LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA V\Data\VV031020\
Data File : VV014822.D
Acq On : 10 Mar 2020 23:29
Operator : SY/MD
Sample : L1840-18
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DBET3

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\SOMVLM030620WMA.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	1.315	63	70	85	rVB	176526	190276	11.96%	1.335%
2	1.576	144	151	166	rVB	141778	177337	11.15%	1.245%
3	2.122	311	321	334	rBV	296791	429071	26.98%	3.011%
4	2.312	376	380	390	rVB5	1445	2007	0.13%	0.014%
5	2.367	393	397	400	rVB6	881	692	0.04%	0.005%
6	2.601	467	470	474	rBV3	794	718	0.05%	0.005%
7	2.913	562	567	570	rBV3	1077	729	0.05%	0.005%
8	2.984	581	589	596	rBV4	2910	5063	0.32%	0.036%
9	3.183	646	651	653	rBV3	957	831	0.05%	0.006%
10	3.367	705	708	712	rBV2	702	577	0.04%	0.004%
11	3.466	735	739	745	rVB2	552	682	0.04%	0.005%
12	3.521	745	756	757	rBV4	641	929	0.06%	0.007%
13	3.544	757	763	767	rBV3	969	1009	0.06%	0.007%
14	3.672	800	803	808	rBV3	884	799	0.05%	0.006%
15	3.740	814	824	842	rBV4	8272	22065	1.39%	0.155%
16	3.913	865	878	909	rBV	108729	324792	20.42%	2.280%
17	4.193	961	965	967	rBV4	700	629	0.04%	0.004%
18	4.241	974	980	981	rBV2	548	518	0.03%	0.004%
19	4.376	1004	1022	1047	rBV	255245	624655	39.27%	4.384%
20	4.527	1066	1069	1074	rBV4	880	572	0.04%	0.004%
21	4.640	1098	1104	1106	rBV4	884	727	0.05%	0.005%
22	4.749	1133	1138	1143	rBV6	794	876	0.06%	0.006%
23	5.074	1219	1239	1264	rBV2	631439	1590499	100.00%	11.163%
24	5.238	1288	1290	1292	rBV3	1076	603	0.04%	0.004%
25	5.386	1333	1336	1340	rBV4	716	639	0.04%	0.004%
26	5.643	1401	1416	1440	rBV	564063	1111873	69.91%	7.804%
27	5.826	1470	1473	1475	rVB3	873	540	0.03%	0.004%
28	5.910	1495	1499	1500	rBV2	980	654	0.04%	0.005%
29	6.006	1525	1529	1530	rBV2	1020	618	0.04%	0.004%
30	6.023	1532	1534	1538	rVV4	984	828	0.05%	0.006%
31	6.096	1539	1557	1580	rVV	356490	722008	45.40%	5.067%
32	6.219	1592	1595	1596	rBV2	990	609	0.04%	0.004%
33	6.379	1641	1645	1649	rBV5	698	784	0.05%	0.006%
34	6.556	1695	1700	1702	rBV3	680	574	0.04%	0.004%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA V\Data\VV031020\
Data File : VV014822.D
Acq On : 10 Mar 2020 23:29
Operator : SY/MD
Sample : L1840-18
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DBET3

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\SOMVLM030620WMA.M
Title : VOC Analysis

35	6.601	1705	1714	1715	rBV5	1794	1807	0.11%	0.013%
36	6.781	1767	1770	1774	rBV2	740	558	0.04%	0.004%
37	6.875	1795	1799	1803	rVB3	712	604	0.04%	0.004%
38	6.907	1803	1809	1812	rBV	484	585	0.04%	0.004%
39	7.010	1829	1841	1858	rBV	194344	342645	21.54%	2.405%
40	7.161	1883	1888	1891	rBV5	932	754	0.05%	0.005%
41	7.212	1902	1904	1907	rVB2	1111	680	0.04%	0.005%
42	7.235	1907	1911	1913	rBV3	1054	734	0.05%	0.005%
43	7.260	1913	1919	1924	rBV5	1300	1836	0.12%	0.013%
44	7.338	1930	1943	1964	rBV	790883	1361353	85.59%	9.555%
45	7.550	2007	2009	2013	rVB3	914	605	0.04%	0.004%
46	7.643	2026	2038	2057	rBV	135504	232702	14.63%	1.633%
47	7.958	2123	2136	2154	rVB4	7278	15074	0.95%	0.106%
48	8.029	2154	2158	2161	rBV2	798	707	0.04%	0.005%
49	8.113	2172	2184	2214	rBV	475441	856071	53.82%	6.008%
50	8.559	2320	2323	2326	rBV3	815	604	0.04%	0.004%
51	8.746	2377	2381	2388	rBV4	1281	1830	0.12%	0.013%
52	8.875	2403	2421	2443	rBV	850214	1374433	86.42%	9.647%
53	9.132	2496	2501	2503	rBV4	829	720	0.05%	0.005%
54	9.244	2526	2536	2547	rBV7	2215	5211	0.33%	0.037%
55	9.399	2579	2584	2585	rBV	731	559	0.04%	0.004%
56	9.572	2628	2638	2650	rBV8	3589	7785	0.49%	0.055%
57	9.627	2650	2655	2663	rVB6	1356	1537	0.10%	0.011%
58	9.707	2676	2680	2684	rBV3	636	654	0.04%	0.005%
59	9.826	2711	2717	2718	rBV3	1299	900	0.06%	0.006%
60	9.958	2750	2758	2760	rBV6	1490	2135	0.13%	0.015%
61	10.035	2777	2782	2786	rBV4	922	1150	0.07%	0.008%
62	10.238	2832	2845	2861	rBV	521524	813431	51.14%	5.709%
63	10.363	2871	2884	2888	rBV5	15094	22358	1.41%	0.157%
64	10.527	2930	2935	2936	rBV3	2418	1875	0.12%	0.013%
65	10.601	2955	2958	2961	rBV4	947	538	0.03%	0.004%
66	10.659	2971	2976	2977	rBV2	1067	862	0.05%	0.006%
67	10.727	2994	2997	3000	rBV3	1032	874	0.05%	0.006%
68	10.755	3000	3006	3016	rVV2	5788	9126	0.57%	0.064%
69	10.881	3040	3045	3050	rBV5	1227	1674	0.11%	0.012%
70	10.936	3054	3062	3071	rVV4	9999	14732	0.93%	0.103%
71	11.055	3089	3099	3112	rBV9	4291	11035	0.69%	0.077%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA V\Data\VV031020\
Data File : VV014822.D
Acq On : 10 Mar 2020 23:29
Operator : SY/MD
Sample : L1840-18
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DBET3

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\SOMVLM030620WMA.M
Title : VOC Analysis

72	11.215	3143	3149	3151	rBV6	3633	3667	0.23%	0.026%
73	11.267	3154	3165	3186	rVV	901054	1393371	87.61%	9.780%
74	11.357	3186	3193	3207	rVB3	11586	19263	1.21%	0.135%
75	11.424	3207	3214	3236	rBV4	7476	19855	1.25%	0.139%
76	11.553	3245	3254	3270	rVB2	36254	66055	4.15%	0.464%
77	11.643	3271	3282	3301	rBV	824541	1293564	81.33%	9.079%
78	11.839	3336	3343	3348	rBV7	4680	7979	0.50%	0.056%
79	11.942	3363	3375	3388	rBV2	61074	117131	7.36%	0.822%
80	12.035	3398	3404	3416	rVB8	6267	10658	0.67%	0.075%
81	12.308	3482	3489	3496	rBV2	6676	10301	0.65%	0.072%
82	12.482	3535	3543	3551	rBV4	17856	26027	1.64%	0.183%
83	12.800	3636	3642	3655	rVB7	13530	23778	1.50%	0.167%
84	12.861	3655	3661	3663	rBV7	3658	4026	0.25%	0.028%
85	12.955	3685	3690	3700	rVB8	6485	9771	0.61%	0.069%
86	13.087	3718	3731	3738	rBV4	11819	24547	1.54%	0.172%
87	13.437	3823	3840	3848	rBV3	37181	82061	5.16%	0.576%
88	13.636	3888	3902	3907	rBV3	12177	32210	2.03%	0.226%
89	13.771	3936	3944	3953	rVB4	23148	36784	2.31%	0.258%
90	13.829	3953	3962	3980	rVB4	44279	88842	5.59%	0.624%
91	14.160	4059	4065	4073	rVB3	12423	15849	1.00%	0.111%
92	14.402	4134	4140	4149	rVB3	15873	22468	1.41%	0.158%
93	14.627	4201	4210	4227	rBV2	151772	269151	16.92%	1.889%
94	14.845	4264	4278	4287	rBV3	74634	156498	9.84%	1.098%
95	14.974	4313	4318	4322	rBV4	8215	11516	0.72%	0.081%
96	15.093	4348	4355	4361	rBV2	34806	52322	3.29%	0.367%
97	15.186	4379	4384	4393	rBV2	15393	22860	1.44%	0.160%
98	15.241	4396	4401	4415	rVB2	24569	42167	2.65%	0.296%
99	15.427	4453	4459	4474	rVB7	15914	29166	1.83%	0.205%
100	15.826	4574	4583	4591	rBV8	26133	49427	3.11%	0.347%

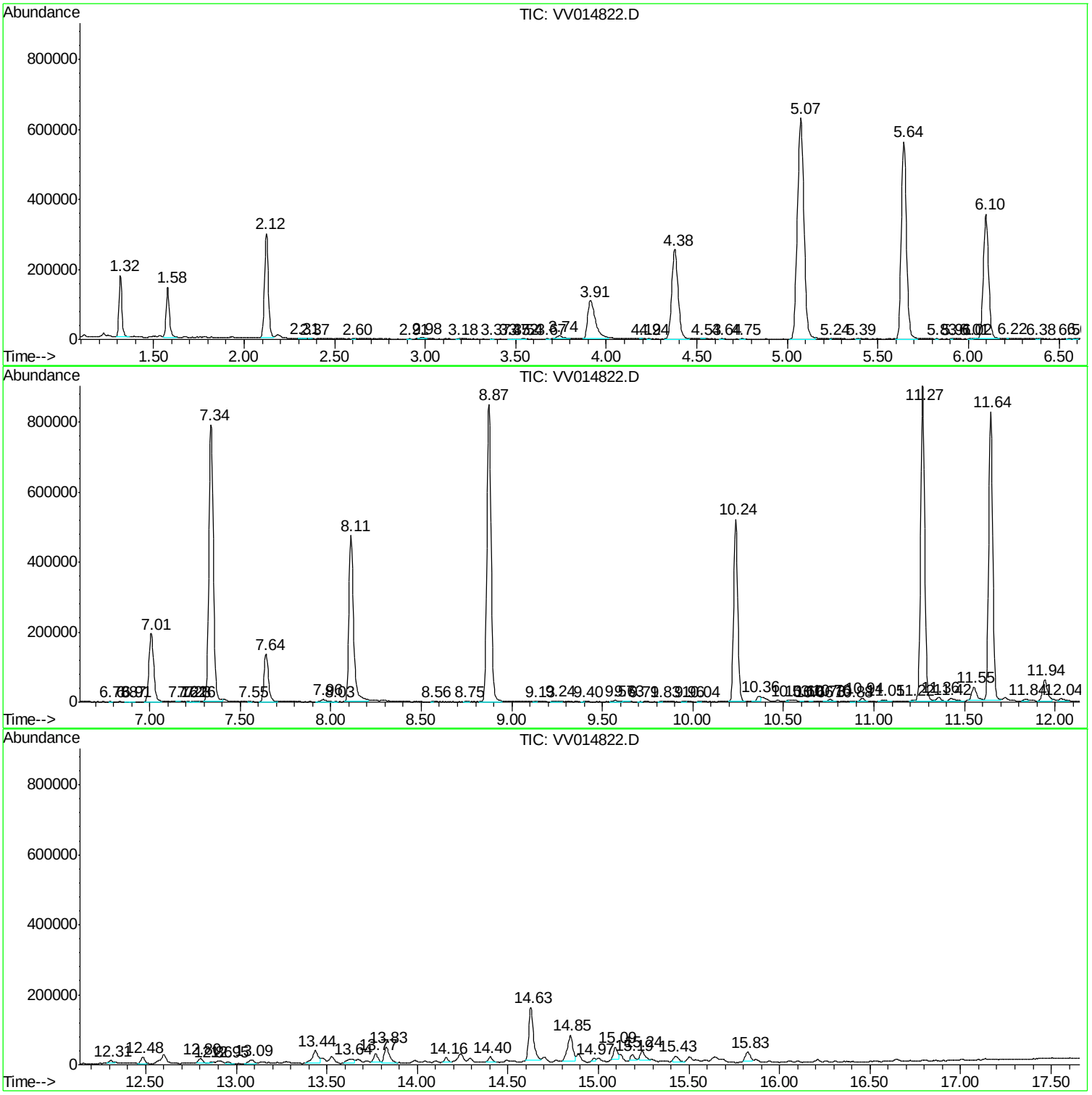
Sum of corrected areas: 14247835

Data Path : Z:\voasrv\HPCHEM1\MSVOA V\Data\VV031020\
Data File : VV014822.D
Acq On : 10 Mar 2020 23:29
Operator : SY/MD
Sample : L1840-18
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DBET3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM030620WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA V\Data\VV031020\
Data File : VV014822.D
Acq On : 10 Mar 2020 23:29
Operator : SY/MD
Sample : L1840-18
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DBET3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM030620WMA.M
Quant Title : VOC Analysis

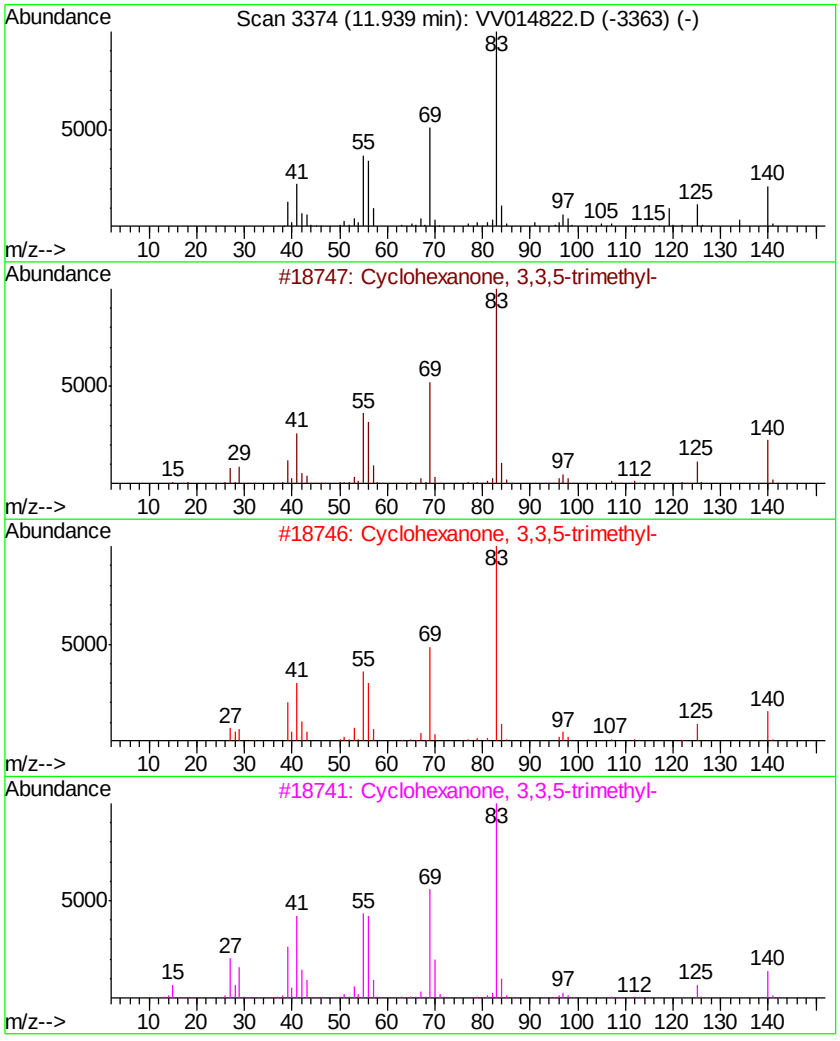
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

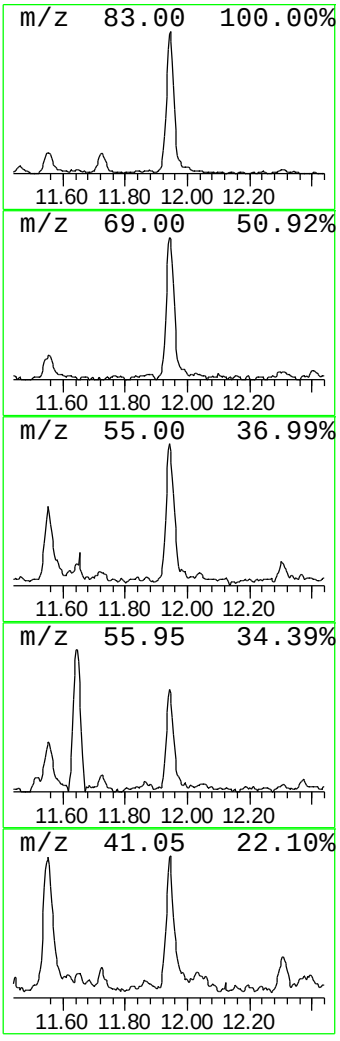
****

Peak Number 2 Cyclohexanone, 3,3,5-trimet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	4.20 ug/L	117131	1,4-Dichlorobenzene-d4	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	96
2	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	94
3	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
4	Cyclohexane, butyl-	140	C10H20	001678-93-9	59
5	Cyclohexane, butyl-	140	C10H20	001678-93-9	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA V\Data\VV031020\
Data File : VV014822.D
Acq On : 10 Mar 2020 23:29
Operator : SY/MD
Sample : L1840-18
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DBET3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM030620WMA.M
Quant Title : VOC Analysis

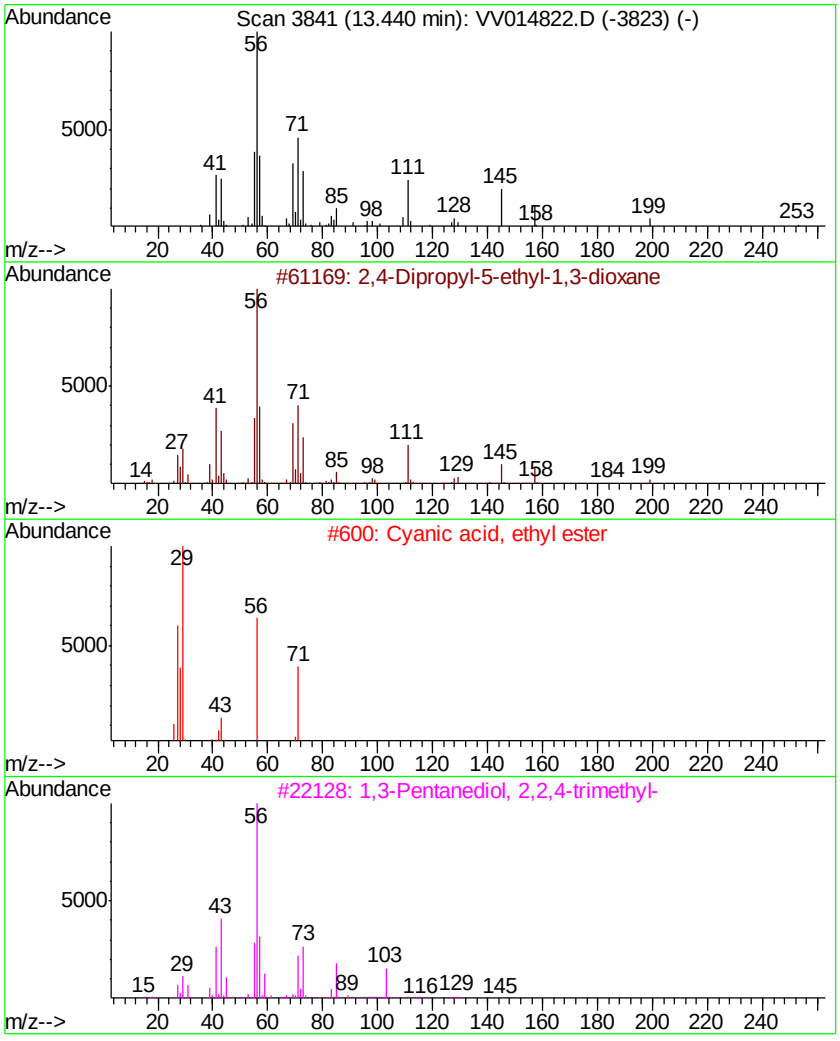
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

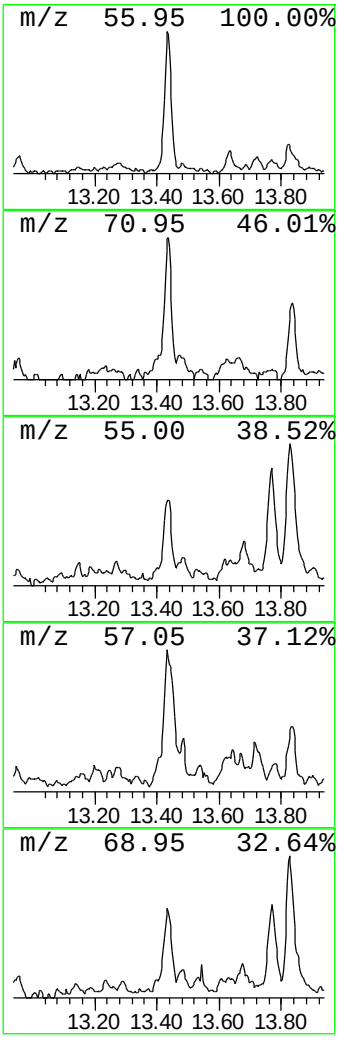
****

Peak Number 3 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	2.94 ug/L	82061	1,4-Dichlorobenzene-d4	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	86
2	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	38
3	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	28
4	1-Heptene, 2,6-dimethyl-	126	C9H18	003074-78-0	27
5	1-Octene, 2-methyl-	126	C9H18	004588-18-5	27





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA V\Data\VV031020\
Data File : VV014822.D
Acq On : 10 Mar 2020 23:29
Operator : SY/MD
Sample : L1840-18
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DBET3

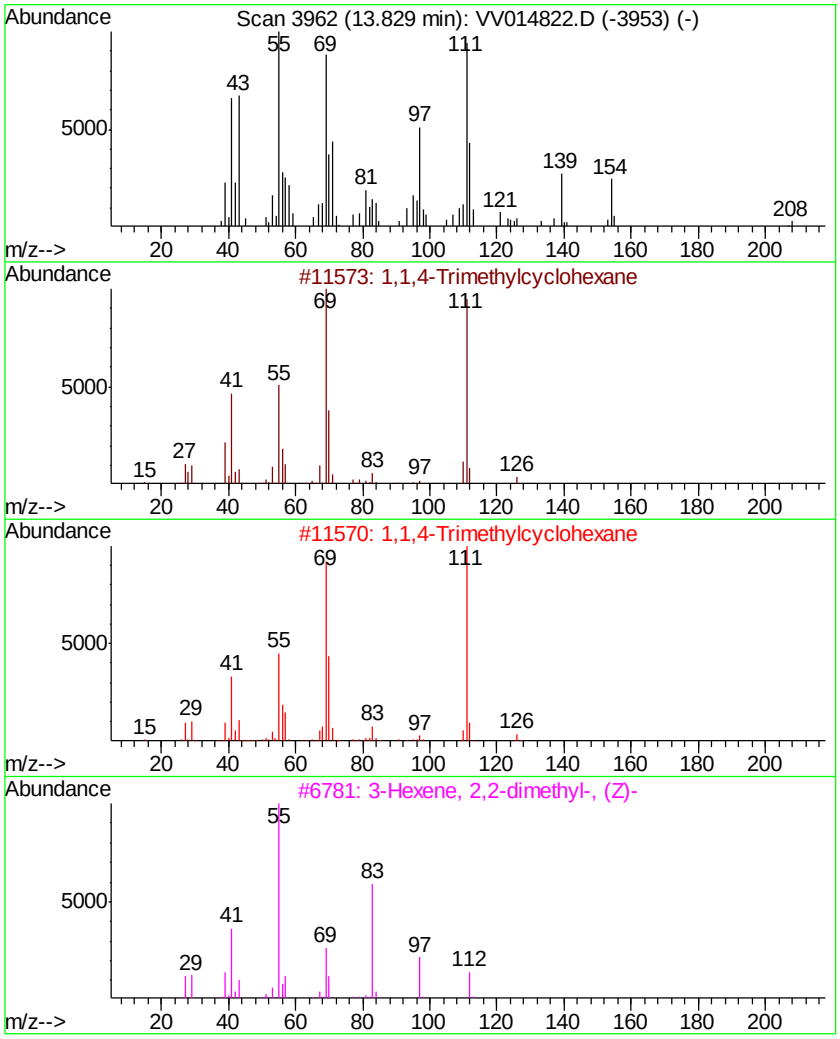
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM030620WMA.M
Quant Title : VOC Analysis

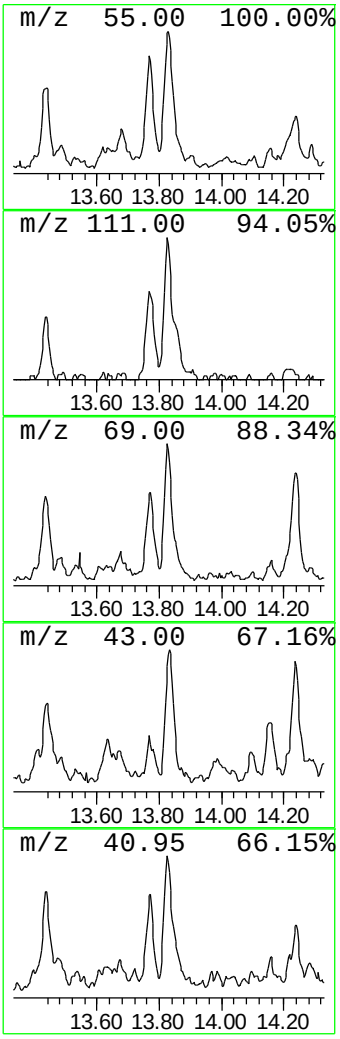
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.19 ug/L	88842	1,4-Dichlorobenzene-d4	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	43
2	1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	43
3	3-Hexene, 2,2-dimethyl-, (Z)-	112	C8H16	000690-92-6	38
4	3-Heptene, 4-methyl-	112	C8H16	004485-16-9	38
5	2-Furanone, 2,5-dihydro-3,5-dime...	112	C6H8O2	1000196-88-1	27





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA V\Data\VV031020\
Data File : VV014822.D
Acq On : 10 Mar 2020 23:29
Operator : SY/MD
Sample : L1840-18
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DBET3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM030620WMA.M
Quant Title : VOC Analysis

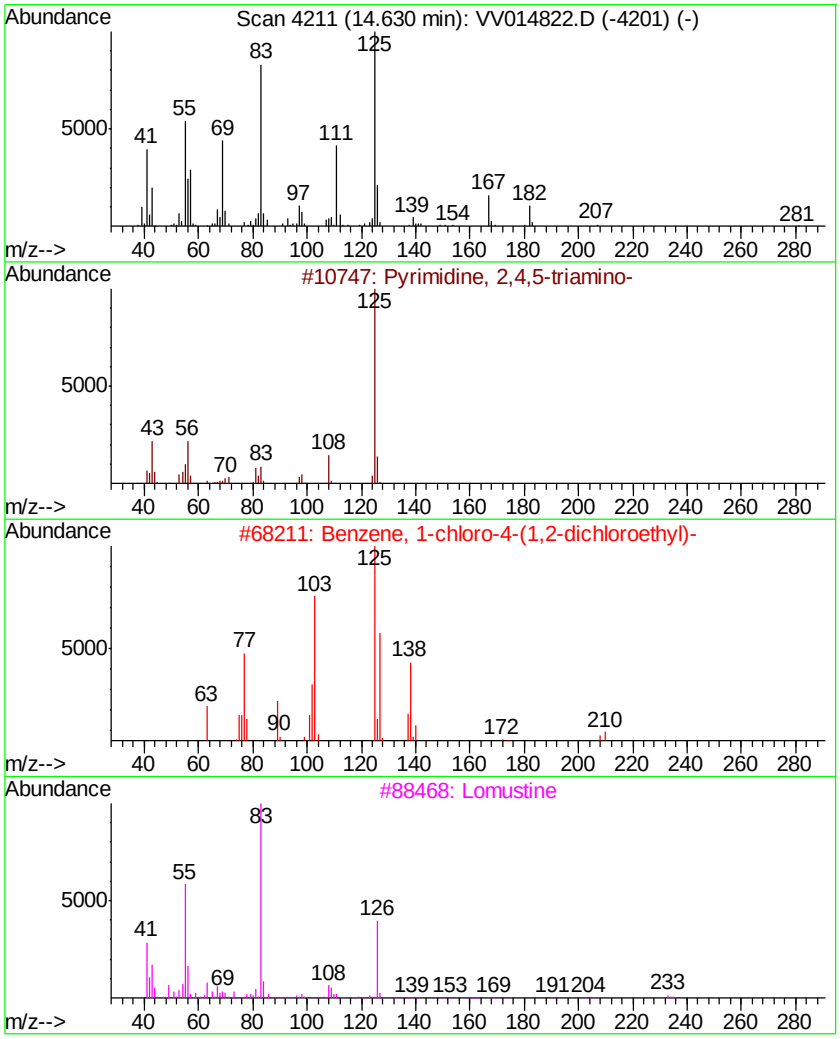
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

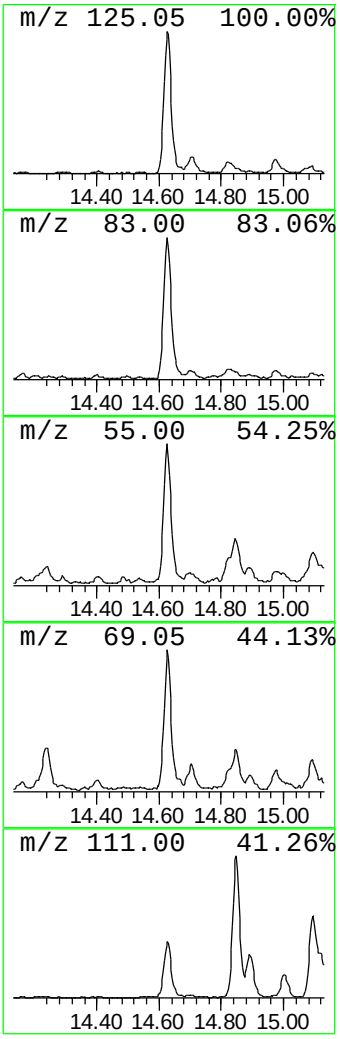
****

Peak Number 5 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	9.66 ug/L	269151	1,4-Dichlorobenzene-d4	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrimidine, 2,4,5-triamino-	125	C4H7N5	003546-50-7	35
2	Benzene, 1-chloro-4-(1,2-dichlor...	208	C8H7Cl3	074298-94-5	30
3	Lomustine	233	C9H16ClN3O2	013010-47-4	27
4	Cyclohexanecarboxylic acid, (1H-...	195	C8H13N5O	1000310-78-1	27
5	Cyclohexanecarboxylic acid, 4-cy...	229	C14H15NO2	1000307-70-6	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA V\Data\VV031020\
Data File : VV014822.D
Acq On : 10 Mar 2020 23:29
Operator : SY/MD
Sample : L1840-18
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DBET3

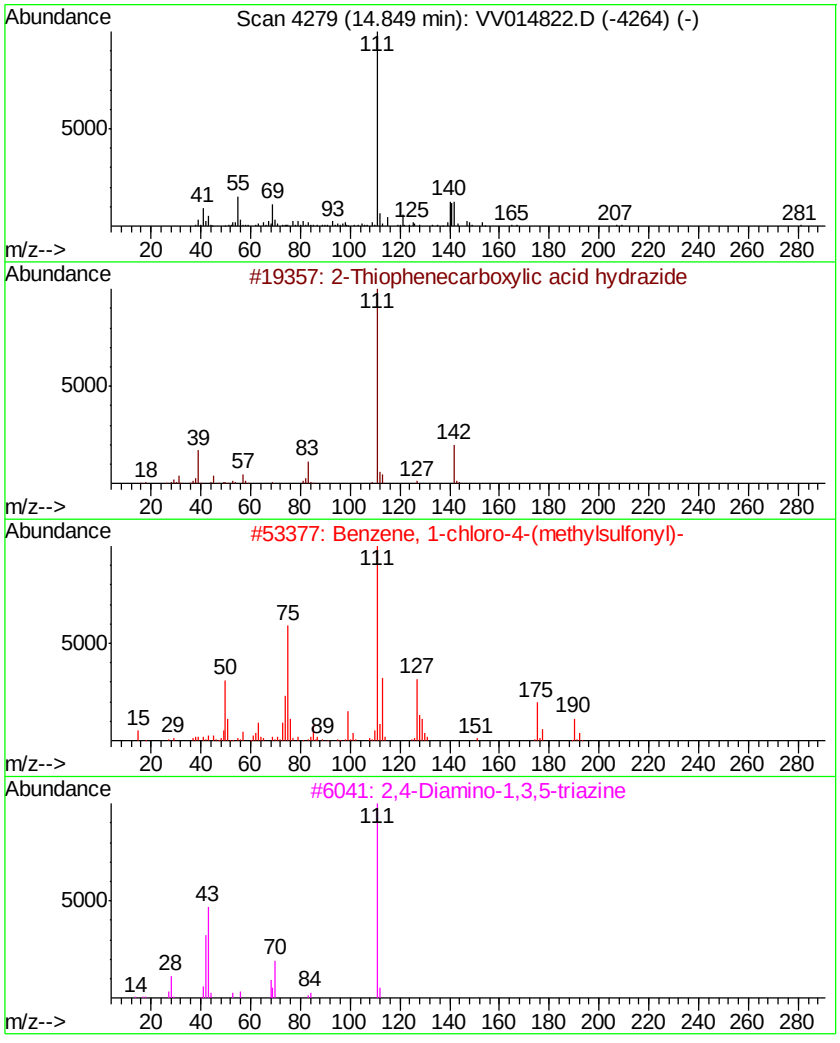
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM030620WMA.M
Quant Title : VOC Analysis

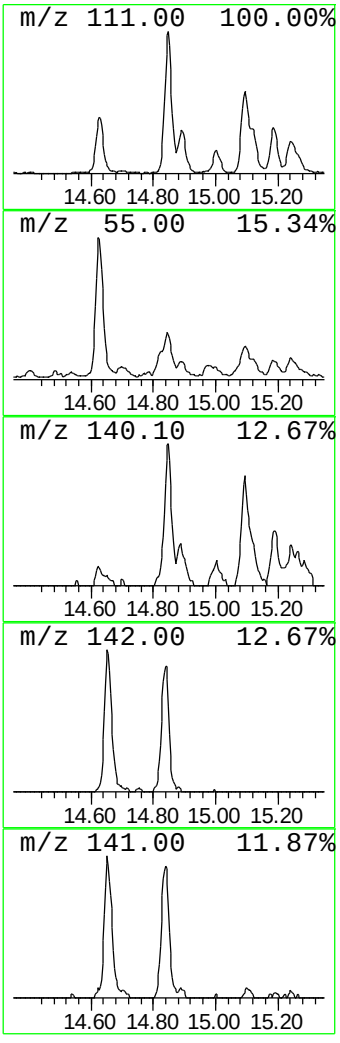
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Thiophenecarboxylic acid ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	5.62 ug/L	156498	1,4-Dichlorobenzene-d4	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiophenecarboxylic acid hydra...	142	C5H6N2OS	002361-27-5	53
2	Benzene, 1-chloro-4-(methylsulfo...	190	C7H7ClO2S	000098-57-7	46
3	2,4-Diamino-1,3,5-triazine	111	C3H5N5	000504-08-5	40
4	2-Thiophenecarboxylic acid hydra...	142	C5H6N2OS	002361-27-5	40
5	Ethylphosphonic acid, di(2-ethyl...	334	C18H39O3P	101883-26-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV031020\
Data File : VV014822.D
Acq On : 10 Mar 2020 23:29
Operator : SY/MD
Sample : L1840-18
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DBET3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM030620WMA.M
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
Cyclohexanone, 3,...	11.94	4.2	ug/L	117131	3	11.27	1393370	50.0
2,4-Dipropyl-5-et...	13.44	2.9	ug/L	82061	3	11.27	1393370	50.0
(DEL) Alkane: Str...	13.83	3.2	ug/L	88842	3	11.27	1393370	50.0
unknown-01	14.63	9.7	ug/L	269151	3	11.27	1393370	50.0
2-Thiophenecarbox...	14.85	5.6	ug/L	156498	3	11.27	1393370	50.0