LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
Data File : VU045256.D
Acq On : 08 Oct 2021 17:03
Operator : SY/MD
Sample : M4000-14ME
Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : EW907ME

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\SFAMULM092321WMA.M
Title : VOC Analysis

Signal : TIC: VU045256.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.456	29	36	51	rBV	90335	143796	10.98%	1.343%
2	1.597	73	80	97	rVB	112972	143935	10.99%	1.344%
3	1.871	159	165	179	rVB	46062	56872	4.34%	0.531%
4	2.520	355	367	387	rBV	208880	361708	27.61%	3.379%
5	2.607	388	394	416	rVB	6999	17640	1.35%	0.165%
6	2.742	433	436	439	rBV2	233	197	0.02%	0.002%
7	2.919	487	491	494	rBV2	194	179	0.01%	0.002%
8	2.967	496	506	515	rVV2	2183	4084	0.31%	0.038%
9	3.028	516	525	542	rVB3	5458	12848	0.98%	0.120%
10	3.289	601	606	611	rBV2	135	181	0.01%	0.002%
11	3.340	619	622	624	rBV2	186	135	0.01%	0.001%
12	3.382	632	635	640	rBV2	175	159	0.01%	0.001%
13	3.485	662	667	669	rBV2	191	196	0.01%	0.002%
14	3.633	706	713	716	rBV	321	384	0.03%	0.004%
15	3.665	717	723	730	rBV4	636	791	0.06%	0.007%
16	3.742	744	747	750	rVV2	149	124	0.01%	0.001%
17	3.803	762	766	769	rBV	141	174	0.01%	0.002%
18	3.961	812	815	822	rVB2	141	120	0.01%	0.001%
19	4.038	835	839	841	rBV	241	228	0.02%	0.002%
20	4.064	844	847	852	rVB2	225	209	0.02%	0.002%
21	4.092	852	856	857	rBV	161	123	0.01%	0.001%
22	4.340	930	933	940	rVB2	228	286	0.02%	0.003%
23	4.375	940	944	947	rBV2	181	167	0.01%	0.002%
24	4.481	974	977	983	rVB2	236	217	0.02%	0.002%
25	4.575	1000	1006	1011	rBV2	173	209	0.02%	0.002%
26	4.645	1011	1028	1071	rBV	119301	370329	28.27%	3.459%
27	4.928	1113	1116	1119	rBV	251	191	0.01%	0.002%
28	4.954	1119	1124	1127	rVV3	209	239	0.02%	0.002%
29	4.990	1131	1135	1140	rVB2	252	244	0.02%	0.002%
30	5.067	1140	1159	1183	rBV	214963	504831	38.54%	4.715%
31	5.205	1199	1202	1209	rVB3	279	252	0.02%	0.002%
32	5.292	1223	1229	1236	rVB3	537	945	0.07%	0.009%
33	5.616	1327	1330	1332	rBV	248	186	0.01%	0.002%
34	5.719	1341	1362	1382	rBV2	520580	1310044	100.00%	12.237%
35	5.980	1432	1443	1465	rBV3	7902	18606	1.42%	0.174%
36	6.250	1511	1527	1547	rBV	359201	709151	54.13%	6.624%

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Sample : M4000-14ME
Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : EW907ME

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\SFAMULM092321WMA.M
Title : VOC Analysis

37	6.321	1547	1549	1556	rVB2	397	347	0.03%	0.003%
38	6.382	1565	1568	1571	rBV	199	122	0.01%	0.001%
39	6.491	1598	1602	1603	rBV	170	120	0.01%	0.001%
40	6.539	1604	1617	1632	rBV	186445	358017	27.33%	3.344%
41	6.694	1650	1665	1684	rBV	302799	610928	46.63%	5.706%
42	6.800	1692	1698	1699	rBV2	665	404	0.03%	0.004%
43	6.912	1726	1733	1736	rBV2	191	264	0.02%	0.002%
44	7.060	1767	1779	1786	rBV4	496	1061	0.08%	0.010%
45	7.195	1810	1821	1829	rBV2	3404	7223	0.55%	0.067%
46	7.401	1881	1885	1890	rBV	265	319	0.02%	0.003%
47	7.497	1912	1915	1922	rVB3	505	554	0.04%	0.005%
48	7.568	1922	1937	1960	rBV	155253	293478	22.40%	2.741%
49	7.649	1960	1962	1964	rBV	187	126	0.01%	0.001%
50	7.694	1968	1976	1988	rVB5	1612	3153	0.24%	0.029%
51	7.851	2021	2025	2026	rBV2	277	214	0.02%	0.002%
52	7.899	2026	2040	2056	rVV	564103	1006967	76.87%	9.406%
53	7.973	2056	2063	2080	rVB3	7974	16734	1.28%	0.156%
54	8.057	2086	2089	2093	rVB2	266	173	0.01%	0.002%
55	8.086	2095	2098	2106	rVB2	156	149	0.01%	0.001%
56	8.128	2108	2111	2114	rBV2	197	137	0.01%	0.001%
57	8.186	2116	2129	2144	rBV	104864	196439	14.99%	1.835%
58	8.359	2179	2183	2185	rBV2	257	161	0.01%	0.002%
59	8.475	2215	2219	2223	rBV	403	314	0.02%	0.003%
60	8.555	2236	2244	2252	rBV3	5248	8234	0.63%	0.077%
61	8.652	2260	2274	2303	rBV	436301	810880	61.90%	7.574%
62	8.864	2337	2340	2346	rVB5	673	758	0.06%	0.007%
63	8.896	2346	2350	2351	rBV2	173	126	0.01%	0.001%
64	8.928	2351	2360	2367	rVV3	2711	3895	0.30%	0.036%
65	8.993	2377	2380	2382	rVB2	255	155	0.01%	0.001%
66	9.079	2400	2407	2410	rVB4	957	1130	0.09%	0.011%
67	9.121	2416	2420	2425	rBV3	372	481	0.04%	0.004%
68	9.166	2427	2434	2442	rVV4	2439	3161	0.24%	0.030%
69	9.211	2445	2448	2454	rVB5	610	640	0.05%	0.006%
70	9.337	2478	2487	2496	rBV6	1252	1914	0.15%	0.018%
71	9.423	2500	2514	2530	rBV	496990	882004	67.33%	8.238%
72	9.571	2551	2560	2569	rVB5	1730	2979	0.23%	0.028%
73	9.610	2569	2572	2575	rBV2	252	259	0.02%	0.002%
74	9.700	2581	2600	2613	rBV7	4852	11606	0.89%	0.108%
75	9.848	2642	2646	2648	rBV	272	218	0.02%	0.002%
76	9.874	2648	2654	2662	rVB6	1138	1840	0.14%	0.017%

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Sample : M4000-14ME
Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : EW907ME

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_U\Method\SFAMULM092321WMA.M
Title : VOC Analysis

77	9.957	2675	2680	2684	rBV4	588	747	0.06%	0.007%
78	10.021	2692	2700	2703	rBV4	3341	4154	0.32%	0.039%
79	10.121	2719	2731	2739	rBV6	2526	4857	0.37%	0.045%
80	10.218	2755	2761	2762	rBV2	973	776	0.06%	0.007%
81	10.253	2763	2772	2785	rVB5	10164	17157	1.31%	0.160%
82	10.356	2787	2804	2808	rBV8	3239	7239	0.55%	0.068%
83	10.398	2810	2817	2828	rVB2	14459	24173	1.85%	0.226%
84	10.468	2830	2839	2850	rVB8	2399	4885	0.37%	0.046%
85	10.536	2854	2860	2861	rBV4	3337	2965	0.23%	0.028%
86	10.626	2883	2888	2895	rVB	4845	5914	0.45%	0.055%
87	10.764	2915	2931	2943	rBV	473816	761722	58.14%	7.115%
88	10.957	2982	2991	2996	rBV8	2045	3294	0.25%	0.031%
89	11.066	3018	3025	3033	rBV7	5023	8412	0.64%	0.079%
90	11.131	3035	3045	3058	rVB8	7975	19415	1.48%	0.181%
91	11.378	3116	3122	3127	rBV5	3884	5625	0.43%	0.053%
92	11.420	3128	3135	3142	rVV2	18407	25092	1.92%	0.234%
93	11.462	3143	3148	3155	rVB7	7172	10389	0.79%	0.097%
94	11.578	3174	3184	3190	rBV8	6352	12085	0.92%	0.113%
95	11.819	3247	3259	3272	rBV	534489	842868	64.34%	7.873%
96	12.198	3365	3377	3390	rBV	592680	939066	71.68%	8.771%
97	12.668	3518	3523	3532	rVB3	15252	22329	1.70%	0.209%
98	13.436	3757	3762	3768	rBV4	14684	21163	1.62%	0.198%
99	13.590	3802	3810	3817	rBV2	27822	47492	3.63%	0.444%
100	14.452	4072	4078	4086	rBV2	20739	26479	2.02%	0.247%

Sum of corrected areas: 10705962

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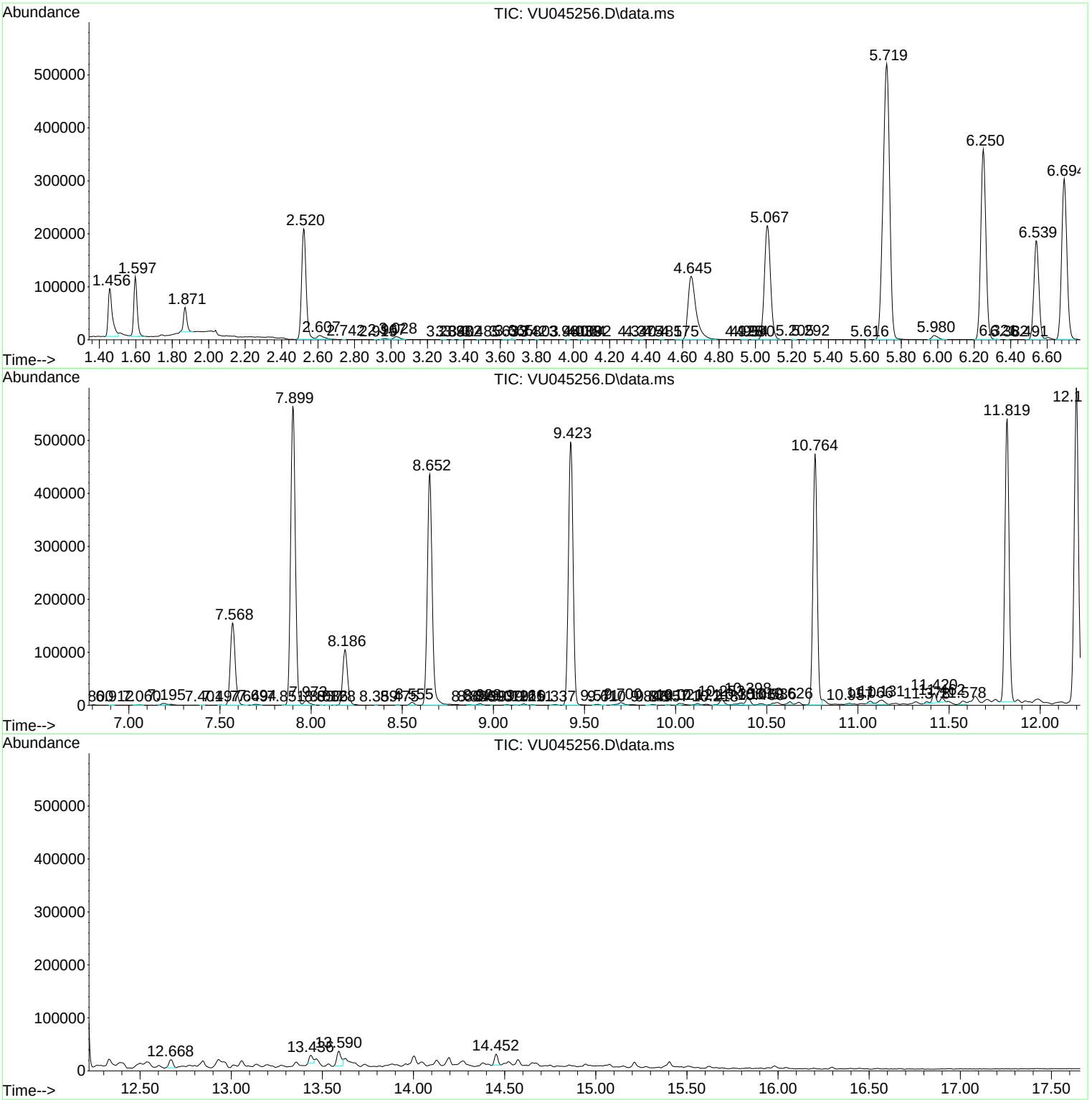
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW907ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
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Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : EW907ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

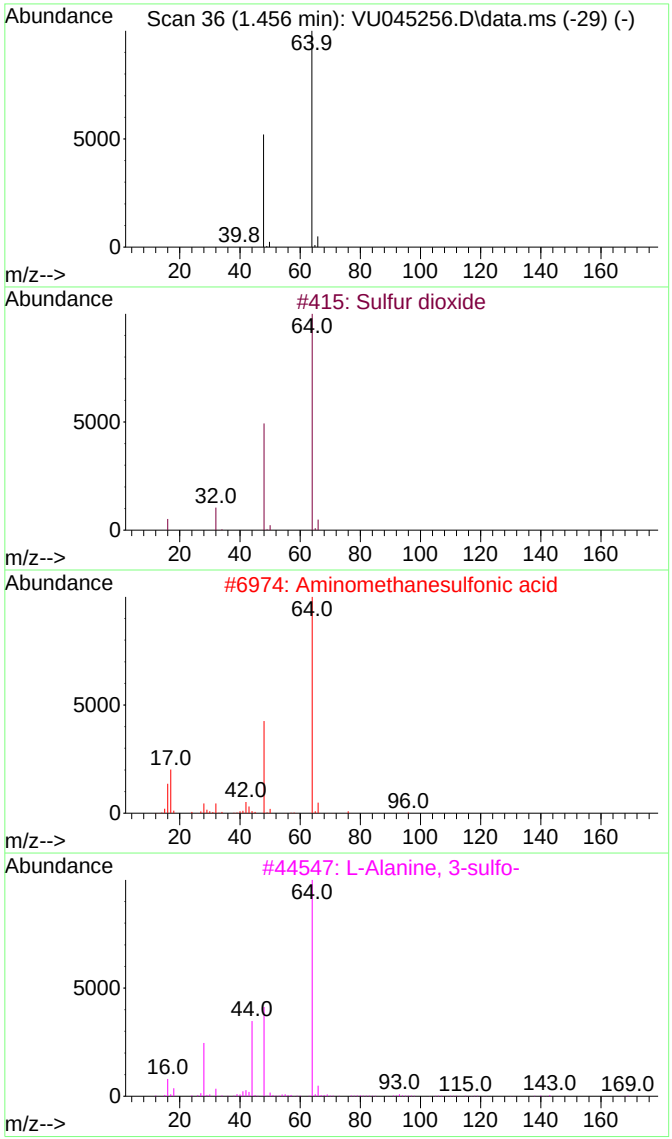
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

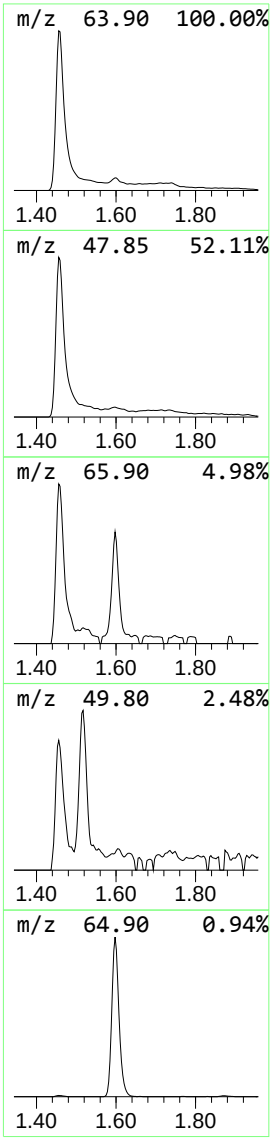
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.456	10.14 ug/L	143796	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





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Operator : SY/MD
Sample : M4000-14ME
Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW907ME

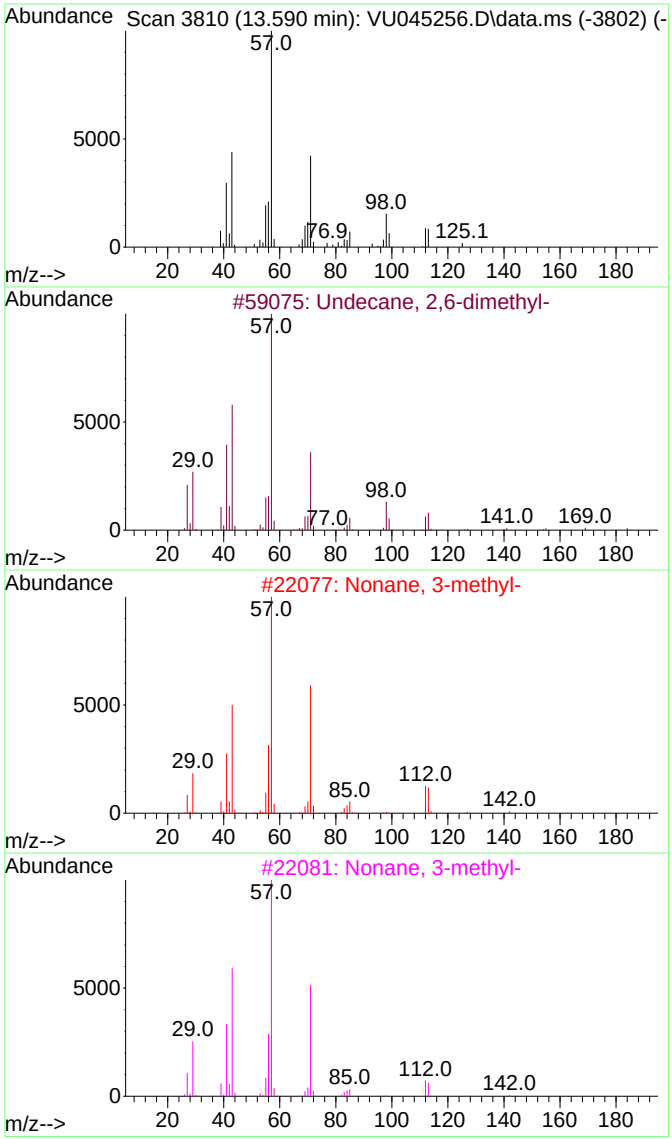
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

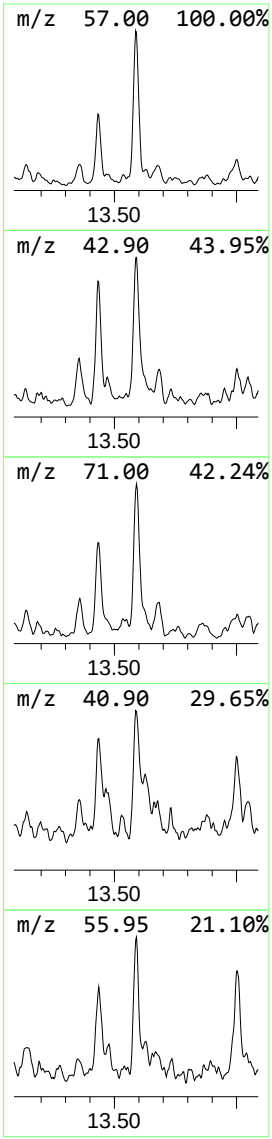
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.590	2.82 ug/L	47492	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	83
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	64
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	59
4	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	53
5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	53





Tentatively Identified Compound (LSC) summary

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Instrument : MSVOA_U
ClientSampleId : EW907ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.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
Sulfur dioxide	1.456	10.1	ug/L	143796	1	6.250	709151	50.0
(DEL) Alkane: S...	13.590	2.8	ug/L	47492	3	11.819	842868	50.0