LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112522\
Data File : VU052136.D
Acq On : 25 Nov 2022 12:03
Operator : JC/MD
Sample : N5711-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0L00

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\SFAMULM112122WMA.M
Title : VOC Analysis

Signal : TIC: VU052136.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	35	43	52	rBV3	10014	20572	1.18%	0.148%
2	1.600	73	81	101	rVB	265832	303481	17.34%	2.187%
3	1.906	167	176	198	rVB	175951	262960	15.03%	1.895%
4	2.379	317	323	333	rVB7	3201	5087	0.29%	0.037%
5	2.565	367	381	393	rBV	379466	619686	35.41%	4.466%
6	2.623	394	399	417	rVB	18516	33860	1.94%	0.244%
7	2.790	441	451	463	rVB3	1985	3966	0.23%	0.029%
8	2.838	463	466	470	rBV2	392	321	0.02%	0.002%
9	2.960	494	504	513	rVB4	1106	2152	0.12%	0.016%
10	3.044	518	530	550	rVV3	18742	39261	2.24%	0.283%
11	3.115	550	552	556	rVV3	557	498	0.03%	0.004%
12	3.186	560	574	588	rVV2	15490	37163	2.12%	0.268%
13	3.276	598	602	613	rBV3	766	1148	0.07%	0.008%
14	3.488	662	668	671	rBV3	400	418	0.02%	0.003%
15	3.652	715	719	724	rVB2	382	450	0.03%	0.003%
16	3.729	740	743	749	rVB2	463	291	0.02%	0.002%
17	3.838	767	777	794	rVB3	4443	10080	0.58%	0.073%
18	3.915	798	801	804	rBV3	323	259	0.01%	0.002%
19	4.060	839	846	849	rVB2	234	289	0.02%	0.002%
20	4.089	849	855	861	rBV2	227	354	0.02%	0.003%
21	4.317	922	926	929	rBV2	329	261	0.01%	0.002%
22	4.362	936	940	945	rBV3	422	394	0.02%	0.003%
23	4.398	948	951	955	rVV2	379	300	0.02%	0.002%
24	4.465	966	972	975	rBV	283	284	0.02%	0.002%
25	4.549	994	998	1004	rBV3	284	289	0.02%	0.002%
26	4.616	1004	1019	1047	rBV	147327	357815	20.45%	2.579%
27	4.938	1114	1119	1121	rBV3	398	330	0.02%	0.002%
28	5.060	1140	1157	1178	rBV	312370	682549	39.01%	4.919%
29	5.211	1201	1204	1208	rVB2	897	610	0.03%	0.004%
30	5.237	1208	1212	1216	rBV3	569	486	0.03%	0.004%
31	5.279	1221	1225	1226	rVV	382	287	0.02%	0.002%
32	5.295	1226	1230	1235	rVB2	796	752	0.04%	0.005%
33	5.722	1342	1363	1393	rBV2	646510	1749846	100.00%	12.610%
34	5.909	1410	1421	1437	rBV	15783	32676	1.87%	0.235%
35	6.047	1460	1464	1469	rVB3	965	879	0.05%	0.006%
36	6.247	1512	1526	1555	rBV	538589	1029983	58.86%	7.422%

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Instrument :
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ClientSampleId :
C0L00

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\SFAMULM112122WMA.M
Title : VOC Analysis

37	6.407	1574	1576	1579	rVB2	500	301	0.02%	0.002%
38	6.536	1607	1616	1619	rBV6	1475	2108	0.12%	0.015%
39	6.587	1628	1632	1633	rBV3	438	282	0.02%	0.002%
40	6.600	1634	1636	1640	rVB2	564	390	0.02%	0.003%
41	6.687	1648	1663	1689	rBV	404057	793103	45.32%	5.715%
42	6.925	1727	1737	1752	rBV2	8077	19490	1.11%	0.140%
43	7.037	1760	1772	1801	rBV	168753	312187	17.84%	2.250%
44	7.156	1807	1809	1812	rBV2	515	347	0.02%	0.003%
45	7.182	1813	1817	1821	rVB5	1149	1046	0.06%	0.008%
46	7.298	1850	1853	1857	rVB2	669	498	0.03%	0.004%
47	7.394	1879	1883	1887	rBV2	455	586	0.03%	0.004%
48	7.562	1922	1935	1960	rBV	199410	353429	20.20%	2.547%
49	7.661	1964	1966	1975	rVB5	827	756	0.04%	0.005%
50	7.735	1978	1989	2002	rBV2	34016	57295	3.27%	0.413%
51	7.896	2023	2039	2068	rBV	770938	1347236	76.99%	9.709%
52	8.176	2109	2126	2146	rBV3	152975	309262	17.67%	2.229%
53	8.311	2166	2168	2173	rVB4	399	315	0.02%	0.002%
54	8.333	2173	2175	2177	rBV2	408	279	0.02%	0.002%
55	8.462	2205	2215	2231	rBV2	38101	63164	3.61%	0.455%
56	8.571	2234	2249	2256	rBV6	7522	16632	0.95%	0.120%
57	8.629	2256	2267	2288	rVV	457390	826545	47.24%	5.956%
58	8.726	2289	2297	2315	rVB	83070	137757	7.87%	0.993%
59	8.832	2322	2330	2347	rVB	47663	78286	4.47%	0.564%
60	8.989	2377	2379	2384	rVB3	521	364	0.02%	0.003%
61	9.018	2384	2388	2389	rBV3	743	461	0.03%	0.003%
62	9.070	2400	2404	2410	rVB3	345	416	0.02%	0.003%
63	9.124	2416	2421	2425	rBV2	402	356	0.02%	0.003%
64	9.208	2435	2447	2461	rBV	114827	181404	10.37%	1.307%
65	9.365	2487	2496	2498	rBV4	2561	3233	0.18%	0.023%
66	9.414	2499	2511	2544	rVB	787014	1299241	74.25%	9.363%
67	9.639	2575	2581	2588	rBV6	1591	1812	0.10%	0.013%
68	9.870	2649	2653	2658	rVB	233	250	0.01%	0.002%
69	9.902	2660	2663	2664	rBV2	516	286	0.02%	0.002%
70	10.073	2708	2716	2727	rBV4	7036	11688	0.67%	0.084%
71	10.320	2788	2793	2798	rBV2	398	392	0.02%	0.003%
72	10.378	2807	2811	2815	rVB2	432	305	0.02%	0.002%
73	10.465	2834	2838	2841	rVB2	371	330	0.02%	0.002%
74	10.488	2841	2845	2847	rBV2	419	371	0.02%	0.003%
75	10.574	2867	2872	2876	rVB2	261	291	0.02%	0.002%
76	10.639	2889	2892	2900	rVB4	593	545	0.03%	0.004%

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Sample : N5711-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0L00

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\SFAMULM112122WMA.M
Title : VOC Analysis

77	10.754	2914	2928	2949	rBV	573886	923626	52.78%	6.656%
78	11.092	3028	3033	3034	rBV	556	469	0.03%	0.003%
79	11.150	3048	3051	3057	rBV3	381	357	0.02%	0.003%
80	11.414	3130	3133	3135	rBV3	518	266	0.02%	0.002%
81	11.500	3157	3160	3163	rBV2	326	283	0.02%	0.002%
82	11.745	3233	3236	3240	rBV	622	541	0.03%	0.004%
83	11.809	3244	3256	3277	rBV	581211	921439	52.66%	6.640%
84	11.986	3308	3311	3315	rVB	859	651	0.04%	0.005%
85	12.015	3315	3320	3323	rBV2	378	406	0.02%	0.003%
86	12.066	3334	3336	3342	rVB3	632	595	0.03%	0.004%
87	12.102	3342	3347	3351	rBV2	393	443	0.03%	0.003%
88	12.192	3361	3375	3409	rBV	596688	999645	57.13%	7.204%
89	12.330	3416	3418	3424	rVB4	557	382	0.02%	0.003%
90	12.388	3432	3436	3438	rBV2	598	349	0.02%	0.003%
91	12.745	3543	3547	3552	rVV3	340	342	0.02%	0.002%
92	12.790	3558	3561	3564	rVB2	516	362	0.02%	0.003%
93	12.857	3578	3582	3586	rBB2	692	442	0.03%	0.003%
94	12.896	3590	3594	3598	rBV2	560	635	0.04%	0.005%
95	13.941	3917	3919	3922	rBV3	397	286	0.02%	0.002%
96	14.574	4113	4116	4118	rBV2	537	319	0.02%	0.002%
97	14.828	4193	4195	4199	rBV	625	437	0.02%	0.003%
98	15.352	4356	4358	4361	rBV3	548	341	0.02%	0.002%
99	15.873	4517	4520	4522	rBV2	785	606	0.03%	0.004%
100	16.011	4561	4563	4566	rBV3	613	482	0.03%	0.003%

Sum of corrected areas: 13876780

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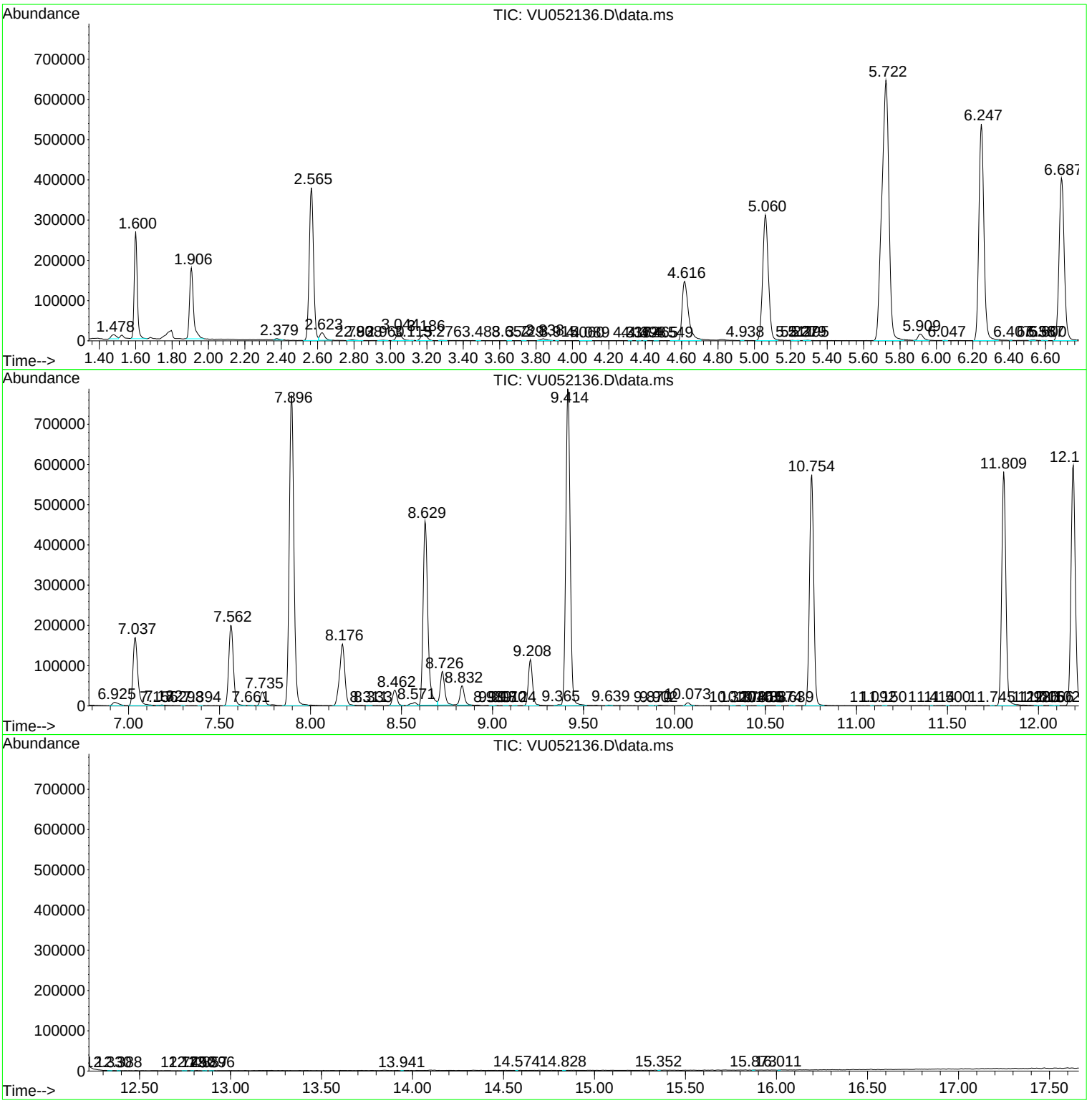
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0L00

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112522\
Data File : VU052136.D
Acq On : 25 Nov 2022 12:03
Operator : JC/MD
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0L00

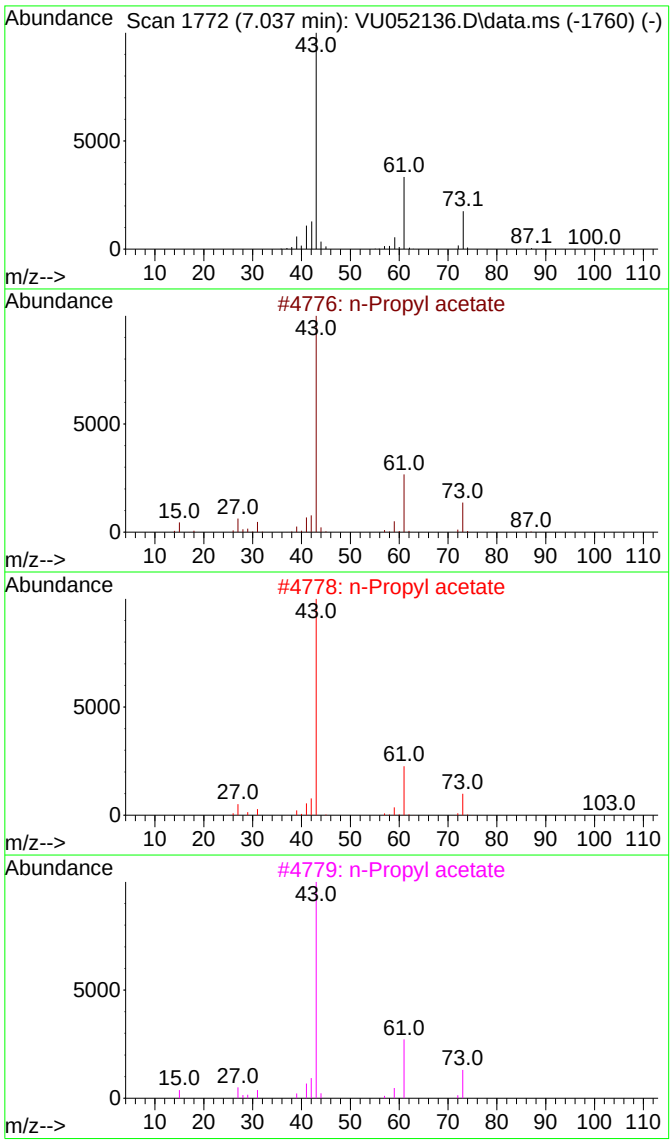
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

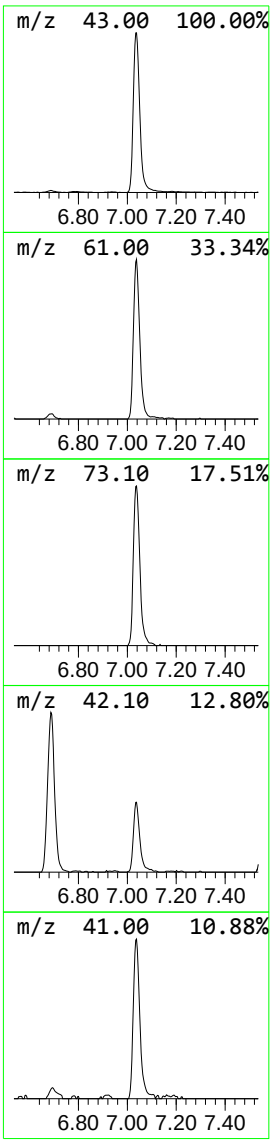
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.037	15.15 ug/L	312187	1,4-Difluorobenzene	6.247

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112522\
Data File : VU052136.D
Acq On : 25 Nov 2022 12:03
Operator : JC/MD
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0L00

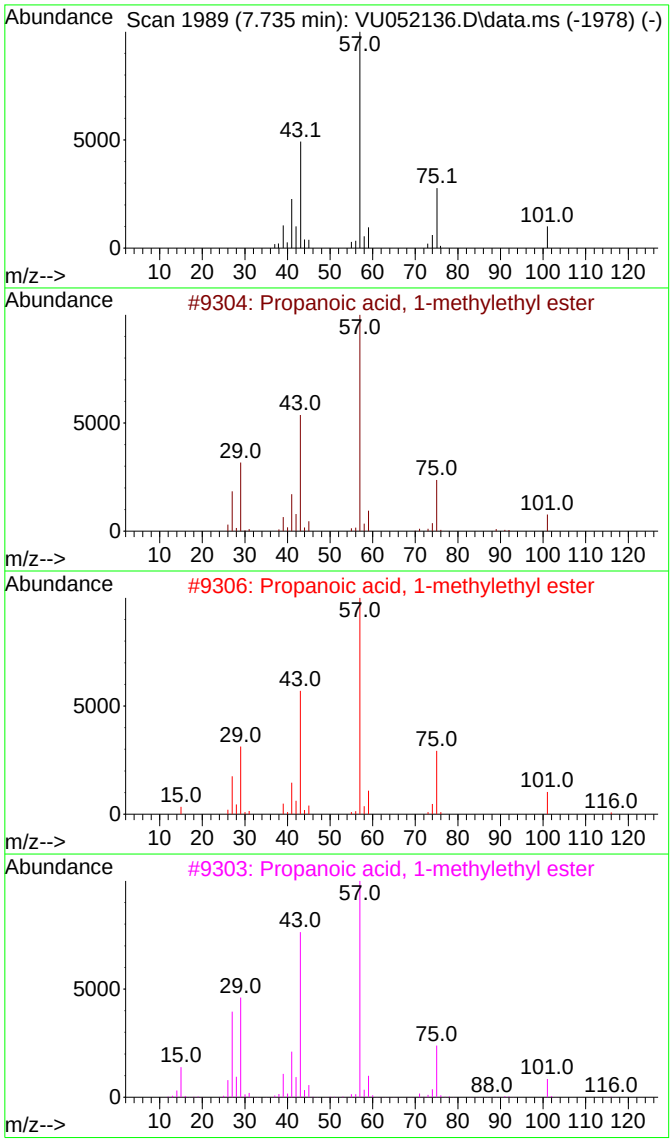
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

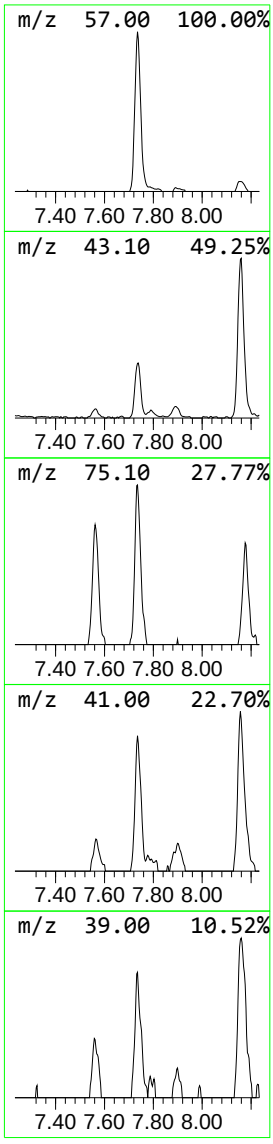
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.735	2.78 ug/L	57295	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50





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Instrument :
MSVOA_U
ClientSampleId :
C0L00

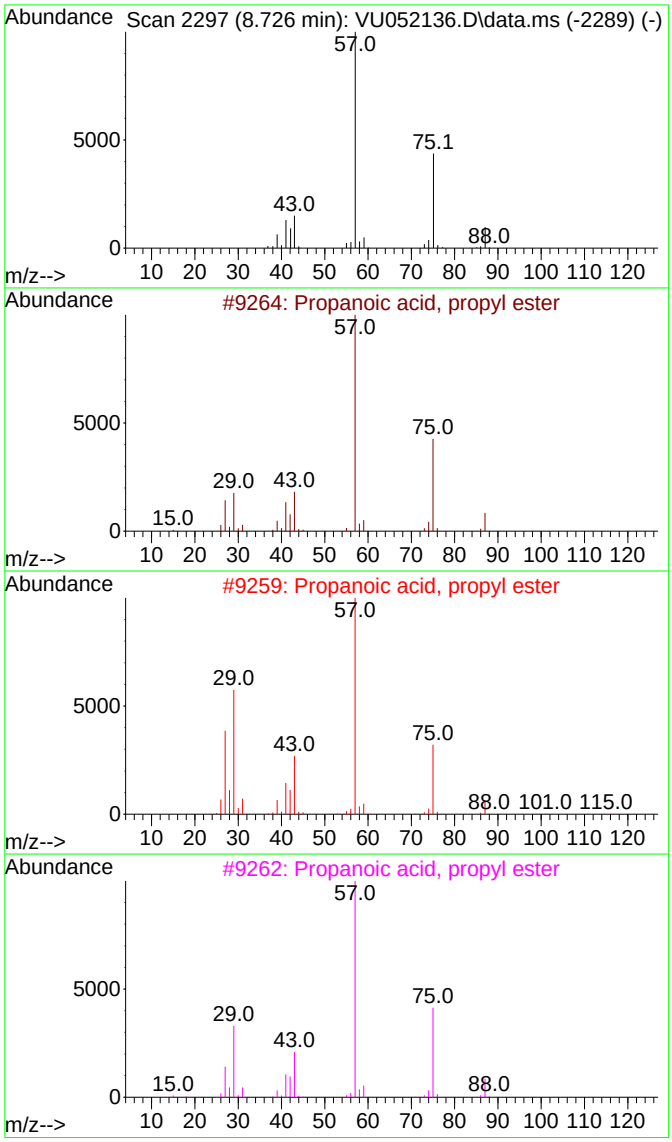
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

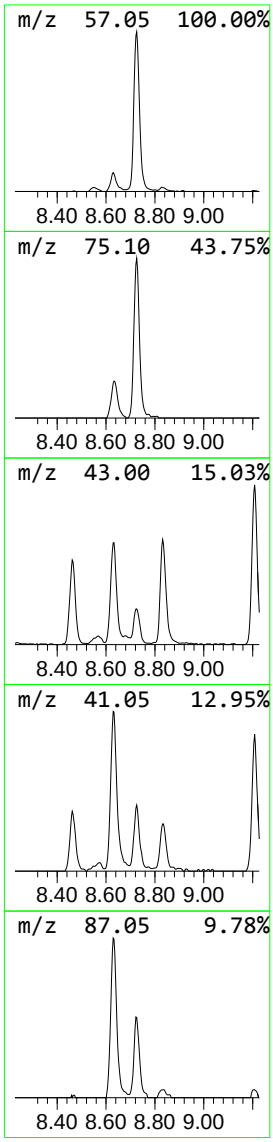
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	5.30 ug/L	137757	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	74
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72





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Instrument :
MSVOA_U
ClientSampleId :
C0L00

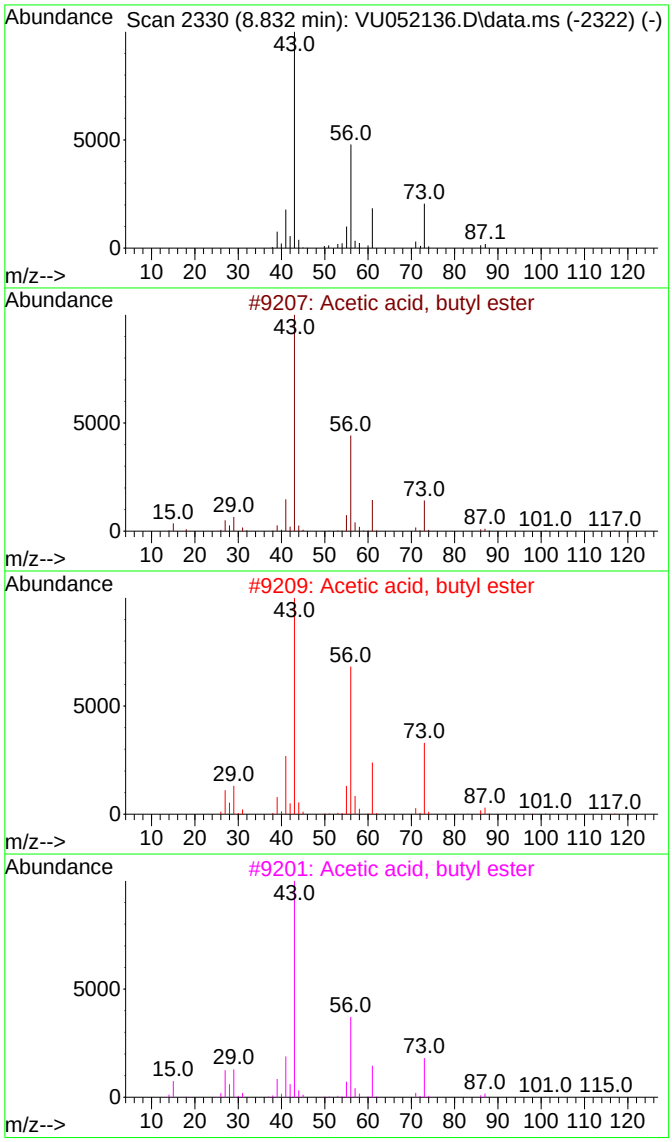
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

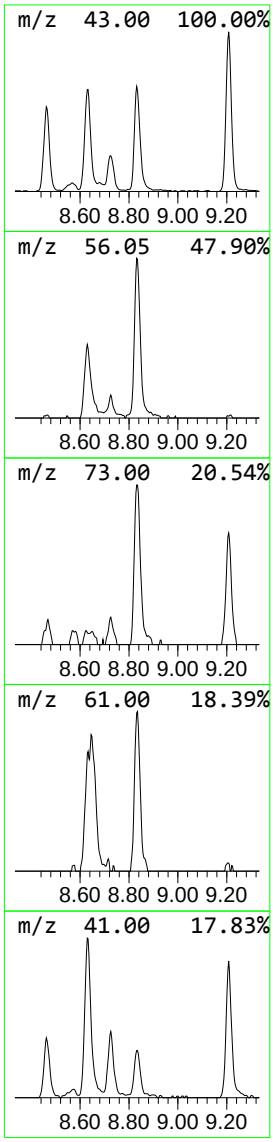
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.832	3.01 ug/L	78286	Chlorobenzene-d5	9.414

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
5	Isobutyl acetate	116	C6H12O2	000110-19-0	39





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Data File : VU052136.D
Acq On : 25 Nov 2022 12:03
Operator : JC/MD
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0L00

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

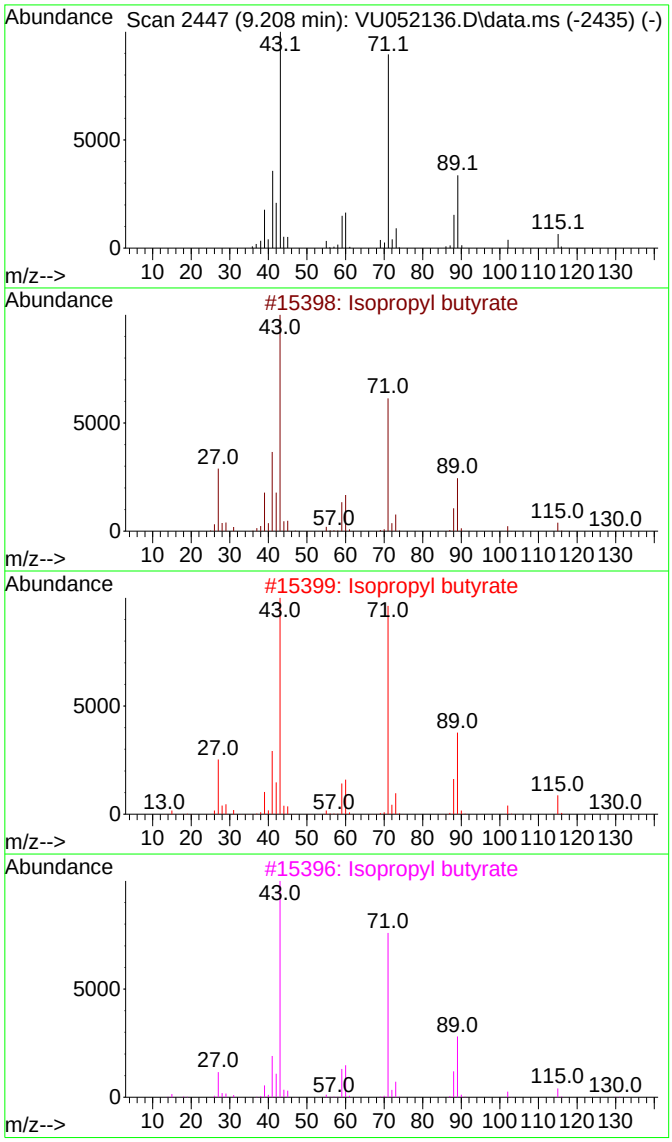
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

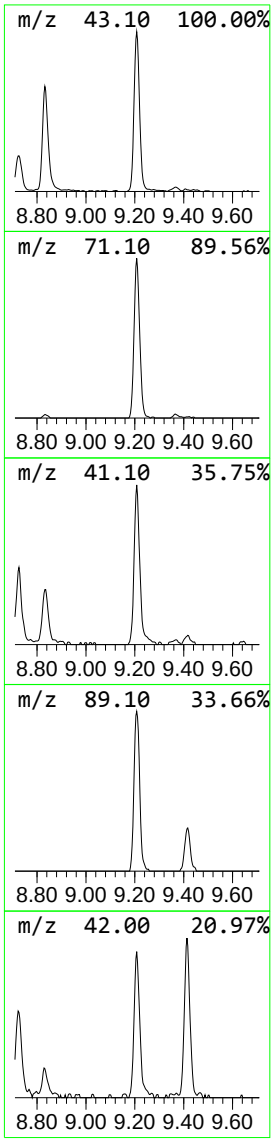
****

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.208	6.98 ug/L	181404	Chlorobenzene-d5	9.414

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	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	78
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112522\
Data File : VU052136.D
Acq On : 25 Nov 2022 12:03
Operator : JC/MD
Sample : N5711-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0L00

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.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	7.037	15.2	ug/L	312187	1	6.247	1029980	50.0
Propanoic acid,...	7.735	2.8	ug/L	57295	1	6.247	1029980	50.0
Propanoic acid,...	8.726	5.3	ug/L	137757	2	9.414	1299240	50.0
Acetic acid, bu...	8.832	3.0	ug/L	78286	2	9.414	1299240	50.0
Isopropyl butyrate	9.208	7.0	ug/L	181404	2	9.414	1299240	50.0