LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042119.D
Acq On : 20 Jan 2021 20:36
Operator : SY/MD
Sample : M1180-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E06

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: VU042119.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.360	3	6	21	rVB2	8240	9267	1.85%	0.179%
2	1.433	23	29	39	rBV	4866	7978	1.60%	0.154%
3	1.482	39	44	48	rBV2	7151	6803	1.36%	0.132%
4	1.591	67	78	86	rVB2	54277	78739	15.75%	1.523%
5	1.909	169	177	187	rVB	40101	50522	10.10%	0.977%
6	2.331	299	308	320	rVB2	16318	28355	5.67%	0.548%
7	2.562	369	380	392	rVB	83981	132363	26.47%	2.560%
8	3.385	611	636	638	rBV5	6989	14971	2.99%	0.290%
9	4.472	958	974	992	rVB7	4636	12307	2.46%	0.238%
10	4.681	1021	1039	1083	rBV3	70756	265724	53.14%	5.139%
11	5.073	1146	1161	1181	rBV	80017	175147	35.03%	3.387%
12	5.729	1346	1365	1389	rBV2	168553	422179	84.43%	8.164%
13	6.182	1494	1506	1515	rBV2	2520	5151	1.03%	0.100%
14	6.256	1516	1529	1546	rVB	149834	276854	55.37%	5.354%
15	6.700	1654	1667	1686	rVB	102041	201607	40.32%	3.899%
16	7.179	1793	1816	1839	rBV	87440	183154	36.63%	3.542%
17	7.571	1925	1938	1955	rBV	61414	107106	21.42%	2.071%
18	7.848	2015	2024	2030	rBV4	6498	11718	2.34%	0.227%
19	7.906	2030	2042	2057	rVB	202879	347667	69.53%	6.723%
20	8.047	2076	2086	2098	rVB3	9334	17502	3.50%	0.338%
21	8.186	2118	2129	2145	rBV	39324	66886	13.38%	1.293%
22	8.497	2213	2226	2239	rBV	15905	27725	5.54%	0.536%
23	8.562	2239	2246	2254	rVB10	3353	5233	1.05%	0.101%
24	8.649	2254	2273	2293	rBV	260011	493242	98.65%	9.539%
25	8.797	2311	2319	2331	rVB6	3454	6848	1.37%	0.132%
26	9.423	2502	2514	2533	rBV	203510	348403	69.68%	6.738%
27	9.649	2576	2584	2593	rVB	19651	28869	5.77%	0.558%
28	9.771	2611	2622	2635	rVB4	6120	11931	2.39%	0.231%
29	9.928	2656	2671	2680	rBV3	4518	8186	1.64%	0.158%
30	10.041	2699	2706	2718	rVB5	3306	5205	1.04%	0.101%
31	10.118	2719	2730	2743	rBV8	3210	7601	1.52%	0.147%
32	10.350	2795	2802	2821	rBV8	2818	6936	1.39%	0.134%
33	10.649	2884	2895	2901	rBV3	5382	8757	1.75%	0.169%
34	10.690	2901	2908	2920	rVB2	12847	20139	4.03%	0.389%
35	10.764	2920	2931	2946	rBV2	78554	127913	25.58%	2.474%
36	10.899	2967	2973	2980	rVB5	4162	6358	1.27%	0.123%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042119.D
Acq On : 20 Jan 2021 20:36
Operator : SY/MD
Sample : M1180-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E06

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	10.973	2984	2996	3009	rBV	14619	25516	5.10%	0.493%
38	11.060	3016	3023	3033	rVB4	2833	5031	1.01%	0.097%
39	11.694	3212	3220	3228	rVB6	3916	5899	1.18%	0.114%
40	11.819	3247	3259	3274	rBV	221735	341016	68.20%	6.595%
41	11.986	3305	3311	3328	rVB2	8866	13483	2.70%	0.261%
42	12.070	3328	3337	3343	rBV4	7540	13794	2.76%	0.267%
43	12.105	3344	3348	3357	rVB5	6937	9524	1.90%	0.184%
44	12.202	3365	3378	3391	rBV	199948	320686	64.14%	6.202%
45	12.330	3404	3418	3428	rBV2	7617	14835	2.97%	0.287%
46	12.520	3467	3477	3492	rBV7	7212	16245	3.25%	0.314%
47	12.777	3550	3557	3566	rBV6	3643	5906	1.18%	0.114%
48	12.893	3585	3593	3600	rVB6	4509	5990	1.20%	0.116%
49	12.954	3603	3612	3623	rBV3	10797	16416	3.28%	0.317%
50	13.214	3683	3693	3705	rBV7	3416	6237	1.25%	0.121%
51	13.619	3811	3819	3826	rVB8	3066	5512	1.10%	0.107%
52	14.201	3990	4000	4013	rVB	58652	86488	17.30%	1.673%
53	14.327	4029	4039	4049	rBV	15414	21949	4.39%	0.424%
54	14.732	4157	4165	4176	rVB3	3457	5439	1.09%	0.105%
55	15.008	4239	4251	4260	rBV4	8116	14814	2.96%	0.286%
56	15.115	4271	4284	4299	rBV3	6335	11916	2.38%	0.230%
57	15.301	4332	4342	4350	rBV7	3829	5963	1.19%	0.115%
58	15.465	4384	4393	4400	rBV4	4556	6543	1.31%	0.127%
59	15.594	4427	4433	4443	rVB7	5341	7649	1.53%	0.148%
60	15.706	4456	4468	4481	rVB2	18163	31813	6.36%	0.615%
61	16.143	4594	4604	4613	rBV2	28529	42195	8.44%	0.816%
62	16.362	4665	4672	4681	rVB9	4238	7012	1.40%	0.136%
63	16.780	4792	4802	4812	rBV	57235	87829	17.57%	1.698%
64	16.899	4827	4839	4852	rBV	336180	500014	100.00%	9.669%

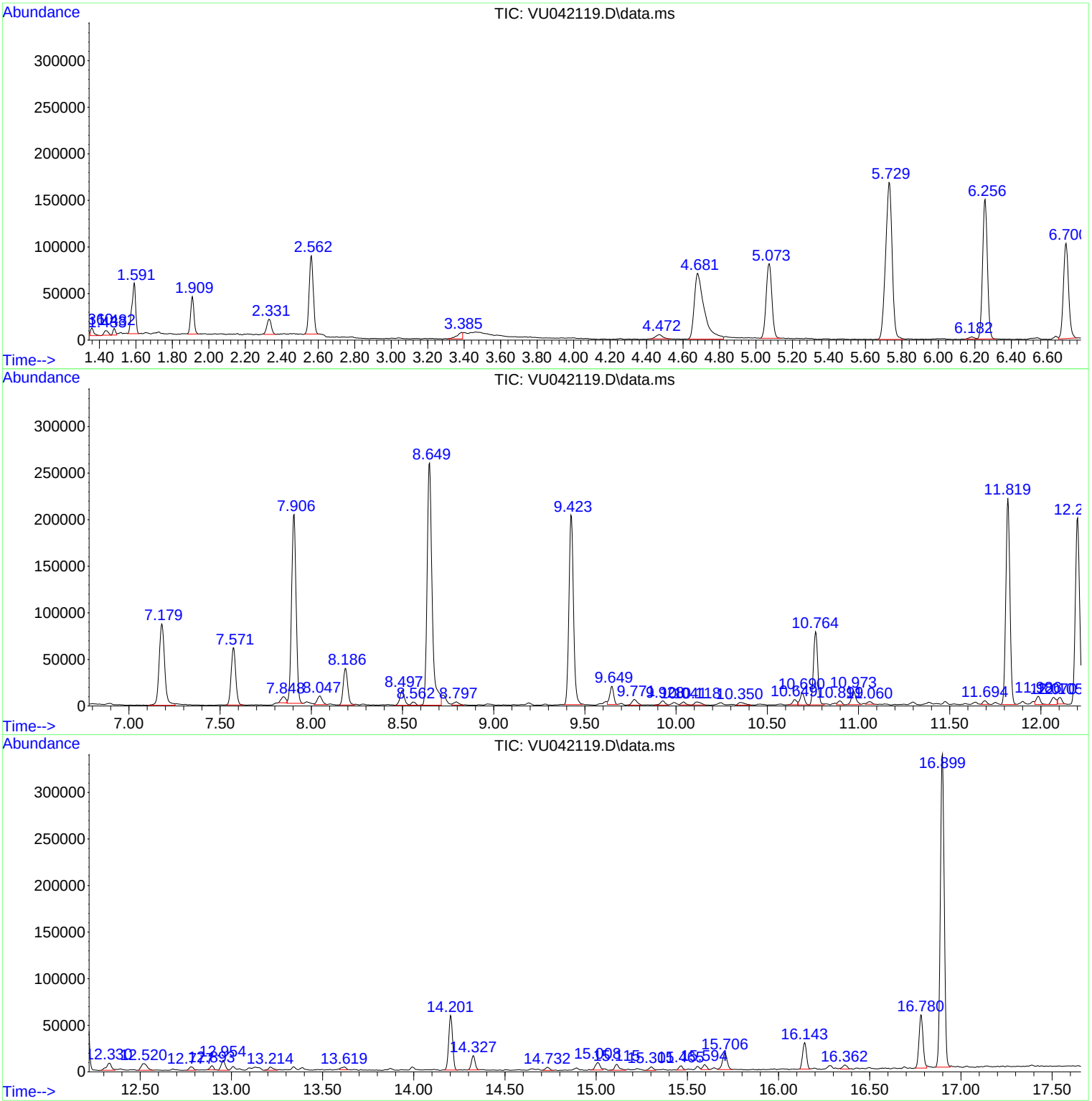
Sum of corrected areas: 5171060

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042119.D
Acq On : 20 Jan 2021 20:36
Operator : SY/MD
Sample : M1180-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E06

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 : VU042119.D
Acq On : 20 Jan 2021 20:36
Operator : SY/MD
Sample : M1180-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E06

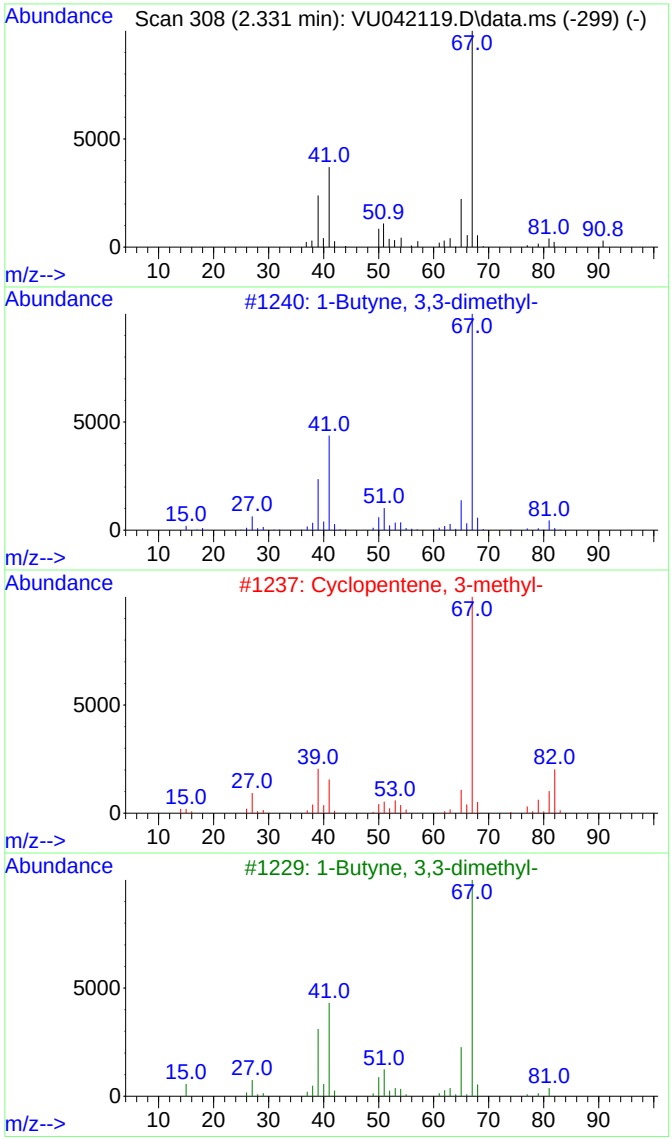
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

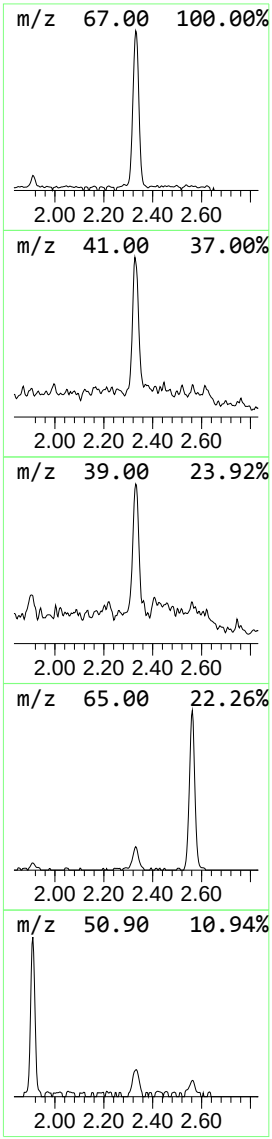
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Butyne, 3,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.331	0.51 ug/L	28355	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butyne, 3,3-dimethyl-	82	C6H10	000917-92-0	78
2	Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	72
3	1-Butyne, 3,3-dimethyl-	82	C6H10	000917-92-0	64
4	1,4-Hexadiene, (Z)-	82	C6H10	007318-67-4	56
5	1-Butyne, 3,3-dimethyl-	82	C6H10	000917-92-0	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042119.D
Acq On : 20 Jan 2021 20:36
Operator : SY/MD
Sample : M1180-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E06

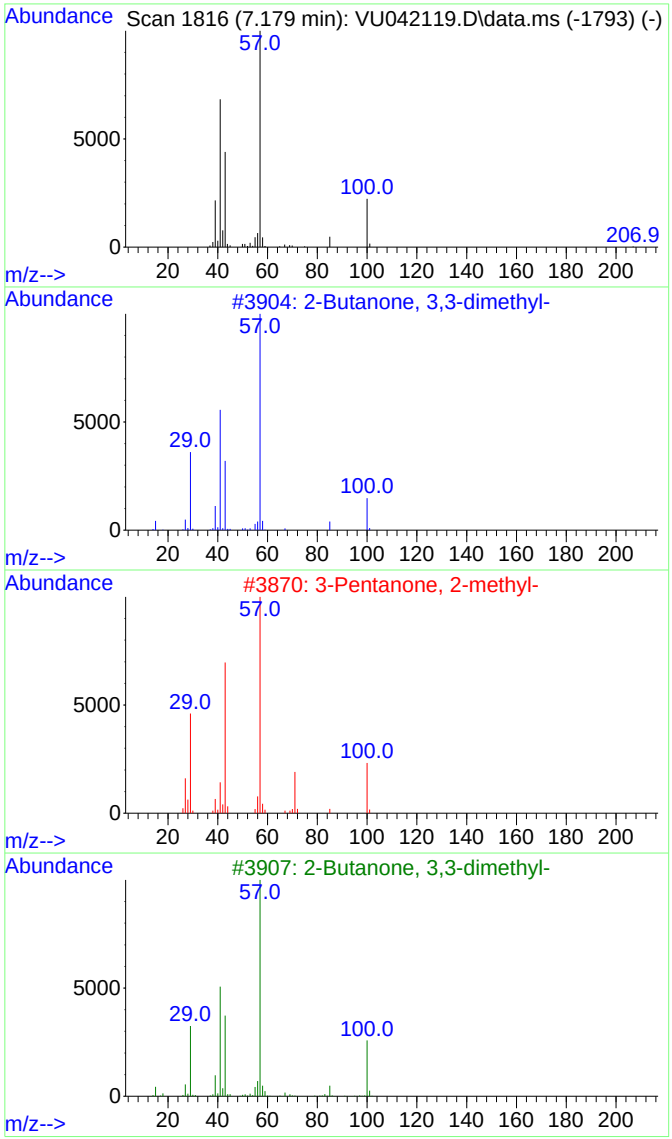
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

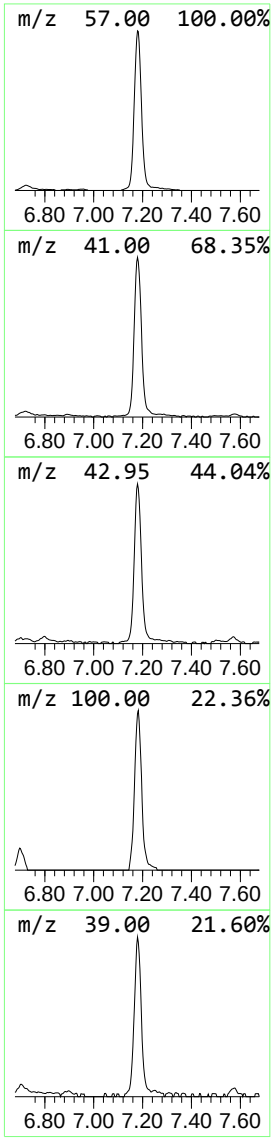
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.179	3.31 ug/L	183154	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	64
2	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	59
3	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	59
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\VU012021\
Data File : VU042119.D
Acq On : 20 Jan 2021 20:36
Operator : SY/MD
Sample : M1180-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E06

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

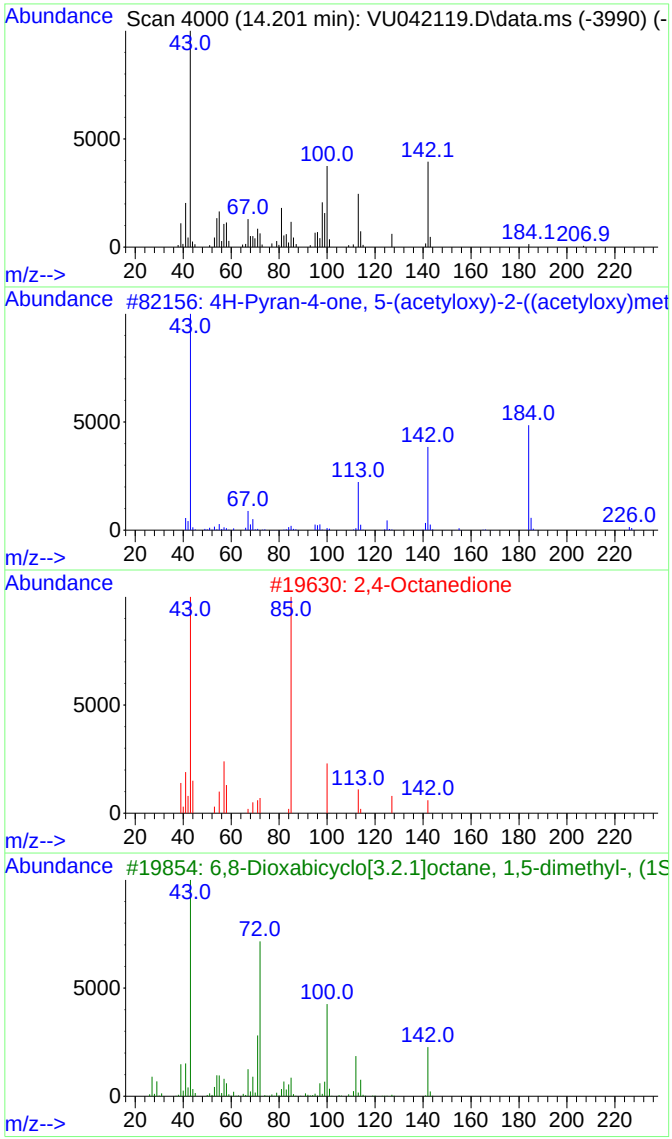
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

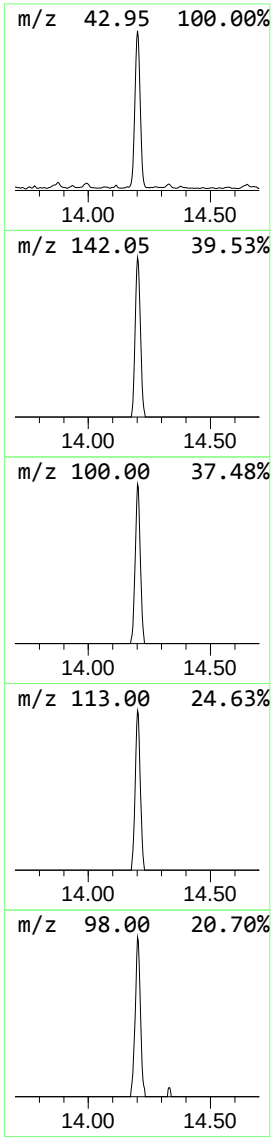
****

Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	1.27 ug/L	86488	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Pyran-4-one, 5-(acetyloxy)-2-...	226	C10H10O6	026209-93-8	38
2	2,4-Octanedione	142	C8H14O2	014090-87-0	38
3	6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	35
4	3-n-Propyl-2,4-pentanedione	142	C8H14O2	001540-35-8	25
5	6-Dodecanone	184	C12H24O	006064-27-3	14





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042119.D
Acq On : 20 Jan 2021 20:36
Operator : SY/MD
Sample : M1180-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E06

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

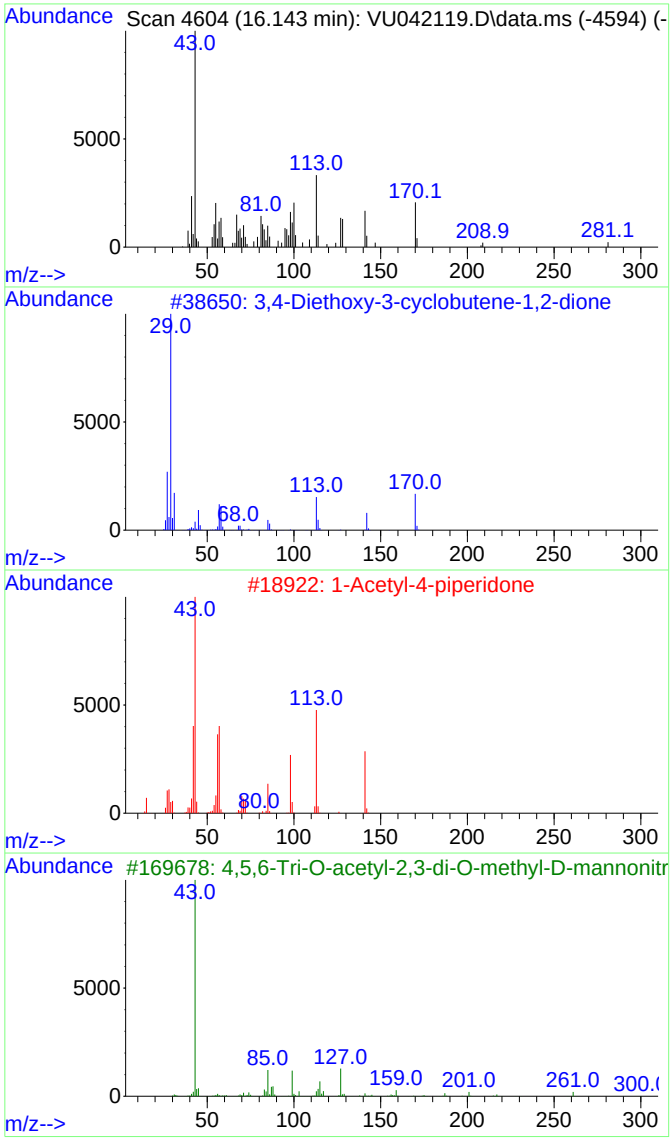
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

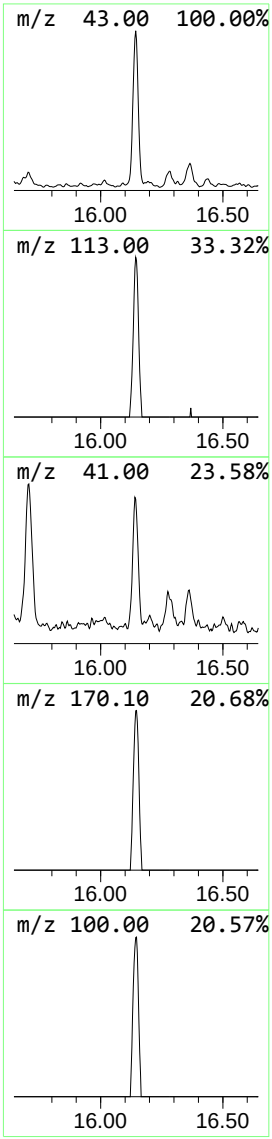
****

Peak Number 5 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.144	0.62 ug/L	42195	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Diethoxy-3-cyclobutene-1,2-d...	170	C8H10O4	005231-87-8	22
2	1-Acetyl-4-piperidone	141	C7H11NO2	032161-06-1	16
3	4,5,6-Tri-O-acetyl-2,3-di-O-meth...	331	C14H21NO8	059061-07-3	14
4	3,4-Diethoxy-3-cyclobutene-1,2-d...	170	C8H10O4	005231-87-8	14
5	Allyl heptanoate	170	C10H18O2	000142-19-8	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042119.D
Acq On : 20 Jan 2021 20:36
Operator : SY/MD
Sample : M1180-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E06

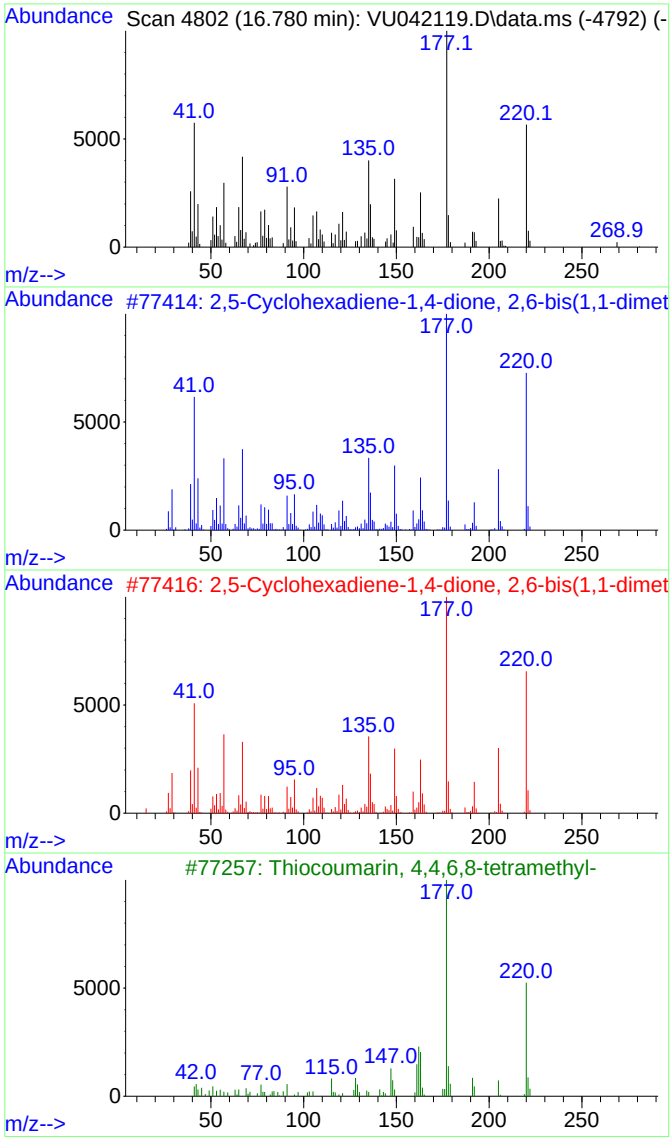
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

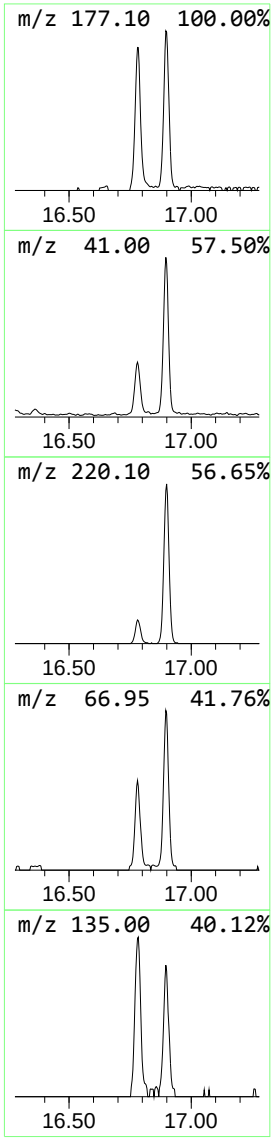
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.780	1.29 ug/L	87829	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	94
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
3	Thiocoumarin, 4,4,6,8-tetramethyl-	220	C13H16OS	1000128-90-3	55
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	55
5	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042119.D
Acq On : 20 Jan 2021 20:36
Operator : SY/MD
Sample : M1180-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E06

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

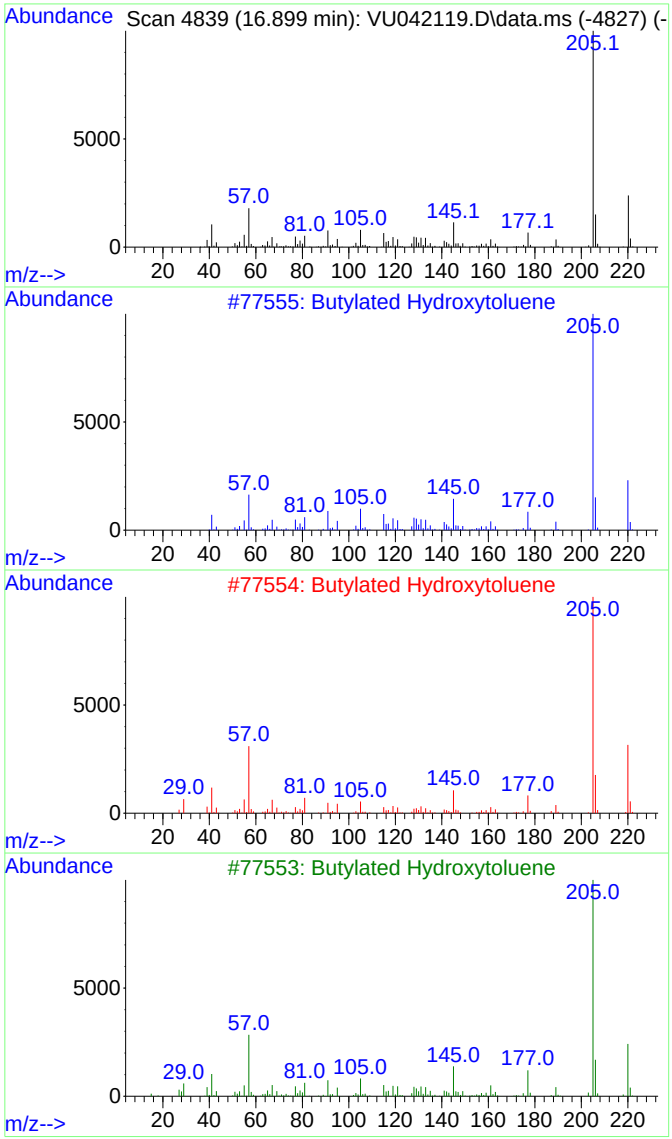
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

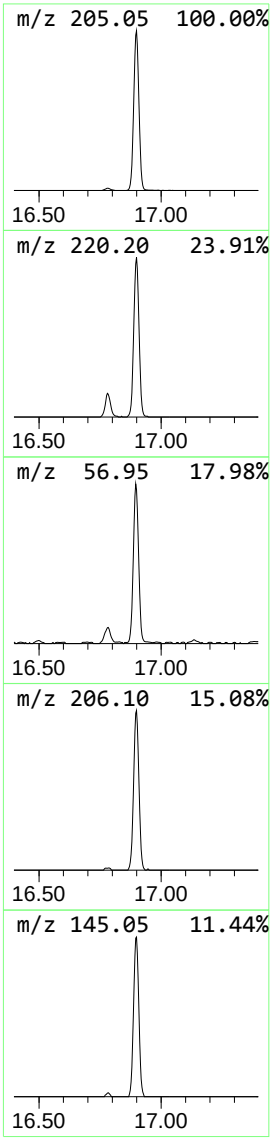
****

Peak Number 7 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.899	7.33 ug/L	500014	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	96
3	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	95
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 : VU042119.D
Acq On : 20 Jan 2021 20:36
Operator : SY/MD
Sample : M1180-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E06

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
1-Butyne, 3,3-d...	2.331	0.5	ug/L	28355	1	6.256	276854	5.0
2-Butanone, 3,3...	7.179	3.3	ug/L	183154	1	6.256	276854	5.0
unknown-01	14.201	1.3	ug/L	86488	3	11.819	341016	5.0
unknown-02	16.144	0.6	ug/L	42195	3	11.819	341016	5.0
2,5-Cyclohexadi...	16.780	1.3	ug/L	87829	3	11.819	341016	5.0
Butylated Hydro...	16.899	7.3	ug/L	500014	3	11.819	341016	5.0