LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032124\
Data File : VV034782.D
Acq On : 21 Mar 2024 12:26
Operator : SY/MD
Sample : PB159661TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB661

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\SFAMVLM022924WMA.M
Title : VOC Analysis

Signal : TIC: VV034782.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.282	68	75	89	rVB	243133	258996	16.85%	2.241%
2	1.532	146	153	168	rVB	206358	238547	15.52%	2.064%
3	2.060	306	317	332	rBV	342944	506184	32.92%	4.380%
4	2.394	417	421	423	rBV2	726	507	0.03%	0.004%
5	2.452	429	439	447	rBV	5993	9556	0.62%	0.083%
6	2.507	453	456	461	rVB2	272	222	0.01%	0.002%
7	2.532	462	464	467	rVB	232	84	0.01%	0.001%
8	2.552	467	470	471	rBV	232	112	0.01%	0.001%
9	2.680	507	510	513	rBV	249	166	0.01%	0.001%
10	2.854	562	564	567	rVB	146	80	0.01%	0.001%
11	2.876	567	571	574	rBV2	180	146	0.01%	0.001%
12	2.889	574	575	576	rBV2	130	29	0.00%	0.000%
13	2.995	604	608	611	rVB3	249	149	0.01%	0.001%
14	3.079	632	634	636	rBV2	126	60	0.00%	0.001%
15	3.114	642	645	646	rBV	106	65	0.00%	0.001%
16	3.140	649	653	656	rVV	198	158	0.01%	0.001%
17	3.191	668	669	670	rBV	131	35	0.00%	0.000%
18	3.236	680	683	686	rBV2	249	139	0.01%	0.001%
19	3.288	697	699	702	rBV	124	79	0.01%	0.001%
20	3.339	712	715	719	rBV2	181	126	0.01%	0.001%
21	3.359	719	721	722	rBV	90	40	0.00%	0.000%
22	3.404	732	735	738	rBV2	178	107	0.01%	0.001%
23	3.423	738	741	742	rBV	127	79	0.01%	0.001%
24	3.458	748	752	754	rBV	249	169	0.01%	0.001%
25	3.494	758	763	765	rBV2	160	159	0.01%	0.001%
26	3.584	787	791	794	rBV2	138	86	0.01%	0.001%
27	3.638	805	808	809	rBV	259	135	0.01%	0.001%
28	3.789	847	855	898	rBV	89922	272570	17.73%	2.358%
29	4.246	982	997	1029	rBV	237072	613385	39.90%	5.307%
30	4.670	1126	1129	1132	rBV2	288	175	0.01%	0.002%
31	4.732	1145	1148	1155	rVB3	430	385	0.03%	0.003%
32	4.802	1165	1170	1174	rBV2	340	398	0.03%	0.003%
33	4.953	1201	1217	1250	rBV2	581633	1537400	100.00%	13.302%
34	5.217	1291	1299	1319	rBV3	7167	18777	1.22%	0.162%
35	5.532	1386	1397	1443	rBV	388314	805896	52.42%	6.973%
36	5.831	1481	1490	1510	rVB4	10915	23684	1.54%	0.205%

LSC Area Percent Report

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Operator : SY/MD
Sample : PB159661TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB661

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\SFAMVLM022924WMA.M
Title : VOC Analysis

37	5.986	1525	1538	1569	rBV	326633	678895	44.16%	5.874%
38	6.275	1625	1628	1629	rBV2	1124	672	0.04%	0.006%
39	6.394	1657	1665	1699	rBV	103119	216788	14.10%	1.876%
40	6.725	1766	1768	1769	rBV	348	109	0.01%	0.001%
41	6.912	1815	1826	1856	rBV	184444	345636	22.48%	2.991%
42	7.121	1883	1891	1910	rBV	25648	45846	2.98%	0.397%
43	7.240	1917	1928	1971	rBV	687063	1222340	79.51%	10.576%
44	7.551	2016	2025	2056	rBV	151583	284829	18.53%	2.464%
45	7.863	2111	2122	2141	rBV	35765	62745	4.08%	0.543%
46	8.024	2163	2172	2198	rBV	299829	593102	38.58%	5.132%
47	8.246	2235	2241	2270	rVB2	28828	57987	3.77%	0.502%
48	8.584	2343	2346	2347	rBV2	437	236	0.02%	0.002%
49	8.619	2347	2357	2377	rVV	102055	169337	11.01%	1.465%
50	8.783	2397	2408	2442	rBV	590636	988534	64.30%	8.553%
51	9.140	2517	2519	2522	rVB	461	207	0.01%	0.002%
52	9.198	2533	2537	2540	rBV2	278	246	0.02%	0.002%
53	9.239	2545	2550	2552	rBV2	425	384	0.02%	0.003%
54	9.294	2565	2567	2570	rBV2	172	89	0.01%	0.001%
55	9.346	2579	2583	2584	rBV2	784	511	0.03%	0.004%
56	9.426	2604	2608	2609	rBV	311	189	0.01%	0.002%
57	9.493	2622	2629	2641	rBV5	5559	9927	0.65%	0.086%
58	9.841	2735	2737	2739	rVB	139	53	0.00%	0.000%
59	9.915	2755	2760	2762	rBV2	265	211	0.01%	0.002%
60	10.021	2789	2793	2794	rBV	148	90	0.01%	0.001%
61	10.149	2822	2833	2852	rBV	410972	649247	42.23%	5.617%
62	10.439	2919	2923	2925	rBV2	263	191	0.01%	0.002%
63	10.474	2932	2934	2935	rBV2	222	81	0.01%	0.001%
64	10.513	2943	2946	2949	rBV2	325	184	0.01%	0.002%
65	10.558	2958	2960	2961	rBV	154	53	0.00%	0.000%
66	10.612	2974	2977	2980	rBV	210	130	0.01%	0.001%
67	10.651	2983	2989	2992	rBV	209	212	0.01%	0.002%
68	10.686	2998	3000	3002	rBV2	233	93	0.01%	0.001%
69	10.818	3039	3041	3046	rBV2	225	152	0.01%	0.001%
70	10.902	3064	3067	3068	rBV	504	297	0.02%	0.003%
71	11.185	3144	3155	3178	rBV	566531	898298	58.43%	7.772%
72	11.471	3241	3244	3246	rBV2	431	277	0.02%	0.002%
73	11.516	3255	3258	3259	rBV	273	128	0.01%	0.001%
74	11.558	3259	3271	3294	rBV	653957	1037622	67.49%	8.978%
75	11.818	3350	3352	3360	rBV3	328	414	0.03%	0.004%
76	11.850	3360	3362	3364	rBV	315	150	0.01%	0.001%

LSC Area Percent Report

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Operator : SY/MD
Sample : PB159661TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB661

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\SFAMVLM022924WMA.M
Title : VOC Analysis

77	12.034	3416	3419	3423	rBV	252	202	0.01%	0.002%
78	12.246	3482	3485	3487	rBV	283	170	0.01%	0.001%
79	12.464	3552	3553	3554	rBV	211	66	0.00%	0.001%
80	12.648	3608	3610	3612	rBV	284	157	0.01%	0.001%
81	12.898	3686	3688	3690	rVB	213	62	0.00%	0.001%
82	13.165	3769	3771	3774	rBV2	238	185	0.01%	0.002%
83	13.291	3809	3810	3813	rBV	308	201	0.01%	0.002%
84	13.683	3929	3932	3934	rBV3	683	500	0.03%	0.004%
85	14.078	4051	4055	4057	rBV2	571	515	0.03%	0.004%
86	14.239	4101	4105	4106	rBV	492	357	0.02%	0.003%

Sum of corrected areas: 11557792

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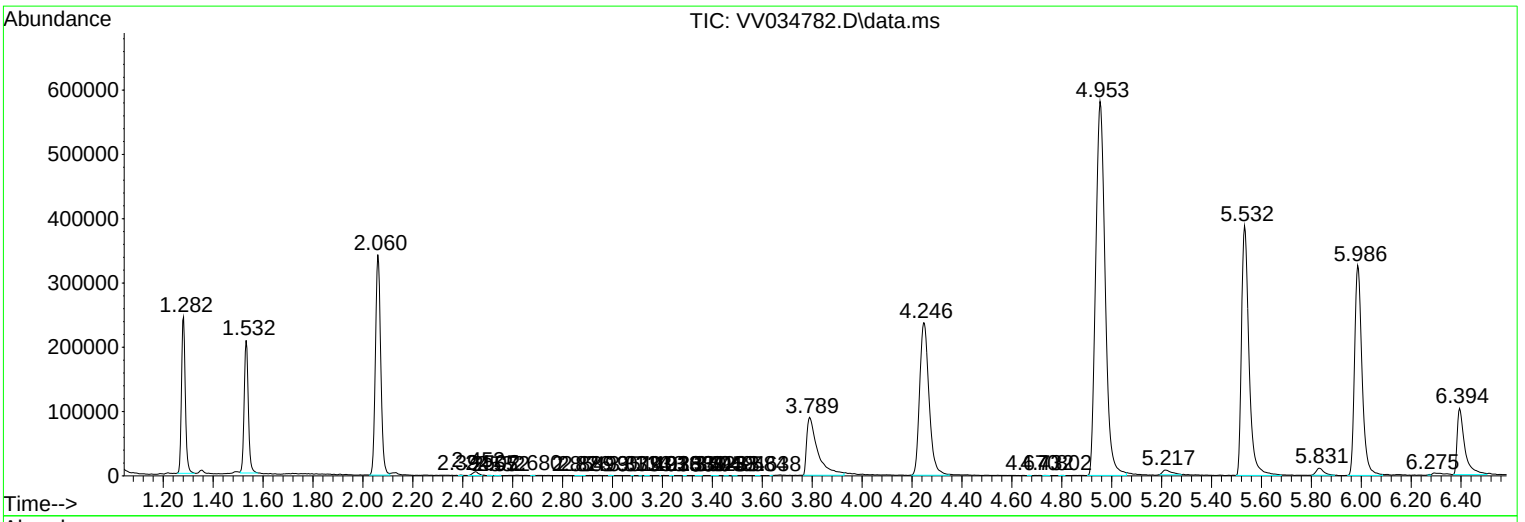
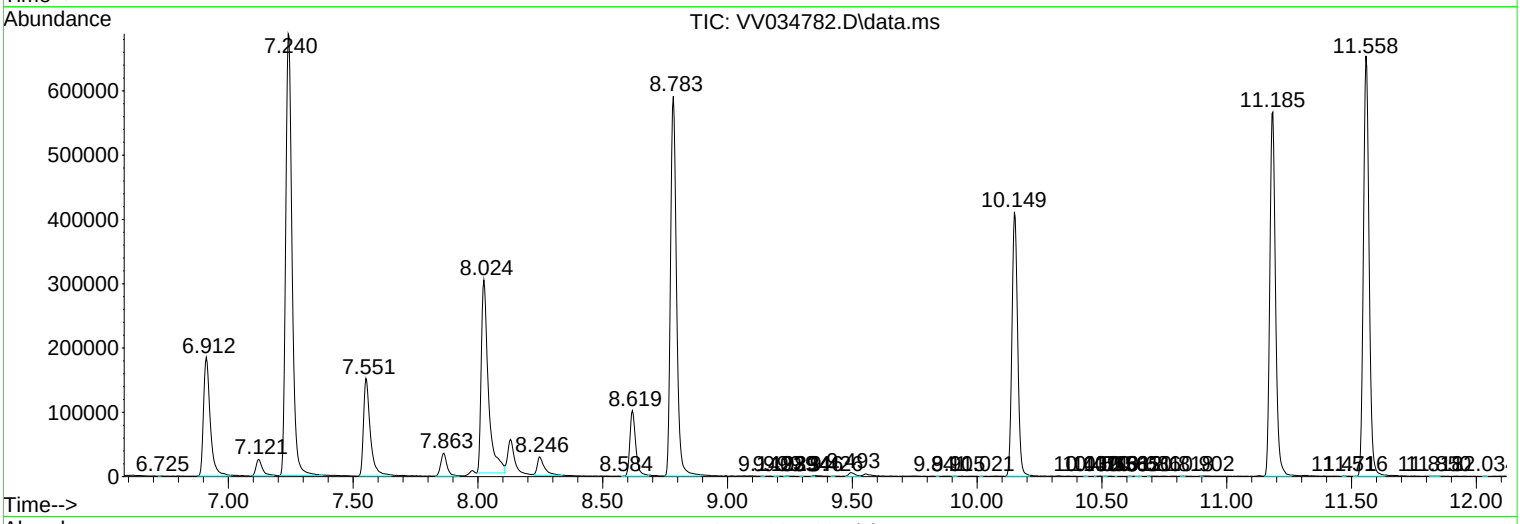
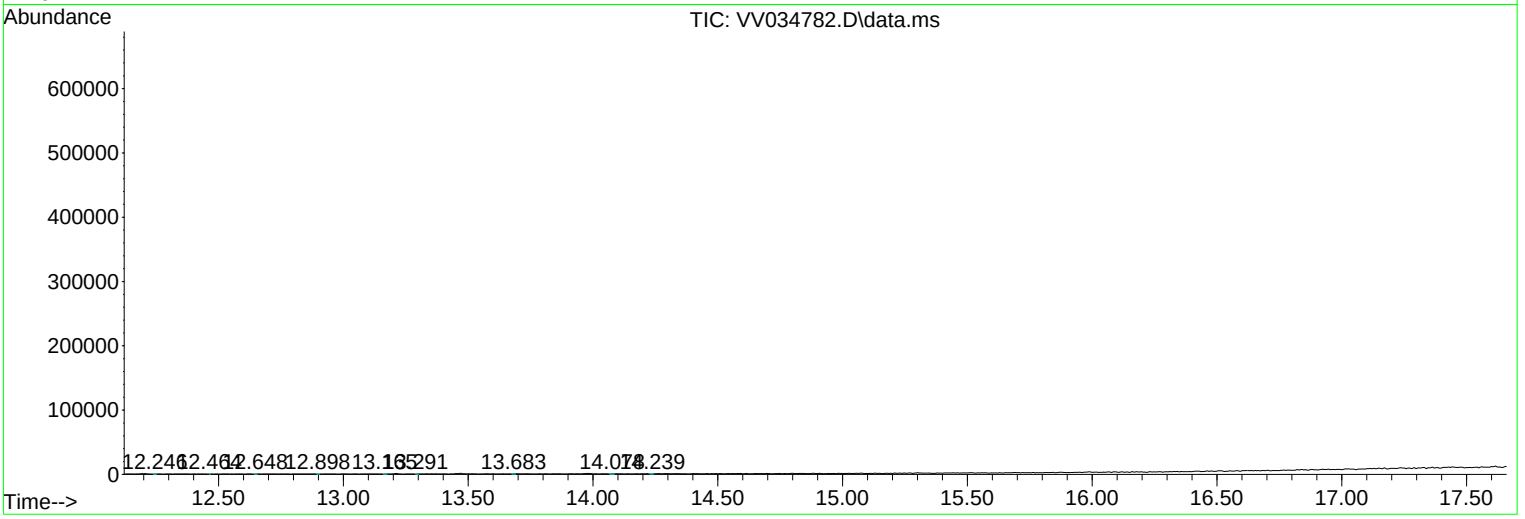
Instrument :
MSVOA_V
ClientSampleId :
VLEB661

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022924WMA.M
Quant Title : VOC Analysis

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032124\
Data File : VV034782.D
Acq On : 21 Mar 2024 12:26
Operator : SY/MD
Sample : PB159661TB 10X
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB661

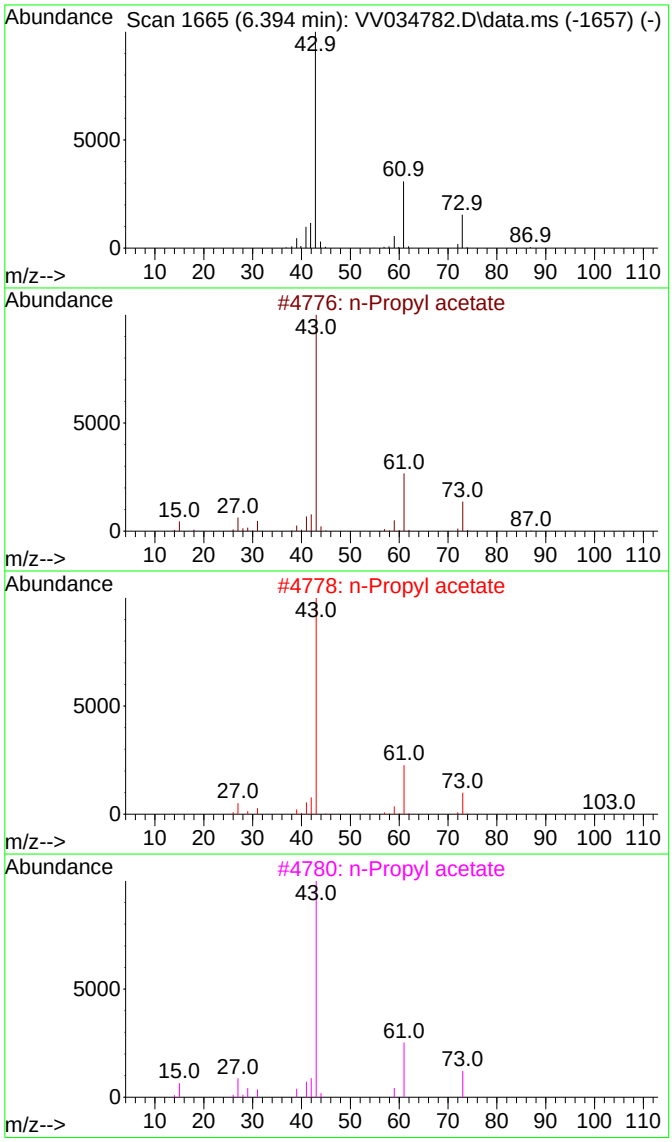
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022924WMA.M
Quant Title : VOC Analysis

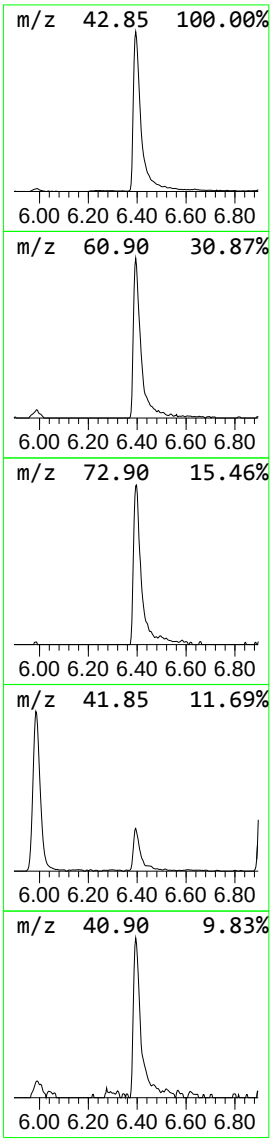
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.394	13.45 ug/L	216788	1,4-Difluorobenzene	5.532

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	72
4	n-Propyl acetate	102	C5H10O2	000109-60-4	64
5	n-Propyl acetate	102	C5H10O2	000109-60-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032124\
Data File : VV034782.D
Acq On : 21 Mar 2024 12:26
Operator : SY/MD
Sample : PB159661TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB661

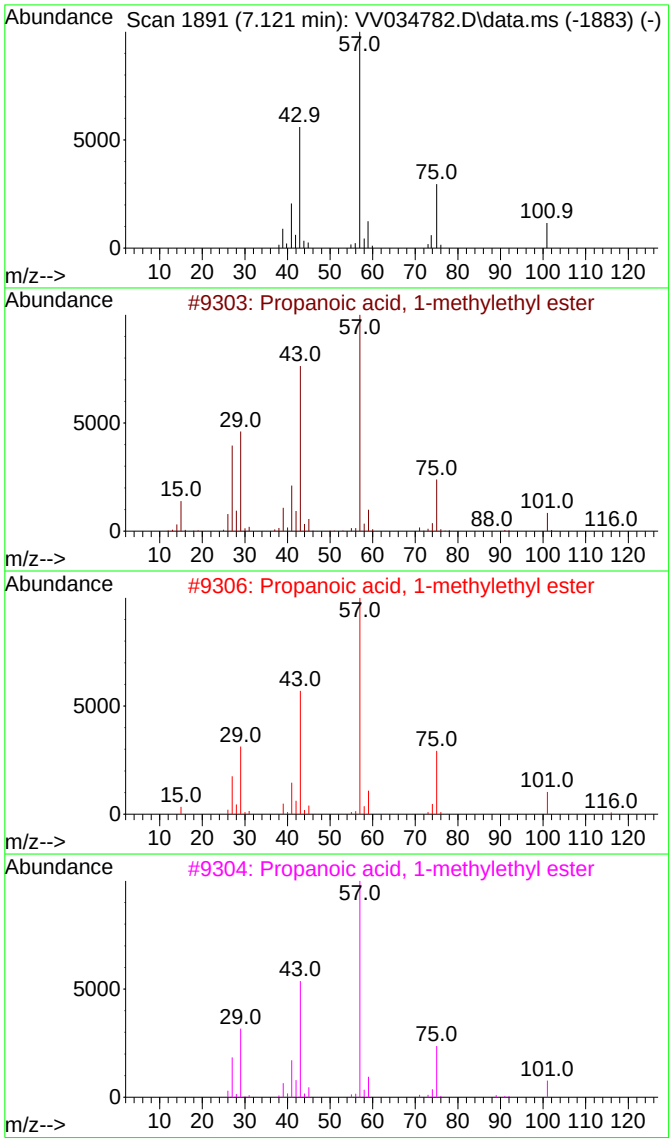
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022924WMA.M
Quant Title : VOC Analysis

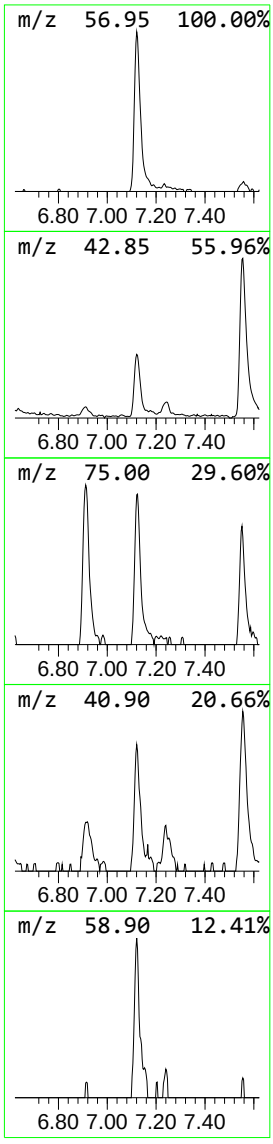
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.121	2.84 ug/L	45846	1,4-Difluorobenzene	5.532

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032124\
Data File : VV034782.D
Acq On : 21 Mar 2024 12:26
Operator : SY/MD
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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB661

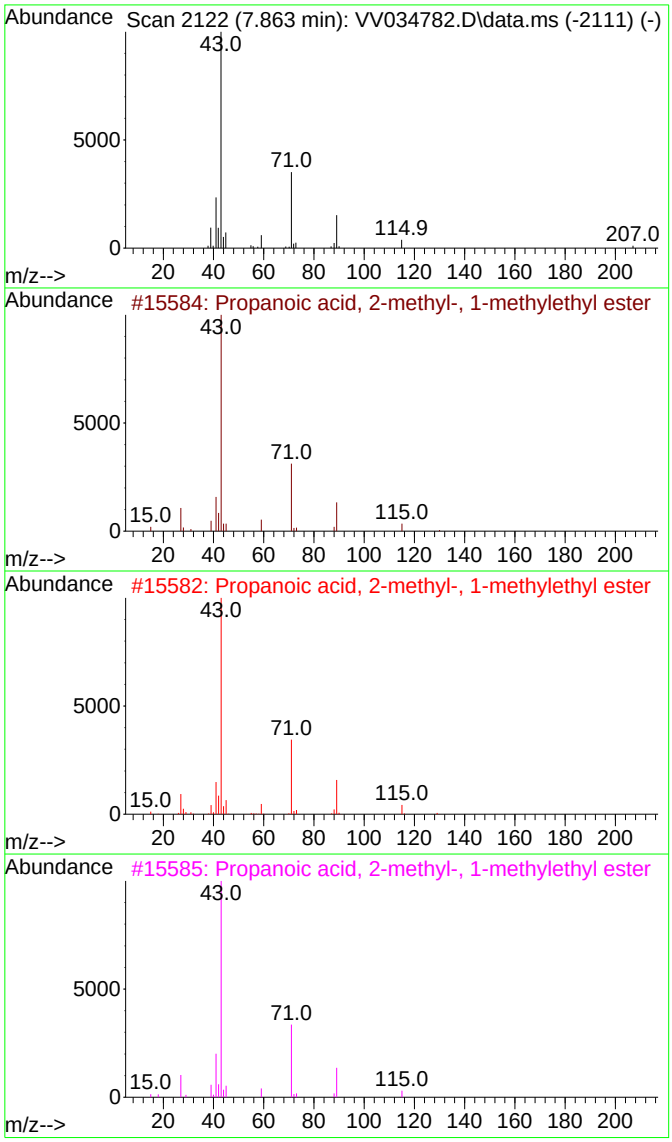
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022924WMA.M
Quant Title : VOC Analysis

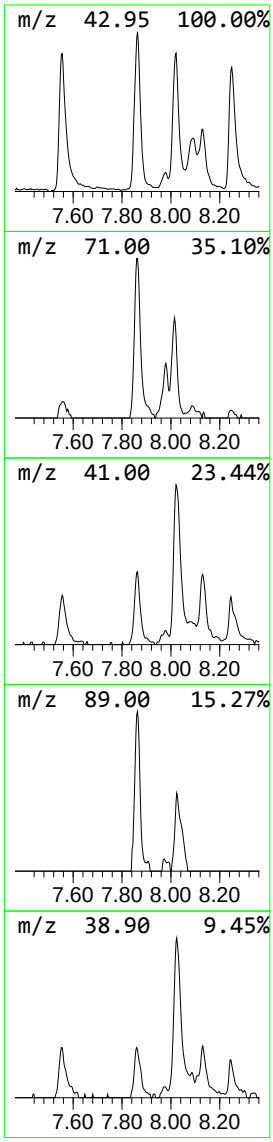
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	3.17 ug/L	62745	Chlorobenzene-d5	8.783

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB661

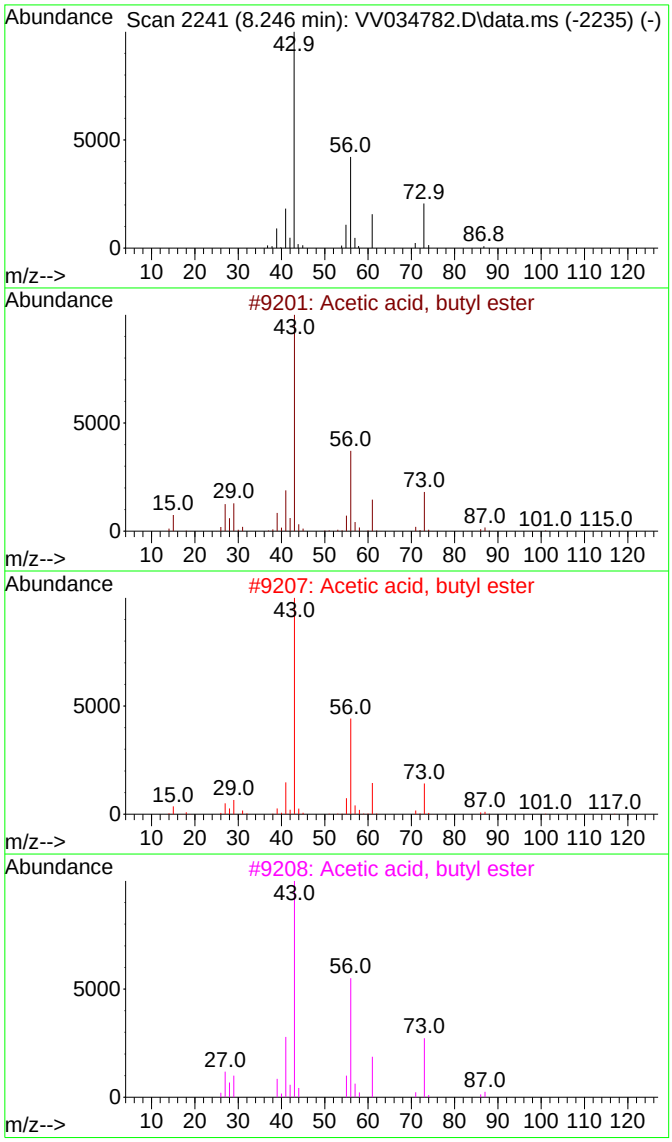
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022924WMA.M
Quant Title : VOC Analysis

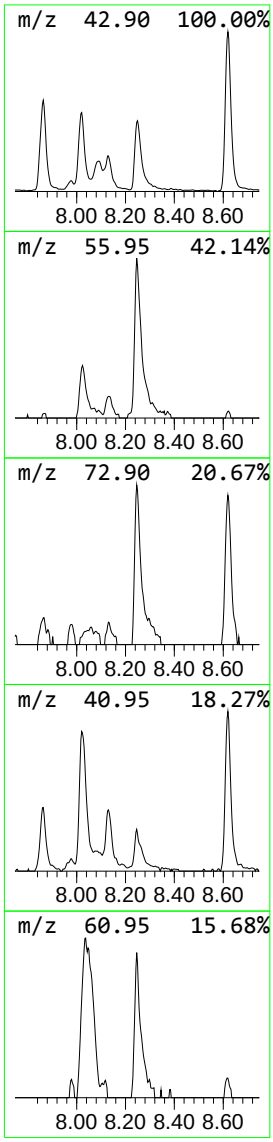
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.246	2.93 ug/L	57987	Chlorobenzene-d5	8.783

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
5	Isobutyl acetate	116	C6H12O2	000110-19-0	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032124\
Data File : VV034782.D
Acq On : 21 Mar 2024 12:26
Operator : SY/MD
Sample : PB159661TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB661

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022924WMA.M
Quant Title : VOC Analysis

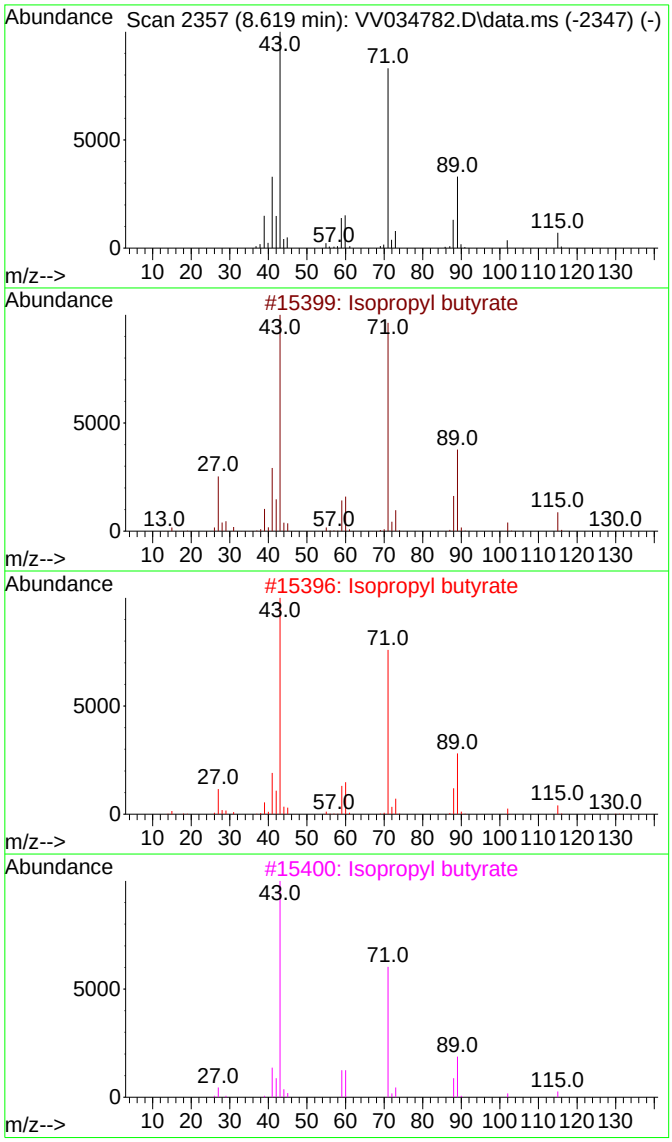
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

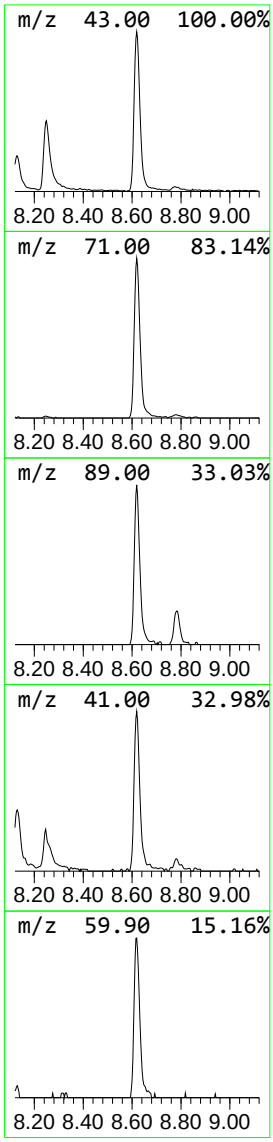
****

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	8.57 ug/L	169337	Chlorobenzene-d5	8.783

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-, propy...	130	C7H14O2	000644-49-5	72
5	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032124\
Data File : VV034782.D
Acq On : 21 Mar 2024 12:26
Operator : SY/MD
Sample : PB159661TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB661

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022924WMA.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	6.394	13.4	ug/L	216788	1	5.532	805896	50.0
Propanoic acid,...	7.121	2.8	ug/L	45846	1	5.532	805896	50.0
Propanoic acid,...	7.863	3.2	ug/L	62745	2	8.783	988534	50.0
Acetic acid, bu...	8.246	2.9	ug/L	57987	2	8.783	988534	50.0
Isopropyl butyrate	8.619	8.6	ug/L	169337	2	8.783	988534	50.0