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Phytochemical characterization and evaluation of the antibacterial activity of *Amruthotharam kwath*, a traditional polyherbal formulation on multidrug resistant clinical isolates from the respiratory tract

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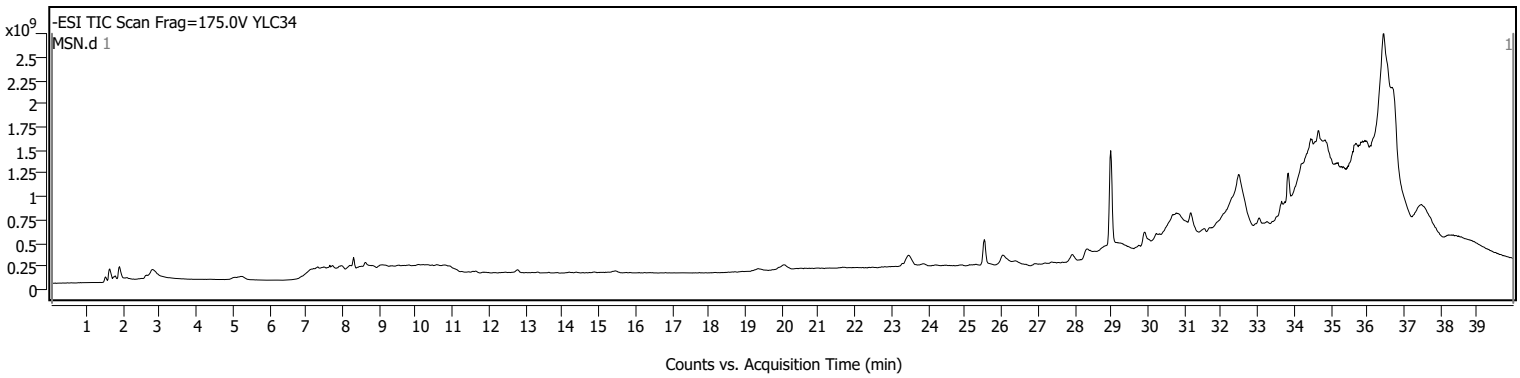
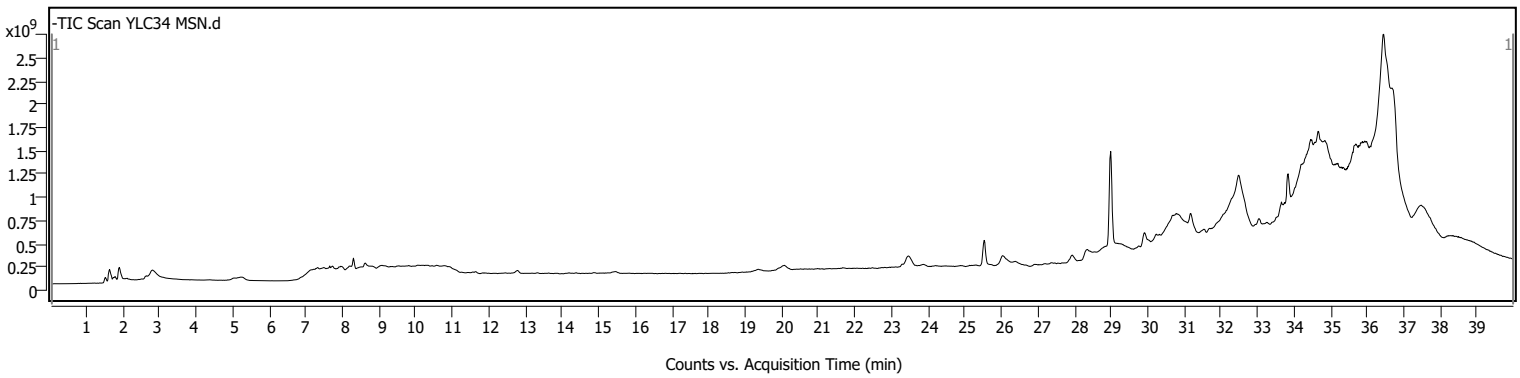
Supplementary Data

Sample Information

Name	Amruthotharam kashayam	**Data File Path**	D:\MassHunter\Data\2022\September\YLC34\YLC34MSN.d
Sample ID	YLC34	**Acq. Time (Local)**	10-02-2023 11:11:09 (UTC+05:30)
Instrument	6545 QTOF	**Method Path (Acq)**	D:\MassHunter\Methods\Generalprofiling 1100 mm.m
MS Type	QTOF	**Version (Acq SW)**	6200 series TOF/6500 series Q-TOF 10.1 (48.0)
Inj. Vol. (uL)	3	**IRM Status**	Success
Position	P1-A2	**Method Path (DA)**	D:\MassHunter\Methods\10.0\Trainingprocessingmethod FBF.m
Plate Pos.		**Target Source Path**	D:\MassHunter\PCDL\Phytoconstitients AK & VK.cdb
Operator		**Result Summary**	76 qualified (96 targets)

Sample Chromatograms





Compound Summary

Cpd	Name	Formula	CAS	RT	Mass	Mass (Tgt)	Diff (Tgt, ppm)	Score	Algorithm
1	6-Gingerol	C17H26O4		9.463	294.1792	294.1831	-13.40	56.05	FBF
2	10-Gingerol	C21H34O4		33.587	350.2420	350.2457	-10.56	40.67	FBF
3	8-Gingerol	C19H30O4		9.862	322.2140	322.2144	-1.34	70.21	FBF
4	1-Dehydro-[10]-gingerdione	C21H30O4		33.654	346.2140	346.2144	-1.20	59.48	FBF
5	6-Shogaol	C17H24O3		30.065	276.1701	276.1725	-8.98	46.29	FBF
6	(10)-SHOGAOL	C21H32O3		34.883	332.2380	332.2351	8.70	77.39	FBF
7	8-Shogaol	C19H28O3		26.410	304.1988	304.2038	-16.59	54.81	FBF
8	6-Paradol	C17H26O3		9.928	278.1854	278.1882	-9.96	81.53	FBF
9	1-Dehydro-6-gingerdione	C17H22O4		31.859	290.1573	290.1518	18.83	42.47	FBF
10	Diacetoxy-6-gingerdiol	C21H32O6		33.271	380.2158	380.2199	-10.67	67.17	FBF
11	Methyldiacetoxy-6-gingerdiol	C22H34O6		35.448	394.2335	394.2355	-5.11	77.35	FBF
12	D-(−)-Quinicacid	C7H12O6		29.766	192.0647	192.0634	6.58	88.67	FBF
13	Protocatechuicacid	C12H21ClN6		32.939	284.1535	284.1516	6.52	51.31	FBF
14	Gentisicacid	C7H6O4		8.101	154.0260	154.0266	-4.20	83.07	FBF
15	Gallicacid	C7H6O5		31.444	170.0201	170.0215	-8.45	41.55	FBF
16	(±)-MalicAcid	C4H6O5		27.706	134.0207	134.0215	-5.94	76.82	FBF
17	Gallocatechin	C15H14O7		20.479	306.0756	306.0740	5.35	64.19	FBF
18	AnacardicacidC15:3	C22H30O3		32.823	342.2133	342.2195	-17.97	59.00	FBF
19	6,2'-Dihydroxyflavanone	C15H12O4		16.458	256.0732	256.0736	-1.31	68.83	FBF
20	Chebulicacid	C14H12O11		28.835	356.0415	356.0380	9.83	72.23	FBF
21	Rutin	C27H30O16		7.220	610.1513	610.1534	-3.37	77.38	FBF
22	Quercetin3-rhamnosyl-(1->2)-rhamnosyl-(1->6)-glucoside	C33H40O20		34.219	756.2089	756.2113	-3.17	43.41	FBF
23	Apigenin	C15H10O5		23.602	270.0535	270.0528	2.44	83.62	FBF
24	4-Methylumbelliferone	C10H8O3		23.868	176.0469	176.0473	-2.58	83.16	FBF
25	Bergapten	C12H8O4		14.082	216.0455	216.0423	15.02	62.77	FBF
26	Sinapicacid	C11H12O5		36.711	224.0681	224.0685	-1.55	65.22	FBF
27	vicenin2	C27H30O15		37.359	594.1699	594.1585	19.21	55.78	FBF
28	Vicenin1	C26H28O14		38.206	564.1486	564.1479	1.18	40.59	FBF
29	Berberine	C20H18NO4		38.372	336.1240	336.1236	1.11	70.11	FBF
30	cis-p-Coumaricacid4-[apiosyl-(1->2)-glucoside]	C20H26O12		2.618	458.1323	458.1424	-22.03	59.07	FBF
31	Monocaffeoyl(-)-tartaricacid	C13H12O9		24.433	312.0475	312.0481	-2.13	75.63	FBF

Target Screening Report

Agilent | Trusted Answers

Compound Summary

Cpd	Name	Formula	CAS	RT	Mass	Mass (Tgt)	Diff (Tgt, ppm)	Score	Algorithm
32	Monocaffeoyl(-)-tartaricacid	C13H12O9		30.713	312.0461	312.0481	-6.52	49.70	FBF
33	Magnoflorine	C20H24NO4		1.871	342.1675	342.1705	-8.90	65.23	FBF
34	AnacardicacidC15:1	C22H34O3		33.072	346.2508	346.2508	-0.10	73.06	FBF
35	1-Caffeoylquinicacid	C16H18O9		37.010	354.0969	354.0951	5.19	47.52	FBF
36	3-Pentadecylphenol	C21H36O		36.694	304.2776	304.2766	3.09	48.49	FBF
37	Desogestrel	C22H30O		33.205	310.2291	310.2297	-1.73	79.31	FBF
38	(-)-Shikimicacid	C7H10O5		7.669	174.0532	174.0528	2.33	45.25	FBF
39	(-)-Shikimicacid	C7H10O5		19.615	174.0539	174.0528	6.10	46.68	FBF
40	trans-caffeicacid	C9H8O4		25.845	180.0384	180.0423	-21.20	45.07	FBF
41	trans-caffeicacid	C9H8O4		30.248	180.0398	180.0423	-13.58	50.05	FBF
42	6-Hydroxyflavanone	C15H12O3		12.819	240.0780	240.0786	-2.70	74.09	FBF
43	(E)-Ferulicacid	C10H10O4		2.851	194.0569	194.0579	-5.23	79.57	FBF
44	(E)-Ferulicacid	C10H10O4		8.018	194.0602	194.0579	12.04	58.22	FBF
45	(E)-Ferulicacid	C10H10O4		22.788	194.0582	194.0579	1.55	54.16	FBF
46	8-Acetyl-7-methoxycoumarin	C12H10O4		11.191	218.0604	218.0579	11.55	65.60	FBF
47	2-Coumaricacid	C9H8O3		33.770	164.0474	164.0473	0.47	70.47	FBF
48	2-Coumaricacid	C9H8O3		36.727	164.0447	164.0473	-15.89	67.12	FBF
49	Diosmetin	C16H12O6		31.527	300.0626	300.0634	-2.70	49.62	FBF
50	Betulinicacid	C30H48O3		35.033	456.3590	456.3603	-2.88	43.79	FBF
51	Apigetrin	C21H20O10		8.284	432.1084	432.1056	6.29	48.21	FBF
52	D-(+)-Catechin	C15H14O6		8.284	290.0857	290.0790	22.84	49.52	FBF
53	D-(+)-Catechin	C15H14O6		30.680	290.0797	290.0790	2.12	52.13	FBF
54	protocatechuicacid-4-glucoside	C13H16O9		11.357	316.0784	316.0794	-3.17	71.77	FBF
55	vanilicacid	C8H8O4		9.031	168.0457	168.0423	20.23	44.30	FBF
56	Methylgallate	C8H8O5		11.091	184.0333	184.0372	-20.87	46.51	FBF
57	Ellagicacid	C14H6O8		23.519	302.0066	302.0063	1.20	83.65	FBF
58	salicylicacidglucoside	C13H16O8		30.214	300.0906	300.0845	20.24	50.16	FBF
59	1-o-Caffeoylglucose	C15H18O9		24.183	342.0923	342.0951	-8.05	69.00	FBF
60	Isopimpinellin	C13H10O5		28.902	246.0526	246.0528	-0.93	47.43	FBF
61	1-Tritriacontanol	C33H68O		36.744	480.5277	480.5270	1.46	61.81	FBF
62	Hirsutrin	C21H20O12		31.693	464.0940	464.0955	-3.18	53.56	FBF
63	Hirsutrin	C21H20O12		38.339	464.0894	464.0955	-13.01	51.62	FBF
64	Isorhamnetin	C16H12O7		35.232	316.0573	316.0583	-3.02	58.17	FBF
65	Kaempferol	C15H10O6		29.882	286.0505	286.0477	9.66	54.23	FBF
66	Ginkgolide-B	C20H24O10		33.404	424.1375	424.1369	1.26	49.31	FBF
67	Quercetin	C15H12O8		30.214	320.0577	320.0532	13.93	54.35	FBF
68	BILOBALIDE	C15H18O8		15.444	326.0973	326.1002	-8.94	43.09	FBF
69	Solanacarpidine	C27H43NO2		34.966	413.3251	413.3294	-10.29	49.80	FBF
70	Asculetine	C9H6O4		11.889	178.0257	178.0266	-4.89	66.97	FBF
71	Aesculin	C15H16O9		34.003	340.0779	340.0794	-4.40	65.88	FBF
72	carpesterol	C37H54O4		13.069	562.4098	562.4022	13.41	62.37	FBF
73	Diosgenin	C27H42O3		34.418	414.3133	414.3134	-0.25	70.73	FBF
74	Diosgenin	C27H42O2		35.082	398.3229	398.3185	11.18	68.31	FBF
75	Campesterol	C28H48O		36.478	400.3702	400.3705	-0.67	57.32	FBF
76	cycloartenol	C30H50O		35.033	426.3918	426.3862	13.23	53.20	FBF

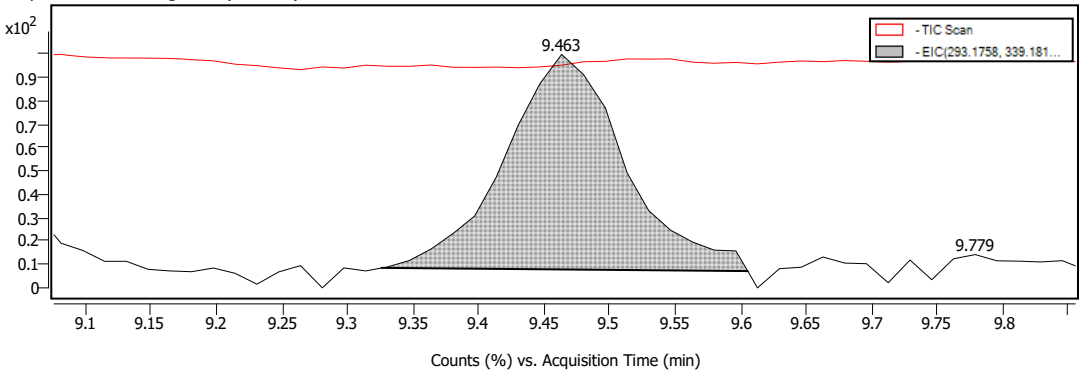
Compound Details

Cpd. 1: 6-Gingerol

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)		CAS	ID Source	Score	Algorithm
6-Gingerol	C17 H26 O4	9.463		294.1792	-13.40		FBF	56.05	FBF

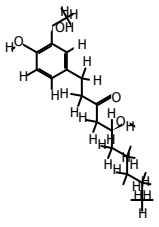
Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	293.1711339.1910 353.2076	56.05				

Compound Chromatograms (overlaid)



Counts (%) vs. Acquisition Time (min)

Structure



Target Screening Report

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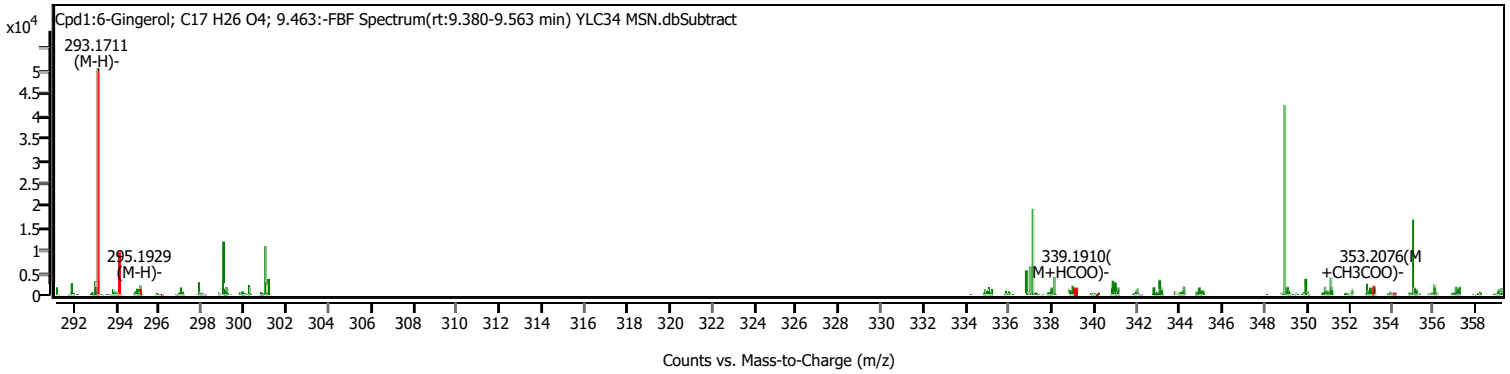
Compound Spectra (overlaid)



Compound ID Table

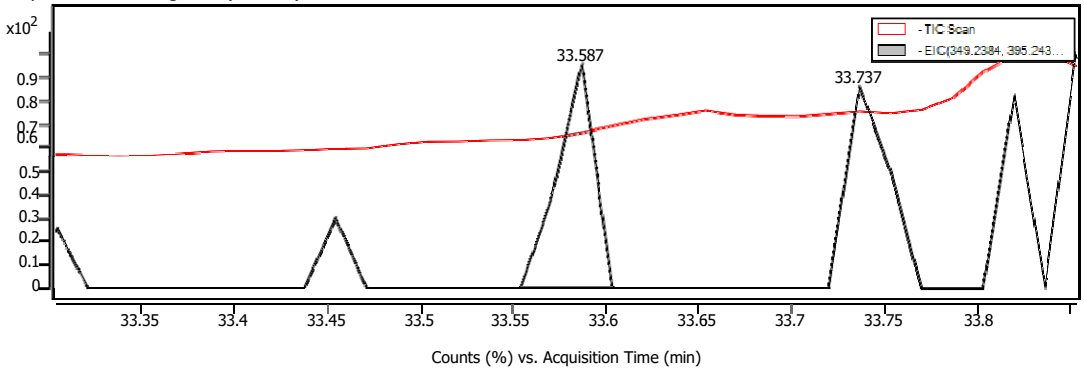
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
6-Gingerol	C17 H26 O4	(M-H)- (M+HCOO)- (M+CH3COO)-	9.463		294.1792		FBF	56.05		56.05

Cpd. 2: 10-Gingerol

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)		CAS	ID Source	Score	Algorithm
10-Gingerol	C21 H34 O4	33.587		350.2420	-10.56		FBF	40.67	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-	349.2348	40.67				

Compound Chromatograms (overlaid)



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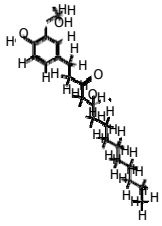
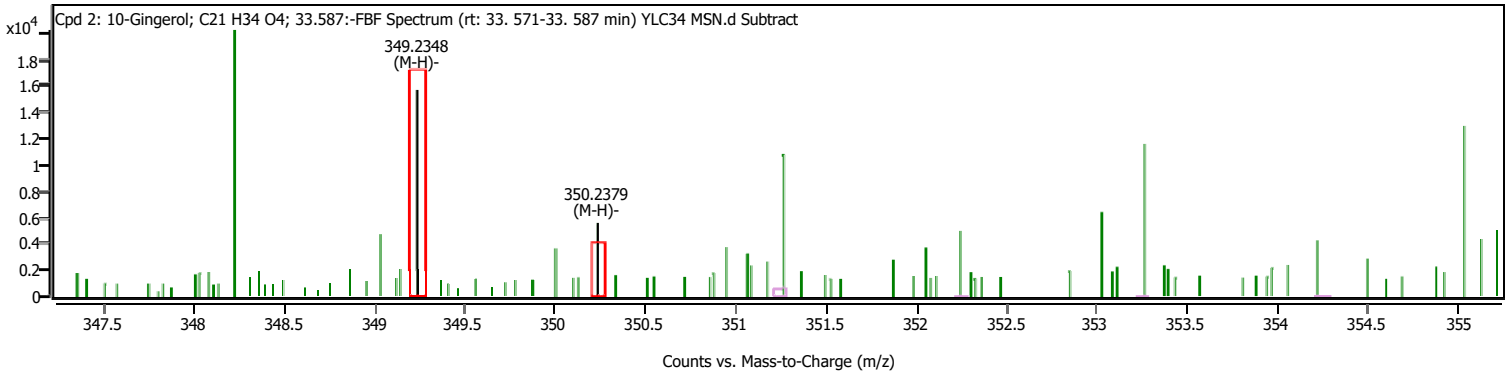


Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
10-Gingerol	C21H34O4	(M-H)-	33.587		350.2420		FBF	40.67		40.67

Cpd.3:8-Gingerol

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)		CAS	ID Source	Score	Algorithm
8-Gingerol	C19 H30 O4	9.862		322.2140	-1.34		FBF	70.21	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+CH3COO)-	321.1978381.2285	70.21				

Target Screening Report

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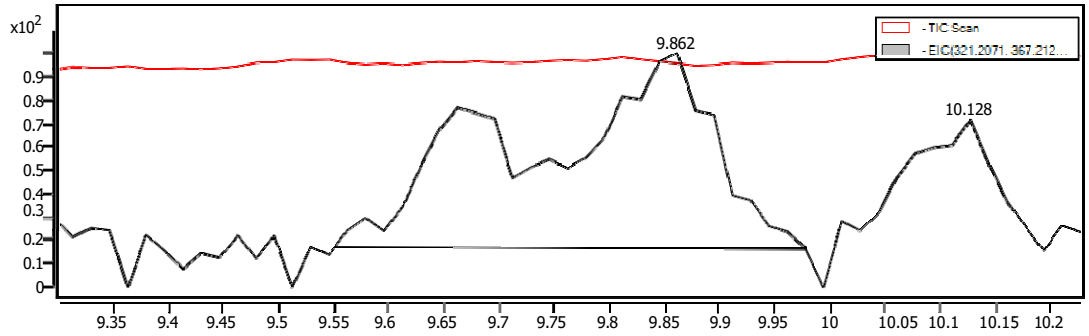
Compound Chromatograms (overlaid)



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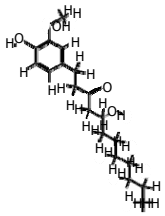
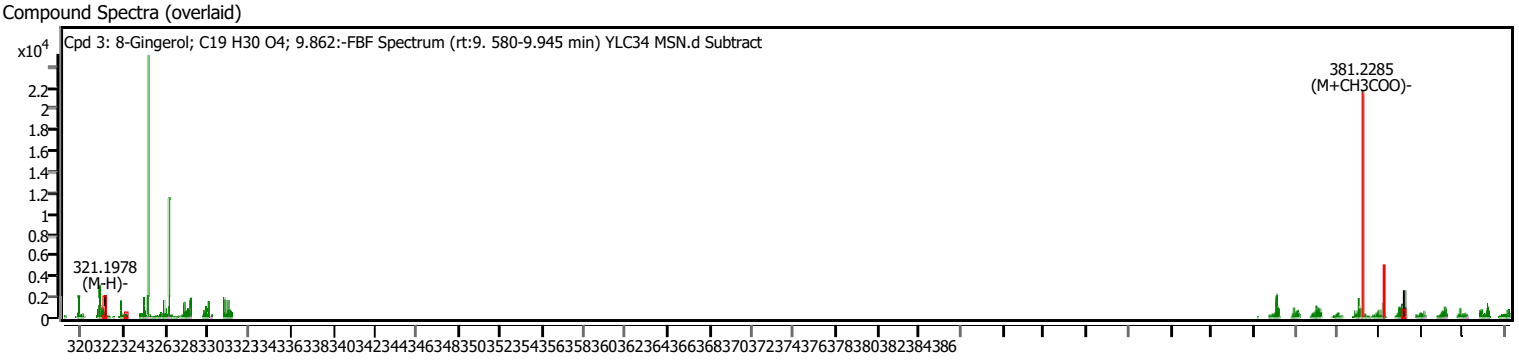


Compound Spectra (overlaid)



Compound ID Table

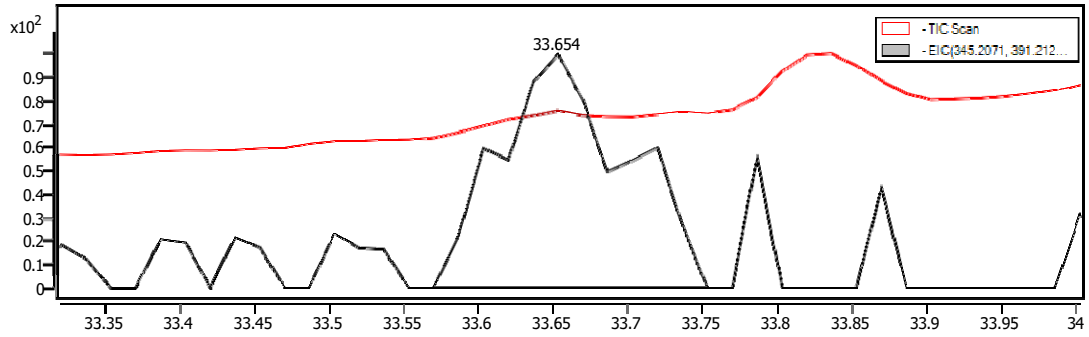
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
8-Gingerol	C19 H30 O4	(M-H)- (M+CH3COO)-	9-862		322.2140		FBF	70.21		70.21

Cpd.4:1-Dehydro-[10]-gingerdione

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
1-Dehydro-[10]-gingerdione	C21H30 O4	33.654		346.2140 -1.20		FBF	59.48	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	345.2090391.2120 405.2116	59.48				

Compound Chromatograms (overlaid)



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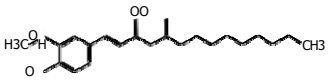
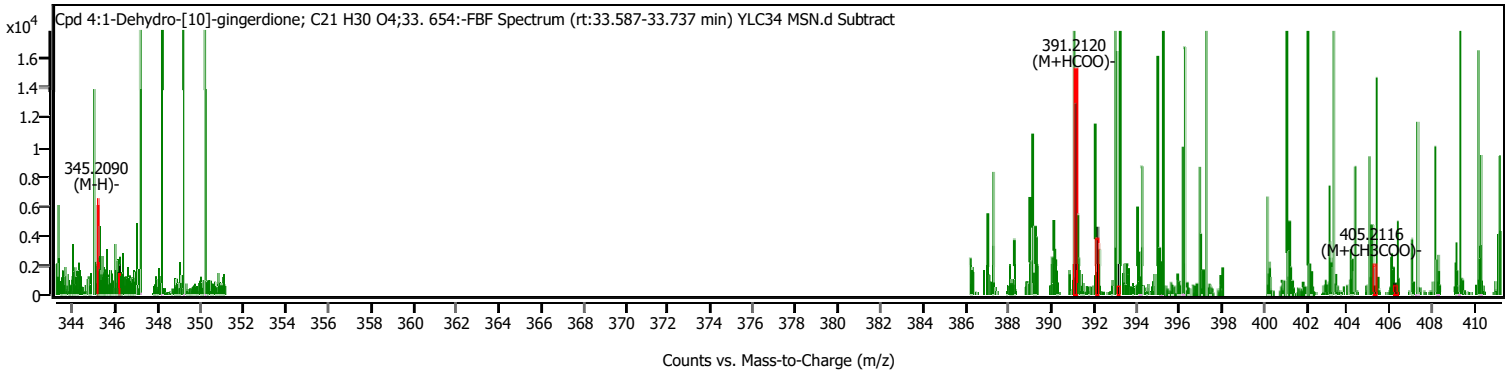


Target Screening Report

Compound Spectra (overlaid)



Compound ID Table

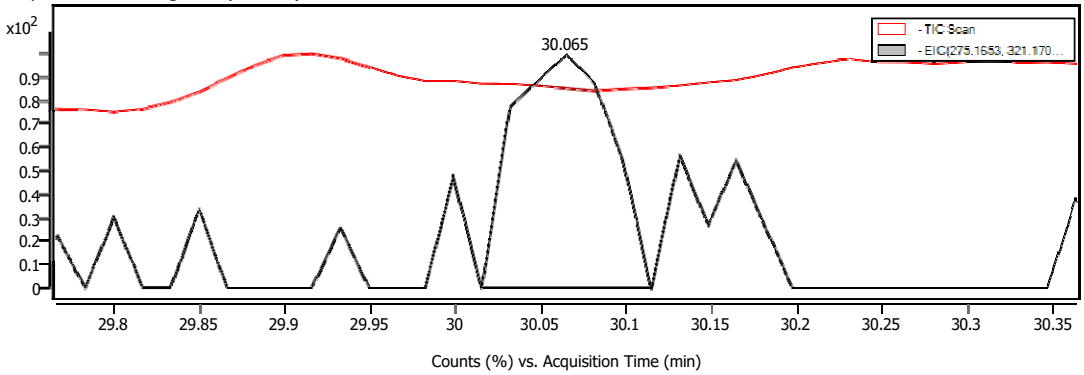
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
1-Dehydro-[10]-gingerdione	C21H30O4	(M-H)- (M+HCOO)- (M+CH3COO)-	33.654		346.2140		FBF	59.48		59.48

Cpd. 5:6-Shogaol

Name	Formula	RT	RI	Mass Diff (Tgt,ppm)	CAS	ID Source	Score	Algorithm
6-Shogaol	C17H24O3	30.065		276.1701 -8.98		FBF	46.29	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+HCOO)-	321.1679	46.29				

Compound Chromatograms (overlaid)



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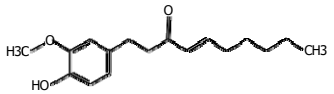
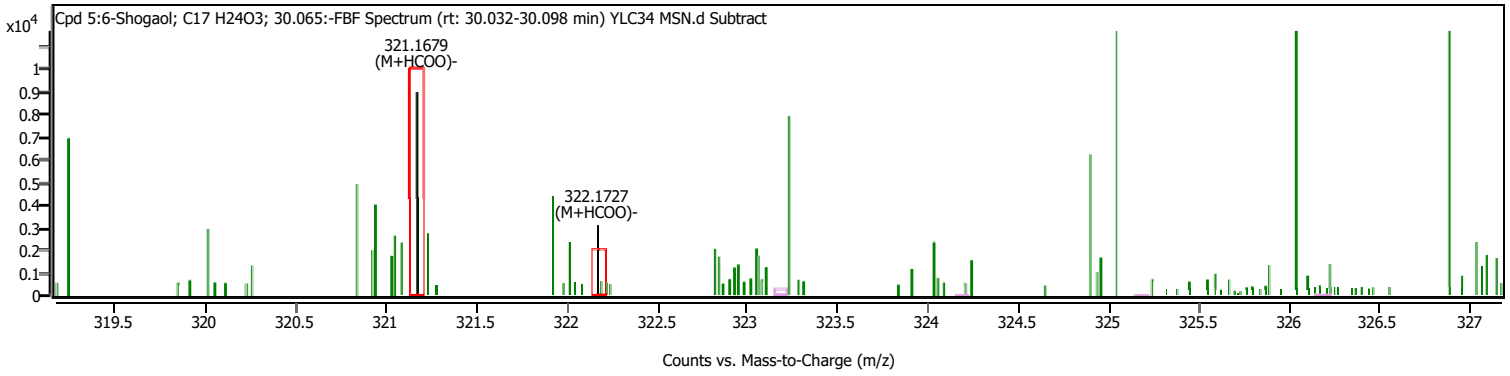


Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
6-Shogaol	C17H24O3	(M+HCOO)-	30.065		276.1701		FBF	46.29		46.29

Cpd.6: (10)-SHOGAOL

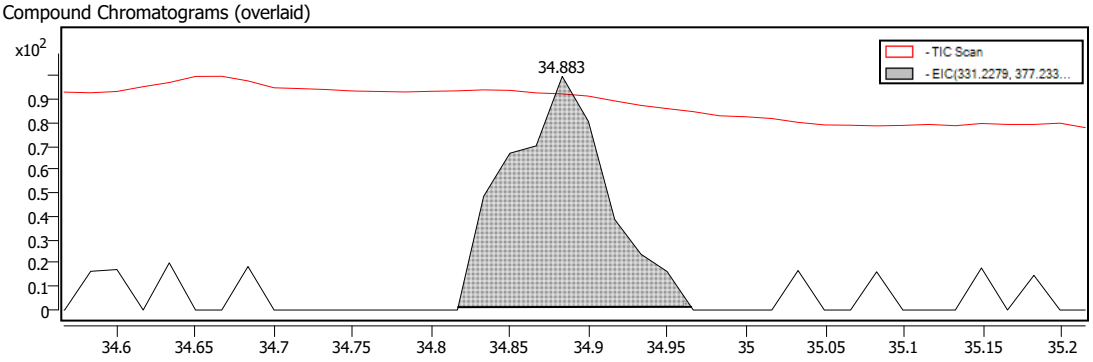
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
(10)-SHOGAOL	C21H32O3	34.883		332.2380 8.70		FBF	77.39	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+CH3COO)-	331.2305391.2602	77.39				

Target Screening Report

Agilent | Trusted Answers

Compound Chromatograms (overlaid)



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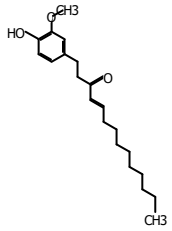
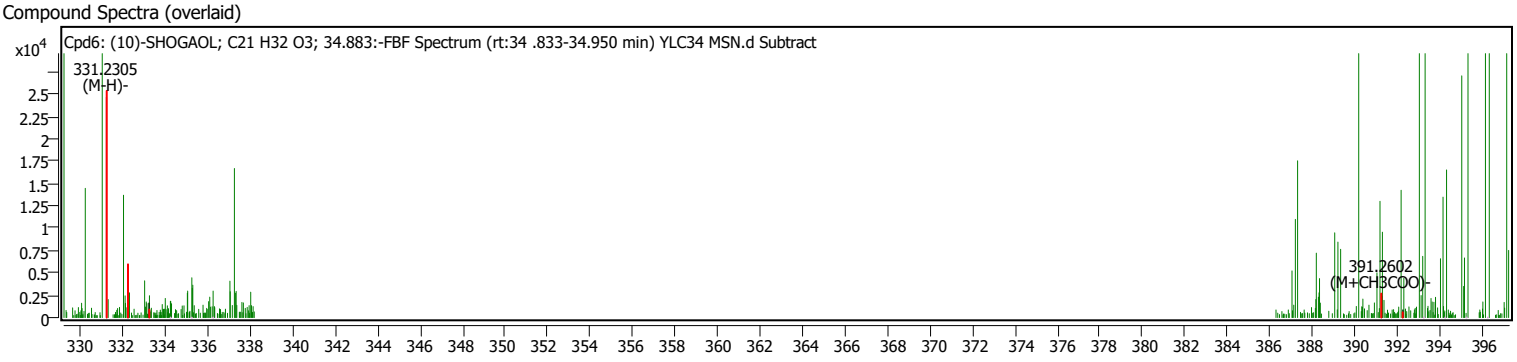


Compound Spectra (overlaid)



Compound ID Table

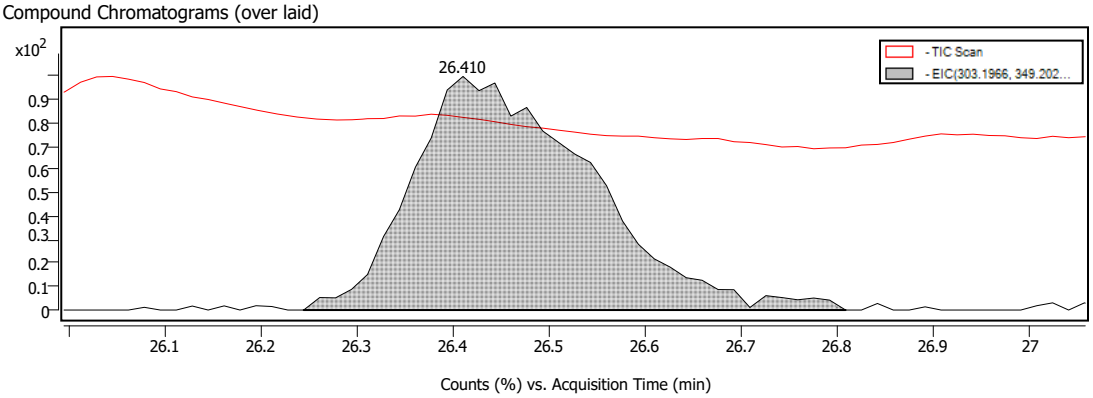
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
(10)-SHOGAOL	C21H32O3	(M-H)- (M+CH3COO)-	34.883		332.2380		FBF	77.39		77.39

Cpd.7:8-Shogaol

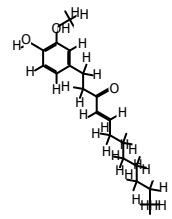
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
8-Shogaol	C19H28O3	26.410		304.1988 -16.59		FBF	54.81	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-	303.1914	54.81				

Compound Chromatograms (over laid)



Structure



TargetScreeningReport

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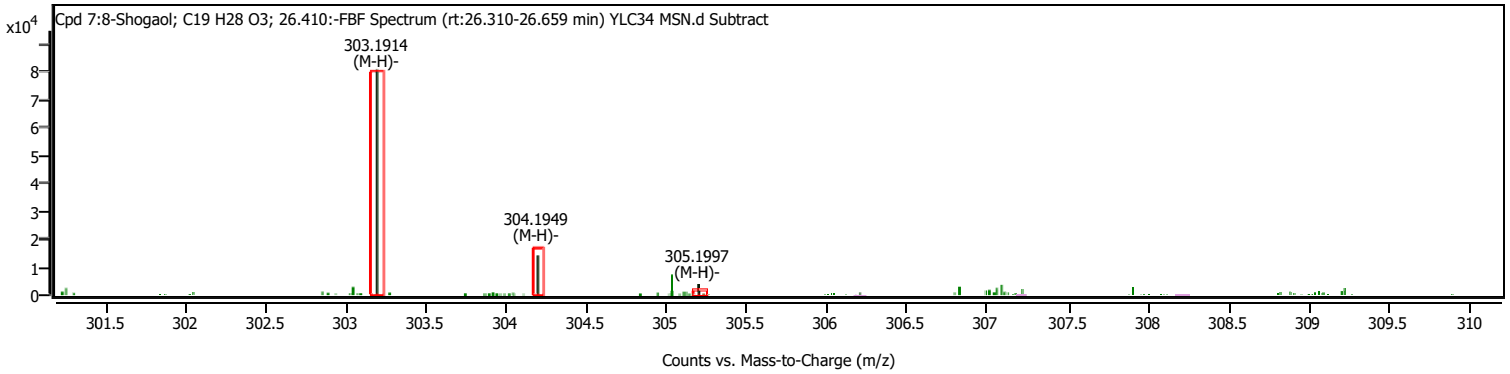
Compound Spectra (overlaid)



Compound ID Table

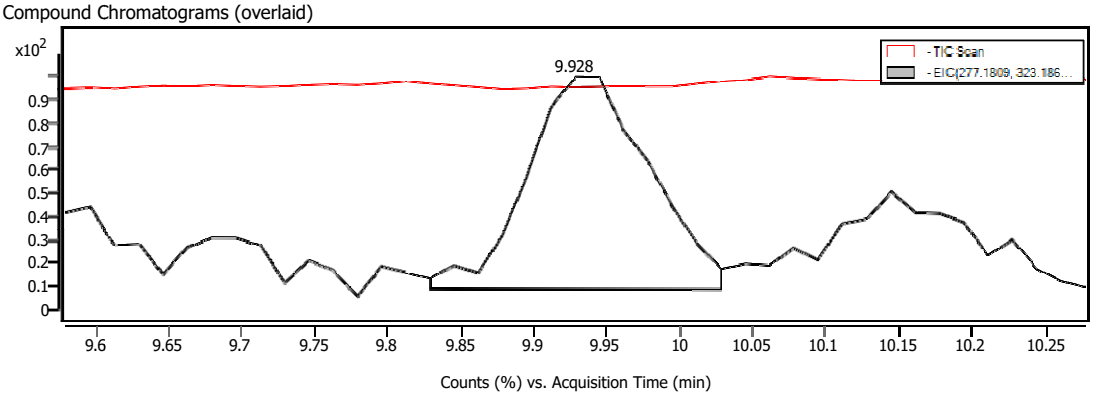
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
8-Shogaol	C19 H28 O3	(M-H)-	26.410		304.1988		FBF	54.81		54.81

Cpd. 8: 6-Paradol

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
6-Paradol	C17 H26 O3	9.928		278.1854 -9.96		FBF	81.53	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+CH3COO)-	277.1735337.1999	81.53				

Compound Chromatograms (overlaid)



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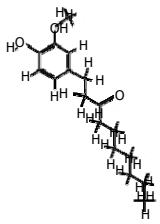
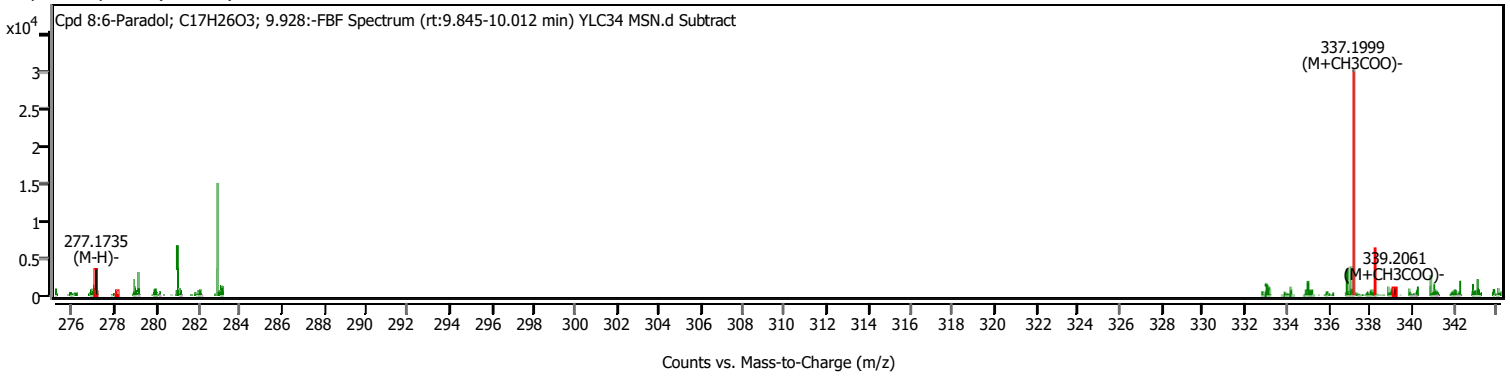


Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
6-Paradol	C17 H26 O3	(M-H)- (M+CH3COO)-	9.928		278.1854		FBF	81.53		81.53

Cpd.9:1-Dehydro-6-gingerdione

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
1-Dehydro-6-gingerdione	C17 H22 O4	31.859		290.1573 18.83		FBF	42.47	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)-	289.1458335.1540	42.47				

Target Screening Report

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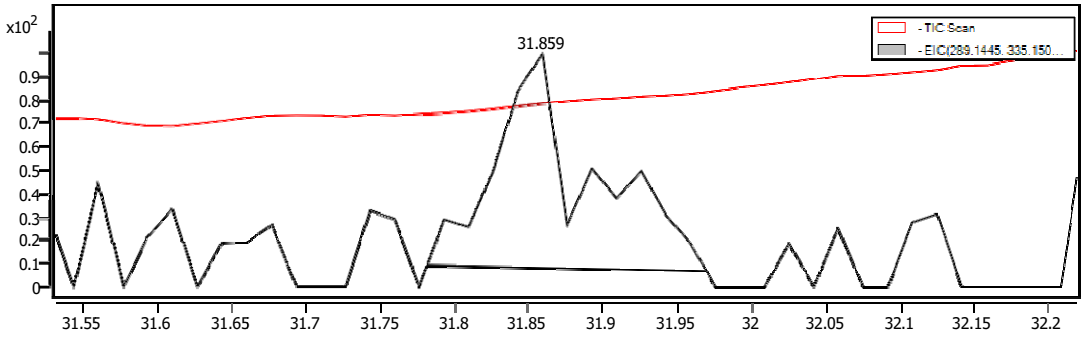
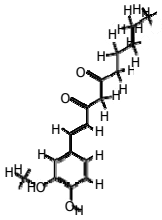
Compound Chromatograms (overlaid)

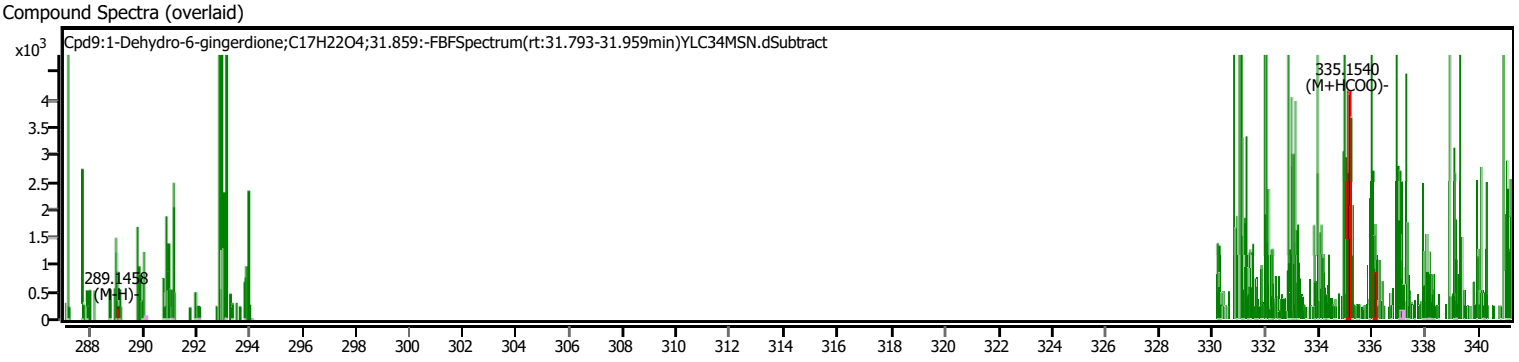


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



Counts vs. Mass-to-Charge (m/z)

CompoundIDTable

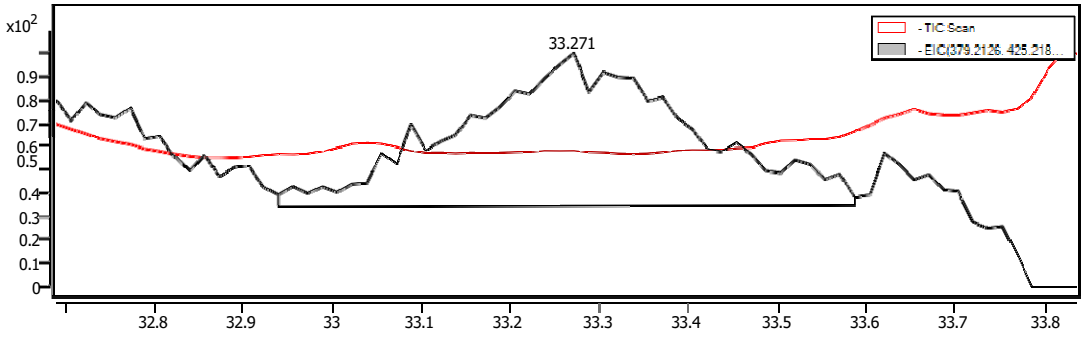
Name	Formula	Species	RT	RTDiff	Mass	CAS	ID Source	Score	Score(Lib)	Score(Tgt)
1-Dehydro-6-gingerdione	C17H22O4	(M-H)- (M+HCOO)-	31.859		290.1573		FBF	42.47		42.47

Cpd.10:Diacetoxy-6-gingerdiol

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)		CAS	IDSource	Score	Algorithm
Diacetoxy-6-gingerdiol	C21H32O6	33.271		380.2158	-10.67		FBF	67.17	FBF

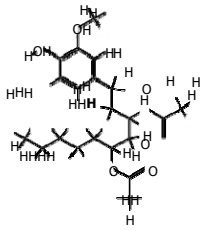
Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	379.2085425.2141 439.2226	67.17				

Compound Chromatograms (overlaid)

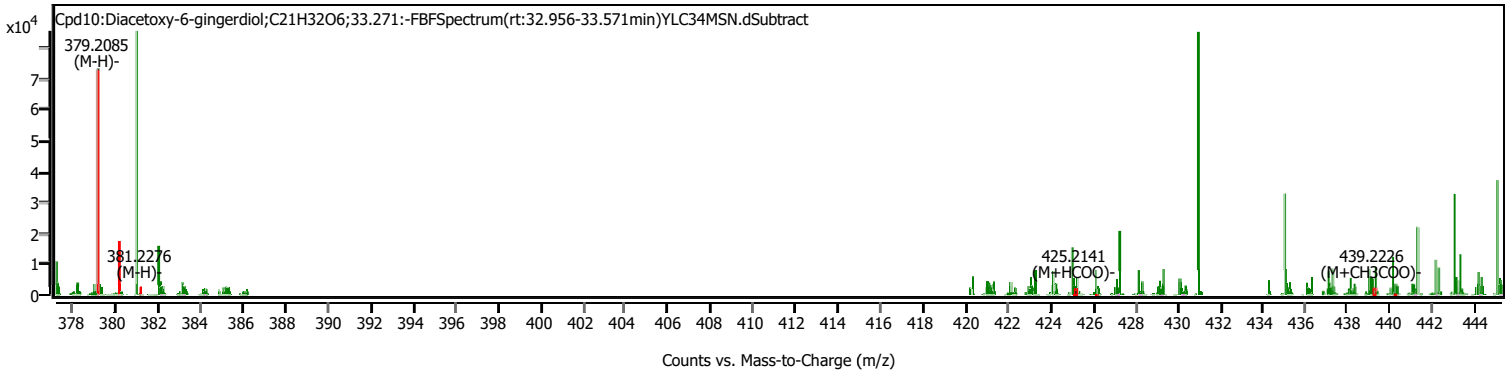


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



Compound ID Table

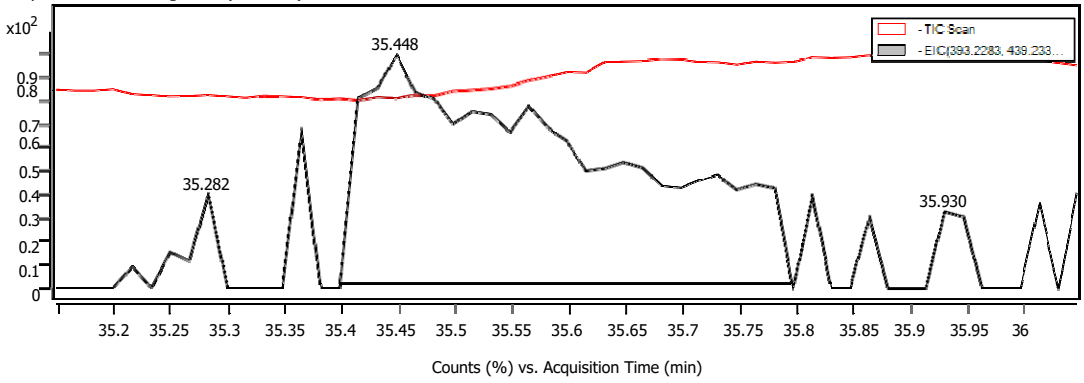
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Diacetoxy-6-gingerdiol	C21 H32 O6	(M-H)- (M+HCOO)- (M+CH3COO)-	33.271		380.2158		FBF	67.17		67.17

Cpd.11:Methyldiacetoxy-6-gingerdiol

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Methyldiacetoxy-6-gingerdiol	C22H34O6	35.448		394.2335 -5.11		FBF	77.35	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+CH3COO)-	393.2273453.2526	77.35				

Compound Chromatograms (overlaid)



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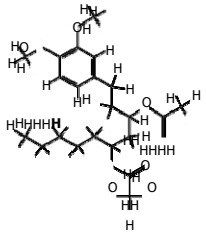
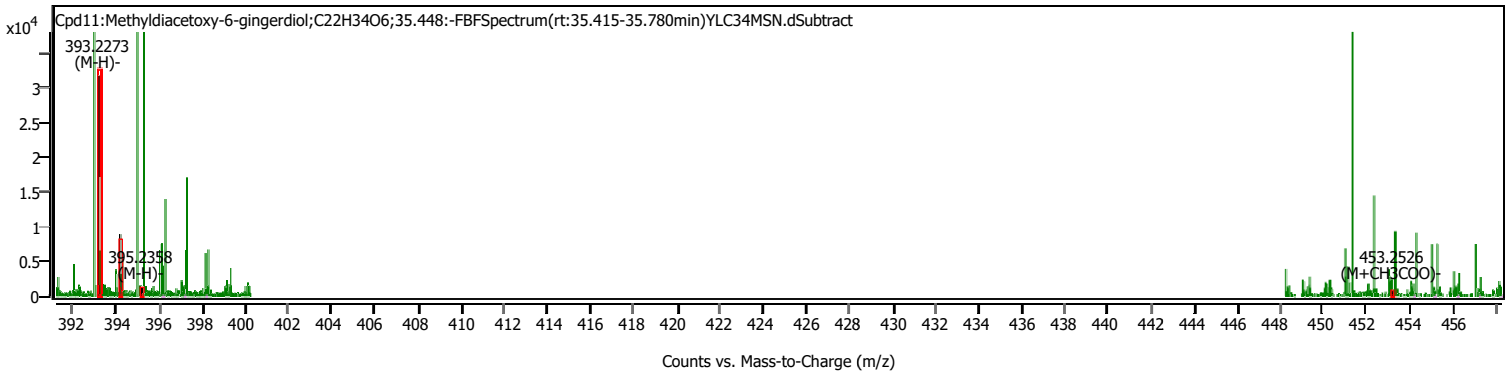


Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Methyldiacetoxy-6-gingerdiol	C22 H34 O6	(M-H)- (M+CH3COO)-	35.448		394.2335		FBF	77.35		77.35

Cpd.12:D-(−)-Quinicacid

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
D-(−)-Quinicacid	C7H12O6	29.766		192.0647 6.58		FBF	88.67	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	191.0617237.0650 251.0783	88.67				

TargetScreeningReport

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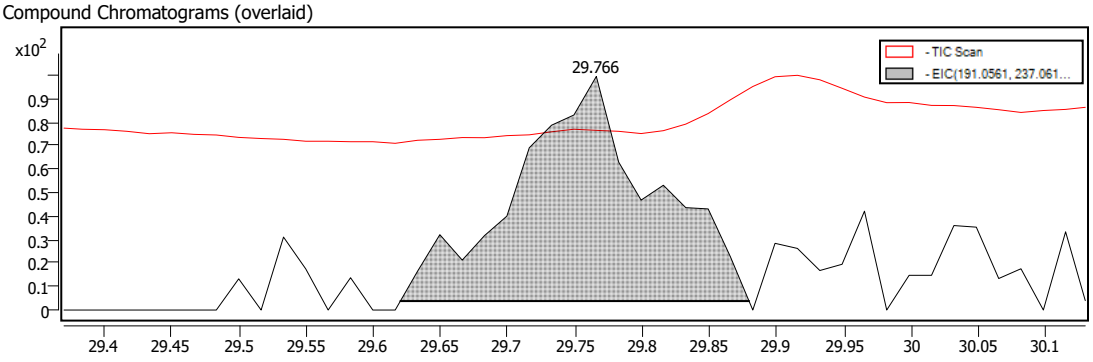
Compound Chromatograms (overlaid)



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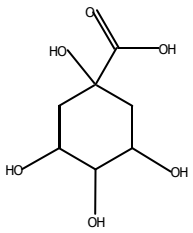
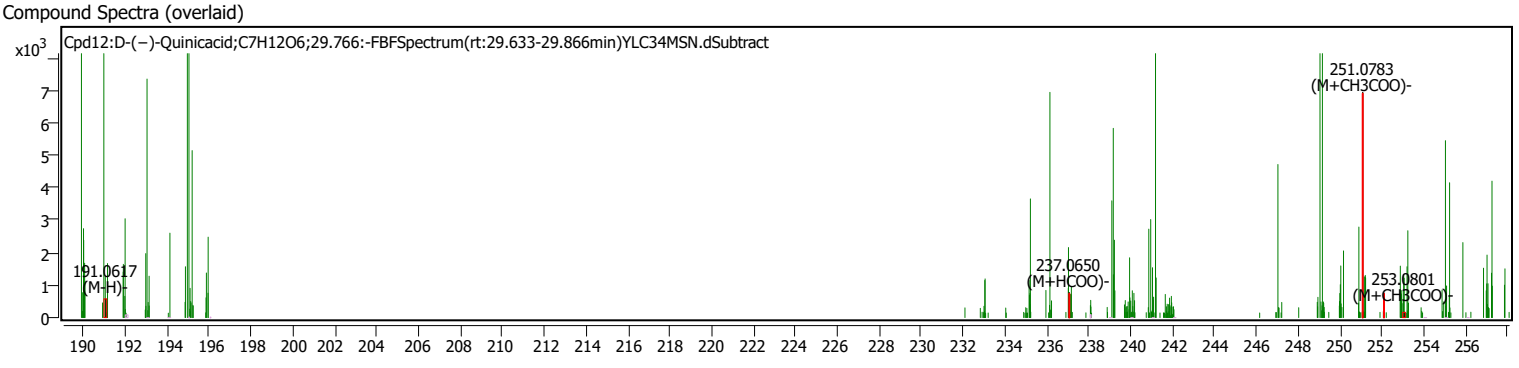


Compound Spectra (overlaid)



Compound ID Table

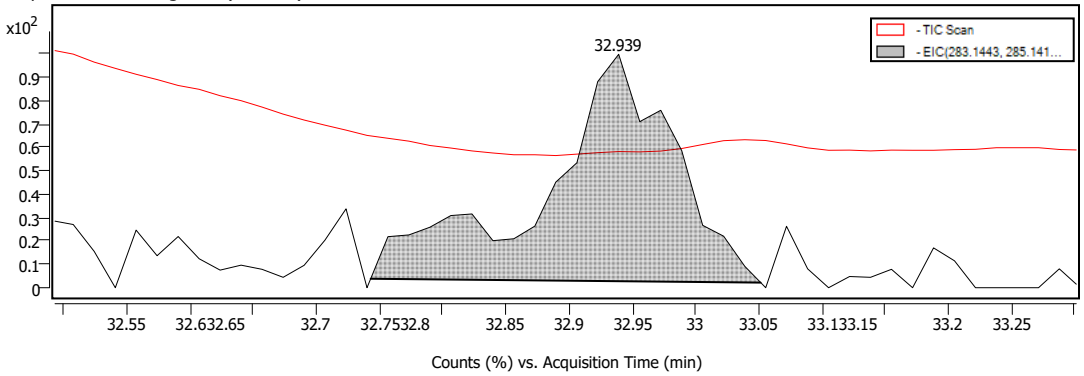
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
D-(−)-Quinicacid	C7 H12 O6	(M-H)- (M+HCOO)- (M+CH3COO)-	29.766		192.0647		FBF	88.67		88.67

Cpd.13:Protocatechuic acid

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)		CAS	ID Source	Score	Algorithm
Protocatechuic acid	C12 H21 Cl N6	32.939		284.1535	6.52		FBF	51.31	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	283.1378329.1619 343.1697	51.31				

Compound Chromatograms (overlaid)



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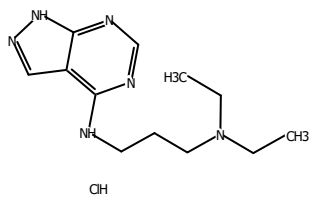
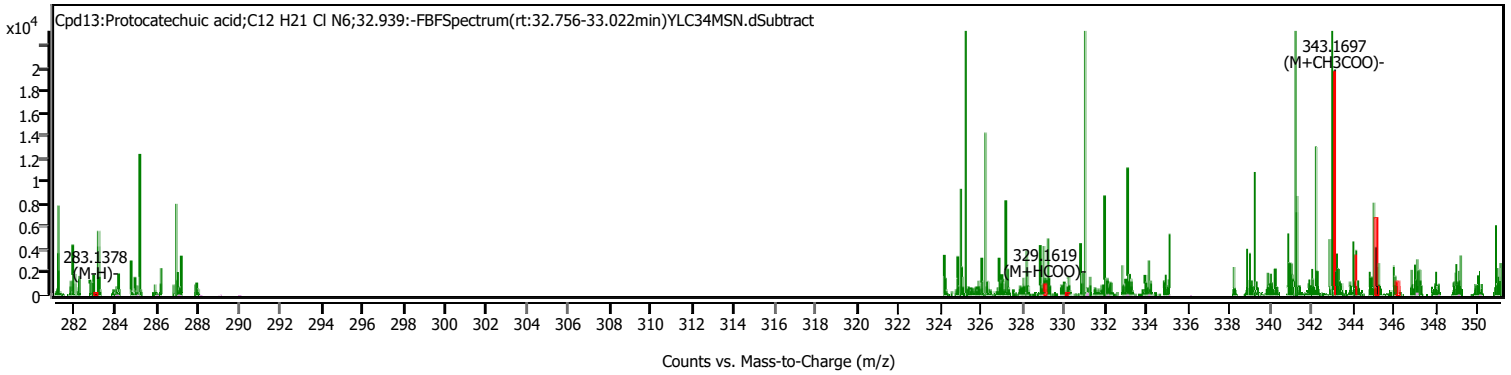


Compound Spectra (overlaid)



Compound ID Table

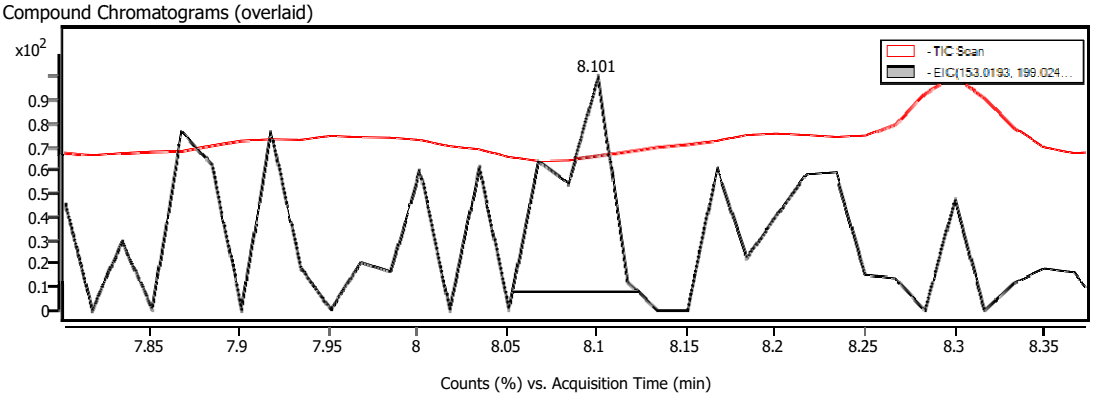
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Protocatechuicacid	C12 H21 Cl N6	(M-H)- (M+HCOO)- (M+CH3COO)-	32.939		284.1535		FBF	51.31		51.31

Cpd.14:Gentisicacid

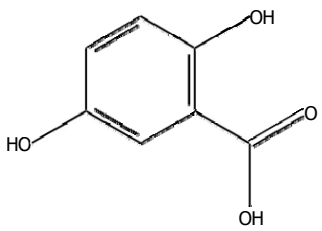
Name	Formula	RT	RI	MassDiff(Tgt,ppm)	CAS	ID Source	Score	Algorithm
Gentisic acid	C7H6O4	8.101		154.0260 -4.20		FBF	83.07	FBF

Species	m/z	Score(Tgt)	Score(Lib)	Score(DB)	Score(MFG)	Score(RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	153.0176199.0238 213.0403	83.07				

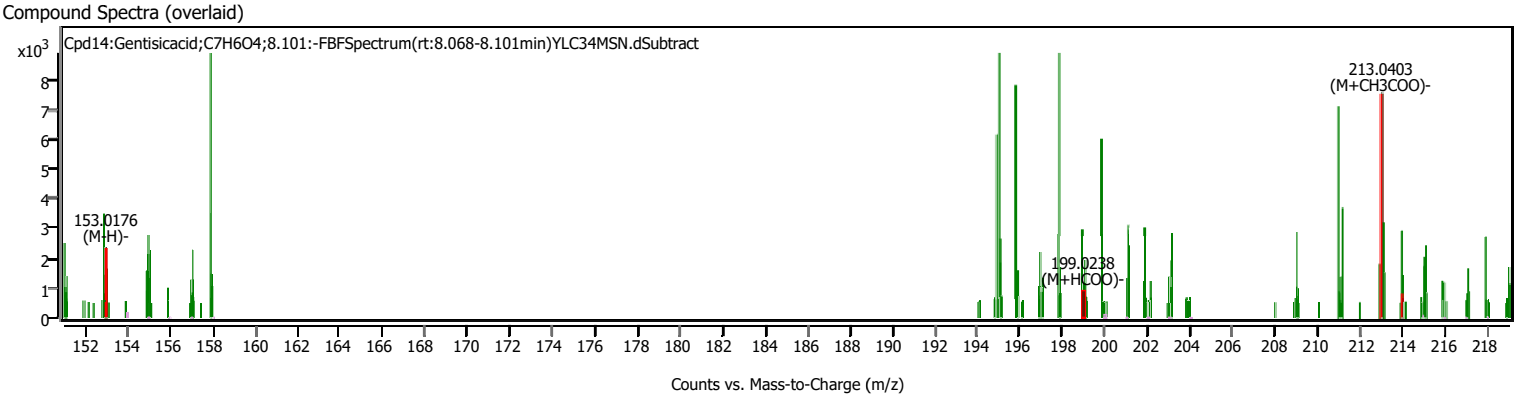
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Gentisicacid	C7H6O4	(M-H)- (M+HCOO)- (M+CH3COO)-	8.101		154.0260		FBF	83.07		83.07

Cpd.15:Gallic acid

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Gallic acid	C7H6O5	31.444		170.0201 -8.45		FBF	41.55	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+CH3COO)-	169.0245229.0310	41.55				

TargetScreeningReport

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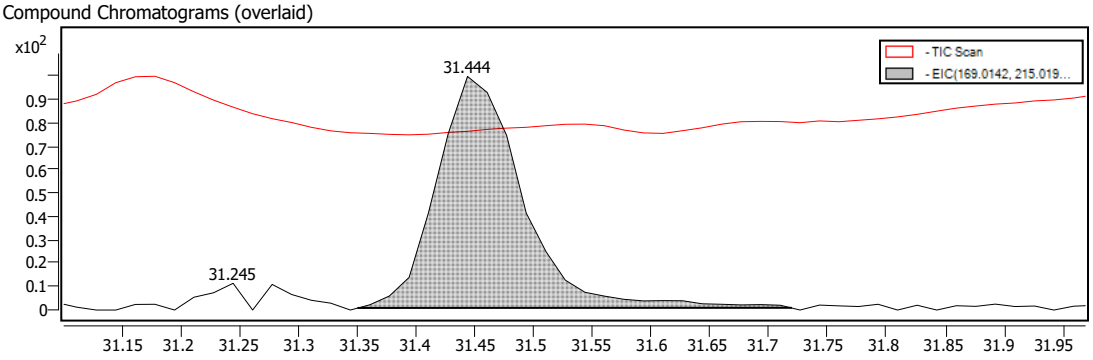
Compound Chromatograms (overlaid)



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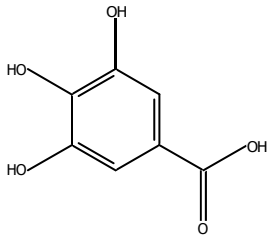
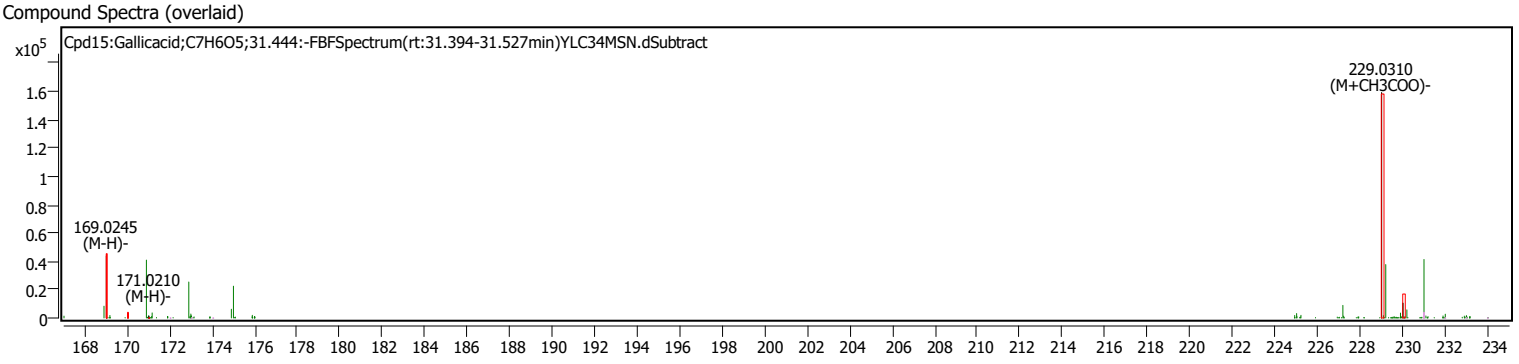


Compound Spectra (overlaid)



Compound ID Table

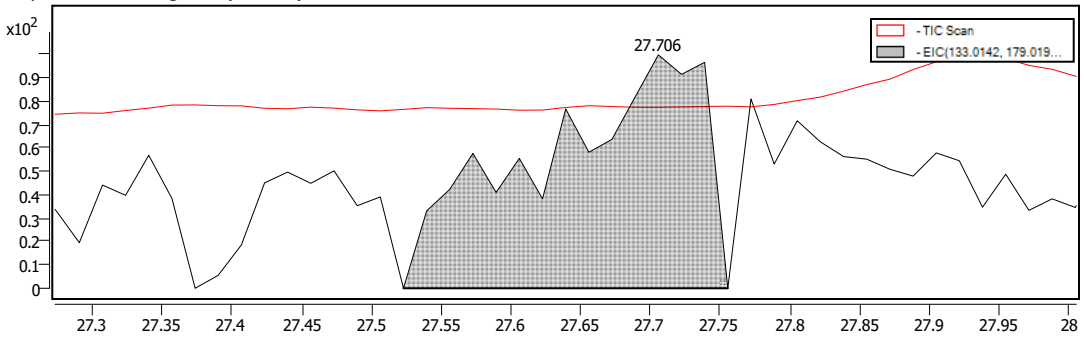
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Gallicacid	C7 H6 O5	(M-H)- (M+CH3COO)-	31.444		170.0201		FBF	41.55		41.55

Cpd.16:(±)-Malic Acid

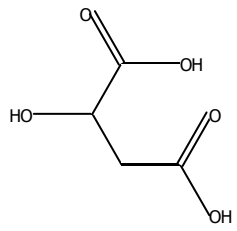
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
(±)-Malic Acid	C4H6O5	27.706		134.0207 -5.94		FBF	76.82	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	133.0171179.0212 193.0269	76.82				

Compound Chromatograms (overlaid)



Structure



TargetScreeningReport

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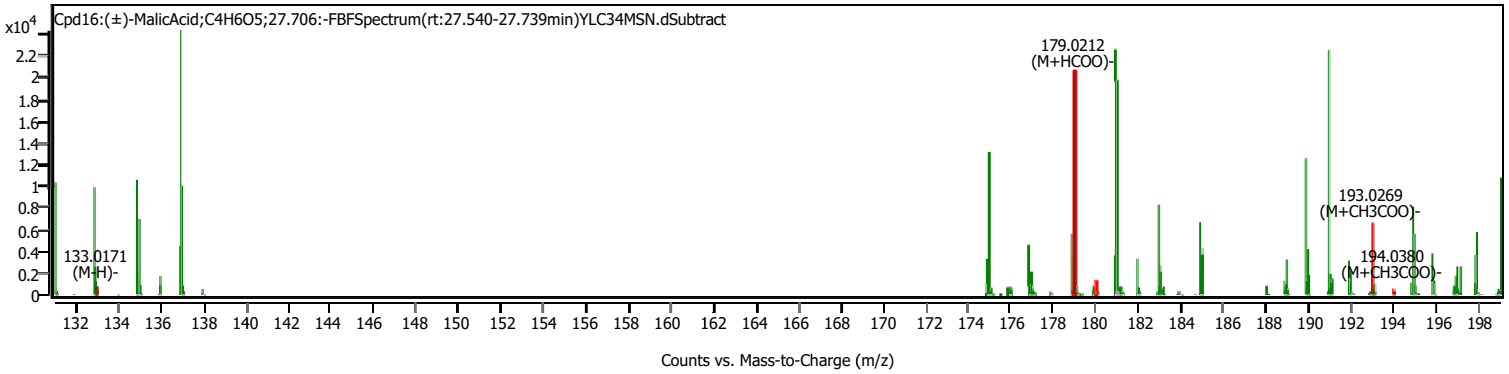
Compound Spectra (overlaid)



Compound ID Table

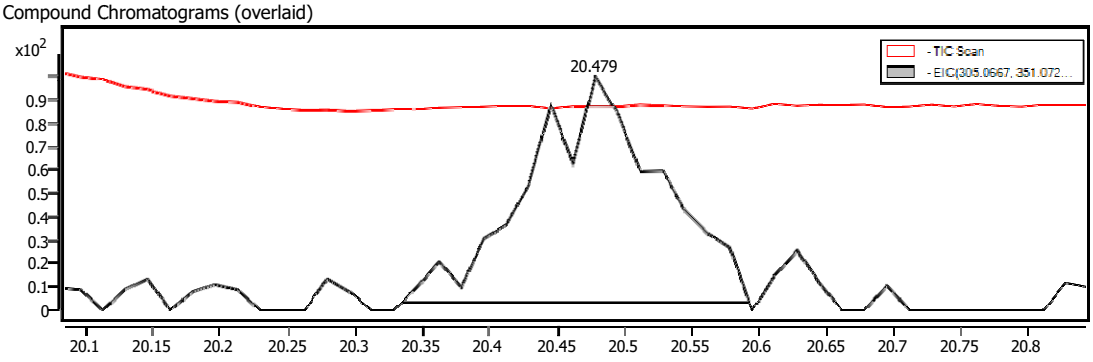
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
(±)-Malic Acid	C4 H6 O5	(M-H)- (M+HCOO)- (M+CH3COO)-	27.706		134.0207		FBF	76.82		76.82

Cpd.17:Gallocatechin

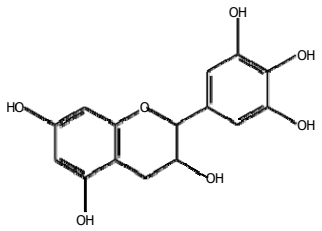
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Gallocatechin	C15H14O7	20.479		306.0756 5.35		FBF	64.19	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	305.0710351.0603 365.0839	64.19				

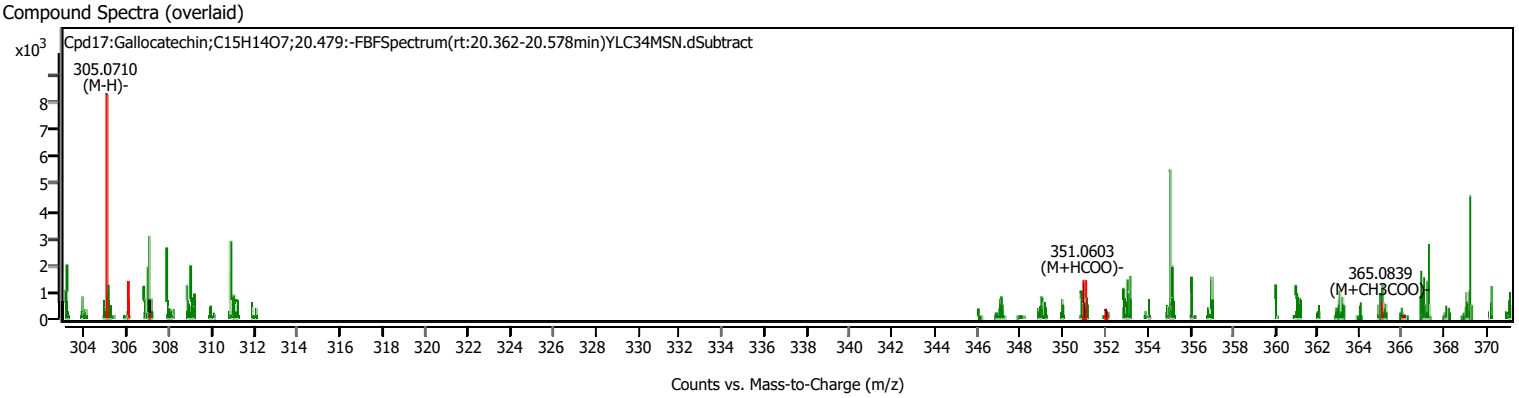
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

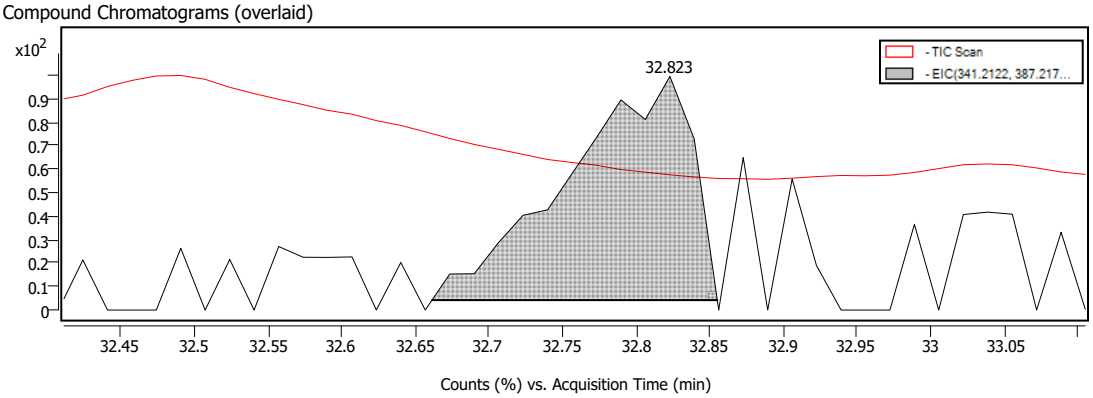
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Gallocatechin	C15 H14 O7	(M-H)- (M+HCOO)- (M+CH3COO)-	20.479		306.0756		FBF	64.19		64.19

Cpd.18:AnacardicacidC15:3

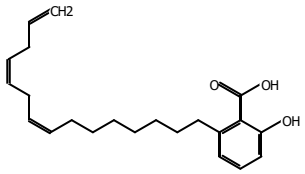
Name	Formula	RT	RI	MassDiff(Tgt, ppm)	CAS	ID Source	Score	Algorithm
AnacardicacidC15:3	C22H30O3	32.823		342.2133 -17.97		FBF	59.00	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+HCOO)- (M+CH3COO)-	387.2156401.2254	59.00				

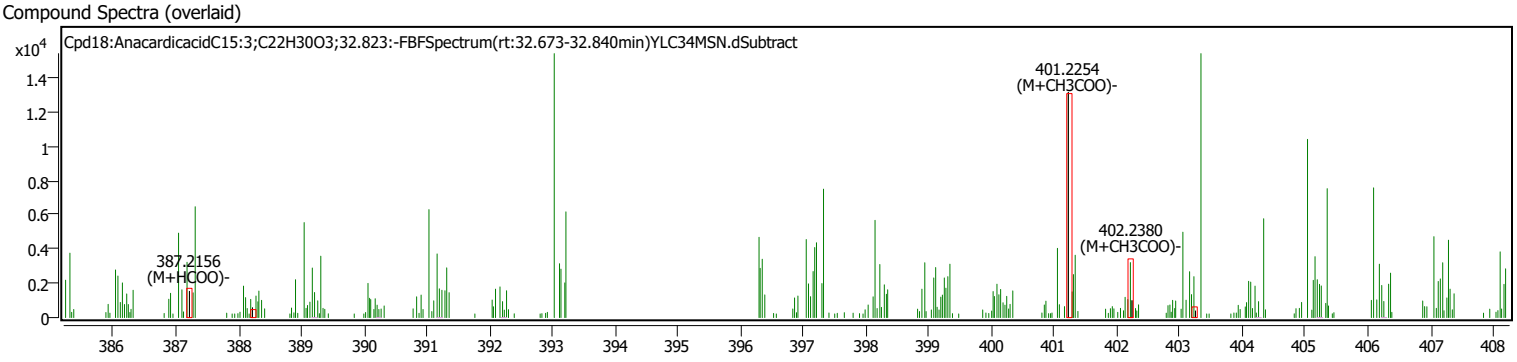
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

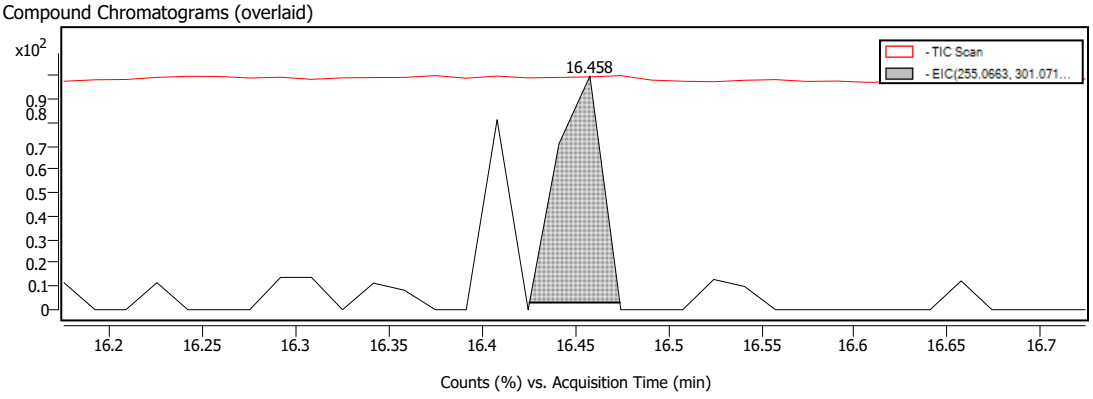
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Anacardic acid C15:3	C22 H30 O3	(M+HCOO)- (M+CH3COO)-	32.823		342.2133		FBF	59.00		59.00

Cpd.19: 6,2'-Dihydroxyflavanone

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
6,2'-Dihydroxyflavanone	C15H12O4	16.458		256.0732 -1.31		FBF	68.83	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+HCOO)-	301.0698	68.83				

Compound Chromatograms (overlaid)



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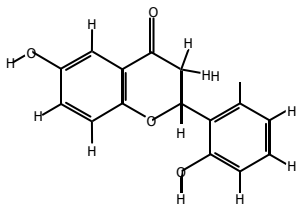
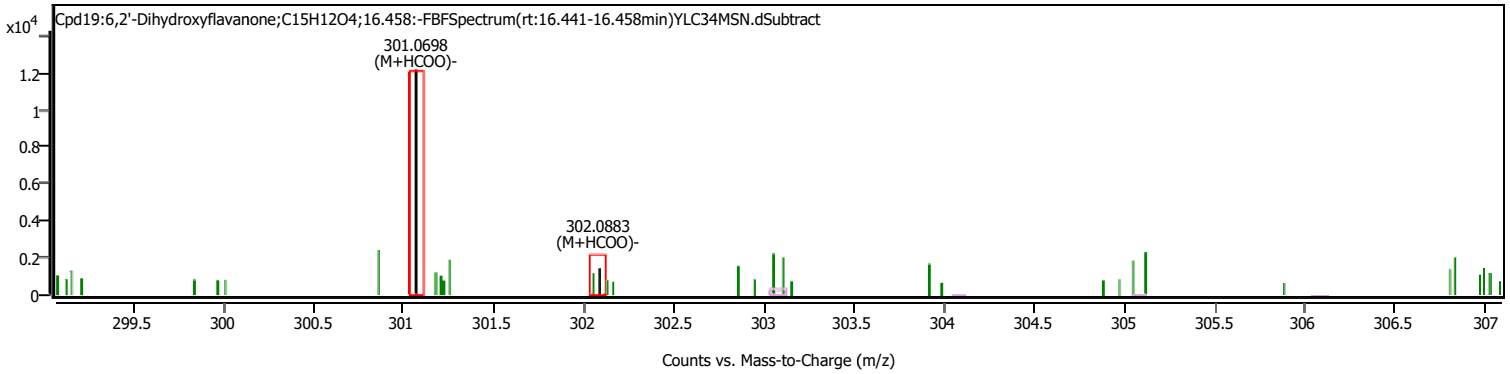


Compound Spectra (overlaid)



Compound ID Table

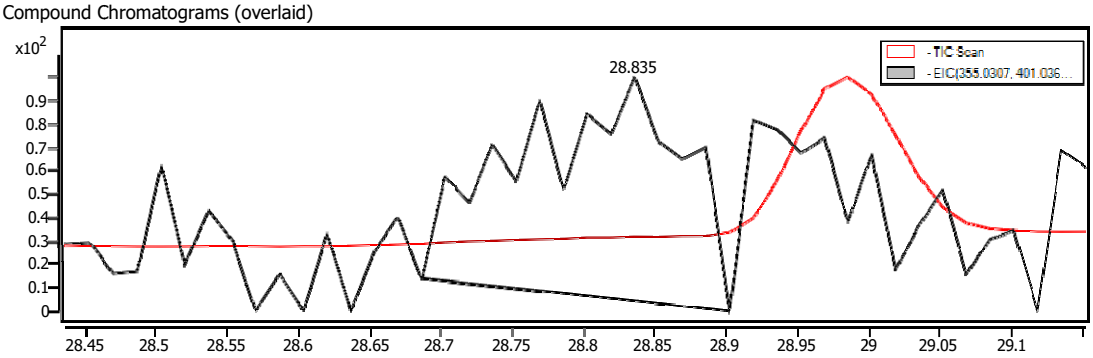
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
6,2'-Dihydroxyflavanone	C15H12O4	(M+HCOO)-	16.458		256.0732		FBF	68.83		68.83

Cpd.20: Chebulic acid

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Chebulic acid	C14H12O11	28.835		356.0415 9.83		FBF	72.23	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	355.0376401.0365 415.0424	72.23				

Compound Chromatograms (overlaid)



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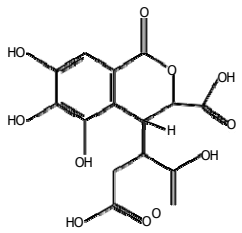
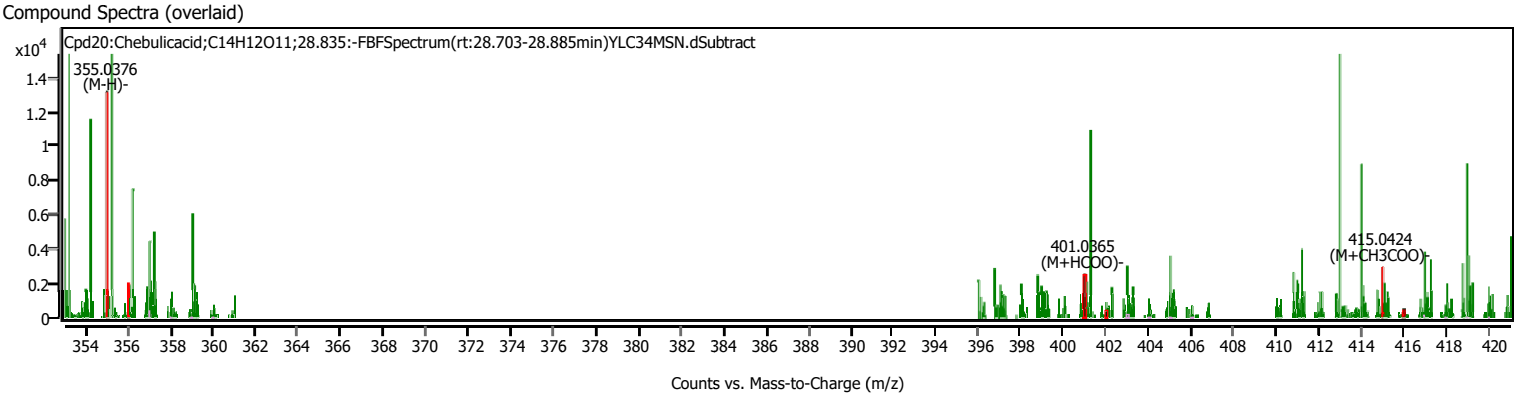


Compound Spectra (overlaid)



Compound ID Table

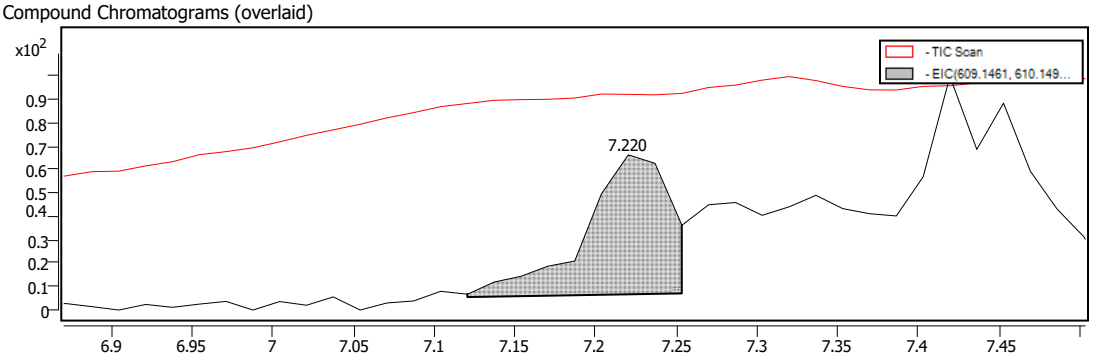
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Chebulic acid	C14H12O11	(M-H)- (M+HCOO)- (M+CH3COO)-	28.835		356.0415		FBF	72.23		72.23

Cpd.21:Rutin

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Rutin	C27H30O16	7.220		610.1513 -3.37		FBF	77.38	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+CH3COO)-	609.1229669.1636	77.38				

Compound Chromatograms (overlaid)



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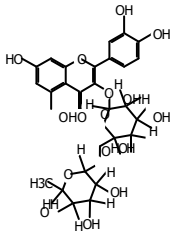
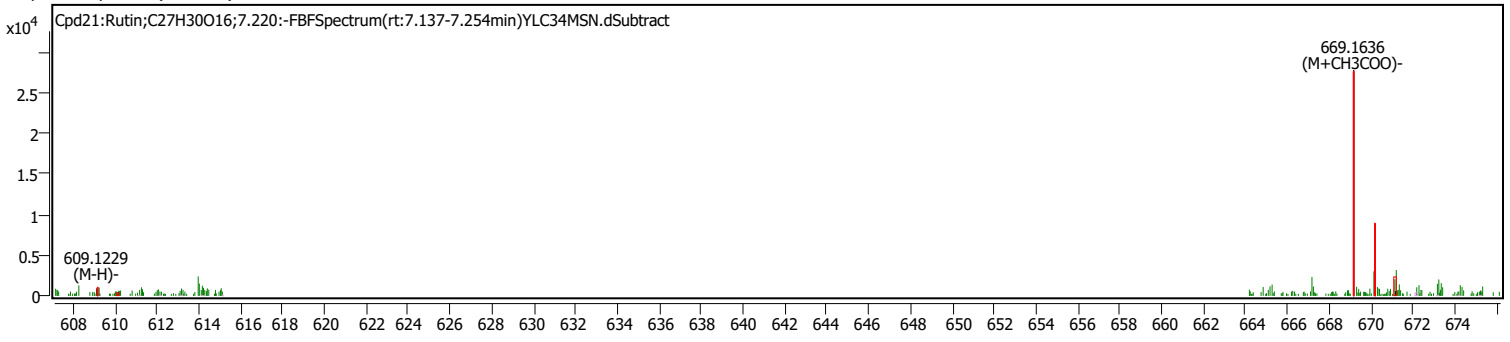


Compound Spectra (overlaid)



Compound ID Table

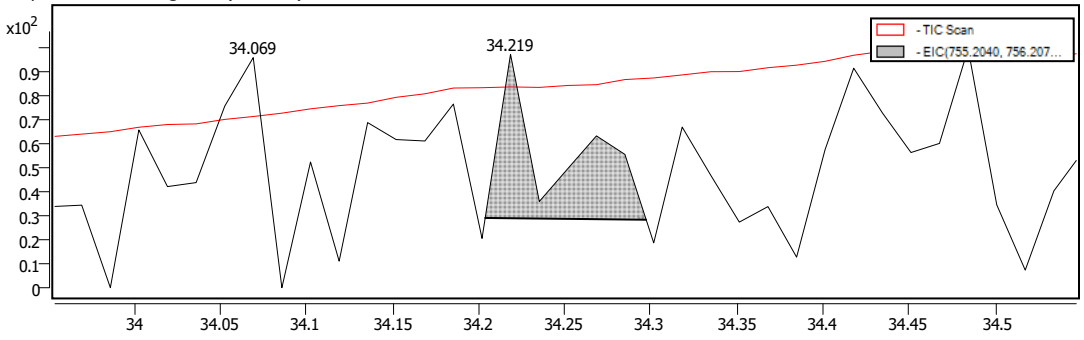
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Rutin	C27 H30 O16	(M-H)- (M+CH3COO)-	7.220		610.1513		FBF	77.38		77.38

Cpd.22:Quercetin3-rhamnosyl-(1->2)-rhamnosyl-(1->6)-glucoside

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)		CAS	ID Source	Score	Algorithm
Quercetin3-rhamnosyl-(1->2)-rhamnosyl-(1->6)-glucoside	C33H40O20	34.219		756.2089	-3.17		FBF	43.41	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+HCOO)- (M+CH3COO)-	801.2156815.2100	43.41				

Compound Chromatograms (overlaid)



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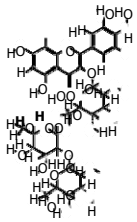
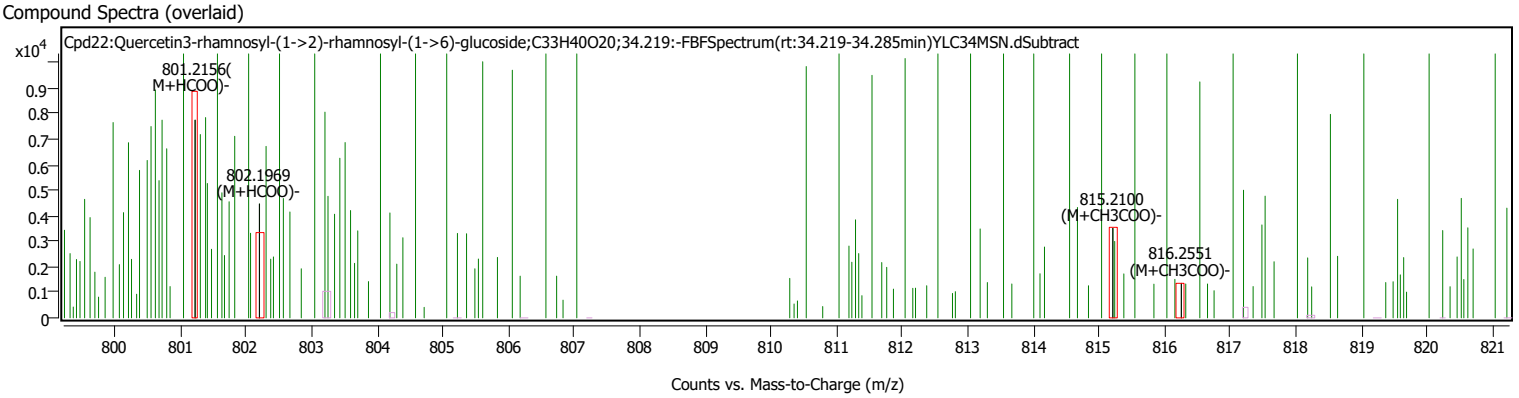


Compound Spectra (overlaid)



Compound ID Table

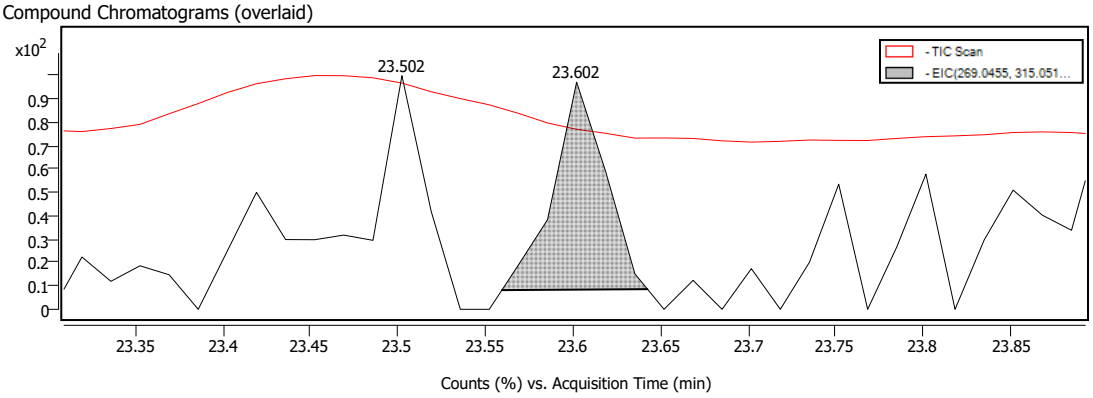
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Quercetin3-rhamnosyl-(1->2)-rhamnosyl-(1->6)-glucoside	C33H40O20	(M+HCOO)-(M+CH3COO)-	34.219		756.2089		FBF	43.41		43.41

Cpd.23:Apigenin

Name	Formula	RT	RI	MassDiff(Tgt,ppm)	CAS	ID Source	Score	Algorithm
Apigenin	C15H10O5	23.602		270.0535	2.44	FBF	83.62	FBF

Species	m/z	Score(Tgt)	Score(Lib)	Score(DB)	Score(MFG)	Score(RT)
(M+HCOO)-	315.0517	83.62				

Compound Chromatograms (overlaid)



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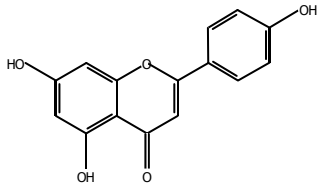
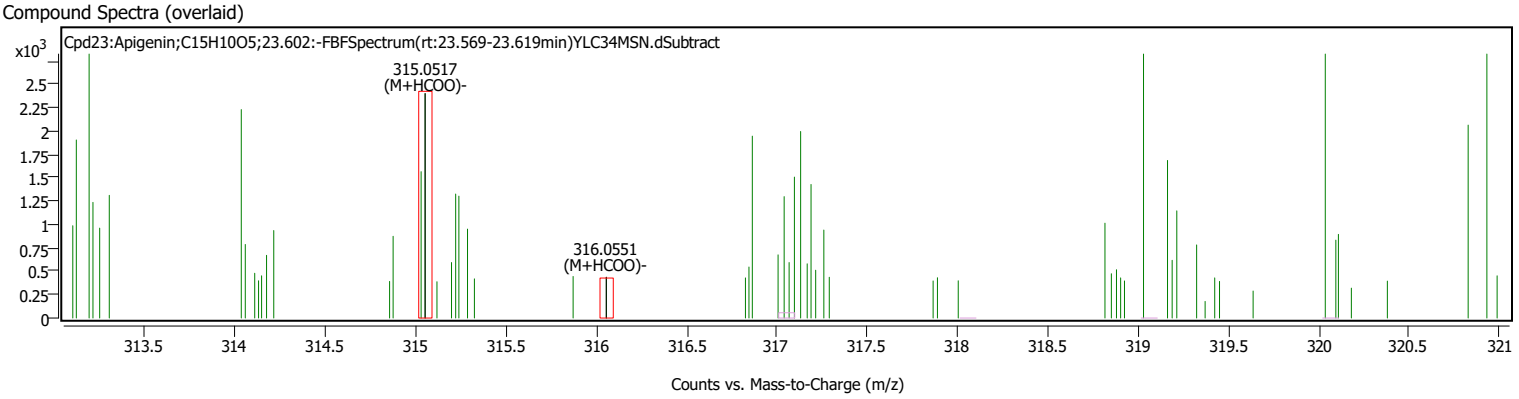


Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RTDiff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Apigenin	C15H10O5	(M+HCOO)-	23.602		270.0535		FBF	83.62		83.62

Cpd.24:4-Methylumbelliferone

Name	Formula	RT	RI	Mass Dif f(Tgt, ppm)	CAS	ID Source	Score	Algorithm
4-Methylumbelliferone	C10H8O3	23.868		176.0469 -2.58		FBF	83.16	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+CH3COO)-	175.0403235.0603	83.16				

TargetScreeningReport

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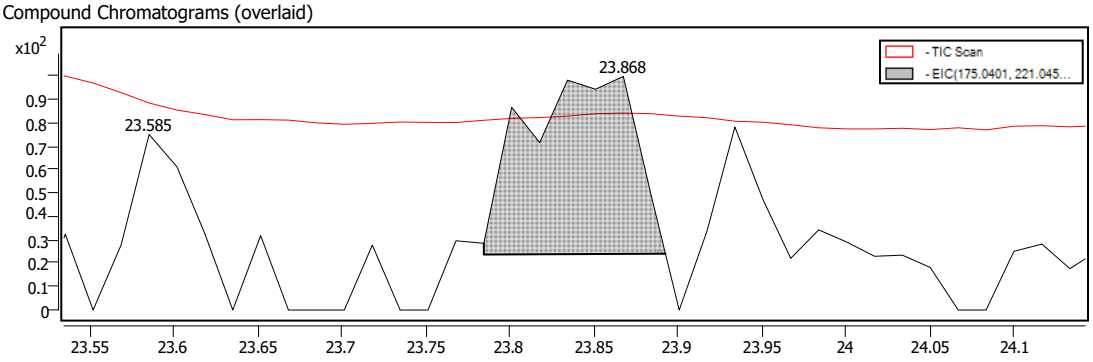
Compound Chromatograms (overlaid)



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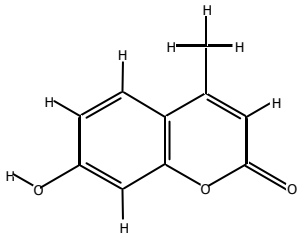
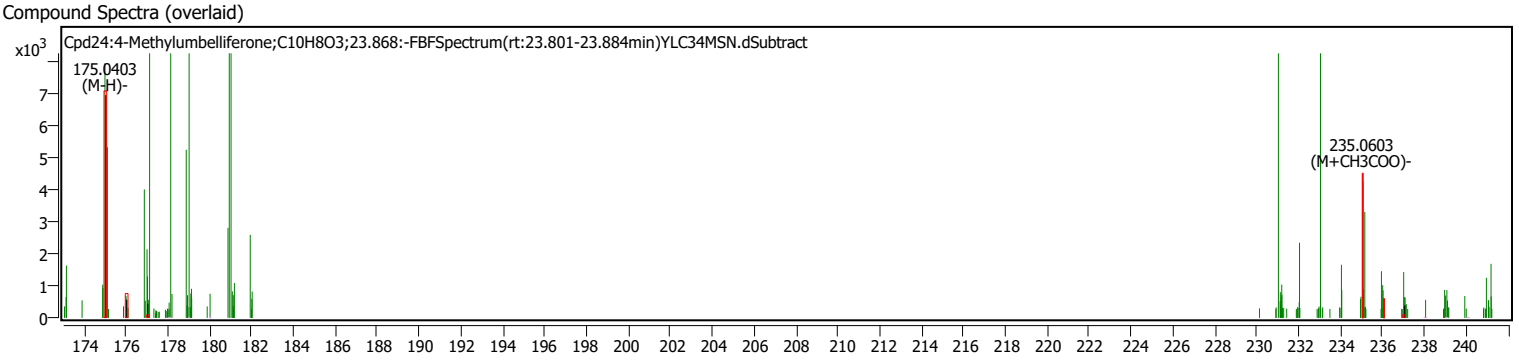


Compound Spectra (overlaid)



Compound ID Table

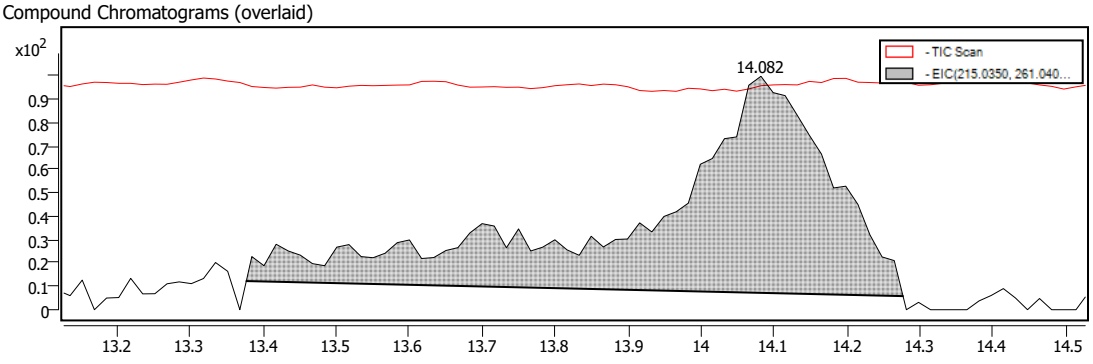
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
4-Methylumbelliferone	C10H8O3	(M-H)- (M+CH3COO)-	23.868		176.0469		FBF	83.16		83.16

Cpd.25:Bergapten

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Bergapten	C12H8O4	14.082		216.0455 15.02		FBF	62.77	FBF

Species	m/z	Score(Tgt)	Score(Lib)	Score(DB)	Score(MFG)	Score(RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	215.0438261.0538 275.0592	62.77				

Compound Chromatograms (overlaid)



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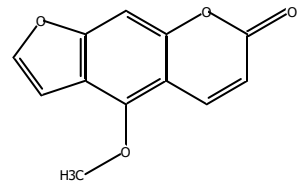
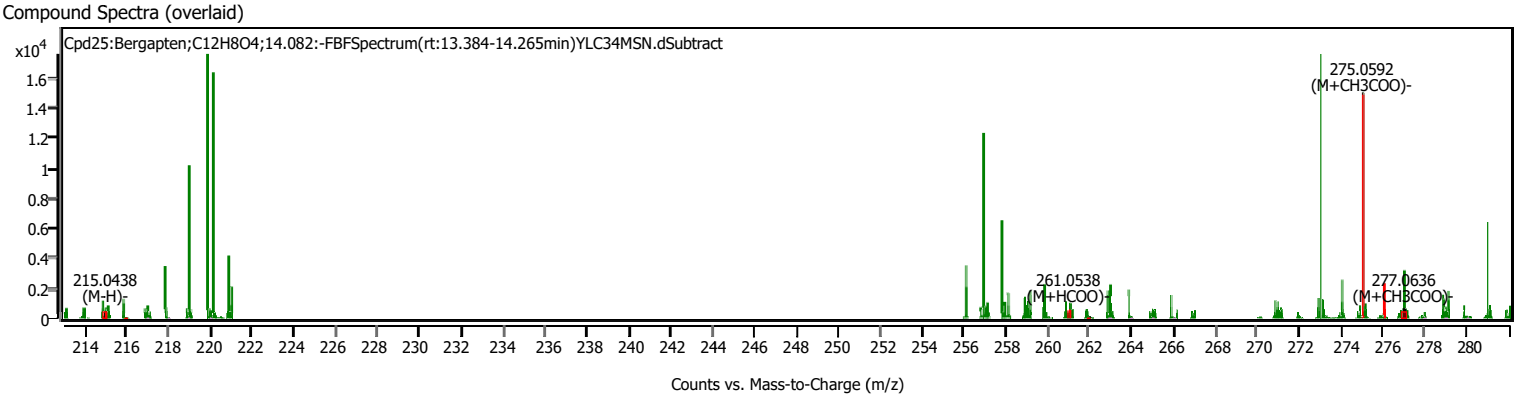


Compound Spectra (overlaid)



Compound ID Table

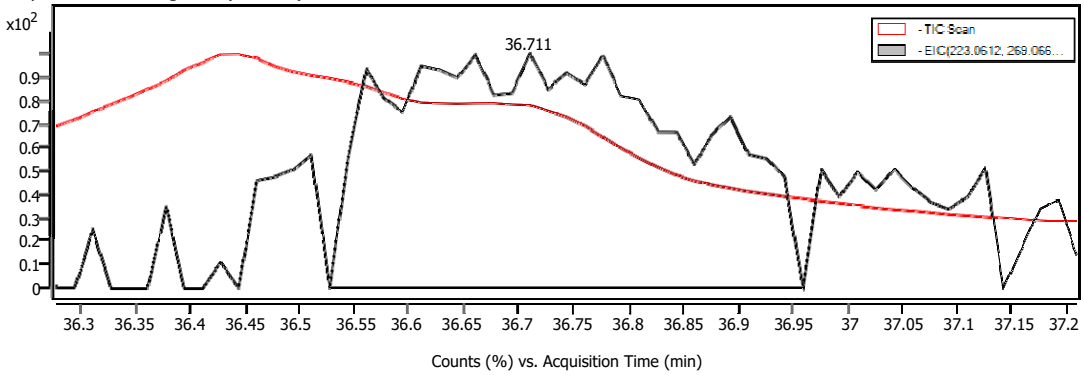
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Bergapten	C12 H8 O4	(M-H)- (M+HCOO)- (M+CH3COO)-	14.082		216.0455		FBF	62.77		62.77

Cpd.26:Sinapic acid

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Sinapicacid	C11H12O5	36.711		224.0681 -1.55		FBF	65.22	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+CH3COO)-	223.0607283.0786	65.22				

Compound Chromatograms (overlaid)



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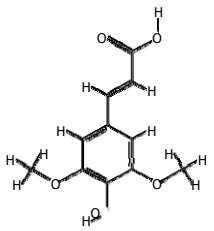
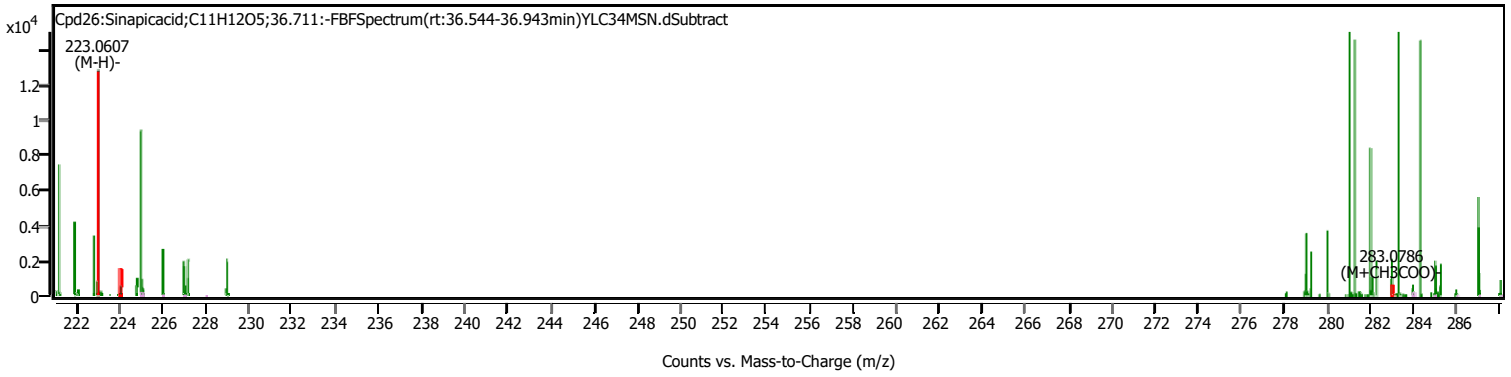


Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Sinapicacid	C11 H12 O5	(M-H)- (M+CH3COO)-	36.711		224.0681		FBF	65.22		65.22

Cpd.27:vicenin2

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
vicenin2	C27H30O15	37.359		594.1699 19.21		FBF	55.78	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+HCOO)- (M+CH3COO)-	639.1719653.1737	55.78				

TargetScreeningReport

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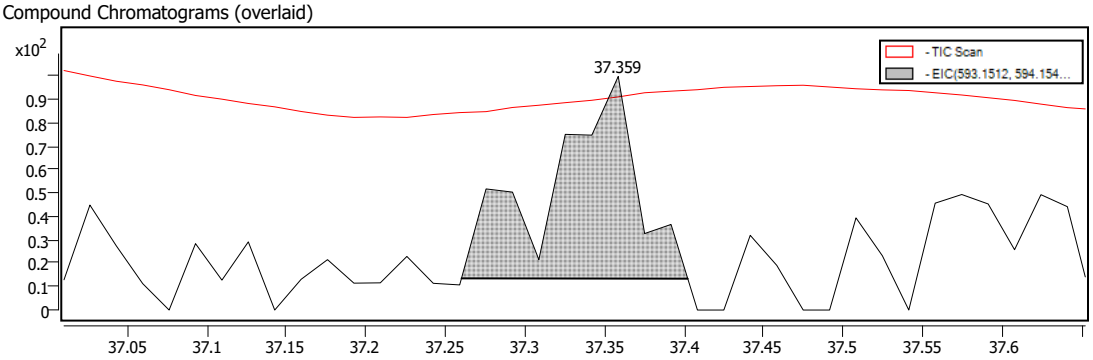
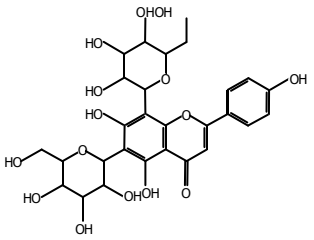
Compound Chromatograms (overlaid)

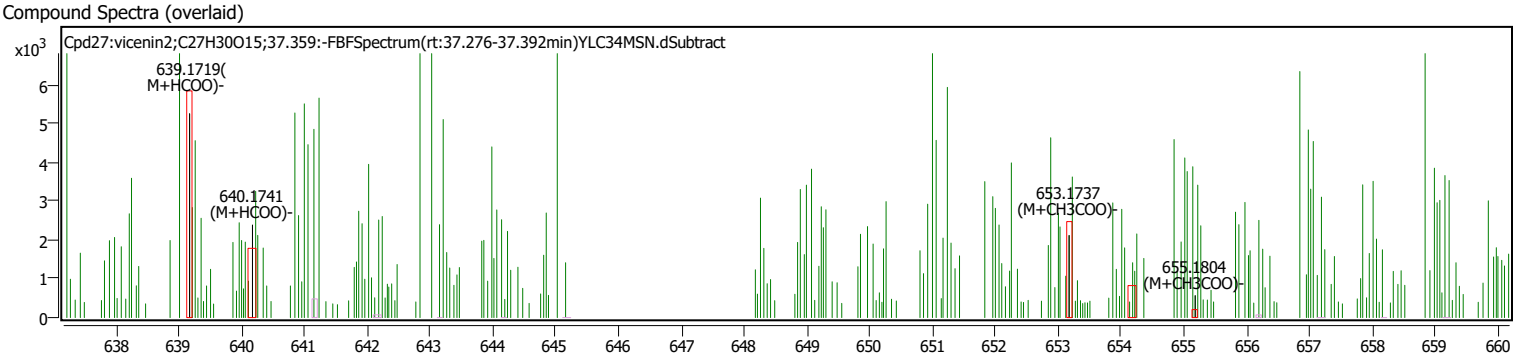


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



Counts vs. Mass-to-Charge (m/z)

Compound ID Table

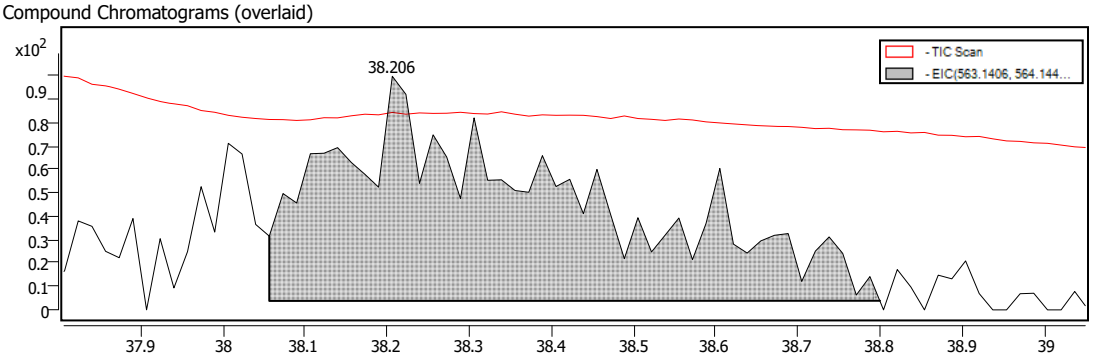
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
vicenin2	C27 H30 O15	(M+HCOO)- (M+CH3COO)-	37.359		594.1699		FBF	55.78		55.78

Cpd.28: Vicenin1

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Vicenin1	C26H28O14	38.206		564.1486	1.18	FBF	40.59	FBF

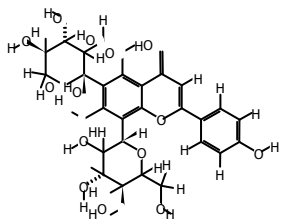
Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+HCOO)- (M+CH3COO)-	609.1516623.1522	40.59				

Compound Chromatograms (overlaid)



Counts (%) vs. Acquisition Time (min)

Structure



TargetScreeningReport

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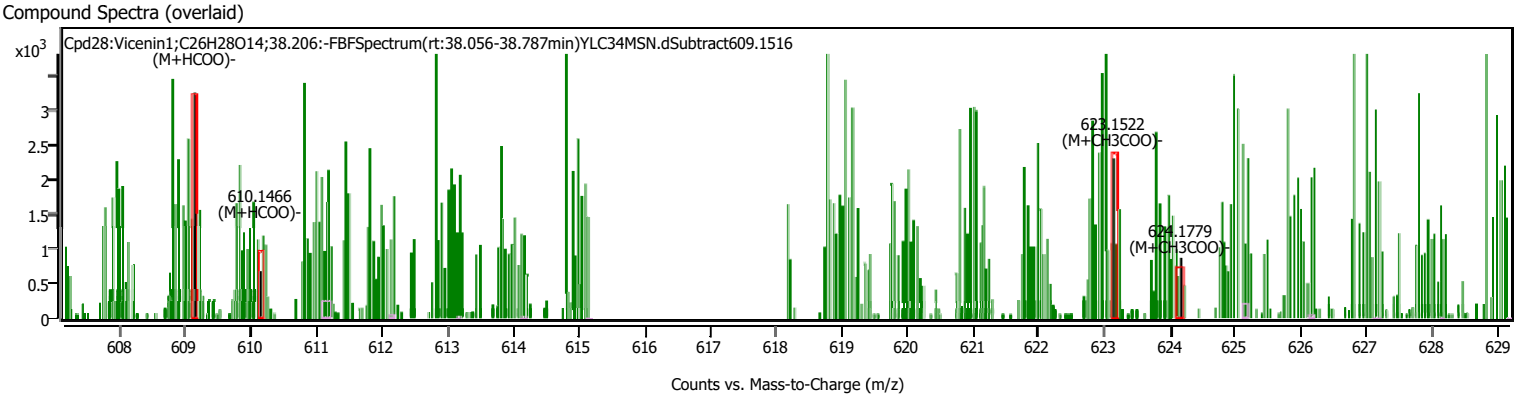
Compound Spectra (overlaid)



Compound ID Table

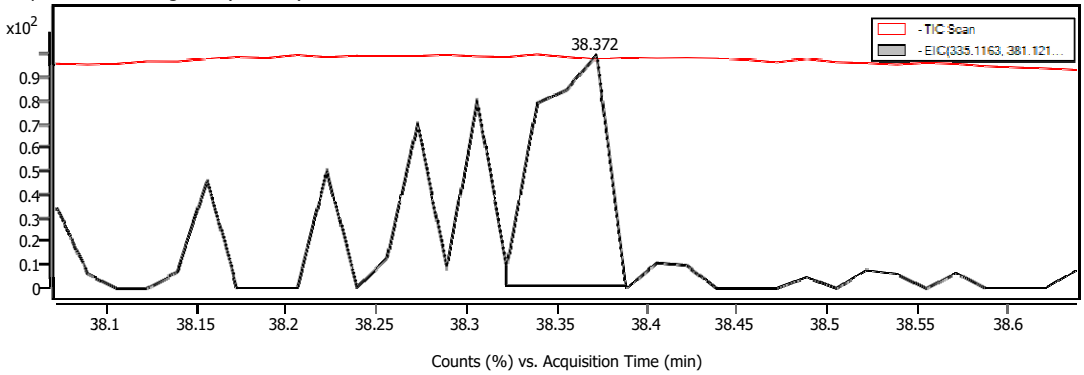
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Vicenin1	C26 H28 O14	(M+HCOO)- (M+CH3COO)-	38.206		564.1486		FBF	40.59		40.59

Cpd.29:Berberine

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Berberine	C20H18NO4	38.372		336.1240	1.11	FBF	70.11	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+HCOO)- (M+CH3COO)-	381.1216395.1489	70.11				

Compound Chromatograms (overlaid)



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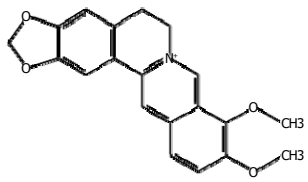
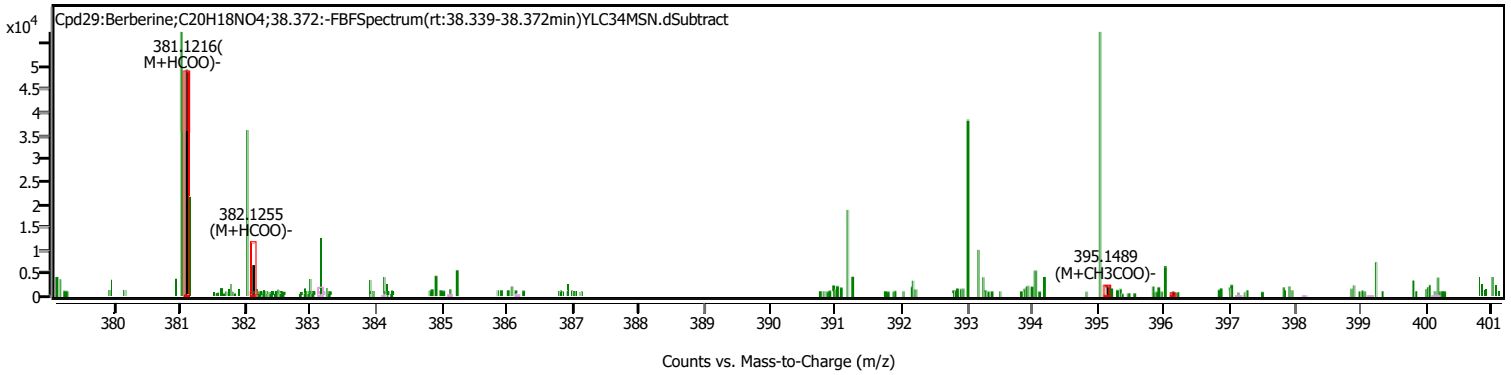


Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Berberine	C20 H18 N O4	(M+HCOO)- (M+CH3COO)-	38.372		336.1240		FBF	70.11		70.11

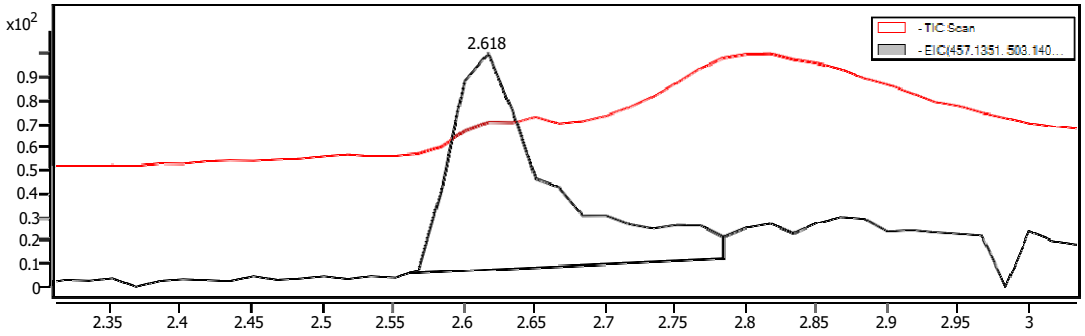
Cpd.30:cis-p-Coumaricacid4-[apiosyl-(1->2)-glucoside]

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
cis-p-Coumaricacid4-[apiosyl-(1- >2)-glucoside]	C20H26 O12	2.618		458.1323	-22.03	FBF	59.07	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	457.1329503.1339 517.1460	59.07				

TargetScreeningReport

Compound Chromatograms (overlaid)



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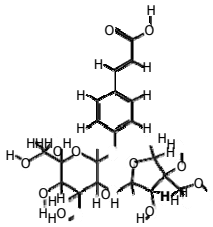
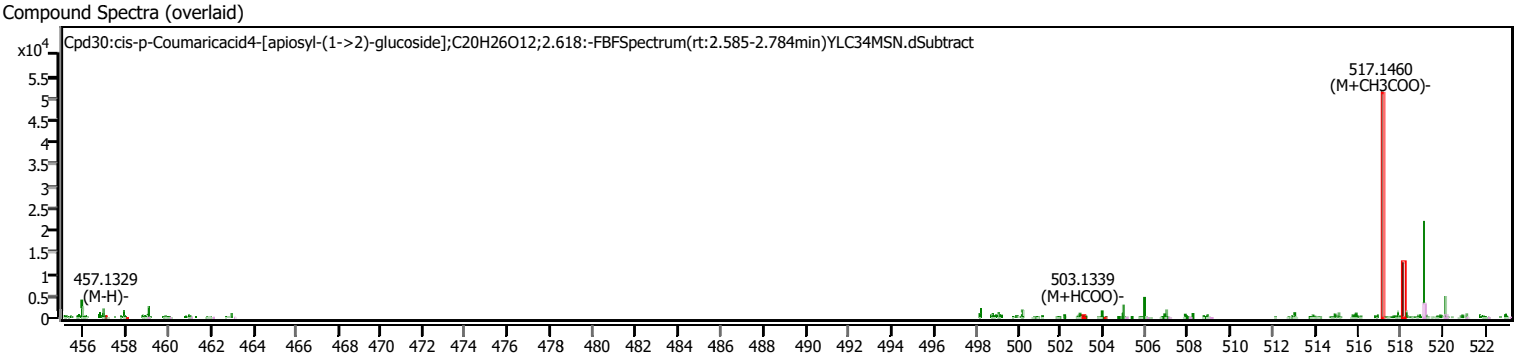


Compound Spectra (overlaid)



Compound ID Table

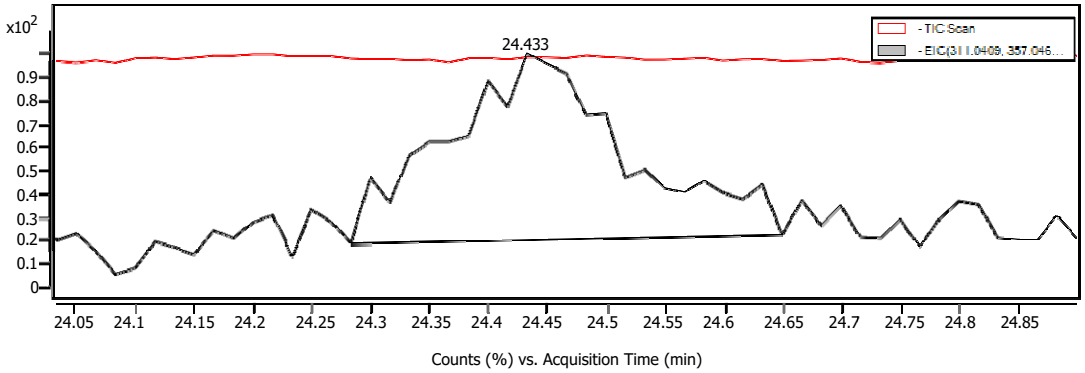
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
cis-p-Coumaricacid4-[apiosyl-(1->2)-glucoside]	C20H26O12	(M-H)- (M+HCOO)- (M+CH3COO)-	2.618		458.1323		FBF	59.07		59.07

Cpd.31:Monocaffeoyl(-)-tartaric acid

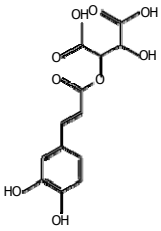
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Monocaffeoyl(-)-tartaricacid	C13H12O9	24.433		312.0475 -2.13		FBF	75.63	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	311.0399357.0453 371.0552	75.63				

Compound Chromatograms (overlaid)



Structure



TargetScreeningReport

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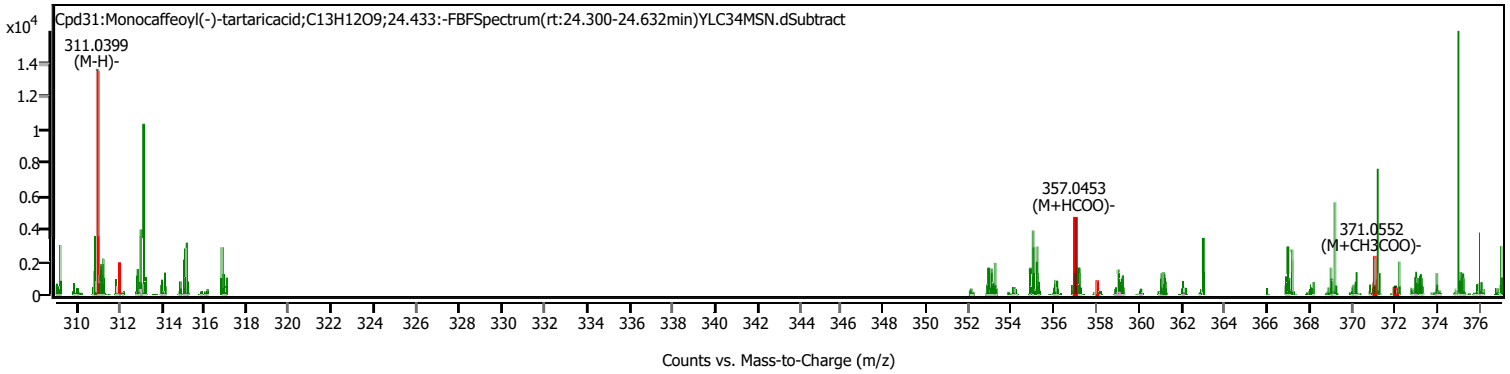
Compound Spectra (overlaid)



Compound ID Table

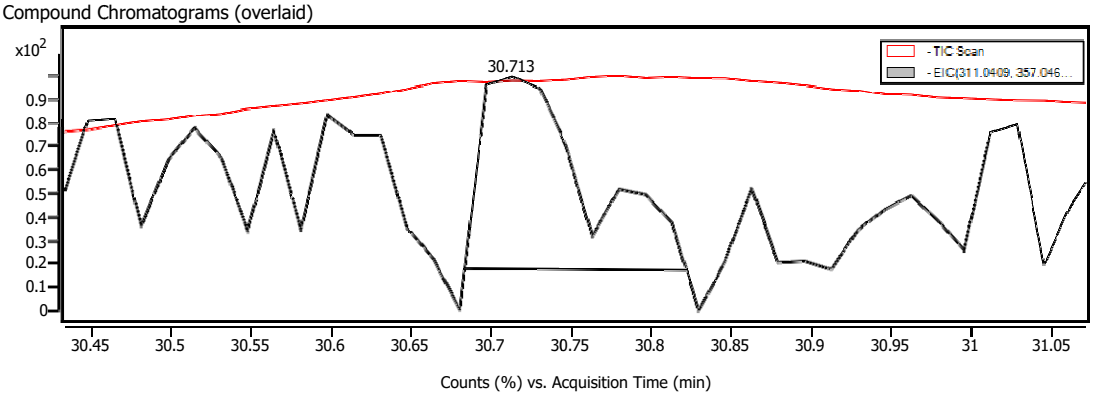
Name	Formula	Species	RT	RTDiff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Monocaffeoyl(-)-tartaricacid	C13H12O9	(M-H)- (M+HCOO)- (M+CH3COO)-	24.433		312.0475		FBF	75.63		75.63
Trans-Caffeoyltartaricacid	C13H12O9	(M-H)- (M+HCOO)- (M+CH3COO)-	24.433		312.0475		FBF	75.63		75.63

Cpd.32:Monocaffeoyl(-)-tartaricacid

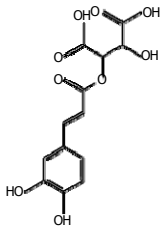
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Monocaffeoyl(-)-tartaricacid	C13H12O9	30.713		312.0461	-6.52	FBF	49.70	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	311.0349357.0523 371.0568	49.70				

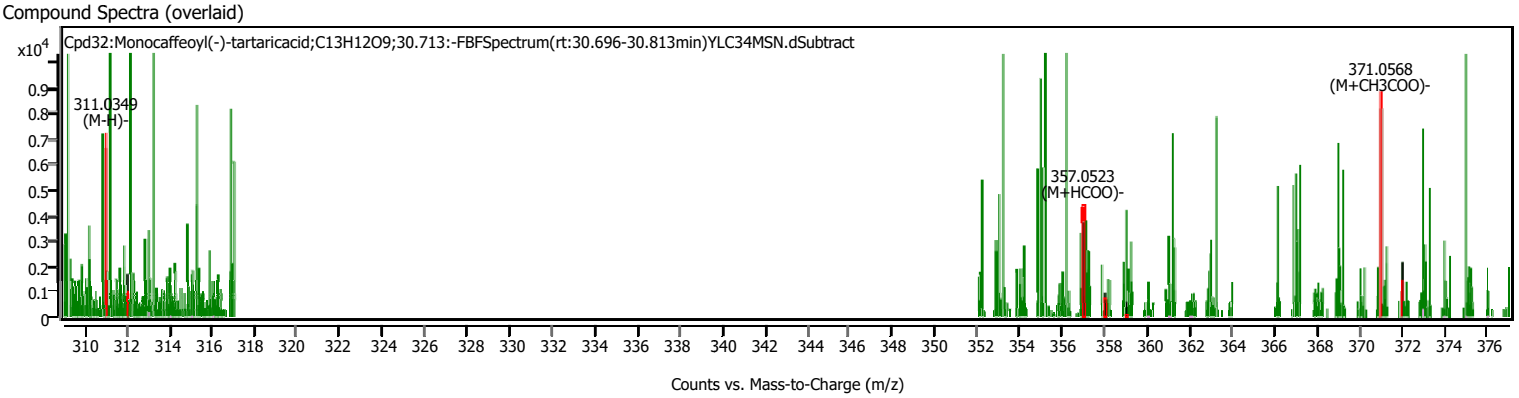
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

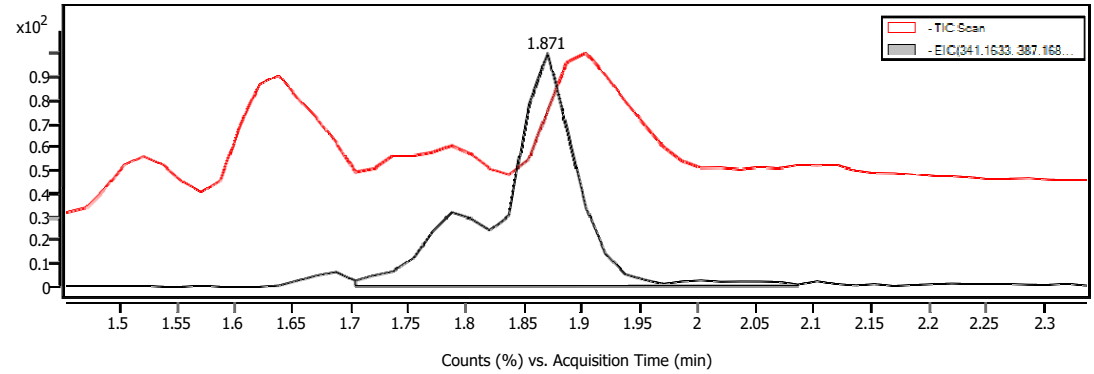
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Monocaffeoyl(-)-tartaricacid	C13 H12 O9	(M-H)- (M+HCOO)- (M+CH3COO)-	30.713		312.0461		FBF	49.70		49.70
Trans-Caffeoyl tartaric acid	C13 H12 O9	(M-H)- (M+HCOO)- (M+CH3COO)-	30.713		312.0461		FBF	49.70		49.70

Cpd.33:Magnoflorine

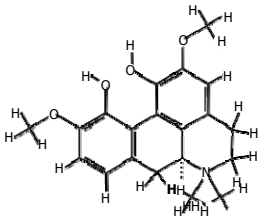
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Magnoflorine	C20H24NO4	1.871		342.1675	-8.90	FBF	65.23	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)- (M+HCOO)- (M+CH3COO)-	341.1587 387.1663 401.1776	65.23				

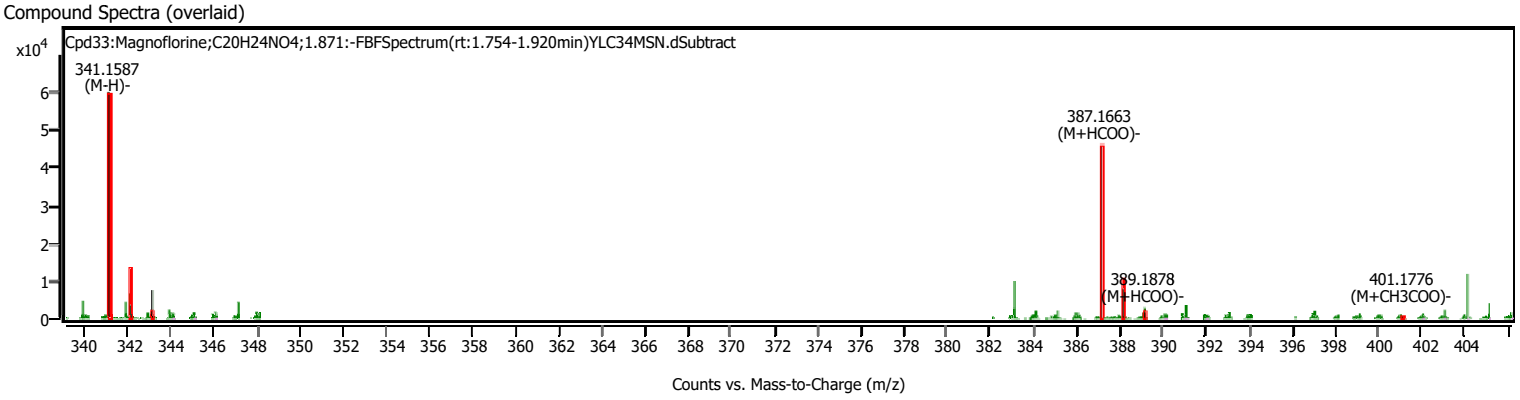
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

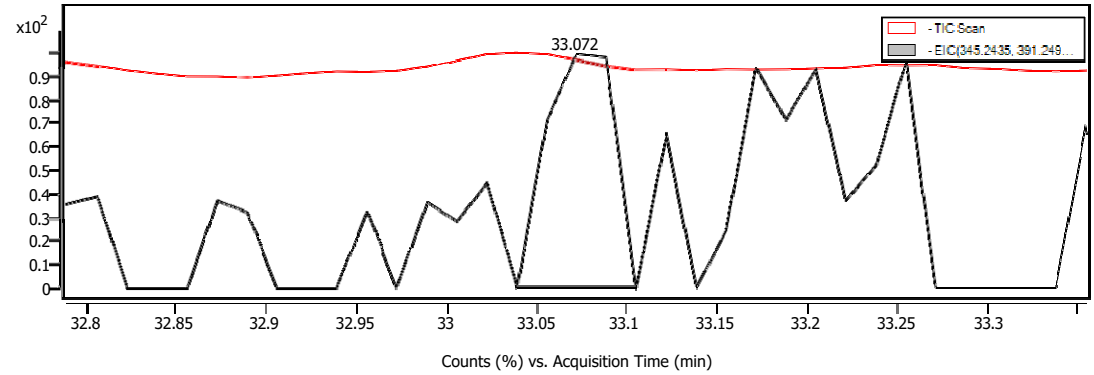
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Magnoflorine	C20 H24 N O4	(M-H)- (M+HCOO)- (M+CH3COO)-	1.871		342.1675		FBF	65.23		65.23

Cpd.34:AnacardicacidC15:1

Name	Formula	RT	RI	Mass Dif f(Tgt, ppm)	CAS	ID Source	Score	Algorithm
AnacardicacidC15:1	C22H34O3	33.072		346.2508 -0.10		FBF	73.06	FBF

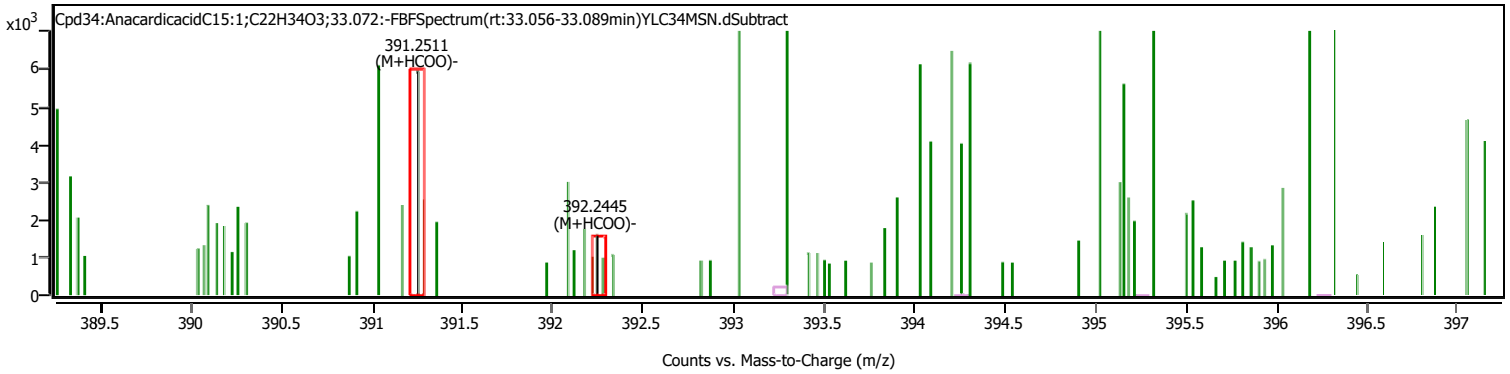
Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+HCOO)-	391.2511	73.06				

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Compound ID Table

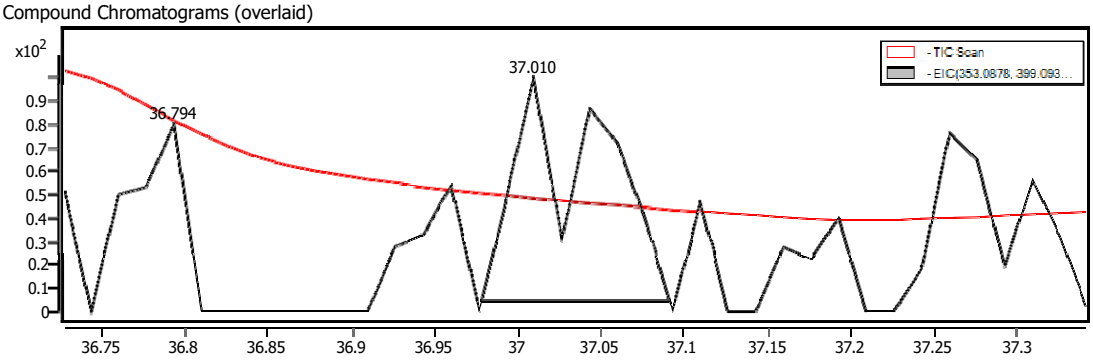
Name	Formula	Species	RT	RTDiff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
AnacardicacidC15:1	C22H34O3	(M+HCOO)-	33.072		346.2508		FBF	73.06		73.06

Cpd.35:1-Caffeoylquinicacid

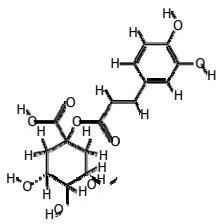
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
1-Caffeoylquinicacid	C16H18O9	37.010		354.0969	5.19	FBF	47.52	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	353.0854399.1017 413.1061	47.52				

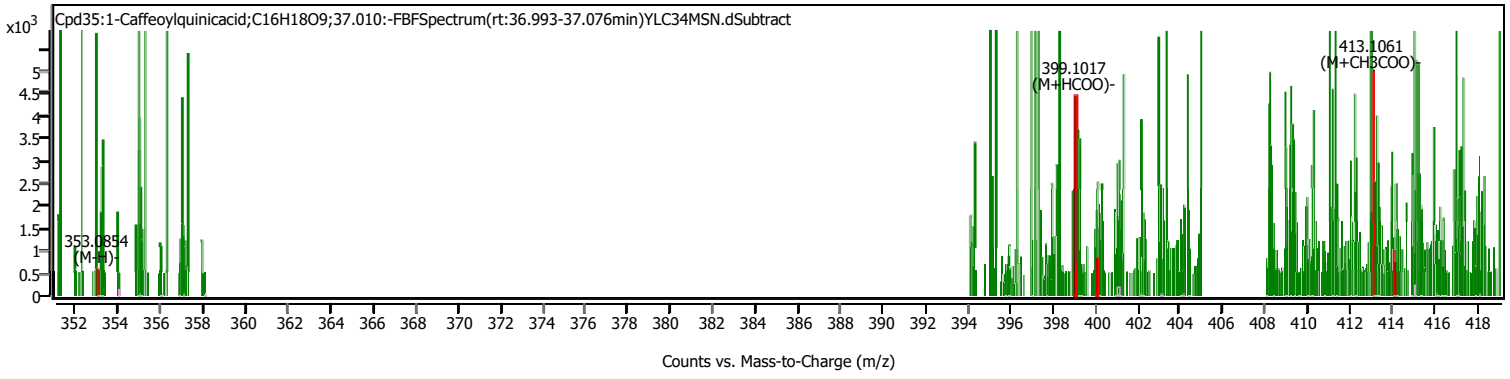
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
1-Caffeoylquinicacid	C16 H18 O9	(M-H)- (M+HCOO)- (M+CH3COO)-	37.010		354.0969		FBF	47.52		47.52

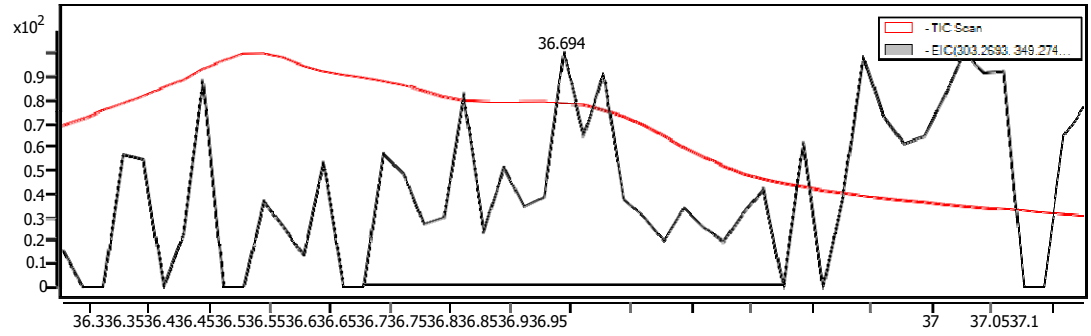
Cpd.36:3-Pentadecylphenol

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
3-Pentadecylphenol	C21H36O	36.694		304.2776	3.09	FBF	48.49	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	303.2707349.2792 363.2861	48.49				

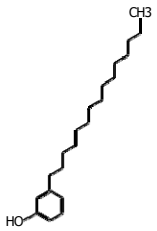
TargetScreeningReport

Compound Chromatograms (overlaid)

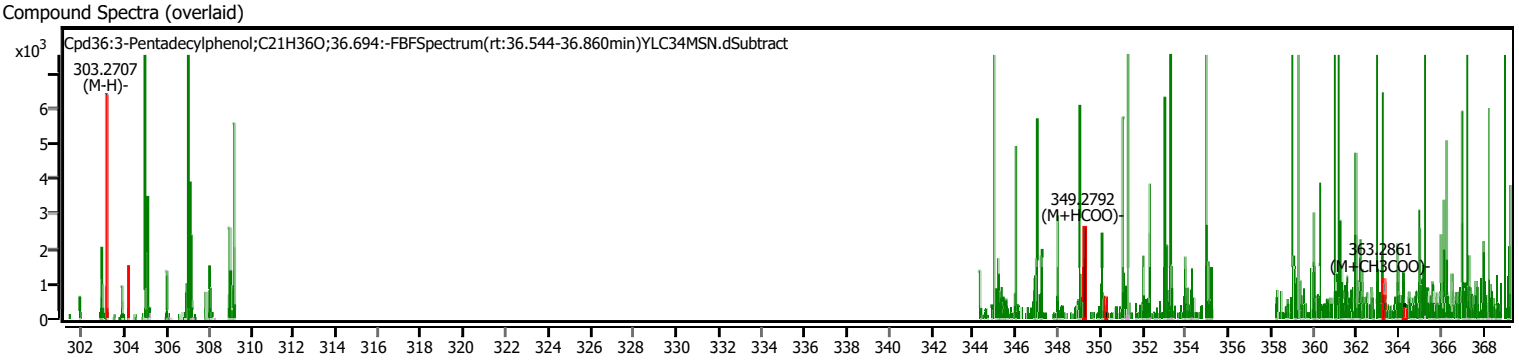


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



Counts vs. Mass-to-Charge (m/z)

Compound ID Table

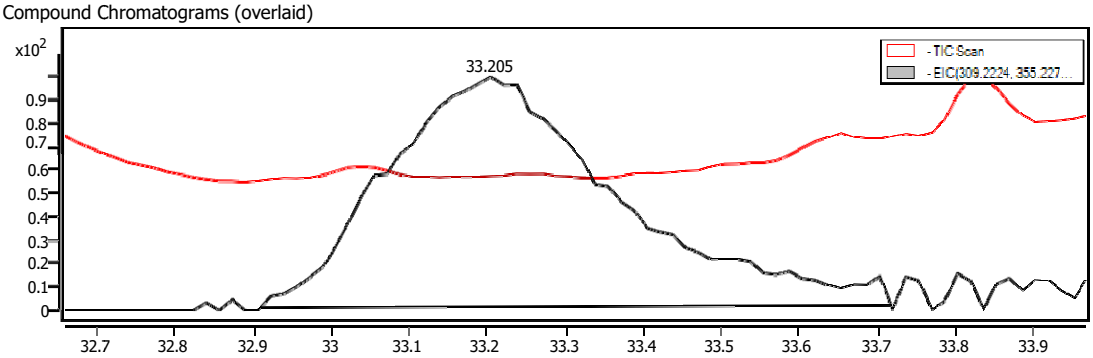
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
3-Pentadecylphenol	C21H36O	(M-H)- (M+HCOO)- (M+CH3COO)-	36.694		304.2776		FBF	48.49		48.49

Cpd.37:Desogestrel

Name	Formula	RT	RI	Mass Diff (Tgt,ppm)	CAS	ID Source	Score	Algorithm
Desogestrel	C22H30O	33.205		310.2291 -1.73		FBF	79.31	FBF

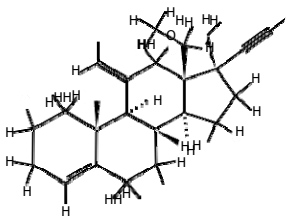
Species	m/z	Score(Tgt)	Score(Lib)	Score(DB)	Score(MFG)	Score(RT)
(M-H)-	309.2219	79.31				

Compound Chromatograms (overlaid)

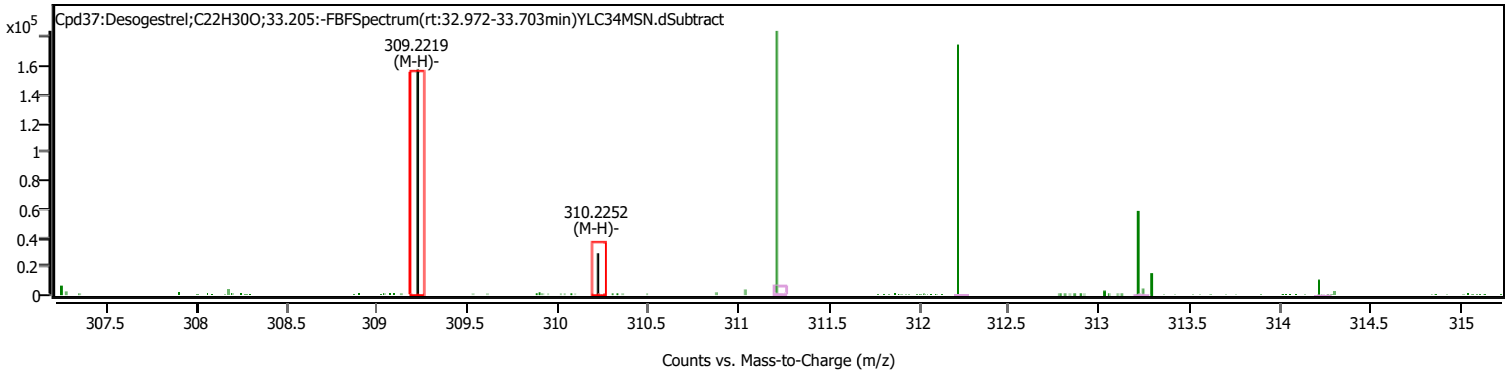


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



Compound ID Table

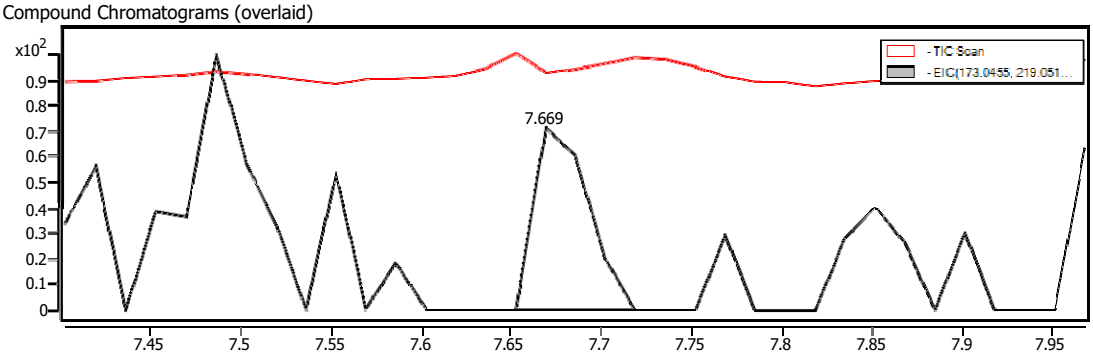
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Desogestrel	C22H30O	(M-H)-	33.205		310.2291		FBF	79.31		79.31

Cpd.38:(-)-Shikimicacid

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
(-)-Shikimicacid	C7H10O5	7.669		174.0532	2.33	FBF	45.25	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	173.0449219.0541 233.0633	45.25				

Compound Chromatograms (overlaid)



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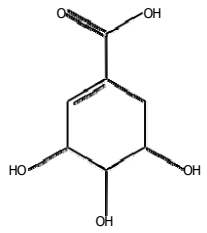
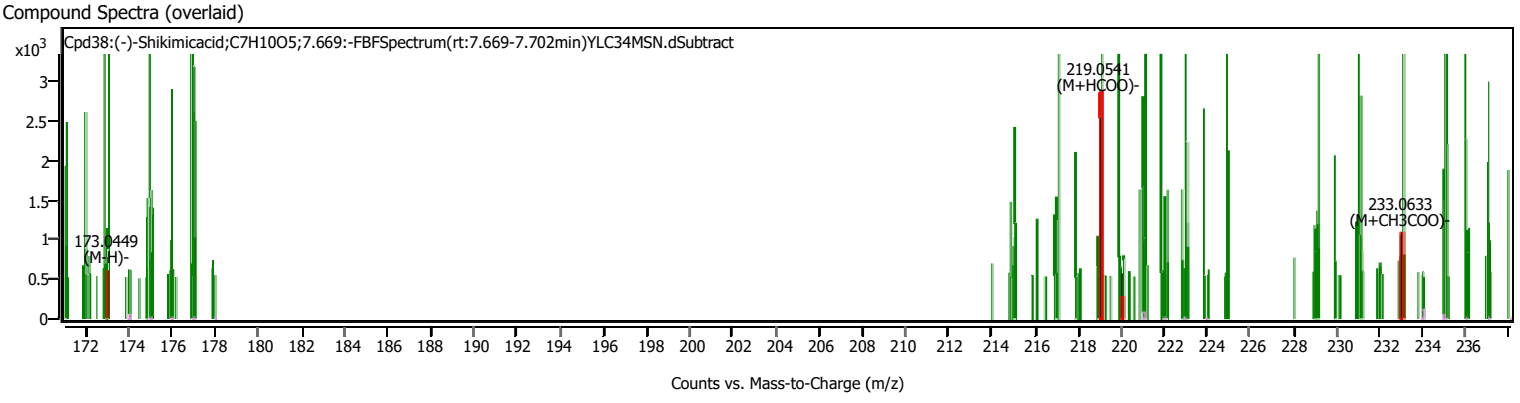


Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
(-)-Shikimicacid	C7 H10 O5	(M-H)- (M+HCOO)- (M+CH3COO)-	7.669		174.0532		FBF	45.25		45.25
(+)-Shikimicacid	C7 H10 O5	(M-H)- (M+HCOO)- (M+CH3COO)-	7.669		174.0532		FBF	45.25		45.25

Cpd.39:(-)-Shikimicacid

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
(-)-Shikimicacid	C7H10O5	19.615		174.0539	6.10	FBF	46.68	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	173.0465219.0521 233.0689	46.68				

TargetScreeningReport

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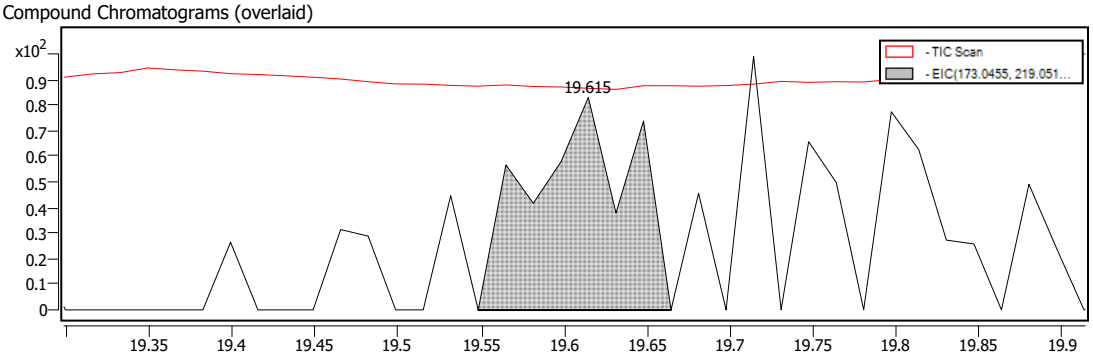
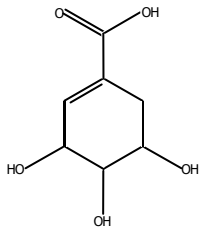
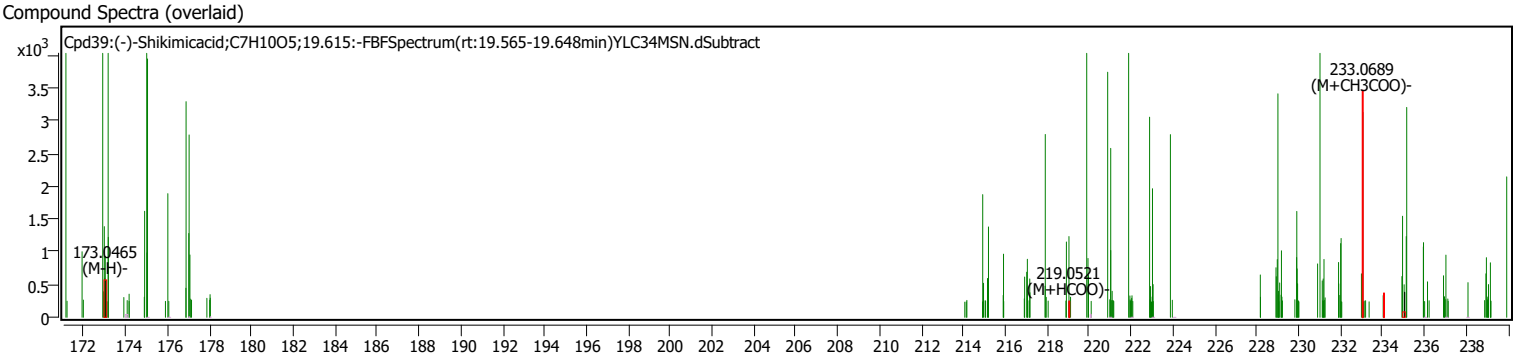
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

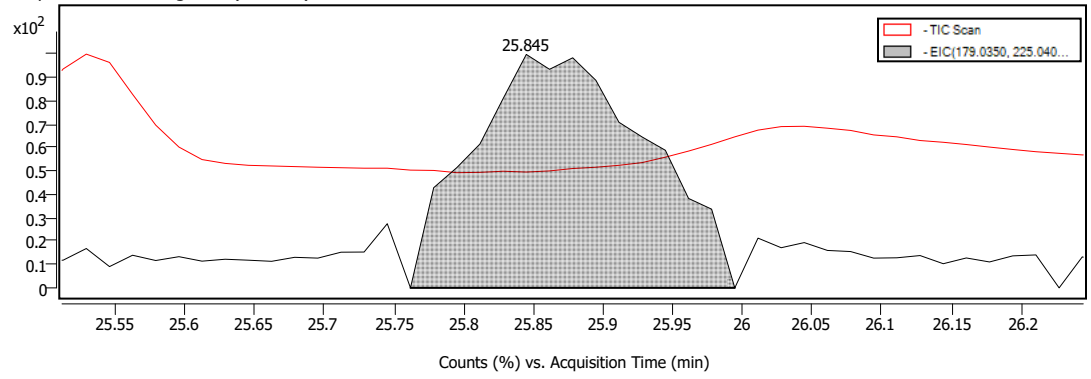
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
(-)-Shikimicacid	C7 H10 O5	(M-H)- (M+HCOO)- (M+CH3COO)-	19.615		174.0539		FBF	46.68		46.68
(+)-Shikimicacid	C7 H10 O5	(M-H)- (M+HCOO)- (M+CH3COO)-	19.615		174.0539		FBF	46.68		46.68

Cpd.40:trans-caffeicacid

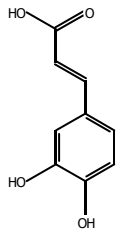
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)		CAS	ID Source	Score	Algorithm
trans-caffeicacid	C9H8O4	25.845		180.0384	-21.20		FBF	45.07	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+HCOO)-	225.0365	45.07				

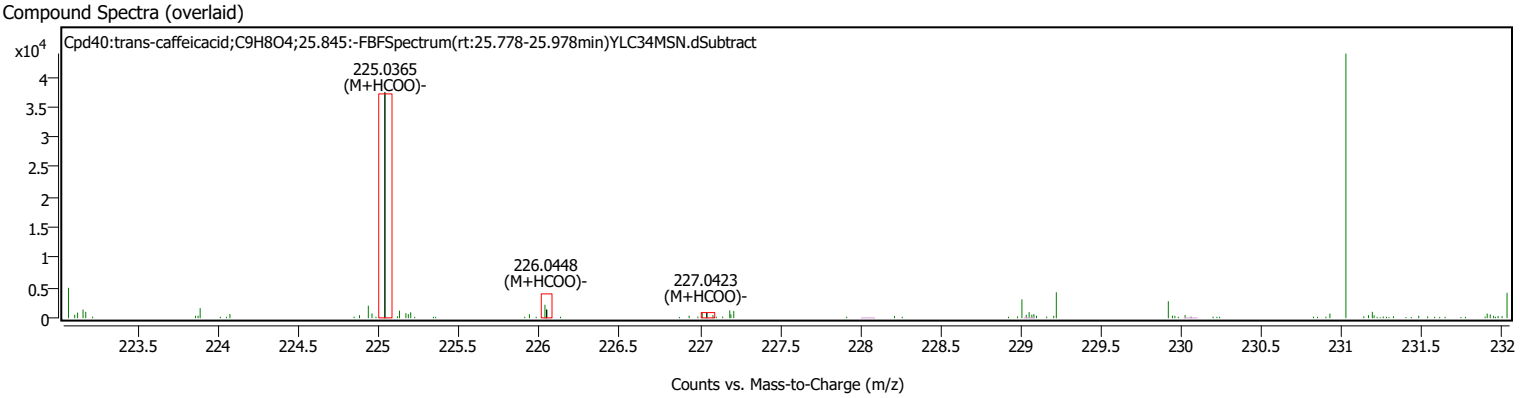
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

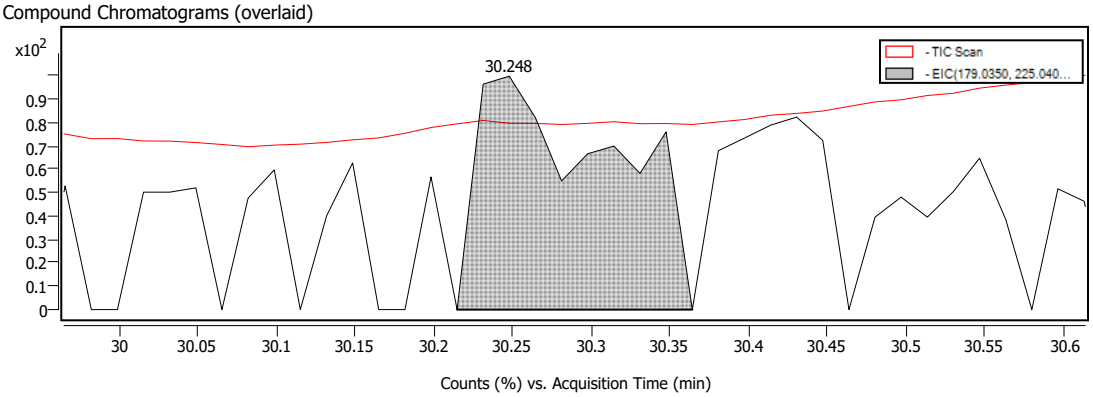
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
trans-caffeicacid	C9H8O4	(M+HCOO)-	25.845		180.0384		FBF	45.07		45.07
Caffeicacid	C9H8O4	(M+HCOO)-	25.845		180.0384		FBF	45.07		45.07

Cpd.41:trans-caffeicacid

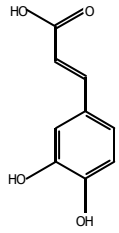
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
trans-caffeicacid	C9H8O4	30.248		180.0398 -13.58		FBF	50.05	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	179.0312225.0382 239.0640	50.05				

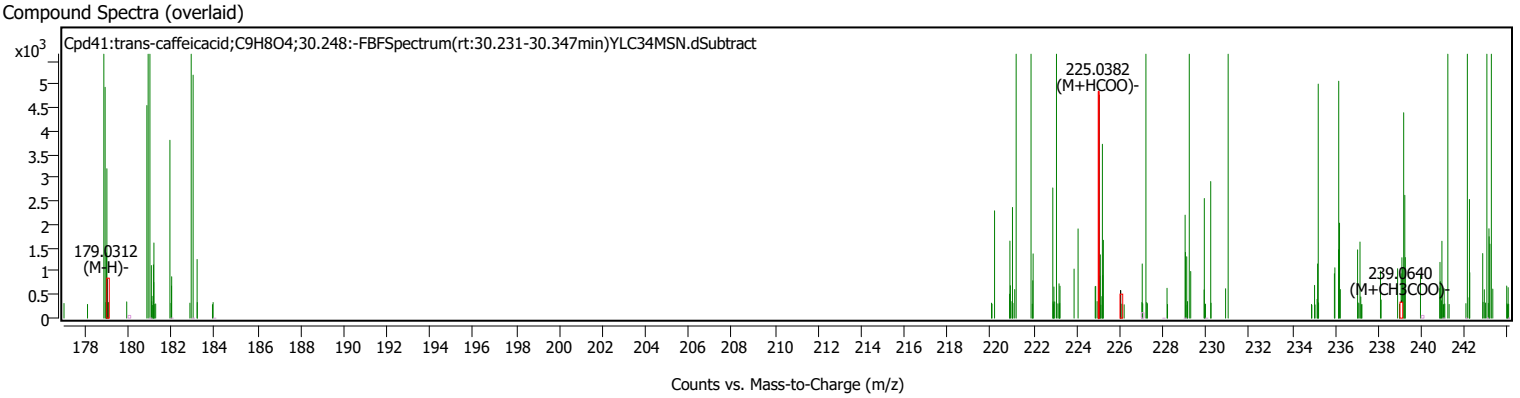
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RTDiff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
trans-caffeic acid	C9H8O4	(M-H)- (M+HCOO)- (M+CH3COO)-	30.248		180.0398		FBF	50.05		50.05
Caffeic acid	C9H8O4	(M-H)- (M+HCOO)- (M+CH3COO)-	30.248		180.0398		FBF	50.05		50.05

Cpd.42:6-Hydroxyflavanone

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
6-Hydroxyflavanone	C15H12O3	12.819		240.0780 -2.70		FBF	74.09	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	239.0660285.0766 299.1004	74.09				

TargetScreeningReport

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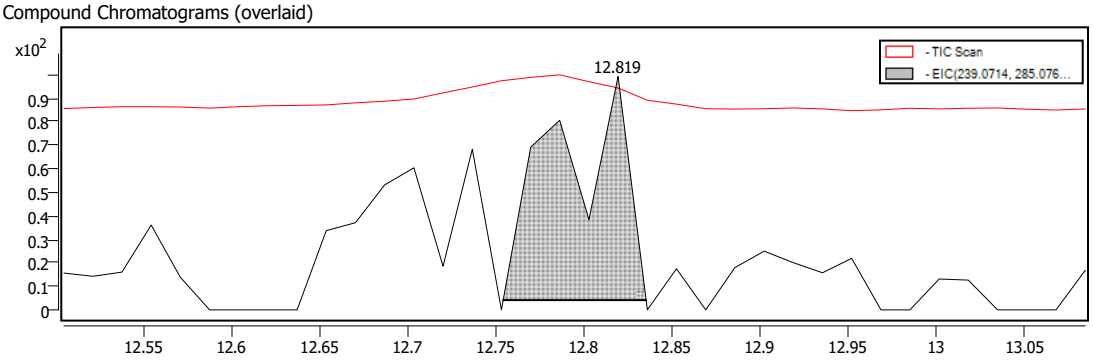
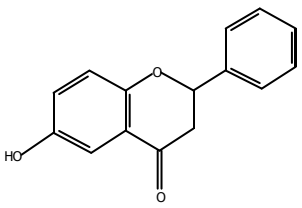
Compound Chromatograms (overlaid)

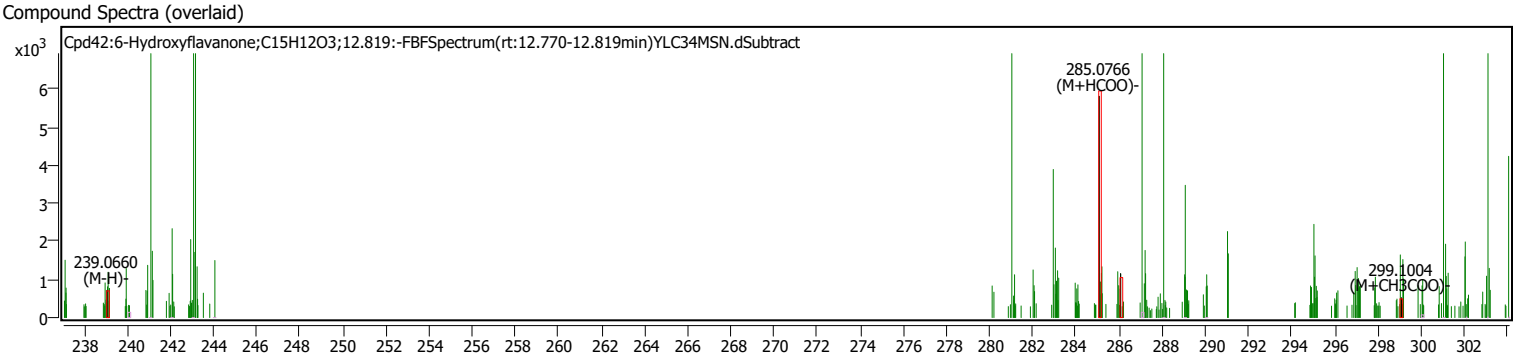


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



Counts vs. Mass-to-Charge (m/z)

Compound ID Table

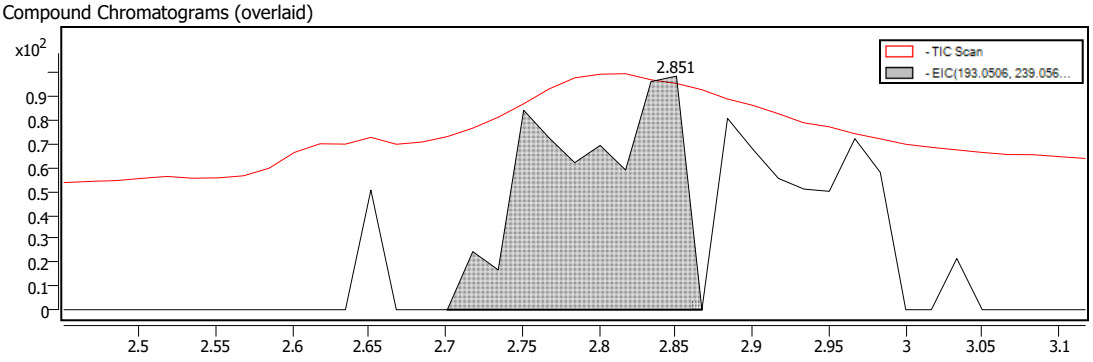
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
6-Hydroxyflavanone	C15 H12 O3	(M-H)- (M+HCOO)- (M+CH3COO)-	12.819		240.0780		FBF	74.09		74.09

Cpd.43:(E)-Ferulic acid

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
(E)-Ferulicacid	C10H10O4	2.851		194.0569 -5.23		FBF	79.57	FBF

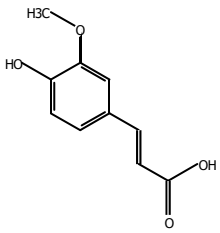
Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)-	193.0505239.0506	79.57				

Compound Chromatograms (overlaid)

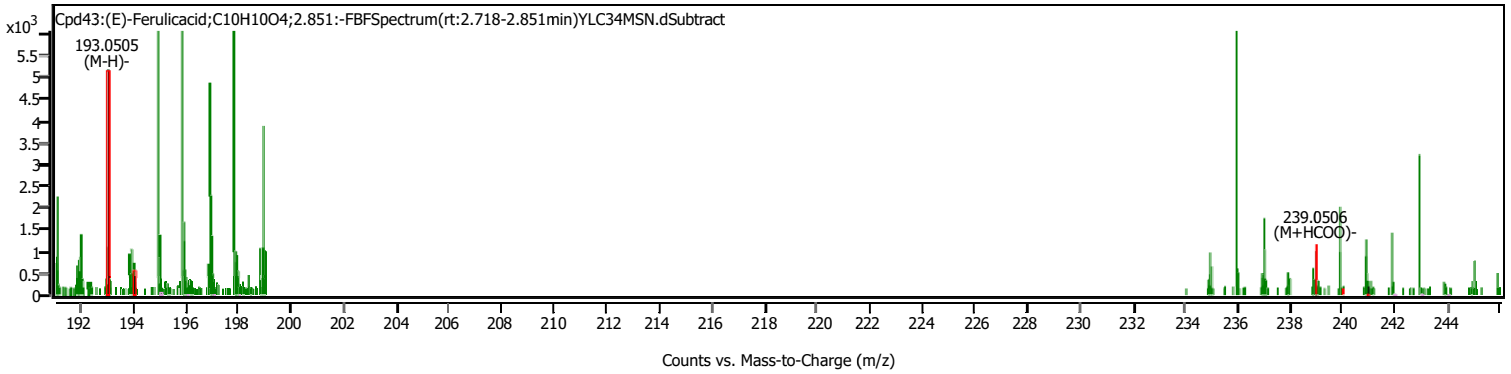


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



Compound ID Table

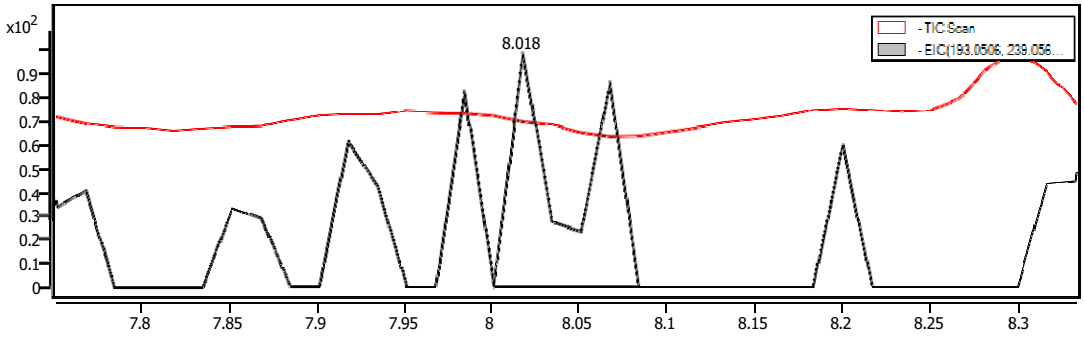
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
(E)-Ferulic acid	C10 H10 O4	(M-H)- (M+HCOO)-	2.851		194.0569		FBF	79.57		79.57
Ferulic acid	C10 H10 O4	(M-H)- (M+HCOO)-	2.851		194.0569		FBF	79.57		79.57
(Z)-ferulic acid	C10 H10 O4	(M-H)- (M+HCOO)-	2.851		194.0569		FBF	79.57		79.57

Cpd.44:(E)-Ferulicacid

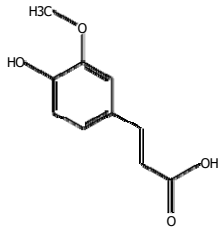
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
(E)-Ferulicacid	C10H10O4	8.018		194.0602	12.04	FBF	58.22	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+CH3COO)-	193.0622253.0696	58.22				

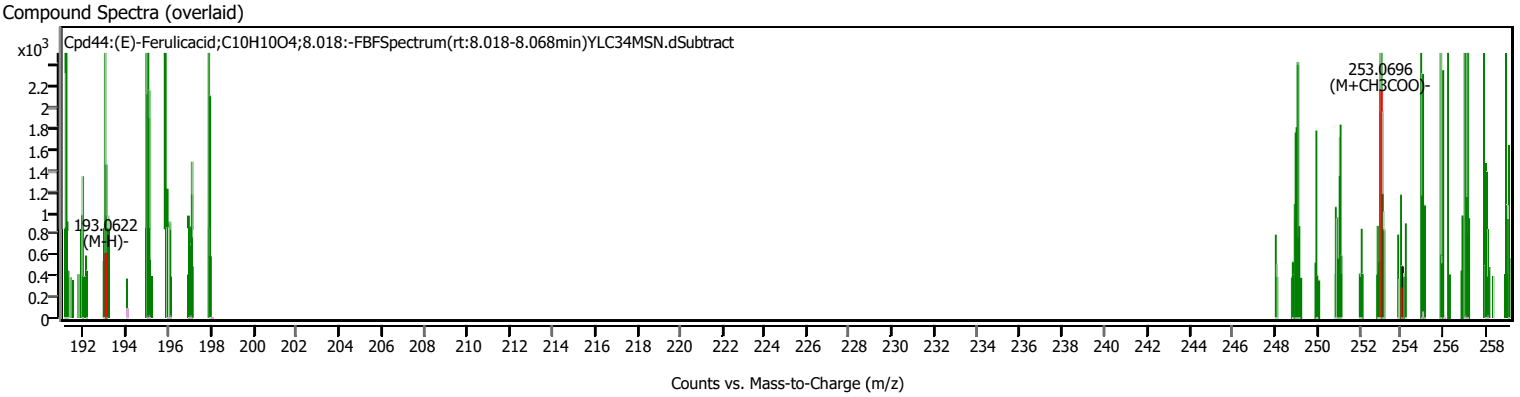
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

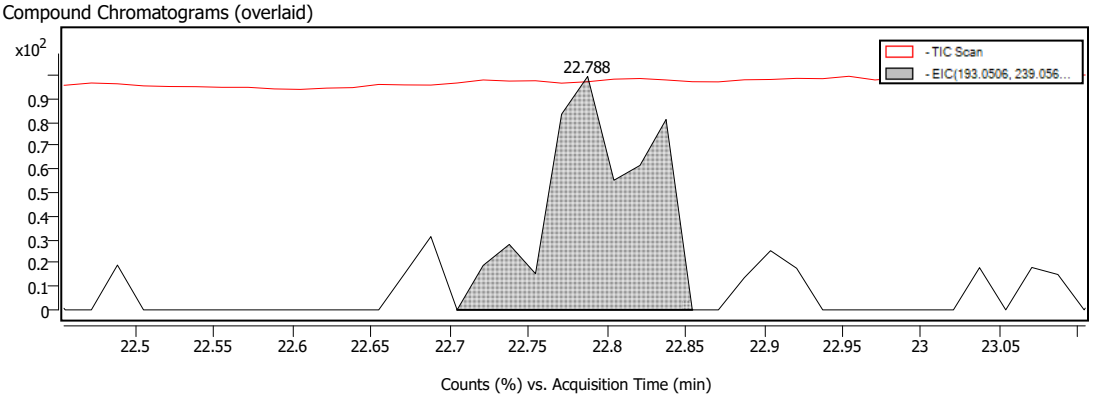
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
(E)-Ferulicacid	C10 H10 O4	(M-H)- (M+CH3COO)-	8.018		194.0602		FBF	58.22		58.22
Ferulicacid	C10 H10 O4	(M-H)- (M+CH3COO)-	8.018		194.0602		FBF	58.22		58.22
(Z)-ferulicacid	C10 H10 O4	(M-H)- (M+CH3COO)-	8.018		194.0602		FBF	58.22		58.22

Cpd.45:(E)-Ferulicacid

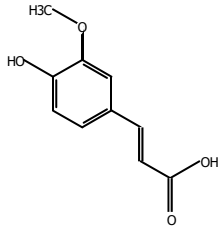
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
(E)-Ferulicacid	C10H10O4	22.788		194.0582	1.55	FBF	54.16	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)-(M+CH3COO)-	193.0503239.0539253.0763	54.16				

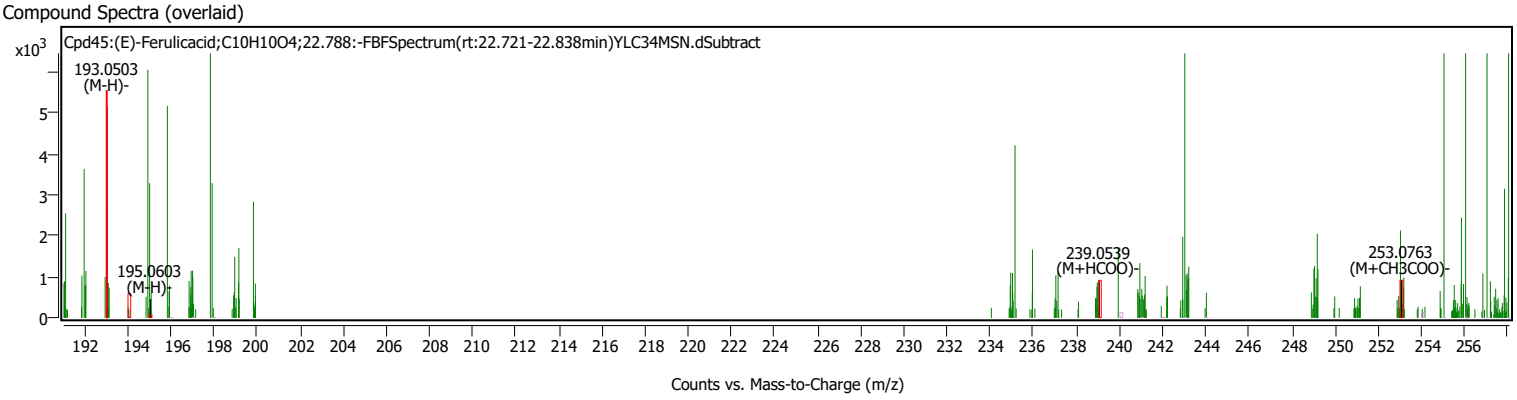
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

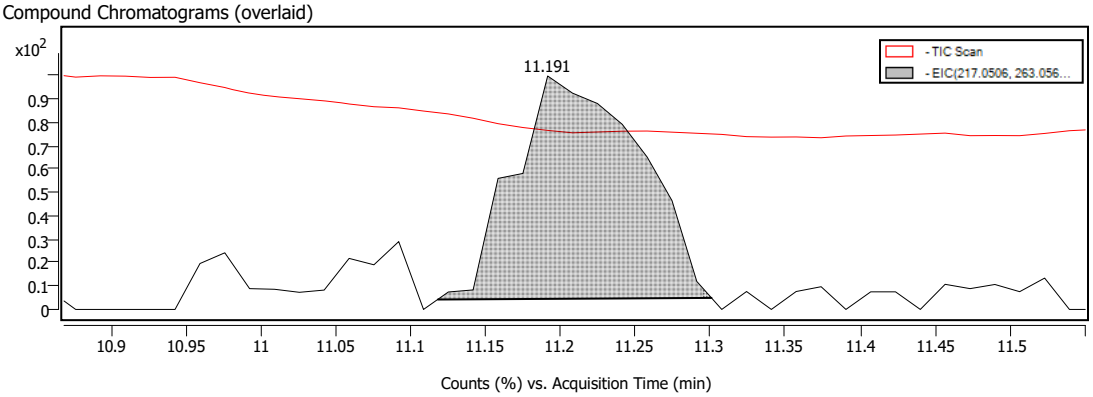
Name	Formula	Species	RT	RTDiff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
(E)-Ferulicacid	C10H10O4	(M-H)-(M+HCOO)-(M+CH3COO)-	22.788		194.0582		FBF	54.16		54.16
Ferulicacid	C10H10O4	(M-H)-(M+HCOO)-(M+CH3COO)-	22.788		194.0582		FBF	54.16		54.16
(Z)-ferulicacid	C10H10O4	(M-H)-(M+HCOO)-(M+CH3COO)-	22.788		194.0582		FBF	54.16		54.16

Cpd.46:8-Acetyl-7-methoxycoumarin

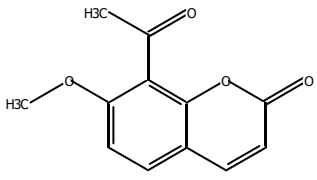
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)		CAS	ID Source	Score	Algorithm
8-Acetyl-7-methoxycoumarin	C12H10O4	11.191		218.0604	11.55		FBF	65.60	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)-(M+CH3COO)-	217.0575263.0494277.0736	65.60				

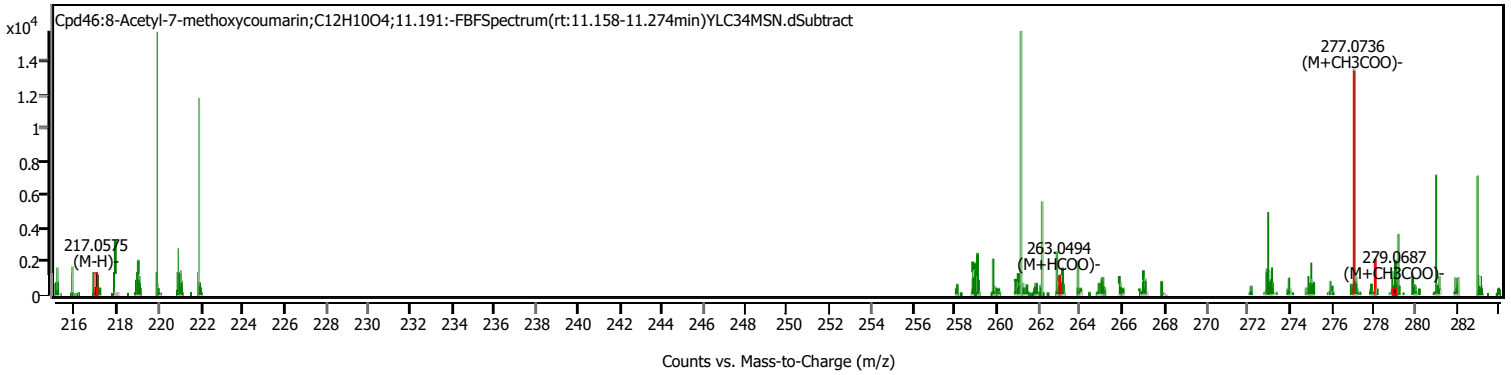
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

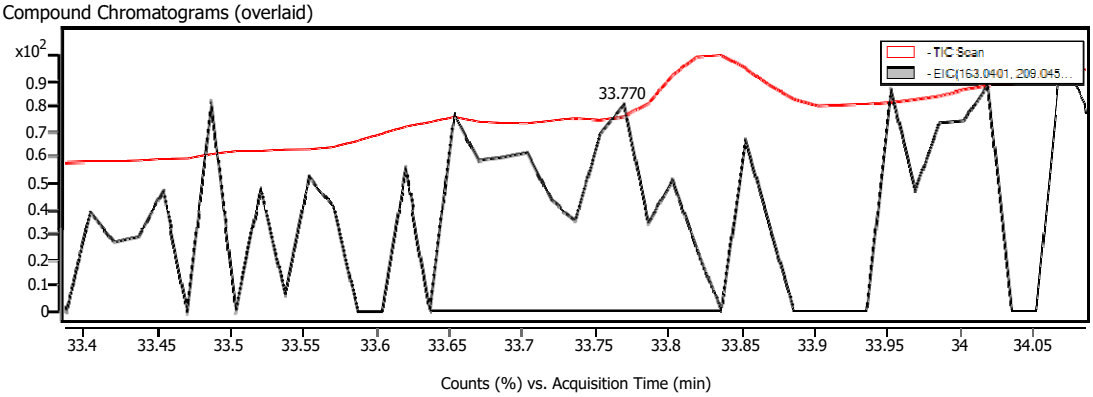
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
8-Acetyl-7-methoxycoumarin	C12 H10 O4	(M-H)- (M+HCOO)- (M+CH3COO)-	11.191		218.0604		FBF	65.60		65.60

Cpd.47:2-Coumaric acid

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
2-Coumaricacid	C9H8O3	33.770		164.0474 0.47		FBF	70.47	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	163.0403209.0400 223.0620	70.47				

Compound Chromatograms (overlaid)



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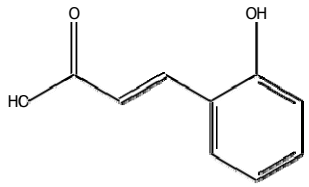
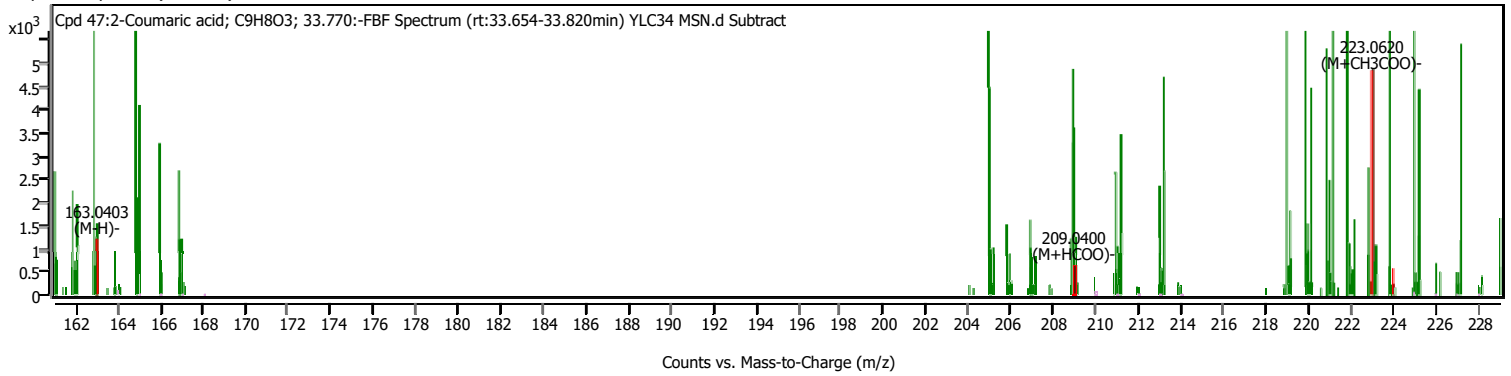


Compound Spectra (overlaid)



Compound ID Table

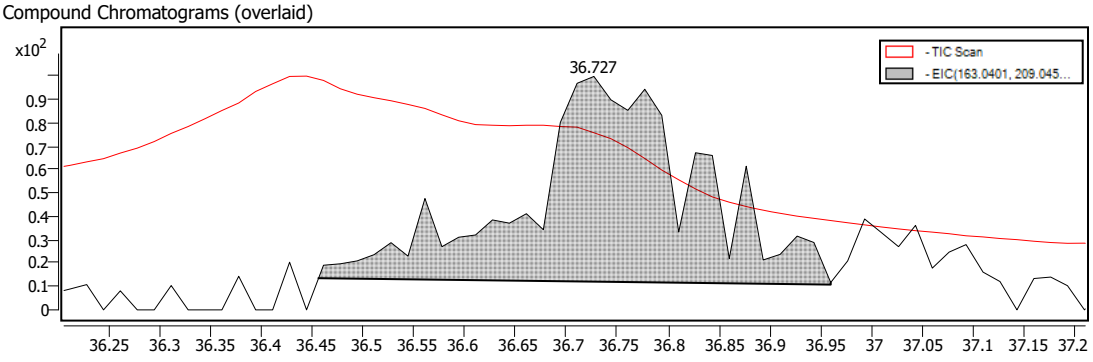
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
2-Coumaric acid	C9H8O3	(M-H)- (M+HCOO)- (M+CH3COO)-	33.770		164.0474		FBF	70.47		70.47
4-Coumaric acid	C9H8O3	(M-H)- (M+HCOO)- (M+CH3COO)-	33.770		164.0474		FBF	70.47		70.47
(E)-p-coumaric acid	C9H8O3	(M-H)- (M+HCOO)- (M+CH3COO)-	33.770		164.0474		FBF	70.47		70.47

Cpd.48:2-Coumaric acid

Name	Formula	RT	RI	Mass Diff (Tgt,ppm)	CAS	ID Source	Score	Algorithm
2-Coumaricacid	C9H8O3	36.727		164.0447 -15.89		FBF	67.12	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	163.0303209.0403 223.0606	67.12				

Compound Chromatograms (overlaid)



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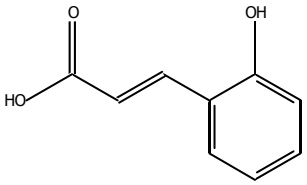
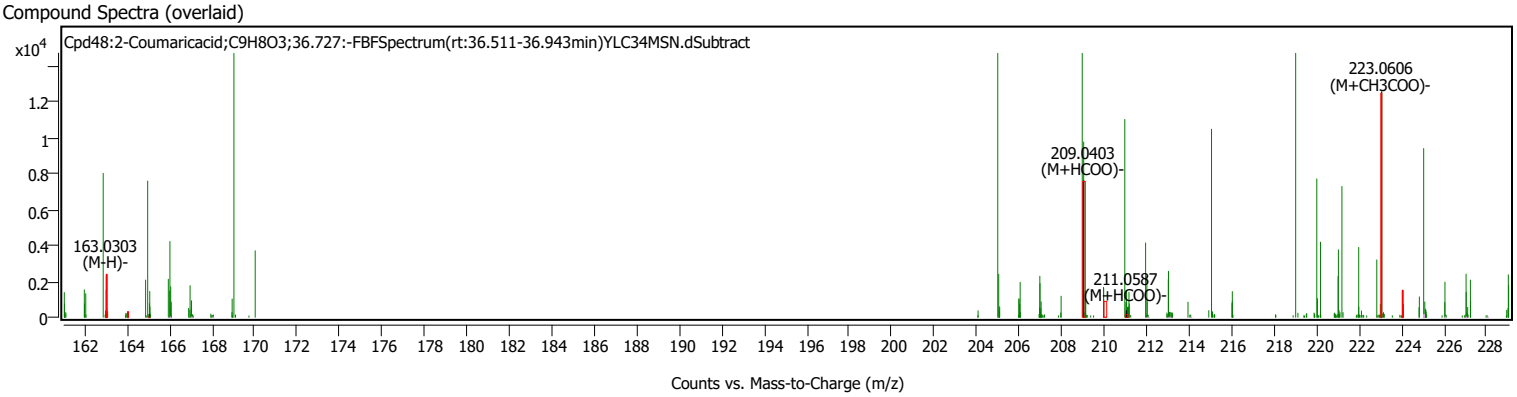


Compound Spectra (overlaid)



Compound ID Table

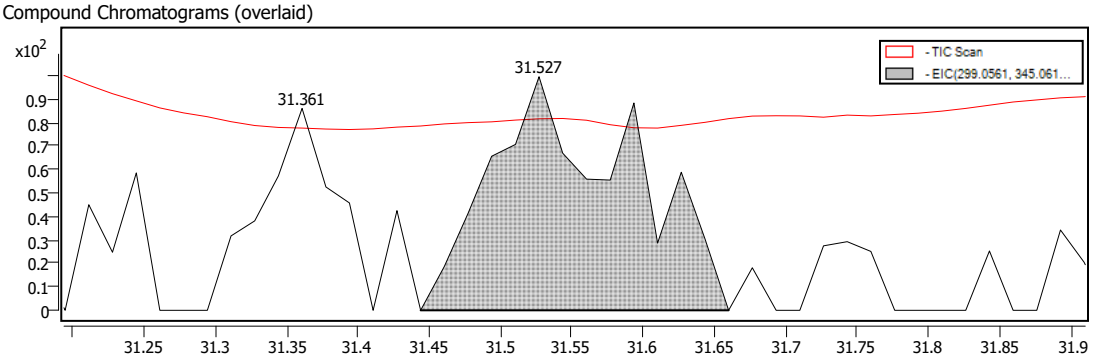
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
2-Coumaricacid	C9H8O3	(M-H)- (M+HCOO)- (M+CH3COO)-	36.727		164.0447		FBF	67.12		67.12
4-Coumaricacid	C9H8O3	(M-H)- (M+HCOO)- (M+CH3COO)-	36.727		164.0447		FBF	67.12		67.12
(E)-p-coumaricacid	C9H8O3	(M-H)- (M+HCOO)- (M+CH3COO)-	36.727		164.0447		FBF	67.12		67.12

Cpd.49:Diosmetin

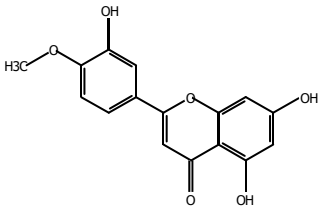
Name	Formula	RT	RI	MassDiff(Tgt,ppm)	CAS	ID Source	Score	Algorithm
Diosmetin	C16H12O6	31.527		300.0626	-2.70	FBF	49.62	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	299.0522345.0761 359.0812	49.62				

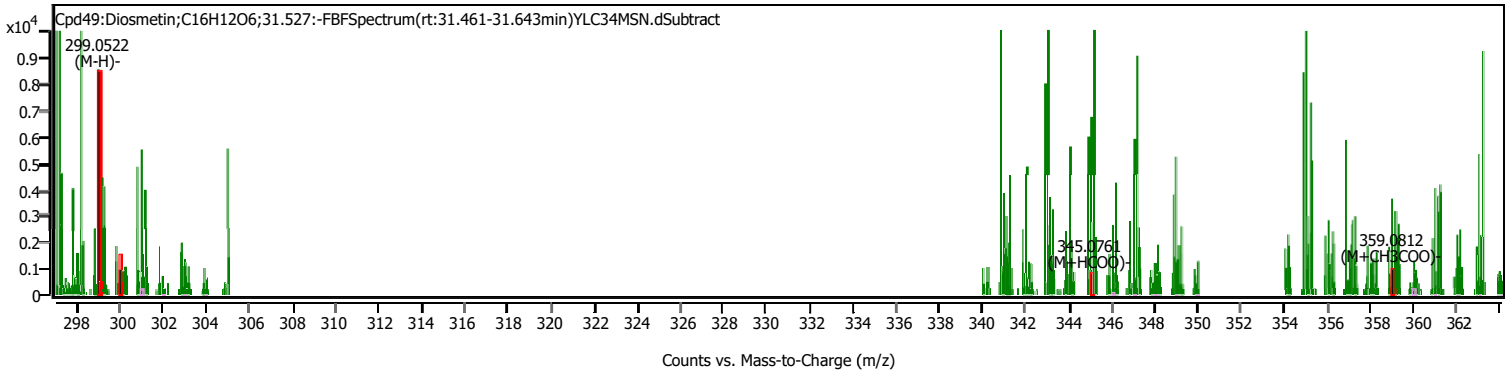
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

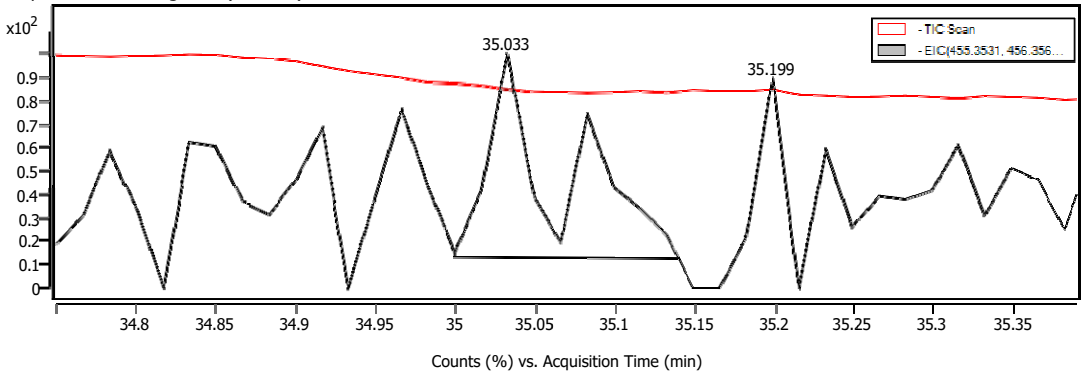
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Diosmetin	C16H12O6	(M-H)- (M+HCOO)- (M+CH3COO)-	31.527		300.0626		FBF	49.62		49.62

Cpd.50:Betulinicacid

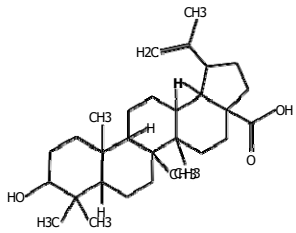
Name	Formula	RT	RI	Mass Diff (Tgt,ppm)	CAS	ID Source	Score	Algorithm
Betulinicacid	C30H48O3	35.033		456.3590 -2.88		FBF	43.79	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-	455.3410	43.79				

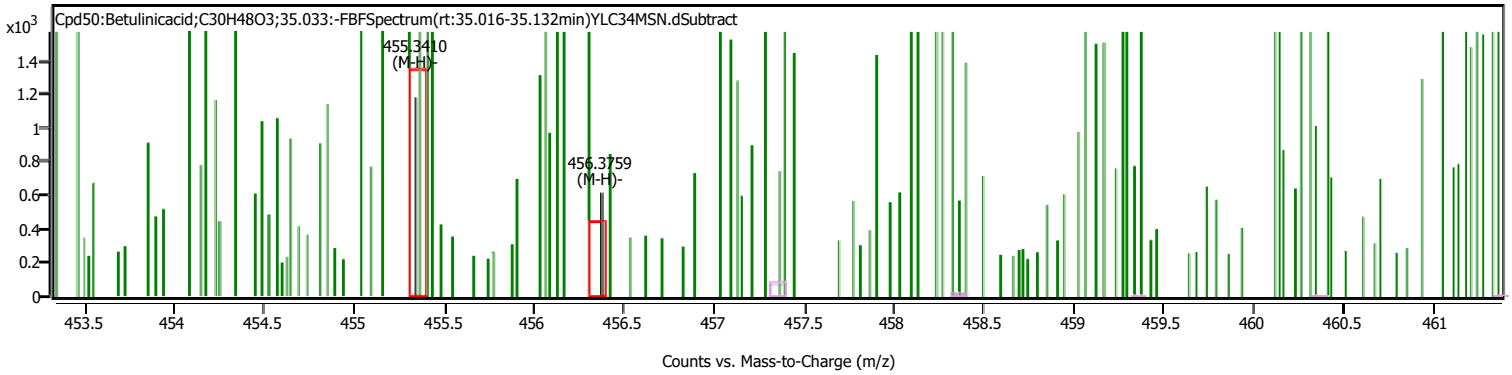
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Betulinicacid	C30H48O3	(M-H)-	35.033		456.3590		FBF	43.79		43.79

Cpd.51:Apigetrin

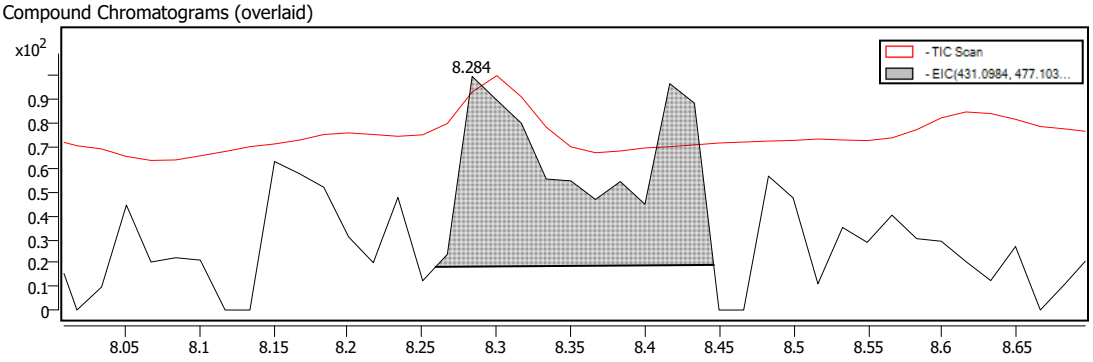
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Apigetrin	C21H20O10	8.284		432.1084 6.29		FBF	48.21	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	431.1008477.1076 491.1062	48.21				

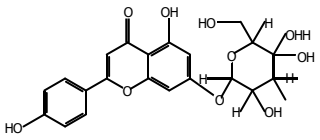
TargetScreeningReport

Agilent | Trusted Answers

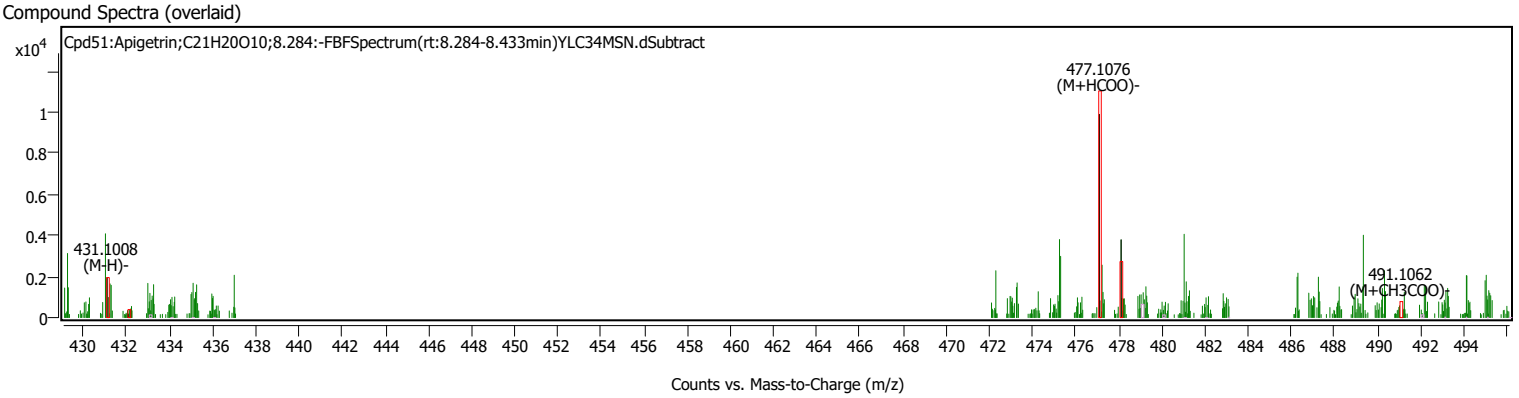
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

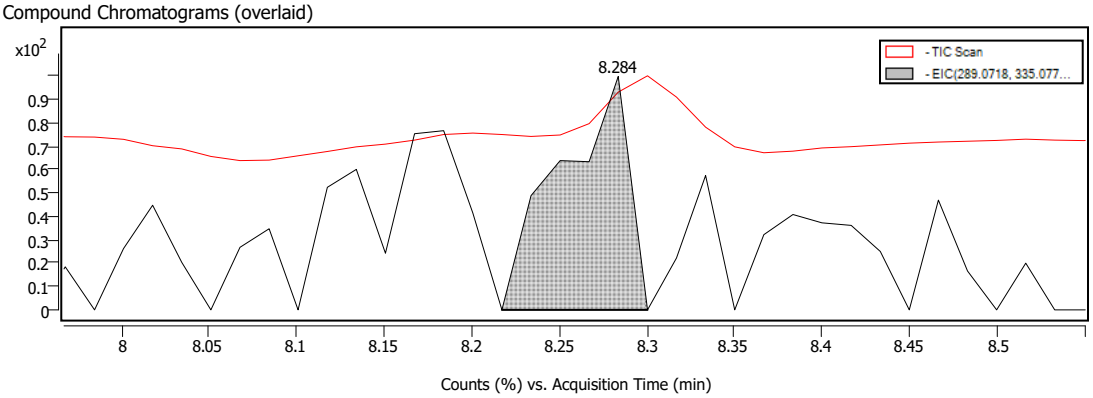
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Apigetrin	C21 H20 O10	(M-H)- (M+HCOO)- (M+CH3COO)-	8.284		432.1084		FBF	48.21		48.21

Cpd.52:D-(+)-Catechin

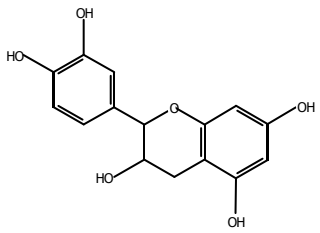
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
D-(+)-Catechin	C15H14O6	8.284		290.0857	22.84	FBF	49.52	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	289.0762335.0920 349.0930	49.52				

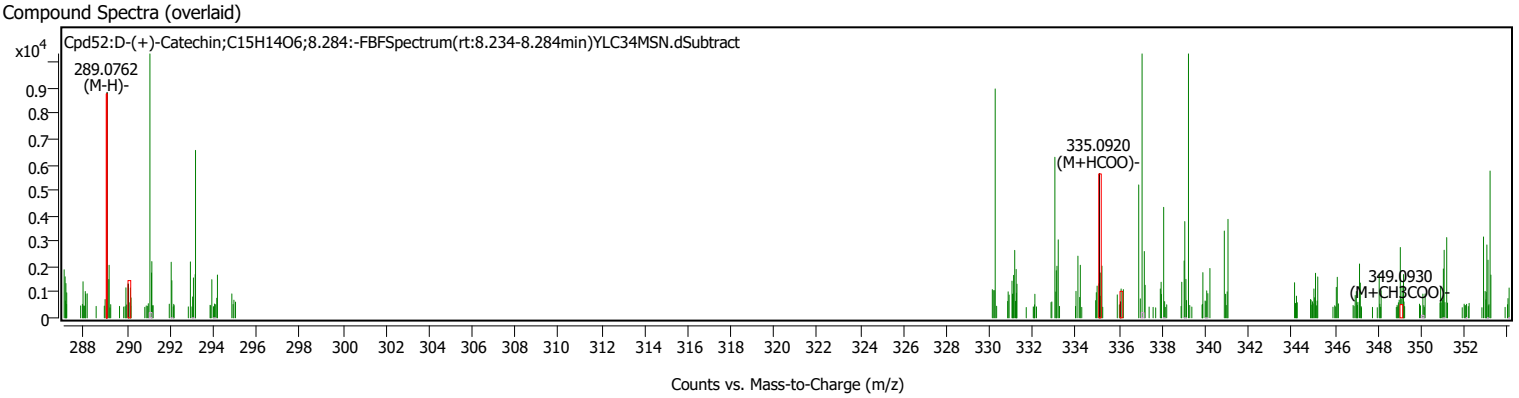
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

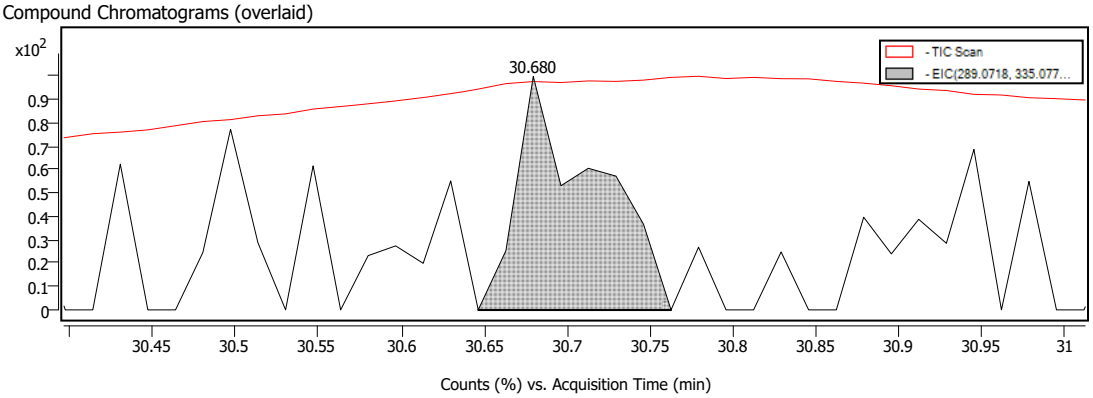
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
D-(+)-Catechin	C15H14O6	(M-H)- (M+HCOO)- (M+CH3COO)-	8.284		290.0857		FBF	49.52		49.52
(−)-Epicatechin	C15H14O6	(M-H)- (M+HCOO)- (M+CH3COO)-	8.284		290.0857		FBF	49.52		49.52
L-(−)-Catechin	C15H14O6	(M-H)- (M+HCOO)- (M+CH3COO)-	8.284		290.0857		FBF	49.52		49.52

Cpd.53:D-(+)-Catechin

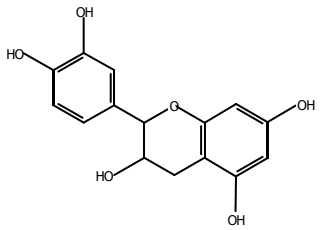
Name	Formula	RT	RI	MassDiff(Tgt,ppm)	CAS	ID Source	Score	Algorithm
D-(+)-Catechin	C15H14O6	30.680		290.0797	2.12	FBF	52.13	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-	289.0730	52.13				

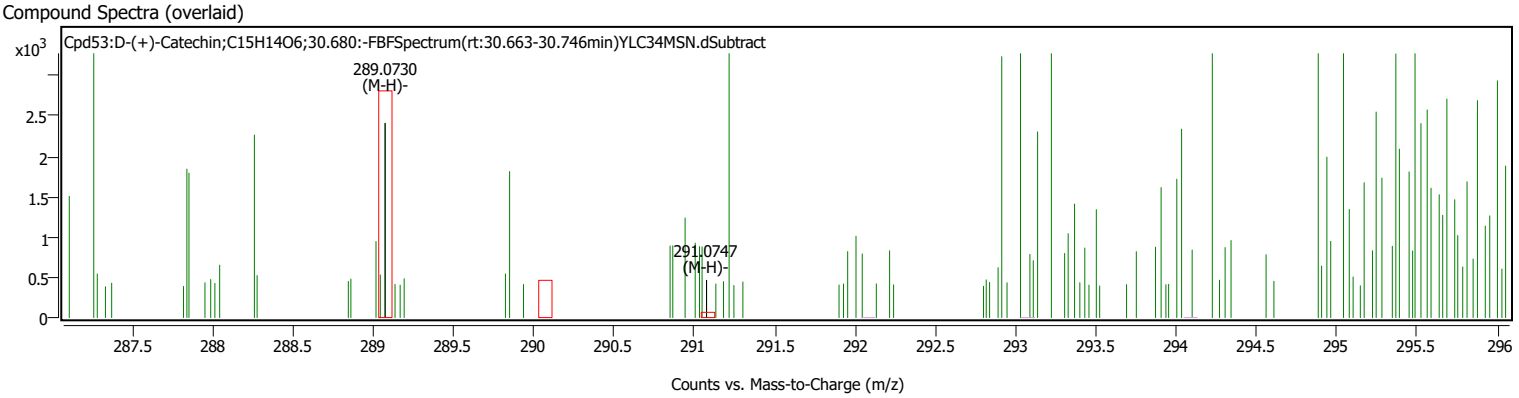
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

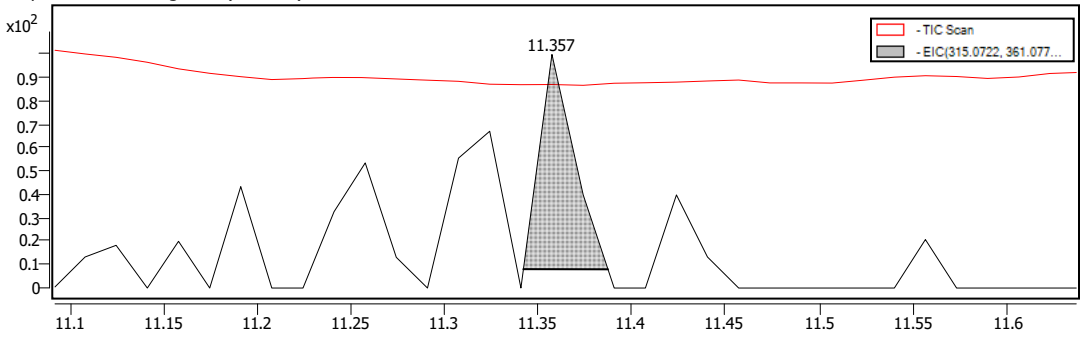
Name	Formula	Species	RT	RTDiff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
D-(+)-Catechin	C15H14O6	(M-H)-	30.680		290.0797		FBF	52.13		52.13
(−)-Epicatechin	C15H14O6	(M-H)-	30.680		290.0797		FBF	52.13		52.13
L-(−)-Catechin	C15H14O6	(M-H)-	30.680		290.0797		FBF	52.13		52.13

Cpd.54:Protocatechuic acid-4-glucoside

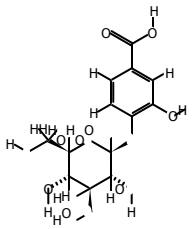
Name	Formula	RT	RI	Mass Dif f(Tgt, ppm)	CAS	ID Source	Score	Algorithm
Protocatechuic acid-4-glucoside	C13H16O9	11.357		316.0784	-3.17	FBF	71.77	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+CH3COO)-	315.0717375.0930	71.77				

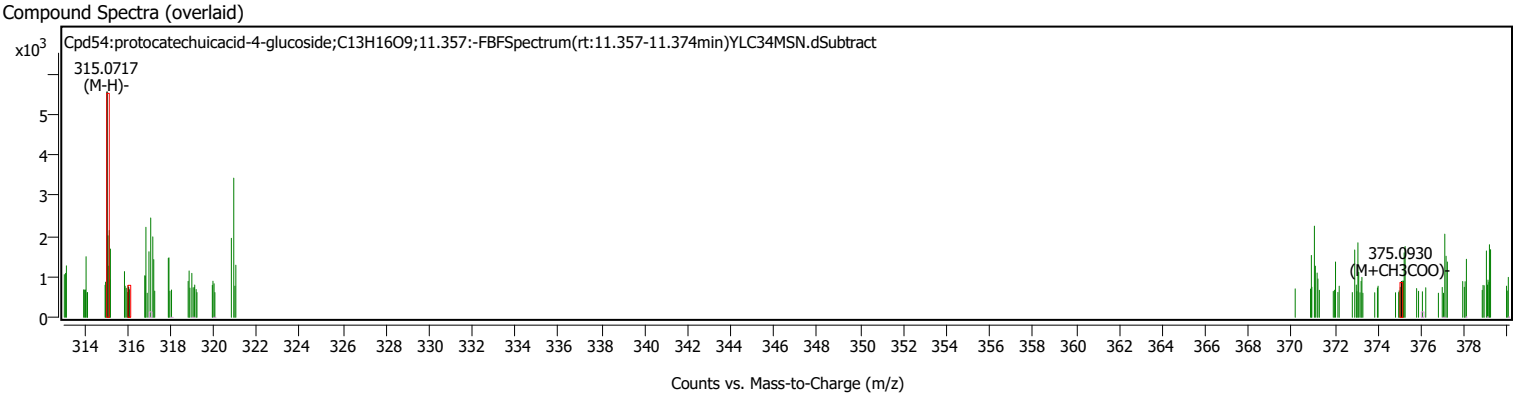
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

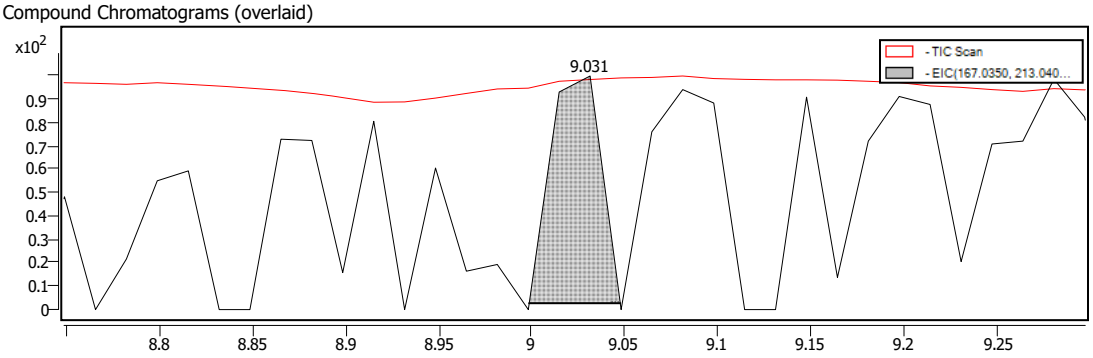
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Protocatechuic acid-4-glucoside	C13H16O9	(M-H)- (M+CH3COO)-	11.357		316.0784		FBF	71.77		71.77

Cpd.55:vanilic acid

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
vanilicacid	C8H8O4	9.031		168.0457 20.23		FBF	44.30	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+CH3COO)-	227.0602	44.30				

Compound Chromatograms (overlaid)



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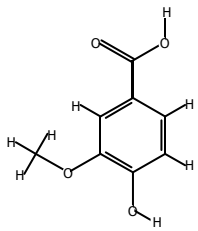
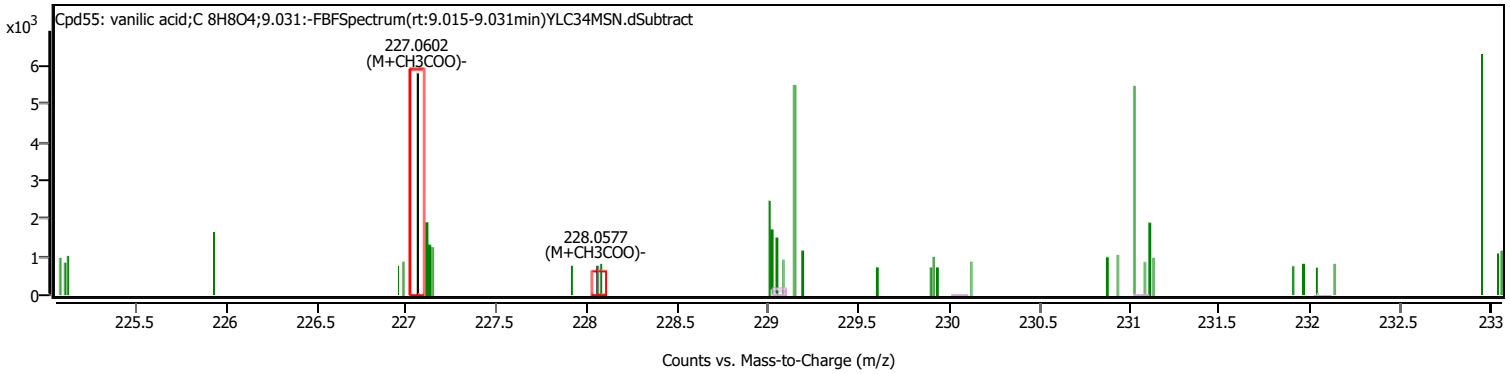


Compound Spectra (overlaid)



Compound ID Table

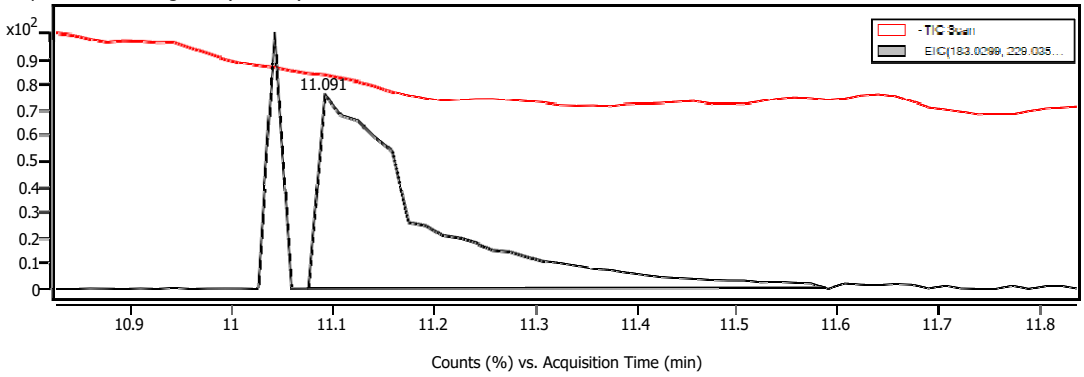
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
vanilicacid	C8H8O4	(M+CH3COO)-	9.031		168.0457		FBF	44.30		44.30

Cpd.56:Methylgallate

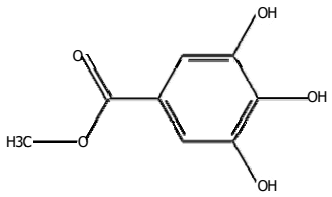
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Methylgallate	C8H8O5	11.091		184.0333 -20.87		FBF	46.51	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	183.0261229.0390 243.0524	46.51				

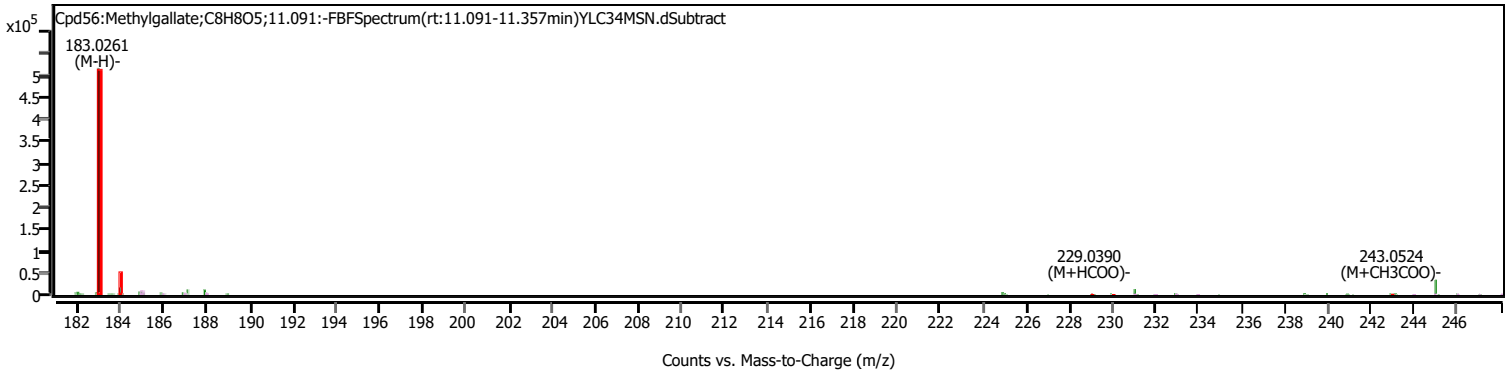
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Methylgallate	C8H8O5	(M-H)- (M+HCOO)- (M+CH3COO)-	11.091		184.0333		FBF	46.51		46.51

Cpd.57:Ellagic acid

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Ellagic acid	C14H6O8	23.519		302.0066 1.20		FBF	83.65	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+HCOO)-	347.0049	83.65				

TargetScreeningReport

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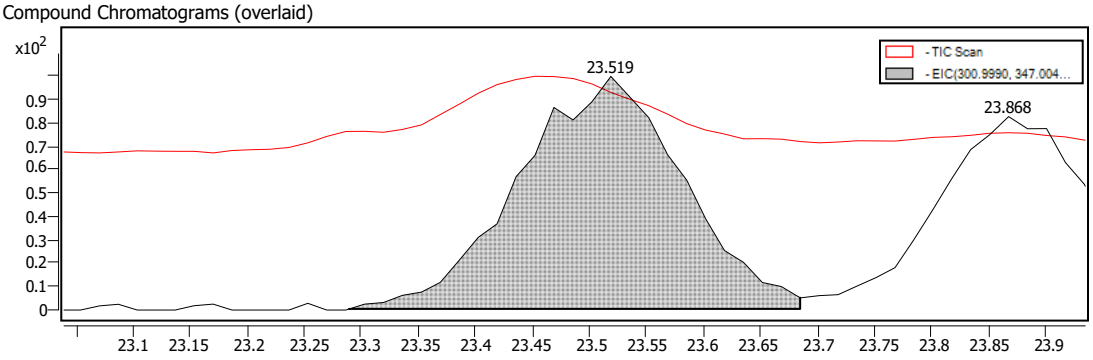
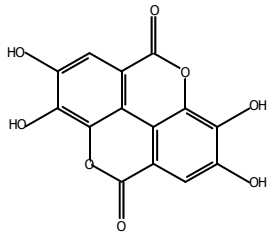
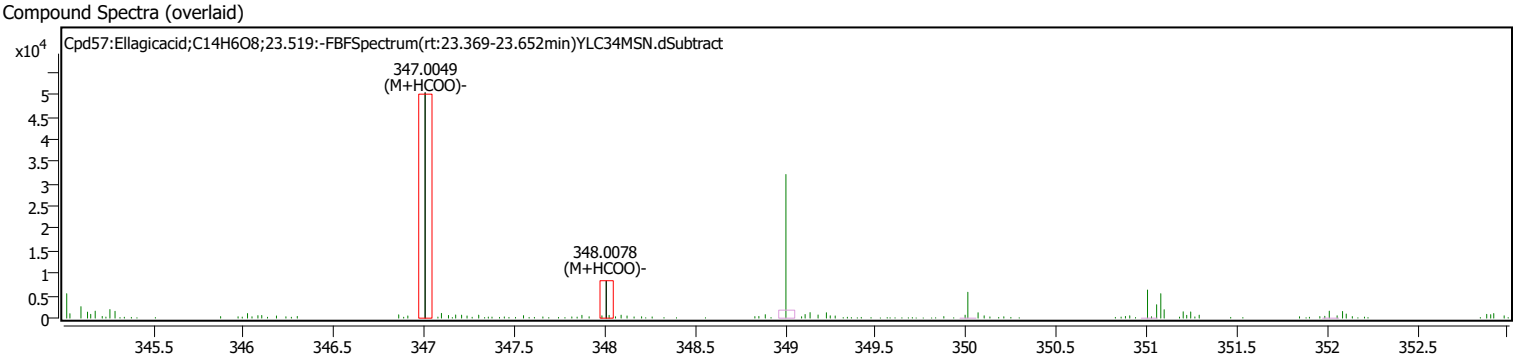
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

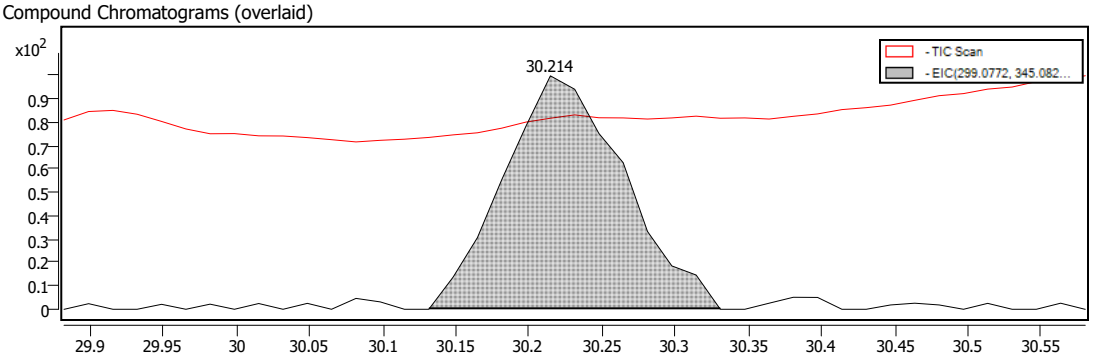
Name	Formula	Species	RT	RTDiff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Ellagicacid	C14H6O8	(M+HCOO)-	23.519		302.0066		FBF	83.65		83.65

Cpd.58:salicylicacidglucoside

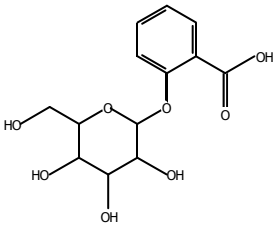
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
salicylicacidglucoside	C13H16O8	30.214		300.0906 20.24		FBF	50.16	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)-	299.0847345.0891	50.16				
(M+CH3COO)-	359.1048					

Compound Chromatograms (overlaid)



Structure



TargetScreeningReport

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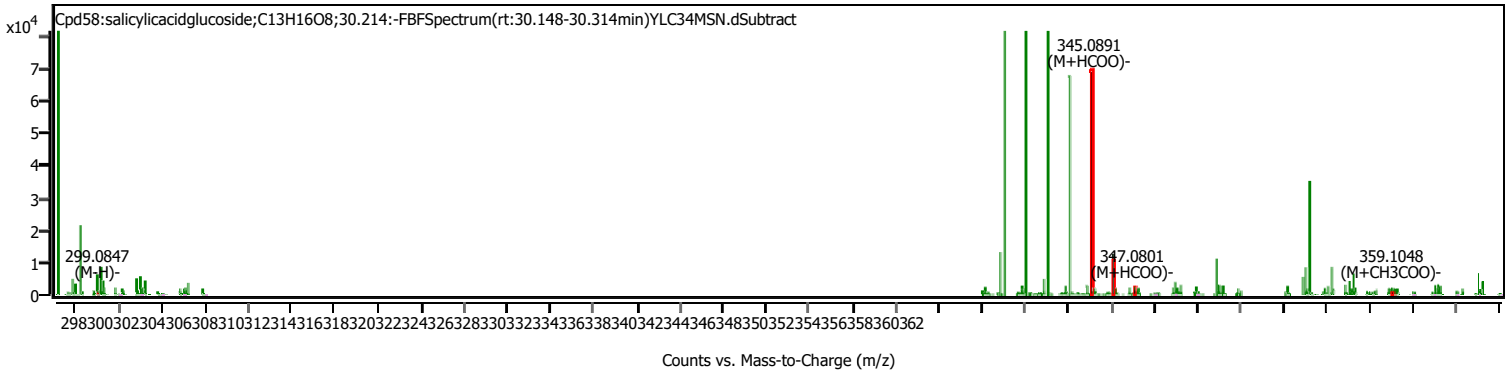
Compound Spectra (overlaid)



Compound ID Table

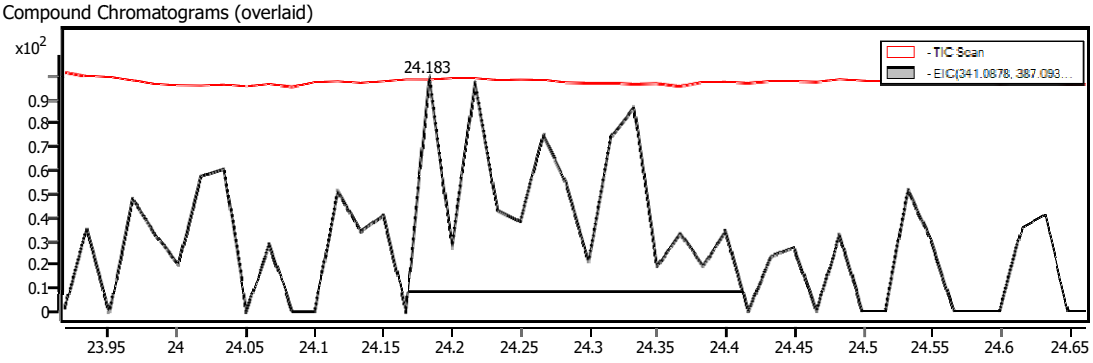
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
salicylic acid glucoside	C13 H16 O8	(M-H)- (M+HCOO)- (M+CH3COO)-	30.214		300.0906		FBF	50.16		50.16

Cpd.59:1-o-Caffeoylglucose

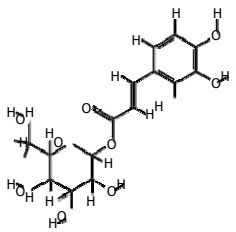
Name	Formula	RT	RI	MassDiff	(Tgt,ppm)	CAS	ID Source	Score	Algorithm
1-o-Caffeoylglucose	C15H18O9	24.183		342.0923	-8.05		FBF	69.00	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	341.0848387.0828 401.1119	69.00				

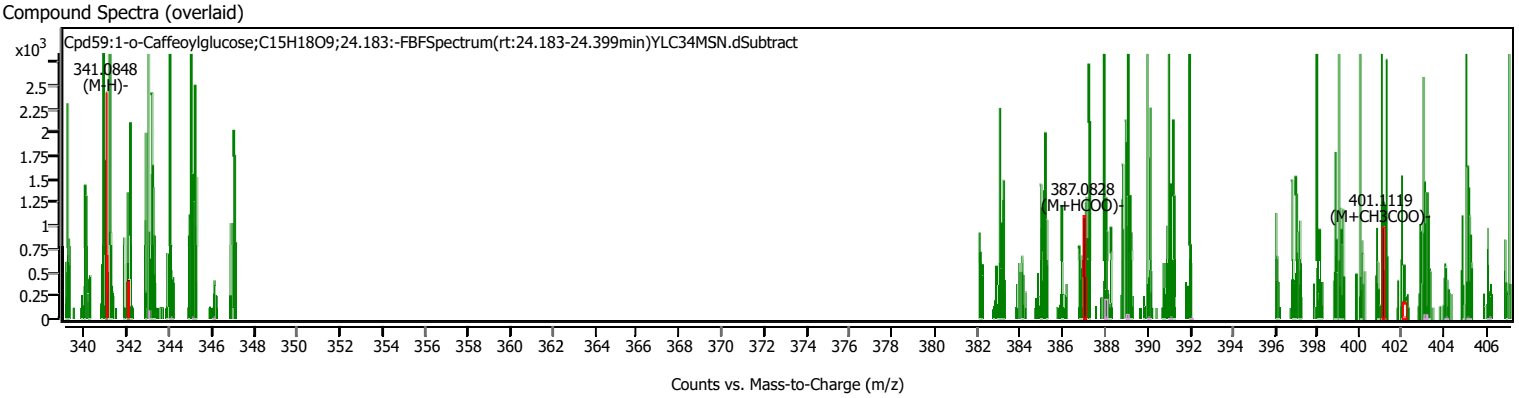
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
1-o-Caffeoylglucose	C15 H18 O9	(M-H)- (M+HCOO)- (M+CH3COO)-	24.183		342.0923		FBF	69.00		69.00

Cpd.60:Isopimpinellin

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Isopimpinellin	C13H10O5	28.902		246.0526 -0.93		FBF	47.43	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+HCOO)-	291.0508	47.43				

TargetScreeningReport

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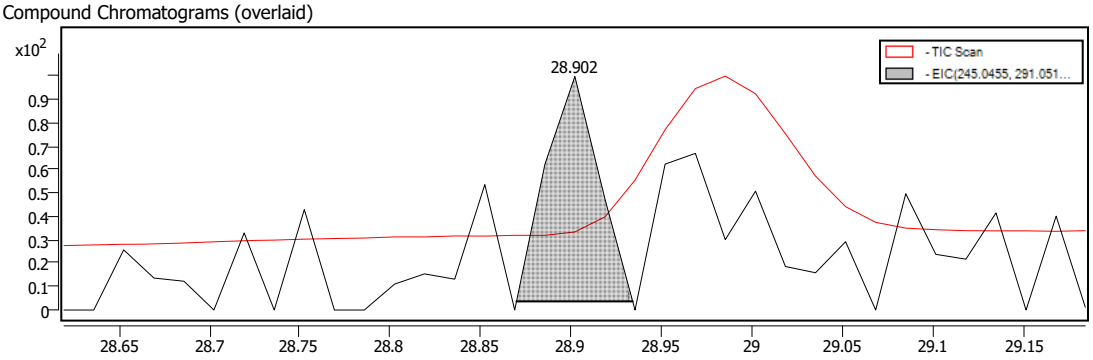
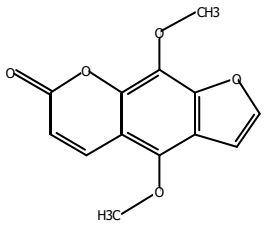
Compound Chromatograms (overlaid)

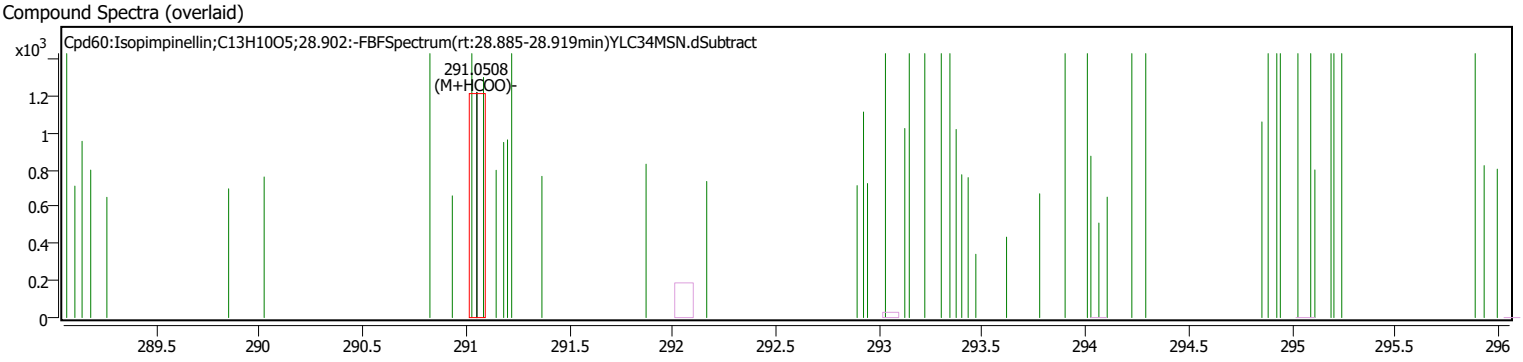


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



Counts vs. Mass-to-Charge (m/z)

Compound ID Table

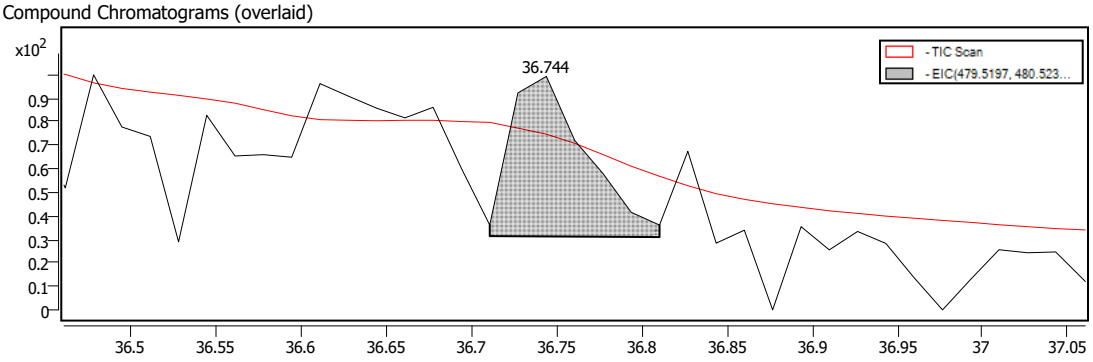
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Isopimpinellin	C13H10O5	(M+HCOO)-	28.902		246.0526		FBF	47.43		47.43

Cpd.61:1-Tritriacontanol

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
1-Tritriacontanol	C33H68O	36.744		480.5277 1.46		FBF	61.81	FBF

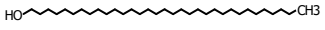
Species	m/z	Score(Tgt)	Score(Lib)	Score(DB)	Score(MFG)	Score(RT)
(M+HCOO)-	525.5262539.5467	61.81				
(M+CH3COO)-						

Compound Chromatograms (overlaid)

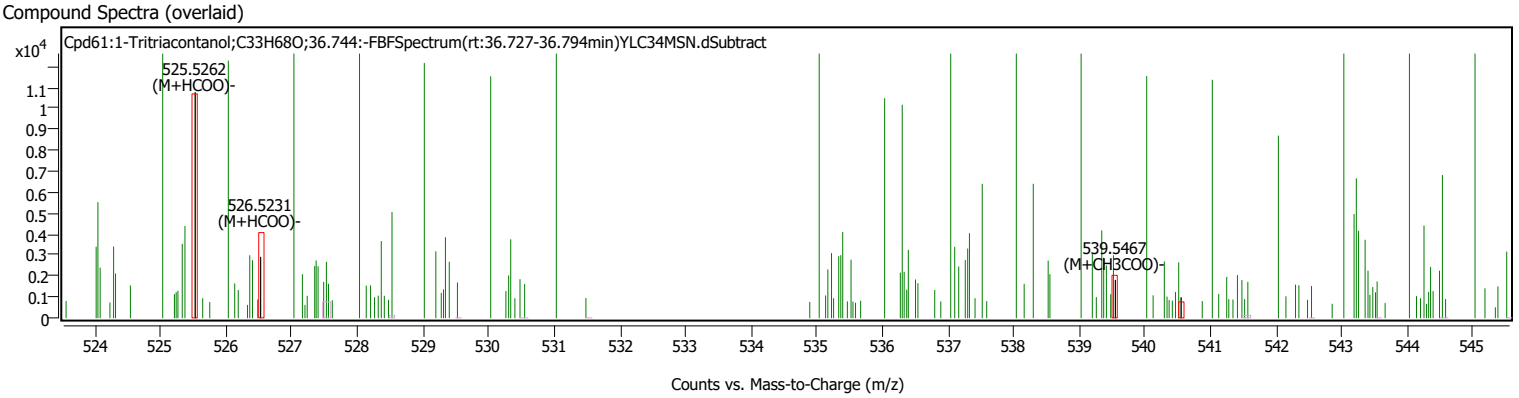


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



Compound ID Table

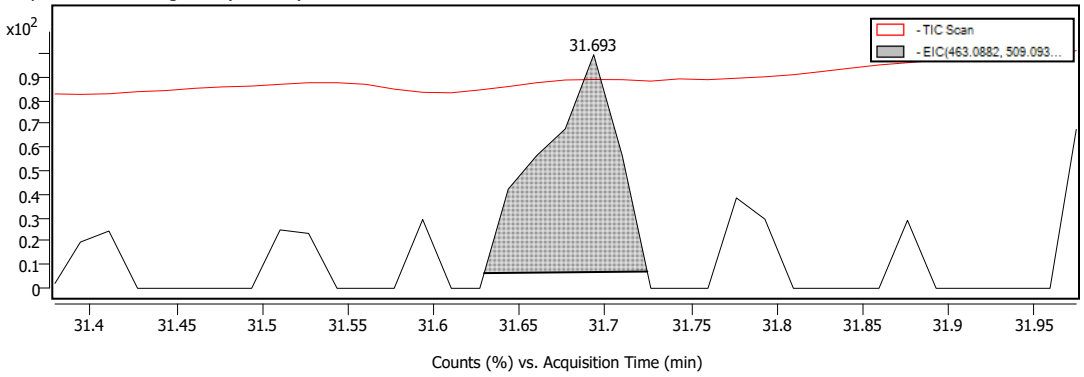
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
1-Tritriacontanol	C33H68O	(M+HCOO)- (M+CH3COO)-	36.744		480.5277		FBF	61.81		61.81

Cpd.62:Hirsutrin

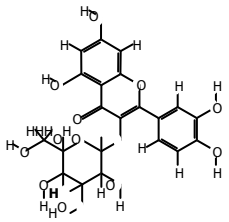
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Hirsutrin	C21H20O12	31.693		464.0940	-3.18	FBF	53.56	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+HCOO)-	509.0919	53.56				

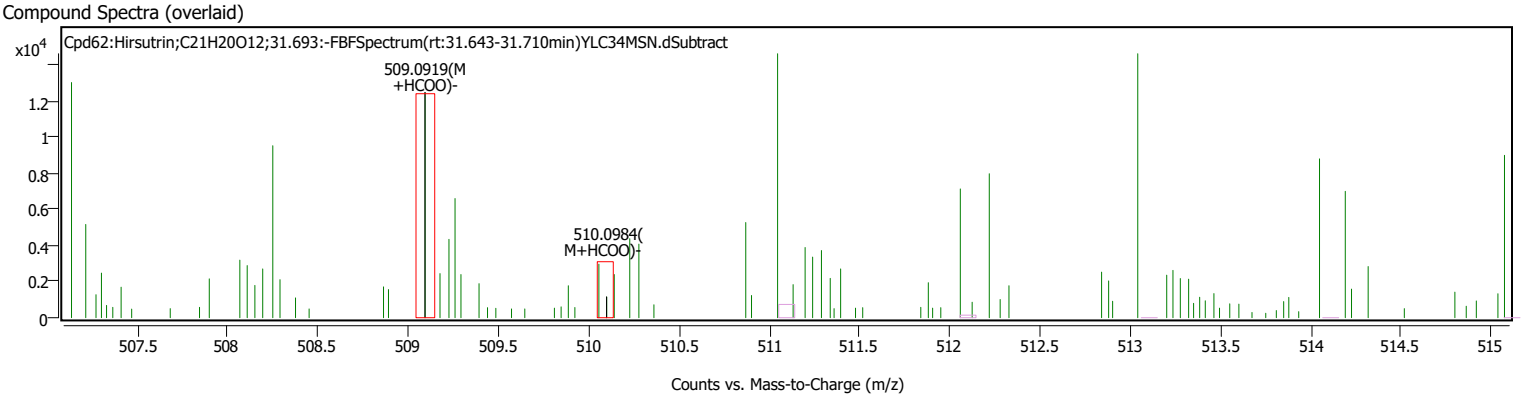
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Hirsutrin	C21H20O12	(M+HCOO)-	31.693		464.0940		FBF	53.56		53.56
isoquercetin	C21H20O12	(M+HCOO)-	31.693		464.0940		FBF	53.56		53.56

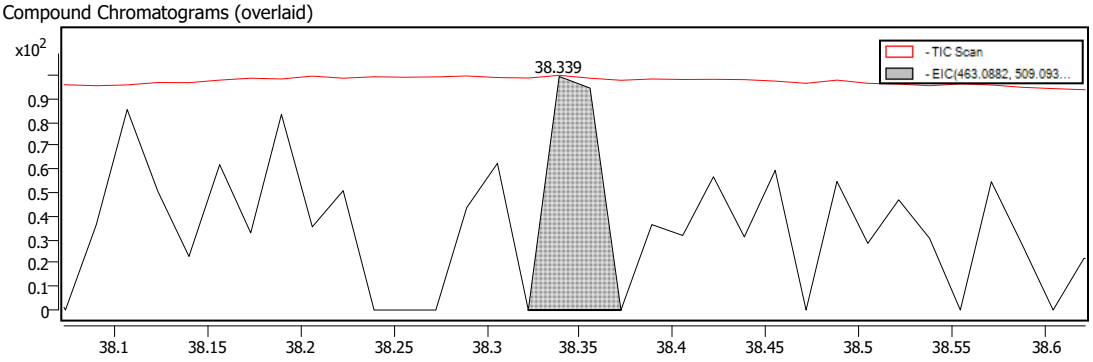
Cpd.63:Hirsutrin

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Hirsutrin	C21H20O12	38.339		464.0894	-13.01	FBF	51.62	FBF

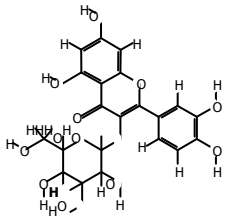
Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)-	463.0856509.0849	51.62				

TargetScreeningReport

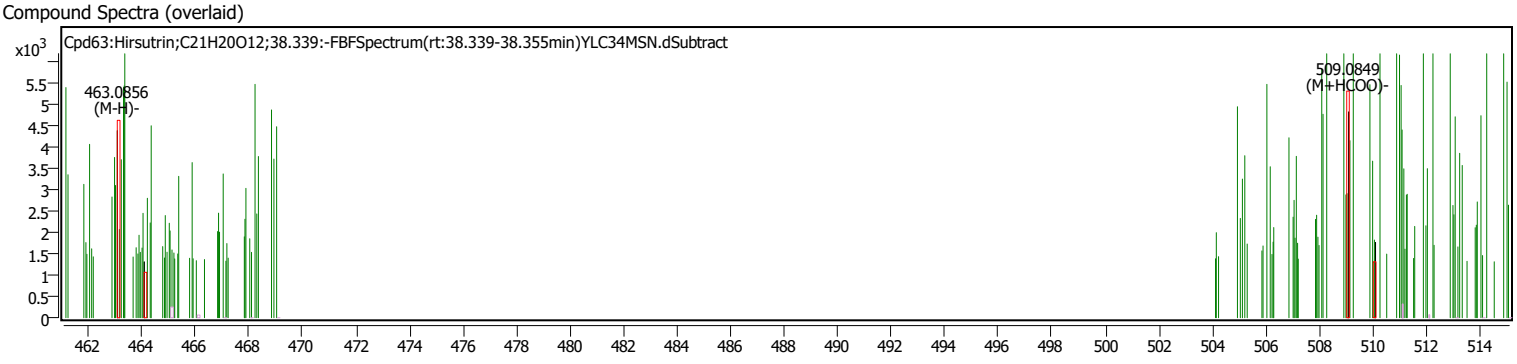
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

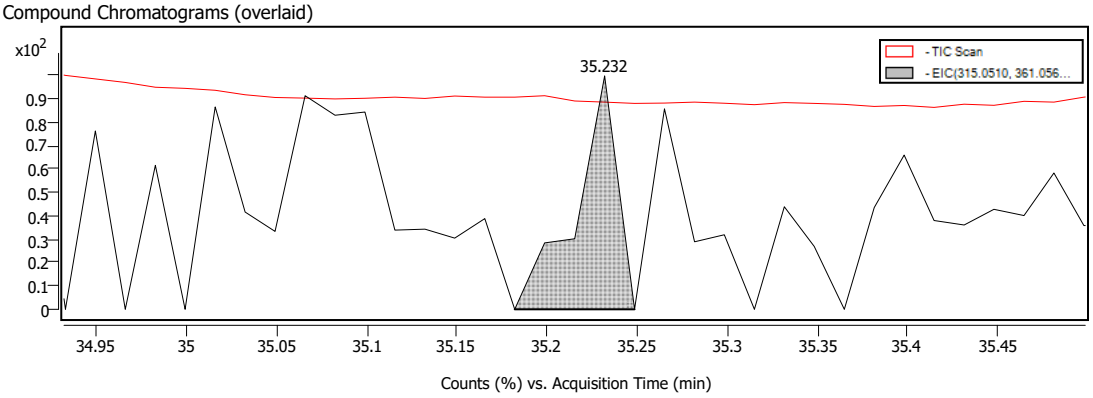
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Hirsutrin	C21 H20 O12	(M-H)- (M+HCOO)-	38.339		464.0894		FBF	51.62		51.62
isoquercetin	C21 H20 O12	(M-H)- (M+HCOO)-	38.339		464.0894		FBF	51.62		51.62

Cpd.64:Isorhamnetin

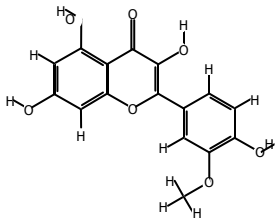
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Isorhamnetin	C16H12O7	35.232		316.0573 -3.02		FBF	58.17	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-	315.0528	58.17				

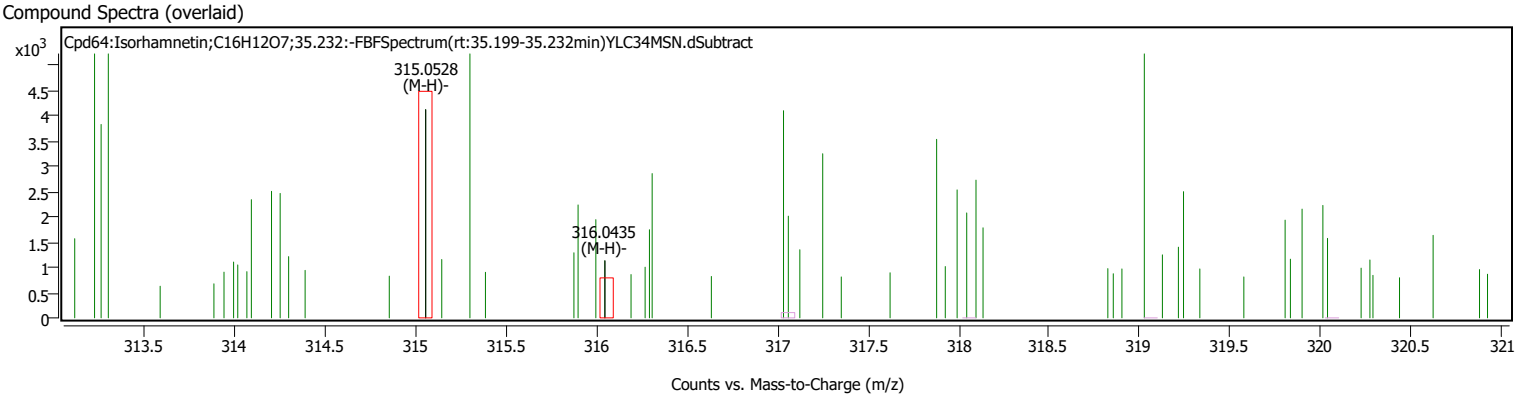
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

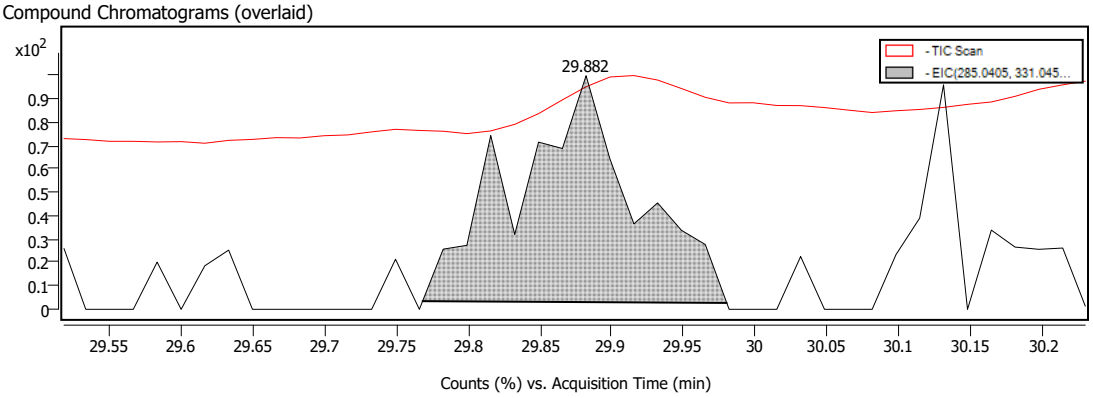
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Isorhamnetin	C16H12O7	(M-H)-	35.232		316.0573		FBF	58.17		58.17

Cpd.65:Kaempferol

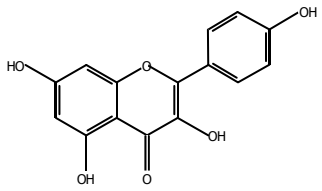
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Kaempferol	C15H10O6	29.882		286.0505 9.66		FBF	54.23	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-	285.0421	54.23				

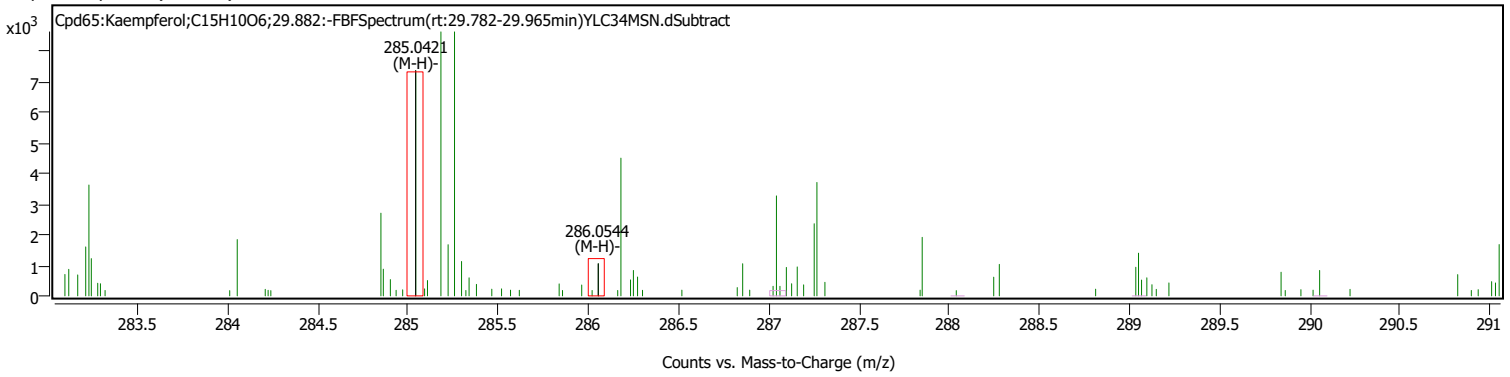
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

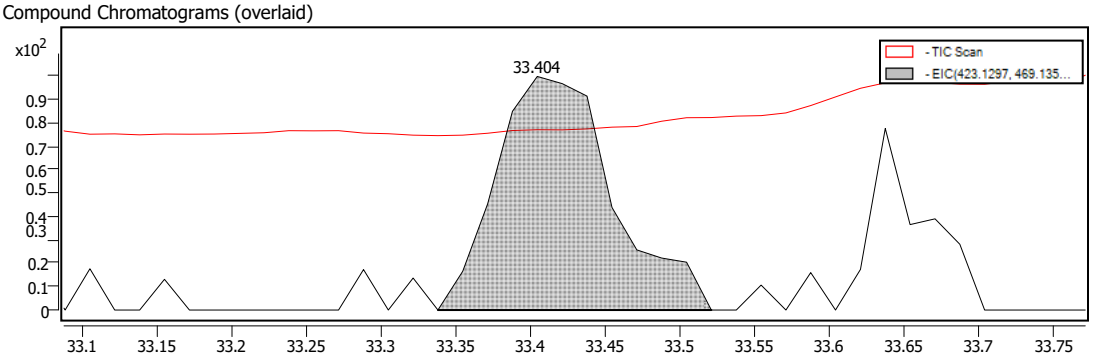
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Kaempferol	C15H10O6	(M-H)-	29.882		286.0505		FBF	54.23		54.23
Luteolin	C15H10O6	(M-H)-	29.882		286.0505		FBF	54.23		54.23

Cpd.66:Ginkgolide-B

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Ginkgolide-B	C20H24O10	33.404		424.1375 1.26		FBF	49.31	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-	423.1281	49.31				

Compound Chromatograms (overlaid)



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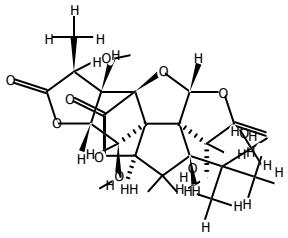
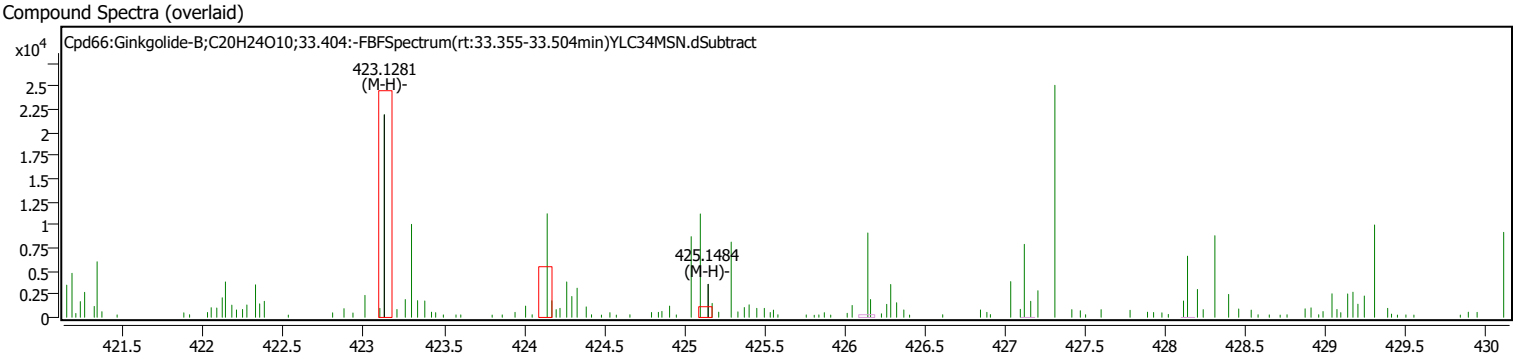


Compound Spectra (overlaid)



Compound ID Table

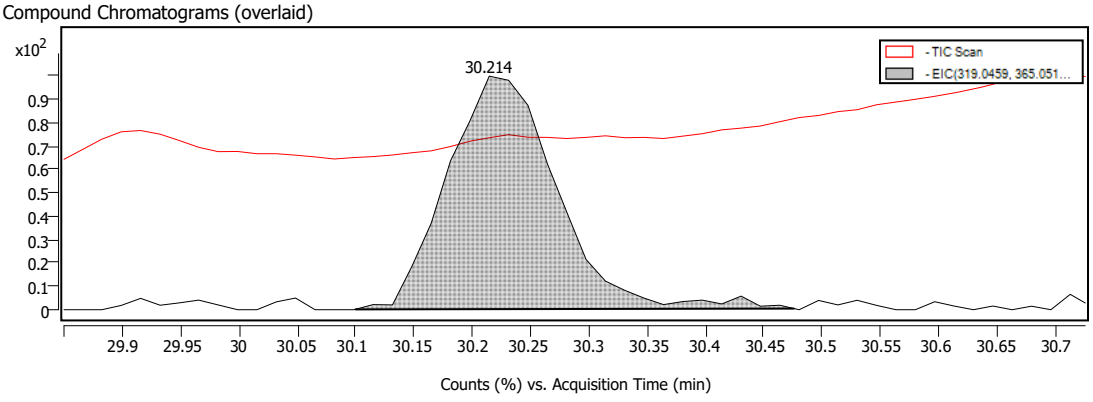
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Ginkgolide-B	C20H24O10	(M-H)-	33.404		424.1375		FBF	49.31		49.31

Cpd.67:Quercetin

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Quercetin	C15H12O8	30.214		320.0577	13.93	FBF	54.35	FBF

Species	m/z	Score(Tgt)	Score(Lib)	Score(DB)	Score(MFG)	Score(RT)
(M+HCOO)- (M+CH3COO)-	365.0498379.0722	54.35				

Compound Chromatograms (overlaid)



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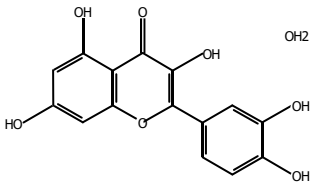
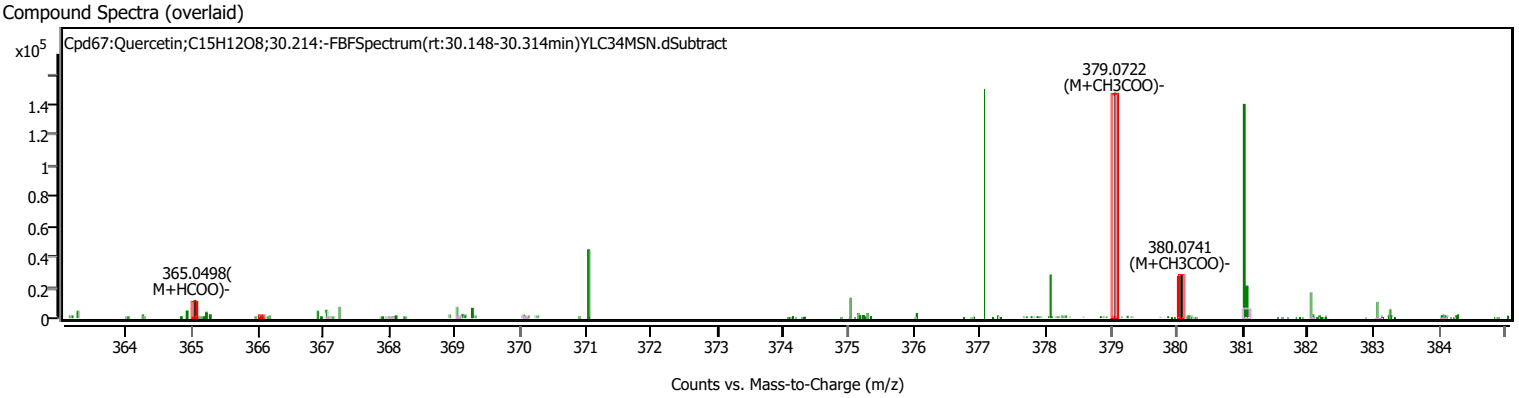


Compound Spectra (overlaid)



Compound ID Table

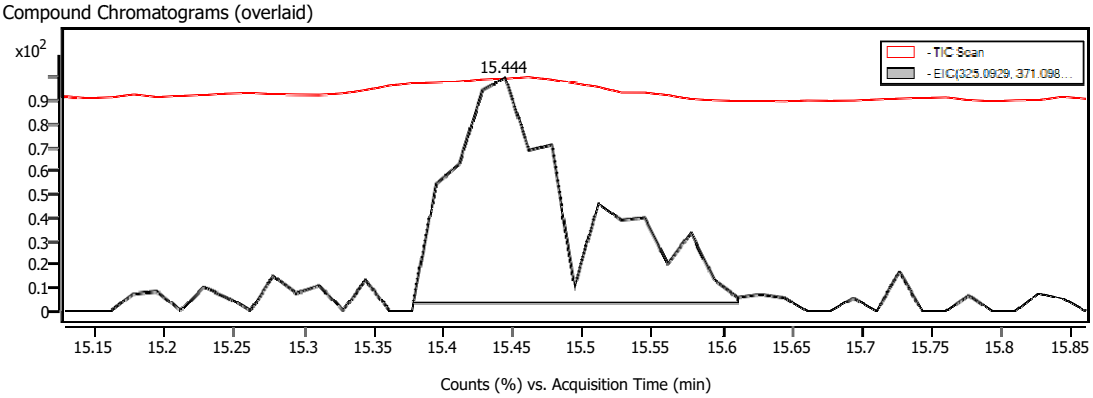
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Quercetin	C15H12O8	(M+HCOO)- (M+CH3COO)-	30.214		320.0577		FBF	54.35		54.35

Cpd.68:BILOBALIDE

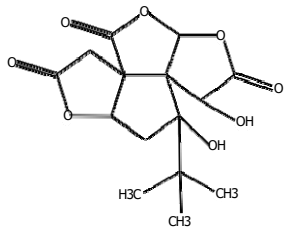
Name	Formula	RT	RI	MassDiff(Tgt,ppm)	CAS	ID Source	Score	Algorithm
BILOBALIDE	C15H18O8	15.444		326.0973 -8.94		FBF	43.09	FBF

Species	m/z	Score(Tgt)	Score(Lib)	Score(DB)	Score(MFG)	Score(RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	325.0886371.0936 385.1201	43.09				

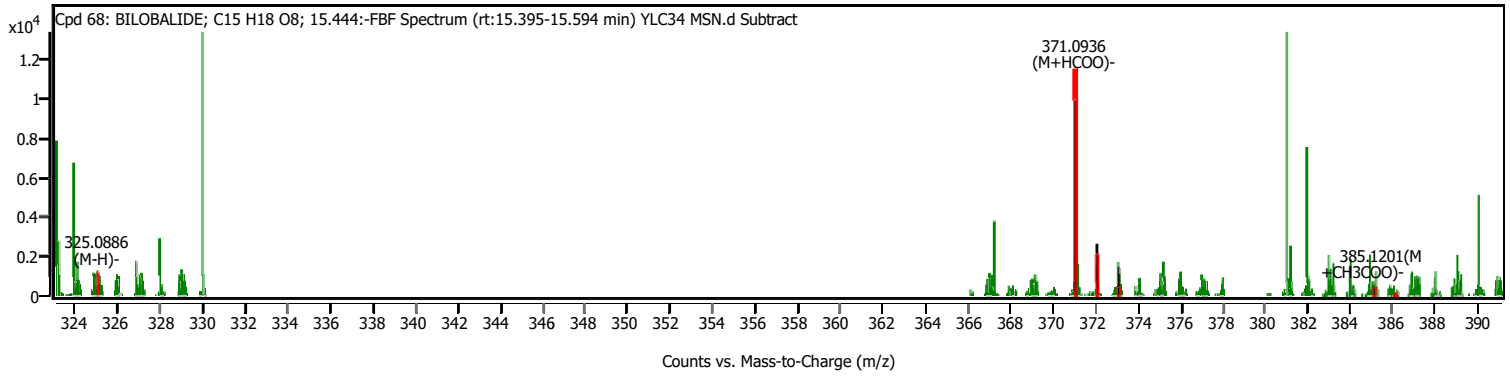
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
BILOBALIDE	C15 H18 O8	(M-H)- (M+HCOO)- (M+CH3COO)-	15.444		326.0973		FBF	43.09		43.09

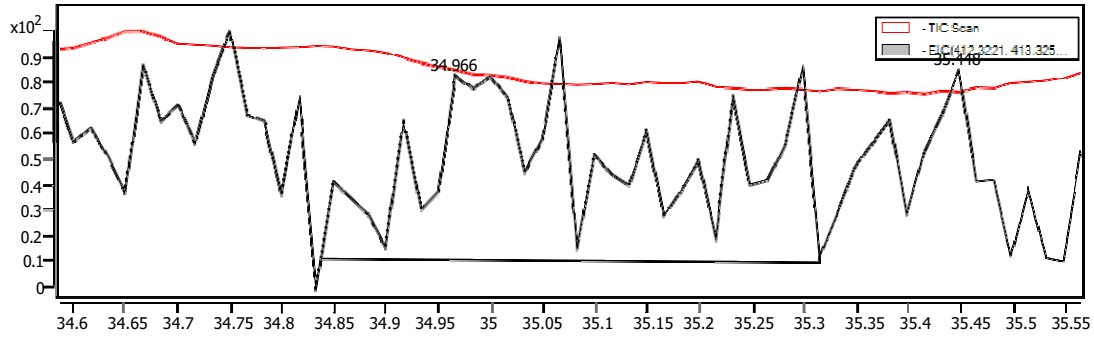
Cpd.69:Solanacarpidine

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Solanacarpidine	C27H43NO2	34.966		413.3251 -10.29		FBF	49.80	FBF

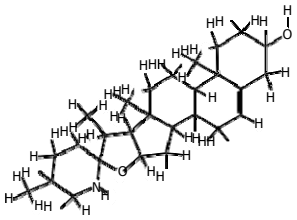
Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)-	412.3091458.3297	49.80				

TargetScreeningReport

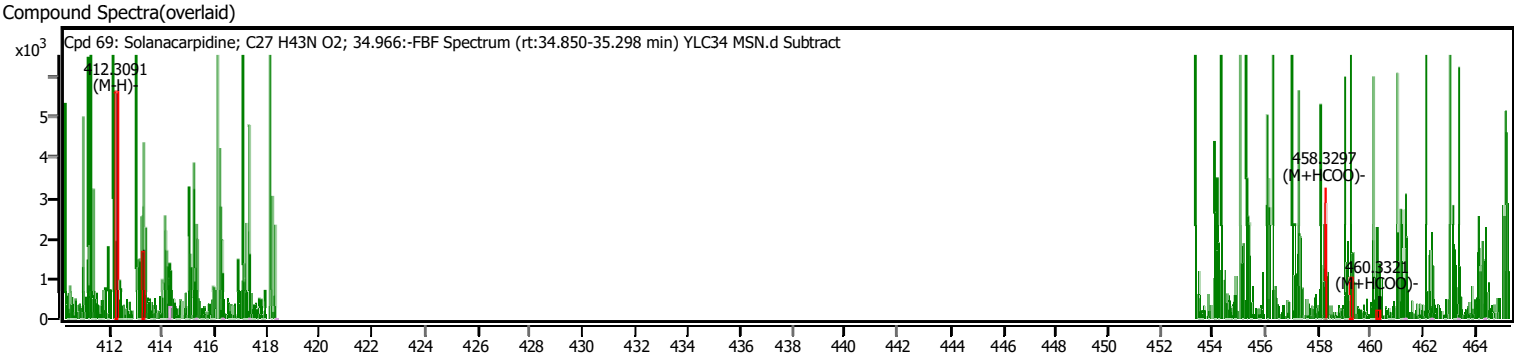
Compound Chromatograms (overlaid)



Structure



Compound Spectra(overlaid)



Compound ID Table

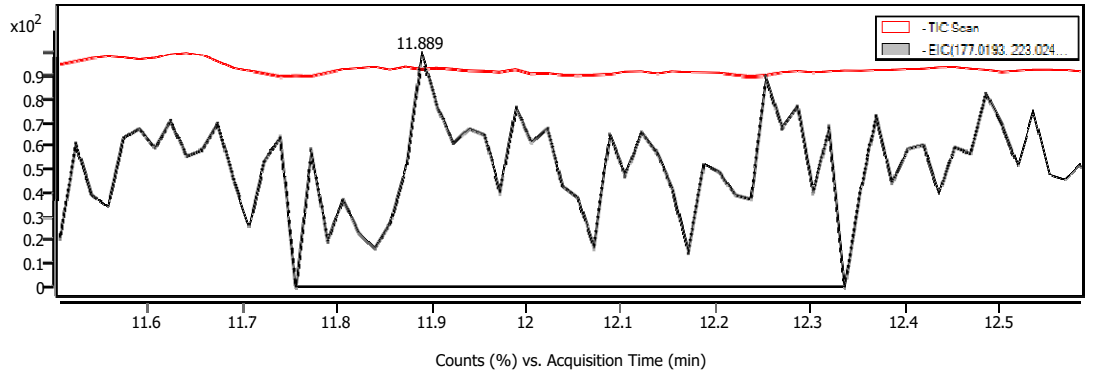
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Solanacarpidine	C27 H43 N O2	(M-H)- (M+HCOO)-	34.966		413.3251		FBF	49.80		49.80

Cpd.70:Asculetine

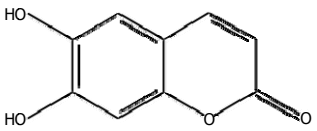
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Asculetine	C9H6O4	11.889		178.0257 -4.89		FBF	66.97	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	177.0160223.0258 237.0535	66.97				

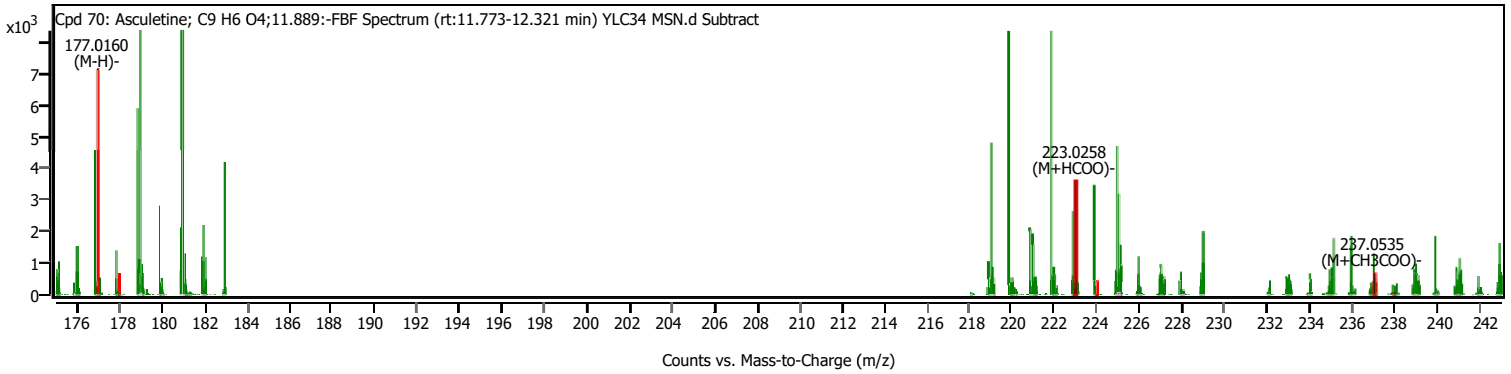
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

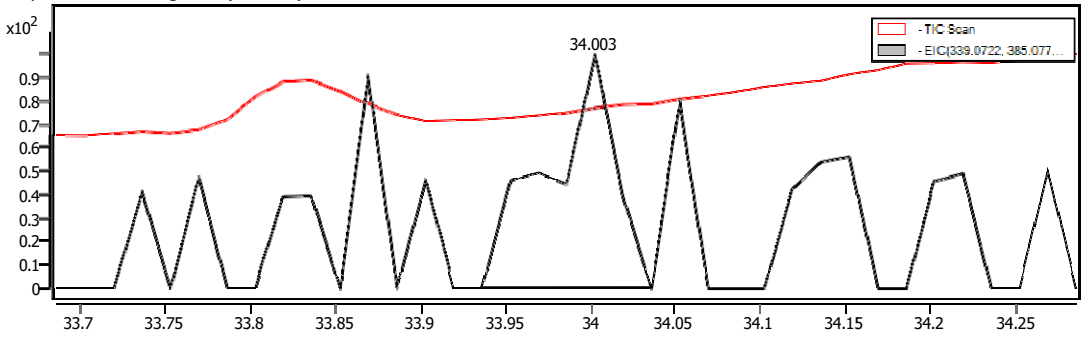
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Asculetine	C9H6O4	(M-H)- (M+HCOO)- (M+CH3COO)-	11.889		178.0257		FBF	66.97		66.97

Cpd.71:Aesculin

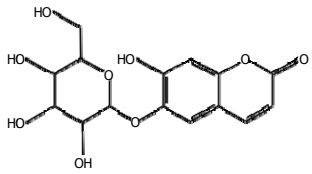
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)		CAS	ID Source	Score	Algorithm
Aesculin	C15H16O9	34.003		340.0779	-4.40		FBF	65.88	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+HCOO)-	385.0746	65.88				

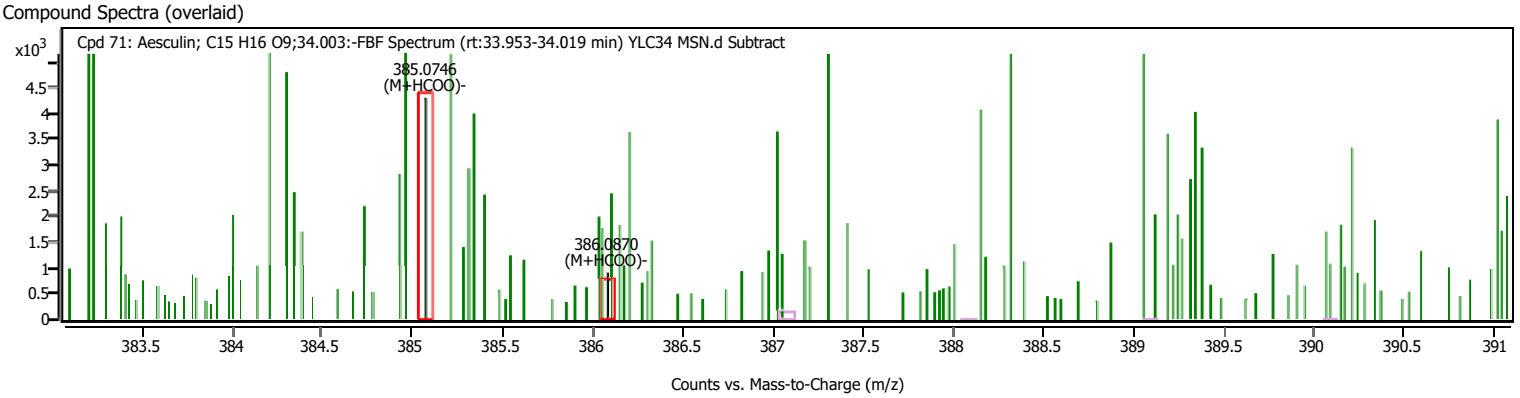
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Aesculin	C15H16O9	(M+HCOO)-	34.003		340.0779		FBF	65.88		65.88

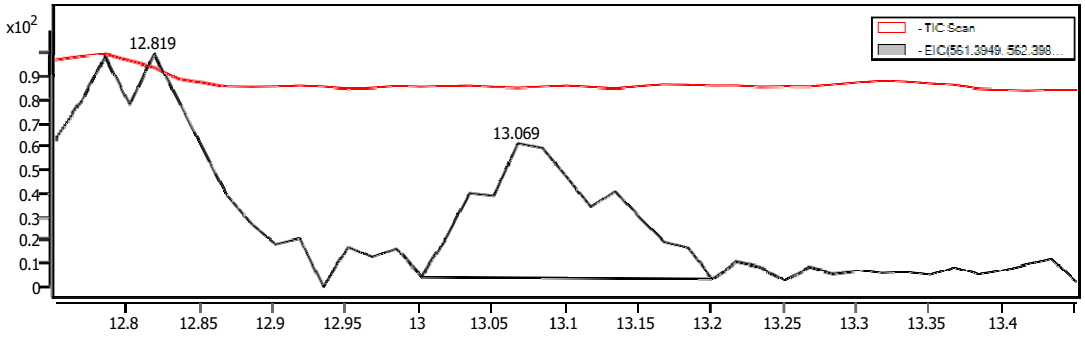
Cpd.72:carpesterol

Name	Formula	RT	RI	Mass Diff (Tgt, ppm)		CAS	ID Source	Score	Algorithm
carpesterol	C37H54O4	13.069		562.4098	13.41		FBF	62.37	FBF

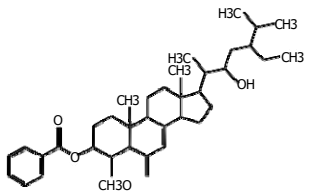
Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	561.3880607.4042 621.4250	62.37				

TargetScreeningReport

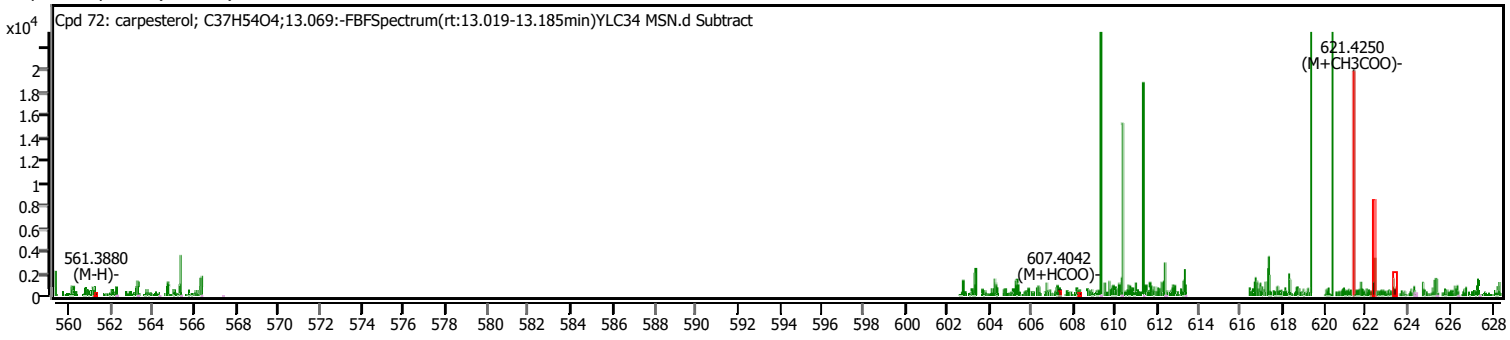
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

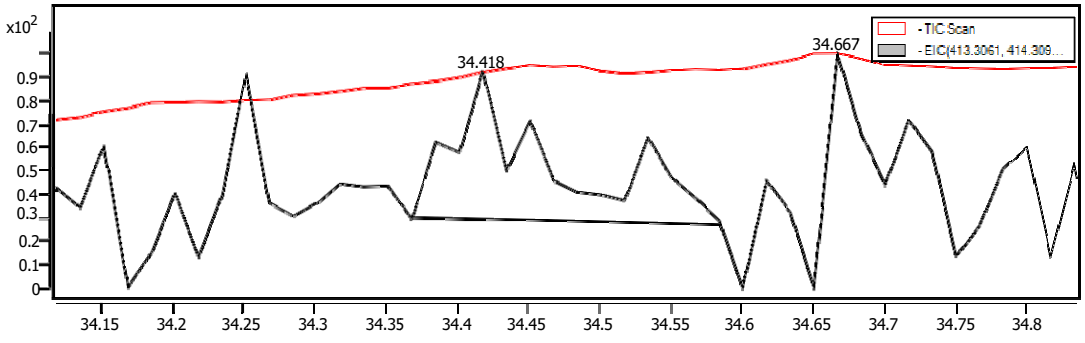
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
carpesterol	C37 H54 O4	(M-H)- (M+HCOO)- (M+CH3COO)-	13.069		562.4098		FBF	62.37		62.37

Cpd.73:Diosgenin

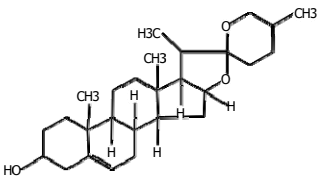
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Diosgenin	C27H42O3	34.418		414.3133	-0.25	FBF	70.73	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+CH3COO)-	413.3094473.3189	70.73				

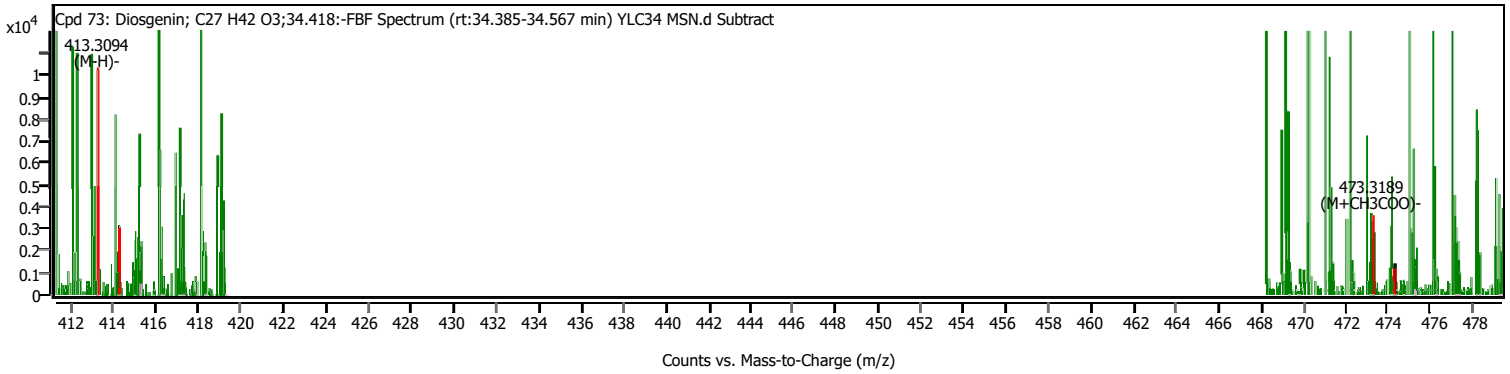
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

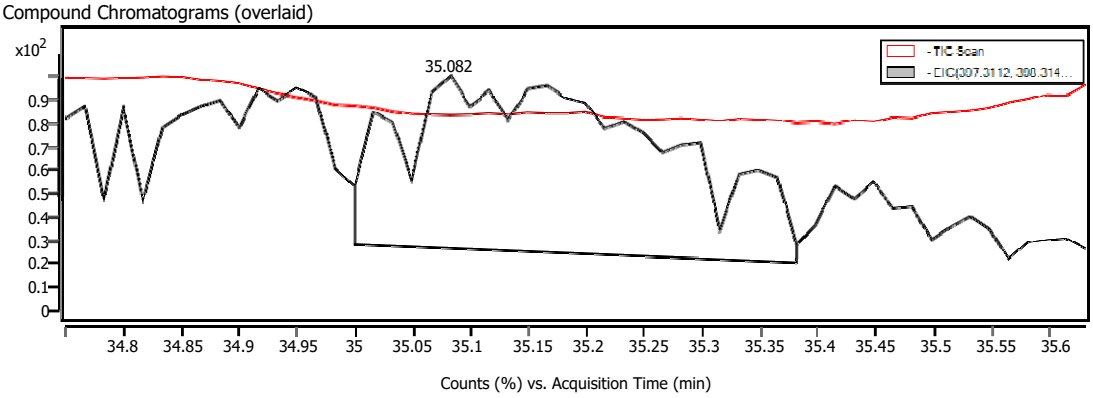
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Diosgenin	C27H42O3	(M-H)- (M+CH3COO)-	34.418		414.3133		FBF	70.73		70.73

Cpd.74:Diosgenin

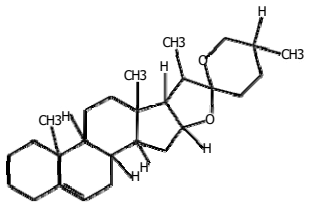
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Diosgenin	C27H42O2	35.082		398.3229	11.18	FBF	68.31	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)-	397.3234443.3165	68.31				

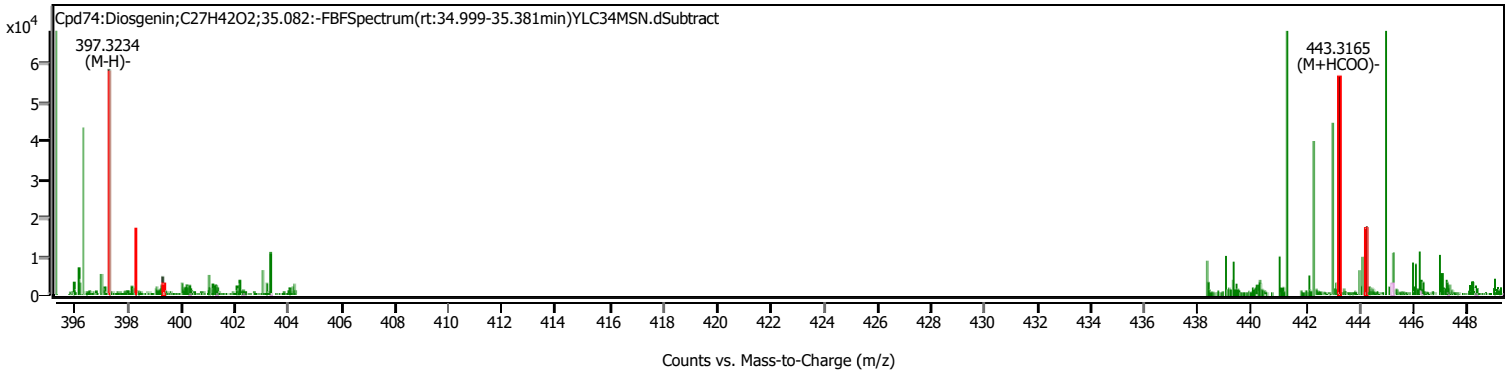
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

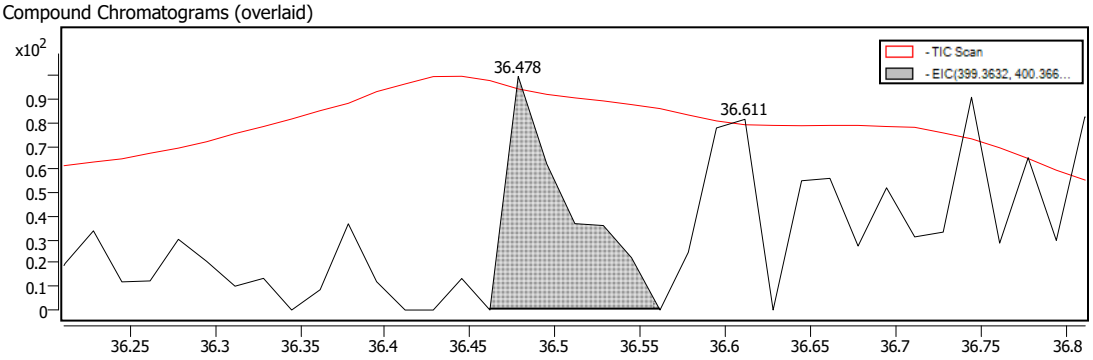
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Diosgenin	C27 H42 O2	(M-H)- (M+HCOO)-	35.082		398.3229		FBF	68.31		68.31

Cpd.75:Campesterol

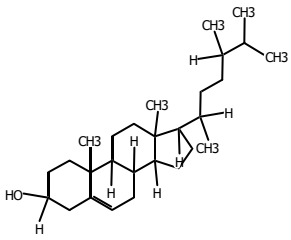
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Campesterol	C28H48O	36.478		400.3702	-0.67	FBF	57.32	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-	399.3614	57.32				

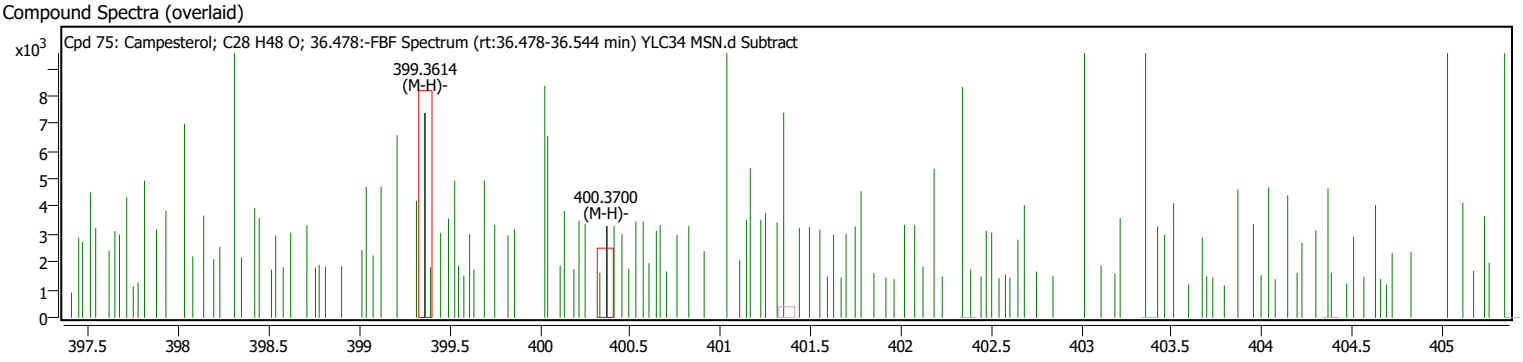
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound ID Table

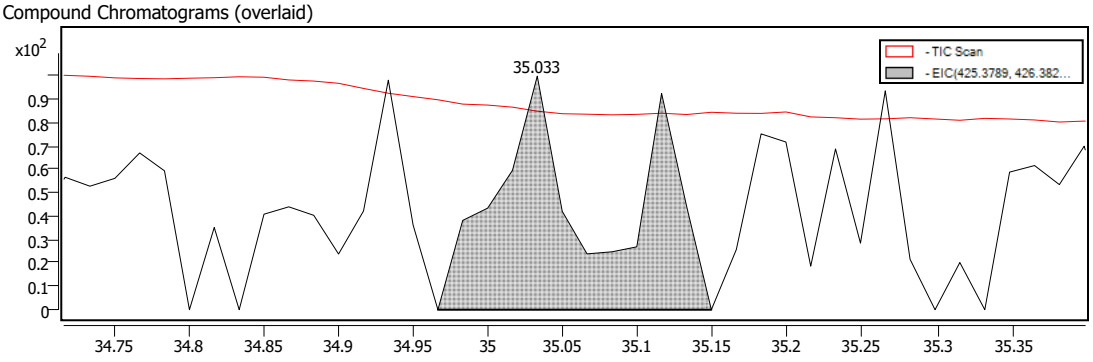
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Campesterol	C28H48O	(M-H)-	36.478		400.3702		FBF	57.32		57.32

Cpd. 76: cycloartenol

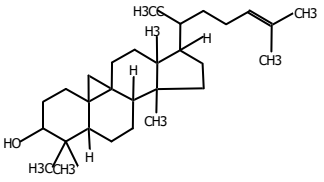
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
cycloartenol	C30H50O	35.033		426.3918	13.23	FBF	53.20	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M-H)-(M+HCOO)- (M+CH3COO)-	425.3958471.3946 485.3924	53.20				

Compound Chromatograms (overlaid)

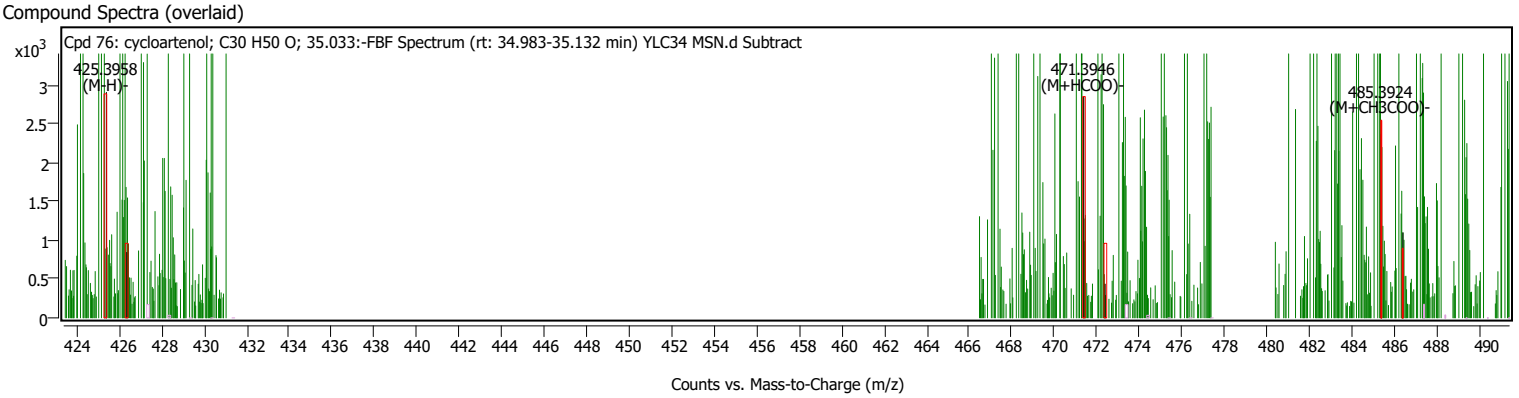


Structure



Target Screening Report

Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib) Score (Tgt)
cycloartenol	C30 H50 O	(M-H)- (M+HCOO)- (M+CH3COO)-	35.033		426.3918		FBF	53.20	53.20

Mass Hunter Qual
10.0(End of Report)