LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025871.D
Acq On : 10 May 2022 19:31
Operator : SY/MD
Sample : N2714-06ME
Misc : 3.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : EW2X7ME

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\SFAMVLM051022WMA.M
Title : VOC Analysis

Signal : TIC: VV025871.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.751	530	532	539	rBV3	444	268	0.53%	0.089%
2	2.989	604	606	609	rVB2	401	210	0.42%	0.070%
3	3.191	667	669	673	rBV	420	294	0.58%	0.097%
4	3.339	713	715	721	rVV2	245	167	0.33%	0.055%
5	3.368	721	724	728	rVB2	387	260	0.51%	0.086%
6	3.400	732	734	740	rVB2	400	450	0.89%	0.149%
7	3.433	740	744	745	rBV2	271	200	0.40%	0.066%
8	3.445	745	748	750	rBV2	214	128	0.25%	0.042%
9	3.516	767	770	773	rBV	237	189	0.37%	0.063%
10	3.590	789	793	797	rVB2	256	203	0.40%	0.067%
11	3.738	836	839	842	rVB2	207	110	0.22%	0.036%
12	3.757	842	845	847	rBV2	189	140	0.28%	0.046%
13	3.802	857	859	864	rVB2	303	157	0.31%	0.052%
14	3.835	867	869	871	rBV	450	226	0.45%	0.075%
15	3.863	877	878	882	rVB	313	153	0.30%	0.051%
16	3.909	887	892	895	rBV	227	190	0.38%	0.063%
17	3.928	895	898	900	rBV	491	363	0.72%	0.120%
18	4.523	1079	1083	1088	rBV3	602	606	1.20%	0.201%
19	4.587	1100	1103	1107	rVB3	441	310	0.61%	0.103%
20	4.664	1124	1127	1129	rBV	349	200	0.40%	0.066%
21	4.716	1141	1143	1146	rVB2	250	127	0.25%	0.042%
22	4.806	1168	1171	1176	rVB2	296	221	0.44%	0.073%
23	4.937	1209	1212	1215	rVB2	319	180	0.36%	0.060%
24	5.050	1236	1247	1273	rBV4	18780	47043	93.17%	15.573%
25	5.211	1294	1297	1301	rBV2	309	246	0.49%	0.081%
26	5.243	1304	1307	1309	rBV	209	161	0.32%	0.053%
27	5.346	1328	1339	1341	rBV3	4499	6726	13.32%	2.227%
28	5.510	1389	1390	1392	rVB3	355	129	0.26%	0.043%
29	5.526	1392	1395	1396	rBV	223	123	0.24%	0.041%
30	5.558	1403	1405	1409	rBV2	420	237	0.47%	0.078%
31	5.584	1409	1413	1414	rBV2	422	298	0.59%	0.099%
32	5.625	1417	1426	1443	rBV3	17893	37688	74.64%	12.477%
33	5.761	1466	1468	1471	rVB2	441	179	0.35%	0.059%
34	5.815	1482	1485	1486	rBV2	220	108	0.21%	0.036%
35	5.873	1500	1503	1504	rBV	294	123	0.24%	0.041%
36	5.886	1504	1507	1508	rBV	272	125	0.25%	0.041%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025871.D
Acq On : 10 May 2022 19:31
Operator : SY/MD
Sample : N2714-06ME
Misc : 3.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EW2X7ME

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\SFAMVLM051022WMA.M
Title : VOC Analysis

37	5.905	1510	1513	1514	rBV	942	539	1.07%	0.178%
38	6.378	1658	1660	1662	rVV	464	165	0.33%	0.055%
39	6.394	1663	1665	1669	rVB2	337	244	0.48%	0.081%
40	6.452	1680	1683	1686	rBV	167	133	0.26%	0.044%
41	6.535	1707	1709	1713	rVB2	350	237	0.47%	0.078%
42	6.568	1717	1719	1723	rVB2	216	109	0.22%	0.036%
43	6.600	1727	1729	1732	rBV2	313	221	0.44%	0.073%
44	6.651	1736	1745	1748	rBV6	1658	2666	5.28%	0.883%
45	6.786	1785	1787	1789	rVB3	376	111	0.22%	0.037%
46	6.844	1803	1805	1806	rBV	244	105	0.21%	0.035%
47	6.879	1813	1816	1819	rBV2	257	184	0.36%	0.061%
48	6.928	1828	1831	1835	rVB3	311	238	0.47%	0.079%
49	6.957	1835	1840	1843	rBV2	241	206	0.41%	0.068%
50	6.998	1844	1853	1866	rBV5	3750	8078	16.00%	2.674%
51	7.130	1891	1894	1895	rVB2	328	109	0.22%	0.036%
52	7.143	1895	1898	1900	rBV3	226	162	0.32%	0.054%
53	7.166	1901	1905	1909	rVB2	392	307	0.61%	0.102%
54	7.272	1936	1938	1942	rVB	336	227	0.45%	0.075%
55	7.323	1945	1954	1972	rBV3	15575	30619	60.64%	10.136%
56	7.561	2025	2028	2031	rBV2	480	359	0.71%	0.119%
57	7.590	2036	2037	2041	rBV	341	182	0.36%	0.060%
58	7.622	2044	2047	2048	rBV	389	235	0.47%	0.078%
59	7.638	2048	2052	2054	rBV3	1821	1606	3.18%	0.532%
60	7.754	2085	2088	2091	rBV2	162	105	0.21%	0.035%
61	7.793	2094	2100	2101	rBV3	544	460	0.91%	0.152%
62	7.799	2101	2102	2104	rVB2	634	171	0.34%	0.057%
63	7.863	2118	2122	2124	rBV2	261	136	0.27%	0.045%
64	7.953	2147	2150	2153	rBV2	260	205	0.41%	0.068%
65	8.146	2200	2210	2213	rBV6	2963	4457	8.83%	1.475%
66	8.304	2257	2259	2263	rBV3	343	250	0.50%	0.083%
67	8.371	2277	2280	2286	rBV	353	349	0.69%	0.116%
68	8.503	2318	2321	2324	rBV	463	223	0.44%	0.074%
69	8.542	2329	2333	2334	rBV	327	173	0.34%	0.057%
70	8.580	2343	2345	2347	rBV	338	156	0.31%	0.052%
71	8.658	2367	2369	2374	rVB	226	143	0.28%	0.047%
72	8.690	2376	2379	2381	rBV	199	152	0.30%	0.050%
73	8.805	2412	2415	2419	rBV2	354	221	0.44%	0.073%
74	8.860	2422	2432	2454	rBV2	25675	50494	100.00%	16.716%
75	8.973	2465	2467	2469	rBV	301	149	0.30%	0.049%
76	9.220	2541	2544	2546	rBV2	217	128	0.25%	0.042%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025871.D
Acq On : 10 May 2022 19:31
Operator : SY/MD
Sample : N2714-06ME
Misc : 3.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EW2X7ME

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\SFAMVLM051022WMA.M
Title : VOC Analysis

77	9.284	2560	2564	2565	rBV2	298	195	0.39%	0.065%
78	9.461	2618	2619	2622	rBV2	257	147	0.29%	0.049%
79	9.477	2622	2624	2629	rVB	252	133	0.26%	0.044%
80	9.538	2639	2643	2645	rBV	327	261	0.52%	0.086%
81	9.561	2648	2650	2653	rBV2	242	130	0.26%	0.043%
82	9.879	2747	2749	2751	rVB	299	111	0.22%	0.037%
83	9.956	2771	2773	2779	rVB	350	310	0.61%	0.103%
84	10.056	2802	2804	2806	rBV	421	185	0.37%	0.061%
85	10.111	2817	2821	2824	rVB3	507	413	0.82%	0.137%
86	10.182	2841	2843	2846	rVB	346	122	0.24%	0.040%
87	10.227	2846	2857	2866	rBV4	11052	18645	36.93%	6.172%
88	10.342	2889	2893	2895	rVB2	300	178	0.35%	0.059%
89	10.432	2917	2921	2924	rBV2	380	263	0.52%	0.087%
90	10.580	2959	2967	2973	rBV5	3169	4155	8.23%	1.376%
91	10.860	3052	3054	3059	rBV	379	222	0.44%	0.073%
92	11.014	3099	3102	3104	rBV	251	105	0.21%	0.035%
93	11.040	3107	3110	3112	rVV	284	149	0.30%	0.049%
94	11.137	3138	3140	3144	rVB	342	159	0.31%	0.053%
95	11.255	3168	3177	3190	rBV	29044	45807	90.72%	15.164%
96	11.628	3285	3293	3307	rBV4	15597	25783	51.06%	8.535%
97	11.905	3377	3379	3383	rBV	241	130	0.26%	0.043%
98	13.198	3779	3781	3785	rVB2	550	233	0.46%	0.077%
99	13.223	3785	3789	3790	rBV	374	266	0.53%	0.088%
100	13.278	3803	3806	3809	rBV3	500	417	0.83%	0.138%

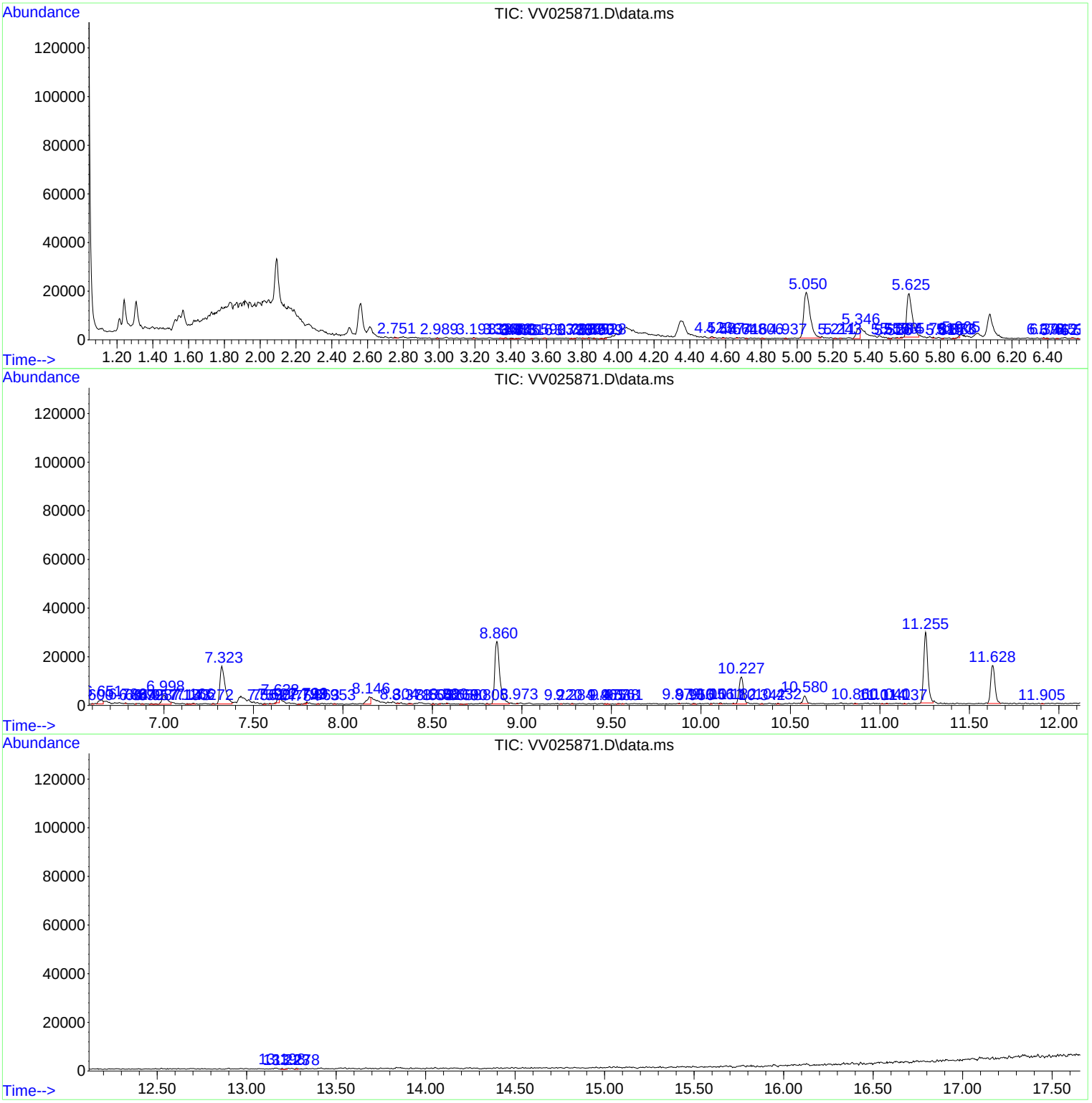
Sum of corrected areas: 302071

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025871.D
Acq On : 10 May 2022 19:31
Operator : SY/MD
Sample : N2714-06ME
Misc : 3.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EW2X7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025871.D
Acq On : 10 May 2022 19:31
Operator : SY/MD
Sample : N2714-06ME
Misc : 3.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EW2X7ME

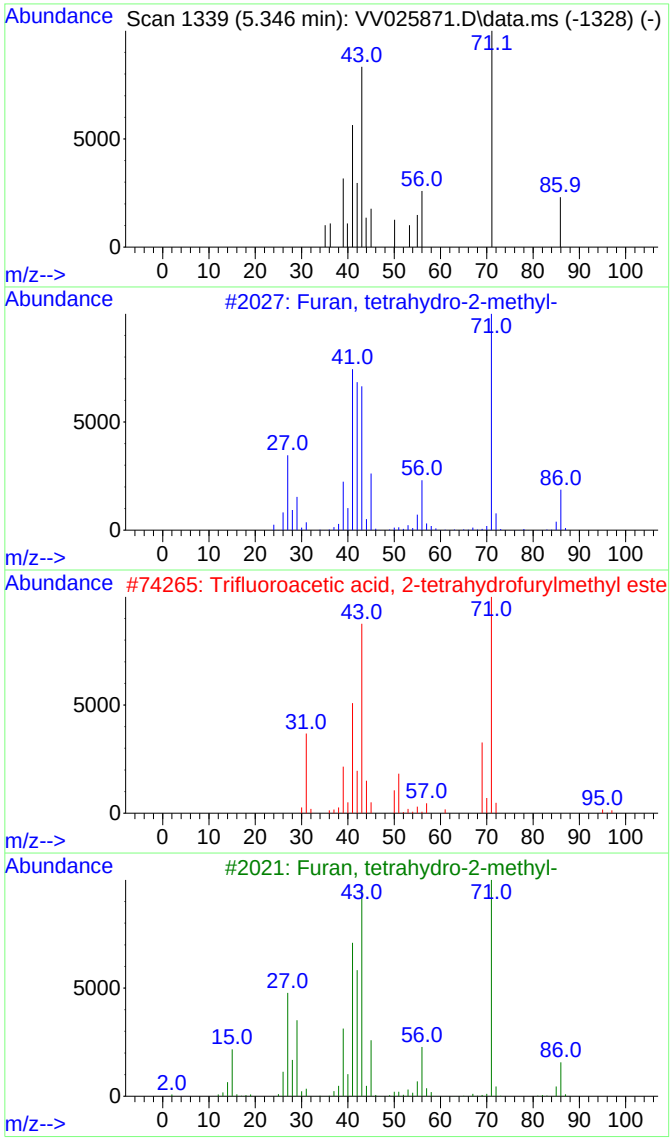
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
Quant Title : VOC Analysis

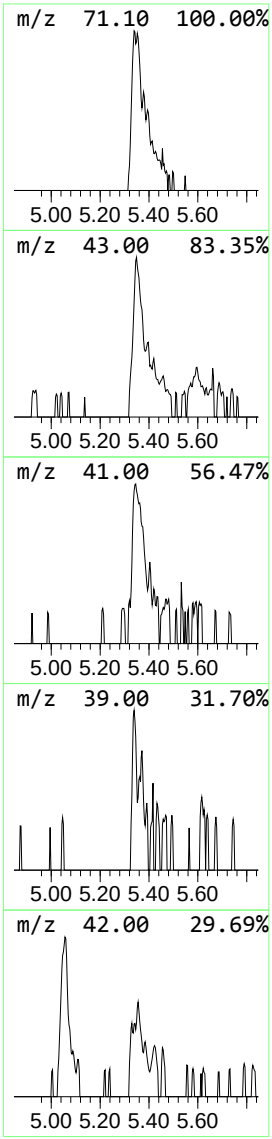
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.346	8.92 ug/L	6726	1,4-Difluorobenzene	5.625

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	42
2	Trifluoroacetic acid, 2-tetrahyd...	198	C7H9F3O3	071239-15-1	33
3	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	28
4	2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	27
5	1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025871.D
Acq On : 10 May 2022 19:31
Operator : SY/MD
Sample : N2714-06ME
Misc : 3.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EW2X7ME

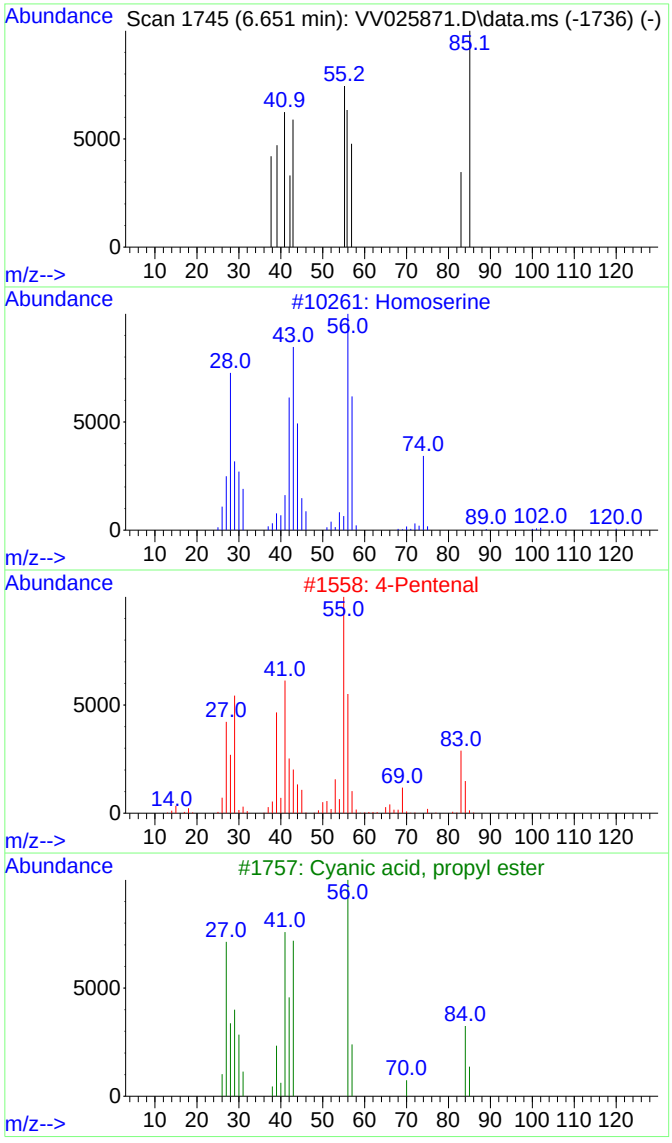
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
Quant Title : VOC Analysis

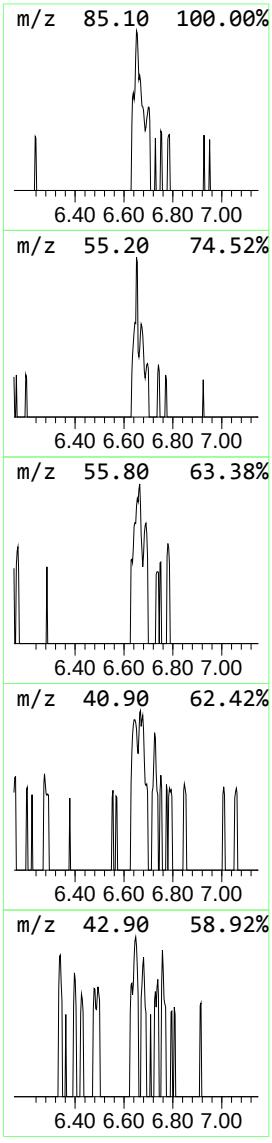
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.651	3.54 ug/L	2666	1,4-Difluorobenzene	5.625

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Homoserine	119	C4H9NO3	000498-19-1	9
2	4-Pentenal	84	C5H8O	002100-17-6	9
3	Cyanic acid, propyl ester	85	C4H7NO	001768-36-1	9
4	Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	9
5	Oxazole, 4,5-dihydro-2-methyl-	85	C4H7NO	001120-64-5	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025871.D
Acq On : 10 May 2022 19:31
Operator : SY/MD
Sample : N2714-06ME
Misc : 3.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EW2X7ME

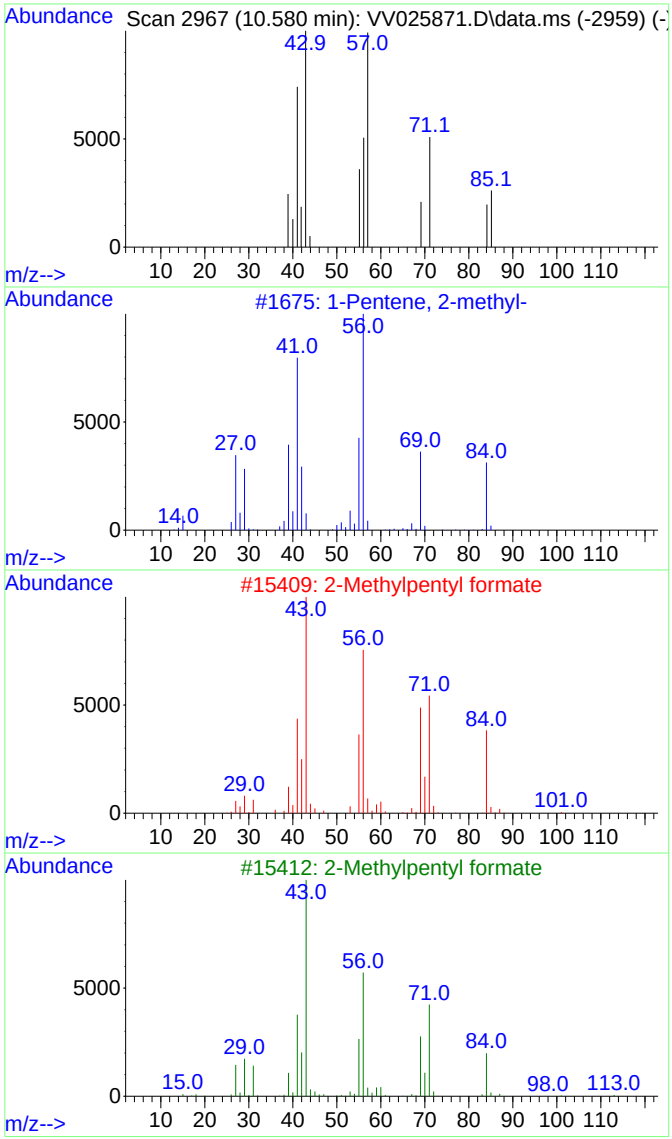
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
Quant Title : VOC Analysis

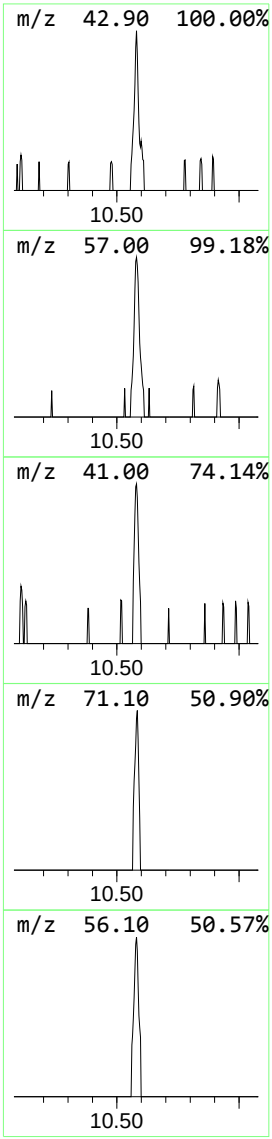
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	4.54 ug/L	4155	1,4-Dichlorobenzene-d4	11.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	35
2	2-Methylpentyl formate	130	C7H14O2	381670-34-4	28
3	2-Methylpentyl formate	130	C7H14O2	381670-34-4	28
4	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	28
5	Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	28





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025871.D
Acq On : 10 May 2022 19:31
Operator : SY/MD
Sample : N2714-06ME
Misc : 3.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EW2X7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.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
unknown-01	5.346	8.9	ug/L	6726	1	5.625	37688	50.0
unknown-02	6.651	3.5	ug/L	2666	1	5.625	37688	50.0
(DEL) Alkane: S...	10.580	4.5	ug/L	4155	3	11.256	45807	50.0