

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
 Data File : VU038955.D
 Acq On : 17 Jun 2020 19:35
 Operator : SY/MD
 Sample : L3040-11
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F9L24

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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	1.620	77	87	97	rBV	122955	150612	10.88%	1.451%
2	1.954	184	191	203	rVB	108948	140243	10.13%	1.351%
3	2.549	368	376	380	rBV4	12709	23064	1.67%	0.222%
4	2.607	384	394	409	rVB	285247	458165	33.09%	4.414%
5	2.816	450	459	462	rBV5	12388	21590	1.56%	0.208%
6	3.137	550	559	562	rBV	11532	20011	1.45%	0.193%
7	3.382	629	635	644	rBV	9302	15331	1.11%	0.148%
8	4.533	974	993	995	rBV3	18355	33982	2.45%	0.327%
9	4.803	1043	1077	1099	rBV2	92368	407183	29.41%	3.923%
10	5.150	1167	1185	1206	rVB	201097	442932	31.99%	4.268%
11	5.796	1364	1386	1406	rBV2	421028	1012368	73.13%	9.754%
12	6.311	1531	1546	1565	rVB	336423	624806	45.13%	6.020%
13	6.748	1668	1682	1697	rBV	250116	478419	34.56%	4.609%
14	7.227	1808	1831	1844	rBV2	56583	127770	9.23%	1.231%
15	7.607	1935	1949	1972	rBV	123495	214106	15.47%	2.063%
16	7.848	2013	2024	2029	rBV4	7957	15339	1.11%	0.148%
17	7.935	2039	2051	2069	rVB	447358	759212	54.84%	7.315%
18	8.214	2126	2138	2150	rBV	84586	136897	9.89%	1.319%
19	8.523	2215	2234	2246	rBV7	5774	14001	1.01%	0.135%
20	8.674	2263	2281	2317	rBV	692406	1384402	100.00%	13.338%
21	8.819	2317	2326	2346	rVB5	16770	33430	2.41%	0.322%
22	9.443	2504	2520	2542	rBV	490187	808797	58.42%	7.793%
23	9.661	2575	2588	2599	rVB	20462	34744	2.51%	0.335%
24	9.790	2611	2628	2635	rBV5	7876	19104	1.38%	0.184%
25	10.256	2756	2773	2787	rBV2	25593	41213	2.98%	0.397%
26	10.362	2798	2806	2825	rVB4	12525	30695	2.22%	0.296%
27	10.700	2904	2911	2922	rVB3	11554	19166	1.38%	0.185%
28	10.774	2922	2934	2948	rBV	213769	345545	24.96%	3.329%
29	10.979	2985	2998	3012	rBV2	17995	30152	2.18%	0.291%
30	11.063	3012	3024	3032	rBV5	12115	20127	1.45%	0.194%
31	11.584	3176	3186	3195	rBV3	11562	19280	1.39%	0.186%
32	11.700	3214	3222	3233	rVB5	19467	27732	2.00%	0.267%
33	11.825	3248	3261	3276	rVB	503487	798942	57.71%	7.698%
34	12.079	3327	3340	3361	rBV3	49861	110122	7.95%	1.061%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038955.D
Acq On : 17 Jun 2020 19:35
Operator : SY/MD
Sample : L3040-11
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9L24

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	12.204	3367	3379	3398	rVB	497810	798307	57.66%	7.691%
36	12.336	3411	3420	3427	rBV2	9816	14672	1.06%	0.141%
37	12.796	3551	3563	3571	rBV4	10551	17790	1.29%	0.171%
38	12.905	3589	3597	3610	rVB5	26425	41381	2.99%	0.399%
39	14.015	3932	3942	3952	rBV6	12472	19499	1.41%	0.188%
40	14.227	3996	4008	4022	rVB6	33174	53133	3.84%	0.512%
41	14.870	4197	4208	4217	rBV3	12471	25035	1.81%	0.241%
42	14.918	4218	4223	4232	rVV7	10786	19019	1.37%	0.183%
43	15.745	4470	4480	4492	rVB6	35816	61991	4.48%	0.597%
44	16.834	4811	4819	4832	rBV3	64667	103692	7.49%	0.999%
45	16.963	4846	4859	4875	rBV	233595	405113	29.26%	3.903%

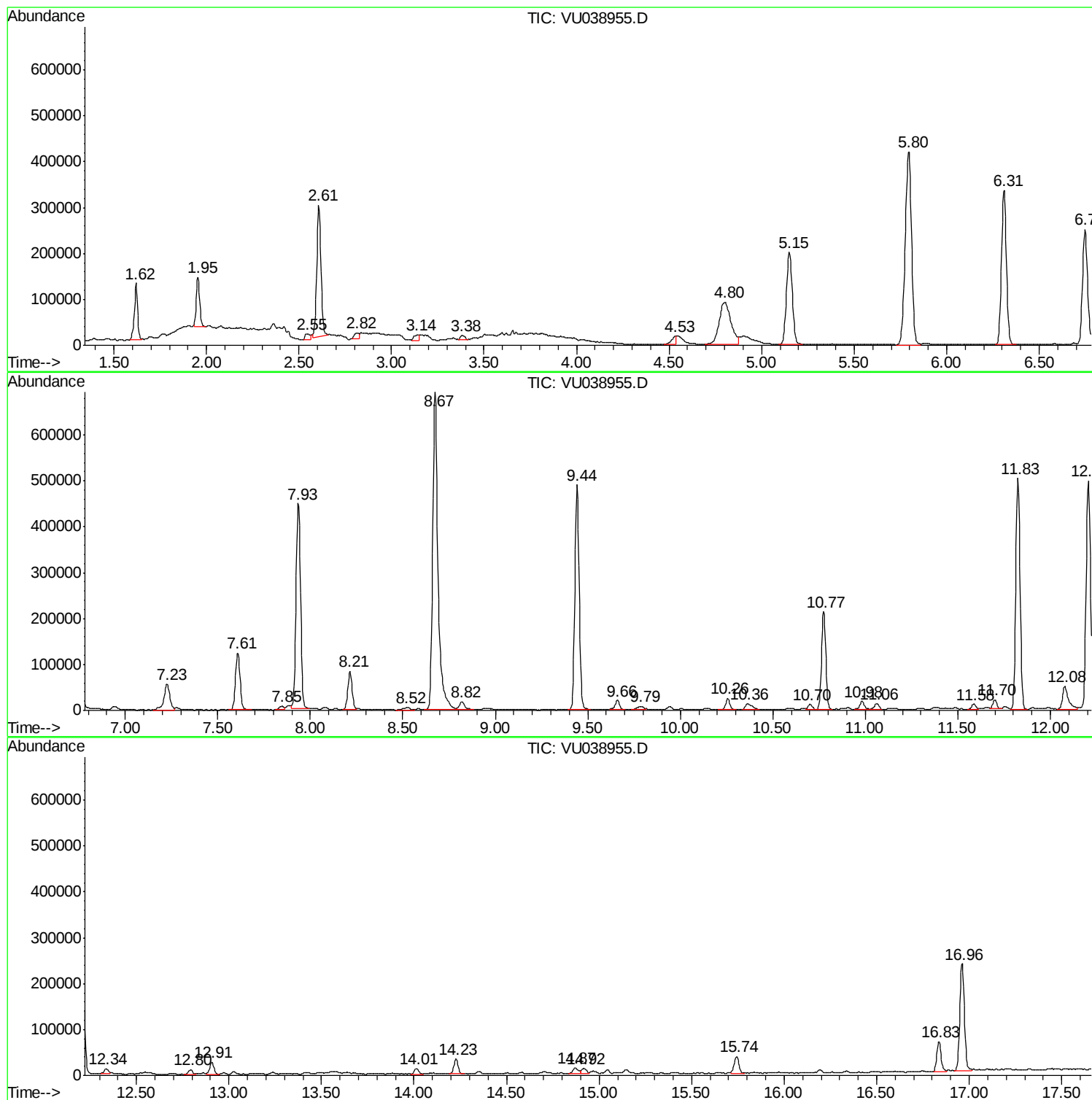
Sum of corrected areas: 10379114

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038955.D
Acq On : 17 Jun 2020 19:35
Operator : SY/MD
Sample : L3040-11
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
F9L24

Quant Method : Z:\V0ASRV\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:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038955.D
Acq On : 17 Jun 2020 19:35
Operator : SY/MD
Sample : L3040-11
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9L24

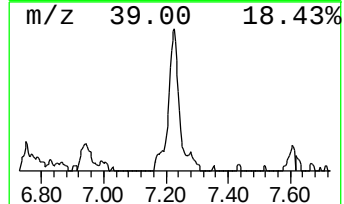
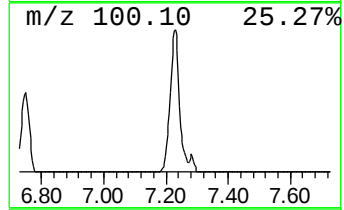
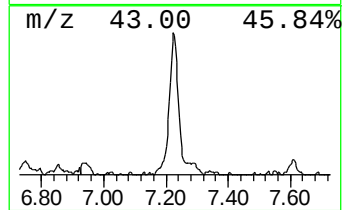
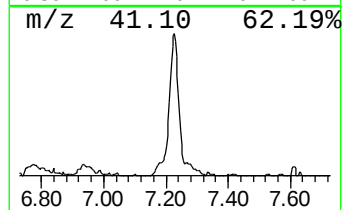
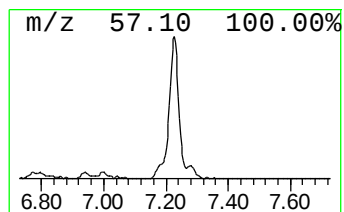
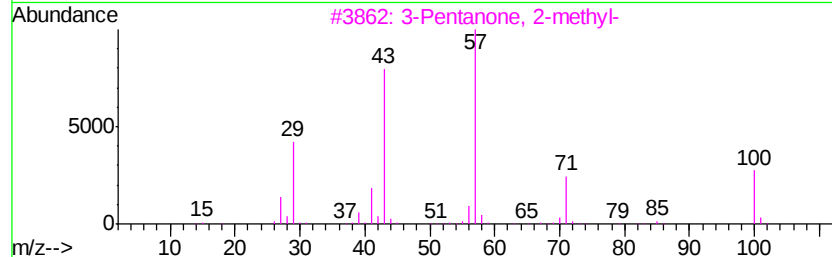
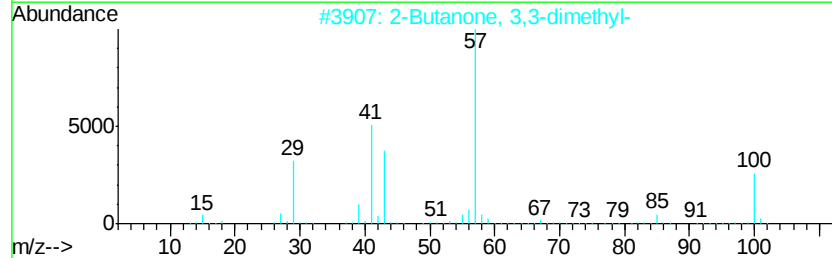
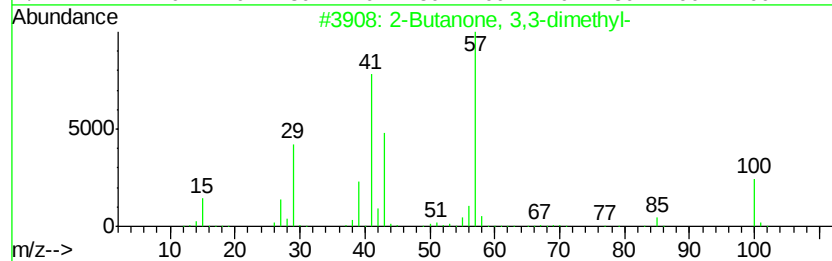
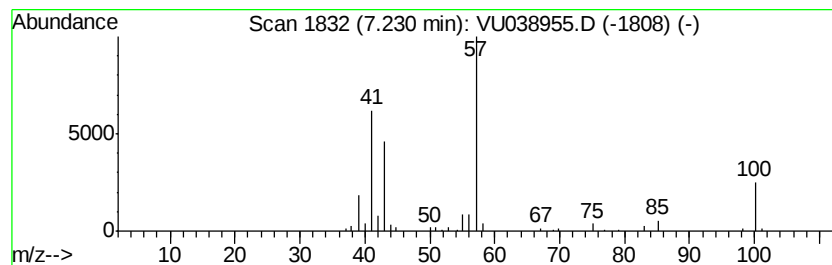
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	1.02 ug/L	127770	1,4-Difluorobenzene	6.31

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	80
3			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	80
4			3-Hexanone	100	C6H12O	000589-38-8	64
5			3-Hexanone	100	C6H12O	000589-38-8	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038955.D
Acq On : 17 Jun 2020 19:35
Operator : SY/MD
Sample : L3040-11
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

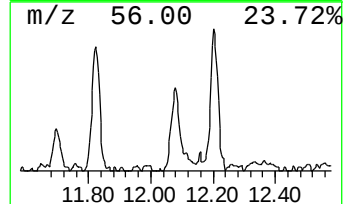
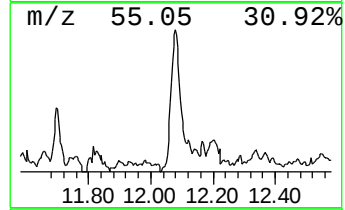
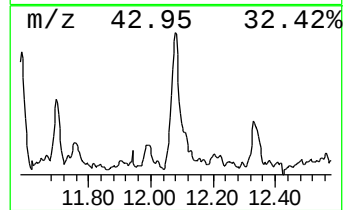
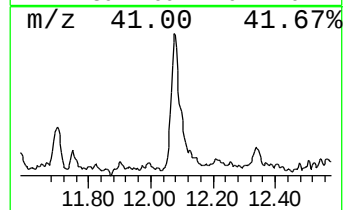
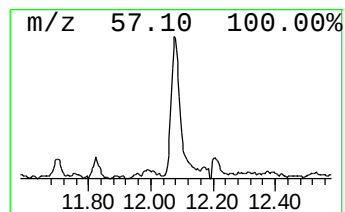
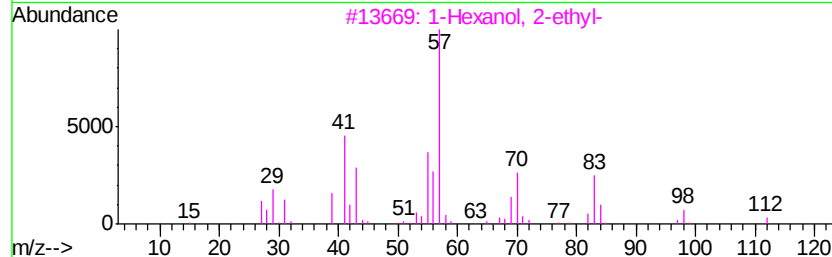
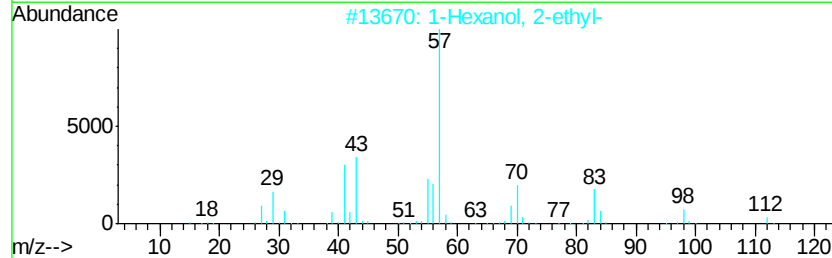
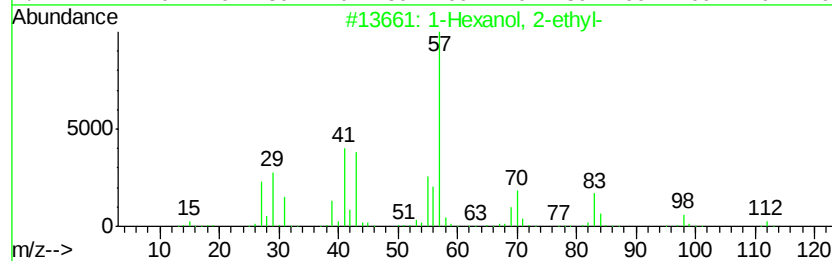
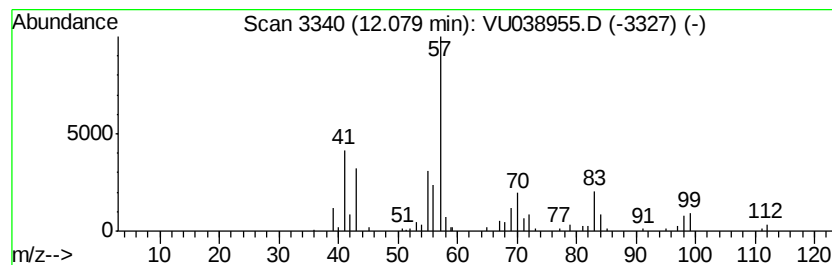
Instrument :
MSVOA_U
ClientSampleId :
F9L24

Quant Method : Z:\V0ASRV\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 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	0.69 ug/L	110122	1,4-Dichlorobenzene-d4	11.82
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7 78
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7 78
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7 59
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7 59
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2 53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038955.D
Acq On : 17 Jun 2020 19:35
Operator : SY/MD
Sample : L3040-11
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9L24

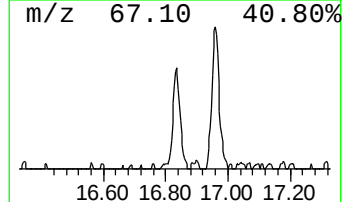
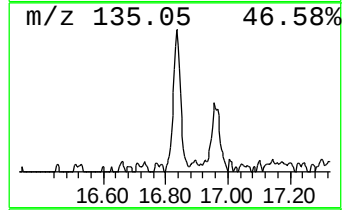
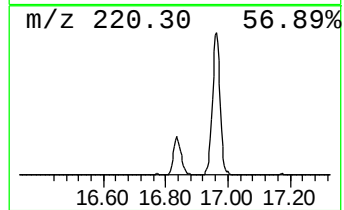
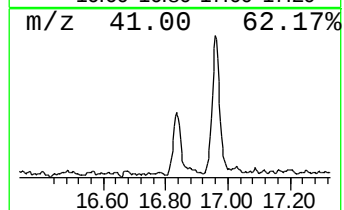
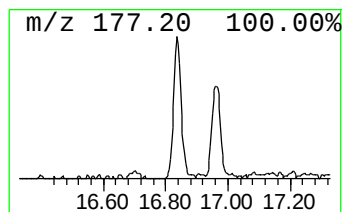
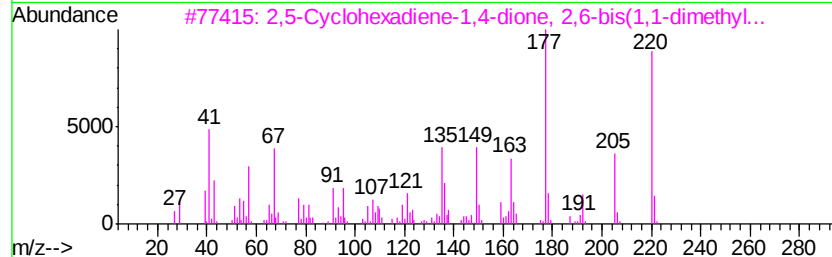
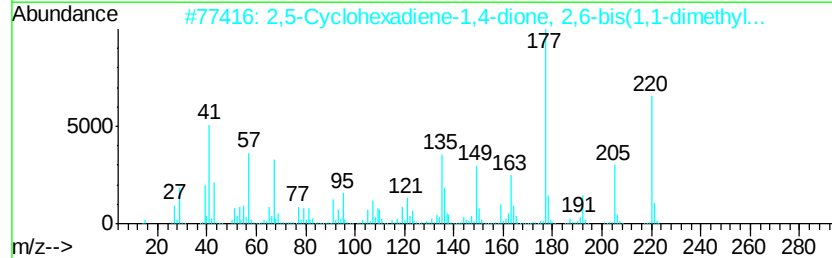
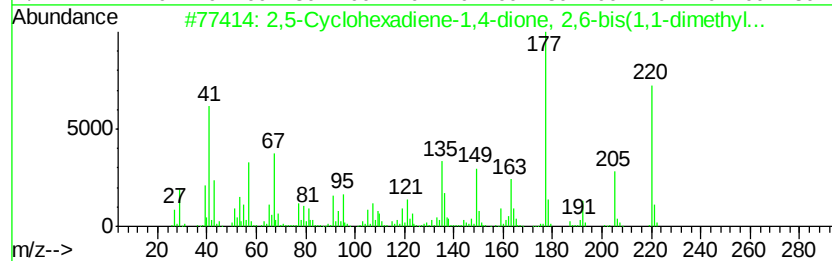
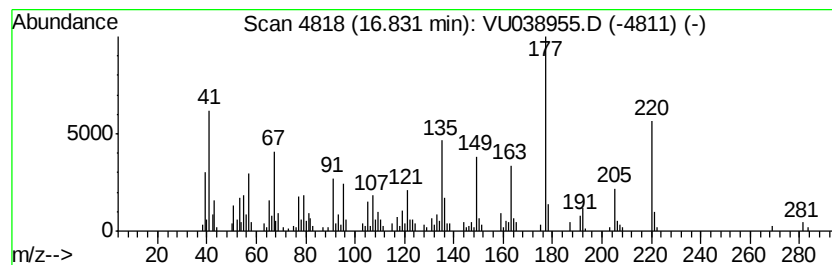
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.83	0.65 ug/L	103692	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
2		2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
3		2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	93
4		Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	45
5		3-Buten-2-one, 4-(2,6,6-trimethyl...	192	C13H20O	014901-07-6	25



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038955.D
Acq On : 17 Jun 2020 19:35
Operator : SY/MD
Sample : L3040-11
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9L24

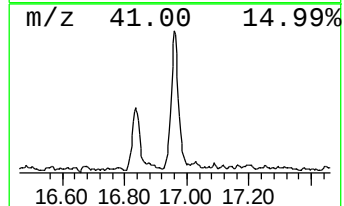
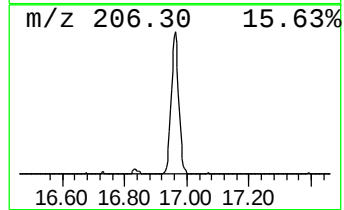
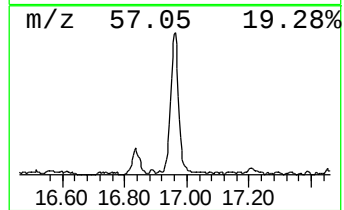
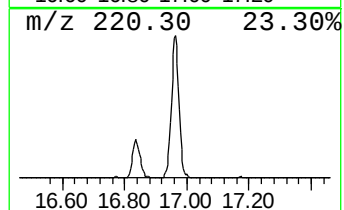
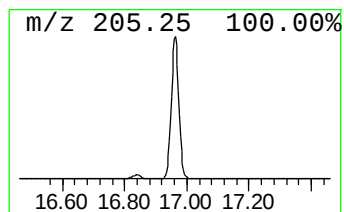
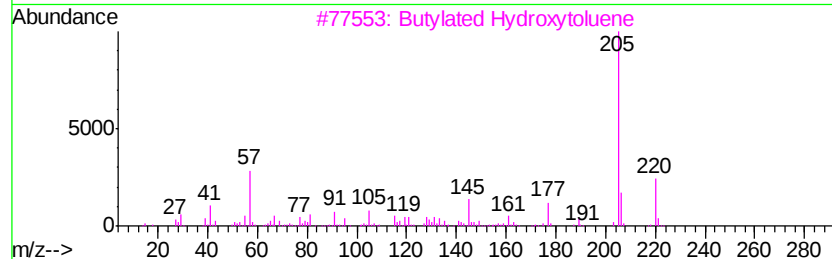
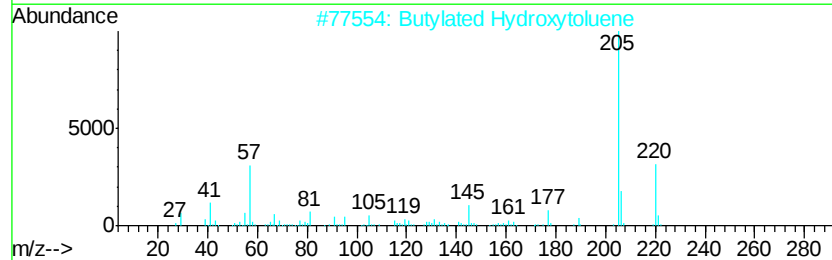
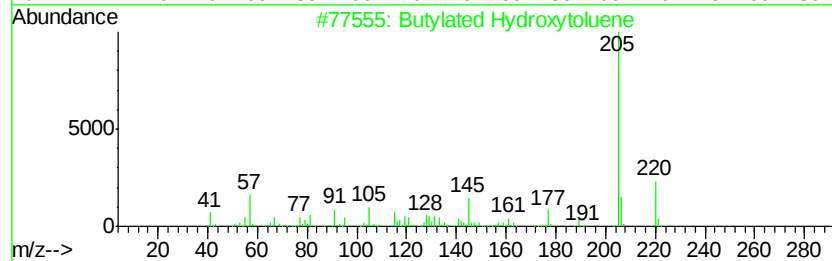
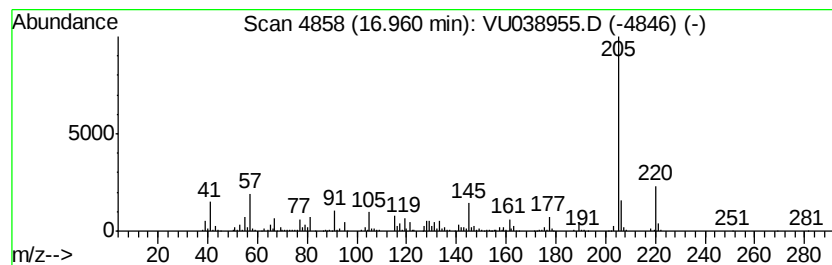
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	2.54 ug/L	405113	1,4-Dichlorobenzene-d4	11.82

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038955.D
Acq On : 17 Jun 2020 19:35
Operator : SY/MD
Sample : L3040-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9L24

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butanone, 3,3-d...	7.23	1.0	ug/L	127770	1	6.31	624806	5.0
1-Hexanol, 2-ethyl-	12.08	0.7	ug/L	110122	3	11.82	798942	5.0
2,5-Cyclohexadien...	16.83	0.7	ug/L	103692	3	11.82	798942	5.0
Butylated Hydroxy...	16.96	2.5	ug/L	405113	3	11.82	798942	5.0