LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
Data File : VU042172.D
Acq On : 22 Jan 2021 16:10
Operator : SY/MD
Sample : M1222-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E14

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: VU042172.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	18	rVB2	9631	10319	1.67%	0.233%
2	1.601	70	81	91	rVB2	45444	60929	9.85%	1.374%
3	1.916	170	179	193	rVB	34689	44552	7.20%	1.004%
4	2.572	372	383	396	rBV	76454	122762	19.84%	2.768%
5	3.253	568	595	616	rBV3	10420	56580	9.14%	1.276%
6	4.462	952	971	985	rBV6	3151	8914	1.44%	0.201%
7	4.649	1014	1029	1076	rBV	42436	160504	25.94%	3.619%
8	5.073	1146	1161	1181	rBV	69609	151797	24.53%	3.422%
9	5.735	1346	1367	1390	rBV2	136043	358792	57.98%	8.089%
10	6.256	1515	1529	1552	rVB	128972	243252	39.31%	5.484%
11	6.700	1654	1667	1688	rVB	89830	173557	28.04%	3.913%
12	7.176	1800	1815	1835	rBV2	33735	70003	11.31%	1.578%
13	7.575	1925	1939	1953	rBV	51187	89921	14.53%	2.027%
14	7.825	1999	2017	2029	rBV	6098	18215	2.94%	0.411%
15	7.906	2029	2042	2056	rVV	172241	297469	48.07%	6.707%
16	7.977	2056	2064	2076	rVV3	6007	12538	2.03%	0.283%
17	8.044	2076	2085	2094	rVB3	4693	8899	1.44%	0.201%
18	8.186	2115	2129	2145	rBV	32957	56072	9.06%	1.264%
19	8.497	2213	2226	2235	rBV2	5501	9784	1.58%	0.221%
20	8.559	2237	2245	2255	rVB5	4631	7286	1.18%	0.164%
21	8.642	2258	2271	2282	rBV	220150	400936	64.79%	9.039%
22	9.423	2501	2514	2535	rBV	183162	308337	49.82%	6.952%
23	9.649	2576	2584	2595	rVB	22399	33395	5.40%	0.753%
24	9.771	2611	2622	2635	rBV6	4059	9843	1.59%	0.222%
25	10.243	2758	2769	2784	rBV	9728	16832	2.72%	0.379%
26	10.690	2901	2908	2920	rVB3	9647	14624	2.36%	0.330%
27	10.764	2920	2931	2948	rVB	70494	117316	18.96%	2.645%
28	10.973	2984	2996	3011	rVB	14097	23952	3.87%	0.540%
29	11.060	3011	3023	3031	rBV8	3141	6262	1.01%	0.141%
30	11.819	3248	3259	3275	rVB	206260	326732	52.80%	7.366%
31	11.902	3275	3285	3293	rBV2	5263	7963	1.29%	0.180%
32	12.070	3325	3337	3366	rBV	82766	170819	27.60%	3.851%
33	12.201	3366	3378	3391	rVB	178809	295586	47.76%	6.664%
34	12.333	3406	3419	3429	rBV	22676	36012	5.82%	0.812%
35	12.893	3586	3593	3602	rBV6	5543	8148	1.32%	0.184%
36	14.201	3988	4000	4012	rVB2	26051	39071	6.31%	0.881%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
Data File : VU042172.D
Acq On : 22 Jan 2021 16:10
Operator : SY/MD
Sample : M1222-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E14

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	14.327	4030	4039	4047	rBV4	5047	7163	1.16%	0.161%
38	15.703	4458	4467	4476	rBV6	8980	14975	2.42%	0.338%
39	16.783	4794	4803	4816	rBV6	10404	16552	2.67%	0.373%
40	16.899	4827	4839	4856	rBV	422593	618858	100.00%	13.952%

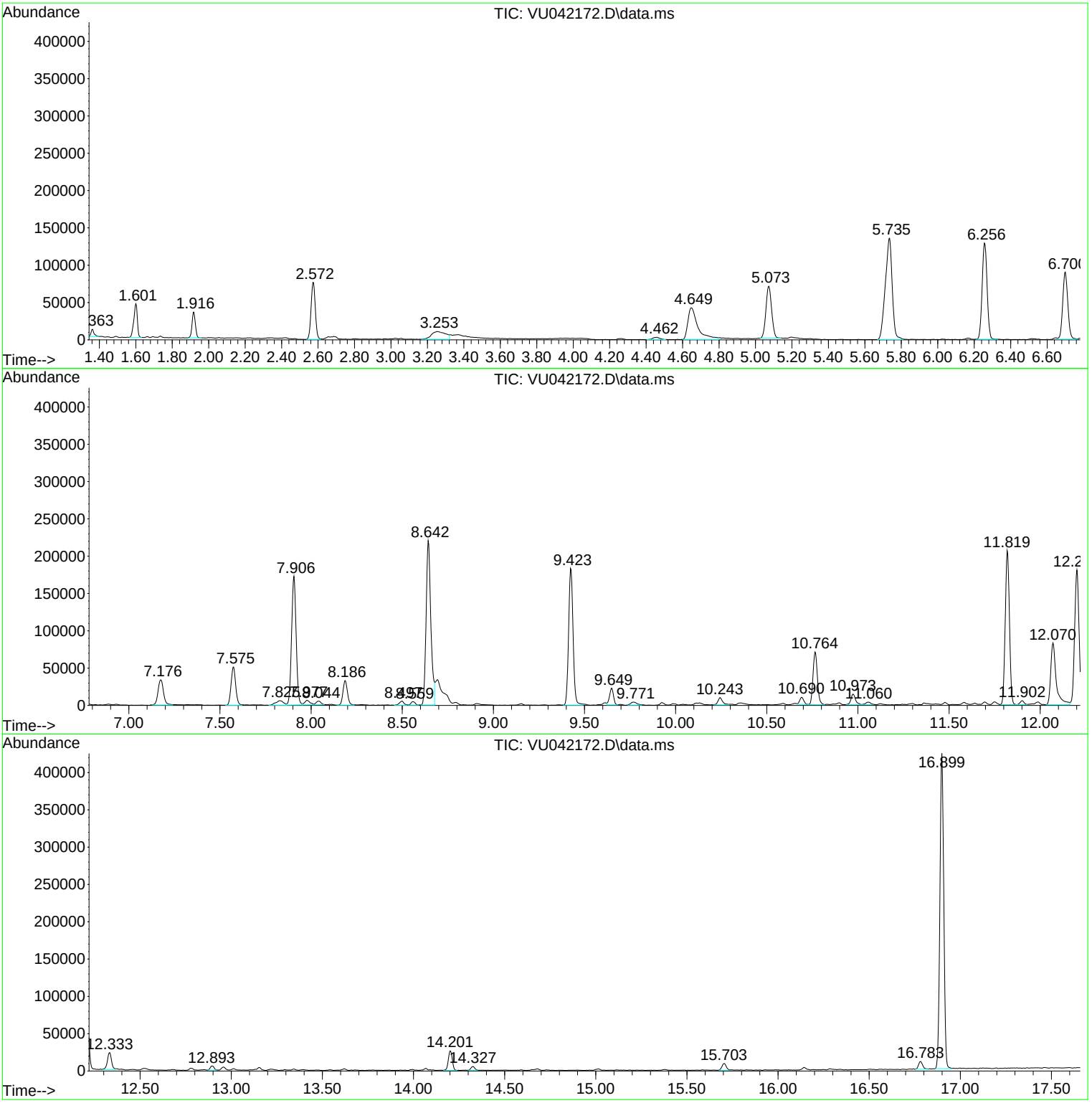
Sum of corrected areas: 4435521

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
Data File : VU042172.D
Acq On : 22 Jan 2021 16:10
Operator : SY/MD
Sample : M1222-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E14

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\VU012221\
Data File : VU042172.D
Acq On : 22 Jan 2021 16:10
Operator : SY/MD
Sample : M1222-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E14

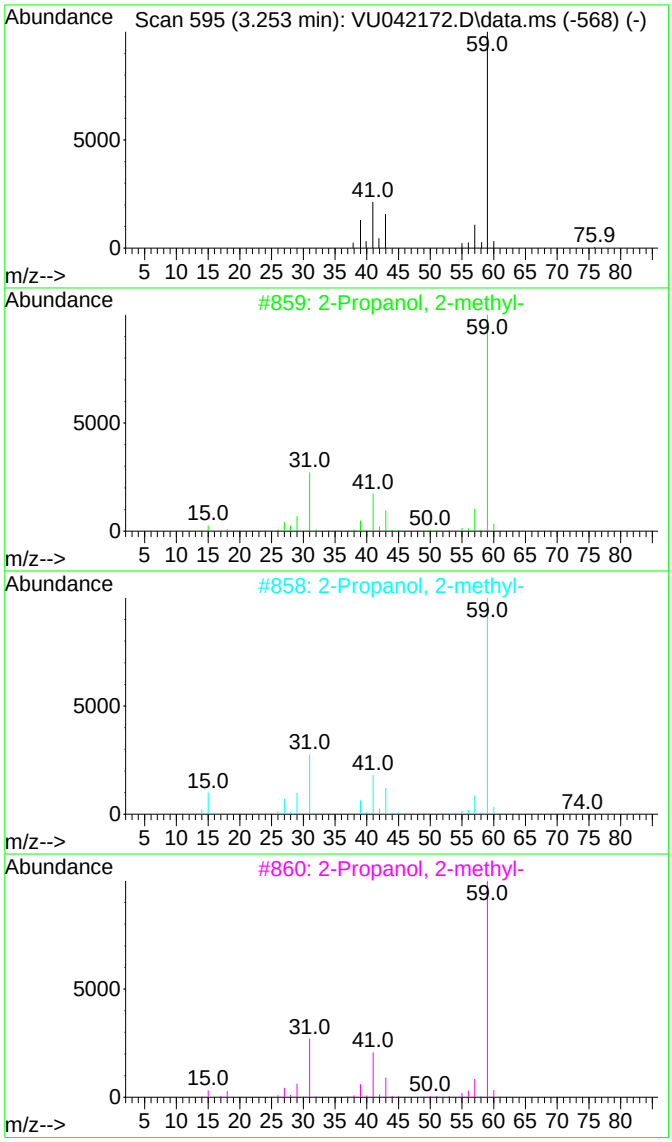
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

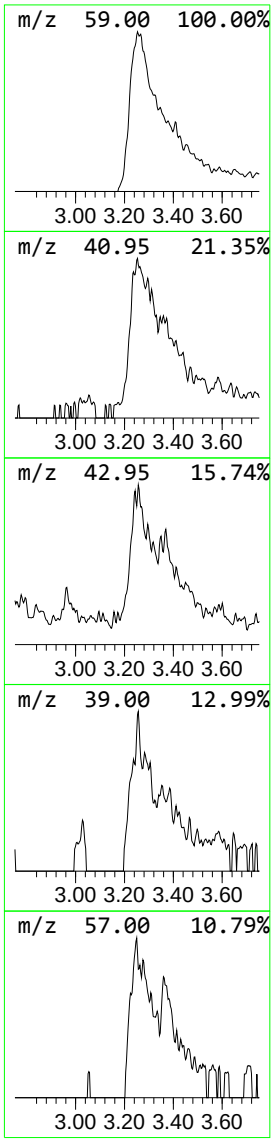
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.253	1.16 ug/L	56580	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	83
2	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	74
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	43
4	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	25
5	3-Pentanol	88	C5H12O	000584-02-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
Data File : VU042172.D
Acq On : 22 Jan 2021 16:10
Operator : SY/MD
Sample : M1222-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E14

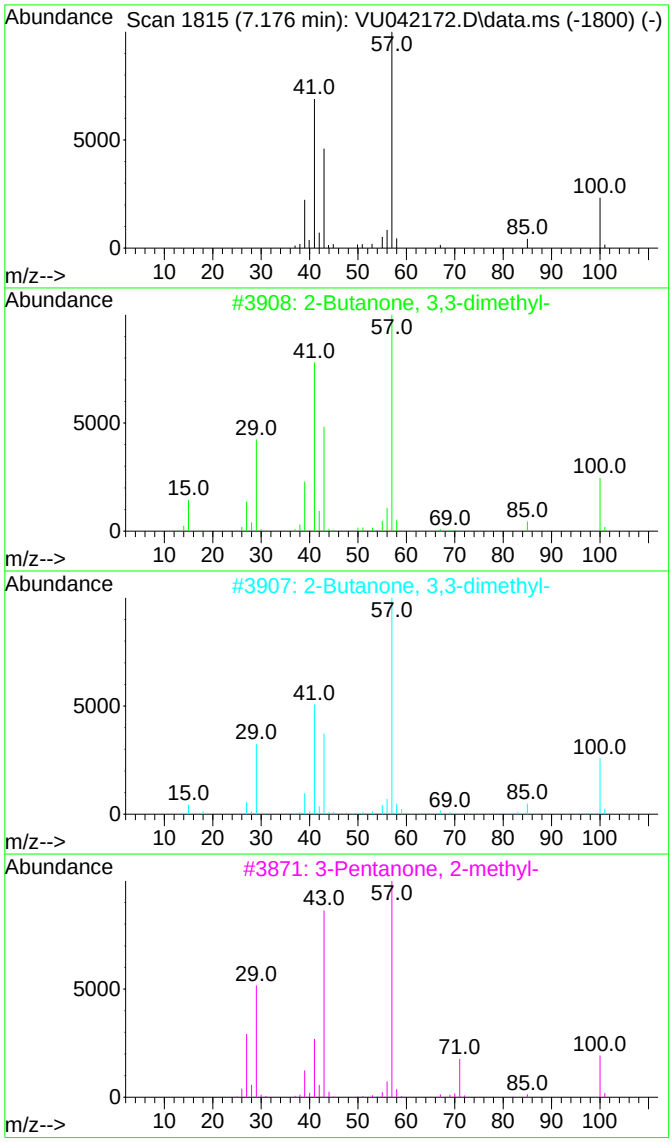
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

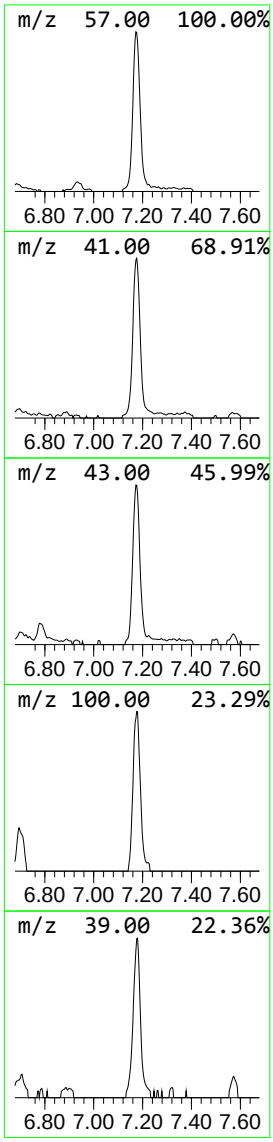
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.176	1.44 ug/L	70003	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	91
2	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	83
3	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
4	Propane, 1-(ethenyloxy)-2-methyl-	100	C6H12O	000109-53-5	59
5	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
Data File : VU042172.D
Acq On : 22 Jan 2021 16:10
Operator : SY/MD
Sample : M1222-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E14

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

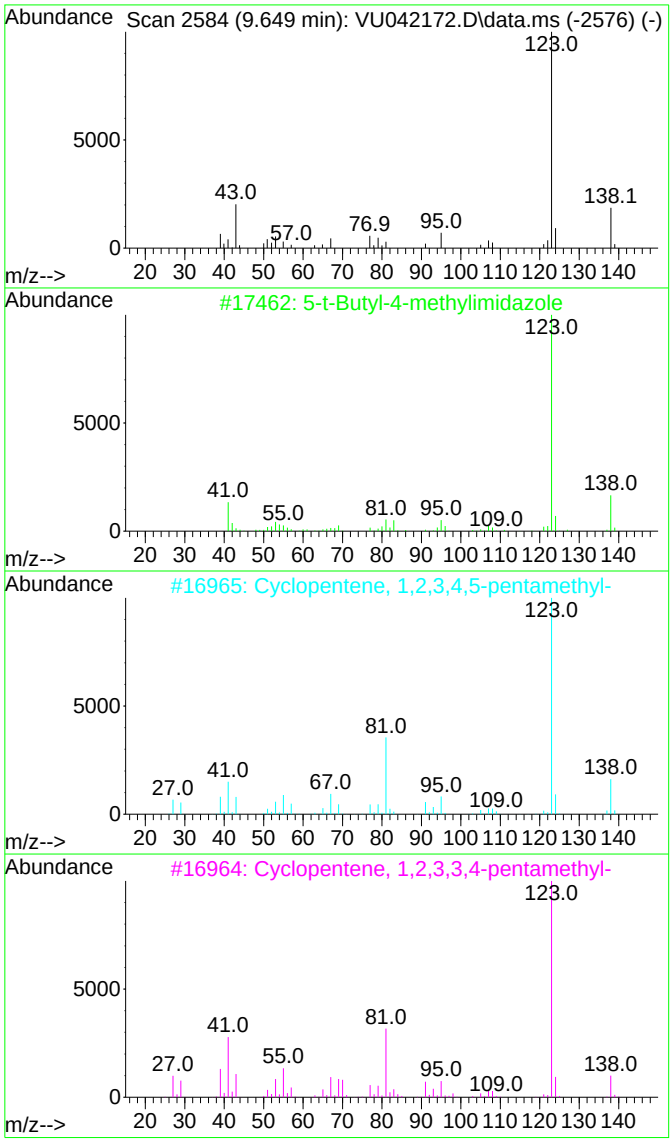
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

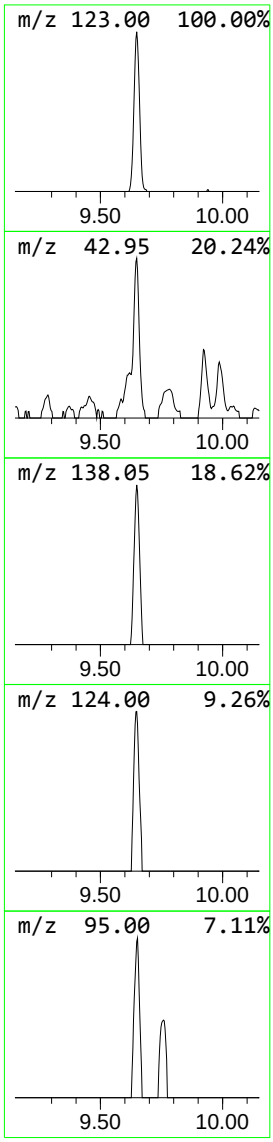
****

Peak Number 4 5-t-Butyl-4-methylimidazole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.649	0.54 ug/L	33395	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-t-Butyl-4-methylimidazole	138	C8H14N2	146979-50-2	90
2	Cyclopentene, 1,2,3,4,5-pentamet...	138	C10H18	1000154-28-6	87
3	Cyclopentene, 1,2,3,3,4-pentamet...	138	C10H18	197390-29-7	86
4	1,3-Benzenediol, 4-ethyl-	138	C8H10O2	002896-60-8	78
5	1,4-Benzenediol, mono-tetradecyl...	306	C20H34O2	013224-40-3	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
Data File : VU042172.D
Acq On : 22 Jan 2021 16:10
Operator : SY/MD
Sample : M1222-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E14

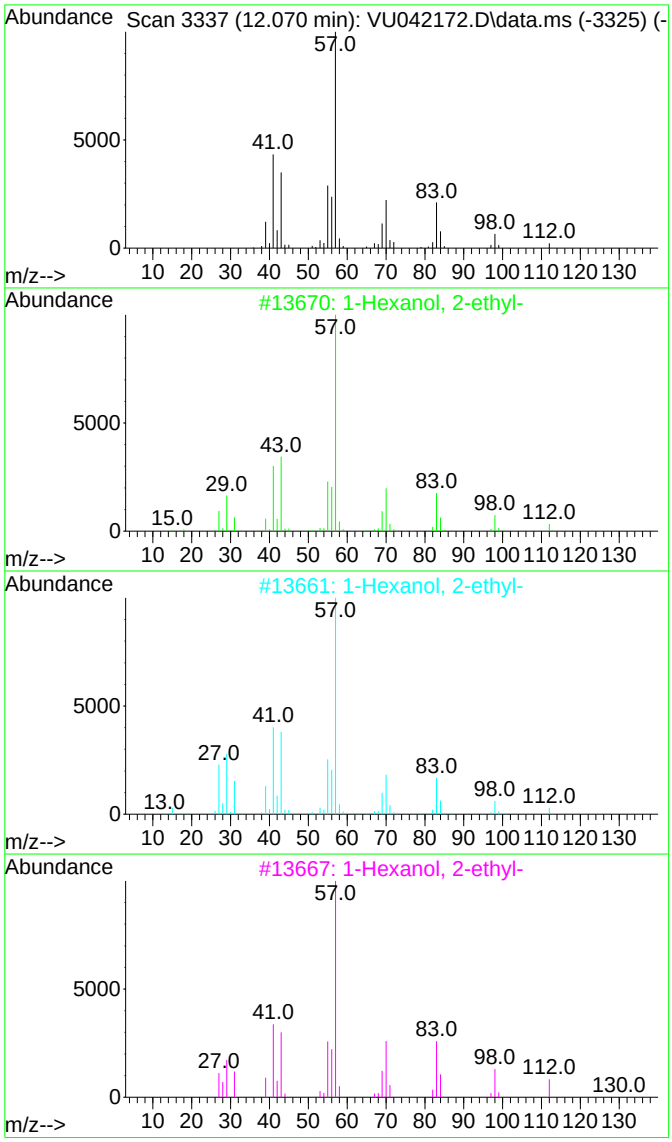
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

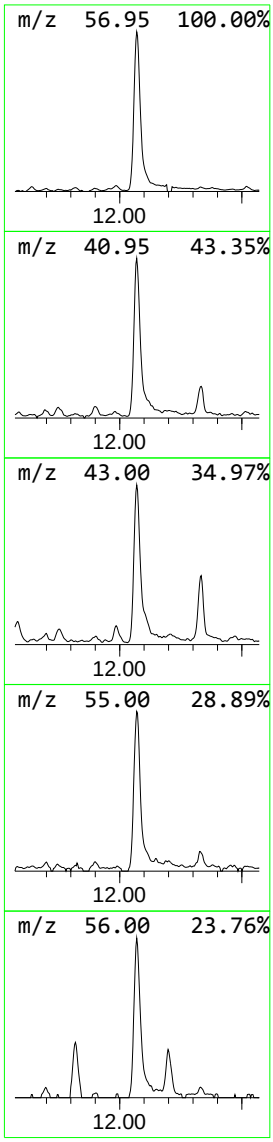
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.070	2.61 ug/L	170819	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	64
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
Data File : VU042172.D
Acq On : 22 Jan 2021 16:10
Operator : SY/MD
Sample : M1222-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E14

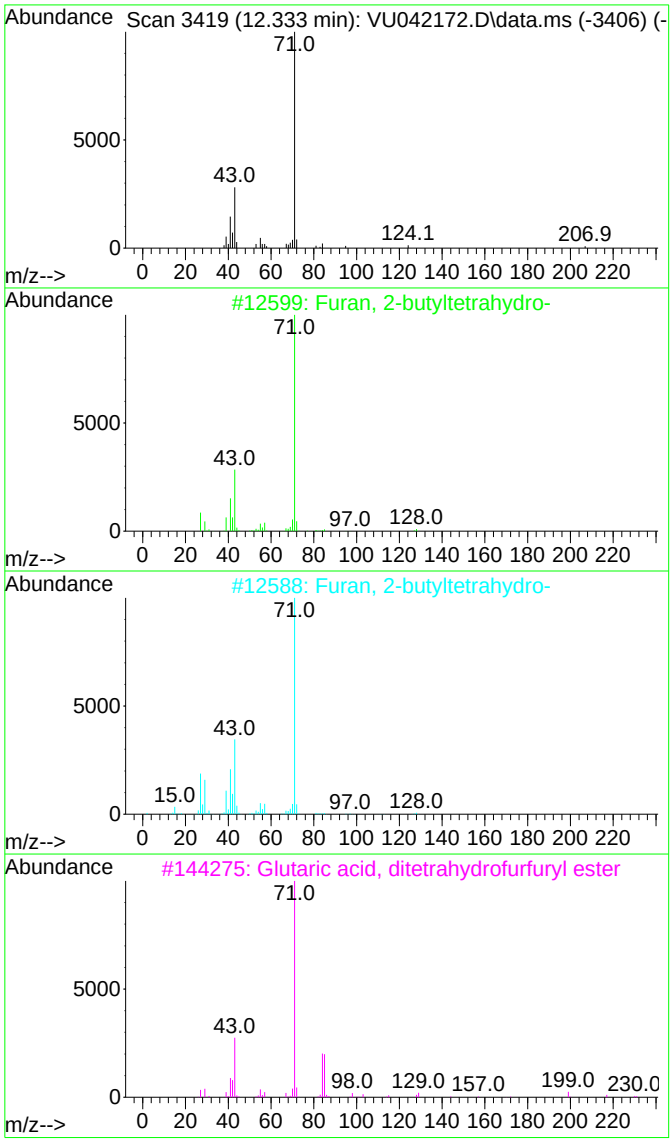
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

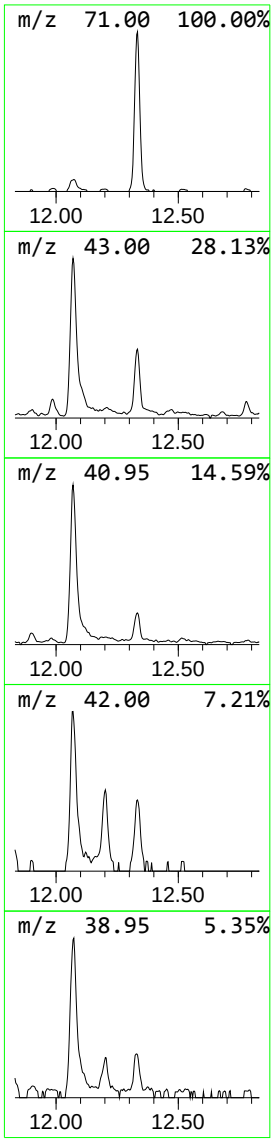
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Furan, 2-butyltetrahydro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.333	0.55 ug/L	36012	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2-butyltetrahydro-	128	C8H16O	001004-29-1	72
2	Furan, 2-butyltetrahydro-	128	C8H16O	001004-29-1	72
3	Glutaric acid, ditetrahydrofurfu...	300	C15H24O6	1000359-67-4	56
4	2,2'-Bifuran, octahydro-	142	C8H14O2	001592-33-2	56
5	Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
Data File : VU042172.D
Acq On : 22 Jan 2021 16:10
Operator : SY/MD
Sample : M1222-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E14

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

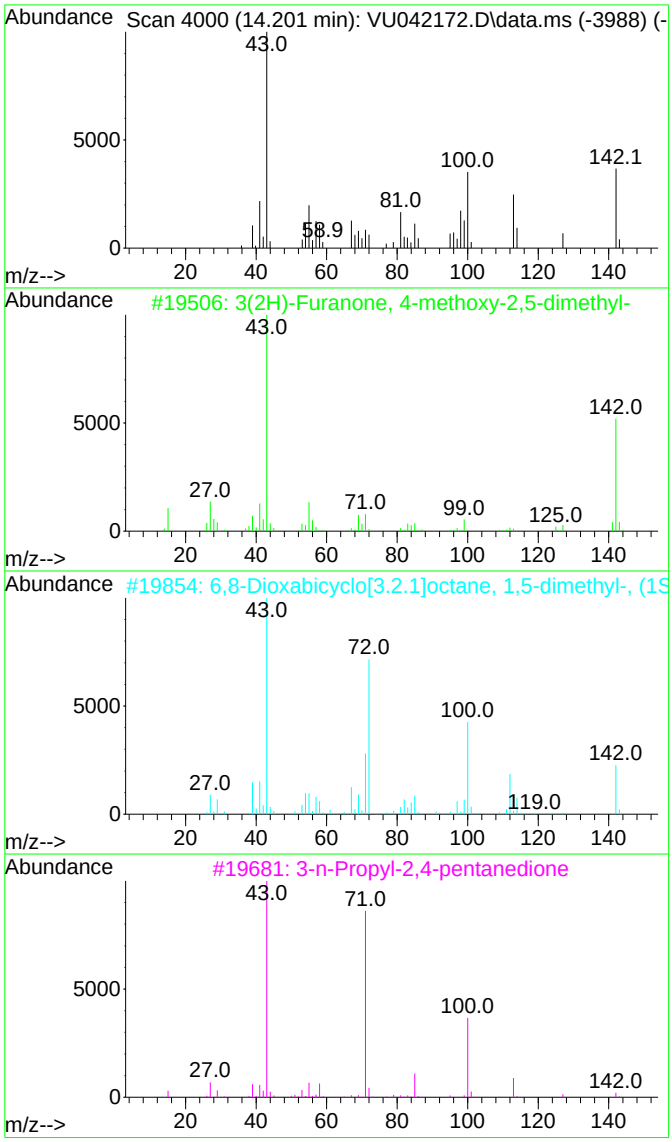
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

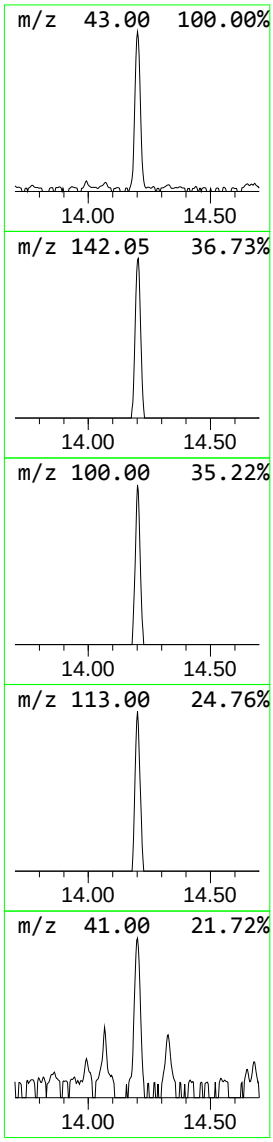
****

Peak Number 7 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	0.60 ug/L	39071	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3(2H)-Furanone, 4-methoxy-2,5-di...	142	C7H10O3	004077-47-8	38
2	6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	37
3	3-n-Propyl-2,4-pentanedione	142	C8H14O2	001540-35-8	32
4	3-n-Propyl-5-methylhexan-2-one	156	C10H20O	1000202-22-8	22
5	1,4,6-Trimethyl-3,7,9-trioxabicy...	172	C9H16O3	062759-58-4	12





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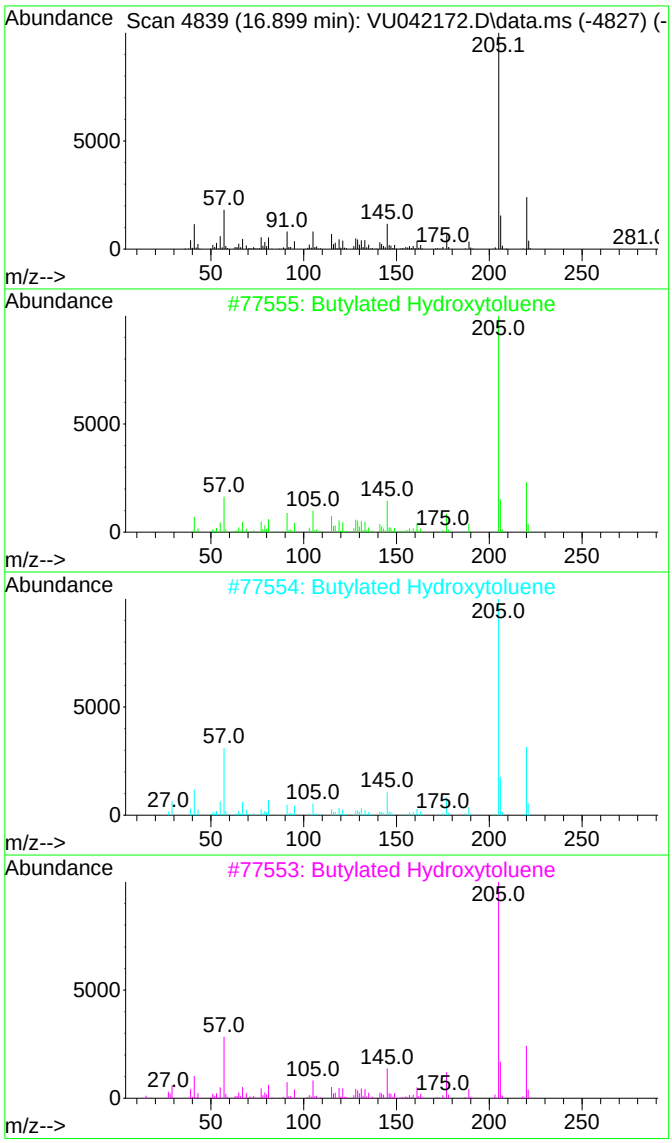
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

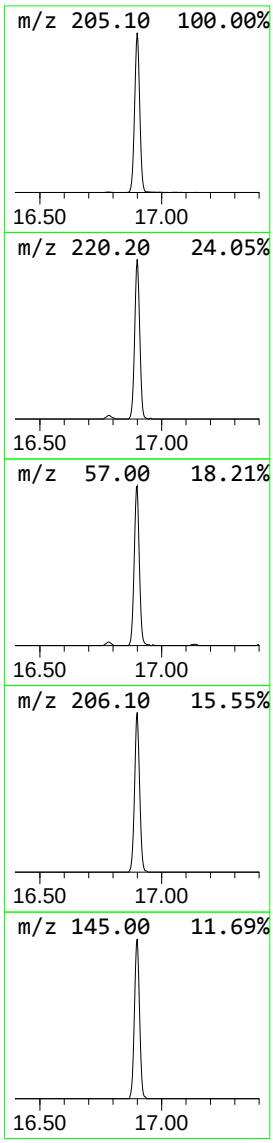
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.899	9.47 ug/L	618858	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\VU012221\
Data File : VU042172.D
Acq On : 22 Jan 2021 16:10
Operator : SY/MD
Sample : M1222-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F1E14

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-Propanol, 2-m...	3.253	1.2	ug/L	56580	1	6.256	243252	5.0
2-Butanone, 3,3...	7.176	1.4	ug/L	70003	1	6.256	243252	5.0
5-t-Butyl-4-met...	9.649	0.5	ug/L	33395	2	9.423	308337	5.0
1-Hexanol, 2-et...	12.070	2.6	ug/L	170819	3	11.819	326732	5.0
Furan, 2-butylt...	12.333	0.6	ug/L	36012	3	11.819	326732	5.0
unknown-01	14.201	0.6	ug/L	39071	3	11.819	326732	5.0
Butylated Hydro...	16.899	9.5	ug/L	618858	3	11.819	326732	5.0