LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049369.D
Acq On : 23 Jun 2022 11:14
Operator : SY/MD
Sample : N3392-20 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : EXEZ5

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: VU049369.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	89	rBV	59140	66115	9.84%	1.010%
2	1.903	169	175	186	rVB	52830	67617	10.06%	1.033%
3	2.565	369	381	393	rBV	103737	168270	25.05%	2.571%
4	2.694	418	421	424	rBV3	265	161	0.02%	0.002%
5	2.893	479	483	487	rBV	477	313	0.05%	0.005%
6	3.044	519	530	541	rBV2	8065	14336	2.13%	0.219%
7	3.108	546	550	555	rVB	329	277	0.04%	0.004%
8	3.186	561	574	593	rVB	31053	72632	10.81%	1.110%
9	3.285	602	605	606	rBV2	191	109	0.02%	0.002%
10	3.337	618	621	623	rVB	218	117	0.02%	0.002%
11	3.385	632	636	638	rBV2	305	162	0.02%	0.002%
12	3.472	660	663	667	rBV	266	188	0.03%	0.003%
13	3.530	678	681	683	rBV2	162	109	0.02%	0.002%
14	3.571	693	694	695	rBV	133	40	0.01%	0.001%
15	3.694	730	732	734	rBV	200	90	0.01%	0.001%
16	3.803	761	766	768	rBV	214	189	0.03%	0.003%
17	3.880	784	790	792	rBV	305	299	0.04%	0.005%
18	3.957	811	814	816	rVB	188	93	0.01%	0.001%
19	3.970	816	818	820	rBV	117	60	0.01%	0.001%
20	4.269	905	911	913	rBV2	257	193	0.03%	0.003%
21	4.285	913	916	919	rBV2	145	108	0.02%	0.002%
22	4.343	931	934	937	rBV	125	73	0.01%	0.001%
23	4.372	937	943	945	rBV	255	272	0.04%	0.004%
24	4.411	951	955	958	rBV2	273	248	0.04%	0.004%
25	4.481	974	977	979	rBV	209	169	0.03%	0.003%
26	4.530	988	992	994	rBV2	201	90	0.01%	0.001%
27	4.539	994	995	996	rBV2	151	43	0.01%	0.001%
28	4.620	1005	1020	1061	rBV2	118545	295043	43.92%	4.508%
29	4.935	1116	1118	1120	rBV	398	221	0.03%	0.003%
30	5.063	1143	1158	1178	rBV	129706	282751	42.09%	4.320%
31	5.153	1184	1186	1190	rBV	254	184	0.03%	0.003%
32	5.237	1210	1212	1215	rBV	312	161	0.02%	0.002%
33	5.282	1220	1226	1230	rBV2	505	551	0.08%	0.008%
34	5.321	1235	1238	1240	rBV2	369	278	0.04%	0.004%
35	5.378	1254	1256	1257	rBV2	126	51	0.01%	0.001%
36	5.404	1263	1264	1270	rBV2	165	84	0.01%	0.001%

LSC Area Percent Report

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Operator : SY/MD
Sample : N3392-20 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ5

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	5.513	1293	1298	1301	rBV2	224	222	0.03%	0.003%
38	5.581	1318	1319	1320	rBV2	106	25	0.00%	0.000%
39	5.639	1335	1337	1339	rVB2	239	119	0.02%	0.002%
40	5.722	1342	1363	1385	rBV2	239136	657094	97.81%	10.039%
41	5.912	1409	1422	1436	rBV2	9255	18921	2.82%	0.289%
42	6.041	1459	1462	1464	rBV2	116	89	0.01%	0.001%
43	6.182	1502	1506	1510	rBV2	163	158	0.02%	0.002%
44	6.250	1512	1527	1548	rBV	291009	553845	82.44%	8.462%
45	6.446	1586	1588	1591	rVB2	216	63	0.01%	0.001%
46	6.478	1592	1598	1601	rBV2	380	340	0.05%	0.005%
47	6.526	1606	1613	1620	rBV5	1665	2581	0.38%	0.039%
48	6.578	1627	1629	1633	rBV2	394	206	0.03%	0.003%
49	6.600	1633	1636	1637	rBV2	218	108	0.02%	0.002%
50	6.629	1643	1645	1648	rBV	180	64	0.01%	0.001%
51	6.690	1650	1664	1687	rVV	173106	336244	50.05%	5.137%
52	6.774	1687	1690	1691	rBV	402	203	0.03%	0.003%
53	6.829	1706	1707	1709	rBV	168	53	0.01%	0.001%
54	6.886	1722	1725	1727	rBV3	317	211	0.03%	0.003%
55	6.925	1727	1737	1756	rVB2	4526	9985	1.49%	0.153%
56	7.038	1761	1772	1796	rBV	107794	189575	28.22%	2.896%
57	7.272	1842	1845	1847	rBV2	224	135	0.02%	0.002%
58	7.340	1863	1866	1871	rVB2	327	258	0.04%	0.004%
59	7.565	1923	1936	1958	rBV	85876	149897	22.31%	2.290%
60	7.697	1969	1977	1979	rBV4	892	1058	0.16%	0.016%
61	7.738	1982	1990	2001	rVB2	19768	31509	4.69%	0.481%
62	7.832	2016	2019	2023	rBV2	301	196	0.03%	0.003%
63	7.896	2026	2039	2059	rBV	276737	479893	71.43%	7.332%
64	8.076	2092	2095	2098	rBV2	363	212	0.03%	0.003%
65	8.176	2108	2126	2143	rBV2	66769	144734	21.54%	2.211%
66	8.465	2206	2216	2229	rBV	25094	40821	6.08%	0.624%
67	8.574	2235	2250	2257	rBV7	4347	9866	1.47%	0.151%
68	8.632	2257	2268	2288	rBV2	297441	542553	80.76%	8.289%
69	8.835	2321	2331	2348	rVB	29563	48882	7.28%	0.747%
70	9.076	2404	2406	2408	rBV2	197	79	0.01%	0.001%
71	9.092	2408	2411	2413	rBV2	210	127	0.02%	0.002%
72	9.211	2437	2448	2464	rBV	72543	114488	17.04%	1.749%
73	9.320	2479	2482	2484	rBV2	246	139	0.02%	0.002%
74	9.369	2491	2497	2499	rBV3	1462	1308	0.19%	0.020%
75	9.417	2499	2512	2541	rVV	407221	671824	100.00%	10.264%
76	9.645	2572	2583	2587	rBV3	1009	1424	0.21%	0.022%

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Acq On : 23 Jun 2022 11:14
Operator : SY/MD
Sample : N3392-20 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ5

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	9.671	2587	2591	2596	rBV2	218	261	0.04%	0.004%
78	9.889	2656	2659	2661	rBV2	244	121	0.02%	0.002%
79	9.918	2661	2668	2670	rBV2	950	874	0.13%	0.013%
80	10.076	2707	2717	2728	rBV3	5186	8215	1.22%	0.126%
81	10.250	2767	2771	2773	rBV	263	142	0.02%	0.002%
82	10.372	2806	2809	2812	rBV	186	147	0.02%	0.002%
83	10.481	2840	2843	2845	rBV2	349	167	0.02%	0.003%
84	10.539	2859	2861	2864	rBV	212	90	0.01%	0.001%
85	10.639	2889	2892	2898	rBV3	386	318	0.05%	0.005%
86	10.754	2916	2928	2947	rBV	272660	443776	66.06%	6.780%
87	10.915	2975	2978	2981	rVB	274	164	0.02%	0.003%
88	10.938	2981	2985	2989	rBV3	396	331	0.05%	0.005%
89	11.330	3105	3107	3110	rBV	246	122	0.02%	0.002%
90	11.391	3123	3126	3129	rVB2	405	231	0.03%	0.004%
91	11.410	3130	3132	3135	rBV	242	110	0.02%	0.002%
92	11.552	3173	3176	3177	rBV2	246	150	0.02%	0.002%
93	11.812	3243	3257	3274	rBV	378585	612085	91.11%	9.351%
94	12.192	3363	3375	3395	rBV	303377	491562	73.17%	7.510%
95	13.224	3693	3696	3703	rVB3	525	444	0.07%	0.007%
96	14.098	3962	3968	3979	rVB2	3499	4868	0.72%	0.074%

Sum of corrected areas: 6545384

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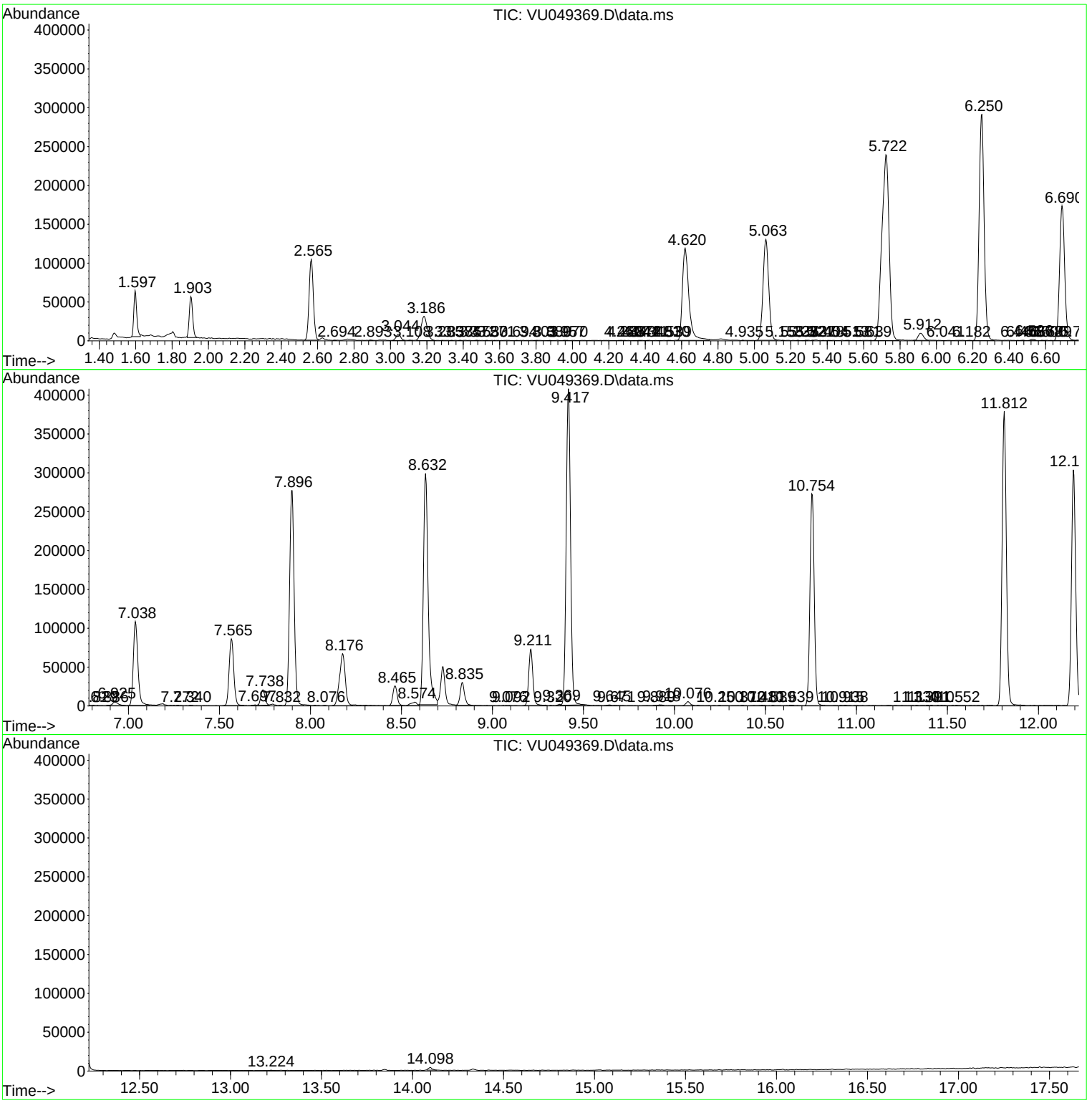
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ5

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
ClientSampleId :
EXEZ5

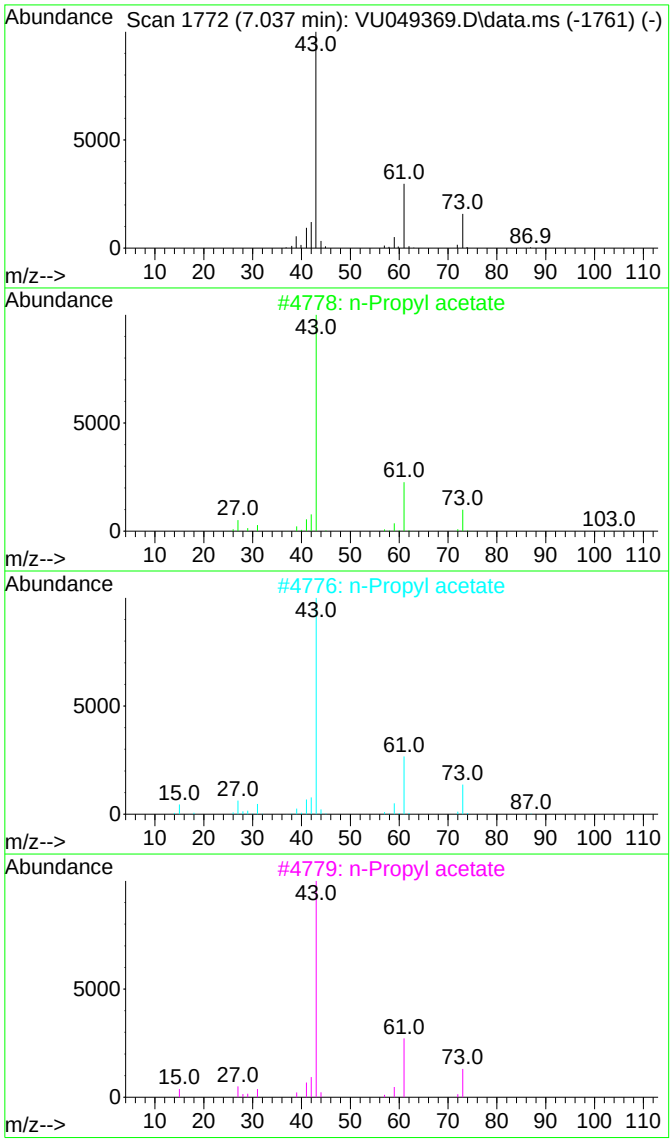
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

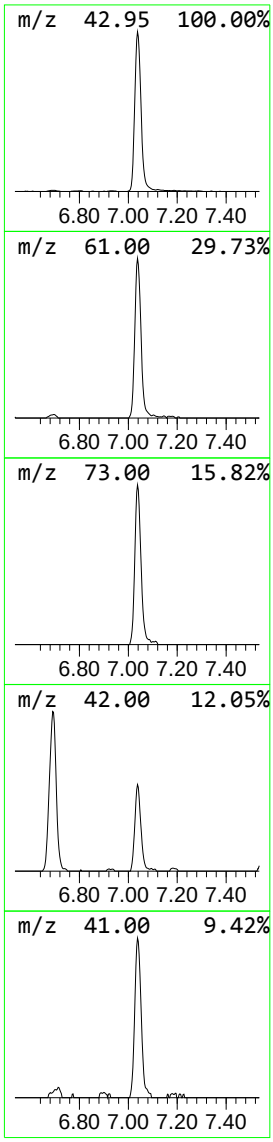
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.037	17.11 ug/L	189575	1,4-Difluorobenzene	6.250

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049369.D
Acq On : 23 Jun 2022 11:14
Operator : SY/MD
Sample : N3392-20 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ5

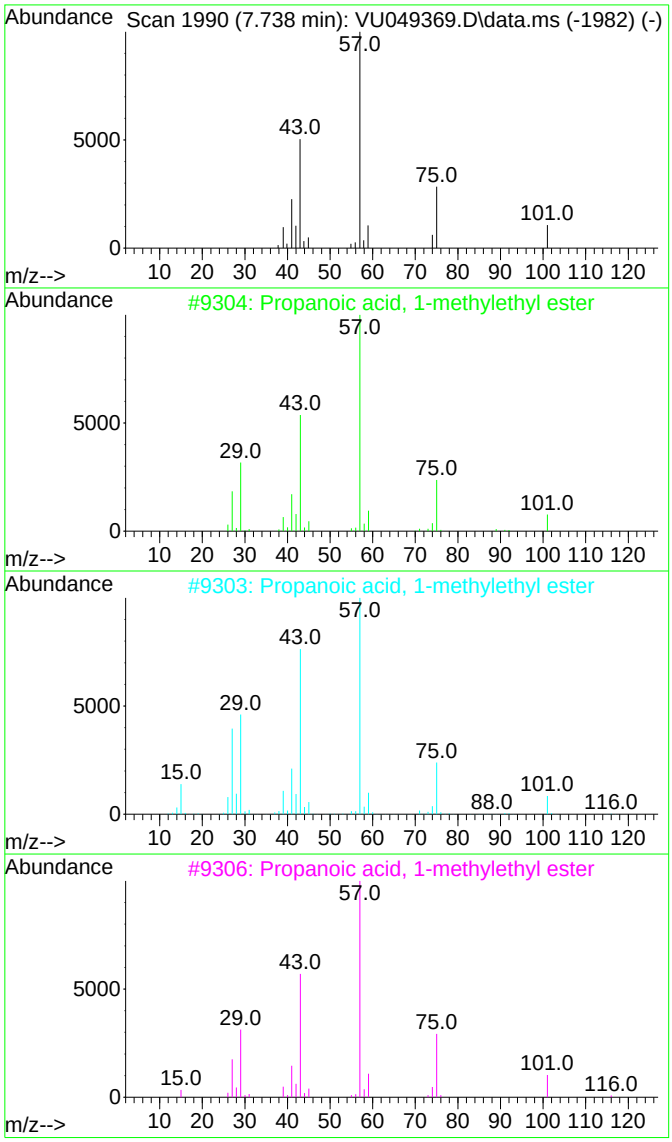
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

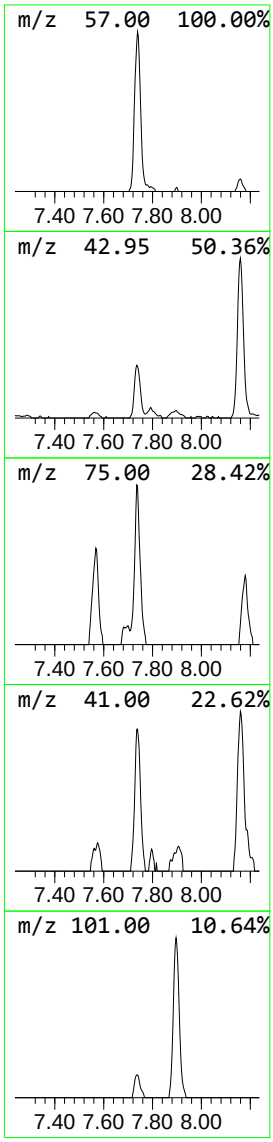
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.738	2.84 ug/L	31509	1,4-Difluorobenzene	6.250

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	83
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59





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Instrument :
MSVOA_U
ClientSampleId :
EXEZ5

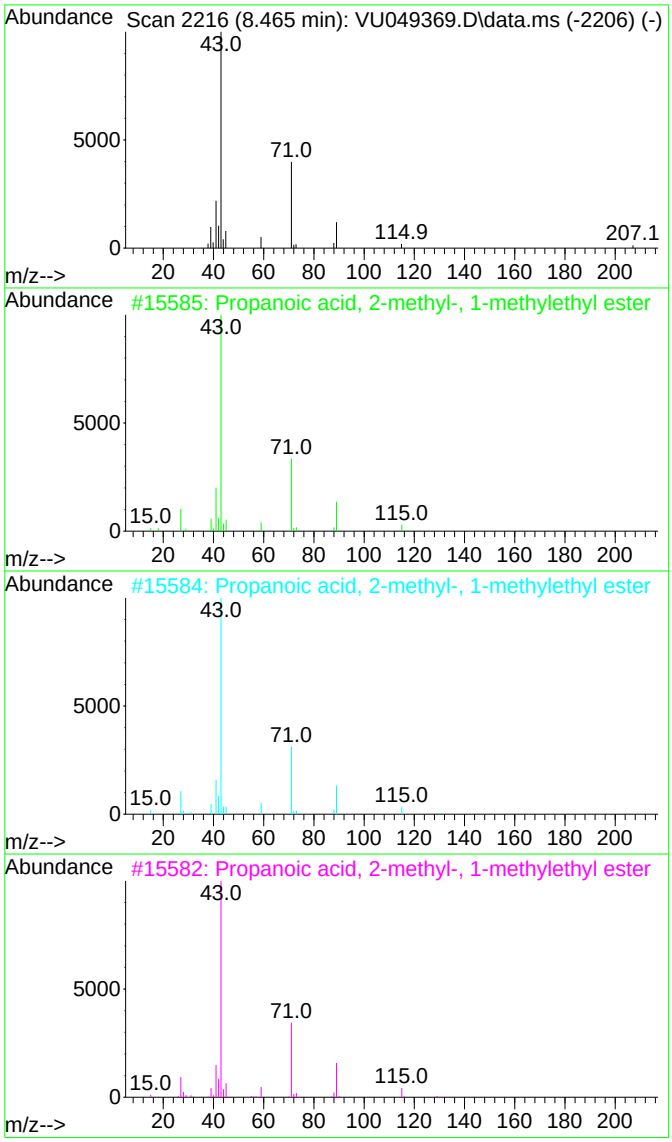
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

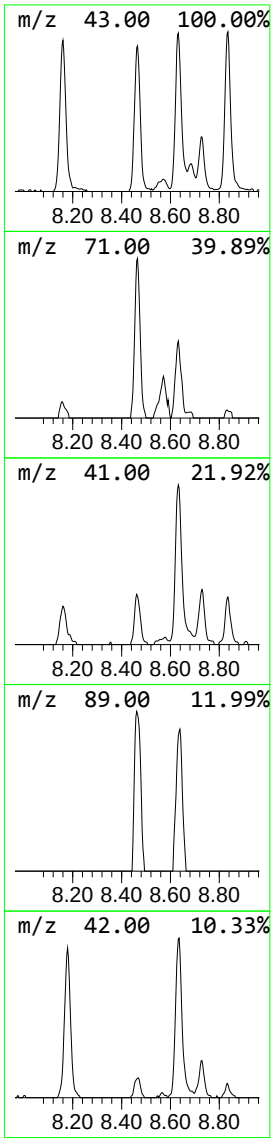
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	3.04 ug/L	40821	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-, propy...	130	C7H14O2	000644-49-5	78
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ5

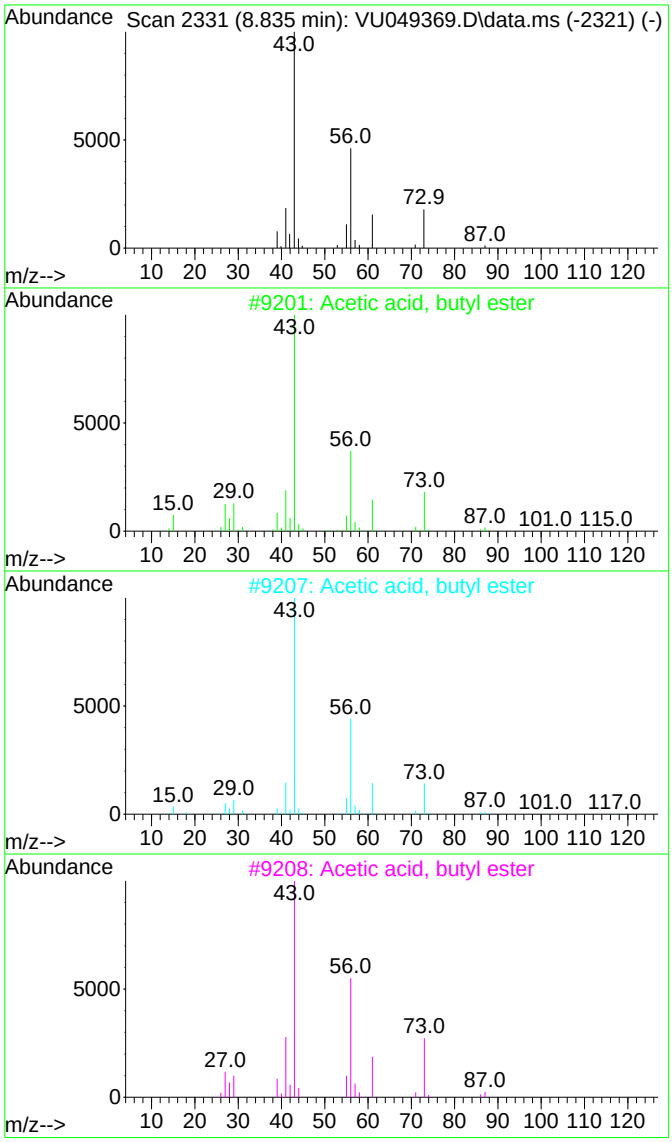
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

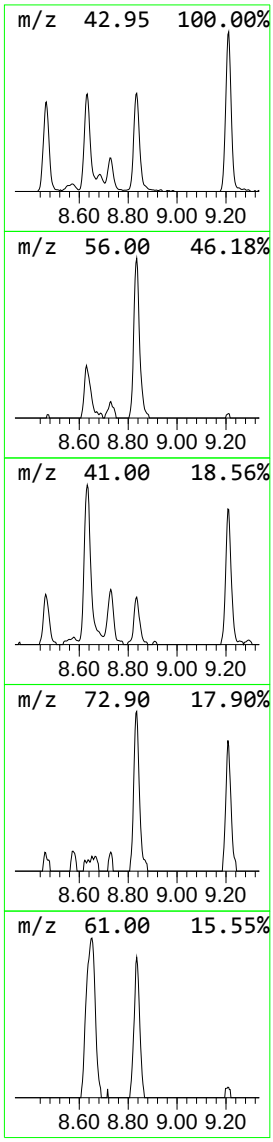
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	3.64 ug/L	48882	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	90
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
5	Isobutyl acetate	116	C6H12O2	000110-19-0	39





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Acq On : 23 Jun 2022 11:14
Operator : SY/MD
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ5

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

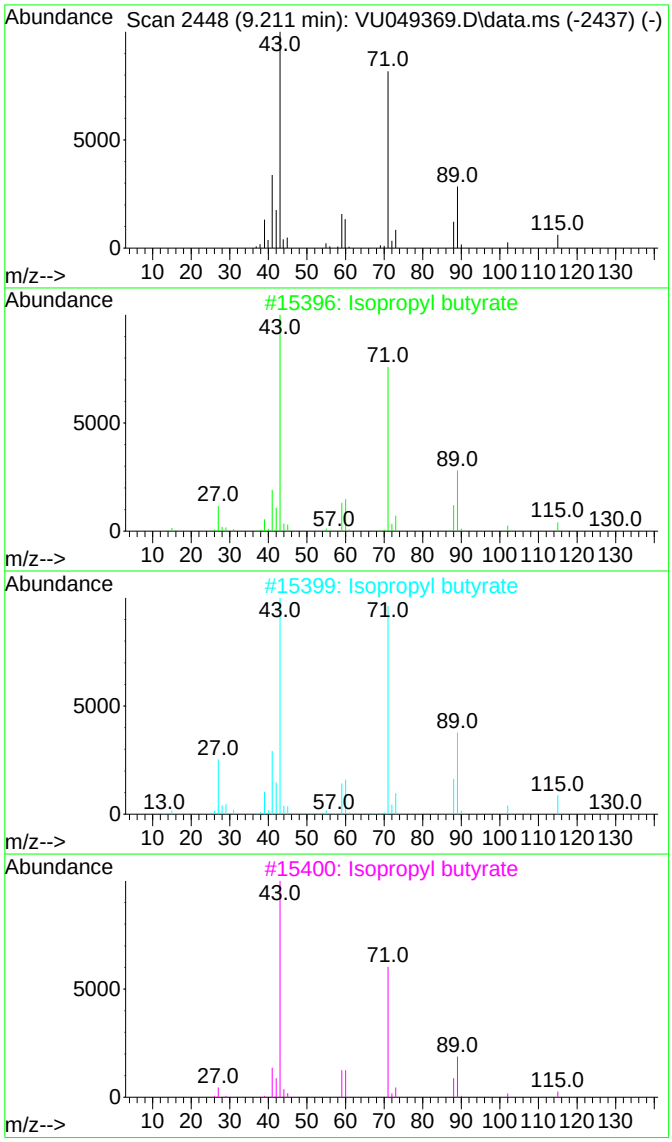
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

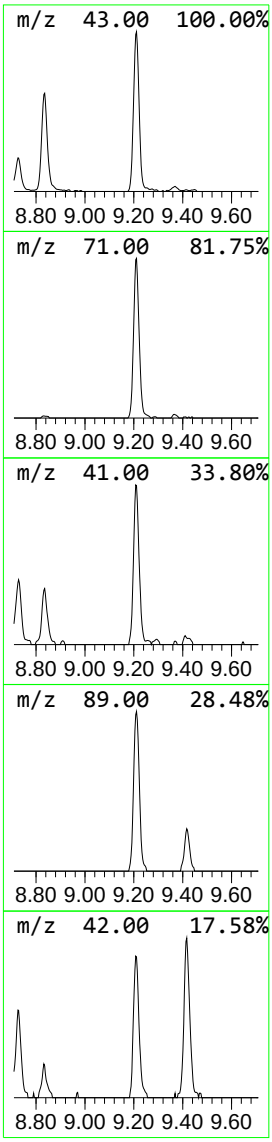
****

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	8.52 ug/L	114488	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	78
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049369.D
Acq On : 23 Jun 2022 11:14
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ5

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	17.1	ug/L	189575	1	6.250	553845	50.0
Propanoic acid,...	7.738	2.8	ug/L	31509	1	6.250	553845	50.0
Propanoic acid,...	8.465	3.0	ug/L	40821	2	9.417	671824	50.0
Acetic acid, bu...	8.835	3.6	ug/L	48882	2	9.417	671824	50.0
Isopropyl butyrate	9.211	8.5	ug/L	114488	2	9.417	671824	50.0