LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101123\
Data File : VU055746.D
Acq On : 11 Oct 2023 14:33
Operator : MD/SY
Sample : 04792-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : EY1B0

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\SFAMULM101023WMA.M
Title : VOC Analysis

Signal : TIC: VU055746.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	88	96	109	rBV	231727	283128	15.84%	1.977%
2	2.557	382	394	413	rBV	357936	606521	33.93%	4.234%
3	2.849	483	485	486	rBV	481	218	0.01%	0.002%
4	2.872	490	492	495	rBV4	362	246	0.01%	0.002%
5	2.911	501	504	506	rBV3	505	339	0.02%	0.002%
6	2.949	514	516	518	rBV2	403	179	0.01%	0.001%
7	3.033	528	542	561	rBV3	48973	106533	5.96%	0.744%
8	3.300	622	625	626	rBV2	227	91	0.01%	0.001%
9	3.354	626	642	653	rBV5	7447	16672	0.93%	0.116%
10	3.422	660	663	667	rBV2	382	371	0.02%	0.003%
11	3.460	673	675	676	rBV	331	97	0.01%	0.001%
12	3.486	682	683	687	rVV2	428	178	0.01%	0.001%
13	3.576	709	711	714	rBV2	281	136	0.01%	0.001%
14	3.628	725	727	733	rVB2	324	201	0.01%	0.001%
15	3.721	754	756	759	rBV2	398	195	0.01%	0.001%
16	3.740	759	762	767	rVB2	483	445	0.02%	0.003%
17	3.775	767	773	776	rBV2	421	467	0.03%	0.003%
18	3.814	781	785	787	rBV2	212	173	0.01%	0.001%
19	3.875	801	804	806	rVB	363	190	0.01%	0.001%
20	3.946	825	826	828	rVB	296	99	0.01%	0.001%
21	3.962	828	831	836	rBV	638	560	0.03%	0.004%
22	3.991	837	840	844	rVB3	237	165	0.01%	0.001%
23	4.042	853	856	857	rBV2	382	212	0.01%	0.001%
24	4.120	878	880	882	rBV2	280	176	0.01%	0.001%
25	4.155	887	891	895	rVB2	258	216	0.01%	0.002%
26	4.181	897	899	902	rVB2	375	198	0.01%	0.001%
27	4.226	908	913	915	rVB	178	142	0.01%	0.001%
28	4.248	915	920	921	rBV2	623	461	0.03%	0.003%
29	4.348	948	951	954	rBV	413	230	0.01%	0.002%
30	4.367	954	957	959	rVV2	677	506	0.03%	0.004%
31	4.425	962	975	995	rVB5	9002	23173	1.30%	0.162%
32	4.499	995	998	1000	rBV3	514	362	0.02%	0.003%
33	4.557	1013	1016	1019	rBV2	339	265	0.01%	0.002%
34	4.615	1022	1034	1072	rVV	156426	448398	25.08%	3.130%
35	5.055	1156	1171	1187	rBV	327726	722952	40.44%	5.047%
36	5.457	1280	1296	1313	rVB4	36970	86445	4.84%	0.603%

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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : EY1B0

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\SFAMULM101023WMA.M
Title : VOC Analysis

37	5.518	1313	1315	1317	rVB2	317	137	0.01%	0.001%
38	5.534	1317	1320	1321	rBV2	406	258	0.01%	0.002%
39	5.586	1334	1336	1338	rBV2	469	296	0.02%	0.002%
40	5.631	1339	1350	1357	rBV8	6708	13443	0.75%	0.094%
41	5.718	1357	1377	1400	rBV2	656163	1787682	100.00%	12.480%
42	6.071	1484	1487	1489	rBV2	306	175	0.01%	0.001%
43	6.119	1500	1502	1507	rVB2	719	600	0.03%	0.004%
44	6.164	1512	1516	1518	rBV2	203	153	0.01%	0.001%
45	6.197	1523	1526	1527	rBV	310	151	0.01%	0.001%
46	6.245	1527	1541	1575	rBV	501921	993273	55.56%	6.934%
47	6.531	1619	1630	1645	rBV9	13449	30303	1.70%	0.212%
48	6.685	1664	1678	1706	rBV	408221	842264	47.11%	5.880%
49	6.910	1743	1748	1750	rBV4	1646	1488	0.08%	0.010%
50	6.984	1769	1771	1772	rBV	302	140	0.01%	0.001%
51	7.068	1784	1797	1806	rBV7	4785	9302	0.52%	0.065%
52	7.377	1880	1893	1910	rVB4	28095	60199	3.37%	0.420%
53	7.473	1916	1923	1925	rBV5	824	926	0.05%	0.006%
54	7.499	1929	1931	1933	rVV3	545	170	0.01%	0.001%
55	7.560	1938	1950	1979	rBV	220079	421777	23.59%	2.944%
56	7.827	2028	2033	2034	rBV3	693	573	0.03%	0.004%
57	7.894	2042	2054	2087	rVB	792718	1397875	78.19%	9.759%
58	8.177	2130	2142	2156	rBV	152673	275077	15.39%	1.920%
59	8.367	2183	2201	2206	rBV7	7405	15675	0.88%	0.109%
60	8.550	2252	2258	2265	rBV7	2559	3577	0.20%	0.025%
61	8.634	2272	2284	2323	rBV2	504544	1165571	65.20%	8.137%
62	9.013	2401	2402	2407	rVB2	453	251	0.01%	0.002%
63	9.036	2407	2409	2412	rVV2	375	251	0.01%	0.002%
64	9.078	2412	2422	2429	rVB8	3312	5999	0.34%	0.042%
65	9.164	2442	2449	2450	rBV2	1010	971	0.05%	0.007%
66	9.315	2493	2496	2499	rBV3	1226	924	0.05%	0.006%
67	9.415	2514	2527	2551	rBV	751761	1294118	72.39%	9.034%
68	9.663	2602	2604	2606	rBV2	814	453	0.03%	0.003%
69	9.695	2606	2614	2623	rVB8	4678	8043	0.45%	0.056%
70	9.762	2633	2635	2638	rBV3	607	272	0.02%	0.002%
71	9.830	2654	2656	2661	rVB3	789	423	0.02%	0.003%
72	9.852	2661	2663	2664	rBV	393	157	0.01%	0.001%
73	9.910	2680	2681	2683	rVB	521	128	0.01%	0.001%
74	10.097	2733	2739	2740	rBV2	1455	1282	0.07%	0.009%
75	10.213	2772	2775	2777	rBV2	330	207	0.01%	0.001%
76	10.306	2800	2804	2808	rBV3	490	488	0.03%	0.003%

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Sample : 04792-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY1B0

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\SFAMULM101023WMA.M
Title : VOC Analysis

77	10.354	2814	2819	2823	rBV3	549	626	0.04%	0.004%
78	10.447	2846	2848	2850	rBV	279	168	0.01%	0.001%
79	10.528	2869	2873	2875	rBV2	394	269	0.02%	0.002%
80	10.547	2875	2879	2880	rBV	294	182	0.01%	0.001%
81	10.592	2891	2893	2895	rBV	407	198	0.01%	0.001%
82	10.663	2912	2915	2917	rBV	508	337	0.02%	0.002%
83	10.688	2921	2923	2929	rVV7	1371	1223	0.07%	0.009%
84	10.753	2930	2943	2967	rVV	664899	1089841	60.96%	7.608%
85	11.010	3021	3023	3025	rBV	373	195	0.01%	0.001%
86	11.058	3036	3038	3041	rBV	419	176	0.01%	0.001%
87	11.094	3047	3049	3051	rBV	266	178	0.01%	0.001%
88	11.187	3075	3078	3080	rBV	377	221	0.01%	0.002%
89	11.203	3080	3083	3086	rBV2	336	247	0.01%	0.002%
90	11.405	3143	3146	3147	rBV2	722	288	0.02%	0.002%
91	11.589	3200	3203	3204	rBV2	698	413	0.02%	0.003%
92	11.811	3259	3272	3297	rBV	769848	1260815	70.53%	8.802%
93	12.190	3377	3390	3411	rBV	780308	1312741	73.43%	9.164%
94	12.418	3458	3461	3464	rBV2	1003	744	0.04%	0.005%
95	12.434	3464	3466	3469	rBV	503	377	0.02%	0.003%
96	12.618	3519	3523	3525	rBV2	662	620	0.03%	0.004%
97	12.807	3580	3582	3585	rBV	394	238	0.01%	0.002%
98	12.862	3594	3599	3606	rVB3	3722	4460	0.25%	0.031%
99	13.328	3735	3744	3754	rVB4	8764	12886	0.72%	0.090%
100	13.528	3803	3806	3811	rBV4	1215	1178	0.07%	0.008%

Sum of corrected areas: 14324613

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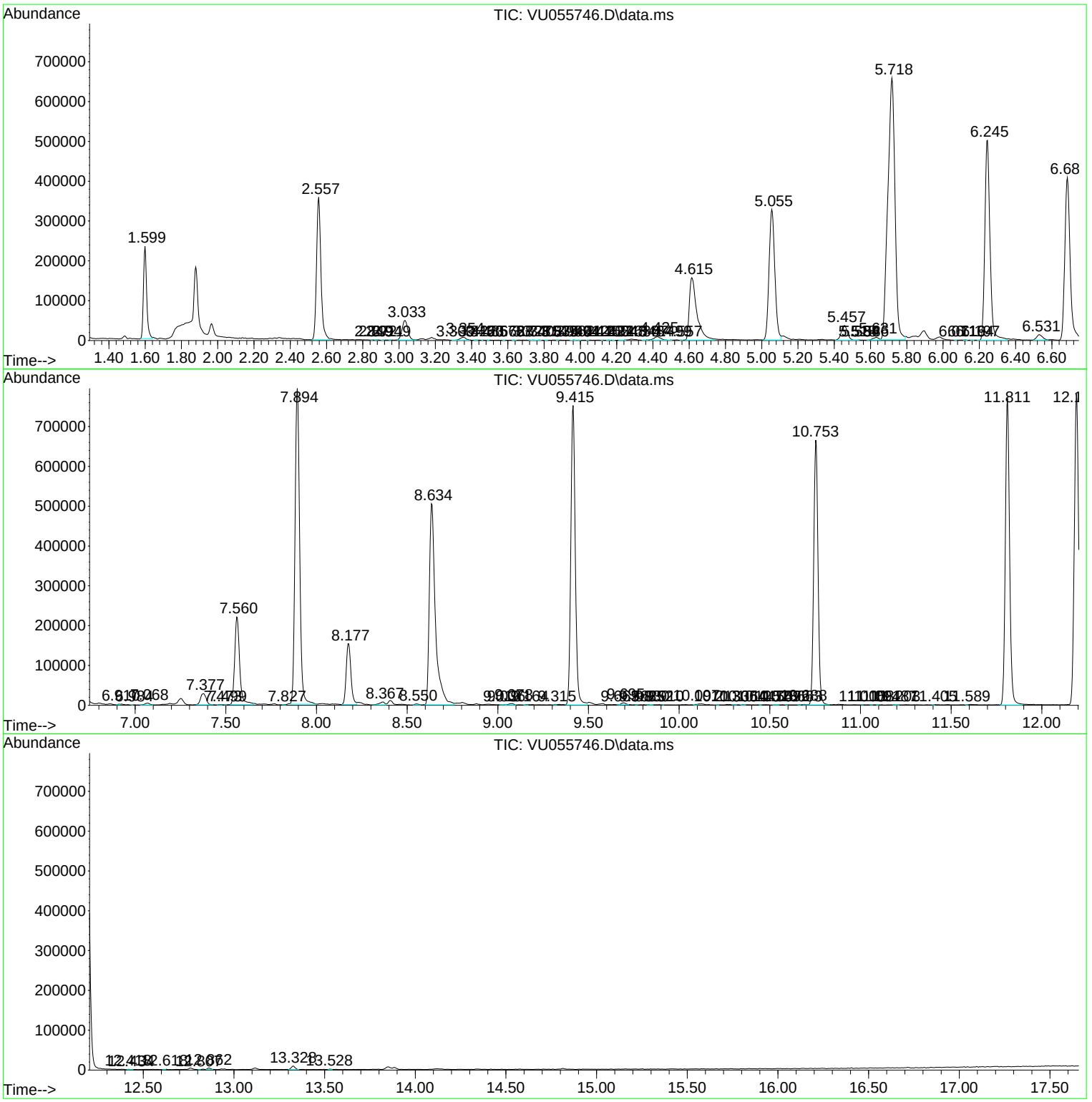
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY1B0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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



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ClientSampleId :
EY1B0

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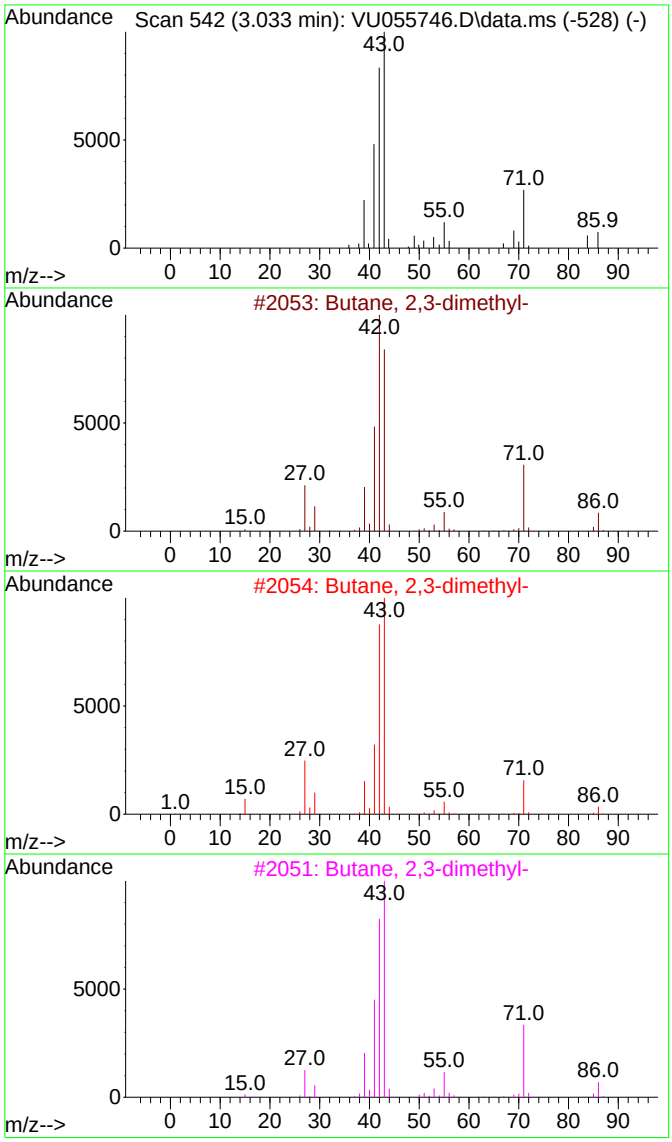
Quant Title : VOC Analysis

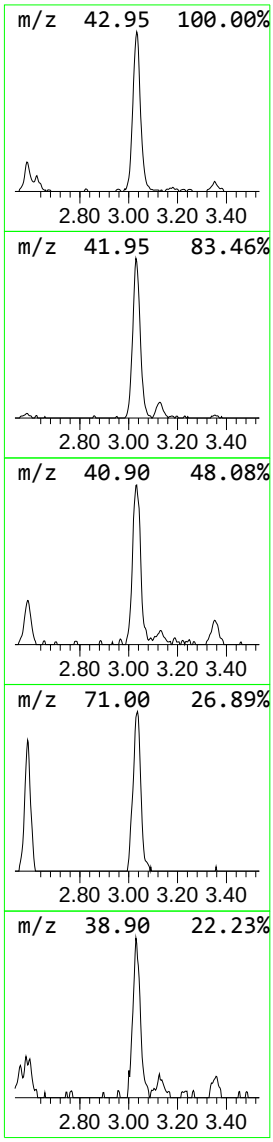
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.033	5.36 ug/L	106533	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
3	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64
4	Pentane, 2-methyl-	86	C6H14	000107-83-5	53
5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	42





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY1B0

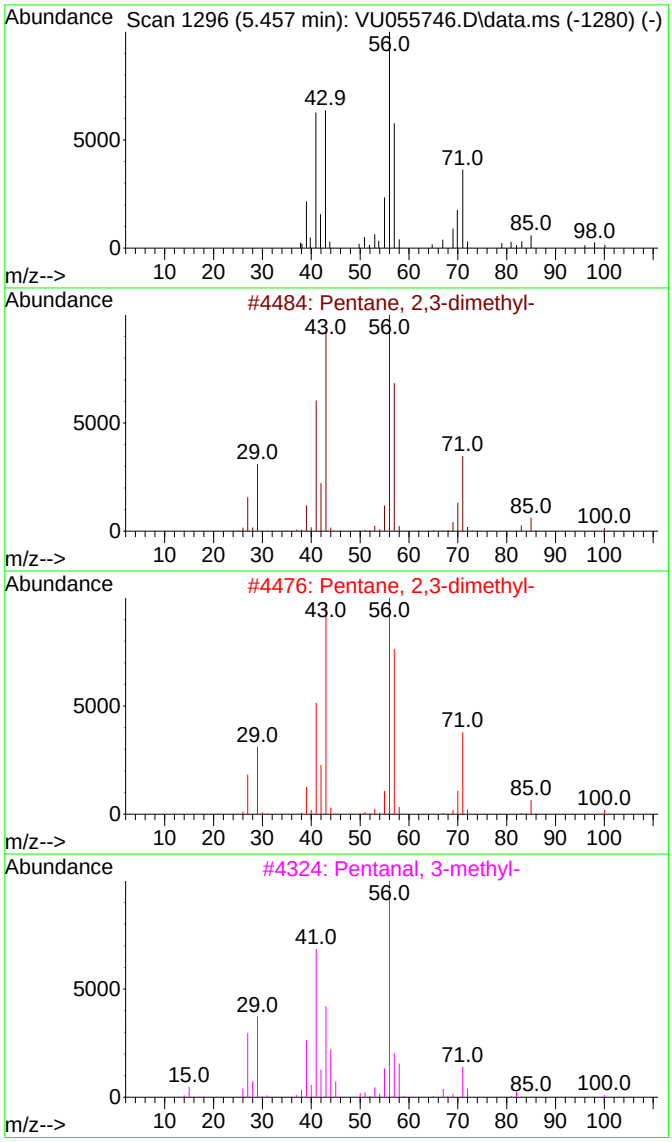
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

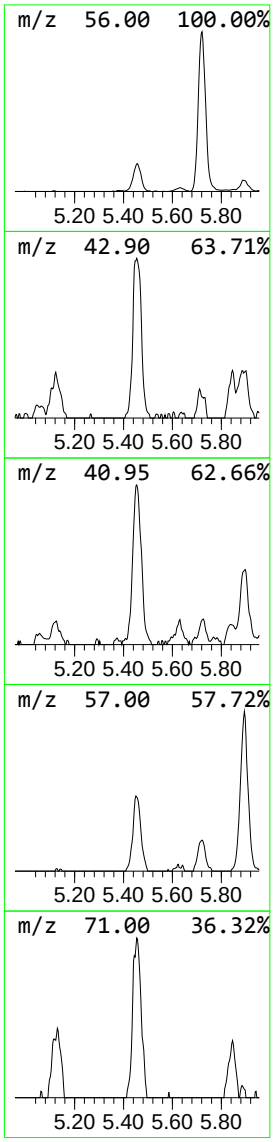
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.457	4.35 ug/L	86445	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	87
2	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	87
3	Pentanal, 3-methyl-	100	C6H12O	015877-57-3	53
4	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	53
5	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	53





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY1B0

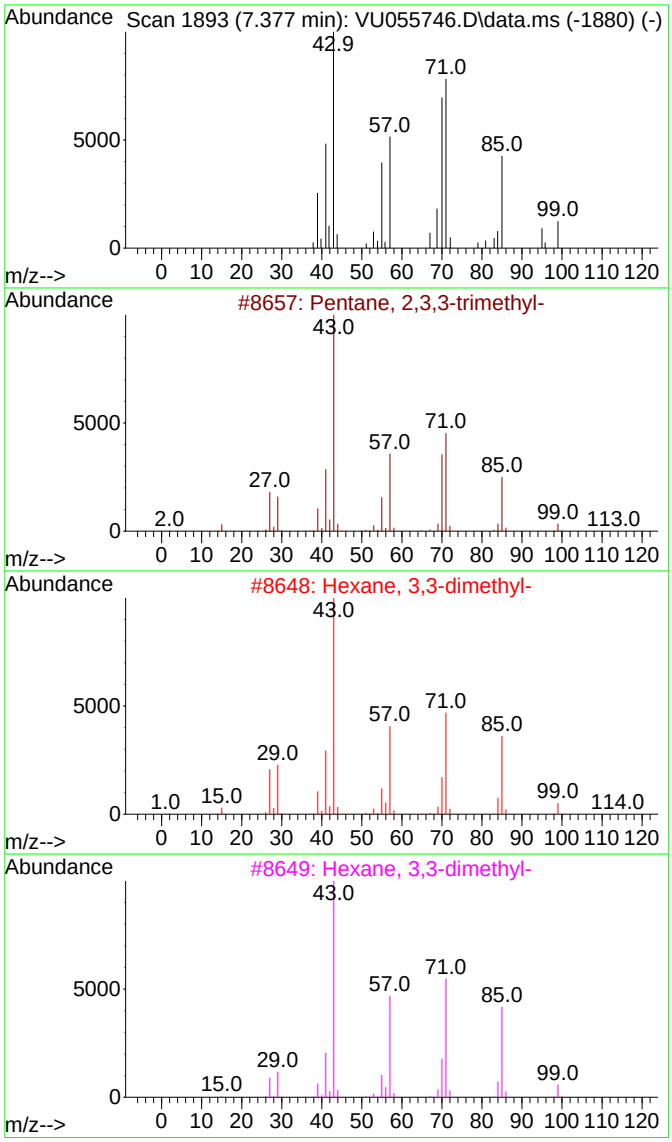
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

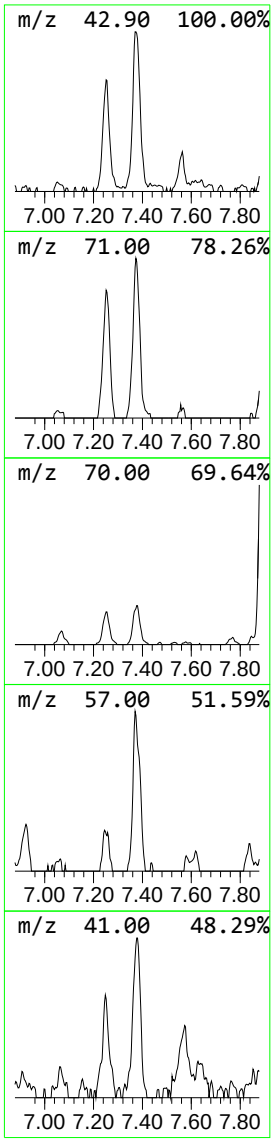
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.377	3.03 ug/L	60199	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
3	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	59
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	56





Tentatively Identified Compound (LSC) summary

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Instrument :
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ClientSampleId :
EY1B0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.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...	3.033	5.4	ug/L	106533	1	6.245	993273	50.0
(DEL) Alkane: S...	5.457	4.3	ug/L	86445	1	6.245	993273	50.0
(DEL) Alkane: S...	7.377	3.0	ug/L	60199	1	6.245	993273	50.0