LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
Data File : VV027062.D
Acq On : 29 Jul 2022 02:32
Operator : SY/MD
Sample : N3820-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXEZ8

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_V\Method\SFAMVLM072822WMA.M
Title : VOC Analysis

Signal : TIC: VV027062.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	74	81	103	rVB	330353	374687	15.05%	1.981%
2	1.561	154	162	177	rBV	254371	310059	12.46%	1.640%
3	2.095	318	328	345	rVB	624411	877602	35.26%	4.641%
4	2.500	444	454	466	rVB2	20165	35165	1.41%	0.186%
5	2.609	478	488	510	rVB	15155	32504	1.31%	0.172%
6	2.793	543	545	551	rVB5	685	561	0.02%	0.003%
7	2.831	555	557	560	rVB3	485	297	0.01%	0.002%
8	2.879	566	572	576	rBV2	546	689	0.03%	0.004%
9	2.902	576	579	584	rVB3	322	343	0.01%	0.002%
10	2.928	584	587	589	rBV	429	332	0.01%	0.002%
11	3.030	611	619	625	rBV4	907	1269	0.05%	0.007%
12	3.339	713	715	723	rVB2	362	354	0.01%	0.002%
13	3.741	836	840	843	rBV3	905	904	0.04%	0.005%
14	3.805	857	860	864	rBV3	341	377	0.02%	0.002%
15	3.895	877	888	941	rBV2	99569	525657	21.12%	2.780%
16	4.339	1010	1026	1052	rBV	391210	975845	39.21%	5.160%
17	4.670	1118	1129	1141	rVB8	2855	6832	0.27%	0.036%
18	4.741	1146	1151	1154	rBV4	308	327	0.01%	0.002%
19	5.040	1226	1244	1287	rBV2	971812	2488809	100.00%	13.161%
20	5.259	1308	1312	1313	rBV2	1170	836	0.03%	0.004%
21	5.291	1314	1322	1341	rVV2	10036	29672	1.19%	0.157%
22	5.558	1403	1405	1407	rBV2	509	307	0.01%	0.002%
23	5.612	1409	1422	1453	rBV	619612	1275710	51.26%	6.746%
24	5.789	1466	1477	1478	rBV5	5812	9279	0.37%	0.049%
25	6.066	1550	1563	1595	rVB	537548	1118439	44.94%	5.914%
26	6.355	1646	1653	1656	rBV3	6001	7867	0.32%	0.042%
27	6.464	1678	1687	1727	rBV	140615	308753	12.41%	1.633%
28	6.831	1797	1801	1804	rVB4	694	624	0.03%	0.003%
29	6.853	1806	1808	1812	rVV3	606	453	0.02%	0.002%
30	6.982	1835	1848	1873	rBV	250863	470453	18.90%	2.488%
31	7.188	1901	1912	1925	rBV	33685	62905	2.53%	0.333%
32	7.313	1939	1951	1978	rBV	1107594	1940442	77.97%	10.261%
33	7.619	2036	2046	2080	rBV	206338	382657	15.38%	2.023%
34	7.738	2080	2083	2089	rBV6	1163	1121	0.05%	0.006%
35	7.812	2103	2106	2109	rBV3	894	528	0.02%	0.003%
36	7.870	2122	2124	2127	rBV2	507	295	0.01%	0.002%

LSC Area Percent Report

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Sample : N3820-01 10X
Misc : 5.0mL/MSVOA_V/WATER
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Instrument :
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ClientSampleId :
EXEZ8

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_V\Method\SFAMVLM072822WMA.M
Title : VOC Analysis

37	7.924	2130	2141	2154	rBV	39432	69878	2.81%	0.370%
38	8.040	2165	2177	2182	rBV4	10000	17298	0.70%	0.091%
39	8.091	2183	2193	2217	rVV	529936	1156867	46.48%	6.117%
40	8.194	2218	2225	2249	rVV2	83553	164431	6.61%	0.869%
41	8.307	2252	2260	2278	rVB	38629	69272	2.78%	0.366%
42	8.509	2320	2323	2327	rBV2	666	400	0.02%	0.002%
43	8.680	2366	2376	2396	rVV	120575	204551	8.22%	1.082%
44	8.850	2416	2429	2452	rBV	1000269	1621293	65.14%	8.573%
45	9.017	2476	2481	2495	rVB4	4496	7189	0.29%	0.038%
46	9.143	2509	2520	2530	rVB5	7657	14398	0.58%	0.076%
47	9.220	2540	2544	2549	rBV4	586	507	0.02%	0.003%
48	9.265	2555	2558	2560	rVB2	749	466	0.02%	0.002%
49	9.294	2560	2567	2572	rVB5	795	993	0.04%	0.005%
50	9.403	2595	2601	2608	rBV4	1628	2519	0.10%	0.013%
51	9.490	2625	2628	2633	rVB3	381	380	0.02%	0.002%
52	9.551	2637	2647	2657	rBV5	7583	13660	0.55%	0.072%
53	9.795	2721	2723	2728	rVB2	470	353	0.01%	0.002%
54	10.027	2792	2795	2801	rVB	663	512	0.02%	0.003%
55	10.085	2808	2813	2815	rBV	361	291	0.01%	0.002%
56	10.213	2841	2853	2872	rBV	786933	1258660	50.57%	6.656%
57	10.455	2924	2928	2934	rVV4	1444	1533	0.06%	0.008%
58	10.484	2934	2937	2939	rVV3	715	391	0.02%	0.002%
59	10.545	2947	2956	2957	rBV2	1006	1195	0.05%	0.006%
60	10.577	2963	2966	2969	rVV4	411	298	0.01%	0.002%
61	10.680	2992	2998	2999	rVV2	426	431	0.02%	0.002%
62	10.689	2999	3001	3005	rVV	489	305	0.01%	0.002%
63	10.741	3009	3017	3026	rVV4	918	1561	0.06%	0.008%
64	10.857	3049	3053	3056	rVB2	784	505	0.02%	0.003%
65	10.924	3065	3074	3081	rBV4	1770	2721	0.11%	0.014%
66	10.966	3084	3087	3091	rVB3	410	310	0.01%	0.002%
67	10.988	3091	3094	3100	rVB3	446	393	0.02%	0.002%
68	11.053	3110	3114	3118	rVB3	561	528	0.02%	0.003%
69	11.156	3142	3146	3151	rBV4	476	450	0.02%	0.002%
70	11.249	3163	3175	3198	rBV	906937	1412484	56.75%	7.469%
71	11.403	3221	3223	3226	rBV2	508	341	0.01%	0.002%
72	11.529	3260	3262	3266	rVB3	624	381	0.02%	0.002%
73	11.548	3266	3268	3271	rBV2	636	410	0.02%	0.002%
74	11.622	3278	3291	3323	rBV	1039915	1626853	65.37%	8.603%
75	11.795	3340	3345	3348	rVB4	547	593	0.02%	0.003%
76	11.988	3401	3405	3407	rBV4	464	382	0.02%	0.002%

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Sample : N3820-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXEZ8

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Title : VOC Analysis

77	12.175	3457	3463	3467	rVB3	605	560	0.02%	0.003%
78	12.316	3503	3507	3510	rBV3	348	315	0.01%	0.002%
79	12.426	3539	3541	3545	rVB2	516	351	0.01%	0.002%
80	12.464	3545	3553	3557	rBV3	544	700	0.03%	0.004%
81	12.490	3557	3561	3566	rVB4	429	426	0.02%	0.002%
82	12.651	3608	3611	3617	rVV4	466	494	0.02%	0.003%
83	13.049	3730	3735	3739	rBV4	438	520	0.02%	0.003%
84	13.149	3761	3766	3769	rBV2	512	460	0.02%	0.002%
85	13.194	3777	3780	3783	rBV3	374	320	0.01%	0.002%
86	13.274	3801	3805	3808	rBV3	462	377	0.02%	0.002%
87	13.307	3812	3815	3820	rBV3	424	361	0.01%	0.002%
88	13.413	3845	3848	3851	rVB2	402	277	0.01%	0.001%
89	13.429	3851	3853	3856	rBV2	588	426	0.02%	0.002%
90	13.516	3874	3880	3884	rBV4	1324	1481	0.06%	0.008%
91	13.750	3951	3953	3958	rVB4	599	466	0.02%	0.002%
92	13.821	3971	3975	3978	rBV4	609	567	0.02%	0.003%
93	13.901	3996	4000	4002	rBV3	492	519	0.02%	0.003%
94	14.294	4120	4122	4125	rBV3	406	274	0.01%	0.001%
95	14.335	4132	4135	4137	rBV	523	334	0.01%	0.002%
96	14.506	4184	4188	4190	rBV3	465	333	0.01%	0.002%
97	14.583	4207	4212	4213	rBV	484	394	0.02%	0.002%
98	15.204	4401	4405	4408	rBV5	974	906	0.04%	0.005%
99	15.390	4460	4463	4464	rBV2	765	440	0.02%	0.002%
100	16.168	4703	4705	4709	rBV4	1192	885	0.04%	0.005%

Sum of corrected areas: 18911123

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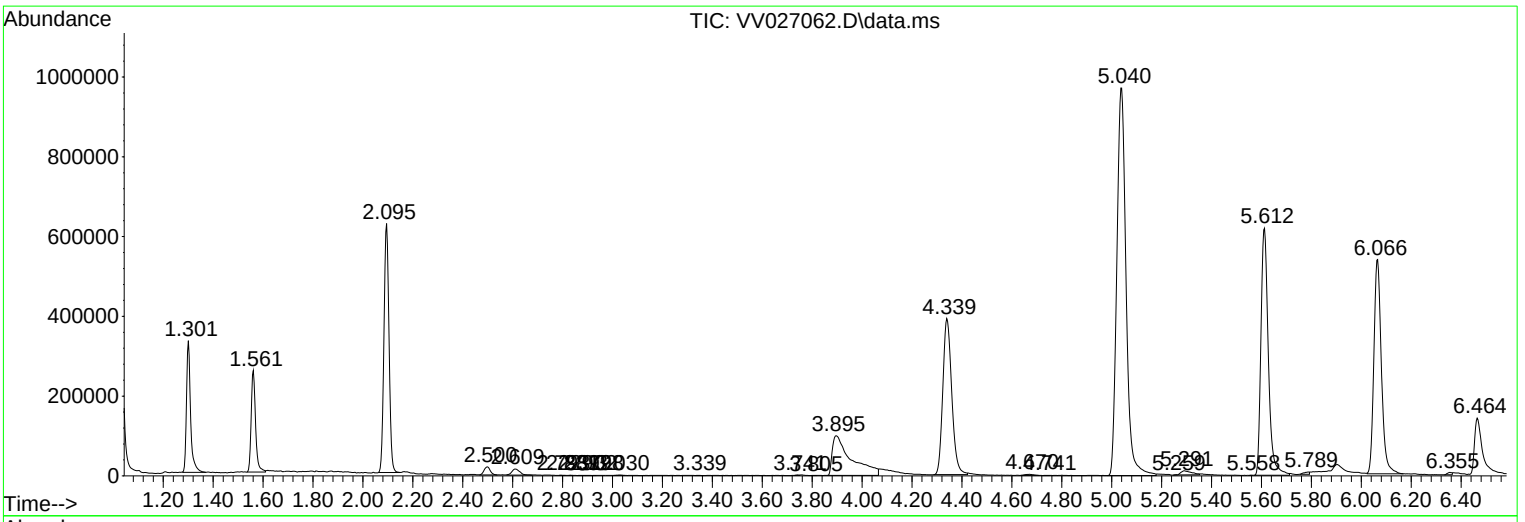
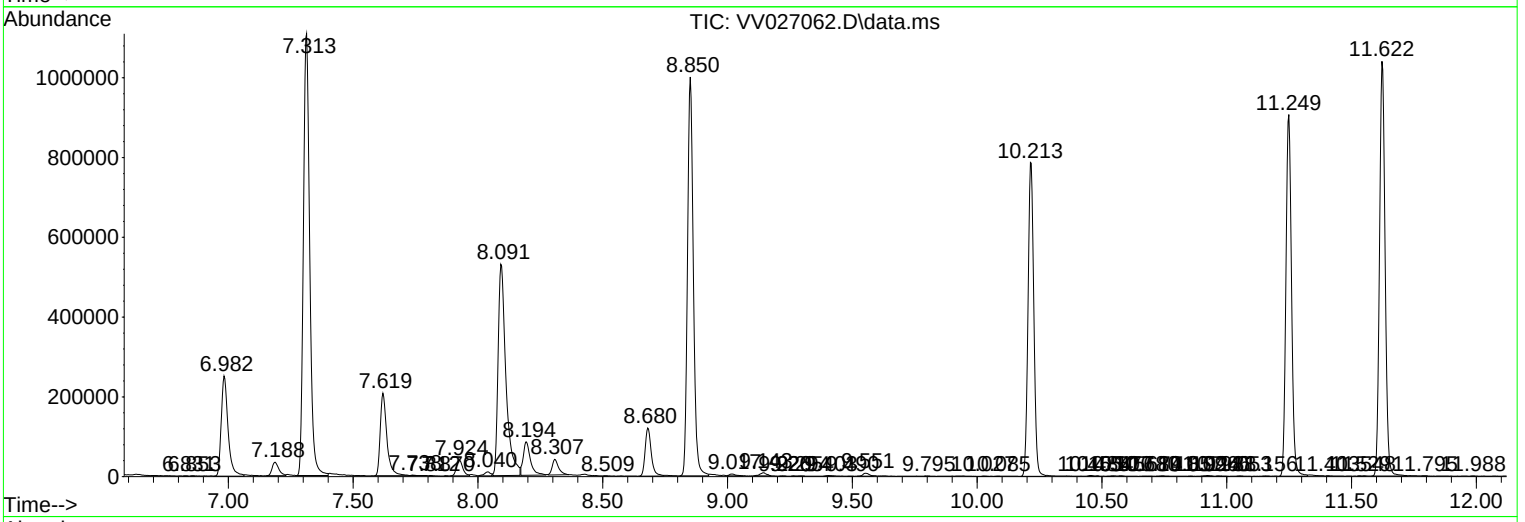
ALS Vial : 32 Sample Multiplier: 1

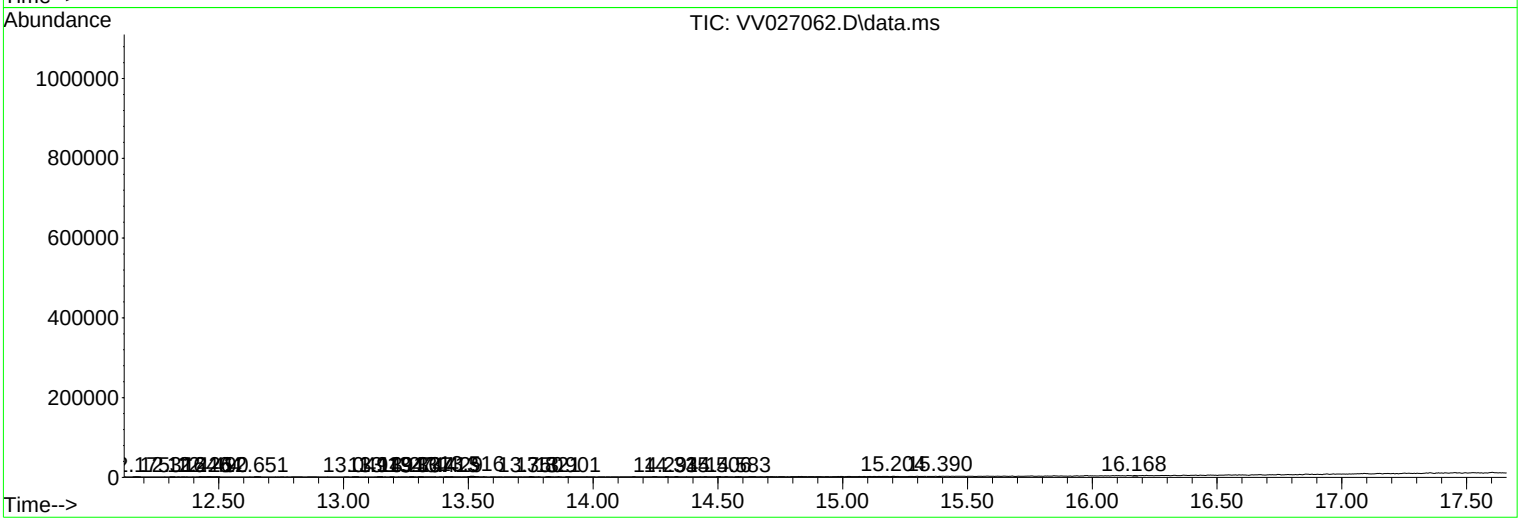
Instrument :
MSVOA_V
ClientSampleId :
EXEZ8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

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







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Instrument :
MSVOA_V
ClientSampleId :
EXEZ8

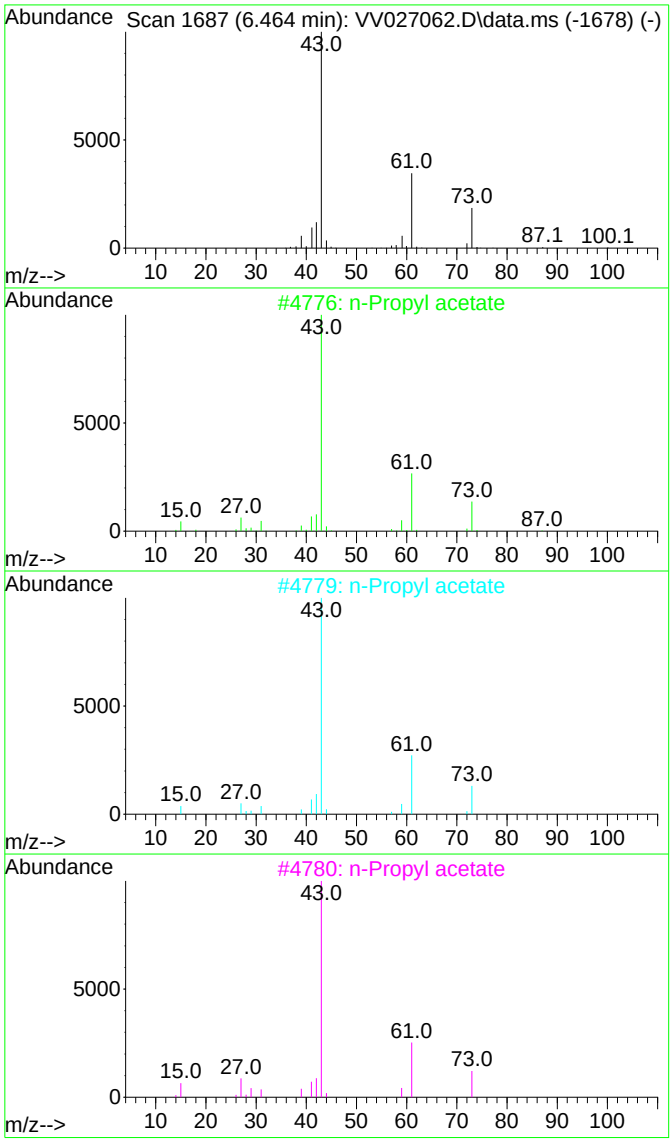
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

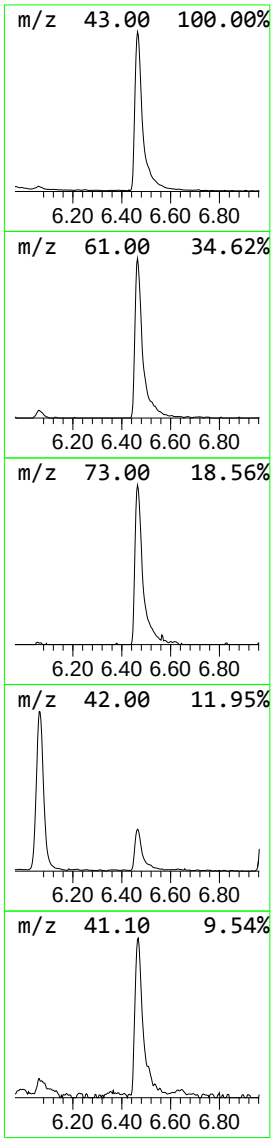
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.464	12.10 ug/L	308753	1,4-Difluorobenzene	5.612

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	72
4	n-Propyl acetate	102	C5H10O2	000109-60-4	72
5	Isopropyl acetate	102	C5H10O2	000108-21-4	36





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MSVOA_V
ClientSampleId :
EXEZ8

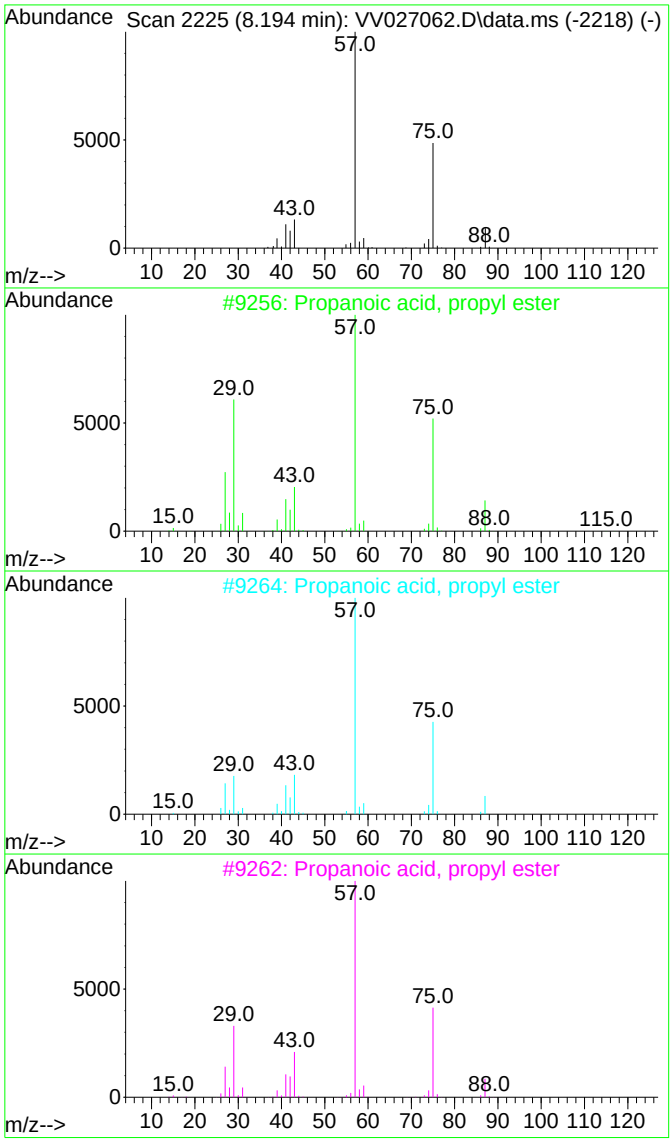
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

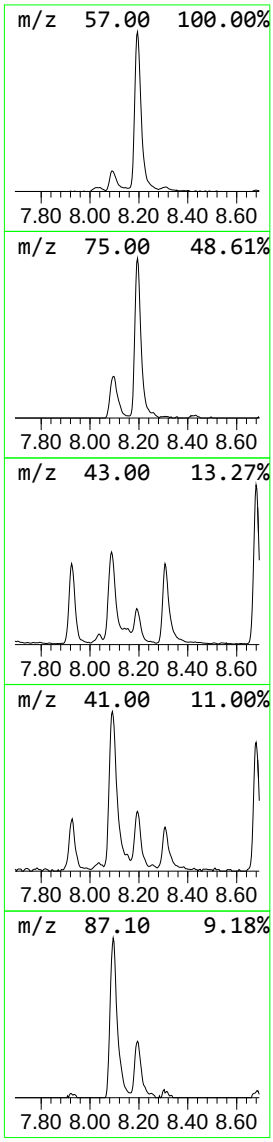
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.194	5.07 ug/L	164431	Chlorobenzene-d5	8.850

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	43
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	38





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ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXEZ8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

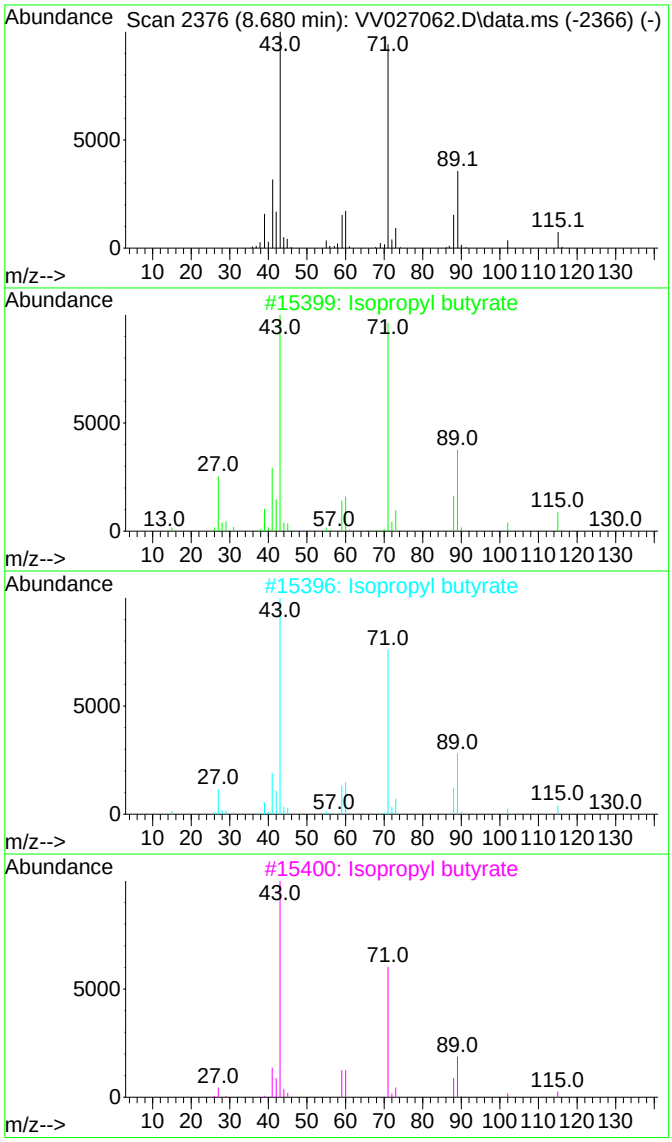
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

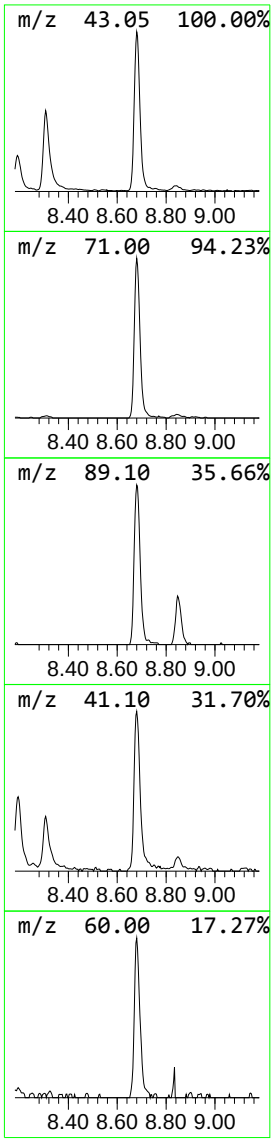
****

Peak Number 4 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.680	6.31 ug/L	204551	Chlorobenzene-d5	8.850

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	83
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64





Tentatively Identified Compound (LSC) summary

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Instrument :
MSVOA_V
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.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	6.464	12.1	ug/L	308753	1	5.612	1275710	50.0
Propanoic acid,...	8.194	5.1	ug/L	164431	2	8.850	1621290	50.0
Isopropyl butyrate	8.680	6.3	ug/L	204551	2	8.850	1621290	50.0