LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111221\
Data File : VX025155.D
Acq On : 12 Nov 2021 15:51
Operator : JC/MD
Sample : M4615-08 10X
Misc : 2.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0V14

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_X\Method\SFAMXLM111121WMA.M
Title : VOC Analysis

Signal : TIC: VX025155.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.367	42	46	54	rVB	97741	101628	14.79%	1.655%
2	1.666	92	95	107	rVB	62723	78167	11.38%	1.273%
3	2.300	194	199	209	rBV	145602	237919	34.62%	3.874%
4	2.392	209	214	223	rVB	28474	54008	7.86%	0.879%
5	2.776	275	277	278	rBV2	643	529	0.08%	0.009%
6	2.867	290	292	294	rBV3	487	312	0.05%	0.005%
7	2.940	296	304	314	rBV	9724	23848	3.47%	0.388%
8	3.099	329	330	334	rBV3	262	258	0.04%	0.004%
9	3.172	340	342	344	rBV3	292	348	0.05%	0.006%
10	3.251	353	355	358	rVB2	330	317	0.05%	0.005%
11	3.312	363	365	367	rVB4	436	327	0.05%	0.005%
12	3.513	397	398	401	rBV3	302	230	0.03%	0.004%
13	3.849	451	453	456	rBV2	204	267	0.04%	0.004%
14	3.940	465	468	469	rBV3	337	275	0.04%	0.004%
15	4.050	484	486	487	rVB2	412	244	0.04%	0.004%
16	4.147	497	502	503	rBV3	273	337	0.05%	0.005%
17	4.318	529	530	533	rVB2	397	307	0.04%	0.005%
18	4.361	533	537	539	rBV2	408	479	0.07%	0.008%
19	4.465	544	554	567	rBV	52297	159816	23.26%	2.602%
20	4.879	620	622	624	rVB3	401	273	0.04%	0.004%
21	4.934	629	631	634	rVB2	222	241	0.04%	0.004%
22	5.056	640	651	669	rVB	88965	270890	39.42%	4.411%
23	5.355	695	700	701	rBV2	270	371	0.05%	0.006%
24	5.452	714	716	718	rBV2	473	334	0.05%	0.005%
25	5.544	730	731	737	rVB4	317	438	0.06%	0.007%
26	5.696	753	756	760	rBV3	242	477	0.07%	0.008%
27	5.763	764	767	769	rBV3	267	310	0.05%	0.005%
28	5.812	773	775	777	rVV2	553	338	0.05%	0.006%
29	5.830	777	778	781	rVV2	271	246	0.04%	0.004%
30	5.970	789	801	815	rBV2	233818	687166	100.00%	11.189%
31	6.190	835	837	840	rBV4	344	288	0.04%	0.005%
32	6.269	846	850	853	rVB3	414	564	0.08%	0.009%
33	6.348	858	863	864	rBV3	548	865	0.13%	0.014%
34	6.598	901	904	905	rBV2	373	324	0.05%	0.005%
35	6.763	920	931	946	rBV	197716	474849	69.10%	7.732%
36	7.049	976	978	980	rBV2	348	299	0.04%	0.005%

LSC Area Percent Report

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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0V14

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_X\Method\SFAMXLM111121WMA.M
Title : VOC Analysis

37	7.312	1011	1021	1031	rBV	141342	311346	45.31%	5.069%
38	7.421	1033	1039	1047	rVB2	18834	39272	5.72%	0.639%
39	7.555	1059	1061	1063	rVB3	438	354	0.05%	0.006%
40	7.592	1063	1067	1072	rBV4	253	634	0.09%	0.010%
41	7.818	1098	1104	1106	rBV4	572	889	0.13%	0.014%
42	7.927	1118	1122	1130	rBV4	960	2029	0.30%	0.033%
43	8.122	1150	1154	1156	rBV3	296	359	0.05%	0.006%
44	8.189	1164	1165	1168	rBV3	299	389	0.06%	0.006%
45	8.324	1180	1187	1201	rBV	112518	185476	26.99%	3.020%
46	8.452	1207	1208	1211	rBV3	429	571	0.08%	0.009%
47	8.574	1225	1228	1233	rBV4	403	934	0.14%	0.015%
48	8.647	1234	1240	1248	rVV	371948	590107	85.88%	9.608%
49	8.720	1248	1252	1257	rVB	4692	7602	1.11%	0.124%
50	8.884	1278	1279	1282	rBV2	245	271	0.04%	0.004%
51	8.952	1284	1290	1299	rVV	82433	122515	17.83%	1.995%
52	9.183	1327	1328	1330	rBV2	276	231	0.03%	0.004%
53	9.244	1336	1338	1340	rBV2	237	232	0.03%	0.004%
54	9.281	1340	1344	1346	rVB2	424	470	0.07%	0.008%
55	9.384	1356	1361	1376	rBV	248906	366036	53.27%	5.960%
56	9.555	1387	1389	1391	rBV3	357	331	0.05%	0.005%
57	9.707	1410	1414	1420	rVB5	1821	2730	0.40%	0.044%
58	9.835	1432	1435	1439	rVB4	727	1294	0.19%	0.021%
59	9.903	1443	1446	1447	rBV3	689	782	0.11%	0.013%
60	10.006	1459	1463	1465	rBV3	602	911	0.13%	0.015%
61	10.055	1465	1471	1488	rVB	426604	568696	82.76%	9.260%
62	10.177	1488	1491	1493	rBV4	844	1018	0.15%	0.017%
63	10.232	1498	1500	1505	rVB5	765	1111	0.16%	0.018%
64	10.360	1517	1521	1526	rVB	7583	9457	1.38%	0.154%
65	10.457	1532	1537	1539	rBV4	682	859	0.13%	0.014%
66	10.591	1553	1559	1563	rVV4	2491	4383	0.64%	0.071%
67	10.646	1566	1568	1569	rVV2	498	311	0.05%	0.005%
68	10.665	1569	1571	1575	rVB4	939	1351	0.20%	0.022%
69	10.780	1583	1590	1594	rBV	6123	9470	1.38%	0.154%
70	10.860	1600	1603	1606	rBV4	2861	3518	0.51%	0.057%
71	10.945	1614	1617	1623	rVB6	1997	3353	0.49%	0.055%
72	11.000	1623	1626	1628	rBV2	1144	1415	0.21%	0.023%
73	11.030	1628	1631	1634	rBV2	2721	3375	0.49%	0.055%
74	11.085	1638	1640	1642	rBV	5046	4321	0.63%	0.070%
75	11.195	1651	1658	1669	rBV	280583	355853	51.79%	5.794%
76	11.317	1674	1678	1681	rBV2	5756	9125	1.33%	0.149%

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ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0V14

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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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Title : VOC Analysis

77	11.433	1693	1697	1700	rBV	8439	10833	1.58%	0.176%
78	11.475	1700	1704	1711	rVB	62294	78542	11.43%	1.279%
79	11.683	1736	1738	1740	rBV2	3195	3054	0.44%	0.050%
80	11.719	1740	1744	1747	rVV	19940	22480	3.27%	0.366%
81	11.841	1761	1764	1766	rBV2	3308	4470	0.65%	0.073%
82	11.945	1777	1781	1784	rBV3	9194	11935	1.74%	0.194%
83	12.024	1789	1794	1800	rVV	484772	610419	88.83%	9.939%
84	12.073	1800	1802	1805	rVV	8527	9413	1.37%	0.153%
85	12.103	1805	1807	1811	rVB	10792	10589	1.54%	0.172%
86	12.323	1838	1843	1849	rVB	438900	551490	80.26%	8.979%
87	12.426	1856	1860	1864	rVB	66546	72950	10.62%	1.188%
88	12.689	1900	1903	1907	rVB4	3250	3815	0.56%	0.062%
89	12.762	1913	1915	1921	rVB2	4595	5987	0.87%	0.097%
90	12.890	1933	1936	1943	rVB6	3342	6429	0.94%	0.105%
91	12.945	1943	1945	1948	rBV3	1394	1342	0.20%	0.022%
92	13.237	1991	1993	1995	rBV3	834	853	0.12%	0.014%
93	13.268	1995	1998	2005	rVB2	5777	7647	1.11%	0.125%
94	13.390	2014	2018	2021	rVB5	976	1368	0.20%	0.022%
95	13.695	2066	2068	2072	rVB4	514	656	0.10%	0.011%
96	13.835	2089	2091	2094	rBV2	457	305	0.04%	0.005%
97	14.042	2122	2125	2127	rVB3	561	589	0.09%	0.010%
98	14.402	2181	2184	2185	rBV3	385	424	0.06%	0.007%
99	14.615	2217	2219	2220	rBV	535	301	0.04%	0.005%
100	15.566	2371	2375	2379	rVB	9889	14496	2.11%	0.236%

Sum of corrected areas: 6141657

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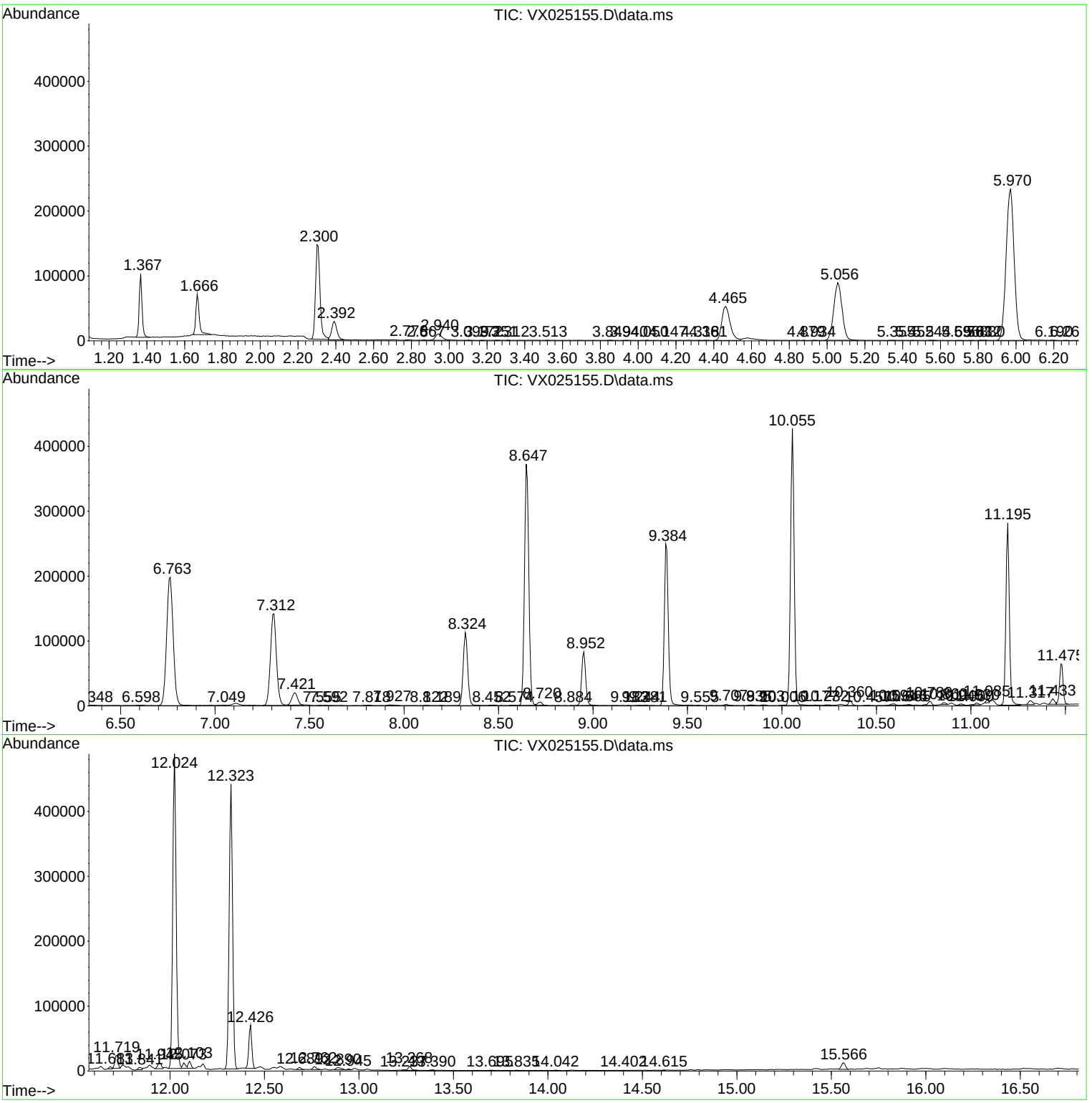
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0V14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

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



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ClientSampleId :
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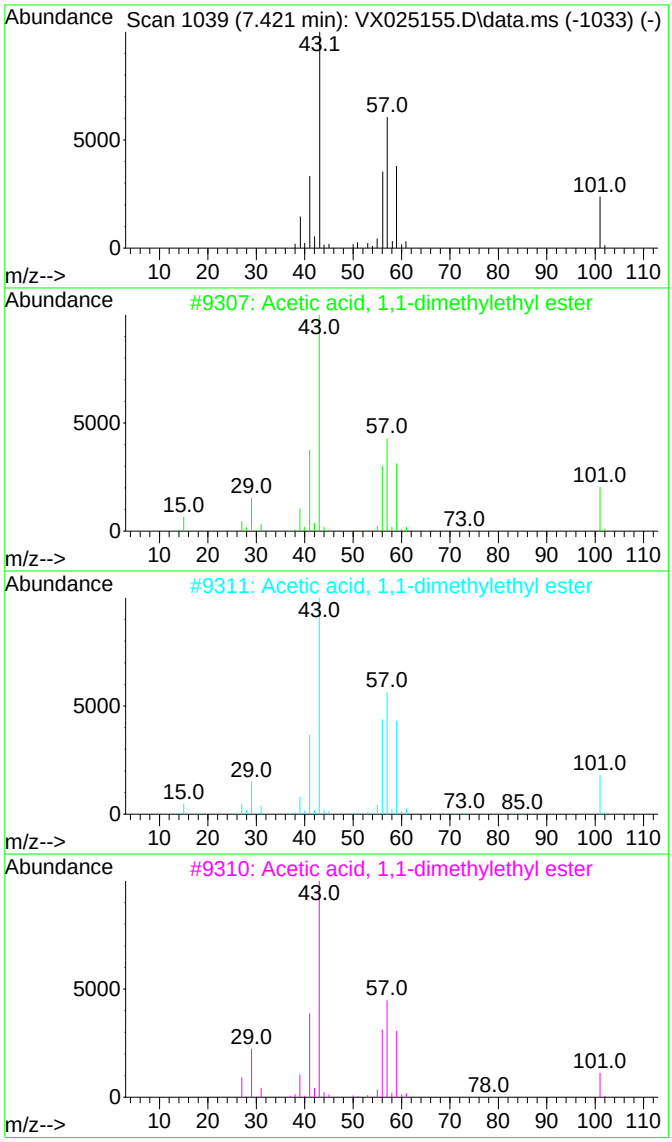
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

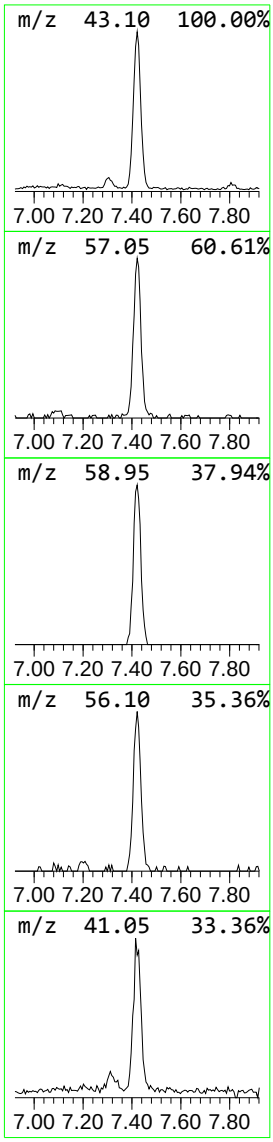
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Acetic acid, 1,1-dimethylet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.421	4.14 ug/L	39272	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	83
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	83
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	72
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	56





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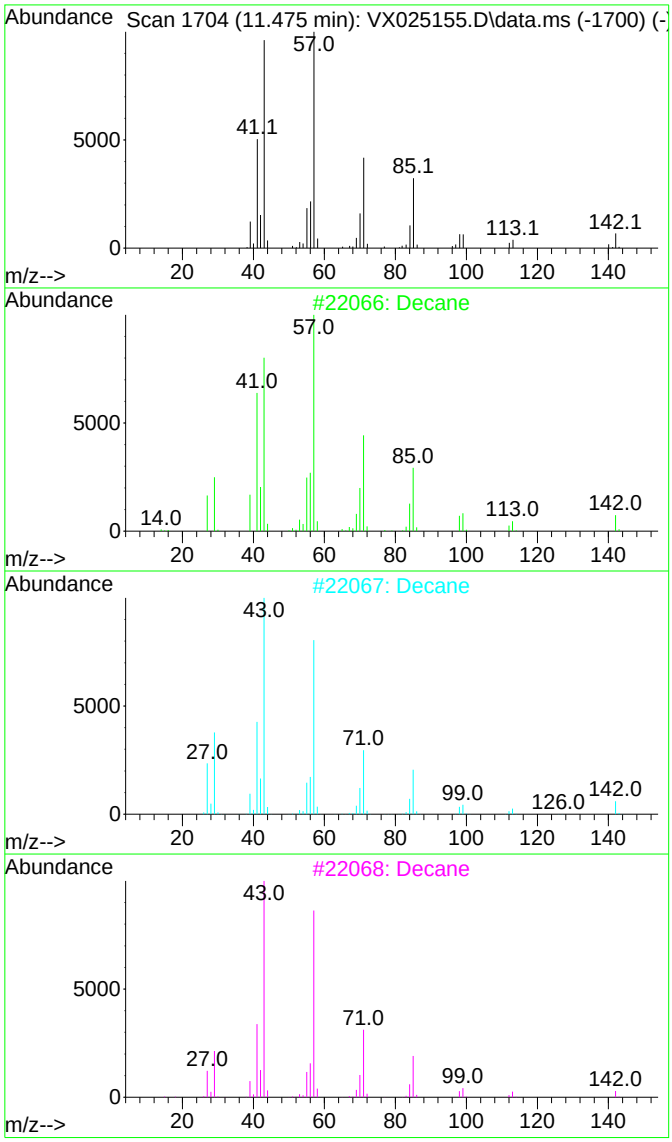
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

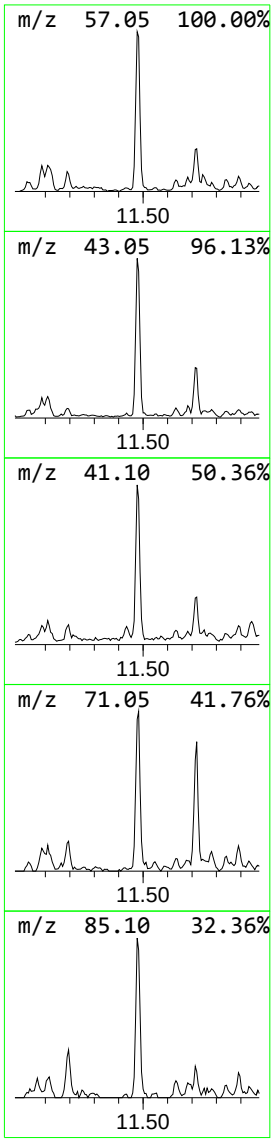
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.475	6.43 ug/L	78542	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	97
2	Decane	142	C10H22	000124-18-5	95
3	Decane	142	C10H22	000124-18-5	94
4	Decane	142	C10H22	000124-18-5	91
5	Nonane	128	C9H20	000111-84-2	78





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0V14

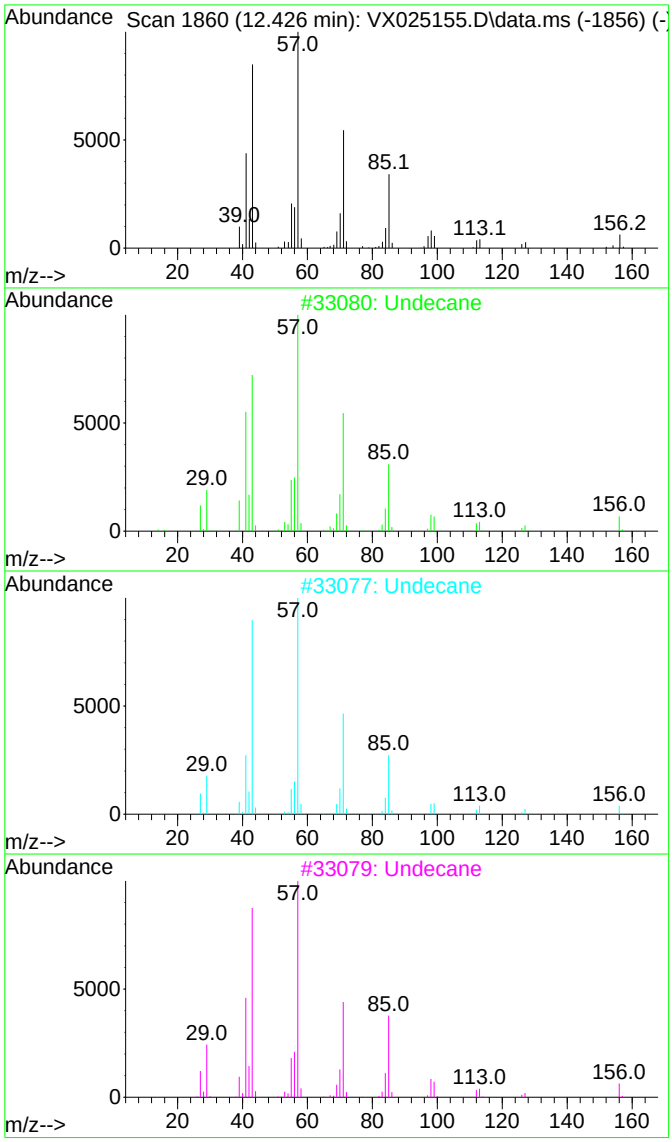
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

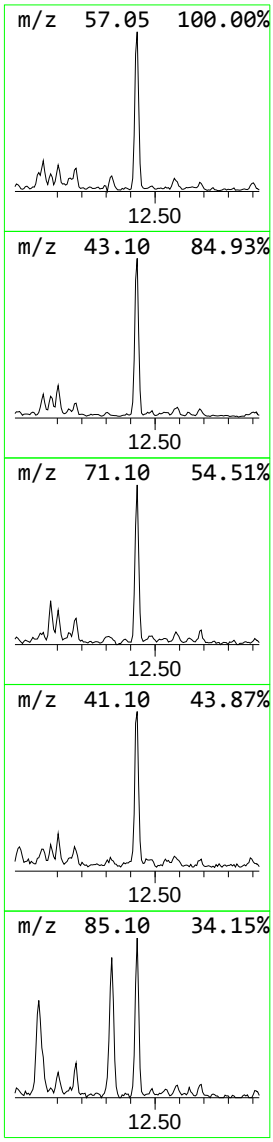
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	5.98 ug/L	72950	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	96
2	Undecane	156	C11H24	001120-21-4	94
3	Undecane	156	C11H24	001120-21-4	93
4	Undecane	156	C11H24	001120-21-4	87
5	Decane	142	C10H22	000124-18-5	86





Tentatively Identified Compound (LSC) summary

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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
Acetic acid, 1,...	7.421	4.1	ug/L	39272	1	6.763	474849	50.0
(DEL) Alkane: S...	11.475	6.4	ug/L	78542	3	12.024	610419	50.0
(DEL) Alkane: S...	12.427	6.0	ug/L	72950	3	12.024	610419	50.0