

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
 Data File : VN065635.D
 Acq On : 27 Jan 2021 17:26
 Operator : JC/MD
 Sample : M1213-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 IDW-BR2-SO-012121

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % of largest Peak

Start Thrs: 0.2

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_N\methods\82N012521W.M
 Title : SW846 8260

Signal : TIC: VN065635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.782	624	635	652	rVB	16911	41483	1.55%	0.319%
2	4.502	840	859	874	rBV2	11724	33500	1.25%	0.257%
3	5.695	1211	1230	1251	rBV2	20411	64498	2.40%	0.495%
4	7.550	1789	1807	1818	rBV	128187	320492	11.95%	2.462%
5	7.624	1818	1830	1854	rVB	251690	599346	22.35%	4.604%
6	7.987	1926	1943	1963	rBV	156861	366613	13.67%	2.816%
7	8.132	1972	1988	2001	rVB3	14826	33774	1.26%	0.259%
8	8.547	2098	2117	2141	rBV	392983	825749	30.79%	6.343%
9	9.151	2294	2305	2317	rBV3	18625	37645	1.40%	0.289%
10	9.235	2317	2331	2360	rBV	970584	1817672	67.77%	13.962%
11	9.872	2515	2529	2545	rBV	177376	310589	11.58%	2.386%
12	10.058	2573	2587	2601	rBV	618901	1142730	42.61%	8.777%
13	10.251	2636	2647	2659	rBV	18941	32465	1.21%	0.249%
14	10.515	2717	2729	2739	rBV	51212	85139	3.17%	0.654%
15	10.608	2747	2758	2774	rBV	110808	187154	6.98%	1.438%
16	10.733	2785	2797	2814	rVV	1651343	2681981	100.00%	20.600%
17	10.823	2815	2825	2841	rVB	172772	289427	10.79%	2.223%
18	11.138	2909	2923	2947	rBV	1094221	1747198	65.15%	13.420%
19	11.376	2984	2997	3017	rBV	532798	925163	34.50%	7.106%
20	11.849	3136	3144	3154	rVB	36785	57645	2.15%	0.443%
21	12.373	3295	3307	3330	rBV	387051	678725	25.31%	5.213%
22	13.312	3588	3599	3619	rBV	433896	740029	27.59%	5.684%

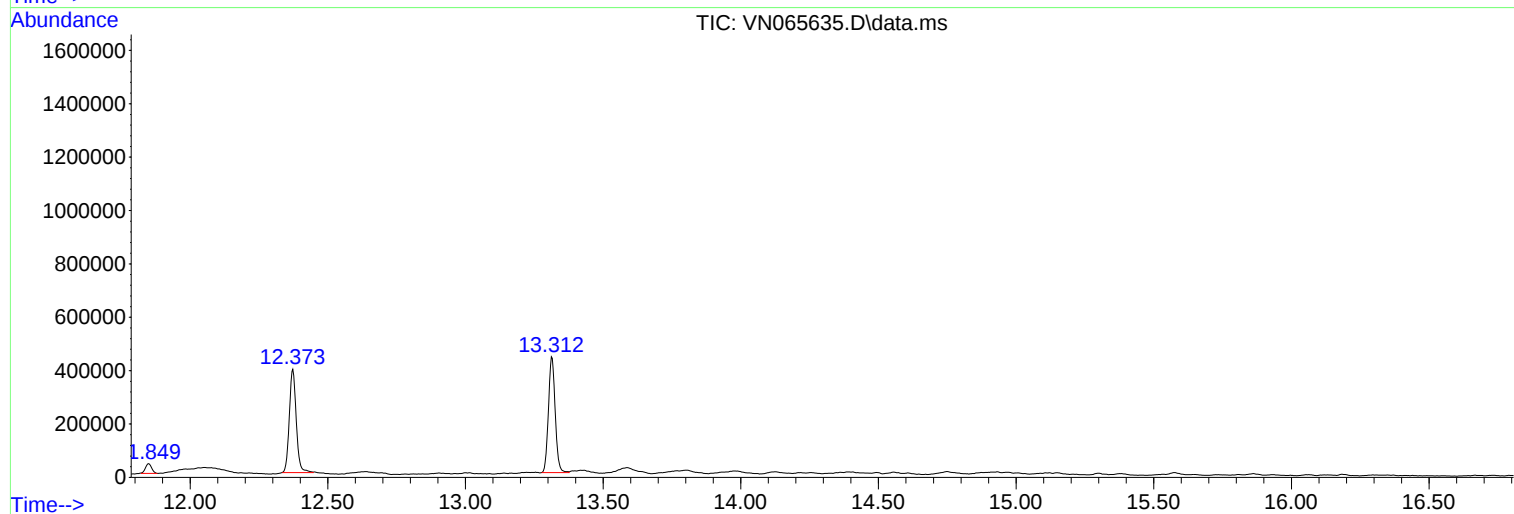
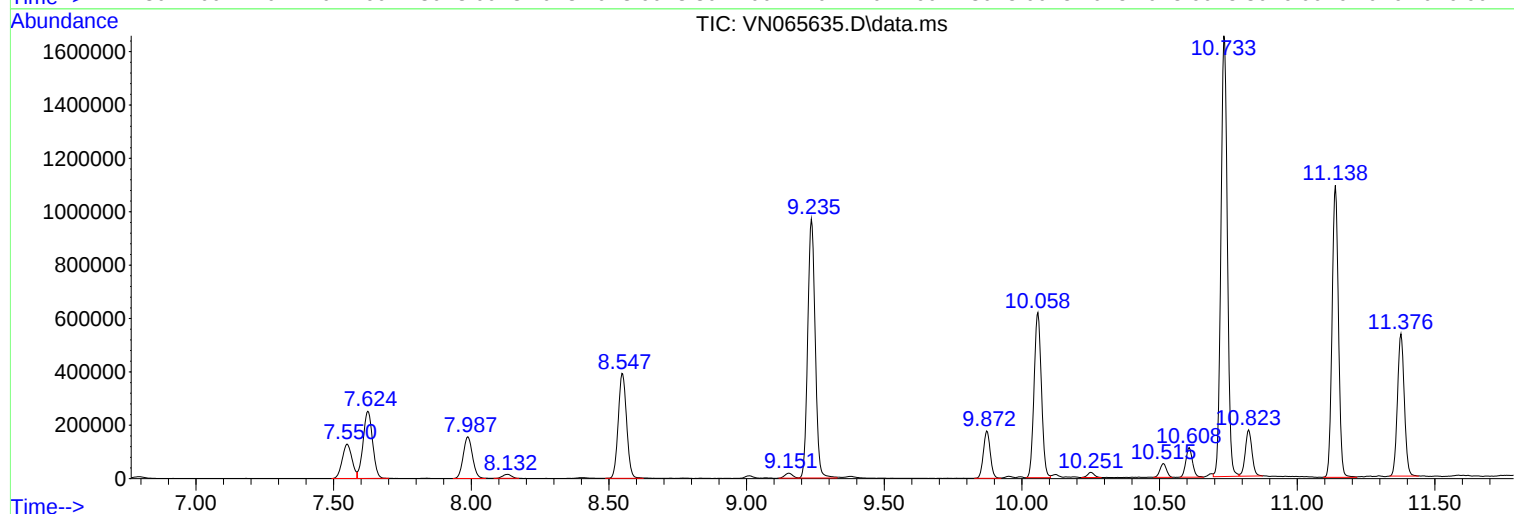
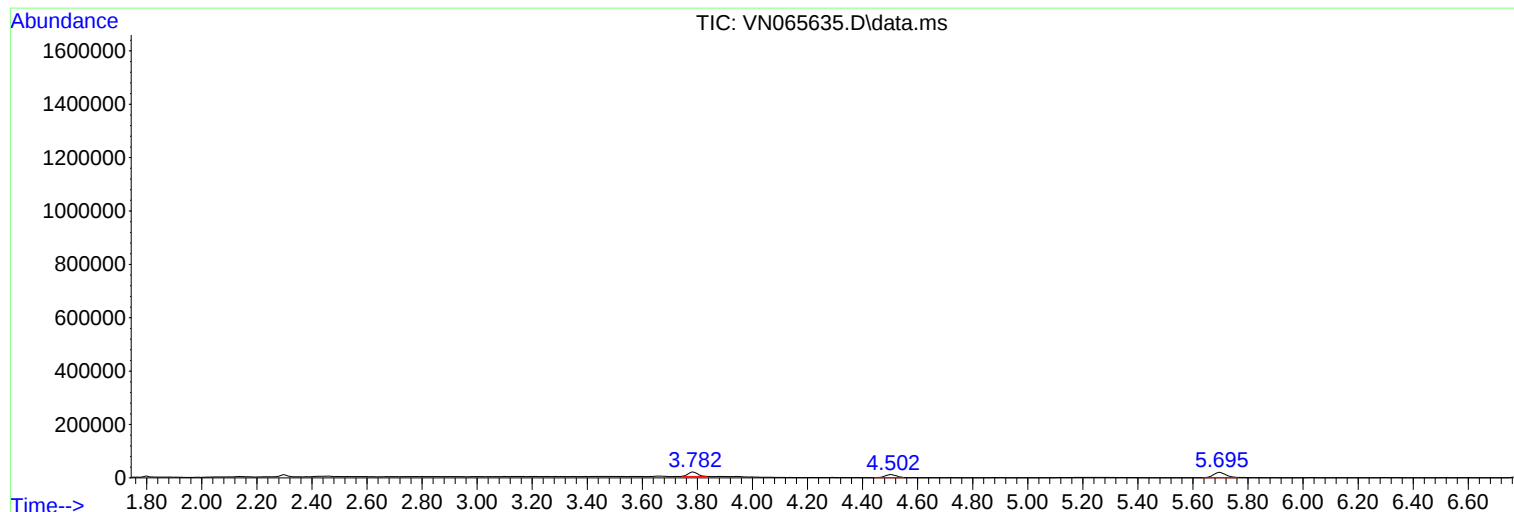
Sum of corrected areas: 13019017

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065635.D
Acq On : 27 Jan 2021 17:26
Operator : JC/MD
Sample : M1213-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-BR2-SO-012121

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065635.D
Acq On : 27 Jan 2021 17:26
Operator : JC/MD
Sample : M1213-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-BR2-SO-012121

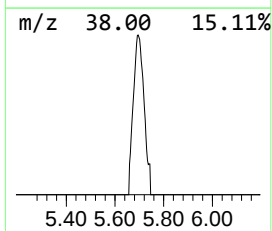
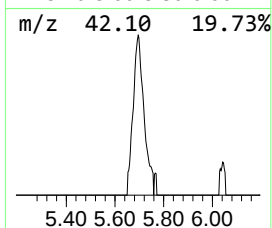
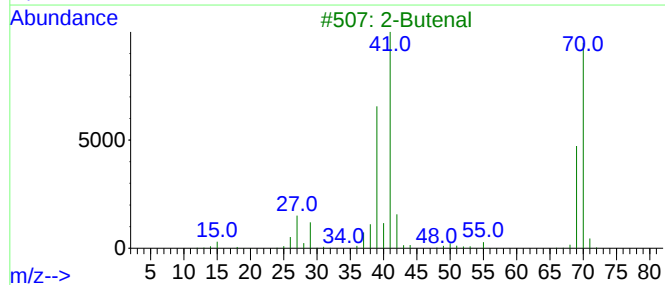
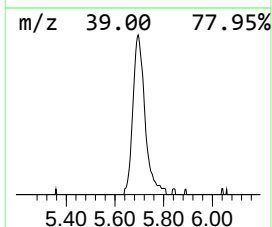
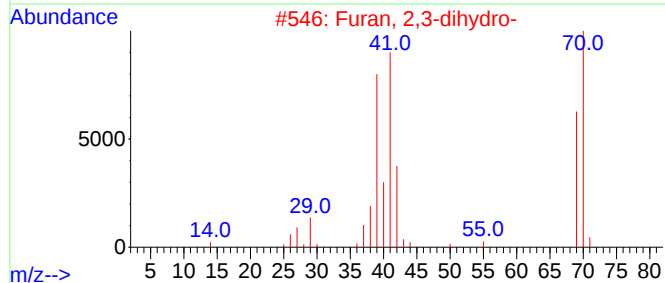
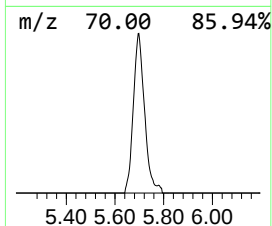
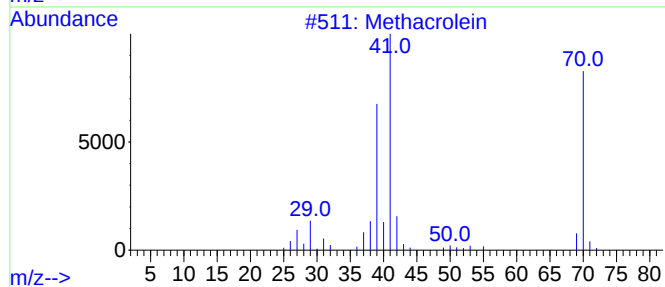
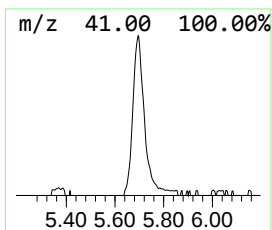
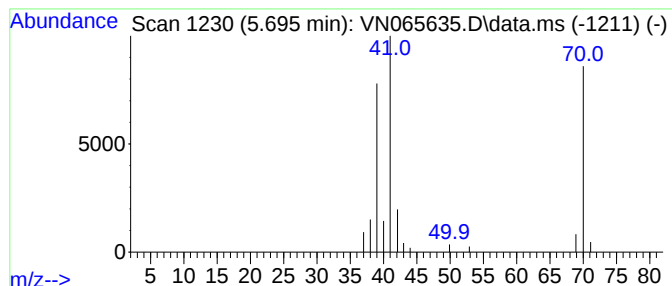
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 1 Methacrolein Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.695	5.38 ug/l	64498	Pentafluorobenzene	7.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methacrolein	70	C4H6O	000078-85-3	91
2			Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	90
3			2-Butenal	70	C4H6O	004170-30-3	90
4			2-Butenal, (E)-	70	C4H6O	000123-73-9	90
5			2-Butenal, (Z)-	70	C4H6O	015798-64-8	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065635.D
Acq On : 27 Jan 2021 17:26
Operator : JC/MD
Sample : M1213-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-BR2-SO-012121

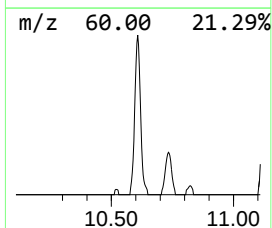
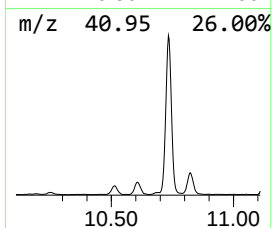
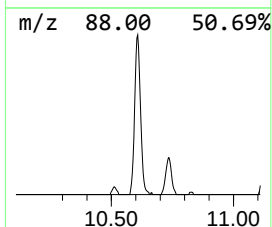
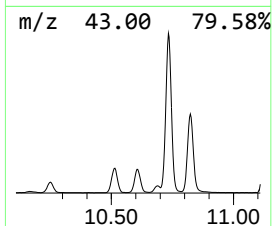
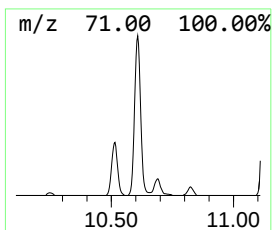
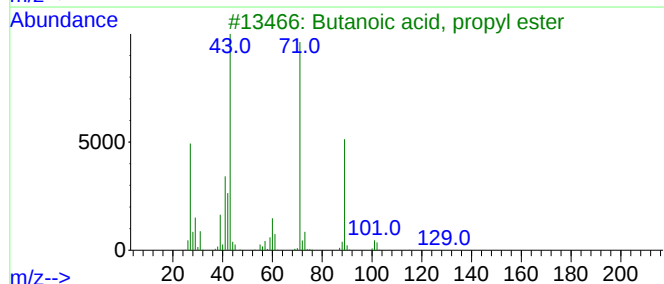
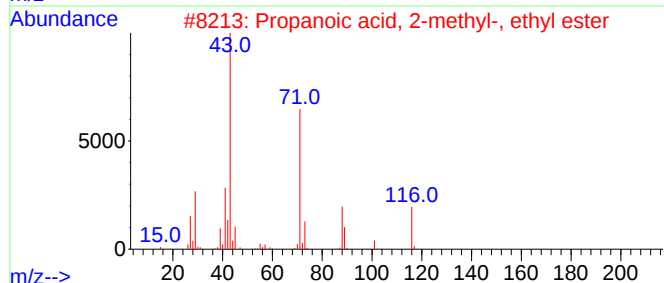
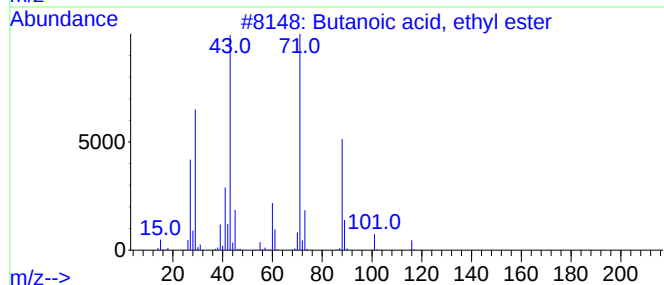
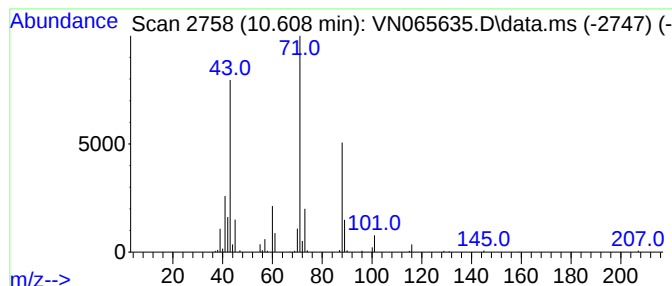
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 2 Butanoic acid, ethyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.608	10.11 ug/l	187154	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	97
2			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	43
4			Propanoic acid, 2-methyl-, 2-met...	158	C9H18O2	002445-69-4	38
5			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065635.D
Acq On : 27 Jan 2021 17:26
Operator : JC/MD
Sample : M1213-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-BR2-SO-012121

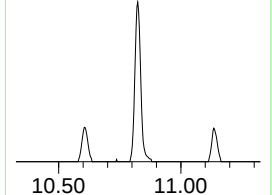
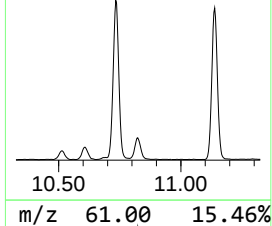
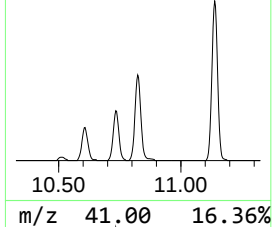
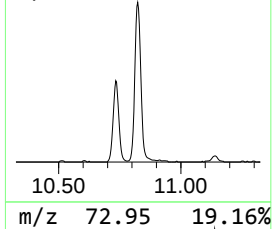
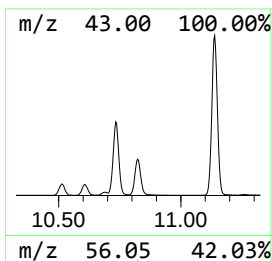
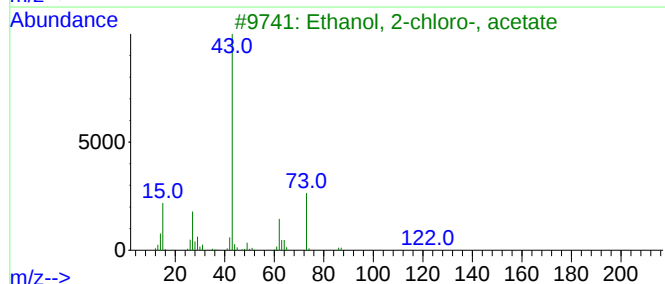
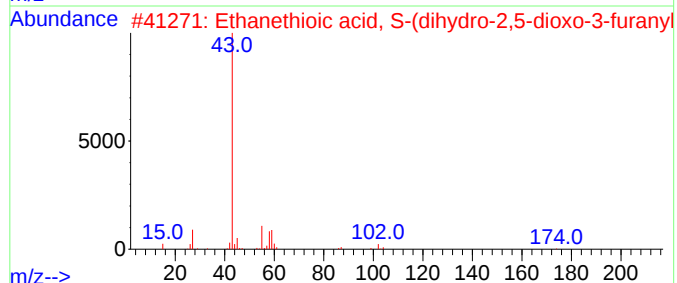
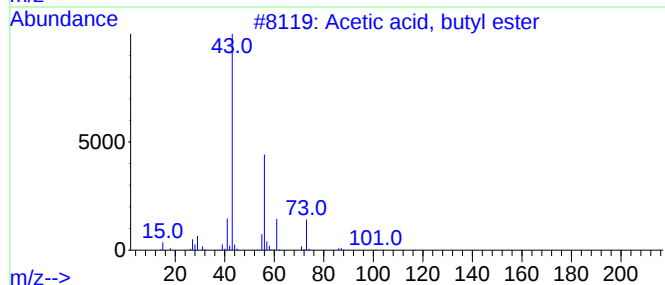
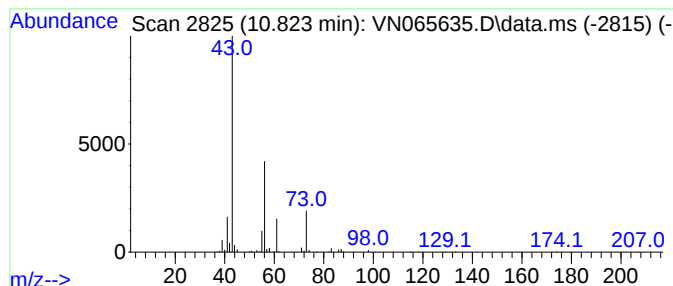
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 3 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.823	15.64 ug/l	289427	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			Ethanethioic acid, S-(dihydro-2,...	174	C6H6O4S	006953-60-2	9
3			Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9
4			Isopropyl acetate	102	C5H10O2	000108-21-4	9
5			Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065635.D
Acq On : 27 Jan 2021 17:26
Operator : JC/MD
Sample : M1213-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-BR2-SO-012121

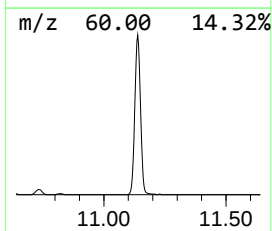
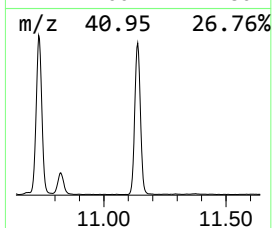
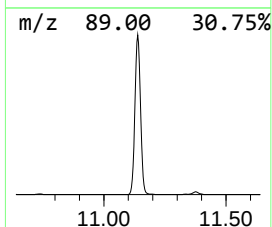
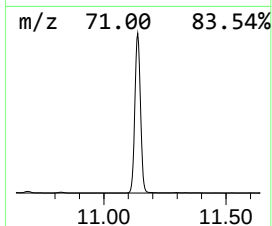
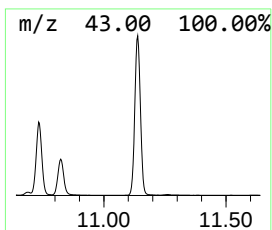
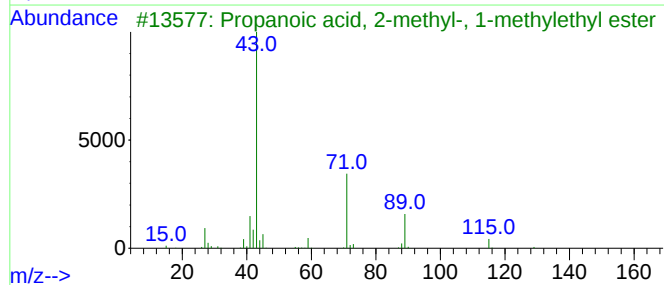
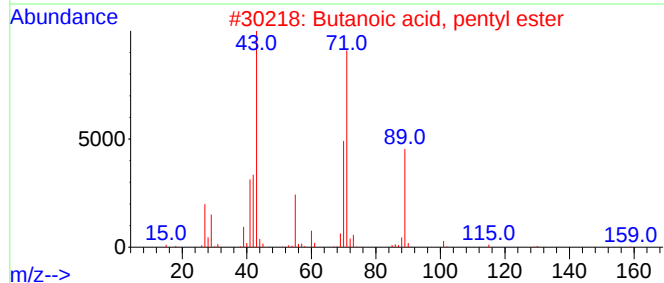
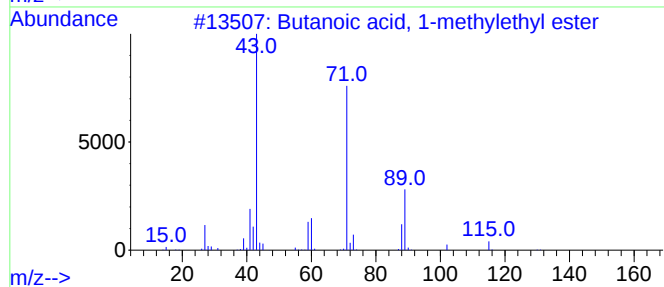
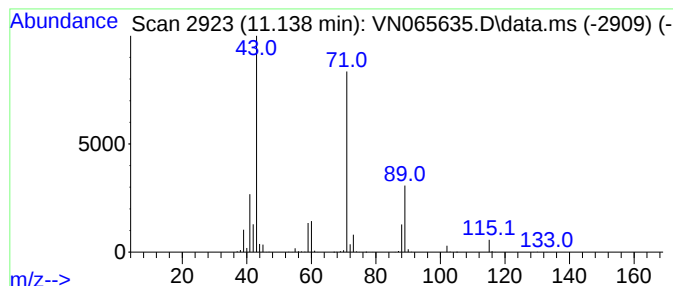
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 4 Butanoic acid, 1-methylethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.139	94.43 ug/l	1747200	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	95
2			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065635.D
Acq On : 27 Jan 2021 17:26
Operator : JC/MD
Sample : M1213-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-BR2-SO-012121

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methacrolein	5.695	5.4	ug/l	64498	1	7.624	599346	50.0
Butanoic acid, ...	10.608	10.1	ug/l	187154	3	11.376	925163	50.0
Acetic acid, bu...	10.823	15.6	ug/l	289427	3	11.376	925163	50.0
Butanoic acid, ...	11.139	94.4	ug/l	1747200	3	11.376	925163	50.0