LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV093024\
Data File : VV037645.D
Acq On : 30 Sep 2024 11:40
Operator : SY/MD
Sample : PB163749TB 10X
Misc : 5mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB749

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_V\Method\SFAMVLM092624WMA.M
Title : VOC Analysis

Signal : TIC: VV037645.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.175	35	42	51	rBV	11940	21921	0.77%	0.102%
2	1.282	67	75	92	rVB	424448	457301	16.09%	2.122%
3	1.532	145	153	171	rVB	344855	409596	14.41%	1.901%
4	2.060	306	317	331	rBV	730346	1063126	37.40%	4.934%
5	3.294	699	701	706	rBV6	920	691	0.02%	0.003%
6	3.597	792	795	799	rVB4	926	737	0.03%	0.003%
7	3.642	805	809	813	rVB5	477	515	0.02%	0.002%
8	3.667	813	817	822	rBV3	541	556	0.02%	0.003%
9	3.725	831	835	839	rVB5	602	499	0.02%	0.002%
10	3.790	847	855	885	rBV2	100669	310099	10.91%	1.439%
11	4.095	949	950	954	rVB3	1130	623	0.02%	0.003%
12	4.240	978	995	1028	rBV	457531	1163311	40.92%	5.399%
13	4.442	1055	1058	1061	rBV2	848	599	0.02%	0.003%
14	4.497	1069	1075	1076	rBV3	815	709	0.02%	0.003%
15	4.526	1080	1084	1090	rVV5	782	946	0.03%	0.004%
16	4.606	1106	1109	1111	rVV2	790	546	0.02%	0.003%
17	4.626	1111	1115	1118	rVV4	782	619	0.02%	0.003%
18	4.722	1140	1145	1150	rBV5	882	911	0.03%	0.004%
19	4.834	1176	1180	1184	rBV4	812	844	0.03%	0.004%
20	4.947	1198	1215	1247	rBV2	1117304	2842879	100.00%	13.193%
21	5.214	1291	1298	1309	rBV5	6824	15000	0.53%	0.070%
22	5.423	1359	1363	1365	rBV4	664	584	0.02%	0.003%
23	5.458	1371	1374	1378	rVB6	1278	888	0.03%	0.004%
24	5.526	1381	1395	1424	rBV	841973	1728231	60.79%	8.020%
25	5.831	1479	1490	1503	rBV7	10753	23029	0.81%	0.107%
26	5.982	1522	1537	1567	rBV	619860	1288705	45.33%	5.981%
27	6.150	1586	1589	1591	rBV3	1065	520	0.02%	0.002%
28	6.397	1659	1666	1691	rBV	80057	177465	6.24%	0.824%
29	6.815	1793	1796	1797	rBV3	1067	550	0.02%	0.003%
30	6.905	1814	1824	1858	rBV	334424	644787	22.68%	2.992%
31	7.121	1882	1891	1911	rBV2	26129	51692	1.82%	0.240%
32	7.236	1916	1927	1963	rBV	1327010	2334381	82.11%	10.834%
33	7.548	2013	2024	2053	rBV2	243504	474756	16.70%	2.203%
34	7.857	2111	2120	2140	rBV	42353	79436	2.79%	0.369%
35	7.950	2146	2149	2152	rBV4	967	894	0.03%	0.004%
36	7.982	2152	2159	2162	rVV6	6969	8687	0.31%	0.040%

LSC Area Percent Report

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Misc : 5mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB749

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_V\Method\SFAMVLM092624WMA.M
Title : VOC Analysis

37	8.024	2163	2172	2198	rVV2	308906	669007	23.53%	3.105%
38	8.130	2200	2205	2227	rVB	57585	112710	3.96%	0.523%
39	8.252	2235	2243	2267	rVB2	23104	49588	1.74%	0.230%
40	8.432	2296	2299	2301	rBV3	930	540	0.02%	0.003%
41	8.551	2331	2336	2338	rBV4	2044	1858	0.07%	0.009%
42	8.616	2344	2356	2376	rBV	120438	206537	7.27%	0.959%
43	8.776	2395	2406	2443	rBV	1344361	2199168	77.36%	10.206%
44	9.500	2623	2631	2642	rBV8	5097	10845	0.38%	0.050%
45	9.696	2690	2692	2697	rVB5	954	698	0.02%	0.003%
46	9.876	2745	2748	2750	rBV4	1107	694	0.02%	0.003%
47	10.021	2789	2793	2795	rBV4	624	587	0.02%	0.003%
48	10.146	2818	2832	2856	rBV	671558	1051775	37.00%	4.881%
49	10.317	2883	2885	2893	rVB5	1066	934	0.03%	0.004%
50	10.423	2915	2918	2920	rBV	822	570	0.02%	0.003%
51	10.532	2947	2952	2956	rVB4	723	735	0.03%	0.003%
52	10.558	2956	2960	2961	rBV2	1012	554	0.02%	0.003%
53	10.587	2967	2969	2975	rVB3	680	478	0.02%	0.002%
54	10.661	2988	2992	2996	rVB4	838	551	0.02%	0.003%
55	10.786	3026	3031	3036	rVB9	1192	1257	0.04%	0.006%
56	10.870	3052	3057	3060	rBV3	761	775	0.03%	0.004%
57	11.069	3116	3119	3122	rBV2	762	630	0.02%	0.003%
58	11.133	3135	3139	3142	rBV3	1633	1411	0.05%	0.007%
59	11.178	3142	3153	3186	rBV	1263349	2022416	71.14%	9.386%
60	11.407	3222	3224	3228	rVB3	1036	558	0.02%	0.003%
61	11.461	3238	3241	3248	rVB4	1189	1270	0.04%	0.006%
62	11.490	3248	3250	3253	rVB2	1121	582	0.02%	0.003%
63	11.554	3253	3270	3303	rBV	1283400	2066662	72.70%	9.591%
64	12.008	3409	3411	3413	rBV2	760	507	0.02%	0.002%
65	12.294	3496	3500	3502	rBV3	890	731	0.03%	0.003%
66	12.336	3511	3513	3517	rVB3	1004	603	0.02%	0.003%
67	12.358	3517	3520	3524	rVB5	669	490	0.02%	0.002%
68	12.435	3541	3544	3548	rBV3	857	669	0.02%	0.003%
69	12.587	3586	3591	3593	rBV4	1235	1124	0.04%	0.005%
70	12.599	3593	3595	3601	rVB5	1147	762	0.03%	0.004%
71	12.661	3612	3614	3618	rVV3	835	635	0.02%	0.003%
72	12.709	3626	3629	3632	rVV4	877	689	0.02%	0.003%
73	12.731	3632	3636	3638	rVV3	813	764	0.03%	0.004%
74	12.747	3638	3641	3645	rVB2	642	543	0.02%	0.003%
75	12.792	3651	3655	3658	rVB3	700	501	0.02%	0.002%
76	12.837	3666	3669	3673	rBV5	481	489	0.02%	0.002%

LSC Area Percent Report

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Misc : 5mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB749

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_V\Method\SFAMVLM092624WMA.M
Title : VOC Analysis

77	12.857	3673	3675	3680	rVB3	825	589	0.02%	0.003%
78	12.898	3685	3688	3693	rVB4	1149	890	0.03%	0.004%
79	12.927	3693	3697	3700	rBV4	950	850	0.03%	0.004%
80	13.040	3730	3732	3737	rVB3	1107	760	0.03%	0.004%
81	13.069	3737	3741	3744	rBV4	563	508	0.02%	0.002%
82	13.172	3769	3773	3775	rBV3	652	548	0.02%	0.003%
83	13.220	3780	3788	3796	rVB10	2782	4782	0.17%	0.022%
84	13.262	3796	3801	3802	rBV4	637	506	0.02%	0.002%
85	13.291	3806	3810	3816	rVB7	790	1010	0.04%	0.005%
86	13.407	3842	3846	3848	rBV3	1340	1014	0.04%	0.005%
87	13.458	3853	3862	3871	rBV8	3637	6511	0.23%	0.030%
88	13.587	3898	3902	3904	rBV4	640	520	0.02%	0.002%
89	13.654	3919	3923	3924	rBV2	769	549	0.02%	0.003%
90	13.673	3924	3929	3930	rBV3	1521	936	0.03%	0.004%
91	13.976	4020	4023	4025	rBV4	957	685	0.02%	0.003%
92	14.053	4044	4047	4051	rBV3	561	496	0.02%	0.002%
93	14.162	4076	4081	4084	rBV4	1332	1163	0.04%	0.005%
94	14.262	4105	4112	4114	rBV4	865	1015	0.04%	0.005%
95	14.394	4151	4153	4157	rBV4	699	569	0.02%	0.003%
96	14.638	4224	4229	4233	rBV6	737	887	0.03%	0.004%
97	14.689	4243	4245	4250	rVB5	1009	610	0.02%	0.003%
98	14.988	4332	4338	4339	rBV5	1151	1194	0.04%	0.006%
99	15.133	4379	4383	4389	rBV6	1823	2051	0.07%	0.010%
100	15.898	4619	4621	4622	rBV2	1605	504	0.02%	0.002%

Sum of corrected areas: 21547677

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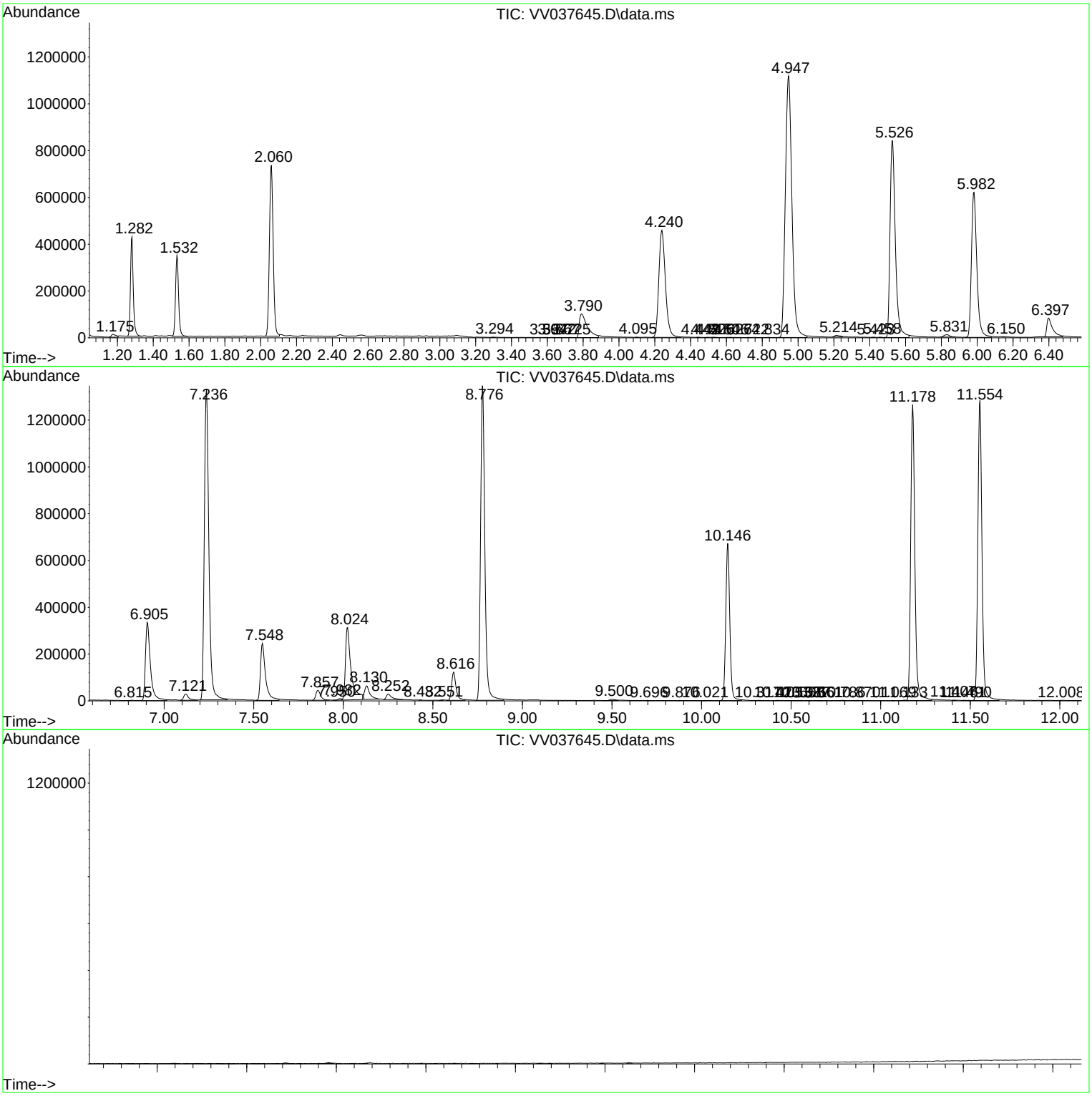
Data File : VV037645.D
Acq On : 30 Sep 2024 11:40
Operator : SY/MD
Sample : PB163749TB 10X
Misc : 5mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB749

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV093024\
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Operator : SY/MD
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Instrument :
MSVOA_V
ClientSampleId :
VLEB749

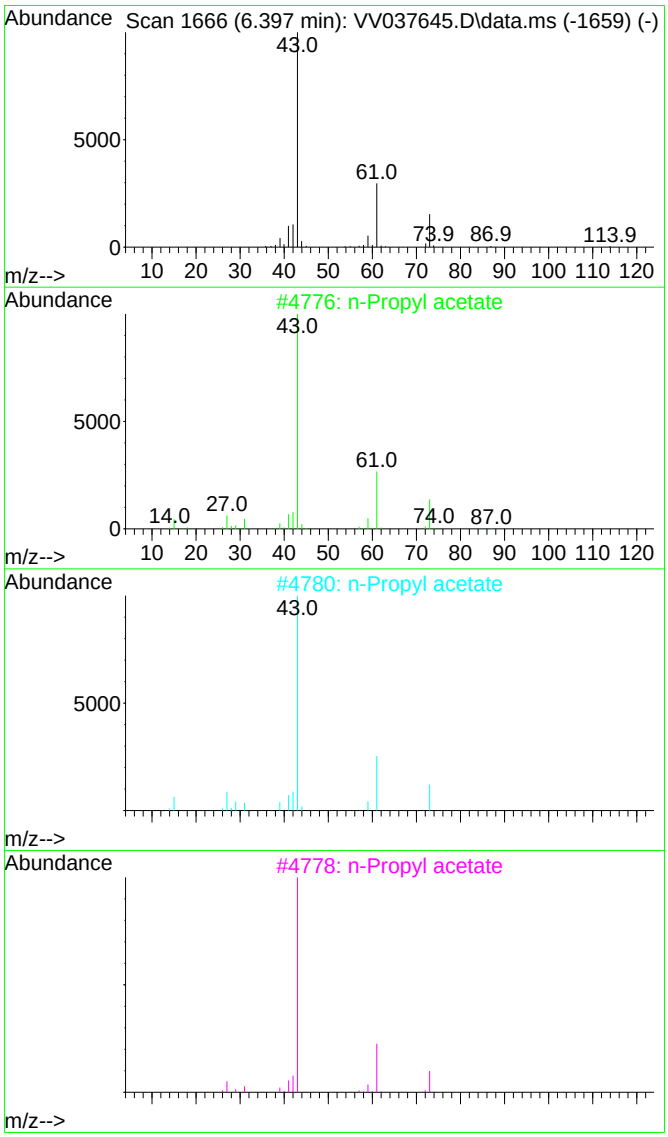
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
Quant Title : VOC Analysis

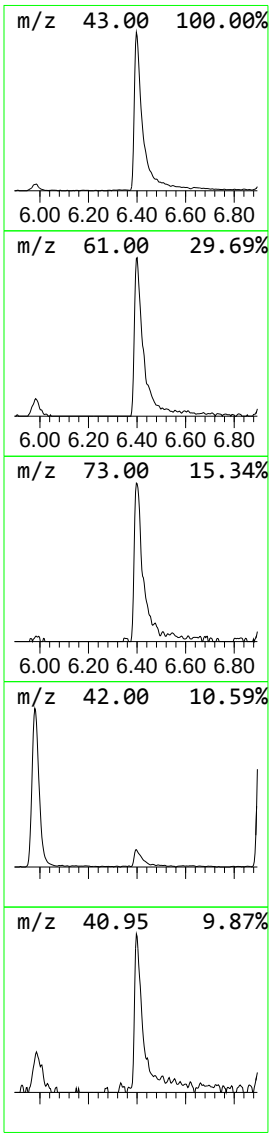
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.397	5.13 ug/L	177465	1,4-Difluorobenzene	5.526

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	n-Propyl acetate	102	C5H10O2	000109-60-4	64
3	n-Propyl acetate	102	C5H10O2	000109-60-4	64
4	n-Propyl acetate	102	C5H10O2	000109-60-4	56
5	n-Propyl acetate	102	C5H10O2	000109-60-4	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV093024\
Data File : VV037645.D
Acq On : 30 Sep 2024 11:40
Operator : SY/MD
Sample : PB163749TB 10X
Misc : 5mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB749

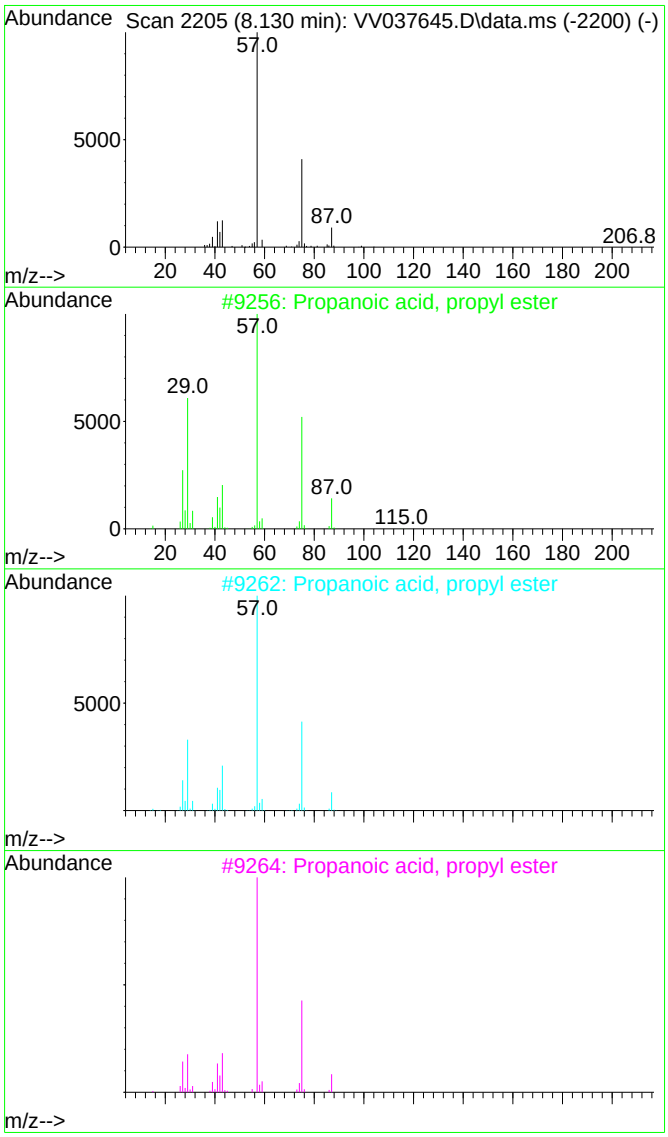
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
Quant Title : VOC Analysis

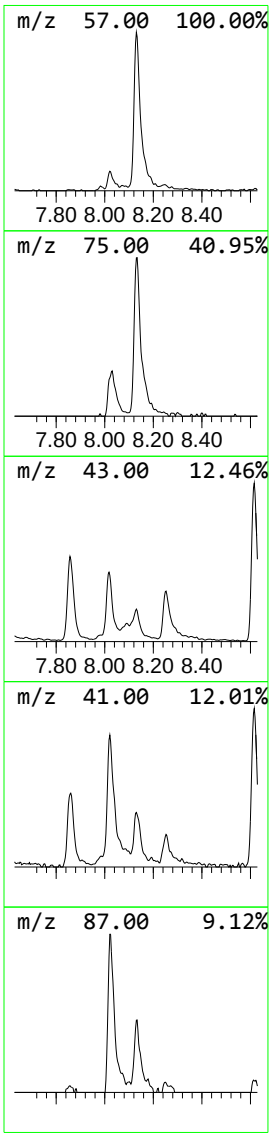
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.130	2.56 ug/L	112710	Chlorobenzene-d5	8.776

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9





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Misc : 5mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB749

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
Quant Title : VOC Analysis

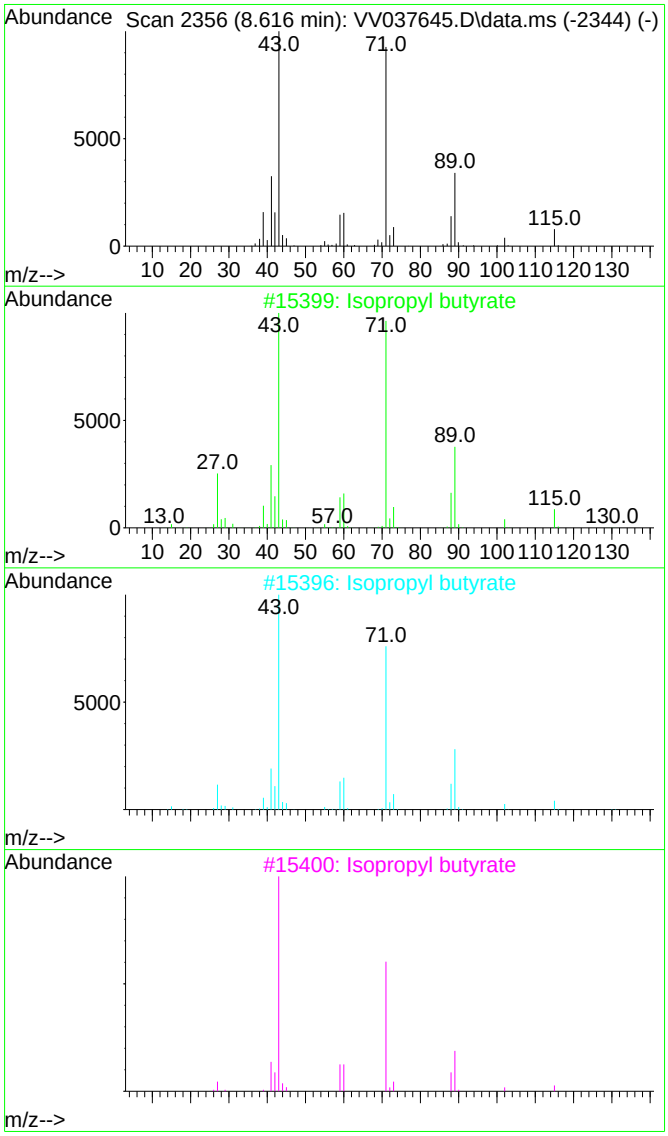
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

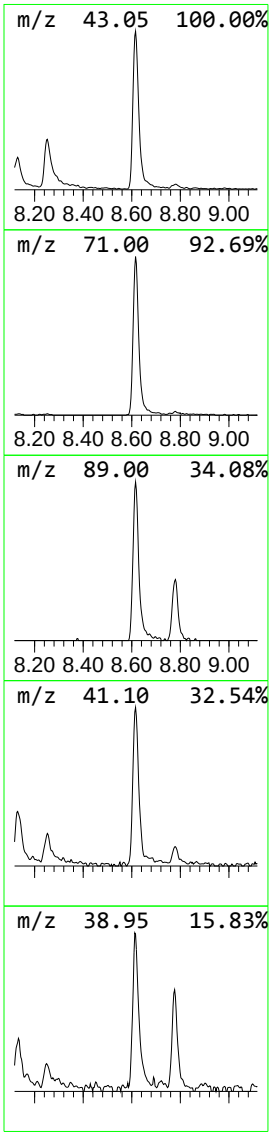
****

Peak Number 4 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.616	4.70 ug/L	206537	Chlorobenzene-d5	8.776

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-, 1-met...	130	C7H14O2	000617-50-5	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV093024\
Data File : VV037645.D
Acq On : 30 Sep 2024 11:40
Operator : SY/MD
Sample : PB163749TB 10X
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ALS Vial : 1 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.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	6.397	5.1	ug/L	177465	1	5.526	1728230	50.0
Propanoic acid,...	8.130	2.6	ug/L	112710	2	8.776	2199170	50.0
Isopropyl butyrate	8.616	4.7	ug/L	206537	2	8.776	2199170	50.0