LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU040920\
Data File : VU037669.D
Acq On : 10 Apr 2020 13:46
Operator : JC/MD
Sample : L2189-01 10X
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFS79

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\SOMULM040920WMA.M
Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.614	77	85	95	rBV	257639	283748	11.66%	1.330%
2	1.926	174	182	199	rVB	203756	285948	11.75%	1.340%
3	2.591	376	389	406	rBV2	405514	689195	28.32%	3.230%
4	2.794	446	452	463	rVB2	5103	8717	0.36%	0.041%
5	2.990	508	513	514	rBV3	861	600	0.02%	0.003%
6	3.077	533	540	550	rVB8	1332	2422	0.10%	0.011%
7	3.138	552	559	561	rBV4	811	786	0.03%	0.004%
8	3.218	568	584	603	rVB2	18215	42774	1.76%	0.200%
9	3.308	609	612	615	rBV3	762	594	0.02%	0.003%
10	3.366	624	630	631	rBV4	693	523	0.02%	0.002%
11	3.385	632	636	637	rBV3	846	611	0.03%	0.003%
12	3.485	663	667	675	rBV5	654	950	0.04%	0.004%
13	3.620	706	709	715	rBV4	850	947	0.04%	0.004%
14	3.913	782	800	822	rVV	250762	595297	24.46%	2.790%
15	4.035	825	838	856	rVB	8273	21900	0.90%	0.103%
16	4.138	866	870	874	rBV3	667	589	0.02%	0.003%
17	4.160	874	877	882	rVV3	527	520	0.02%	0.002%
18	4.376	940	944	948	rBV2	629	565	0.02%	0.003%
19	4.475	970	975	979	rBV3	640	744	0.03%	0.003%
20	4.665	1019	1034	1062	rBV	267209	640098	26.30%	3.000%
21	4.839	1085	1088	1094	rBV6	874	1065	0.04%	0.005%
22	5.102	1153	1170	1194	rBV	354878	777950	31.96%	3.646%
23	5.353	1229	1248	1266	rBV	1086310	2433999	100.00%	11.408%
24	5.585	1317	1320	1323	rBV2	726	592	0.02%	0.003%
25	5.758	1352	1374	1401	rVV2	779093	2055586	84.45%	9.635%
26	5.890	1413	1415	1421	rBV6	684	590	0.02%	0.003%
27	6.073	1464	1472	1475	rBV5	1697	2007	0.08%	0.009%
28	6.141	1488	1493	1496	rBV5	903	822	0.03%	0.004%
29	6.279	1521	1536	1556	rBV	707981	1312669	53.93%	6.153%
30	6.405	1571	1575	1577	rVV3	699	517	0.02%	0.002%
31	6.491	1597	1602	1605	rVV3	695	576	0.02%	0.003%
32	6.562	1613	1624	1634	rBV8	5182	11315	0.46%	0.053%
33	6.723	1657	1674	1694	rBV	494709	954526	39.22%	4.474%
34	6.835	1700	1709	1713	rBV5	2066	2841	0.12%	0.013%

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ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFS79

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\SOMULM040920WMA.M
Title : VOC Analysis

35	6.877	1719	1722	1726	rVB4	823	532	0.02%	0.002%
36	6.945	1729	1743	1758	rBV3	36037	69346	2.85%	0.325%
37	7.073	1778	1783	1790	rBV5	569	616	0.03%	0.003%
38	7.205	1816	1824	1831	rBV9	3375	5703	0.23%	0.027%
39	7.363	1862	1873	1887	rVV2	7818	15130	0.62%	0.071%
40	7.540	1915	1928	1933	rBV4	13836	25082	1.03%	0.118%
41	7.591	1933	1944	1958	rVB	310488	534476	21.96%	2.505%
42	7.742	1978	1991	2005	rVB2	31948	60318	2.48%	0.283%
43	7.922	2032	2047	2064	rVV	969860	1651214	67.84%	7.739%
44	8.202	2120	2134	2151	rBV	227075	372057	15.29%	1.744%
45	8.421	2199	2202	2208	rVB4	1091	1276	0.05%	0.006%
46	8.494	2214	2225	2233	rBV3	2850	5082	0.21%	0.024%
47	8.572	2237	2249	2260	rVB6	7910	12699	0.52%	0.060%
48	8.655	2260	2275	2304	rBV	795718	1382227	56.79%	6.479%
49	8.797	2317	2319	2324	rVB2	861	603	0.02%	0.003%
50	8.826	2324	2328	2329	rBV	807	515	0.02%	0.002%
51	8.874	2340	2343	2346	rVB5	826	539	0.02%	0.003%
52	8.983	2375	2377	2385	rVB3	1006	974	0.04%	0.005%
53	9.028	2385	2391	2394	rBV4	745	966	0.04%	0.005%
54	9.102	2412	2414	2420	rBV4	535	524	0.02%	0.002%
55	9.337	2481	2487	2493	rVV4	1675	1799	0.07%	0.008%
56	9.437	2504	2518	2538	rBV	991368	1630552	66.99%	7.642%
57	9.536	2544	2549	2557	rVB10	3406	5194	0.21%	0.024%
58	9.713	2598	2604	2612	rVB6	2199	3393	0.14%	0.016%
59	9.867	2647	2652	2657	rBV5	586	641	0.03%	0.003%
60	9.951	2675	2678	2681	rBV3	769	644	0.03%	0.003%
61	10.118	2720	2730	2739	rBV7	2436	3704	0.15%	0.017%
62	10.276	2765	2779	2797	rBV	320817	520777	21.40%	2.441%
63	10.504	2844	2850	2858	rBV7	1928	3217	0.13%	0.015%
64	10.559	2860	2867	2877	rVV3	11430	17207	0.71%	0.081%
65	10.658	2893	2898	2906	rVB6	1748	2722	0.11%	0.013%
66	10.771	2920	2933	2948	rBV	653907	1041798	42.80%	4.883%
67	10.906	2967	2975	2984	rVB	4391	7898	0.32%	0.037%
68	10.999	2998	3004	3005	rBV4	3230	2472	0.10%	0.012%
69	11.044	3006	3018	3033	rVB	373575	629538	25.86%	2.951%
70	11.170	3055	3057	3061	rVB2	985	599	0.02%	0.003%
71	11.205	3061	3068	3074	rBV5	2485	3397	0.14%	0.016%

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ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFS79

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\SOMULM040920WMA.M
Title : VOC Analysis

72	11.247	3074	3081	3088	rVB4	2311	2551	0.10%	0.012%
73	11.308	3094	3100	3105	rBV5	1438	1791	0.07%	0.008%
74	11.391	3121	3126	3130	rBV5	833	961	0.04%	0.005%
75	11.478	3148	3153	3162	rBV7	2026	2881	0.12%	0.014%
76	11.543	3169	3173	3178	rVB6	674	707	0.03%	0.003%
77	11.636	3193	3202	3204	rBV3	3287	4138	0.17%	0.019%
78	11.723	3222	3229	3235	rVV6	1476	2229	0.09%	0.010%
79	11.826	3248	3261	3280	rVV	1032032	1604687	65.93%	7.521%
80	11.906	3282	3286	3296	rVV8	1431	2360	0.10%	0.011%
81	11.990	3309	3312	3320	rVB4	543	609	0.03%	0.003%
82	12.067	3333	3336	3337	rVV3	1080	722	0.03%	0.003%
83	12.108	3339	3349	3359	rVB6	17733	28730	1.18%	0.135%
84	12.205	3366	3379	3395	rBV	924714	1485837	61.05%	6.964%
85	12.797	3557	3563	3566	rBV3	1714	1925	0.08%	0.009%
86	12.887	3577	3591	3601	rBV2	16473	27033	1.11%	0.127%
87	12.944	3607	3609	3611	rBV2	937	583	0.02%	0.003%
88	13.096	3653	3656	3658	rBV	799	526	0.02%	0.002%
89	13.166	3675	3678	3680	rBV3	1214	867	0.04%	0.004%
90	13.305	3718	3721	3725	rBV4	854	718	0.03%	0.003%
91	13.504	3780	3783	3785	rBV3	790	519	0.02%	0.002%
92	13.719	3846	3850	3855	rBV4	960	1098	0.05%	0.005%
93	13.838	3883	3887	3889	rVV3	649	606	0.02%	0.003%
94	13.867	3893	3896	3901	rVV3	1031	771	0.03%	0.004%
95	14.118	3966	3974	3983	rVB4	2673	4519	0.19%	0.021%
96	14.163	3986	3988	3993	rBV3	638	558	0.02%	0.003%
97	14.379	4053	4055	4062	rBV4	840	888	0.04%	0.004%
98	14.626	4124	4132	4143	rVB2	4766	7054	0.29%	0.033%
99	14.899	4213	4217	4220	rBV4	1187	902	0.04%	0.004%
100	15.253	4325	4327	4330	rBV4	984	639	0.03%	0.003%

Sum of corrected areas: 21335423

LSC Report - Integrated Chromatogram

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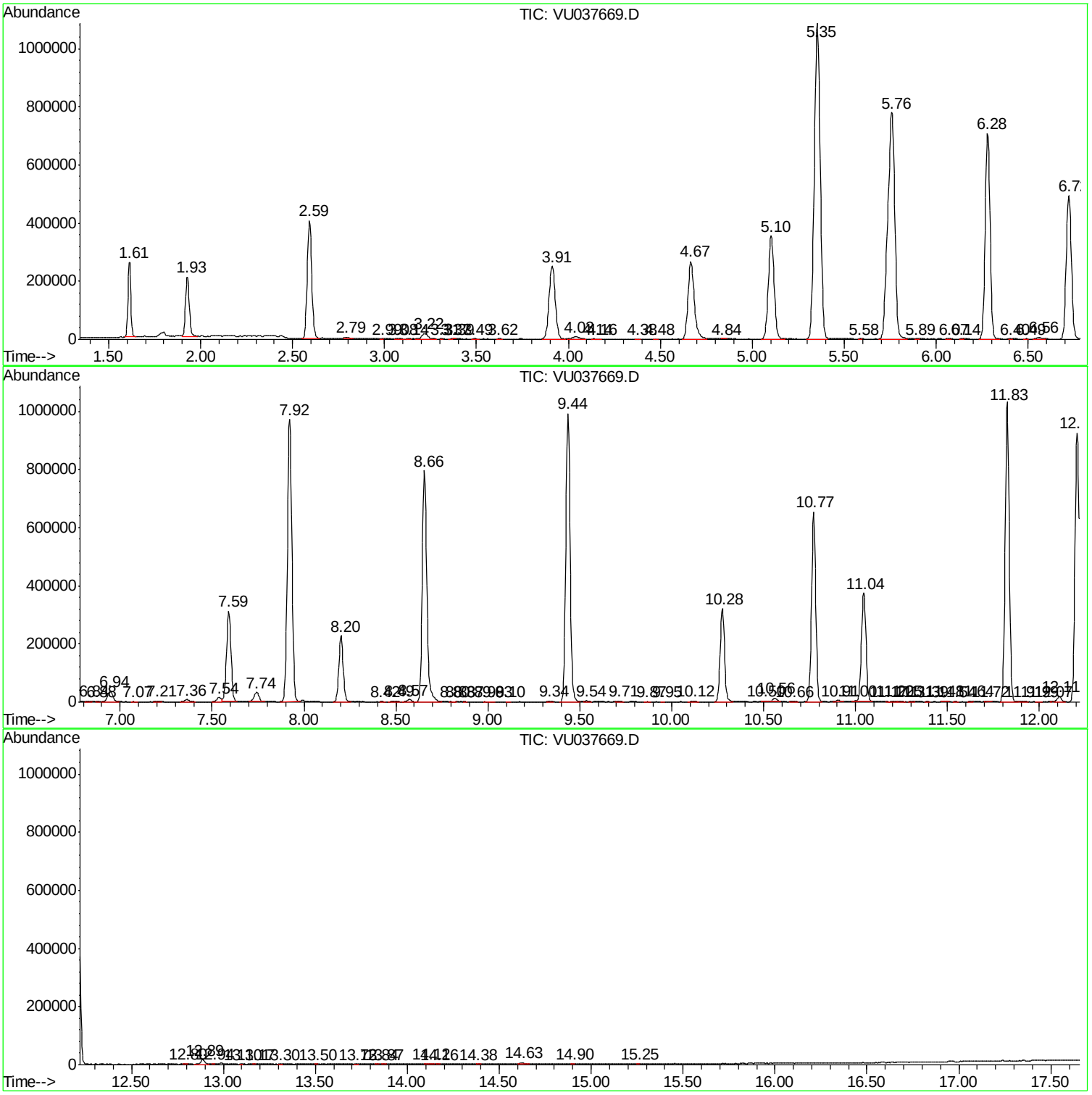
Instrument : MSVOA_U
ClientSampleId : BFS79

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040920WMA.M
Quant Title : VOC Analysis

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



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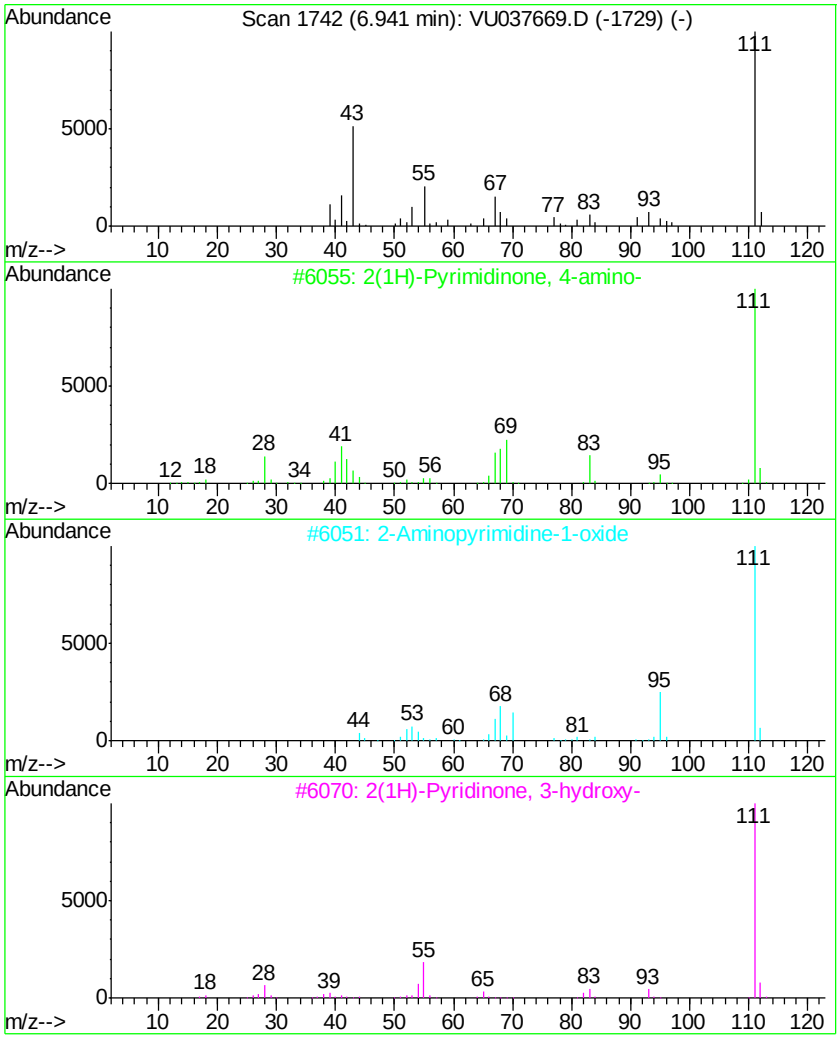
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

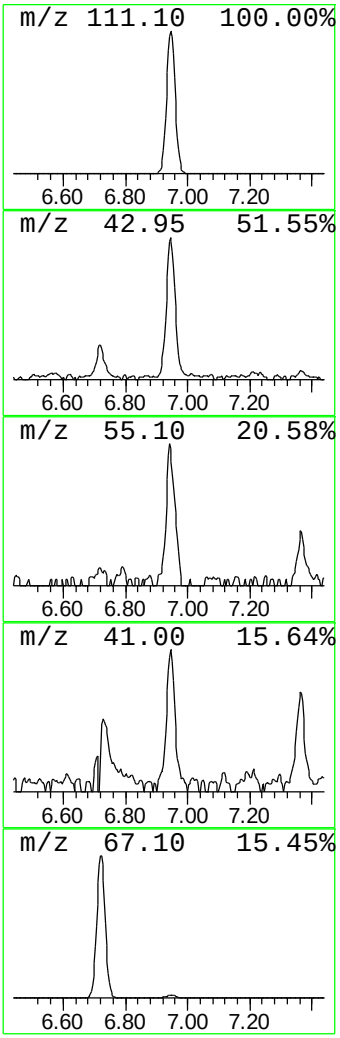
****

Peak Number 1 2(1H)-Pyrimidinone, 4-amino- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	2.64 ug/L	69346	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	59
2	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	56
3	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	53
4	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	45
5	Isocytosine	111	C4H5N3O	000108-53-2	42





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040920WMA.M
Quant Title : VOC Analysis

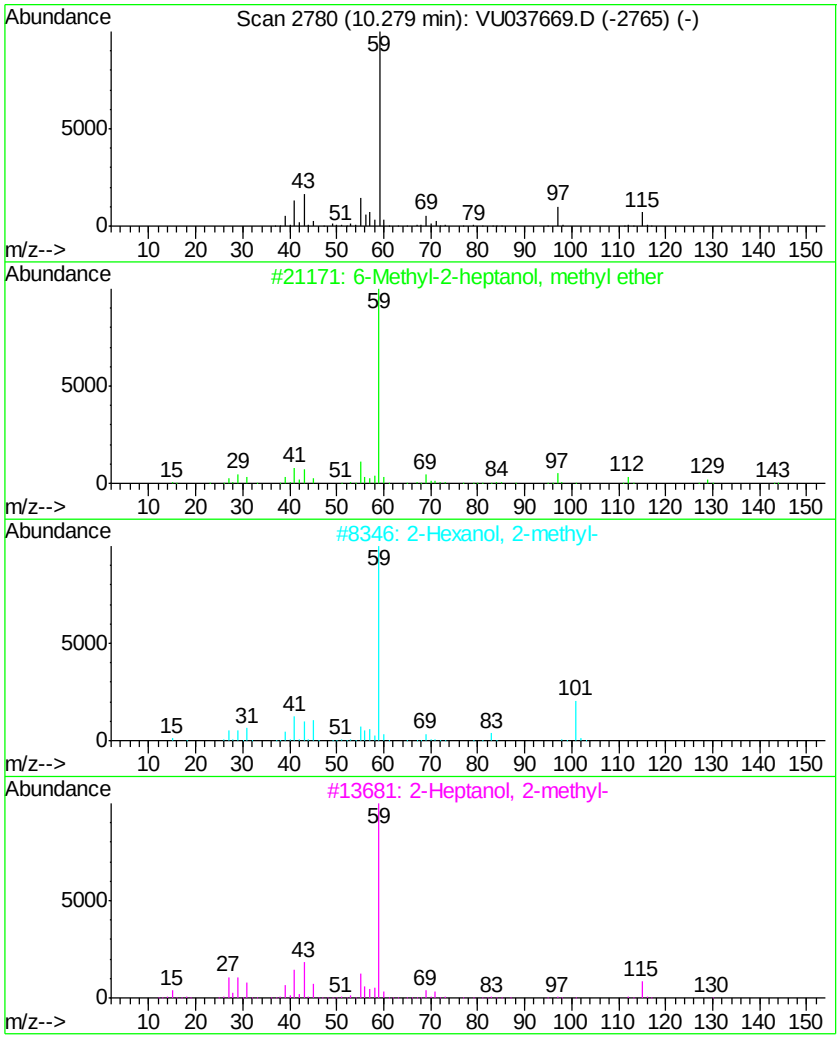
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

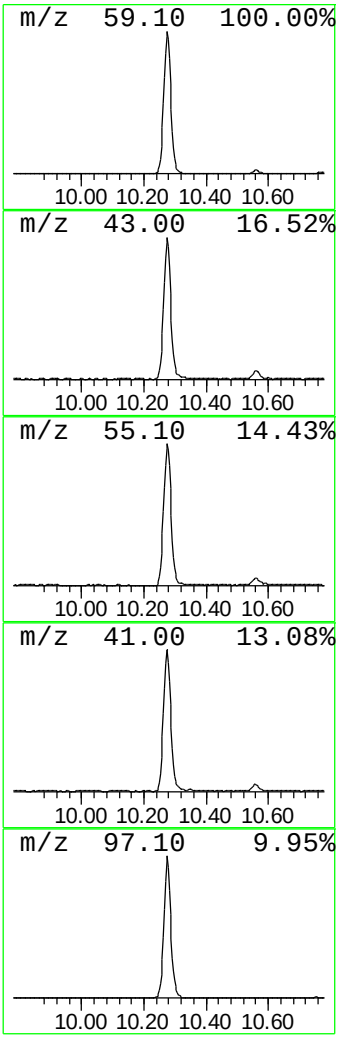
****

Peak Number 3 6-Methyl-2-heptanol, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	15.97 ug/L	520777	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	64
3	2-Heptanol, 2-methyl-	130	C8H18O	000625-25-2	64
4	2-Hexanol, methyl ether	116	C7H16O	1000333-92-0	50
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	50





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Quant Title : VOC Analysis

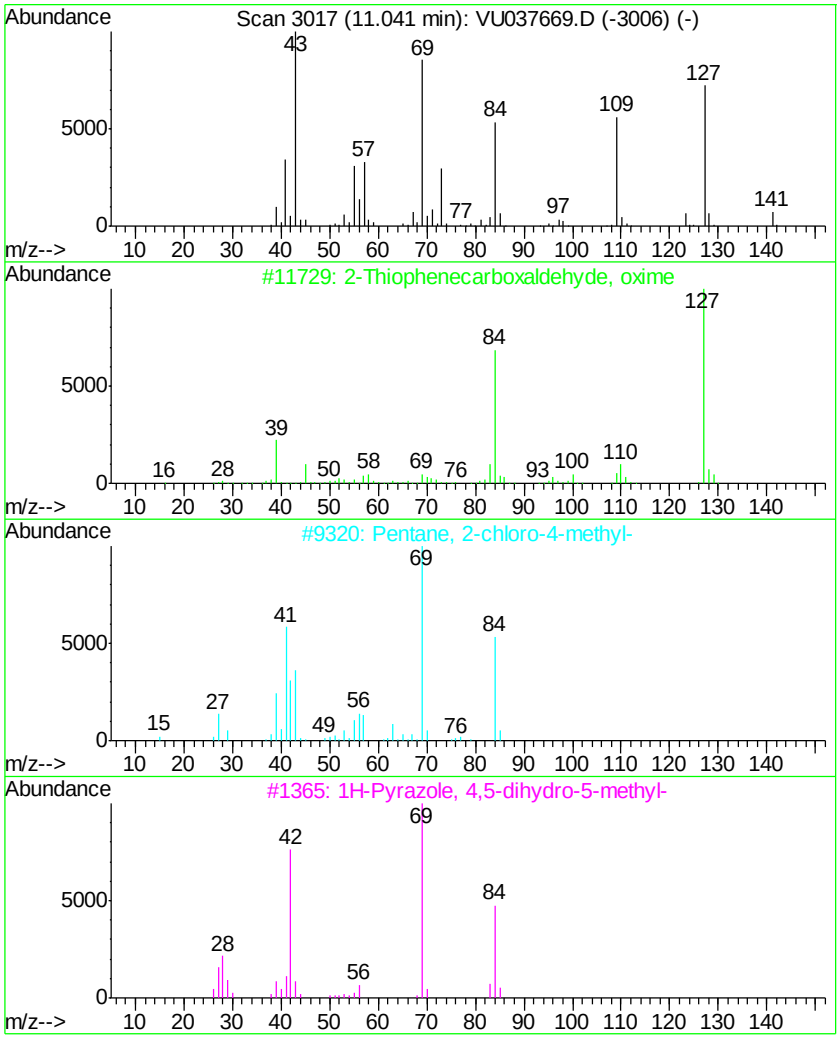
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

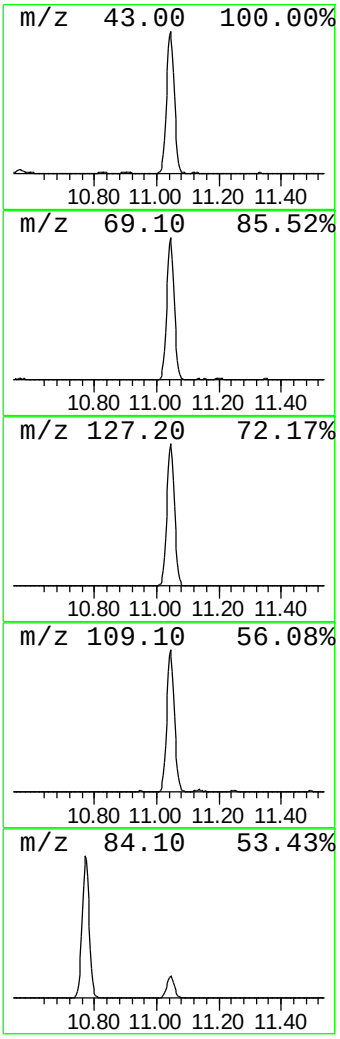
****

Peak Number 4 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	19.62 ug/L	629538	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	35
2	Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	27
3	1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	27
4	Formic acid, 4-methylpent-2-yl e...	130	C7H14O2	1000367-94-0	25
5	4-Piperidinone, 1,3-dimethyl-	127	C7H13NO	004629-80-5	22





Tentatively Identified Compound (LSC) summary

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Quant Title : VOC Analysis

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2(1H)-Pyrimidinon...	6.94	2.6	ug/L	69346	1	6.28	1312670	50.0
6-Methyl-2-heptan...	10.28	16.0	ug/L	520777	2	9.44	1630550	50.0
unknown-01	11.04	19.6	ug/L	629538	3	11.83	1604690	50.0