LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042124.D
Acq On : 20 Jan 2021 23:09
Operator : SY/MD
Sample : M1180-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E10

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: VU042124.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	69	79	89	rVB	50865	60725	8.23%	1.066%
2	1.909	169	177	187	rVB	39051	48704	6.60%	0.855%
3	2.163	249	256	266	rBV3	7045	12944	1.75%	0.227%
4	2.562	370	380	393	rVB	80592	126256	17.11%	2.217%
5	4.453	951	968	970	rBV6	5763	11495	1.56%	0.202%
6	4.719	1032	1051	1084	rBV	33434	142671	19.33%	2.506%
7	5.073	1144	1161	1182	rVB	83235	186635	25.29%	3.278%
8	5.729	1347	1365	1389	rBV2	168486	411626	55.78%	7.229%
9	6.256	1516	1529	1546	rVB	142506	270078	36.60%	4.743%
10	6.700	1654	1667	1688	rVV	100197	195235	26.46%	3.429%
11	6.806	1689	1700	1714	rVV3	6515	13493	1.83%	0.237%
12	7.186	1808	1818	1832	rVB2	19189	37015	5.02%	0.650%
13	7.575	1926	1939	1952	rBV	59392	102718	13.92%	1.804%
14	7.813	2001	2013	2021	rBV5	4384	9527	1.29%	0.167%
15	7.903	2029	2041	2055	rVB	195834	333749	45.23%	5.861%
16	8.047	2079	2086	2096	rVB3	4782	9325	1.26%	0.164%
17	8.189	2118	2130	2142	rBV	38506	62975	8.53%	1.106%
18	8.501	2211	2227	2237	rBV3	5604	11461	1.55%	0.201%
19	8.562	2237	2246	2260	rVB6	5344	9814	1.33%	0.172%
20	8.652	2260	2274	2284	rBV	231613	423202	57.35%	7.432%
21	8.706	2286	2291	2310	rVB4	43087	88109	11.94%	1.547%
22	9.423	2502	2514	2541	rBV	200464	336992	45.67%	5.918%
23	9.623	2556	2576	2577	rBV8	4122	7985	1.08%	0.140%
24	9.648	2577	2584	2593	rVB2	11122	16840	2.28%	0.296%
25	9.780	2610	2625	2641	rBV3	8860	22473	3.05%	0.395%
26	9.925	2659	2670	2683	rBV	15646	27130	3.68%	0.476%
27	10.137	2719	2736	2755	rVB5	6194	16939	2.30%	0.297%
28	10.243	2755	2769	2785	rBV	30398	55389	7.51%	0.973%
29	10.353	2795	2803	2825	rVB7	5992	13935	1.89%	0.245%
30	10.693	2901	2909	2921	rVB	17601	27119	3.67%	0.476%
31	10.764	2921	2931	2943	rBV	77109	123535	16.74%	2.170%
32	10.899	2966	2973	2981	rVB7	5113	8284	1.12%	0.145%
33	10.973	2981	2996	3011	rBV2	26085	44871	6.08%	0.788%
34	11.057	3013	3022	3036	rVB3	13165	21695	2.94%	0.381%
35	11.478	3144	3153	3162	rBV2	9568	13934	1.89%	0.245%
36	11.581	3174	3185	3195	rBV2	13220	21659	2.93%	0.380%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042124.D
Acq On : 20 Jan 2021 23:09
Operator : SY/MD
Sample : M1180-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E10

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	11.697	3213	3221	3230	rVB7	5959	9789	1.33%	0.172%
38	11.819	3247	3259	3277	rVB	218837	342382	46.40%	6.013%
39	11.986	3306	3311	3323	rVB4	5250	8265	1.12%	0.145%
40	12.070	3325	3337	3367	rBV	392318	737962	100.00%	12.960%
41	12.201	3367	3378	3399	rVB	195801	334064	45.27%	5.867%
42	12.330	3411	3418	3424	rBV	10880	16342	2.21%	0.287%
43	12.362	3425	3428	3444	rVB2	9415	14210	1.93%	0.250%
44	12.780	3549	3558	3567	rBV	15102	22099	2.99%	0.388%
45	12.893	3585	3593	3603	rVB5	8687	13479	1.83%	0.237%
46	12.957	3603	3613	3621	rBV6	5658	9507	1.29%	0.167%
47	13.153	3668	3674	3685	rVB	6542	9263	1.26%	0.163%
48	13.619	3810	3819	3829	rVB2	14287	20344	2.76%	0.357%
49	14.066	3948	3958	3968	rBV8	4984	8414	1.14%	0.148%
50	14.201	3988	4000	4012	rVB	57004	86278	11.69%	1.515%
51	14.645	4131	4138	4146	rBV5	5043	8604	1.17%	0.151%
52	15.703	4458	4467	4476	rVB5	12019	17181	2.33%	0.302%
53	16.143	4594	4604	4617	rBV2	19886	28658	3.88%	0.503%
54	16.780	4792	4802	4815	rBV3	47681	75225	10.19%	1.321%
55	16.899	4827	4839	4855	rBV	411774	605398	82.04%	10.632%

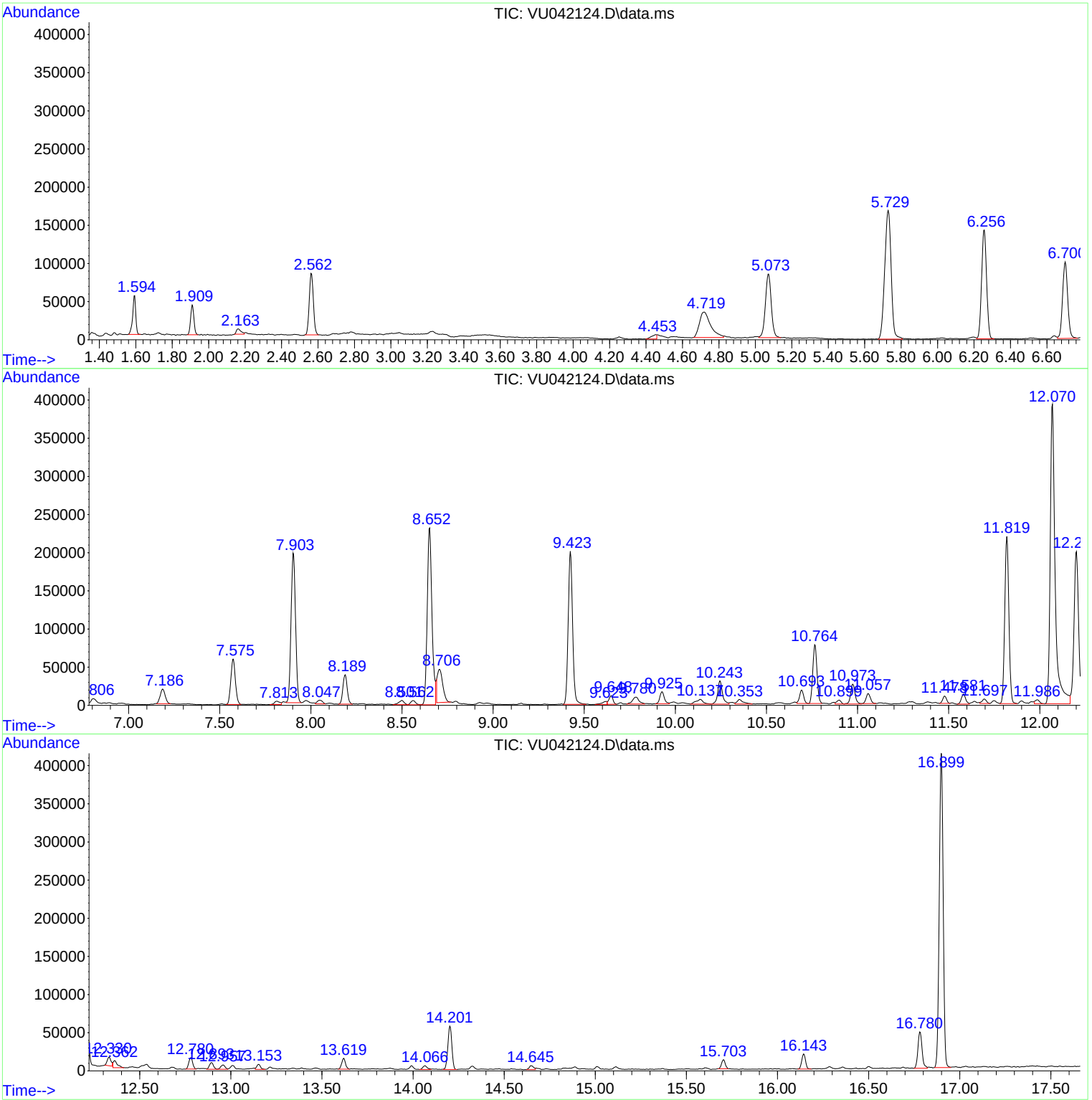
Sum of corrected areas: 5694001

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042124.D
Acq On : 20 Jan 2021 23:09
Operator : SY/MD
Sample : M1180-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E10

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 : VU042124.D
Acq On : 20 Jan 2021 23:09
Operator : SY/MD
Sample : M1180-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E10

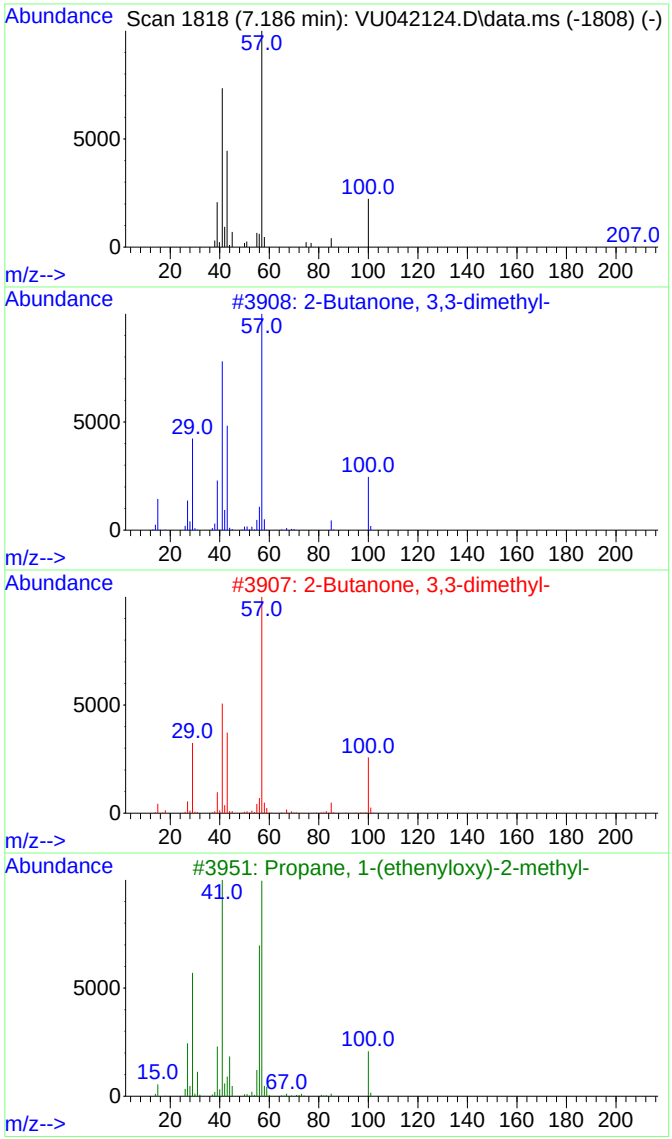
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

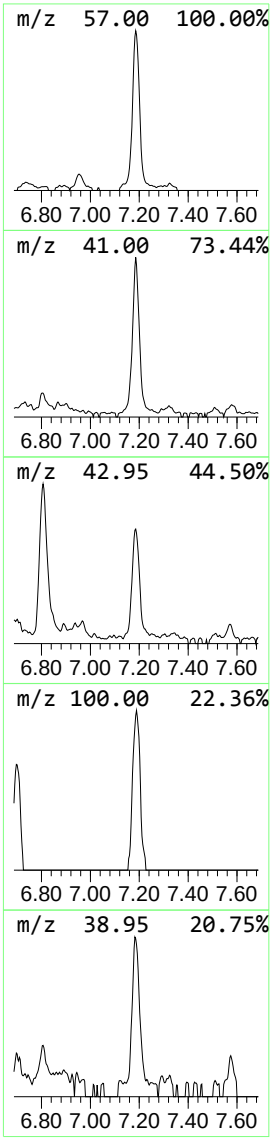
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Butanone, 3,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.186	0.69 ug/L	37015	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	86
2	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	78
3	Propane, 1-(ethenyloxy)-2-methyl-	100	C6H12O	000109-53-5	59
4	Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	50
5	Propane, 1-bromo-2-methyl-	136	C4H9Br	000078-77-3	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042124.D
Acq On : 20 Jan 2021 23:09
Operator : SY/MD
Sample : M1180-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E10

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

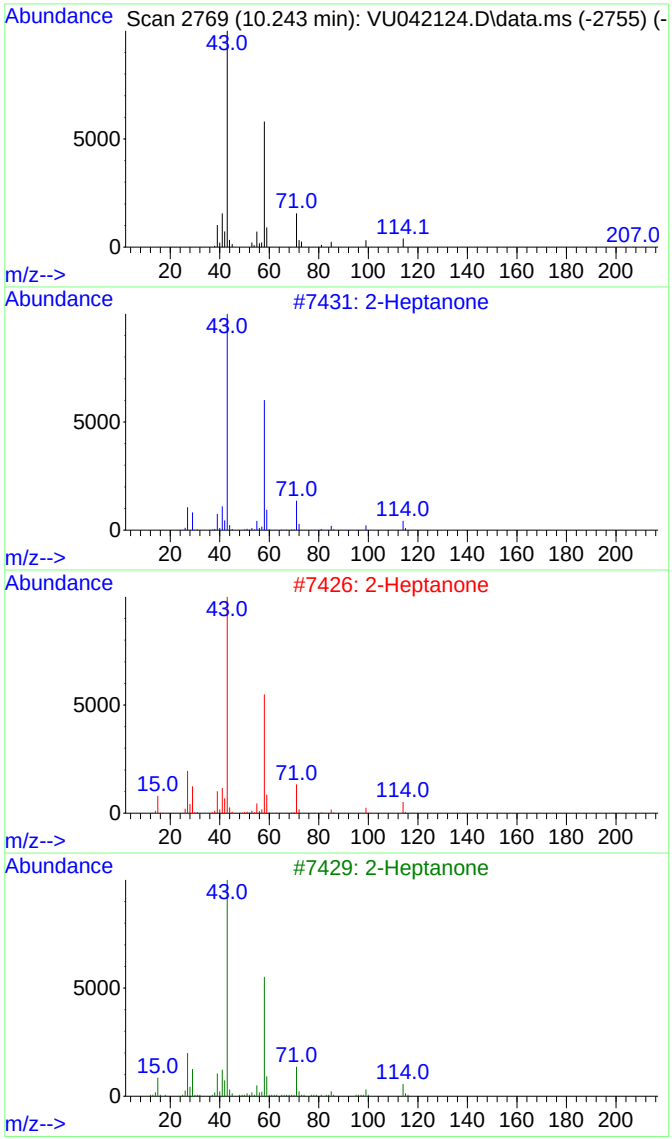
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

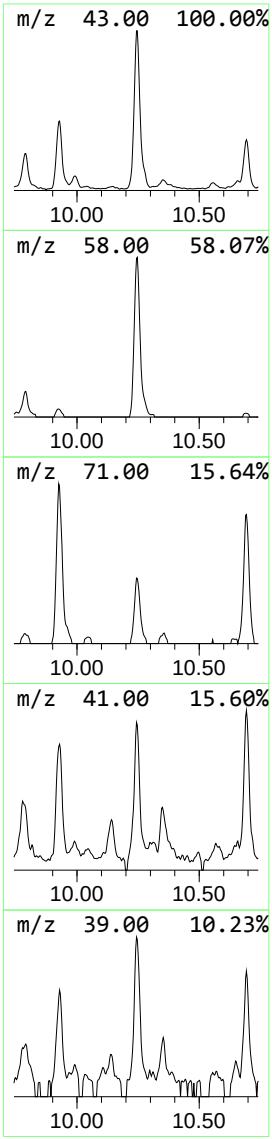
****

Peak Number 3 2-Heptanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.243	0.82 ug/L	55389	Chlorobenzene-d5	9.423

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	90
3	2-Heptanone	114	C7H14O	000110-43-0	90
4	2-Heptanone	114	C7H14O	000110-43-0	78
5	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042124.D
Acq On : 20 Jan 2021 23:09
Operator : SY/MD
Sample : M1180-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E10

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

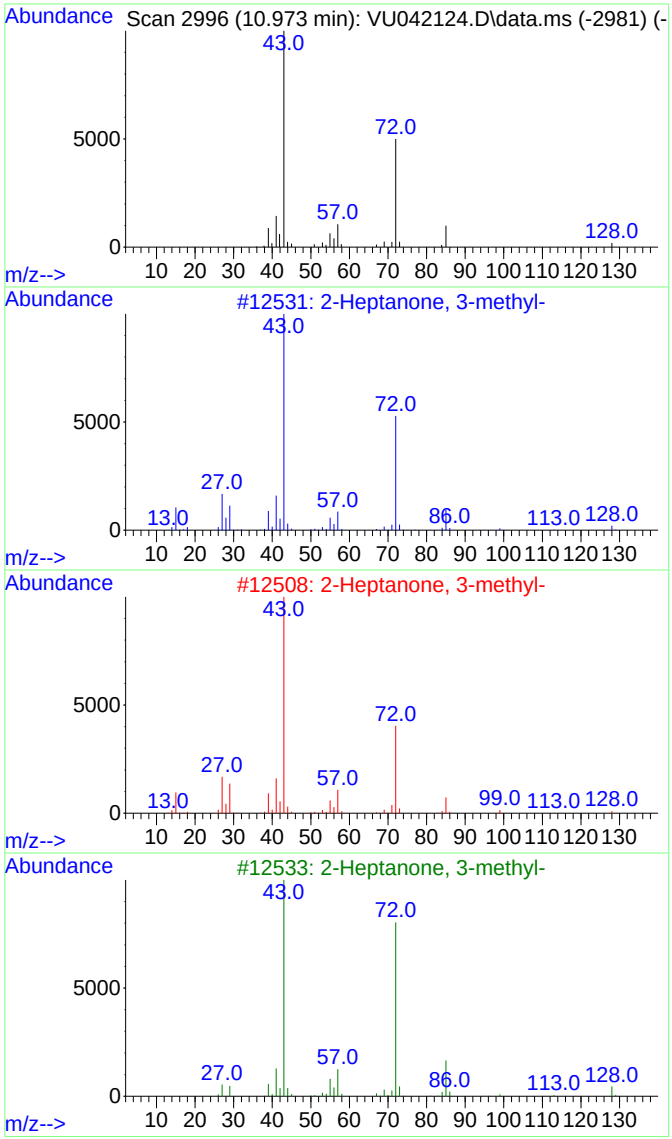
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

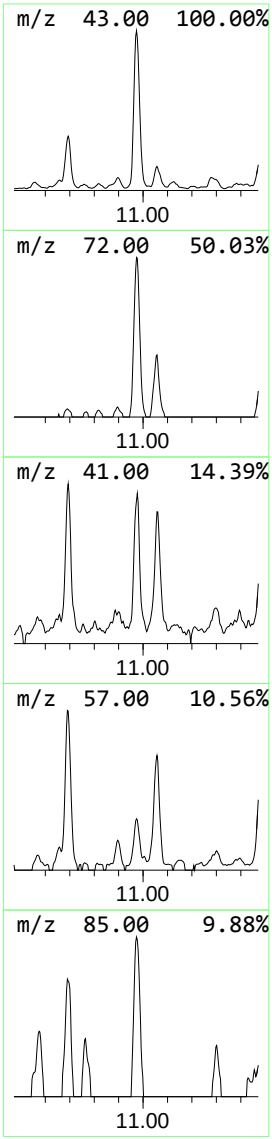
****

Peak Number 4 2-Heptanone, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.973	0.66 ug/L	44871	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 3-methyl-	128	C8H16O	002371-19-9	91
2	2-Heptanone, 3-methyl-	128	C8H16O	002371-19-9	91
3	2-Heptanone, 3-methyl-	128	C8H16O	002371-19-9	90
4	2-Heptanone, 3-methyl-	128	C8H16O	002371-19-9	80
5	2-Hexanone, 3,4-dimethyl-	128	C8H16O	019550-10-8	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042124.D
Acq On : 20 Jan 2021 23:09
Operator : SY/MD
Sample : M1180-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E10

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

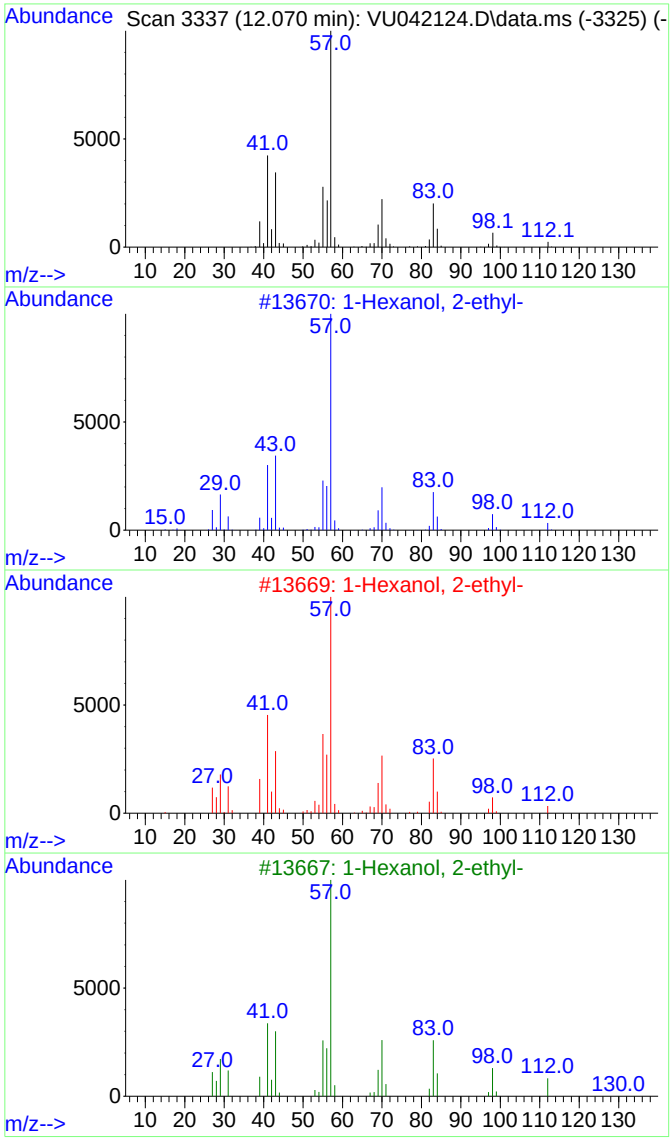
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

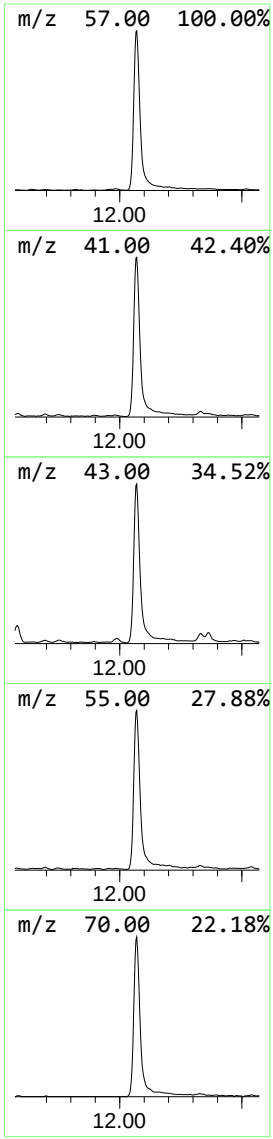
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.070	10.78 ug/L	737962	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	83
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	74
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042124.D
Acq On : 20 Jan 2021 23:09
Operator : SY/MD
Sample : M1180-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E10

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

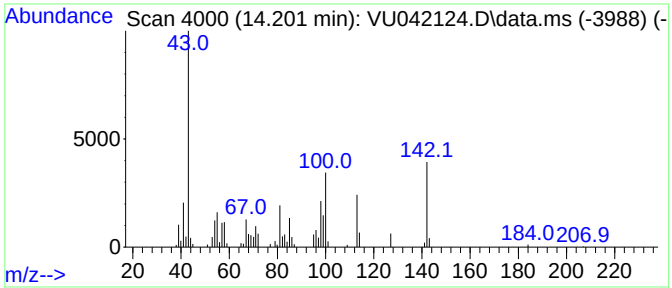
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

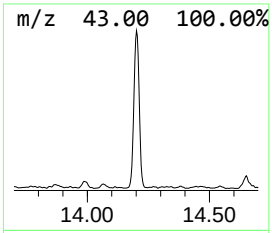
****

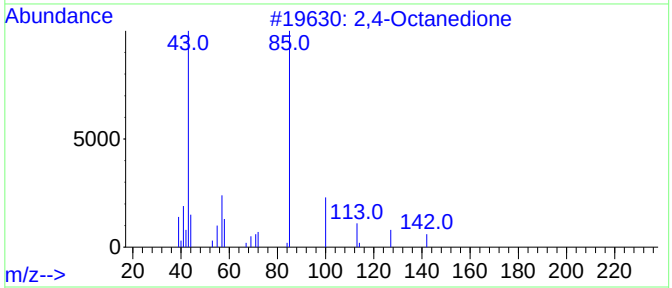
Peak Number 6 unknown-01 Concentration Rank 4

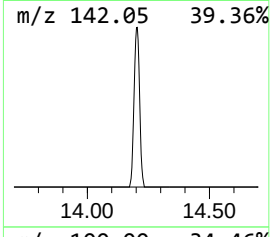
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	1.26 ug/L	86278	1,4-Dichlorobenzene-d4	11.819

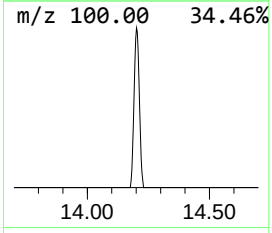
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Octanedione	142	C8H14O2	014090-87-0	47
2	4H-Pyran-4-one, 5-(acetyloxy)-2-...	226	C10H10O6	026209-93-8	38
3	6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	32
4	6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	25
5	6-Dodecanone	184	C12H24O	006064-27-3	14

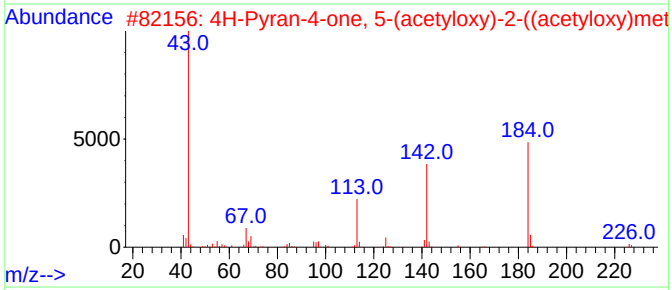


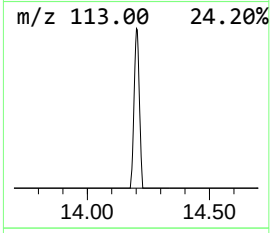


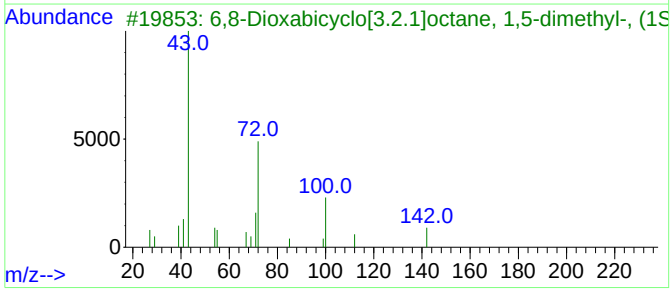


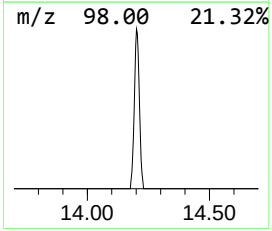












Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042124.D
Acq On : 20 Jan 2021 23:09
Operator : SY/MD
Sample : M1180-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E10

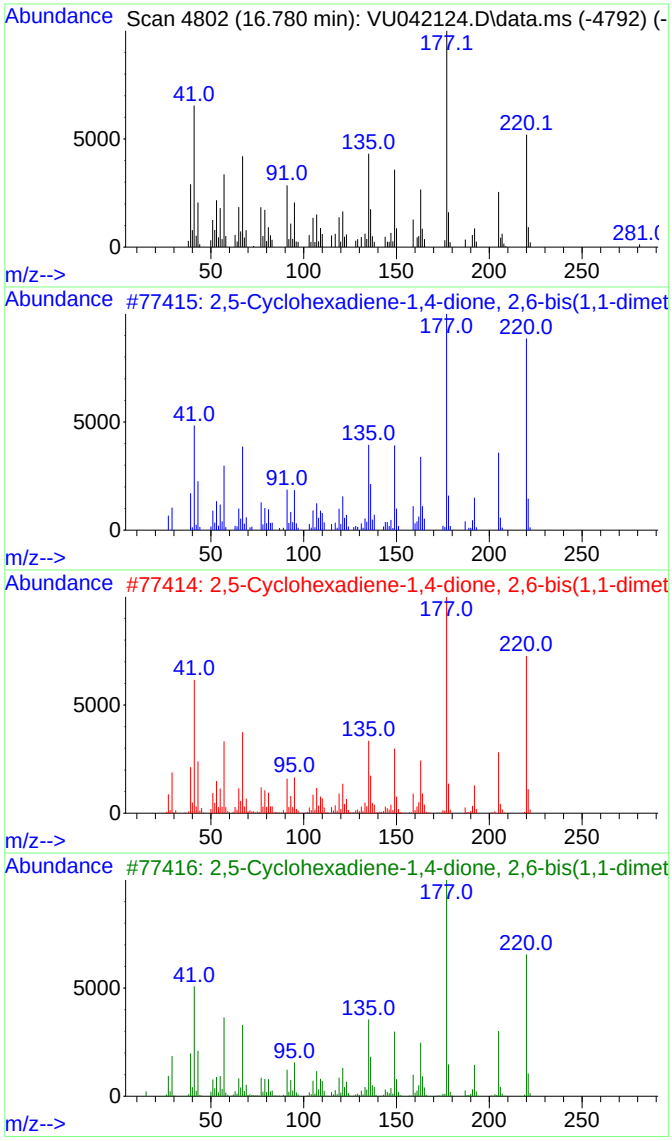
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

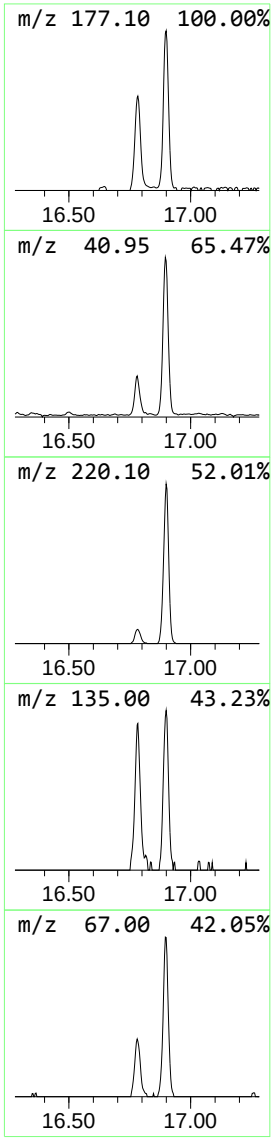
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.780	1.10 ug/L	75225	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	97
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	97
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	90
4	trans-.beta.-Ionone	192	C13H20O	000079-77-6	38
5	trans-.beta.-Ionone	192	C13H20O	000079-77-6	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042124.D
Acq On : 20 Jan 2021 23:09
Operator : SY/MD
Sample : M1180-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E10

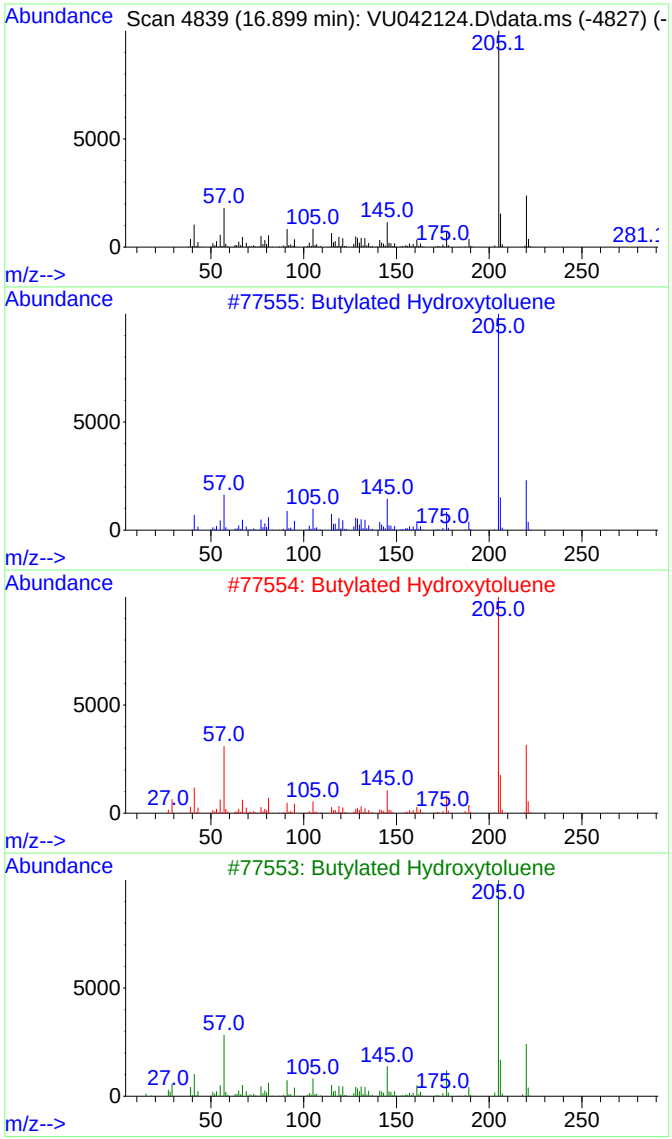
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

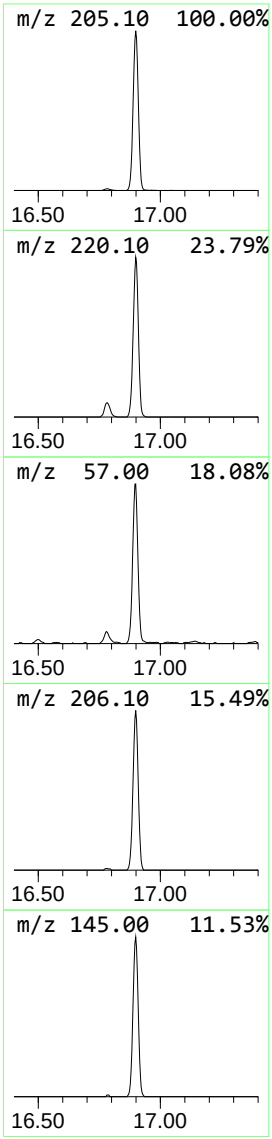
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Butylated Hydroxytoluene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.899	8.84 ug/L	605398	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, 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\VU012021\
Data File : VU042124.D
Acq On : 20 Jan 2021 23:09
Operator : SY/MD
Sample : M1180-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E10

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	0.7	ug/L	37015	1	6.256	270078	5.0
2-Heptanone	10.243	0.8	ug/L	55389	2	9.423	336992	5.0
2-Heptanone, 3-...	10.973	0.7	ug/L	44871	3	11.819	342382	5.0
1-Hexanol, 2-et...	12.070	10.8	ug/L	737962	3	11.819	342382	5.0
unknown-01	14.201	1.3	ug/L	86278	3	11.819	342382	5.0
2,5-Cyclohexadi...	16.780	1.1	ug/L	75225	3	11.819	342382	5.0
Butylated Hydro...	16.899	8.8	ug/L	605398	3	11.819	342382	5.0