LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV071521\
Data File : VV021664.D
Acq On : 15 Jul 2021 11:48
Operator : SY/MD
Sample : M3033-04
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BG7M4

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\SFAMVLM062921WMA.M
Title : VOC Analysis

Signal : TIC: VV021664.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.105	15	20	31	rVB	80697	74150	2.58%	0.390%
2	1.304	75	82	95	rVB	247531	260198	9.05%	1.368%
3	1.561	155	162	175	rVB	180863	208909	7.26%	1.098%
4	2.105	321	331	344	rBV	379835	551052	19.16%	2.897%
5	2.757	517	534	562	rBV	435425	879495	30.57%	4.624%
6	3.034	605	620	657	rBV	1450079	2876695	100.00%	15.124%
7	3.352	716	719	721	rBV2	663	479	0.02%	0.003%
8	3.442	745	747	748	rBV	482	218	0.01%	0.001%
9	3.635	804	807	811	rBV3	420	300	0.01%	0.002%
10	3.654	811	813	815	rBV2	456	242	0.01%	0.001%
11	3.757	826	845	869	rBV	717311	1814207	63.07%	9.538%
12	3.867	869	879	922	rVB	149563	389689	13.55%	2.049%
13	4.236	990	994	996	rBV2	569	370	0.01%	0.002%
14	4.346	1012	1028	1058	rBV	279447	696411	24.21%	3.661%
15	4.674	1119	1130	1145	rVB5	9751	23705	0.82%	0.125%
16	4.812	1169	1173	1176	rBV2	425	279	0.01%	0.001%
17	4.866	1187	1190	1192	rBV3	299	163	0.01%	0.001%
18	4.883	1192	1195	1197	rVV4	677	338	0.01%	0.002%
19	4.902	1199	1201	1204	rVB	653	367	0.01%	0.002%
20	5.043	1225	1245	1271	rBV2	692243	1782131	61.95%	9.370%
21	5.455	1371	1373	1375	rBV2	378	193	0.01%	0.001%
22	5.612	1410	1422	1452	rBV	464080	940207	32.68%	4.943%
23	5.828	1485	1489	1492	rVB3	694	508	0.02%	0.003%
24	5.905	1501	1513	1530	rBV2	22091	47761	1.66%	0.251%
25	6.066	1549	1563	1591	rBV	393516	812704	28.25%	4.273%
26	6.384	1658	1662	1663	rBV	337	247	0.01%	0.001%
27	6.416	1670	1672	1678	rVB3	623	483	0.02%	0.003%
28	6.448	1678	1682	1684	rBV2	647	460	0.02%	0.002%
29	6.490	1691	1695	1698	rBV	588	545	0.02%	0.003%
30	6.567	1715	1719	1720	rBV2	505	327	0.01%	0.002%
31	6.812	1793	1795	1799	rVB2	703	344	0.01%	0.002%
32	6.831	1799	1801	1803	rBV	89	40	0.00%	0.000%
33	6.844	1803	1805	1807	rBV	260	93	0.00%	0.000%
34	6.905	1820	1824	1827	rVB3	324	239	0.01%	0.001%
35	6.934	1830	1833	1835	rBV3	509	272	0.01%	0.001%
36	6.985	1837	1849	1873	rBV	240831	439508	15.28%	2.311%

LSC Area Percent Report

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Sample : M3033-04
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BG7M4

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\SFAMVLM062921WMA.M
Title : VOC Analysis

37	7.313	1939	1951	1970	rBV	845247	1484097	51.59%	7.803%
38	7.622	2037	2047	2071	rBV	162368	285285	9.92%	1.500%
39	7.870	2122	2124	2125	rBV	287	97	0.00%	0.001%
40	8.037	2171	2176	2181	rBV4	676	841	0.03%	0.004%
41	8.085	2181	2191	2235	rBV	462890	874501	30.40%	4.598%
42	8.551	2330	2336	2339	rBV4	713	682	0.02%	0.004%
43	8.616	2354	2356	2359	rBV	436	293	0.01%	0.002%
44	8.718	2386	2388	2390	rBV	329	167	0.01%	0.001%
45	8.792	2410	2411	2413	rBV	375	106	0.00%	0.001%
46	8.853	2417	2430	2460	rBV	701415	1143099	39.74%	6.010%
47	9.120	2512	2513	2514	rBV	382	135	0.00%	0.001%
48	9.197	2532	2537	2541	rVB3	711	519	0.02%	0.003%
49	9.268	2556	2559	2561	rBV3	354	197	0.01%	0.001%
50	9.326	2574	2577	2579	rBV	215	120	0.00%	0.001%
51	9.390	2594	2597	2599	rBV2	319	178	0.01%	0.001%
52	9.419	2602	2606	2609	rBV3	281	234	0.01%	0.001%
53	9.519	2634	2637	2639	rBV2	262	129	0.00%	0.001%
54	9.545	2642	2645	2649	rBV3	581	623	0.02%	0.003%
55	9.606	2662	2664	2669	rBV	318	272	0.01%	0.001%
56	9.651	2676	2678	2679	rBV	178	47	0.00%	0.000%
57	9.693	2689	2691	2695	rVB	279	174	0.01%	0.001%
58	9.818	2729	2730	2731	rBV	152	41	0.00%	0.000%
59	9.911	2757	2759	2762	rVB	357	177	0.01%	0.001%
60	9.924	2762	2763	2765	rBV	369	190	0.01%	0.001%
61	9.995	2783	2785	2788	rVB2	476	262	0.01%	0.001%
62	10.014	2788	2791	2793	rBV	498	300	0.01%	0.002%
63	10.217	2841	2854	2876	rBV	540449	854228	29.69%	4.491%
64	10.513	2944	2946	2947	rBV	363	125	0.00%	0.001%
65	10.522	2947	2949	2951	rVV	307	170	0.01%	0.001%
66	10.651	2987	2989	2995	rVB2	575	512	0.02%	0.003%
67	10.921	3066	3073	3083	rVB4	3727	5832	0.20%	0.031%
68	10.979	3088	3091	3095	rVB2	440	235	0.01%	0.001%
69	11.030	3103	3107	3111	rBV3	602	637	0.02%	0.003%
70	11.082	3120	3123	3126	rBV2	738	547	0.02%	0.003%
71	11.149	3136	3144	3155	rBV8	2433	4391	0.15%	0.023%
72	11.249	3164	3175	3199	rBV	764065	1178915	40.98%	6.198%
73	11.519	3257	3259	3261	rBV2	209	101	0.00%	0.001%
74	11.541	3261	3266	3267	rBV2	954	800	0.03%	0.004%
75	11.625	3280	3292	3314	rBV	868470	1372826	47.72%	7.218%
76	12.101	3434	3440	3443	rBV4	712	670	0.02%	0.004%

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ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BG7M4

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\SFAMVLM062921WMA.M
Title : VOC Analysis

77	12.249	3479	3486	3490	rBV3	1185	1370	0.05%	0.007%
78	12.355	3513	3519	3525	rBV7	1573	2159	0.08%	0.011%
79	12.522	3568	3571	3575	rVB	479	375	0.01%	0.002%
80	12.541	3575	3577	3578	rBV	326	139	0.00%	0.001%

Sum of corrected areas: 19020127

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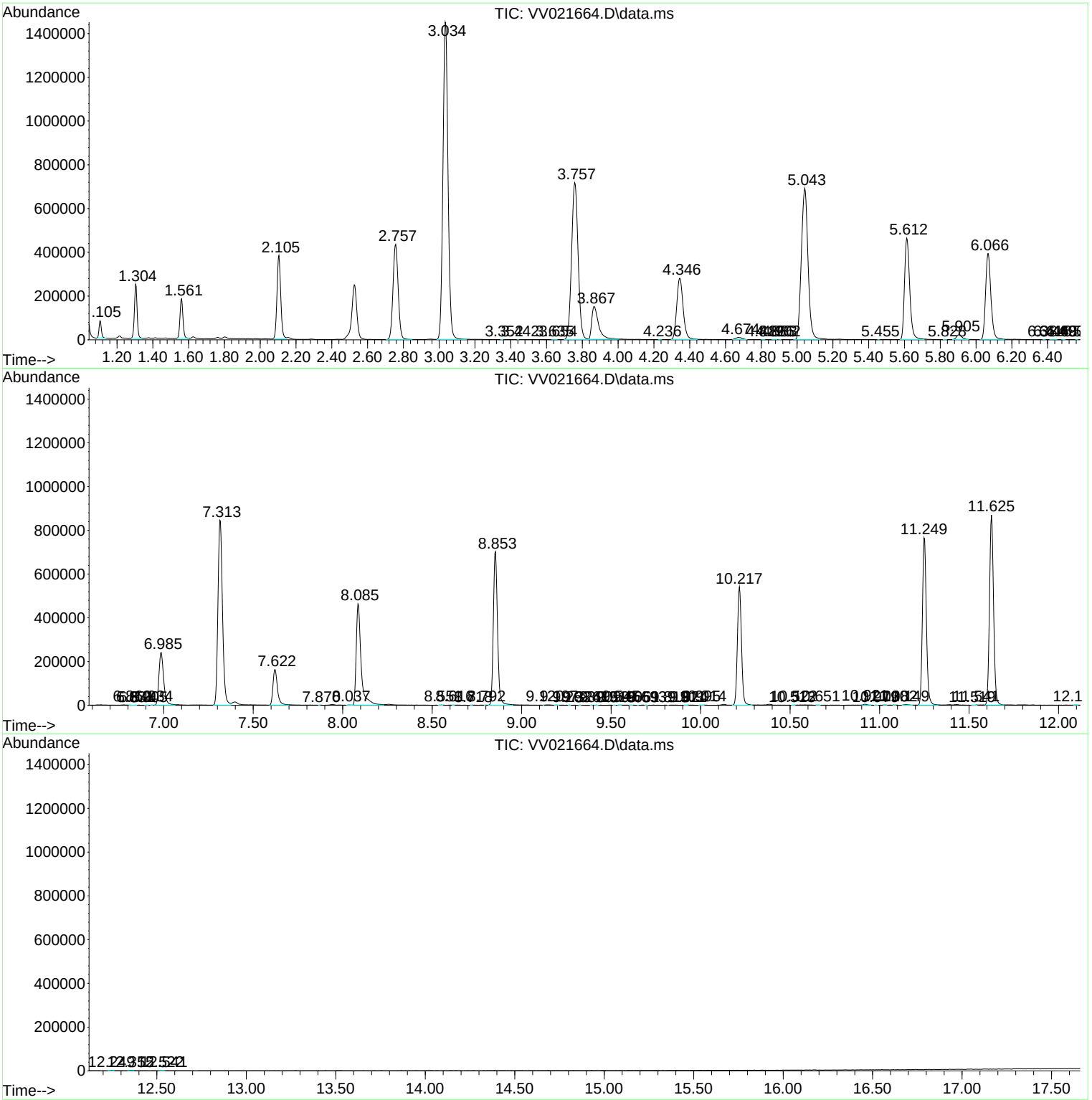
Sample : M3033-04
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG7M4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV071521\
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Operator : SY/MD
Sample : M3033-04
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BG7M4

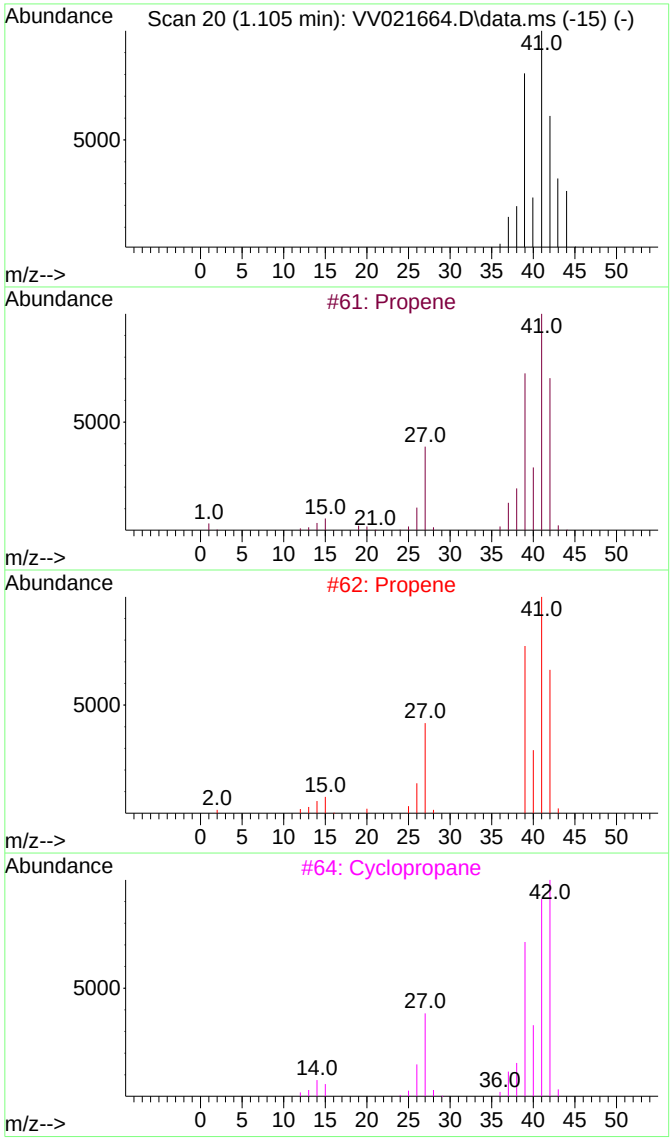
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
Quant Title : VOC Analysis

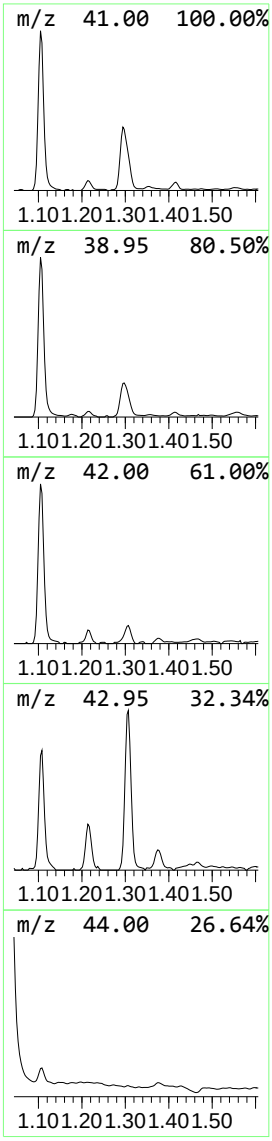
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.105	3.94 ug/L	74150	1,4-Difluorobenzene	5.612

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Propene	42	C3H6	000115-07-1	42
3	Cyclopropane	42	C3H6	000075-19-4	9
4	Cyclopropane	42	C3H6	000075-19-4	7
5	Cyclopropene	40	C3H4	002781-85-3	5





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Operator : SY/MD
Sample : M3033-04
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BG7M4

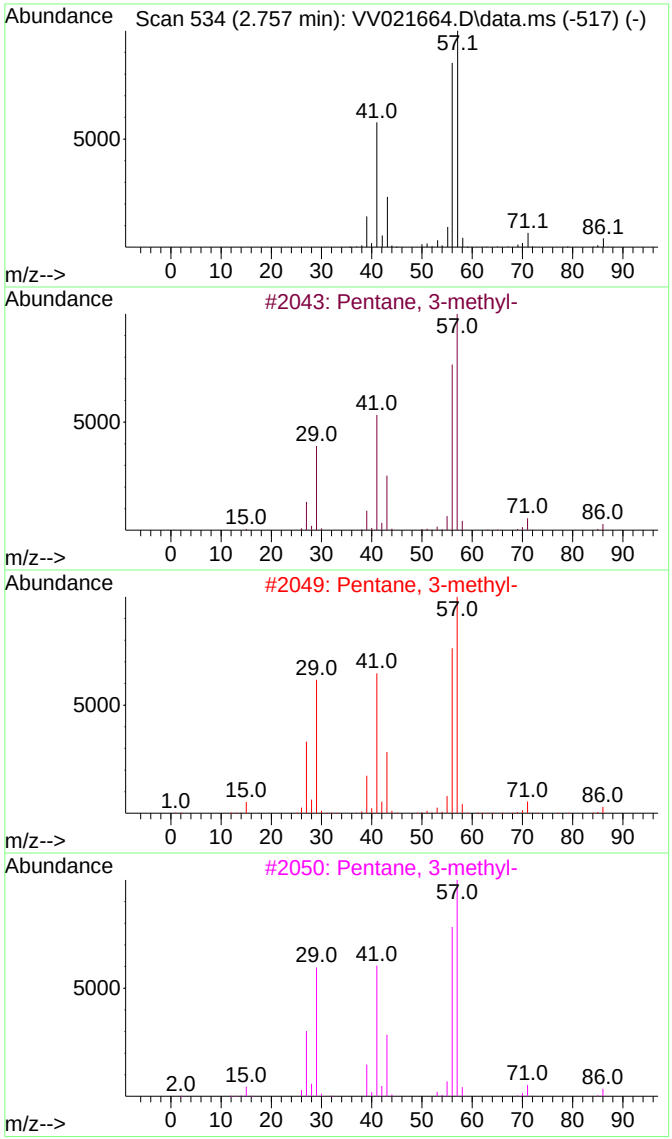
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
Quant Title : VOC Analysis

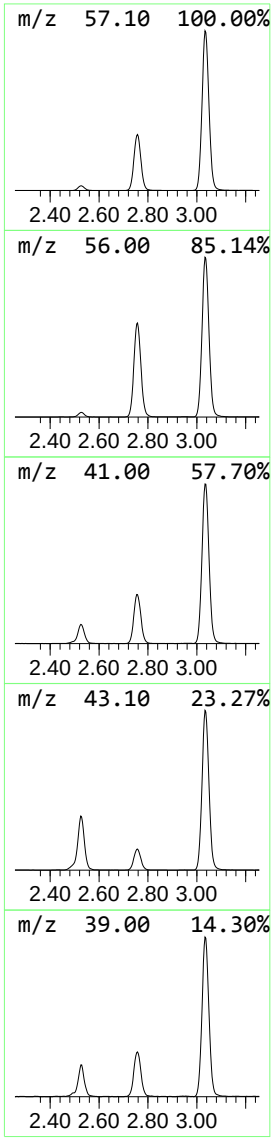
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.757	46.77 ug/L	879495	1,4-Difluorobenzene	5.612

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
3	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
4	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV071521\
Data File : VV021664.D
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Operator : SY/MD
Sample : M3033-04
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BG7M4

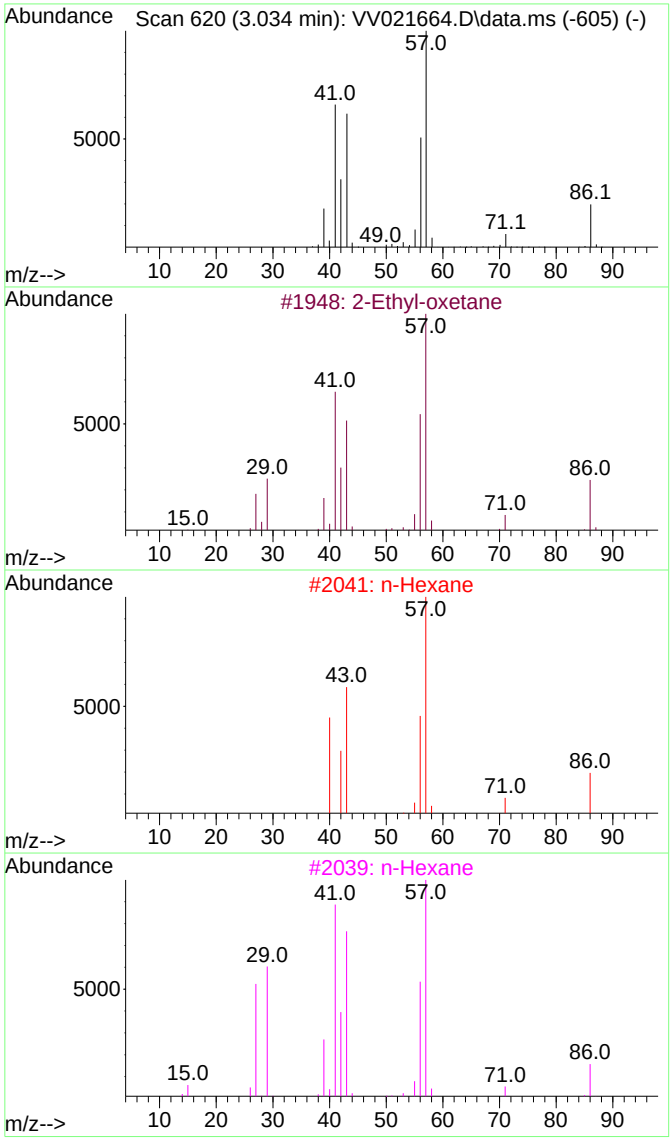
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
Quant Title : VOC Analysis

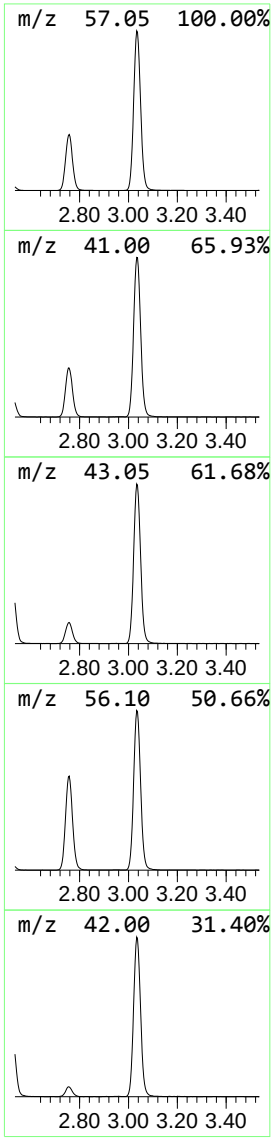
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Ethyl-oxetane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.034	152.98 ug/L	2876700	1,4-Difluorobenzene	5.612

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	90
2	n-Hexane	86	C6H14	000110-54-3	87
3	n-Hexane	86	C6H14	000110-54-3	78
4	n-Hexane	86	C6H14	000110-54-3	78
5	n-Hexane	86	C6H14	000110-54-3	59





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Instrument : MSVOA_V
ClientSampleId : BG7M4

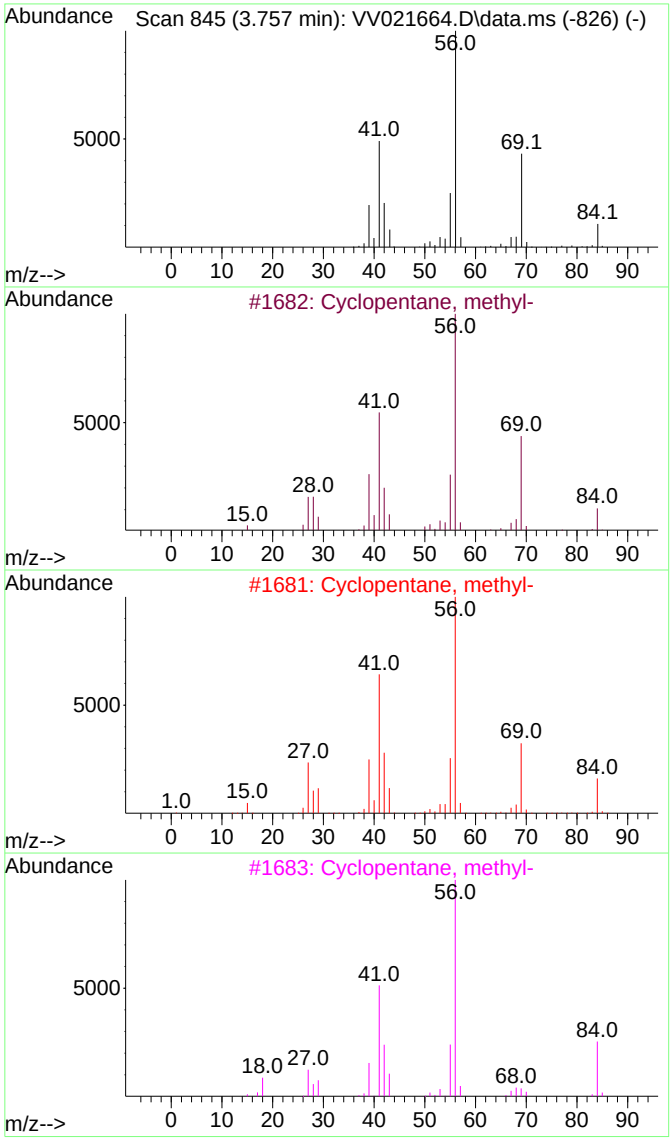
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
Quant Title : VOC Analysis

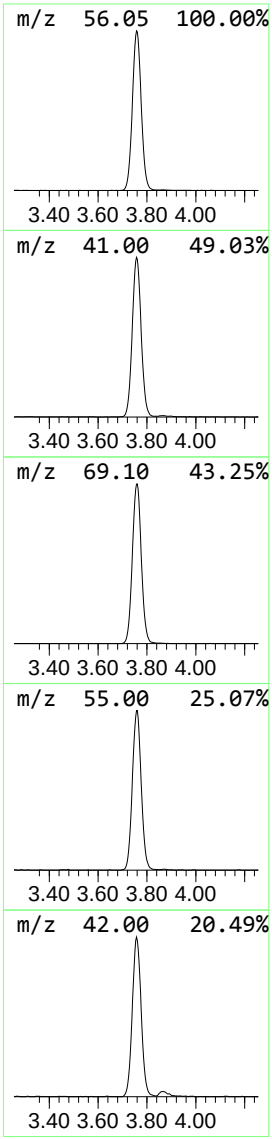
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Cyclic3.757 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.757	96.48 ug/L	1814210	1,4-Difluorobenzene	5.612

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	80
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	78





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ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BG7M4

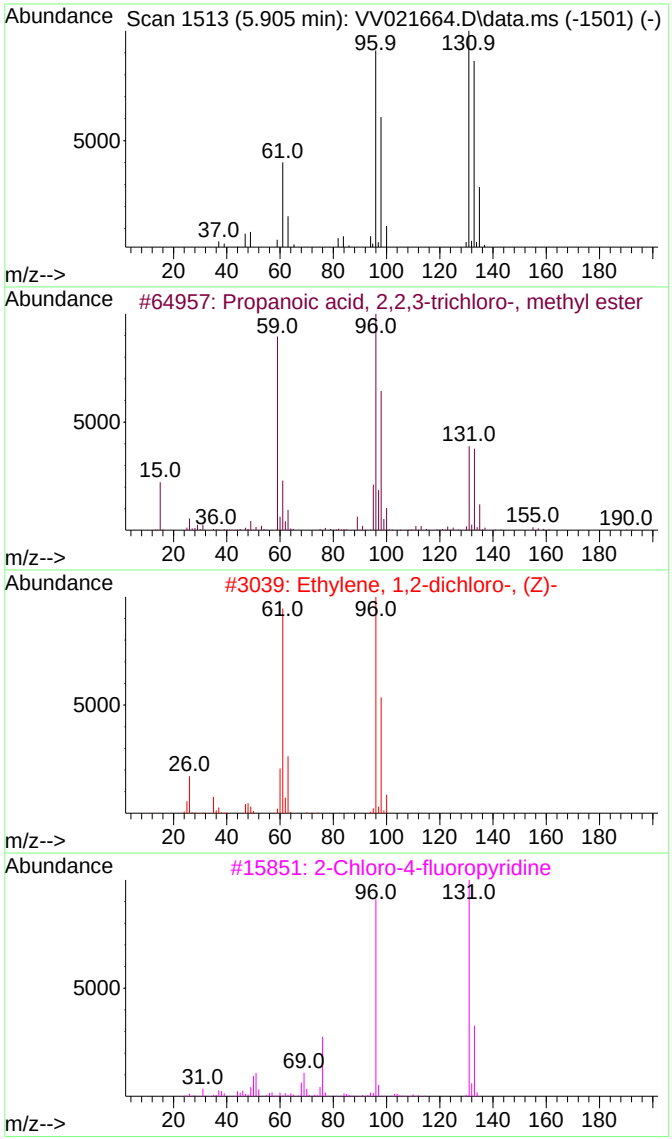
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
Quant Title : VOC Analysis

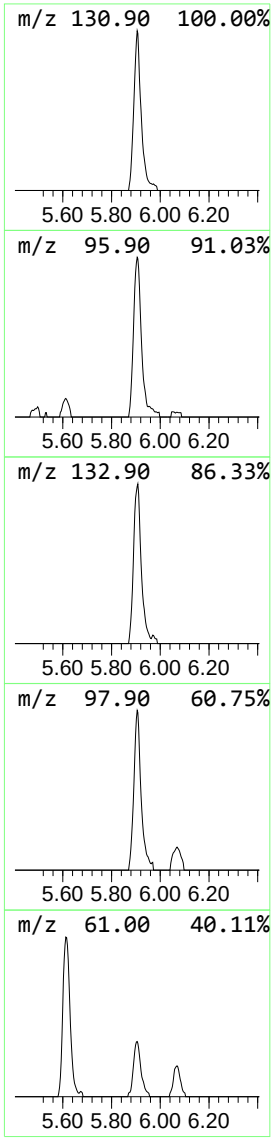
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 2,2,3-trich... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.905	2.54 ug/L	47761	1,4-Difluorobenzene	5.612

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2	Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3	2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	32
4	4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27
5	Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25





Tentatively Identified Compound (LSC) summary

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ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BG7M4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.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
(DEL) Alkane: S...	1.105	3.9	ug/L	74150	1	5.612	940207	50.0
(DEL) Alkane: S...	2.757	46.8	ug/L	879495	1	5.612	940207	50.0
2-Ethyl-oxetane	3.034	153.0	ug/L	2876700	1	5.612	940207	50.0
(DEL) Alkane: C...	3.757	96.5	ug/L	1814210	1	5.612	940207	50.0
Propanoic acid,...	5.905	2.5	ug/L	47761	1	5.612	940207	50.0