LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041223\
Data File : VU053667.D
Acq On : 12 Apr 2023 17:17
Operator : JC/MD
Sample : 02255-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AN5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Title : VOC Analysis

Signal : TIC: VU053667.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	103	rVB	111696	136436	17.40%	2.038%
2	1.909	169	177	195	rVB	80711	118884	15.16%	1.776%
3	2.562	368	380	393	rBV	165690	274988	35.07%	4.108%
4	2.694	416	421	423	rBV2	573	596	0.08%	0.009%
5	3.002	514	517	520	rBV	323	200	0.03%	0.003%
6	3.041	520	529	539	rVV4	3007	5567	0.71%	0.083%
7	3.240	588	591	595	rBV2	318	230	0.03%	0.003%
8	3.478	664	665	669	rBV2	244	133	0.02%	0.002%
9	3.999	822	827	830	rBV2	237	237	0.03%	0.004%
10	4.080	850	852	861	rVB2	359	338	0.04%	0.005%
11	4.121	863	865	868	rBV2	208	135	0.02%	0.002%
12	4.170	877	880	883	rBV	291	223	0.03%	0.003%
13	4.324	926	928	931	rBV	289	193	0.02%	0.003%
14	4.520	988	989	990	rBV	179	39	0.00%	0.001%
15	4.613	1006	1018	1046	rBV	64770	154825	19.74%	2.313%
16	5.057	1140	1156	1175	rBV2	145377	313429	39.97%	4.682%
17	5.430	1270	1272	1274	rBV	193	109	0.01%	0.002%
18	5.520	1295	1300	1309	rVB2	321	438	0.06%	0.007%
19	5.610	1327	1328	1329	rBV2	137	40	0.01%	0.001%
20	5.639	1334	1337	1339	rBV	282	184	0.02%	0.003%
21	5.719	1341	1362	1383	rBV2	288993	784142	100.00%	11.713%
22	5.864	1406	1407	1410	rVB	461	157	0.02%	0.002%
23	6.041	1458	1462	1464	rVB2	588	423	0.05%	0.006%
24	6.060	1465	1468	1470	rBV2	351	300	0.04%	0.004%
25	6.105	1479	1482	1489	rBV3	359	421	0.05%	0.006%
26	6.243	1511	1525	1542	rBV	291360	547998	69.89%	8.186%
27	6.449	1586	1589	1592	rBV	251	205	0.03%	0.003%
28	6.526	1606	1613	1622	rVB5	3366	5704	0.73%	0.085%
29	6.684	1649	1662	1684	rBV	178816	344037	43.87%	5.139%
30	6.922	1729	1736	1753	rBV	3393	6327	0.81%	0.095%
31	7.034	1757	1771	1784	rBV	50975	89968	11.47%	1.344%
32	7.192	1812	1820	1830	rVB5	1076	1666	0.21%	0.025%
33	7.308	1852	1856	1862	rBV2	255	274	0.03%	0.004%
34	7.417	1887	1890	1892	rBV2	213	134	0.02%	0.002%
35	7.465	1903	1905	1909	rVB2	310	234	0.03%	0.003%
36	7.494	1910	1914	1916	rBV2	236	159	0.02%	0.002%

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Instrument :
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ClientSampleId :
C0AN5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Title : VOC Analysis

37	7.504	1916	1917	1921	rVB2	251	90	0.01%	0.001%
38	7.562	1923	1935	1960	rBV	97962	178047	22.71%	2.660%
39	7.694	1971	1976	1979	rBV4	912	1069	0.14%	0.016%
40	7.732	1980	1988	2000	rVV3	15030	24058	3.07%	0.359%
41	7.893	2024	2038	2063	rBV	381532	658635	83.99%	9.838%
42	8.173	2111	2125	2143	rBV2	72938	135838	17.32%	2.029%
43	8.321	2169	2171	2175	rBV2	266	206	0.03%	0.003%
44	8.462	2205	2215	2227	rVB2	18872	30575	3.90%	0.457%
45	8.549	2235	2242	2244	rBV4	1964	2428	0.31%	0.036%
46	8.626	2256	2266	2288	rBV	206506	365864	46.66%	5.465%
47	8.722	2291	2296	2315	rVB	27892	41732	5.32%	0.623%
48	8.832	2323	2330	2343	rVB	9979	15879	2.03%	0.237%
49	9.005	2381	2384	2388	rBV2	286	278	0.04%	0.004%
50	9.057	2399	2400	2401	rBV	191	66	0.01%	0.001%
51	9.150	2427	2429	2430	rBV	225	65	0.01%	0.001%
52	9.208	2437	2447	2465	rVB	49293	78130	9.96%	1.167%
53	9.359	2491	2494	2498	rBV4	956	986	0.13%	0.015%
54	9.414	2499	2511	2535	rVB	402378	672006	85.70%	10.038%
55	9.600	2568	2569	2570	rBV	279	85	0.01%	0.001%
56	9.639	2578	2581	2586	rVB	670	482	0.06%	0.007%
57	9.677	2586	2593	2594	rBV2	349	344	0.04%	0.005%
58	9.890	2657	2659	2663	rBV	207	133	0.02%	0.002%
59	9.922	2664	2669	2680	rVB3	1067	1330	0.17%	0.020%
60	10.073	2708	2716	2726	rVB3	2493	3754	0.48%	0.056%
61	10.230	2760	2765	2768	rVB2	273	279	0.04%	0.004%
62	10.256	2769	2773	2778	rBV2	325	301	0.04%	0.004%
63	10.279	2778	2780	2783	rBV	196	86	0.01%	0.001%
64	10.587	2874	2876	2877	rBV	155	50	0.01%	0.001%
65	10.674	2902	2903	2904	rBV	219	67	0.01%	0.001%
66	10.751	2915	2927	2944	rBV	254748	408659	52.12%	6.104%
67	11.028	3008	3013	3015	rBV	358	334	0.04%	0.005%
68	11.340	3108	3110	3113	rBV	197	140	0.02%	0.002%
69	11.748	3234	3237	3243	rVB3	780	606	0.08%	0.009%
70	11.809	3243	3256	3273	rBV	424070	677829	86.44%	10.125%
71	12.002	3314	3316	3317	rBV	146	47	0.01%	0.001%
72	12.189	3362	3374	3394	rBV	369750	603720	76.99%	9.018%
73	12.716	3534	3538	3543	rBV	239	314	0.04%	0.005%
74	13.375	3740	3743	3745	rBV2	336	209	0.03%	0.003%
75	13.674	3833	3836	3841	rBV2	413	537	0.07%	0.008%

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C0AN5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Title : VOC Analysis

Sum of corrected areas: 6694631

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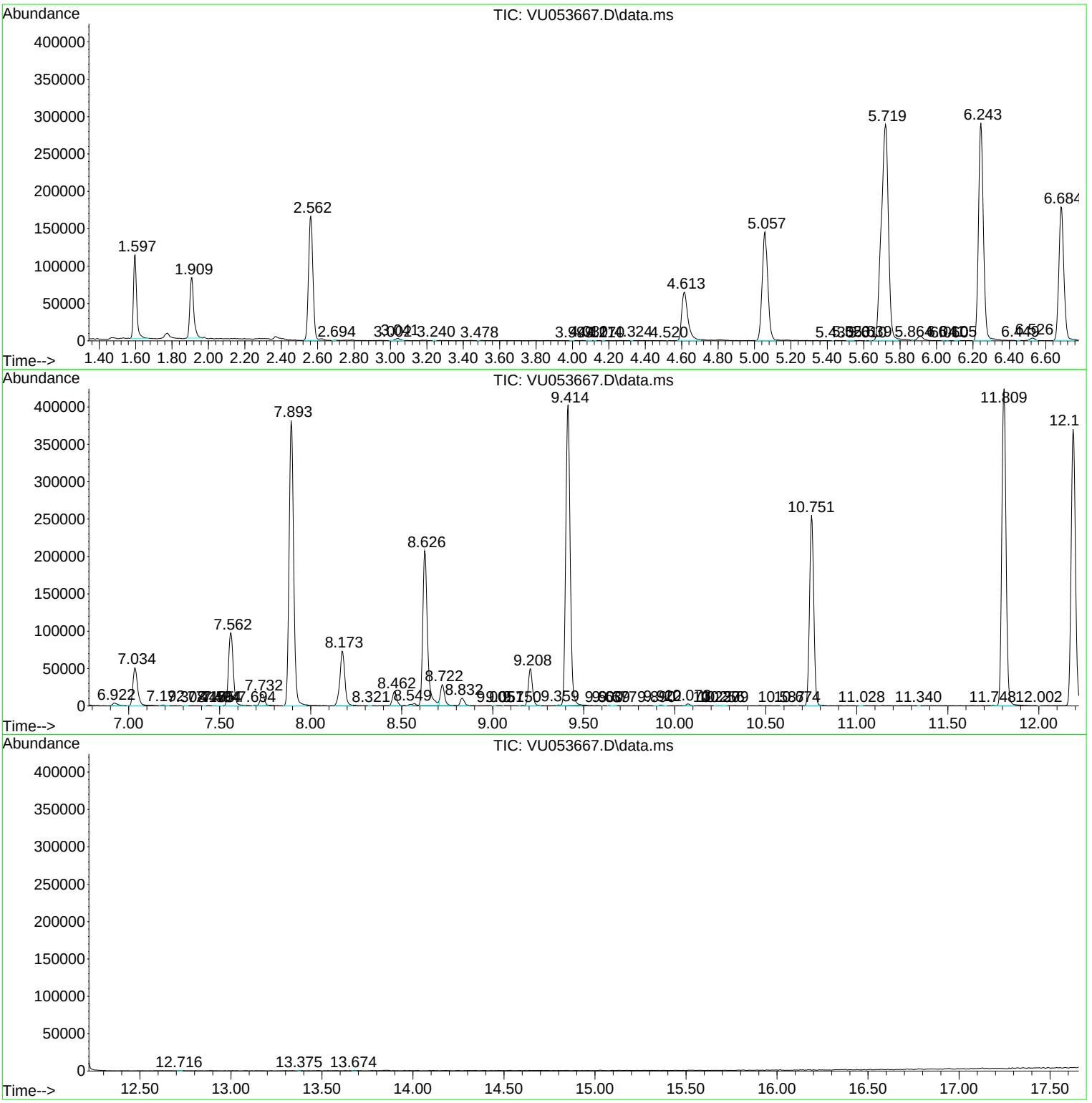
Instrument :
MSVOA_U
ClientSampleId :
C0AN5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

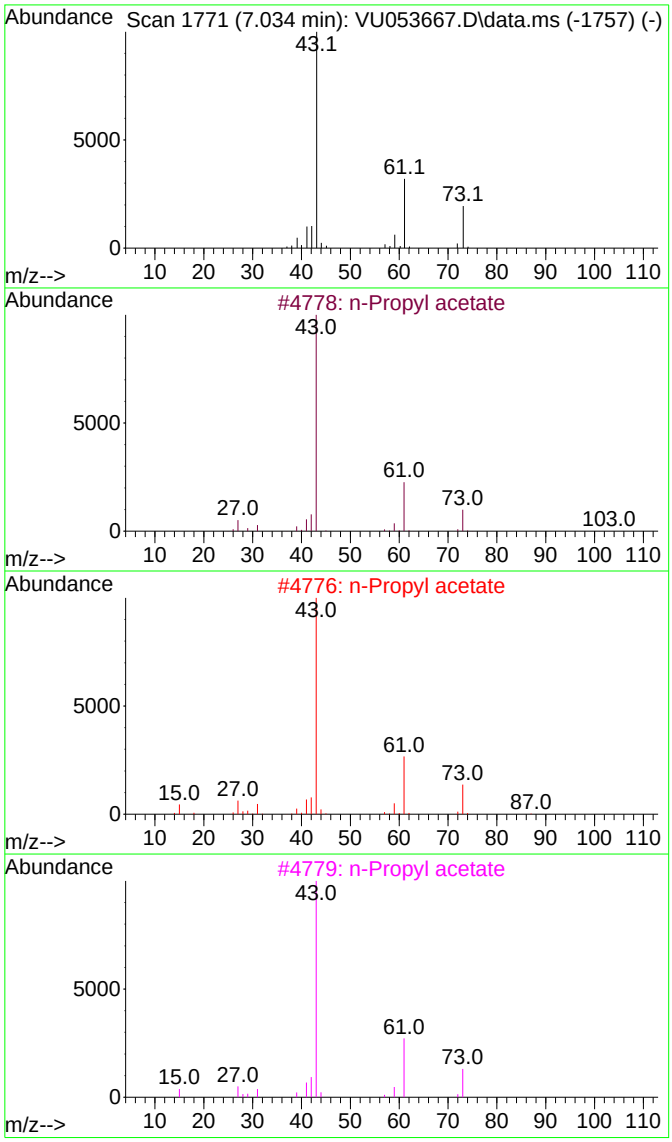
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

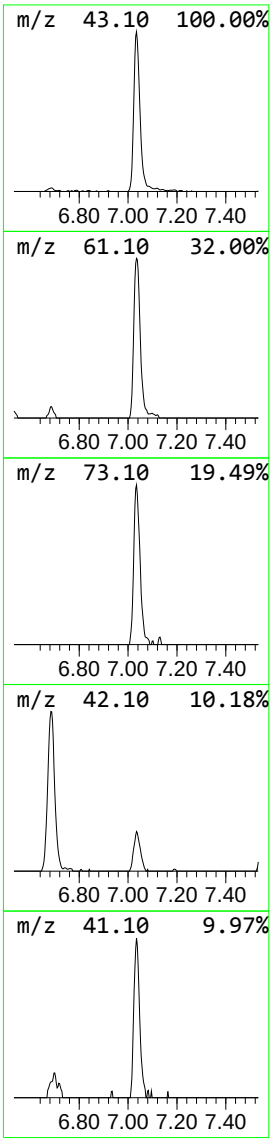
****

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.034	8.21 ug/L	89968	1,4-Difluorobenzene	6.243

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	n-Propyl acetate	102	C5H10O2	000109-60-4	83
3	n-Propyl acetate	102	C5H10O2	000109-60-4	78
4	n-Propyl acetate	102	C5H10O2	000109-60-4	56
5	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	38





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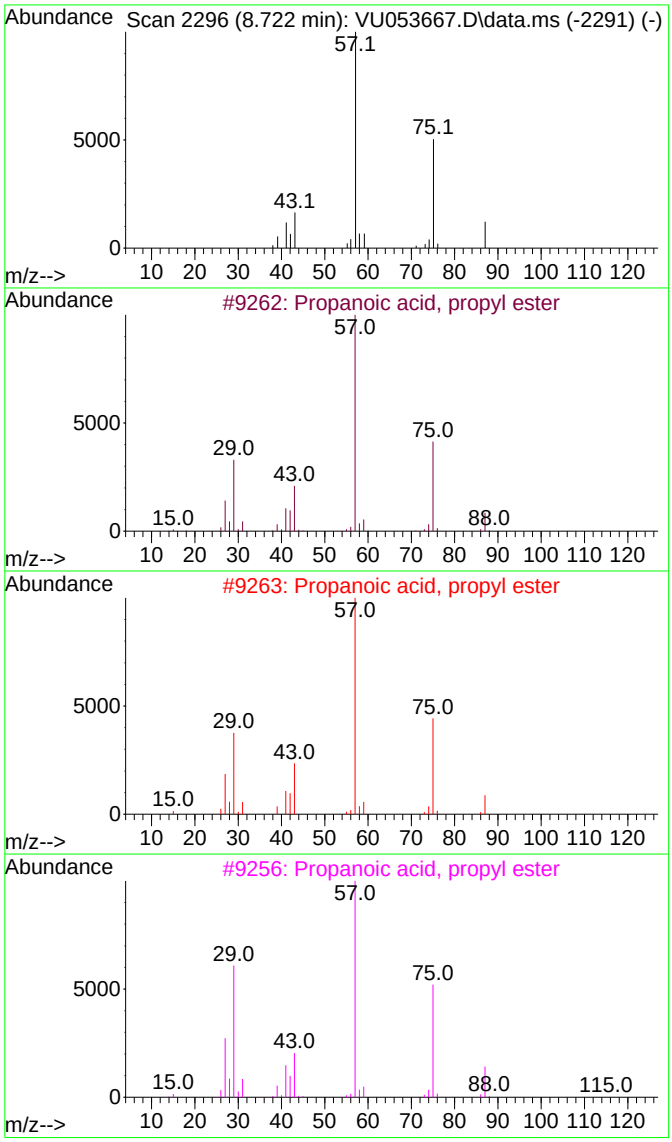
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

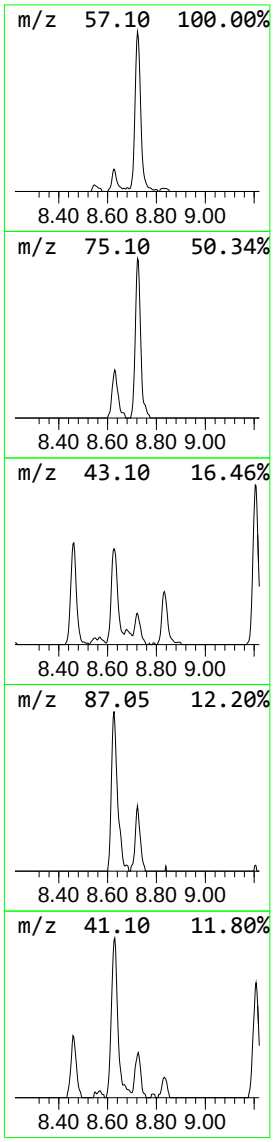
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.722	3.11 ug/L	41732	Chlorobenzene-d5	9.414

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40





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Instrument :
MSVOA_U
ClientSampleId :
C0AN5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

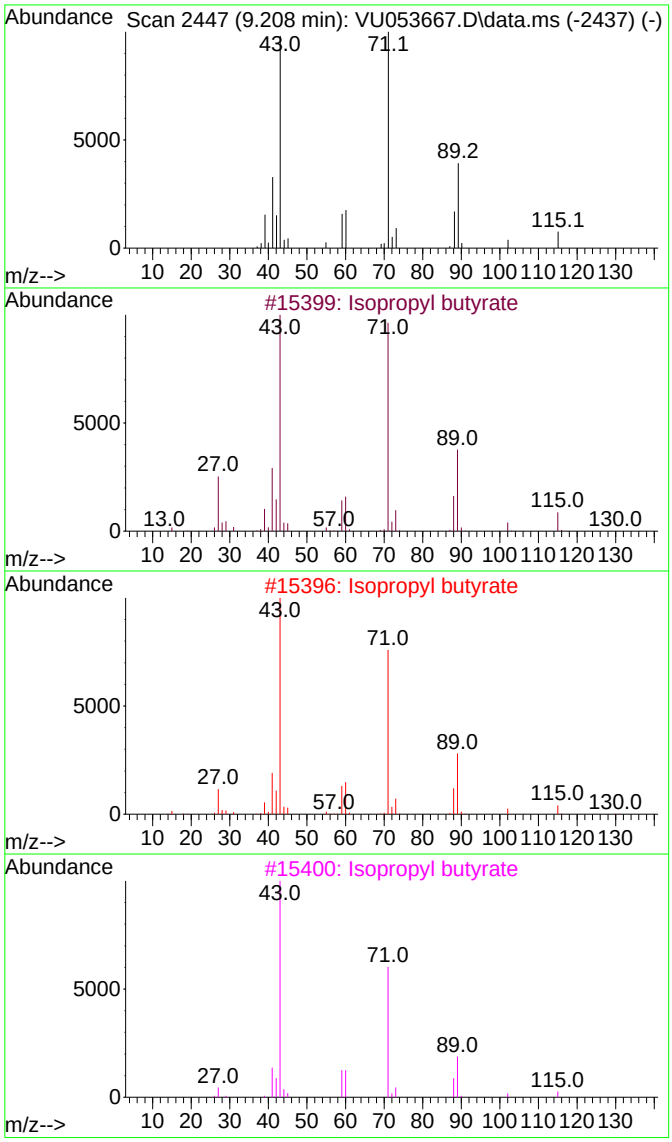
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

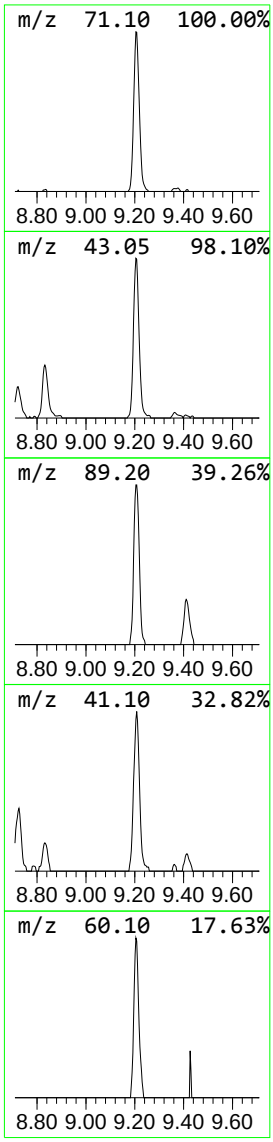
****

Peak Number 4 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.208	5.81 ug/L	78130	Chlorobenzene-d5	9.414

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72





Tentatively Identified Compound (LSC) summary

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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	7.034	8.2	ug/L	89968	1	6.243	547998	50.0
Propanoic acid,...	8.722	3.1	ug/L	41732	2	9.414	672006	50.0
Isopropyl butyrate	9.208	5.8	ug/L	78130	2	9.414	672006	50.0