LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038950.D
Acq On : 17 Jun 2020 17:39
Operator : SY/MD
Sample : L3040-06
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L16

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	1.649	86	96	105	rBV	129655	155542	12.39%	1.211%
2	1.883	150	169	170	rBV	17875	41981	3.35%	0.327%
3	1.967	188	195	208	rBV	107928	135891	10.83%	1.058%
4	2.141	245	249	261	rBV2	16575	33844	2.70%	0.264%
5	2.623	389	399	417	rVB	307674	507158	40.41%	3.949%
6	3.282	594	604	606	rBV	10627	17283	1.38%	0.135%
7	4.514	970	987	1013	rBV8	18969	60470	4.82%	0.471%
8	4.803	1052	1077	1115	rBV	102562	455769	36.32%	3.549%
9	5.147	1166	1184	1202	rBV2	195823	448668	35.75%	3.493%
10	5.623	1323	1332	1349	rBV4	5286	12722	1.01%	0.099%
11	5.803	1369	1388	1416	rBV2	432060	1026256	81.78%	7.990%
12	6.317	1535	1548	1569	rVB	354818	653911	52.11%	5.091%
13	6.755	1670	1684	1708	rBV	252908	507937	40.48%	3.955%
14	7.234	1821	1833	1847	rVB2	37353	73250	5.84%	0.570%
15	7.613	1937	1951	1964	rVB	125711	216542	17.26%	1.686%
16	7.848	2012	2024	2034	rBV2	13664	27626	2.20%	0.215%
17	7.941	2040	2053	2068	rVB	451959	761917	60.71%	5.932%
18	8.082	2089	2097	2108	rVB2	11202	19360	1.54%	0.151%
19	8.218	2127	2139	2153	rBV2	84633	141720	11.29%	1.103%
20	8.523	2220	2234	2245	rBV5	7144	18671	1.49%	0.145%
21	8.591	2245	2255	2265	rVB6	13033	21184	1.69%	0.165%
22	8.677	2265	2282	2292	rBV	715457	1254940	100.00%	9.771%
23	8.816	2320	2325	2337	rVB5	13599	22672	1.81%	0.177%
24	8.947	2353	2366	2376	rBV4	6931	15100	1.20%	0.118%
25	9.443	2508	2520	2536	rBV	504510	836509	66.66%	6.513%
26	9.661	2583	2588	2596	rVB2	14316	19549	1.56%	0.152%
27	9.793	2617	2629	2644	rBV4	12123	28769	2.29%	0.224%
28	9.941	2658	2675	2687	rBV	41901	69842	5.57%	0.544%
29	10.150	2725	2740	2751	rVB5	16326	34844	2.78%	0.271%
30	10.256	2755	2773	2790	rBV	98547	170315	13.57%	1.326%
31	10.365	2799	2807	2829	rVB10	13755	35400	2.82%	0.276%
32	10.703	2904	2912	2922	rVB2	24454	38529	3.07%	0.300%
33	10.774	2923	2934	2948	rBV	209236	342347	27.28%	2.666%
34	10.983	2984	2999	3014	rBV	44197	75025	5.98%	0.584%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038950.D
Acq On : 17 Jun 2020 17:39
Operator : SY/MD
Sample : L3040-06
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L16

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	11.066	3015	3025	3037	rBV4	15293	25654	2.04%	0.200%
36	11.484	3145	3155	3163	rBV4	18574	26516	2.11%	0.206%
37	11.587	3176	3187	3198	rBV	148403	234715	18.70%	1.827%
38	11.661	3203	3210	3216	rVV4	14972	28690	2.29%	0.223%
39	11.700	3217	3222	3231	rVV8	15185	24219	1.93%	0.189%
40	11.754	3232	3239	3248	rVV8	9382	17097	1.36%	0.133%
41	11.825	3248	3261	3277	rVB	547044	866383	69.04%	6.746%
42	11.986	3308	3311	3324	rVB5	10487	14209	1.13%	0.111%
43	12.076	3327	3339	3367	rBV	208716	475624	37.90%	3.703%
44	12.205	3368	3379	3400	rVB	509882	846458	67.45%	6.591%
45	12.340	3412	3421	3426	rBV2	19038	30485	2.43%	0.237%
46	12.372	3427	3431	3451	rVB4	17129	29565	2.36%	0.230%
47	12.549	3482	3486	3496	rVB6	9775	15323	1.22%	0.119%
48	12.793	3550	3562	3572	rBV	182800	284032	22.63%	2.211%
49	12.838	3572	3576	3590	rVV4	15813	32029	2.55%	0.249%
50	12.905	3590	3597	3610	rVV6	22790	40242	3.21%	0.313%
51	12.973	3610	3618	3627	rVV7	9426	15658	1.25%	0.122%
52	13.028	3627	3635	3643	rVB4	9377	13239	1.05%	0.103%
53	13.166	3667	3678	3689	rVB	13062	21927	1.75%	0.171%
54	13.233	3691	3699	3712	rBV	6722	12699	1.01%	0.099%
55	13.639	3818	3825	3835	rVB3	13748	18137	1.45%	0.141%
56	14.015	3934	3942	3950	rBV9	11251	16780	1.34%	0.131%
57	14.092	3954	3966	3973	rBV10	11084	19831	1.58%	0.154%
58	14.227	3997	4008	4021	rBV	96160	149648	11.92%	1.165%
59	14.349	4040	4046	4057	rVB7	8568	13882	1.11%	0.108%
60	14.680	4141	4149	4161	rBV7	8727	19462	1.55%	0.152%
61	14.873	4200	4209	4214	rBV4	9426	16355	1.30%	0.127%
62	14.921	4218	4224	4234	rVB7	15062	24534	1.95%	0.191%
63	15.745	4463	4480	4492	rVB8	21539	40640	3.24%	0.316%
64	16.192	4610	4619	4632	rBV4	25698	39440	3.14%	0.307%
65	16.835	4810	4819	4834	rBV3	71572	117110	9.33%	0.912%
66	16.963	4845	4859	4876	rBV	613548	1031416	82.19%	8.031%

Sum of corrected areas: 12843542

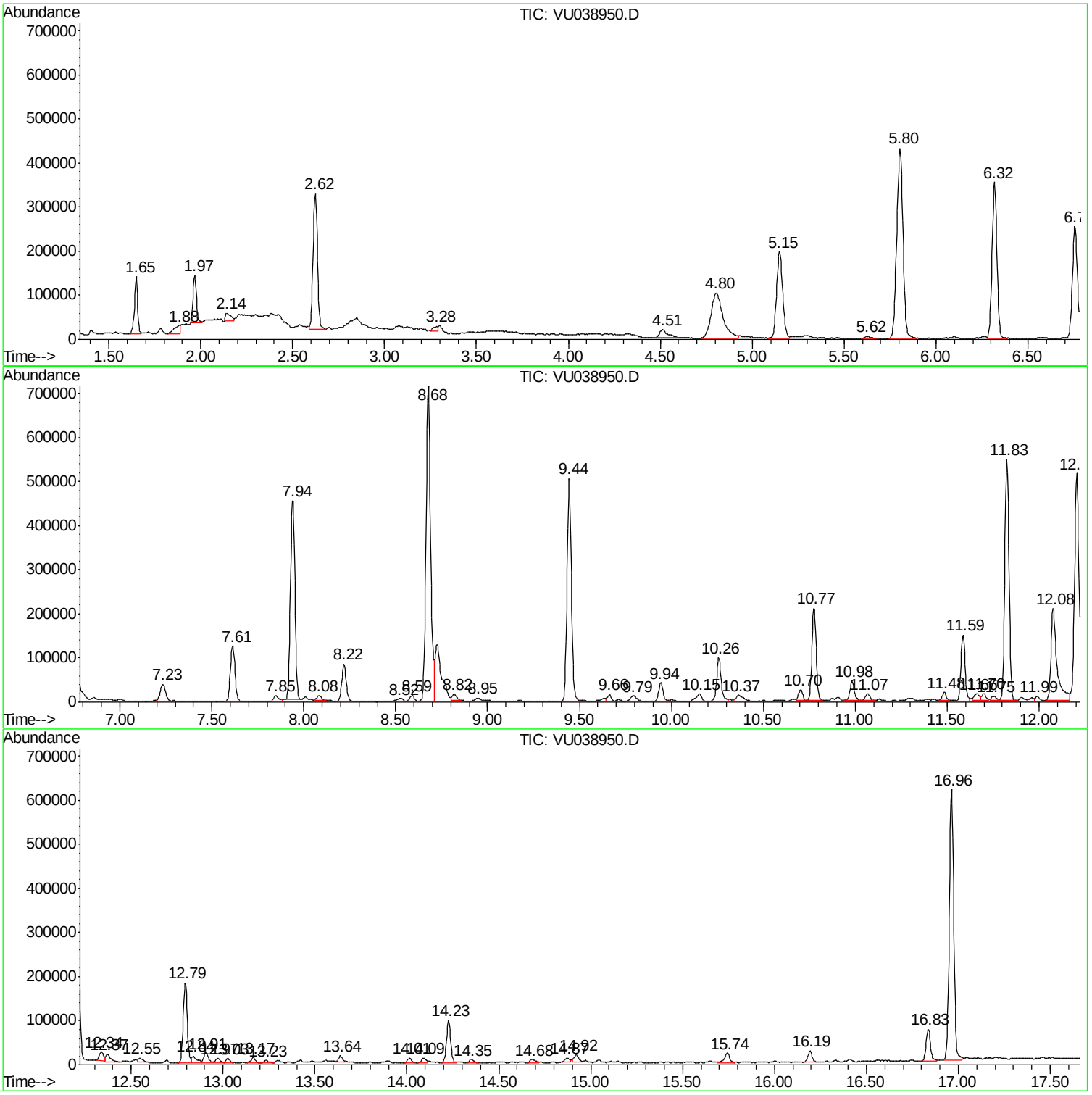
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038950.D
Acq On : 17 Jun 2020 17:39
Operator : SY/MD
Sample : L3040-06
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L16

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 : VU038950.D
Acq On : 17 Jun 2020 17:39
Operator : SY/MD
Sample : L3040-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L16

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

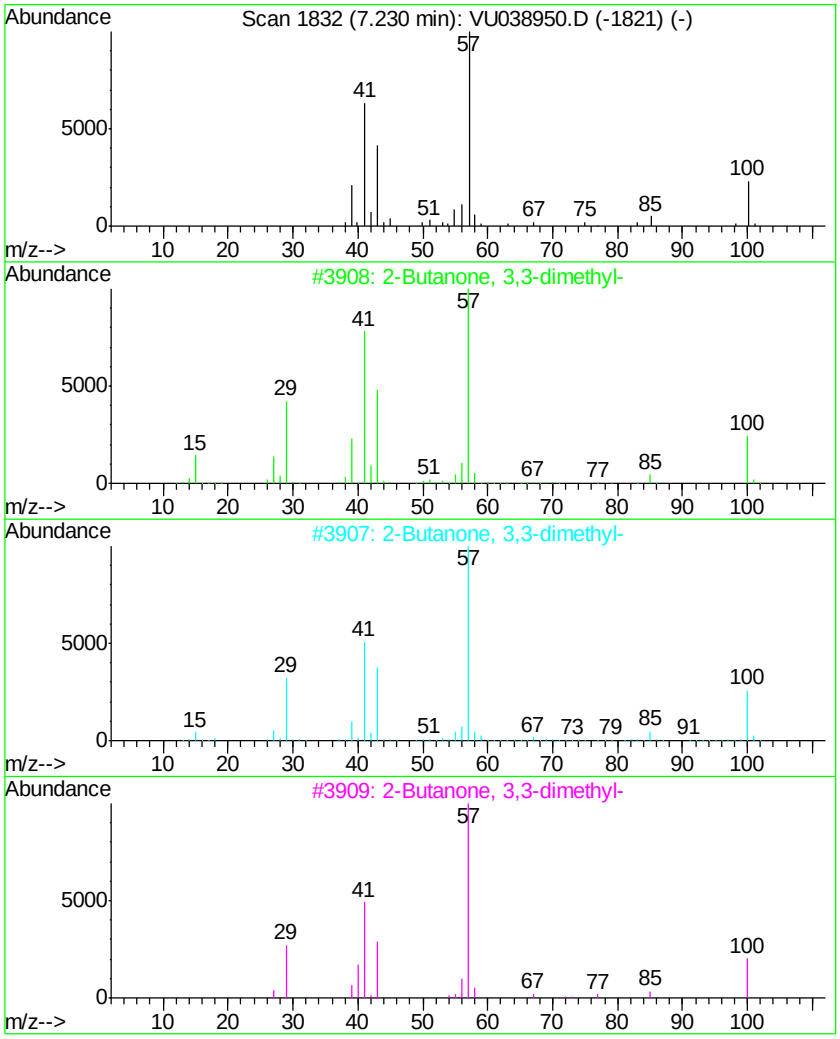
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

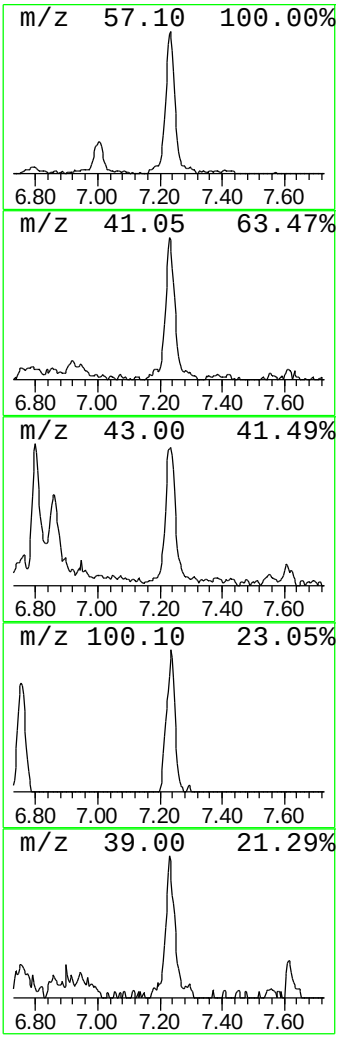
****

Peak Number 1 2-Butanone, 3,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	0.56 ug/L	73250	1,4-Difluorobenzene	6.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	80
2	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	80
3	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	64
4	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
5	3-Hexanone	100	C6H12O	000589-38-8	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038950.D
Acq On : 17 Jun 2020 17:39
Operator : SY/MD
Sample : L3040-06
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L16

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

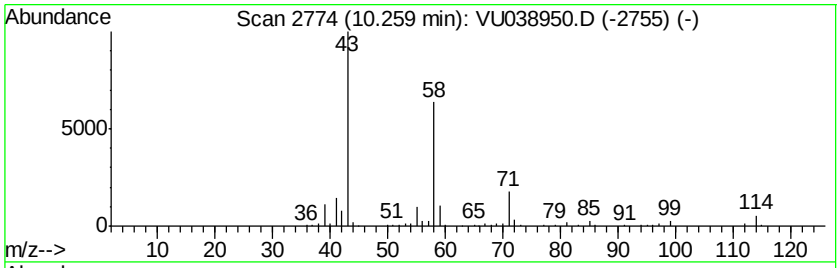
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

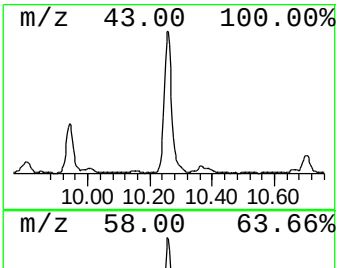
****

Peak Number 3 2-Heptanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	1.02 ug/L	170315	Chlorobenzene-d5	9.44

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	90
4	2-Heptanone	114	C7H14O	000110-43-0	80
5	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038950.D
Acq On : 17 Jun 2020 17:39
Operator : SY/MD
Sample : L3040-06
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L16

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

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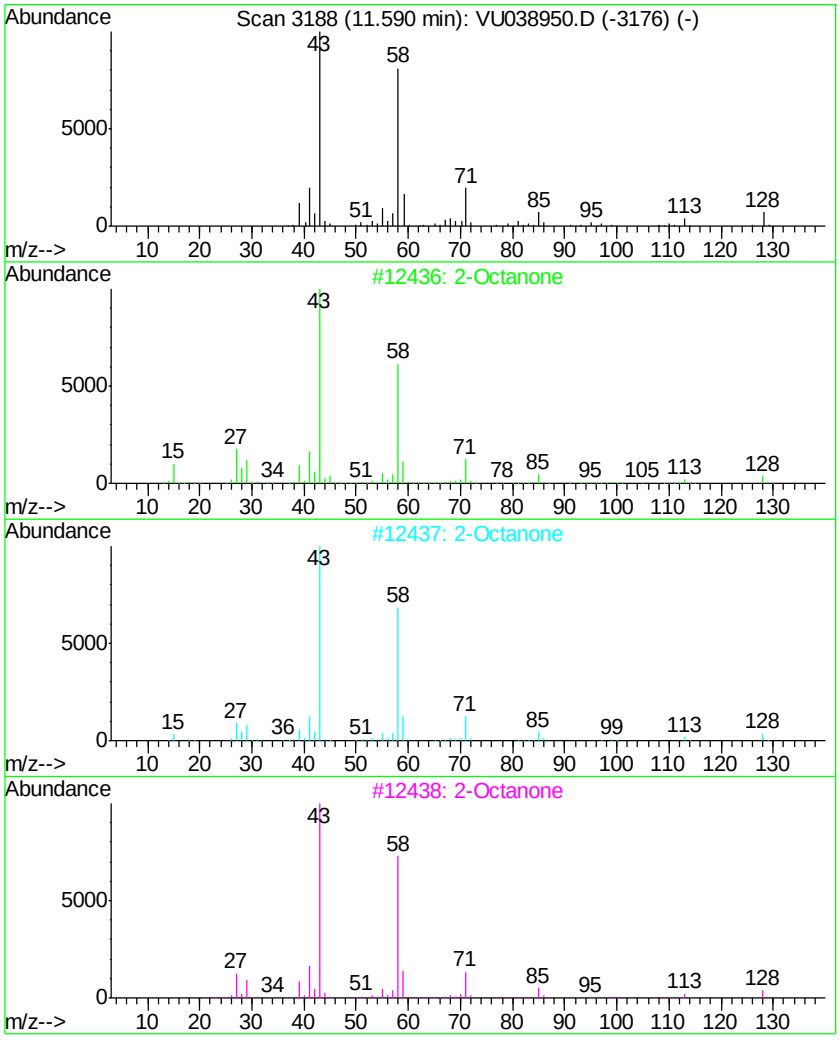
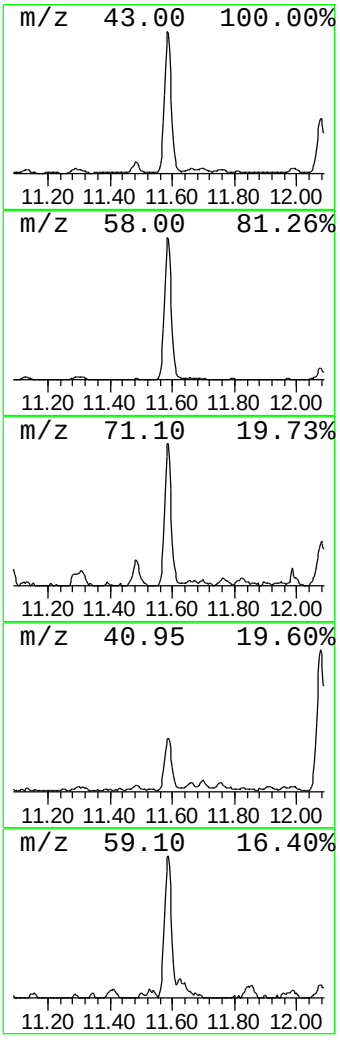
Peak Number 4 2-Octanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	1.35 ug/L	234715	1,4-Dichlorobenzene-d4	11.83

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	91
4	2-Octanone	128	C8H16O	000111-13-7	91
5	2-Octanone	128	C8H16O	000111-13-7	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038950.D
Acq On : 17 Jun 2020 17:39
Operator : SY/MD
Sample : L3040-06
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L16

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

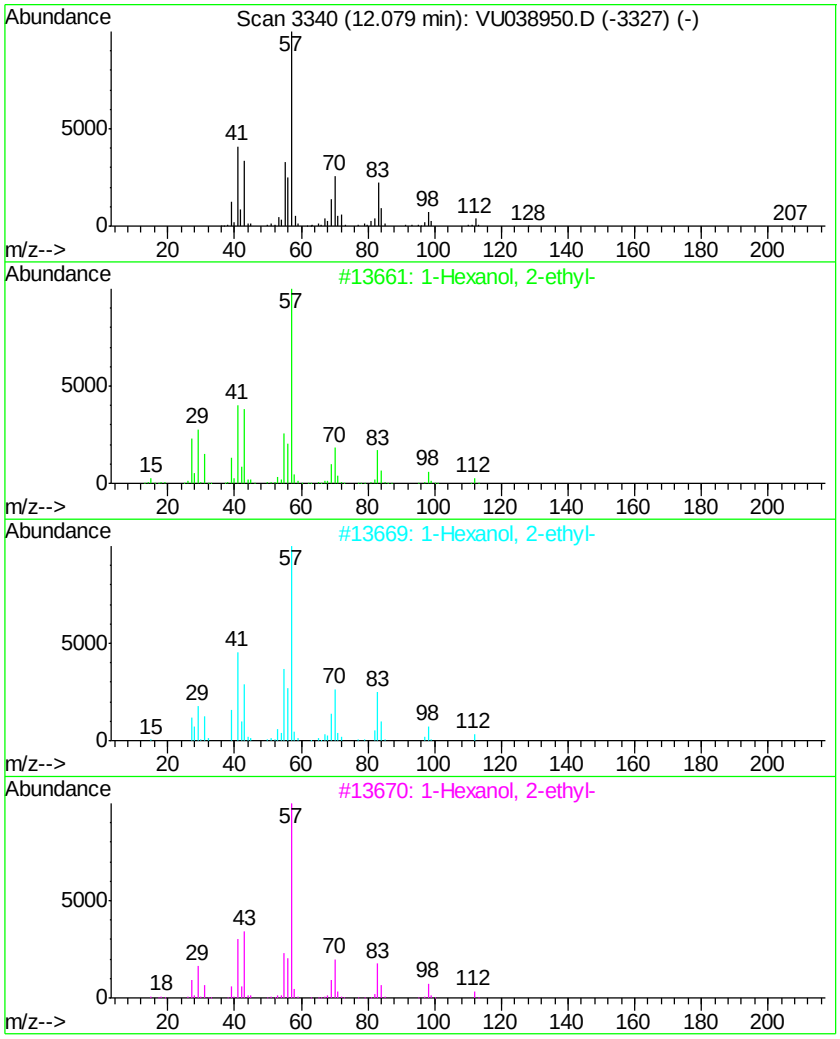
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

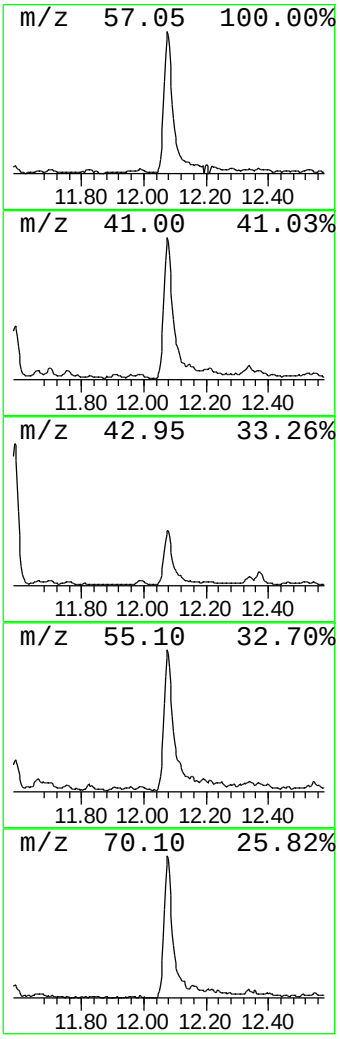
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	2.74 ug/L	475624	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	83
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038950.D
Acq On : 17 Jun 2020 17:39
Operator : SY/MD
Sample : L3040-06
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L16

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

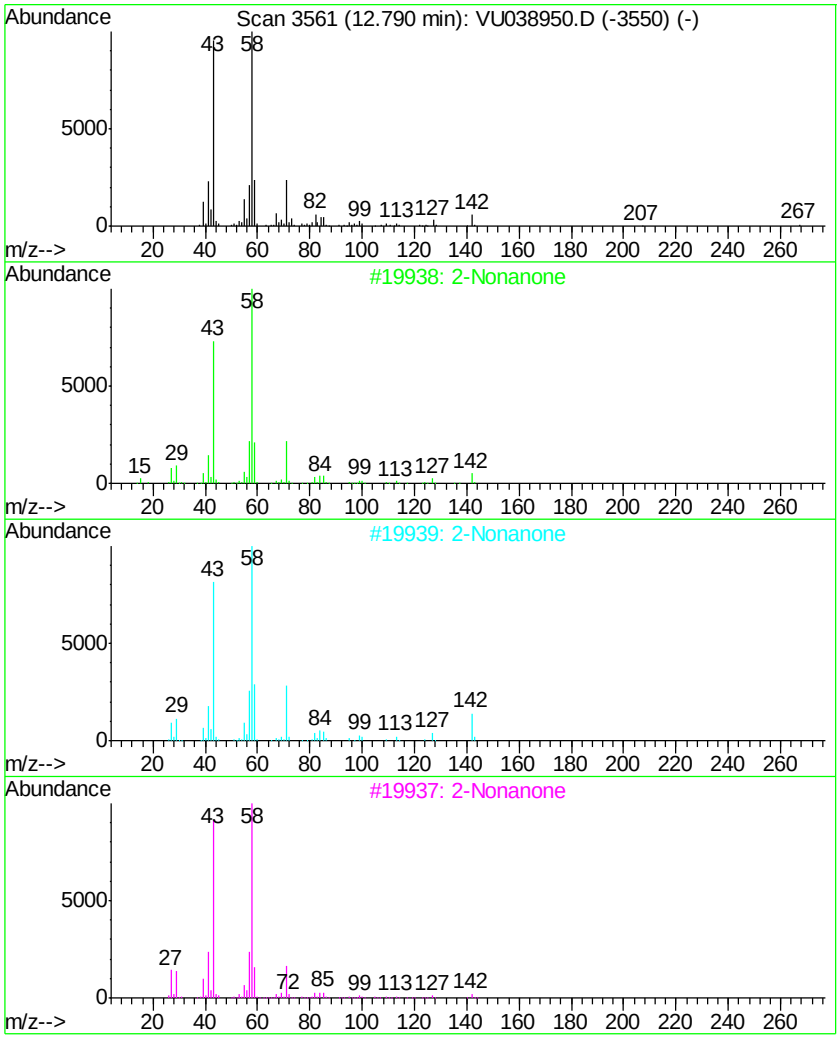
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

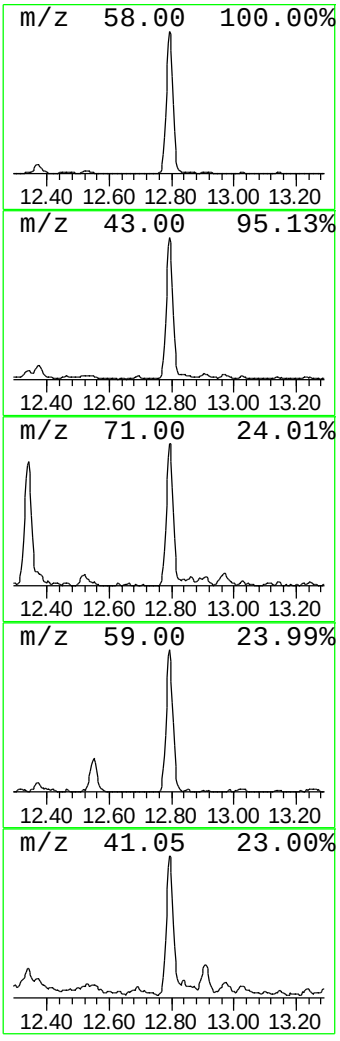
****

Peak Number 6 2-Nonanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	1.64 ug/L	284032	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone	142	C9H18O	000821-55-6	97
2	2-Nonanone	142	C9H18O	000821-55-6	91
3	2-Nonanone	142	C9H18O	000821-55-6	87
4	2-Dodecanone	184	C12H24O	006175-49-1	72
5	2-Decanone	156	C10H20O	000693-54-9	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038950.D
Acq On : 17 Jun 2020 17:39
Operator : SY/MD
Sample : L3040-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L16

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

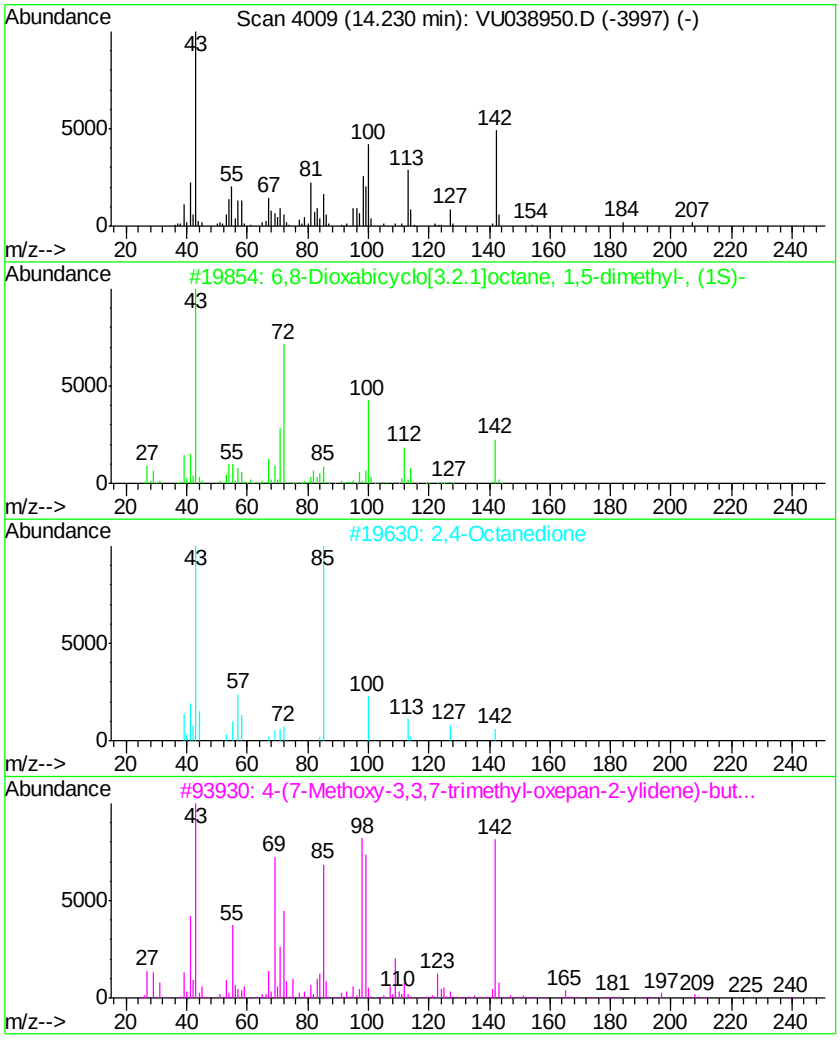
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

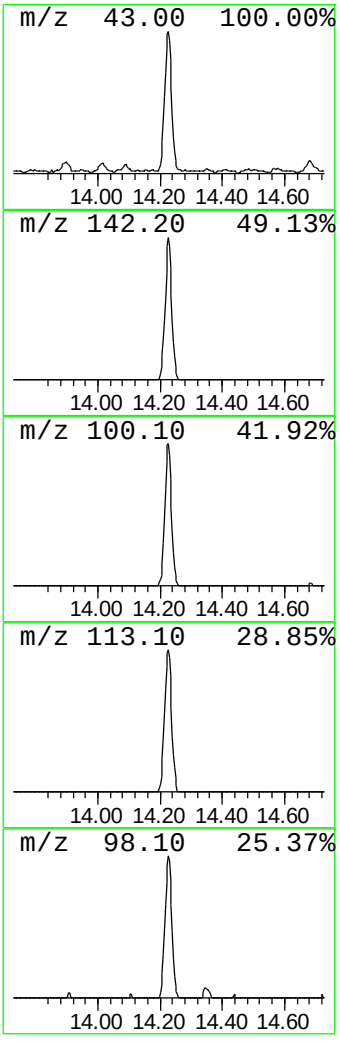
****

Peak Number 7 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	0.86 ug/L	149648	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	2,4-Octanedione	142	C8H14O2	014090-87-0	32
3	4-(7-Methoxy-3,3,7-trimethyl-oxe...	240	C14H24O3	107675-07-0	32
4	3-n-Propyl-2,4-pentanedione	142	C8H14O2	001540-35-8	25
5	1,4,6-Trimethyl-3,7,9-trioxabicy...	172	C9H16O3	062759-58-4	22





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038950.D
Acq On : 17 Jun 2020 17:39
Operator : SY/MD
Sample : L3040-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L16

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

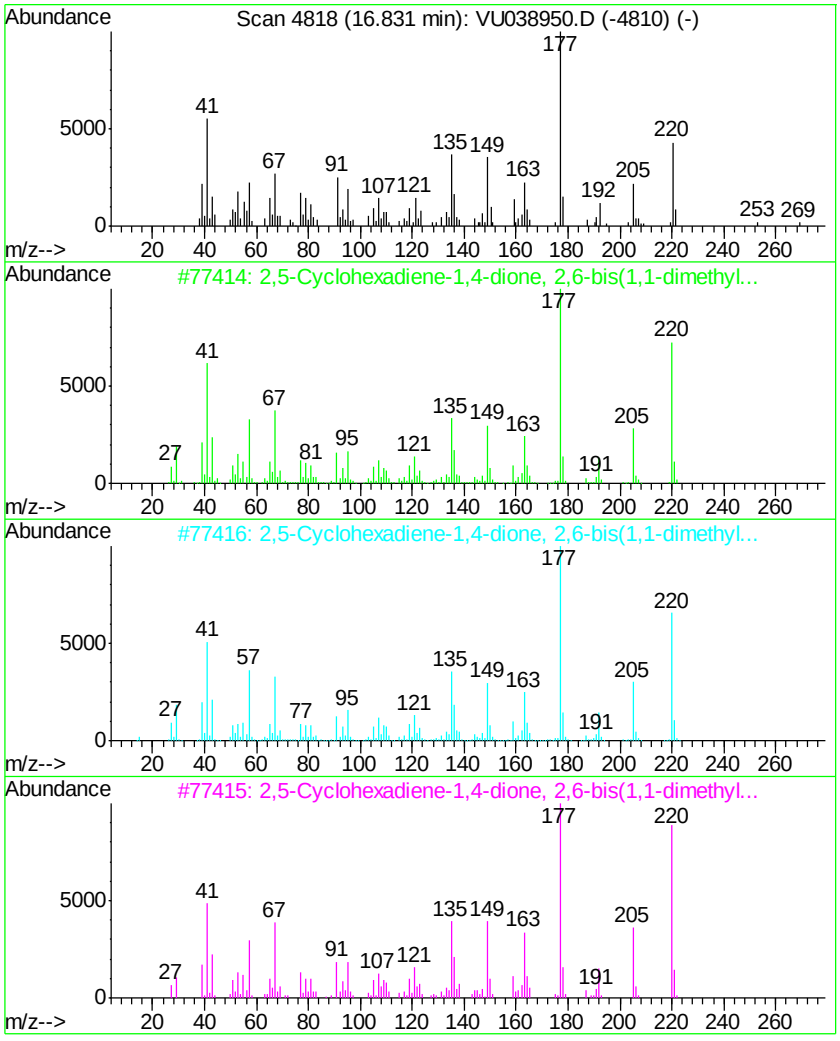
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

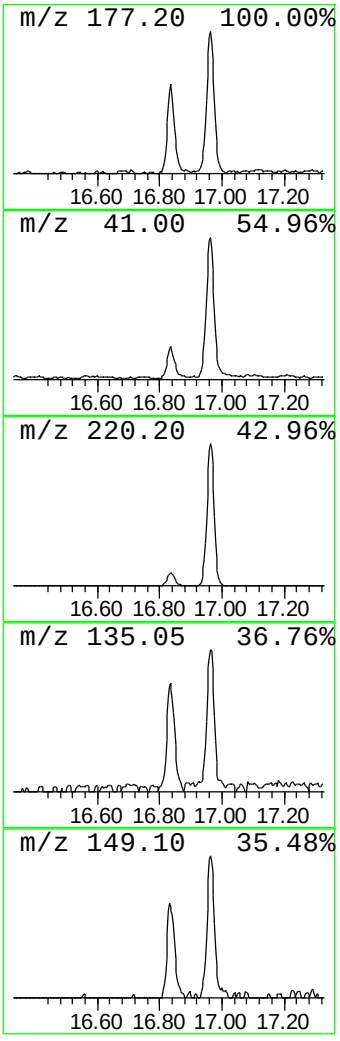
****

Peak Number 8 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.83	0.68 ug/L	117110	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	99
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	97
4	trans-.beta.-Ionone	192	C13H20O	000079-77-6	43
5	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	42





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038950.D
Acq On : 17 Jun 2020 17:39
Operator : SY/MD
Sample : L3040-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L16

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

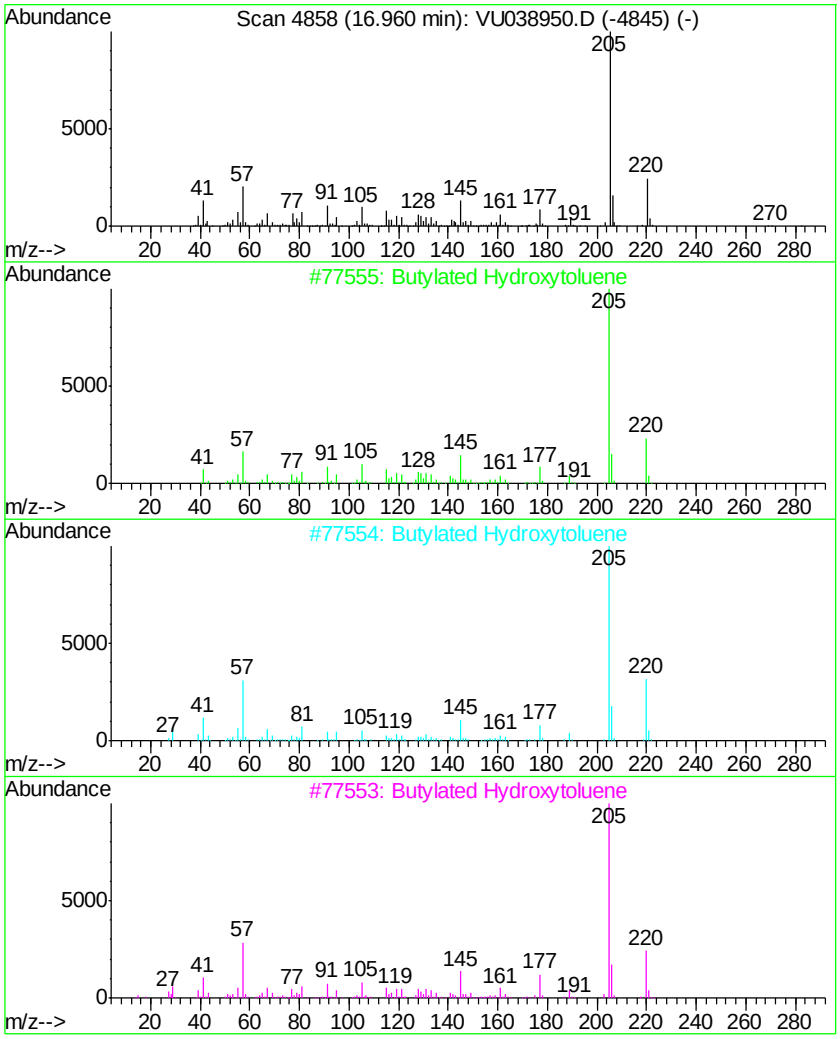
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

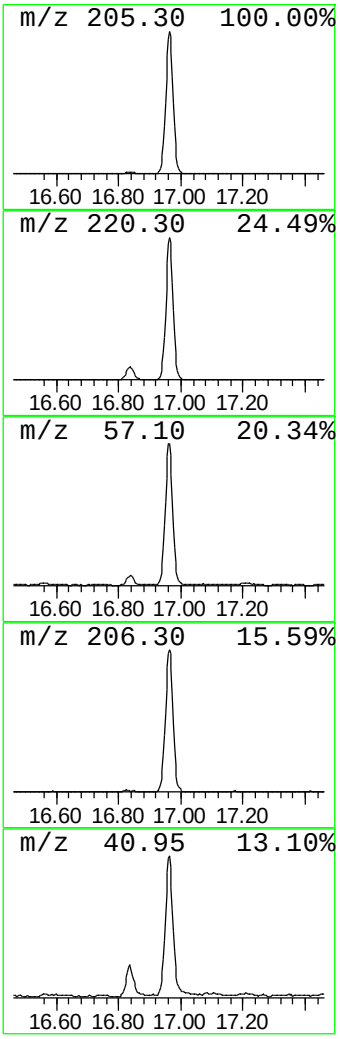
****

Peak Number 9 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	5.95 ug/L	1031420	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	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
5	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038950.D
Acq On : 17 Jun 2020 17:39
Operator : SY/MD
Sample : L3040-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L16

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...	7.23	0.6	ug/L	73250	1	6.32	653911	5.0
2-Heptanone	10.26	1.0	ug/L	170315	2	9.44	836509	5.0
2-Octanone	11.59	1.4	ug/L	234715	3	11.83	866383	5.0
1-Hexanol, 2-ethyl-	12.08	2.7	ug/L	475624	3	11.83	866383	5.0
2-Nonanone	12.79	1.6	ug/L	284032	3	11.83	866383	5.0
unknown-01	14.23	0.9	ug/L	149648	3	11.83	866383	5.0
2,5-Cyclohexadien...	16.83	0.7	ug/L	117110	3	11.83	866383	5.0
Butylated Hydroxy...	16.96	6.0	ug/L	1031420	3	11.83	866383	5.0