LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU042420\
Data File : VU037879.D
Acq On : 24 Apr 2020 18:19
Operator : JC/MD
Sample : L2395-13
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0D98

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\SOMULM042320WMA.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	1.369	5	9	17	rBV3	6624	7076	0.01%	0.003%
2	1.485	37	45	57	rBV2	21593	51088	0.06%	0.019%
3	1.613	76	85	106	rBV2	455506	530413	0.59%	0.198%
4	1.697	108	111	119	rVB3	5401	5629	0.01%	0.002%
5	1.929	175	183	199	rVB	265314	354914	0.39%	0.133%
6	2.186	259	263	275	rVB2	18960	30257	0.03%	0.011%
7	2.269	280	289	298	rBV	24514	33895	0.04%	0.013%
8	2.604	376	393	434	rBV2	30005029	53003254	58.67%	19.823%
9	2.790	442	451	458	rBV3	4219	7564	0.01%	0.003%
10	3.076	522	540	568	rBV	5892542	11177526	12.37%	4.180%
11	3.211	574	582	583	rBV7	3489	3346	0.00%	0.001%
12	3.395	619	639	667	rBV	298285	705987	0.78%	0.264%
13	3.916	780	801	830	rBV	817297	1935251	2.14%	0.724%
14	4.179	875	883	892	rBV6	1317	2105	0.00%	0.001%
15	4.710	1022	1048	1111	rBV3	39343538	90348110	100.00%	33.790%
16	5.022	1135	1145	1155	rBV3	18985	39266	0.04%	0.015%
17	5.105	1155	1171	1193	rVB2	443189	1147316	1.27%	0.429%
18	5.359	1228	1250	1282	rBV	24602206	56117548	62.11%	20.988%
19	5.768	1353	1377	1390	rBV2	891135	2563157	2.84%	0.959%
20	5.829	1390	1396	1421	rVB2	133290	280506	0.31%	0.105%
21	6.288	1523	1539	1561	rVB	679191	1497918	1.66%	0.560%
22	6.755	1676	1684	1709	rVB	834543	1491779	1.65%	0.558%
23	7.282	1837	1848	1863	rVB4	28419	51749	0.06%	0.019%
24	7.594	1932	1945	1961	rBV	414990	702173	0.78%	0.263%
25	7.822	2005	2016	2030	rVB2	36352	63438	0.07%	0.024%
26	7.925	2034	2048	2059	rVV	1349385	2261309	2.50%	0.846%
27	7.996	2059	2070	2085	rVV	1206872	2001776	2.22%	0.749%
28	8.057	2085	2089	2097	rVB8	2559	3144	0.00%	0.001%
29	8.202	2123	2134	2150	rVB	293535	479668	0.53%	0.179%
30	8.423	2189	2203	2218	rBV	1703520	2833136	3.14%	1.060%
31	8.513	2219	2231	2241	rVV	246149	418982	0.46%	0.157%
32	8.575	2241	2250	2262	rVB	160611	269123	0.30%	0.101%
33	8.655	2262	2275	2298	rBV	998725	1727584	1.91%	0.646%
34	8.796	2309	2319	2328	rVB3	28294	47051	0.05%	0.018%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU042420\
Data File : VU037879.D
Acq On : 24 Apr 2020 18:19
Operator : JC/MD
Sample : L2395-13
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0D98

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\SOMULM042320WMA.M
Title : VOC Analysis

35	9.060	2391	2401	2416	rVB4	9589	15918	0.02%	0.006%
36	9.185	2431	2440	2449	rVB3	5310	9103	0.01%	0.003%
37	9.301	2467	2476	2479	rBV7	2538	4271	0.00%	0.002%
38	9.337	2479	2487	2491	rBV3	13964	21590	0.02%	0.008%
39	9.436	2504	2518	2533	rBV	1233427	1998781	2.21%	0.748%
40	9.555	2541	2555	2558	rBV	678890	1035057	1.15%	0.387%
41	9.587	2558	2565	2580	rVV	2518478	4059390	4.49%	1.518%
42	9.710	2582	2603	2616	rVV	6559433	10709700	11.85%	4.005%
43	9.780	2616	2625	2652	rVB	459397	787699	0.87%	0.295%
44	9.992	2683	2691	2703	rVB9	4226	7821	0.01%	0.003%
45	10.118	2715	2730	2755	rVB	6165564	9747960	10.79%	3.646%
46	10.259	2765	2774	2777	rBV6	2136	3404	0.00%	0.001%
47	10.301	2782	2787	2796	rVB4	6497	9571	0.01%	0.004%
48	10.362	2796	2806	2814	rBV5	14271	22660	0.03%	0.008%
49	10.501	2830	2849	2859	rBV	92611	166661	0.18%	0.062%
50	10.562	2859	2868	2883	rVV3	17750	31557	0.03%	0.012%
51	10.661	2889	2899	2910	rVB4	12452	21135	0.02%	0.008%
52	10.771	2913	2933	2947	rBV	809063	1310846	1.45%	0.490%
53	10.838	2947	2954	2966	rVB	39789	62571	0.07%	0.023%
54	10.912	2966	2977	2995	rBV3	45514	100874	0.11%	0.038%
55	11.009	2999	3007	3013	rBV	27641	42502	0.05%	0.016%
56	11.102	3028	3036	3044	rBV	16771	24466	0.03%	0.009%
57	11.250	3075	3082	3087	rBV7	2684	3896	0.00%	0.001%
58	11.304	3091	3099	3111	rVB2	14118	22568	0.02%	0.008%
59	11.401	3123	3129	3136	rBV8	3894	6182	0.01%	0.002%
60	11.481	3144	3154	3163	rBV2	25439	40815	0.05%	0.015%
61	11.542	3163	3173	3183	rVB2	37973	62008	0.07%	0.023%
62	11.652	3198	3207	3218	rVB10	8576	13615	0.02%	0.005%
63	11.732	3228	3232	3233	rBV4	3428	2297	0.00%	0.001%
64	11.825	3246	3261	3277	rVV	1264045	2040012	2.26%	0.763%
65	11.906	3277	3286	3303	rVB4	11180	25733	0.03%	0.010%
66	12.079	3332	3340	3341	rBV5	5633	5987	0.01%	0.002%
67	12.108	3342	3349	3364	rVB6	23499	41504	0.05%	0.016%
68	12.205	3365	3379	3392	rBV	1201900	1928423	2.13%	0.721%
69	12.468	3456	3461	3465	rBV5	2435	2824	0.00%	0.001%
70	12.507	3470	3473	3481	rVV4	3264	4276	0.00%	0.002%
71	12.581	3490	3496	3506	rVB4	5327	8239	0.01%	0.003%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU042420\
Data File : VU037879.D
Acq On : 24 Apr 2020 18:19
Operator : JC/MD
Sample : L2395-13
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0D98

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\SOMULM042320WMA.M
Title : VOC Analysis

72	12.700	3527	3533	3538	rBV6	1437	2208	0.00%	0.001%
73	12.825	3557	3572	3586	rVB7	25091	46845	0.05%	0.018%
74	12.970	3607	3617	3626	rBV2	21512	37632	0.04%	0.014%
75	13.185	3676	3684	3693	rBV5	15530	22252	0.02%	0.008%
76	13.237	3693	3700	3707	rBV6	5651	8145	0.01%	0.003%
77	13.314	3719	3724	3733	rVB8	2682	4174	0.00%	0.002%
78	13.430	3755	3760	3765	rBV7	2057	2574	0.00%	0.001%
79	13.475	3766	3774	3781	rVB8	4632	7362	0.01%	0.003%
80	13.533	3782	3792	3804	rBV4	74128	121010	0.13%	0.045%
81	13.725	3841	3852	3860	rBV3	70320	110349	0.12%	0.041%
82	13.764	3861	3864	3875	rVB5	17098	23507	0.03%	0.009%
83	13.867	3887	3896	3903	rBV5	7540	13629	0.02%	0.005%
84	13.970	3920	3928	3940	rVB6	6634	11152	0.01%	0.004%
85	14.053	3946	3954	3958	rVV9	4040	5385	0.01%	0.002%
86	14.111	3962	3972	3982	rVV	90084	150524	0.17%	0.056%
87	14.153	3982	3985	3993	rVB4	12355	13459	0.01%	0.005%
88	14.233	4002	4010	4018	rVB4	6161	9337	0.01%	0.003%
89	14.311	4029	4034	4038	rBV7	2400	2520	0.00%	0.001%
90	14.356	4042	4048	4058	rVB9	2950	4229	0.00%	0.002%
91	14.545	4101	4107	4108	rBV3	2332	2274	0.00%	0.001%
92	14.912	4216	4221	4227	rVB8	2078	2993	0.00%	0.001%
93	15.259	4320	4329	4340	rVB	24869	38332	0.04%	0.014%
94	15.449	4378	4388	4398	rVB3	15642	26453	0.03%	0.010%
95	15.999	4555	4559	4568	rVB2	7893	10614	0.01%	0.004%
96	16.311	4653	4656	4666	rVB9	4662	5255	0.01%	0.002%
97	16.455	4694	4701	4711	rBV10	7801	12266	0.01%	0.005%
98	16.497	4711	4714	4722	rVB8	3789	4359	0.00%	0.002%
99	16.664	4761	4766	4770	rBV7	4543	5816	0.01%	0.002%
100	17.153	4909	4918	4929	rVB3	47296	81252	0.09%	0.030%

Sum of corrected areas: 267380861

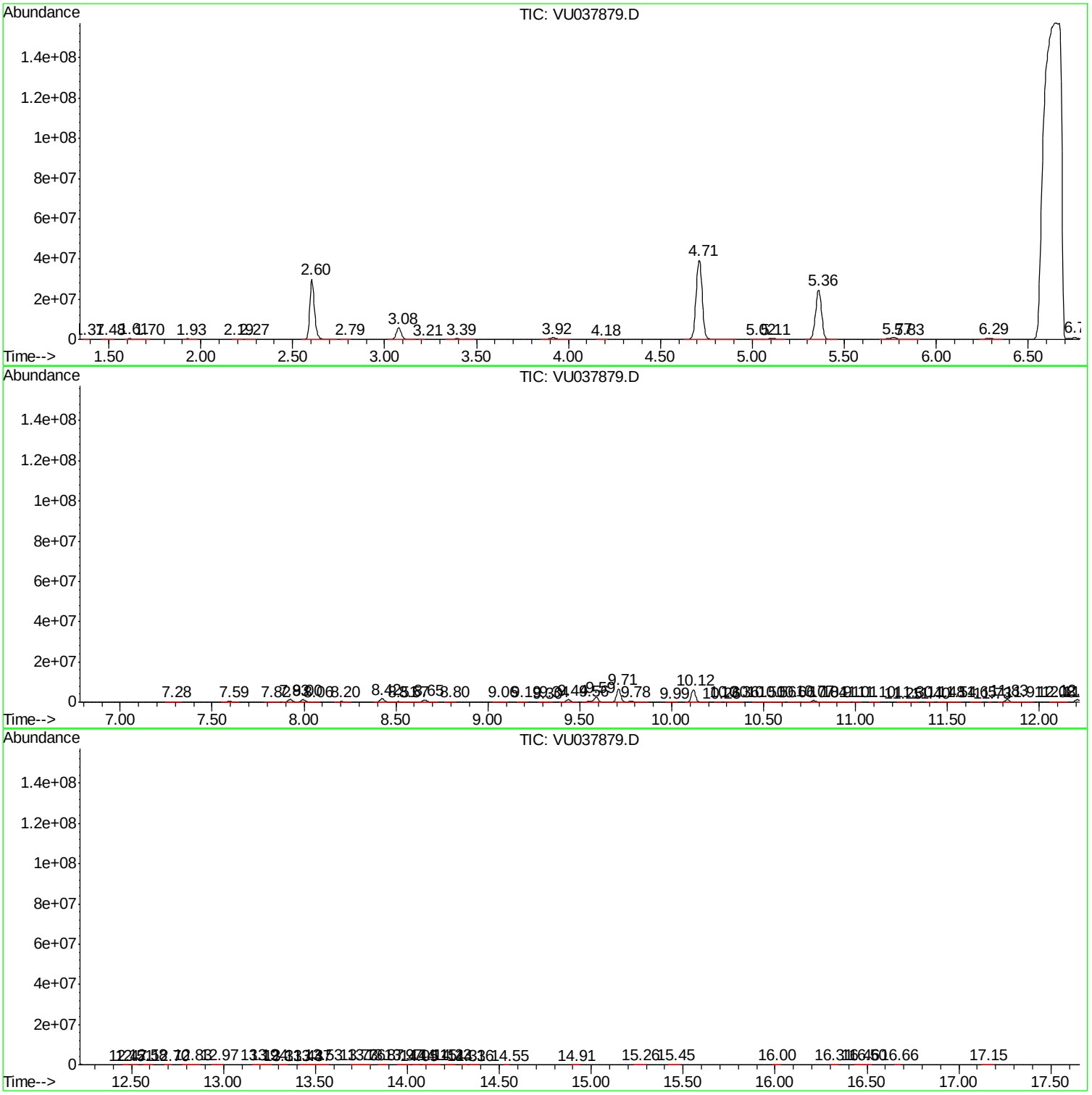
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU042420\
Data File : VU037879.D
Acq On : 24 Apr 2020 18:19
Operator : JC/MD
Sample : L2395-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0D98

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042320WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU042420\
Data File : VU037879.D
Acq On : 24 Apr 2020 18:19
Operator : JC/MD
Sample : L2395-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0D98

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042320WMA.M
Quant Title : VOC Analysis

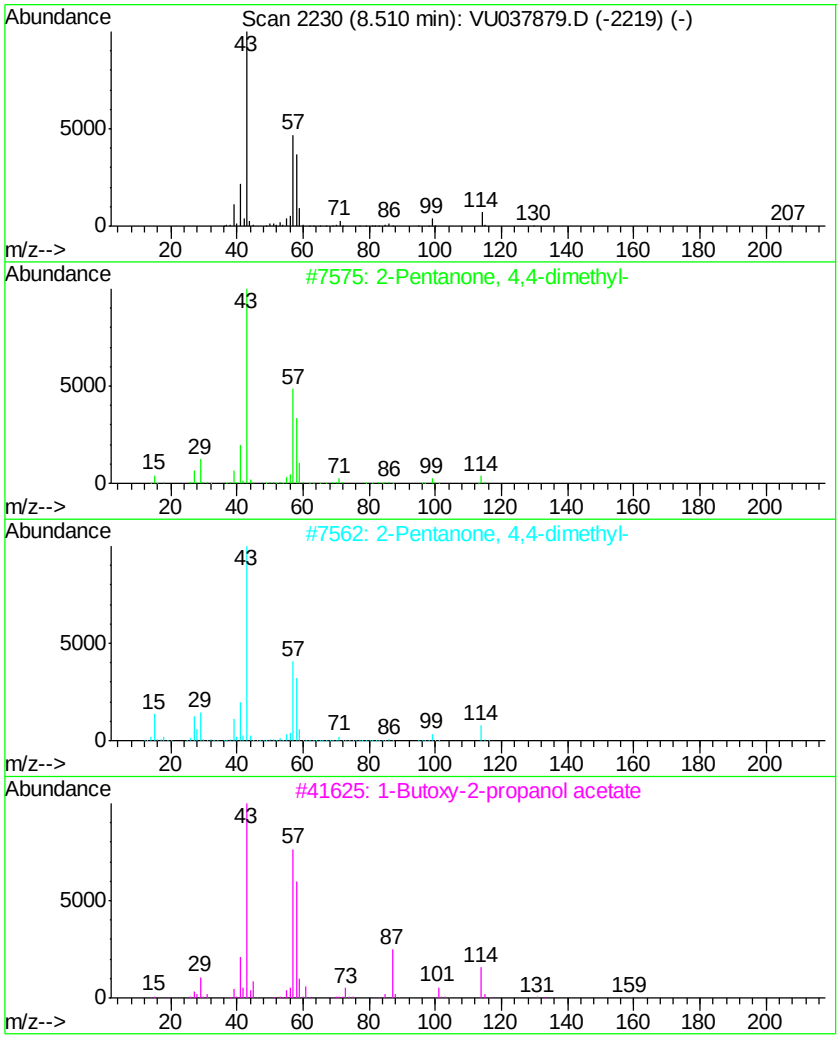
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

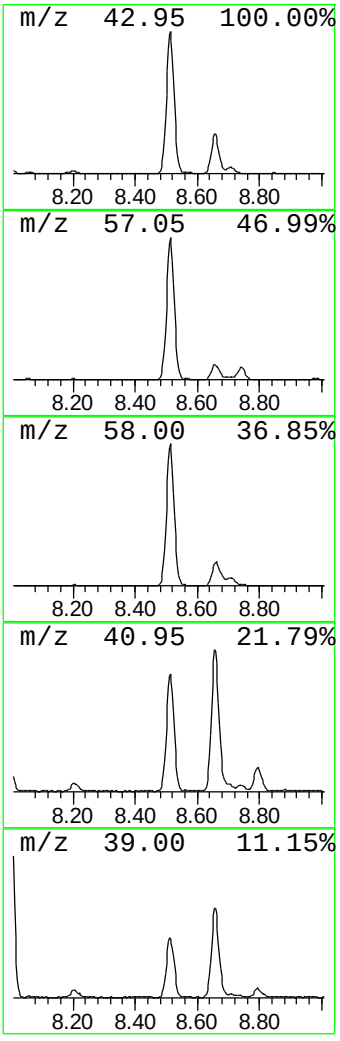
****

Peak Number 2 2-Pentanone, 4,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.51	10.48 ug/L	418982	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	91
2	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	91
3	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	72
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	64
5	2-Heptanone	114	C7H14O	000110-43-0	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU042420\
Data File : VU037879.D
Acq On : 24 Apr 2020 18:19
Operator : JC/MD
Sample : L2395-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0D98

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042320WMA.M
Quant Title : VOC Analysis

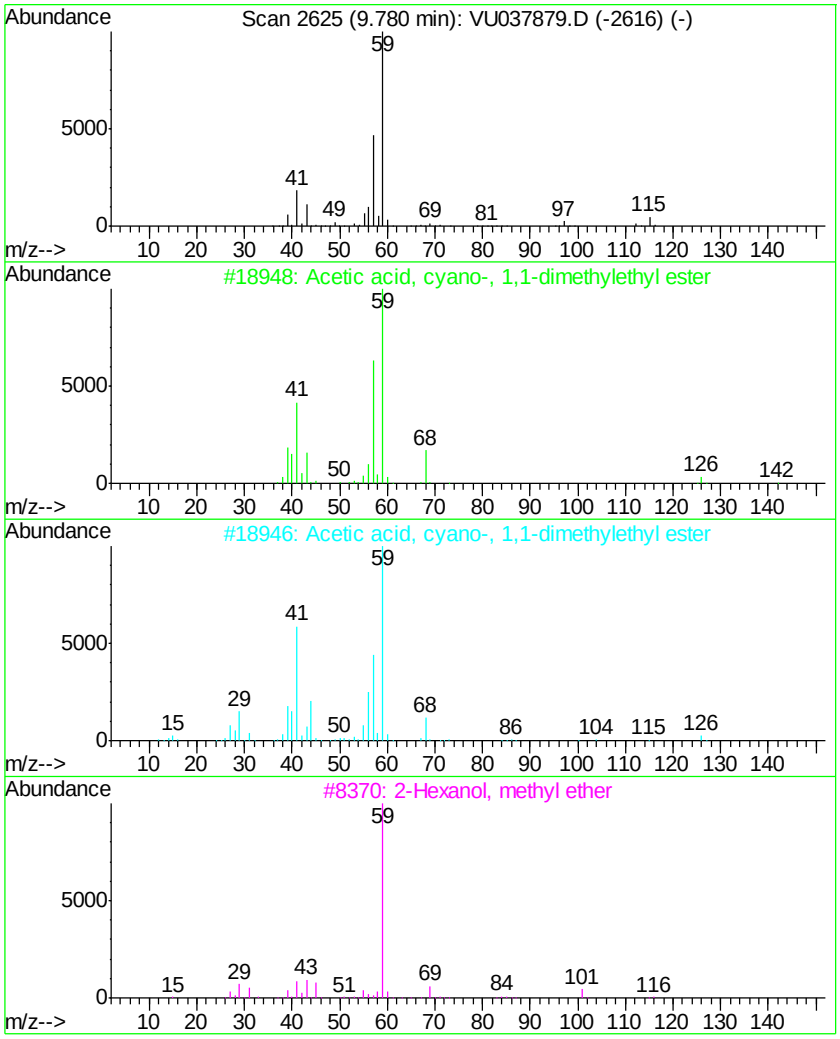
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

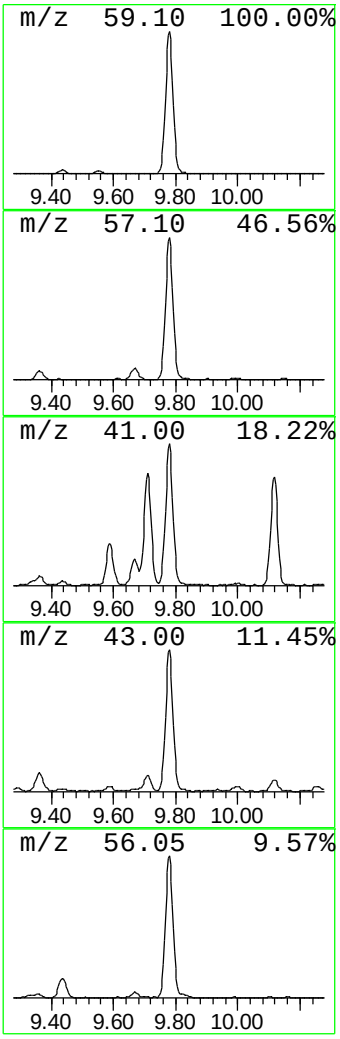
****

Peak Number 3 Acetic acid, cyano-, 1,1-di... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.78	19.70 ug/L	787699	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	50
3	2-Hexanol, methyl ether	116	C7H16O	1000333-92-0	45
4	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	9
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU042420\
Data File : VU037879.D
Acq On : 24 Apr 2020 18:19
Operator : JC/MD
Sample : L2395-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0D98

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042320WMA.M
Quant Title : VOC Analysis

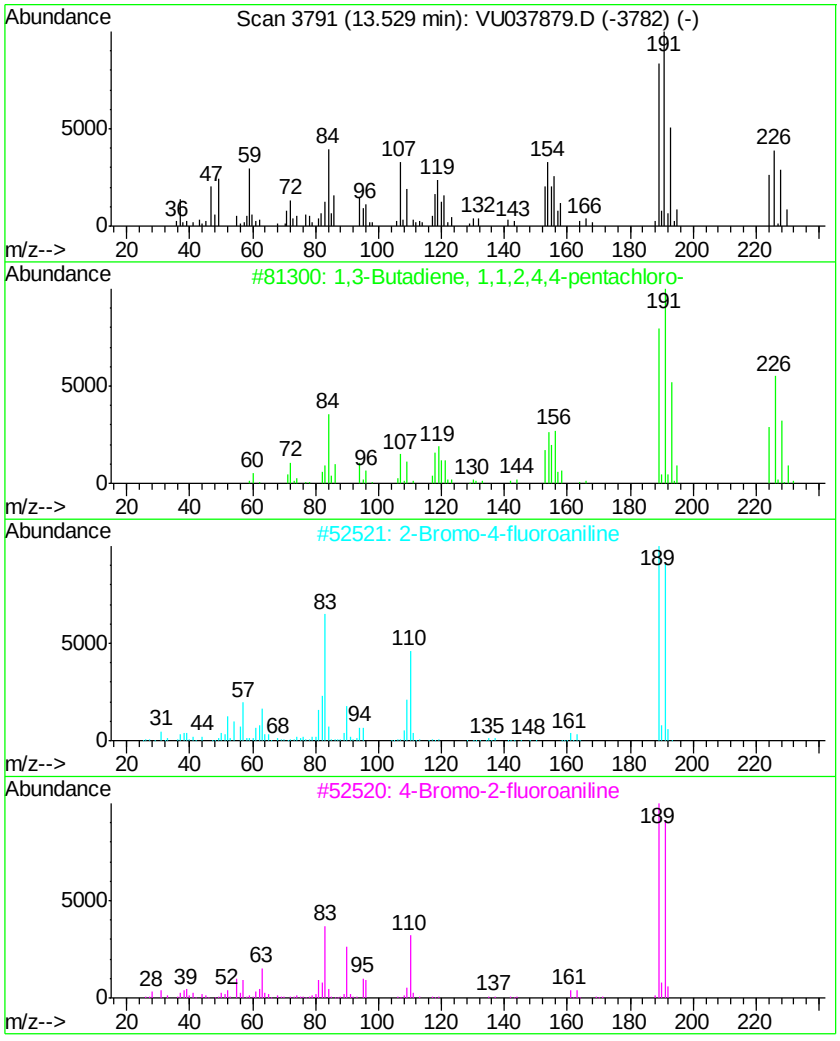
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

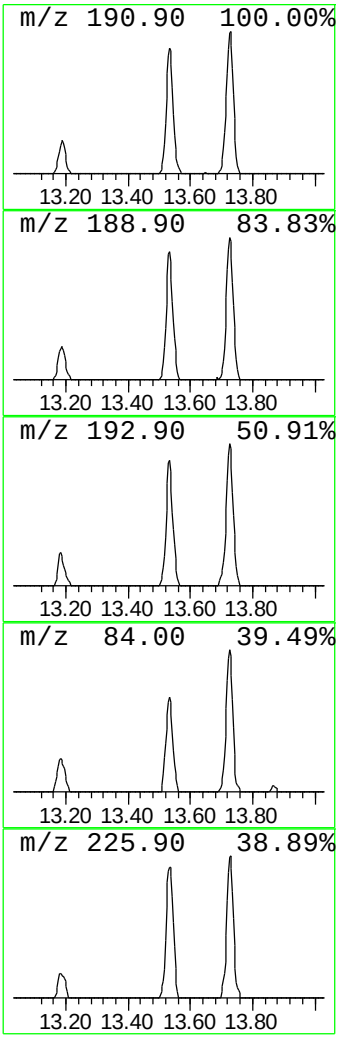
****

Peak Number 4 1,3-Butadiene, 1,1,2,4,4-pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	2.97 ug/L	121010	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HCl5	021400-41-9	99
2	2-Bromo-4-fluoroaniline	189	C6H5BrFN	001003-98-1	25
3	4-Bromo-2-fluoroaniline	189	C6H5BrFN	000367-24-8	22
4	4-Bromo-2-fluoroaniline	189	C6H5BrFN	000367-24-8	22
5	2-Chloro-4,6-dimethylquinoline	191	C11H10ClN	003913-18-6	14





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU042420\
Data File : VU037879.D
Acq On : 24 Apr 2020 18:19
Operator : JC/MD
Sample : L2395-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0D98

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042320WMA.M
Quant Title : VOC Analysis

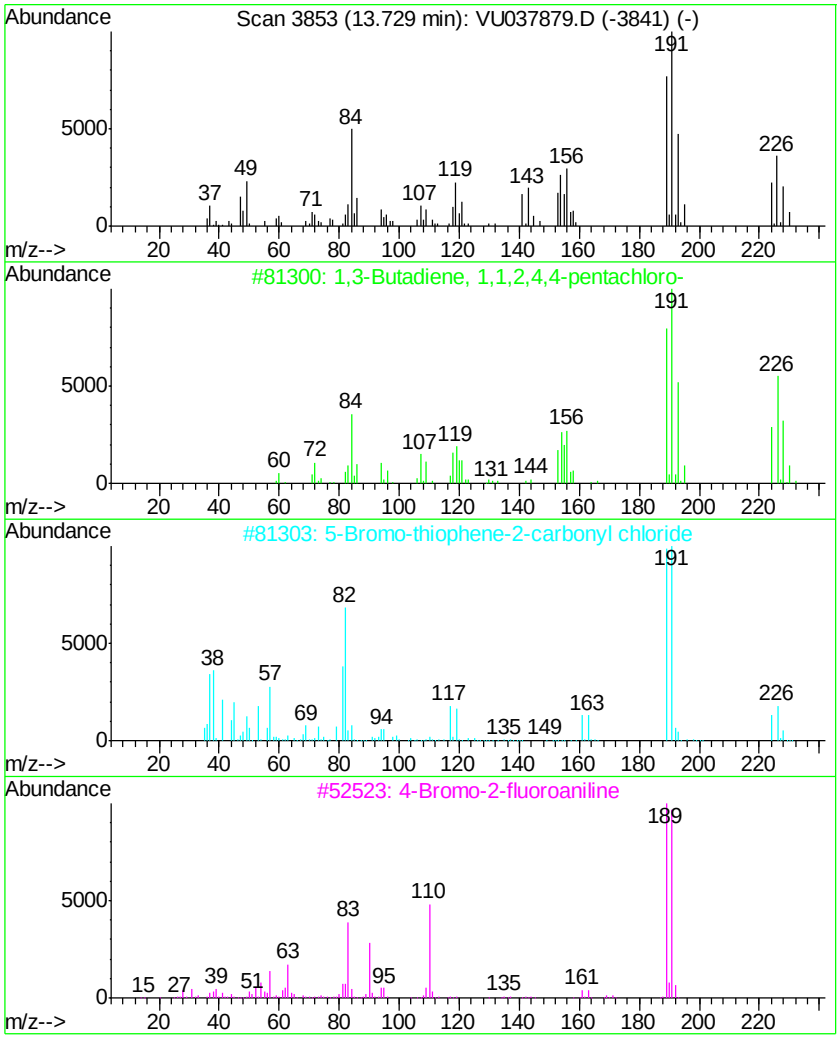
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

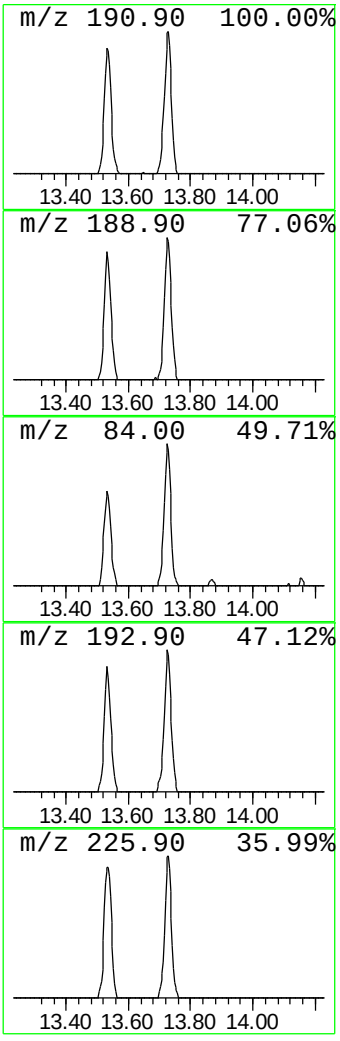
****

Peak Number 5 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	2.70 ug/L	110349	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HCl5	021400-41-9	91
2	5-Bromo-thiophene-2-carbonyl chl...	224	C5H2BrClOS	1000296-94-3	37
3	4-Bromo-2-fluoroaniline	189	C6H5BrFN	000367-24-8	25
4	4-Bromo-2-fluoroaniline	189	C6H5BrFN	000367-24-8	22
5	2-Bromo-4-fluoroaniline	189	C6H5BrFN	001003-98-1	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU042420\
Data File : VU037879.D
Acq On : 24 Apr 2020 18:19
Operator : JC/MD
Sample : L2395-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0D98

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042320WMA.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
2-Pentanone, 4,4-...	8.51	10.5	ug/L	418982	2	9.44	1998780	50.0
Acetic acid, cyan...	9.78	19.7	ug/L	787699	2	9.44	1998780	50.0
1,3-Butadiene, 1,...	13.53	3.0	ug/L	121010	3	11.83	2040010	50.0
unknown-01	13.73	2.7	ug/L	110349	3	11.83	2040010	50.0