LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048490.D
Acq On : 10 May 2022 14:51
Operator : SY/MD
Sample : N2736-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW7

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\SFAMULM050622WMA.M
Title : VOC Analysis

Signal : TIC: VU048490.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	26	rVB	480597	426864	43.93%	5.013%
2	1.600	74	81	94	rVB	125769	141033	14.51%	1.656%
3	1.912	171	178	191	rVB	87639	116407	11.98%	1.367%
4	2.205	264	269	280	rVB3	8467	11554	1.19%	0.136%
5	2.485	346	356	362	rBV2	6331	11241	1.16%	0.132%
6	2.568	371	382	395	rBV	181658	295521	30.41%	3.471%
7	2.681	410	417	430	rVB5	9180	16100	1.66%	0.189%
8	2.748	434	438	444	rBV3	394	417	0.04%	0.005%
9	2.989	510	513	514	rBV2	473	295	0.03%	0.003%
10	3.022	515	523	526	rBV4	6123	8920	0.92%	0.105%
11	3.231	582	588	590	rBV5	1003	1077	0.11%	0.013%
12	3.266	597	599	601	rBV	144	81	0.01%	0.001%
13	3.449	653	656	661	rVB	234	141	0.01%	0.002%
14	3.507	671	674	680	rBV2	205	223	0.02%	0.003%
15	3.578	692	696	697	rBV2	352	193	0.02%	0.002%
16	3.636	711	714	717	rBV2	256	171	0.02%	0.002%
17	3.690	728	731	733	rBV	370	261	0.03%	0.003%
18	3.723	740	741	745	rVB2	327	164	0.02%	0.002%
19	3.800	761	765	766	rBV	157	129	0.01%	0.002%
20	3.842	773	778	781	rVB4	436	405	0.04%	0.005%
21	3.874	786	788	790	rVV	180	97	0.01%	0.001%
22	3.912	797	800	805	rBV2	331	291	0.03%	0.003%
23	4.096	848	857	859	rBV3	346	544	0.06%	0.006%
24	4.134	867	869	870	rBV	400	196	0.02%	0.002%
25	4.166	871	879	881	rBV2	1781	2001	0.21%	0.024%
26	4.250	895	905	906	rBV4	1246	1353	0.14%	0.016%
27	4.340	930	933	936	rBV2	597	416	0.04%	0.005%
28	4.388	945	948	950	rBV	213	139	0.01%	0.002%
29	4.427	956	960	962	rBV3	532	505	0.05%	0.006%
30	4.452	966	968	969	rBV	295	144	0.01%	0.002%
31	4.530	982	992	1007	rBV4	14398	30172	3.10%	0.354%
32	4.620	1008	1020	1050	rBV	131059	320767	33.01%	3.767%
33	4.787	1070	1072	1076	rBV3	477	277	0.03%	0.003%
34	4.977	1128	1131	1133	rBV2	335	222	0.02%	0.003%
35	5.063	1142	1158	1177	rBV	192842	417839	43.00%	4.907%
36	5.234	1209	1211	1216	rVB2	352	281	0.03%	0.003%

LSC Area Percent Report

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Sample : N2736-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW7

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\SFAMULM050622WMA.M
Title : VOC Analysis

37	5.269	1216	1222	1224	rBV	421	358	0.04%	0.004%
38	5.285	1224	1227	1229	rBV2	565	435	0.04%	0.005%
39	5.324	1235	1239	1242	rBV	301	291	0.03%	0.003%
40	5.391	1246	1260	1275	rVV5	18758	43300	4.46%	0.509%
41	5.636	1328	1336	1343	rBV7	1224	2182	0.22%	0.026%
42	5.726	1343	1364	1371	rBV2	350269	971726	100.00%	11.413%
43	6.144	1490	1494	1495	rBV	587	406	0.04%	0.005%
44	6.185	1504	1507	1509	rBV	136	84	0.01%	0.001%
45	6.198	1509	1511	1513	rBV	194	110	0.01%	0.001%
46	6.250	1513	1527	1550	rVV	278555	531429	54.69%	6.241%
47	6.690	1650	1664	1682	rBV	233094	456810	47.01%	5.365%
48	6.838	1706	1710	1712	rBV3	631	435	0.04%	0.005%
49	6.996	1748	1759	1775	rBV3	16223	30315	3.12%	0.356%
50	7.066	1779	1781	1785	rBV	163	98	0.01%	0.001%
51	7.185	1802	1818	1828	rBV10	5706	14998	1.54%	0.176%
52	7.253	1837	1839	1842	rVB2	366	155	0.02%	0.002%
53	7.275	1842	1846	1850	rVB2	279	275	0.03%	0.003%
54	7.292	1850	1851	1852	rBV2	247	78	0.01%	0.001%
55	7.333	1860	1864	1871	rBV2	258	258	0.03%	0.003%
56	7.394	1873	1883	1892	rVV6	3522	5387	0.55%	0.063%
57	7.449	1897	1900	1903	rBV3	364	304	0.03%	0.004%
58	7.491	1904	1913	1924	rVB4	5718	9664	0.99%	0.114%
59	7.565	1924	1936	1949	rBV2	91903	168447	17.33%	1.978%
60	7.687	1967	1974	1987	rVB5	6632	11236	1.16%	0.132%
61	7.899	2026	2040	2054	rBV	379754	651094	67.00%	7.647%
62	8.134	2112	2113	2116	rBV	214	120	0.01%	0.001%
63	8.179	2116	2127	2140	rBV2	68031	116112	11.95%	1.364%
64	8.410	2195	2199	2200	rBV2	1266	973	0.10%	0.011%
65	8.478	2215	2220	2222	rBV4	3248	3178	0.33%	0.037%
66	8.574	2237	2250	2259	rBV	180534	300719	30.95%	3.532%
67	8.632	2259	2268	2310	rVB	412084	755571	77.76%	8.874%
68	8.864	2337	2340	2344	rBV3	342	315	0.03%	0.004%
69	8.886	2344	2347	2348	rBV2	312	173	0.02%	0.002%
70	8.967	2368	2372	2373	rBV2	420	265	0.03%	0.003%
71	9.127	2420	2422	2428	rBV4	543	409	0.04%	0.005%
72	9.272	2459	2467	2475	rVB4	5240	8903	0.92%	0.105%
73	9.333	2475	2486	2498	rBV8	8026	15513	1.60%	0.182%
74	9.417	2498	2512	2550	rBV	372198	647802	66.67%	7.608%
75	9.574	2554	2561	2566	rBV3	5673	8218	0.85%	0.097%
76	9.697	2590	2599	2608	rVB6	2838	4284	0.44%	0.050%

LSC Area Percent Report

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Data File : VU048490.D
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Operator : SY/MD
Sample : N2736-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : EXEW7

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\SFAMULM050622WMA.M
Title : VOC Analysis

77	9.880	2649	2656	2665	rVB8	2720	4567	0.47%	0.054%
78	9.947	2665	2677	2690	rBV8	6059	14758	1.52%	0.173%
79	10.082	2714	2719	2725	rBV3	685	848	0.09%	0.010%
80	10.253	2765	2772	2775	rBV3	979	1101	0.11%	0.013%
81	10.307	2787	2789	2793	rVB2	497	291	0.03%	0.003%
82	10.359	2795	2805	2815	rBV3	12228	23114	2.38%	0.271%
83	10.613	2880	2884	2885	rBV2	409	336	0.03%	0.004%
84	10.648	2887	2895	2905	rVB7	8519	14080	1.45%	0.165%
85	10.754	2909	2928	2943	rBV	360018	583809	60.08%	6.857%
86	11.063	3017	3024	3040	rVB7	10408	16467	1.69%	0.193%
87	11.127	3040	3044	3047	rBV	414	351	0.04%	0.004%
88	11.176	3057	3059	3060	rBV	419	179	0.02%	0.002%
89	11.217	3069	3072	3076	rBV	503	365	0.04%	0.004%
90	11.330	3097	3107	3108	rBV6	2088	2565	0.26%	0.030%
91	11.385	3120	3124	3125	rBV3	1264	776	0.08%	0.009%
92	11.558	3175	3178	3181	rBV4	446	295	0.03%	0.003%
93	11.645	3199	3205	3213	rBV9	5453	8303	0.85%	0.098%
94	11.748	3228	3237	3245	rBV2	20126	32399	3.33%	0.381%
95	11.812	3246	3257	3273	rVB	375076	593767	61.10%	6.974%
96	12.192	3364	3375	3392	rVB	404453	637473	65.60%	7.487%
97	12.307	3404	3411	3423	rBV10	2980	5633	0.58%	0.066%
98	12.526	3477	3479	3482	rBV	416	286	0.03%	0.003%
99	12.635	3510	3513	3516	rBV2	772	565	0.06%	0.007%
100	12.680	3522	3527	3535	rVB6	2483	3317	0.34%	0.039%

Sum of corrected areas: 8514516

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Data File : VU048490.D
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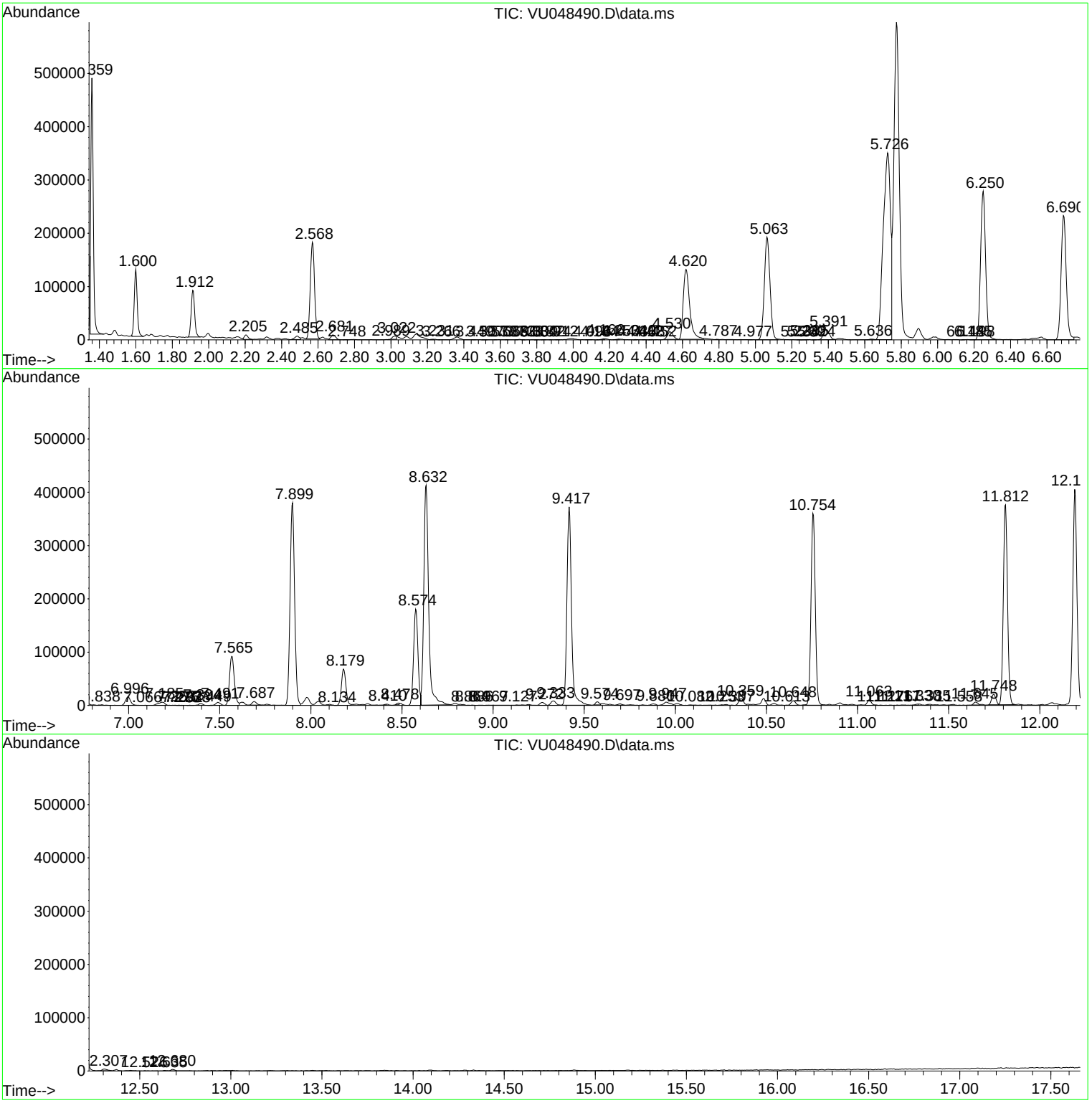
Operator : SY/MD
Sample : N2736-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048490.D
Acq On : 10 May 2022 14:51
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ClientSampleId :
EXEW7

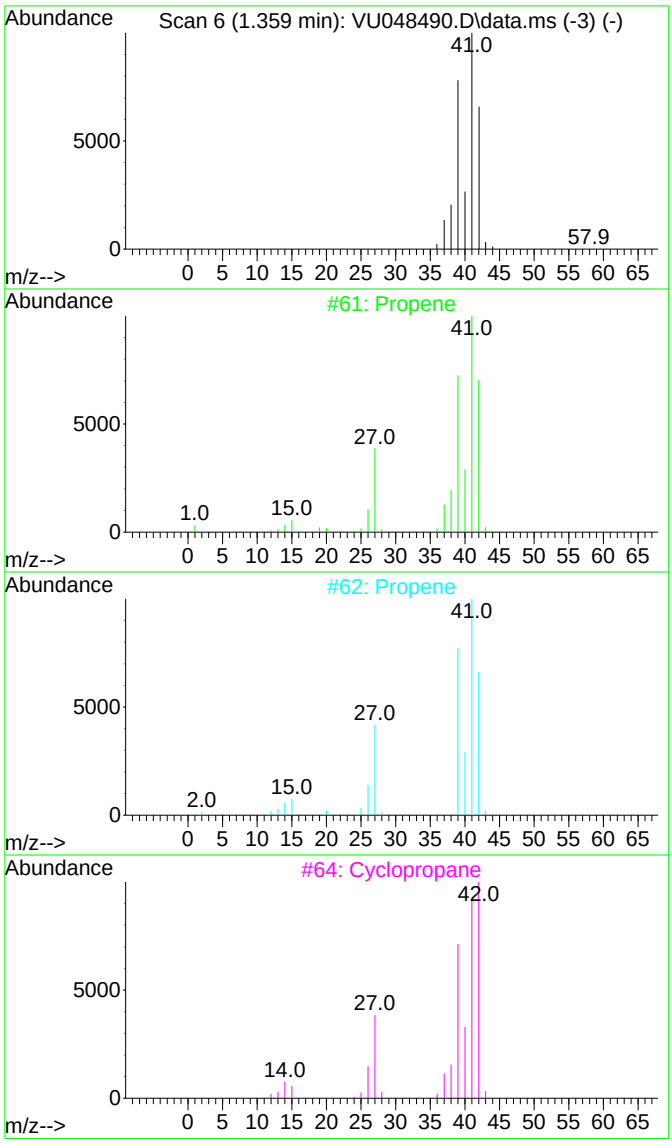
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

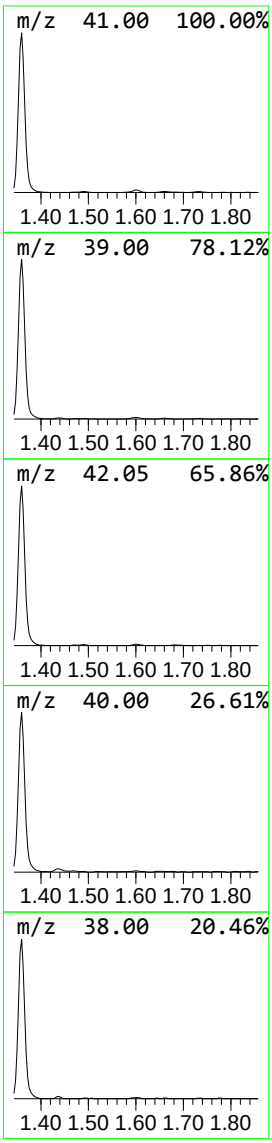
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	40.16 ug/L	426864	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Propene	42	C3H6	000115-07-1	59
3	Cyclopropane	42	C3H6	000075-19-4	10
4	Cyclopropene	40	C3H4	002781-85-3	10
5	Cyclopropane	42	C3H6	000075-19-4	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048490.D
Acq On : 10 May 2022 14:51
Operator : SY/MD
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW7

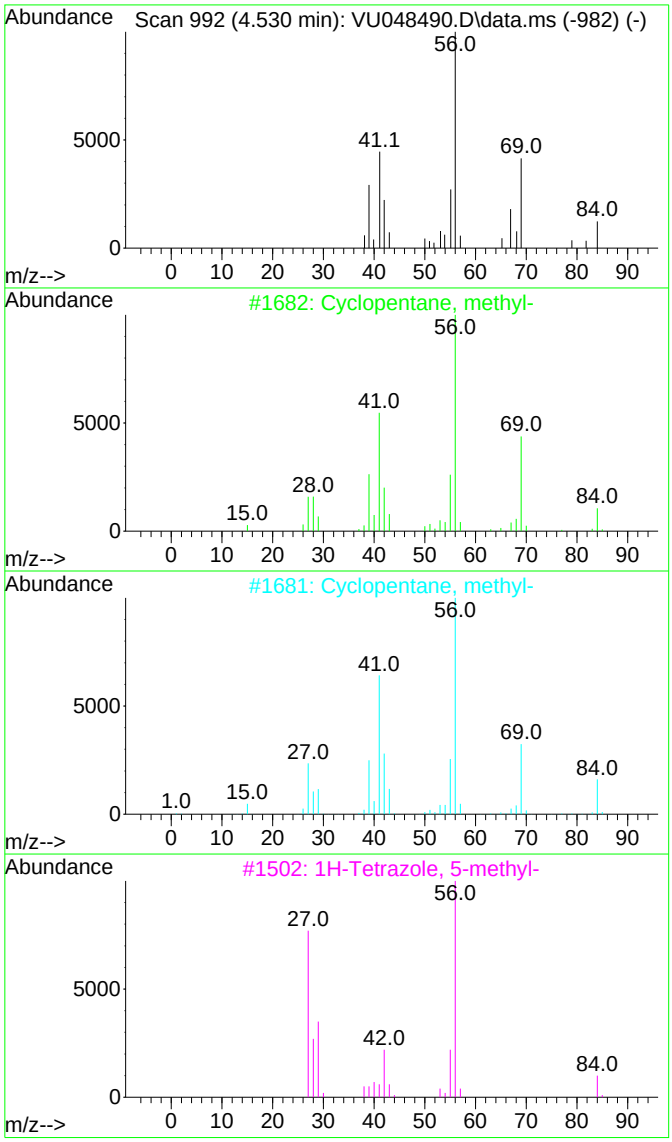
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

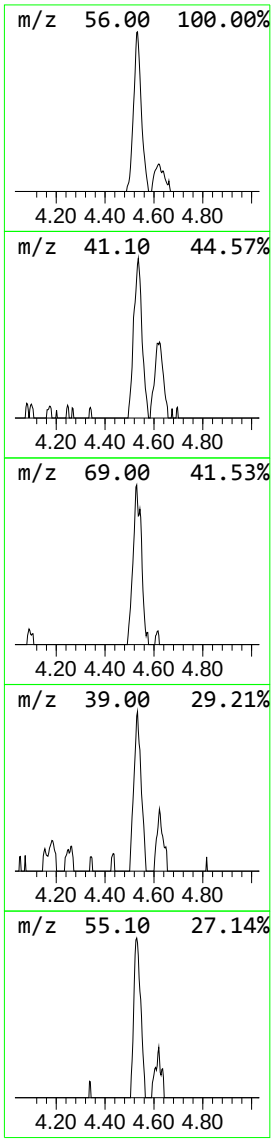
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Cyclic4.530 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.530	2.84 ug/L	30172	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	83
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	83
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	64
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	64





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Data File : VU048490.D
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Instrument :
MSVOA_U
ClientSampleId :
EXEW7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

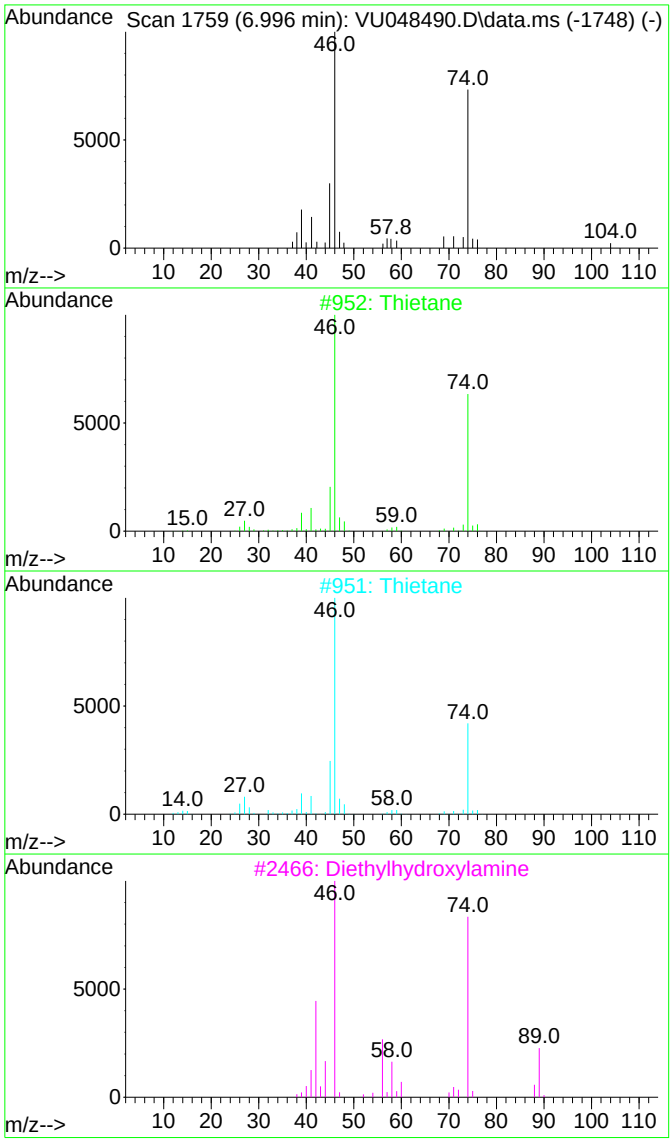
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

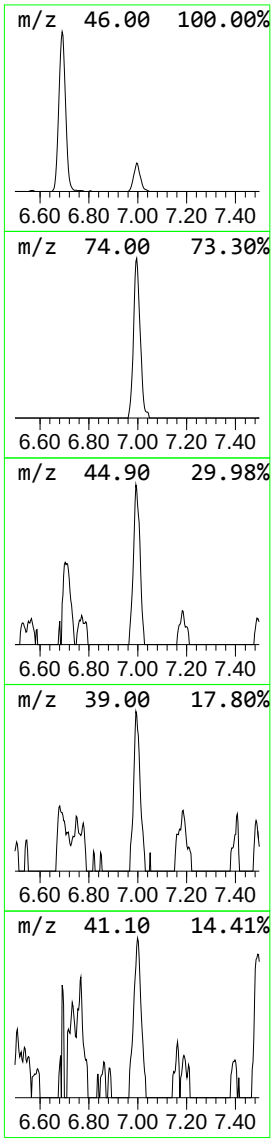
****

Peak Number 3 Thietane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.996	2.85 ug/L	30315	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thietane	74	C3H6S	000287-27-4	90
2	Thietane	74	C3H6S	000287-27-4	74
3	Diethylhydroxylamine	89	C4H11NO	003710-84-7	39
4	Allyl mercaptan	74	C3H6S	000870-23-5	38
5	Dihydro-3-(2H)-thiophenone	102	C4H6OS	001003-04-9	23





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW7

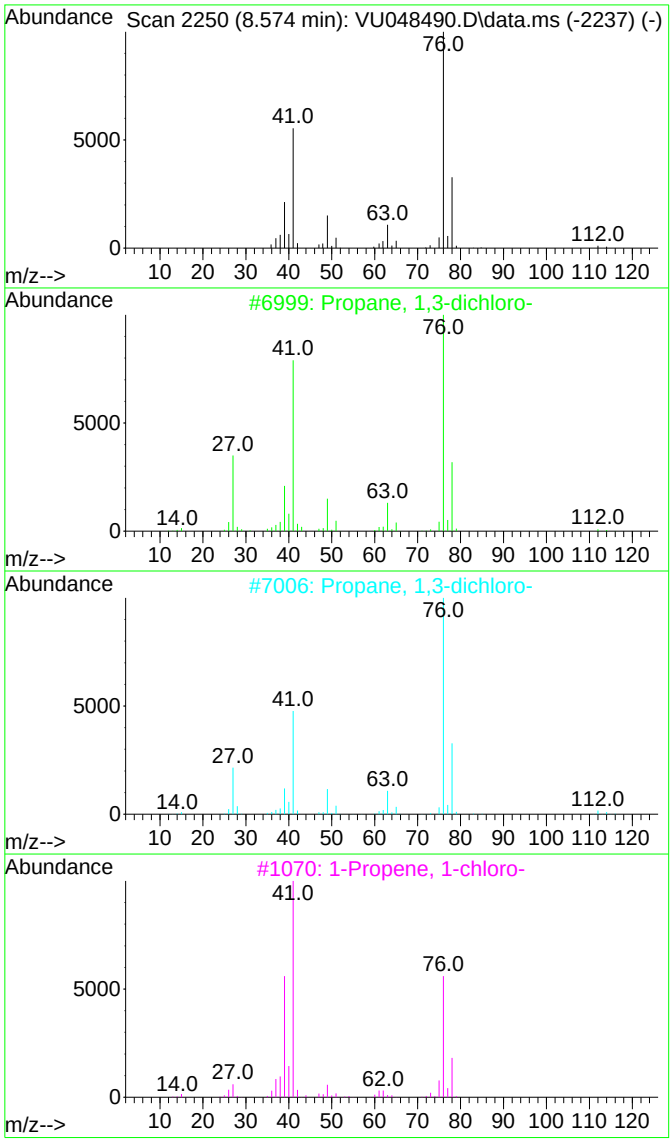
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

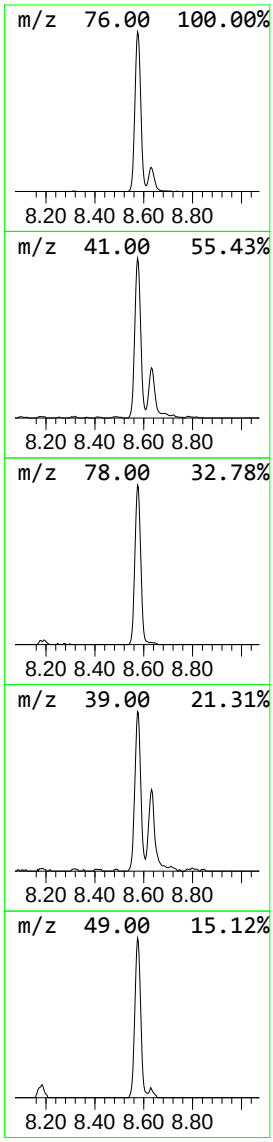
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propane, 1,3-dichloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.574	23.21 ug/L	300719	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	91
2	Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	83
3	1-Propene, 1-chloro-	76	C3H5Cl	000590-21-6	83
4	Allyl chloride	76	C3H5Cl	000107-05-1	78
5	Propanal, 2,3-dichloro-2-methyl-	140	C4H6Cl2O	010141-22-7	64





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Data File : VU048490.D
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Operator : SY/MD
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW7

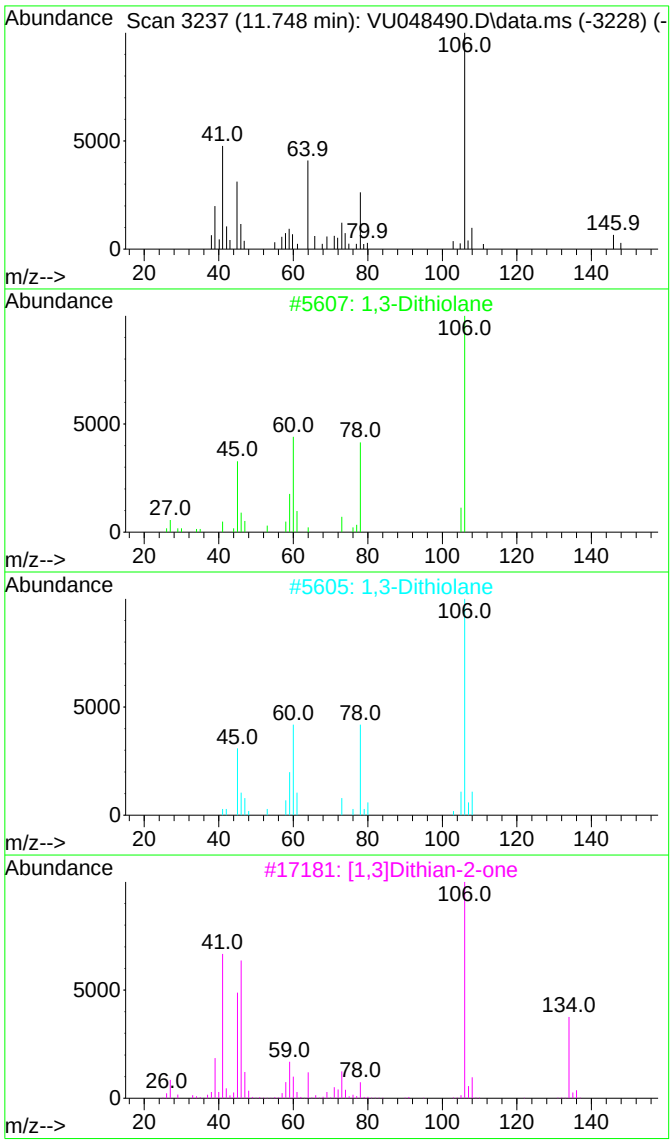
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

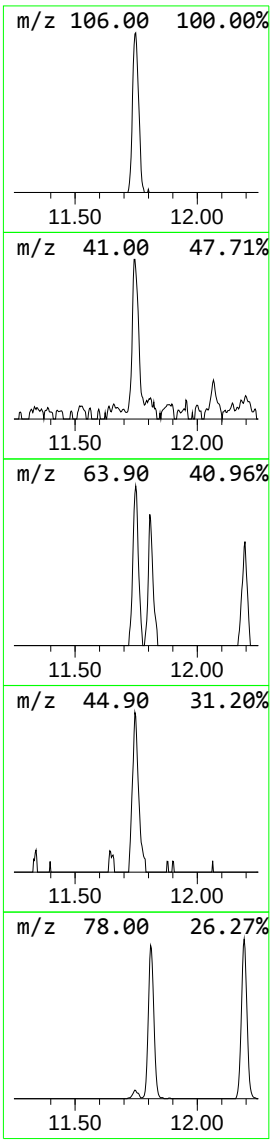
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.748	2.73 ug/L	32399	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dithiolane	106	C3H6S2	004829-04-3	27
2	1,3-Dithiolane	106	C3H6S2	004829-04-3	16
3	[1,3]Dithian-2-one	134	C4H6OS2	035345-24-5	12
4	Benzenemethanamine, .alpha.-meth...	121	C8H11N	003886-69-9	9
5	1-Azonia-2-boratacyclopropane, 1...	279	C8H16BF6NSi	1000161-95-9	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048490.D
Acq On : 10 May 2022 14:51
Operator : SY/MD
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.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...	1.359	40.2	ug/L	426864	1	6.250	531429	50.0
(DEL) Alkane: C...	4.530	2.8	ug/L	30172	1	6.250	531429	50.0
Thietane	6.996	2.9	ug/L	30315	1	6.250	531429	50.0
Propane, 1,3-di...	8.574	23.2	ug/L	300719	2	9.417	647802	50.0
unknown-01	11.748	2.7	ug/L	32399	3	11.812	593767	50.0