LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049360.D
Acq On : 22 Jun 2022 18:30
Operator : SY/MD
Sample : N3392-15 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ0

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\SFAMULM061022WMA.M
Title : VOC Analysis

Signal : TIC: VU049360.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	74	80	97	rBV	65991	73327	10.79%	1.089%
2	1.899	167	174	188	rVB	54562	72128	10.61%	1.071%
3	2.562	369	380	393	rBV	112068	177667	26.14%	2.639%
4	2.626	394	400	409	rVB2	3062	4407	0.65%	0.065%
5	2.771	434	445	447	rBV4	1252	1620	0.24%	0.024%
6	3.044	519	530	547	rVB2	16380	31107	4.58%	0.462%
7	3.115	547	552	557	rBV3	288	343	0.05%	0.005%
8	3.182	558	573	598	rVB	24776	61223	9.01%	0.909%
9	3.404	635	642	644	rBV2	224	274	0.04%	0.004%
10	3.459	652	659	664	rBV3	306	423	0.06%	0.006%
11	3.526	678	680	684	rVB2	204	134	0.02%	0.002%
12	3.546	684	686	688	rBV2	212	146	0.02%	0.002%
13	3.571	691	694	695	rBV	265	129	0.02%	0.002%
14	3.661	719	722	725	rBV	209	123	0.02%	0.002%
15	3.678	725	727	735	rVB2	278	221	0.03%	0.003%
16	3.816	768	770	777	rVB	344	211	0.03%	0.003%
17	3.899	793	796	799	rBV3	258	184	0.03%	0.003%
18	3.960	812	815	817	rBV	178	141	0.02%	0.002%
19	4.147	871	873	878	rBV2	258	192	0.03%	0.003%
20	4.211	890	893	896	rVV2	249	207	0.03%	0.003%
21	4.375	942	944	949	rBV2	149	122	0.02%	0.002%
22	4.420	954	958	960	rBV2	194	168	0.02%	0.002%
23	4.513	982	987	992	rBV	401	374	0.06%	0.006%
24	4.546	992	997	1000	rBV2	363	281	0.04%	0.004%
25	4.620	1007	1020	1048	rBV	118668	291513	42.88%	4.330%
26	4.986	1131	1134	1137	rVB	220	134	0.02%	0.002%
27	5.063	1141	1158	1178	rBV	136164	294440	43.31%	4.374%
28	5.157	1185	1187	1191	rVB2	540	342	0.05%	0.005%
29	5.198	1197	1200	1202	rVV2	255	144	0.02%	0.002%
30	5.420	1265	1269	1274	rBV2	218	192	0.03%	0.003%
31	5.488	1288	1290	1294	rVB	216	148	0.02%	0.002%
32	5.632	1331	1335	1339	rBV2	382	373	0.05%	0.006%
33	5.722	1342	1363	1388	rVV2	246565	679784	100.00%	10.098%
34	5.912	1412	1422	1433	rBV2	9208	17288	2.54%	0.257%
35	6.005	1447	1451	1452	rBV2	249	128	0.02%	0.002%
36	6.063	1466	1469	1475	rVB2	221	217	0.03%	0.003%

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Instrument :
MSVOA_U
ClientSampleId :
EXEZ0

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\SFAMULM061022WMA.M
Title : VOC Analysis

37	6.095	1475	1479	1483	rBV2	326	210	0.03%	0.003%
38	6.118	1483	1486	1488	rBV2	237	203	0.03%	0.003%
39	6.247	1514	1526	1546	rBV	299038	552213	81.23%	8.203%
40	6.523	1607	1612	1613	rBV2	1482	1202	0.18%	0.018%
41	6.626	1642	1644	1647	rBV2	349	203	0.03%	0.003%
42	6.690	1647	1664	1684	rVV	180240	346529	50.98%	5.147%
43	6.867	1717	1719	1723	rBV3	368	204	0.03%	0.003%
44	6.922	1727	1736	1753	rBV	5616	12197	1.79%	0.181%
45	7.038	1758	1772	1789	rBV	89147	157260	23.13%	2.336%
46	7.311	1853	1857	1860	rVB3	621	422	0.06%	0.006%
47	7.353	1864	1870	1873	rBV3	437	403	0.06%	0.006%
48	7.398	1878	1884	1890	rBV2	498	508	0.07%	0.008%
49	7.436	1890	1896	1907	rVB5	1001	1413	0.21%	0.021%
50	7.513	1915	1920	1923	rBV	245	233	0.03%	0.003%
51	7.565	1924	1936	1956	rVV	91494	159339	23.44%	2.367%
52	7.658	1963	1965	1969	rBV3	314	179	0.03%	0.003%
53	7.687	1969	1974	1980	rBV3	709	961	0.14%	0.014%
54	7.738	1981	1990	2000	rVB2	19992	32979	4.85%	0.490%
55	7.896	2020	2039	2061	rBV	285955	502114	73.86%	7.458%
56	8.176	2105	2126	2142	rBV3	69199	142690	20.99%	2.120%
57	8.349	2177	2180	2184	rBV2	444	323	0.05%	0.005%
58	8.391	2189	2193	2197	rBV3	379	328	0.05%	0.005%
59	8.465	2204	2216	2230	rBV	25348	41887	6.16%	0.622%
60	8.571	2236	2249	2256	rBV8	4549	10536	1.55%	0.157%
61	8.632	2256	2268	2289	rVV	332866	594378	87.44%	8.829%
62	8.726	2291	2297	2310	rVB	49220	75462	11.10%	1.121%
63	8.832	2322	2330	2348	rVB2	19926	34024	5.01%	0.505%
64	8.954	2364	2368	2376	rVB3	415	498	0.07%	0.007%
65	8.989	2376	2379	2380	rBV2	217	136	0.02%	0.002%
66	9.037	2390	2394	2395	rBV	240	198	0.03%	0.003%
67	9.098	2411	2413	2415	rVB	293	137	0.02%	0.002%
68	9.211	2436	2448	2462	rBV	74149	116659	17.16%	1.733%
69	9.417	2500	2512	2531	rBV	391926	645362	94.94%	9.586%
70	9.571	2555	2560	2565	rVB2	338	290	0.04%	0.004%
71	9.610	2568	2572	2575	rVV2	311	271	0.04%	0.004%
72	9.648	2575	2584	2591	rVV6	865	1662	0.24%	0.025%
73	9.780	2622	2625	2630	rVB	343	232	0.03%	0.003%
74	9.922	2662	2669	2680	rBV5	834	1573	0.23%	0.023%
75	10.002	2690	2694	2697	rBV	206	186	0.03%	0.003%
76	10.021	2697	2700	2702	rBV	222	158	0.02%	0.002%

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Sample : N3392-15 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ0

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\SFAMULM061022WMA.M
Title : VOC Analysis

77	10.076	2707	2717	2726	rVV3	4852	7783	1.14%	0.116%
78	10.124	2729	2732	2742	rVB2	233	307	0.05%	0.005%
79	10.304	2786	2788	2791	rVB	288	126	0.02%	0.002%
80	10.446	2829	2832	2834	rBV2	223	144	0.02%	0.002%
81	10.478	2839	2842	2849	rVB3	382	375	0.06%	0.006%
82	10.529	2855	2858	2859	rBV2	307	186	0.03%	0.003%
83	10.671	2895	2902	2907	rBV2	299	450	0.07%	0.007%
84	10.754	2916	2928	2949	rBV	288070	467717	68.80%	6.948%
85	10.841	2952	2955	2959	rBV3	469	415	0.06%	0.006%
86	11.147	3047	3050	3051	rBV	221	133	0.02%	0.002%
87	11.259	3081	3085	3090	rBV2	275	323	0.05%	0.005%
88	11.378	3119	3122	3126	rBV	274	224	0.03%	0.003%
89	11.610	3191	3194	3198	rVB2	381	278	0.04%	0.004%
90	11.767	3240	3243	3244	rBV	236	126	0.02%	0.002%
91	11.812	3244	3257	3281	rVV	376358	606824	89.27%	9.014%
92	11.973	3305	3307	3311	rBV	240	145	0.02%	0.002%
93	12.095	3343	3345	3349	rVB3	441	307	0.05%	0.005%
94	12.192	3362	3375	3395	rBV	310045	498334	73.31%	7.402%
95	12.343	3418	3422	3426	rBV2	399	379	0.06%	0.006%
96	12.674	3522	3525	3526	rBV	407	239	0.04%	0.004%
97	12.751	3546	3549	3550	rBV2	317	186	0.03%	0.003%
98	13.192	3684	3686	3692	rBV2	275	278	0.04%	0.004%
99	13.622	3815	3820	3823	rBV2	682	762	0.11%	0.011%
100	13.915	3909	3911	3916	rBV3	407	467	0.07%	0.007%

Sum of corrected areas: 6732125

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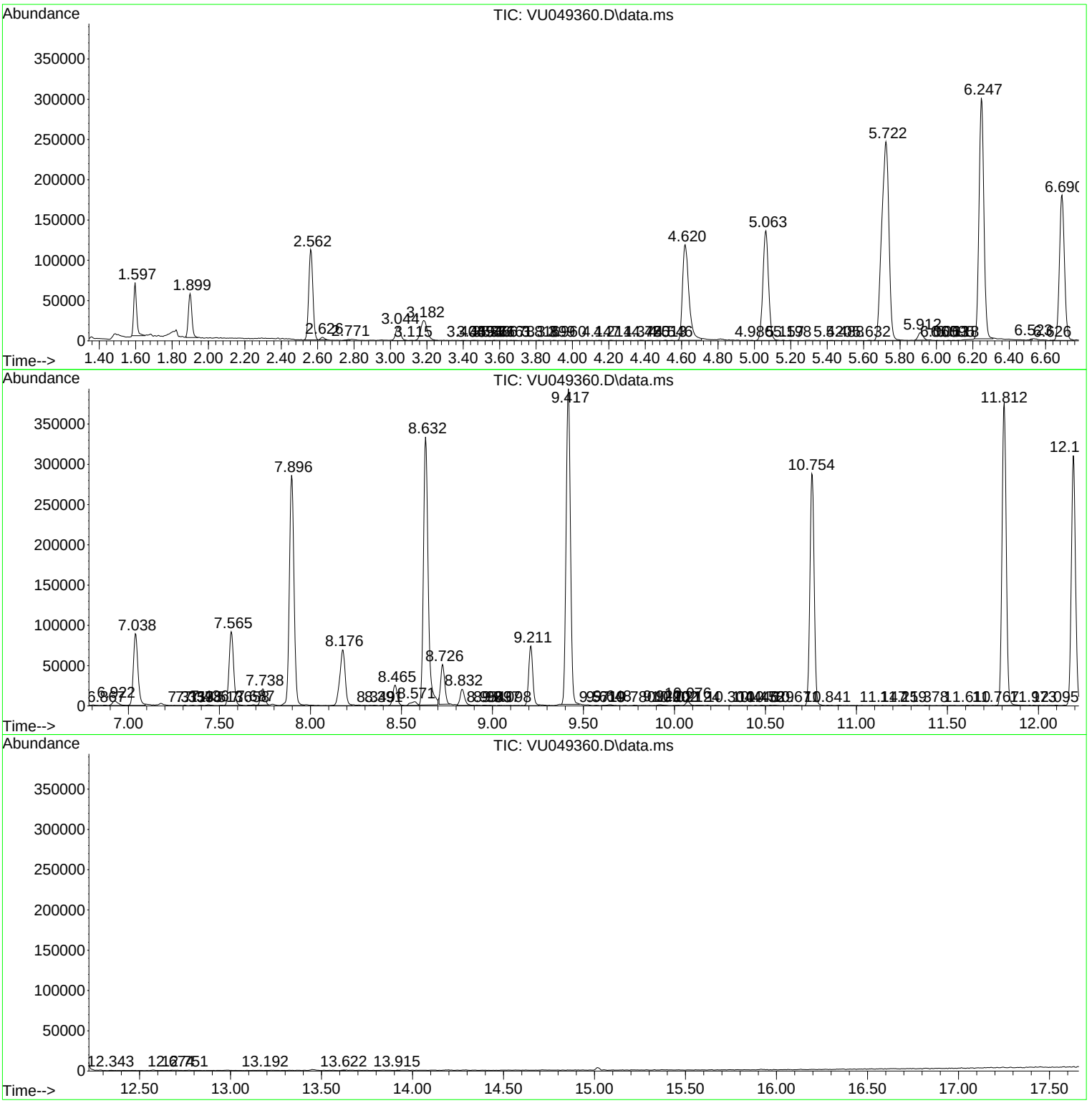
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
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Instrument :
MSVOA_U
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EXEZ0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

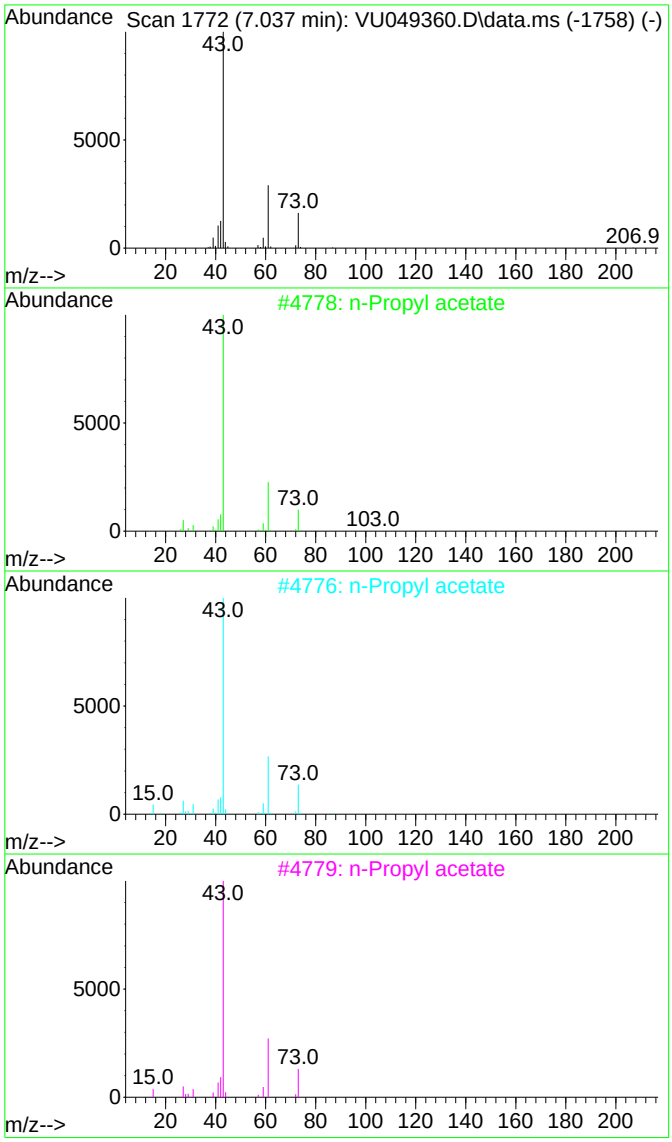
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

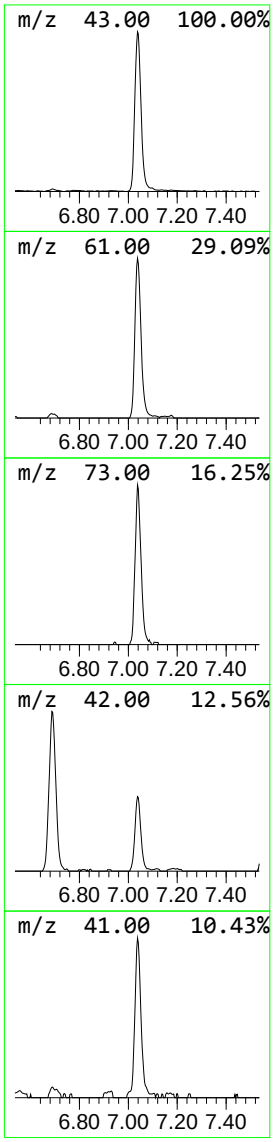
****

Peak Number 3 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.037	14.24 ug/L	157260	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	83
3	n-Propyl acetate	102	C5H10O2	000109-60-4	78
4	n-Propyl acetate	102	C5H10O2	000109-60-4	64
5	n-Propyl acetate	102	C5H10O2	000109-60-4	50





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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ0

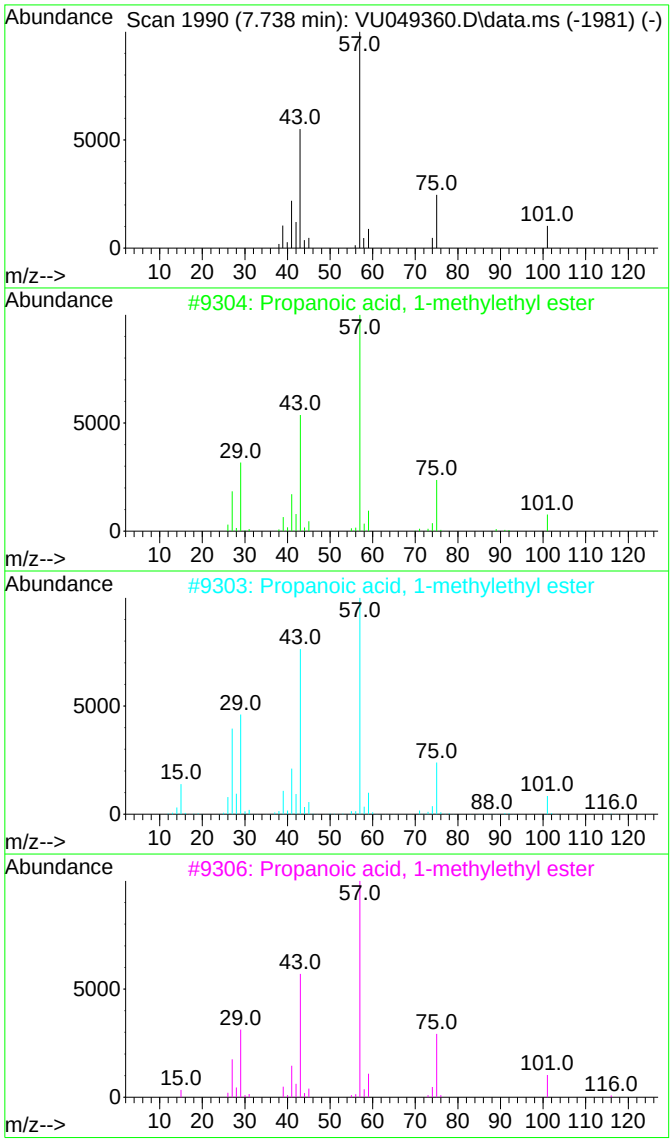
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

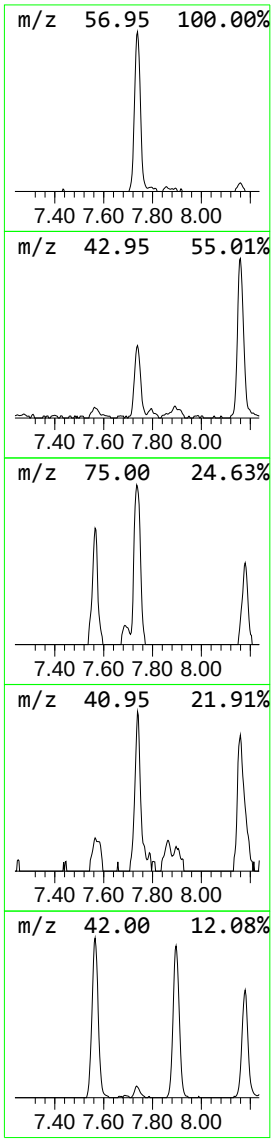
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.738	2.99 ug/L	32979	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	78
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56





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MSVOA_U
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EXEZ0

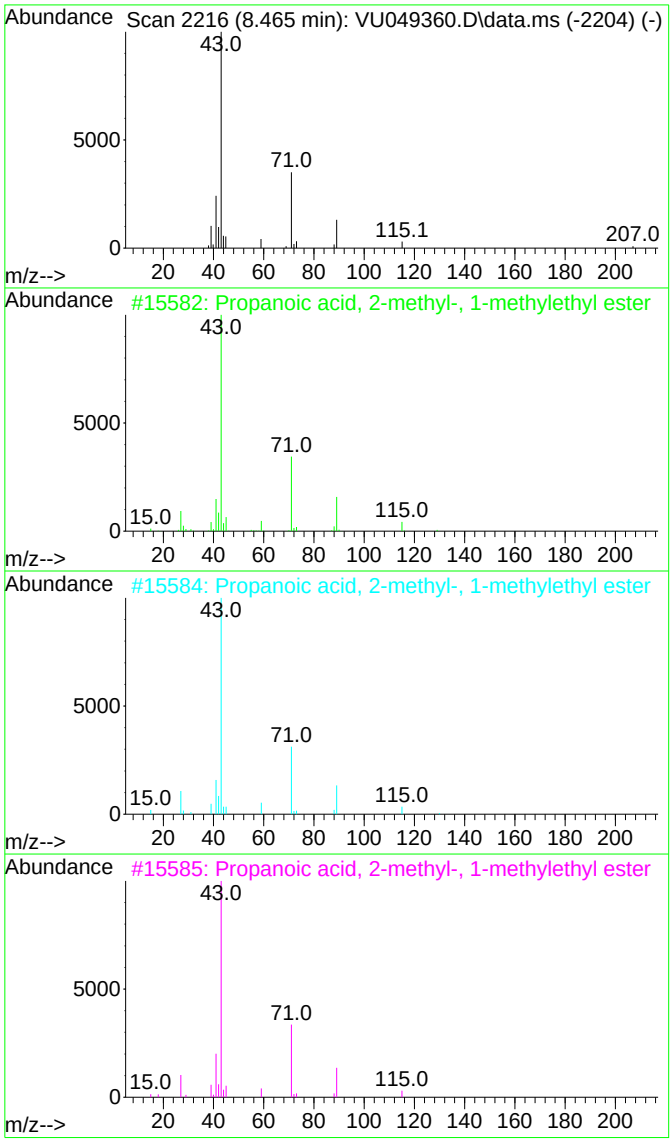
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

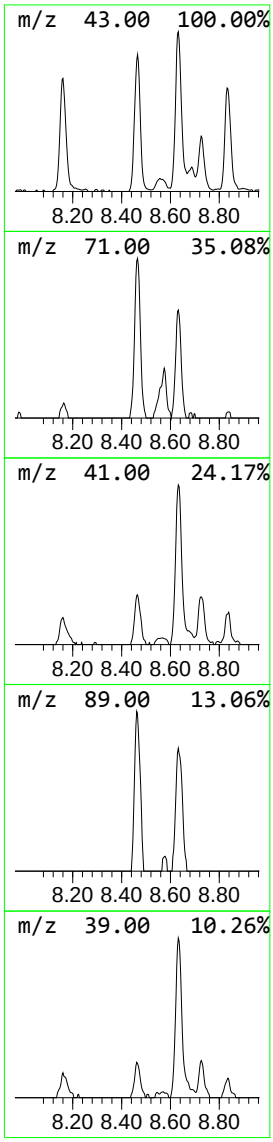
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	3.25 ug/L	41887	Chlorobenzene-d5	9.417

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	83
5	Isopropyl butyrate	130	C7H14O2	000638-11-9	72





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MSVOA_U
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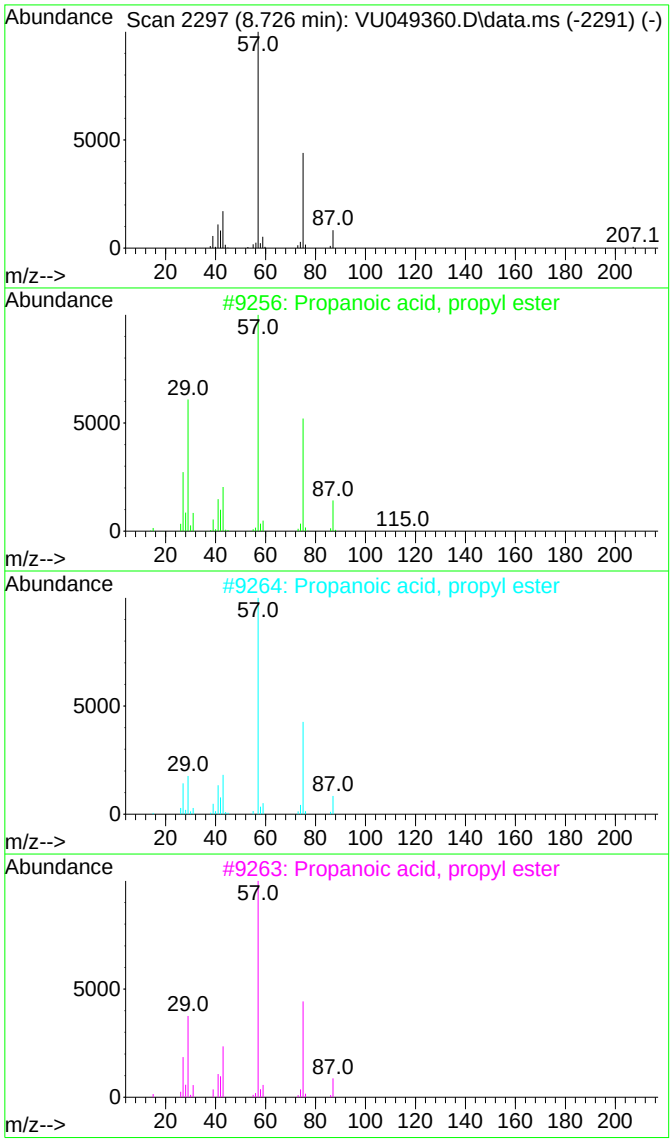
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

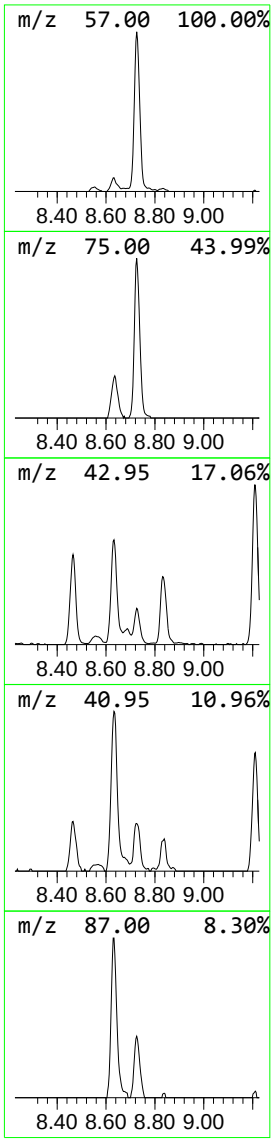
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	5.85 ug/L	75462	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	47
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	47
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	40
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	38





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Data File : VU049360.D
Acq On : 22 Jun 2022 18:30
Operator : SY/MD
Sample : N3392-15 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ0

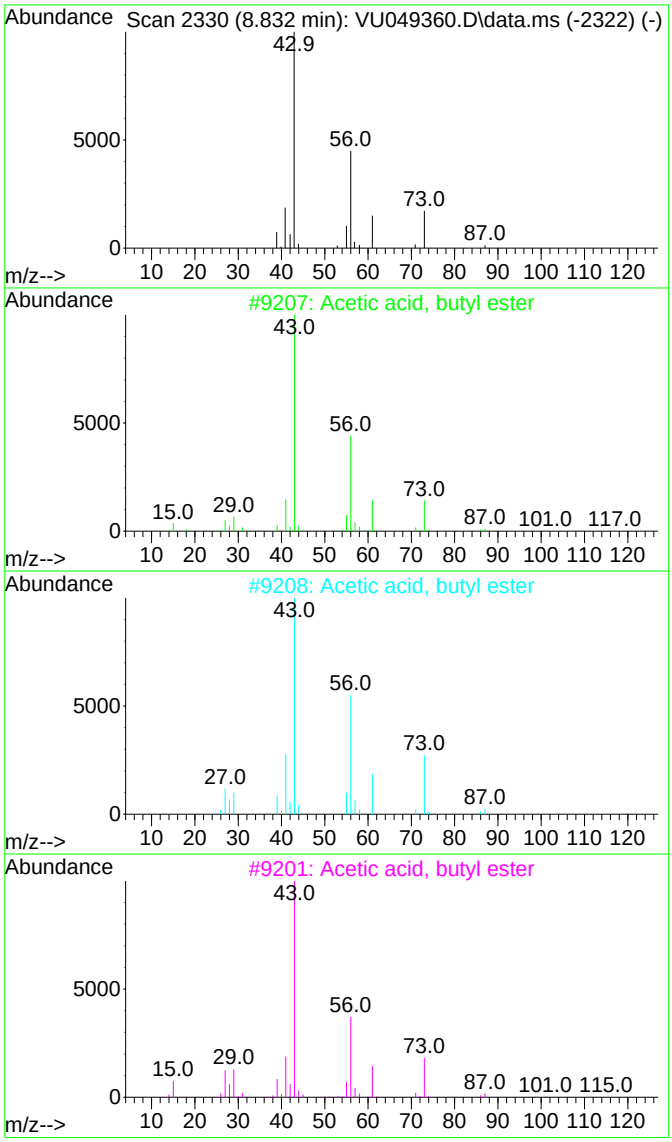
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

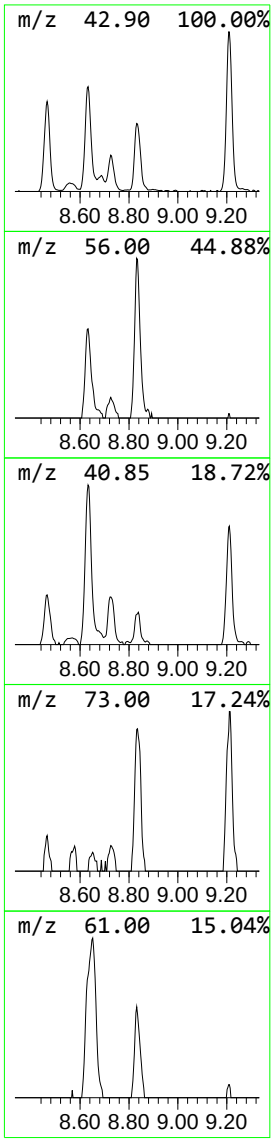
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.832	2.64 ug/L	34024	Chlorobenzene-d5	9.417

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	74
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	43
4	1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	23
5	Ethane, diazo-	56	C2H4N2	001117-96-0	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049360.D
Acq On : 22 Jun 2022 18:30
Operator : SY/MD
Sample : N3392-15 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

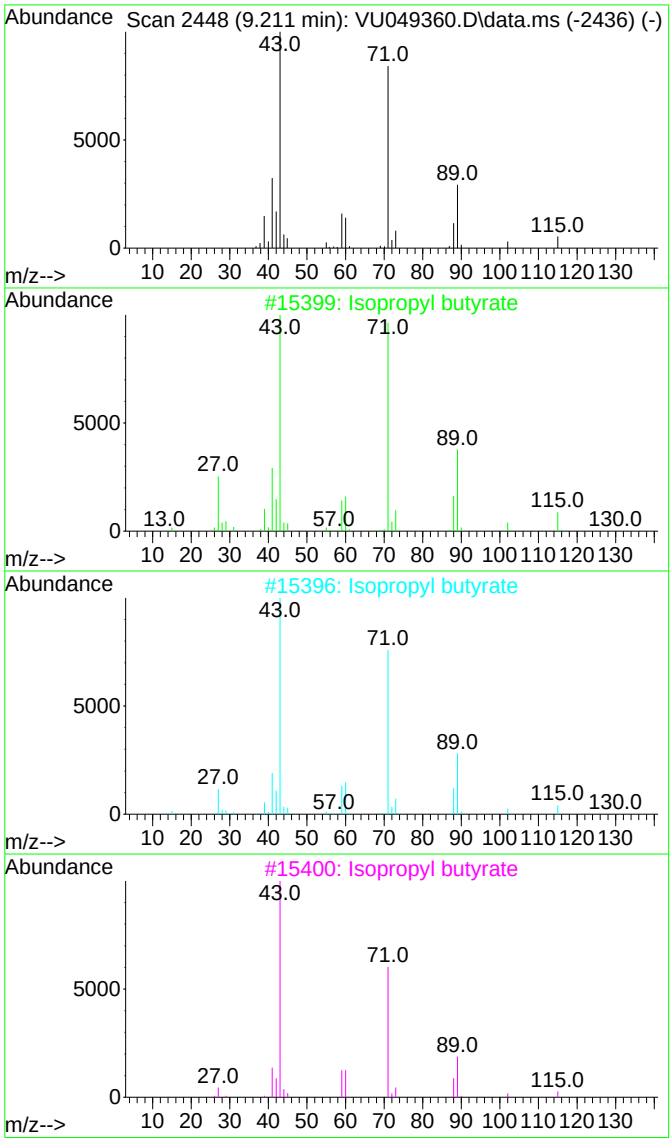
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

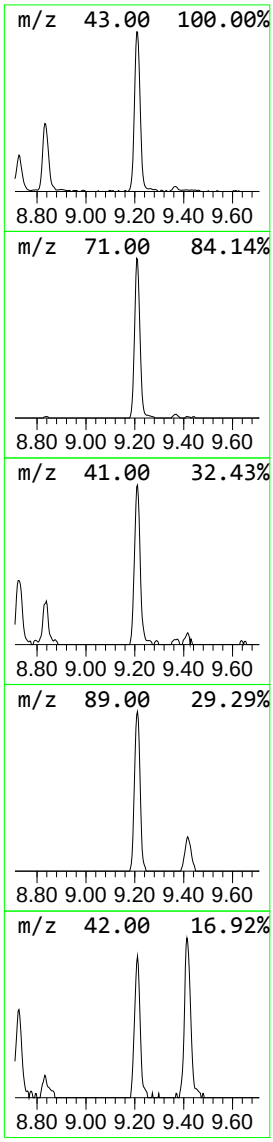
****

Peak Number 9 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	9.04 ug/L	116659	Chlorobenzene-d5	9.417

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	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_U\Data\VU062222\
Data File : VU049360.D
Acq On : 22 Jun 2022 18:30
Operator : SY/MD
Sample : N3392-15 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.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	14.2	ug/L	157260	1	6.247	552213	50.0
Propanoic acid,...	7.738	3.0	ug/L	32979	1	6.247	552213	50.0
Propanoic acid,...	8.465	3.3	ug/L	41887	2	9.417	645362	50.0
Propanoic acid,...	8.726	5.8	ug/L	75462	2	9.417	645362	50.0
Acetic acid, bu...	8.832	2.6	ug/L	34024	2	9.417	645362	50.0
Isopropyl butyrate	9.211	9.0	ug/L	116659	2	9.417	645362	50.0