LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042123.D
Acq On : 20 Jan 2021 22:45
Operator : SY/MD
Sample : M1180-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E09

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\SOMUTR012021WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC: VU042123.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.440	24	31	39	rVB2	3383	5769	1.00%	0.114%
2	1.591	69	78	86	rVB	50049	59653	10.37%	1.182%
3	1.910	170	177	190	rVB	40681	50072	8.71%	0.992%
4	2.045	209	219	229	rBV3	3834	8541	1.48%	0.169%
5	2.562	370	380	394	rVB	82750	128763	22.39%	2.551%
6	4.717	1027	1050	1087	rBV	38443	167243	29.08%	3.313%
7	5.070	1147	1160	1178	rVB	82349	176931	30.76%	3.505%
8	5.726	1343	1364	1388	rBV2	177247	419565	72.95%	8.312%
9	6.253	1516	1528	1545	rVV	145137	271741	47.25%	5.384%
10	6.700	1654	1667	1688	rBV	100853	196166	34.11%	3.886%
11	6.806	1692	1700	1717	rVV3	5336	10952	1.90%	0.217%
12	7.186	1801	1818	1836	rBV	17126	34809	6.05%	0.690%
13	7.575	1925	1939	1953	rBV	60730	105402	18.33%	2.088%
14	7.813	2003	2013	2023	rBV2	10791	20499	3.56%	0.406%
15	7.903	2029	2041	2057	rVB	201576	342228	59.50%	6.780%
16	8.051	2079	2087	2098	rVB4	5015	8913	1.55%	0.177%
17	8.189	2119	2130	2144	rBV	38818	64201	11.16%	1.272%
18	8.504	2215	2228	2236	rVB5	3113	6207	1.08%	0.123%
19	8.559	2236	2245	2255	rBV5	5885	9259	1.61%	0.183%
20	8.652	2260	2274	2284	rBV	242017	436852	75.95%	8.655%
21	8.700	2285	2289	2313	rVV5	48622	88147	15.33%	1.746%
22	8.925	2345	2359	2368	rBV4	3115	7150	1.24%	0.142%
23	9.424	2501	2514	2535	rBV	203636	335446	58.32%	6.646%
24	9.649	2576	2584	2593	rVB2	10379	15870	2.76%	0.314%
25	9.781	2609	2625	2639	rVB4	5952	14325	2.49%	0.284%
26	9.929	2658	2671	2683	rBV2	15530	27242	4.74%	0.540%
27	10.141	2719	2737	2748	rBV5	5090	11702	2.03%	0.232%
28	10.247	2754	2770	2783	rBV	21868	39715	6.90%	0.787%
29	10.353	2796	2803	2811	rBV7	4678	6948	1.21%	0.138%
30	10.694	2900	2909	2921	rVB2	12804	19885	3.46%	0.394%
31	10.765	2921	2931	2945	rBV	77394	123377	21.45%	2.444%
32	10.974	2982	2996	3010	rVV	19125	31774	5.52%	0.629%
33	11.057	3013	3022	3034	rVB3	8556	14378	2.50%	0.285%
34	11.475	3146	3152	3163	rVB3	6736	9860	1.71%	0.195%
35	11.578	3176	3184	3196	rBV	12883	19391	3.37%	0.384%
36	11.819	3247	3259	3273	rVB	219038	341875	59.44%	6.773%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042123.D
Acq On : 20 Jan 2021 22:45
Operator : SY/MD
Sample : M1180-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E09

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\SOMUTR012021WMA.M
Title : TRACE VOA SOM01.0

37	11.983	3305	3310	3323	rVB7	3669	6328	1.10%	0.125%
38	12.070	3324	3337	3366	rBV	308929	575174	100.00%	11.395%
39	12.202	3367	3378	3395	rVB	200885	331481	57.63%	6.567%
40	12.330	3411	3418	3425	rBV	5525	8619	1.50%	0.171%
41	12.536	3477	3482	3494	rVB5	4301	6789	1.18%	0.135%
42	12.781	3549	3558	3568	rBV	12003	17434	3.03%	0.345%
43	12.893	3583	3593	3605	rVB6	8158	13611	2.37%	0.270%
44	13.616	3810	3818	3827	rVB2	8178	11528	2.00%	0.228%
45	14.202	3989	4000	4012	rBV	48974	73245	12.73%	1.451%
46	14.652	4131	4140	4148	rBV7	4642	8501	1.48%	0.168%
47	15.703	4455	4467	4476	rBV8	11934	19000	3.30%	0.376%
48	16.144	4596	4604	4613	rVB3	13948	19829	3.45%	0.393%
49	16.780	4792	4802	4814	rBV2	64085	97143	16.89%	1.925%
50	16.896	4828	4838	4850	rVB	153560	228000	39.64%	4.517%

Sum of corrected areas: 5047533

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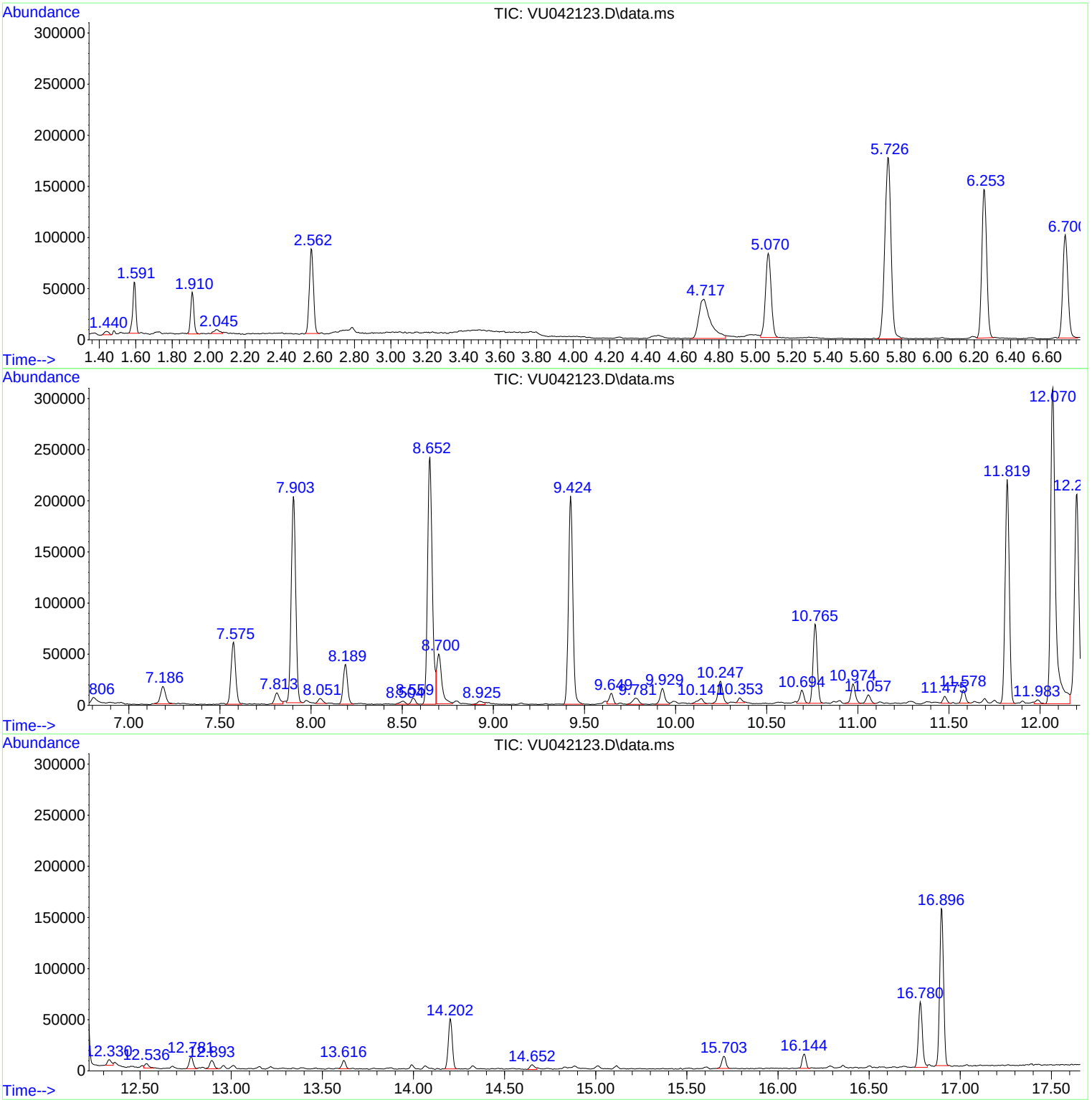
Data File : VU042123.D
Acq On : 20 Jan 2021 22:45
Operator : SY/MD
Sample : M1180-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E09

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.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\VU012021\
Data File : VU042123.D
Acq On : 20 Jan 2021 22:45
Operator : SY/MD
Sample : M1180-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E09

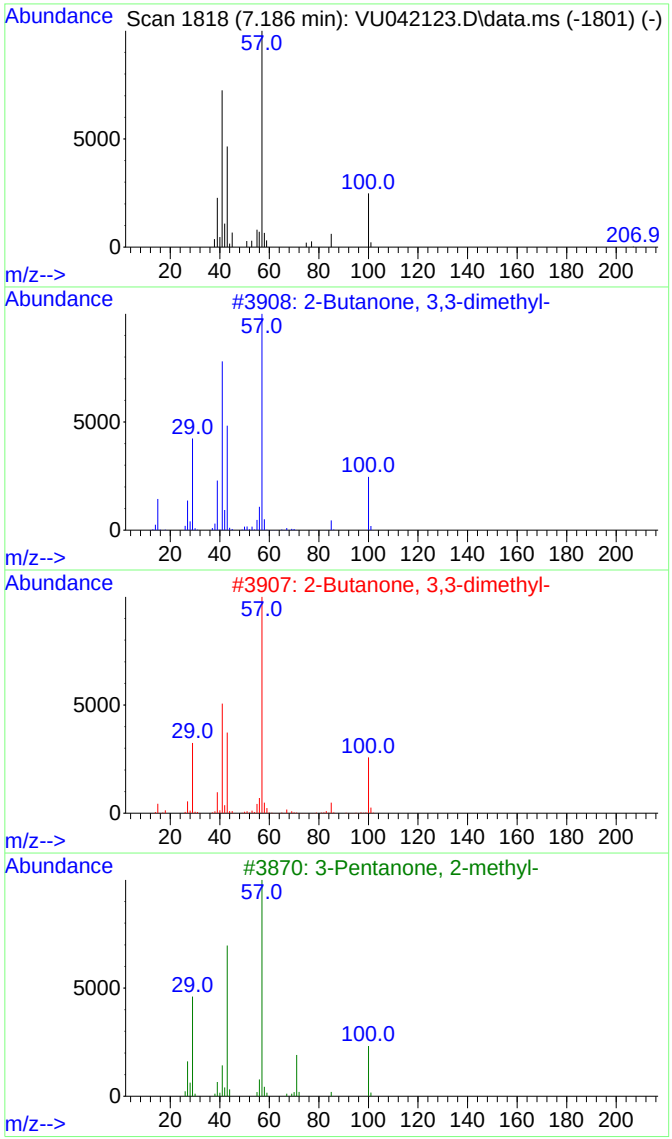
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

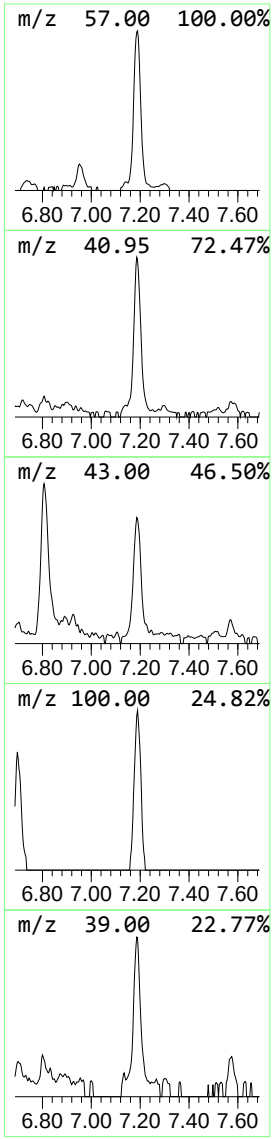
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.186	0.64 ug/L	34809	1,4-Difluorobenzene	6.257

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	59
4	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	58
5	Propane, 1-(ethenyloxy)-2-methyl-	100	C6H12O	000109-53-5	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042123.D
Acq On : 20 Jan 2021 22:45
Operator : SY/MD
Sample : M1180-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E09

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

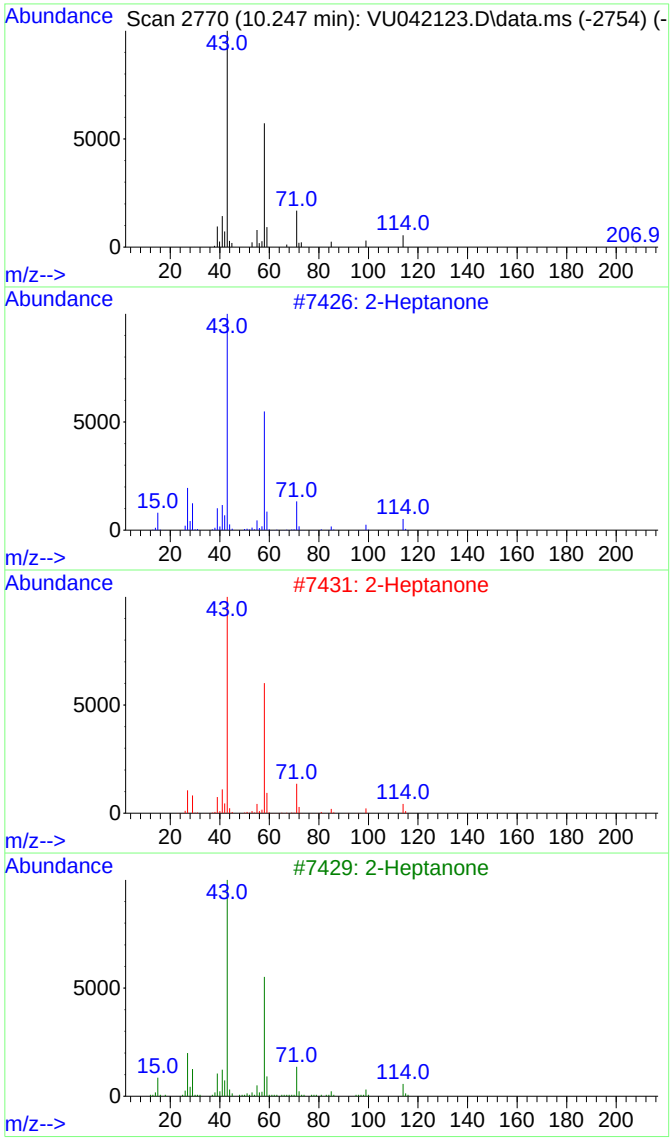
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

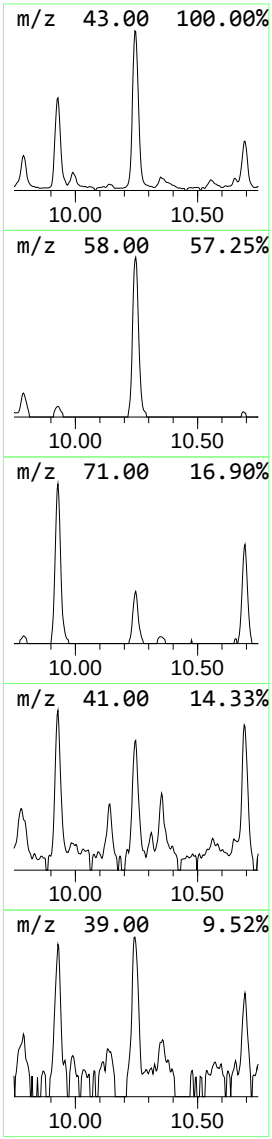
****

Peak Number 3 2-Heptanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.247	0.59 ug/L	39715	Chlorobenzene-d5	9.424

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-Heptanone	114	C7H14O	000110-43-0	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042123.D
Acq On : 20 Jan 2021 22:45
Operator : SY/MD
Sample : M1180-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E09

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

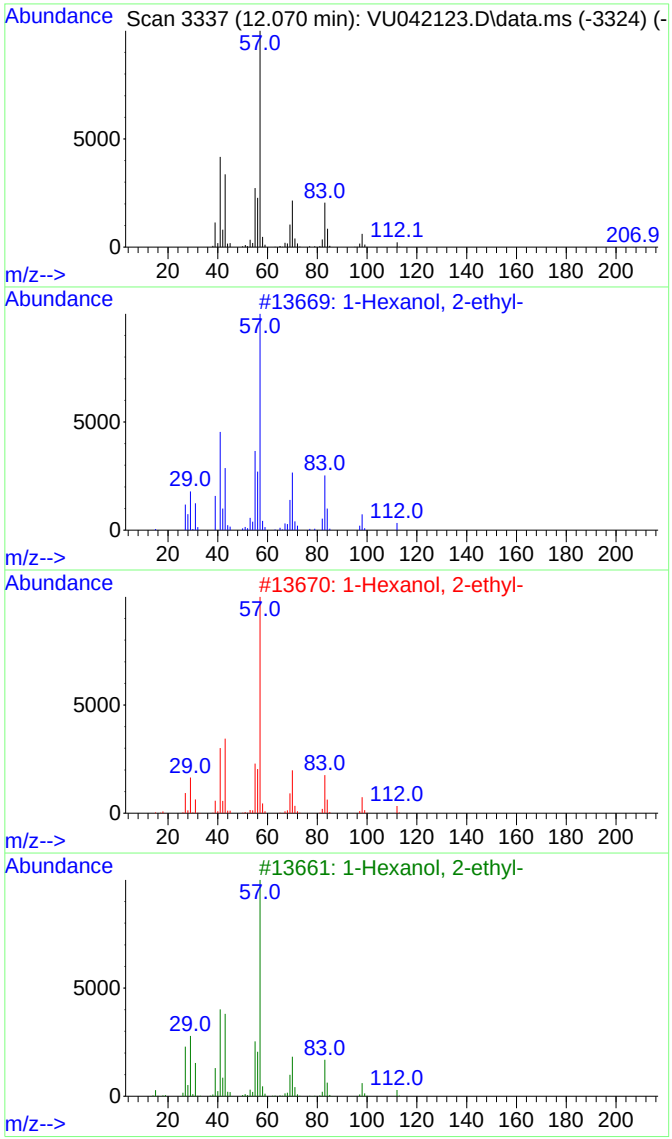
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

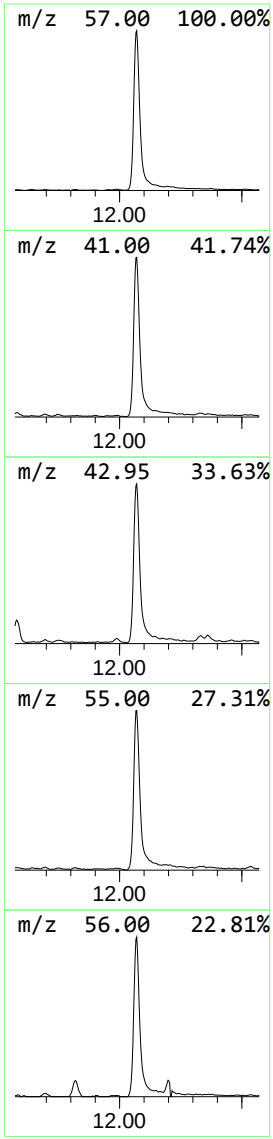
****

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.070	8.41 ug/L	575174	1,4-Dichlorobenzene-d4	11.819

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	83
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042123.D
Acq On : 20 Jan 2021 22:45
Operator : SY/MD
Sample : M1180-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E09

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

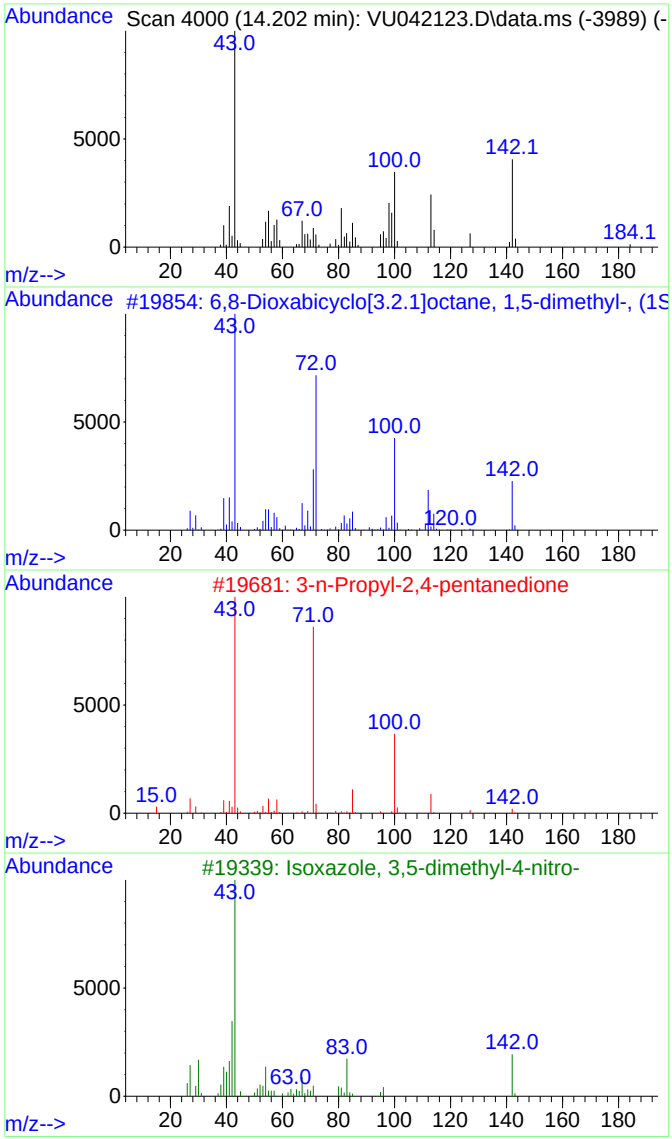
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

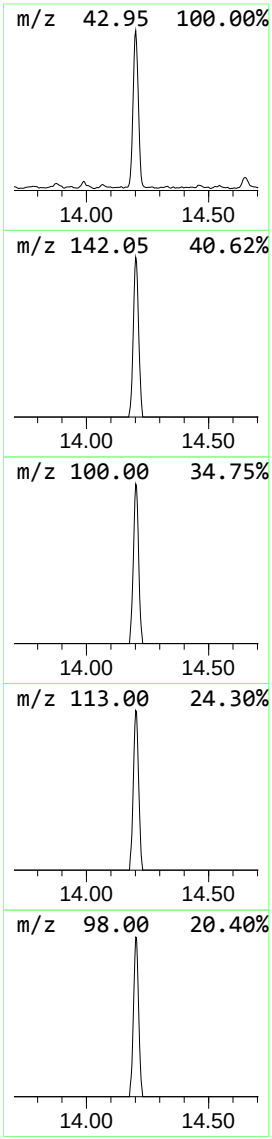
****

Peak Number 5 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.202	1.07 ug/L	73245	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	25
2	3-n-Propyl-2,4-pentanedione	142	C8H14O2	001540-35-8	16
3	Isoxazole, 3,5-dimethyl-4-nitro-	142	C5H6N2O3	001123-49-5	12
4	7-Oxabicyclo[4.1.0]heptan-1-ol, ...	156	C8H12O3	014161-46-7	10
5	6-Dodecanone	184	C12H24O	006064-27-3	10





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Acq On : 20 Jan 2021 22:45
Operator : SY/MD
Sample : M1180-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E09

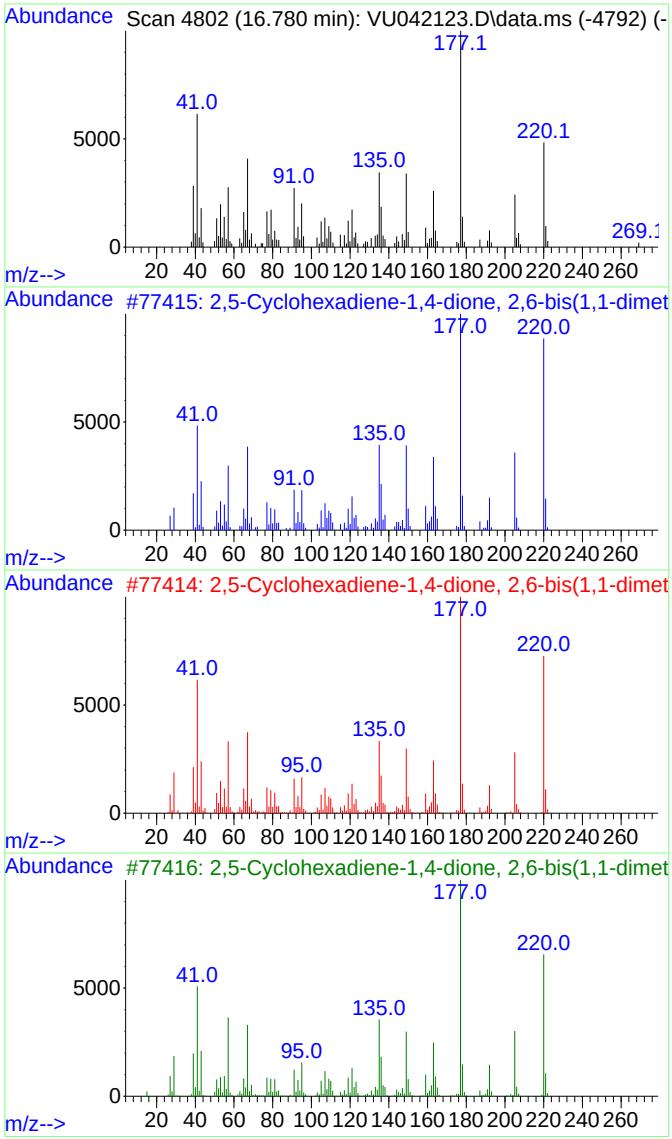
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

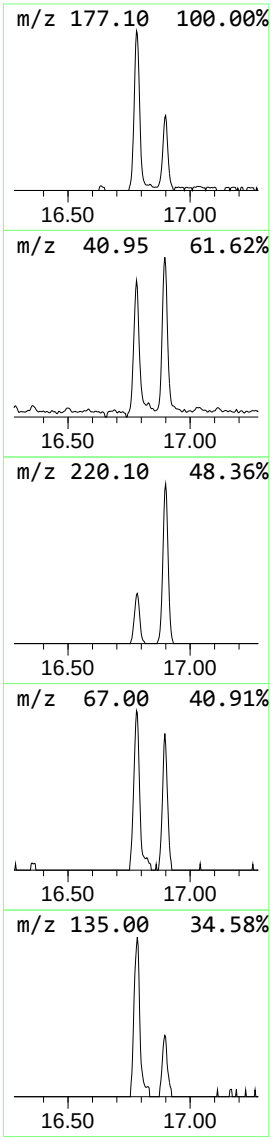
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.780	1.42 ug/L	97143	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	87
4	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	60
5	Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	47





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ClientSampleId : F1E09

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

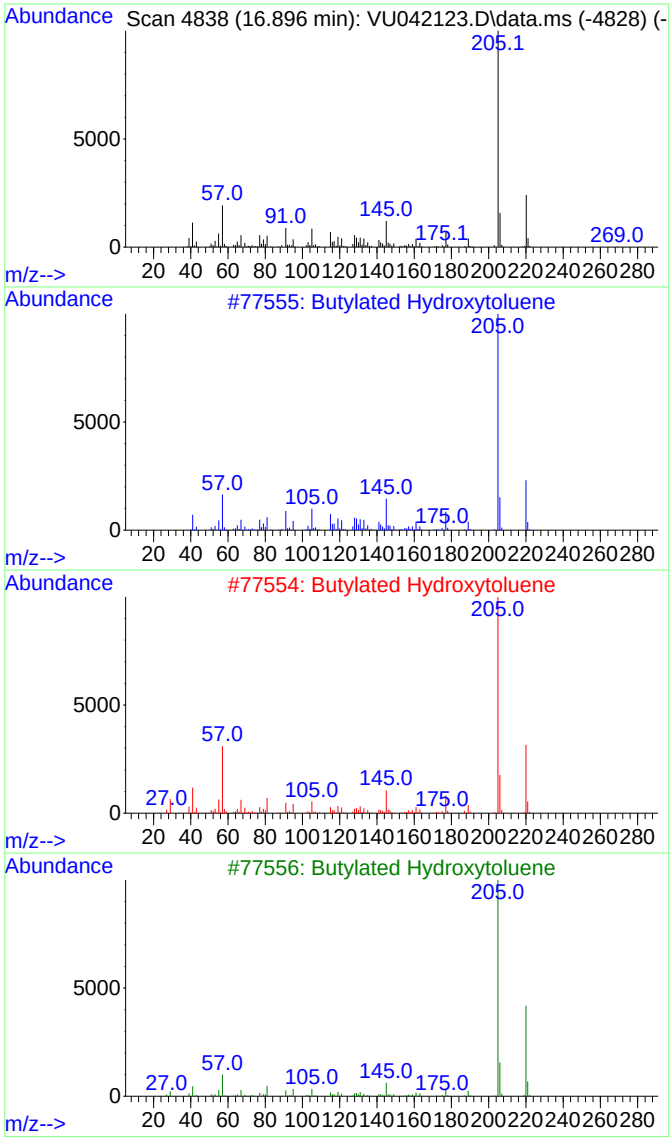
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

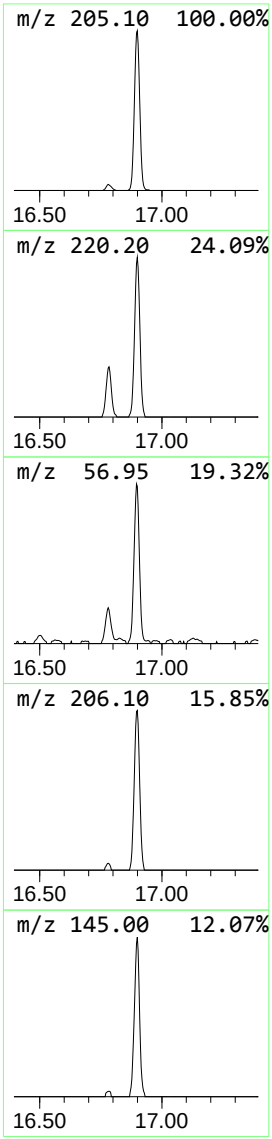
****

Peak Number 7 Butylated Hydroxytoluene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.896	3.33 ug/L	228000	1,4-Dichlorobenzene-d4	11.819

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	94
4	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
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\VU012021\
Data File : VU042123.D
Acq On : 20 Jan 2021 22:45
Operator : SY/MD
Sample : M1180-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E09

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.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...	7.186	0.6	ug/L	34809	1	6.257	271741	5.0
2-Heptanone	10.247	0.6	ug/L	39715	2	9.424	335446	5.0
1-Hexanol, 2-et...	12.070	8.4	ug/L	575174	3	11.819	341875	5.0
unknown-01	14.202	1.1	ug/L	73245	3	11.819	341875	5.0
2,5-Cyclohexadi...	16.780	1.4	ug/L	97143	3	11.819	341875	5.0
Butylated Hydro...	16.896	3.3	ug/L	228000	3	11.819	341875	5.0