LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049355.D
Acq On : 22 Jun 2022 16:33
Operator : SY/MD
Sample : N3392-09 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY4

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: VU049355.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	93	rBV	69871	77076	10.26%	1.095%
2	1.906	170	176	192	rVB	62683	80780	10.76%	1.147%
3	2.565	370	381	394	rBV	119827	192118	25.58%	2.729%
4	2.771	439	445	447	rBV2	1100	1042	0.14%	0.015%
5	3.047	521	531	543	rVB4	3424	6431	0.86%	0.091%
6	3.186	559	574	595	rVB	20167	47718	6.35%	0.678%
7	3.263	596	598	600	rBV2	184	62	0.01%	0.001%
8	3.436	649	652	654	rBV2	253	157	0.02%	0.002%
9	3.469	660	662	665	rBV2	226	110	0.01%	0.002%
10	3.485	665	667	670	rBV2	268	155	0.02%	0.002%
11	3.726	738	742	745	rBV2	300	243	0.03%	0.003%
12	3.983	820	822	823	rBV	180	75	0.01%	0.001%
13	4.054	840	844	846	rBV2	166	130	0.02%	0.002%
14	4.102	856	859	862	rBV3	263	195	0.03%	0.003%
15	4.118	862	864	866	rVB	162	47	0.01%	0.001%
16	4.256	904	907	910	rBV	139	95	0.01%	0.001%
17	4.337	927	932	938	rBV2	240	280	0.04%	0.004%
18	4.388	946	948	952	rVB	244	142	0.02%	0.002%
19	4.433	958	962	964	rBV2	208	173	0.02%	0.002%
20	4.623	1007	1021	1054	rBV2	125048	317945	42.33%	4.516%
21	5.063	1143	1158	1175	rBV	145178	316273	42.11%	4.492%
22	5.231	1208	1210	1212	rBV	232	102	0.01%	0.001%
23	5.263	1218	1220	1223	rVB	312	152	0.02%	0.002%
24	5.292	1223	1229	1230	rBV4	661	537	0.07%	0.008%
25	5.350	1243	1247	1249	rBV	194	157	0.02%	0.002%
26	5.514	1295	1298	1304	rBV2	134	113	0.02%	0.002%
27	5.539	1304	1306	1309	rBV	211	105	0.01%	0.001%
28	5.613	1325	1329	1333	rBV3	254	203	0.03%	0.003%
29	5.636	1334	1336	1339	rBV2	189	102	0.01%	0.001%
30	5.726	1342	1364	1392	rVV2	273345	751091	100.00%	10.668%
31	5.915	1414	1423	1433	rBV2	8077	15671	2.09%	0.223%
32	6.250	1515	1527	1541	rBV	296155	560072	74.57%	7.955%
33	6.690	1650	1664	1687	rBV	195554	379835	50.57%	5.395%
34	7.041	1762	1773	1793	rBV	113215	203121	27.04%	2.885%
35	7.269	1840	1844	1845	rBV	458	289	0.04%	0.004%
36	7.311	1854	1857	1861	rBV2	568	443	0.06%	0.006%

LSC Area Percent Report

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Operator : SY/MD
Sample : N3392-09 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY4

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	7.340	1864	1866	1867	rBV	223	86	0.01%	0.001%
38	7.407	1882	1887	1888	rBV2	399	346	0.05%	0.005%
39	7.440	1888	1897	1907	rVB6	2334	4103	0.55%	0.058%
40	7.494	1909	1914	1919	rBV4	464	532	0.07%	0.008%
41	7.565	1923	1936	1953	rBV	102431	181242	24.13%	2.574%
42	7.681	1969	1972	1974	rBV3	706	562	0.07%	0.008%
43	7.739	1981	1990	2001	rVB	18260	29362	3.91%	0.417%
44	7.896	2019	2039	2056	rBV	319078	560448	74.62%	7.961%
45	8.060	2087	2090	2091	rBV2	408	227	0.03%	0.003%
46	8.089	2098	2099	2100	rVB2	207	40	0.01%	0.001%
47	8.118	2106	2108	2109	rBV	151	38	0.01%	0.001%
48	8.179	2109	2127	2149	rBV2	76305	158212	21.06%	2.247%
49	8.337	2173	2176	2182	rBV3	352	436	0.06%	0.006%
50	8.427	2202	2204	2205	rBV	201	70	0.01%	0.001%
51	8.465	2206	2216	2231	rVB2	20369	33388	4.45%	0.474%
52	8.575	2236	2250	2256	rBV7	6123	11514	1.53%	0.164%
53	8.632	2256	2268	2288	rVV	333695	599576	79.83%	8.516%
54	8.726	2290	2297	2314	rVB	65866	106134	14.13%	1.508%
55	8.835	2323	2331	2348	rVB2	26806	43506	5.79%	0.618%
56	8.989	2377	2379	2384	rBV3	186	194	0.03%	0.003%
57	9.054	2397	2399	2403	rBV3	290	177	0.02%	0.003%
58	9.211	2437	2448	2463	rBV	68347	107582	14.32%	1.528%
59	9.320	2480	2482	2485	rBV2	226	142	0.02%	0.002%
60	9.417	2500	2512	2535	rBV	407789	666887	88.79%	9.472%
61	9.639	2578	2581	2585	rBV4	906	616	0.08%	0.009%
62	9.671	2589	2591	2594	rBV	133	60	0.01%	0.001%
63	9.687	2594	2596	2598	rBV2	407	192	0.03%	0.003%
64	10.073	2710	2716	2727	rBB5	3666	5229	0.70%	0.074%
65	10.156	2740	2742	2745	rBV	234	145	0.02%	0.002%
66	10.224	2761	2763	2767	rBV	276	185	0.02%	0.003%
67	10.292	2782	2784	2786	rBV	253	121	0.02%	0.002%
68	10.410	2819	2821	2825	rVB2	291	132	0.02%	0.002%
69	10.433	2825	2828	2830	rBV2	254	194	0.03%	0.003%
70	10.755	2916	2928	2945	rBV	287390	470394	62.63%	6.681%
71	11.005	3003	3006	3008	rBV	246	182	0.02%	0.003%
72	11.639	3199	3203	3207	rBV	549	420	0.06%	0.006%
73	11.812	3245	3257	3273	rBV	370973	593909	79.07%	8.436%
74	12.192	3362	3375	3392	rBV	314281	510146	67.92%	7.246%
75	12.529	3477	3480	3482	rBV2	391	324	0.04%	0.005%

LSC Area Percent Report

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Operator : SY/MD
Sample : N3392-09 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY4

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

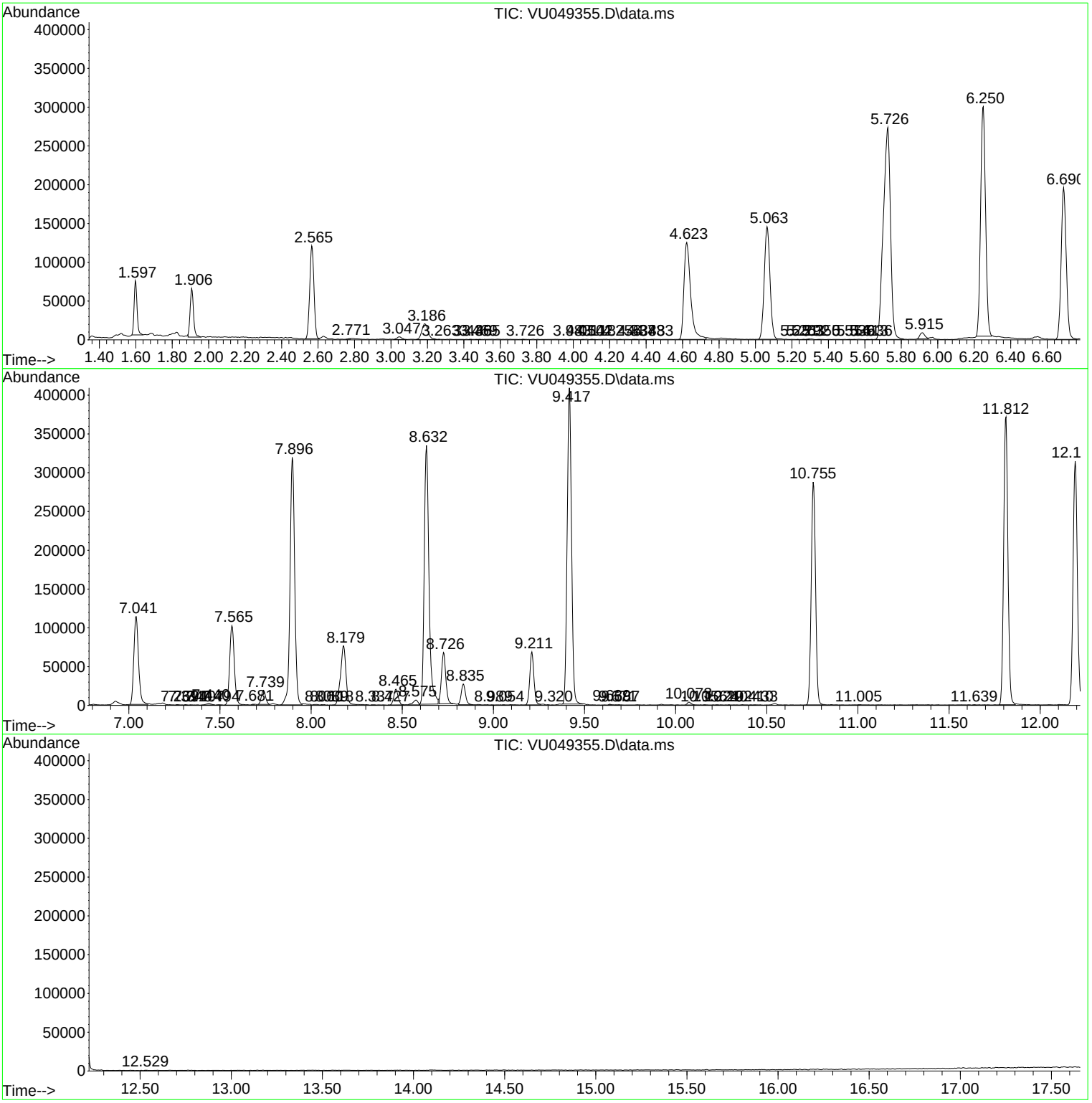
Sum of corrected areas: 7040293

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049355.D
Acq On : 22 Jun 2022 16:33
Operator : SY/MD
Sample : N3392-09 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY4

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\
Data File : VU049355.D
Acq On : 22 Jun 2022 16:33
Operator : SY/MD
Sample : N3392-09 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY4

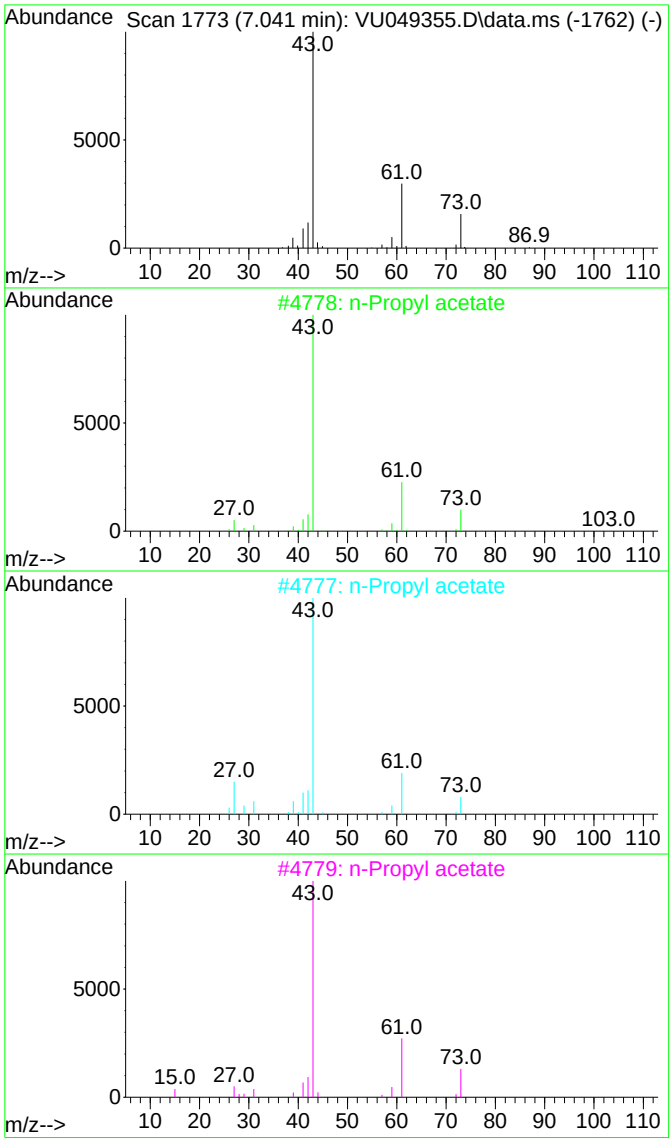
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

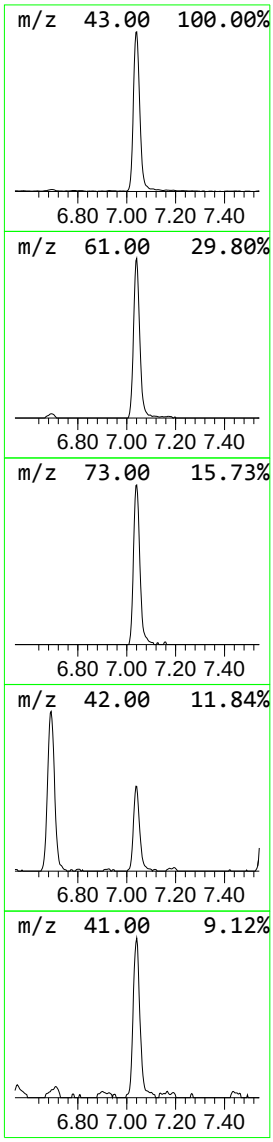
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	18.13 ug/L	203121	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	78
3	n-Propyl acetate	102	C5H10O2	000109-60-4	78
4	n-Propyl acetate	102	C5H10O2	000109-60-4	78
5	n-Propyl acetate	102	C5H10O2	000109-60-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049355.D
Acq On : 22 Jun 2022 16:33
Operator : SY/MD
Sample : N3392-09 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY4

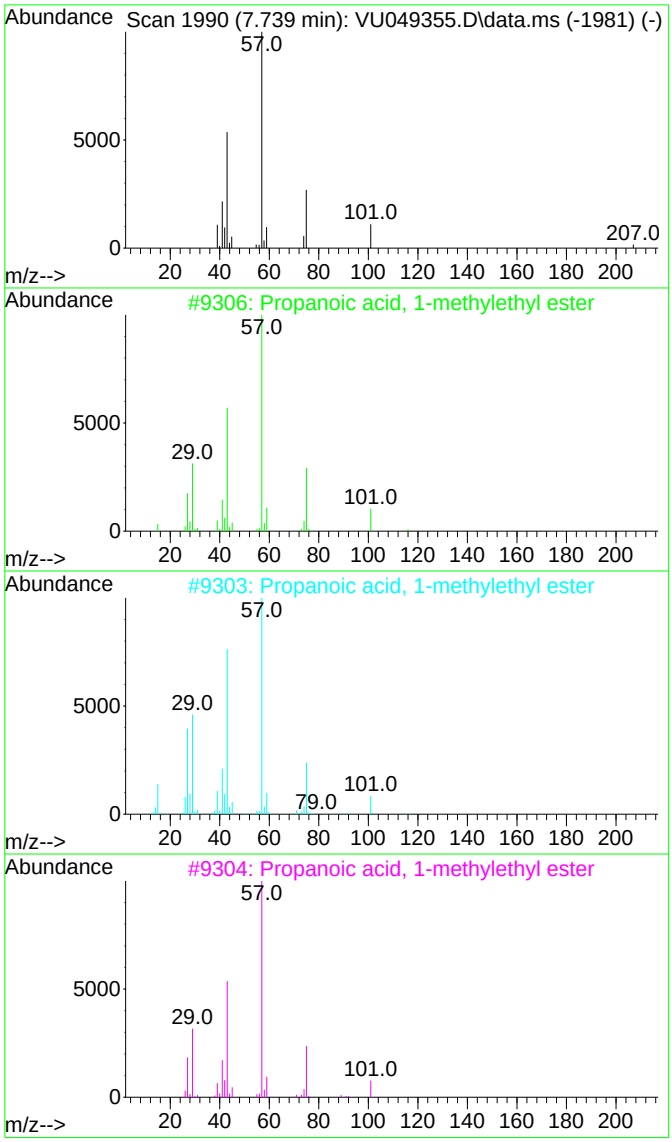
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

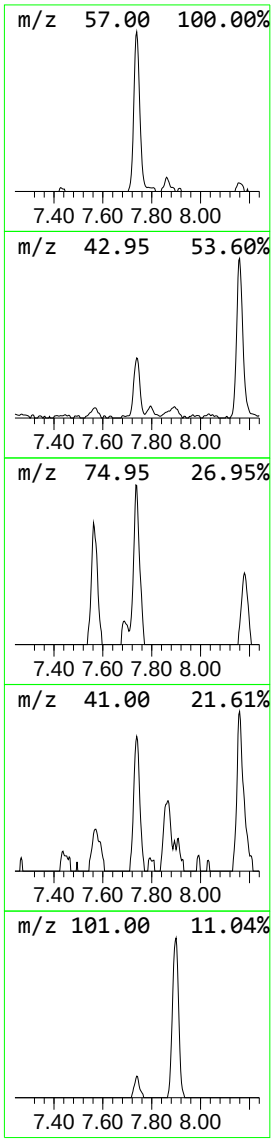
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.739	2.62 ug/L	29362	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	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049355.D
Acq On : 22 Jun 2022 16:33
Operator : SY/MD
Sample : N3392-09 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY4

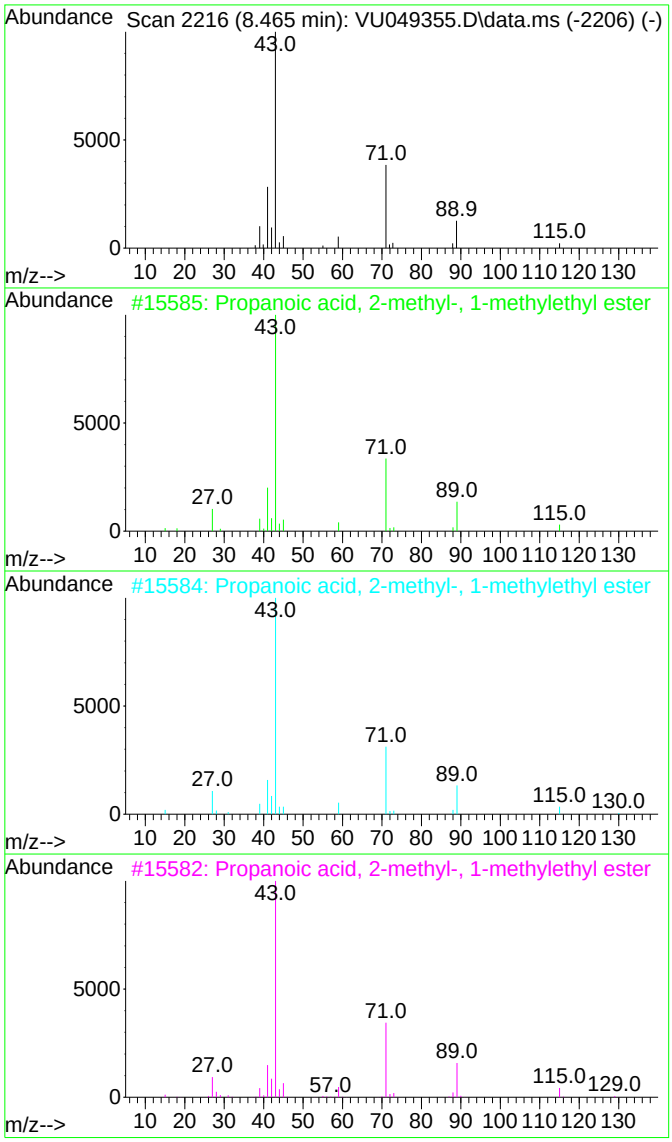
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

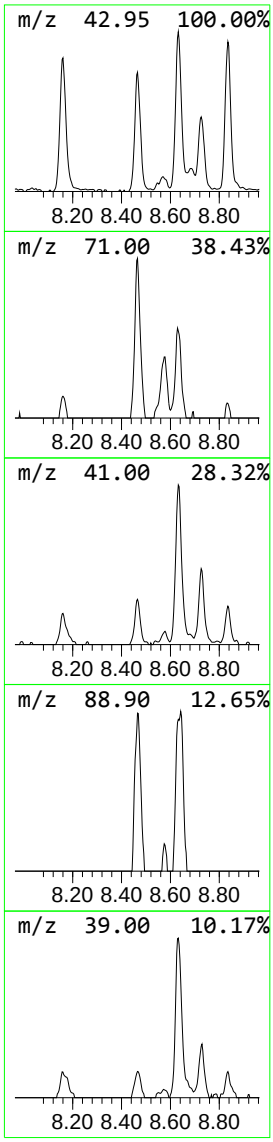
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	2.50 ug/L	33388	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	78





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MSVOA_U
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EXEY4

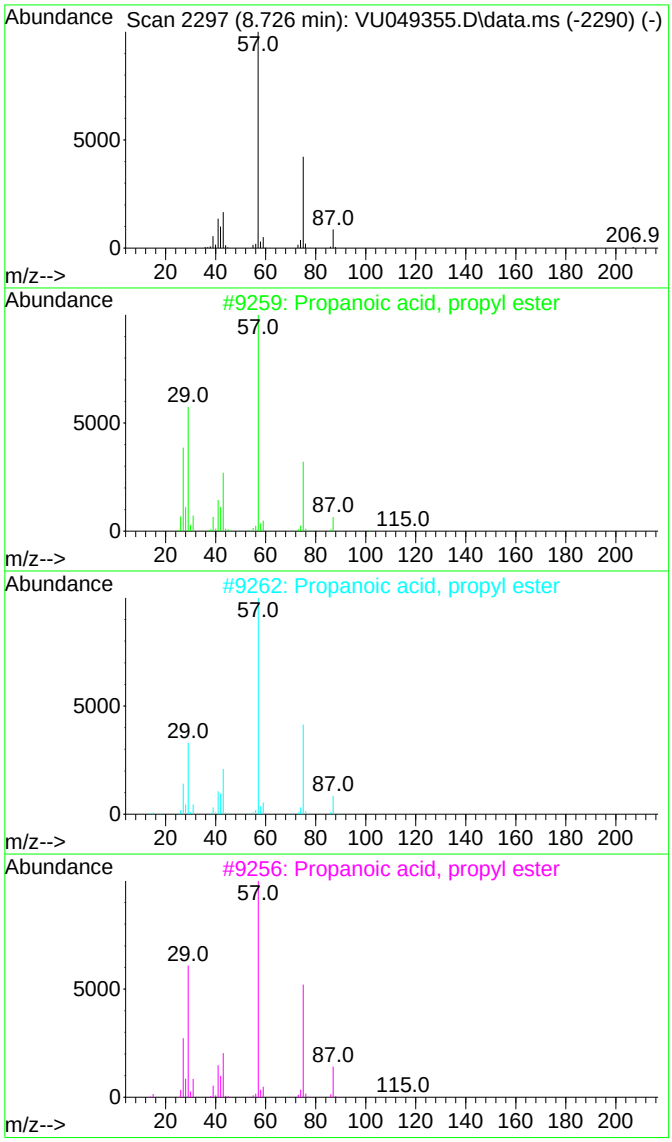
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

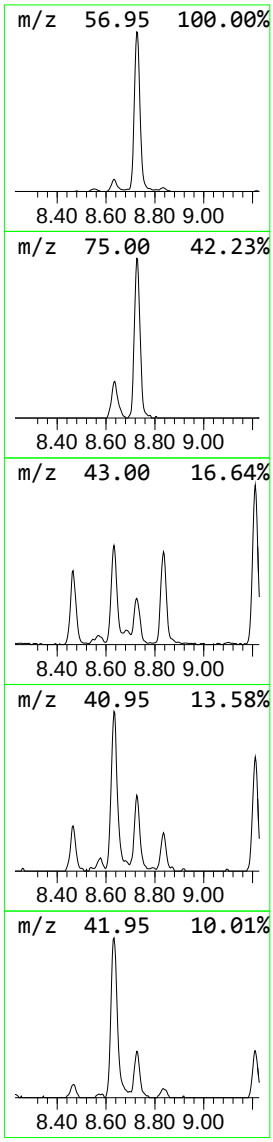
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	7.96 ug/L	106134	Chlorobenzene-d5	9.417

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	78
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64





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Acq On : 22 Jun 2022 16:33
Operator : SY/MD
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY4

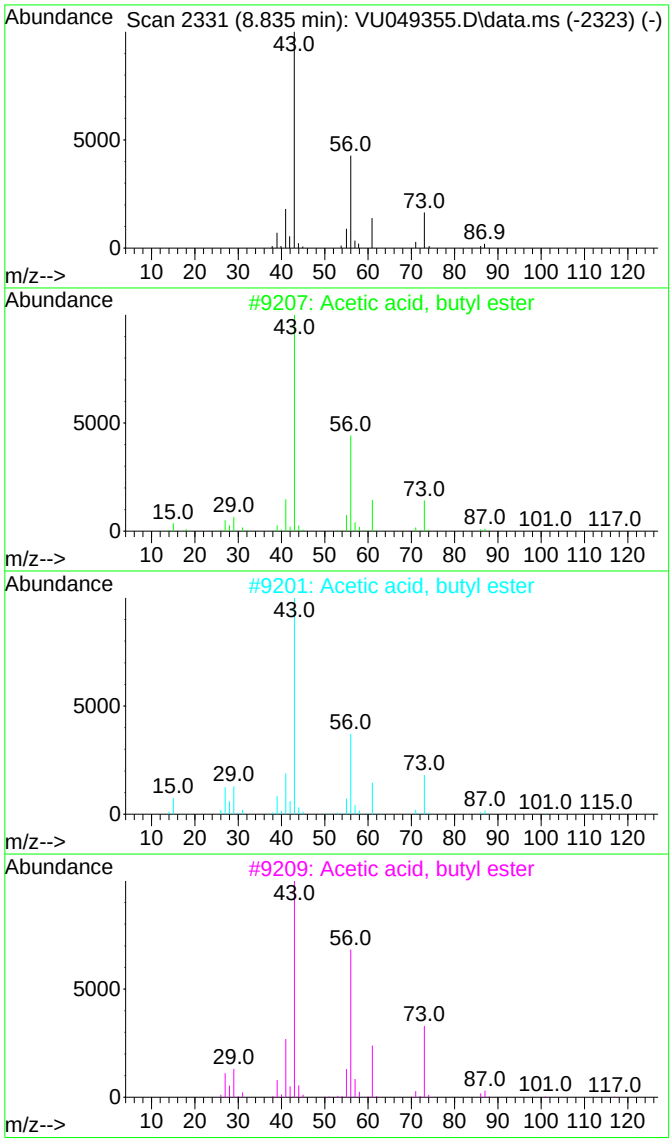
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

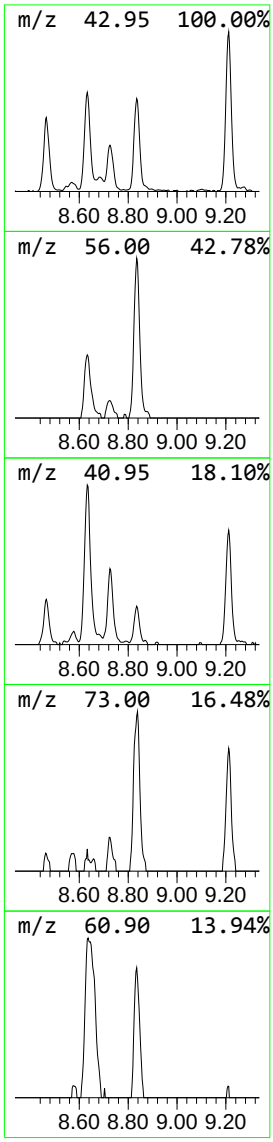
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	3.26 ug/L	43506	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	64
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	47
5	Isobutyl acetate	116	C6H12O2	000110-19-0	39





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY4

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

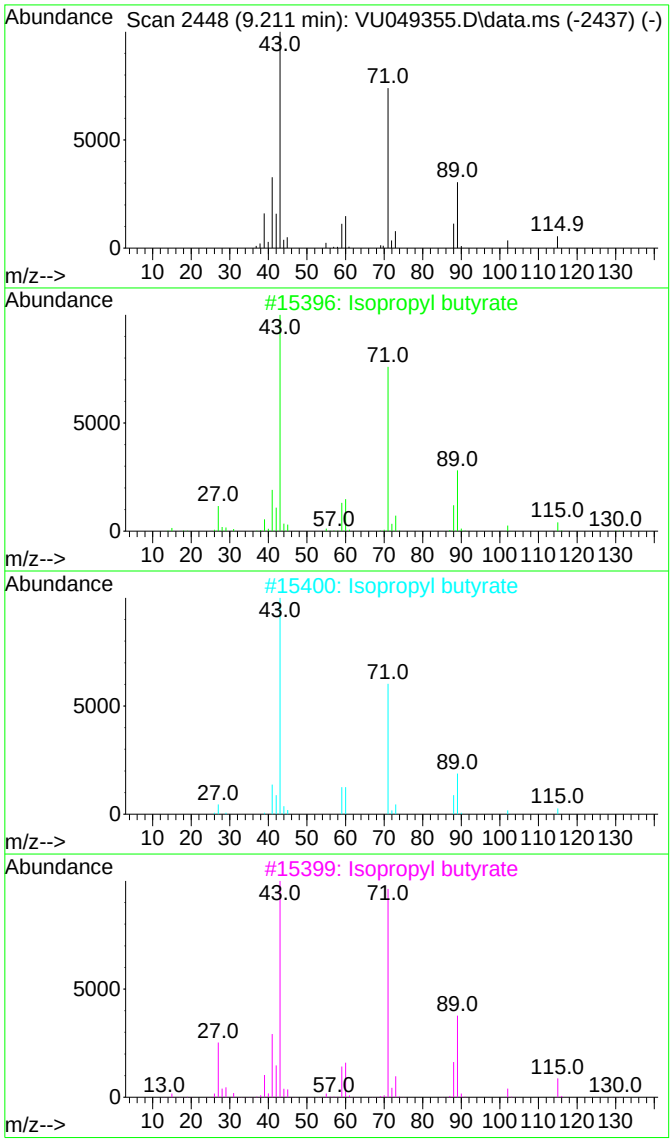
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

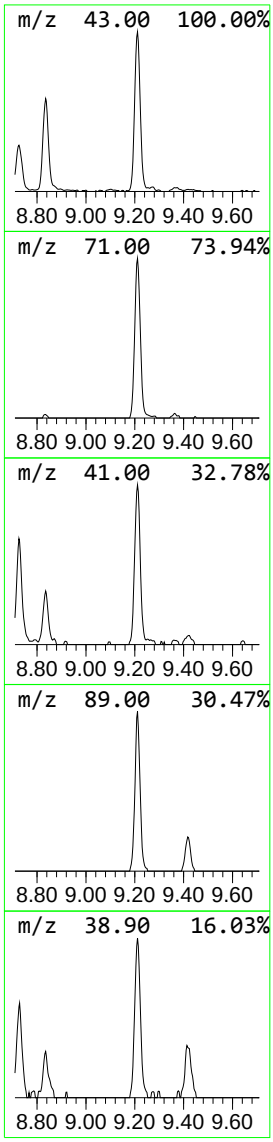
****

Peak Number 8 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	8.07 ug/L	107582	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	83
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049355.D
Acq On : 22 Jun 2022 16:33
Operator : SY/MD
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY4

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	7.041	18.1	ug/L	203121	1	6.250	560072	50.0
Propanoic acid,...	7.739	2.6	ug/L	29362	1	6.250	560072	50.0
Propanoic acid,...	8.465	2.5	ug/L	33388	2	9.417	666887	50.0
Propanoic acid,...	8.726	8.0	ug/L	106134	2	9.417	666887	50.0
Acetic acid, bu...	8.835	3.3	ug/L	43506	2	9.417	666887	50.0
Isopropyl butyrate	9.211	8.1	ug/L	107582	2	9.417	666887	50.0