LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV042624\
Data File : VV035431.D
Acq On : 26 Apr 2024 16:52
Operator : SY/MD
Sample : PB160522TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
LEB522

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\SFAMVLM042624WMA.M
Title : VOC Analysis

Signal : TIC: VV035431.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.188	42	46	49	rBV	2524	2246	0.13%	0.015%
2	1.278	67	74	89	rVB	266599	286077	15.96%	1.957%
3	1.532	145	153	166	rBV	236733	272301	15.19%	1.863%
4	2.056	306	316	332	rBV	434945	626768	34.97%	4.287%
5	2.445	429	437	447	rBV2	7050	10724	0.60%	0.073%
6	2.558	460	472	484	rBV	5182	11161	0.62%	0.076%
7	2.802	542	548	554	rBV2	387	404	0.02%	0.003%
8	2.847	558	562	564	rBV	390	266	0.01%	0.002%
9	2.899	574	578	585	rVB2	212	290	0.02%	0.002%
10	2.934	585	589	593	rBV2	420	316	0.02%	0.002%
11	3.127	636	649	650	rBV3	1023	1357	0.08%	0.009%
12	3.185	665	667	672	rVB4	334	246	0.01%	0.002%
13	3.278	694	696	702	rVB2	457	365	0.02%	0.002%
14	3.384	726	729	734	rVV2	353	248	0.01%	0.002%
15	3.500	762	765	768	rBV2	317	222	0.01%	0.002%
16	3.799	849	858	895	rBV	96010	331247	18.48%	2.266%
17	4.243	980	996	1030	rBV	276961	723452	40.37%	4.948%
18	4.674	1126	1130	1137	rBV4	269	309	0.02%	0.002%
19	4.806	1166	1171	1174	rBV2	243	273	0.02%	0.002%
20	4.851	1179	1185	1187	rBV2	327	373	0.02%	0.003%
21	4.953	1200	1217	1253	rBV2	682164	1792190	100.00%	12.259%
22	5.220	1291	1300	1314	rBV2	7898	19682	1.10%	0.135%
23	5.397	1353	1355	1359	rVB4	659	385	0.02%	0.003%
24	5.529	1385	1396	1436	rBV	574220	1201552	67.04%	8.219%
25	5.834	1480	1491	1506	rVV5	8205	18880	1.05%	0.129%
26	5.986	1525	1538	1576	rVV	389060	809254	45.15%	5.535%
27	6.137	1582	1585	1588	rBV4	579	525	0.03%	0.004%
28	6.304	1631	1637	1638	rBV2	2998	2466	0.14%	0.017%
29	6.397	1657	1666	1694	rBV	117642	251290	14.02%	1.719%
30	6.822	1795	1798	1802	rBV3	648	561	0.03%	0.004%
31	6.912	1816	1826	1853	rBV	199943	386874	21.59%	2.646%
32	7.121	1883	1891	1906	rBV	28672	51433	2.87%	0.352%
33	7.239	1917	1928	1966	rBV	802250	1418441	79.15%	9.702%
34	7.551	2014	2025	2050	rBV2	165421	317190	17.70%	2.170%
35	7.860	2112	2121	2149	rVB2	38251	70015	3.91%	0.479%
36	7.976	2149	2157	2162	rBV3	8778	13191	0.74%	0.090%

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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
LEB522

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\SFAMVLM042624WMA.M
Title : VOC Analysis

37	8.027	2163	2173	2198	rVV2	303879	708111	39.51%	4.844%
38	8.130	2200	2205	2223	rVB2	69106	120828	6.74%	0.826%
39	8.249	2235	2242	2269	rVB	31404	65445	3.65%	0.448%
40	8.503	2319	2321	2324	rVB2	434	234	0.01%	0.002%
41	8.522	2324	2327	2330	rBV3	396	240	0.01%	0.002%
42	8.619	2348	2357	2382	rBV	114780	193073	10.77%	1.321%
43	8.783	2397	2408	2447	rBV	902261	1508489	84.17%	10.318%
44	9.191	2531	2535	2536	rBV2	419	329	0.02%	0.002%
45	9.243	2547	2551	2556	rBV2	366	286	0.02%	0.002%
46	9.272	2556	2560	2563	rVB2	289	243	0.01%	0.002%
47	9.294	2563	2567	2571	rBV3	540	451	0.03%	0.003%
48	9.323	2574	2576	2578	rVB2	548	230	0.01%	0.002%
49	9.346	2578	2583	2585	rBV3	533	414	0.02%	0.003%
50	9.423	2605	2607	2613	rVB2	400	267	0.01%	0.002%
51	9.452	2613	2616	2621	rVB3	395	269	0.02%	0.002%
52	9.500	2621	2631	2649	rBV3	5040	10965	0.61%	0.075%
53	9.628	2668	2671	2676	rVB3	610	480	0.03%	0.003%
54	9.725	2698	2701	2707	rVB2	417	378	0.02%	0.003%
55	9.757	2708	2711	2713	rBV	404	251	0.01%	0.002%
56	9.792	2716	2722	2725	rVB3	363	345	0.02%	0.002%
57	9.924	2758	2763	2766	rBV3	299	270	0.02%	0.002%
58	9.947	2766	2770	2773	rVB2	361	222	0.01%	0.002%
59	9.989	2779	2783	2786	rBV3	330	249	0.01%	0.002%
60	10.082	2808	2812	2815	rBV2	327	271	0.02%	0.002%
61	10.149	2820	2833	2858	rBV	547194	875078	48.83%	5.986%
62	10.429	2916	2920	2923	rBV2	437	370	0.02%	0.003%
63	10.474	2931	2934	2936	rBV3	522	347	0.02%	0.002%
64	10.503	2940	2943	2950	rVB4	583	569	0.03%	0.004%
65	10.571	2960	2964	2967	rBV	269	224	0.01%	0.002%
66	10.587	2967	2969	2972	rVB3	390	226	0.01%	0.002%
67	10.693	2999	3002	3008	rBV3	275	310	0.02%	0.002%
68	10.722	3008	3011	3015	rBV2	361	277	0.02%	0.002%
69	10.792	3028	3033	3038	rVB5	557	668	0.04%	0.005%
70	10.944	3077	3080	3084	rVB2	379	279	0.02%	0.002%
71	11.034	3106	3108	3110	rBV2	370	238	0.01%	0.002%
72	11.133	3132	3139	3143	rBV4	1111	1412	0.08%	0.010%
73	11.181	3143	3154	3177	rBV	802755	1277336	71.27%	8.737%
74	11.349	3204	3206	3209	rVB3	643	305	0.02%	0.002%
75	11.493	3249	3251	3255	rBV2	275	254	0.01%	0.002%
76	11.558	3259	3271	3298	rBV	741880	1203657	67.16%	8.233%

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Instrument :
MSVOA_V
ClientSampleId :
LEB522

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\SFAMVLM042624WMA.M
Title : VOC Analysis

77	11.850	3360	3362	3365	rVB3	524	244	0.01%	0.002%
78	11.940	3388	3390	3396	rVB2	349	310	0.02%	0.002%
79	11.966	3396	3398	3402	rBV3	502	314	0.02%	0.002%
80	12.017	3410	3414	3416	rBV2	497	309	0.02%	0.002%
81	12.114	3440	3444	3446	rBV2	418	305	0.02%	0.002%
82	12.194	3466	3469	3473	rVB2	264	251	0.01%	0.002%
83	12.342	3511	3515	3518	rBV2	417	379	0.02%	0.003%
84	12.413	3535	3537	3544	rVB2	443	289	0.02%	0.002%
85	12.593	3589	3593	3597	rBV3	567	543	0.03%	0.004%
86	12.728	3630	3635	3641	rBV2	513	519	0.03%	0.004%
87	12.792	3651	3655	3657	rBV2	455	292	0.02%	0.002%
88	12.927	3693	3697	3699	rBV	457	322	0.02%	0.002%
89	13.008	3719	3722	3724	rBV	474	261	0.01%	0.002%
90	13.204	3775	3783	3793	rBV3	6216	9738	0.54%	0.067%
91	13.339	3821	3825	3829	rBV2	340	278	0.02%	0.002%
92	13.468	3852	3865	3869	rBV3	1018	2024	0.11%	0.014%
93	13.689	3925	3934	3944	rVB5	2484	3813	0.21%	0.026%
94	13.924	4002	4007	4008	rBV	289	249	0.01%	0.002%
95	14.033	4037	4041	4042	rBV	443	298	0.02%	0.002%
96	14.197	4089	4092	4096	rBV2	408	311	0.02%	0.002%
97	14.342	4131	4137	4141	rBV5	470	635	0.04%	0.004%
98	14.545	4195	4200	4203	rBV3	491	437	0.02%	0.003%
99	14.786	4271	4275	4281	rBV4	594	776	0.04%	0.005%
100	14.853	4292	4296	4297	rBV3	552	431	0.02%	0.003%

Sum of corrected areas: 14619792

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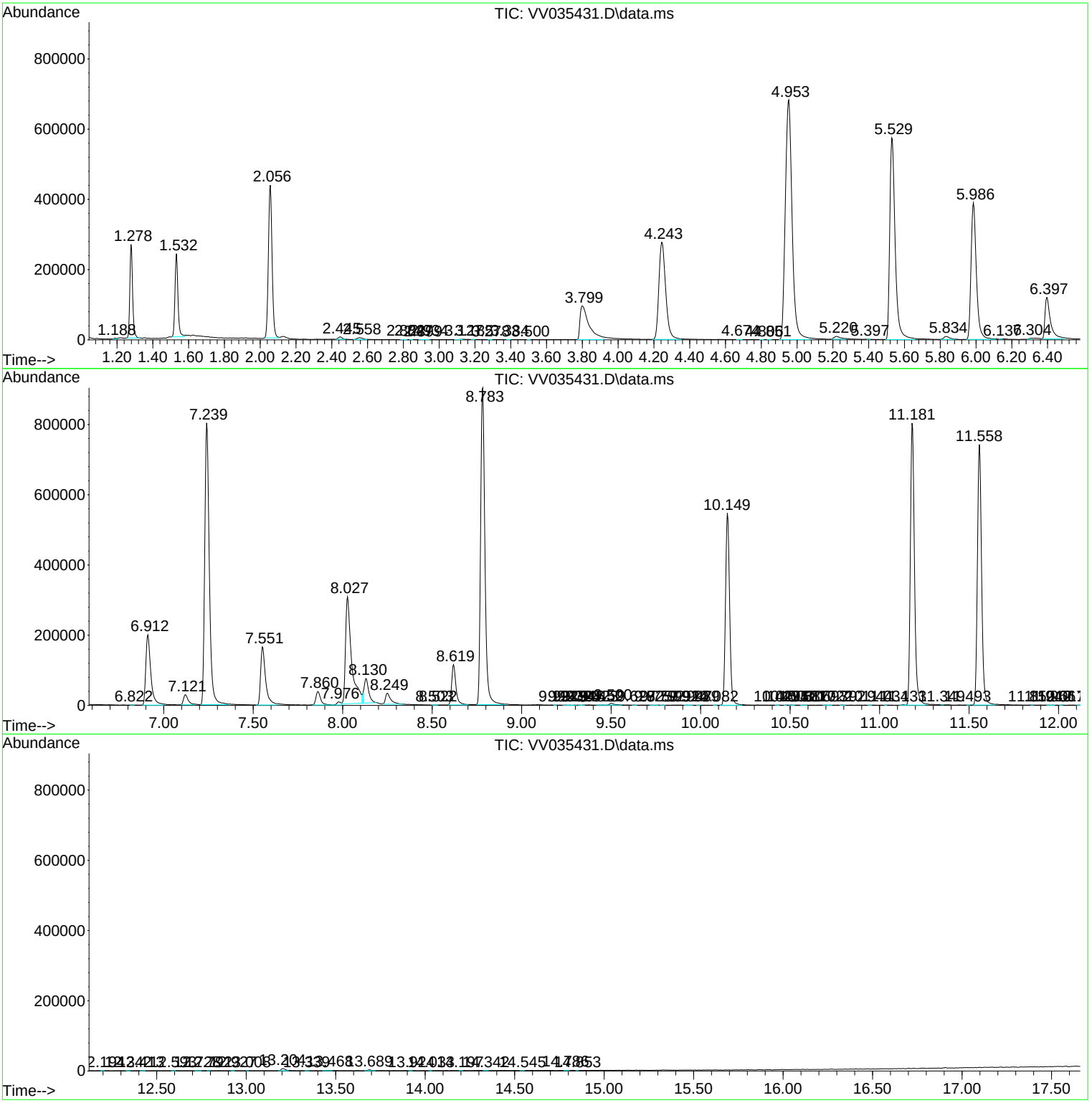
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
LEB522

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042624WMA.M
Quant Title : VOC Analysis

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



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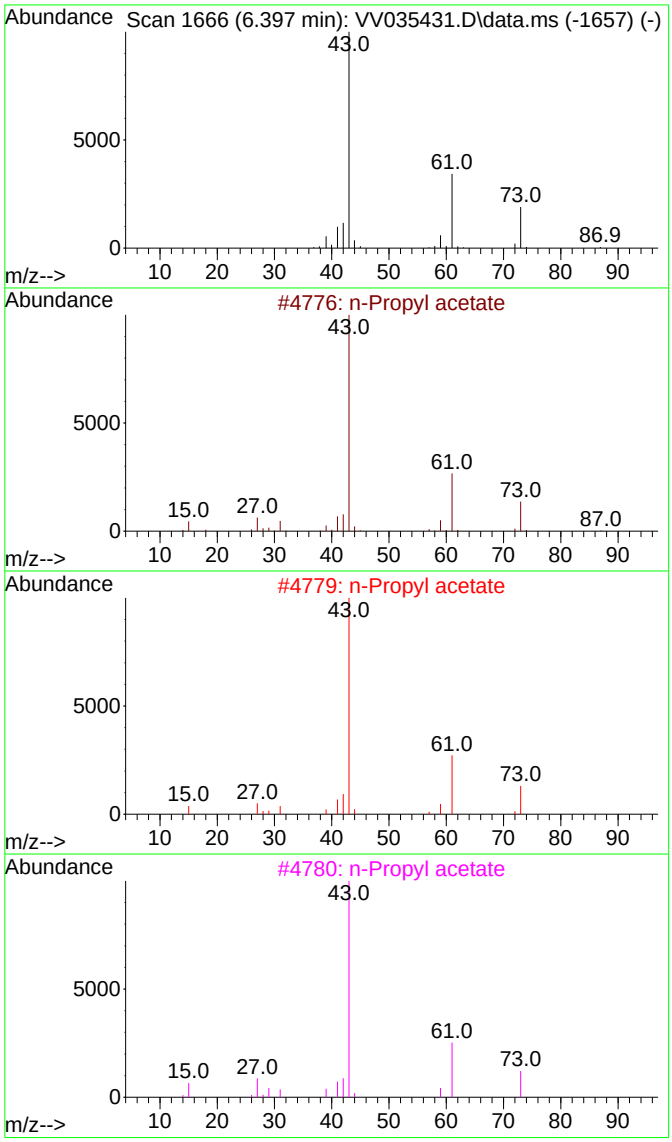
Quant Title : VOC Analysis

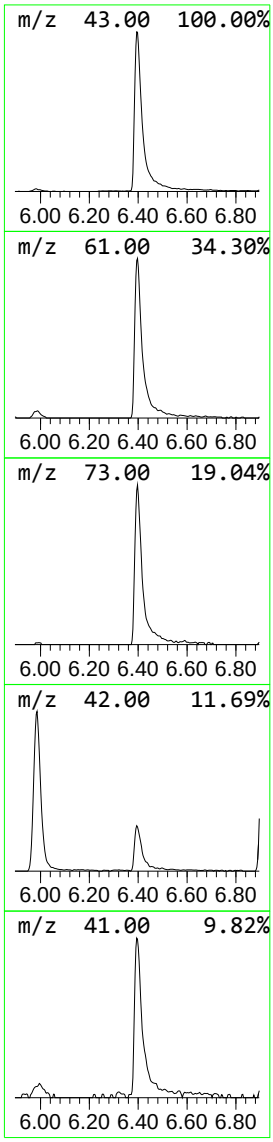
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.397	10.46 ug/L	251290	1,4-Difluorobenzene	5.529

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	64
5	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36





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Instrument :
MSVOA_V
ClientSampleId :
LEB522

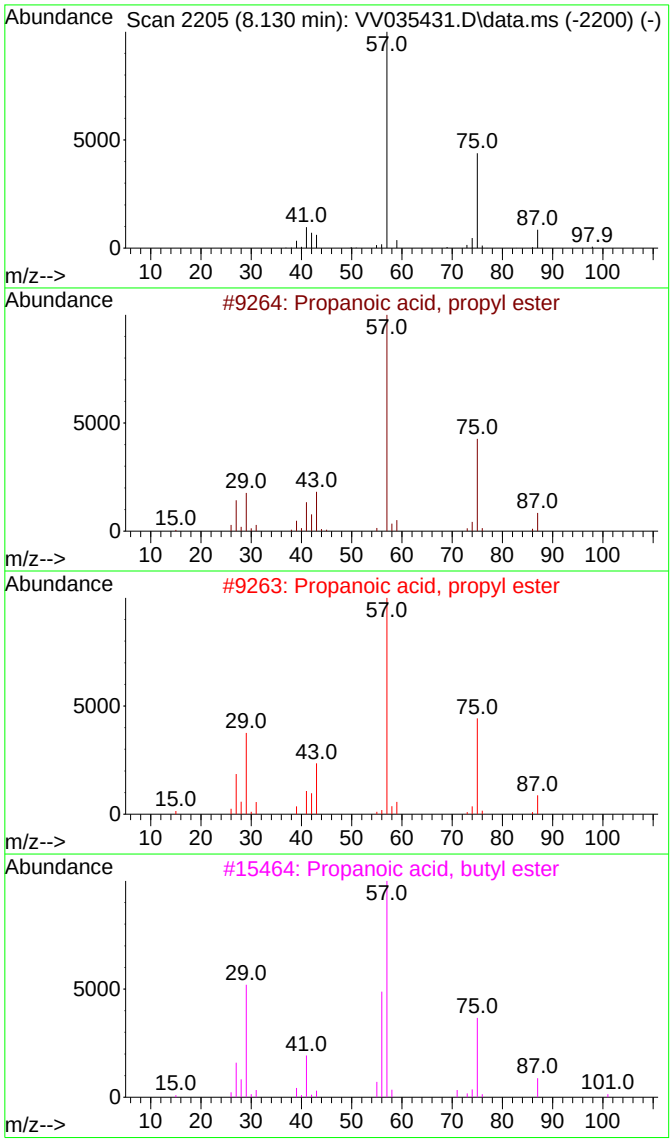
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042624WMA.M
Quant Title : VOC Analysis

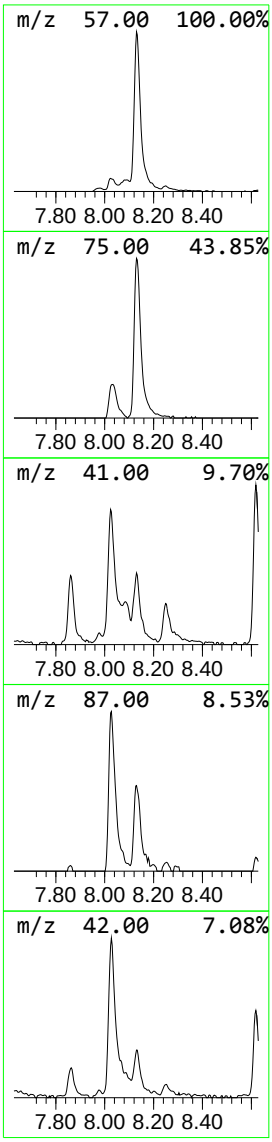
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.130	4.00 ug/L	120828	Chlorobenzene-d5	8.783

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	50
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	40
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	39





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MSVOA_V
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042624WMA.M
Quant Title : VOC Analysis

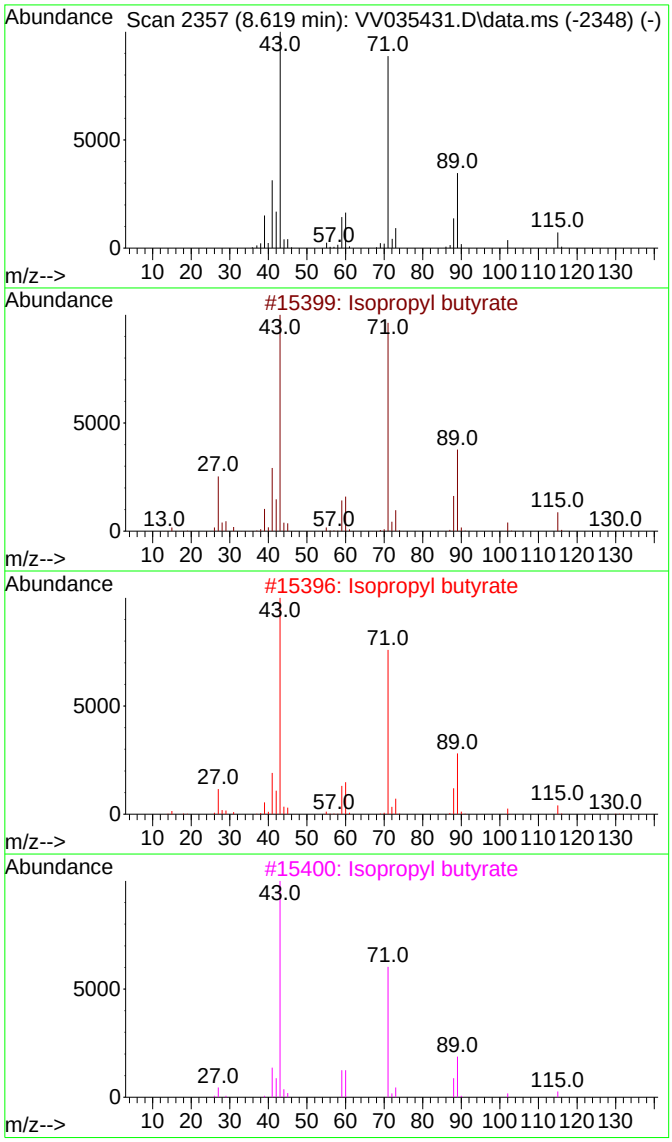
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

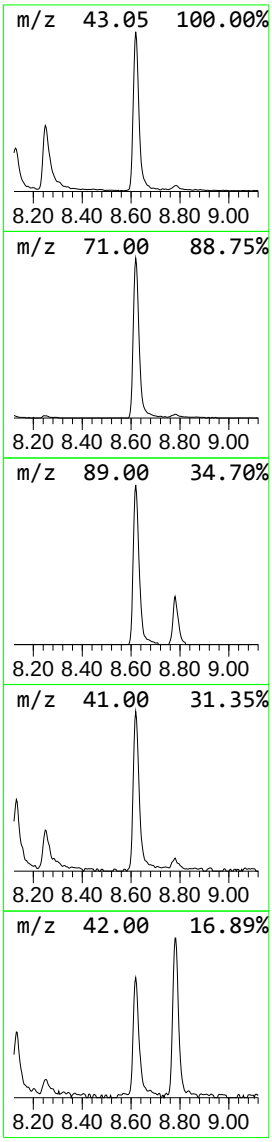
****

Peak Number 4 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	6.40 ug/L	193073	Chlorobenzene-d5	8.783

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, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM042624WMA.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	6.397	10.5	ug/L	251290	1	5.529	1201550	50.0
Propanoic acid,...	8.130	4.0	ug/L	120828	2	8.783	1508490	50.0
Isopropyl butyrate	8.619	6.4	ug/L	193073	2	8.783	1508490	50.0