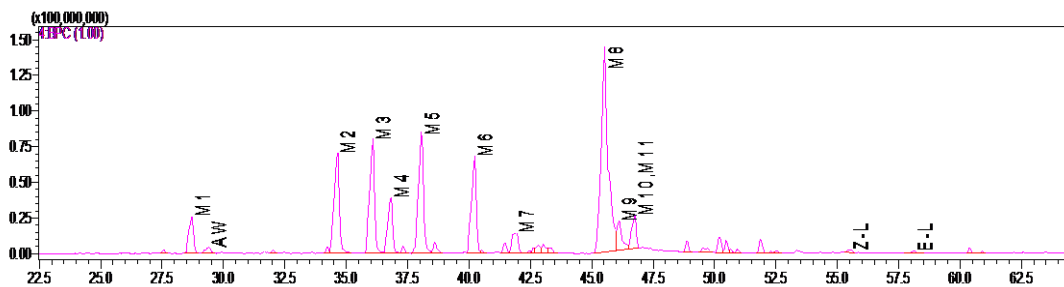


Supplementary File

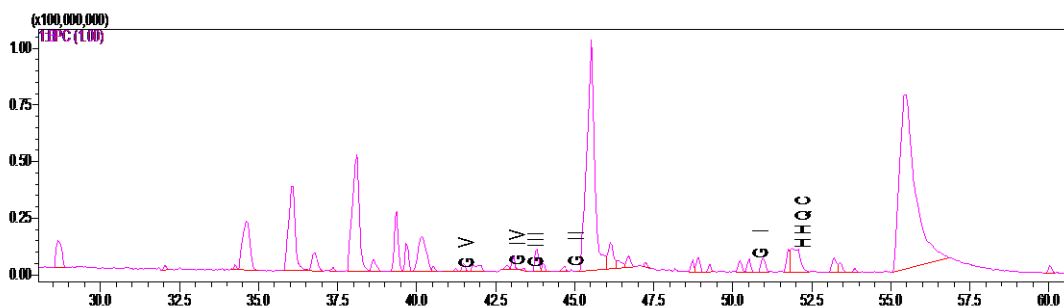
1. The HRMS data of 19 reference compounds	S2–S8
2. The HRMS data of DBT1 boiling samples	S9–S35
3. The HRMS data of DBT2 boiling samples	S36–S51
4. The HRMS data of DBT1 urine samples	S52–S66
5. The HRMS data of DBT2 urine samples	S67–S77
6. The supplemental data of tables S1–S6	S78–S87

1. The HRMS data of 19 reference compounds

In PI model.



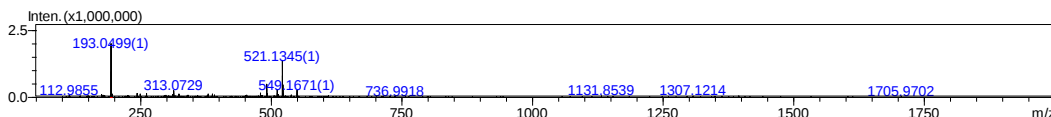
In NI model.



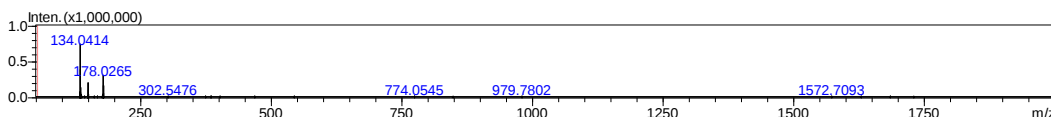
Reference compounds

D1Ferulic acid in NI mode

Event#: 4 MS(E-) Ret. Time : 29.162 Scan# : 2853



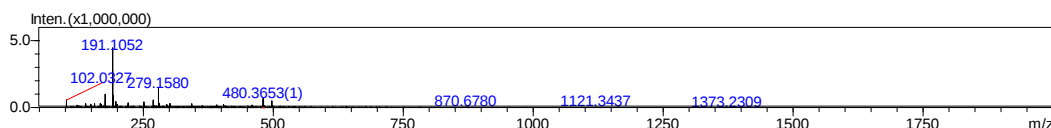
Event#: 5 MS/MS(E-) Ret. Time : 29.162 Scan# : 2854 Precursor : 193.0499 Cutoff : 53



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	65.37	C10 H10 O4	[M-H]-	193.0501	193.0506	-0.5	-2.59	68.08	6.0

D2 Z-ligustilide in PI mode

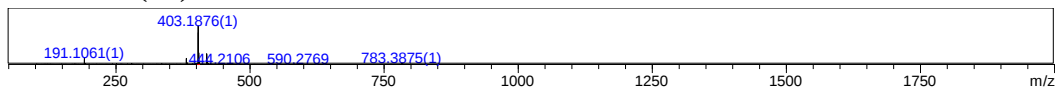
Event#: 1 MS(E+) Ret. Time : 58.102 Scan# : 5719



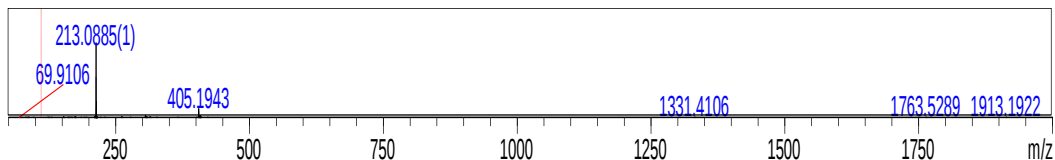
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	57.22	C12 H14 O2	[M+H]+	191.1066	191.1067	-0.1	-0.52	57.22	6.0

E-L

Event#: 1 MS(E+) Ret. Time : 62.323 Scan# : 6138



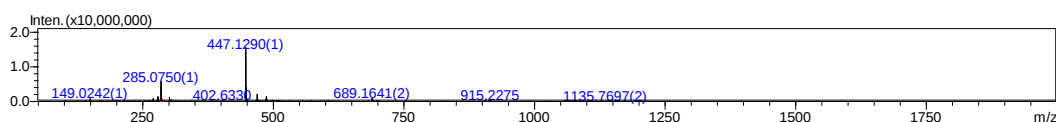
Event#: 2 MS/MS(E+) Ret. Time : 62.323 Scan# : 6138 Precursor : 403.1876 Cutoff : 111



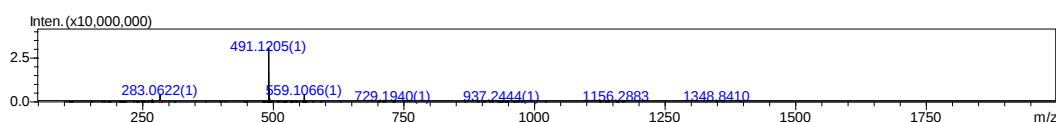
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	52.67	C12 H14 O2	[M+H] ⁺	191.1061	191.1067	-0.6	-3.14	55.64	6.0

D3 Calycosin-7-O- β -D-glucopyranoside

Event#: 1 MS(E+) Ret. Time : 28.595 Scan# : 2794



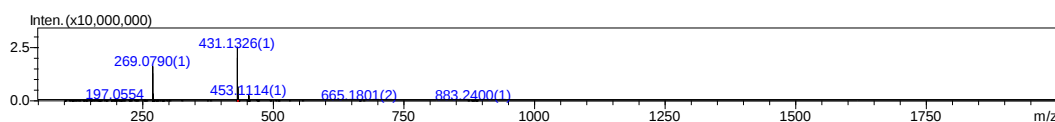
Event#: 4 MS(E-) Ret. Time : 28.595 Scan# : 2797



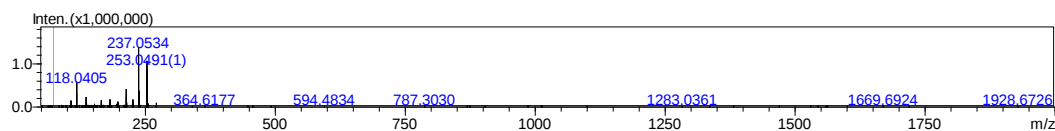
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	93.45	C22 H22 O10	[M+H] ⁺	447.1290	447.1286	0.4	0.89	93.45	12.0

D4 ononin

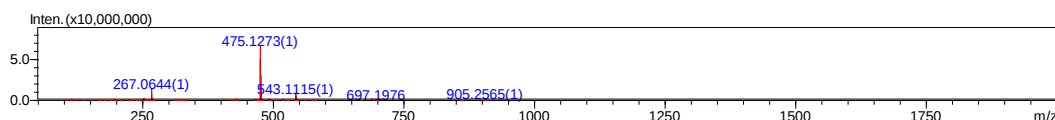
Event#: 1 MS(E+) Ret. Time : 34.545 Scan# : 3382



Event#: 2 MS/MS(E+) Ret. Time : 34.665 Scan# : 3395 Precursor : 269.0803 Cutoff : 74



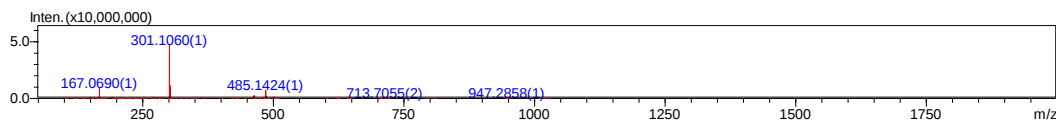
Event#: 4 MS(E-) Ret. Time : 34.545 Scan# : 3385



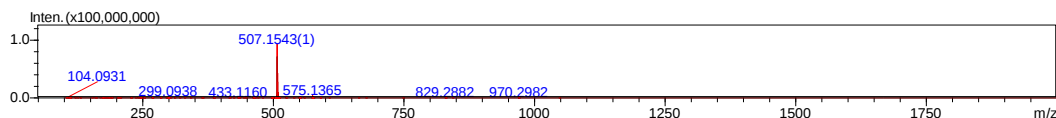
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	93.09	C22 H22 O9	[M+H] ⁺	431.1326	431.1337	-1.1	-2.55	96.84	12.0

D5 astrapterocarpan-7-O- β -D-glucopyranoside

Event#: 1 MS(E+) Ret. Time : 36.038 Scan# : 3530



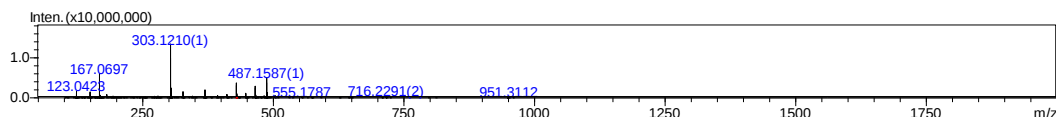
Event#: 4 MS(E-) Ret. Time : 36.038 Scan# : 3533



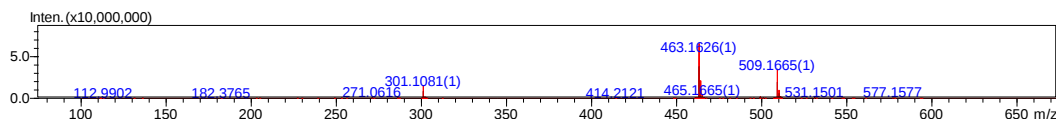
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	81.60	C ₂₃ H ₂₆ O ₁₀	[M+Na] ⁺	485.1400	485.1418	-1.8	-3.71	87.53	11.0

D6 astraisoflavan-7-O- β -D-glucopyranoside

Event#: 1 MS(E+) Ret. Time : 36.785 Scan# : 3604



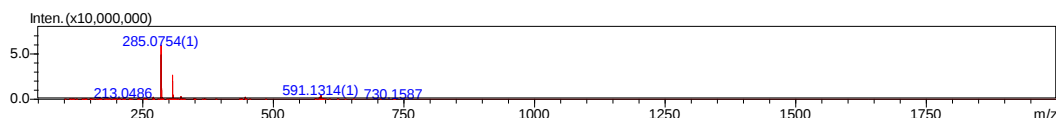
Event#: 4 MS(E-) Ret. Time : 36.785 Scan# : 3607



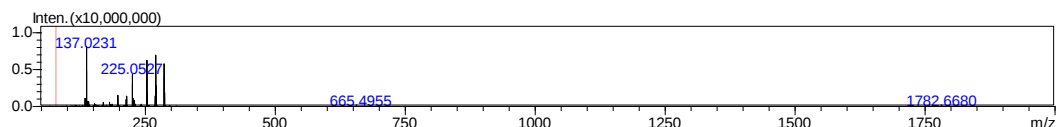
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	87.96	C ₂₃ H ₂₈ O ₁₀	[M+Na] ⁺	487.1574	487.1575	-0.1	-0.21	87.96	10.0

D7 calycosin

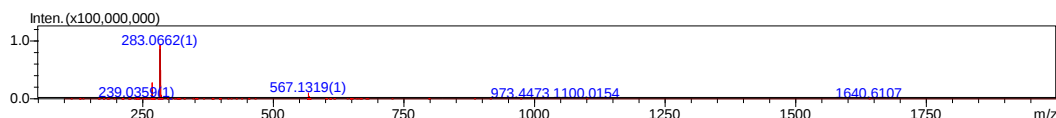
Event#: 1 MS(E+) Ret. Time : 38.055 Scan# : 3730



Event#: 2 MS/MS(E+) Ret. Time : 38.055 Scan# : 3731 Precursor : 285.0754 Cutoff : 78



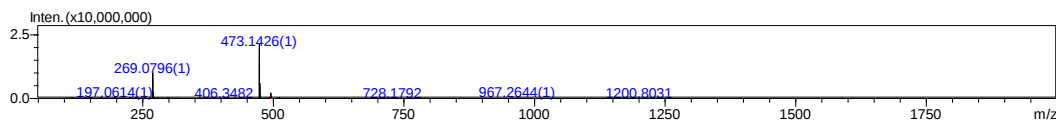
Event#: 4 MS(E-) Ret. Time : 38.055 Scan# : 3733



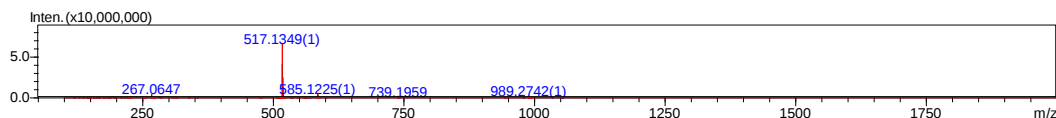
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	85.82	C ₁₆ H ₁₂ O ₅	[M+H] ⁺	285.0754	285.0758	-0.4	-1.40	86.69	11.0

D8 6"-O-acetyl-ononin

Event#: 1 MS(E+) Ret. Time : 40.123 Scan# : 3935



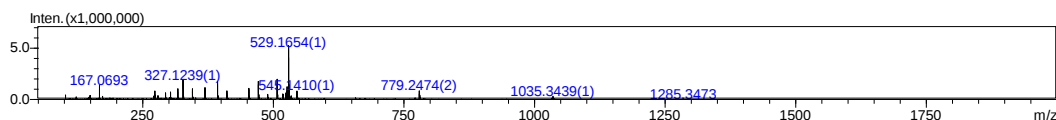
Event#: 4 MS(E-) Ret. Time : 40.123 Scan# : 3938



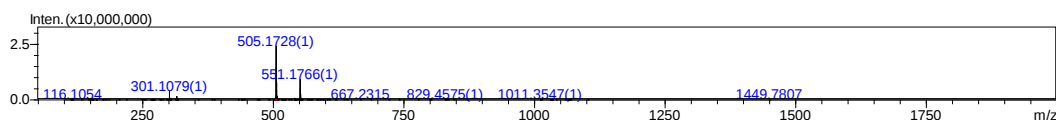
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	85.99	C ₂₄ H ₂₄ O ₁₀	[M+H] ⁺	473.1432	473.1442	-1.0	-2.11	88.44	13.0

D9 6"-O-acetyl-astraisoflavan-7-O-β-D-glucopyranoside

Event#: 1 MS(E+) Ret. Time : 41.942 Scan# : 4116



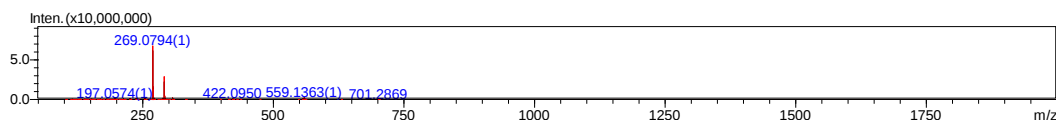
Event#: 4 MS(E-) Ret. Time : 41.942 Scan# : 4118



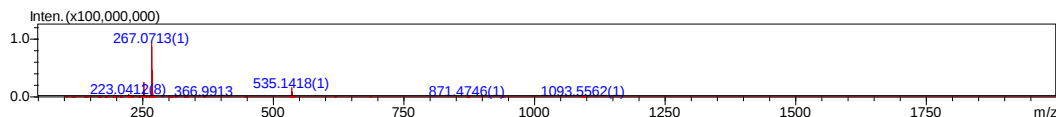
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	91.36	C ₂₅ H ₃₀ O ₁₁	[M+Na] ⁺	529.1691	529.1680	1.1	2.08	93.90	11.0

D10 formononetein

Event#: 1 MS(E+) Ret. Time : 45.410 Scan# : 4459



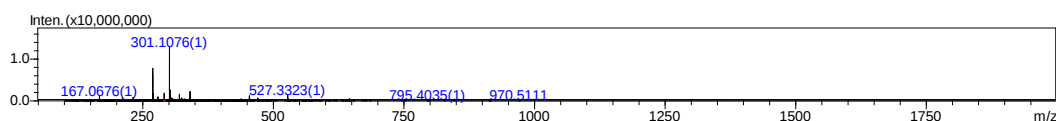
Event#: 4 MS(E-) Ret. Time : 45.410 Scan# : 4462



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	75.86	C ₁₆ H ₁₂ O ₄	[M+H] ⁺	269.0795	269.0808	-1.3	-4.83	83.89	11.0

D11 astrapterocarpan

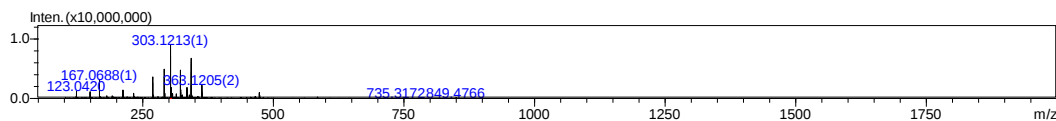
Event#: 1 MS(E+) Ret. Time : 46.062 Scan# : 4524



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	78.61	C ₁₇ H ₁₆ O ₅	[M+H] ⁺	301.1076	301.1071	0.5	1.66	79.93	10.0

D12 astraisoflavan

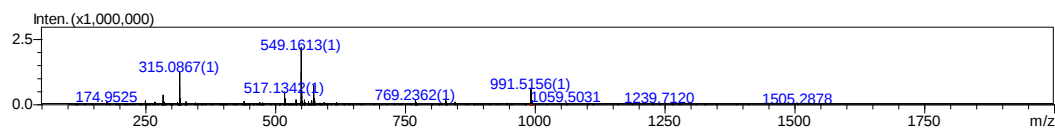
Event#: 1 MS(E+) Ret. Time : 46.655 Scan# : 4583



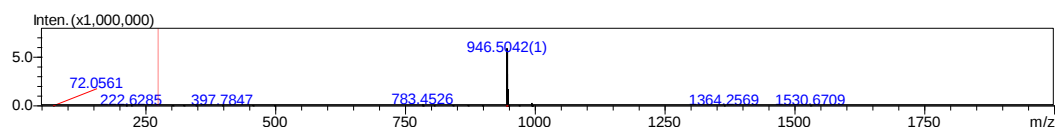
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	64.21	C17 H18 O5	[M+H] ⁺	303.1213	303.1227	-1.4	-4.62	70.60	9.0

ZG-V

Event#: 4 MS(E-) Ret. Time : 41.110 Scan# : 4036



Event#: 5 MS/MS(E-) Ret. Time : 41.110 Scan# : 4037 Precursor : 991.5156 Cutoff : 274

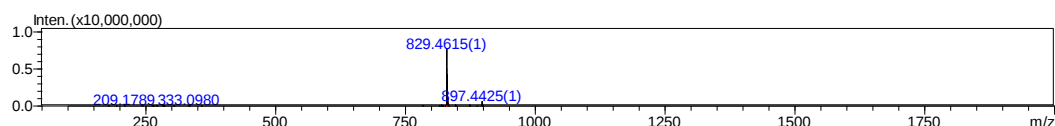


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
3	36.36	C47 H78 O19	[M+HCOO] ⁻	991.5156	991.5119	3.7	3.73	39.03	9.0

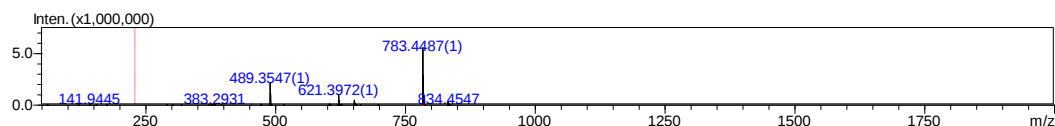
C6H10O5

ZG-IV

Event#: 4 MS(E-) Ret. Time : 42.775 Scan# : 4201



Event#: 5 MS/MS(E-) Ret. Time : 42.775 Scan# : 4202 Precursor : 829.7059 Cutoff : 229

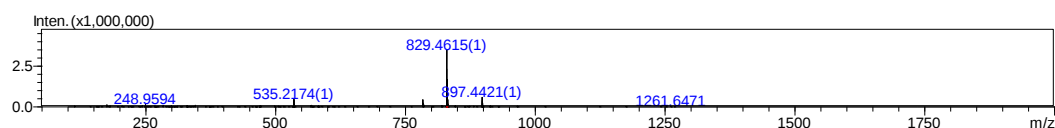


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	90.31	C42 H70 O16	[M-H] ⁻	829.4615	829.4591	2.4	2.89	94.78	8.0
2	90.31	C41 H68 O14	[M+HCOO] ⁻	829.4615	829.4591	2.4	2.89	94.78	8.0

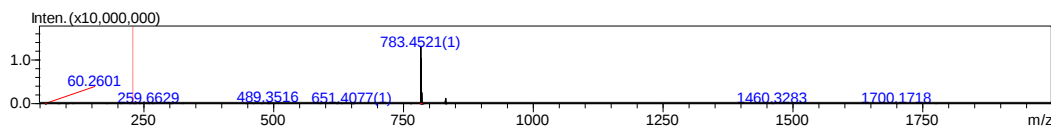
C2H2O

GIII

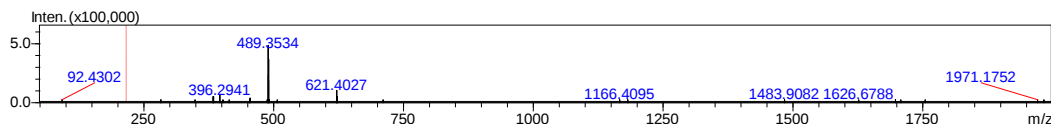
Event#: 4 MS(E-) Ret. Time : 43.410 Scan# : 4264



Event#: 5 MS/MS(E-) Ret. Time : 43.410 Scan# : 4265 Precursor : 829.4617 Cutoff : 229



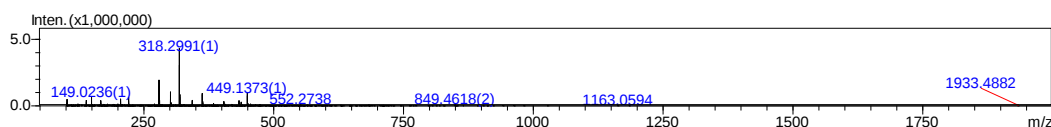
Event#: 6 MS3(E-) Ret. Time : 43.410 Scan# : 4266 Precursor : 783.4520 Cutoff : 216



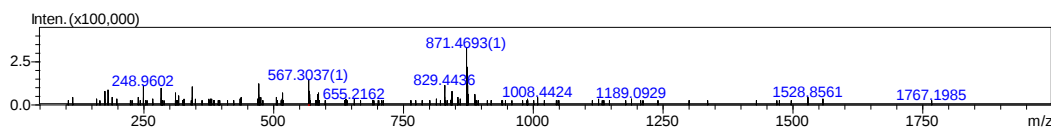
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	59.30	C42 H70 O16 [M-H]-		829.4585	829.4591	-0.6	-0.72	59.30	8.0
2	59.30	C41 H68 O14 [M+HCOO]-		829.4585	829.4591	-0.6	-0.72	59.30	8.0

ZG-II

Event#: 1 MS(E+) Ret. Time : 44.628 Scan# : 4382



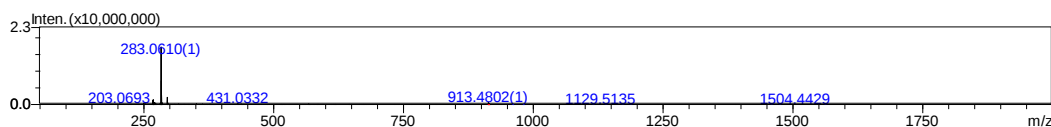
Event#: 4 MS(E-) Ret. Time : 44.628 Scan# : 4385



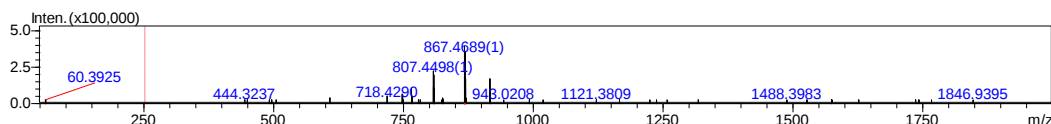
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
5	44.80	C43 H70 O15 [M+HCOO]-		871.4693	871.4697	-0.4	-0.46	44.80	9.0

ZG-I

Event#: 4 MS(E-) Ret. Time : 50.525 Scan# : 4970



Event#: 5 MS/MS(E-) Ret. Time : 50.525 Scan# : 4971 Precursor : 913.4805 Cutoff : 252

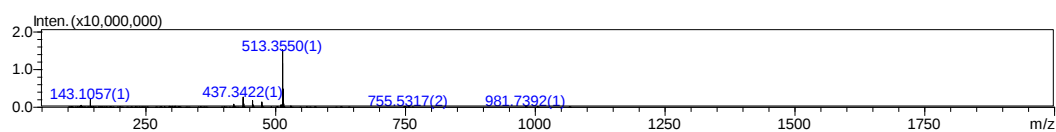


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	46.02	C45 H72 O16 [M+HCOO]-		913.4802	913.4802	0.0	0.00	46.02	10.0

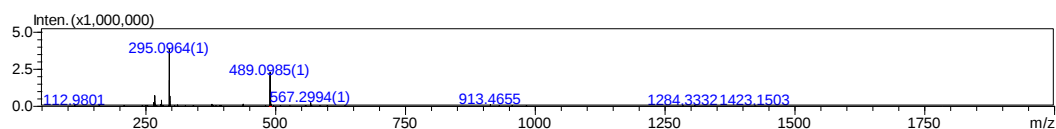
C2H2O

HHQC

Event#: 1 MS(E+) Ret. Time : 51.855 Scan# : 5099



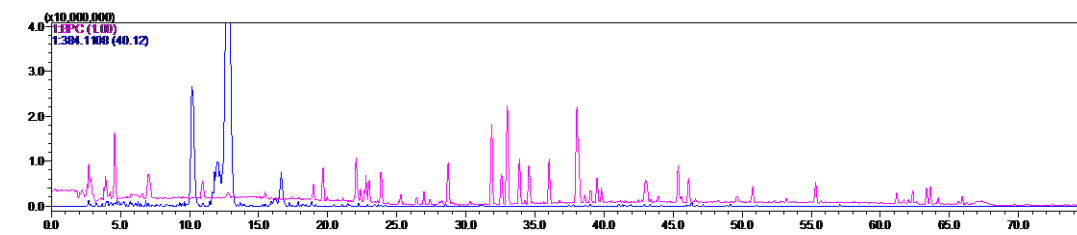
Event#: 4 MS(E-) Ret. Time : 52.482 Scan# : 5164



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	94.74	C30 H50 O5	[M+Na] ⁺	513.3550	513.3550	0.0	0.00	94.74	6.0

2. The HRMS data of DBT1 boiling samples

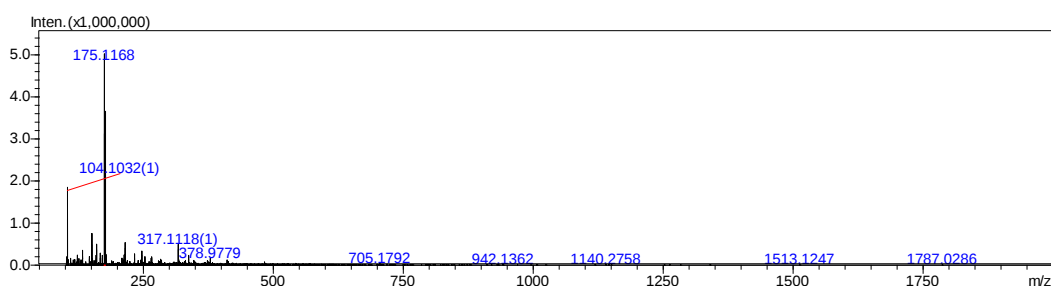
In PI and NI model.



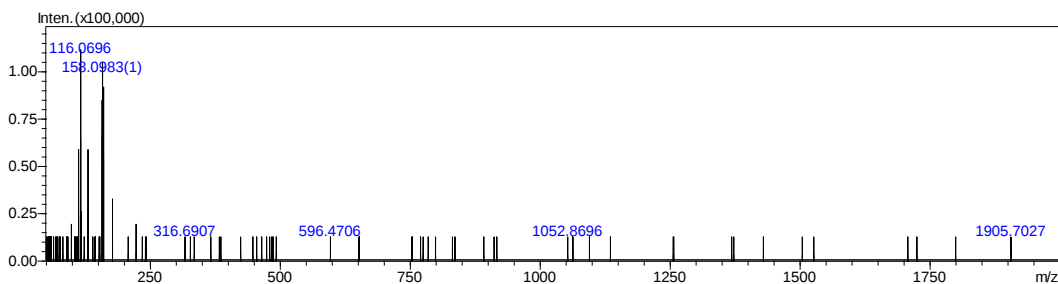
X24+A5+Z11+Y23=69

C1 A1

Event#: 1 MS(E+) Ret. Time : 2.280 -> 2.572 Scan# : 224 -> 253



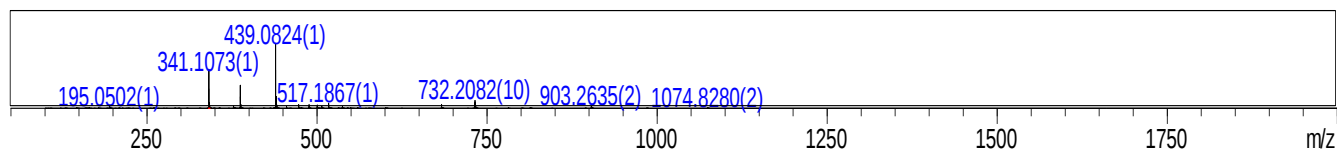
MS/MS(E+) Ret. Time : 2.280 -> 2.572 Scan# : 225 -> 254 Precursor : 175.1180 Cutoff : 48



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	18.01	C6 H14 N4 O2	[M+H] ⁺	175.1168	175.1190	-2.2	-12.56	54.29	2.0

C2 A4

Event#: 4 MS(E-) Ret. Time : 2.692 Scan# : 267

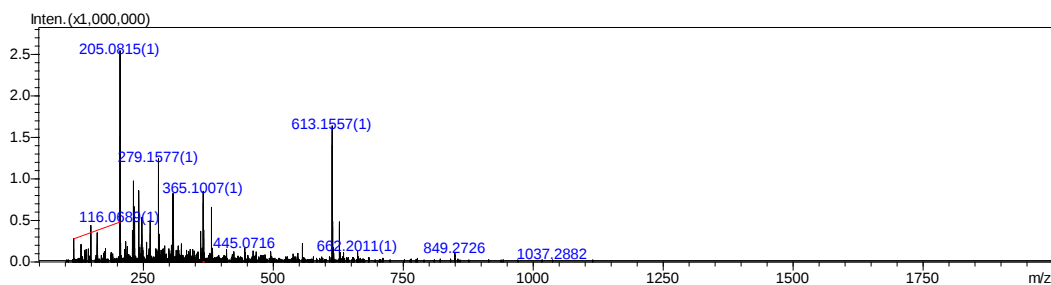


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	52.45	C6 H12 O7	[M-H] ⁻	195.0502	195.0510	-0.8	-4.10	56.86	1.0

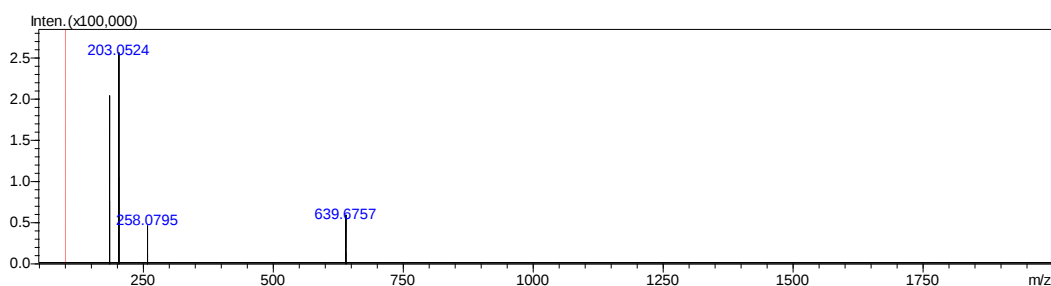
C3

T1

Event#: 1 MS(E+) Ret. Time : 3.095 Scan# : 305



MS/MS(E+) Ret. Time : 3.095 Scan# : 306 Precursor : 365.1008 Cutoff : 101

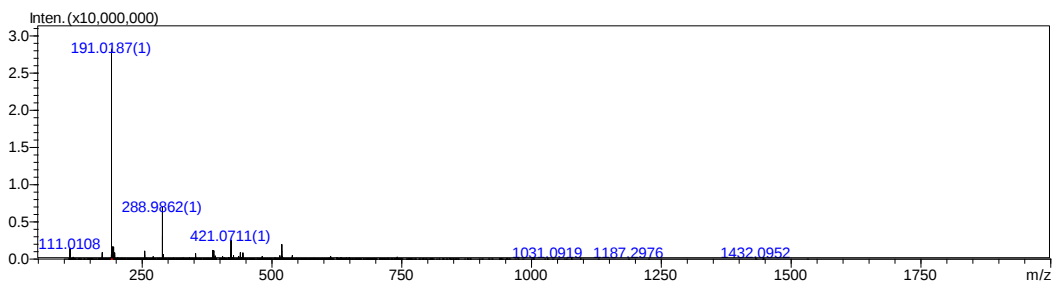


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	47.34	C21 H16 O6	[M+H] ⁺	365.1007	365.1020	-1.3	-3.56	50.58	14.0
2	46.62	C19 H18 O6	[M+Na] ⁺	365.1007	365.0996	1.1	3.01	49.09	11.0
3	17.33	C28 H12 O	[M+H] ⁺	365.1007	365.0961	4.6	12.60	52.40	23.0
4	13.68	C12 H22 O11	[M+Na] ⁺	365.1007	365.1054	-4.7	-12.87	42.30	2.0

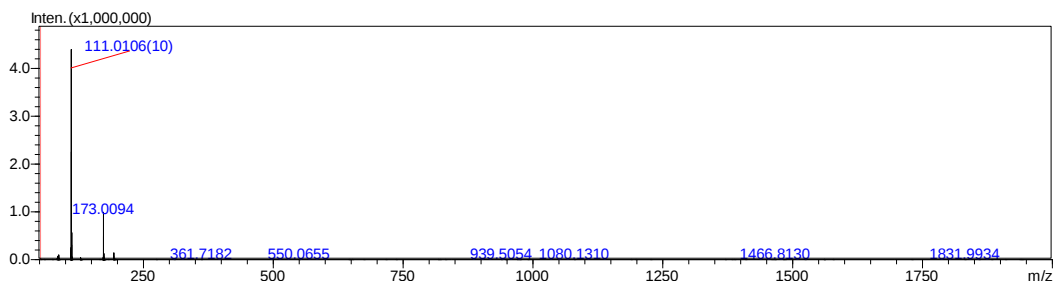
C4

A2 Citric acid

Event#: 4 MS(E-) Ret. Time : 3.682 -> 4.437 Scan# : 365 -> 440



MS/MS(E-) Ret. Time : 3.682 -> 4.437 Scan# : 366 -> 441 Precursor : 191.0181 Cutoff : 52

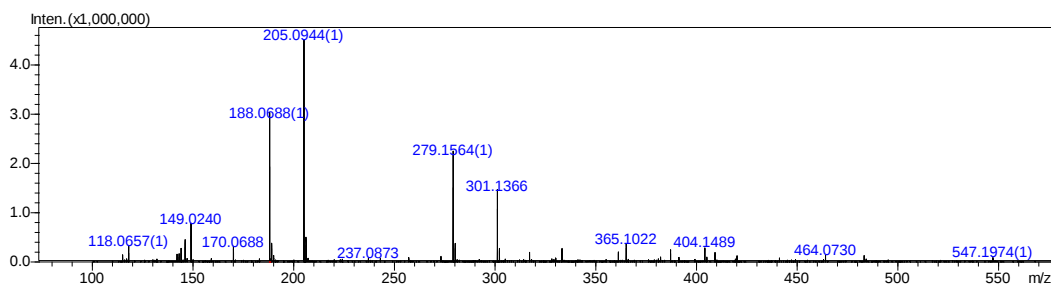


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	73.92	C6 H8 O7	[M-H] ⁻	191.0187	191.0197	-1.0	-5.24	84.39	3.0

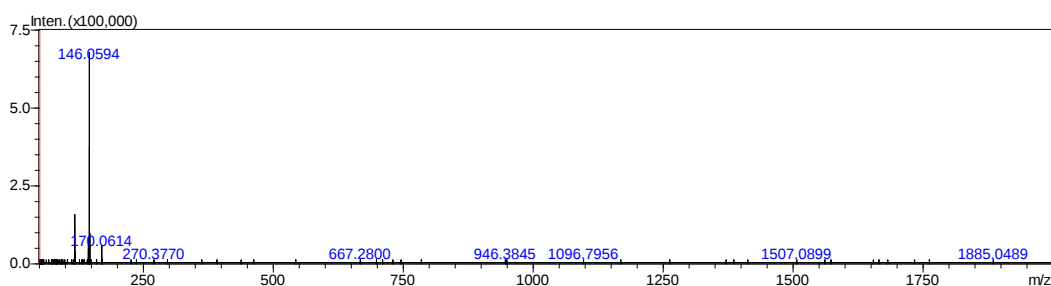
C9

A3

Event#: 1 MS(E+) Ret. Time : 10.773 -> 11.005 Scan# : 1062 -> 1085



MS/MS(E+) Ret. Time : 10.773 -> 11.005 Scan# : 1063 -> 1086 Precursor : 188.0702 Cutoff : 52

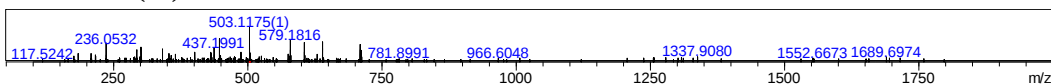


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	73.75	C9 H11 N O2	[M+Na] ⁺	188.0688	188.0682	0.6	3.19	78.02	5.0

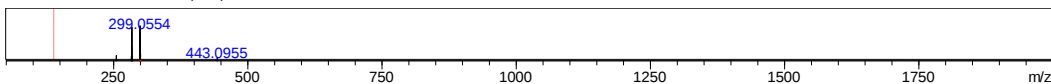
C18

Y1

Event#: 4 MS(E-) Ret. Time : 23.590 Scan# : 2321



Event#: 5 MS/MS(E-) Ret. Time : 23.590 Scan# : 2322 Precursor : 503.1172 Cutoff : 139



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	42.44	C24 H24 O12	[M-H] ⁻	503.1175	503.1195	-2.0	-3.98	45.85	13.0

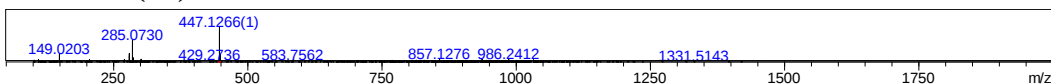
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	51.24	C16 H12 O6	[M-H] ⁻	299.0554	299.0561	-0.7	-2.34	53.02	11.0

C16H12O5

C23

Y2 calycosin-glucoside

Event#: 1 MS(E+) Ret. Time : 28.830 Scan# : 2834

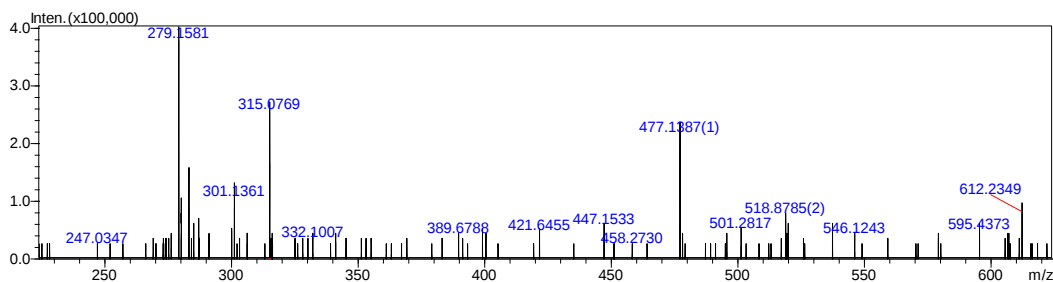


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	91.01	C22 H22 O10	[M+H] ⁺	447.1266	447.1286	-2.0	-4.47	99.66	12.0

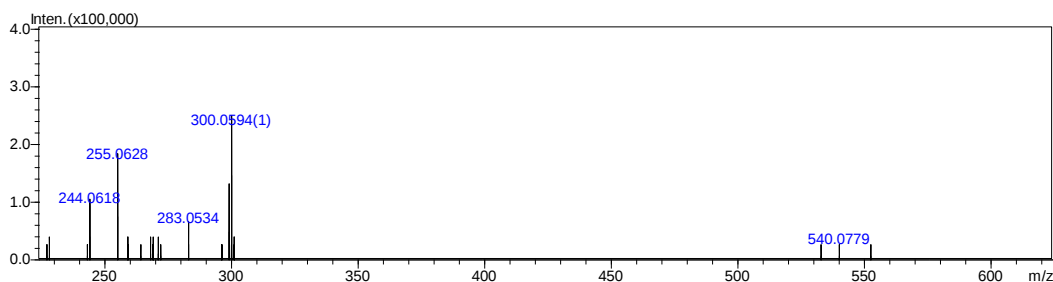
C24

Y3

Event#: 1 MS(E+) Ret. Time : 29.233 Scan# : 2874



MS/MS(E+) Ret. Time : 29.233 Scan# : 2875 Precursor : 315.0768 Cutoff : 87

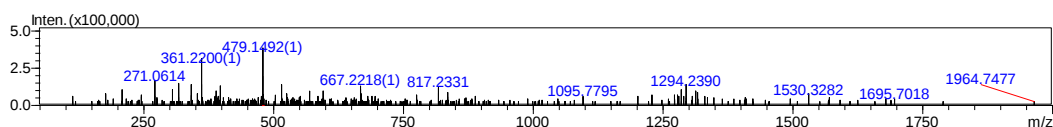


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	41.50	C23 H24 O11	[M+H] ⁺	477.1387	477.1391	-0.4	-0.84	41.50	12.0
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	31.05	C17 H14 O6	[M+H] ⁺	315.0872	315.0863	0.9	2.86	32.57	11.0
C6H10O5		C17H14O6							
		(16H12O5)							
		CH2O							

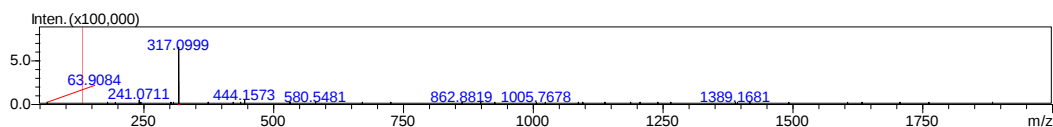
C26

Y4

Event#: 4 MS(E-) Ret. Time : 30.653 Scan# : 3017



Event#: 5 MS/MS(E-) Ret. Time : 30.653 Scan# : 3018 Precursor : 479.1494 Cutoff : 132

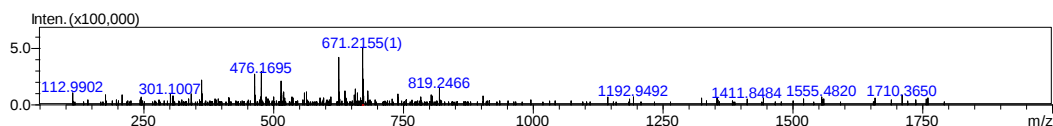


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	28.90	C30 H24 O6	[M-H] ⁻	479.1492	479.1500	-0.8	-1.67	29.39	19.0
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	0.00	C24 H14 O	[M-H] ⁻	317.0999	317.0972	2.7	8.51	0.00	18.0
C6H10O5									

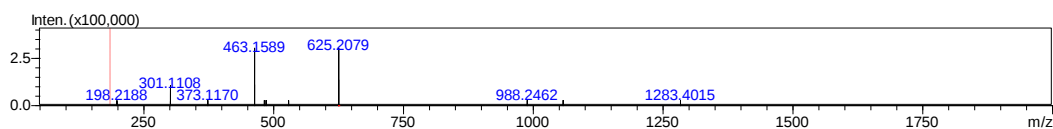
C27

Y5

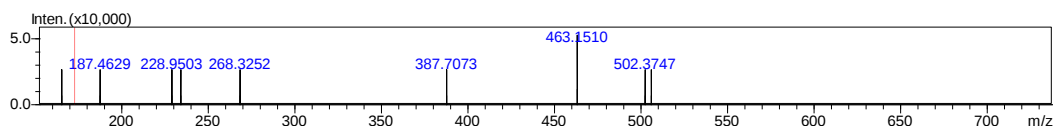
Event#: 4 MS(E-) Ret. Time : 30.773 Scan# : 3029



Event#: 5 MS/MS(E-) Ret. Time : 30.773 Scan# : 3030 Precursor : 671.2156 Cutoff : 185



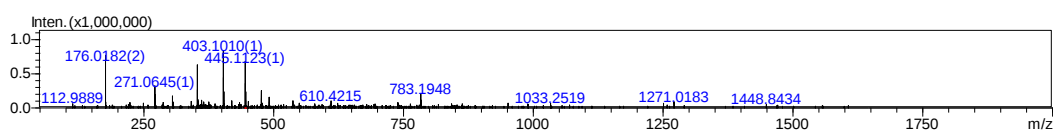
Event#: 6 MS3(E-) Ret. Time : 30.773 Scan# : 3031 Precursor : 625.2078 Cutoff : 173



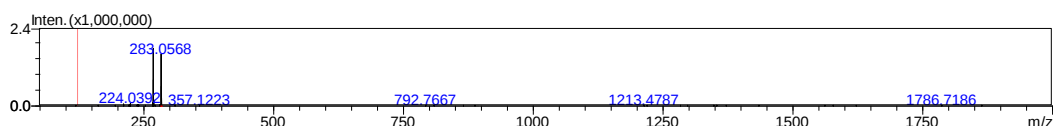
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
4	52.07	C29 H38 O15 [M+HCOO]-		671.2155	671.2193	-3.8	-5.66	62.43	11.0	
5	0.00	C29 H38 O15 [M-H]-		625.2079	625.2138	-5.9	-9.44	0.00	11.0	
1	0.00	C23 H28 O10 [M-H]-		463.1589	463.1610	-2.1	-4.53	0.00	10.0	
1	0.00	C17 H18 O5 [M-H]-		301.1108	301.1081	2.7	8.97	0.00	9.0	

C29 Y6

Event#: 4 MS(E-) Ret. Time : 31.348 Scan# : 3086



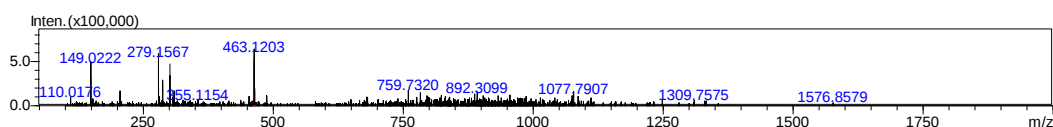
Event#: 5 MS/MS(E-) Ret. Time : 31.348 Scan# : 3087 Precursor : 445.1123 Cutoff : 123



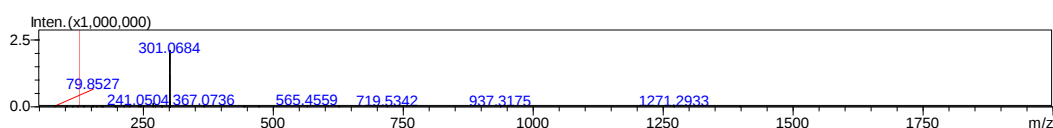
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	67.00	C22 H22 O10 [M-H]-		445.1123	445.1140	-1.7	-3.82	72.08	12.0	
2	9.46	C16 H12 O5 [M-H]-		283.0568	283.0612	-4.4	-15.54	37.49	11.0	

C30 Y7 M=300

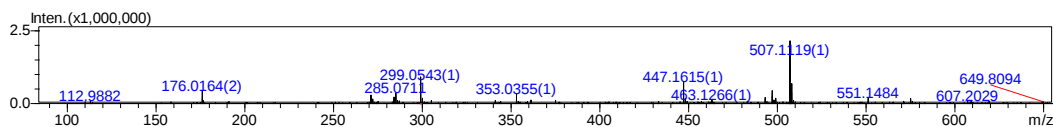
Event#: 1 MS(E+) Ret. Time : 32.078 Scan# : 3155



Event#: 2 MS/MS(E+) Ret. Time : 32.078 Scan# : 3156 Precursor : 463.1203 Cutoff : 128



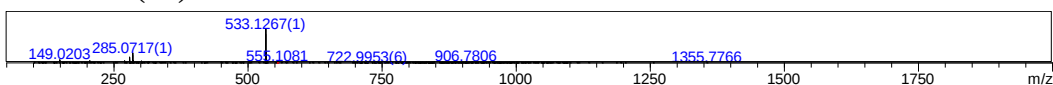
Event#: 4 MS(E-) Ret. Time : 32.078 Scan# : 3158



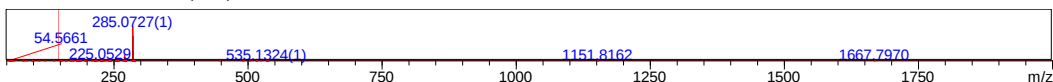
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
2	40.84	C22 H22 O11	[M+H] ⁺	463.1203	463.1235	-3.2	-6.91	57.61	12.0	
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
2	30.14	C16 H12 O6	[M+H] ⁺	301.0684	301.0707	-2.3	-7.64	47.39	11.0	
C6H10O5										

C31 Y8 532=284+ 248==162+86==

Event#: 1 MS(E+) Ret. Time : 32.662 Scan# : 3213



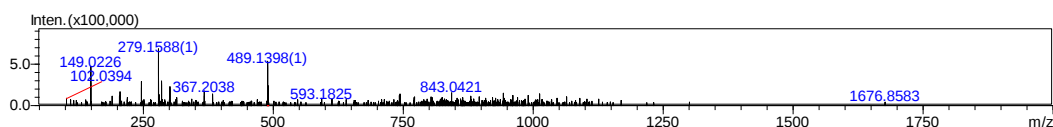
Event#: 2 MS/MS(E+) Ret. Time : 32.542 Scan# : 3202 Precursor : 533.1259 Cutoff : 147



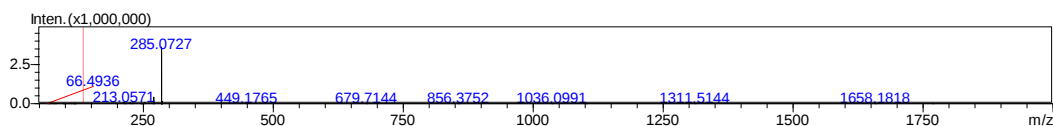
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	82.95	C23 H26 O13	[M+Na] ⁺	533.1267	533.1266	0.1	0.19	82.95	11.0	
2	76.61	C25 H24 O13	[M+H] ⁺	533.1267	533.1290	-2.3	-4.31	83.52	14.0	
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
3	18.81	C16 H12 O5	[M+H] ⁺	285.0717	285.0758	-4.1	-14.38	66.43	11.0	
C9H12O8 ---H2O C6H10O5 C3H2O3-										

C32 Y9

Event#: 1 MS(E+) Ret. Time : 34.207 Scan# : 3366



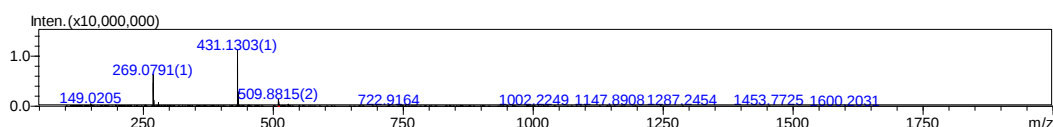
Event#: 2 MS/MS(E+) Ret. Time : 34.207 Scan# : 3367 Precursor : 489.1398 Cutoff : 135



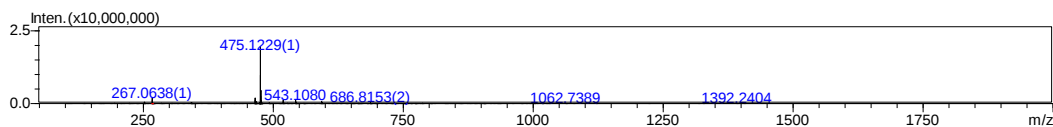
1	49.97	C24 H24 O11	[M+H] ⁺	489.1398	489.1391	0.7	1.43	50.51	13.0	
C16H12O5 C8H16O7+										

C33 Y10 ononin

Event#: 1 MS(E+) Ret. Time : 34.550 Scan# : 3400



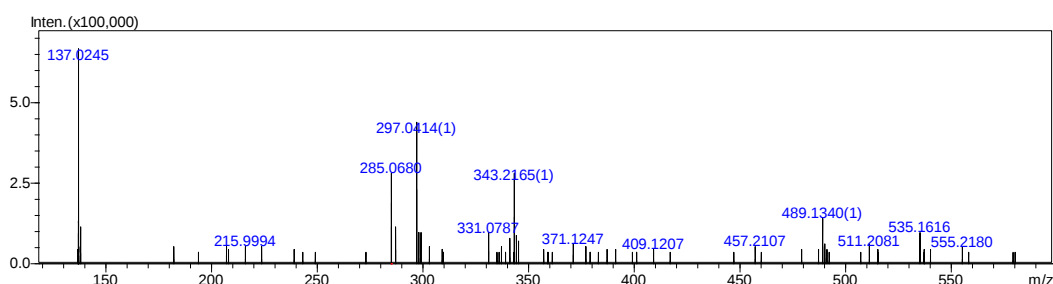
Event#: 4 MS(E-) Ret. Time : 34.550 Scan# : 3403



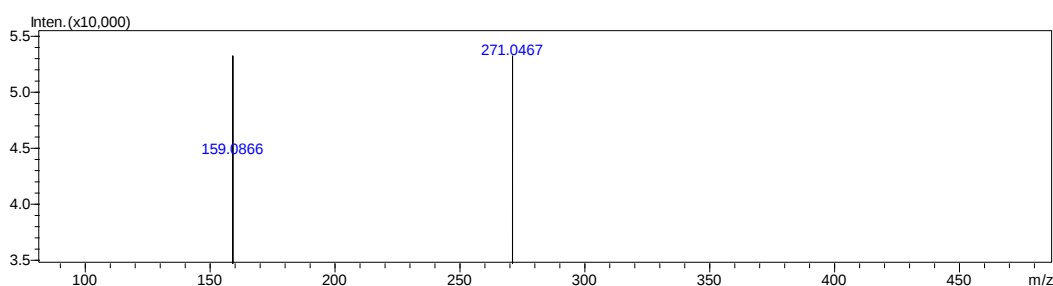
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	66.82	C29 H18 O4	[M+H] ⁺	431.1303	431.1278	2.5	5.80	81.48	21.0
2	56.98	C22 H22 O9	[M+H]⁺	431.1303	431.1337	-3.4	-7.89	93.25	12.0
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	75.50	C22 H22 O9	[M+HCOO] ⁻	475.1229	475.1246	-1.7	-3.58	80.71	12.0

C34 Y11 (286+204)

Event#: 4 MS(E-) Ret. Time : 35.348 Scan# : 3482



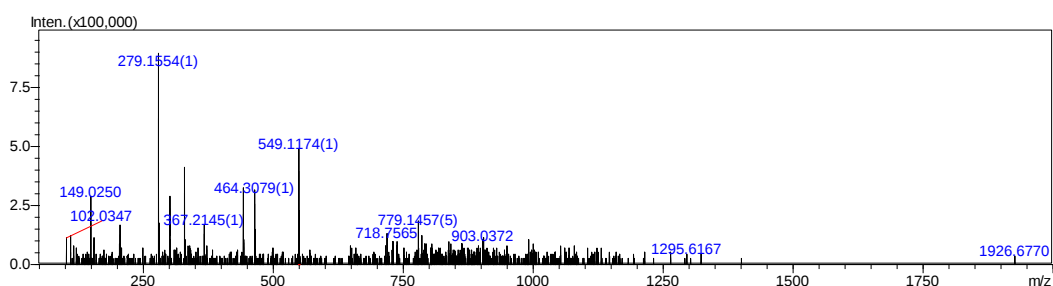
MS/MS(E-) Ret. Time : 35.348 Scan# : 3483 Precursor : 285.0680 Cutoff : 78



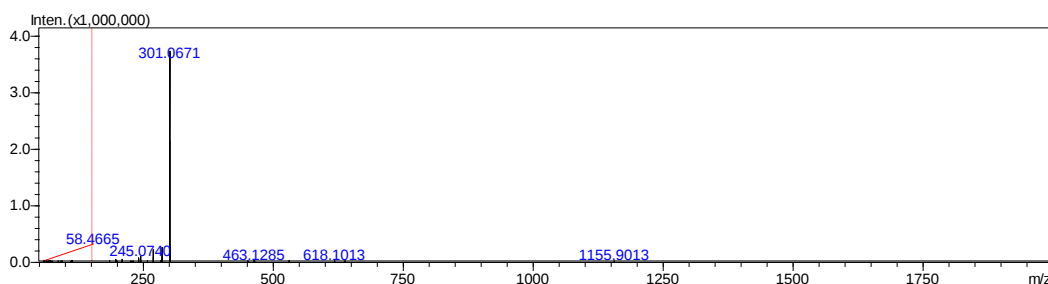
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
4	7.73	C24 H26 O11	[M-H] ⁻	489.1340	489.1402	-6.2	-12.68	23.53	12.0
		C8H16O7 ⁺							
		C16H12O5							

C35 Y12

Event#: 1 MS(E+) Ret. Time : 35.580 Scan# : 3502



MS/MS(E+) Ret. Time : 35.580 Scan# : 3503 Precursor : 549.1174 Cutoff : 151

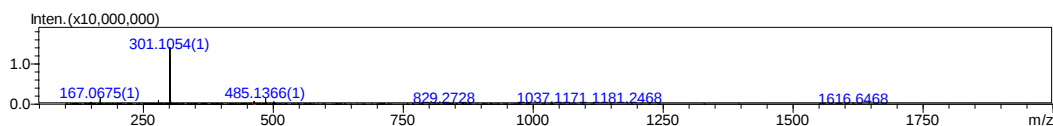


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
4	20.29	C25 H24 O14	[M+H] ⁺	549.1174	549.1239	-6.5	-11.84	57.82	14.0

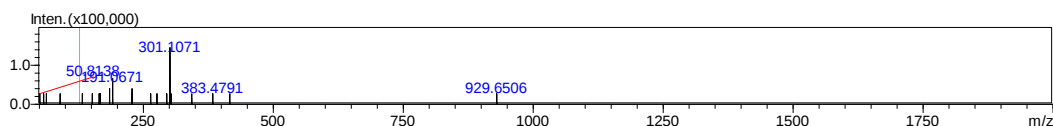
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
3	17.81	C16 H12 O6	[M+H] ⁺	301.0671	301.0707	-3.6	-11.96	51.21	11.0

C36 Y13

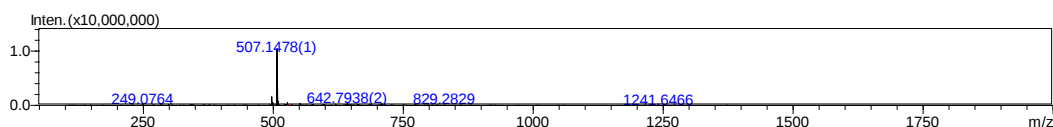
Event#: 1 MS(E+) Ret. Time : 36.027 Scan# : 3546



Event#: 2 MS/MS(E+) Ret. Time : 36.027 Scan# : 3547 Precursor : 463.1591 Cutoff : 128



Event#: 4 MS(E-) Ret. Time : 36.027 Scan# : 3549



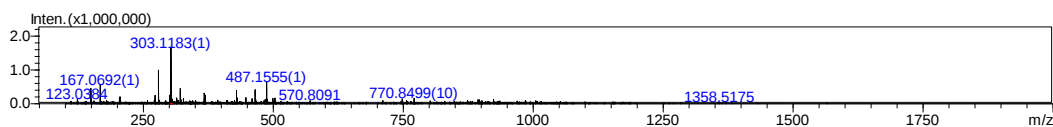
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	35.85	C23 H26 O10	[M+H] ⁺	463.1615	463.1599	1.6	3.45	38.19	11.0

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	27.23	C17 H16 O5	[M+H] ⁺	301.1071	301.1071	0.0	0.00	27.23	10.0

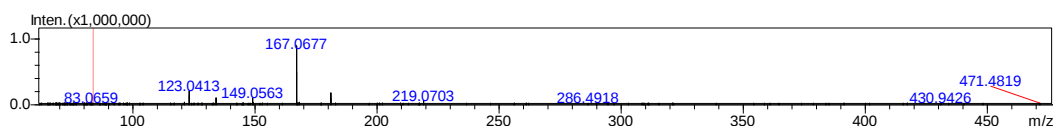
C6H10O5---H2O

C37 Y14

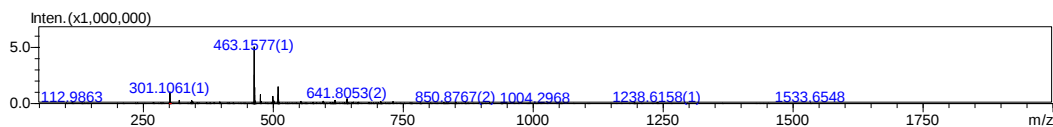
Event#: 1 MS(E+) Ret. Time : 36.773 Scan# : 3620



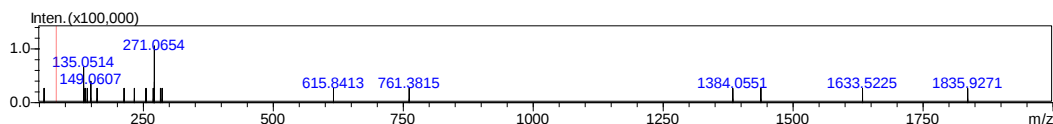
Event#: 2 MS/MS(E+) Ret. Time : 36.773 Scan# : 3621 Precursor : 303.1185 Cutoff : 83



Event#: 4 MS(E-) Ret. Time : 36.773 Scan# : 3623



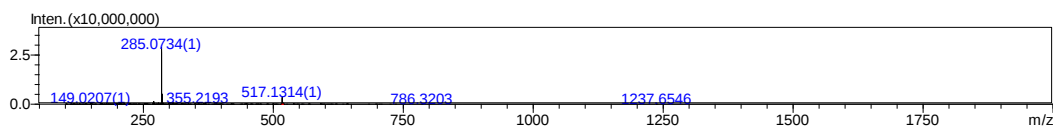
Event#: 5 MS/MS(E-) Ret. Time : 36.773 Scan# : 3624 Precursor : 301.1061 Cutoff : 83



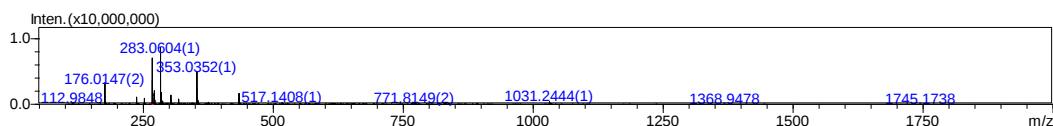
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	65.33	C23 H28 O10	[M-H]-	463.1577	463.1610	-3.3	-7.13	95.10	10.0

C38 Y15 calycosin (DZ)

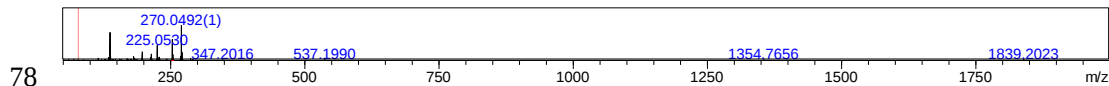
Event#: 1 MS(E+) Ret. Time : 38.035 Scan# : 3745



Event#: 4 MS(E-) Ret. Time : 38.035 Scan# : 3748



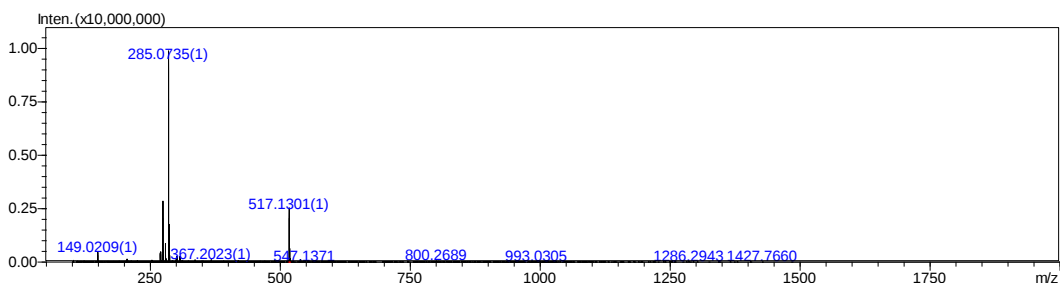
Event#: 2 MS/MS(E+) Ret. Time : 37.915 Scan# : 3734 Precursor : 285.0744 Cutoff :



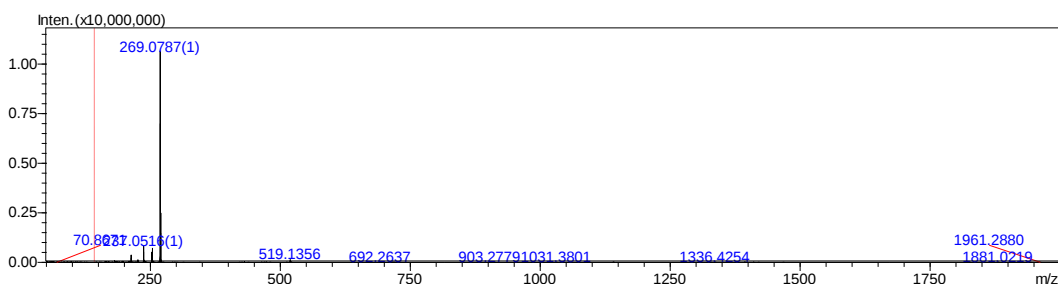
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	82.64	C16 H12 O5	[M+H]+	285.0744	285.0758	-1.4	-4.91	91.59	11.0

C38 C43 Y16 517=269+ 248==162+86==

Event#: 1 MS(E+) Ret. Time : 38.035 -> 39.452 Scan# : 3745 -> 3885



MS/MS(E+) Ret. Time : 38.035 -> 39.452 Scan# : 3746 -> 3886 Precursor : 517.1313 Cutoff : 143



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	95.25	C23 H26 O12	[M+Na]+	517.1301	517.1316	-1.5	-2.90	100.00	11.0

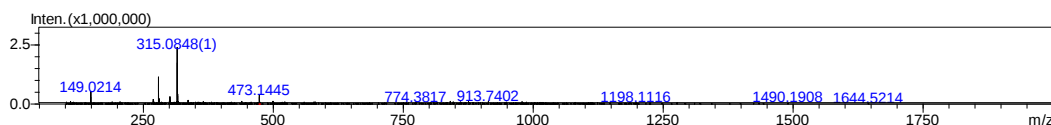
3 62.40 C25 H24 O12 [M+H]+ 517.1301 517.1341 -4.0 -7.73 99.53 14.0

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	72.73	C14 H14 O4	[M+Na]+	269.0787	269.0784	0.3	1.11	72.93	8.0
2	46.45	C16 H12 O4	[M+H]+	269.0787	269.0808	-2.1	-7.80	74.91	11.0

C9H12O8 ---H2O=== C9H14O9

C39 Y17

Event#: 1 MS(E+) Ret. Time : 38.653 Scan# : 3806

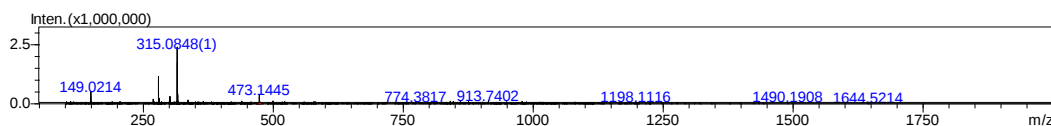


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	72.52	C15 H16 O6	[M+Na]+	315.0844	315.0839	0.5	1.59	73.60	8.0
2	63.21	C17 H14 O6	[M+H]+	315.0844	315.0863	-1.9	-6.03	79.31	11.0

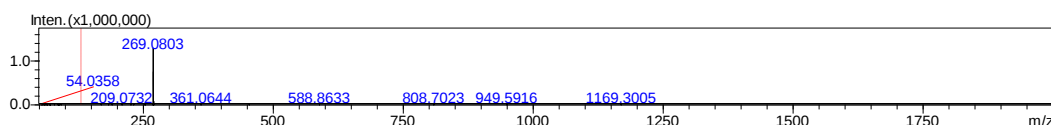
(C16 H12 O5) CH2O

C40 Y18

Event#: 1 MS(E+) Ret. Time : 38.653 Scan# : 3806



Event#: 2 MS/MS(E+) Ret. Time : 38.653 Scan# : 3807 Precursor : 473.1445 Cutoff : 130

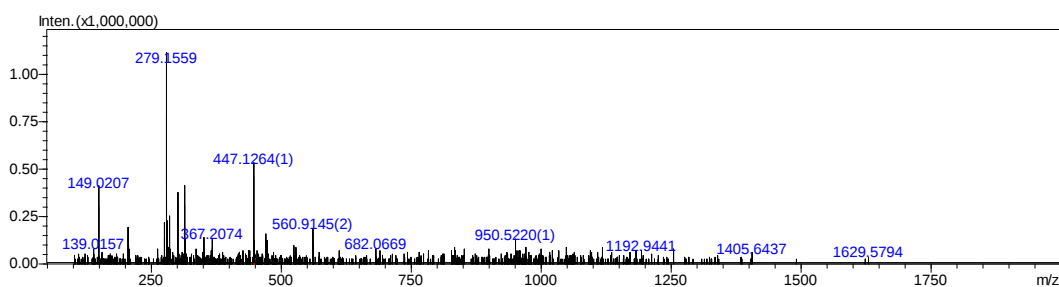


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	22.21	C24 H24 O10	[M+H]+	473.1445	473.1442	0.3	0.63	22.21	13.0

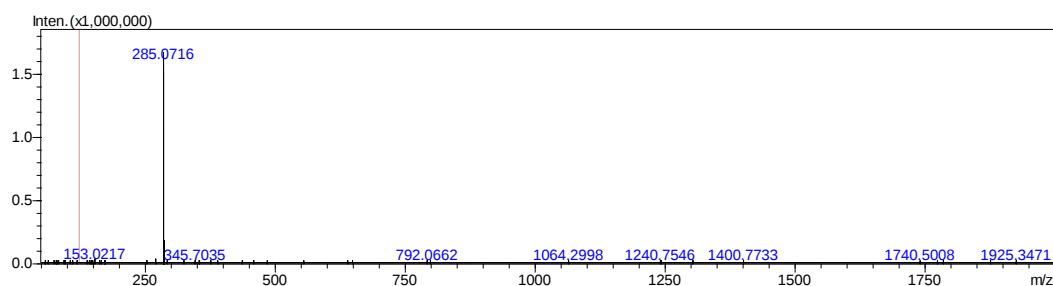
C41

Y19

Event#: 1 MS(E+) Ret. Time : 38.773 Scan# : 3818



MS/MS(E+) Ret. Time : 38.773 Scan# : 3819 Precursor : 447.1264 Cutoff : 123



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	45.08	C22 H22 O10	[M+H] ⁺	447.1264	447.1286	-2.2	-4.92	49.97	12.0

C6H10O5
C16H12O5

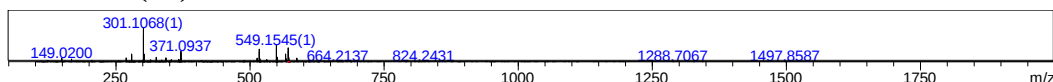
C42

Y20

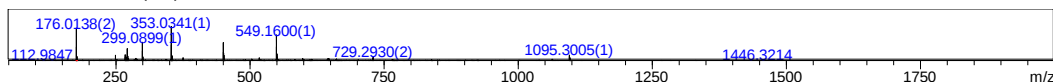
300

532=284+ 248==162+86==

Event#: 1 MS(E+) Ret. Time : 38.997 Scan# : 3840



Event#: 4 MS(E-) Ret. Time : 38.997 Scan# : 3843



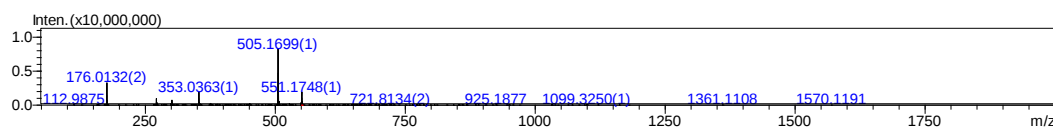
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	82.39	C17 H16 O5	[M+H] ⁺	301.1068	301.1071	-0.3	-1.00	82.39	10.0

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
5	38.51	C26 H28 O13	[M+H] ⁺	549.1545	549.1603	-5.8	-10.56	100.00	13.0

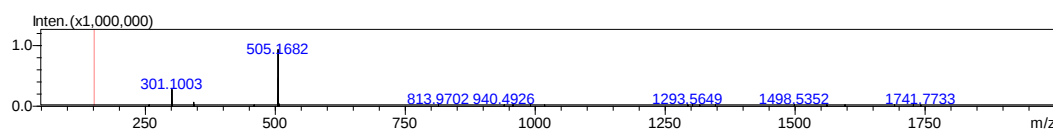
C44

Y21

Event#: 4 MS(E-) Ret. Time : 39.683 Scan# : 3911



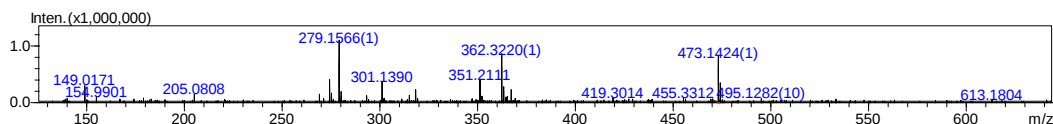
Event#: 5 MS/MS(E-) Ret. Time : 39.683 Scan# : 3912 Precursor : 551.1747 Cutoff : 152



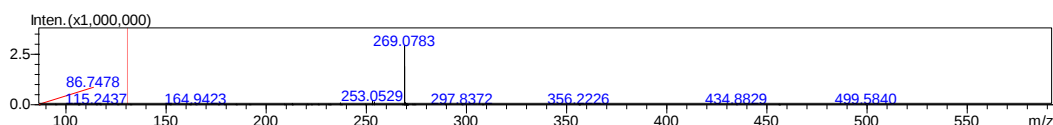
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	92.99	C25 H30 O11	[M-H]-	505.1699	505.1715	-1.6	-3.17	98.32	11.0
		C8H14O7		C17H18O5					

C46 Y22

Event#: 1 MS(E+) Ret. Time : 40.138 Scan# : 3953



Event#: 2 MS/MS(E+) Ret. Time : 40.138 Scan# : 3954 Precursor : 473.1422 Cutoff : 130

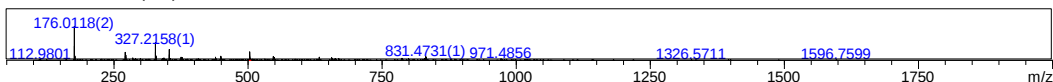


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	63.78	C22 H26 O10	[M+Na]+	473.1424	473.1418	0.6	1.27	64.22	10.0
2	63.47	C24 H24 O10	[M+H]+	473.1424	473.1442	-1.8	-3.80	68.25	13.0
		C16H12O4		C6H16O7					

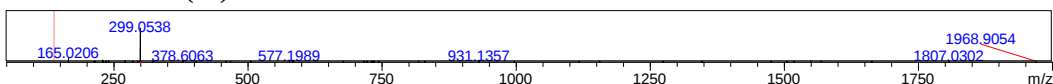
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	16.74	C16 H12 O4	[M+H]+	269.0783	269.0808	-2.5	-9.29	35.55	11.0
		C8H14O7							

C47 Y23

Event#: 4 MS(E-) Ret. Time : 40.430 Scan# : 3985



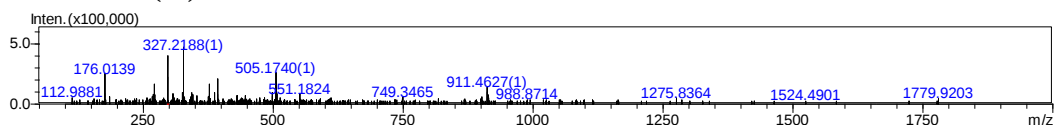
Event#: 5 MS/MS(E-) Ret. Time : 40.430 Scan# : 3986 Precursor : 503.1153 Cutoff : 139



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	0.00	C16 H12 O6	[M-H]-	299.0538	299.0561	-2.3	-7.69	0.00	11.0
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	45.39	C31 H20 O7	[M-H]-	503.1154	503.1136	1.8	3.58	48.52	22.0
4	37.04	C24 H24 O12	[M-H]-	503.1154	503.1195	-4.1	-8.15	63.32	13.0
		C8H14O7		C16H12O6					

Y24

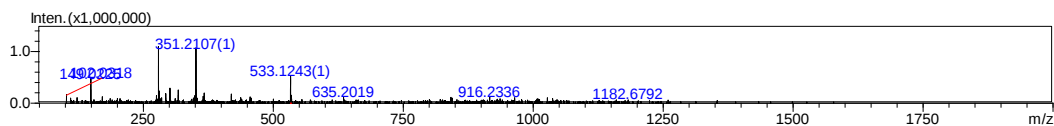
Event#: 4 MS(E-) Ret. Time : 41.675 Scan# : 4108



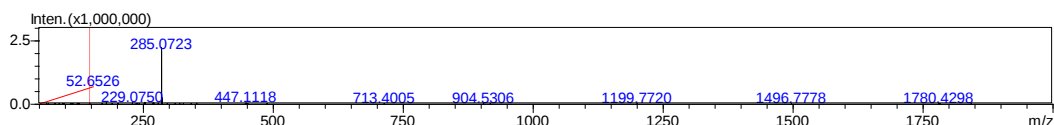
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	24.09	C25 H30 O11	[M-H]-	505.1740	505.1715	2.5	4.95	26.73	11.0
		C8H16O7							

C51 Y25 532=284+ 248==162+86==

Event#: 1 MS(E+) Ret. Time : 41.950 Scan#: 4132



Event#: 2 MS/MS(E+) Ret. Time : 41.950 Scan#: 4133 Precursor : 533.1244 Cutoff : 147

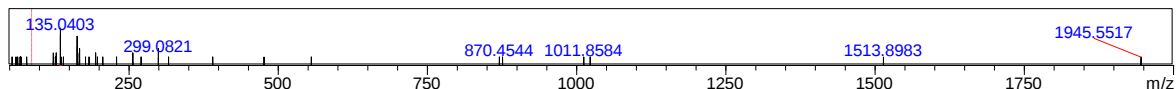


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
4	26.13	C25 H24 O13	[M+H] ⁺	533.1243	533.1290	-4.7	-8.82	50.45	14.0
5	9.41	C16 H30 O18	[M+Na] ⁺	533.1243	533.1324	-8.1	-15.19	35.96	2.0
6	5.32	C18 H28 O18	[M+H] ⁺	533.1243	533.1348	-10.5	-19.70	37.62	5.0

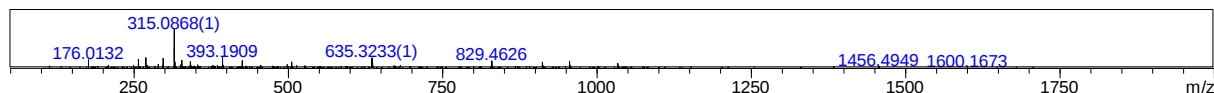
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	22.07	C16 H12 O5	[M+H] ⁺	285.0723	285.0758	-3.5	-12.28	65.07	11.0

C50 Y26

Event#: 2 MS/MS(E+) Ret. Time : 41.778 Scan#: 4116 Precursor : 317.1023 Cutoff : 87



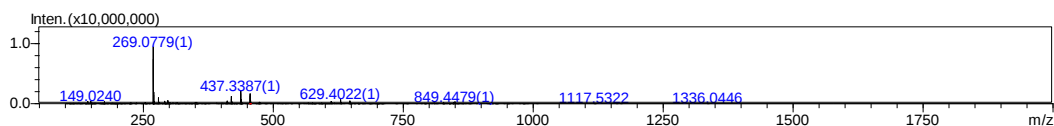
Event#: 4 MS(E-) Ret. Time : 41.778 Scan#: 4118



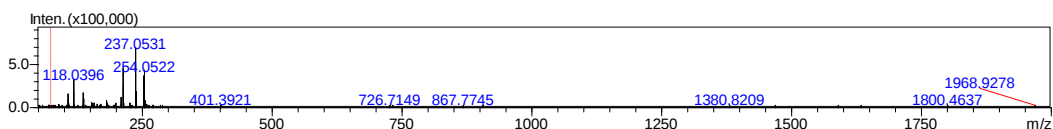
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	74.37	C17 H16 O6	[M-H] ⁻	315.0868	315.0874	-0.6	-1.90	76.09	10.0

C56 Y27 formononetin

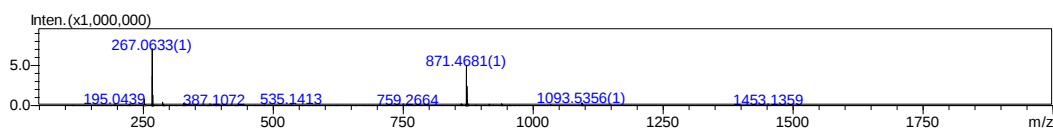
Event#: 1 MS(E+) Ret. Time : 45.315 Scan#: 4465



Event#: 2 MS/MS(E+) Ret. Time : 45.255 Scan#: 4460 Precursor : 269.0791 Cutoff : 74



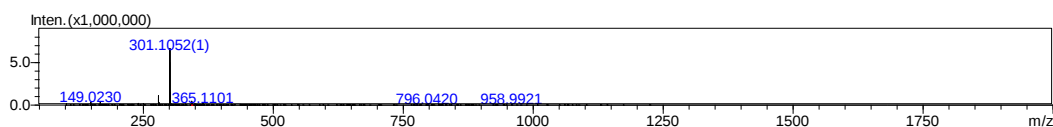
Event#: 4 MS(E-) Ret. Time : 45.315 Scan# : 4468



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	61.30	C16 H12 O4	[M+H] ⁺	269.0791	269.0808	-1.7	-6.32	79.82	11.0

C58 Y28 astrapterocarpan

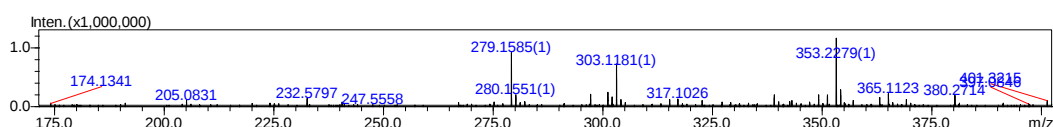
Event#: 1 MS(E+) Ret. Time : 46.158 Scan# : 4547



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	56.73	C17 H16 O5	[M+H] ⁺	301.1052	301.1071	-1.9	-6.31	73.77	10.0

C59 Y29 astraisoflavan

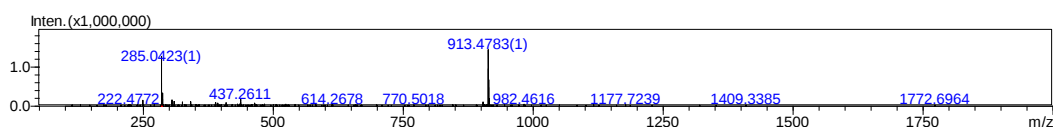
Event#: 1 MS(E+) Ret. Time : 46.708 Scan# : 4601



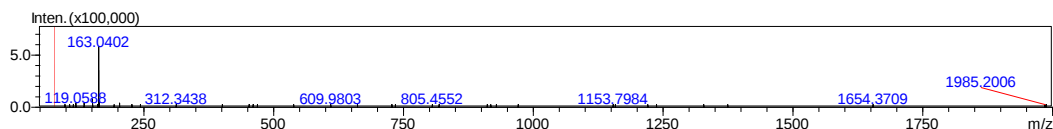
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	12.80	C17 H18 O5	[M+H] ⁺	303.1181	303.1227	-4.6	-15.18	48.89	9.0

C62 Y30 286

Event#: 4 MS(E-) Ret. Time : 49.432 Scan# : 4872



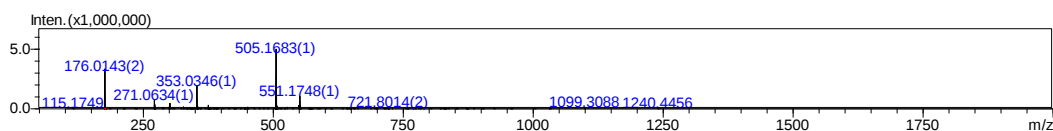
Event#: 5 MS/MS(E-) Ret. Time : 49.432 Scan# : 4873 Precursor : 285.0422 Cutoff : 78



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	26.48	C15 H10 O6	[M-H] ⁻	285.0423	285.0405	1.8	6.31	34.43	11.0

C45 Z1

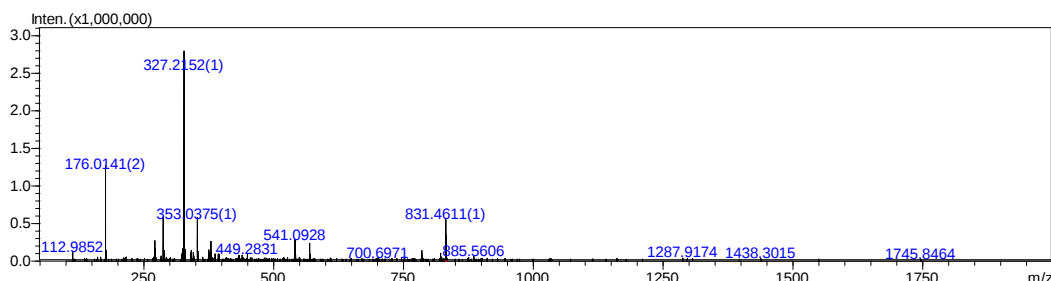
Event#: 4 MS(E-) Ret. Time : 39.743 Scan# : 3917



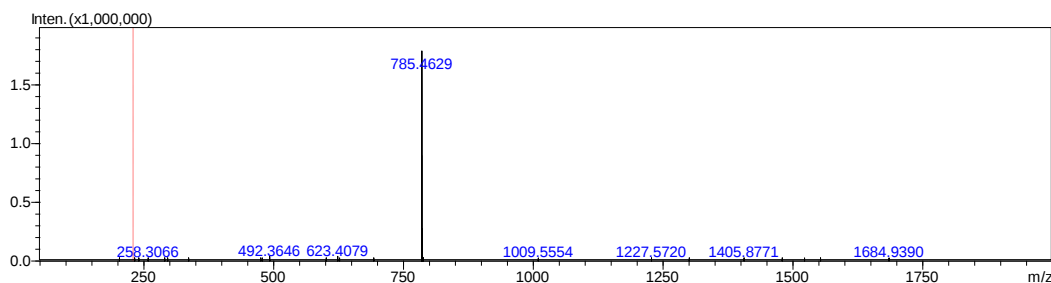
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
10	0.00	C48 H78 O19 [M-H]-		957.5126	957.5065	6.1	6.37	0.00	10.0	

C48 Z1

Event#: 4 MS(E-) Ret. Time : 40.825 Scan# : 4024



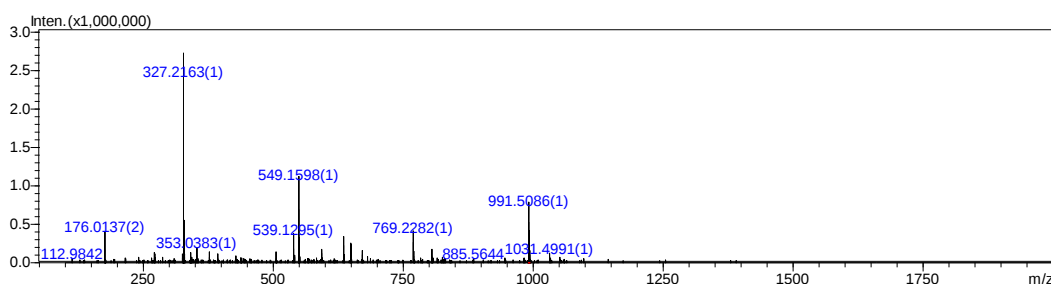
MS/MS(E-) Ret. Time : 40.825 Scan# : 4025 Precursor : 831.4614 Cutoff : 230



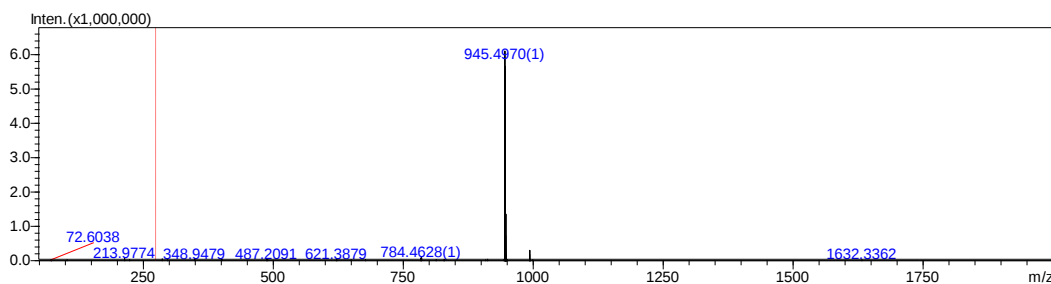
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
7	0.00	C41 H70 O14 [M-H]-		785.4629	785.4693	-6.4	-8.15	0.00	7.0	

C49 Z2 ZG-V

Event#: 4 MS(E-) Ret. Time : 41.108 Scan# : 4052



MS/MS(E-) Ret. Time : 41.108 Scan# : 4053 Precursor : 991.5089 Cutoff : 274

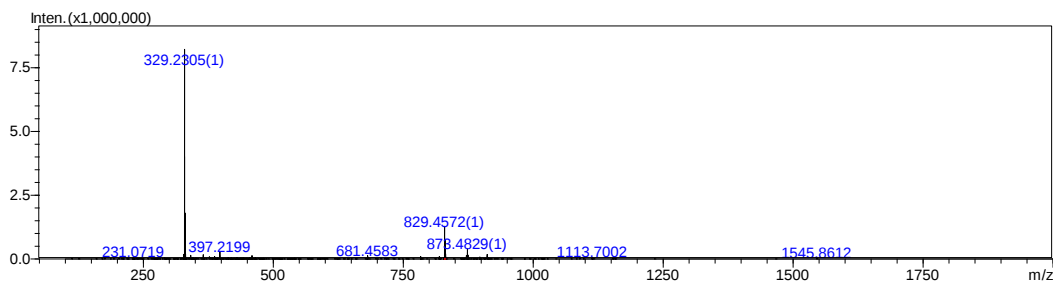


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	68.58	C48 H80 O21 [M-H]-		991.5086	991.5119	-3.3	-3.33	72.82	9.0	
2	68.58	C46 H76 O19 [M+CH3COO]-		991.5086	991.5119	-3.3	-3.33	72.82	9.0	
3	68.58	C47 H78 O19 [M+HCOO]-		991.5086	991.5119	-3.3	-3.33	72.82	9.0	

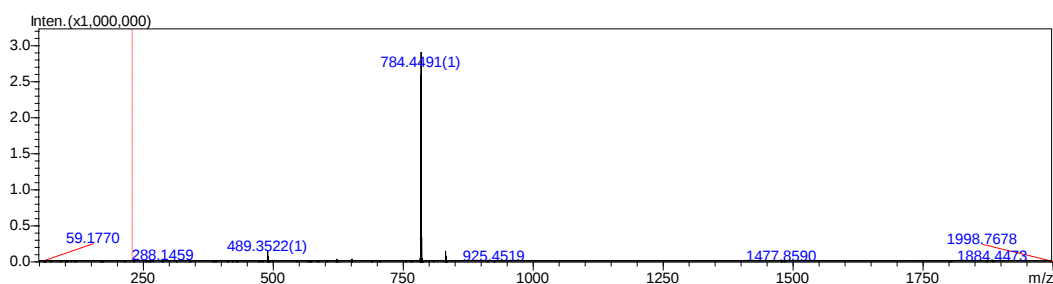
C53

Z3 ZG-IV

Event#: 4 MS(E-) Ret. Time : 42.612 -> 43.135 Scan# : 4200 -> 4252



MS/MS(E-) Ret. Time : 42.612 -> 43.135 Scan# : 4201 -> 4253 Precursor : 829.4586 Cutoff : 229

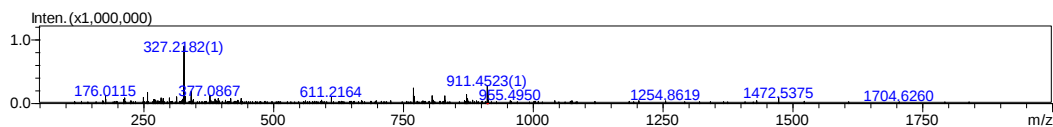


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	81.60	C41 H68 O14	[M+HCOO]-	829.4572	829.4591	-1.9	-2.29	84.32	8.0

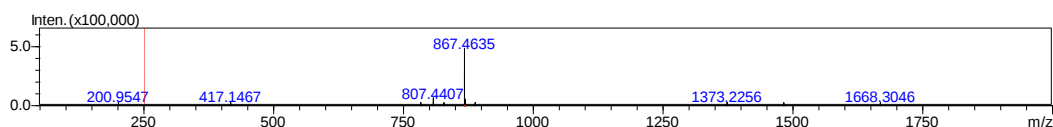
C52

Z4 =G I

Event#: 4 MS(E-) Ret. Time : 42.062 Scan# : 4145



Event#: 5 MS/MS(E-) Ret. Time : 42.062 Scan# : 4146 Precursor : 911.4525 Cutoff : 252

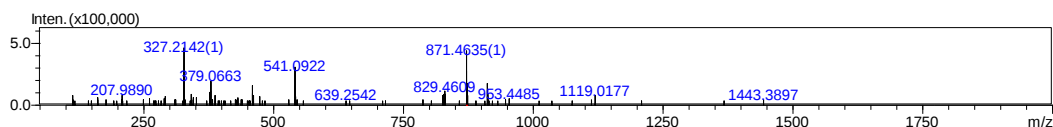


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
14	0.00	C45 H72 O16	[M-H]-	867.4635	867.4748	-11.3	-13.03	0.00	10.0

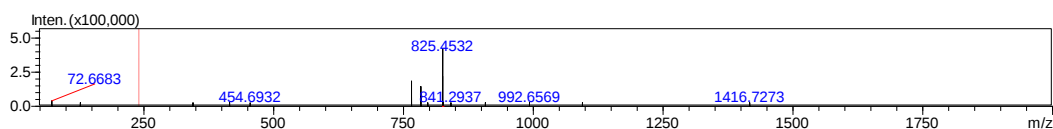
C54

Z5 ISO ZG II

Event#: 4 MS(E-) Ret. Time : 42.560 Scan# : 4194



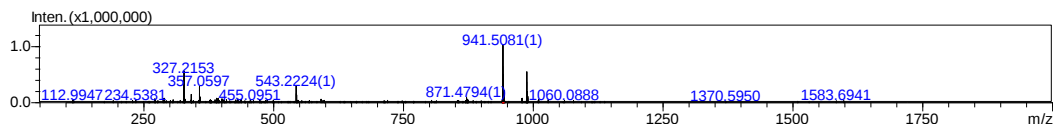
Event#: 5 MS/MS(E-) Ret. Time : 42.560 Scan# : 4195 Precursor : 871.4641 Cutoff : 241



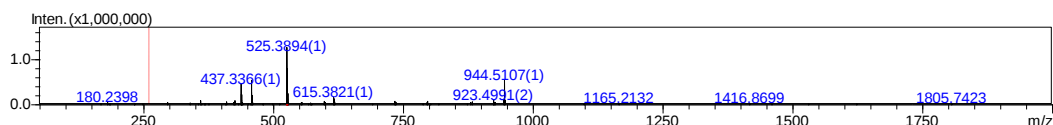
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score DBE
14	0.00	C43 H70 O15 [M-H]-		825.4532	825.4642	-11.0	-13.33	0.00 9.0

C55 Z6 Bb

Event#: 4 MS(E-) Ret. Time : 44.190 Scan# : 4357



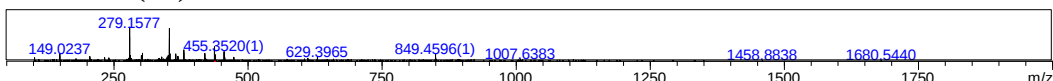
Event#: 5 MS/MS(E-) Ret. Time : 44.190 Scan# : 4358 Precursor : 941.5081 Cutoff : 260



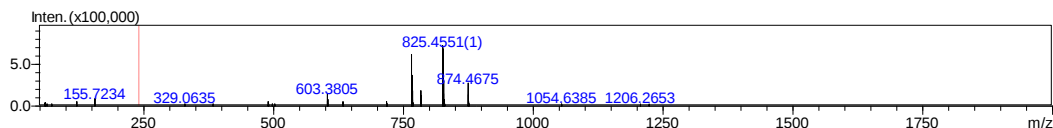
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score DBE
1	44.34	C48 H78 O18 [M-H]-		941.5081	941.5115	-3.4	-3.61	47.43 10.0

C60 Z7 G-II

Event#: 1 MS(E+) Ret. Time : 46.768 Scan# : 4607



Event#: 5 MS/MS(E-) Ret. Time : 46.708 Scan# : 4605 Precursor : 871.4660 Cutoff : 241



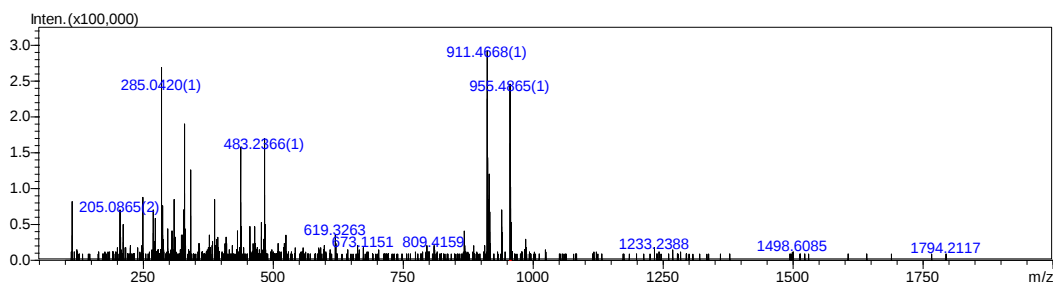
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score DBE
1	54.12	C43 H70 O15 [M+Na]+		849.4596	849.4607	-1.1	-1.29	54.52 9.0

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score DBE
1	66.10	C44 H72 O17 [M-H]-		871.4656	871.4697	-4.1	-4.70	72.83 9.0

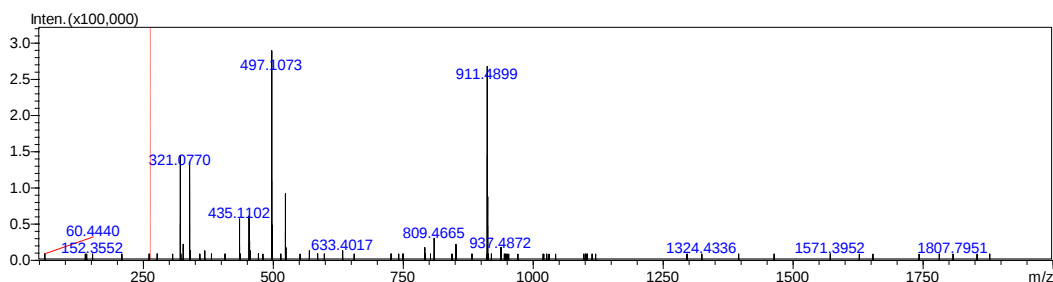
2	66.10	C43 H70 O15 [M+HCOO]-		871.4656	871.4697	-4.1	-4.70	72.83 9.0
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C61 Z8 ==G I

Event#: 4 MS(E-) Ret. Time : 47.172 -> 48.985 Scan# : 4649 -> 4828

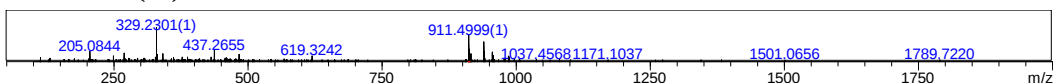


MS/MS(E-) Ret. Time : 47.172 -> 48.985 Scan# : 4650 -> 4829 Precursor : 955.4807 Cutoff : 264

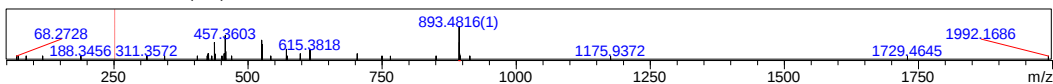


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	54.01	C45 H70 O16 [M+HCOO]-		911.4668	911.4646	2.2	2.41	55.98	11.0

Event#: 4 MS(E-) Ret. Time : 47.223 Scan# : 4655



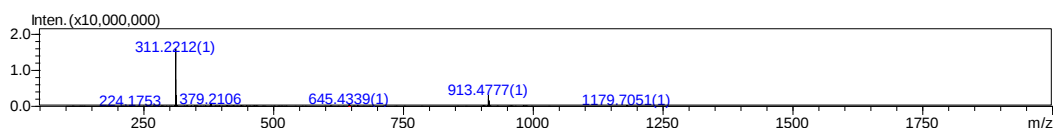
Event#: 5 MS/MS(E-) Ret. Time : 47.223 Scan# : 4656 Precursor : 911.5002 Cutoff : 252



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
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C64 Z9 i-ZG--I

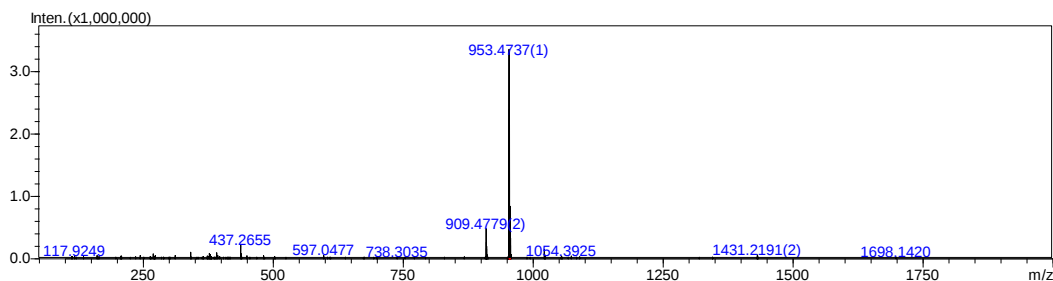
Event#: 4 MS(E-) Ret. Time : 50.713 Scan# : 4997



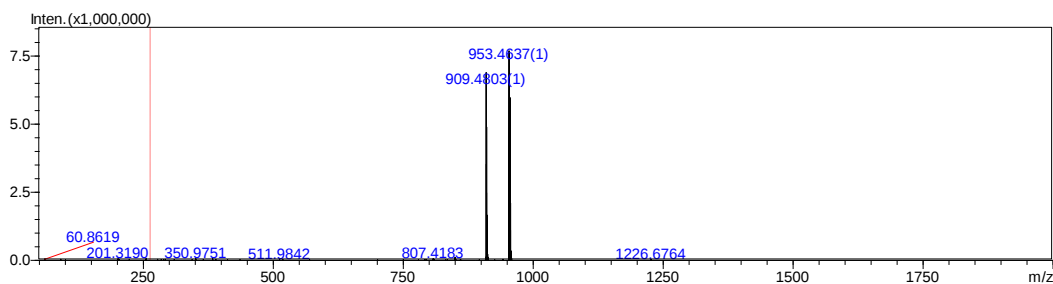
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	95.07	C46 H74 O18 [M-H]-		913.4777	913.4802	-2.5	-2.74	99.40	10.0
2	95.07	C44 H70 O16 [M+CH3COO]-		913.4777	913.4802	-2.5	-2.74	99.40	10.0
3	95.07	C45 H72 O16 [M+HCOO]-		913.4777	913.4802	-2.5	-2.74	99.40	10.0

C65 Z10

Event#: 4 MS(E-) Ret. Time : 51.607 Scan# : 5085



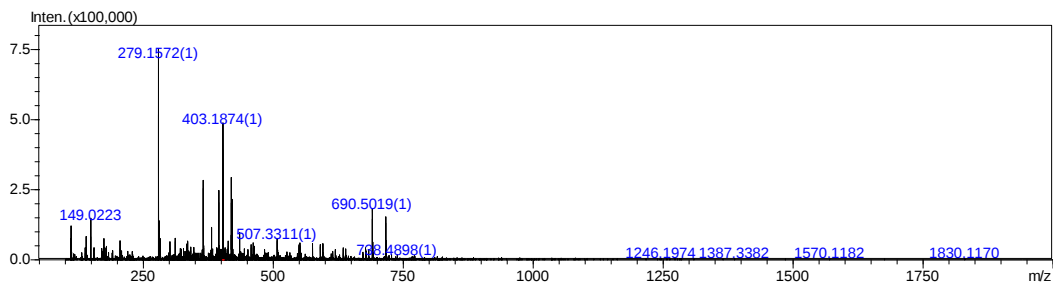
MS/MS(E-) Ret. Time : 51.607 Scan# : 5086 Precursor : 953.9829 Cutoff : 264

[illegible]

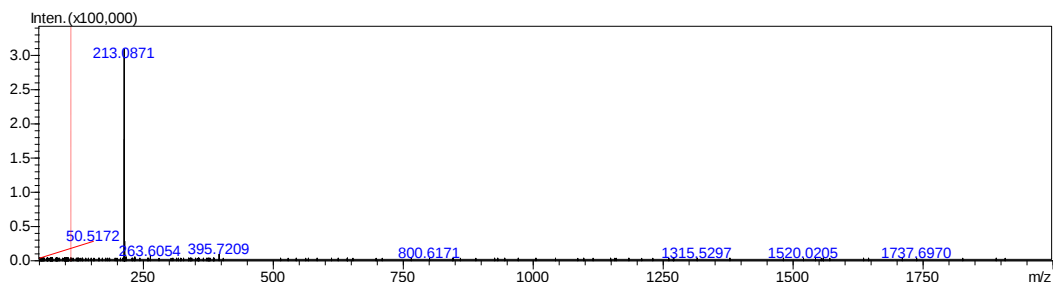
C67

$$Z_-$$

Event#: 1 MS(E+) Ret. Time : 59.933 -> 62.997 Scan# : 5900 -> 6204



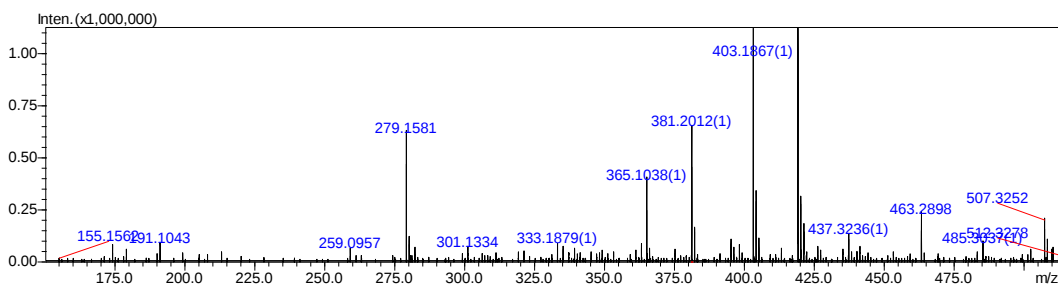
MS/MS(E+) Ret. Time : 59.933 -> 62.997 Scan# : 5901 -> 6205 Precursor : 403.1850 Cutoff : 111



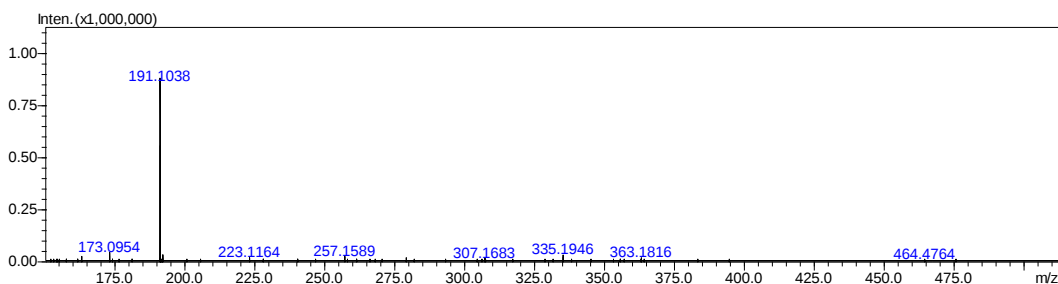
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	36.86	C12 H14 O2	[M+Na] ⁺	213.0871	213.0886	-1.5	-7.04	52.96	6.0

C68 E-

Event#: 1 MS(E+) Ret. Time : 61.708 -> 62.542 Scan# : 6077 -> 6159



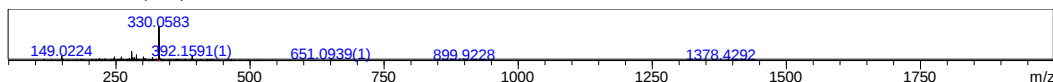
MS/MS(E+) Ret. Time : 61.708 -> 62.542 Scan# : 6078 -> 6160 Precursor : 381.2017 Cutoff : 105



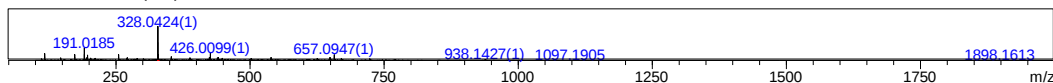
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	78.12	C ₂₄ H ₂₈ O ₄	[M+Na] ⁺	403.1867	403.1880	-1.3	-3.22	82.71	11.0	
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	59.05	C ₂₂ H ₃₀ O ₄	[M+Na] ⁺	381.2012	381.2036	-2.4	-6.30	76.69	8.0	
2	18.30	C ₂₄ H ₂₈ O ₄	[M+H] ⁺	381.2012	381.2060	-4.8	-12.59	55.30	11.0	
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
2	12.97	C ₁₂ H ₁₄ O ₂	[M+H] ⁺	191.1038	191.1067	-2.9	-15.17	49.46	6.0	

C5 X1 =

Event#: 1 MS(E+) Ret. Time : 4.498 Scan# : 443



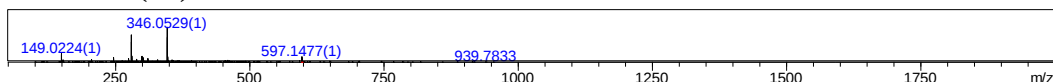
Event#: 4 MS(E-) Ret. Time : 4.498 Scan# : 446



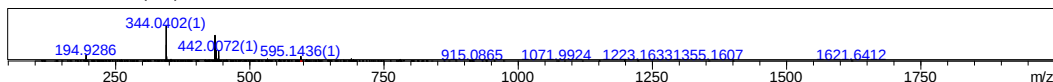
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	61.39	C ₁₁ H ₁₁ N ₃ O ₉	[M+H] ⁺	330.0583	330.0568	1.5	4.54	67.35	8.0	

C6 X2 =

Event#: 1 MS(E+) Ret. Time : 6.480 Scan# : 638



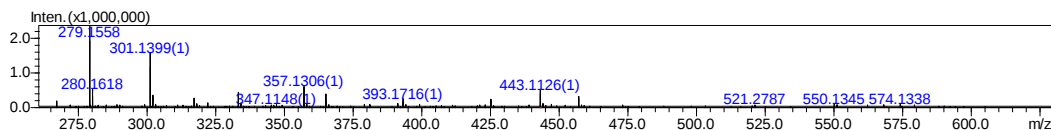
Event#: 4 MS(E-) Ret. Time : 6.480 Scan# : 641



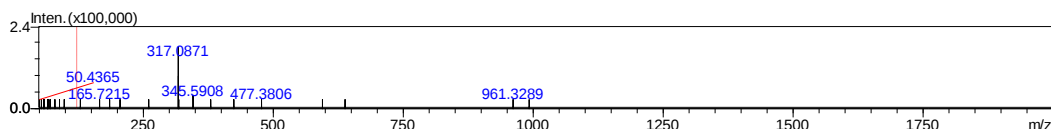
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
3	65.91	C ₁₁ H ₁₁ N ₃ O ₁₀	[M+H] ⁺	346.0529	346.0517	1.2	3.47	70.25	8.0	

C7

Event#: 1 MS(E+) Ret. Time : 9.227 Scan# : 910



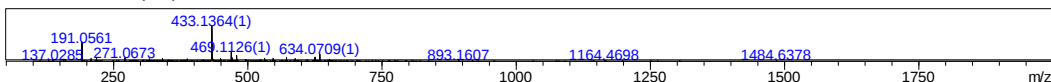
Event#: 2 MS/MS(E+) Ret. Time : 9.227 Scan# : 911 Precursor : 443.1126 Cutoff : 122



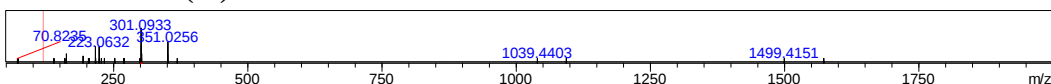
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	59.89	C26 H18 O7	[M+H] ⁺	443.1126	443.1125	0.1	0.23	59.89	18.0

C8 X3

Event#: 4 MS(E-) Ret. Time : 9.398 Scan# : 929



Event#: 5 MS/MS(E-) Ret. Time : 9.398 Scan# : 930 Precursor : 433.1364 Cutoff : 119



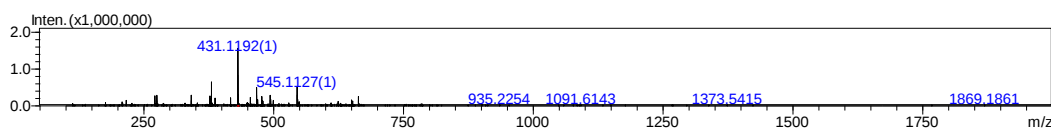
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	71.60	C18 H26 O12	[M-H] ⁻	433.1364	433.1352	1.2	2.77	74.91	6.0

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	37.82	C13 H18 O8	[M-H] ⁻	301.0933	301.0929	0.4	1.33	38.13	5.0

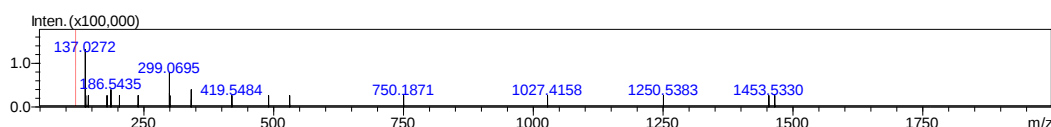
C5H10O5

C10 X3 benzoic acid+xylan

Event#: 4 MS(E-) Ret. Time : 11.125 Scan# : 1099



Event#: 5 MS/MS(E-) Ret. Time : 11.125 Scan# : 1100 Precursor : 431.1190 Cutoff : 119

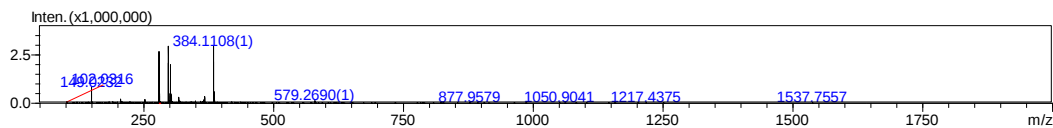


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	89.05	C18 H24 O12	[M-H] ⁻	431.1192	431.1195	-0.3	-0.70	89.05	7.0

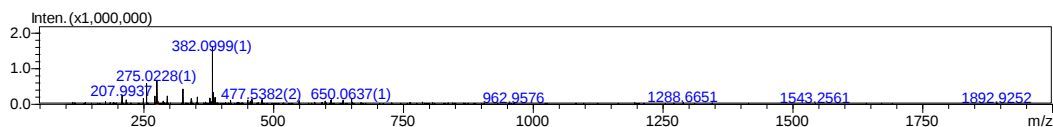
C5H8O4 C13H16O8

C11 X4 =

Event#: 1 MS(E+) Ret. Time : 12.653 Scan# : 1248



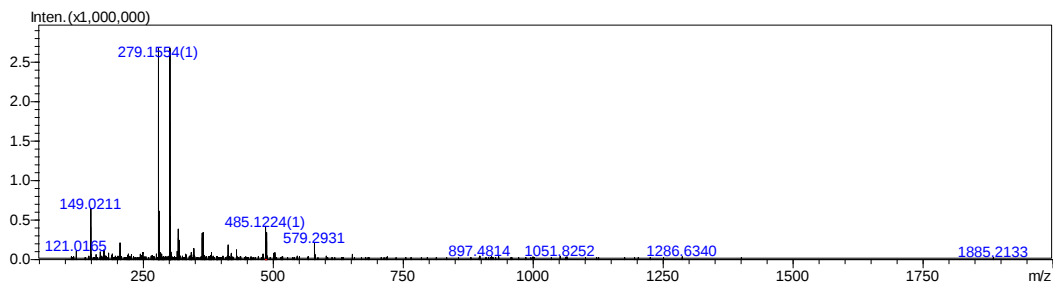
Event#: 4 MS(E-) Ret. Time : 12.653 Scan# : 1251



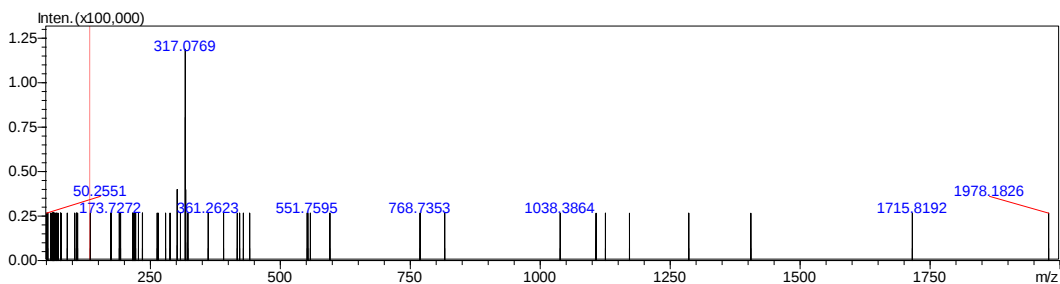
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	79.82	C13 H21 N O12	[M+H] ⁺	384.1127	384.1137	-1.0 -2.60	83.14	4.0		

C12 X5

Event#: 1 MS(E+) Ret. Time : 13.847 Scan# : 1366



MS/MS(E+) Ret. Time : 13.847 Scan# : 1367 Precursor : 485.1225 Cutoff : 134

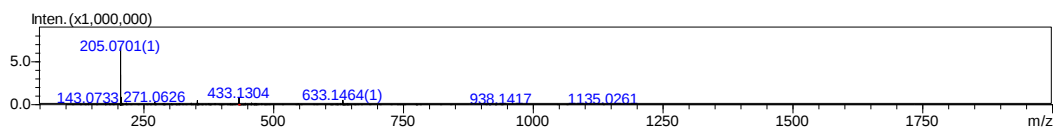


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	15.37	C26 H22 O8	[M+Na] ⁺	485.1224	485.1207	1.7 3.50	16.39	16.0		
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
2	10.77	C20 H12 O4	[M+H] ⁺	317.0769	317.0808	-3.9 -12.30	31.80	15.0		

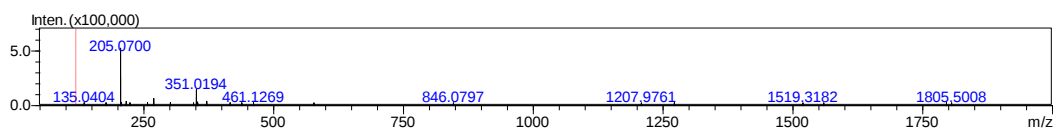
+C6H12O5

C13 X8

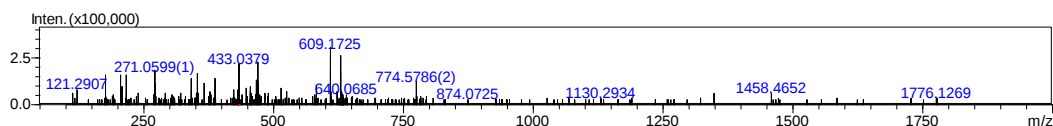
Event#: 4 MS(E-) Ret. Time : 17.807 Scan# : 1758



Event#: 5 MS/MS(E-) Ret. Time : 17.807 Scan# : 1759 Precursor : 433.1305 Cutoff : 119



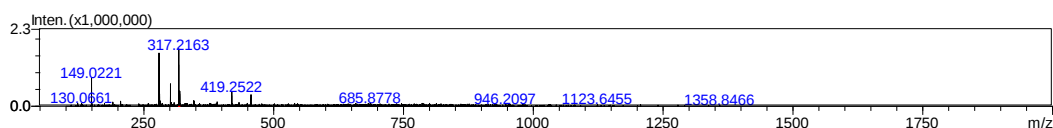
Event#: 4 MS(E-) Ret. Time : 18.557 Scan# : 1832



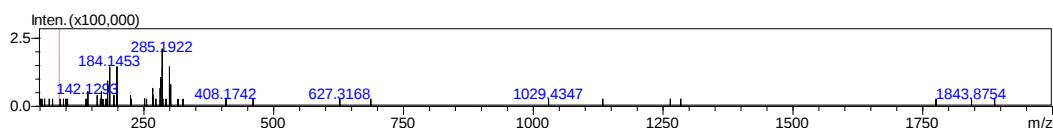
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	35.69	C8 H14 O6	[M-H]-	205.0701	205.0718	-1.7	-8.29	62.50	2.0

C14 X9 lambertianic acid

Event#: 1 MS(E+) Ret. Time : 21.147 Scan# : 2082

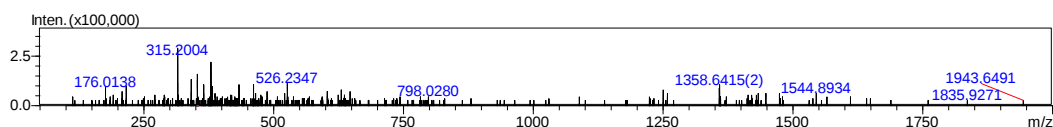


Event#: 2 MS/MS(E+) Ret. Time : 21.147 Scan# : 2083 Precursor : 317.2162 Cutoff : 87



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	5.39	C20 H28 O3	[M+H]+	317.2163	317.2111	5.2	16.39	23.48	7.0

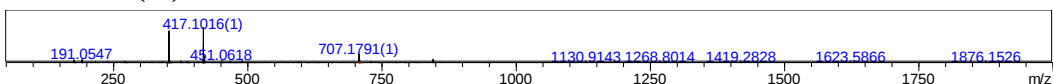
Event#: 4 MS(E-) Ret. Time : 22.590 Scan# : 2223



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	20.54	C20 H28 O3	[M-H]-	315.2004	315.1966	3.8	12.06	59.51	7.0

C15 X10 =

Event#: 4 MS(E-) Ret. Time : 22.132 Scan# : 2180

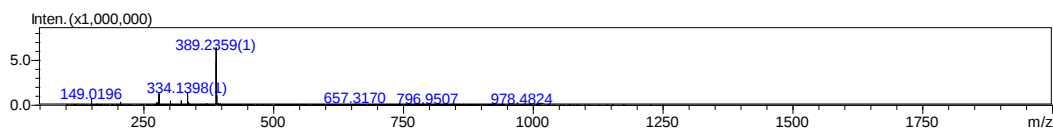


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	78.66	C17 H22 O12	[M-H]-	417.1016	417.1038	-2.2	-5.27	90.10	7.0

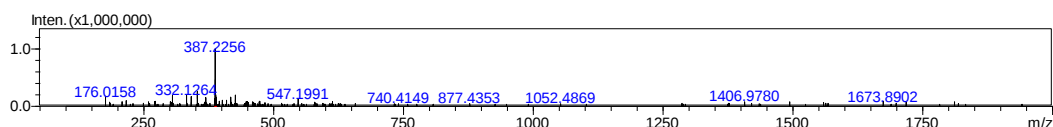
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	35.52	C7 H12 O6	[M-H]-	191.0547	191.0561	-1.4	-7.33	53.25	2.0

C10H12O7

C16 X11 Cyclopentaneacetic acid =
 Event#: 1 MS(E+) Ret. Time : 22.950 Scan# : 2256

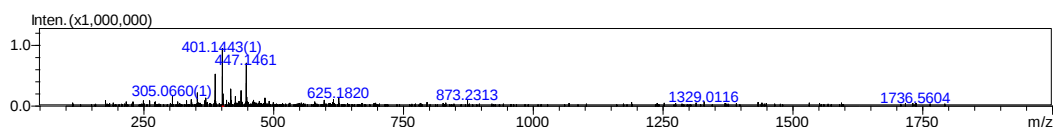


Event#: 4 MS(E-) Ret. Time : 22.950 Scan# : 2259

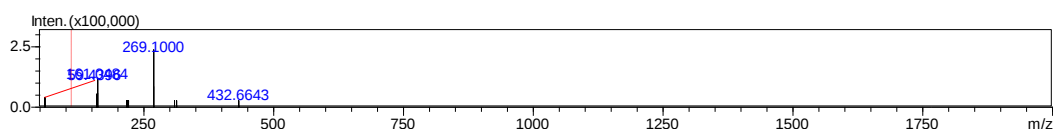


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	4.02	C27 H32 O2	[M-H]-	387.2256	387.2330	-7.4	-19.11	25.57	12.0
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	22.96	C23 H32 O5	[M+H]+	389.2359	389.2323	3.6	9.25	48.33	8.0

C17 X12 +xylan =
 Event#: 4 MS(E-) Ret. Time : 23.012 Scan# : 2264



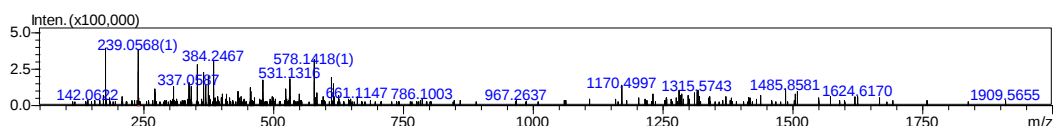
Event#: 5 MS/MS(E-) Ret. Time : 23.012 Scan# : 2265 Precursor : 401.1442 Cutoff : 111



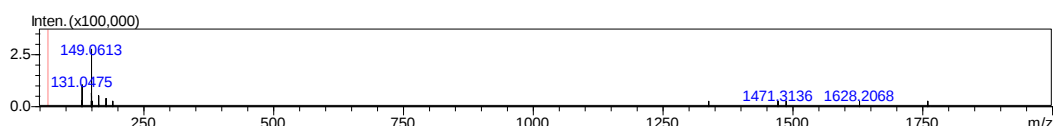
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	58.11	C18 H26 O10	[M-H]-	401.1443	401.1453	-1.0	-2.49	60.36	6.0
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	0.00	C13 H18 O6	[M-H]-	269.1000	269.1031	-3.1	-11.52	0.00	5.0

C5H8O4 xylan

C19 X13 (4-formyl-2,6-dimethoxyphenoxoy)Acetic acid =
 Event#: 4 MS(E-) Ret. Time : 24.347 Scan# : 2395



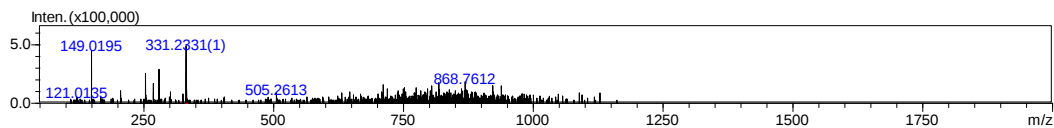
Event#: 5 MS/MS(E-) Ret. Time : 24.347 Scan# : 2396 Precursor : 239.0567 Cutoff : 66



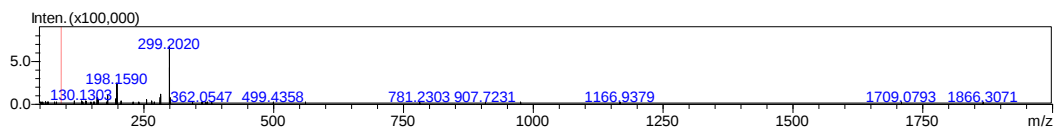
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	62.78	C11 H12 O6	[M-H]-	239.0568	239.0561	0.7	2.93	65.96	6.0

C20 X14 Testosterone acetate

Event#: 1 MS(E+) Ret. Time : 25.662 Scan# : 2521



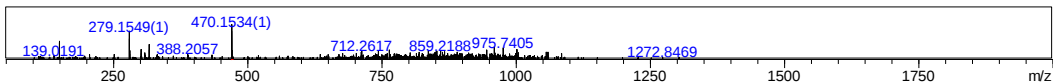
Event#: 2 MS/MS(E+) Ret. Time : 25.662 Scan# : 2522 Precursor : 331.2330 Cutoff : 91



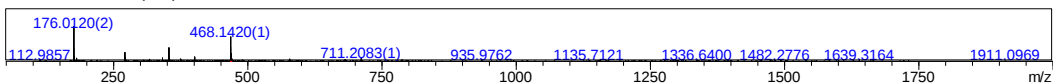
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	50.18	C21 H30 O3	[M+H] ⁺	331.2296	331.2268	2.8	8.45	90.41	7.0
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	33.48	C20 H26 O2	[M+H] ⁺	299.2020	299.2006	1.4	4.68	36.88	8.0

C21 X15

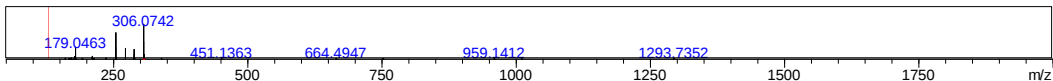
Event#: 1 MS(E+) Ret. Time : 26.743 Scan# : 2628



Event#: 4 MS(E-) Ret. Time : 26.743 Scan# : 2631



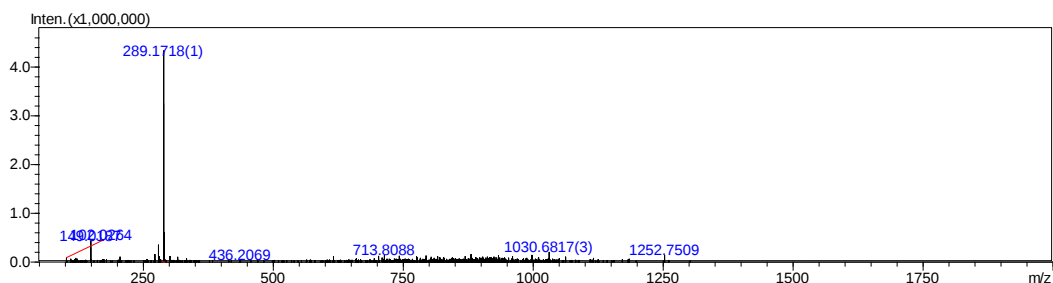
Event#: 5 MS/MS(E-) Ret. Time : 26.743 Scan# : 2632 Precursor : 468.1417 Cutoff : 129



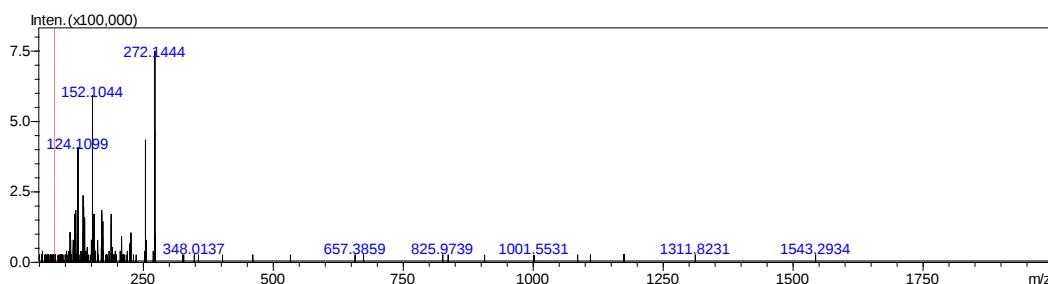
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	49.45	C18 H23 N5 O10	[M+H] ⁺	470.1534	470.1518	1.6	3.40	52.61	10.0
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
7	23.10	C18 H23 N5 O10	[M-H] ⁻	468.1420	468.1372	4.8	10.25	58.74	10.0

C22 X16

Event#: 1 MS(E+) Ret. Time : 26.967 Scan# : 2650



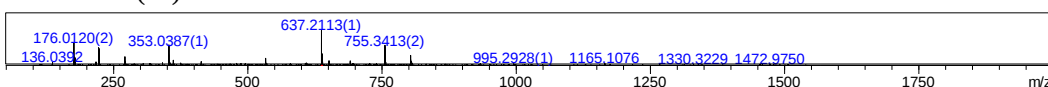
MS/MS(E+) Ret. Time : 26.967 Scan# : 2651 Precursor : 289.4785 Cutoff : 80



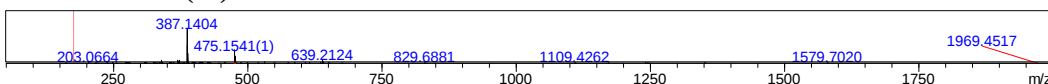
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	47.38	C13 H24 N2 O5	[M+H] ⁺	289.1747	289.1758	-1.1	-3.80	50.94	3.0

C25 X18

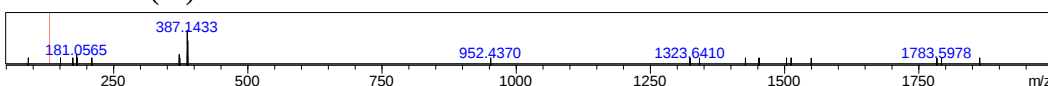
Event#: 4 MS(E-) Ret. Time : 30.070 Scan# : 2959



Event#: 5 MS/MS(E-) Ret. Time : 30.070 Scan# : 2960 Precursor : 637.2112 Cutoff : 176



Event#: 6 MS3(E-) Ret. Time : 30.070 Scan# : 2961 Precursor : 475.1541 Cutoff : 131



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	73.32	C30 H38 O15	[M-H] ⁻	637.2113	637.2138	-2.5	-3.92	79.09	12.0

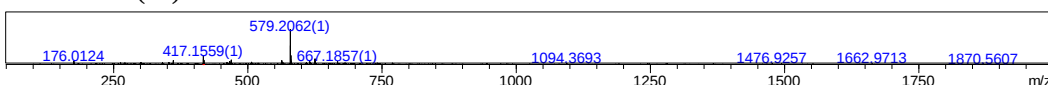
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
5	11.69	C24 H28 O10	[M-H] ⁻	475.1541	475.1610	-6.9	-14.52	41.85	11.0

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
4	27.11	C21 H24 O7	[M-H] ⁻	387.1404	387.1449	-4.5	-11.62	75.98	10.0

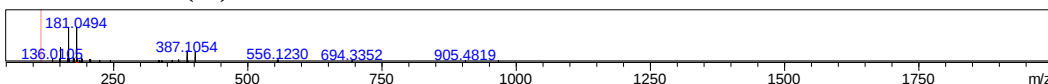
C3H6O3

C28 X19

Event#: 4 MS(E-) Ret. Time : 31.005 Scan# : 3052



Event#: 5 MS/MS(E-) Ret. Time : 31.005 Scan# : 3053 Precursor : 417.1560 Cutoff : 115



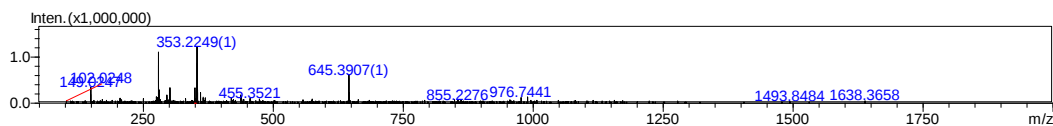
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	73.85	C23 H36 N2 O15	[M-H] ⁻	579.2062	579.2043	1.9	3.28	78.31	7.0

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
4	17.39	C17 H26 N2 O10	[M-H] ⁻	417.1559	417.1515	4.4	10.55	45.14	6.0

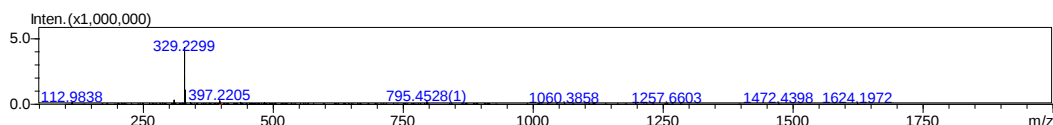
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	54.29	C15 H20 N2 O10	[M-H] ⁻	387.1054	387.1045	0.9	2.32	56.14	7.0

C57 X20 Hexanedioic acid

Event#: 1 MS(E+) Ret. Time : 45.935 Scan# : 4525



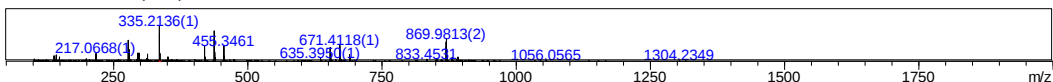
Event#: 4 MS(E-) Ret. Time : 45.935 Scan# : 4528



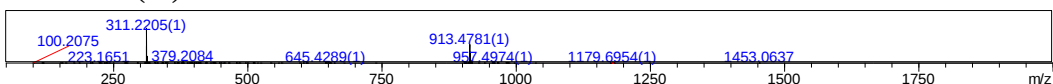
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	32.21	C18 H34 O5	[M-H]-	329.2299	329.2333	-3.4	-10.33	82.34	2.0

C63 X21

Event#: 1 MS(E+) Ret. Time : 50.670 Scan# : 4990



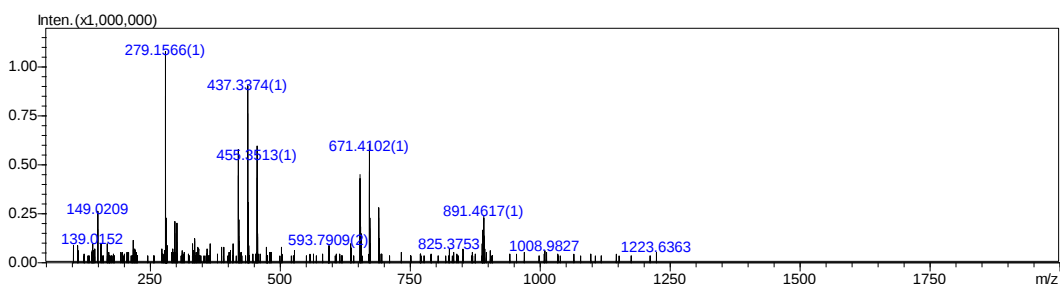
Event#: 4 MS(E-) Ret. Time : 50.670 Scan# : 4992



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	88.60	C18 H32 O4	[M-H]-	311.2212	311.2228	-1.6	-5.14	100.00	3.0

C66 X21

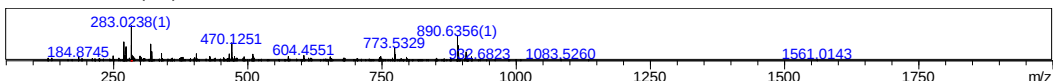
Event#: 1 MS(E+) Ret. Time : 52.363 Scan# : 5156



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	62.38	C28 H46 O2	[M+Na]+	437.3374	437.3390	-1.6	-3.66	66.82	6.0

C69 X23

Event#: 4 MS(E-) Ret. Time : 69.377 Scan# : 6837



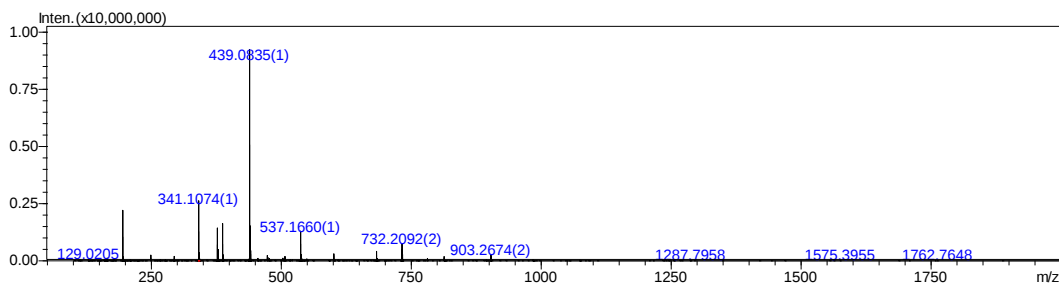
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	44.73	C15 H8 O6	[M-H]-	283.0238	283.0248	-1.0	-3.53	47.74	12.0

3. The HRMS data of DBT2 boiling samples

X13+D4+Z7+Y19+6=49

c03 T1

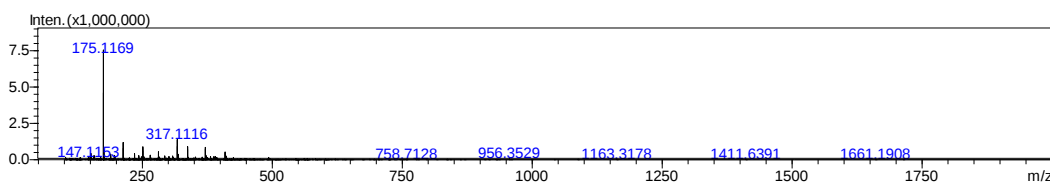
Event#: 4 MS(E-) Ret. Time : 1.293 -> 2.695 Scan# : 127 -> 265



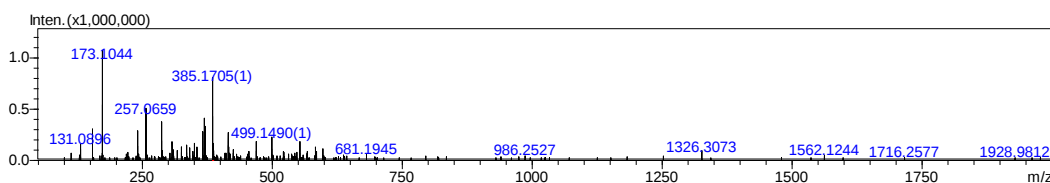
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	83.58	C12 H22 O11	[M-H]-	341.1074	341.1089	-1.5	-4.40	91.34	2.0	

c01 A1

Event#: 1 MS(E+) Ret. Time : 2.395 Scan# : 232



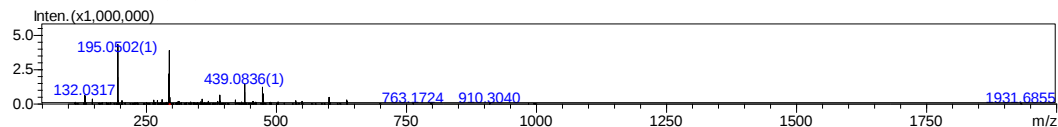
Event#: 4 MS(E-) Ret. Time : 2.395 Scan# : 235



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	60.64	C6 H14 N4 O2	[M-H]-	173.1044	173.1044	0.0	0.00	60.64	2.0	

c02 A4

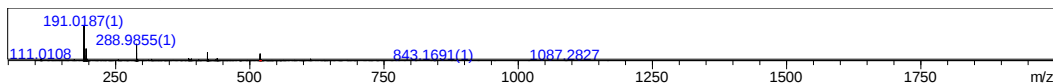
Event#: 4 MS(E-) Ret. Time : 2.575 Scan# : 253



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	46.80	C6 H12 O7	[M-H]-	195.0502	195.0510	-0.8	-4.10	50.73	1.0	

c04 A2

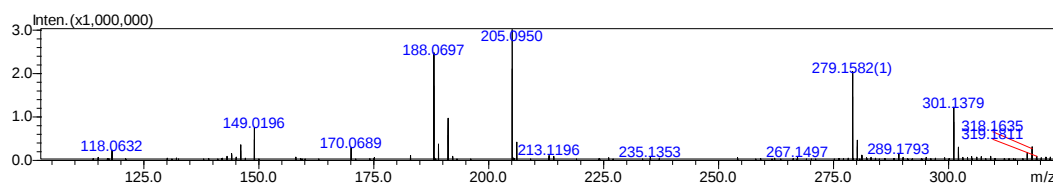
Event#: 4 MS(E-) Ret. Time : 3.643 Scan# : 358



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	82.32	C6 H8 O7	[M-H]-	191.0187	191.0197	-1.0	-5.24	93.97	3.0

c09 A3

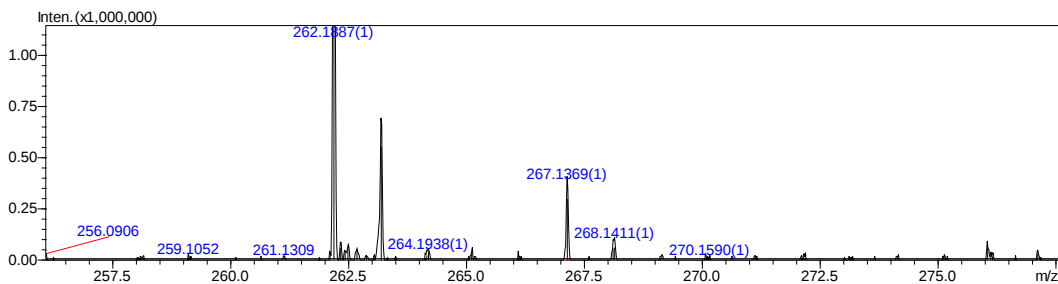
Event#: 1 MS(E+) Ret. Time : 10.842 Scan# : 1059



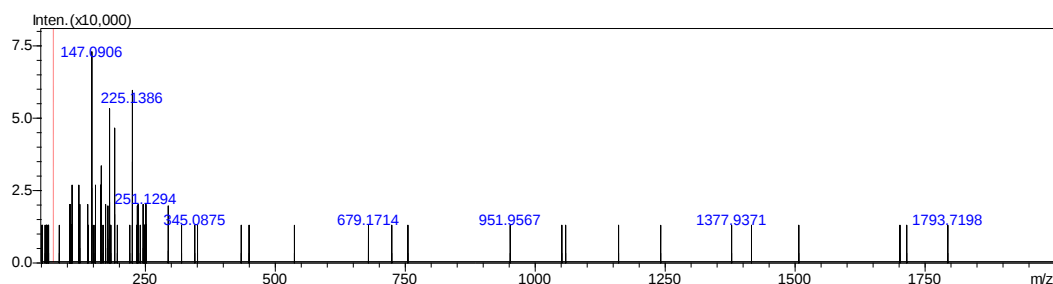
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	69.53	C9 H11 N O2	[M+Na]+	188.0674	188.0682	-0.8	-4.25	75.68	5.0

c08

Event#: 1 MS(E+) Ret. Time : 8.643 -> 9.345 Scan# : 843 -> 912



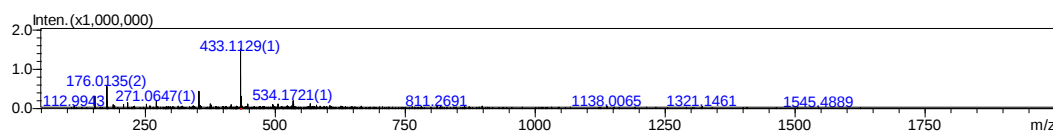
MS/MS(E+) Ret. Time : 8.643 -> 9.345 Scan# : 844 -> 913 Precursor : 267.1328 Cutoff : 73



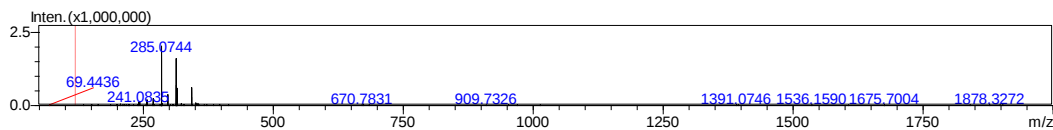
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	57.25	C18 H18 O2	[M+H]+	267.1369	267.1380	-1.1	-4.12	62.09	10.0

c012 Y01

Event#: 4 MS(E-) Ret. Time : 21.207 Scan# : 2069



Event#: 5 MS/MS(E-) Ret. Time : 21.207 Scan# : 2070 Precursor : 433.1129 Cutoff : 119

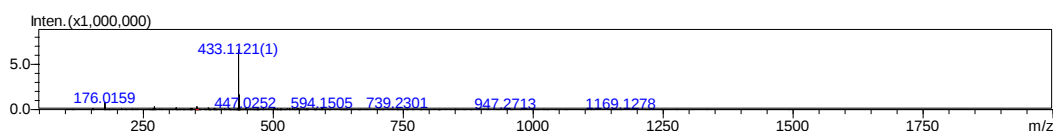


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	66.52	C21 H22 O10	[M-H]-	433.1129	433.1140	-1.1	-2.54	69.18	11.0
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	19.29	C16 H14 O5	[M-H]-	285.0744	285.0768	-2.4	-8.42	34.56	10.0

C5H10O6

c013 Y2

Event#: 4 MS(E-) Ret. Time : 21.322 Scan# : 2080

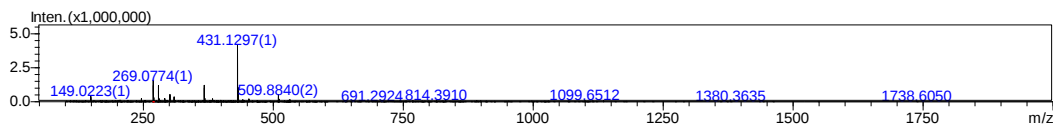


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	88.43	C21 H22 O10	[M-H]-	433.1121	433.1140	-1.9	-4.39	96.62	11.0

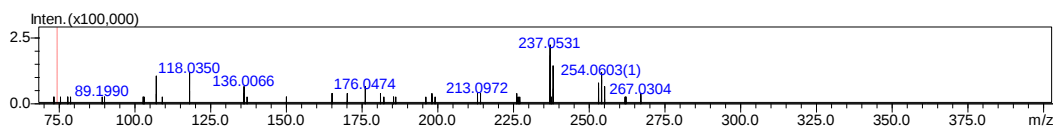
C15H12O5

c018 Y3 ononin

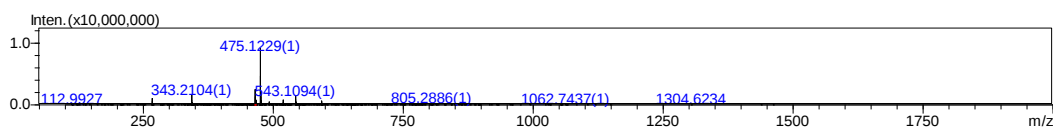
Event#: 1 MS(E+) Ret. Time : 34.517 Scan# : 3373



Event#: 2 MS/MS(E+) Ret. Time : 34.517 Scan# : 3374 Precursor : 269.0774 Cutoff : 74



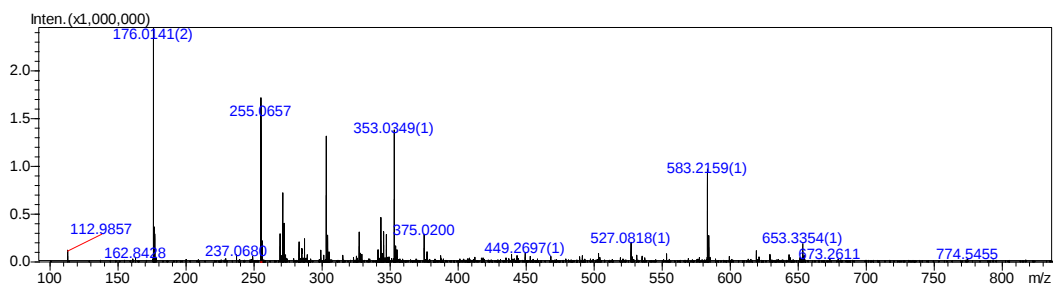
Event#: 4 MS(E-) Ret. Time : 34.517 Scan# : 3376



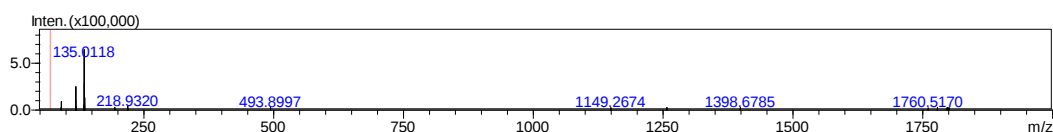
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	87.28	C22 H22 O9	[M+H]+	431.1322	431.1337	-1.5	-3.48	93.05	12.0

c019 Y3 C15 H12 O4

Event#: 4 MS(E-) Ret. Time : 37.480 -> 39.977 Scan#: 3669 -> 3917



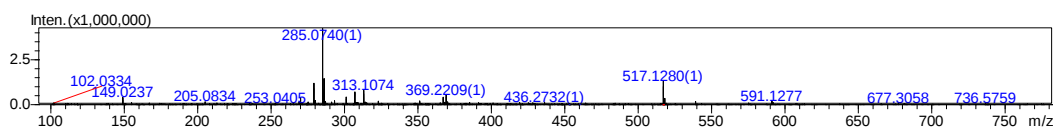
Event#: 5 MS/MS(E-) Ret. Time : 37.480 Scan#: 3670 Precursor : 255.0657 Cutoff : 70



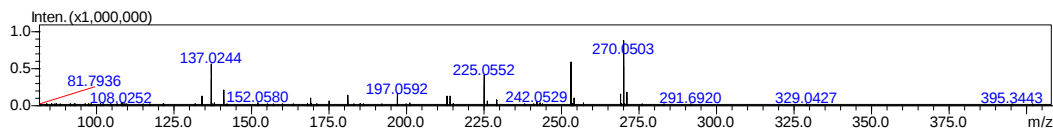
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	59.93	C15 H12 O4	[M-H]-	255.0657	255.0663	-0.6	-2.35	62.02	10.0

c20 Y4 calycosin

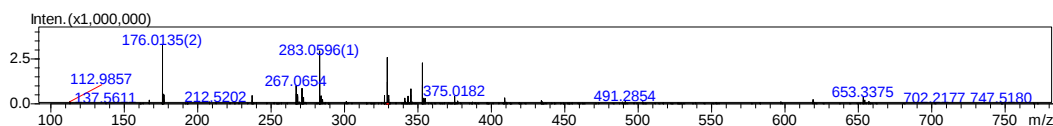
Event#: 1 MS(E+) Ret. Time : 38.072 Scan#: 3725



Event#: 2 MS/MS(E+) Ret. Time : 37.952 Scan#: 3714 Precursor : 285.0741 Cutoff : 78



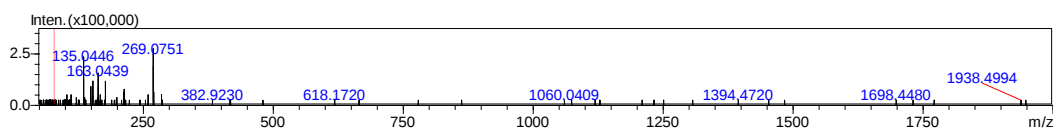
Event#: 4 MS(E-) Ret. Time : 38.072 Scan#: 3728



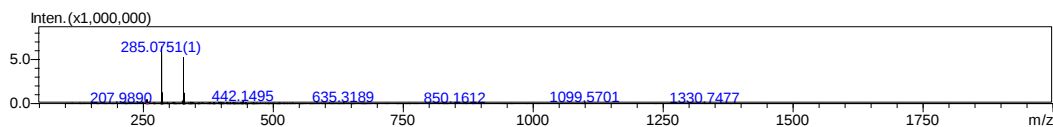
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	51.62	C16 H12 O5	[M-H]-	283.0596	283.0612	-1.6	-5.65	61.82	11.0

c025 Y5

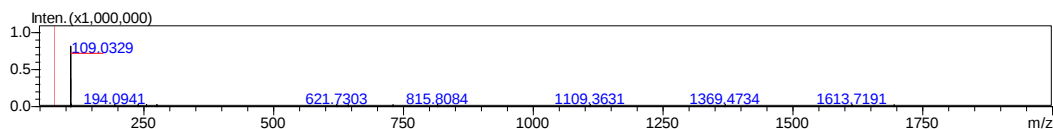
Event#: 2 MS/MS(E+) Ret. Time : 41.273 Scan#: 4043 Precursor : 287.0885 Cutoff : 79



Event#: 4 MS(E-) Ret. Time : 41.273 Scan# : 4045



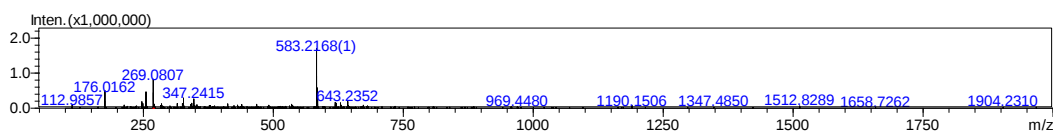
Event#: 5 MS/MS(E-) Ret. Time : 41.222 Scan# : 4040 Precursor : 285.0750 Cutoff : 78



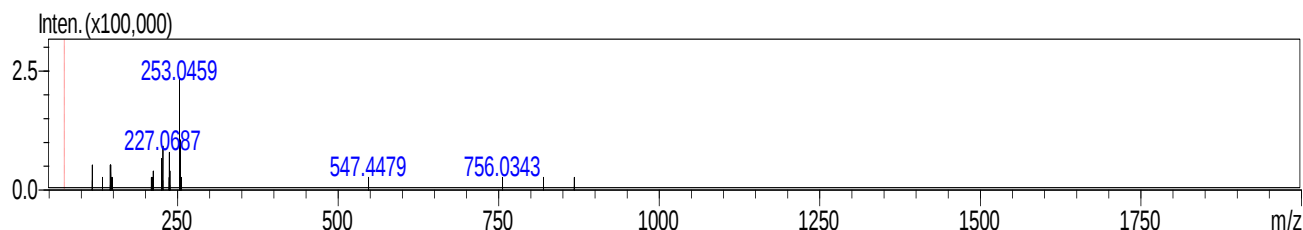
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	47.28	C16 H14 O5	[M-H]-	285.0751	285.0768	-1.7	-5.96	58.80	10.0

c021 Y7

Event#: 4 MS(E-) Ret. Time : 39.917 Scan# : 3911



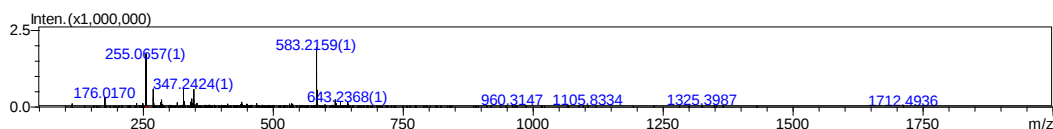
Event#: 5 MS/MS(E-) Ret. Time : 39.917 Scan# : 3912 Precursor : 269.0807 Cutoff : 74



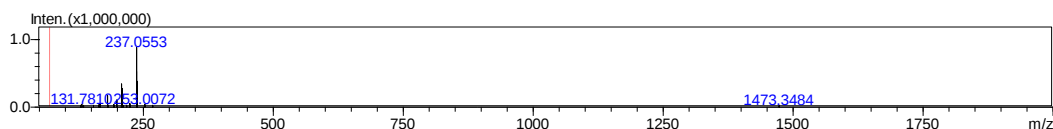
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	40.72	C16 H14 O4	[M-H]-	269.0807	269.0819	-1.2	-4.46	44.58	10.0

c022 Y8

Event#: 4 MS(E-) Ret. Time : 39.977 Scan# : 3917



Event#: 5 MS/MS(E-) Ret. Time : 39.977 Scan# : 3918 Precursor : 255.0657 Cutoff : 70

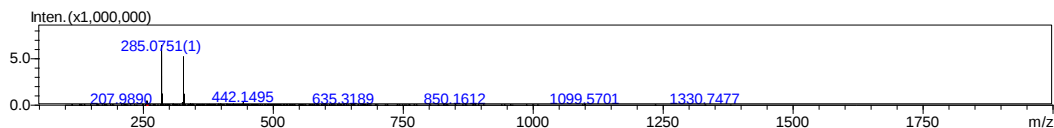


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	52.28	C15 H12 O4	[M-H]-	255.0657	255.0663	-0.6	-2.35	54.10	10.0

C15 H12 O4

c025 Y9

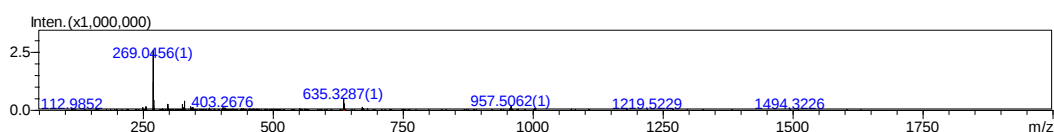
Event#: 4 MS(E-) Ret. Time : 41.273 Scan# : 4045



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	47.28	C16 H14 O5	[M-H]-	285.0751	285.0768	-1.7	-5.96	58.80	10.0

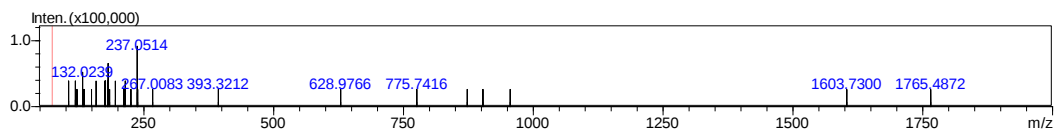
c026 Y10 (genistein)

Event#: 4 MS(E-) Ret. Time : 41.772 Scan# : 4094



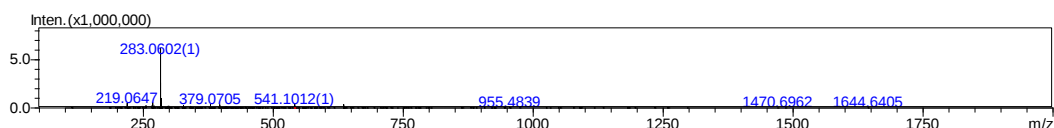
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	60.17	C15 H10 O5	[M-H]-	269.0456	269.0455	0.1	0.37	60.17	11.0

Event#: 5 MS/MS(E-) Ret. Time : 41.712 Scan# : 4089 Precursor : 269.0527 Cutoff : 74



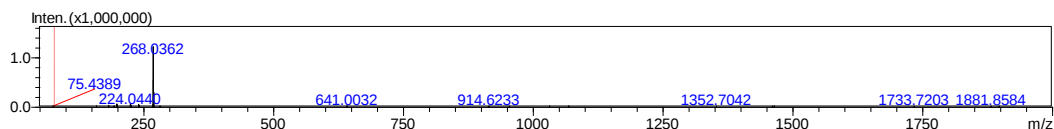
c027 Y11 isomer of calycosin

Event#: 4 MS(E-) Ret. Time : 42.243 Scan# : 4141



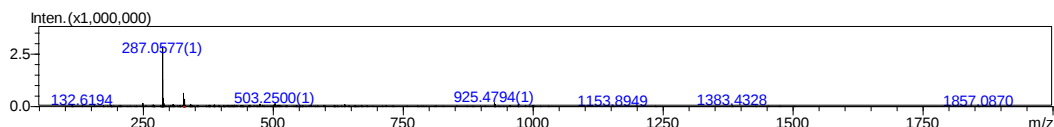
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	67.47	C16 H12 O5	[M-H]-	283.0602	283.0612	-1.0	-3.53	72.02	11.0

Event#: 5 MS/MS(E-) Ret. Time : 42.363 Scan# : 4154 Precursor : 283.0599 Cutoff : 78



c030 Y12

Event#: 4 MS(E-) Ret. Time : 44.690 Scan# : 4383

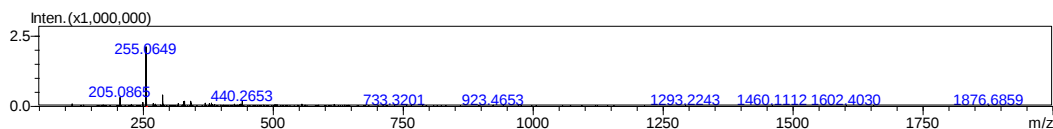


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
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1 57.35 C₁₅H₁₂O₆ [M-H]⁻ 287.0577 287.0561 1.6 5.57 68.03 10.0

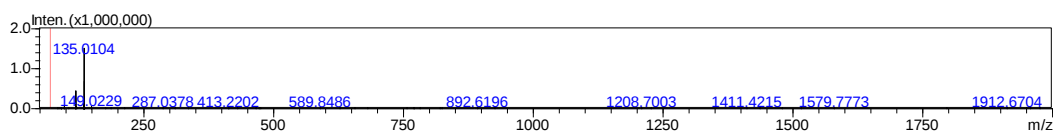
c031 Y13 Liquiritigenin C₁₅H₁₂O₄

Event#: 4 MS(E⁻) Ret. Time : 44.982 Scan# : 4412



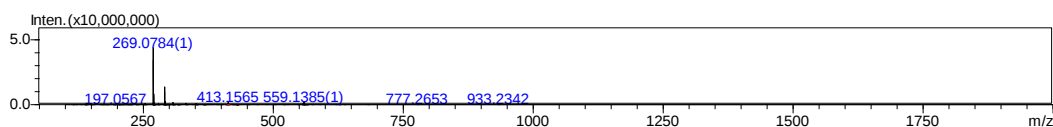
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	38.99	C ₁₅ H ₁₂ O ₄	[M-H] ⁻	255.0649	255.0663	-1.4	-5.49	45.81	10.0

Event#: 5 MS/MS(E⁻) Ret. Time : 44.982 Scan# : 4413 Precursor : 256.0677 Cutoff : 70

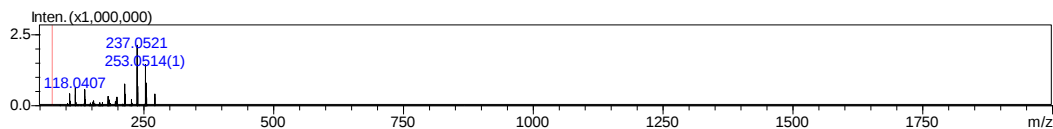


c032 Y14 formononetin

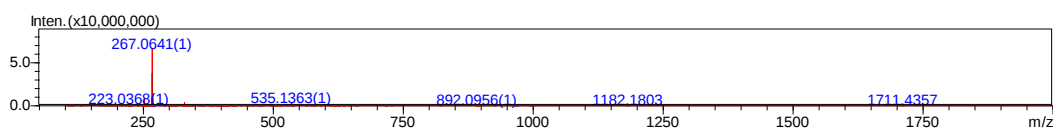
Event#: 1 MS(E⁺) Ret. Time : 45.393 Scan# : 4450



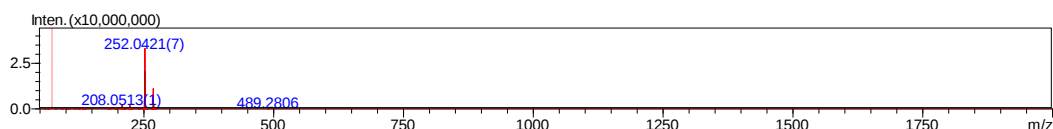
Event#: 2 MS/MS(E⁺) Ret. Time : 45.453 Scan# : 4457 Precursor : 269.0790 Cutoff : 74



Event#: 4 MS(E⁻) Ret. Time : 45.393 Scan# : 4453



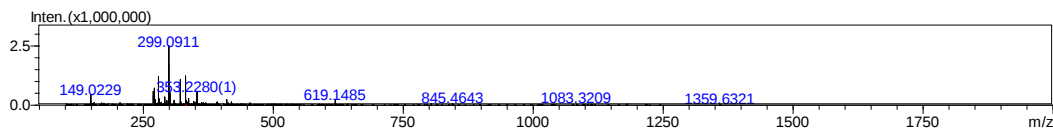
Event#: 5 MS/MS(E⁻) Ret. Time : 45.333 Scan# : 4448 Precursor : 267.2028 Cutoff : 73



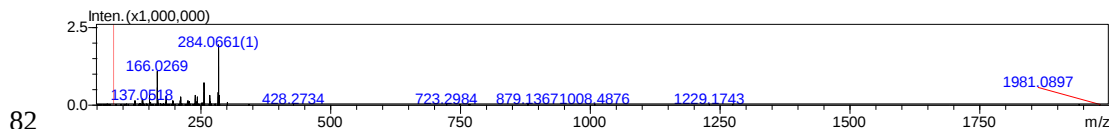
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	39.84	C ₁₆ H ₁₂ O ₄	[M+H] ⁺	269.0784	269.0808	-2.4	-8.92	78.43	11.0

c033 Y15 astrapterocarpan

Event#: 1 MS(E+) Ret. Time : 45.745 Scan# : 4485



Event#: 2 MS/MS(E+) Ret. Time : 45.805 Scan# : 4492 Precursor : 299.0888 Cutoff :

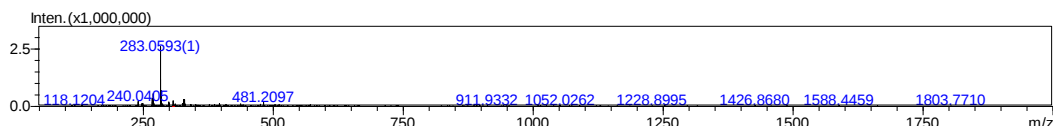


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	38.67	C17 H14 O5	[M+H] ⁺	299.0911	299.0914	-0.3	-1.00	38.67	11.0

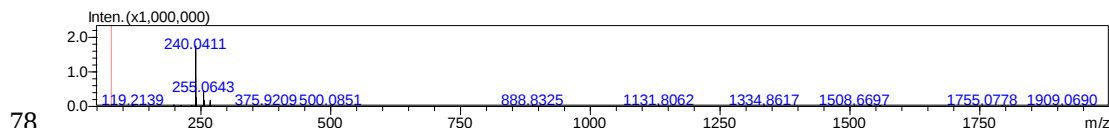
C17H16O5

c034 Y16 wogonin

Event#: 4 MS(E-) Ret. Time : 46.080 Scan# : 4520



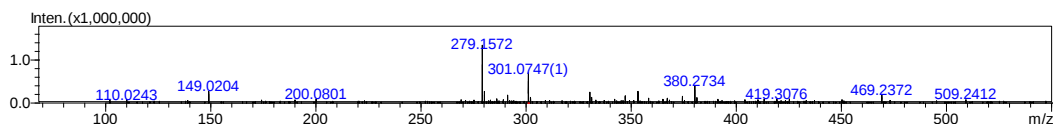
Event#: 5 MS/MS(E-) Ret. Time : 46.028 Scan# : 4516 Precursor : 283.0606 Cutoff :



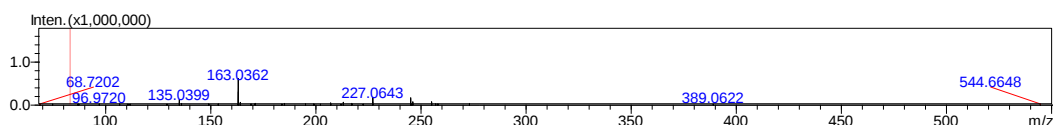
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	34.44	C16 H12 O5	[M-H] ⁻	283.0599	283.0612	-1.3	-4.59	37.84	11.0

c036 Y17

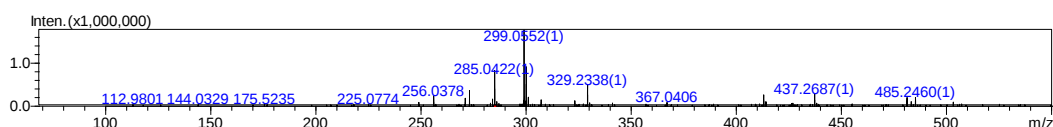
Event#: 1 MS(E+) Ret. Time : 47.772 Scan# : 4685



Event#: 2 MS/MS(E+) Ret. Time : 47.772 Scan# : 4686 Precursor : 301.0748 Cutoff : 83



Event#: 4 MS(E-) Ret. Time : 47.772 Scan# : 4688

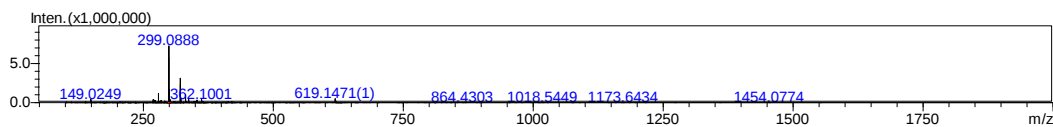


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	59.51	C16 H12 O6	[M-H] ⁻	299.0552	299.0561	-0.9	-3.01	62.66	11.0
C16 H12 O5									

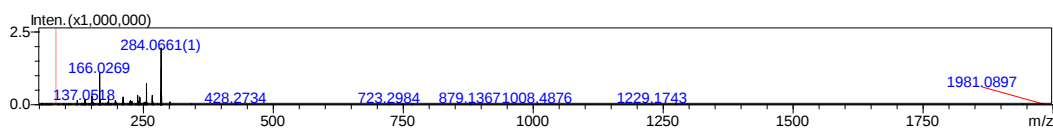
c033

Y6

Event#: 1 MS(E+) Ret. Time : 45.805 Scan# : 4491



Event#: 2 MS/MS(E+) Ret. Time : 45.805 Scan# : 4492 Precursor : 299.0888 Cutoff : 82

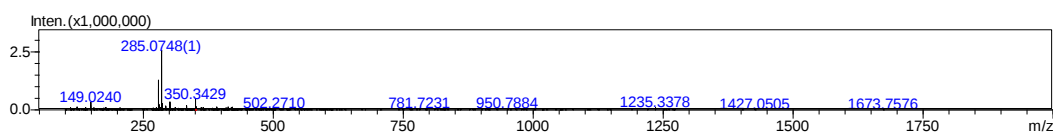


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	88.60	C15 H16 O5	[M+Na] ⁺	299.0888	299.0890	-0.2	-0.67	88.60	8.0
2	50.90	C17 H14 O5	[M+H] ⁺	299.0888	299.0914	-2.6	-8.69	95.86	11.0

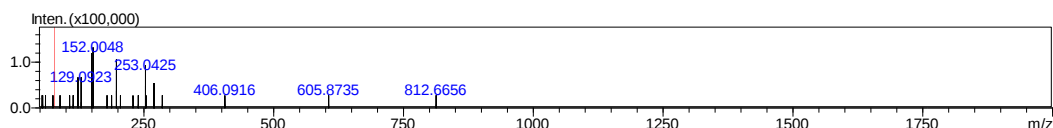
c040

Y18

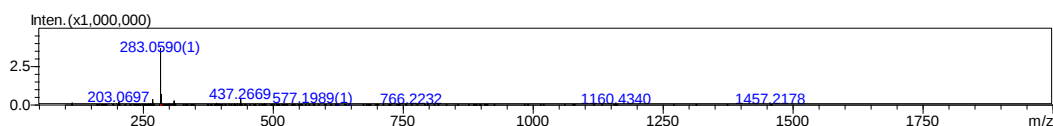
Event#: 1 MS(E+) Ret. Time : 50.435 Scan# : 4947



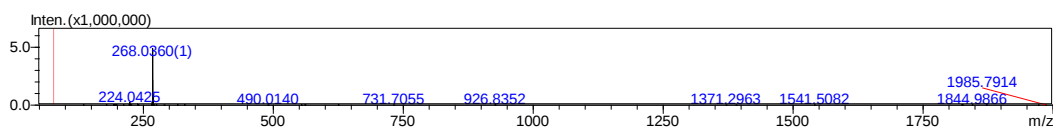
Event#: 2 MS/MS(E+) Ret. Time : 50.375 Scan# : 4942 Precursor : 285.0750 Cutoff : 78



Event#: 4 MS(E-) Ret. Time : 50.375 Scan# : 4944

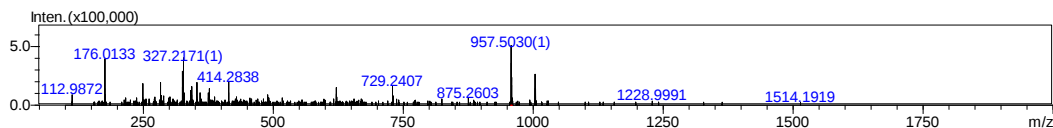


Event#: 5 MS/MS(E-) Ret. Time : 50.375 Scan# : 4945 Precursor : 283.0590 Cutoff : 78

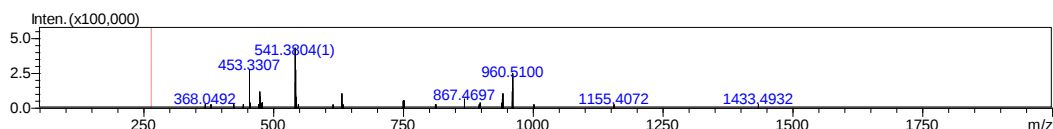


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	79.60	C16 H12 O5	[M+H] ⁺	285.0748	285.0758	-1.0	-3.51	84.93	11.0

c023 Z1 Ba
Event#: 4 MS(E-) Ret. Time : 39.745 Scan# : 3894

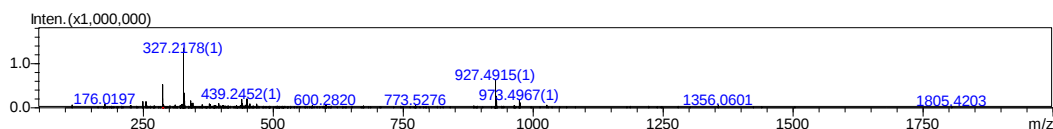


Event#: 5 MS/MS(E-) Ret. Time : 39.745 Scan# : 3895 Precursor : 957.5031 Cutoff : 265



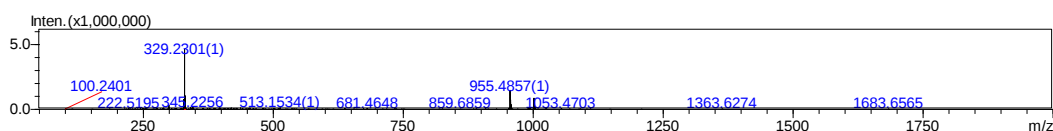
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	51.55	C48 H78 O19	[M-H]-	957.5030	957.5065	-3.5	-3.66	55.22	10.0

c024 Z2 Akebia saponin D
Event#: 4 MS(E-) Ret. Time : 40.903 Scan# : 4008



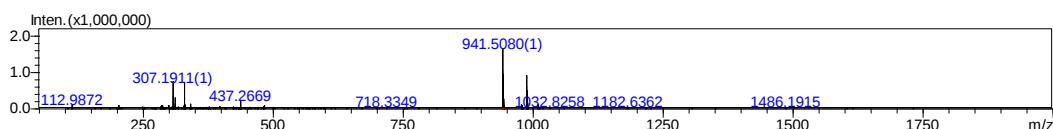
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	63.25	C47 H76 O18	[M-H]-	927.4915	927.4959	-4.4	-4.74	69.77	10.0

c029 Z3 人参皂苷 Ro
Event#: 4 MS(E-) Ret. Time : 43.197 Scan# : 4235

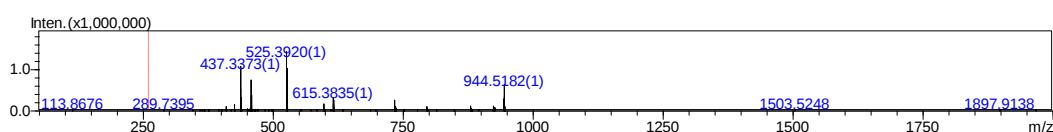


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
4	50.61	C48 H76 O19	[M-H]-	955.4857	955.4908	-5.1	-5.34	58.45	11.0

c035 Z4 Bb
Event#: 4 MS(E-) Ret. Time : 47.592 Scan# : 4670



Event#: 5 MS/MS(E-) Ret. Time : 47.592 Scan# : 4671 Precursor : 941.5083 Cutoff : 260

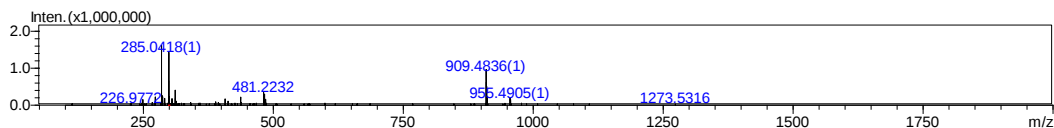


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	82.82	C48 H78 O18	[M-H]-	941.5080	941.5115	-3.5	-3.72	88.86	10.0

c037

Z5

Event#: 4 MS(E-) Ret. Time : 47.943 Scan# : 4705



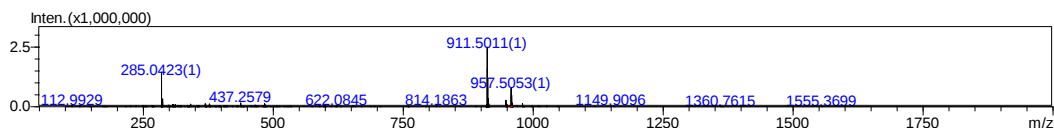
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
4	59.79	C47 H74 O17	[M-H]-	909.4836	909.4853	-1.7	-1.87	61.12	11.0

c038

Z6

Castaraleside H

Event#: 4 MS(E-) Ret. Time : 48.347 Scan# : 4745



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	78.66	C46 H74 O15	[M+HCOO]-	911.5011	911.5010	0.1	0.11	78.66	10.0

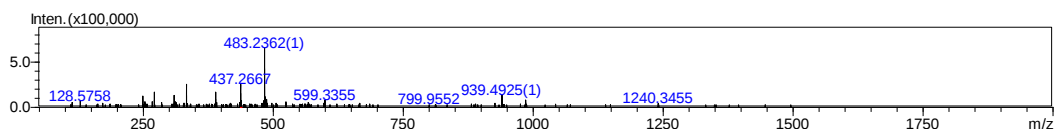
G—I? ? ?

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	86.89	C46 H74 O15	[M+HCOO]-	911.5012	911.5010	0.2	0.22	86.89	10.0
2	86.89	C47 H76 O17	[M-H]-	911.5012	911.5010	0.2	0.22	86.89	10.0

c039

Z7

Event#: 4 MS(E-) Ret. Time : 50.065 Scan# : 4914

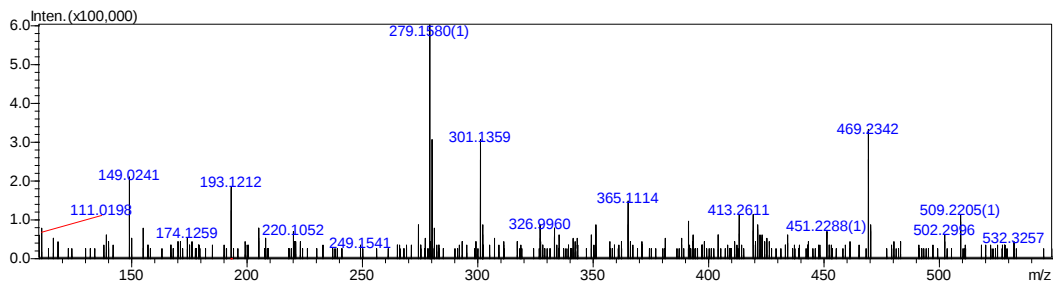


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	33.31	C48 H76 O18	[M-H]-	939.4925	939.4959	-3.4	-3.62	35.64	11.0

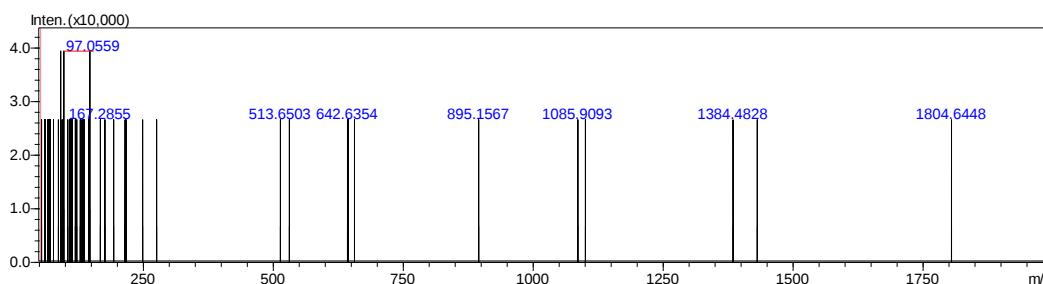
c042

D1 A

Event#: 1 MS(E+) Ret. Time : 51.560 Scan# : 5058



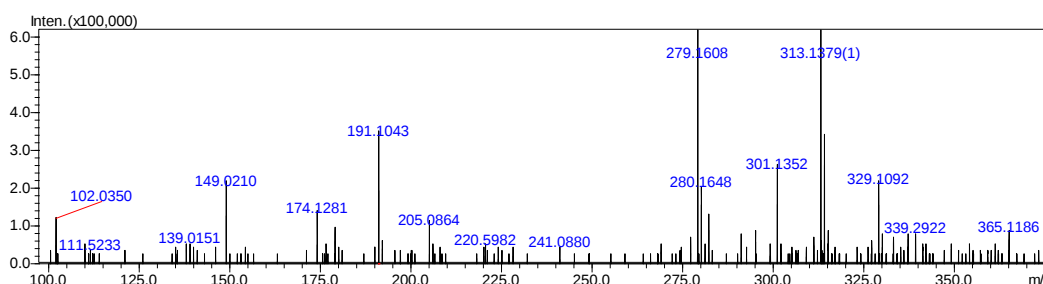
MS/MS(E+) Ret. Time : 51.560 Scan# : 5059 Precursor : 193.1212 Cutoff : 53



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	71.30	C12 H16 O2	[M+H] ⁺	193.1212	193.1223	-1.1	-5.70	85.91	5.0

c043 D2

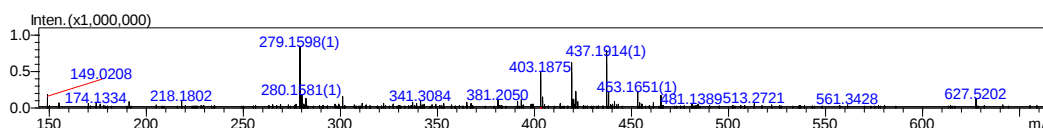
Event#: 1 MS(E+) Ret. Time : 55.212 Scan# : 5417



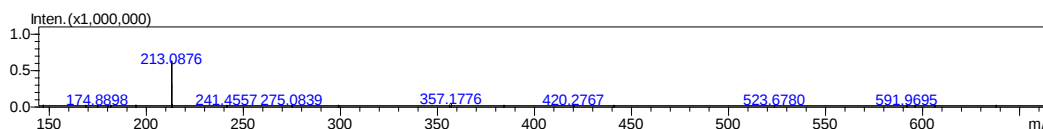
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	85.23	C10 H16 O2	[M+Na] ⁺	191.1043	191.1043	0.0	0.00	85.23	3.0
2	4.70	C12 H14 O2	[M+H] ⁺	191.1043	191.1067	-2.4	-12.56	14.18	6.0

c044 D3 Z-

Event#: 1 MS(E+) Ret. Time : 59.250 Scan# : 5814



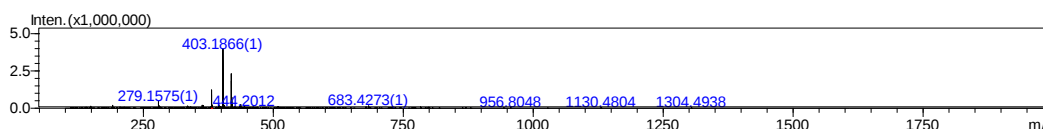
Event#: 2 MS/MS(E+) Ret. Time : 59.250 Scan# : 5815 Precursor : 403.1875 Cutoff : 111



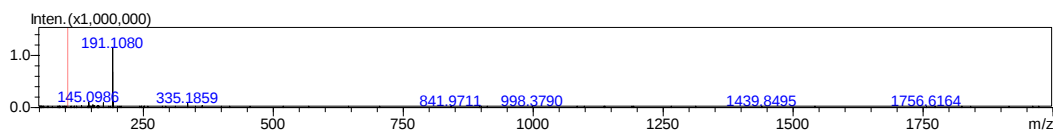
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	0.00	C12 H14 O2	[M+Na] ⁺	213.0876	213.0886	-1.0	-4.69	0.00	6.0

c045 D4 E-

Event#: 1 MS(E+) Ret. Time : 61.765 Scan# : 6063



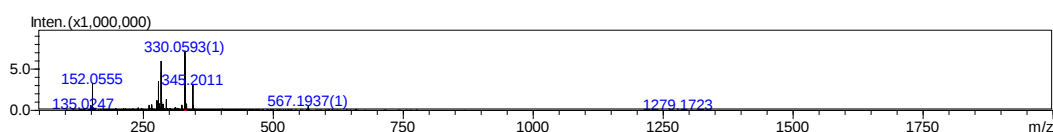
Event#: 2 MS/MS(E+) Ret. Time : 61.765 Scan# : 6064 Precursor : 381.2059 Cutoff : 105



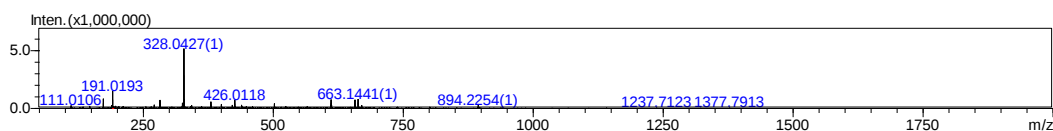
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	38.11	C12 H14 O2	[M+H] ⁺	191.1080	191.1067	1.3	6.80	52.94	6.0
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	42.13	C12 H14 O2	[M+Na] ⁺	213.0893	213.0886	0.7	3.29	44.69	6.0

c05 X1

Event#: 1 MS(E+) Ret. Time : 4.477 Scan# : 437



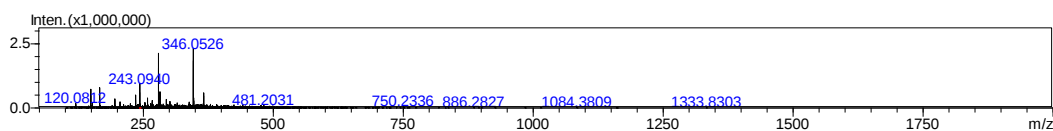
Event#: 4 MS(E-) Ret. Time : 4.477 Scan# : 440



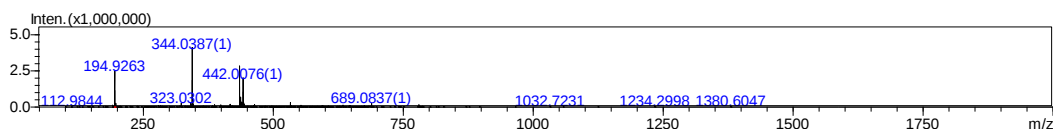
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	99.45	C11 H11 N3 O9	[M-H] ⁻	328.0427	328.0423	0.4	1.22	100.00	8.0

c06 X2

Event#: 1 MS(E+) Ret. Time : 6.172 Scan# : 602



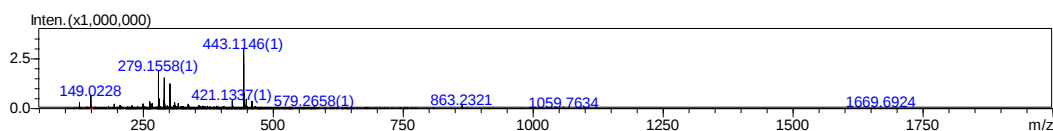
Event#: 4 MS(E-) Ret. Time : 6.172 Scan# : 605



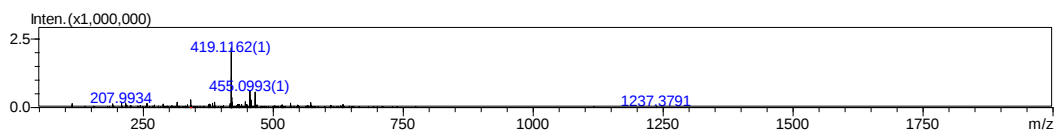
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	81.82	C11 H11 N3 O10	[M-H] ⁻	344.0387	344.0372	1.5	4.36	89.32	8.0

c07 X4

Event#: 1 MS(E+) Ret. Time : 9.120 Scan# : 890



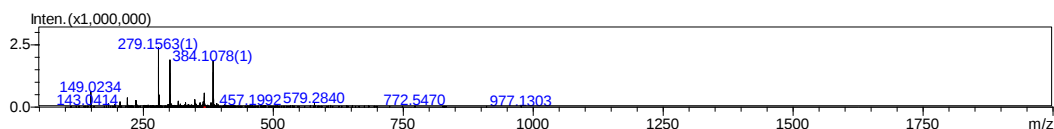
Event#: 4 MS(E-) Ret. Time : 9.120 Scan# : 892



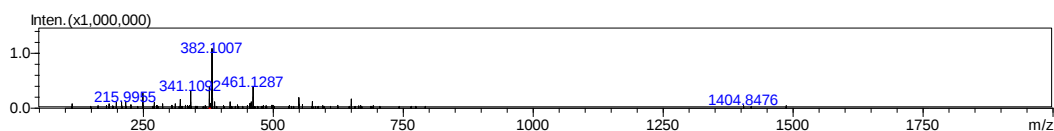
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	84.70	C17 H24 O12	[M+Na] ⁺	443.1146	443.1160	-1.4	-3.16	89.54	6.0	

c010 X5

Event#: 1 MS(E+) Ret. Time : 12.765 Scan# : 1250



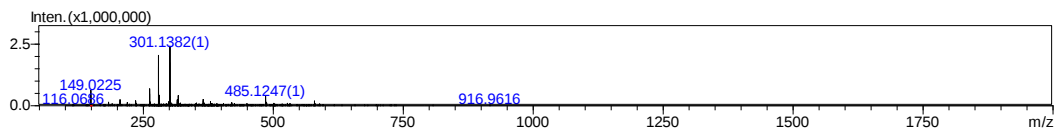
Event#: 4 MS(E-) Ret. Time : 12.765 Scan# : 1253



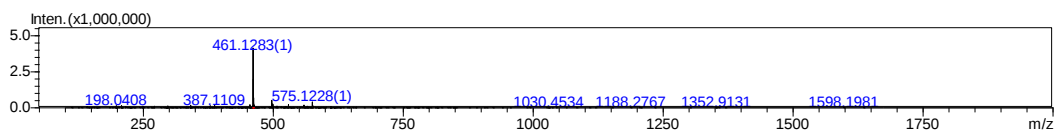
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	63.30	C13 H21 N O12	[M-H] ⁻	382.1007	382.0991	1.6	4.19	68.79	4.0	

c011 X6

Event#: 1 MS(E+) Ret. Time : 13.840 Scan# : 1355



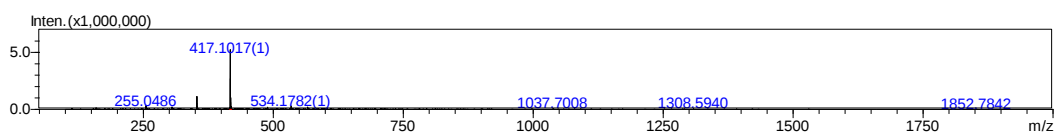
Event#: 4 MS(E-) Ret. Time : 13.840 Scan# : 1358



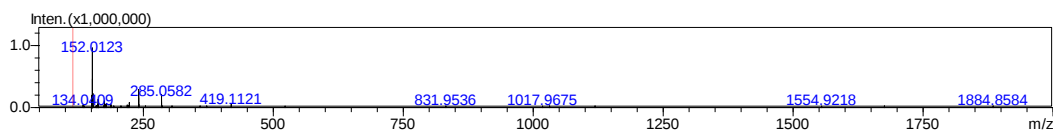
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	69.28	C19 H26 O13	[M-H] ⁻	461.1283	461.1301	-1.8	-3.90	74.69	7.0	

c014 X7+

Event#: 4 MS(E-) Ret. Time : 22.020 Scan# : 2147



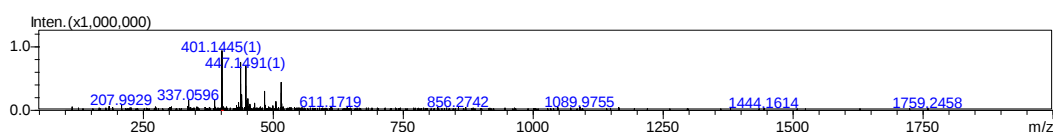
Event#: 5 MS/MS(E-) Ret. Time : 22.020 Scan#: 2148 Precursor : 417.1018 Cutoff : 115



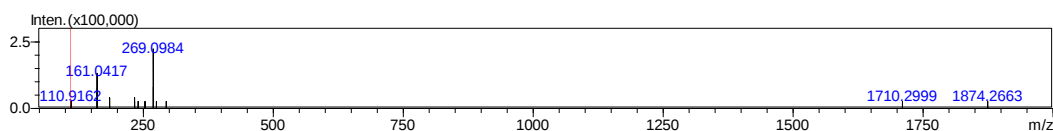
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	86.57	C17 H22 O12	[M-H]-	417.1017	417.1038	-2.1	-5.03	96.51	7.0	
4	9.29	C12 H14 O8	[M-H]-	285.0582	285.0616	-3.4	-11.93	26.65	6.0	

c015 X8 =

Event#: 4 MS(E-) Ret. Time : 23.018 Scan#: 2243



Event#: 5 MS/MS(E-) Ret. Time : 23.018 Scan#: 2244 Precursor : 401.1445 Cutoff : 111

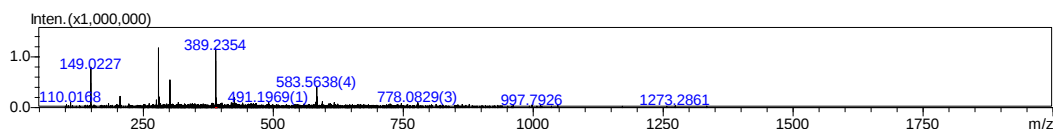


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	86.04	C18 H26 O10	[M-H]-	401.1445	401.1453	-0.8	-1.99	88.22	6.0	

C5H8O4 xylan

c016 X9 =

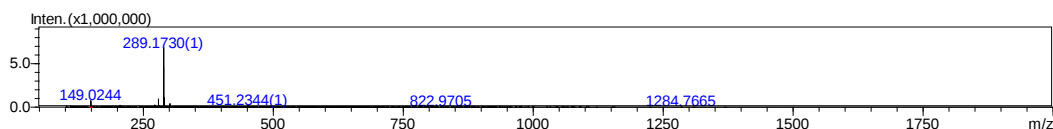
Event#: 1 MS(E+) Ret. Time : 23.080 Scan#: 2246



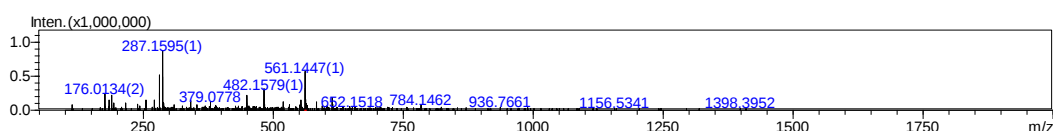
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	59.93	C23 H32 O5	[M+H]+	389.2325	389.2323	0.2	0.51	59.93	8.0	

c017 X10 =

Event#: 1 MS(E+) Ret. Time : 26.998 Scan#: 2628



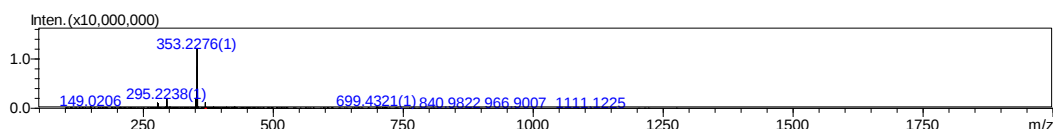
Event#: 4 MS(E-) Ret. Time : 26.998 Scan#: 2630



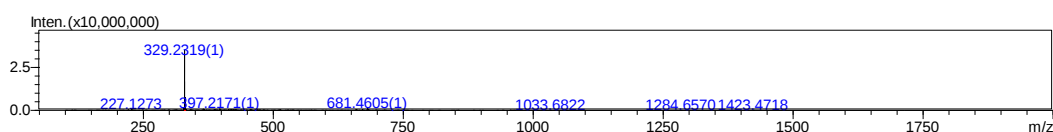
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	35.86	C13 H24 N2 O5	[M+H] ⁺	289.1730	289.1758	-2.8 -9.68	83.01	3.0	
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	54.79	C13 H24 N2 O5	[M-H] ⁻	287.1595	287.1612	-1.7 -5.92	67.81	3.0	

c028 X11 Hexanedioic acid =

Event#: 1 MS(E⁺) Ret. Time : 42.965 Scan# : 4209



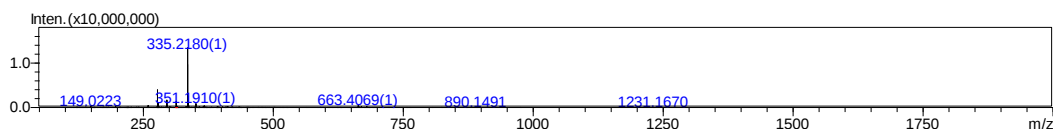
Event#: 4 MS(E⁻) Ret. Time : 42.965 Scan# : 4212



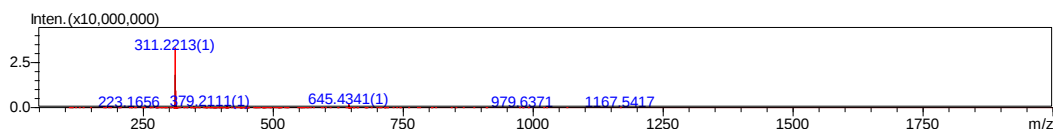
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
3	55.25	C18 H34 O5	[M+Na] ⁺	353.2276	353.2298	-2.2 -6.23	71.10	2.0	
1	80.09	C18 H34 O5	[M-H] ⁻	329.2319	329.2333	-1.4 -4.25	87.18	2.0	

c041 X12 =

Event#: 1 MS(E⁺) Ret. Time : 50.667 Scan# : 4970



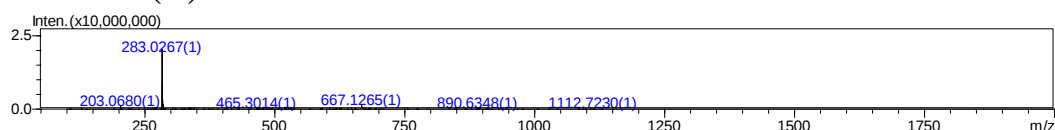
Event#: 4 MS(E⁻) Ret. Time : 50.667 Scan# : 4973



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	79.68	C18 H32 O4	[M+Na] ⁺	335.2180	335.2193	-1.3 -3.88	85.86	3.0	
3	51.89	C19 H28 N4	[M+Na] ⁺	335.2180	335.2206	-2.6 -7.76	83.15	8.0	
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	75.98	C18 H32 O4	[M-H] ⁻	311.2213	311.2228	-1.5 -4.82	84.01	3.0	
4	44.87	C19 H28 N4	[M-H] ⁻	311.2213	311.2241	-2.8 -9.00	89.75	8.0	

c046 X13

Event#: 4 MS(E⁻) Ret. Time : 69.093 Scan# : 6786

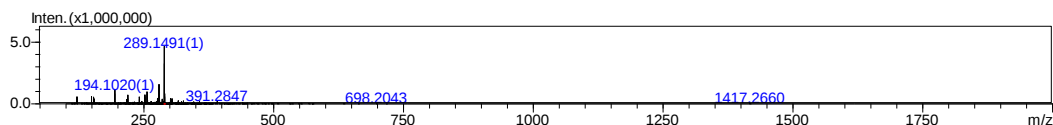


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	61.26	C15 H8 O6	[M-H] ⁻	283.0257	283.0248	0.9 3.18	64.79	12.0	

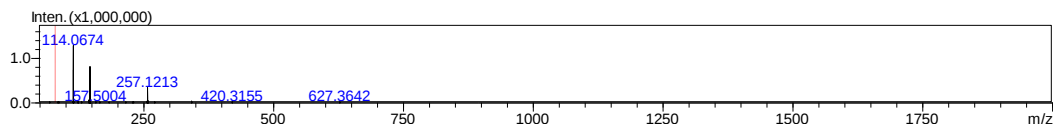
4. The HRMS data of DBT1 urine samples

M1

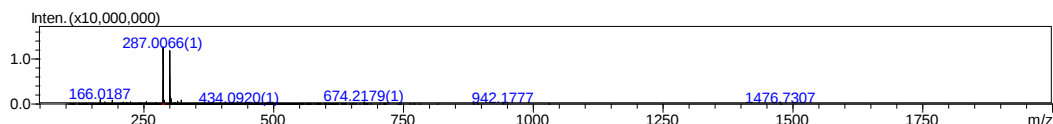
Event#: 1 MS(E+) Ret. Time : 4.130 Scan# : 403



Event#: 2 MS/MS(E+) Ret. Time : 4.130 Scan# : 404 Precursor : 289.1490 Cutoff : 80



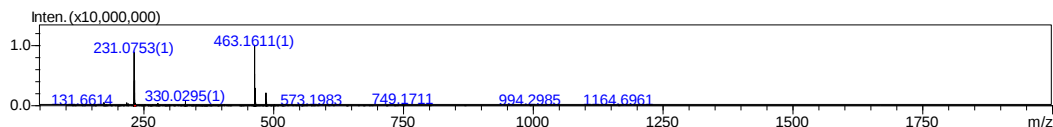
Event#: 4 MS(E-) Ret. Time : 4.130 Scan# : 406



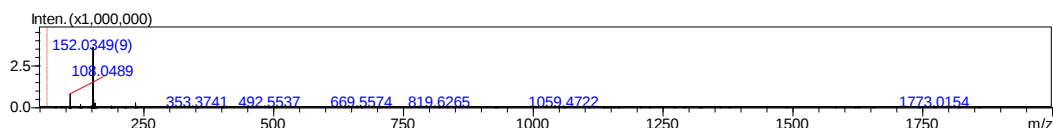
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	45.75	C10 H8 O10	[M-H]-	287.0066	287.0045	2.1	7.32	68.49	7.0
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	10.69	C17 H20 O4	[M+H]+	289.1491	289.1434	5.7	19.71	75.76	8.0

M2

Event#: 4 MS(E-) Ret. Time : 28.110 Scan# : 2764



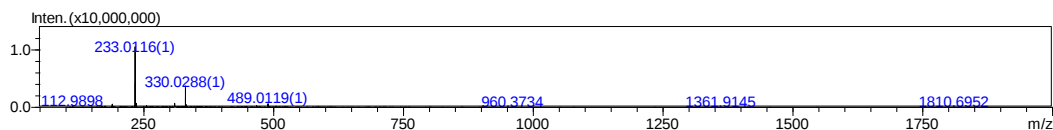
Event#: 5 MS/MS(E-) Ret. Time : 28.110 Scan# : 2765 Precursor : 231.9906 Cutoff : 64



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	67.52	C12 H12 N2 O3	[M+H]+	233.0909	233.0921	-1.2	-5.15	76.29	8.0

M3

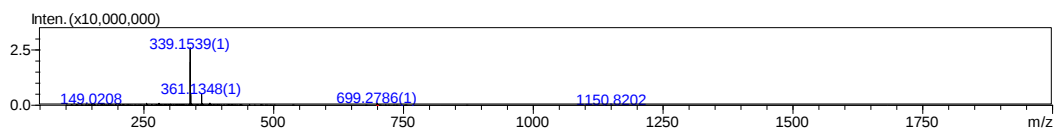
Event#: 4 MS(E-) Ret. Time : 28.848 Scan# : 2838



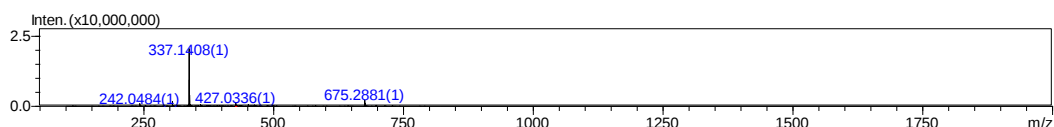
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	51.23	C12 H2 N4 O2	[M-H]-	233.0116	233.0105	1.1	4.72	56.48	14.0

M4

Event#: 1 MS(E+) Ret. Time : 29.415 Scan# : 2891



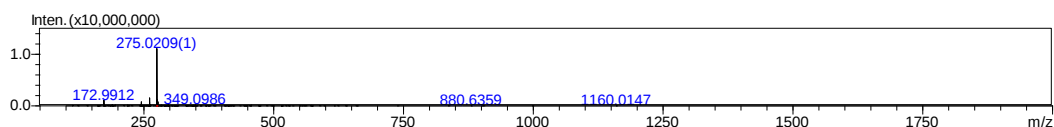
Event#: 4 MS(E-) Ret. Time : 29.415 Scan# : 2894



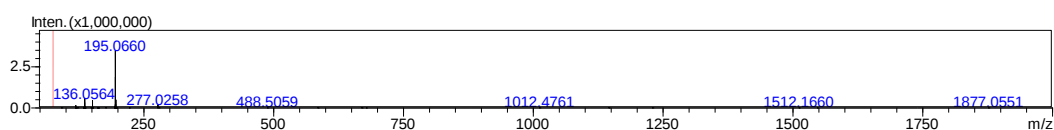
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	67.69	C16 H22 N2 O6	[M-H]-	337.1407	337.1405	0.2	0.59	67.69	7.0

M5

Event#: 4 MS(E-) Ret. Time : 31.338 Scan# : 3083



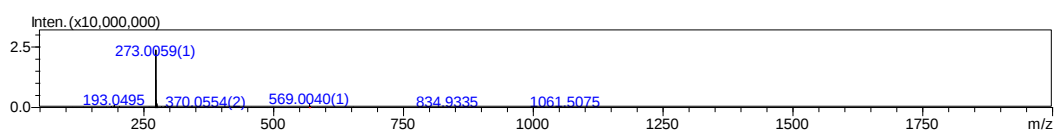
Event#: 5 MS/MS(E-) Ret. Time : 31.338 Scan# : 3084 Precursor : 275.0209 Cutoff : 76



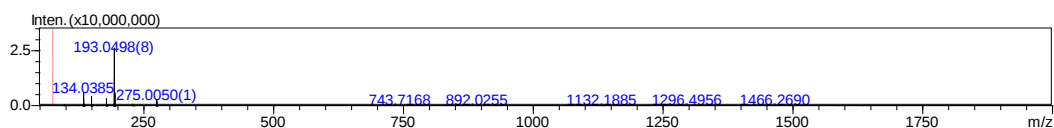
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	57.28	C13 H8 O7	[M-H]-	275.0209	275.0197	1.2	4.36	62.53	10.0

M6

Event#: 4 MS(E-) Ret. Time : 32.678 Scan# : 3216



Event#: 5 MS/MS(E-) Ret. Time : 32.858 Scan# : 3235 Precursor : 273.0063 Cutoff : 75

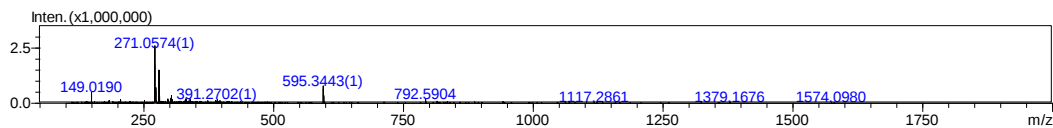


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	39.52	C13 H6 O7	[M-H]-	273.0063	273.0041	2.2	8.06	66.53	11.0

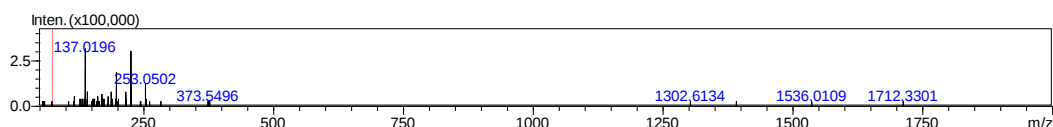
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	50.55	C15 H12 O5	[M+H]+	273.0750	273.0758	-0.8	-2.93	53.11	10.0

M7

Event#: 1 MS(E+) Ret. Time : 33.038 Scan# : 3249



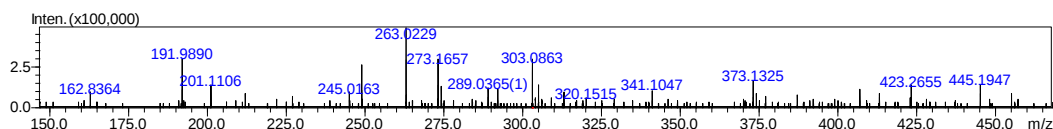
Event#: 2 MS/MS(E+) Ret. Time : 33.038 Scan# : 3250 Precursor : 271.0574 Cutoff : 75



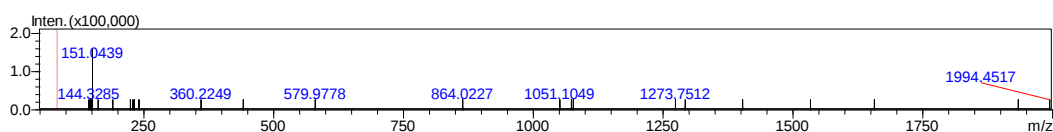
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
3	29.45	C15 H10 O5	[M+H] ⁺	271.0585	271.0601	-1.6	-5.90	36.36	11.0

M8

Event#: 4 MS(E-) Ret. Time : 36.155 Scan# : 3559



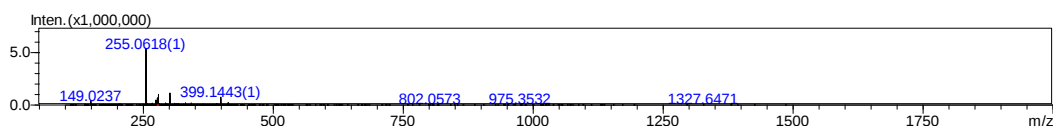
Event#: 5 MS/MS(E-) Ret. Time : 36.155 Scan# : 3560 Precursor : 303.0865 Cutoff : 83



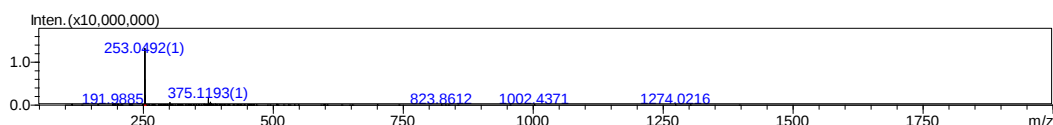
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	15.77	C16 H16 O6	[M-H] ⁻	303.0863	303.0874	-1.1	-3.63	16.88	9.0
2	15.77	C15 H14 O4	[M+HCOO] ⁻	303.0863	303.0874	-1.1	-3.63	16.88	9.0

M9

Event#: 1 MS(E+) Ret. Time : 36.705 Scan# : 3611



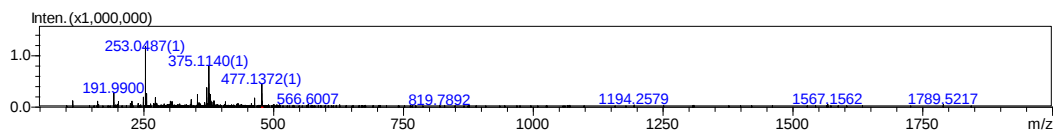
Event#: 4 MS(E-) Ret. Time : 36.705 Scan# : 3613



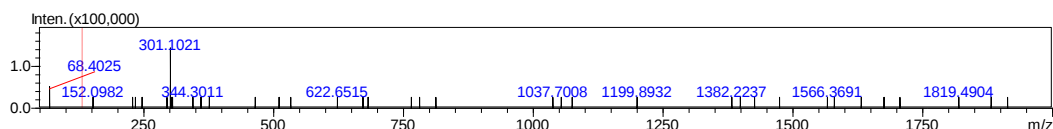
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	73.78	C15 H10 O4	[M-H] ⁻	253.0492	253.0506	-1.4	-5.53	87.11	11.0

M10

Event#: 4 MS(E-) Ret. Time : 36.808 Scan# : 3624



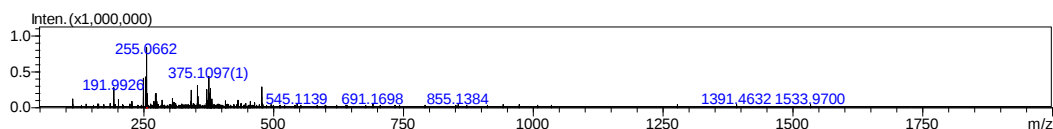
Event#: 5 MS/MS(E-) Ret. Time : 36.808 Scan# : 3625 Precursor : 477.1372 Cutoff : 132



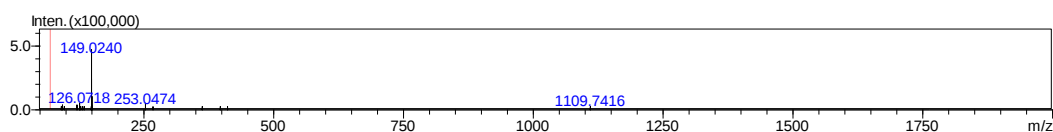
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
4	43.96	C23 H26 O11	[M-H]-	477.1372	477.1402	-3.0	-6.29	57.01	11.0

M11

Event#: 4 MS(E-) Ret. Time : 36.868 Scan# : 3629



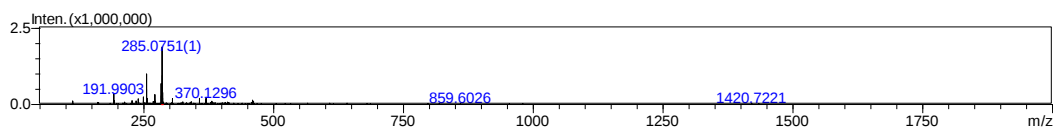
Event#: 5 MS/MS(E-) Ret. Time : 36.868 Scan# : 3630 Precursor : 255.0662 Cutoff : 70



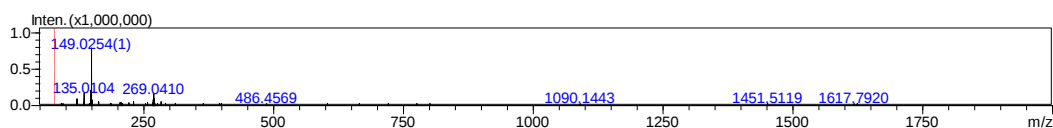
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	53.81	C15 H12 O4	[M-H]-	255.0662	255.0663	-0.1	-0.39	53.81	10.0

M13

Event#: 4 MS(E-) Ret. Time : 37.435 Scan# : 3686



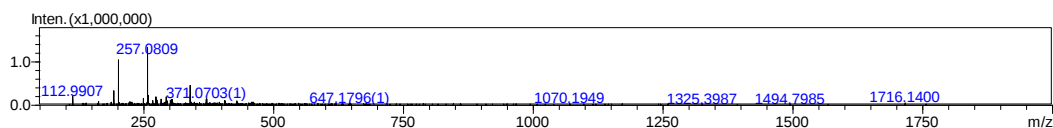
Event#: 5 MS/MS(E-) Ret. Time : 37.435 Scan# : 3687 Precursor : 285.0751 Cutoff : 78



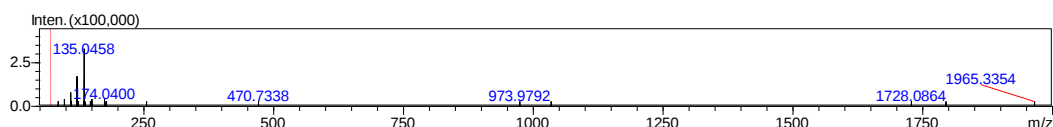
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	54.35	C16 H14 O5	[M-H]-	285.0751	285.0768	-1.7	-5.96	67.60	10.0

M14

Event#: 4 MS(E-) Ret. Time : 37.195 Scan# : 3662



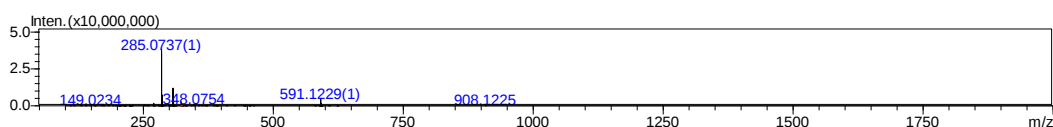
Event#: 5 MS/MS(E-) Ret. Time : 37.195 Scan# : 3663 Precursor : 257.0808 Cutoff : 71



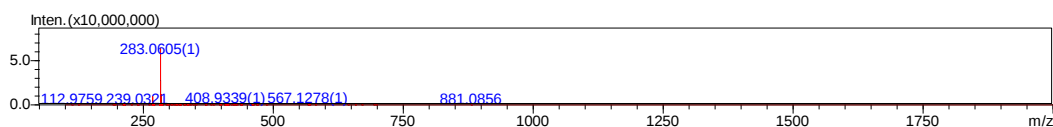
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	24.88	C15 H14 O4	[M-H]-	257.0809	257.0819	-1.0	-3.89	26.81	9.0

M15

Event#: 1 MS(E+) Ret. Time : 38.070 Scan# : 3746



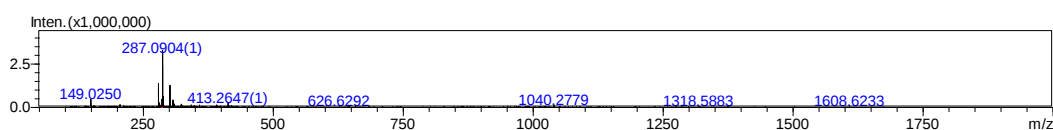
Event#: 4 MS(E-) Ret. Time : 38.070 Scan# : 3749



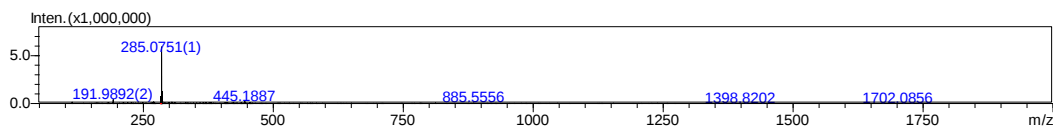
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	71.00	C16 H12 O5	[M-H]-	283.0605	283.0612	-0.7	-2.47	73.71	11.0

M16

Event#: 1 MS(E+) Ret. Time : 38.362 Scan# : 3775



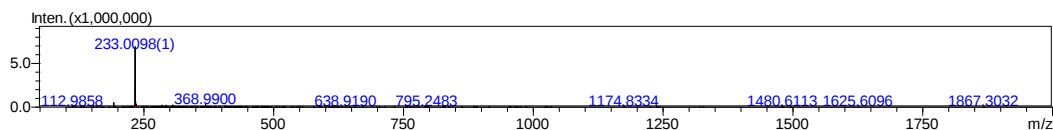
Event#: 4 MS(E-) Ret. Time : 38.362 Scan# : 3778



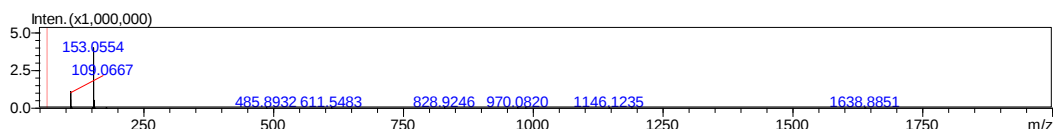
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	48.12	C16 H14 O5	[M-H]-	285.0751	285.0768	-1.7	-5.96	59.85	10.0

M17

Event#: 4 MS(E-) Ret. Time : 39.367 Scan# : 3876



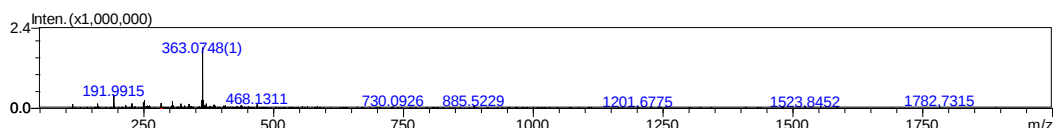
Event#: 5 MS/MS(E-) Ret. Time : 39.367 Scan# : 3877 Precursor : 233.0098 Cutoff : 64



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	72.09	C11 H6 O6	[M-H]-	233.0098	233.0092	0.6	2.57	75.04	9.0
4	54.66	C12 H2 N4 O2	[M-H]-	233.0098	233.0105	-0.7	-3.00	57.54	14.0

M18

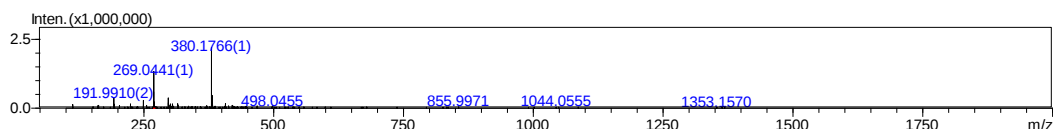
Event#: 4 MS(E-) Ret. Time : 40.260 Scan# : 3965



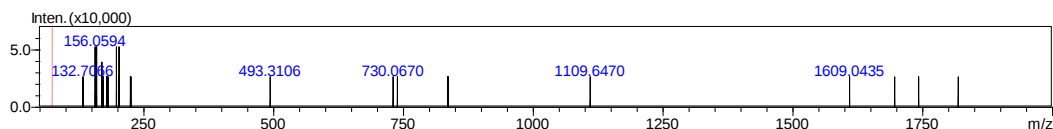
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	53.49	C13 H18 O7 S	[M+HCOO]-	363.0748	363.0755	-0.7	-1.93	54.76	5.0
4	40.39	C17 H16 O9	[M-H]-	363.0748	363.0722	2.6	7.16	59.06	10.0
5	40.39	C16 H14 O7	[M+HCOO]-	363.0748	363.0722	2.6	7.16	59.06	10.0

M19

Event#: 4 MS(E-) Ret. Time : 41.755 Scan# : 4112



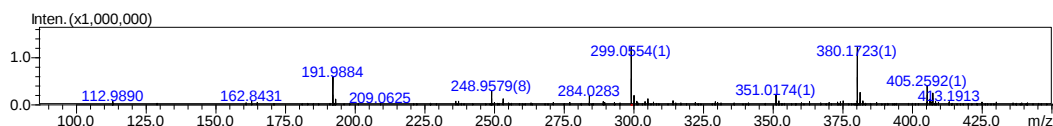
Event#: 5 MS/MS(E-) Ret. Time : 41.755 Scan# : 4113 Precursor : 269.0441 Cutoff : 74



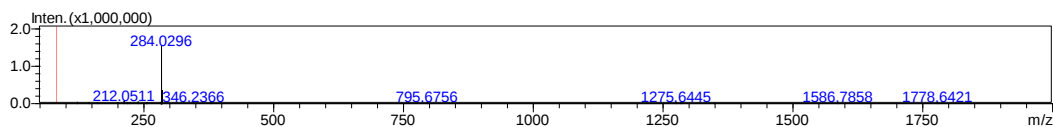
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	40.88	C15 H10 O5	[M-H]-	269.0441	269.0455	-1.4	-5.20	46.46	11.0

M20

Event#: 4 MS(E-) Ret. Time : 42.365 Scan# : 4172



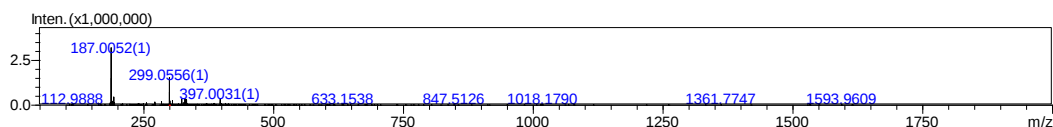
Event#: 5 MS/MS(E-) Ret. Time : 42.365 Scan# : 4173 Precursor : 299.0555 Cutoff : 82



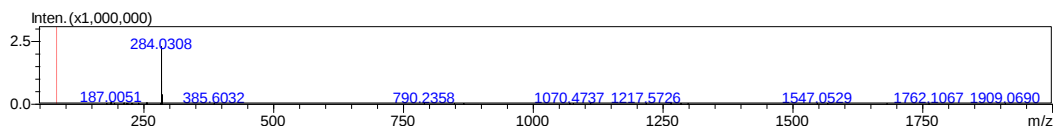
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	51.88	C16 H12 O6	[M-H]-	299.0554	299.0561	-0.7	-2.34	53.67	11.0

M21

Event#: 4 MS(E-) Ret. Time : 42.923 Scan# : 4227



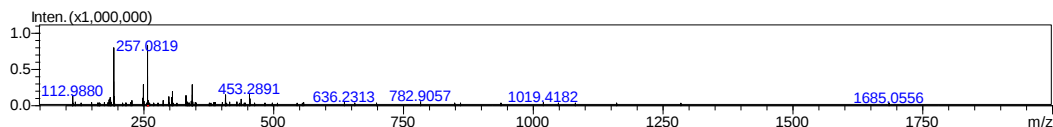
Event#: 5 MS/MS(E-) Ret. Time : 42.923 Scan# : 4228 Precursor : 299.0556 Cutoff : 82



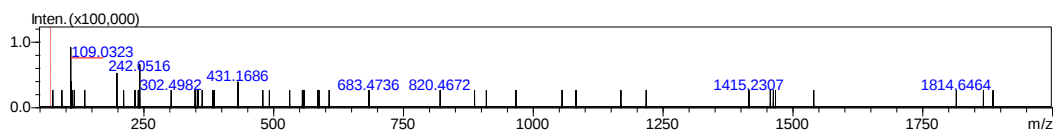
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	52.63	C16 H12 O6	[M-H]-	299.0556	299.0561	-0.5	-1.67	53.53	11.0

M22

Event#: 4 MS(E-) Ret. Time : 44.315 Scan# : 4364



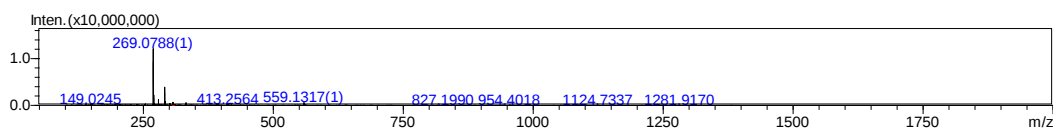
Event#: 5 MS/MS(E-) Ret. Time : 44.315 Scan# : 4365 Precursor : 257.0819 Cutoff : 71



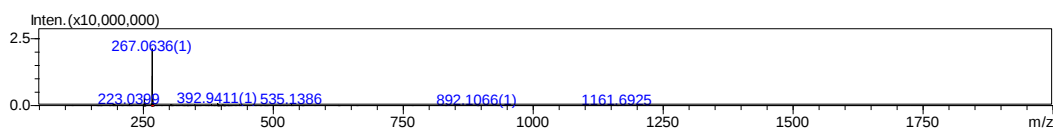
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	53.92	C15 H14 O4	[M-H]-	257.0819	257.0819	0.0	0.00	53.92	9.0

M23

Event#: 1 MS(E+) Ret. Time : 45.328 Scan# : 4461



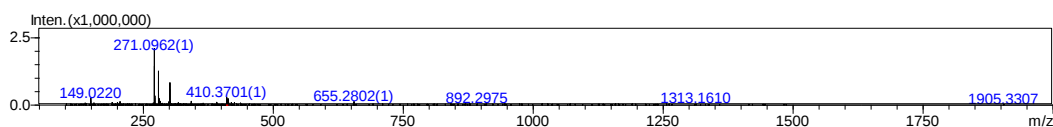
Event#: 4 MS(E-) Ret. Time : 45.328 Scan# : 4463



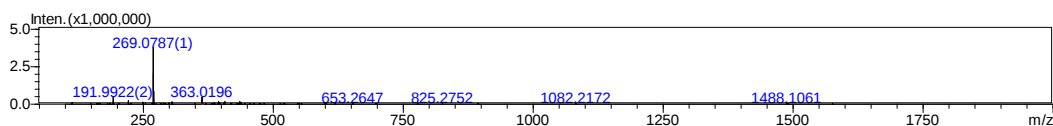
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
3	63.60	C16 H12 O4	[M+H] ⁺	269.0793	269.0808	-1.5	-5.57	75.44	11.0

M24

Event#: 1 MS(E+) Ret. Time : 45.732 Scan# : 4501



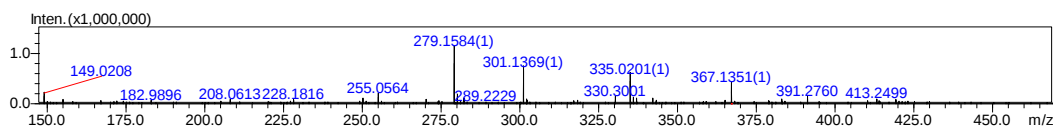
Event#: 4 MS(E-) Ret. Time : 45.732 Scan# : 4504



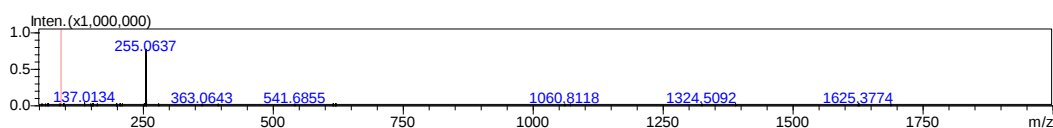
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	43.94	C16 H14 O4	[M-H] ⁻	269.0798	269.0819	-2.1	-7.80	70.87	10.0

M25

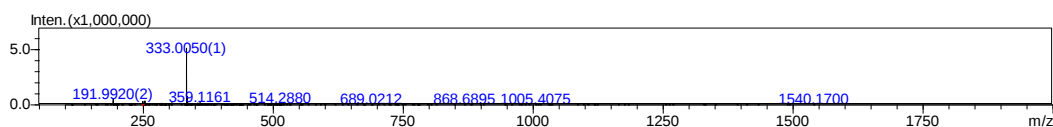
Event#: 1 MS(E+) Ret. Time : 46.290 Scan# : 4556



Event#: 2 MS/MS(E+) Ret. Time : 46.170 Scan# : 4545 Precursor : 335.0203 Cutoff : 92



Event#: 4 MS(E-) Ret. Time : 46.170 Scan# : 4547

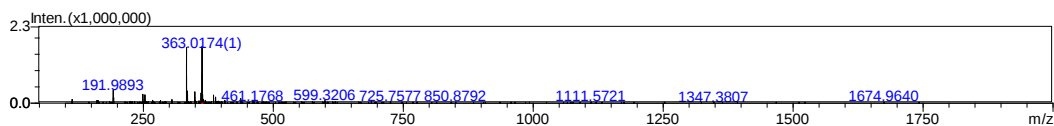


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	63.03	C15 H10 O4	[M+H] ⁺	255.0637	255.0652	-1.5	-5.88	77.62	11.0

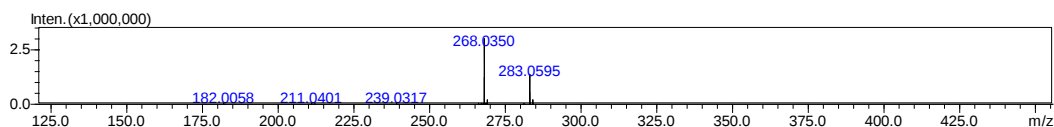
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	47.61	C15 H10 O7 S	[M+H] ⁺	335.0201	335.0220	-1.9	-5.67	57.15	11.0

M26

Event#: 4 MS(E-) Ret. Time : 47.862 Scan# : 4714



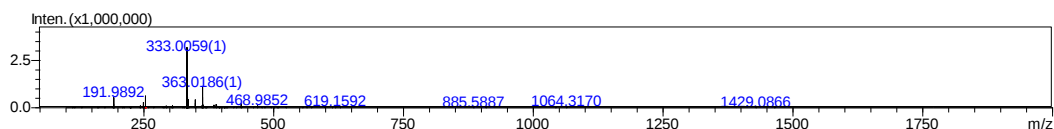
Event#: 5 MS/MS(E-) Ret. Time : 47.862 Scan# : 4715 Precursor : 363.0175 Cutoff : 100



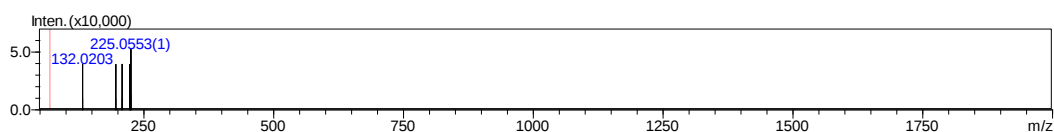
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	73.29	C16 H12 O8 S[M-H]-		363.0174	363.0180	-0.6	-1.65	74.50	11.0

M27

Event#: 4 MS(E-) Ret. Time : 47.922 Scan# : 4719



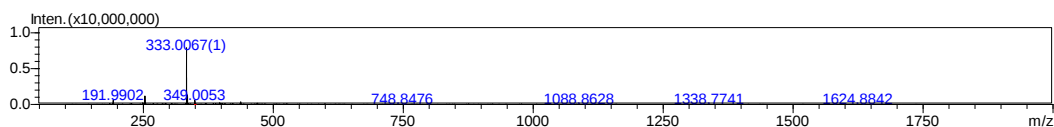
Event#: 5 MS/MS(E-) Ret. Time : 47.922 Scan# : 4720 Precursor : 253.0469 Cutoff : 70



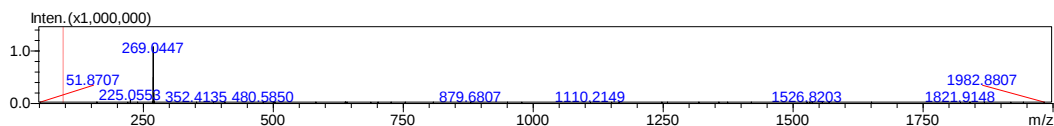
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	70.96	C15 H10 O7 S[M-H]-		333.0059	333.0074	-1.5	-4.50	77.76	11.0

M28

Event#: 4 MS(E-) Ret. Time : 48.205 Scan# : 4748



Event#: 5 MS/MS(E-) Ret. Time : 48.205 Scan# : 4749 Precursor : 349.0053 Cutoff : 96

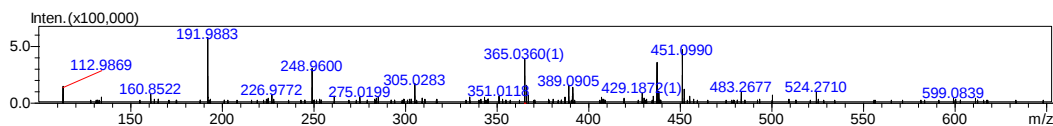


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
4	31.44	C15 H10 O8 S[M-H]-		349.0053	349.0024	2.9	8.31	55.25	11.0

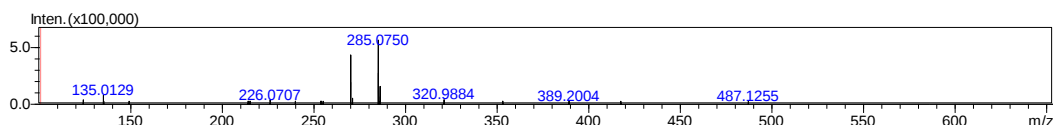
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	58.01	C15 H10 O7 S[M-H]-		333.0067	333.0074	-0.7	-2.10	59.65	11.0

M30

Event#: 4 MS(E-) Ret. Time : 49.193 Scan# : 4844



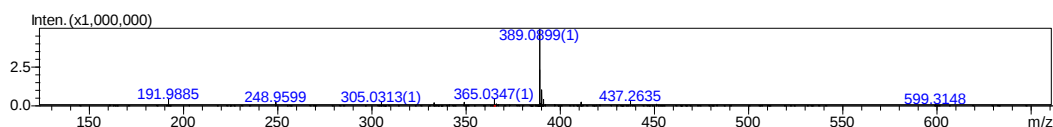
Event#: 5 MS/MS(E-) Ret. Time : 49.193 Scan# : 4845 Precursor : 365.0361 Cutoff : 101



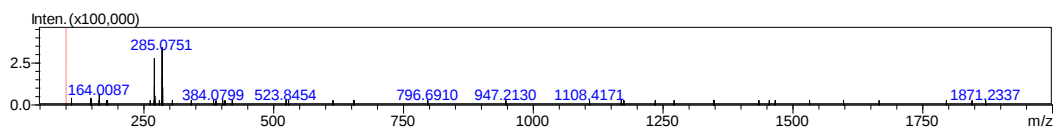
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	23.06	C16 H14 O8 S[M-H]-		365.0360	365.0337	2.3	6.30	29.95	10.0

M29

Event#: 4 MS(E-) Ret. Time : 48.747 Scan# : 4800



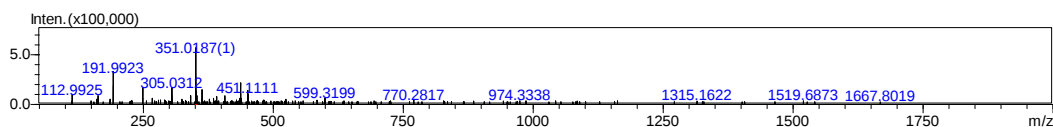
Event#: 5 MS/MS(E-) Ret. Time : 48.747 Scan# : 4801 Precursor : 365.0349 Cutoff : 101



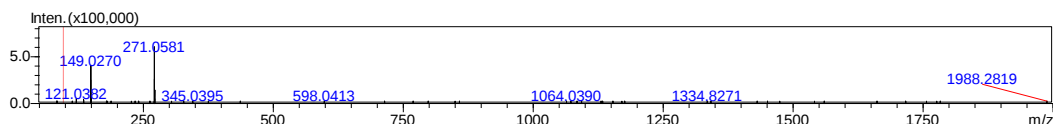
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	38.94	C16 H14 O8 S[M-H]-		365.0347	365.0337	1.0	2.74	40.72	10.0

M31

Event#: 4 MS(E-) Ret. Time : 49.623 Scan# : 4886



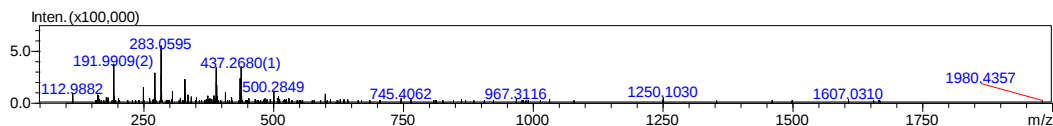
Event#: 5 MS/MS(E-) Ret. Time : 49.623 Scan# : 4887 Precursor : 351.0188 Cutoff : 97



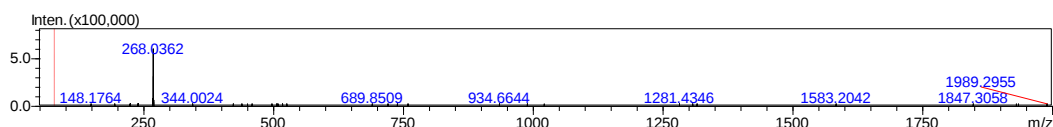
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	41.71	C15 H12 O8 S[M-H]-		351.0187	351.0180	0.7	1.99	42.76	10.0

M32

Event#: 4 MS(E-) Ret. Time : 50.467 Scan# : 4968



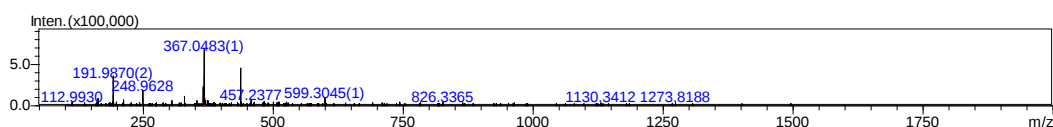
Event#: 5 MS/MS(E-) Ret. Time : 50.467 Scan# : 4969 Precursor : 283.0595 Cutoff : 78



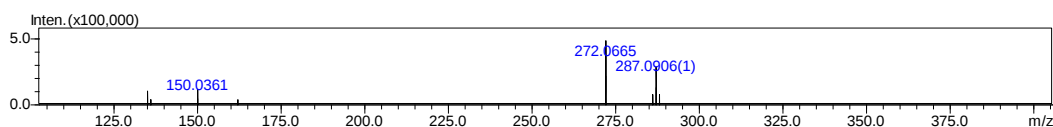
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	46.79	C16 H12 O5	[M-H]-	283.0595	283.0612	-1.7	-6.01	58.56	11.0

M33

Event#: 4 MS(E-) Ret. Time : 50.973 Scan# : 5019



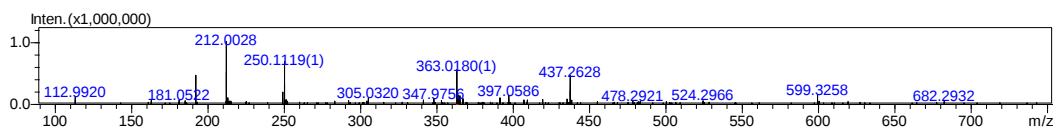
Event#: 5 MS/MS(E-) Ret. Time : 50.973 Scan# : 5020 Precursor : 367.0485 Cutoff : 101



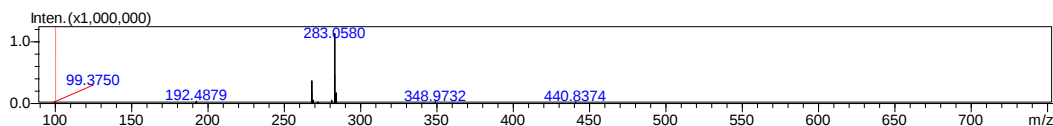
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	55.98	C16 H16 O8 S	[M-H]-	367.0483	367.0493	-1.0	-2.72	58.50	9.0

M34

Event#: 4 MS(E-) Ret. Time : 51.515 Scan# : 5072



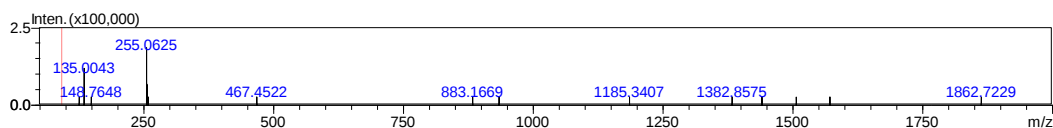
Event#: 5 MS/MS(E-) Ret. Time : 51.515 Scan# : 5073 Precursor : 363.0182 Cutoff : 100



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	46.31	C16 H12 O8 S	[M-H]-	363.0180	363.0180	0.0	0.00	46.31	11.0

M35

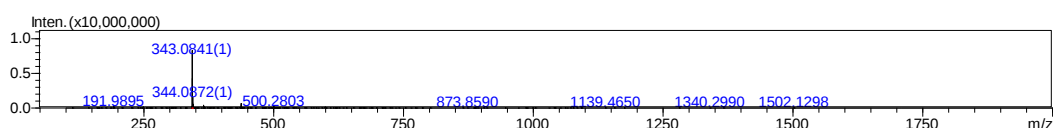
Event#: 5 MS/MS(E-) Ret. Time : 52.563 Scan# : 5175 Precursor : 335.0251 Cutoff : 92



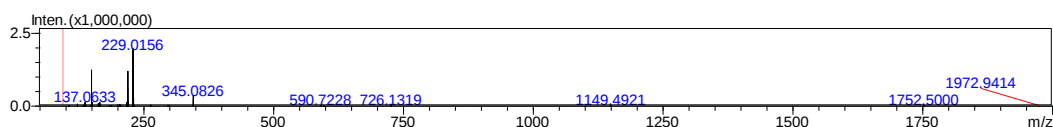
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	31.53	C15 H12 O7 S	[M-H]-	335.0250	335.0231	1.9	5.67	37.85	10.0	
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	13.95	C21 H42 O7 S	[M-H]-	437.2628	437.2578	5.0	11.43	38.55	1.0	

M36

Event#: 4 MS(E-) Ret. Time : 53.637 Scan# : 5280



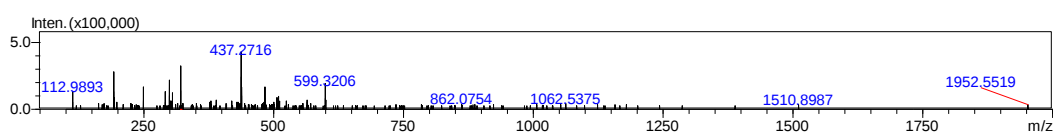
Event#: 5 MS/MS(E-) Ret. Time : 53.637 Scan# : 5281 Precursor : 343.0843 Cutoff : 94



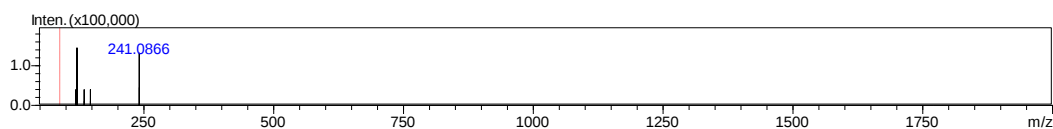
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	30.24	C18 H16 O7	[M-H]-	343.0835	343.0823	1.2	3.50	32.26	11.0	
2	30.24	C17 H14 O5	[M+HCOO]-	343.0835	343.0823	1.2	3.50	32.26	11.0	

M37

Event#: 4 MS(E-) Ret. Time : 55.165 Scan# : 5431



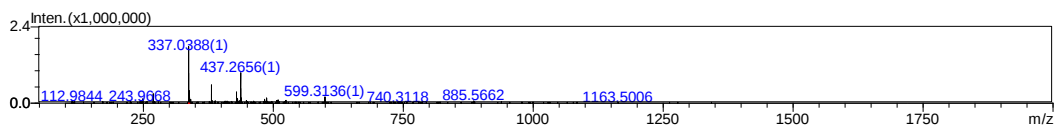
Event#: 5 MS/MS(E-) Ret. Time : 55.165 Scan# : 5432 Precursor : 321.0398 Cutoff : 88



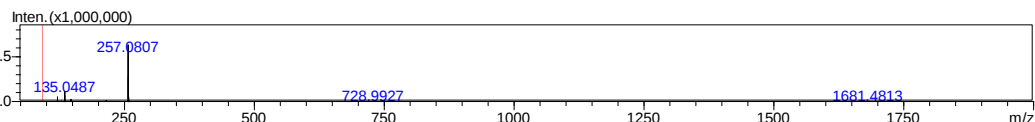
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	0.00	C18 H10 O6	[M-H]-	321.0417	321.0405	1.2	3.74	0.00	14.0	
4	0.00	C15 H14 O6 S	[M-H]-	321.0417	321.0438	-2.1	-6.54	0.00	9.0	

M38

Event#: 4 MS(E-) Ret. Time : 59.468 Scan# : 5856



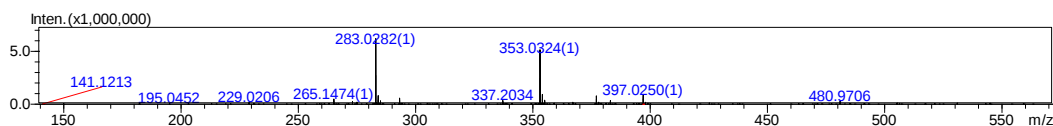
Event#: 5 MS/MS(E-) Ret. Time : 59.468 Scan# : 5857 Precursor : 337.0389 Cutoff : 93



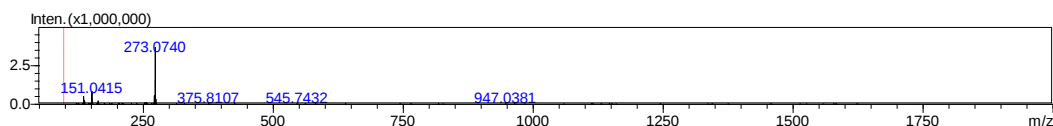
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	78.95	C15 H14 O7 S	[M-H]-	337.0388	337.0387	0.1	0.30	78.95	9.0

M43

Event#: 4 MS(E-) Ret. Time : 71.557 Scan# : 7045



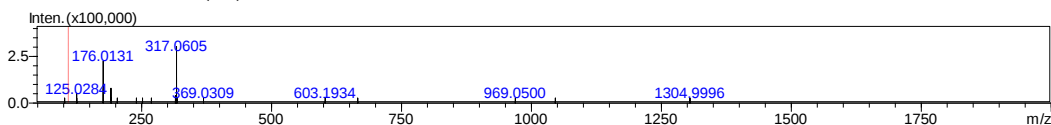
Event#: 5 MS/MS(E-) Ret. Time : 72.485 Scan# : 7137 Precursor : 353.0319 Cutoff : 97



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	85.66	C15 H14 O8 S	[M-H]-	353.0324	353.0337	-1.3	-3.68	91.81	9.0

M44

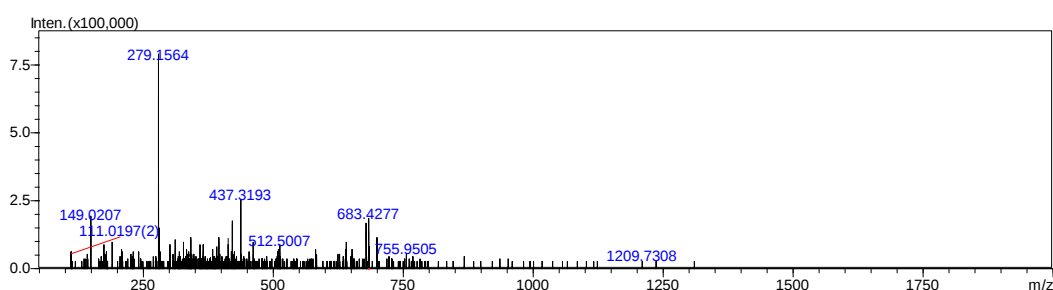
Event#: 5 MS/MS(E-) Ret. Time : 71.557 Scan# : 7046 Precursor : 397.0250 Cutoff : 109



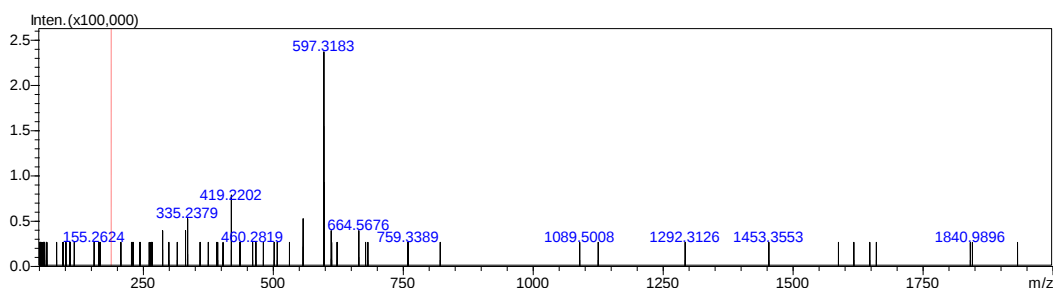
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	56.86	C16 H14 O10 S	[M-H]-	397.0250	397.0235	1.5	3.78	61.10	10.0

M39

Event#: 1 MS(E+) Ret. Time : 61.838 Scan# : 6087



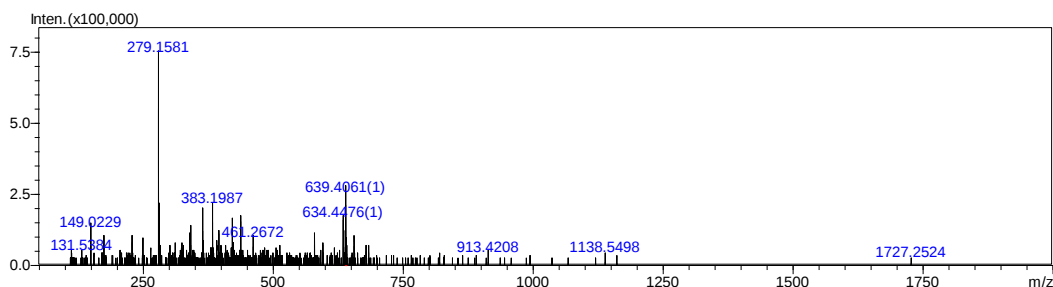
MS/MS(E+) Ret. Time : 61.838 Scan# : 6088 Precursor : 683.4276 Cutoff : 189



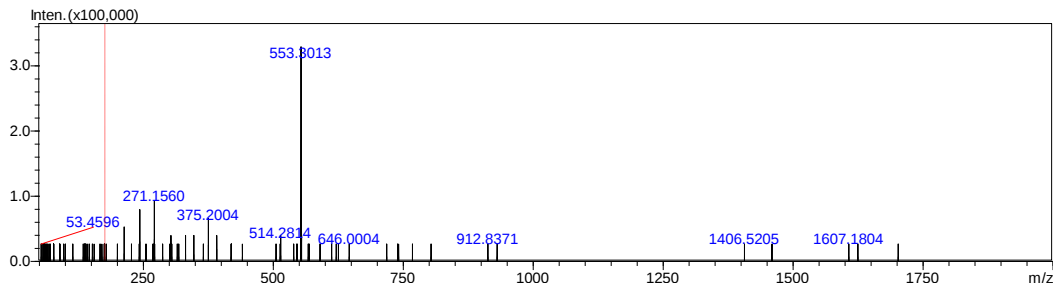
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	0.00	C42 H60 O6	[M+Na] ⁺	683.4277	683.4282	-0.5	-0.73	0.00	13.0
2	0.00	C35 H64 O11	[M+Na]⁺	683.4277	683.4341	-6.4	-9.36	0.00	4.0

M40

Event#: 1 MS(E+) Ret. Time : 62.002 Scan# : 6103



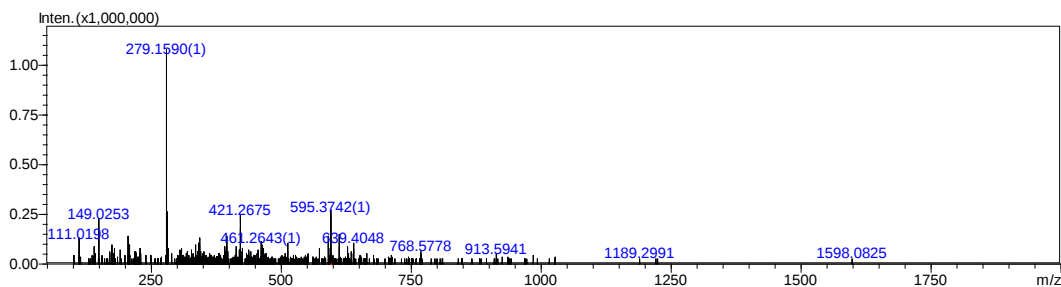
MS/MS(E+) Ret. Time : 62.002 Scan# : 6104 Precursor : 639.4062 Cutoff : 176



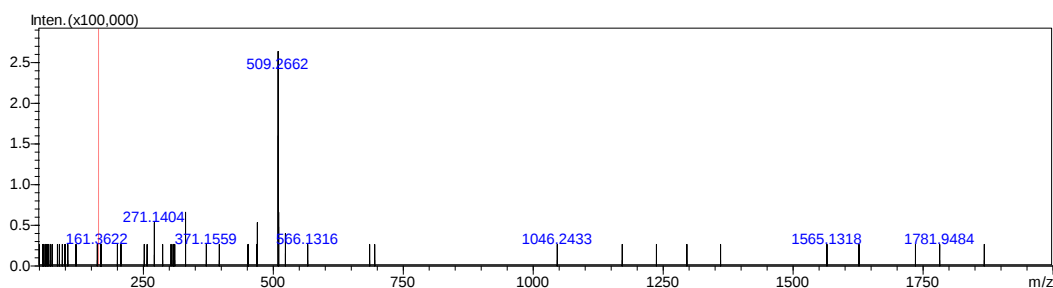
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
8	0.00	C44 H56 O2	[M+Na] ⁺	639.4061	639.4173	-11.2	-17.52	0.00	17.0
7	1.92	C42 H54 O5	[M+H] ⁺	639.4061	639.4044	1.7	2.66	2.00	16.0
6	2.45	C40 H56 O5	[M+Na] ⁺	639.4061	639.4020	4.1	6.41	3.23	13.0
5	3.83	C47 H52	[M+Na] ⁺	639.4061	639.3961	10.0	15.64	15.34	22.0
4	4.21	C35 H58 O10	[M+H]⁺	639.4061	639.4103	-4.2	-6.57	5.67	7.0
3	4.51	C49 H50	[M+H] ⁺	639.4061	639.3985	7.6	11.89	12.90	25.0
2	5.45	C31 H58 O13	[M+H] ⁺	639.4061	639.3950	11.1	17.36	26.73	3.0
1	6.02	C33 H60 O10	[M+Na] ⁺	639.4061	639.4079	-1.8	-2.82	6.31	4.0

M41

Event#: 1 MS(E+) Ret. Time : 62.113 Scan# : 6114



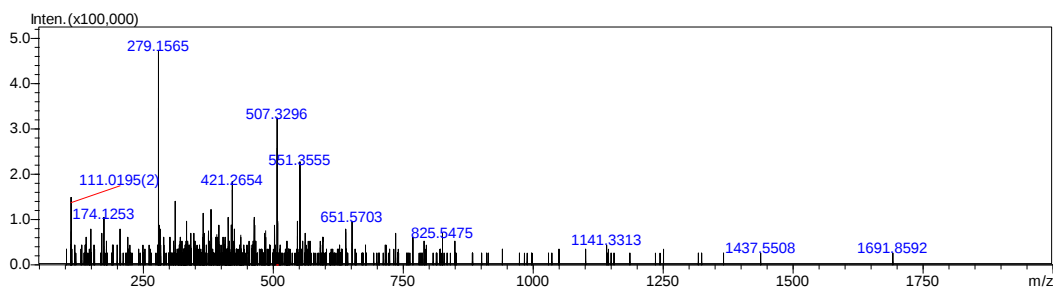
MS/MS(E+) Ret. Time : 62.113 Scan# : 6115 Precursor : 595.3742 Cutoff : 164



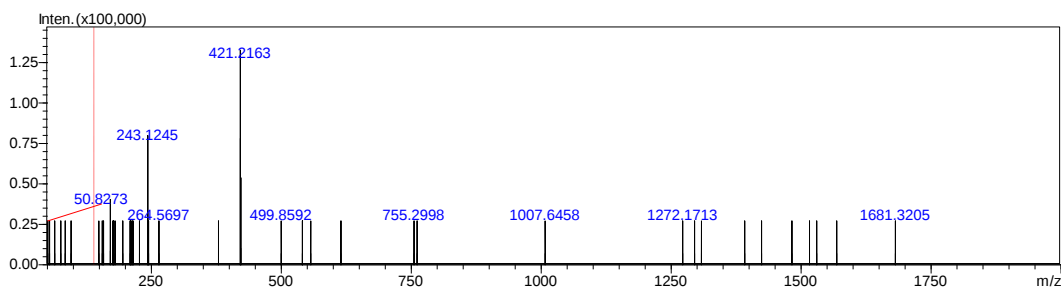
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	15.05	C38 H52 O4	[M+Na] ⁺	595.3742	595.3758	-1.6	-2.69	15.72	13.0
2	11.49	C29 H54 O12	[M+H] ⁺	595.3742	595.3688	5.4	9.07	23.30	3.0
3	7.41	C27 H56 O12	[M+Na] ⁺	595.3742	595.3664	7.8	13.10	23.34	0.0
4	6.99	C31 H56 O9	[M+Na] ⁺	595.3742	595.3817	-7.5	-12.60	21.15	4.0
5	3.80	C33 H54 O9	[M+H]⁺	595.3742	595.3841	-9.9	-16.63	17.02	7.0

M42

Event#: 1 MS(E+) Ret. Time : 62.413 Scan# : 6144



MS/MS(E+) Ret. Time : 62.413 Scan# : 6145 Precursor : 507.3294 Cutoff : 140

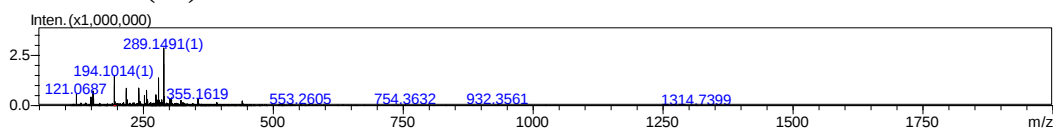


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	41.90	C27 H48 O7	[M+Na] ⁺	507.3296	507.3292	0.4	0.79	41.90	4.0
2	29.20	C29 H46 O7	[M+H]⁺	507.3296	507.3316	-2.0	-3.94	31.52	7.0

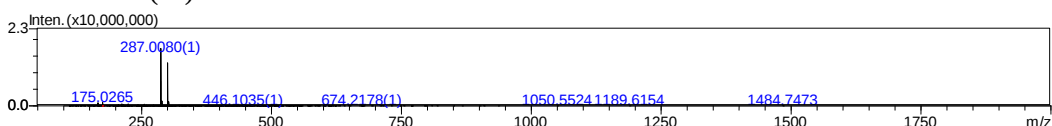
5. The HRMS data of DBT2 urine samples

m1

Event#: 1 MS(E+) Ret. Time : 4.132 Scan# : 403



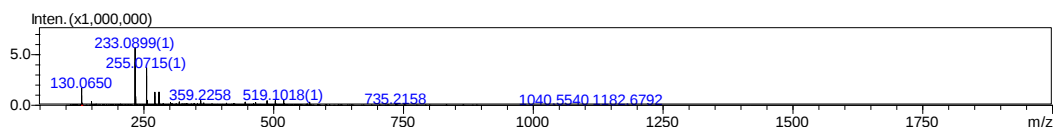
Event#: 4 MS(E-) Ret. Time : 4.132 Scan# : 406



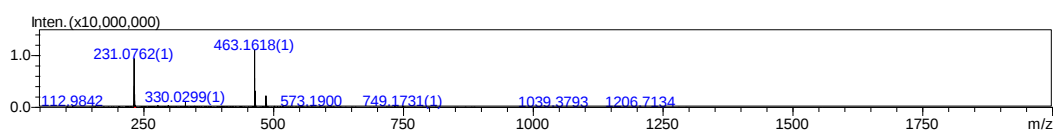
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	44.14	C10 H8 O10	[M-H]-	287.0065	287.0045	2.0	6.97	62.79	7.0

m2

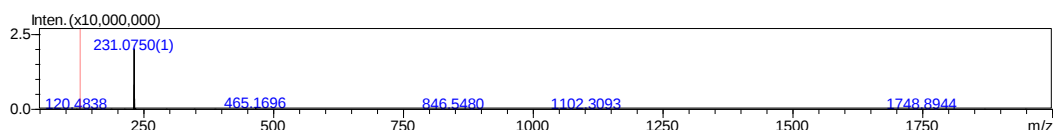
Event#: 1 MS(E+) Ret. Time : 28.200 Scan# : 2772



Event#: 4 MS(E-) Ret. Time : 28.200 Scan# : 2774



Event#: 5 MS/MS(E-) Ret. Time : 28.147 Scan# : 2770 Precursor : 463.1629 Cutoff : 128

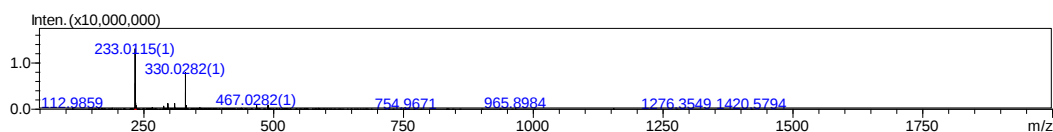
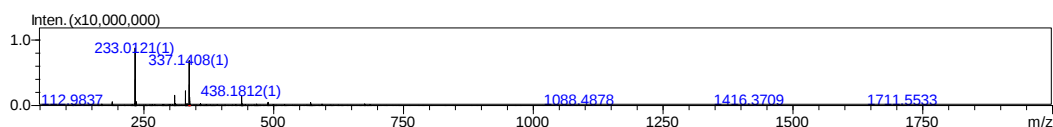


2M-H

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	84.13	C12 H12 N2 O3	[M-H]-	231.0768	231.0775	-0.7	-3.03	88.63	8.0

m3

Event#: 4 MS(E-) Ret. Time : 29.298 Scan# : 2883

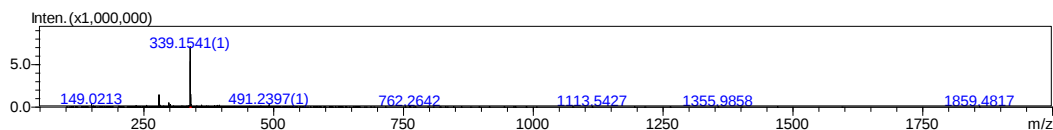


2M-H

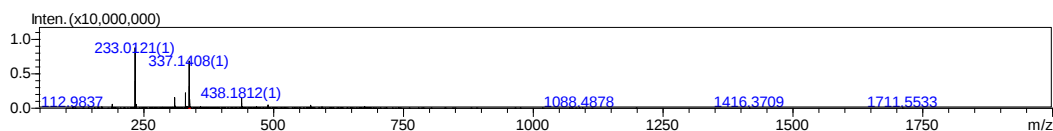
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	56.14	C12 H2 N4 O2	[M-H]-	233.0115	233.0105	1.0	4.29	61.17	14.0

m4

Event#: 1 MS(E+) Ret. Time : 29.298 Scan# : 2880



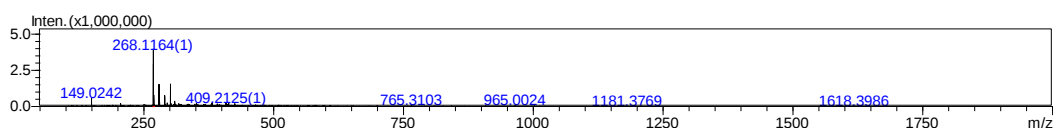
Event#: 4 MS(E-) Ret. Time : 29.298 Scan# : 2883



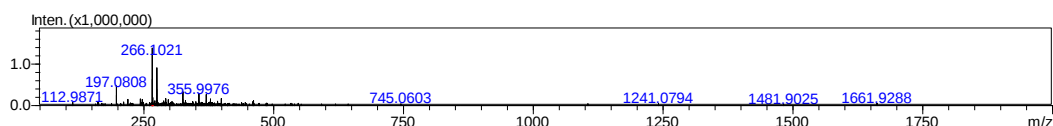
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	62.13	C16 H22 N2 O6	[M-H]-	337.1408	337.1405	0.3	0.89	62.13	7.0

m5

Event#: 1 MS(E+) Ret. Time : 31.083 Scan# : 3056



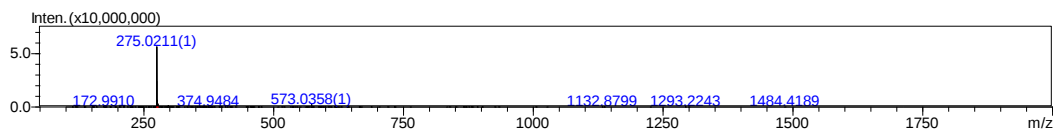
Event#: 4 MS(E-) Ret. Time : 31.083 Scan# : 3059



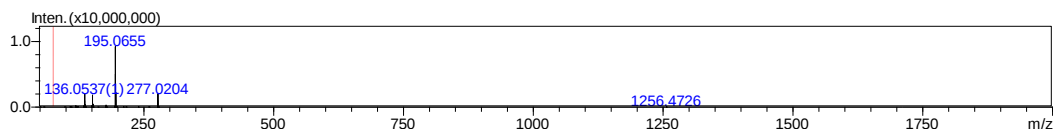
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	35.90	C13 H17 N O5	[M-H]-	266.1021	266.1034	-1.3	-4.89	35.90	6.0

m6

Event#: 4 MS(E-) Ret. Time : 31.970 Scan# : 3146



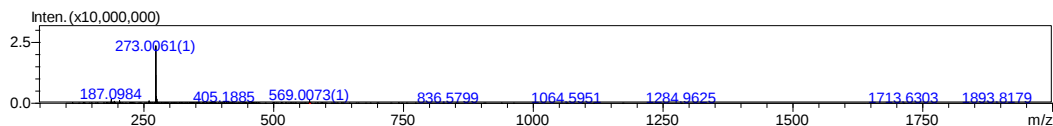
Event#: 5 MS/MS(E-) Ret. Time : 31.970 Scan# : 3147 Precursor : 275.3296 Cutoff : 76



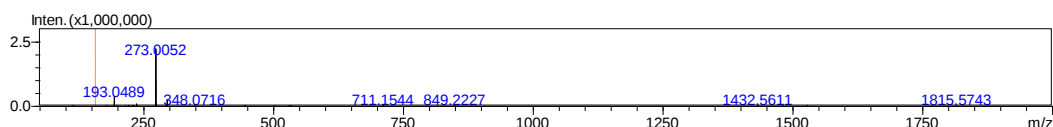
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	65.68	C13 H8 O7	[M-H]-	275.0211	275.0197	1.4	5.09	65.68	7.0

m07

Event#: 4 MS(E-) Ret. Time : 32.927 Scan# : 3240



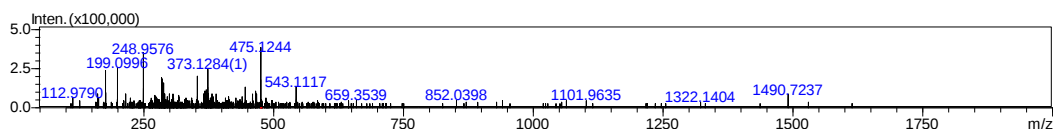
Event#: 5 MS/MS(E-) Ret. Time : 32.927 Scan# : 3241 Precursor : 569.0071 Cutoff : 157



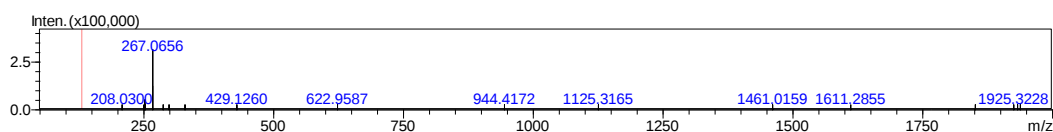
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	55.73	C13 H6 O7	[M-H]-	273.0056	273.0041	1.5	5.49	65.49	11.0

m08

Event#: 4 MS(E-) Ret. Time : 34.518 Scan# : 3397



Event#: 5 MS/MS(E-) Ret. Time : 34.518 Scan# : 3398 Precursor : 475.1243 Cutoff : 131



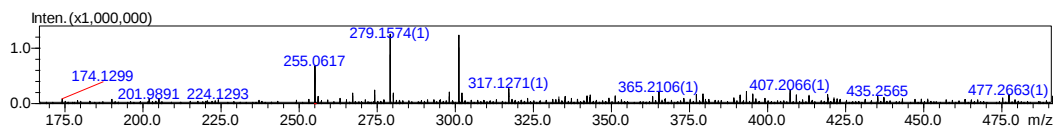
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	0.00	C16 H12 O4	[M-H]-	267.0656	267.0663	-0.7	-2.62	0.00	11.0

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	29.80	C23 H24 O11	[M-H]-	475.1244	475.1246	-0.2	-0.42	29.80	12.0
2	29.80	C22 H22 O9	[M+HCOO]-	475.1244	475.1246	-0.2	-0.42	29.80	12.0

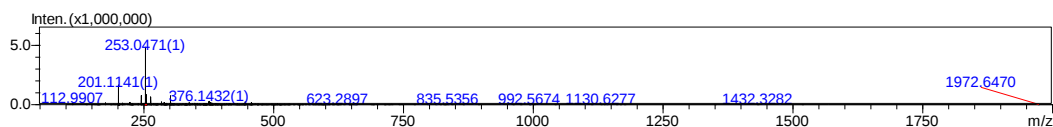
C6H12O6 C7H16O8

m09

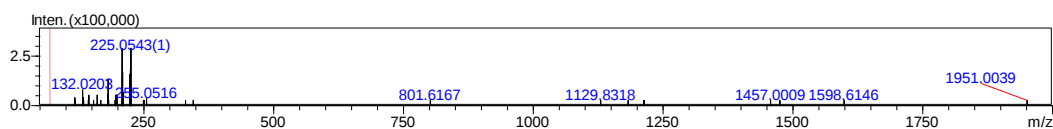
Event#: 1 MS(E+) Ret. Time : 36.583 Scan# : 3598



Event#: 4 MS(E-) Ret. Time : 36.583 Scan# : 3601



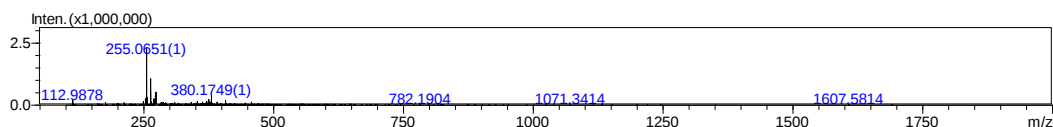
Event#: 5 MS/MS(E-) Ret. Time : 36.583 Scan# : 3602 Precursor : 253.0470 Cutoff : 70



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
2	52.81	C15 H10 O4	[M+H] ⁺	255.0637	255.0652	-1.5	-5.88	65.04	11.0

m10

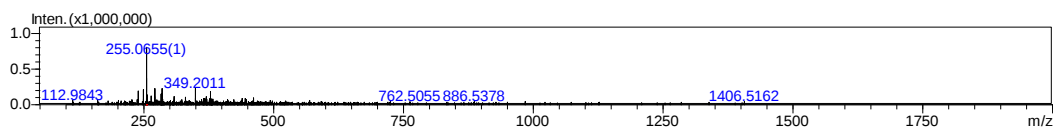
Event#: 4 MS(E-) Ret. Time : 36.918 Scan# : 3634



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	51.19	C15 H12 O4	[M-H] ⁻	255.0651	255.0663	-1.2	-4.70	56.41	10.0

m11

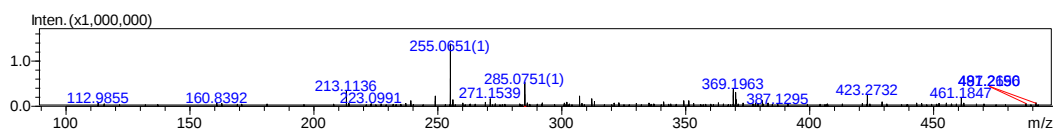
Event#: 4 MS(E-) Ret. Time : 37.442 Scan# : 3686



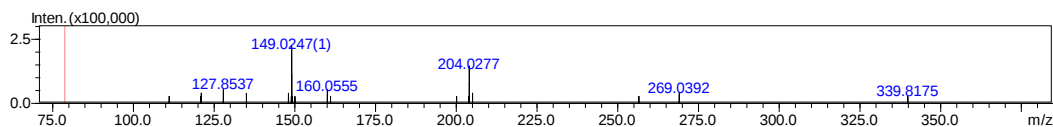
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	49.24	C15 H12 O4	[M-H] ⁻	255.0655	255.0663	-0.8	-3.14	52.02	10.0

m12

Event#: 4 MS(E-) Ret. Time : 37.502 Scan# : 3692



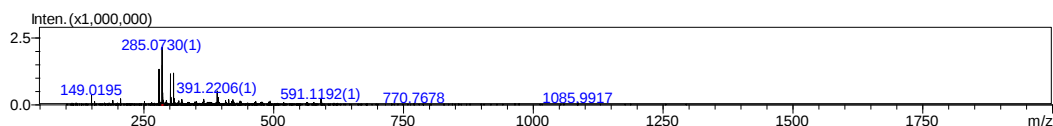
Event#: 5 MS/MS(E-) Ret. Time : 37.502 Scan# : 3693 Precursor : 285.0750 Cutoff : 78



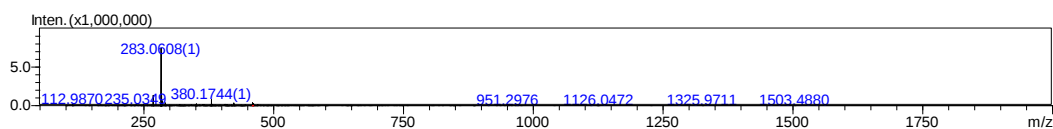
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	41.72	C16 H14 O5	[M-H] ⁻	285.0751	285.0768	-1.7	-5.96	51.89	10.0

m13

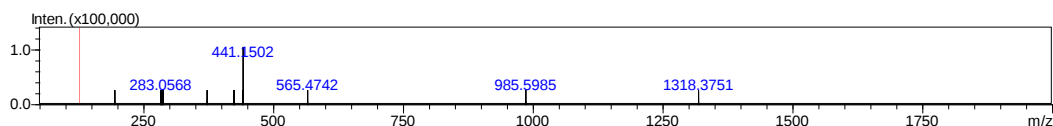
Event#: 1 MS(E+) Ret. Time : 38.033 Scan# : 3742



Event#: 4 MS(E-) Ret. Time : 37.973 Scan# : 3739



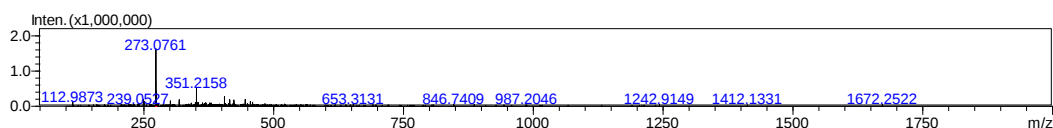
ven#: 5 MS/MS(E-) Ret. Time : 37.973 Scan# : 3740 Precursor : 459.1729 Cutoff : 127



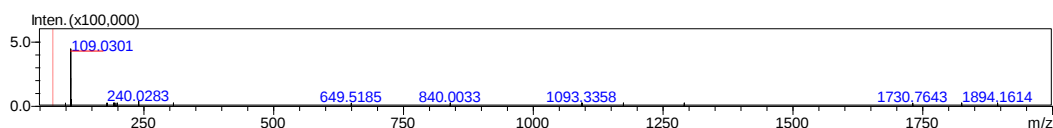
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	58.71	C16 H12 O5	[M-H]-	283.0608	283.0612	-0.4	-1.41	59.32	11.0

m14

Event#: 4 MS(E-) Ret. Time : 39.047 Scan# : 3844



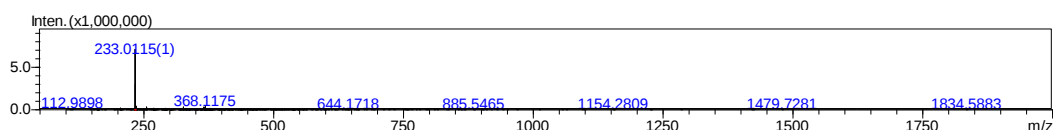
Event#: 5 MS/MS(E-) Ret. Time : 39.047 Scan# : 3845 Precursor : 273.0760 Cutoff : 75



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	67.76	C15 H14 O5	[M-H]-	273.0761	273.0768	-0.7	-2.56	70.51	9.0

m15

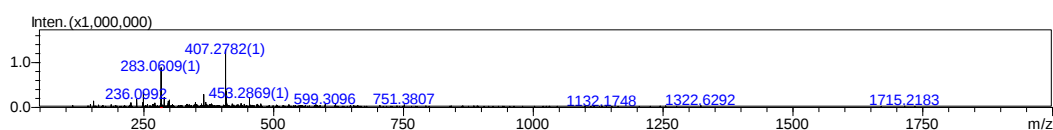
Event#: 4 MS(E-) Ret. Time : 40.128 Scan# : 3952



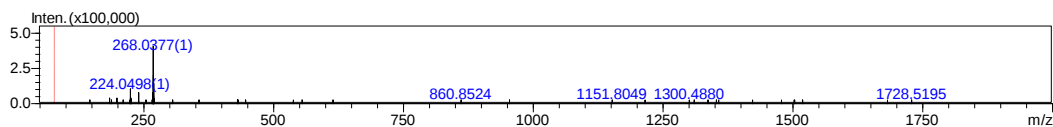
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	50.48	C12 H2 N4 O2	[M-H]-	233.0115	233.0105	1.0	4.29	55.01	14.0

m16

Event#: 4 MS(E-) Ret. Time : 41.630 Scan# : 4101



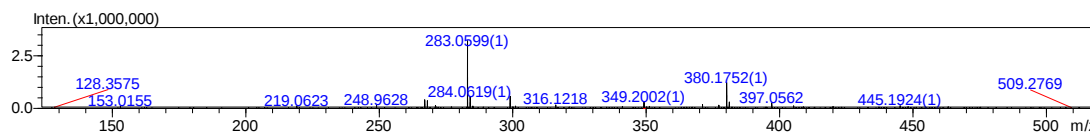
Event#: 5 MS/MS(E-) Ret. Time : 41.630 Scan# : 4102 Precursor : 283.0609 Cutoff : 78



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	45.89	C16 H12 O5	[M-H]-	283.0609	283.0612	-0.3	-1.06	45.96	11.0

m17

Event#: 4 MS(E-) Ret. Time : 42.180 Scan# : 4155

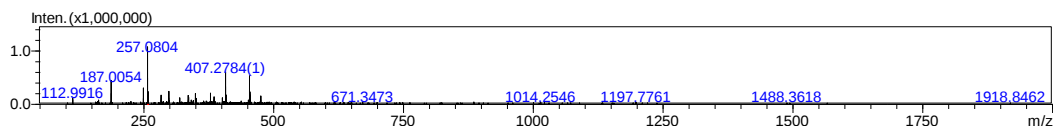


Event#: 5 MS/MS(E-) Ret. Time : 42.180 Scan# : 4156 Precursor : 349.2003 Cutoff : 96

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	54.91	C16 H12 O5	[M-H]-	283.0603	283.0612	-0.9	-3.18	58.08	11.0

m18

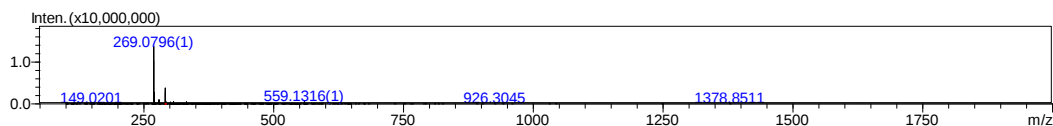
Event#: 4 MS(E-) Ret. Time : 44.327 Scan# : 4367



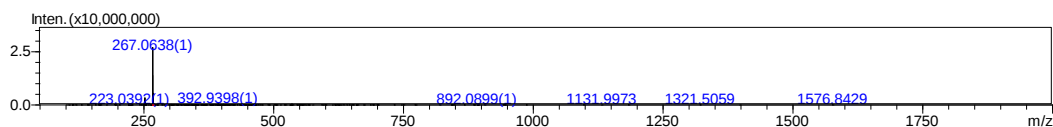
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	31.69	C15 H14 O4	[M-H]-	257.0804	257.0819	-1.5	-5.83	38.79	9.0

m19

vent#: 1 MS(E+) Ret. Time : 45.322 Scan# : 4463



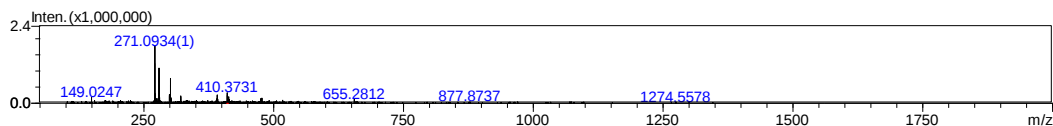
vent#: 4 MS(E-) Ret. Time : 45.322 Scan# : 4465



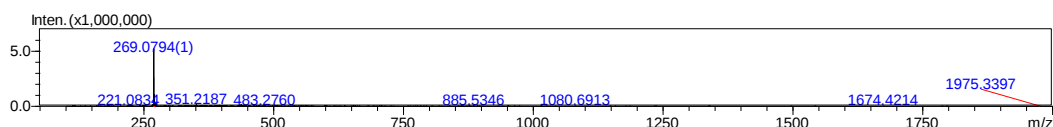
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	73.96	C16 H12 O4	[M+H]+	269.0796	269.0808	-1.2	-4.46	80.96	11.0

m20

Event#: 1 MS(E+) Ret. Time : 45.733 Scan# : 4504



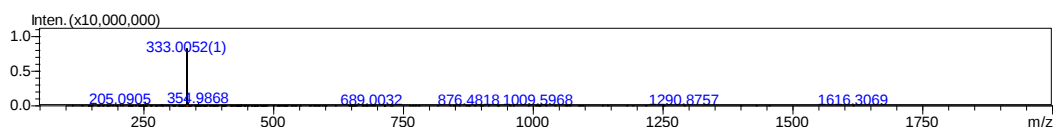
Event#: 4 MS(E-) Ret. Time : 45.673 Scan# : 4501



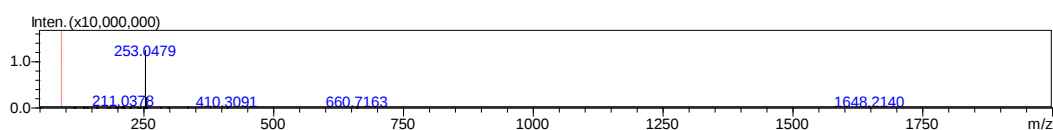
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	67.33	C16 H14 O4	[M-H]-	269.0804	269.0819	-1.5	-5.57	79.87	10.0

m21

Event#: 4 MS(E-) Ret. Time : 47.175 Scan# : 4650



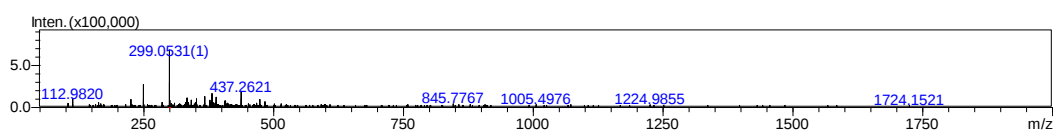
Event#: 5 MS/MS(E-) Ret. Time : 47.175 Scan# : 4651 Precursor : 333.0054 Cutoff : 92



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	64.86	C15 H10 O7 S	[M-H]-	333.0052	333.0074	-2.2	-6.61	87.76	11.0

m22

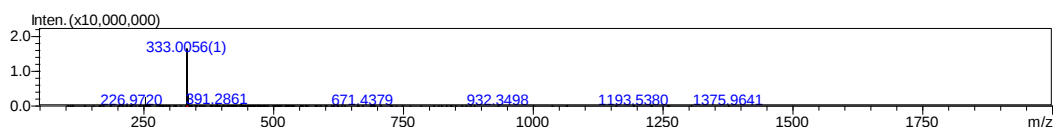
Event#: 4 MS(E-) Ret. Time : 47.775 Scan# : 4709



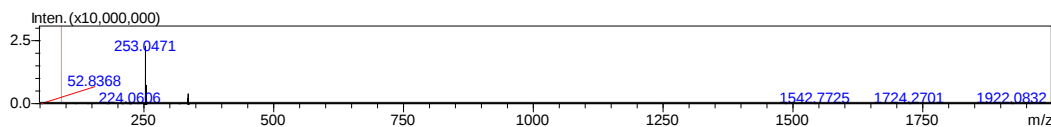
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	41.92	C16 H12 O6	[M-H]-	299.0556	299.0561	-0.5	-1.67	42.64	11.0

m23

Event#: 4 MS(E-) Ret. Time : 49.072 Scan# : 4838



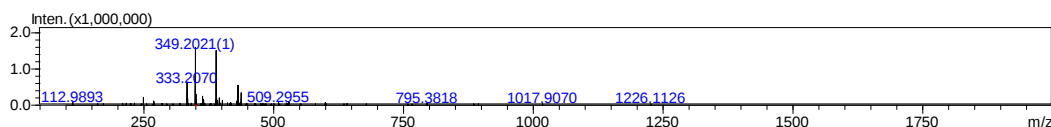
Event#: 5 MS/MS(E-) Ret. Time : 49.072 Scan# : 4839 Precursor : 333.0055 Cutoff : 92



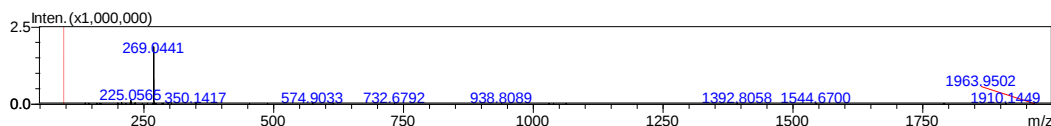
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	71.66	C15 H10 O7 S[M-H]-		333.0056	333.0074	-1.8	-5.41	83.42	11.0

m25

Event#: 4 MS(E-) Ret. Time : 49.810 Scan# : 4911



Event#: 5 MS/MS(E-) Ret. Time : 49.810 Scan# : 4912 Precursor : 349.0033 Cutoff : 96

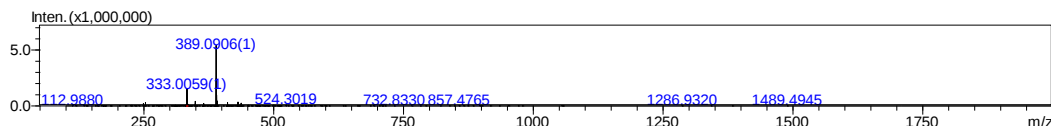


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	37.85	C15 H10 O8 S[M-H]-		349.0033	349.0024	0.9	2.58	39.41	11.0

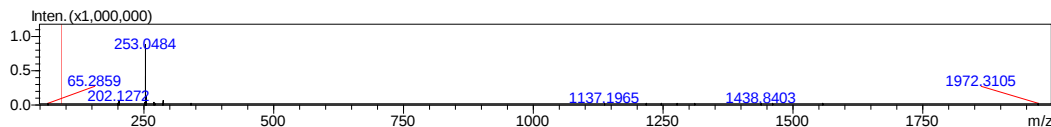
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	27.31	C15 H10 O5 [M-H]-		269.0438	269.0455	-1.7	-6.32	35.56	11.0

m24

Event#: 4 MS(E-) Ret. Time : 49.543 Scan# : 4884



Event#: 5 MS/MS(E-) Ret. Time : 49.698 Scan# : 4901 Precursor : 333.2078 Cutoff : 92

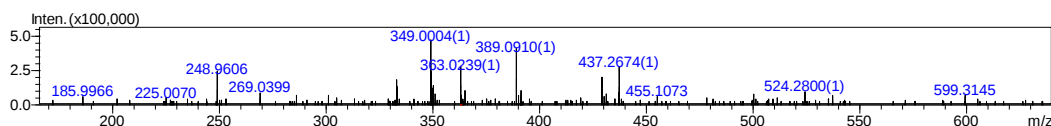


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	36.99	C15 H10 O4 [M-H]-		253.0484	253.0506	-2.2	-8.69	69.66	11.0

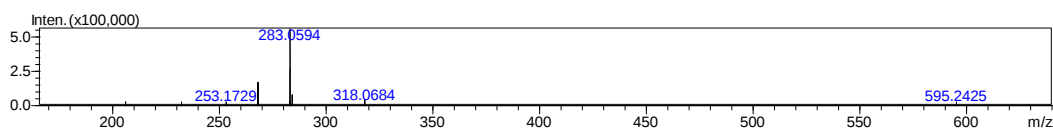
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	78.22	C15 H10 O7 S[M-H]-		333.0059	333.0074	-1.5	-4.50	85.72	11.0

m26

Event#: 4 MS(E-) Ret. Time : 49.930 Scan# : 4923



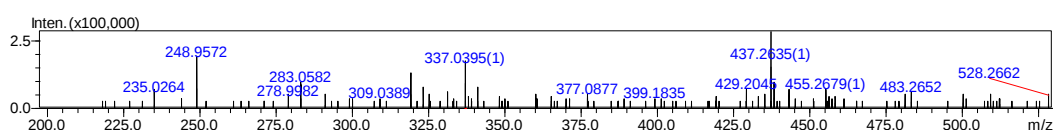
Event#: 5 MS/MS(E-) Ret. Time : 49.930 Scan# : 4924 Precursor : 363.0240 Cutoff : 100



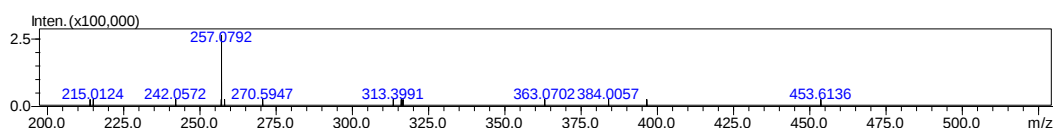
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
12	6.04	C16 H12 O8 S[M-H]-		363.0239	363.0180	5.9	16.25	25.87	11.0
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
4	13.46	C16 H12 O8 S[M-H]-		363.0184	363.0180	0.4	1.10	13.50	11.0

m27

Event#: 4 MS(E-) Ret. Time : 50.325 Scan# : 4962



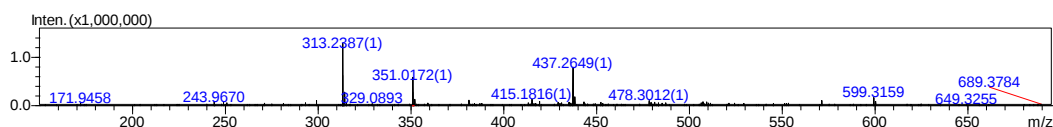
Event#: 5 MS/MS(E-) Ret. Time : 50.325 Scan# : 4963 Precursor : 337.0397 Cutoff : 93



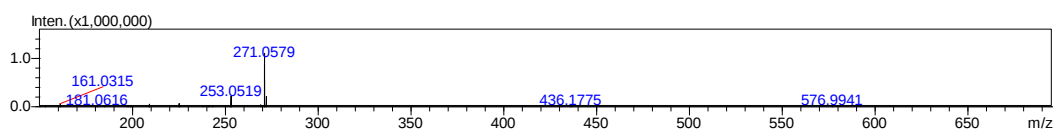
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	48.84	C15 H14 O7 S[M-H]-		337.0395	337.0387	0.8	2.37	50.58	9.0

m28

Event#: 4 MS(E-) Ret. Time : 55.693 Scan# : 5491

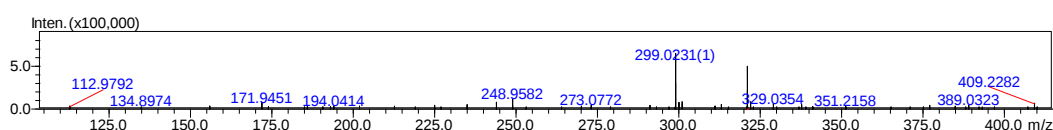


Event#: 5 MS/MS(E-) Ret. Time : 55.693 Scan# : 5492 Precursor : 351.0172 Cutoff : 97



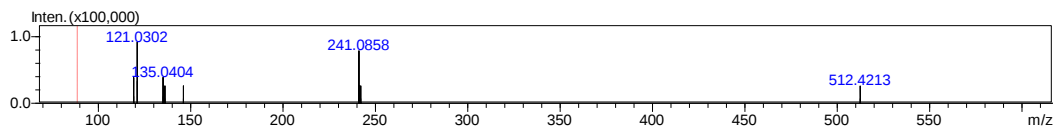
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	53.68	C15 H12 O8 S[M-H]-		351.0172	351.0180	-0.8	-2.28	55.46	10.0

Event#: 4 MS(E-) Ret. Time : 57.015 Scan# : 5622



m29

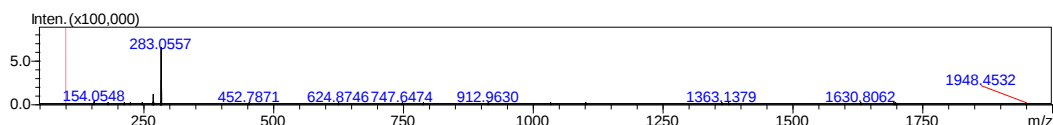
Event#: 5 MS/MS(E-) Ret. Time : 57.015 Scan#: 5623 Precursor : 321.0414 Cutoff : 88



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	0.00	C15 H14 O6 S[M-H]-		321.0414	321.0438	-2.4	-7.48	0.00	9.0

M033

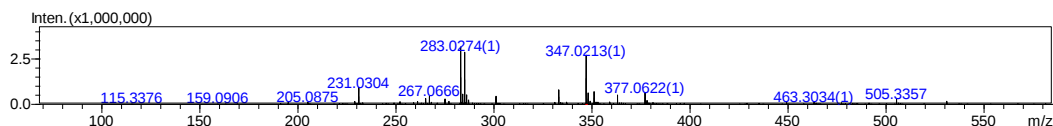
Event#: 5 MS/MS(E-) Ret. Time : 72.797 Scan#: 7175 Precursor : 363.0198 Cutoff : 100



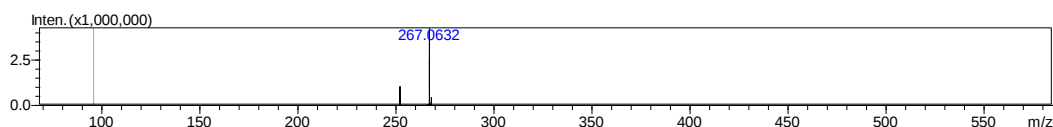
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	29.40	C16 H12 O8 S[M-H]-		363.0197	363.0180	1.7	4.68	32.38	11.0

m34

Event#: 4 MS(E-) Ret. Time : 73.543 Scan#: 7249



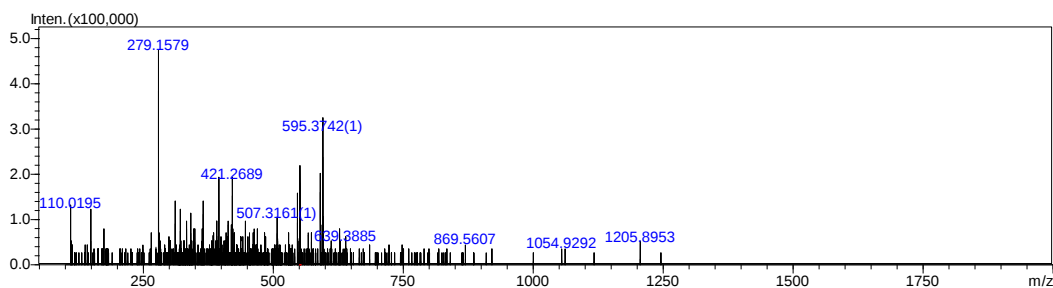
Event#: 5 MS/MS(E-) Ret. Time : 73.543 Scan#: 7250 Precursor : 347.0214 Cutoff : 96



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	60.34	C16 H12 O7 S[M-H]-		347.0213	347.0231	-1.8	-5.19	68.49	11.0

m31

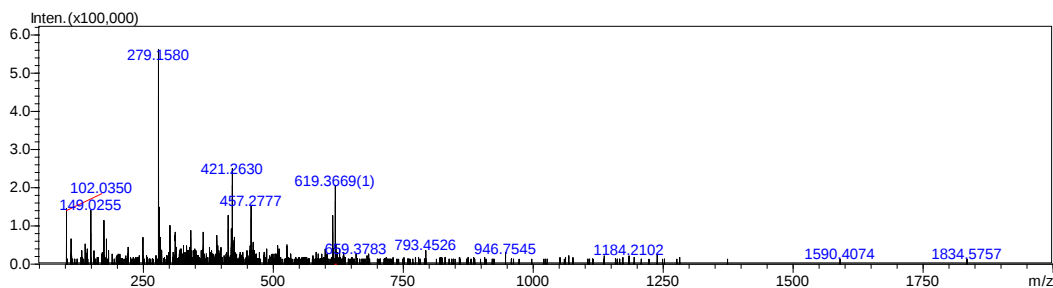
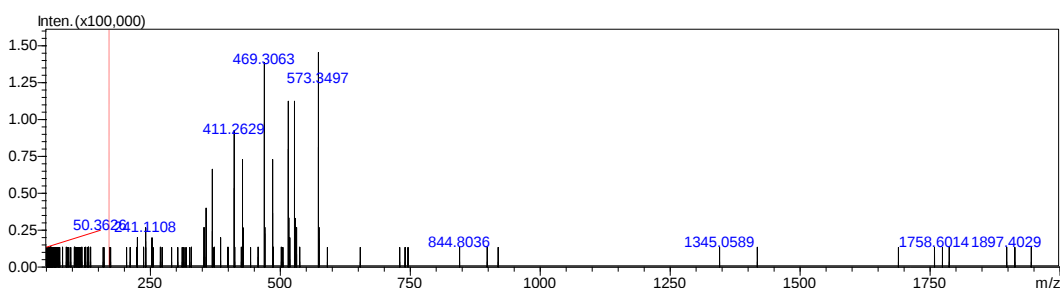
Event#: 1 MS(E+) Ret. Time : 62.218 Scan#: 6133



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	11.03	C29 H54 O12 [M+H]+		595.3742	595.3688	5.4	9.07	22.37	3.0
2	9.28	C27 H56 O12 [M+Na]+		595.3742	595.3664	7.8	13.10	29.24	0.0
3	6.34	C38 H52 O4 [M+Na]+		595.3742	595.3758	-1.6	-2.69	6.62	13.0

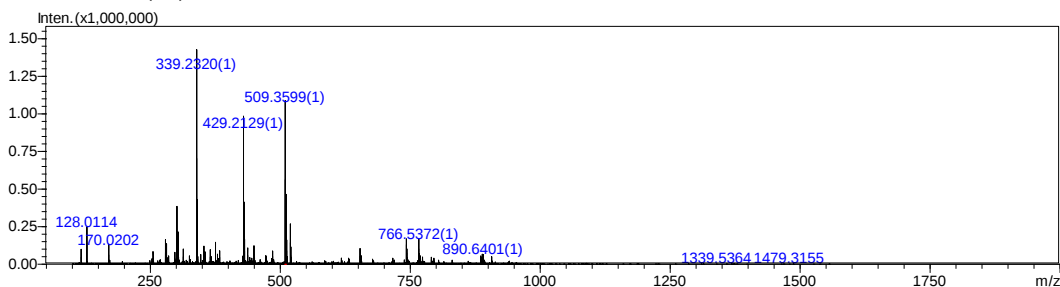
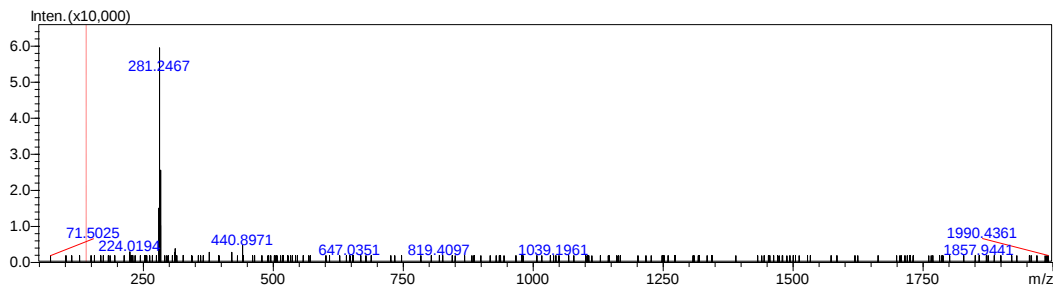
4	3.26	C31 H56 O9	[M+Na] ⁺	595.3742	595.3817	-7.5	-12.60	9.87	4.0
5	2.98	C40 H50 O4	[M+H] ⁺	595.3742	595.3782	-4.0	-6.72	4.10	16.0
6	1.99	C36 H50 O7	[M+H] ⁺	595.3742	595.3629	11.3	18.98	12.40	12.0
7	1.58	C33 H54 O9	[M+H]⁺	595.3742	595.3841	-9.9	-16.63	7.09	7.0

m30

Event#: 1 MS(E⁺) Ret. Time : 59.728 -> 59.995 Scan# : 5887 -> 5913MS/MS(E⁺) Ret. Time : 59.728 -> 59.995 Scan# : 5888 -> 5914 Precursor : 619.3650 Cutoff : 171

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	24.07	C29 H56 O12	[M+Na] ⁺	619.3669	619.3664	0.5	0.81	24.07	2.0	
2	8.39	C38 H50 O7	[M+H] ⁺	619.3669	619.3629	4.0	6.46	11.12	14.0	
3	5.59	C36 H52 O7	[M+Na]⁺	619.3669	619.3605	6.4	10.33	14.29	11.0	

m32

Event#: 4 MS(E⁻) Ret. Time : 63.292 -> 68.353 Scan# : 6241 -> 6739MS/MS(E⁻) Ret. Time : 63.292 -> 68.353 Scan# : 6242 -> 6740 Precursor : 509.3632 Cutoff : 140

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso	Score	DBE
1	22.16	C33 H50 O4	[M-H]⁻	509.3599	509.3636	-3.7	-7.26	32.89	9.0	

6. The supplemental data of tables S1–S6

Table S1. The ion fragment of 19 kinds of reference compounds by HPLC-IT-TOF-MSⁿ.

NO.	T _R (min)	[M+H] ⁺	[M-H] [−]	Predicted Formula	Fragment ions	Error (ppm)	The name of the reference compounds
1 (T1)	28.595	447.1290		C ₂₂ H ₂₂ O ₁₀	447,285,270,225	0.89	Calycosin-7-O-β-D-glucopyranoside
2(AW)	29.162		193.0501	C ₁₀ H ₁₀ O ₄	193,178,134	−2.59	Ferulic acid
3(T2)	34.545		431.1326	C ₂₂ H ₂₂ O ₉	431,269,253,237,118	−2.55	Ononin
4 (T3)	36.038	485.1400	[M+Na] ⁺	C ₂₃ H ₂₆ O ₁₀	485,463,323,301	−3.71	Astrapterocarpan-7-O-β-D-glucopyranoside
5 (T4)	36.785	487.1574	[M+Na] ⁺	C ₂₃ H ₂₈ O ₁₀	487,303,167	−0.21	Astraisoflavan-7-O-β-D-glucopyranoside
6 (T5)	38.055	285.0754		C ₁₆ H ₁₂ O ₅	285,270,225, 137	−1.40	Calycosin
7 (T6)	40.123	473.1432		C ₂₄ H ₂₄ O ₁₀	473,269	−2.11	6"-O-acetyl-ononin
8(T7)	41.942	529.1691	[M+Na] ⁺	C ₂₅ H ₃₀ O ₁₁	529,507,303	2.08	6"-O-acetyl-astraisoflavan-7-O-β-D-glucopyranoside
9(T8)	45.410	269.0795		C ₁₆ H ₁₂ O ₄	269,270,237	−4.83	Formononetin
10(T9)	46.062	301.1076		C ₁₇ H ₁₆ O ₅		1.66	(6aR,11aR)-3-hydroxy-9,10-dimethoxypterocarpan; Astrapterocarpan
11(T10)	46.655	303.1213		C ₁₇ H ₁₈ O ₅	303,167,123	−4.62	(3R)-7,2'-dihydroxy-3',4'-dimethoxyisoflavan; Astraisoflavan
12(G V)	41.110	[M+HCOO] [−]	991.5156	C ₄₇ H ₇₈ O ₁₉	991,783,397	3.73	Astragaloside V, VI, VII
13(GIV)	42.775	[M+HCOO] [−]	829.4615	C ₄₁ H ₆₈ O ₁₄	829,783,621,489,383	2.89	Astragaloside IV
14(GIII)	43.410	[M+HCOO] [−]	829.4585	C ₄₁ H ₆₈ O ₁₄	829,783,651,489	−0.72	Astragaloside III
15(G II)	44.628	[M+HCOO] [−]	871.4693	C ₄₃ H ₇₀ O ₁₅	871,765,717	−0.46	Astragaloside II
16(G I)	50.525	[M+HCOO] [−]	913.4802	C ₄₅ H ₇₂ O ₁₆	913,867,807	0.00	Astragaloside I
17(HHQC)	51.855	513.3550	[M+Na] ⁺	C ₃₀ H ₅₀ O ₅	513,515,405,229	0.00	Cycloastragenol(HHQC)
18(ZL)	55.477	191.1056		C ₁₂ H ₁₄ O ₂	191,173,117	−5.76	Z-ligustilide
19(EL)	58.102	191.1066		C ₁₂ H ₁₄ O ₂	191,173	−0.52	E-ligustilide

Table S2. The identified proposed compounds from DBT1 boiled sample by HPLC-IT-TOF-MSⁿ.

NO.	T _R (min)	[M+H] ⁺	[M-H] ⁻	Predicted Formula	Fragment ions	Error ppm	Identification	T	IT	S
C1	2.280	175.1168		C ₆ H ₁₄ N ₄ O ₂		-12.56	Arginine	●		
C2	2.692		195.0502	C ₆ H ₁₂ O ₇		-4.10	Gluconic acid	●		
C3	3.095	365.1007		C ₁₂ H ₂₂ O ₁₁		-12.87	D(+)-sucrose	●		
C4	3.682		191.0187	C ₆ H ₈ O ₇		-5.24	Citric acid	●		
C5	4.498	330.0583		C ₁₁ H ₁₁ N ₃ O ₉		4.54	--	●		
C6	6.480	346.0529		C ₁₁ H ₁₁ N ₃ O ₁₀		3.47	--	●		
C7	9.063		433.1364	C ₁₈ H ₂₆ O ₁₂	301,191	4.91	--			⊙
C8	9.398		433.1364	C ₁₈ H ₂₆ O ₁₂	433,351,301,223	2.77	--			⊙
C9	10.773	188.0688		C ₉ H ₁₁ NO ₂	146	3.19	L-phenylalanine	●		
C10	11.125		431.1192	C ₁₈ H ₂₄ O ₁₂	431,299	-0.70	--			⊙
C11	12.653	384.1127		C ₁₃ H ₂₁ NO ₁₂		-2.60	--	●		
C12	13.847	485.1224	[M+Na] ⁺	C ₂₆ H ₂₂ O ₈	485,317	3.50	--			⊙
C13	17.807		205.0701	C ₈ H ₁₄ O ₆		-8.29	--			⊙
C14	21.147		315.2004	C ₂₀ H ₂₈ O ₃		12.06	--			⊙
C15	22.132		417.1016	C ₁₇ H ₂₂ O ₁₂		-5.27	--		★	
C16	22.950	389.2359		C ₂₃ H ₃₂ O ₅		9.25	--	●		
C17	23.012		401.1443	C ₁₈ H ₂₆ O ₁₀	401,269	-2.49	--	●		
C18	23.590		503.1175	C ₂₄ H ₂₄ O ₁₂	503,443,299	-3.98	6''-O-acetyl-pratensein-7-O-β-D-glucoside			⊙
C19	24.347		239.0568	C ₁₁ H ₁₂ O ₆		2.93	--			⊙
C20	25.662	331.2296		C ₂₁ H ₃₀ O ₃	331,299	8.45	--			⊙
C21	26.743	470.1534		C ₁₈ H ₂₃ N ₅ O ₁₀		3.40	--			⊙
C22	26.967	289.1747		C ₁₃ H ₂₄ N ₂ O ₅	289,272,152	-3.80	--	●		
C23	28.830	447.1266		C ₂₂ H ₂₂ O ₁₀	447,285	-4.47	Calycosin-7-O-β-D-glucoside			⊙
C24	29.233	477.1387		C ₂₃ H ₂₄ O ₁₁	477,315,300,283,255	-0.84	4-methoxy-maackiain-7-O-β-D-glucoside			⊙
C25	30.070		637.2113	C ₃₀ H ₃₈ O ₁₅	637,475,387	-3.92	--			⊙

Table S2. Cont.

NO.	T _R (min)	[M+H] ⁺	[M-H] ⁻	Predicted Formula	Fragment ions	Error ppm	Identification	T	IT	S
C26	30.653		479.1492	C ₃₀ H ₂₄ O ₆	479,317	-1.67	--			⊙
C27	30.773	[M+HCOO] ⁻	671.2155	C ₂₉ H ₃₈ O ₁₅	671,625,463,301	-5.66	Astraisoflavan-di-7-O-β-D-glucoside			⊙
C28	31.005		579.2062	C ₂₃ H ₃₆ N ₂ O ₁₅	579,417,387	3.28	--			⊙
C29	31.348		445.1123	C ₂₂ H ₂₂ O ₁₀	445,283	-3.82	Glycetein-4'-O-β-D-glucoside			⊙
C30	32.078	463.1203		C ₂₂ H ₂₂ O ₁₁	463,301	-6.91	Kaempferide-7-O-β-D-glucoside			⊙
C31	32.662	533.1267		C ₂₅ H ₂₄ O ₁₃	533,285	-4.31	6"-O-malonate-calycosin-7-O-β-D-glucoside			⊙
C32	34.207	489.1398		C ₂₄ H ₂₄ O ₁₁	489,285	1.43	6"-O-acetyl-calycosin-7-O-β-D-glucoside			⊙
C33	34.550	431.1303		C ₂₂ H ₂₂ O ₉	431,269	-7.89	Ononin		★	
C34	35.348		489.1340	C ₂₄ H ₂₆ O ₁₁	489,285,271,159	-12.68	6"-O-acetyl-isosakuranetin-7-O-β-D-glucoside			⊙
C35	35.580	549.1174		C ₂₅ H ₂₄ O ₁₄	549,301	-11.84	6"-O-malonate-kaempferide-7-O-β-D-glucoside			⊙
C36	36.027	463.1615		C ₂₃ H ₂₆ O ₁₀	485(+Na ⁺),463,301	3.45	Astrapterocarpan-7-O-β-D-glucopyranoside			⊙
C37	36.773		463.1577	C ₂₃ H ₂₈ O ₁₀	463,301,271	-7.13	Astraisoflavan-7-O-β-D-glucopyranoside			⊙
C38	38.035	285.0744		C ₁₆ H ₁₂ O ₅	285,270,225,137	-4.91	Calycosin		★	
C39	38.653	315.0844		C ₁₇ H ₁₄ O ₆		-6.03	4-methoxy-maackiain or the isomer			⊙
C40	38.653	473.1445		C ₂₄ H ₂₄ O ₁₀	473,269	0.63	The isomer of 6"-O-acetyl-ononin			⊙
C41	38.773	447.1264		C ₂₂ H ₂₂ O ₁₀	447,285	-4.92	Glycetein-7-O-β-D-glucoside			⊙
C42	38.997	549.1545		C ₂₆ H ₂₈ O ₁₃	549,301	-10.56	6"-O-malonate-astrapterocarpan-glucoside			⊙
C43	39.452	517.1301		C ₂₅ H ₂₄ O ₁₂	517,269	-7.73	6"-O-malonate-ononin			⊙
C44	39.683		505.1699	C ₂₅ H ₃₀ O ₁₁	505,301	-3.17	6"-O-acetyl-astraisoflavan-7-O-β-D-glucoside			⊙
C45	39.743		957.5126	C ₄₈ H ₇₈ O ₁₉		6.37	Soyasaponin Ba		★	
C46	40.138	473.1424		C ₂₄ H ₂₄ O ₁₀	473,269	-3.80	6"-O-acetyl-ononin			⊙
C47	40.430		503.1154	C ₂₄ H ₂₄ O ₁₂	503,299	-8.15	6"-O-acetyl-kaempferide-7-O-β-D-glucoside			⊙
C48	40.825		785.4629	C ₄₁ H ₇₀ O ₁₄		-8.15	Cyclocanthoside E			⊙
C49	41.108		991.5086	C ₄₈ H ₈₀ O ₂₁		-3.33	Astragaloside V			⊙
C50	41.778		315.0868	C ₁₇ H ₁₆ O ₆	315,253	-1.90	Astragaluquinone or isomer			⊙

Table S2. Cont.

NO.	T _R (min)	[M+H] ⁺	[M-H] ⁻	Predicted Formula	Fragment ions	Error ppm	Identification	T	IT	S
C51	41.950	533.1243		C ₂₅ H ₂₄ O ₁₃	533,285	-8.82	6"-O-malonate-glycetein-7-O-β-D-glucoside			◎
C52	42.062		867.4635	C ₄₅ H ₇₂ O ₁₆		-13.03	Isoastragaloside I			◎
C53	42.612	[M+HCOO] ⁻	829.4572	C ₄₁ H ₆₈ O ₁₄		-2.29	Astragaloside IV			◎
C54	42.560		825.4532	C ₄₃ H ₇₀ O ₁₅	871,825	-13.33	Isoastragaloside II			◎
C55	44.190		941.5081	C ₄₈ H ₇₈ O ₁₈	941,525,437	-3.61	Soyasaponin Bb		★	
C56	45.315	269.0791		C ₁₆ H ₁₂ O ₄	269,254,237,118	-6.32	formononetin		★	
C57	45.935		329.2299	C ₁₈ H ₃₄ O ₅		-10.33	--			◎
C58	46.158	301.1052		C ₁₇ H ₁₆ O ₅		-6.31	Astraoptercarpan			◎
C59	46.708	303.1181		C ₁₇ H ₁₈ O ₅		-15.18	Astraisoflavan			◎
C60	46.768	[M+HCOO] ⁻	871.4656	C ₄₃ H ₇₀ O ₁₅	871,825,603	-4.70	Astragaloside II			◎
C61	47.172	[M+HCOO] ⁻	911.4668	C ₄₅ H ₇₀ O ₁₆	955,911	2.41	--			◎
C62	49.432		285.0423	C ₁₅ H ₁₀ O ₆	285,163	6.31	Kaempferol or isomer			◎
C63	50.670		311.2212	C ₁₈ H ₃₂ O ₄		-5.14	--	●		
C64	50.713	[M+HCOO] ⁻	913.4777	C ₄₅ H ₇₂ O ₁₆		-2.74	Astragaloside I			◎
C65	51.607	[M+HCOO] ⁻	953.4637	C ₄₇ H ₇₂ O ₁₇	953,909	-12.06	--			◎
C66	52.363	437.3374	[M+Na] ⁺	C ₂₈ H ₄₆ O ₂		-3.66	--			◎
C67	59.933	213.0871	[M+Na] ⁺	C ₁₂ H ₁₄ O ₂	403[2M+Na] ⁺ ,213,191	-7.04	Z-ligustilide		★	
C68	61.708	403.1867	[2M+Na] ⁺	C ₁₂ H ₁₄ O ₂	403,381,191	-3.22	E-ligustilide		★	
C69	69.377		283.0238	C ₁₅ H ₈ O ₆	283,203,147	-3.53	--	●		

T(●)The same unidentified proposed compounds of two kinds DBT; IT(★) The same identified proposed compounds of two kinds DBT; S(◎) The special proposed compounds of two kinds DBT in respectively.

Table S3. The identified compounds from DBT2 boiled sample by HPLC-IT-TOF-MSⁿ.

NO.	T _R (min)	[M+H] ⁺	[M-H] ⁻	Predicted Formula	Fragment ions	Error ppm	Identification	T	IT	S
c1	2.395		173.1044	C ₆ H ₁₄ N ₄ O ₂		0.00	Arginine	●		
c2	2.575		195.0502	C ₆ H ₁₂ O ₇		-4.10	Gluconic acid	●		
c3	2.695		341.1074	C ₁₂ H ₂₂ O ₁₁		-4.40	D(+)sucrose	●		
c4	3.643		191.0187	C ₆ H ₈ O ₇	191,173	-5.24	Citric acid	●		
c5	4.477		328.0427	C ₁₁ H ₁₁ N ₃ O ₉		1.22	--	●		
c6	6.172		344.0387	C ₁₁ H ₁₁ N ₃ O ₁₀		4.36	--	●		
c7	9.120	443.1146	[M+Na] ⁺	C ₁₇ H ₂₄ O ₁₂		-3.16	--			⊙
c8	9.345	267.1369		C ₁₈ H ₁₈ O ₂	267,225	-4.12	Magnolol			⊙
c9	10.842	188.0674		C ₉ H ₁₁ NO ₂		-4.25	L-phenylalanine	●		
c10	12.765		382.1007	C ₁₃ H ₂₁ NO ₁₂		4.19	--	●		
c11	13.840		461.1283	C ₁₉ H ₂₆ O ₁₃	461,167	-3.90	--			⊙
c12	21.207		433.1129	C ₂₁ H ₂₂ O ₁₀	433,285	-2.54	--			⊙
c13	21.322		433.1121	C ₂₁ H ₂₂ O ₁₀	433,285,241	-4.39	--			⊙
c14	22.020		417.1017	C ₁₇ H ₂₂ O ₁₂	417,285,152	-5.03	--		★	
c15	23.018		401.1445	C ₁₈ H ₂₆ O ₁₀	401,269,161	-1.99	--	●		
c16	23.080	389.2325		C ₂₃ H ₃₂ O ₅		0.51	--	●		
c17	26.998		287.1595	C ₁₃ H ₂₄ N ₂ O ₅		-5.92	--	●		
c18	34.517	431.1322		C ₂₂ H ₂₂ O ₉	431,269,237,118	-3.48	Ononin		★	
c19	37.480		255.0657	C ₁₅ H ₁₂ O ₄	255,135	-2.35	Isoliquiritigenin			⊙
c20	38.072		283.0596	C ₁₆ H ₁₂ O ₅	283,268,240	-5.65	Calycosin		★	
c21	39.917		269.0807	C ₁₆ H ₁₄ O ₄	269,253,227	-4.46	Isomer of alpinetin			⊙
c22	39.977		255.0657	C ₁₅ H ₁₂ O ₄	255,237	-2.35	Liquiritigenin			⊙
c23	39.745		957.5030	C ₄₈ H ₇₈ O ₁₉	957,541,453	-3.66	Soyasaponin Ba		★	
c24	40.903		927.4915	C ₄₇ H ₇₆ O ₁₈		-4.74	Akebia saponin D			⊙
c25	41.273		285.0751	C ₁₆ H ₁₄ O ₅	285,194,109	-5.96	Isomer of isosakuranetin			⊙

Table S3. Cont.

NO.	T _R (min)	[M+H] ⁺	[M-H] ⁻	Predicted Formula	Fragment ions	Error ppm	Identification	T	IT	S
c26	41.772		269.0456	C ₁₅ H ₁₀ O ₅	269,237	0.37	Genistein			⊙
c27	42.243		283.0602	C ₁₆ H ₁₂ O ₅	283,268,224	-3.53	Glycetein			⊙
c28	42.965		329.2319	C ₁₈ H ₃₄ O ₅		-4.25	--			⊙
c29	43.197		955.4857	C ₄₈ H ₇₆ O ₁₉		-5.34	--			⊙
c30	44.690		287.0577	C ₁₅ H ₁₂ O ₆		5.57	Dihydro-kaempferol			⊙
c31	44.982		255.0649	C ₁₅ H ₁₂ O ₄	256,135	-5.49	Isomer of Liquiritigenin			⊙
c32	45.393	269.0784		C ₁₆ H ₁₂ O ₄	269,253,237	-8.92	Formononetin		★	
c33	45.745	299.0911		C ₁₇ H ₁₄ O ₅	299,284,166		Pterocarpin			⊙
c34	46.080		283.0599	C ₁₆ H ₁₂ O ₅	283,255,240	-4.59	The isomer of glycetein			⊙
c35	47.592		941.5080	C ₄₈ H ₇₈ O ₁₈	947,525,437	-3.72	Soyasaponin Bb		★	
c36	47.772		299.0552	C ₁₆ H ₁₂ O ₆		-3.01	Kaempferide or isomer			⊙
c37	47.943		909.4836	C ₄₇ H ₇₄ O ₁₇		-1.87	Acetylastragaloside I			⊙
c38	48.347	[M+HCOO] ⁻	911.5011	C ₄₆ H ₇₄ O ₁₅		0.11	Castaraleside H			⊙
c39	50.065		939.4925	C ₄₈ H ₇₆ O ₁₈		-3.62	--			⊙
c40	50.435	285.0748		C ₁₆ H ₁₂ O ₅	285,253,152	-3.51	Isomer of calycosin			⊙
c41	50.667	335.2180	[M+Na] ⁺	C ₁₈ H ₃₂ O ₄		-3.88	--	●		
c42	51.560	193.1212		C ₁₂ H ₁₆ O ₂		-5.70	Senkyunolide A			⊙
c43	55.212	191.1043		C ₁₂ H ₁₄ O ₂		-12.56	n-butyl-phthalide			⊙
c44	59.250	213.0876	[M+Na] ⁺	C ₁₂ H ₁₄ O ₂	403,213	-4.69	Z-ligustilide		★	
c45	61.765	213.0893	[M+Na] ⁺	C ₁₂ H ₁₄ O ₂	381,191,213	3.29	E-ligustilide		★	
c46	69.093		283.0257	C ₁₅ H ₈ O ₆		3.18	--	●		

T(●)The same unidentified proposed compounds of two kinds DBT; IT(★) The same identified proposed compounds of two kinds DBT; S(⊙) The special proposed compounds of two kinds DBT in respectively.

Table S4. The identified proposed metabolites from the urine sample after administrated DBT1 to rats.

NO.	T _R (min)	[M+H] ⁺	[M-H] ⁻	Predicted Formula	Fragment ions	Error ppm	Identification	T	IT	S
M1	4.130		287.0066	C ₁₀ H ₈ O ₁₀		7.32	--	●		
M2	28.110	233.0909		C ₁₂ H ₁₂ N ₂ O ₃	233, 130	-5.15	--	●		
M3	28.848		233.0116	C ₁₂ H ₂ N ₄ O ₂	233,169	4.72	--	●		
M4	29.415		337.1407	C ₁₆ H ₂₂ N ₂ O ₆	337.193	0.59	--	●		
M5	31.338		275.0209	C ₁₃ H ₈ O ₇	275,195	4.36	--	●		
M6	32.678		273.0063	C ₁₃ H ₆ O ₇	273,193	8.06	--	●		
M7	33.038	271.0585		C ₁₅ H ₁₀ O ₅		-5.90	Hydroxyl-daidzein			⊙
M8	36.155		303.0863	C ₁₆ H ₁₆ O ₆	303,151	-3.63	hydroxyl-calycosin, di-reduction(C ² =C ³ ; C ⁴ =O)			⊙
M9	36.705		253.0492	C ₁₅ H ₁₀ O ₄		-5.53	Daidzein		★	
M10	36.808		477.1372	C ₂₃ H ₂₆ O ₁₁	477,301	-6.29	Astraisoflavan, glucuronidation			⊙
M11	36.868		255.0662	C ₁₅ H ₁₂ O ₄	255,149	-0.39	Daidzein, reduction(C ² =C ³)		★	
M12	37.255	385.1478		C ₁₈ H ₂₄ O ₉		-3.89	Hydro-ligustilide, glucuronidation			⊙
M13	37.435		285.0751	C ₁₆ H ₁₄ O ₅	285,269,149	-5.96	Calycosin, reduction(C ² =C ³)		★	
M14	37.195		257.0809	C ₁₅ H ₁₄ O ₄		-3.89	Daidzein, di-reduction(C ² =C ³ ; C ⁴ =O)			⊙
M15	38.070		283.0605	C ₁₆ H ₁₂ O ₅	283,268,211	-2.47	Calycosin		★	
M16	38.362		285.0751	C ₁₆ H ₁₄ O ₅	285,270	-5.96	Calycosin, reduction(C ⁴ =O)			⊙
M17	39.367		233.0098	C ₁₂ H ₂ N ₄ O ₂		-3.00	--	●		
M18	40.260	[M+HCOO] ⁻	363.0748	C ₁₆ H ₁₄ O ₇		7.16	Dihydroxy-calycosin, reduction(C ² =C ³)			⊙
M19	41.755		269.0441	C ₁₅ H ₁₀ O ₅		-5.20	Hydroxy-daidzein			⊙
M20	42.365		299.0554	C ₁₆ H ₁₂ O ₆	299,284	-2.34	Hydroxy-calycosin, or isomer			⊙
M21	42.923		299.0556	C ₁₆ H ₁₂ O ₆	299,284	-1.67	Hydroxy-calycosin			⊙
M22	44.315		257.0819	C ₁₅ H ₁₄ O ₄		0.00	Isoliquiritigenin, reduction(C=C)		★	
M23	45.328	269.0793		C ₁₆ H ₁₂ O ₄	269,253,237	-5.57	Formononetin		★	
M24	45.732		269.0798	C ₁₆ H ₁₄ O ₄	269,254,135	-7.80	Formononetin, reduction(C ² =C ³)		★	
M25	46.290	335.0201		C ₁₅ H ₁₀ O ₇ S	335,255	-5.67	Daidzein, sulfation		★	

Table S4. Cont.

NO.	T _R (min)	[M+H] ⁺	[M-H] ⁻	Predicted Formula	Fragment ions	Error ppm	Identification	T	IT	S
M26	47.862		363.0174	C ₁₆ H ₁₂ O ₈ S	363,268	-1.65	Calycosin, sulfation			☉
M27	47.922		333.0059	C ₁₅ H ₁₀ O ₇ S	333,253,225	-4.50	Daidzein, sulfation			☉
M28	48.205		349.0053	C ₁₅ H ₁₀ O ₈ S	349,269	8.31	Hydroxy-daidzein, sulfation		★	
M29	48.747		365.0347	C ₁₆ H ₁₄ O ₈ S	365,285	2.74	Calycosin, reduction(C ² =C ³), sulfation			☉
M30	49.193		365.0360	C ₁₆ H ₁₄ O ₈ S	365,285	6.30	Calycosin, reduction(C ² =C ³), sulfation			☉
M31	49.623		351.0187	C ₁₅ H ₁₂ O ₈ S	351,271,149	1.99	Hydroxy-daidzein, reduction(C ² =C ³), sulfation			☉
M32	50.467		283.0595	C ₁₆ H ₁₂ O ₅	283,268	-6.01	Isomer of calycosin			☉
M33	50.973		367.0483	C ₁₆ H ₁₆ O ₈ S	367,272,150	-2.72	Calycosin, di-reduction(C ² =C ³ ; C ⁴ =O), sulfation			☉
M34	51.515		363.0180	C ₁₆ H ₁₂ O ₈ S	363,283	0.00	Calycosin, sulfation		★	
M35	52.563		335.0250	C ₁₅ H ₁₂ O ₇ S	335,255,135	5.67	Daidzein, reduction(C ² =C ³), sulfation			☉
M36	53.637		343.0835	C ₁₈ H ₁₆ O ₇		3.50	--			☉
M37	55.165		321.0417	C ₁₅ H ₁₄ O ₆ S	321,241	-6.54	Equol, sulfation	●		
M38	59.468		337.0388	C ₁₅ H ₁₄ O ₇ S	337,257,243	0.30	Daidzein, di-reduction(C ² =C ³ ; C ⁴ =O), sulfation			☉
M39	61.838	683.4277		C ₃₅ H ₆₄ O ₁₁		-9.57	Related to astragaloside			☉
M40	62.002	639.4061		C ₃₅ H ₅₈ O ₁₀		-6.57	Related to astragaloside			☉
M41	62.113	595.3742		C ₃₃ H ₅₄ O ₉		-16.63	Related to astragaloside	●		
M42	62.414	507.3296		C ₂₉ H ₄₆ O ₇		-3.94	Related to astragaloside			☉
M43	71.557		353.0324	C ₁₅ H ₁₄ O ₈ S	353,273	-3.68	Hydroxy-daidzein, di-reduction(C ² =C ³ ; C ⁴ =O) sulfation			☉
M44	71.557		397.0250	C ₁₆ H ₁₄ O ₁₀ S	397,317	3.78	Dihydroxy-calycosin, reduction(C ² =C ³), sulfation			☉

T(●)The same unidentified metabolites from the urine administrated two kinds DBT; IT(★) The same standard metabolites from the urine administrated two kinds DBT; S(☉) The special metabolites from the urine administrated two kinds DBT in respectively.

Table S5. The identified proposed metabolites from the urine sample after administrated by DBT2 to rats.

NO.	T _R (min)	[M+H] ⁺	[M-H] ⁻	Predicted Formula	Fragment ions	Error ppm	Identification	T	IT	S
m1	4.132		287.0065	C ₁₀ H ₈ O ₁₀		6.97	--	●		
m2	28.200		231.0768	C ₁₂ H ₁₂ N ₂ O ₃	463,231	-3.03	--	●		
m3	29.298		233.0115	C ₁₂ H ₂ N ₄ O ₂	233,169	4.29	--	●		
m4	29.298		337.1408	C ₁₆ H ₂₂ N ₂ O ₆	337,253	0.89	--	●		
m5	31.083	268.1164	266.1021	C ₁₃ H ₁₇ NO ₅		-4.89	--			⊙
m6	31.970		275.0211	C ₁₃ H ₈ O ₇	275,195	5.09	--	●		
m7	32.927		273.0056	C ₁₃ H ₆ O ₇	273,193	5.49	--	●		
m8	34.518	[M+HCOO] ⁻	475.1244	C ₂₂ H ₂₂ O ₉	475,267	-0.42	Isomer of ononin			⊙
m9	36.583	255.0637		C ₁₅ H ₁₀ O ₄	255,199	-5.88	daidzein		★	
m10	36.918		255.0651	C ₁₅ H ₁₂ O ₄	255,149	-4.70	Daidzein, reduction(C ² =C ³)		★	
m11	37.442		255.0655	C ₁₅ H ₁₂ O ₄		-3.14	Daidzein, reduction(C ⁴ =O)			⊙
m12	37.502		285.0751	C ₁₆ H ₁₄ O ₅	285,269,149	-5.96	Calycosin, reduction(C ² =C ³)		★	
m13	38.033		283.0608	C ₁₆ H ₁₂ O ₅	283,268	-1.41	Calycosin		★	
m14	39.047		273.0761	C ₁₅ H ₁₄ O ₅	273,240,109	-2.56	hydroxy-daidzein, di-reduction (C ² =C ³ ; C ⁴ =O)			⊙
m15	40.128		233.0115	C ₁₂ H ₂ N ₄ O ₂		4.29	--	●		
m16	41.630		283.0609	C ₁₆ H ₁₂ O ₅	283,268,224	-1.06	Isomer of calycosin			⊙
m17	42.180		283.0603	C ₁₆ H ₁₂ O ₅	283,268,224	-3.18	Isomer of calycosin			⊙
m18	44.327		257.0804	C ₁₅ H ₁₄ O ₄	257,240	-5.83	Isoliquiritigenin, reduction(C=C)		★	
m19	45.322	269.0796		C ₁₆ H ₁₂ O ₄	269,253,237	-4.46	Formononetin		★	
m20	45.733		269.0804	C ₁₆ H ₁₄ O ₄	269,254,135	-5.57	Formononetin, reduction(C ² =C ³)		★	
m21	47.175		333.0052	C ₁₅ H ₁₀ O ₇ S	333,253	-6.61	daidzein, sulfation		★	
m22	47.775		299.0556	C ₁₆ H ₁₂ O ₆	299,256	-1.67	Hydroxy-calycosin			⊙
m23	49.072		333.0056	C ₁₅ H ₁₀ O ₇ S	333,253,208	-5.41	daidzein, sulfation			⊙
m24	49.543		333.0059	C ₁₅ H ₁₀ O ₇ S	333,253	-4.50	Isomer of daidzein, sulfation			⊙
m25	49.810		349.0033	C ₁₅ H ₁₀ O ₈ S	349,269,225	2.58	Hydroxy-daidzein, sulfation		★	

Table S5. Cont.

NO.	T _R (min)	[M+H] ⁺	[M-H] ⁻	Predicted Formula	Fragment ions	Error ppm	Identification	T	IT	S
m26	49.930		363.0184	C ₁₆ H ₁₂ O ₈ S	363,283	1.10	Calycosin, sulfation		★	
m27	50.325		337.0395	C ₁₅ H ₁₄ O ₇ S	337,257	2.37	Daidzein, di-reduction(C ² =C ³ ; C ⁴ =O), sulfation			◎
m28	55.693		351.0172	C ₁₅ H ₁₂ O ₈ S	351,271	-2.28	Hydroxy-daidzein, reduction(C ² =C ³), sulfation			◎
m29	57.015		321.0414	C ₁₅ H ₁₄ O ₆ S	321,241	-7.48	Equol, sulfation	●		
m30	59.728	619.3669	[M+Na] ⁺	C ₃₆ H ₅₂ O ₇		10.33	Related to astragaloside			◎
m31	62.218	595.3742		C ₃₃ H ₅₄ O ₉		-16.63	Related to astragaloside	●		
m32	63.292		509.3599	C ₃₃ H ₅₀ O ₄		-7.26	Related to astragaloside			◎
m33	72.797		363.0197	C ₁₆ H ₁₂ O ₈ S	363,283	4.68	Calycosin, sulfation			◎
m34	73.543		347.0213	C ₁₆ H ₁₂ O ₇ S	347,267	-5.19	Formononetin, sulfation			◎

T(●) The same unidentified metabolites from the urine administrated two kinds DBT; IT(★) The same standard metabolites from the urine administrated two kinds DBT; S(◎) The special metabolites from the urine administrated two kinds DBT in respectively.

Table S6. The number comparison of the identified compounds between DBT1 and DBT2.

N.	ID.	S-ID.	T.ID.	S%	H+S	S%
DBT1	69	21	115-21=94	22.34	56	59.57
DBT2	46					
DBT1-U	44	19	75-19=56	33.93	48	85.71
DBT2-U	31					

ID.: Identified proposed compounds; S-ID.: Identified the common proposed compounds between two DBT; T.ID.: Identified the unfamiliar proposed compounds between two DBT; H+S: The total isoflavones and the total saponins; S%: The ratio about the selective compounds in the total identified proposed compounds number.