LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
Data File : VX039301.D
Acq On : 18 Dec 2023 11:14
Operator : JC/MD
Sample : PB157840TB 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB840

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_X\Method\SFAMXLM120523WMA.M
Title : VOC Analysis

Signal : TIC: VX039301.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	23	26	33	rBV3	5404	12700	1.36%	0.167%
2	1.368	42	46	56	rVB	105344	111074	11.93%	1.465%
3	1.666	91	95	106	rBV	65726	98425	10.58%	1.298%
4	2.307	194	200	208	rBV	199533	306367	32.92%	4.039%
5	2.569	241	243	247	rVB	369	367	0.04%	0.005%
6	2.605	247	249	252	rBV2	325	327	0.04%	0.004%
7	2.660	256	258	261	rVB	337	323	0.03%	0.004%
8	2.691	261	263	268	rBV2	497	863	0.09%	0.011%
9	2.788	273	279	288	rBV2	9598	19240	2.07%	0.254%
10	2.947	300	305	312	rVB3	2251	5511	0.59%	0.073%
11	3.081	325	327	329	rBV	298	363	0.04%	0.005%
12	3.355	369	372	376	rBV2	243	353	0.04%	0.005%
13	3.489	392	394	398	rVV2	361	381	0.04%	0.005%
14	3.593	404	411	415	rVV3	1143	2831	0.30%	0.037%
15	3.648	418	420	422	rVV2	297	247	0.03%	0.003%
16	3.684	425	426	429	rVV	294	281	0.03%	0.004%
17	4.007	478	479	484	rBV2	233	275	0.03%	0.004%
18	4.245	514	518	521	rBV2	670	1250	0.13%	0.016%
19	4.452	544	552	567	rBV	86391	245505	26.38%	3.237%
20	4.855	617	618	624	rBV	286	315	0.03%	0.004%
21	5.056	640	651	669	rBV	116219	364020	39.11%	4.800%
22	5.471	717	719	721	rBV2	343	324	0.03%	0.004%
23	5.550	729	732	734	rVV2	271	320	0.03%	0.004%
24	5.568	734	735	738	rVB2	478	283	0.03%	0.004%
25	5.970	789	801	821	rBV2	307030	930667	100.00%	12.271%
26	6.348	856	863	873	rBV2	5363	14860	1.60%	0.196%
27	6.476	880	884	887	rBV2	341	508	0.05%	0.007%
28	6.617	905	907	909	rBV	297	293	0.03%	0.004%
29	6.653	912	913	915	rVV	257	241	0.03%	0.003%
30	6.763	919	931	953	rBV	216323	523854	56.29%	6.907%
31	7.129	990	991	993	rBV2	345	228	0.02%	0.003%
32	7.312	1012	1021	1040	rBV	188028	426473	45.82%	5.623%
33	7.647	1071	1076	1082	rBV	3712	6679	0.72%	0.088%
34	7.799	1095	1101	1120	rBV	83285	150090	16.13%	1.979%
35	8.153	1155	1159	1160	rBV3	174	245	0.03%	0.003%
36	8.202	1163	1167	1170	rBV2	303	527	0.06%	0.007%

LSC Area Percent Report

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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB840

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_X\Method\SFAMXLM120523WMA.M
Title : VOC Analysis

37	8.324	1181	1187	1200	rBV	140138	227195	24.41%	2.996%
38	8.549	1218	1224	1234	rBV	15783	26982	2.90%	0.356%
39	8.647	1234	1240	1250	rBV	456277	726926	78.11%	9.585%
40	8.818	1266	1268	1271	rVB4	475	340	0.04%	0.004%
41	8.952	1284	1290	1303	rBV2	121991	184976	19.88%	2.439%
42	9.244	1332	1338	1346	rBV	16858	25609	2.75%	0.338%
43	9.311	1346	1349	1351	rBV2	2355	2847	0.31%	0.038%
44	9.385	1356	1361	1373	rVV	407842	594729	63.90%	7.842%
45	9.482	1373	1377	1388	rVV	37891	57532	6.18%	0.759%
46	9.580	1389	1393	1404	rVB	24816	36347	3.91%	0.479%
47	9.695	1410	1412	1416	rVB4	882	1073	0.12%	0.014%
48	9.848	1436	1437	1439	rVV	462	235	0.03%	0.003%
49	9.915	1443	1448	1459	rVV	55360	75863	8.15%	1.000%
50	9.994	1459	1461	1463	rVV	337	238	0.03%	0.003%
51	10.055	1465	1471	1491	rVV	461096	642495	69.04%	8.471%
52	10.189	1491	1493	1494	rVV	455	439	0.05%	0.006%
53	10.238	1498	1501	1502	rBV2	333	322	0.03%	0.004%
54	10.299	1505	1511	1516	rBV5	751	1862	0.20%	0.025%
55	10.512	1541	1546	1550	rBV4	1128	1472	0.16%	0.019%
56	10.640	1564	1567	1571	rVV2	4365	6173	0.66%	0.081%
57	10.683	1572	1574	1579	rVB	1789	2354	0.25%	0.031%
58	10.787	1589	1591	1593	rVB2	248	255	0.03%	0.003%
59	10.963	1618	1620	1626	rVB2	651	800	0.09%	0.011%
60	11.092	1636	1641	1644	rBV2	969	1602	0.17%	0.021%
61	11.189	1652	1657	1667	rBV	355298	456178	49.02%	6.015%
62	11.311	1675	1677	1680	rBV3	560	582	0.06%	0.008%
63	11.409	1691	1693	1697	rBV2	168	256	0.03%	0.003%
64	11.445	1697	1699	1704	rBV4	546	818	0.09%	0.011%
65	11.756	1746	1750	1755	rVB4	988	1304	0.14%	0.017%
66	11.969	1781	1785	1788	rBV3	892	1276	0.14%	0.017%
67	12.024	1788	1794	1808	rBV	473123	633396	68.06%	8.351%
68	12.317	1837	1842	1854	rBV	485829	630759	67.77%	8.317%
69	12.536	1874	1878	1882	rBV2	273	392	0.04%	0.005%
70	12.762	1912	1915	1921	rVV	709	993	0.11%	0.013%
71	13.116	1970	1973	1977	rVB3	787	796	0.09%	0.010%
72	13.353	2009	2012	2015	rBV2	190	245	0.03%	0.003%
73	13.390	2015	2018	2022	rVV2	274	319	0.03%	0.004%
74	13.420	2022	2023	2026	rVB	347	225	0.02%	0.003%
75	13.445	2026	2027	2030	rBV2	233	229	0.02%	0.003%
76	13.591	2048	2051	2055	rBV4	1115	1377	0.15%	0.018%

LSC Area Percent Report

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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB840

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_X\Method\SFAMXLM120523WMA.M
Title : VOC Analysis

77	13.670	2061	2064	2066	rBV	232	295	0.03%	0.004%
78	13.731	2070	2074	2076	rVV2	241	228	0.02%	0.003%
79	13.780	2079	2082	2089	rVV	767	1254	0.13%	0.017%
80	13.963	2109	2112	2118	rVB2	753	1032	0.11%	0.014%
81	14.012	2118	2120	2121	rBV2	265	218	0.02%	0.003%
82	14.134	2137	2140	2144	rVB3	781	986	0.11%	0.013%
83	14.207	2151	2152	2157	rBB2	254	309	0.03%	0.004%
84	14.286	2163	2165	2167	rBV	221	253	0.03%	0.003%
85	14.353	2173	2176	2177	rVB2	345	282	0.03%	0.004%
86	14.378	2177	2180	2181	rBV	294	306	0.03%	0.004%
87	14.493	2196	2199	2200	rBV	367	299	0.03%	0.004%
88	14.530	2203	2205	2208	rVB2	288	342	0.04%	0.005%
89	14.743	2238	2240	2242	rBV2	287	282	0.03%	0.004%
90	14.890	2262	2264	2268	rVV2	347	499	0.05%	0.007%
91	15.152	2305	2307	2309	rVB2	343	257	0.03%	0.003%
92	15.249	2322	2323	2326	rBV	261	239	0.03%	0.003%
93	15.377	2342	2344	2345	rBV	537	300	0.03%	0.004%
94	15.768	2406	2408	2409	rBV	301	287	0.03%	0.004%
95	15.804	2413	2414	2417	rBV2	300	265	0.03%	0.003%
96	15.969	2439	2441	2447	rBV3	387	480	0.05%	0.006%
97	16.249	2485	2487	2488	rBV	354	274	0.03%	0.004%
98	16.298	2493	2495	2498	rVV2	417	455	0.05%	0.006%
99	16.664	2554	2555	2558	rBV2	328	347	0.04%	0.005%
100	16.749	2566	2569	2572	rVB2	364	416	0.04%	0.005%

Sum of corrected areas: 7584326

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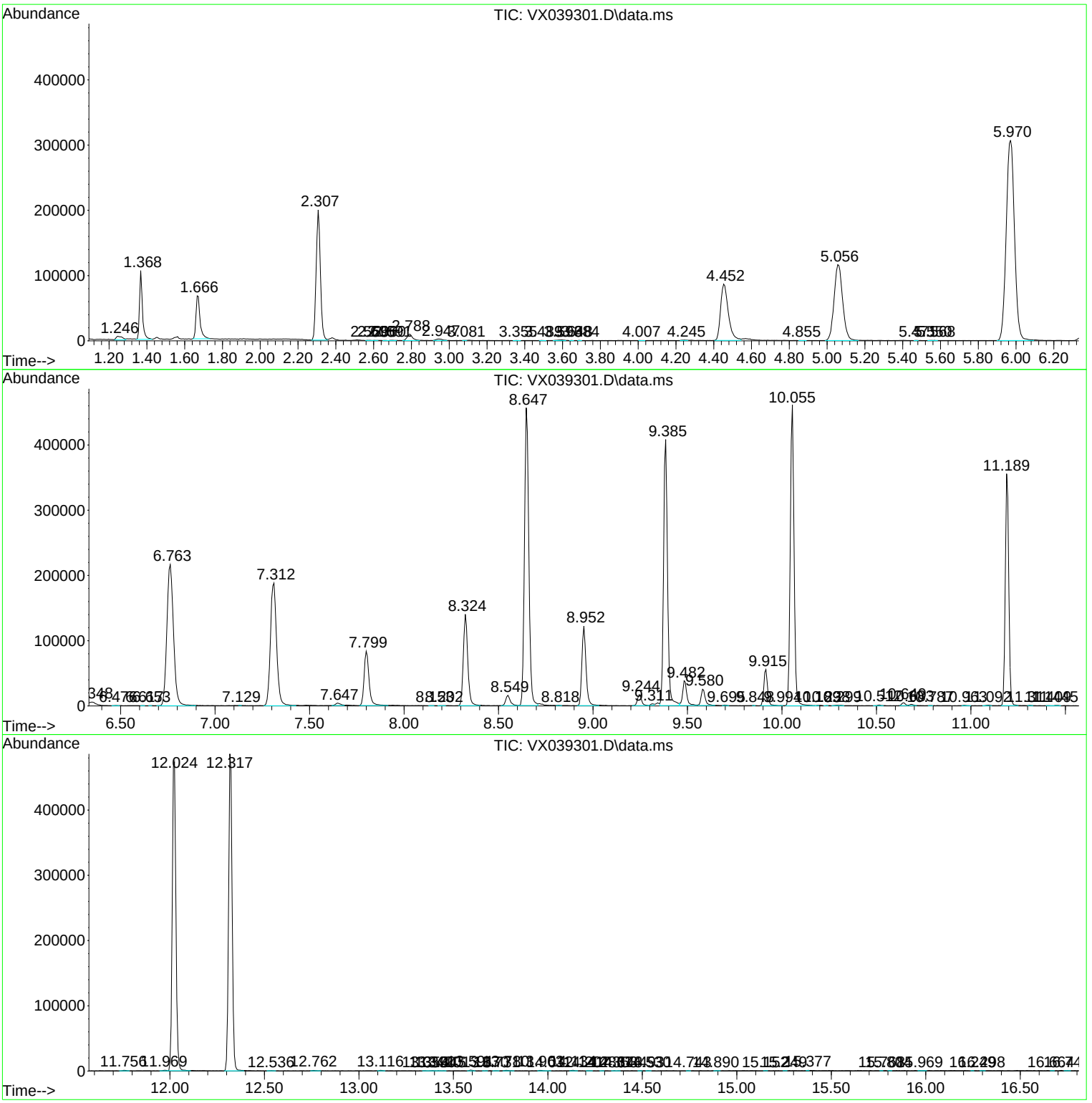
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB840

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
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Instrument :
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ClientSampleId :
VLEB840

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

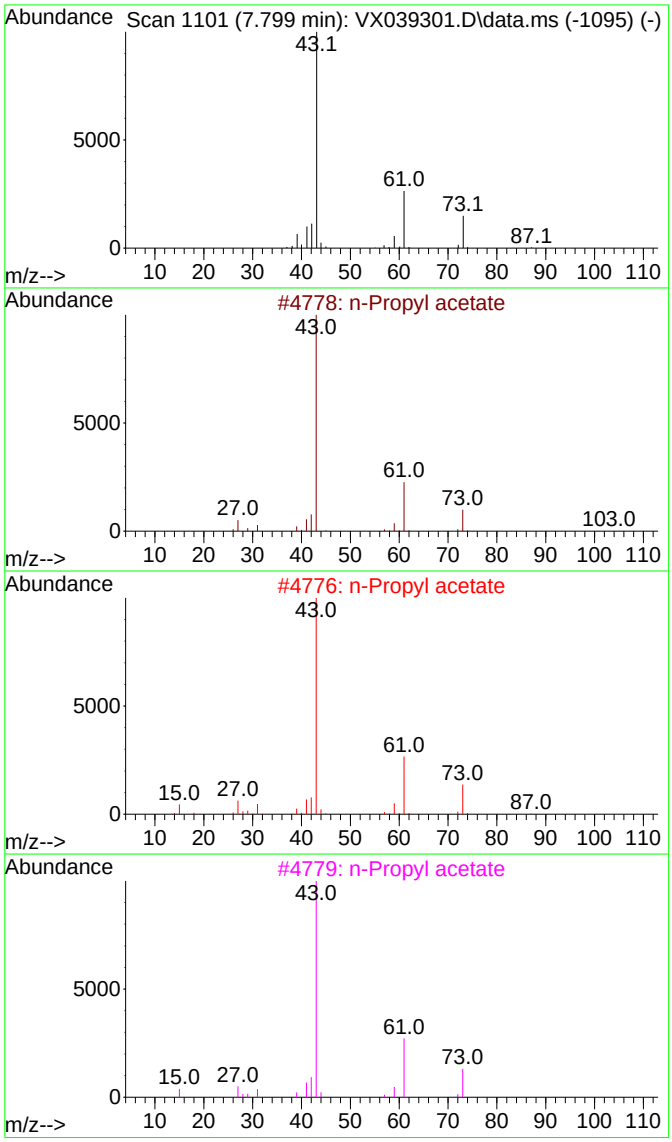
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

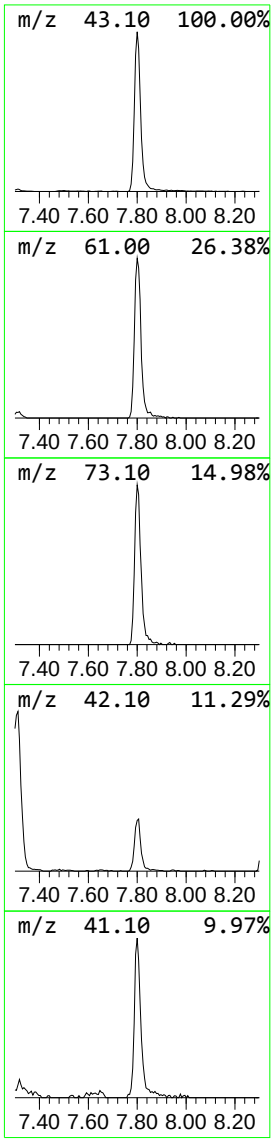
****

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	14.33 ug/L	150090	1,4-Difluorobenzene	6.763

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	78
3	n-Propyl acetate	102	C5H10O2	000109-60-4	78
4	n-Propyl acetate	102	C5H10O2	000109-60-4	78
5	n-Propyl acetate	102	C5H10O2	000109-60-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
Data File : VX039301.D
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB840

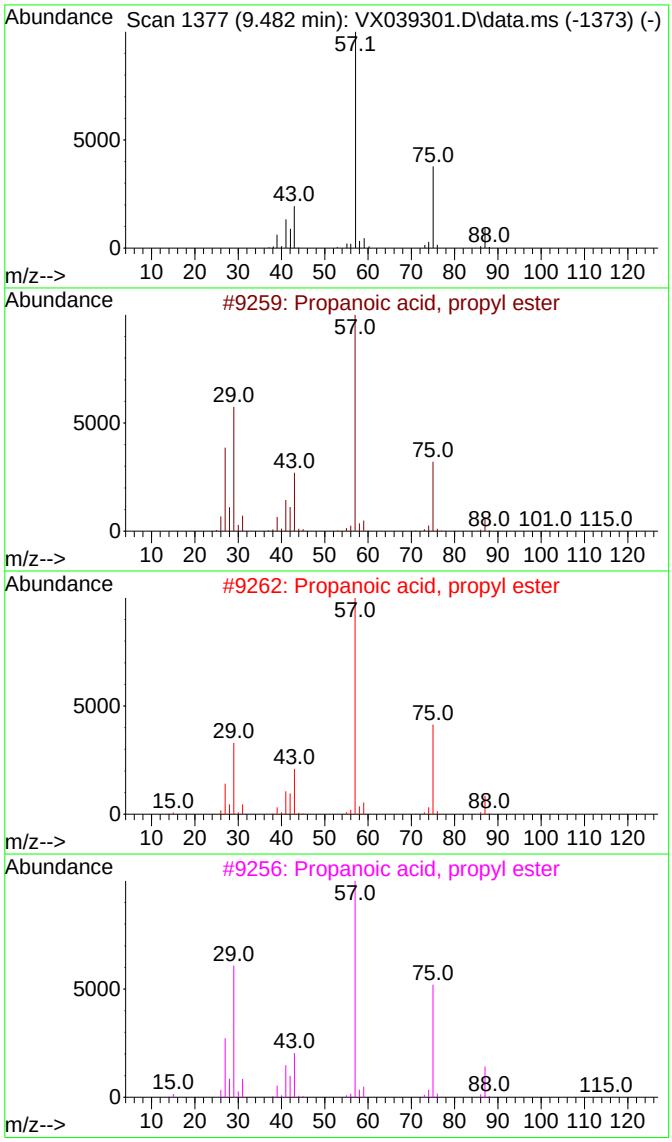
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

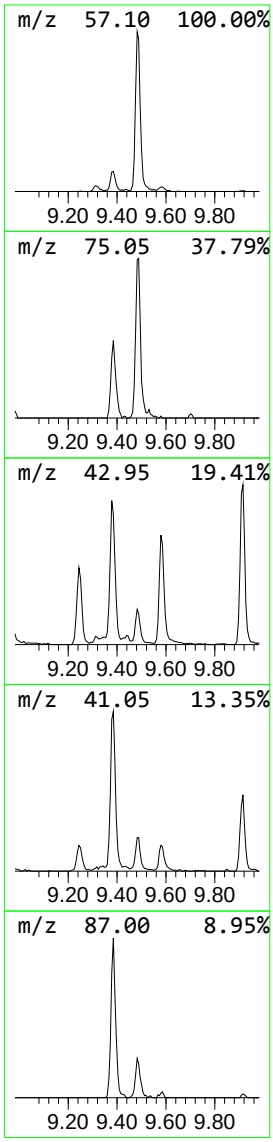
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	4.48 ug/L	57532	Chlorobenzene-d5	10.055

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	78
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78





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Instrument :
MSVOA_X
ClientSampleId :
VLEB840

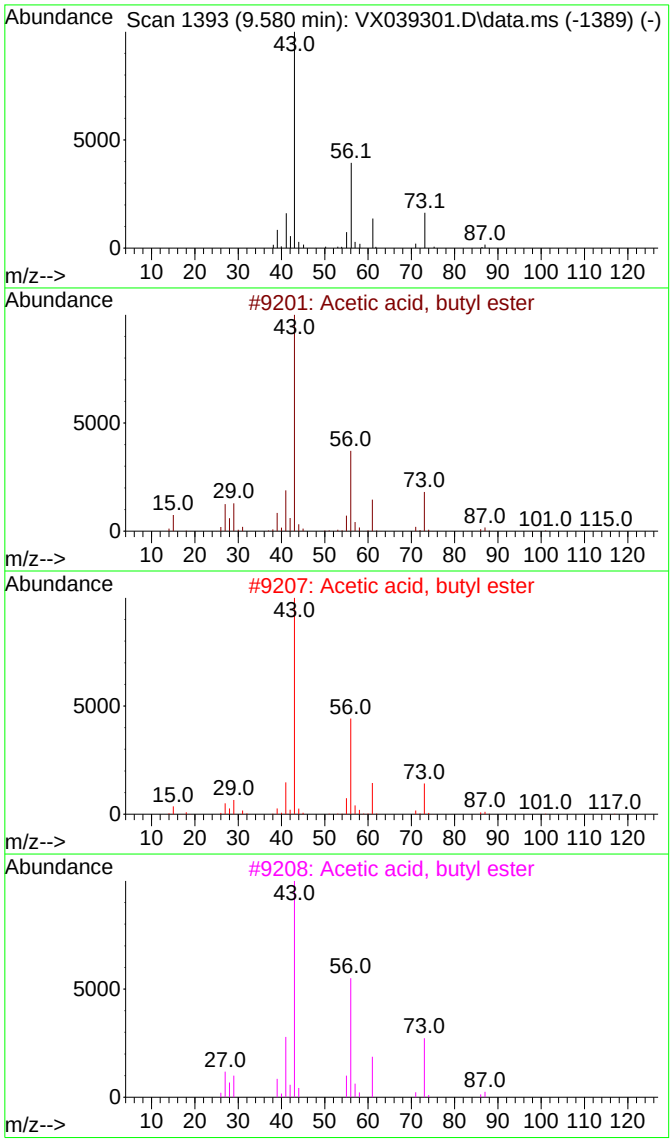
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

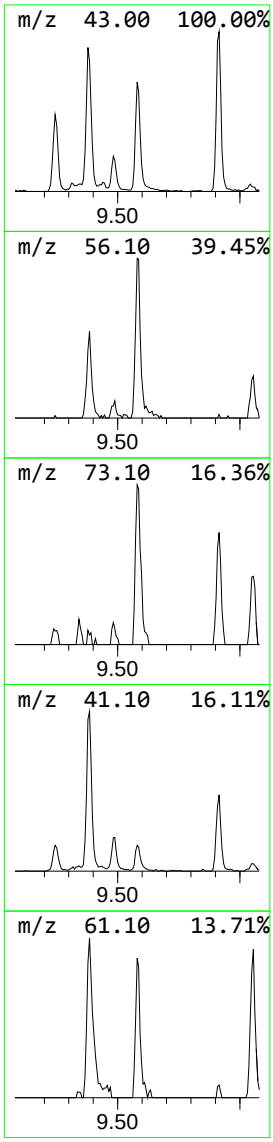
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	2.83 ug/L	36347	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	39
5	1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	23





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB840

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

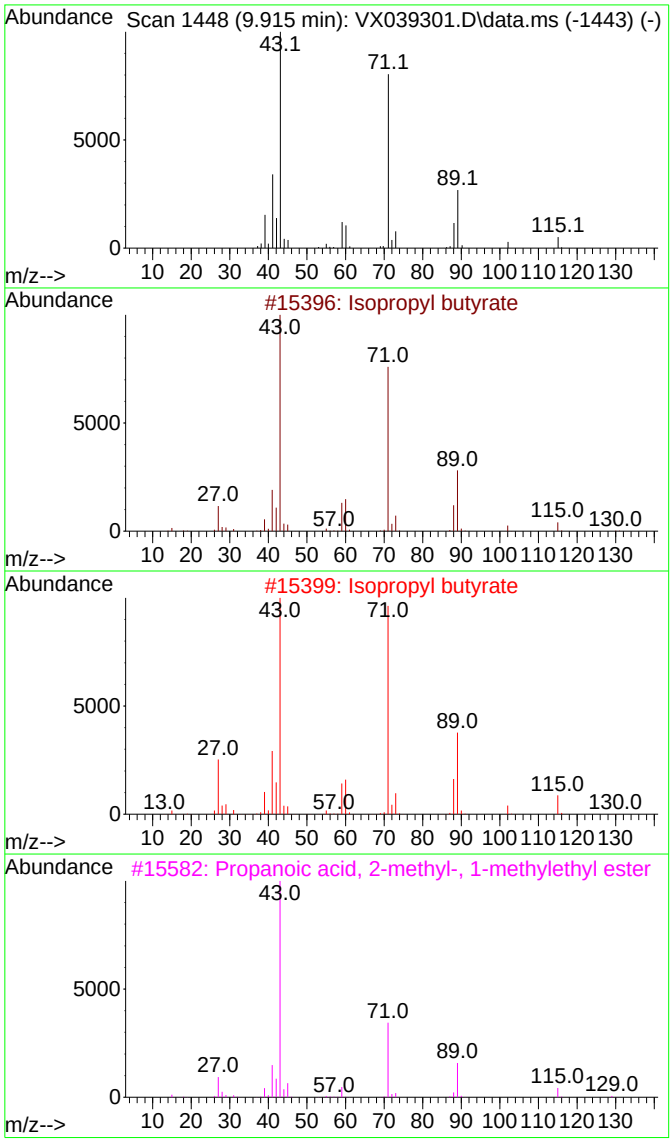
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

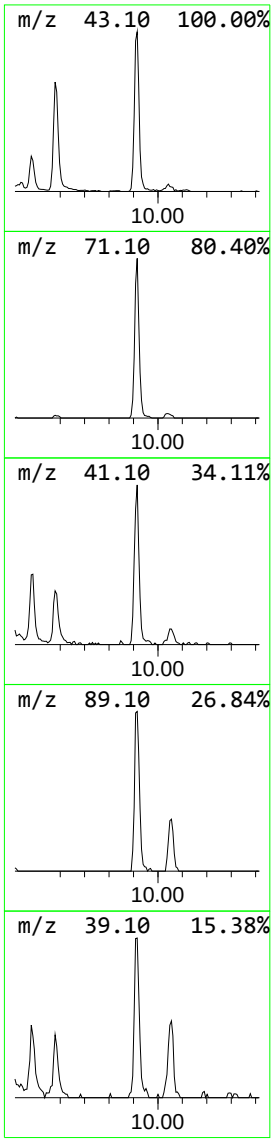
****

Peak Number 5 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	5.90 ug/L	75863	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64





Tentatively Identified Compound (LSC) summary

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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB840

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
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	7.799	14.3	ug/L	150090	1	6.763	523854	50.0
Propanoic acid,...	9.482	4.5	ug/L	57532	2	10.055	642495	50.0
Acetic acid, bu...	9.580	2.8	ug/L	36347	2	10.055	642495	50.0
Isopropyl butyrate	9.915	5.9	ug/L	75863	2	10.055	642495	50.0