LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
Data File : VU033927.D
Acq On : 23 Aug 2019 02:10
Operator : JC/SP
Sample : K4485-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F2B75

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\SOMULM082219WMA.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	1.174	22	26	29	rBV2	7988	7879	0.32%	0.032%
2	1.286	54	61	70	rBV2	15512	26507	1.07%	0.106%
3	1.389	85	93	103	rBV	367635	383574	15.53%	1.534%
4	1.547	138	142	160	rVB2	27403	35783	1.45%	0.143%
5	1.633	164	169	172	rVV	17365	18318	0.74%	0.073%
6	1.666	172	179	197	rVB	276689	350322	14.18%	1.401%
7	1.871	238	243	256	rVB6	8467	14336	0.58%	0.057%
8	1.932	256	262	268	rBV6	6086	8372	0.34%	0.033%
9	2.113	308	318	330	rVB	95412	135792	5.50%	0.543%
10	2.174	332	337	345	rVB	7307	8509	0.34%	0.034%
11	2.254	351	362	370	rBV	562374	850006	34.41%	3.400%
12	2.302	370	377	386	rVV	433701	664978	26.92%	2.660%
13	2.360	386	395	408	rVB	809547	1253346	50.74%	5.013%
14	2.428	408	416	422	rBV2	27189	42316	1.71%	0.169%
15	2.601	460	470	482	rVB2	6266	11502	0.47%	0.046%
16	2.682	491	495	504	rVB6	2270	3611	0.15%	0.014%
17	2.813	528	536	545	rVV8	2030	4425	0.18%	0.018%
18	2.961	573	582	594	rVB5	2721	5245	0.21%	0.021%
19	3.781	828	837	839	rBV3	1955	2854	0.12%	0.011%
20	4.093	923	934	935	rBV5	2543	3179	0.13%	0.013%
21	4.148	939	951	972	rBV	234829	672612	27.23%	2.690%
22	4.620	1075	1098	1124	rVV	408607	970719	39.30%	3.882%
23	4.710	1124	1126	1133	rVV5	1313	1395	0.06%	0.006%
24	4.810	1151	1157	1158	rBV2	2016	2045	0.08%	0.008%
25	4.968	1200	1206	1211	rVV7	1276	1675	0.07%	0.007%
26	5.315	1290	1314	1353	rBV2	827196	2470148	100.00%	9.880%
27	5.575	1392	1395	1398	rVV3	1333	1192	0.05%	0.005%
28	5.620	1398	1409	1425	rVB4	9143	22225	0.90%	0.089%
29	5.768	1445	1455	1471	rBV2	10241	24335	0.99%	0.097%
30	5.862	1471	1484	1516	rBV	704687	1401188	56.72%	5.604%
31	6.164	1565	1578	1599	rBV5	41240	89182	3.61%	0.357%
32	6.309	1606	1623	1641	rBV	564994	1142902	46.27%	4.571%
33	6.399	1641	1651	1672	rVV	207367	425462	17.22%	1.702%
34	6.482	1674	1677	1689	rVV	11824	22608	0.92%	0.090%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
Data File : VU033927.D
Acq On : 23 Aug 2019 02:10
Operator : JC/SP
Sample : K4485-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F2B75

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\SOMULM082219WMA.M
Title : VOC Analysis

35	6.556	1689	1700	1729	rVB	240526	462582	18.73%	1.850%
36	6.765	1755	1765	1769	rBV2	9826	16857	0.68%	0.067%
37	7.209	1890	1903	1930	rBV	277602	521633	21.12%	2.086%
38	7.321	1930	1938	1945	rVB7	4142	7213	0.29%	0.029%
39	7.447	1967	1977	1991	rBV	16753	29776	1.21%	0.119%
40	7.546	1994	2008	2023	rBV	1081678	1918498	77.67%	7.673%
41	7.617	2023	2030	2052	rVB	104708	204556	8.28%	0.818%
42	7.829	2084	2096	2116	rBV	204179	361110	14.62%	1.444%
43	8.074	2164	2172	2181	rBV9	1428	2367	0.10%	0.009%
44	8.148	2189	2195	2198	rBV5	2220	3190	0.13%	0.013%
45	8.209	2204	2214	2229	rBV5	37721	71479	2.89%	0.286%
46	8.292	2229	2240	2252	rBV	787181	1362565	55.16%	5.450%
47	8.347	2253	2257	2275	rVB	109160	186243	7.54%	0.745%
48	8.579	2326	2329	2347	rVB	2880	5990	0.24%	0.024%
49	8.665	2349	2356	2367	rVB6	3081	5091	0.21%	0.020%
50	8.778	2383	2391	2395	rVV6	1526	1872	0.08%	0.007%
51	8.826	2402	2406	2413	rVB6	1359	1694	0.07%	0.007%
52	8.890	2422	2426	2432	rVB6	1256	1039	0.04%	0.004%
53	8.926	2432	2437	2441	rBV6	1709	2169	0.09%	0.009%
54	9.070	2460	2482	2505	rBV	1074450	1842772	74.60%	7.370%
55	9.167	2505	2512	2526	rVV3	20424	46576	1.89%	0.186%
56	9.234	2526	2533	2541	rVB2	8991	14880	0.60%	0.060%
57	9.328	2551	2562	2564	rBV6	8217	14969	0.61%	0.060%
58	9.360	2565	2572	2583	rVB	28469	48445	1.96%	0.194%
59	9.572	2631	2638	2640	rBV4	1718	1735	0.07%	0.007%
60	9.591	2641	2644	2648	rVV3	1100	1144	0.05%	0.005%
61	9.681	2662	2672	2688	rBV4	29228	65888	2.67%	0.264%
62	9.765	2689	2698	2706	rBV2	16895	31595	1.28%	0.126%
63	9.903	2730	2741	2766	rBV	300535	512464	20.75%	2.050%
64	10.041	2776	2784	2807	rVB2	47279	94058	3.81%	0.376%
65	10.138	2807	2814	2832	rVB5	13340	24366	0.99%	0.097%
66	10.218	2836	2839	2844	rVB4	1897	1501	0.06%	0.006%
67	10.292	2858	2862	2863	rBV4	1403	1035	0.04%	0.004%
68	10.414	2887	2900	2919	rBV	791073	1269818	51.41%	5.079%
69	10.482	2919	2921	2928	rVB4	1266	972	0.04%	0.004%
70	10.559	2929	2945	2959	rBV7	26958	76005	3.08%	0.304%
71	10.665	2972	2978	2993	rVB2	12666	21349	0.86%	0.085%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
Data File : VU033927.D
Acq On : 23 Aug 2019 02:10
Operator : JC/SP
Sample : K4485-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F2B75

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\SOMULM082219WMA.M
Title : VOC Analysis

72	10.755	3002	3006	3011	rVB5	3260	2939	0.12%	0.012%
73	10.791	3011	3017	3023	rBV6	2589	3441	0.14%	0.014%
74	10.894	3043	3049	3052	rBV6	1694	1988	0.08%	0.008%
75	10.932	3052	3061	3076	rVB3	10742	22481	0.91%	0.090%
76	11.012	3079	3086	3090	rBV7	4027	5933	0.24%	0.024%
77	11.099	3105	3113	3116	rBV2	41274	53783	2.18%	0.215%
78	11.138	3117	3125	3138	rVV	467630	722141	29.23%	2.888%
79	11.196	3139	3143	3149	rVV4	26908	39234	1.59%	0.157%
80	11.241	3149	3157	3180	rVV2	143925	351757	14.24%	1.407%
81	11.337	3181	3187	3203	rVB4	16699	36548	1.48%	0.146%
82	11.466	3215	3227	3246	rVV	1075012	1674722	67.80%	6.698%
83	11.553	3250	3254	3263	rVB5	4829	6863	0.28%	0.027%
84	11.620	3269	3275	3295	rVB8	18626	37501	1.52%	0.150%
85	11.749	3305	3315	3324	rBV4	23002	49856	2.02%	0.199%
86	11.842	3332	3344	3363	rBV	999929	1605505	65.00%	6.421%
87	12.135	3426	3435	3444	rVB8	6766	11444	0.46%	0.046%
88	12.189	3444	3452	3456	rBV9	3554	6093	0.25%	0.024%
89	12.305	3483	3488	3491	rBV6	1296	1426	0.06%	0.006%
90	12.356	3502	3504	3510	rBV7	1680	1370	0.06%	0.005%
91	12.450	3523	3533	3545	rBV2	18391	39897	1.62%	0.160%
92	12.942	3676	3686	3687	rBV4	2463	3697	0.15%	0.015%
93	13.106	3731	3737	3739	rBV6	1461	1613	0.07%	0.006%
94	13.125	3740	3743	3744	rBV3	1621	955	0.04%	0.004%
95	13.289	3789	3794	3799	rBV8	1331	1764	0.07%	0.007%
96	13.373	3816	3820	3825	rBV5	884	867	0.04%	0.003%
97	14.012	4015	4019	4025	rVB6	1325	1373	0.06%	0.005%
98	14.655	4216	4219	4226	rBV6	734	834	0.03%	0.003%
99	15.083	4348	4352	4356	rVB5	1110	1015	0.04%	0.004%
100	15.112	4356	4361	4364	rBV5	1418	1369	0.06%	0.005%

Sum of corrected areas: 25002447

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
Data File : VU033927.D
Acq On : 23 Aug 2019 02:10
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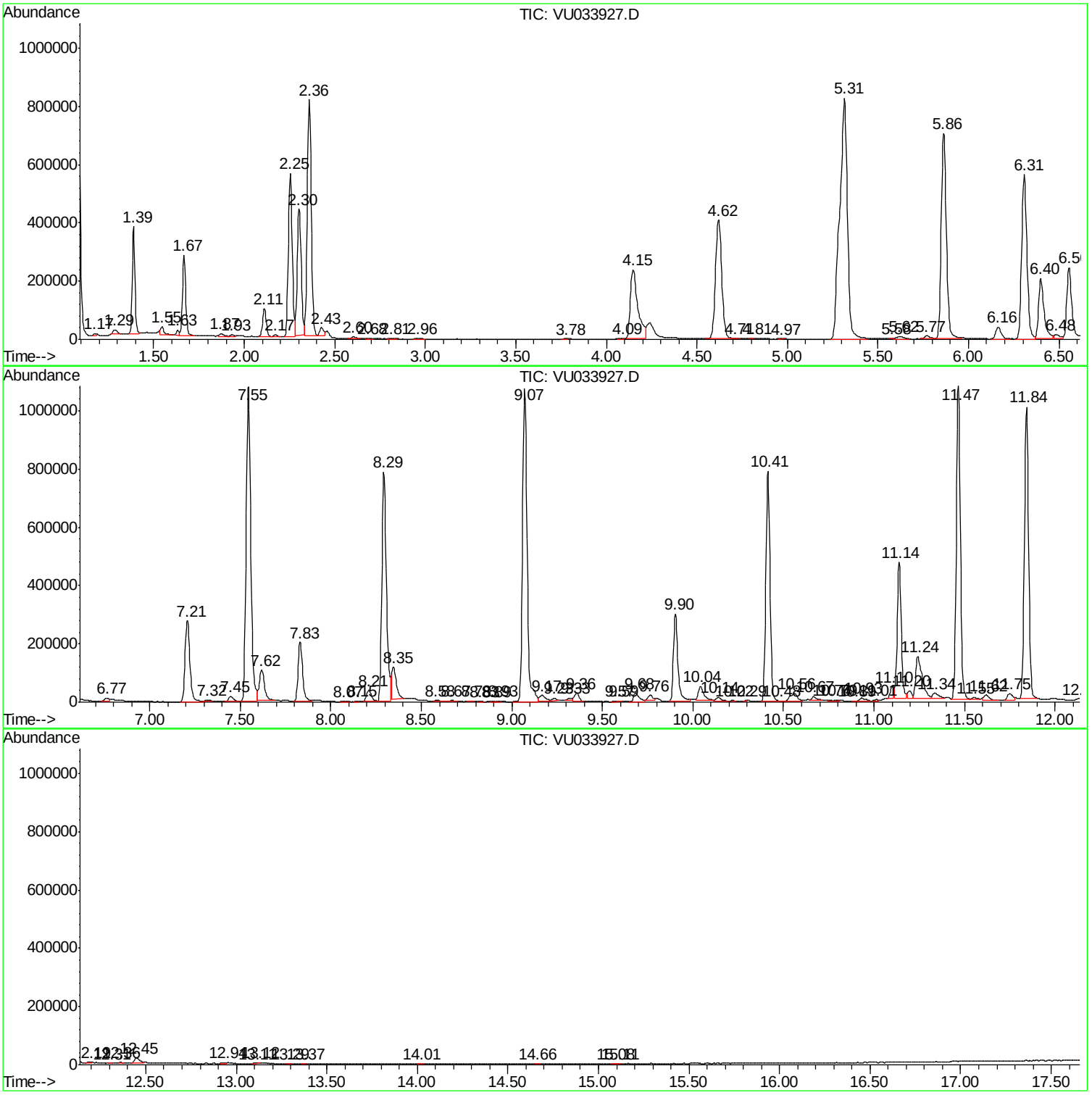
Sample : K4485-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F2B75

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
Data File : VU033927.D
Acq On : 23 Aug 2019 02:10
Operator : JC/SP
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ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F2B75

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

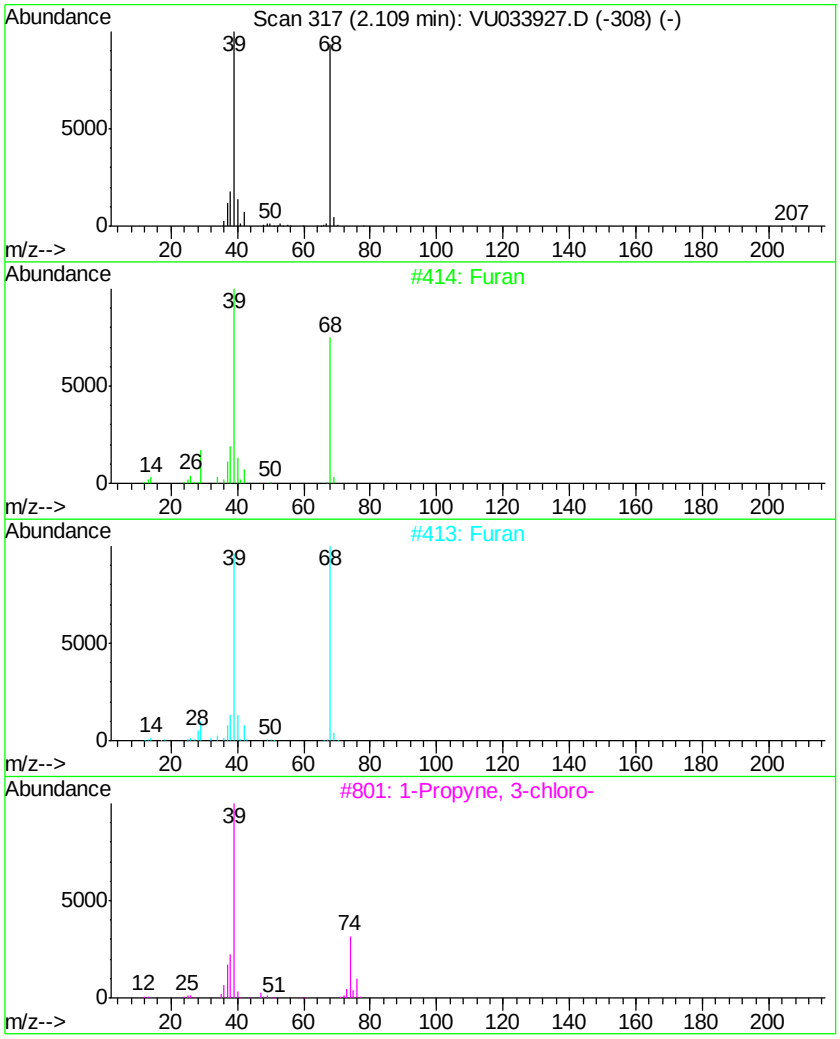
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

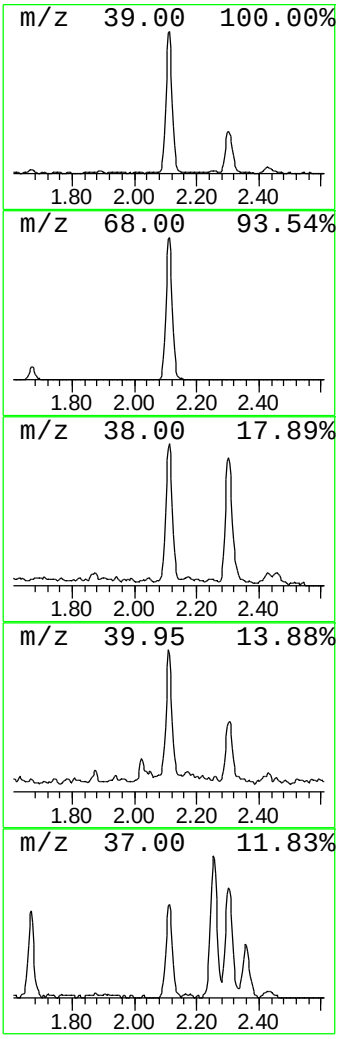
****

Peak Number 1 Furan Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.11	4.85 ug/L	135792	1,4-Difluorobenzene	5.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan	68	C4H4O	000110-00-9	91
2	Furan	68	C4H4O	000110-00-9	90
3	1-Propyne, 3-chloro-	74	C3H3Cl	000624-65-7	39
4	1H-Imidazole	68	C3H4N2	000288-32-4	9
5	1-Propyne, 3-chloro-	74	C3H3Cl	000624-65-7	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU082219\
Data File : VU033927.D
Acq On : 23 Aug 2019 02:10
Operator : JC/SP
Sample : K4485-09
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F2B75

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

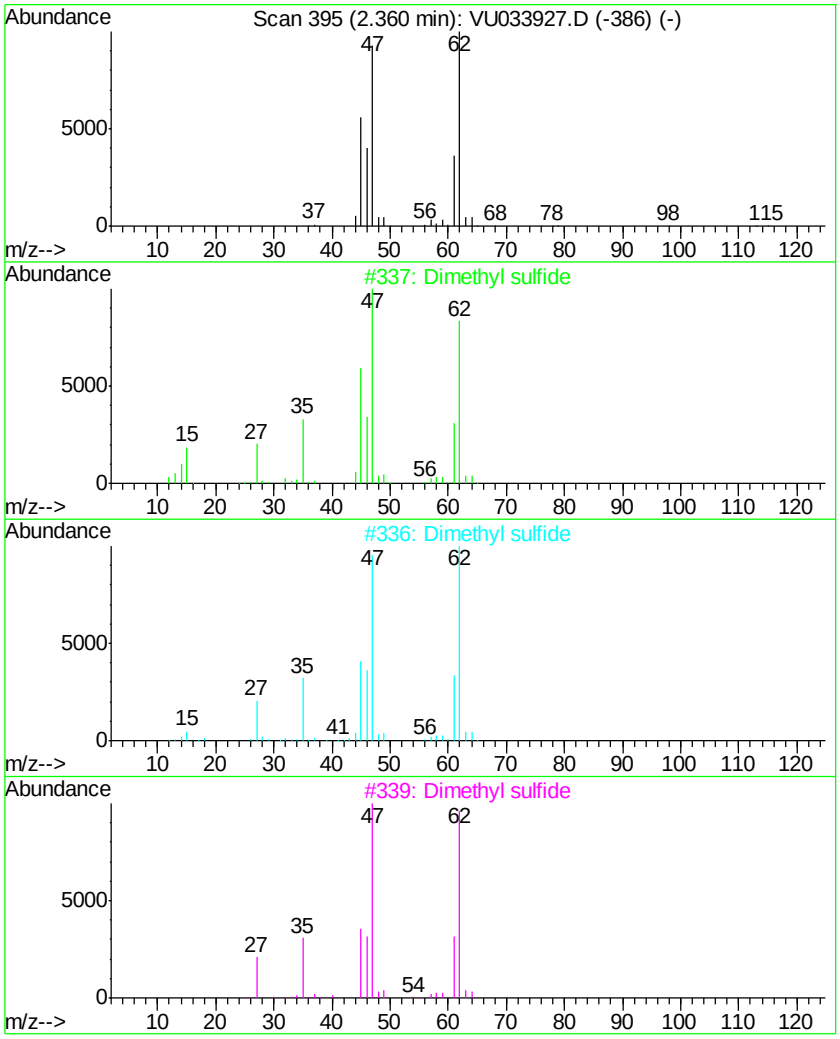
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

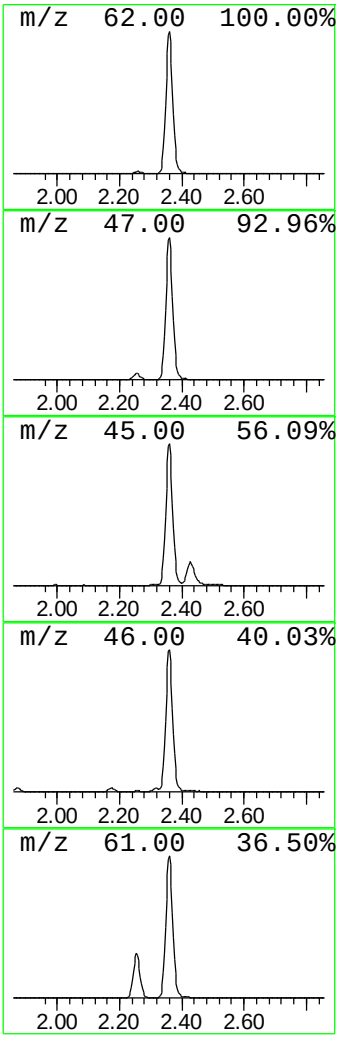
****

Peak Number 2 Dimethyl sulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.36	44.72 ug/L	1253350	1,4-Difluorobenzene	5.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl sulfide	62	C2H6S	000075-18-3	94
2	Dimethyl sulfide	62	C2H6S	000075-18-3	94
3	Dimethyl sulfide	62	C2H6S	000075-18-3	91
4	Dimethyl sulfide	62	C2H6S	000075-18-3	91
5	Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
Data File : VU033927.D
Acq On : 23 Aug 2019 02:10
Operator : JC/SP
Sample : K4485-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F2B75

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

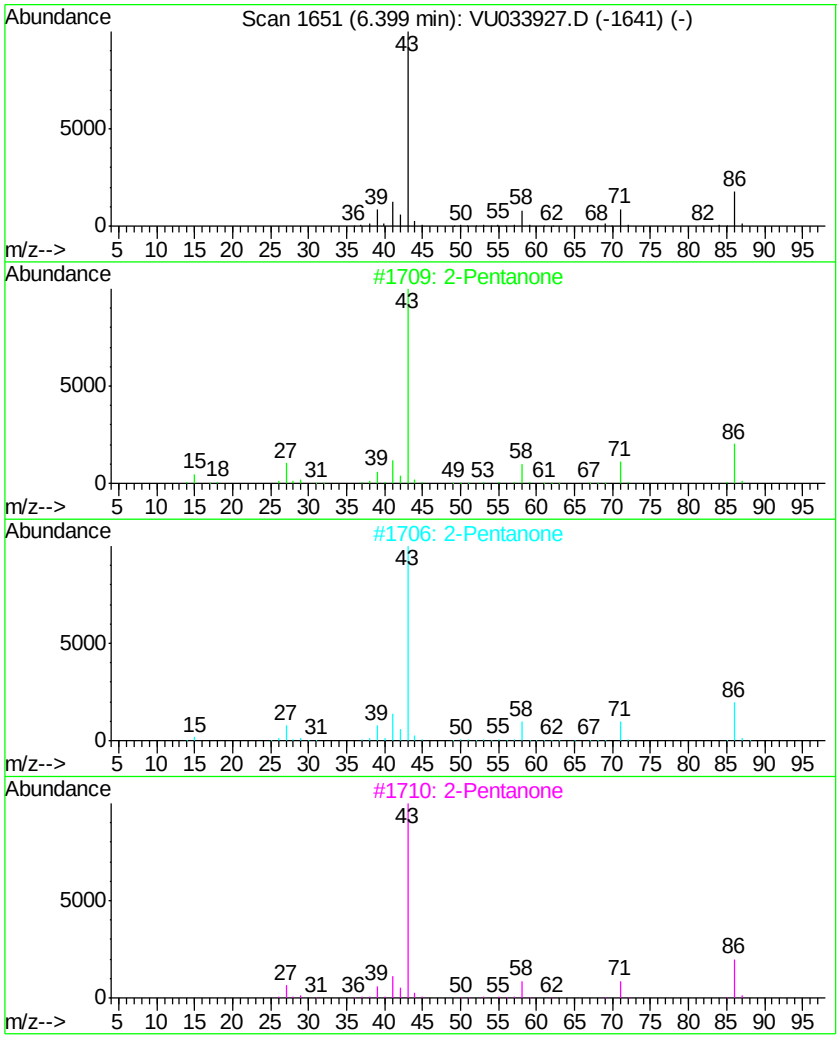
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

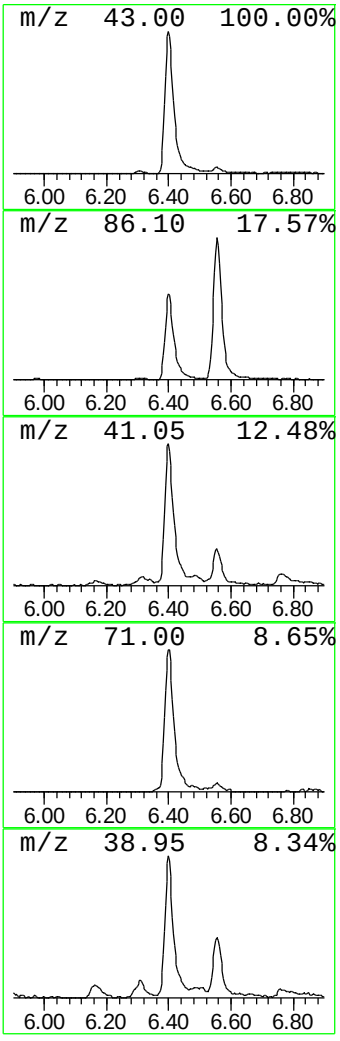
****

Peak Number 3 2-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	15.18 ug/L	425462	1,4-Difluorobenzene	5.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	86
2	2-Pentanone	86	C5H10O	000107-87-9	83
3	2-Pentanone	86	C5H10O	000107-87-9	74
4	2,3-Butanedione	86	C4H6O2	000431-03-8	53
5	2,3-Butanedione	86	C4H6O2	000431-03-8	37





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
Data File : VU033927.D
Acq On : 23 Aug 2019 02:10
Operator : JC/SP
Sample : K4485-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F2B75

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

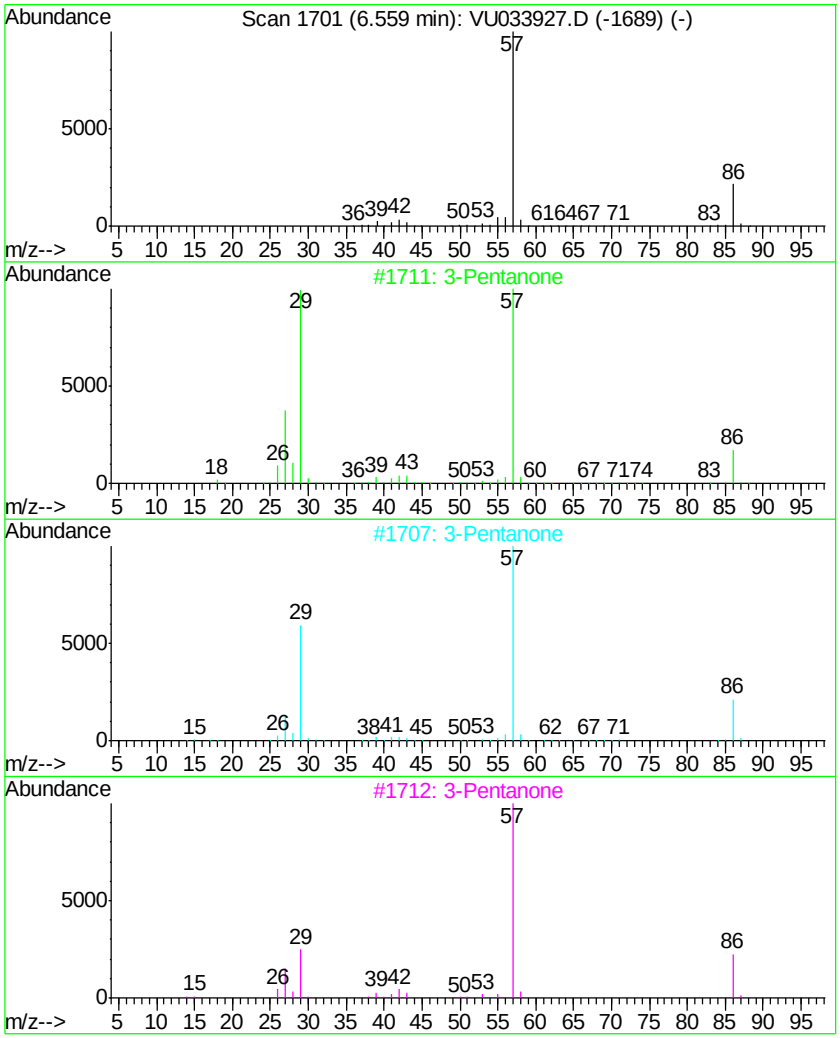
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

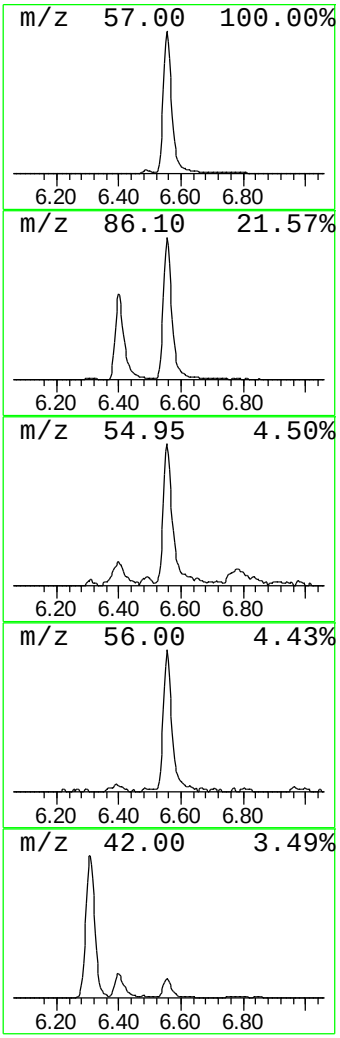
****

Peak Number 4 3-Pentanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	16.51 ug/L	462582	1,4-Difluorobenzene	5.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	80
2	3-Pentanone	86	C5H10O	000096-22-0	80
3	3-Pentanone	86	C5H10O	000096-22-0	59
4	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9
5	Neopentane	72	C5H12	000463-82-1	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
Data File : VU033927.D
Acq On : 23 Aug 2019 02:10
Operator : JC/SP
Sample : K4485-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F2B75

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

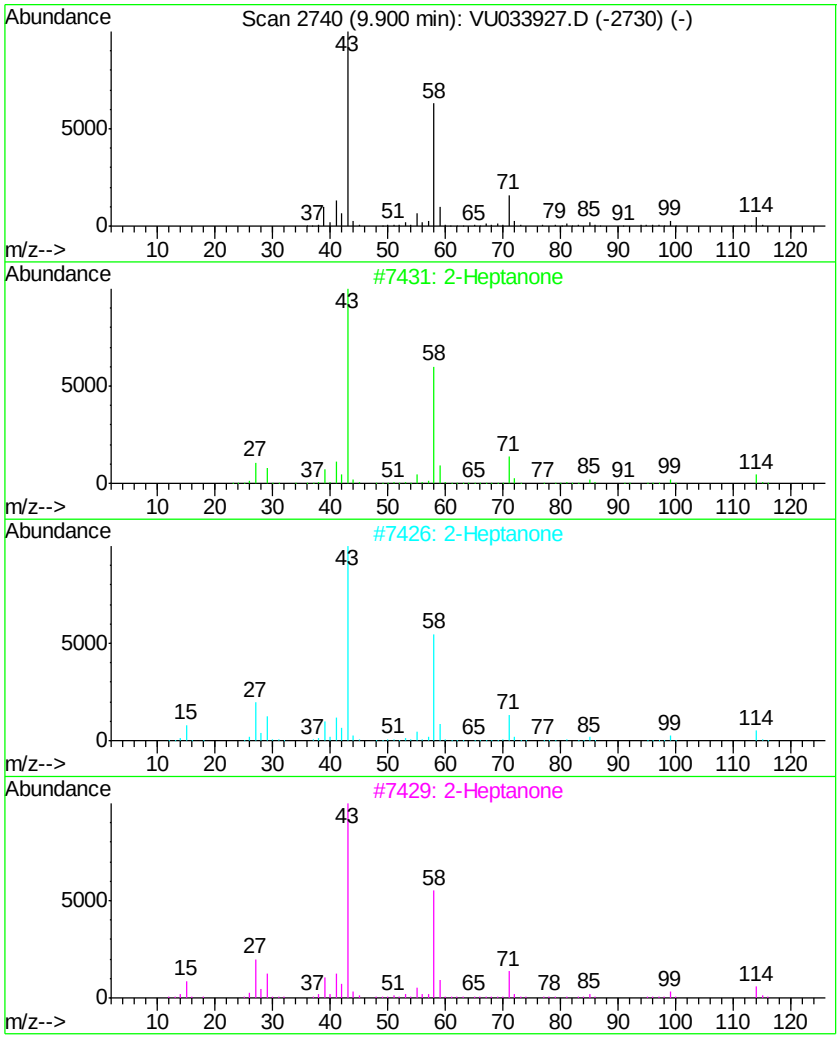
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

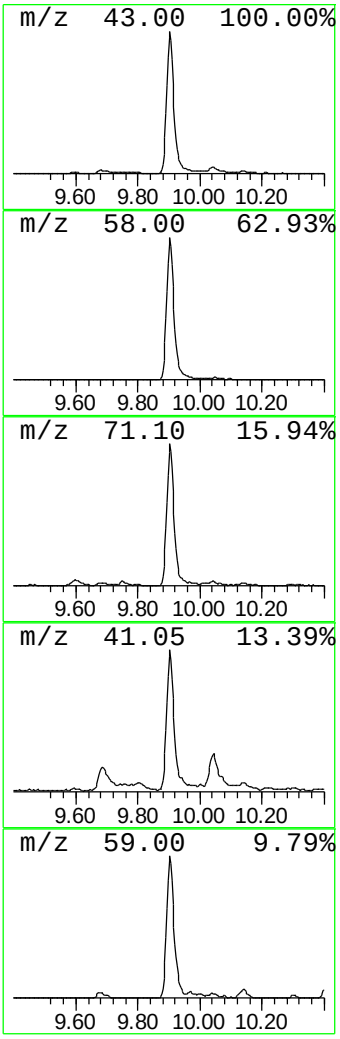
****

Peak Number 6 2-Heptanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.90	13.90 ug/L	512464	Chlorobenzene-d5	9.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	91
2	2-Heptanone	114	C7H14O	000110-43-0	91
3	2-Heptanone	114	C7H14O	000110-43-0	91
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78
5	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU082219\
Data File : VU033927.D
Acq On : 23 Aug 2019 02:10
Operator : JC/SP
Sample : K4485-09
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F2B75

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

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

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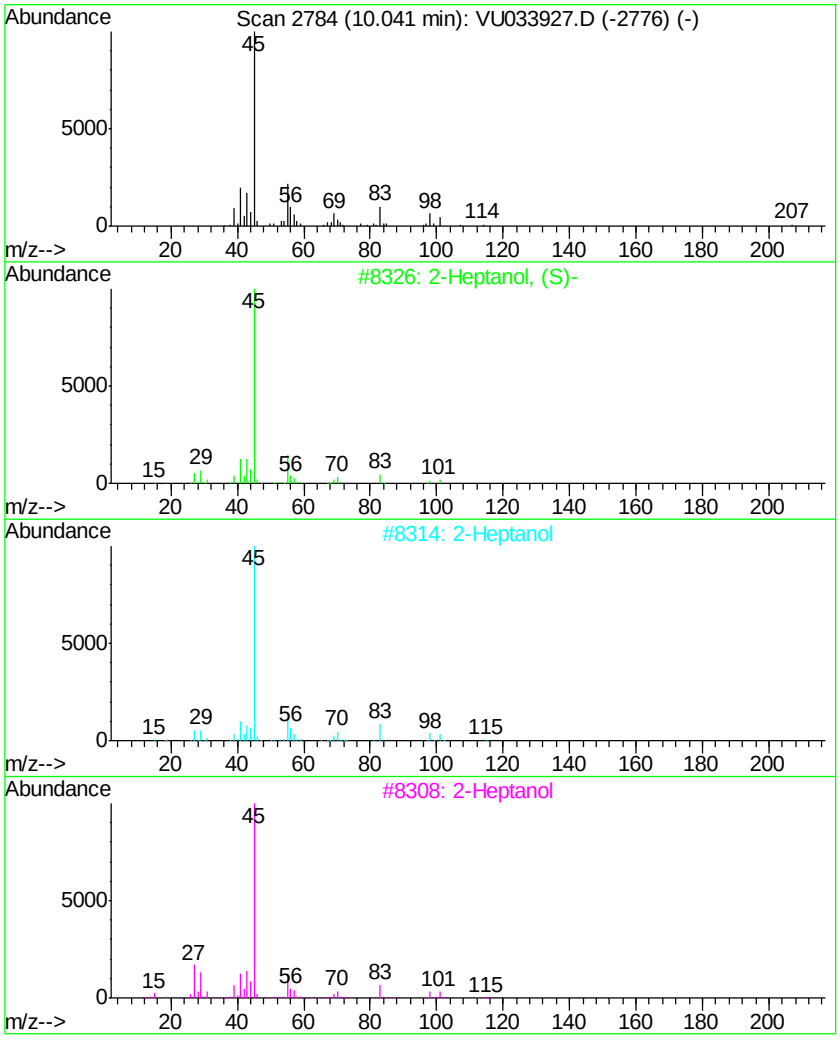
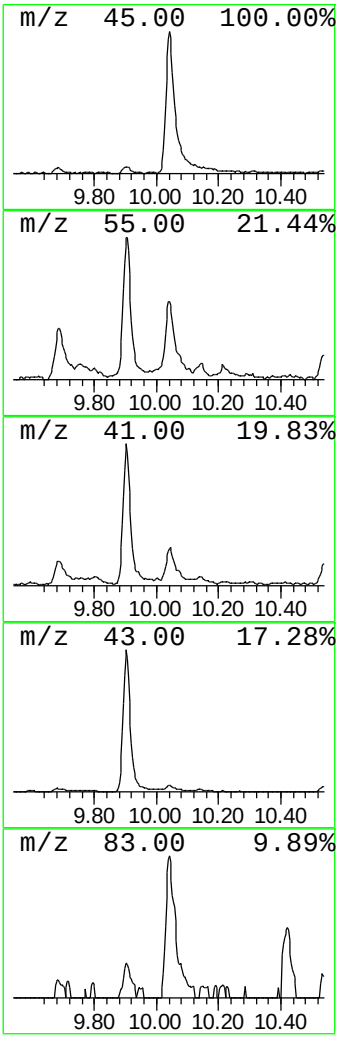
Peak Number 7 2-Heptanol, (S)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.04	2.55 ug/L	94058	Chlorobenzene-d5	9.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanol, (S)-	116	C7H16O	006033-23-4	78
2	2-Heptanol	116	C7H16O	000543-49-7	78
3	2-Heptanol	116	C7H16O	000543-49-7	72
4	2-Heptanol	116	C7H16O	000543-49-7	64
5	2-Octanol	130	C8H18O	000123-96-6	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
Data File : VU033927.D
Acq On : 23 Aug 2019 02:10
Operator : JC/SP
Sample : K4485-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F2B75

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

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

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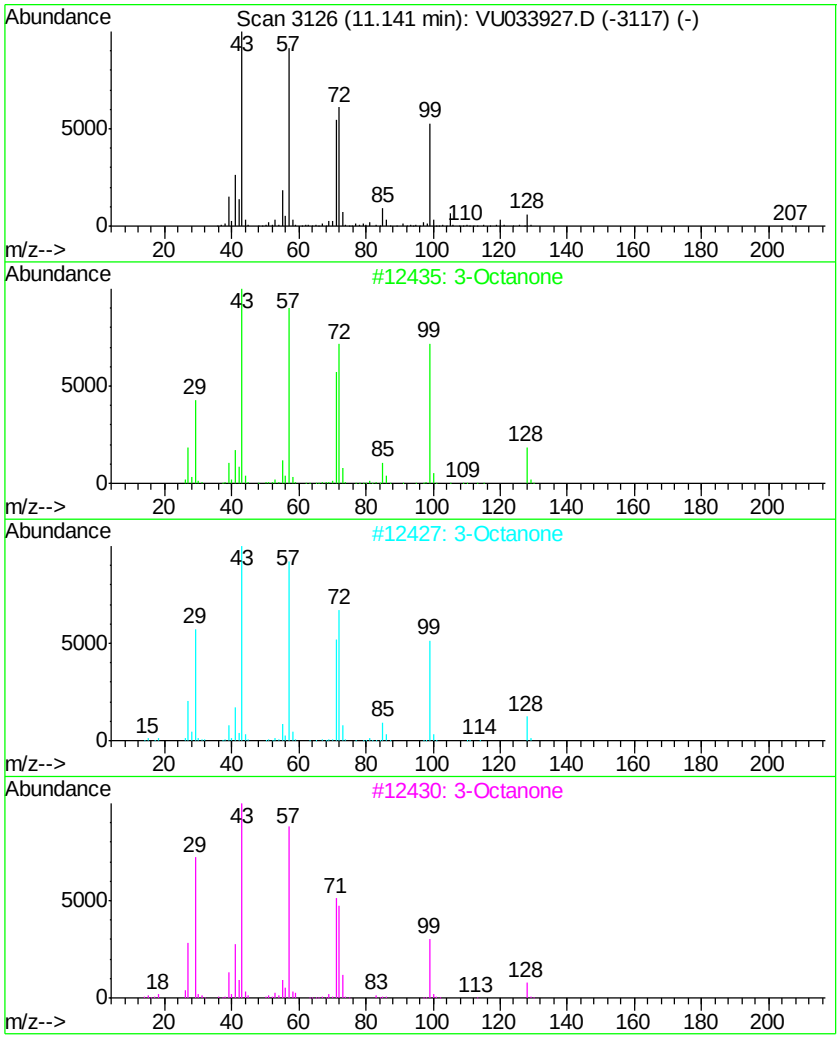
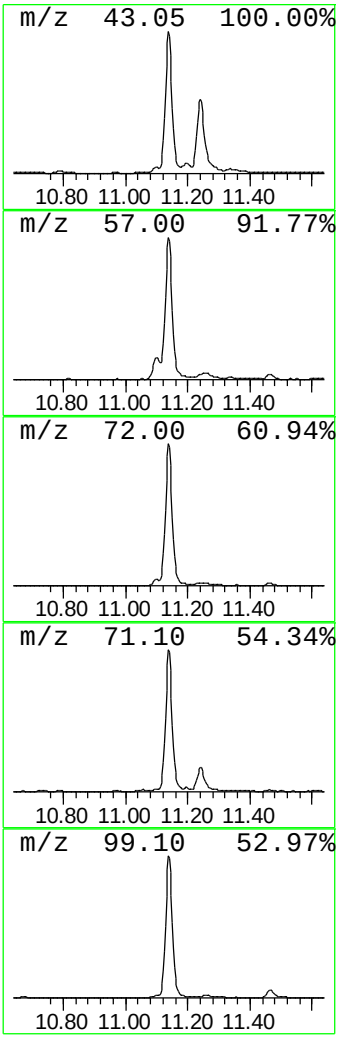
Peak Number 8 3-Octanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	21.56 ug/L	722141	1,4-Dichlorobenzene-d4	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone	128	C8H16O	000106-68-3	93
2	3-Octanone	128	C8H16O	000106-68-3	90
3	3-Octanone	128	C8H16O	000106-68-3	53
4	3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	52
5	3-Octanone	128	C8H16O	000106-68-3	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
Data File : VU033927.D
Acq On : 23 Aug 2019 02:10
Operator : JC/SP
Sample : K4485-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F2B75

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

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

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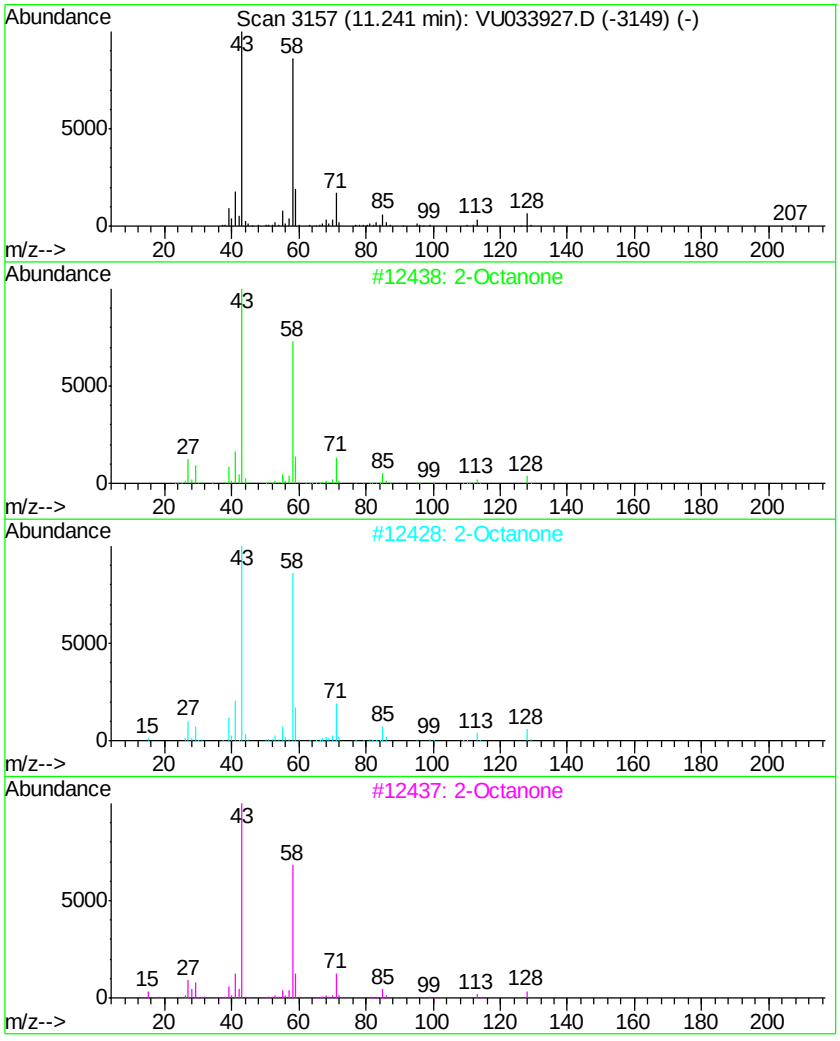
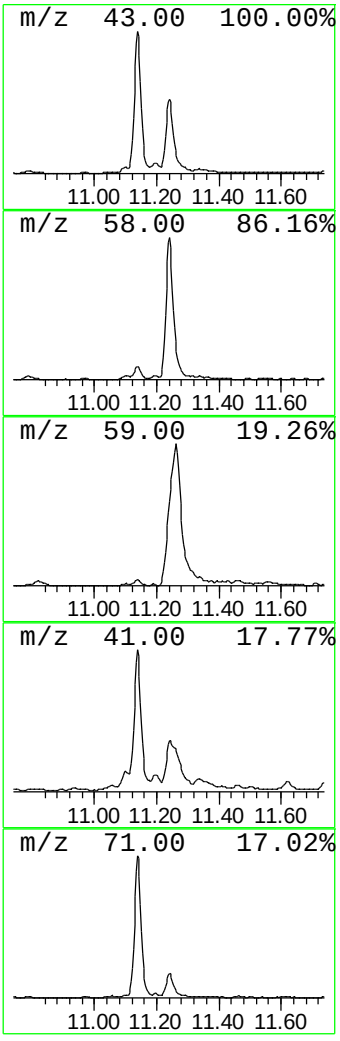
Peak Number 9 2-Octanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	10.50 ug/L	351757	1,4-Dichlorobenzene-d4	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	91
2	2-Octanone	128	C8H16O	000111-13-7	91
3	2-Octanone	128	C8H16O	000111-13-7	90
4	2-Octanone	128	C8H16O	000111-13-7	72
5	2-Octanone	128	C8H16O	000111-13-7	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU082219\
Data File : VU033927.D
Acq On : 23 Aug 2019 02:10
Operator : JC/SP
Sample : K4485-09
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F2B75

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.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
Furan	2.11	4.8	ug/L	135792	1	5.86	1401190	50.0
Dimethyl sulfide	2.36	44.7	ug/L	1253350	1	5.86	1401190	50.0
2-Pentanone	6.40	15.2	ug/L	425462	1	5.86	1401190	50.0
3-Pentanone	6.56	16.5	ug/L	462582	1	5.86	1401190	50.0
2-Heptanone	9.90	13.9	ug/L	512464	2	9.07	1842770	50.0
2-Heptanol, (S)-	10.04	2.5	ug/L	94058	2	9.07	1842770	50.0
3-Octanone	11.14	21.6	ug/L	722141	3	11.47	1674720	50.0
2-Octanone	11.24	10.5	ug/L	351757	3	11.47	1674720	50.0