

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU111618\
 Data File : VU028185.D
 Acq On : 16 Nov 2018 15:49
 Operator : MD/SY
 Sample : J5960-07
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AK9

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\SOMUTR111418WMA.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	1.395	59	69	81	rBV2	94736	142865	17.09%	2.022%
2	1.685	151	159	179	rVB	65636	87321	10.44%	1.236%
3	2.276	332	343	352	rBV	124376	185717	22.21%	2.628%
4	2.325	352	358	370	rVB	37937	60066	7.18%	0.850%
5	2.450	386	397	409	rBV2	34236	61961	7.41%	0.877%
6	2.556	423	430	440	rVB3	5620	8979	1.07%	0.127%
7	2.839	500	518	535	rBV	96615	210059	25.12%	2.973%
8	3.993	856	877	905	rBV2	159344	443753	53.07%	6.279%
9	4.196	924	940	981	rBV2	130169	485753	58.09%	6.874%
10	4.649	1065	1081	1100	rBV2	103258	241574	28.89%	3.418%
11	4.993	1171	1188	1208	rVB2	35130	79618	9.52%	1.127%
12	5.341	1272	1296	1319	rBV3	204813	580519	69.42%	8.215%
13	5.887	1448	1466	1491	rBV	214152	421410	50.40%	5.963%
14	6.334	1591	1605	1621	rBV	145136	287141	34.34%	4.063%
15	6.787	1730	1746	1776	rBV2	225802	535342	64.02%	7.576%
16	7.231	1868	1884	1901	rBV3	62655	116367	13.92%	1.647%
17	7.566	1974	1988	2006	rBV	250063	436724	52.23%	6.180%
18	7.852	2067	2077	2094	rBV2	37515	66635	7.97%	0.943%
19	8.315	2209	2221	2254	rBV	464527	836186	100.00%	11.833%
20	8.469	2261	2269	2283	rVB4	9486	17806	2.13%	0.252%
21	9.090	2450	2462	2482	rBV	309000	515073	61.60%	7.289%
22	10.035	2746	2756	2773	rVB4	10589	19346	2.31%	0.274%
23	10.430	2869	2879	2892	rBV	106146	170252	20.36%	2.409%
24	11.485	3194	3207	3228	rBV	289584	464174	55.51%	6.568%
25	11.745	3281	3288	3299	rBV4	5723	10094	1.21%	0.143%
26	11.861	3310	3324	3346	rBV	231257	380297	45.48%	5.382%
27	12.572	3536	3545	3558	rBV7	6175	11245	1.34%	0.159%
28	13.990	3975	3986	4000	rBV	51048	82634	9.88%	1.169%
29	14.568	4158	4166	4189	rBV8	6390	17178	2.05%	0.243%
30	15.353	4399	4410	4419	rBV10	10729	17739	2.12%	0.251%
31	16.430	4734	4745	4756	rBV5	41720	72886	8.72%	1.031%

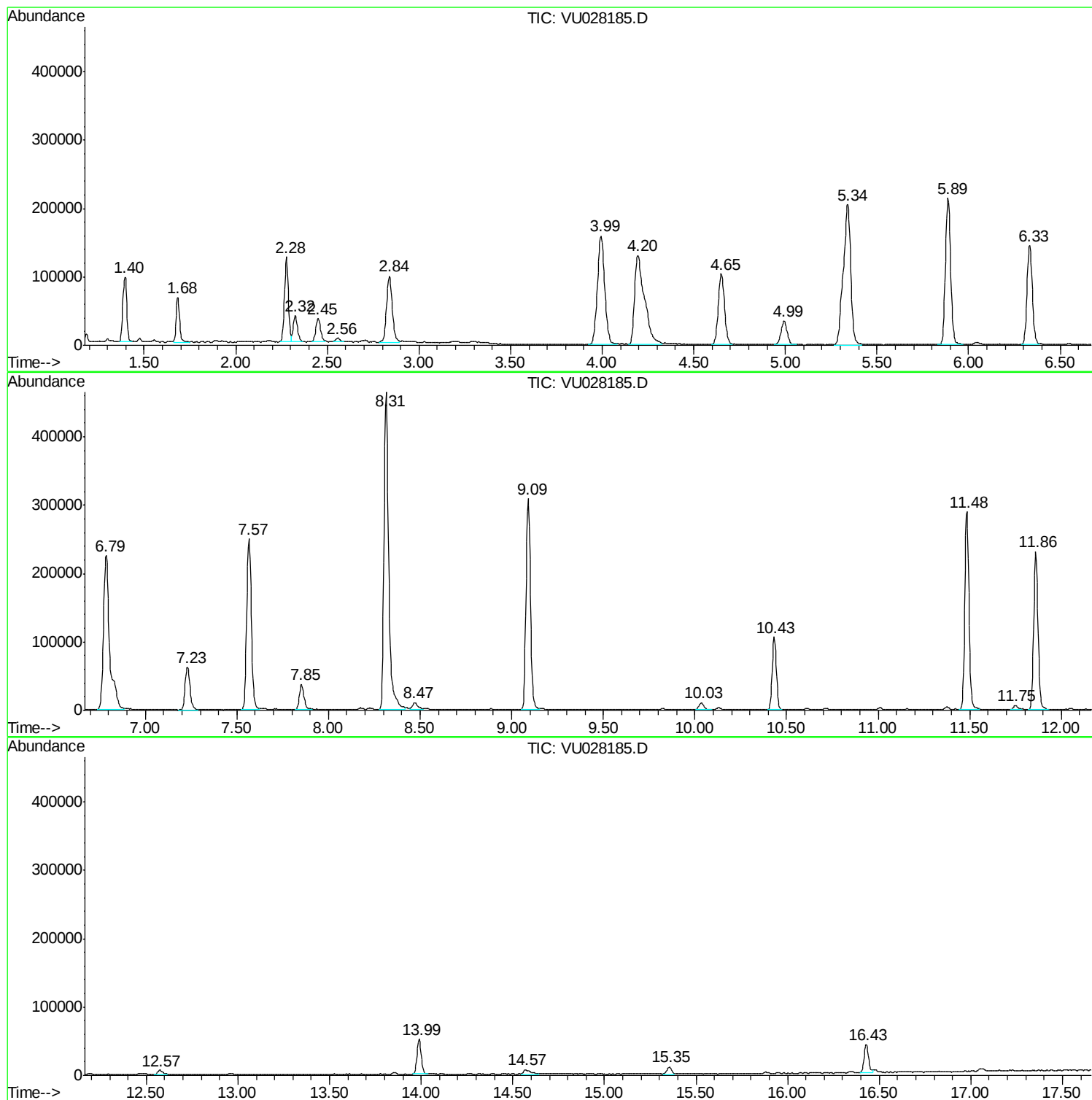
Sum of corrected areas: 7066714

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU111618\
Data File : VU028185.D
Acq On : 16 Nov 2018 15:49
Operator : MD/SY
Sample : J5960-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0AK9

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111418WMA.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\VU111618\
Data File : VU028185.D
Acq On : 16 Nov 2018 15:49
Operator : MD/SY
Sample : J5960-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AK9

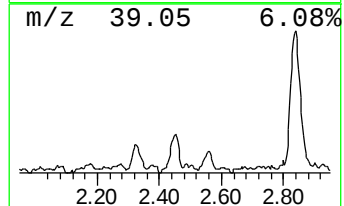
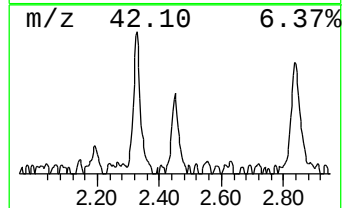
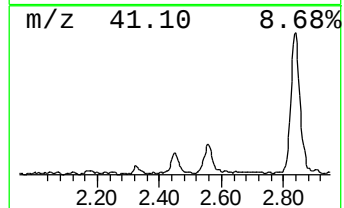
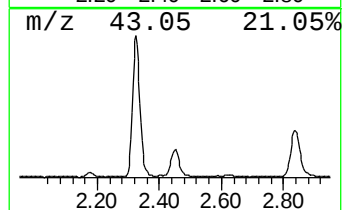
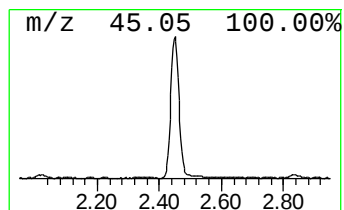
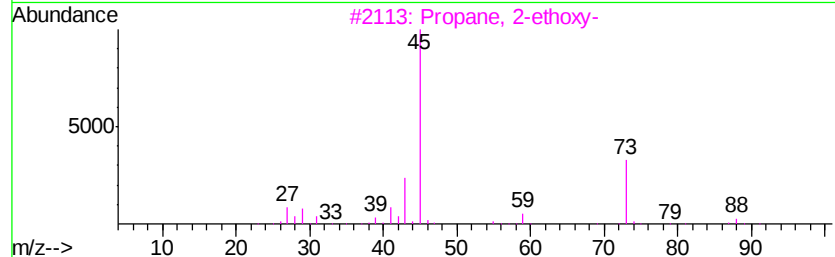
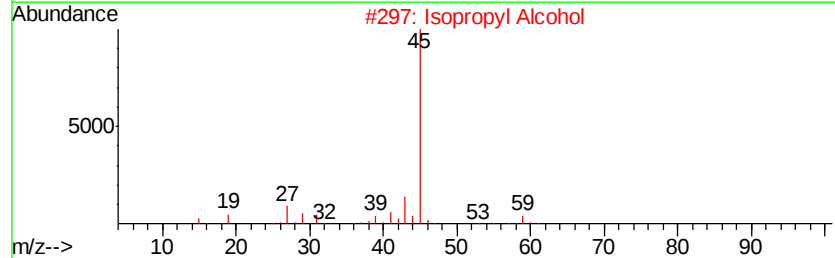
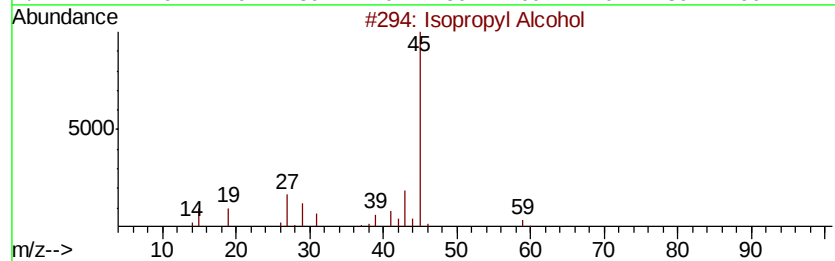
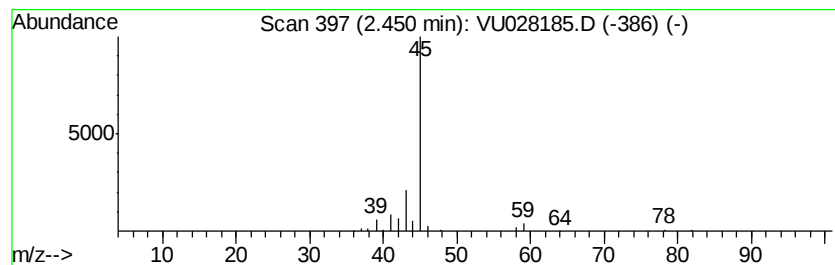
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111418WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	0.74 ug/L	61961	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	64
3		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
4		2-Pentanol	88	C5H12O	006032-29-7	9
5		Isopropyl Alcohol	60	C3H8O	000067-63-0	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU111618\
Data File : VU028185.D
Acq On : 16 Nov 2018 15:49
Operator : MD/SY
Sample : J5960-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AK9

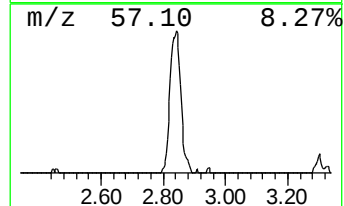
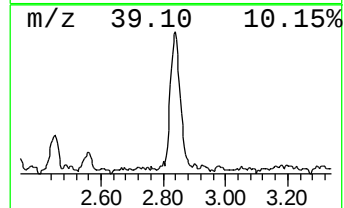
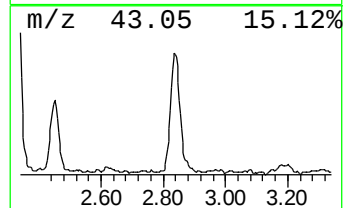
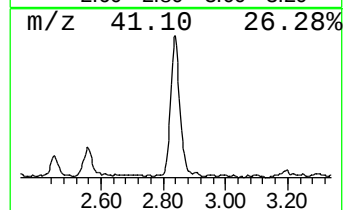
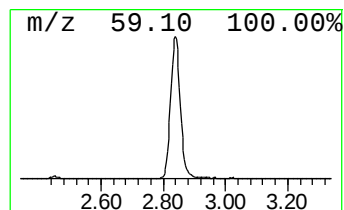
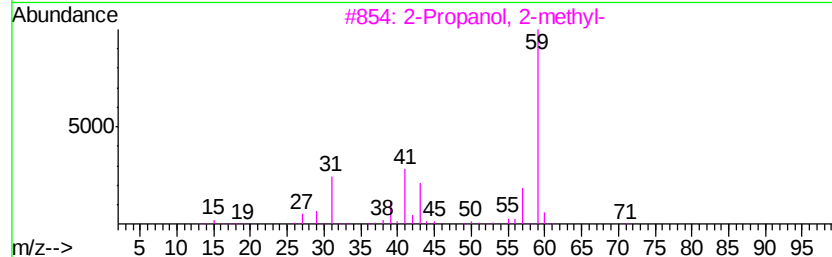
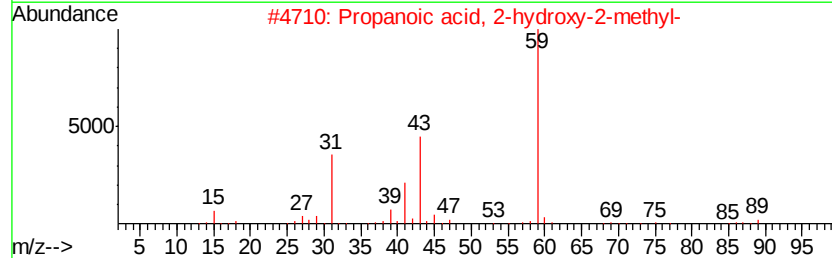
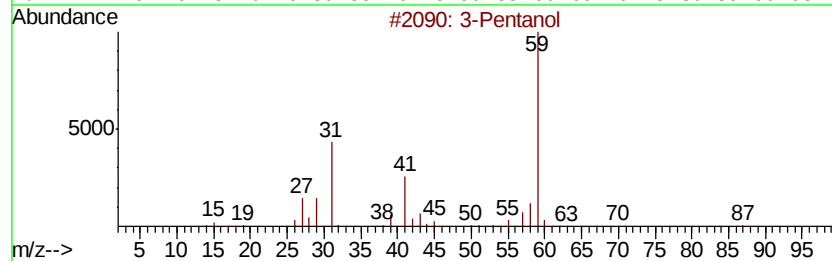
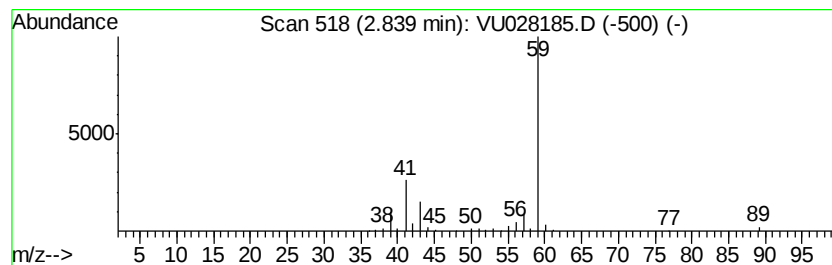
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111418WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 3-Pentanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	2.49 ug/L	210059	1,4-Difluorobenzene	5.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol	88	C5H12O	000584-02-1	56
2			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	56
3			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56
4			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56
5			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU111618\
Data File : VU028185.D
Acq On : 16 Nov 2018 15:49
Operator : MD/SY
Sample : J5960-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AK9

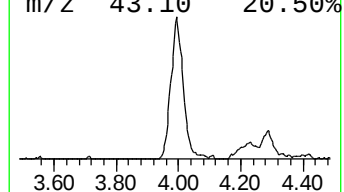
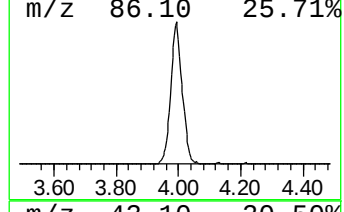
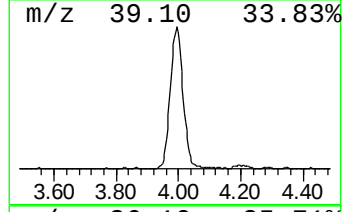
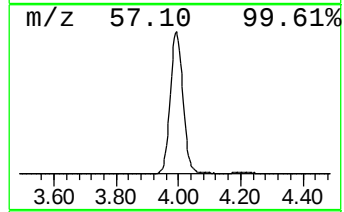
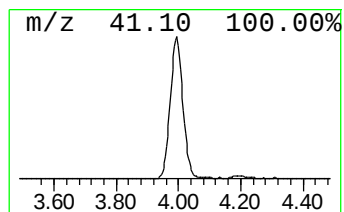
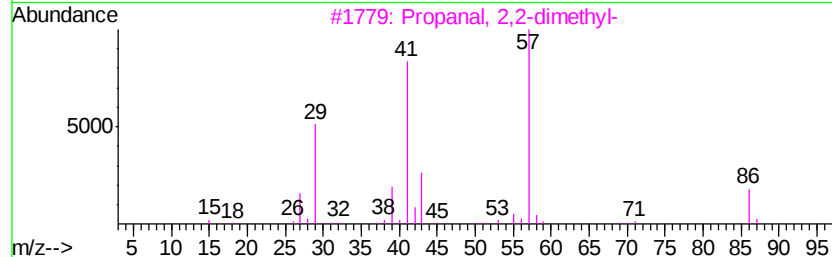
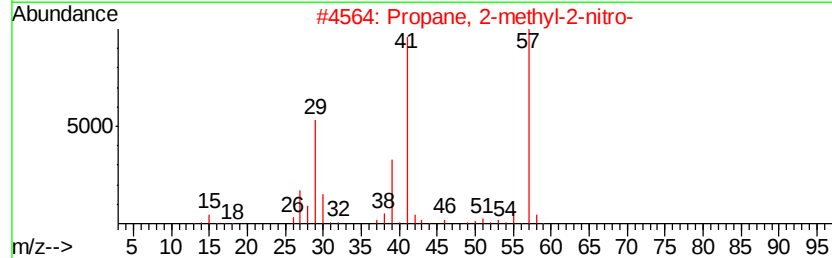
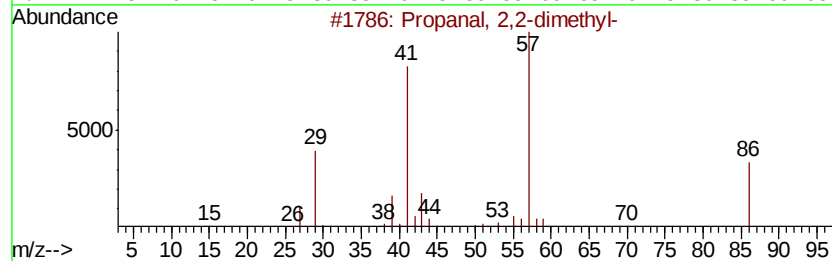
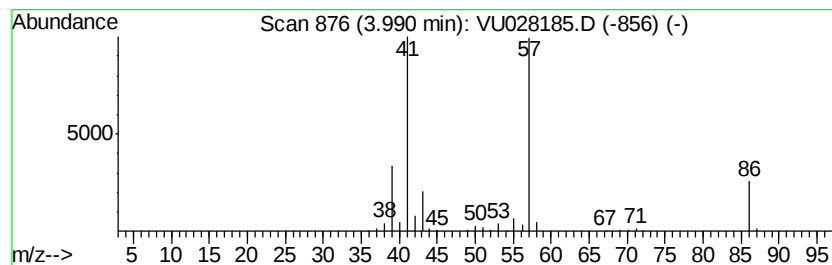
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111418WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Propanal, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	5.27 ug/L	443753	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	64
2		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	53
3		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	50
4		3-Heptanone, 5-ethyl-4-methyl-	156	C10H20O	027607-63-2	42
5		3-Pentanone	86	C5H10O	000096-22-0	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU111618\
Data File : VU028185.D
Acq On : 16 Nov 2018 15:49
Operator : MD/SY
Sample : J5960-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

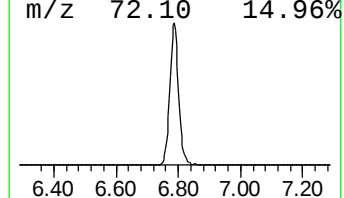
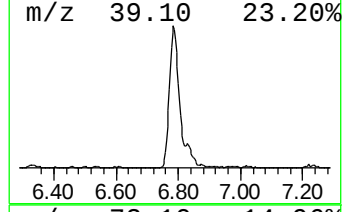
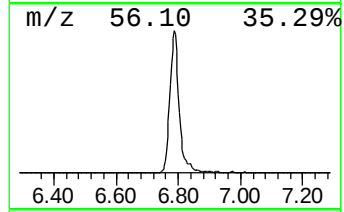
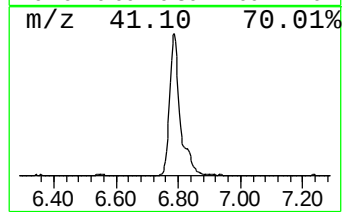
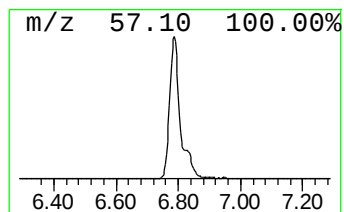
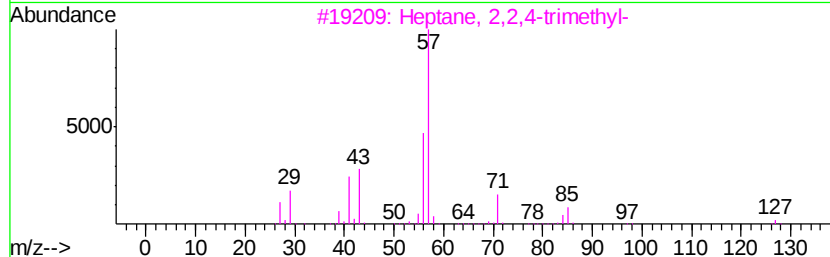
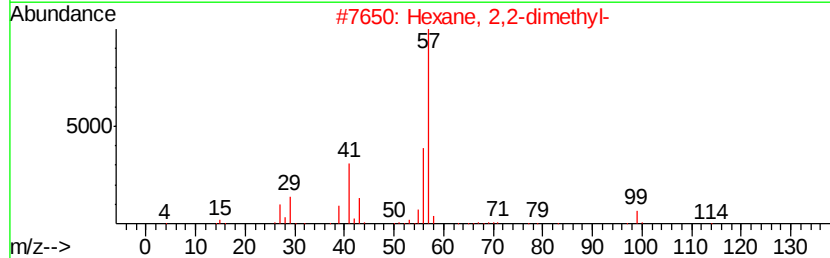
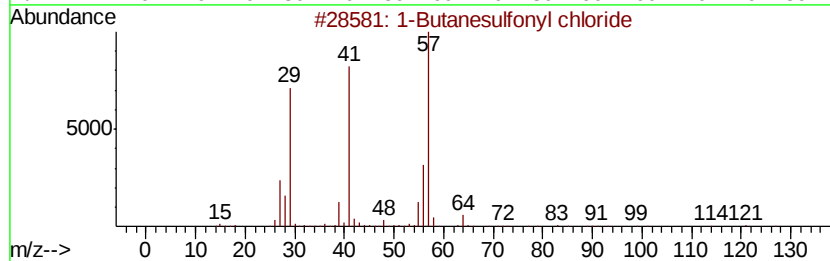
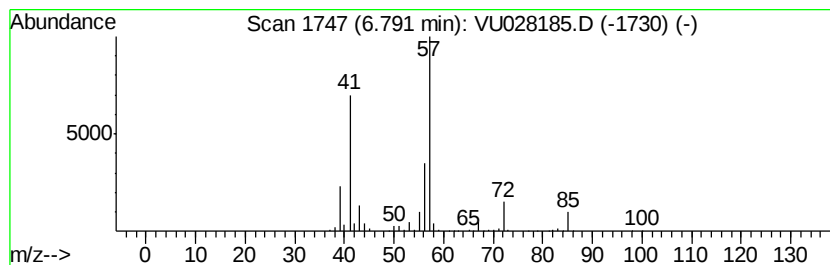
Instrument :
MSVOA_U
ClientSampled :
C0AK9

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111418WMA.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 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
6.79	6.35 ug/L	535342	1,4-Difluorobenzene	5.89		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	38
2		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	38
3		Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	36
4		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	33
5		2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	33



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU111618\
Data File : VU028185.D
Acq On : 16 Nov 2018 15:49
Operator : MD/SY
Sample : J5960-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

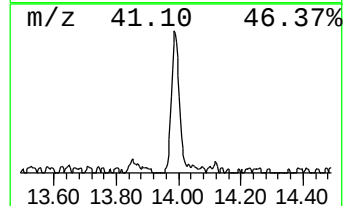
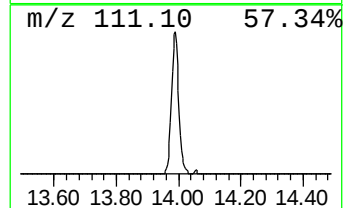
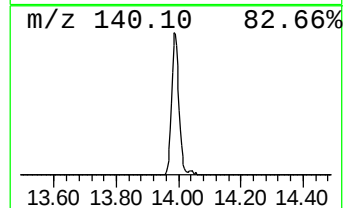
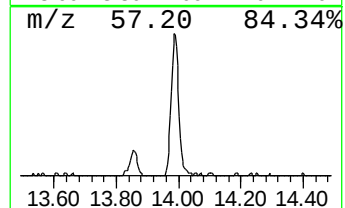
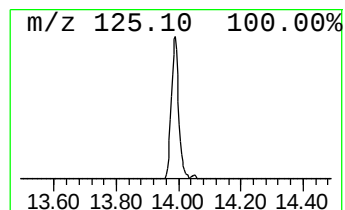
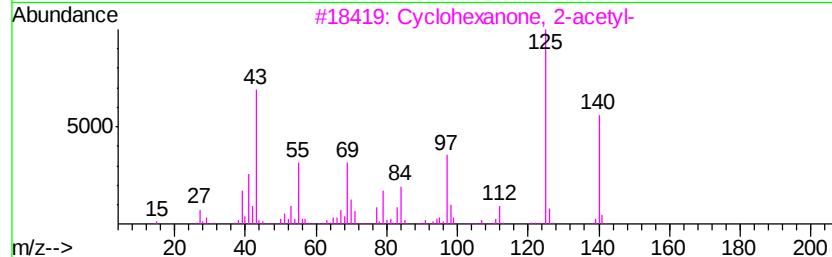
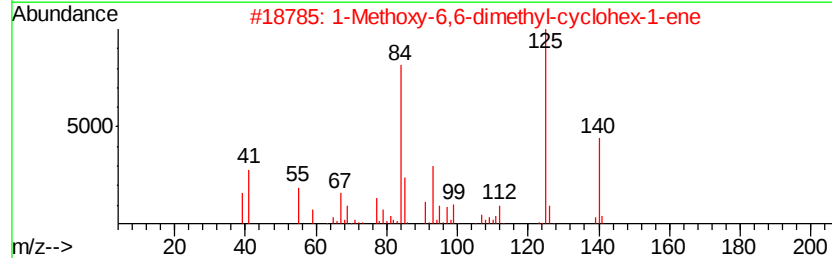
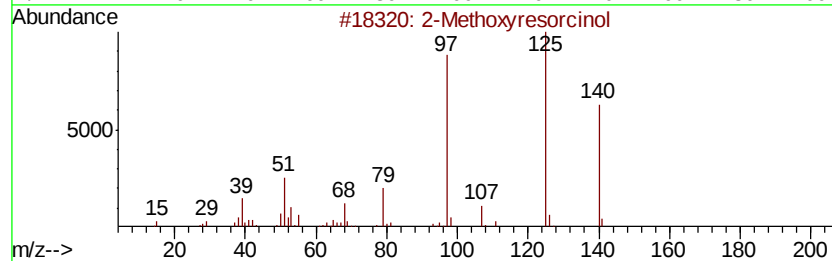
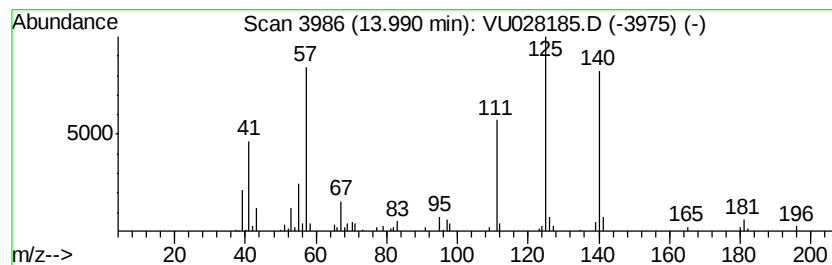
Instrument :
MSVOA_U
ClientSampleId :
C0AK9

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111418WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 2-Methoxyresorcinol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.99	0.89 ug/L	82634	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methoxyresorcinol	140	C7H8O3	029267-67-2	53
2	1-Methoxy-6,6-dimethyl-cyclohex-...	140	C9H16O	073741-66-9	53
3	Cyclohexanone, 2-acetyl-	140	C8H12O2	000874-23-7	53
4	1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	53
5	3-Amino-5-t-butyliisoxazole	140	C7H12N2O	055809-36-4	52



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU111618\
Data File : VU028185.D
Acq On : 16 Nov 2018 15:49
Operator : MD/SY
Sample : J5960-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AK9

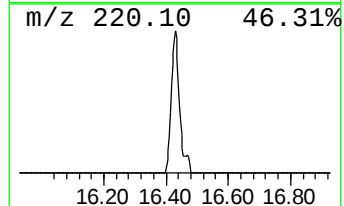
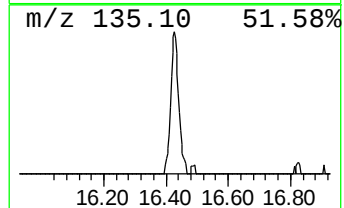
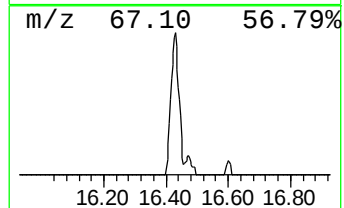
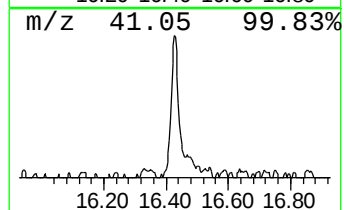
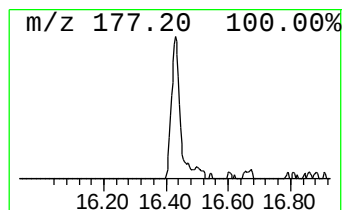
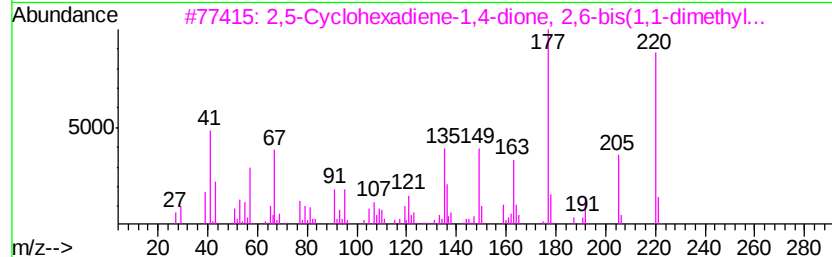
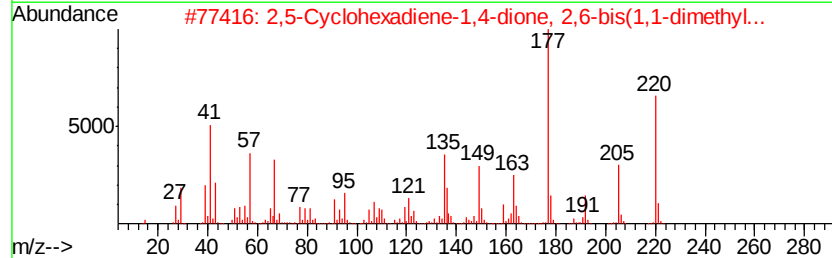
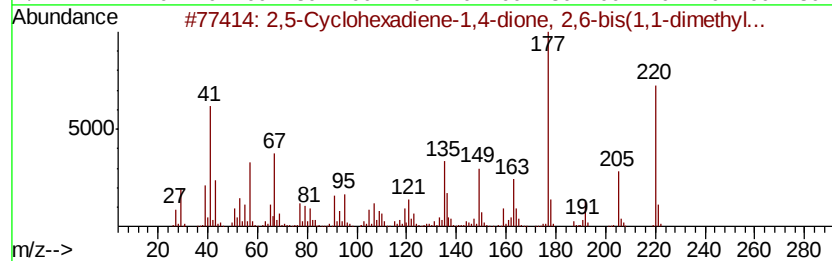
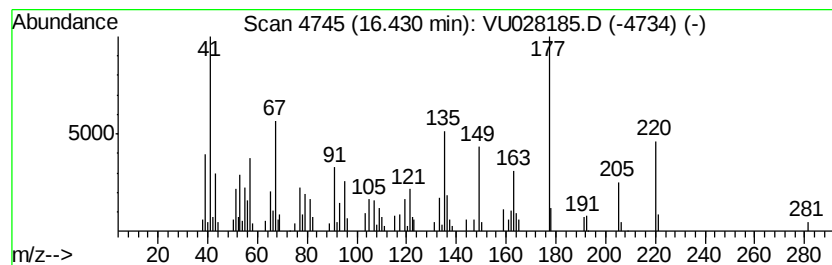
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111418WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	0.79 ug/L	72886	1,4-Dichlorobenzene-d4	11.48

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	91
3		2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	86
4		Dimethyl 5-methylisophthalate	208	C11H12O4	017649-58-0	27
5		4-Propylbenzaldehyde diethyl acetal	222	C14H22O2	089557-35-7	27



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU111618\
Data File : VU028185.D
Acq On : 16 Nov 2018 15:49
Operator : MD/SY
Sample : J5960-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AK9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111418WMA.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
Isopropyl Alcohol	2.45	0.7	ug/L	61961	1	5.89	421410	5.0
3-Pentanol	2.84	2.5	ug/L	210059	1	5.89	421410	5.0
Propanal, 2,2-dim...	3.99	5.3	ug/L	443753	1	5.89	421410	5.0
unknown-01	6.79	6.3	ug/L	535342	1	5.89	421410	5.0
2-Methoxyresorcinol	13.99	0.9	ug/L	82634	3	11.48	464174	5.0
2,5-Cyclohexadien...	16.43	0.8	ug/L	72886	3	11.48	464174	5.0