LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022222\
Data File : VU047234.D
Acq On : 22 Feb 2022 16:13
Operator : SY/MD
Sample : N1621-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBD34

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\SFAMULM021022WMA.M
Title : VOC Analysis

Signal : TIC: VU047234.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	75	82	101	rVB	145919	172314	12.47%	1.343%
2	1.919	172	180	199	rVB	134824	179424	12.99%	1.399%
3	2.575	371	384	404	rBV	261916	439909	31.84%	3.430%
4	2.765	440	443	447	rBV	457	412	0.03%	0.003%
5	2.794	447	452	453	rBV2	628	483	0.03%	0.004%
6	2.858	470	472	474	rVB2	549	207	0.01%	0.002%
7	2.880	474	479	480	rBV2	346	254	0.02%	0.002%
8	2.935	493	496	499	rBV4	361	291	0.02%	0.002%
9	3.051	519	532	549	rVB	23669	46346	3.35%	0.361%
10	3.138	557	559	562	rBV	285	163	0.01%	0.001%
11	3.157	562	565	568	rBV3	440	253	0.02%	0.002%
12	3.263	595	598	605	rVB3	321	324	0.02%	0.003%
13	3.347	622	624	628	rVB2	338	249	0.02%	0.002%
14	3.408	640	643	647	rBV2	423	346	0.03%	0.003%
15	3.433	647	651	655	rVV3	259	297	0.02%	0.002%
16	3.459	655	659	667	rVB4	302	428	0.03%	0.003%
17	3.511	673	675	680	rVB4	458	316	0.02%	0.002%
18	3.546	685	686	693	rVB3	486	304	0.02%	0.002%
19	3.594	693	701	702	rBV2	366	295	0.02%	0.002%
20	3.700	730	734	737	rBV3	244	213	0.02%	0.002%
21	3.732	741	744	748	rVB2	281	207	0.01%	0.002%
22	3.768	753	755	761	rVB3	263	284	0.02%	0.002%
23	3.806	761	767	769	rBV2	191	169	0.01%	0.001%
24	3.822	769	772	774	rBV3	485	358	0.03%	0.003%
25	3.912	795	800	809	rVB3	319	408	0.03%	0.003%
26	4.006	826	829	832	rBV	201	169	0.01%	0.001%
27	4.086	852	854	858	rVV	232	177	0.01%	0.001%
28	4.369	939	942	947	rVB3	279	272	0.02%	0.002%
29	4.430	958	961	964	rVV	329	245	0.02%	0.002%
30	4.453	967	968	974	rVB3	276	190	0.01%	0.001%
31	4.507	981	985	987	rBV2	374	270	0.02%	0.002%
32	4.572	999	1005	1007	rBV3	341	329	0.02%	0.003%
33	4.629	1007	1023	1054	rBV	183530	479422	34.70%	3.738%
34	4.877	1096	1100	1102	rVB3	260	211	0.02%	0.002%
35	4.945	1117	1121	1125	rVB3	276	240	0.02%	0.002%
36	5.067	1141	1159	1185	rBV	255920	560072	40.53%	4.366%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022222\
Data File : VU047234.D
Acq On : 22 Feb 2022 16:13
Operator : SY/MD
Sample : N1621-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBD34

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\SFAMULM021022WMA.M
Title : VOC Analysis

37	5.218	1204	1206	1209	rVB3	589	280	0.02%	0.002%
38	5.234	1209	1211	1215	rVB2	471	218	0.02%	0.002%
39	5.334	1240	1242	1248	rVB2	451	290	0.02%	0.002%
40	5.366	1248	1252	1256	rVB2	252	162	0.01%	0.001%
41	5.449	1275	1278	1281	rVB2	256	184	0.01%	0.001%
42	5.530	1301	1303	1309	rVB2	270	220	0.02%	0.002%
43	5.575	1313	1317	1324	rVB2	333	302	0.02%	0.002%
44	5.610	1324	1328	1333	rVB3	239	236	0.02%	0.002%
45	5.633	1333	1335	1338	rBV2	379	215	0.02%	0.002%
46	5.729	1342	1365	1393	rBV2	507945	1381726	100.00%	10.772%
47	5.861	1401	1406	1409	rBV4	206	192	0.01%	0.001%
48	5.916	1410	1423	1430	rBV3	2783	4852	0.35%	0.038%
49	5.970	1436	1440	1444	rBV4	454	357	0.03%	0.003%
50	6.018	1450	1455	1457	rBV	223	172	0.01%	0.001%
51	6.038	1457	1461	1462	rBV3	486	338	0.02%	0.003%
52	6.250	1514	1527	1563	rVB	444509	847659	61.35%	6.608%
53	6.694	1650	1665	1683	rBV	336653	642853	46.53%	5.012%
54	6.764	1684	1687	1691	rBV6	839	738	0.05%	0.006%
55	6.890	1723	1726	1728	rBV3	439	300	0.02%	0.002%
56	7.041	1759	1773	1794	rBV	149002	261827	18.95%	2.041%
57	7.134	1799	1802	1805	rBV3	288	191	0.01%	0.001%
58	7.147	1805	1806	1808	rVV2	347	175	0.01%	0.001%
59	7.182	1808	1817	1830	rVB5	4111	7166	0.52%	0.056%
60	7.243	1834	1836	1839	rBV2	294	165	0.01%	0.001%
61	7.288	1847	1850	1854	rBV2	304	252	0.02%	0.002%
62	7.472	1906	1907	1912	rVB3	225	177	0.01%	0.001%
63	7.568	1922	1937	1954	rBV	203653	356468	25.80%	2.779%
64	7.687	1965	1974	1978	rBV3	2604	3881	0.28%	0.030%
65	7.739	1981	1990	2001	rVB	21037	34394	2.49%	0.268%
66	7.787	2003	2005	2007	rBV2	654	378	0.03%	0.003%
67	7.822	2013	2016	2020	rBB3	265	187	0.01%	0.001%
68	7.845	2020	2023	2025	rVB3	410	229	0.02%	0.002%
69	7.899	2025	2040	2056	rBV	664693	1132582	81.97%	8.830%
70	7.970	2056	2062	2074	rVB	10271	16475	1.19%	0.128%
71	8.041	2082	2084	2088	rVB3	359	227	0.02%	0.002%
72	8.070	2091	2093	2095	rBV4	541	315	0.02%	0.002%
73	8.179	2111	2127	2151	rBV	144679	250141	18.10%	1.950%
74	8.404	2194	2197	2202	rVB3	452	421	0.03%	0.003%
75	8.472	2205	2218	2235	rBV3	15715	30670	2.22%	0.239%
76	8.575	2235	2250	2257	rBV	15194	25324	1.83%	0.197%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022222\
Data File : VU047234.D
Acq On : 22 Feb 2022 16:13
Operator : SY/MD
Sample : N1621-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBD34

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\SFAMULM021022WMA.M
Title : VOC Analysis

77	8.632	2257	2268	2286	rVV	649521	1071217	77.53%	8.351%
78	8.726	2287	2297	2315	rVB	233525	367628	26.61%	2.866%
79	8.835	2321	2331	2342	rVB	23977	38869	2.81%	0.303%
80	8.909	2351	2354	2356	rVB2	355	180	0.01%	0.001%
81	9.031	2390	2392	2397	rVB3	415	296	0.02%	0.002%
82	9.060	2398	2401	2403	rBV2	296	194	0.01%	0.002%
83	9.115	2414	2418	2421	rBV2	269	228	0.02%	0.002%
84	9.173	2432	2436	2437	rBV2	363	201	0.01%	0.002%
85	9.211	2437	2448	2465	rVV	136747	208913	15.12%	1.629%
86	9.321	2472	2482	2484	rBV2	1459	2337	0.17%	0.018%
87	9.417	2500	2512	2544	rVB	638734	1048589	75.89%	8.175%
88	10.073	2709	2716	2729	rVB2	5011	7455	0.54%	0.058%
89	10.674	2895	2903	2911	rBV3	2417	3804	0.28%	0.030%
90	10.758	2916	2929	2946	rVV	527917	840276	60.81%	6.551%
91	10.896	2959	2972	2987	rVB2	10853	19200	1.39%	0.150%
92	11.812	3244	3257	3271	rBV	750934	1165777	84.37%	9.088%
93	12.192	3362	3375	3392	rBV	726323	1150499	83.27%	8.969%
94	12.272	3398	3400	3404	rBV2	430	327	0.02%	0.003%
95	12.404	3439	3441	3446	rBV5	444	345	0.02%	0.003%
96	12.671	3521	3524	3529	rBV3	396	270	0.02%	0.002%
97	12.774	3549	3556	3567	rVB	6489	10221	0.74%	0.080%
98	13.365	3738	3740	3743	rVB	523	253	0.02%	0.002%
99	14.327	4036	4039	4046	rVB4	981	777	0.06%	0.006%
100	14.912	4218	4221	4224	rBV2	637	485	0.04%	0.004%

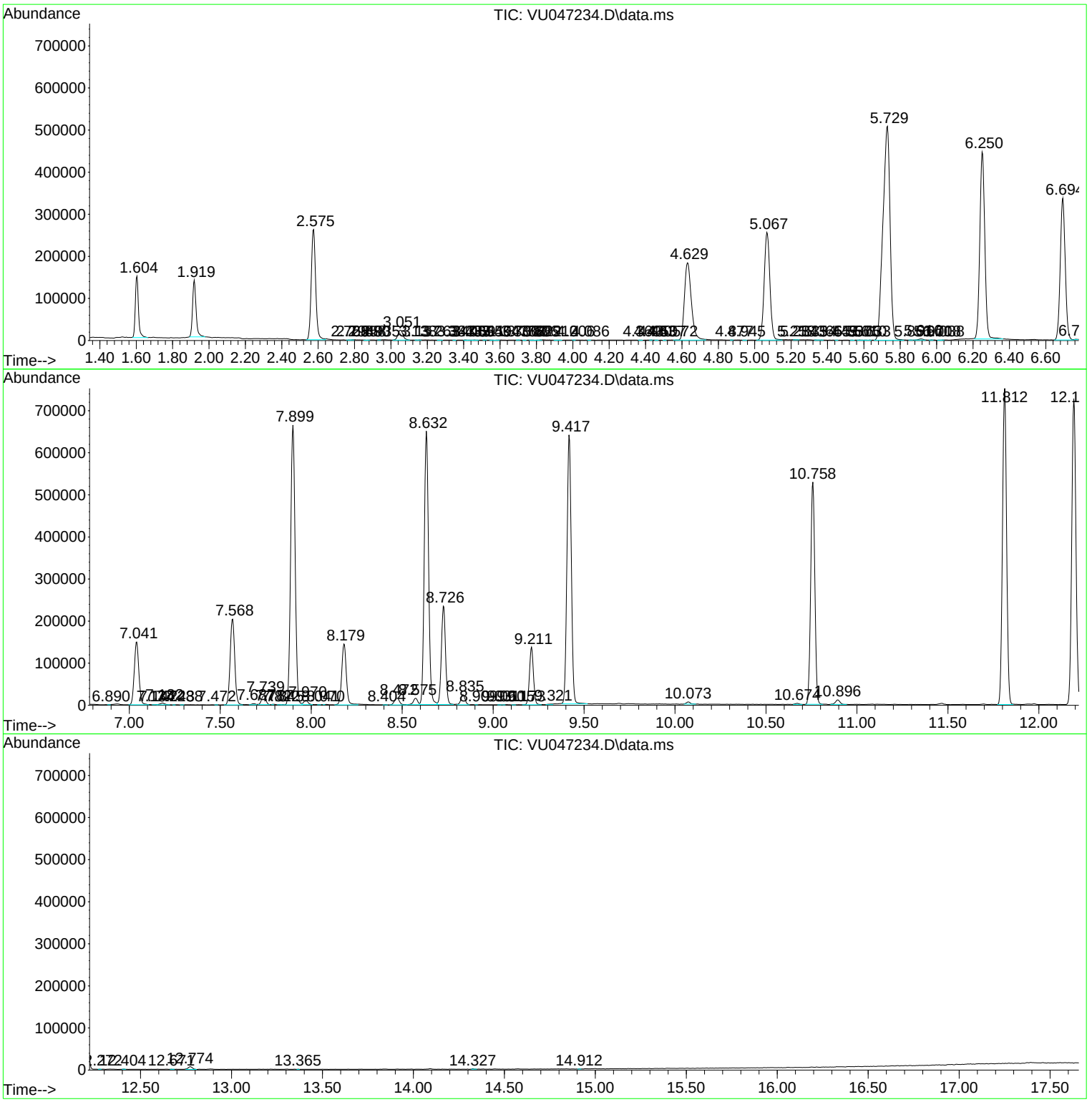
Sum of corrected areas: 12827131

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022222\
Data File : VU047234.D
Acq On : 22 Feb 2022 16:13
Operator : SY/MD
Sample : N1621-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBD34

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022222\
Data File : VU047234.D
Acq On : 22 Feb 2022 16:13
Operator : SY/MD
Sample : N1621-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBD34

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

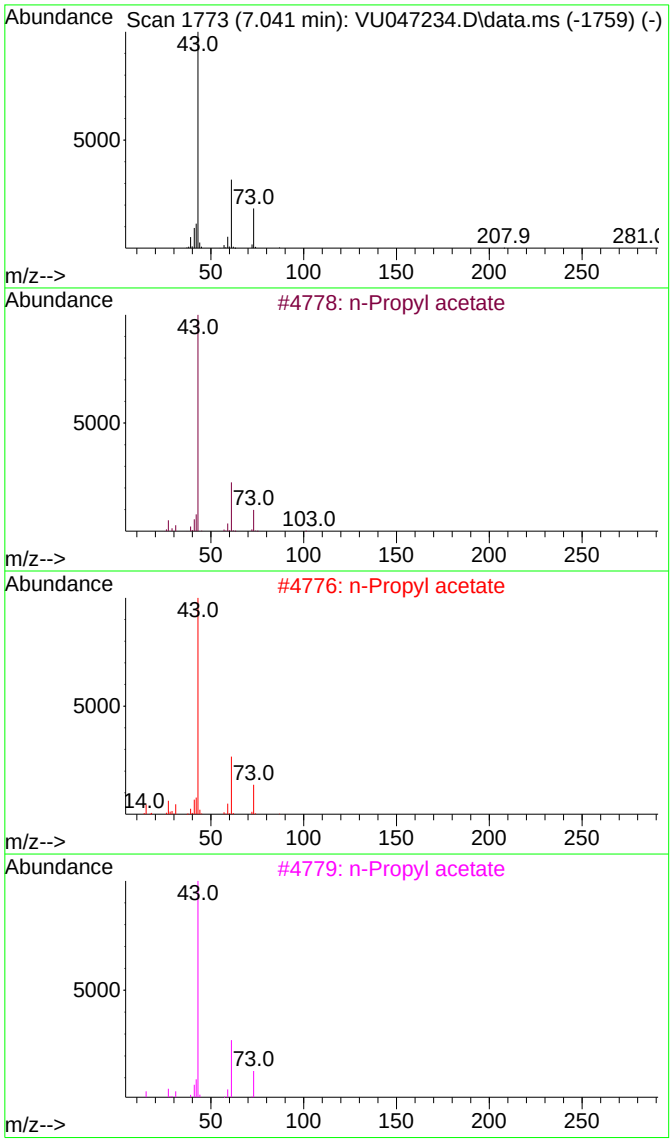
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

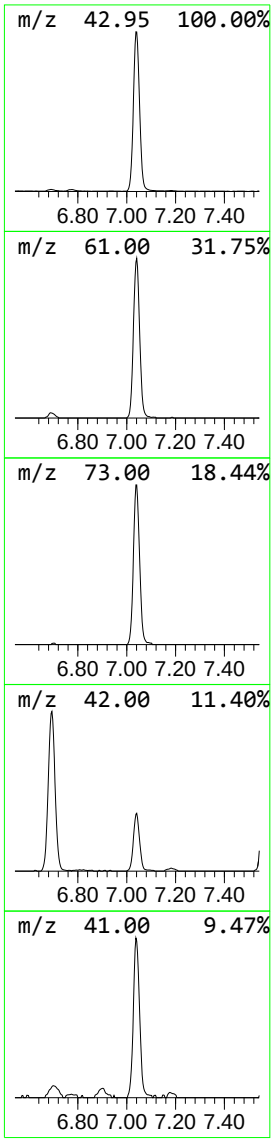
****

Peak Number 2 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	15.44 ug/L	261827	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	50
5	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022222\
Data File : VU047234.D
Acq On : 22 Feb 2022 16:13
Operator : SY/MD
Sample : N1621-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBD34

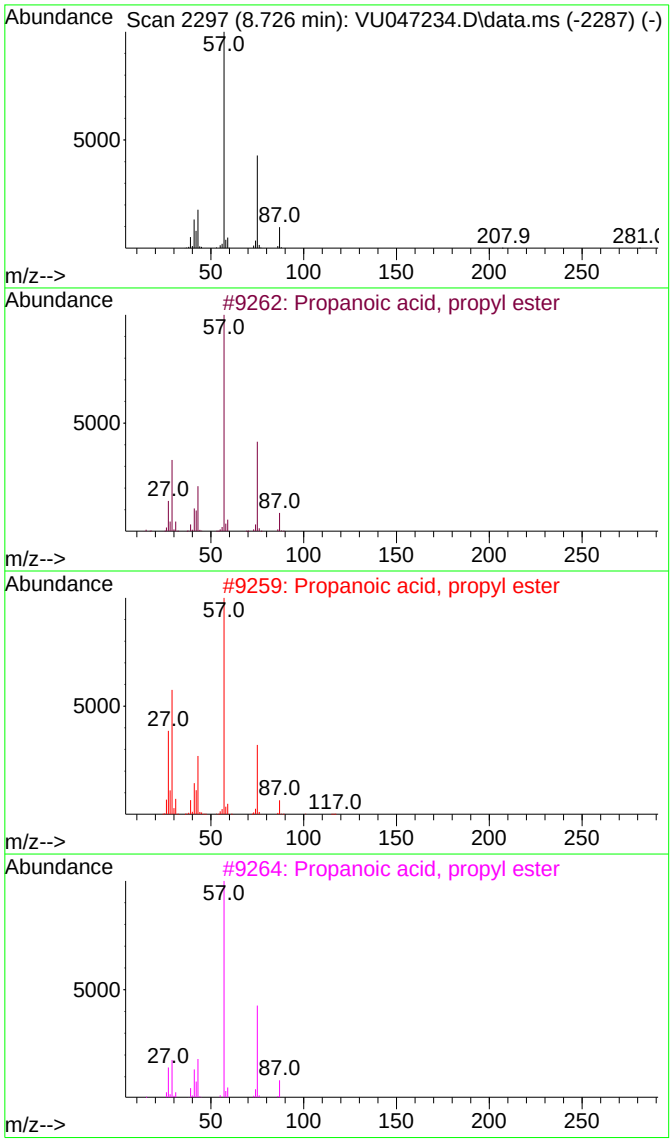
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

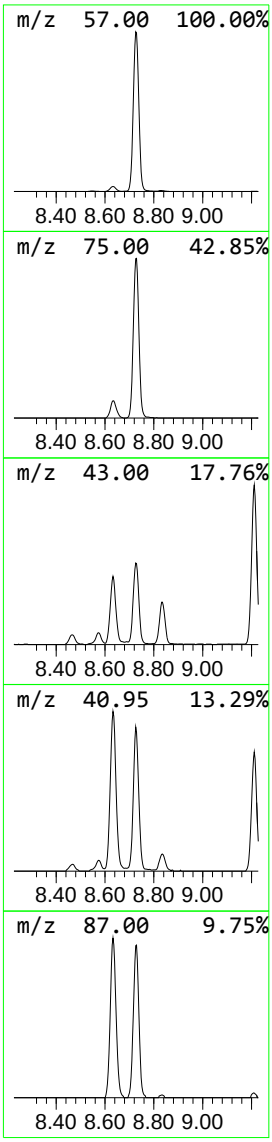
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	17.53 ug/L	367628	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	83
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022222\
Data File : VU047234.D
Acq On : 22 Feb 2022 16:13
Operator : SY/MD
Sample : N1621-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBD34

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

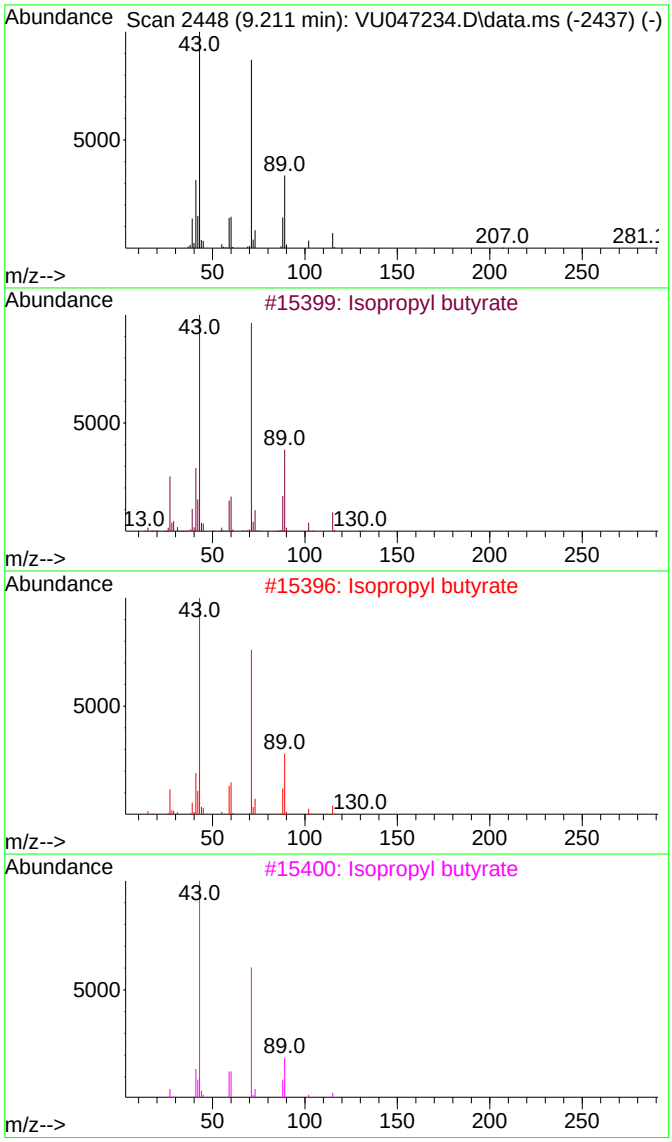
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

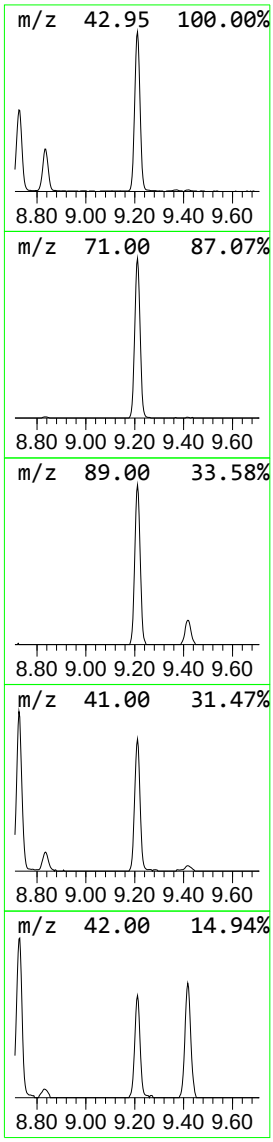
****

Peak Number 5 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	9.96 ug/L	208913	Chlorobenzene-d5	9.417

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	78
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	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\VU022222\
Data File : VU047234.D
Acq On : 22 Feb 2022 16:13
Operator : SY/MD
Sample : N1621-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBD34

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.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	15.4	ug/L	261827	1	6.250	847659	50.0
Propanoic acid,...	8.726	17.5	ug/L	367628	2	9.417	1048590	50.0
Isopropyl butyrate	9.211	10.0	ug/L	208913	2	9.417	1048590	50.0