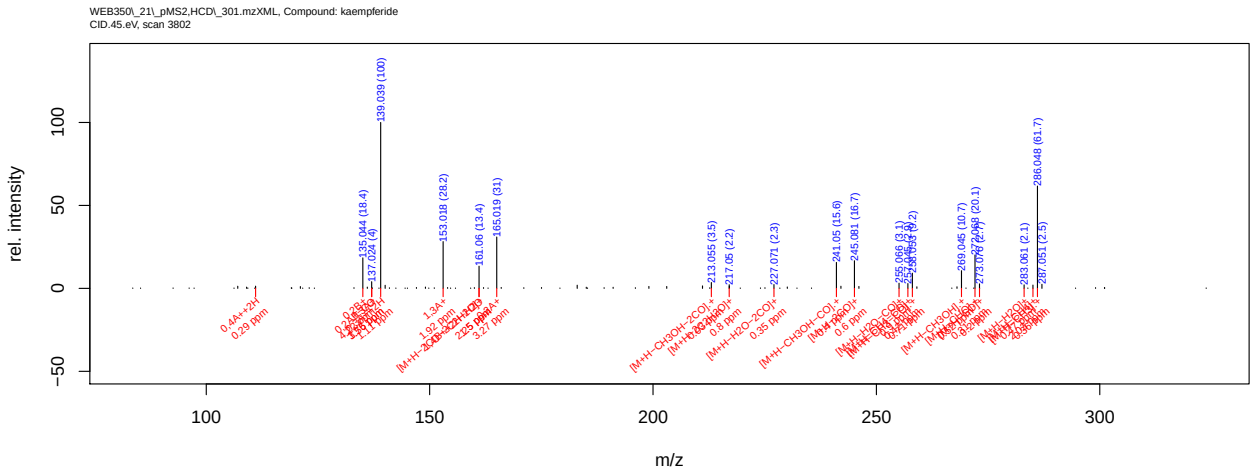
	mz	int	ppm	fragment
1	69.00	1.5	0.99	1,3A+-2CO-C2H4
2	81.03	1.1	8.07	C5H5O+
3	124.02	3.4	0.27	1,4A.+
4	137.02	3.6	2.75	0,2A+-CO
5	137.02	3.6	0.56	0,3A+
6	139.04	1.3	0.21	0,3A++2H
7	151.04	2.4	2.73	0,2B+
8	153.02	100.0	0.82	1,3A+
9	163.04	1.2	3.00	1,3B+-2H
10	165.02	1.3	1.79	0,2A+
11	170.02	2.4	2.21	C7H6O5+
12	189.05	3.7	1.58	[M+H-CH4-4CO]+
13	191.03	1.1	1.94	AC+
14	203.03	18.3	1.26	[M+H-CH4-2CO-C2H2O]+
15	217.05	41.1	1.36	[M+H-CH4-3CO]+
16	217.05	41.1	1.36	[M+H-H2O-2CO-C2H2]+
17	219.03	7.1	1.36	[M+H-H2O-CO-2C2H2]+
18	229.05	33.2	1.09	[M+H-CH3OH-2CO].+
19	245.04	41.9	1.19	[M+H-CH4-2CO]+
20	245.04	41.9	1.19	[M+H-H2O-CO-C2H2]+
21	246.05	8.8	0.24	[M+H-CH3-2CO].+
22	256.04	2.2	0.97	[M+H-CH3-H2O-CO].+
23	257.04	7.3	1.02	[M+H-CH3OH-CO].+
24	273.04	13.0	1.00	[M+H-CH4-CO]+
25	274.05	6.3	0.71	[M+H-CH3-CO].+
26	285.04	11.0	1.06	[M+H-CH3OH].+
27	301.03	2.9	0.64	[M+H-CH4]+
28	302.04	5.6	0.88	[M+H-CH3].+

isorhamnetin.HCD.100eV



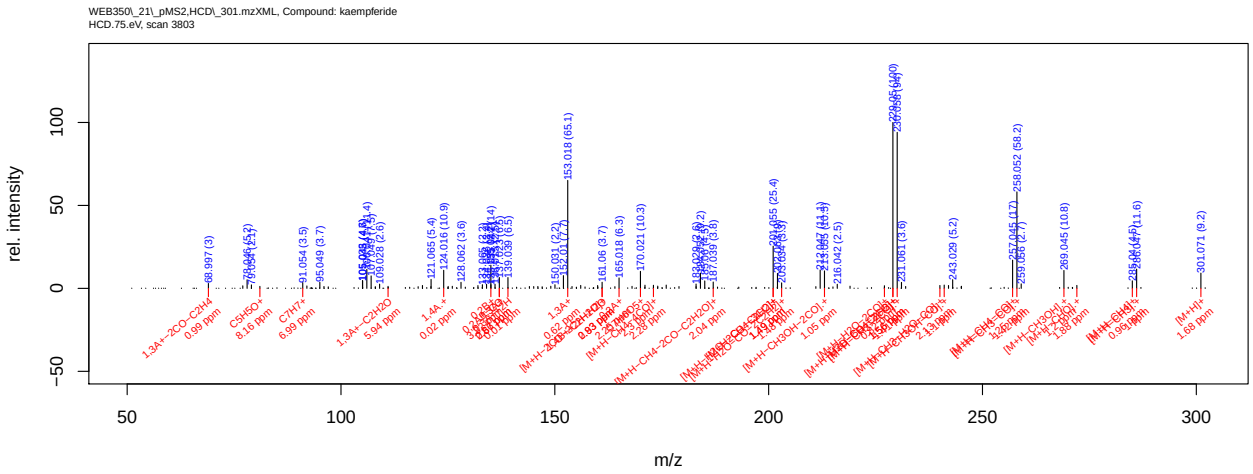
	mz	int	ppm	fragment
1	69.00	8.2	1.43	1,3A+-2CO-C2H4
2	81.03	6.9	8.35	C5H5O+
3	89.04	1.9	7.90	C7H5+
4	97.03	3.4	0.83	1,3A+-2CO
5	111.01	5.7	4.98	1,3A+-C2H2O
6	124.02	13.9	0.65	1,4A.+
7	137.02	13.0	2.19	0,2A+-CO
8	137.02	13.0	0.00	0,3A+
9	151.04	1.2	4.15	0,2B+
10	153.02	100.0	0.22	1,3A+
11	159.04	2.5	0.64	1,4B++2H
12	163.04	5.3	2.44	1,3B+-2H
13	165.02	1.0	2.16	0,2A+
14	170.02	3.5	2.75	C7H6O5+
15	189.05	10.6	2.23	[M+H-CH4-4CO]+
16	191.03	1.9	1.22	AC+
17	203.03	36.8	1.86	[M+H-CH4-2CO-C2H2O]+
18	217.05	56.0	2.06	[M+H-CH4-3CO]+
19	217.05	56.0	2.06	[M+H-H2O-2CO-C2H2]+
20	219.03	13.3	1.64	[M+H-H2O-CO-2C2H2]+
21	229.05	14.8	2.02	[M+H-CH3OH-2CO].+
22	245.04	34.3	1.94	[M+H-CH4-2CO]+
23	245.04	34.3	1.94	[M+H-H2O-CO-C2H2]+
24	257.04	1.6	1.49	[M+H-CH3OH-CO].+
25	273.04	1.9	2.79	[M+H-CH4-CO]+
26	285.04	3.0	0.85	[M+H-CH3OH].+

kaempferide.CID.45eV



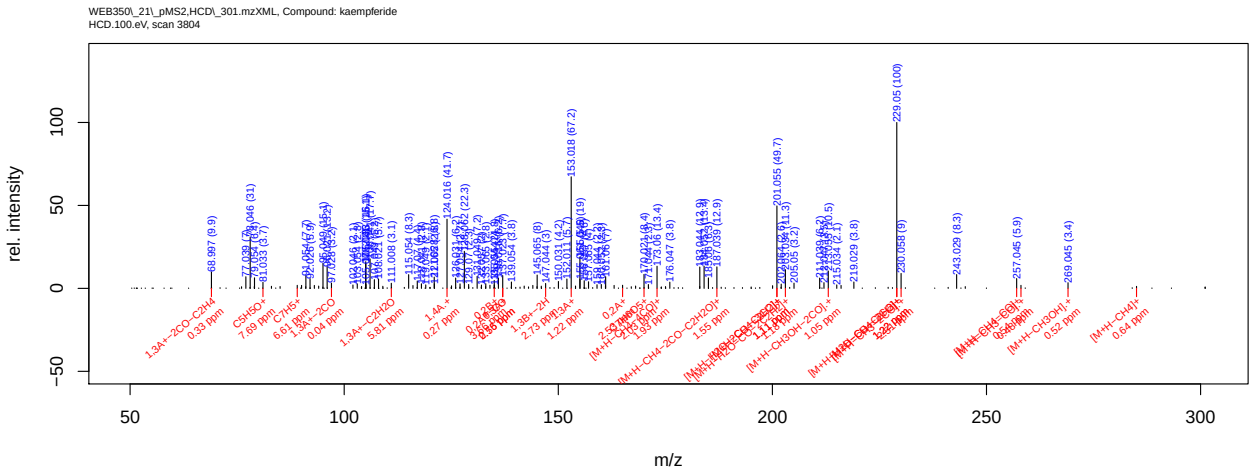
	mz	int	ppm	fragment
1	111.04	1.3	0.29	0,4A++2H
2	135.04	18.4	4.22	0,2B+
3	137.02	4.0	3.75	0,2A+-CO
4	137.02	4.0	1.56	0,3A+
5	139.04	100.0	1.11	0,3A++2H
6	153.02	28.2	1.92	1,3A+
7	161.06	13.4	2.25	1,4B++2H-H2O
8	161.06	13.4	1.50	[M+H-2CO-2C2H2O]+
9	165.02	31.0	3.27	0,2A+
10	213.06	3.5	0.03	[M+H-CH3OH-2CO].+
11	217.05	2.2	0.80	[M+H-2C2H2O]+
12	227.07	2.3	0.35	[M+H-H2O-2CO]+
13	241.05	15.6	0.40	[M+H-CH3OH-CO].+
14	245.08	16.7	0.60	[M+H-2CO]+
15	255.07	3.1	0.90	[M+H-H2O-CO]+
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	0.99	1,3A+-2CO-C2H4
2	81.03	1.2	8.16	C5H5O+
3	91.05	3.5	6.99	C7H7+
4	111.01	1.2	5.94	1,3A+-C2H2O
5	124.02	10.9	0.02	1,4A.+
6	135.04	14.0	3.32	0,2B+
7	137.02	6.5	2.86	0,2A+-CO
8	137.02	6.5	0.67	0,3A+
9	139.04	6.5	0.01	0,3A++2H
10	153.02	65.1	0.62	1,3A+
11	161.06	3.7	0.93	1,4B++2H-H2O
12	161.06	3.7	2.83	[M+H-2CO-2C2H2O]+
13	165.02	6.3	2.25	0,2A+
14	170.02	10.3	2.30	C7H6O5+
15	173.06	1.9	2.28	[M+H-CH4-4CO]+
16	187.04	3.8	2.04	[M+H-CH4-2CO-C2H2O]+
17	201.05	25.4	1.49	[M+H-CH4-3CO]+
18	201.05	25.4	1.49	[M+H-H2O-2CO-C2H2]+
19	203.03	3.3	1.48	[M+H-H2O-CO-2C2H2]+
20	213.05	10.5	1.05	[M+H-CH3OH-2CO].+
21	227.07	1.6	0.82	[M+H-H2O-2CO]+
22	229.05	100.0	1.56	[M+H-CH4-2CO]+
23	229.05	100.0	1.56	[M+H-H2O-CO-C2H2]+
24	230.06	94.0	1.41	[M+H-CH3-2CO].+
25	240.04	1.8	2.13	[M+H-CH3-H2O-CO].+
26	241.05	2.0	1.10	[M+H-CH3OH-CO].+
27	257.04	17.0	1.25	[M+H-CH4-CO]+
28	258.05	58.2	1.42	[M+H-CH3-CO].+
29	269.04	10.8	1.20	[M+H-CH3OH].+
30	272.07	1.8	1.88	[M+H-CHO].+
31	285.04	4.5	0.96	[M+H-CH4]+
32	286.05	11.6	1.00	[M+H-CH3].+
33	301.07	9.2	1.68	[M+H]+

kaempferide.HCD.100eV



	mz	int	ppm	fragment
1	69.00	9.9	0.33	1,3A+-2CO-C2H4
2	81.03	3.7	7.69	C5H5O+
3	89.04	1.8	6.61	C7H5+
4	97.03	3.2	0.04	1,3A+-2CO
5	111.01	3.1	5.81	1,3A+-C2H2O
6	124.02	41.7	0.27	1,4A.+
7	135.04	4.8	3.66	0,2B+
8	137.02	7.7	2.75	0,2A+-CO
9	137.02	7.7	0.56	0,3A+
10	147.04	3.0	2.73	1,3B+-2H
11	153.02	67.2	1.22	1,3A+
12	165.02	1.9	2.53	0,2A+
13	170.02	8.4	2.03	C7H6O5+
14	173.06	13.4	1.93	[M+H-CH4-4CO]+
15	187.04	12.9	1.55	[M+H-CH4-2CO-C2H2O]+
16	201.05	49.7	1.11	[M+H-CH4-3CO]+
17	201.05	49.7	1.11	[M+H-H2O-2CO-C2H2]+
18	203.03	11.3	1.18	[M+H-H2O-CO-2C2H2]+
19	213.05	10.5	1.05	[M+H-CH3OH-2CO].+
20	229.05	100.0	1.22	[M+H-CH4-2CO]+
21	229.05	100.0	1.22	[M+H-H2O-CO-C2H2]+
22	230.06	9.0	2.51	[M+H-CH3-2CO].+
23	257.04	5.9	0.54	[M+H-CH4-CO]+
24	258.05	1.8	0.48	[M+H-CH3-CO].+
25	269.04	3.4	0.52	[M+H-CH3OH].+
26	285.04	1.2	0.64	[M+H-CH4]+

Table 1: Fragment table for method *CID.45*

	fragment	naringenin	eriodictyol	ponciretin	hesperetin	homoeriodictyol	apigenin	luteolin	acacetin	diosmetin	chrysoeriol	kaempferol	quercetin	myricetin	kaempferide	isorhamnetin
1	$[M+H]^+$						271 (2)									
2	$[M+H-CH_3]^{\bullet+}$								270 (100)	286 (100)	286 (100)				286 (62)	302 (100)
3	$[M+H-CH_4]^+$														285 (2)	
4	$[M+H-H_2O]^+$	255 (1)	271 (18)	269 (1)	285 (10)	285 (4)	253 (1)	269 (9)				269 (32)	285 (63)	301 (40)	283 (2)	299 (3)
5	$[M+H-CO]^+$						243 (7)	259 (9)				259 (24)	275 (14)	291 (6)	273 (3)	
6	$[M+H-CHO]^{\bullet+}$						242 (14)	258 (47)				258 (46)	274 (20)	290 (22)	272 (20)	288 (3)
7	$[M+H-CH_3OH]^{\bullet+}$														269 (11)	285 (36)
8	$[M+H-2H_2O]^+$		253 (4)											283 (4)		
9	$[M+H-C_2H_2O]^+$	231 (4)	247 (3)	245 (3)	261 (2)	261 (2)	229 (21)	245 (13)	243 (1)			245 (4)				
10	$[M+H-CH_3-CO]^{\bullet+}$								242 (7)						258 (9)	274 (5)
11	$[M+H-CO_2]^+$											243 (5)				
12	$[M+H-CH_4-CO]^+$														257 (3)	
13	$[M+H-H_2O-CO]^+$						225 (13)	241 (13)				241 (99)	257 (100)	273 (100)	255 (3)	271 (5)
14	$[M+H-2CO]^+$							231 (2)				231 (40)	247 (37)	263 (25)	245 (17)	261 (8)
15	$[M+H-CH_3OH-CO]^{\bullet+}$							227 (3)							241 (16)	257 (8)
16	$[M+H-H_2O-2CO]^+$							213 (2)				213 (77)	229 (70)	245 (32)	227 (2)	243 (2)
17	$[M+H-2C_2H_2O]^+$	189 (5)	205 (3)	203 (4)	219 (2)	219 (1)	187 (3)	203 (4)				203 (7)	219 (4)	235 (4)	217 (2)	
18	$[M+H-CH_3OH-2CO]^{\bullet+}$											199 (3)	215 (2)	231 (2)	213 (4)	229 (3)
19	$[M+H-2C_2H_2O-H_2O]^+$		187 (4)		201 (1)											
20	$[M+H-CH_4-4CO]^+$		161 (2)													
21	$[M+H-2CO-2C_2H_2O]^+$											147 (13)	163 (7)	179 (7)	161 (13)	177 (2)
22	AC^+	179 (4)	179 (20)	179 (5)	179 (28)	179 (30)							191 (1)			
23	$0,2A^+$											165 (100)	165 (59)	165 (41)	165 (31)	165 (6)
24	$0,2A^+-CO$											137 (11)	137 (23)	137 (6)	137 (4)	
25	$0,2B^+$						121 (6)	137 (7)				121 (36)	137 (23)	153 (35)	135 (18)	151 (2)
26	$0,3A^+$							137 (7)				137 (11)	137 (23)	137 (6)	137 (4)	
27	$0,3A^++2H$														139 (100)	139 (9)
28	$0,4A^++2H$														111 (1)	
29	$0,4B^+$						163 (6)	179 (7)								
30	$0,4B^+-H_2O$						145 (13)									
31	$1,3A^+$	153 (100)	153 (31)	153 (77)	153 (21)	153 (57)	153 (100)	153 (100)	153 (5)			153 (61)	153 (20)	153 (35)	153 (28)	153 (4)
32	$1,3A^+-C_2H_2O$											111 (19)	111 (7)	111 (4)		
33	$1,3B^+$						119 (12)	135 (11)	133 (2)							
34	$1,3B^+-2H$											133 (25)	149 (10)	165 (41)		163 (2)
35	$1,4A^++2H$											127 (2)	127 (1)	127 (4)		
36	$1,4B^+-2H$	147 (84)	163 (100)	161 (100)	177 (100)	177 (100)										
37	$1,4B^++2H-H_2O$											147 (13)			161 (13)	
38	$1,4B^+-2H-H_2O$		145 (5)													
39	$1,4B^+-2H-CO$	119 (3)	135 (1)	133 (4)												
40	$C_7H_7^+$						91 (1)									

Table 2: Fragment table for method *HCD.75*

	fragment	naringenin	eriodictyol	ponciretin	hesperetin	homoeriodictyol	apigenin	luteolin	acacetin	diosmetin	chrysoeriol	kaempferol	quercetin	myricetin	kaempferide	isorhamnetin
1	$[M+H]^+$						271 (84)	287 (66)	285 (4)			287 (25)	303 (8)	319 (1)	301 (9)	
2	$[M+H-CH_3]^{\bullet+}$								270 (9)	286 (20)	286 (18)				286 (12)	302 (6)
3	$[M+H-CH_4]^+$				287 (1)										285 (5)	301 (3)
4	$[M+H-H_2O]^+$						253 (3)	269 (6)				269 (2)	285 (6)	301 (1)		
5	$[M+H-CO]^+$						243 (7)					259 (3)				
6	$[M+H-CHO]^{\bullet+}$						242 (1)	258 (3)				258 (10)	274 (4)		272 (2)	
7	$[M+H-CH_3OH]^{\bullet+}$														269 (11)	285 (11)
8	$[M+H-C_2H_2O]^+$						229 (4)									
9	$[M+H-CH_3-CO]^{\bullet+}$								242 (100)	258 (100)	258 (100)				258 (58)	274 (6)
10	$[M+H-CH_4-CO]^+$								241 (1)	257 (7)	257 (7)				257 (17)	273 (13)
11	$[M+H-H_2O-CO]^+$						225 (4)	241 (16)				241 (5)	257 (13)	273 (6)		
12	$[M+H-2CO]^+$											231 (5)	247 (2)			
13	$[M+H-CH_3OH-CO]^{\bullet+}$														241 (2)	257 (7)
14	$[M+H-CH_3-H_2O-CO]^{\bullet+}$														240 (2)	256 (2)
15	$[M+H-CH_3-2CO]^{\bullet+}$											216 (2)	232 (2)		230 (94)	246 (9)
16	$[M+H-H_2O-CO-C_2H_2]^+$									229 (12)	229 (13)				229 (100)	245 (42)
17	$[M+H-CH_4-2CO]^+$									229 (12)	229 (13)				229 (100)	245 (42)
18	$[M+H-H_2O-2CO]^+$						197 (4)	213 (7)				213 (20)	229 (49)	245 (22)	227 (2)	
19	$[M+H-3CO]^+$											203 (2)		235 (2)		
20	$[M+H-2C_2H_2O]^+$						187 (2)	203 (2)					219 (1)			
21	$[M+H-CH_3OH-2CO]^{\bullet+}$							199 (1)						231 (1)	213 (11)	229 (33)
22	$[M+H-H_2O-CO-2C_2H_2]^+$														203 (3)	219 (7)
23	$[M+H-H_2O-2CO-C_2H_2]^+$												203 (3)	219 (8)	201 (25)	217 (41)
24	$[M+H-CH_4-3CO]^+$												203 (3)	219 (8)	201 (25)	217 (41)
25	$[M+H-CH_4-2CO-C_2H_2O]^+$														187 (4)	203 (18)
26	$[M+H-CH_4-4CO]^+$													191 (2)	173 (2)	189 (4)
27	$[M+H-2CO-2C_2H_2O]^+$						131 (2)	147 (1)				147 (9)	163 (7)	179 (9)	161 (4)	
28	AC^+		179 (1)		179 (2)	179 (2)							191 (2)	191 (2)		191 (1)
29	$0,2A^+$											165 (11)	165 (9)	165 (6)	165 (6)	165 (1)
30	$0,2A^+-CO$											137 (14)	137 (47)	137 (15)	137 (7)	137 (4)
31	$0,2B^+$						121 (16)	137 (12)					137 (47)	153 (100)	135 (14)	151 (2)
32	$0,3A^+$							137 (12)				137 (14)	137 (47)	137 (15)	137 (7)	137 (4)
33	$0,3A^++2H$													139 (3)	139 (7)	139 (1)
34	$0,4A^++2H$					111 (2)										
35	$0,4B^+$						163 (8)	179 (3)								
36	$0,4B^+-H_2O$						145 (17)	161 (16)								
37	$1,3A^+$	153 (100)	153 (100)	153 (100)	153 (100)	153 (100)	153 (100)	153 (100)	153 (11)	153 (8)	153 (8)		153 (100)	153 (100)	153 (65)	153 (100)
38	$1,3A^+-CO$						125 (1)	125 (2)						125 (3)		
39	$1,3A^+-C_2H_2O$		111 (2)	111 (1)	111 (1)		111 (2)	111 (2)				111 (5)	111 (6)	111 (6)	111 (1)	
40	$1,3A^+-2CO$	97 (3)	97 (4)	97 (3)	97 (4)	97 (4)	97 (2)	97 (2)				97 (2)	97 (2)	97 (3)		
41	$1,3A^+-2CO-C_2H_4$	69 (2)	69 (2)	69 (2)	69 (2)	69 (2)	69 (4)	69 (5)				69 (7)	69 (8)	69 (8)	69 (3)	69 (1)
42	$1,3B^+$						119 (49)	135 (40)	133 (3)							
43	$1,3B^+-2H$											133 (3)	149 (3)	165 (6)		163 (1)
44	$1,4A^++2H$							127 (1)				127 (1)	127 (3)	127 (2)		
45	$1,4A^{\bullet+}$													124 (2)	124 (11)	124 (3)
46	$1,4A^+$						125 (1)	125 (2)						125 (3)		
47	$1,4B^++2H$												145 (2)	161 (2)		
48	$1,4B^+-2H$	147 (15)	163 (10)	161 (10)	177 (4)	177 (2)										
49	$1,4B^++2H-H_2O$											147 (9)			161 (4)	
50	$1,4B^+-2H-H_2O$		145 (7)													
51	$1,4B^+-2H-CO$	119 (32)	135 (29)	133 (36)	149 (15)	149 (11)										
52	$1,4B^+-2H-CO-CH_3$			118 (11)	134 (11)	134 (7)										
53	$1,4B^+-2H-CO-CH_2O$			103 (6)												
54	$1,4B^+-2H-2CO$	91 (24)														
55	$1,4B^+-2H-2CO-CH_3$			90 (3)												
56	$1,4B^+-2H-C_2H_2O-H_2O$				117 (15)	117 (32)										
57	$1,4B^+-2H-H_2O-CO$		117 (18)													
58	$C_7H_6O_5^+$													170 (1)	170 (10)	170 (2)
59	$C_7H_7^+$	91 (24)		91 (1)	91 (3)	91 (2)	91 (26)					91 (2)	91 (2)	91 (2)	91 (4)	
60	$C_7H_5^+$		89 (23)		89 (29)	89 (24)		89 (17)								
61	$C_5H_5O^+$						81 (1)	81 (2)				81 (3)	81 (8)	81 (5)	81 (1)	81 (1)

Table 3: Fragment table for method *HCD.100*

	fragment	naringenin	eriodictyol	ponciretin	hesperetin	homoeriodictyol	apigenin	luteolin	acacetin	diosmetin	chrysoeriol	kaempferol	quercetin	myricetin	kaempferide	isorhamnetin
1	$[M+H]^+$						271 (2)	287 (2)								
2	$[M+H-CH_4]^+$														285 (1)	
3	$[M+H-H_2O]^+$											269 (2)	285 (3)			
4	$[M+H-CO]^+$						243 (2)									
5	$[M+H-CHO]^{\bullet+}$						242 (2)	258 (2)								
6	$[M+H-CH_3OH]^{\bullet+}$														269 (3)	285 (3)
7	$[M+H-CH_3-CO]^{\bullet+}$								242 (49)	258 (49)	258 (46)				258 (2)	
8	$[M+H-CH_4-CO]^+$								241 (7)	257 (38)	257 (37)				257 (6)	273 (2)
9	$[M+H-H_2O-CO]^+$							241 (4)				241 (1)	257 (2)			
10	$[M+H-CH_3OH-CO]^{\bullet+}$															257 (2)
11	$[M+H-CH_3-2CO]^{\bullet+}$							216 (1)				216 (2)			230 (9)	
12	$[M+H-H_2O-CO-C_2H_2]^+$								213 (6)	229 (75)	229 (76)				229 (100)	245 (34)
13	$[M+H-CH_4-2CO]^+$								213 (6)	229 (75)	229 (76)				229 (100)	245 (34)
14	$[M+H-H_2O-2CO]^+$						197 (3)	213 (4)				213 (12)	229 (16)	245 (6)		
15	$[M+H-2C_2H_2O]^+$						187 (1)	203 (3)				203 (1)	219 (2)			
16	$[M+H-CH_3OH-2CO]^{\bullet+}$									213 (4)	213 (4)				213 (10)	229 (15)
17	$[M+H-H_2O-CO-2C_2H_2]^+$									203 (29)	203 (31)				203 (11)	219 (13)
18	$[M+H-H_2O-2CO-C_2H_2]^+$							187 (2)	185 (1)	201 (7)	201 (6)	187 (2)	203 (10)	219 (21)	201 (50)	217 (56)
19	$[M+H-CH_4-3CO]^+$							187 (2)	185 (1)	201 (7)	201 (6)	187 (2)	203 (10)	219 (21)	201 (50)	217 (56)
20	$[M+H-2C_2H_2O-H_2O]^+$						169 (2)	185 (2)								
21	$[M+H-CH_4-2CO-C_2H_2O]^+$									187 (6)	187 (5)				187 (13)	203 (37)
22	$[M+H-CH_4-4CO]^+$						143 (1)			173 (3)	173 (2)	159 (1)	175 (1)	191 (2)	173 (13)	189 (11)
23	$[M+H-2CO-2C_2H_2O]^+$						131 (5)	147 (3)		161 (4)	161 (5)	147 (8)	163 (5)	179 (9)		
24	AC^+				179 (2)	179 (1)								191 (2)		191 (2)
25	$0,2A^+$											165 (2)	165 (3)	165 (4)	165 (2)	165 (1)
26	$0,2A^+-CO$											137 (12)	137 (38)	137 (32)	137 (8)	137 (13)
27	$0,2B^+$						121 (25)	137 (16)				121 (69)	137 (38)	153 (100)	135 (5)	151 (1)
28	$0,3A^+$				137 (3)	137 (2)		137 (16)		137 (1)	137 (2)	137 (12)	137 (38)	137 (32)	137 (8)	137 (13)
29	$0,3A^++2H$													139 (3)		
30	$0,4B^+$						163 (2)									
31	$0,4B^+-H_2O$						145 (41)	161 (29)								
32	$1,3A^+$	153 (69)	153 (50)	153 (100)	153 (63)	153 (58)	153 (84)	153 (87)	153 (100)	153 (100)	153 (100)	153 (100)	153 (100)	153 (100)	153 (67)	153 (100)
33	$1,3A^+-CO$	125 (1)		125 (1)	125 (1)		125 (3)	125 (2)				125 (2)	125 (1)	125 (5)		
34	$1,3A^+-C_2H_2O$	111 (2)	111 (2)	111 (4)	111 (2)	111 (2)	111 (4)	111 (3)		111 (1)	111 (1)	111 (4)	111 (5)	111 (7)	111 (3)	111 (6)
35	$1,3A^+-2CO$	97 (10)	97 (8)	97 (15)	97 (9)	97 (9)	97 (9)	97 (9)	97 (1)	97 (2)	97 (2)	97 (9)	97 (10)	97 (14)	97 (3)	97 (3)
36	$1,3A^+-2CO-C_2H_4$	69 (9)	69 (8)	69 (13)	69 (9)	69 (8)	69 (24)	69 (22)	69 (1)	69 (2)	69 (2)	69 (33)	69 (31)	69 (29)	69 (10)	69 (8)
37	$1,3B^+$						119 (35)									
38	$1,3B^+-2H$											133 (1)	149 (4)	165 (4)	147 (3)	163 (5)
39	$1,4A^++2H$							127 (2)				127 (2)	127 (6)	127 (4)		
40	$1,4A^{\bullet+}$							124 (2)	124 (4)	124 (4)	124 (5)	124 (1)	124 (3)	124 (15)	124 (42)	124 (14)
41	$1,4A^+$	125 (1)		125 (1)	125 (1)		125 (3)	125 (2)				125 (2)	125 (1)	125 (5)		
42	$1,4B^++2H$												145 (4)	161 (4)		159 (2)
43	$1,4B^+-2H$	147 (3)	163 (1)	161 (3)												
44	$1,4B^++2H-H_2O$											147 (8)				
45	$1,4B^+-2H-H_2O$		145 (1)													
46	$1,4B^+-2H-CO$	119 (34)	135 (16)	133 (36)	149 (5)	149 (3)										
47	$1,4B^+-2H-CO-CH_3$			118 (57)	134 (20)	134 (13)										
48	$1,4B^+-2H-CO-CH_2O$			103 (27)												
49	$1,4B^+-2H-2CO$	91 (100)														
50	$1,4B^+-2H-2CO-CH_3$			90 (49)												
51	$1,4B^+-2H-C_2H_2O-H_2O$				117 (13)	117 (26)										
52	$1,4B^+-2H-H_2O-CO$		117 (21)													
53	$C_7H_6O_5^+$								170 (1)	170 (1)	170 (1)			170 (3)	170 (8)	170 (3)
54	$C_7H_7^+$	91 (100)		91 (5)	91 (7)	91 (5)										
55	$C_7H_5^+$		89 (100)	89 (22)	89 (100)	89 (100)	89 (7)	89 (100)	89 (3)		89 (1)	89 (6)	89 (9)	89 (7)	89 (2)	89 (2)
56	$C_5H_5O^+$	81 (1)	81 (1)	81 (1)	81 (2)	81 (1)	81 (3)	81 (8)				81 (12)	81 (39)	81 (24)	81 (4)	81 (7)

Table 4: Fragment table for type *flavanon*

	fragment	naringenin_CID.45	eriodictyol_CID.45	ponciretin_CID.45	hesperetin_CID.45	homoeriodictyol_CID.45	naringenin_HCD.75	eriodictyol_HCD.75	ponciretin_HCD.75	hesperetin_HCD.75	homoeriodictyol_HCD.75	naringenin_HCD.100	eriodictyol_HCD.100	ponciretin_HCD.100	hesperetin_HCD.100	homoeriodictyol_HCD.100
1	$[M+H-CH_4]^+$									287 (1)						
2	$[M+H-H_2O]^+$	255 (1)	271 (18)	269 (1)	285 (10)	285 (4)										
3	$[M+H-2H_2O]^+$		253 (4)													
4	$[M+H-C_2H_2O]^+$	231 (4)	247 (3)	245 (3)	261 (2)	261 (2)										
5	$[M+H-2C_2H_2O]^+$	189 (5)	205 (3)	203 (4)	219 (2)	219 (1)										
6	$[M+H-2C_2H_2O-H_2O]^+$		187 (4)		201 (1)											
7	$[M+H-CH_4-4CO]^+$		161 (2)													
8	AC^+	179 (4)	179 (20)	179 (5)	179 (28)	179 (30)		179 (1)		179 (2)	179 (2)				179 (2)	179 (1)
9	$0,3A^+$														137 (3)	137 (2)
10	$0,4A^+ + 2H$										111 (2)					
11	$1,3A^+$	153 (100)	153 (31)	153 (77)	153 (21)	153 (57)	153 (100)	153 (100)	153 (100)	153 (100)	153 (100)	153 (69)	153 (50)	153 (100)	153 (63)	153 (58)
12	$1,3A^+ - CO$											125 (1)		125 (1)	125 (1)	
13	$1,3A^+ - C_2H_2O$							111 (2)	111 (1)	111 (1)		111 (2)	111 (2)	111 (4)	111 (2)	111 (2)
14	$1,3A^+ - 2CO$						97 (3)	97 (4)	97 (3)	97 (4)	97 (4)	97 (10)	97 (8)	97 (15)	97 (9)	97 (9)
15	$1,3A^+ - 2CO - C_2H_4$						69 (2)	69 (2)	69 (2)	69 (2)	69 (2)	69 (9)	69 (8)	69 (13)	69 (9)	69 (8)
16	$1,4A^+$											125 (1)		125 (1)	125 (1)	
17	$1,4B^+ - 2H$	147 (84)	163 (100)	161 (100)	177 (100)	177 (100)	147 (15)	163 (10)	161 (10)	177 (4)	177 (2)	147 (3)	163 (1)	161 (3)		
18	$1,4B^+ - 2H - H_2O$		145 (5)					145 (7)					145 (1)			
19	$1,4B^+ - 2H - CO$	119 (3)	135 (1)	133 (4)			119 (32)	135 (29)	133 (36)	149 (15)	149 (11)	119 (34)	135 (16)	133 (36)	149 (5)	149 (3)
20	$1,4B^+ - 2H - CO - CH_3$								118 (11)	134 (11)	134 (7)			118 (57)	134 (20)	134 (13)
21	$1,4B^+ - 2H - CO - CH_2O$								103 (6)					103 (27)		
22	$1,4B^+ - 2H - 2CO$						91 (24)					91 (100)				
23	$1,4B^+ - 2H - 2CO - CH_3$								90 (3)					90 (49)		
24	$1,4B^+ - 2H - C_2H_2O - H_2O$									117 (15)	117 (32)				117 (13)	117 (26)
25	$1,4B^+ - 2H - H_2O - CO$							117 (18)					117 (21)			
26	$C_7H_7^+$						91 (24)		91 (1)	91 (3)	91 (2)	91 (100)		91 (5)	91 (7)	91 (5)
27	$C_7H_5^+$							89 (23)		89 (29)	89 (24)		89 (100)	89 (22)	89 (100)	89 (100)
28	$C_5H_5O^+$											81 (1)	81 (1)	81 (1)	81 (2)	81 (1)

Table 5: Fragment table for type *flavone*

	fragment	apigenin_CID.45	luteolin_CID.45	acacetin_CID.45	diosmetin_CID.45	chrysoeriol_CID.45	apigenin_HCD.75	luteolin_HCD.75	acacetin_HCD.75	diosmetin_HCD.75	chrysoeriol_HCD.75	apigenin_HCD.100	luteolin_HCD.100	acacetin_HCD.100	diosmetin_HCD.100	chrysoeriol_HCD.100
1	$[M+H]^+$	271 (2)					271 (84)	287 (66)	285 (4)			271 (2)	287 (2)			
2	$[M+H-CH_3]^{\bullet+}$			270 (100)	286 (100)	286 (100)			270 (9)	286 (20)	286 (18)					
3	$[M+H-H_2O]^+$	253 (1)	269 (9)				253 (3)	269 (6)								
4	$[M+H-CO]^+$	243 (7)	259 (9)				243 (7)					243 (2)				
5	$[M+H-CHO]^{\bullet+}$	242 (14)	258 (47)				242 (1)	258 (3)				242 (2)	258 (2)			
6	$[M+H-C_2H_2O]^+$	229 (21)	245 (13)	243 (1)			229 (4)									
7	$[M+H-CH_3-CO]^{\bullet+}$			242 (7)					242 (100)	258 (100)	258 (100)			242 (49)	258 (49)	258 (46)
8	$[M+H-CH_4-CO]^+$								241 (1)	257 (7)	257 (7)			241 (7)	257 (38)	257 (37)
9	$[M+H-H_2O-CO]^+$	225 (13)	241 (13)				225 (4)	241 (16)					241 (4)			
10	$[M+H-2CO]^+$		231 (2)													
11	$[M+H-CH_3OH-CO]^{\bullet+}$		227 (3)													
12	$[M+H-CH_3-2CO]^{\bullet+}$												216 (1)			
13	$[M+H-H_2O-CO-C_2H_2]^+$									229 (12)	229 (13)			213 (6)	229 (75)	229 (76)
14	$[M+H-CH_4-2CO]^+$									229 (12)	229 (13)			213 (6)	229 (75)	229 (76)
15	$[M+H-H_2O-2CO]^+$		213 (2)				197 (4)	213 (7)				197 (3)	213 (4)			
16	$[M+H-2C_2H_2O]^+$	187 (3)	203 (4)				187 (2)	203 (2)				187 (1)	203 (3)			
17	$[M+H-CH_3OH-2CO]^{\bullet+}$							199 (1)							213 (4)	213 (4)
18	$[M+H-H_2O-CO-2C_2H_2]^+$														203 (29)	203 (31)
19	$[M+H-H_2O-2CO-C_2H_2]^+$												187 (2)	185 (1)	201 (7)	201 (6)
20	$[M+H-CH_4-3CO]^+$												187 (2)	185 (1)	201 (7)	201 (6)
21	$[M+H-2C_2H_2O-H_2O]^+$											169 (2)	185 (2)			
22	$[M+H-CH_4-2CO-C_2H_2O]^+$														187 (6)	187 (5)
23	$[M+H-CH_4-4CO]^+$											143 (1)			173 (3)	173 (2)
24	$[M+H-2CO-2C_2H_2O]^+$						131 (2)	147 (1)				131 (5)	147 (3)		161 (4)	161 (5)
25	$0,2B^+$	121 (6)	137 (7)				121 (16)	137 (12)				121 (25)	137 (16)			
26	$0,3A^+$		137 (7)					137 (12)					137 (16)		137 (1)	137 (2)
27	$0,4B^+$	163 (6)	179 (7)				163 (8)	179 (3)				163 (2)				
28	$0,4B^+-H_2O$	145 (13)					145 (17)	161 (16)				145 (41)	161 (29)			
29	$1,3A^+$	153 (100)	153 (100)	153 (5)			153 (100)	153 (100)	153 (11)	153 (8)	153 (8)	153 (84)	153 (87)	153 (100)	153 (100)	153 (100)
30	$1,3A^+-CO$						125 (1)	125 (2)				125 (3)	125 (2)			
31	$1,3A^+-C_2H_2O$						111 (2)	111 (2)				111 (4)	111 (3)		111 (1)	111 (1)
32	$1,3A^+-2CO$						97 (2)	97 (2)				97 (9)	97 (9)	97 (1)	97 (2)	97 (2)
33	$1,3A^+-2CO-C_2H_4$						69 (4)	69 (5)				69 (24)	69 (22)	69 (1)	69 (2)	69 (2)
34	$1,3B^+$	119 (12)	135 (11)	133 (2)			119 (49)	135 (40)	133 (3)			119 (35)				
35	$1,4A^++2H$							127 (1)					127 (2)			
36	$1,4A^{\bullet+}$												124 (2)	124 (4)	124 (4)	124 (5)
37	$1,4A^+$						125 (1)	125 (2)				125 (3)	125 (2)			
38	$C_7H_6O_5^+$													170 (1)	170 (1)	170 (1)
39	$C_7H_7^+$	91 (1)					91 (26)									
40	$C_7H_5^+$							89 (17)				89 (7)	89 (100)	89 (3)		89 (1)
41	$C_5H_5O^+$						81 (1)	81 (2)				81 (3)	81 (8)			

Table 6: Fragment table for type *flavonole*

	fragment	kaempferol_CID.45	quercetin_CID.45	myricetin_CID.45	kaempferide_CID.45	isorhamnetin_CID.45	kaempferol_HCD.75	quercetin_HCD.75	myricetin_HCD.75	kaempferide_HCD.75	isorhamnetin_HCD.75	kaempferol_HCD.100	quercetin_HCD.100	myricetin_HCD.100	kaempferide_HCD.100	isorhamnetin_HCD.100
1	$[M+H]^+$						287 (25)	303 (8)	319 (1)	301 (9)						
2	$[M+H-CH_3]^{\bullet+}$				286 (62)	302 (100)				286 (12)	302 (6)					
3	$[M+H-CH_4]^+$				285 (2)					285 (5)	301 (3)				285 (1)	
4	$[M+H-H_2O]^+$	269 (32)	285 (63)	301 (40)	283 (2)	299 (3)	269 (2)	285 (6)	301 (1)			269 (2)	285 (3)			
5	$[M+H-CO]^+$	259 (24)	275 (14)	291 (6)	273 (3)		259 (3)									
6	$[M+H-CHO]^{\bullet+}$	258 (46)	274 (20)	290 (22)	272 (20)	288 (3)	258 (10)	274 (4)		272 (2)						
7	$[M+H-CH_3OH]^{\bullet+}$				269 (11)	285 (36)				269 (11)	285 (11)				269 (3)	285 (3)
8	$[M+H-2H_2O]^+$			283 (4)												
9	$[M+H-C_2H_2O]^+$	245 (4)														
10	$[M+H-CH_3-CO]^{\bullet+}$				258 (9)	274 (5)				258 (58)	274 (6)				258 (2)	
11	$[M+H-CO_2]^+$	243 (5)														
12	$[M+H-CH_4-CO]^+$				257 (3)					257 (17)	273 (13)				257 (6)	273 (2)
13	$[M+H-H_2O-CO]^+$	241 (99)	257 (100)	273 (100)	255 (3)	271 (5)	241 (5)	257 (13)	273 (6)			241 (1)	257 (2)			
14	$[M+H-2CO]^+$	231 (40)	247 (37)	263 (25)	245 (17)	261 (8)	231 (5)	247 (2)								
15	$[M+H-CH_3OH-CO]^{\bullet+}$				241 (16)	257 (8)				241 (2)	257 (7)					257 (2)
16	$[M+H-CH_3-H_2O-CO]^{\bullet+}$									240 (2)	256 (2)					
17	$[M+H-CH_3-2CO]^{\bullet+}$						216 (2)	232 (2)		230 (94)	246 (9)	216 (2)			230 (9)	
18	$[M+H-H_2O-CO-C_2H_2]^+$									229 (100)	245 (42)				229 (100)	245 (34)
19	$[M+H-CH_4-2CO]^+$									229 (100)	245 (42)				229 (100)	245 (34)
20	$[M+H-H_2O-2CO]^+$	213 (77)	229 (70)	245 (32)	227 (2)	243 (2)	213 (20)	229 (49)	245 (22)	227 (2)		213 (12)	229 (16)	245 (6)		
21	$[M+H-3CO]^+$						203 (2)		235 (2)							
22	$[M+H-2C_2H_2O]^+$	203 (7)	219 (4)	235 (4)	217 (2)			219 (1)				203 (1)	219 (2)			
23	$[M+H-CH_3OH-2CO]^{\bullet+}$	199 (3)	215 (2)	231 (2)	213 (4)	229 (3)			231 (1)	213 (11)	229 (33)				213 (10)	229 (15)
24	$[M+H-H_2O-CO-2C_2H_2]^+$									203 (3)	219 (7)				203 (11)	219 (13)
25	$[M+H-H_2O-2CO-C_2H_2]^+$							203 (3)	219 (8)	201 (25)	217 (41)	187 (2)	203 (10)	219 (21)	201 (50)	217 (56)
26	$[M+H-CH_4-3CO]^+$							203 (3)	219 (8)	201 (25)	217 (41)	187 (2)	203 (10)	219 (21)	201 (50)	217 (56)
27	$[M+H-CH_4-2CO-C_2H_2O]^+$									187 (4)	203 (18)				187 (13)	203 (37)
28	$[M+H-CH_4-4CO]^+$								191 (2)	173 (2)	189 (4)	159 (1)	175 (1)	191 (2)	173 (13)	189 (11)
29	$[M+H-2CO-2C_2H_2O]^+$	147 (13)	163 (7)	179 (7)	161 (13)	177 (2)	147 (9)	163 (7)	179 (9)	161 (4)		147 (8)	163 (5)	179 (9)		
30	AC^+		191 (1)					191 (2)	191 (2)		191 (1)			191 (2)		191 (2)
31	$0,2A^+$	165 (100)	165 (59)	165 (41)	165 (31)	165 (6)	165 (11)	165 (9)	165 (6)	165 (6)	165 (1)	165 (2)	165 (3)	165 (4)	165 (2)	165 (1)
32	$0,2A^+-CO$	137 (11)	137 (23)	137 (6)	137 (4)		137 (14)	137 (47)	137 (15)	137 (7)	137 (4)	137 (12)	137 (38)	137 (32)	137 (8)	137 (13)
33	$0,2B^+$	121 (36)	137 (23)	153 (35)	135 (18)	151 (2)		137 (47)	153 (100)	135 (14)	151 (2)	121 (69)	137 (38)	153 (100)	135 (5)	151 (1)
34	$0,3A^+$	137 (11)	137 (23)	137 (6)	137 (4)		137 (14)	137 (47)	137 (15)	137 (7)	137 (4)	137 (12)	137 (38)	137 (32)	137 (8)	137 (13)
35	$0,3A^++2H$				139 (100)	139 (9)			139 (3)	139 (7)	139 (1)			139 (3)		
36	$0,4A^++2H$				111 (1)											
37	$1,3A^+$	153 (61)	153 (20)	153 (35)	153 (28)	153 (4)		153 (100)	153 (100)	153 (65)	153 (100)	153 (100)	153 (100)	153 (100)	153 (67)	153 (100)
38	$1,3A^+-CO$								125 (3)			125 (2)	125 (1)	125 (5)		
39	$1,3A^+-C_2H_2O$	111 (19)	111 (7)	111 (4)			111 (5)	111 (6)	111 (6)	111 (1)		111 (4)	111 (5)	111 (7)	111 (3)	111 (6)
40	$1,3A^+-2CO$						97 (2)	97 (2)	97 (3)			97 (9)	97 (10)	97 (14)	97 (3)	97 (3)
41	$1,3A^+-2CO-C_2H_4$						69 (7)	69 (8)	69 (8)	69 (3)	69 (1)	69 (33)	69 (31)	69 (29)	69 (10)	69 (8)
42	$1,3B^+-2H$	133 (25)	149 (10)	165 (41)		163 (2)	133 (3)	149 (3)	165 (6)		163 (1)	133 (1)	149 (4)	165 (4)	147 (3)	163 (5)
43	$1,4A^++2H$	127 (2)	127 (1)	127 (4)			127 (1)	127 (3)	127 (2)			127 (2)	127 (6)	127 (4)		
44	$1,4A^{\bullet+}$								124 (2)	124 (11)	124 (3)	124 (1)	124 (3)	124 (15)	124 (42)	124 (14)
45	$1,4A^+$								125 (3)			125 (2)	125 (1)	125 (5)		
46	$1,4B^++2H$							145 (2)	161 (2)				145 (4)	161 (4)		159 (2)
47	$1,4B^++2H-H_2O$	147 (13)			161 (13)		147 (9)			161 (4)		147 (8)				
48	$C_7H_6O_5^+$								170 (1)	170 (10)	170 (2)			170 (3)	170 (8)	170 (3)
49	$C_7H_7^+$						91 (2)	91 (2)	91 (2)	91 (4)						
50	$C_7H_5^+$											89 (6)	89 (9)	89 (7)	89 (2)	89 (2)
51	$C_5H_5O^+$						81 (3)	81 (8)	81 (5)	81 (1)	81 (1)	81 (12)	81 (39)	81 (24)	81 (4)	81 (7)