LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043747.D
Acq On : 14 May 2021 11:40
Operator : SY/MD
Sample : M2350-02DL 20X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 60 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L5DL

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\SFAMULM051421WMA.M
Title : VOC Analysis

Signal : TIC: VU043747.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	94	rVB	242494	265604	14.61%	1.709%
2	1.912	169	178	196	rVB	168442	227649	12.52%	1.465%
3	2.572	370	383	398	rBV2	383927	648330	35.67%	4.173%
4	2.771	434	445	447	rBV3	1333	2093	0.12%	0.013%
5	2.867	473	475	480	rVB	300	212	0.01%	0.001%
6	2.954	496	502	505	rBV2	558	531	0.03%	0.003%
7	3.054	521	533	547	rVB2	7052	13115	0.72%	0.084%
8	3.192	563	576	587	rBV	5471	12497	0.69%	0.080%
9	3.317	613	615	622	rVB	301	265	0.01%	0.002%
10	3.353	622	626	627	rBV	425	253	0.01%	0.002%
11	3.363	627	629	636	rVB2	385	332	0.02%	0.002%
12	3.453	652	657	660	rBV2	198	239	0.01%	0.002%
13	3.806	760	767	769	rBV2	248	301	0.02%	0.002%
14	3.877	772	789	812	rBV	102271	241795	13.30%	1.556%
15	4.002	815	828	841	rBV3	3122	6748	0.37%	0.043%
16	4.208	887	892	898	rBV2	180	210	0.01%	0.001%
17	4.266	906	910	915	rBV2	311	310	0.02%	0.002%
18	4.536	988	994	998	rBV2	234	276	0.02%	0.002%
19	4.626	1007	1022	1052	rBV	200119	484228	26.64%	3.117%
20	4.816	1077	1081	1084	rVV3	360	350	0.02%	0.002%
21	4.845	1088	1090	1099	rVB3	376	342	0.02%	0.002%
22	4.890	1100	1104	1107	rBV2	283	220	0.01%	0.001%
23	5.073	1143	1161	1186	rBV	312216	684586	37.66%	4.406%
24	5.160	1186	1188	1191	rVV2	437	318	0.02%	0.002%
25	5.224	1204	1208	1211	rBV2	575	425	0.02%	0.003%
26	5.240	1211	1213	1217	rVB4	449	255	0.01%	0.002%
27	5.324	1221	1239	1267	rBV	469757	1055410	58.06%	6.793%
28	5.523	1296	1301	1304	rBV3	268	226	0.01%	0.001%
29	5.559	1310	1312	1318	rVB2	245	253	0.01%	0.002%
30	5.732	1344	1366	1396	rVV2	676878	1817644	100.00%	11.699%
31	5.970	1437	1440	1443	rBV3	413	300	0.02%	0.002%
32	6.044	1458	1463	1466	rBV5	512	635	0.03%	0.004%
33	6.092	1474	1478	1482	rVB3	408	340	0.02%	0.002%
34	6.131	1482	1490	1494	rBV3	463	559	0.03%	0.004%
35	6.256	1513	1529	1548	rBV	559739	1048210	57.67%	6.746%
36	6.423	1578	1581	1584	rBV3	305	265	0.01%	0.002%

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ALS Vial : 60 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L5DL

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\SFAMULM051421WMA.M
Title : VOC Analysis

37	6.533	1606	1615	1626	rVB4	3129	5820	0.32%	0.037%
38	6.697	1651	1666	1688	rBV	415927	812480	44.70%	5.229%
39	6.919	1725	1735	1748	rVB2	11951	22143	1.22%	0.143%
40	6.970	1748	1751	1755	rVB2	345	241	0.01%	0.002%
41	7.044	1770	1774	1779	rBV2	585	513	0.03%	0.003%
42	7.179	1813	1816	1818	rBV2	574	369	0.02%	0.002%
43	7.343	1858	1867	1880	rVB2	5839	10576	0.58%	0.068%
44	7.520	1911	1922	1927	rBV3	11596	18649	1.03%	0.120%
45	7.571	1927	1938	1959	rVB	223291	390162	21.47%	2.511%
46	7.665	1964	1967	1970	rVV	336	307	0.02%	0.002%
47	7.684	1970	1973	1974	rVV2	618	429	0.02%	0.003%
48	7.719	1974	1984	1998	rVB2	11513	20785	1.14%	0.134%
49	7.793	2004	2007	2010	rBV	329	250	0.01%	0.002%
50	7.906	2025	2042	2056	rBV	821402	1402748	77.17%	9.028%
51	7.976	2057	2064	2077	rVB	12904	22711	1.25%	0.146%
52	8.185	2115	2129	2148	rBV	156414	261035	14.36%	1.680%
53	8.385	2187	2191	2199	rBV	608	794	0.04%	0.005%
54	8.468	2214	2217	2218	rBV	419	283	0.02%	0.002%
55	8.552	2240	2243	2246	rBV	343	249	0.01%	0.002%
56	8.639	2256	2270	2304	rBV	560686	1006745	55.39%	6.480%
57	8.861	2336	2339	2342	rBV2	230	218	0.01%	0.001%
58	8.890	2345	2348	2353	rVB2	458	425	0.02%	0.003%
59	9.324	2478	2483	2490	rVB2	457	674	0.04%	0.004%
60	9.423	2500	2514	2540	rBV	792693	1291436	71.05%	8.312%
61	9.700	2592	2600	2608	rVB4	1156	1869	0.10%	0.012%
62	9.771	2618	2622	2627	rBV2	259	323	0.02%	0.002%
63	9.816	2632	2636	2642	rVB2	246	347	0.02%	0.002%
64	10.063	2709	2713	2718	rVB2	262	242	0.01%	0.002%
65	10.099	2718	2724	2726	rBV3	614	517	0.03%	0.003%
66	10.272	2763	2778	2799	rVV	67721	150159	8.26%	0.966%
67	10.346	2799	2801	2803	rVV2	769	519	0.03%	0.003%
68	10.359	2803	2805	2812	rVV3	985	809	0.04%	0.005%
69	10.555	2858	2866	2876	rBV6	2039	4294	0.24%	0.028%
70	10.674	2892	2903	2912	rVB3	5542	8562	0.47%	0.055%
71	10.761	2916	2930	2953	rBV	588668	940734	51.76%	6.055%
72	10.886	2959	2969	2973	rBV6	2381	4107	0.23%	0.026%
73	10.996	2997	3003	3005	rVV2	1048	1118	0.06%	0.007%
74	11.034	3005	3015	3030	rVB	118421	200417	11.03%	1.290%
75	11.089	3030	3032	3036	rBV3	319	261	0.01%	0.002%
76	11.124	3037	3043	3050	rBV8	1858	2411	0.13%	0.016%

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ALS Vial : 60 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L5DL

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\SFAMULM051421WMA.M
Title : VOC Analysis

77	11.201	3060	3067	3075	rVB5	1413	1908	0.10%	0.012%
78	11.240	3075	3079	3083	rVB3	786	587	0.03%	0.004%
79	11.291	3090	3095	3098	rBV2	504	518	0.03%	0.003%
80	11.349	3108	3113	3118	rVB3	412	474	0.03%	0.003%
81	11.462	3140	3148	3161	rVB8	3500	5833	0.32%	0.038%
82	11.584	3182	3186	3193	rVB2	649	819	0.05%	0.005%
83	11.703	3215	3223	3229	rBV4	2319	3360	0.18%	0.022%
84	11.754	3235	3239	3243	rBV3	337	363	0.02%	0.002%
85	11.819	3245	3259	3282	rVV	739863	1170368	64.39%	7.533%
86	11.947	3287	3299	3303	rVV6	1932	3963	0.22%	0.026%
87	11.980	3305	3309	3318	rVB3	3248	4170	0.23%	0.027%
88	12.105	3341	3348	3355	rVB6	4193	5970	0.33%	0.038%
89	12.198	3359	3377	3398	rBV	765686	1231547	67.76%	7.926%
90	12.336	3414	3420	3425	rVB5	1499	1749	0.10%	0.011%
91	12.391	3431	3437	3438	rBV3	492	389	0.02%	0.003%
92	12.523	3473	3478	3480	rBV2	317	262	0.01%	0.002%
93	12.555	3486	3488	3495	rVB2	295	247	0.01%	0.002%
94	12.629	3505	3511	3513	rBV2	465	445	0.02%	0.003%
95	12.648	3515	3517	3522	rVB3	632	434	0.02%	0.003%
96	12.754	3546	3550	3553	rBV2	313	267	0.01%	0.002%
97	13.160	3671	3676	3681	rVB4	566	611	0.03%	0.004%
98	13.426	3755	3759	3764	rBV3	449	376	0.02%	0.002%
99	13.770	3863	3866	3868	rBV2	338	233	0.01%	0.001%
100	14.468	4080	4083	4086	rBV2	332	222	0.01%	0.001%

Sum of corrected areas: 15537172

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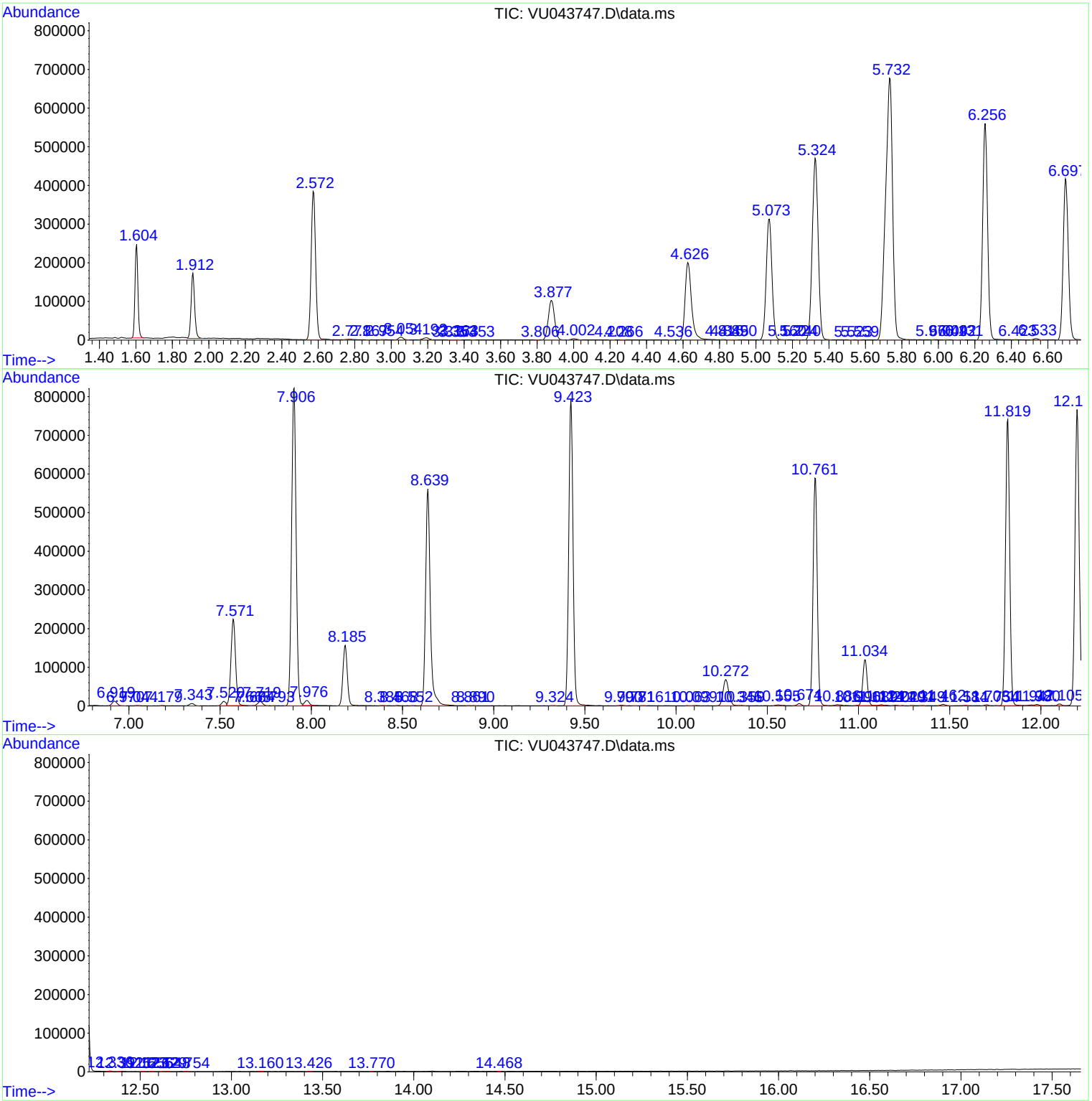
Instrument :
MSVOA_U
ClientSampleId :
BG6L5DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 60 Sample Multiplier: 1

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ClientSampleId : BG6L5DL

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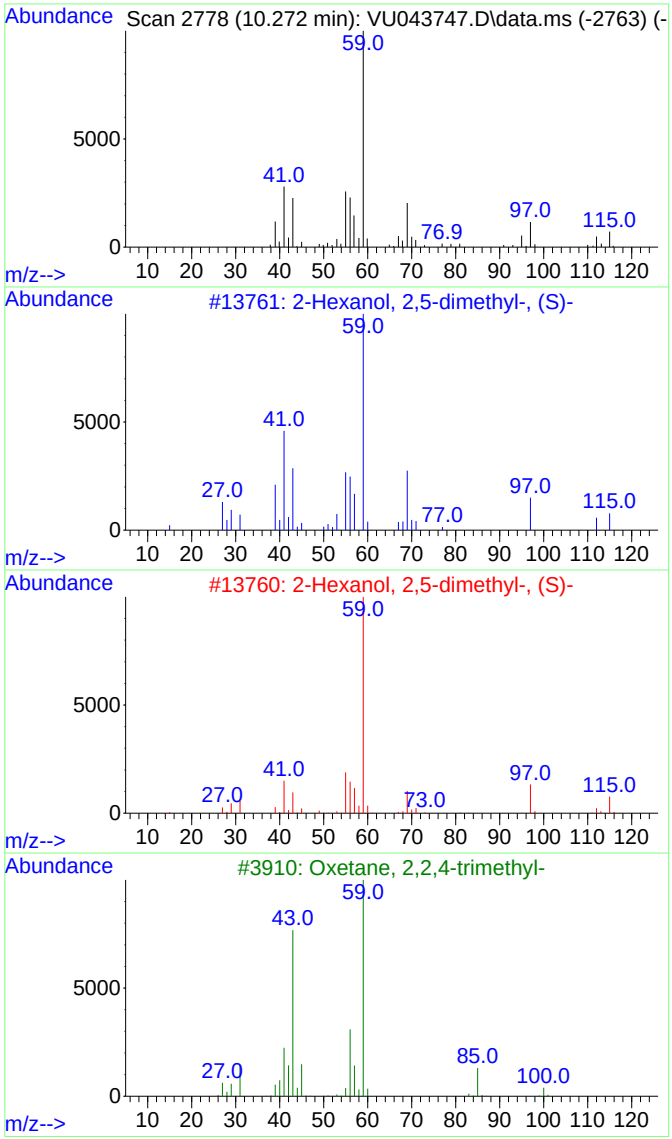
Quant Title : VOC Analysis

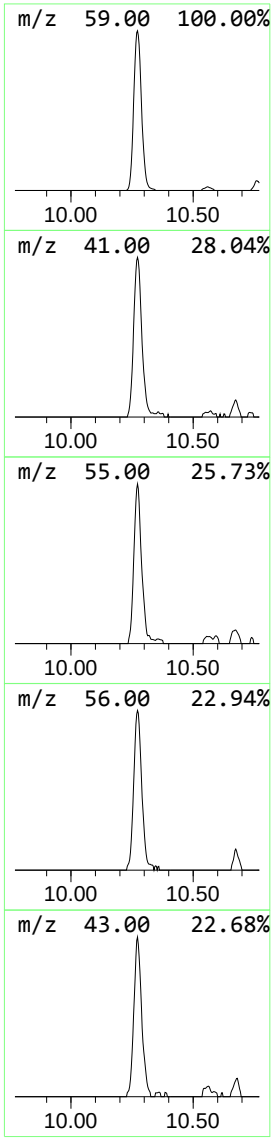
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.272	5.81 ug/L	150159	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	78
2	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	72
3	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	64
4	dl-Erythro-O-methylthreonine	133	C5H11NO3	1000214-70-7	64
5	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	40





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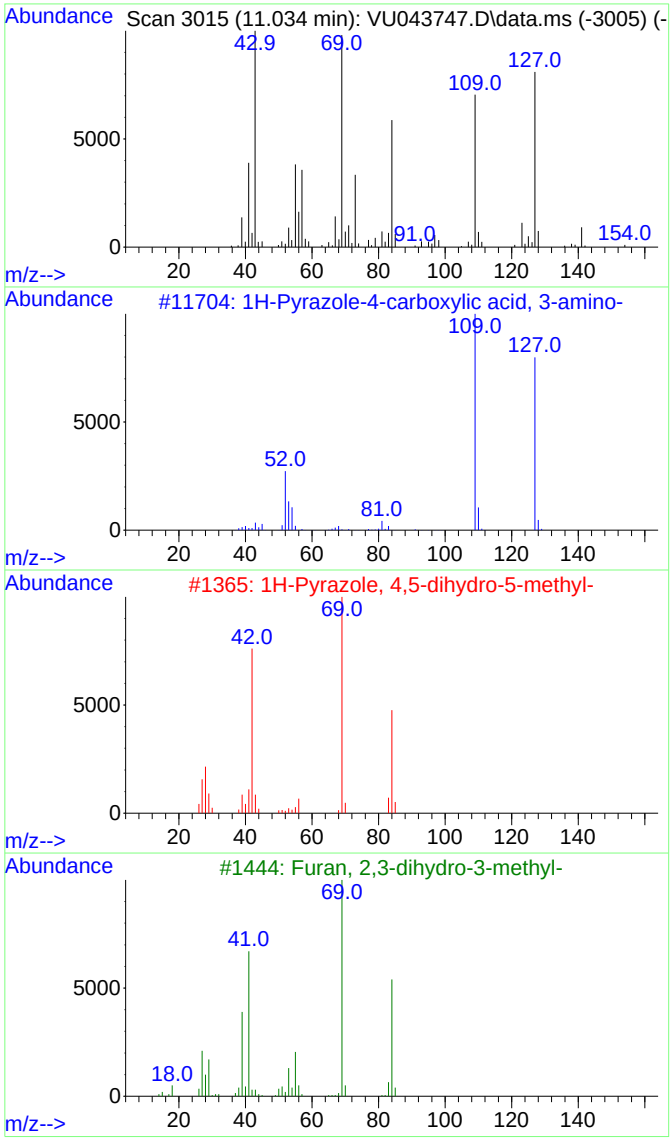
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

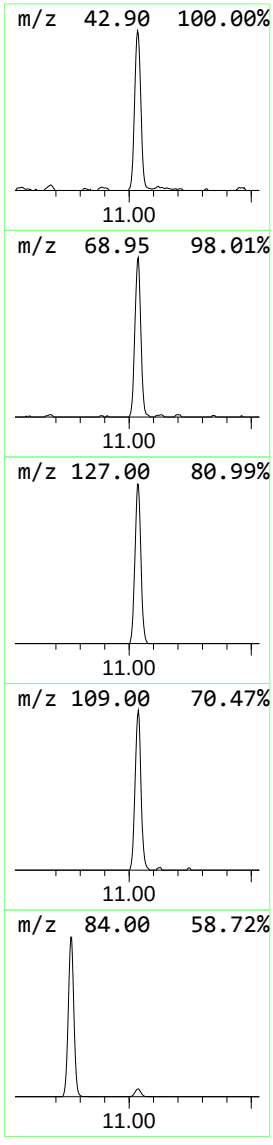
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.034	8.56 ug/L	200417	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2	041680-34-6	35
2	1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	27
3	Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	27
4	Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	27
5	3,5,5-Trimethylcyclohexyl propyl...	250	C12H24FO2P	1000298-30-8	25





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Hexanol, 2,5-...	10.272	5.8	ug/L	150159	2	9.423	1291440	50.0
unknown-01	11.034	8.6	ug/L	200417	3	11.819	1170370	50.0