

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
 Data File : VX022295.D
 Acq On : 01 Jun 2021 17:00
 Operator : JC/MD
 Sample : M2529-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 41815

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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_X\Method\82X051921W.M
 Title : SW846 8260

Signal : TIC: VX022295.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.148	7	10	18	rVB	172345	155826	4.08%	1.271%
2	1.368	40	46	53	rBV	53063	70088	1.84%	0.572%
3	1.453	56	60	78	rVV	3195611	3818011	100.00%	31.133%
4	2.069	154	161	174	rBV	127547	197850	5.18%	1.613%
5	2.300	193	199	207	rVV	264353	415450	10.88%	3.388%
6	2.386	207	213	226	rVB	210440	340148	8.91%	2.774%
7	2.550	230	240	252	rVB	56281	101175	2.65%	0.825%
8	3.581	399	409	422	rBV2	27196	66137	1.73%	0.539%
9	3.885	447	459	479	rVB	608527	1628039	42.64%	13.275%
10	4.245	505	518	525	rBV2	15102	45479	1.19%	0.371%
11	4.385	532	541	556	rVB	75689	206739	5.41%	1.686%
12	5.397	696	707	716	rBV	45006	130708	3.42%	1.066%
13	5.562	725	734	753	rVB2	75940	220970	5.79%	1.802%
14	5.964	789	800	806	rBV3	53066	133737	3.50%	1.091%
15	6.050	806	814	824	rVB2	107421	284832	7.46%	2.323%
16	6.769	919	932	942	rBV	135306	321897	8.43%	2.625%
17	6.879	942	950	961	rVB	52952	122652	3.21%	1.000%
18	7.220	996	1006	1016	rBV	46691	106528	2.79%	0.869%
19	8.653	1234	1241	1247	rBV	283863	438042	11.47%	3.572%
20	8.720	1247	1252	1269	rVB	495315	783900	20.53%	6.392%
21	9.573	1387	1392	1399	rBV	32284	70009	1.83%	0.571%
22	10.055	1466	1471	1480	rVB	194224	282331	7.39%	2.302%
23	10.159	1480	1488	1491	rBV	49755	66991	1.75%	0.546%
24	10.195	1491	1494	1501	rVB	33103	45685	1.20%	0.373%
25	10.305	1506	1512	1518	rVB	154782	222846	5.84%	1.817%
26	10.646	1563	1568	1578	rVB	66426	91813	2.40%	0.749%
27	11.085	1634	1640	1645	rBV	110980	140621	3.68%	1.147%
28	11.689	1734	1739	1743	rBV	77153	93213	2.44%	0.760%
29	11.988	1780	1788	1790	rBV4	24505	51355	1.35%	0.419%
30	12.024	1790	1794	1802	rVB	112215	139338	3.65%	1.136%
31	12.219	1822	1826	1834	rBV2	26369	51483	1.35%	0.420%
32	13.774	2072	2081	2089	rVB2	17194	40659	1.06%	0.332%
33	14.621	2216	2220	2222	rBV	61069	90225	2.36%	0.736%
34	14.847	2254	2257	2261	rVB4	41735	47931	1.26%	0.391%
35	15.036	2284	2288	2294	rBV3	23231	47256	1.24%	0.385%
36	15.182	2308	2312	2314	rBV4	36623	56044	1.47%	0.457%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
Data File : VX022295.D
Acq On : 01 Jun 2021 17:00
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_X\Method\82X051921W.M
Title : SW846 8260

37	15.213	2314	2317	2320	rVB2	59870	71422	1.87%	0.582%
38	15.420	2347	2351	2356	rVB	136657	195454	5.12%	1.594%
39	15.487	2357	2362	2366	rBV4	60254	133825	3.51%	1.091%
40	15.615	2380	2383	2387	rVB3	52840	64851	1.70%	0.529%
41	15.749	2400	2405	2412	rVB3	166522	276449	7.24%	2.254%
42	16.097	2458	2462	2468	rBV6	31834	65428	1.71%	0.534%
43	16.420	2512	2515	2526	rBV5	28268	82868	2.17%	0.676%
44	16.554	2534	2537	2542	rVB4	33954	56775	1.49%	0.463%
45	16.712	2558	2563	2569	rVB3	101881	190542	4.99%	1.554%

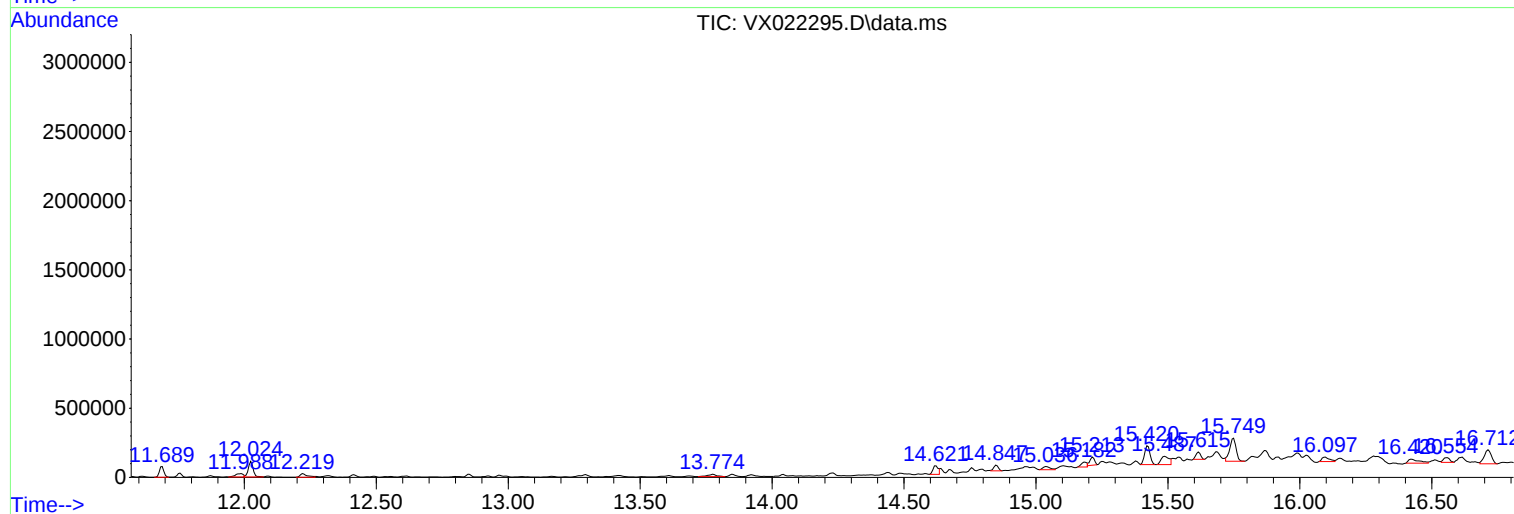
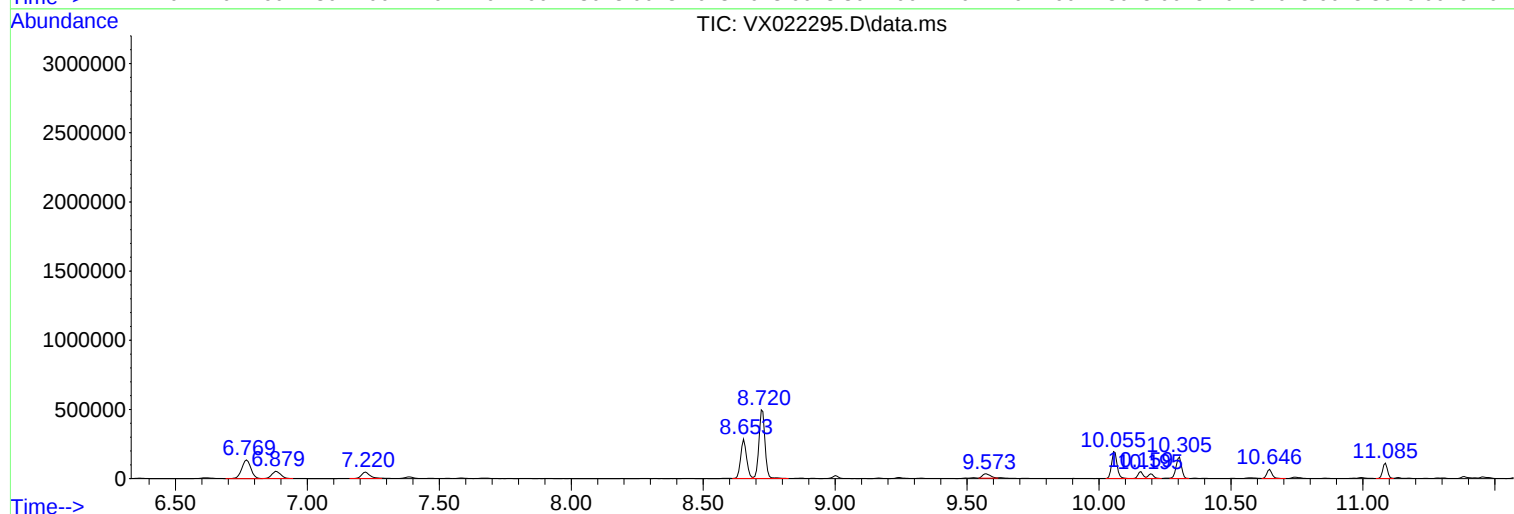
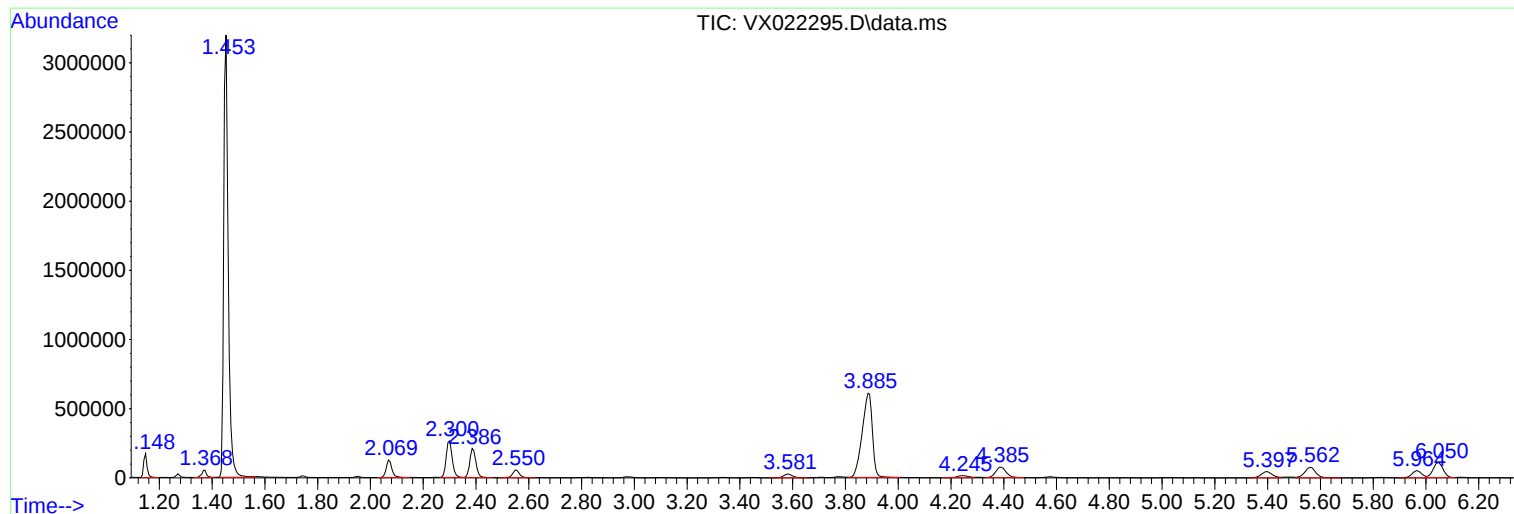
Sum of corrected areas: 12263622

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
Data File : VX022295.D
Acq On : 01 Jun 2021 17:00
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
Data File : VX022295.D
Acq On : 01 Jun 2021 17:00
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

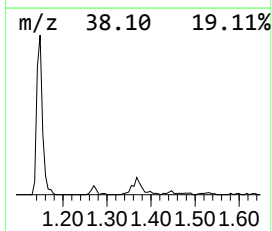
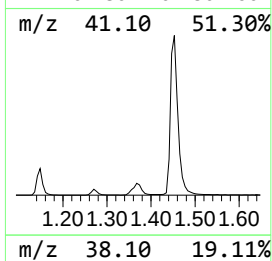
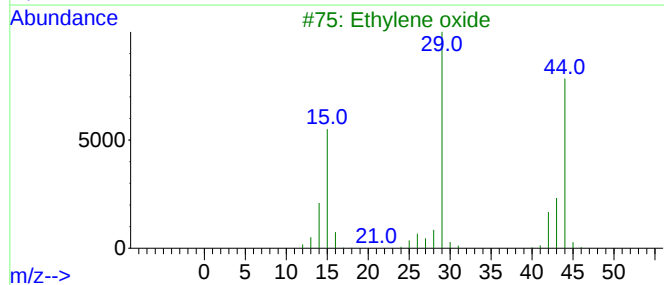
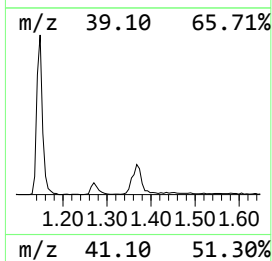
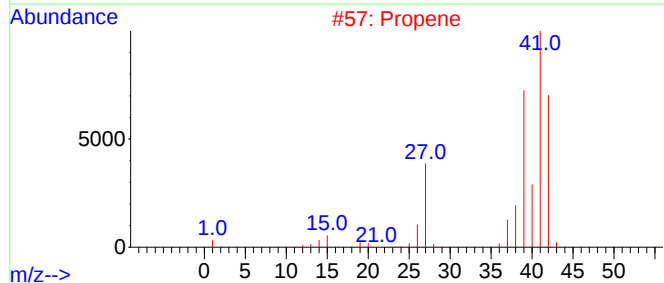
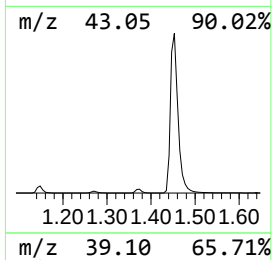
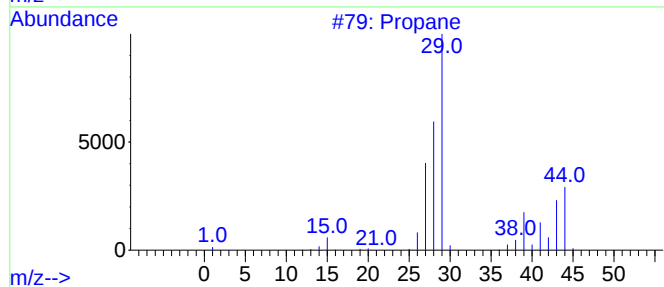
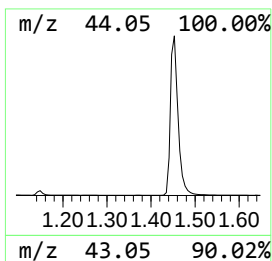
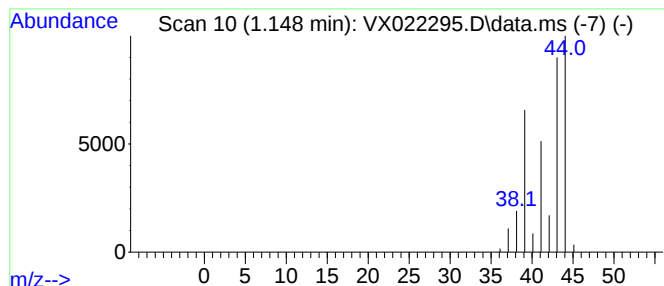
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.148	35.26 ug/l	155826	Pentafluorobenzene	5.568

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane		44	C3H8	000074-98-6	83
2	Propene		42	C3H6	000115-07-1	9
3	Ethylene oxide		44	C2H4O	000075-21-8	5
4	Acetaldehyde		44	C2H4O	000075-07-0	5
5	Ethyne, fluoro-		44	C2HF	002713-09-9	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
Data File : VX022295.D
Acq On : 01 Jun 2021 17:00
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

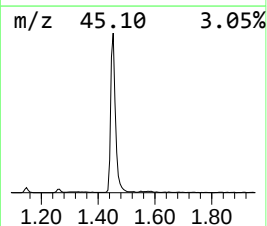
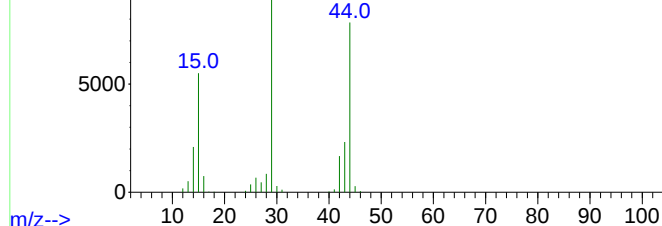
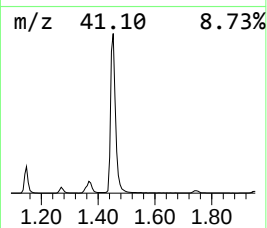
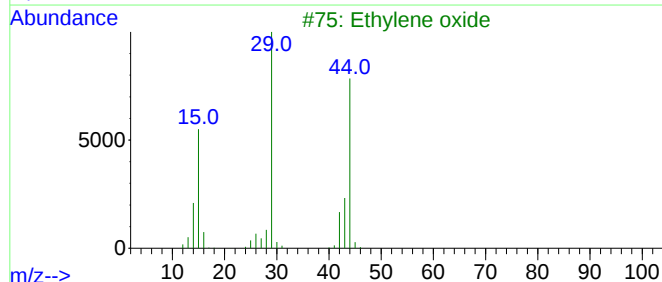
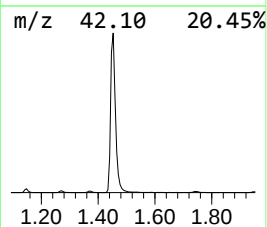
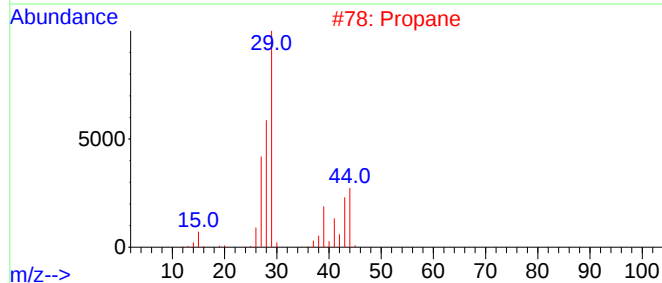
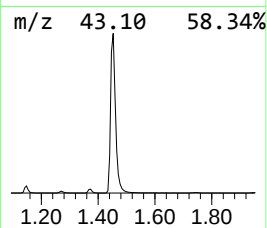
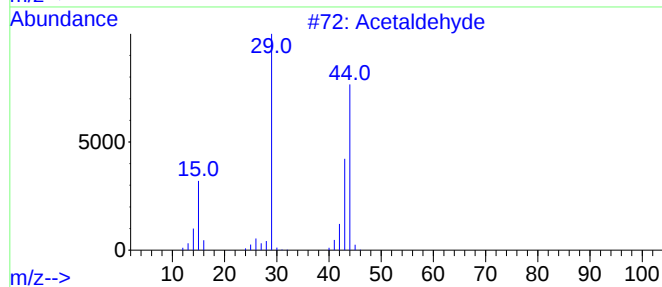
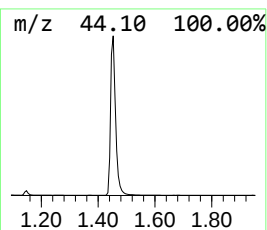
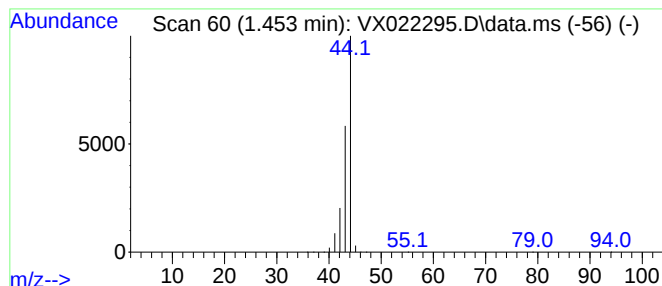
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	863.92 ug/l	3818010	Pentafluorobenzene	5.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Ethyne, fluoro-	44	C2HF	002713-09-9	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
Data File : VX022295.D
Acq On : 01 Jun 2021 17:00
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

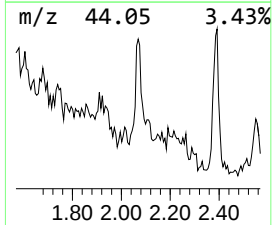
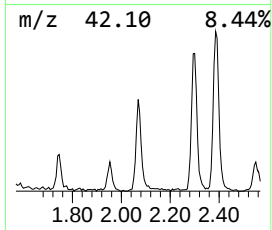
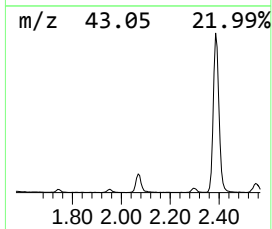
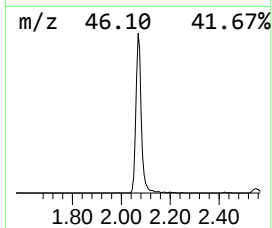
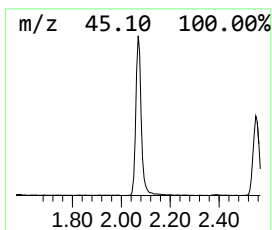
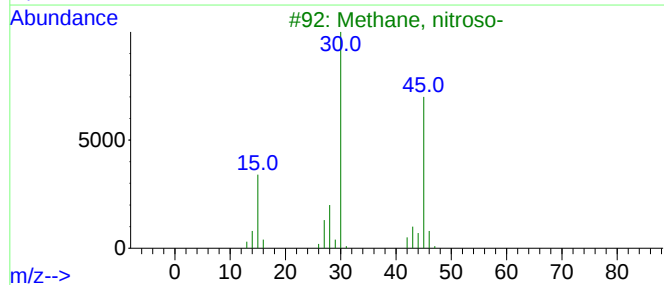
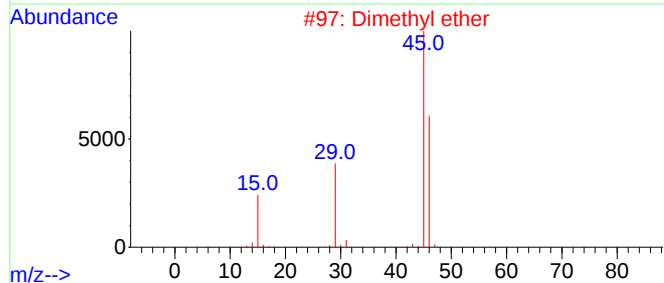
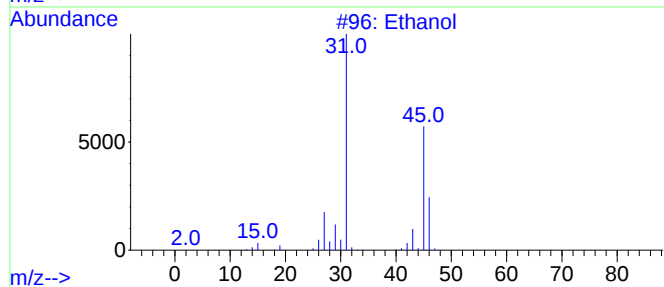
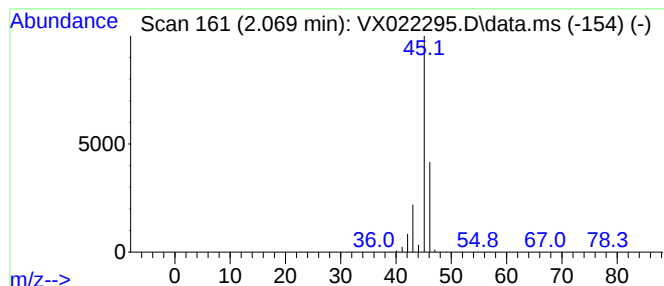
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	44.77 ug/l	197850	Pentafluorobenzene	5.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
Data File : VX022295.D
Acq On : 01 Jun 2021 17:00
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

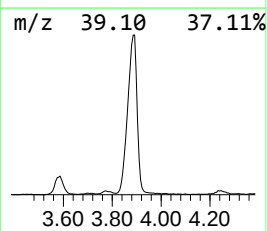
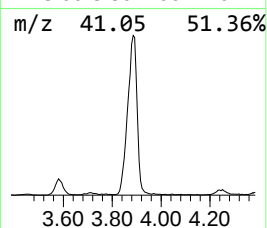
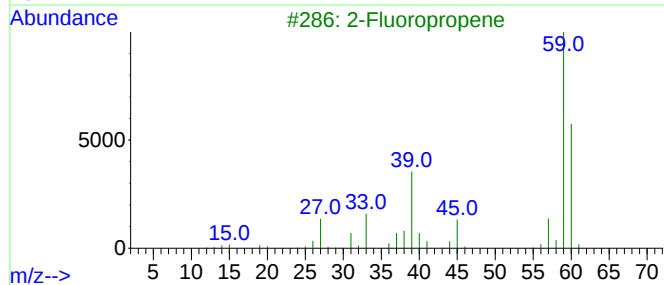
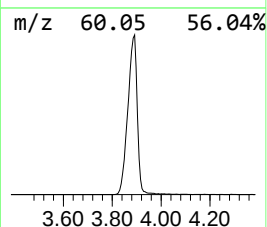
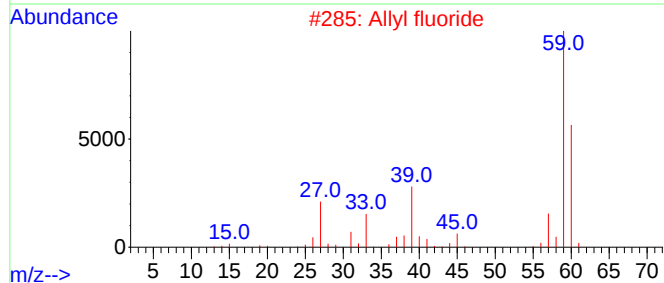
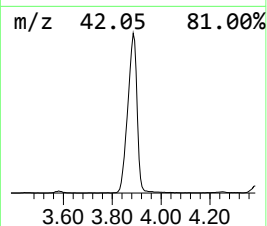
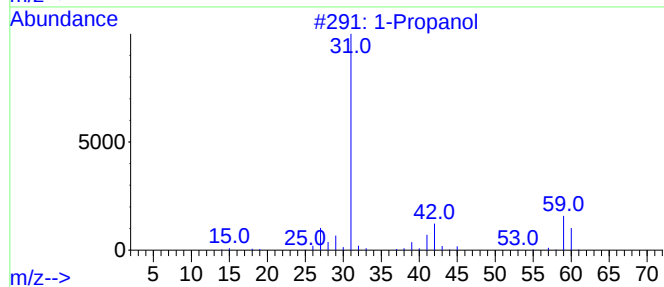
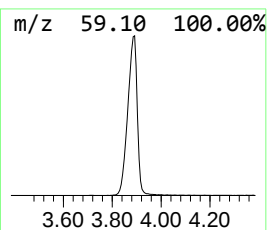
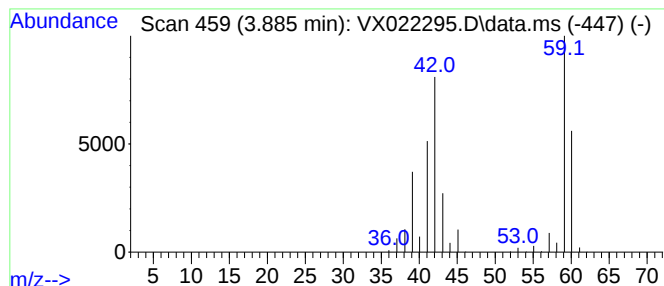
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.885	368.38 ug/l	1628040	Pentafluorobenzene	5.568

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	78
2		Allyl fluoride	60	C3H5F	000818-92-8	47
3		2-Fluoropropene	60	C3H5F	001184-60-7	43
4		Cyclopropane	42	C3H6	000075-19-4	16
5		Acetaldoxime	59	C2H5NO	000107-29-9	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
Data File : VX022295.D
Acq On : 01 Jun 2021 17:00
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

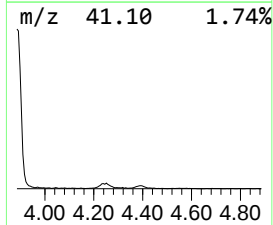
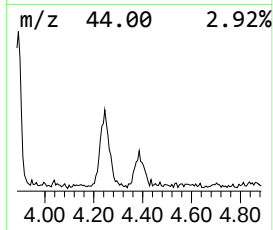
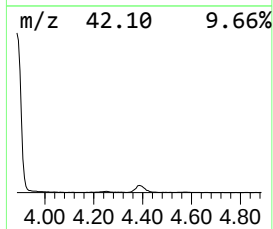
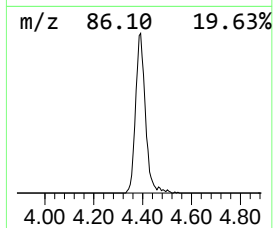
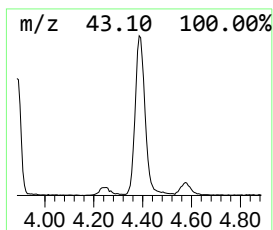
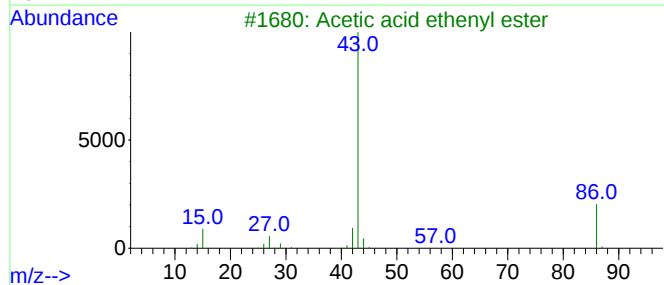
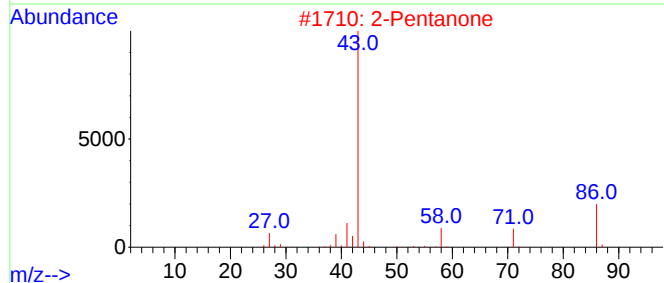
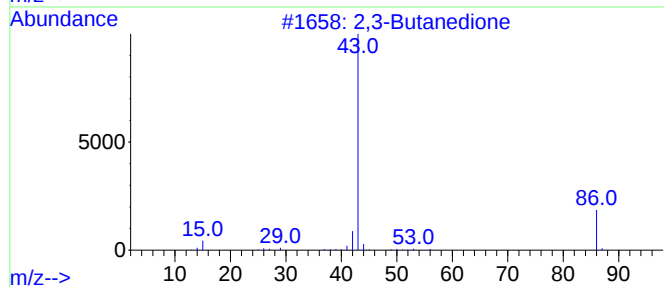
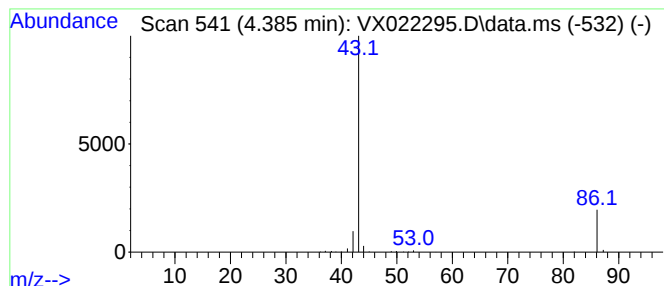
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 5 2,3-Butanedione Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.385	46.78 ug/l	206739	Pentafluorobenzene	5.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione			86	C4H6O2	000431-03-8	86
2	2-Pentanone			86	C5H10O	000107-87-9	56
3	Acetic acid ethenyl ester			86	C4H6O2	000108-05-4	9
4	Azetidine, 1-nitroso-			86	C3H6N2O	015216-10-1	7
5	Ethanone, 1-oxiranyl-			86	C4H6O2	004401-11-0	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
Data File : VX022295.D
Acq On : 01 Jun 2021 17:00
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

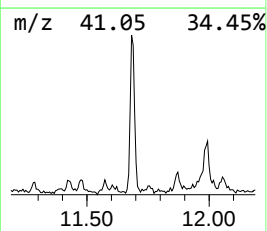
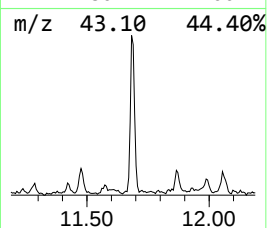
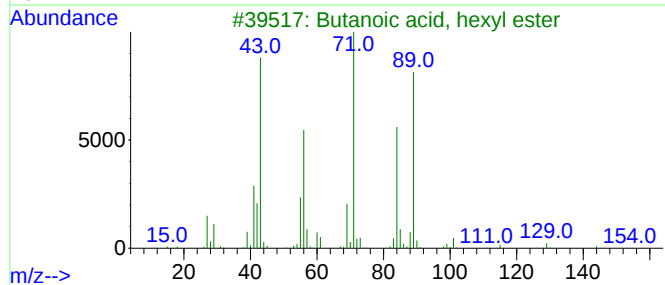
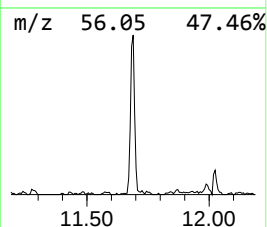
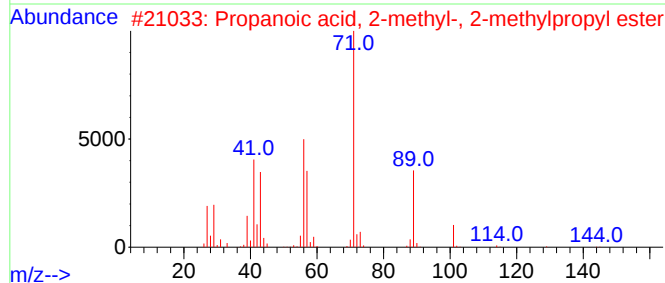
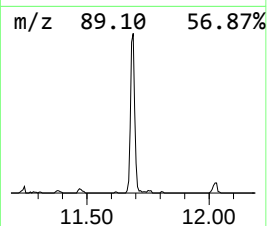
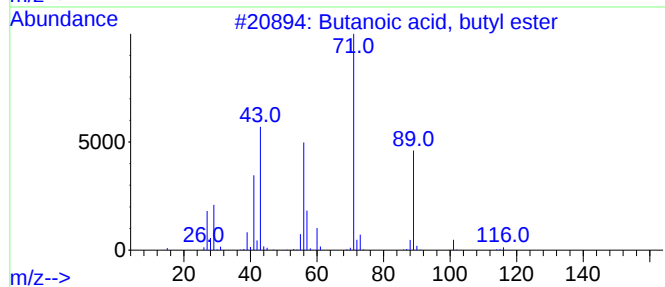
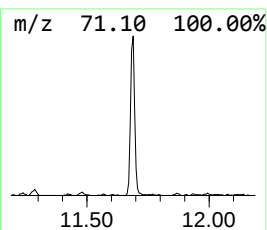
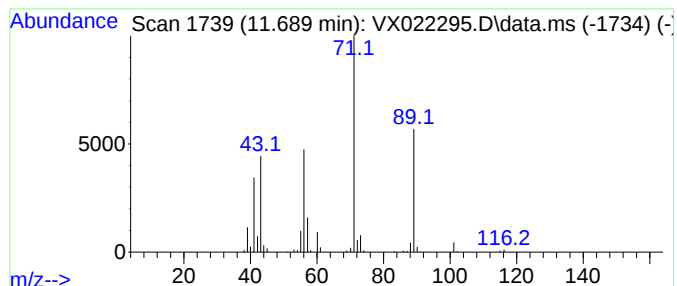
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 6 Butanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.689	33.45 ug/l	93213	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	86
2			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
4			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
Data File : VX022295.D
Acq On : 01 Jun 2021 17:00
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

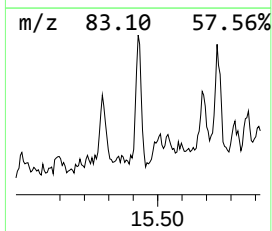
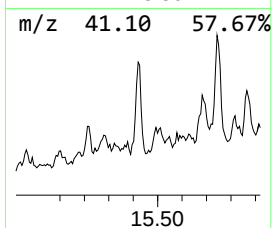
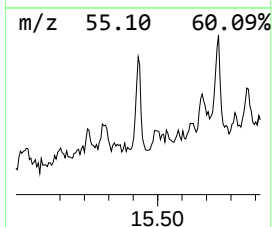
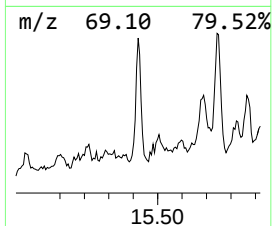
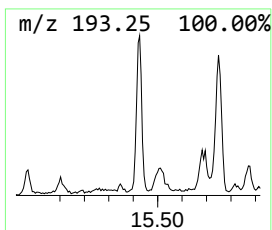
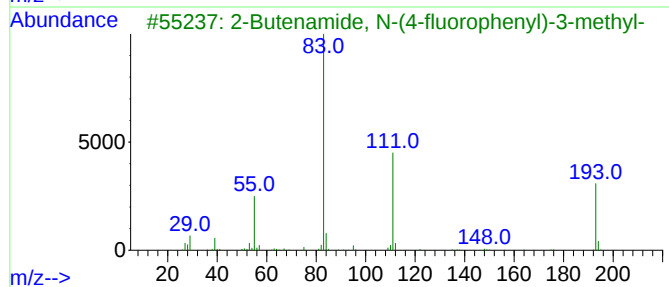
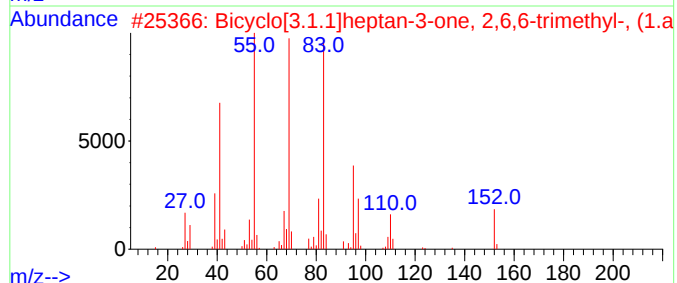
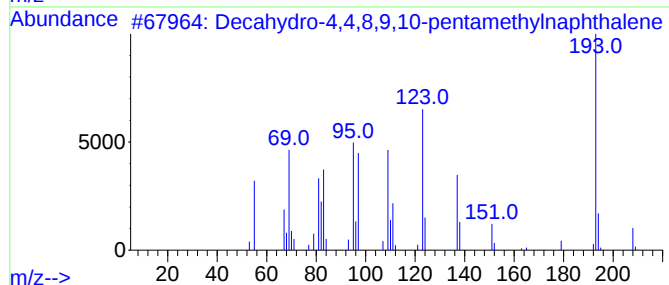
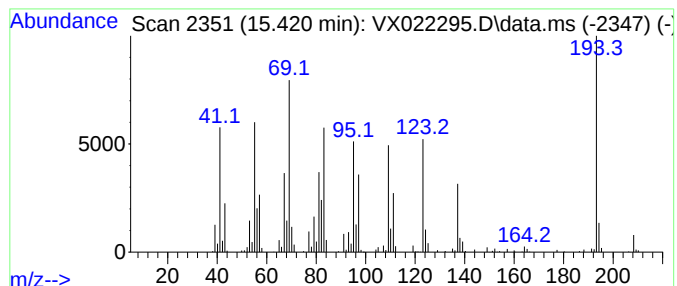
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 7 Decahydro-4,4,8,9,10-pentam... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.420	70.14 ug/l	195454	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	83
2			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	27
3			2-Butenamide, N-(4-fluorophenyl)...	193	C11H12FNO	1000307-26-7	25
4			4-Hexen-1-ol, 5-methyl-2-(1-meth...	154	C10H18O	058461-27-1	14
5			6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
Data File : VX022295.D
Acq On : 01 Jun 2021 17:00
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

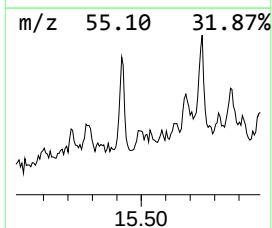
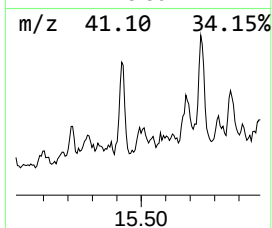
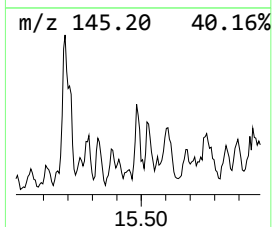
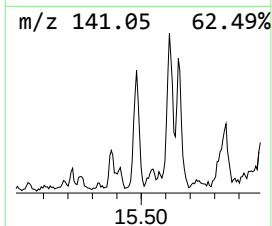
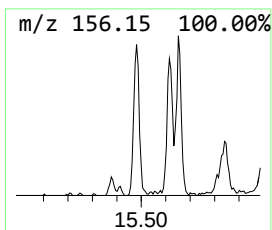
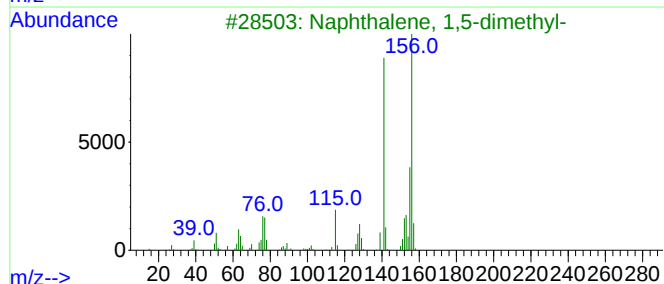
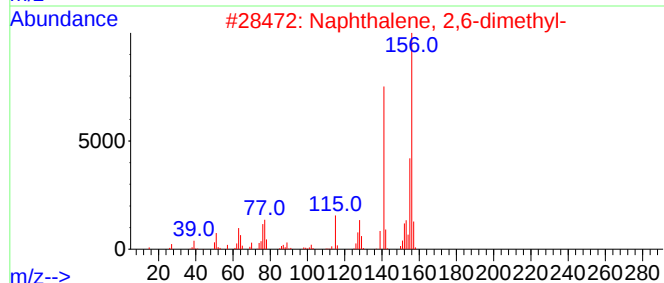
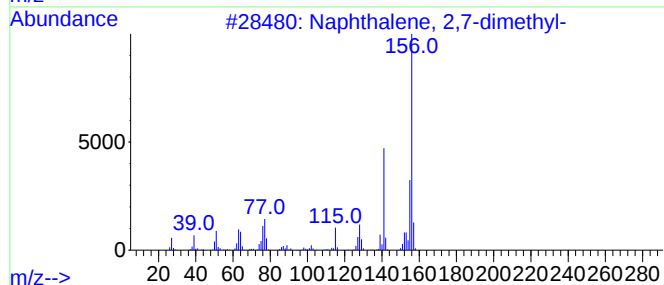
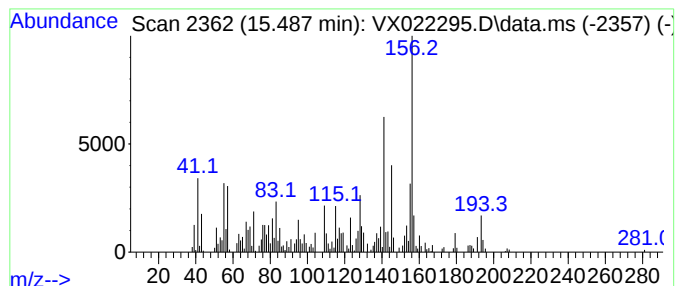
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2,7-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.487	48.02 ug/l	133825	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	93
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	92
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	92
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	91
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
Data File : VX022295.D
Acq On : 01 Jun 2021 17:00
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

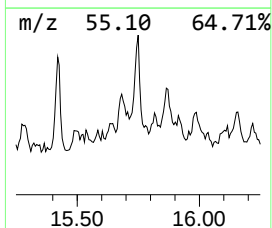
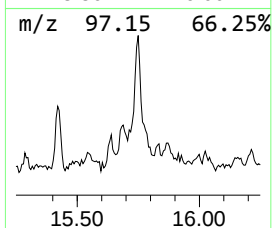
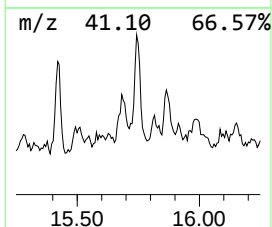
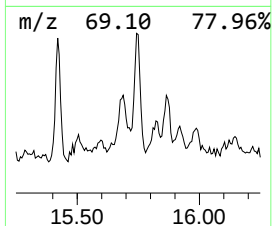
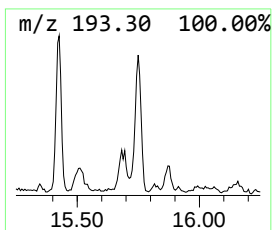
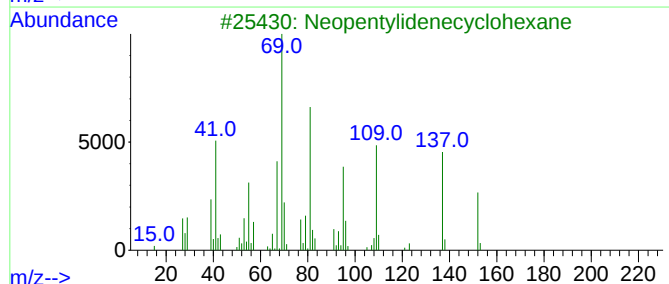
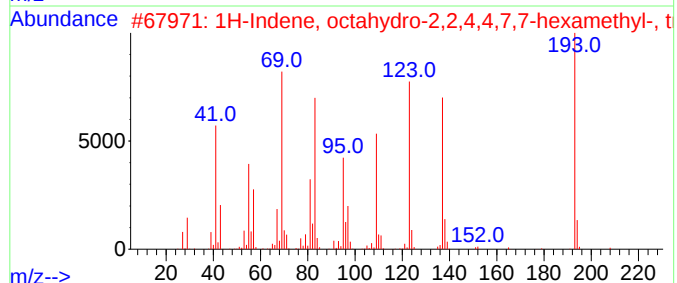
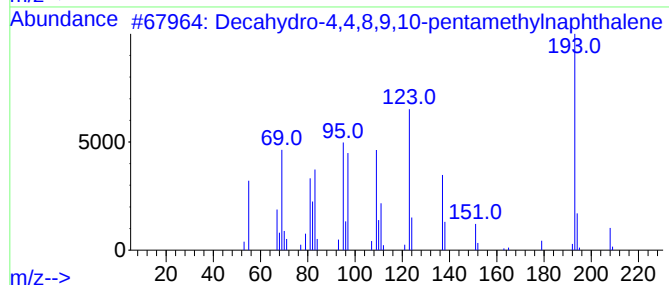
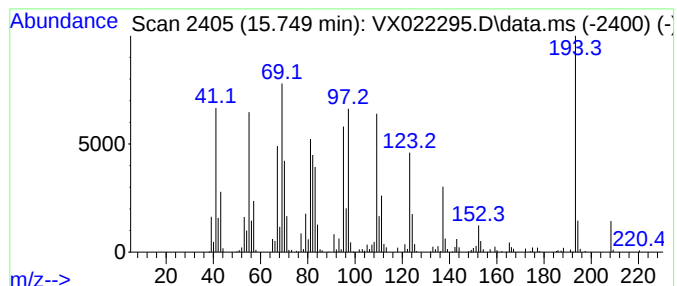
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 9 unknown15.749 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.749	99.20 ug/l	276449	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	58
2			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	27
3			Neopentylidenecyclohexane	152	C11H20	039546-80-0	27
4			Bicyclo[3.1.1]heptane-2-carboxal...	152	C10H16O	004764-14-1	22
5			2-Acetyl-4,4-dimethyl-cyclopent...	152	C9H12O2	081979-96-6	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
Data File : VX022295.D
Acq On : 01 Jun 2021 17:00
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

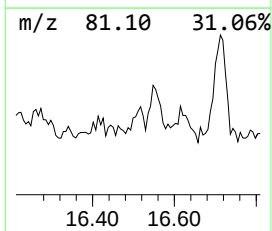
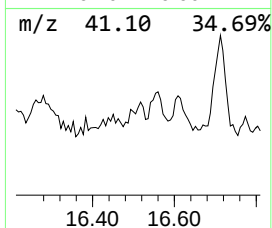
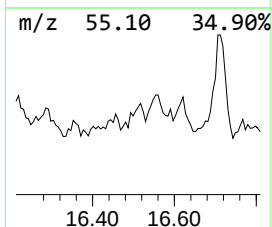
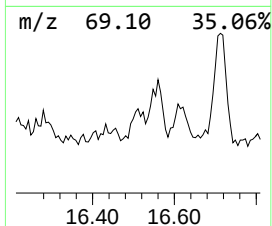
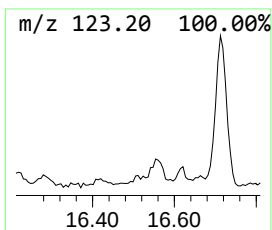
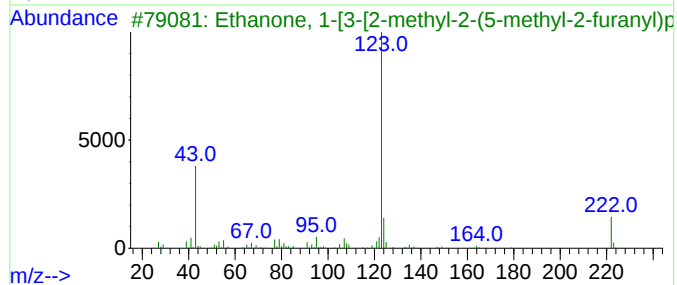
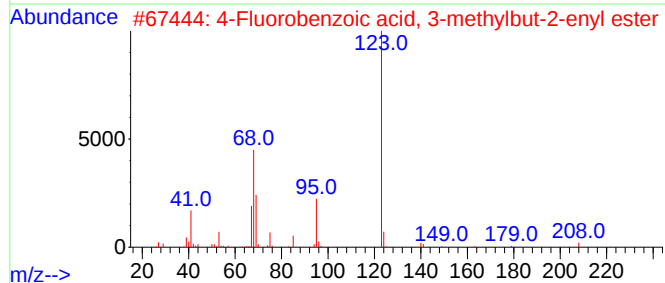
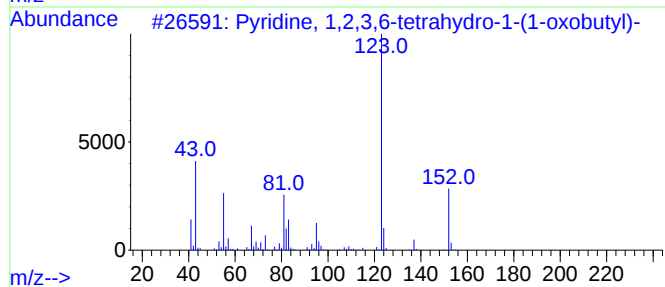
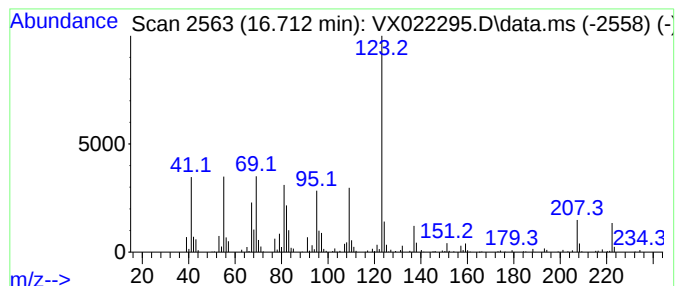
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 10 Pyridine, 1,2,3,6-tetrahydr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.712	68.37 ug/l	190542	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyridine, 1,2,3,6-tetrahydro-1-(...	153	C9H15NO	057150-46-6	53
2			4-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	1000299-15-1	47
3			Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	46
4			Benzene, 1,4-dimethoxy-	138	C8H10O2	000150-78-7	43
5			Benzamide, 4-fluoro-N-methallyl-	193	C11H12FNO	1000340-31-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060121\
Data File : VX022295.D
Acq On : 01 Jun 2021 17:00
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.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
Propane	1.148	35.3	ug/l	155826	1	5.568	220970	50.0
Acetaldehyde	1.453	863.9	ug/l	3818010	1	5.568	220970	50.0
Ethanol	2.069	44.8	ug/l	197850	1	5.568	220970	50.0
1-Propanol	3.885	368.4	ug/l	1628040	1	5.568	220970	50.0
2,3-Butanedione	4.385	46.8	ug/l	206739	1	5.568	220970	50.0
Butanoic acid, ...	11.689	33.5	ug/l	93213	4	12.024	139338	50.0
Decahydro-4,4,8...	15.420	70.1	ug/l	195454	4	12.024	139338	50.0
Naphthalene, 2,...	15.487	48.0	ug/l	133825	4	12.024	139338	50.0
unknown15.749	15.749	99.2	ug/l	276449	4	12.024	139338	50.0
Pyridine, 1,2,3...	16.712	68.4	ug/l	190542	4	12.024	139338	50.0