LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038952.D
Acq On : 17 Jun 2020 18:25
Operator : SY/MD
Sample : L3040-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L18

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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\SOMUTR061720WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.626	79	89	101	rVB	128222	166280	13.63%	1.496%
2	1.948	182	189	197	rBV	104910	129845	10.64%	1.168%
3	2.601	382	392	407	rVB	277012	454803	37.27%	4.091%
4	2.826	457	462	473	rVB2	10948	19978	1.64%	0.180%
5	2.893	477	483	487	rBV7	9678	14642	1.20%	0.132%
6	3.363	621	629	637	rBV	8449	14376	1.18%	0.129%
7	4.530	966	992	1010	rBV10	11434	46312	3.80%	0.417%
8	4.787	1043	1072	1116	rBV2	98058	453107	37.13%	4.076%
9	5.125	1162	1177	1192	rVB	203601	435751	35.71%	3.920%
10	5.780	1362	1381	1403	rBV2	441690	1014471	83.14%	9.126%
11	6.301	1529	1543	1558	rVB	339429	632072	51.80%	5.686%
12	6.739	1667	1679	1700	rVB	248046	478945	39.25%	4.309%
13	6.845	1705	1712	1725	rVB2	9213	16736	1.37%	0.151%
14	7.224	1820	1830	1844	rVB2	32062	63453	5.20%	0.571%
15	7.604	1936	1948	1964	rVB2	122900	210490	17.25%	1.894%
16	7.932	2038	2050	2064	rVB	451749	760051	62.29%	6.837%
17	8.076	2087	2095	2105	rVB3	9026	14480	1.19%	0.130%
18	8.211	2124	2137	2152	rBV	85423	141501	11.60%	1.273%
19	8.523	2218	2234	2245	rBV5	6849	16219	1.33%	0.146%
20	8.674	2266	2281	2293	rBV	687140	1220203	100.00%	10.977%
21	8.816	2318	2325	2337	rVB4	14942	25115	2.06%	0.226%
22	9.440	2507	2519	2538	rBV	495314	815536	66.84%	7.337%
23	9.658	2568	2587	2597	rVB2	27327	48435	3.97%	0.436%
24	9.787	2614	2627	2646	rBV5	13291	30002	2.46%	0.270%
25	9.941	2659	2675	2685	rBV2	29465	47901	3.93%	0.431%
26	10.150	2723	2740	2748	rBV4	10956	22098	1.81%	0.199%
27	10.256	2759	2773	2785	rBV2	25001	48533	3.98%	0.437%
28	10.362	2798	2806	2820	rVB7	12295	20826	1.71%	0.187%
29	10.700	2903	2911	2922	rVB3	22116	35787	2.93%	0.322%
30	10.774	2922	2934	2952	rBV	208655	345375	28.30%	3.107%
31	10.980	2982	2998	3011	rBV2	37100	65828	5.39%	0.592%
32	11.063	3013	3024	3037	rVB4	16670	28733	2.35%	0.258%
33	11.481	3145	3154	3163	rBV3	13009	20376	1.67%	0.183%
34	11.584	3175	3186	3196	rBV	24239	37833	3.10%	0.340%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038952.D
Acq On : 17 Jun 2020 18:25
Operator : SY/MD
Sample : L3040-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L18

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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\SOMUTR061720WMA.M
Title : TRACE VOA SOM01.0

35	11.700	3213	3222	3231	rVB3	20035	30362	2.49%	0.273%
36	11.825	3248	3261	3277	rVB	517057	816481	66.91%	7.345%
37	11.989	3307	3312	3325	rVB8	7841	12520	1.03%	0.113%
38	12.076	3325	3339	3361	rBV	240269	517101	42.38%	4.652%
39	12.205	3368	3379	3394	rVB	512017	836080	68.52%	7.521%
40	12.336	3413	3420	3427	rBV	11816	15900	1.30%	0.143%
41	12.793	3552	3562	3572	rBV2	27412	42699	3.50%	0.384%
42	12.909	3589	3598	3609	rVB5	22437	33334	2.73%	0.300%
43	13.420	3745	3757	3767	rBV10	8424	17985	1.47%	0.162%
44	13.639	3818	3825	3835	rVB3	22848	35180	2.88%	0.316%
45	14.012	3934	3941	3953	rBV5	12615	19305	1.58%	0.174%
46	14.227	3996	4008	4019	rBV3	57551	90990	7.46%	0.819%
47	14.680	4139	4149	4164	rBV3	7969	21457	1.76%	0.193%
48	14.877	4196	4210	4215	rBV7	10231	21470	1.76%	0.193%
49	14.922	4217	4224	4233	rVB10	9698	17889	1.47%	0.161%
50	15.742	4471	4479	4490	rVB10	15533	25719	2.11%	0.231%
51	16.192	4612	4619	4631	rVB5	14664	22985	1.88%	0.207%
52	16.838	4809	4820	4832	rBV2	94722	155863	12.77%	1.402%
53	16.963	4847	4859	4875	rBV	284908	486563	39.88%	4.377%

Sum of corrected areas: 11115976

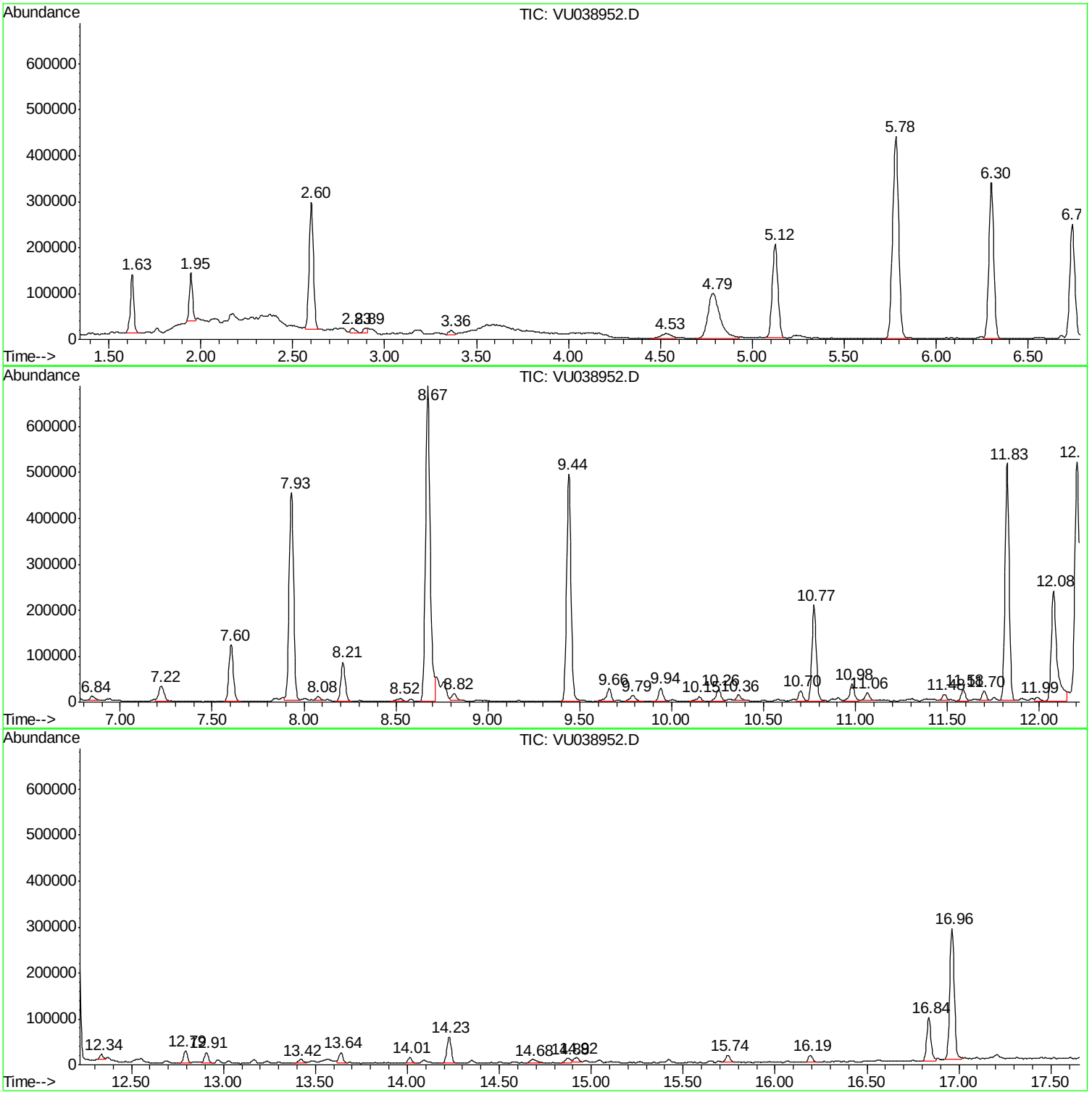
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038952.D
Acq On : 17 Jun 2020 18:25
Operator : SY/MD
Sample : L3040-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038952.D
Acq On : 17 Jun 2020 18:25
Operator : SY/MD
Sample : L3040-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

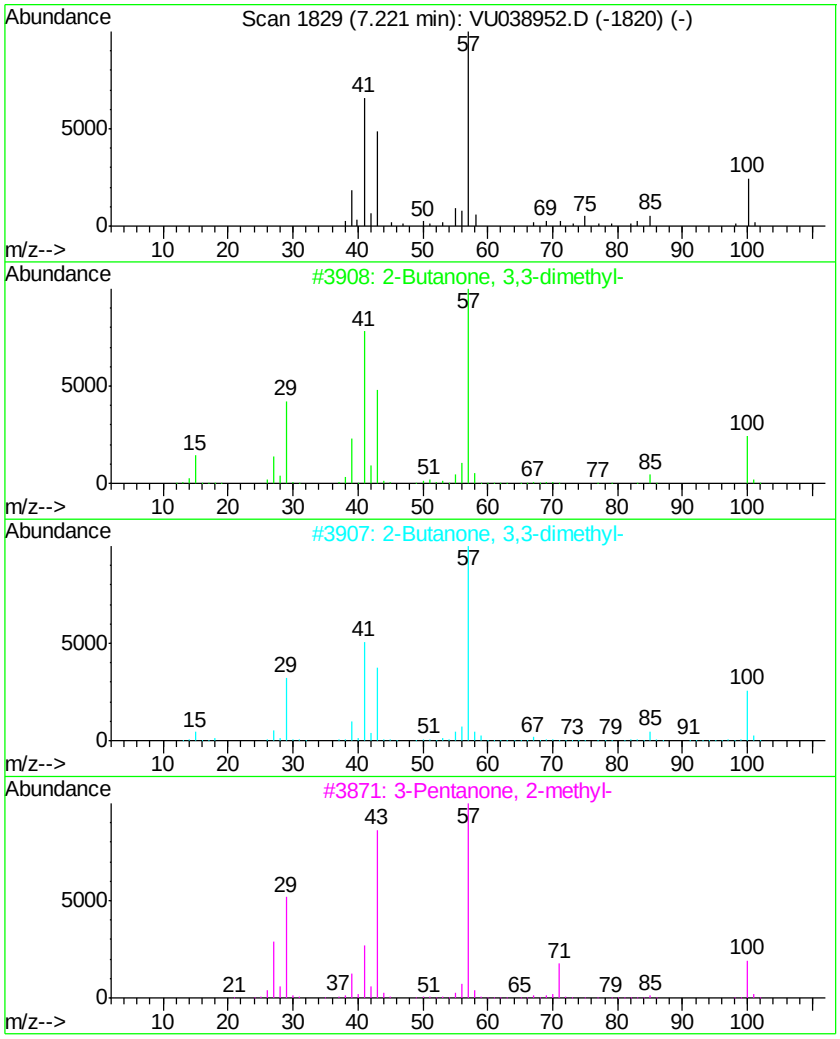
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

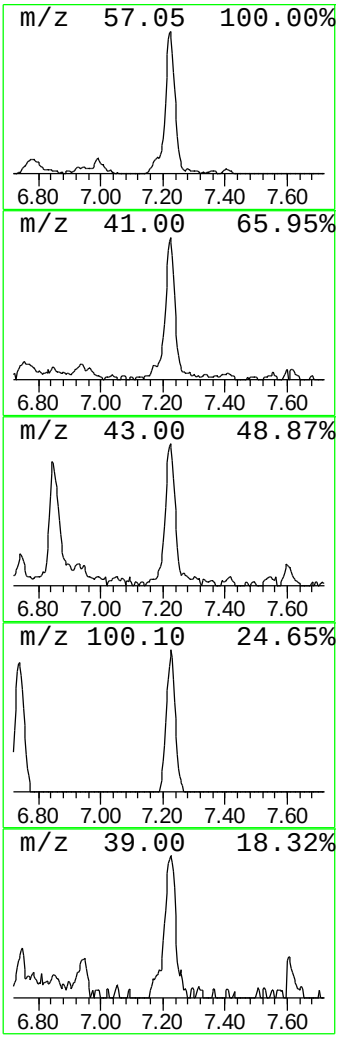
****

Peak Number 1 2-Butanone, 3,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	0.50 ug/L	63453	1,4-Difluorobenzene	6.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	83
2	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	80
3	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	72
4	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	53
5	3-Hexanone	100	C6H12O	000589-38-8	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038952.D
Acq On : 17 Jun 2020 18:25
Operator : SY/MD
Sample : L3040-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

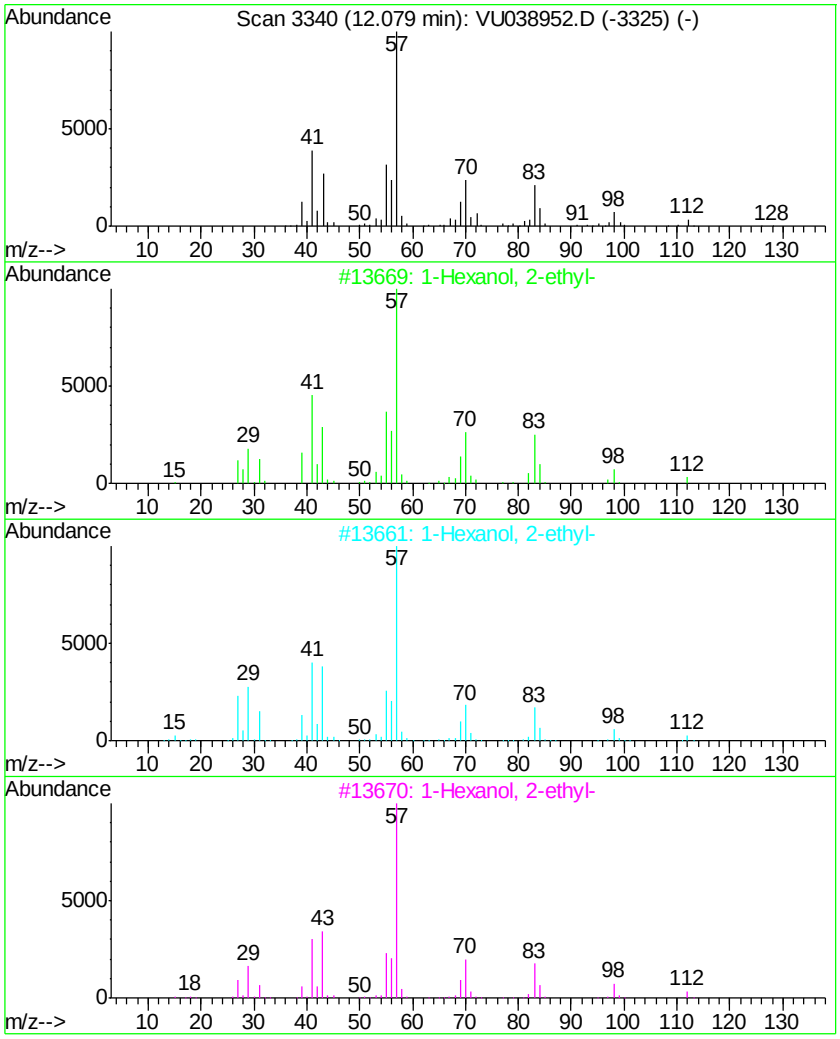
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

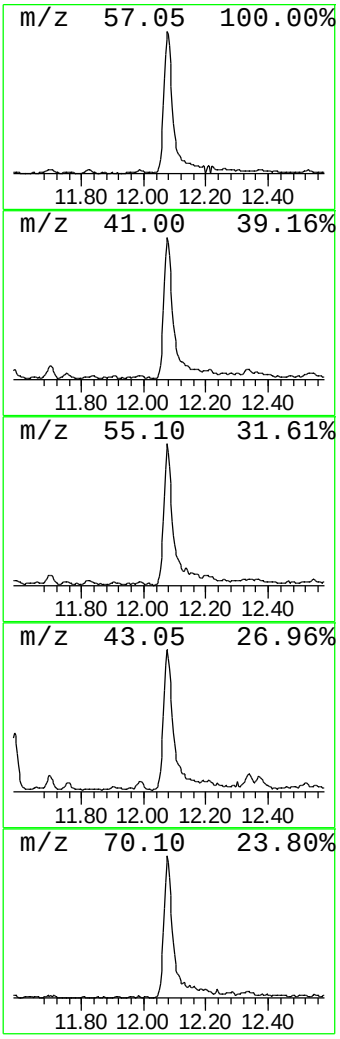
****

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	3.17 ug/L	517101	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	53





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038952.D
Acq On : 17 Jun 2020 18:25
Operator : SY/MD
Sample : L3040-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

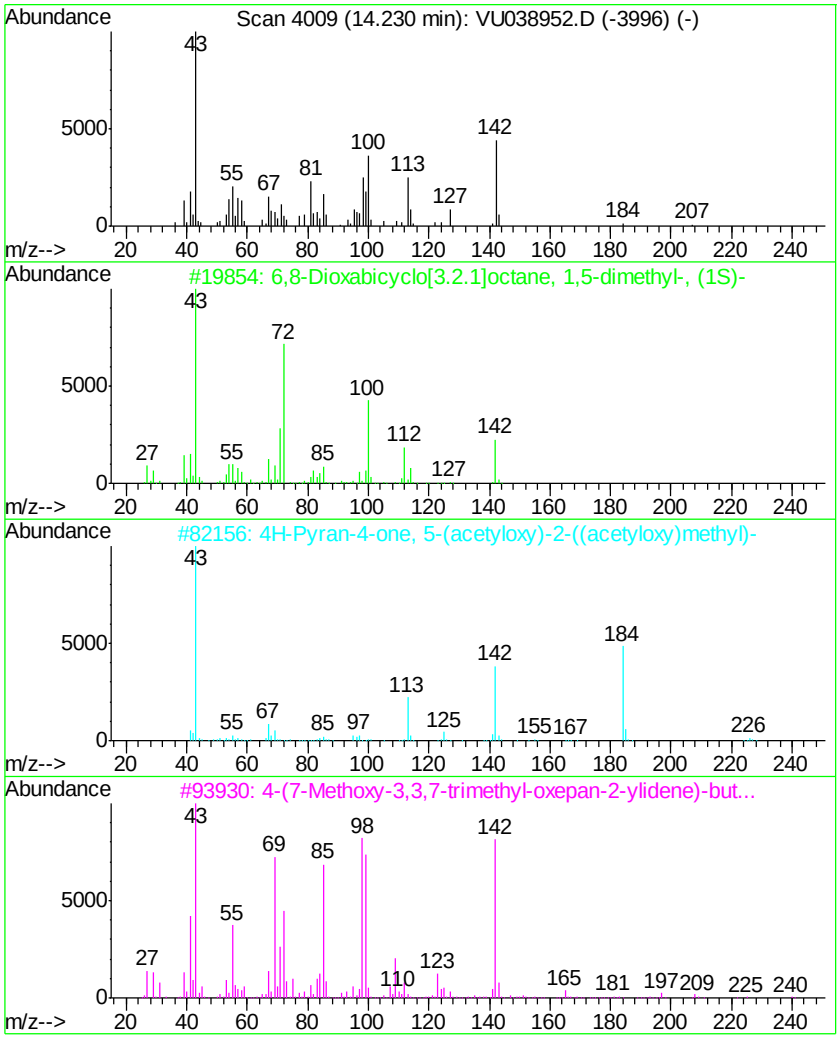
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

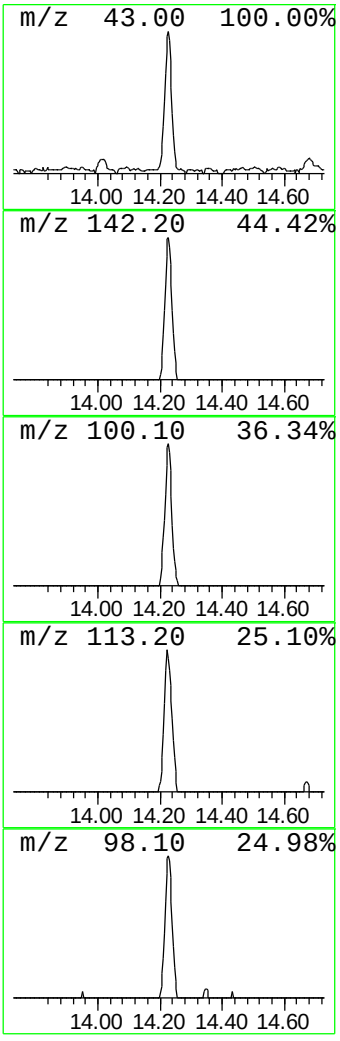
****

Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	0.56 ug/L	90990	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	35
2	4H-Pyran-4-one, 5-(acetyloxy)-2-...	226	C10H10O6	026209-93-8	32
3	4-(7-Methoxy-3,3,7-trimethyl-oxe...	240	C14H24O3	107675-07-0	23
4	2,4,6-Heptanetrione	142	C7H10O3	000626-53-9	17
5	Alloxan	142	C4H2N2O4	000050-71-5	12





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038952.D
Acq On : 17 Jun 2020 18:25
Operator : SY/MD
Sample : L3040-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

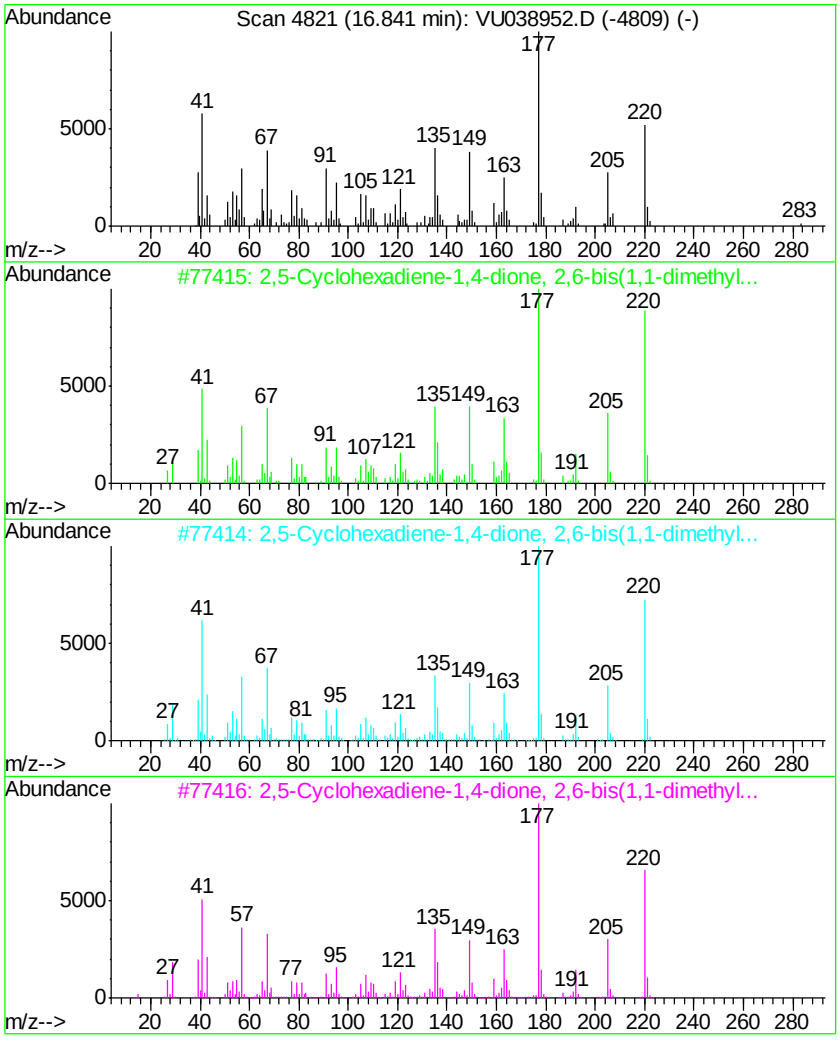
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

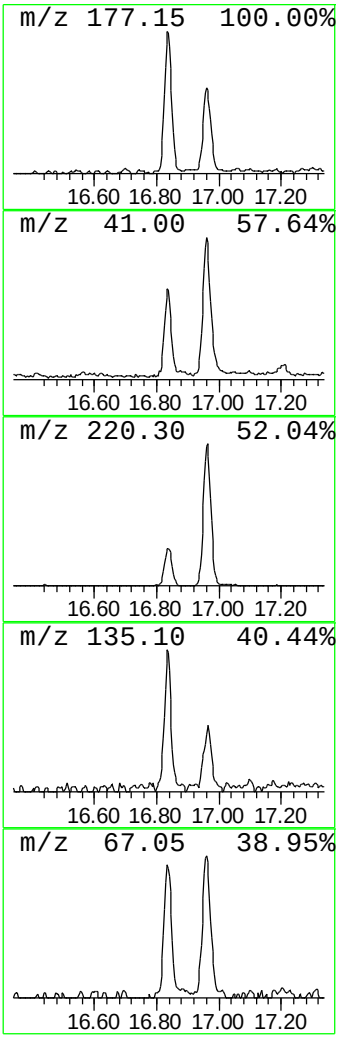
****

Peak Number 5 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.84	0.95 ug/L	155863	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
4	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	47
5	2H-1-Benzopyran, 3,5,6,8a-tetrah...	192	C13H20O	041678-29-9	42





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038952.D
Acq On : 17 Jun 2020 18:25
Operator : SY/MD
Sample : L3040-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

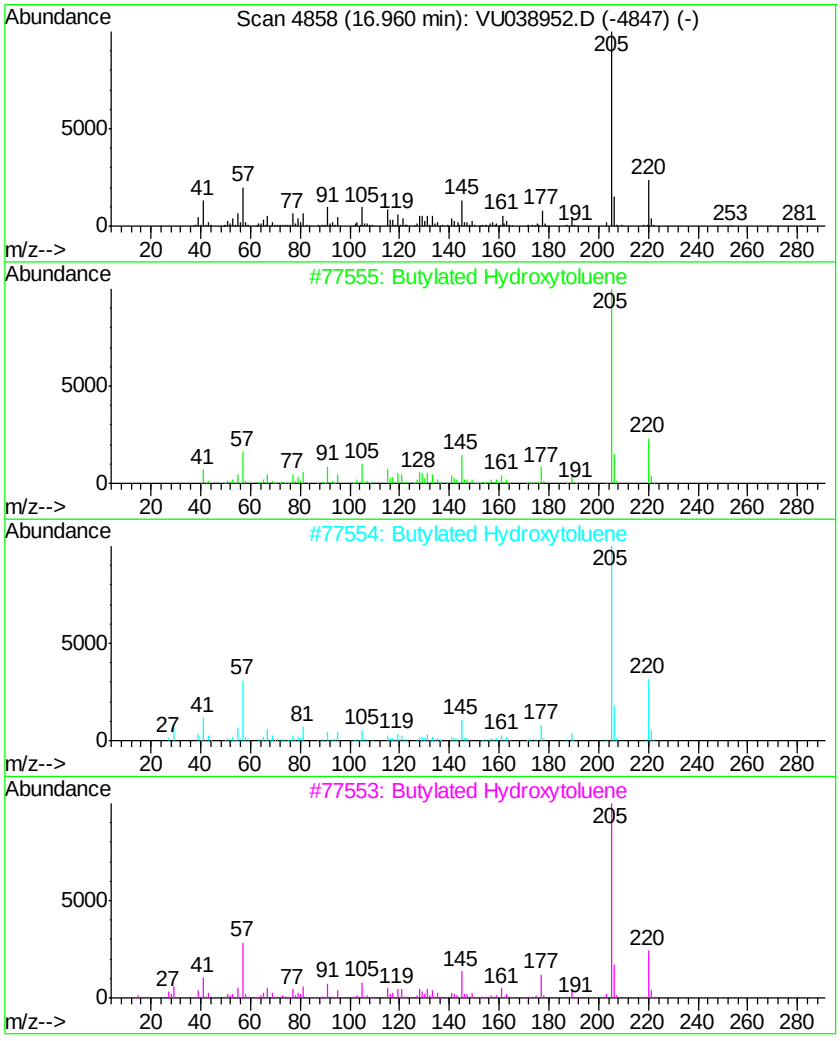
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

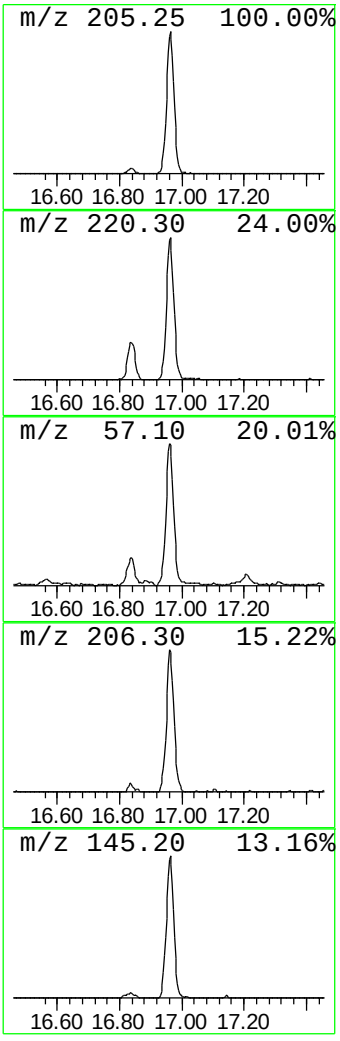
****

Peak Number 6 Butylated Hydroxytoluene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	2.98 ug/L	486563	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
3	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	95
4	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	93
5	Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038952.D
Acq On : 17 Jun 2020 18:25
Operator : SY/MD
Sample : L3040-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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-Butanone, 3,3-d...	7.22	0.5	ug/L	63453	1	6.30	632072	5.0
1-Hexanol, 2-ethyl-	12.08	3.2	ug/L	517101	3	11.83	816481	5.0
unknown-01	14.23	0.6	ug/L	90990	3	11.83	816481	5.0
2,5-Cyclohexadien...	16.84	0.9	ug/L	155863	3	11.83	816481	5.0
Butylated Hydroxy...	16.96	3.0	ug/L	486563	3	11.83	816481	5.0