

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052622\
 Data File : VX029009.D
 Acq On : 26 May 2022 19:09
 Operator : JC/MD
 Sample : N3053-05 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 52322-G

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\82X051222W.M
 Title : SW846 8260

Signal : TIC: VX029009.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	73	rBV	199263	242487	2.95%	1.169%
2	2.081	152	163	189	rBV	4143837	8222001	100.00%	39.649%
3	2.380	206	212	230	rVB	124330	206107	2.51%	0.994%
4	3.855	445	454	476	rBV	76878	218774	2.66%	1.055%
5	4.562	559	570	584	rBV2	30419	91527	1.11%	0.441%
6	4.714	584	595	612	rVV	148185	422934	5.14%	2.039%
7	5.391	694	706	721	rBV2	218111	635779	7.73%	3.066%
8	5.556	721	733	752	rVB	347771	984350	11.97%	4.747%
9	5.830	770	778	789	rBV	36615	101701	1.24%	0.490%
10	5.958	789	799	817	rVB	224872	596562	7.26%	2.877%
11	6.763	920	931	950	rBV	567222	1334541	16.23%	6.436%
12	7.214	997	1005	1022	rBV	212098	475336	5.78%	2.292%
13	8.653	1233	1241	1249	rBV	1167961	1839325	22.37%	8.870%
14	10.055	1465	1471	1485	rBV	1279896	1672695	20.34%	8.066%
15	10.579	1552	1557	1565	rBV	62556	92926	1.13%	0.448%
16	11.085	1634	1640	1652	rBV	994533	1312504	15.96%	6.329%
17	12.024	1788	1794	1802	rBV	1359896	1668758	20.30%	8.047%
18	15.560	2368	2374	2386	rBV	418521	618837	7.53%	2.984%

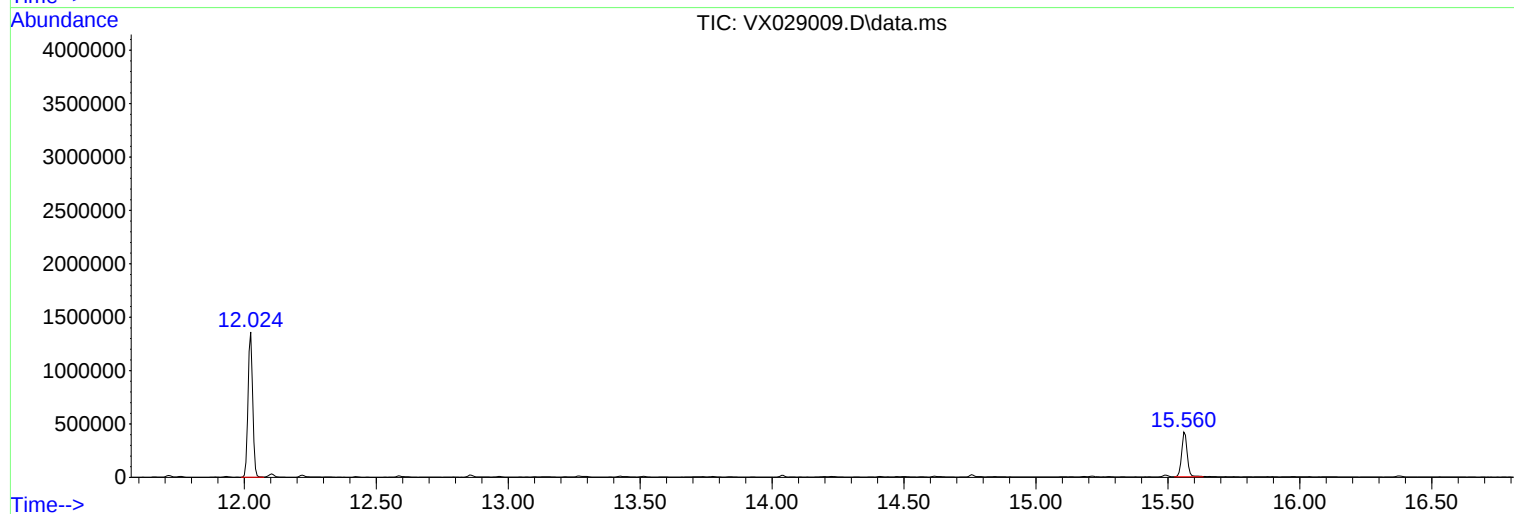
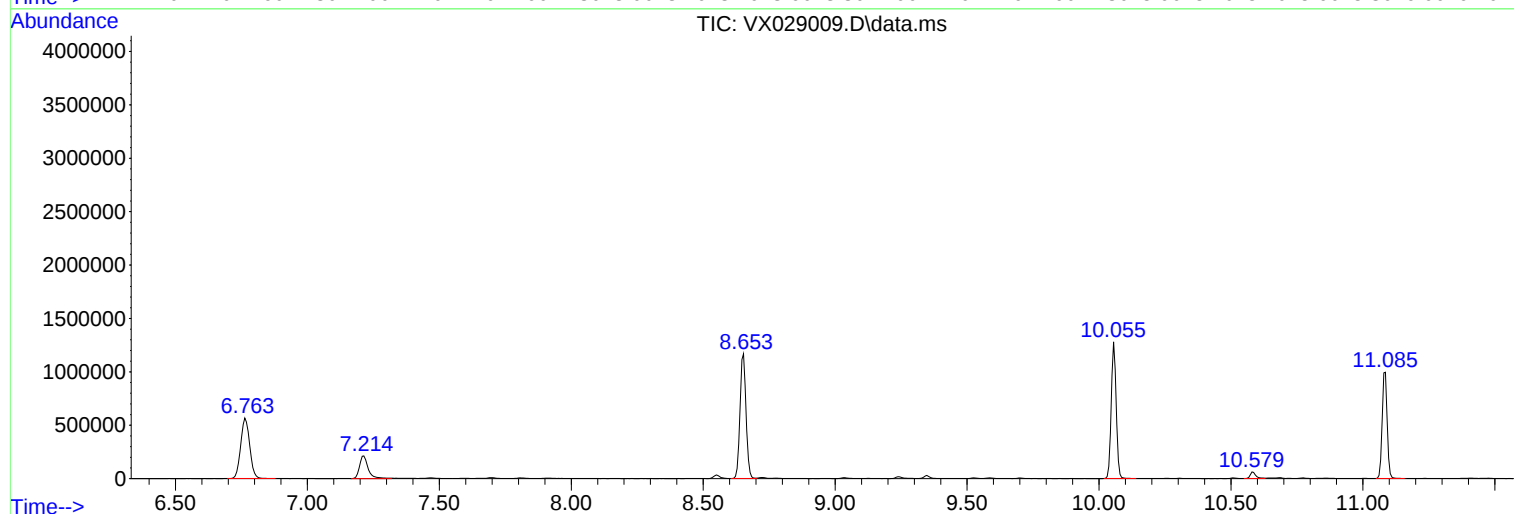
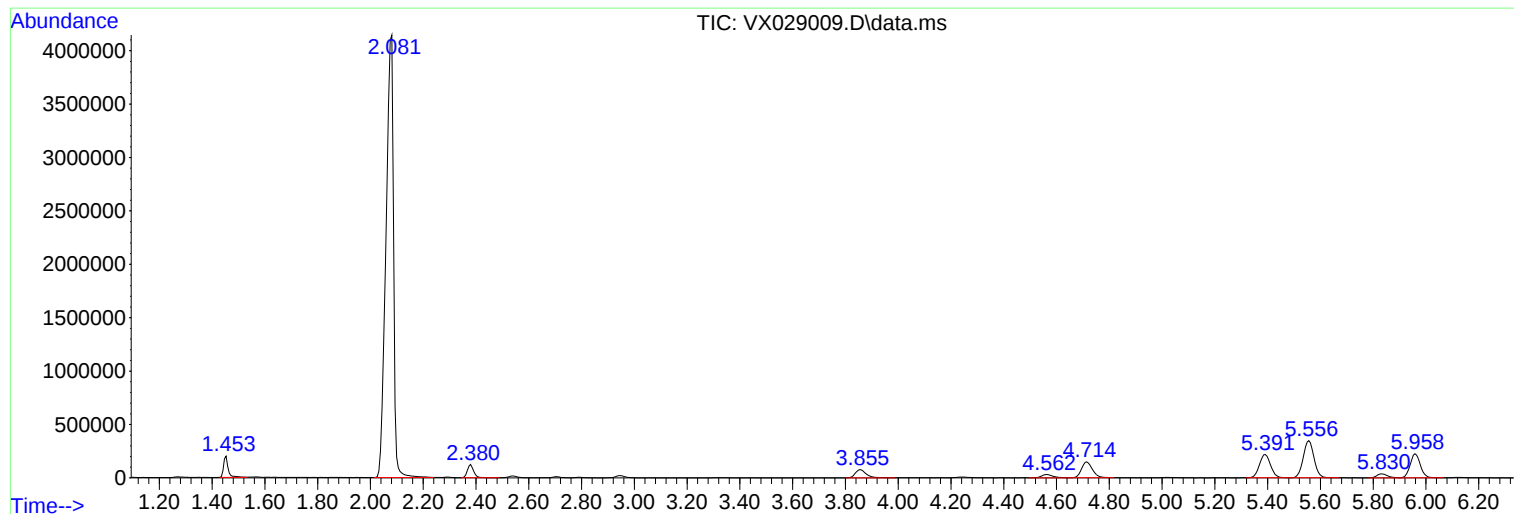
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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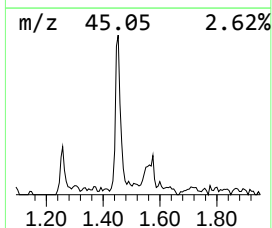
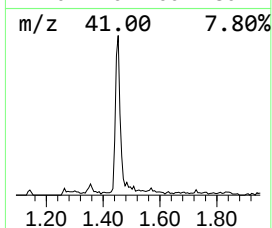
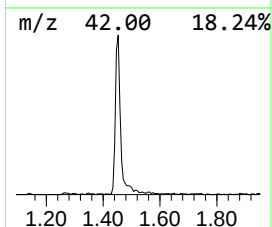
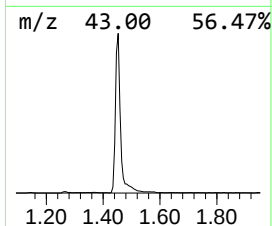
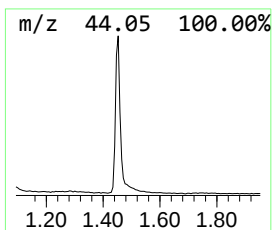
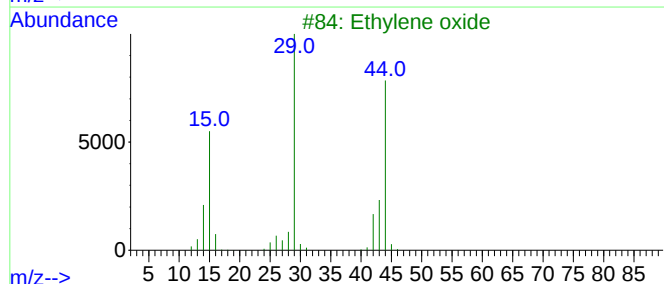
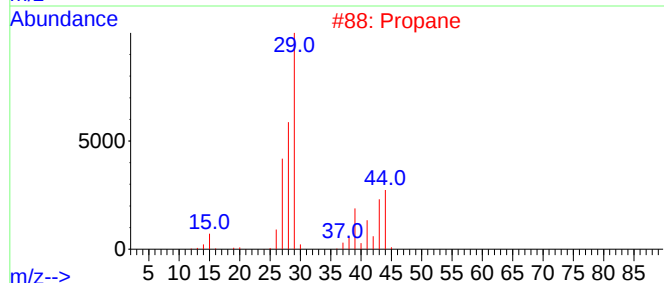
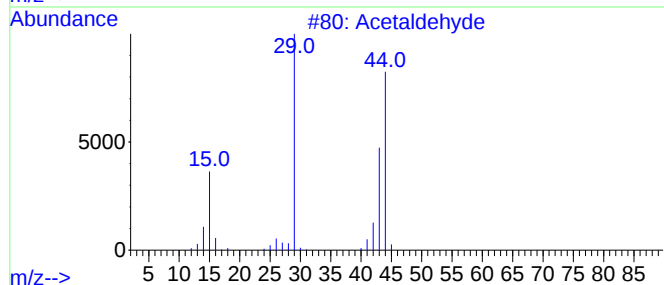
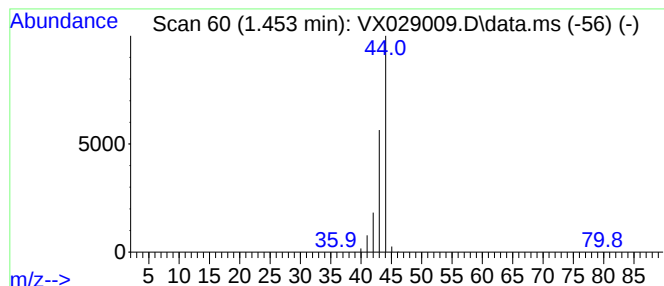
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetaldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	12.32 ug/l	242487	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
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			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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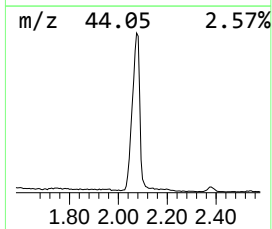
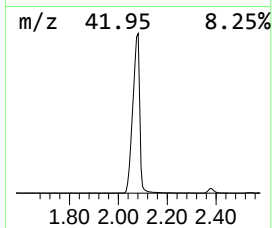
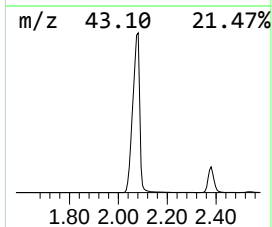
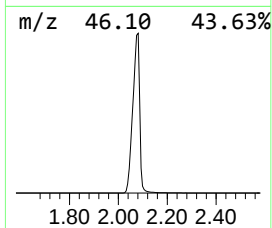
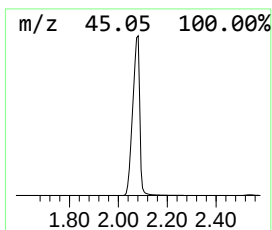
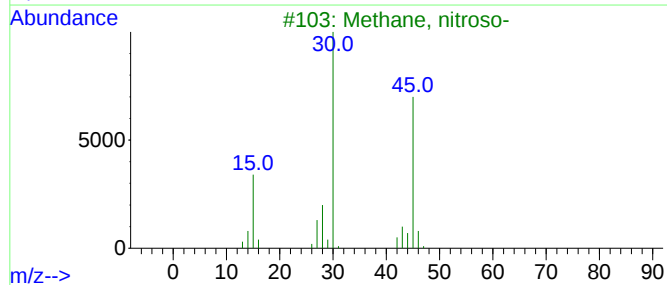
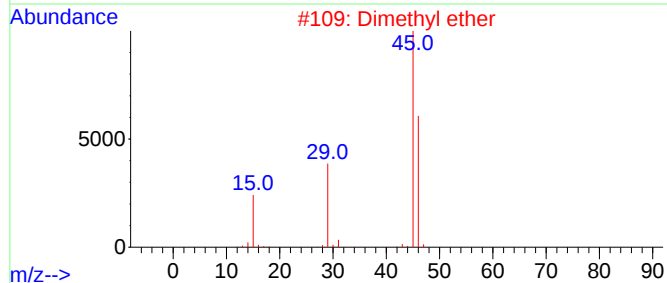
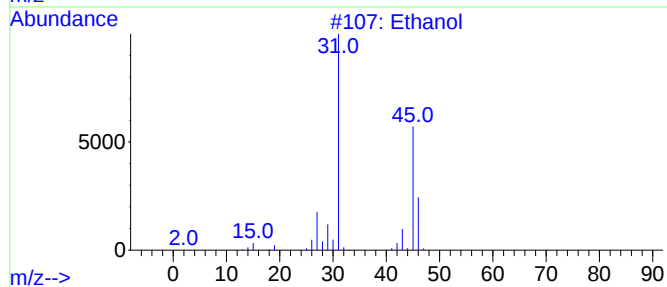
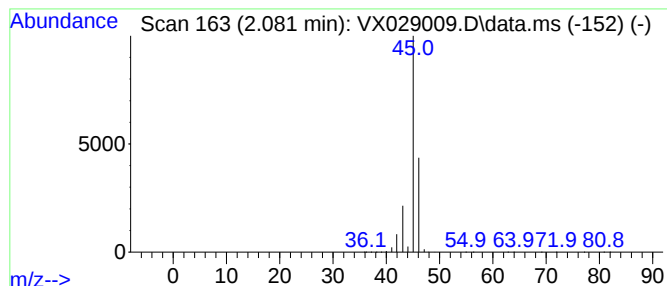
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.081	417.64 ug/l	8222000	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	83
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



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
52322-G

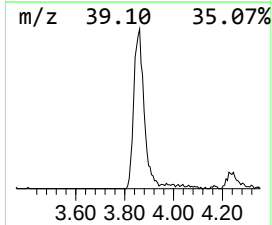
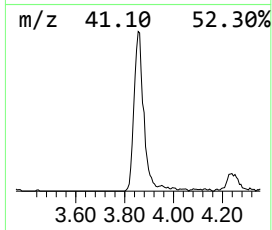
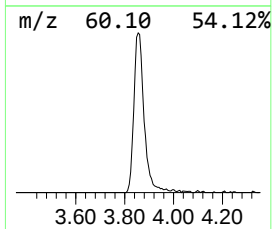
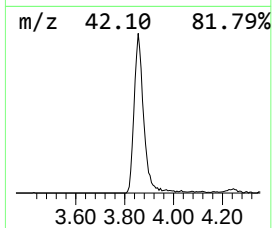
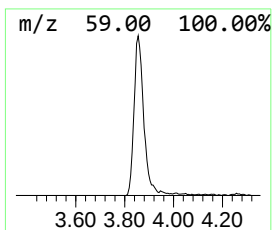
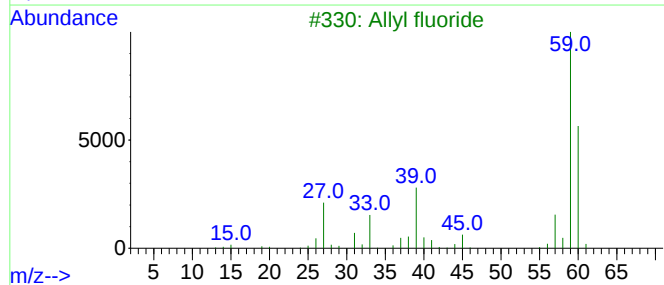
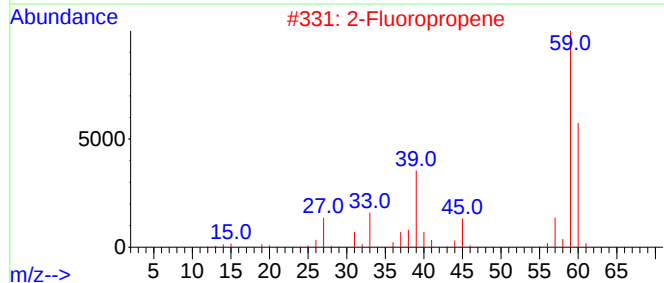
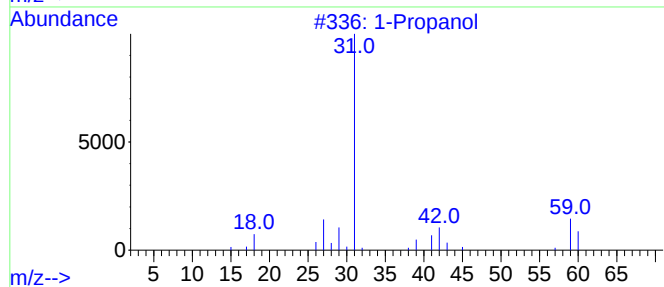
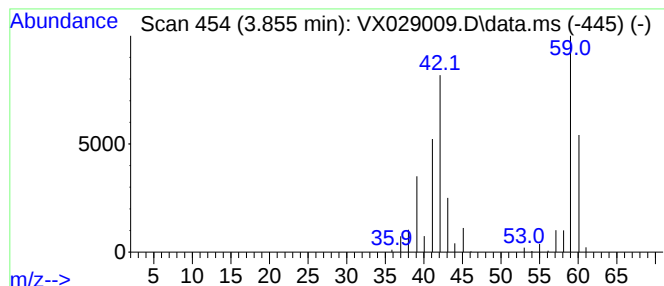
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Propanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.855	11.11 ug/l	218774	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	72
2		2-Fluoropropene	60	C3H5F	001184-60-7	49
3		Allyl fluoride	60	C3H5F	000818-92-8	43
4		1,2-Butanediol	90	C4H10O2	000584-03-2	17
5		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	17



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
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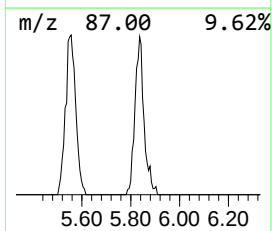
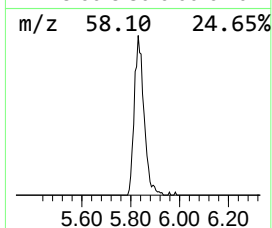
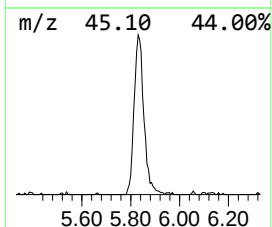
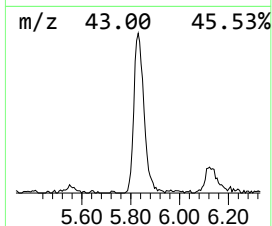
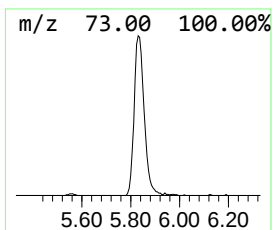
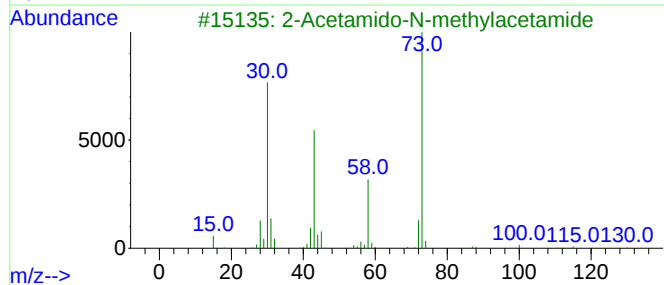
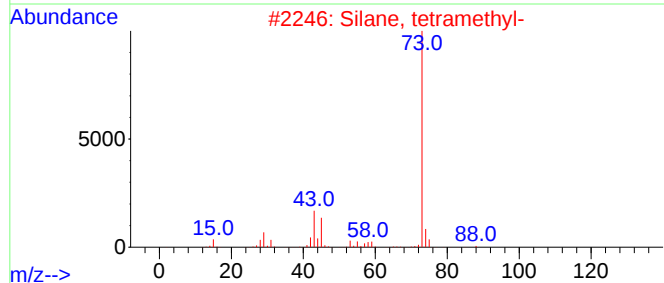
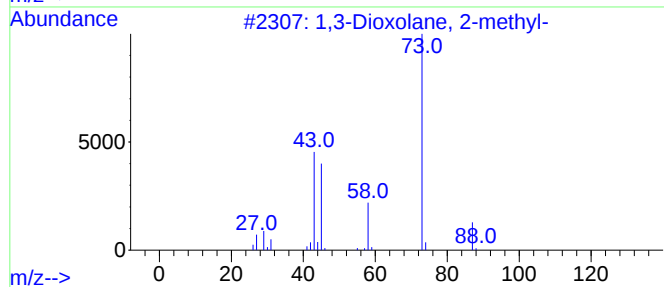
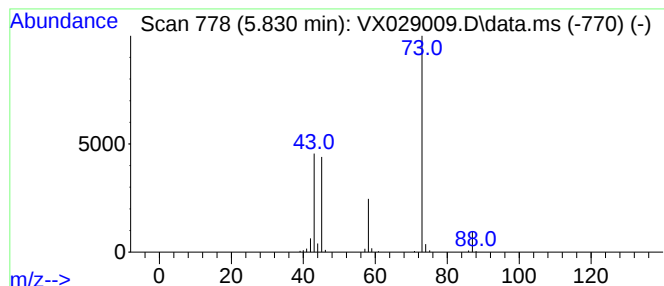
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,3-Dioxolane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.830	5.17 ug/l	101701	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	27
3			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	23
4			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9
5			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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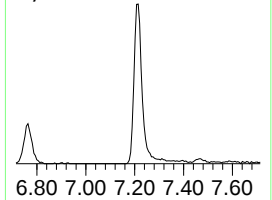
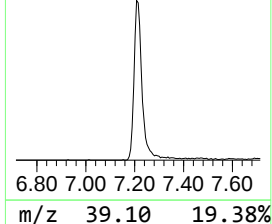
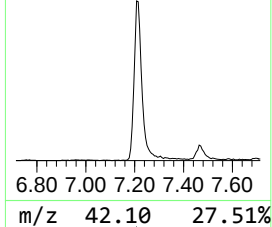
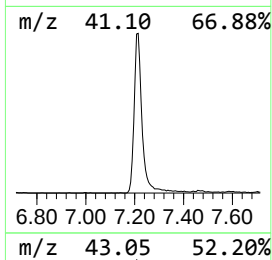
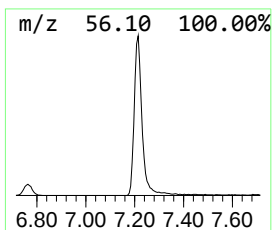
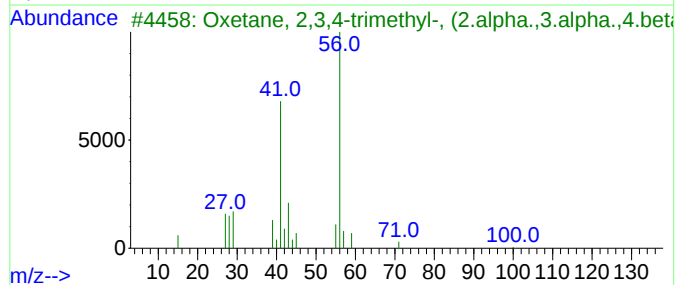
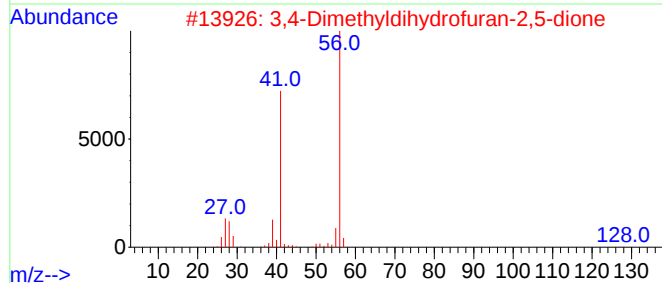
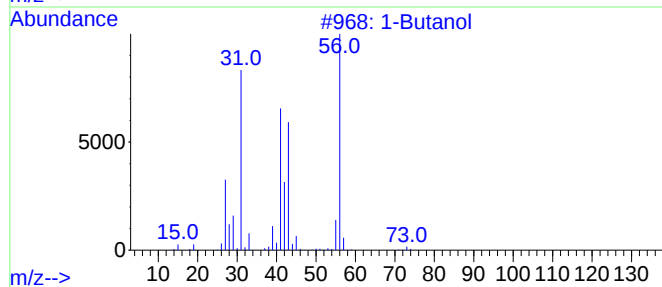
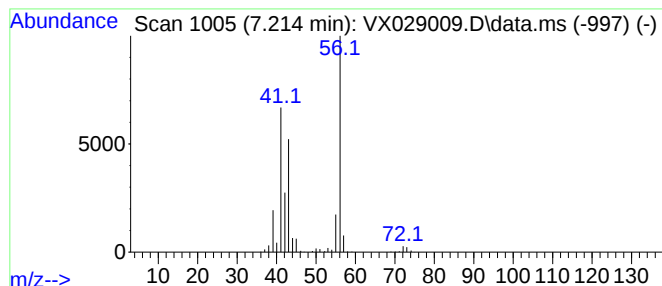
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	17.81 ug/l	475336	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	50
3			Oxetane, 2,3,4-trimethyl-, (2.alpha...	100	C6H12O	032347-12-9	9
4			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9
5			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9



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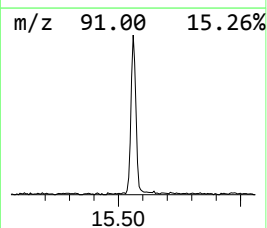
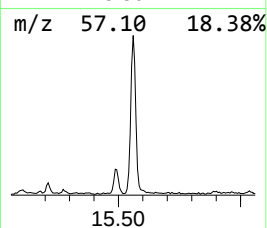
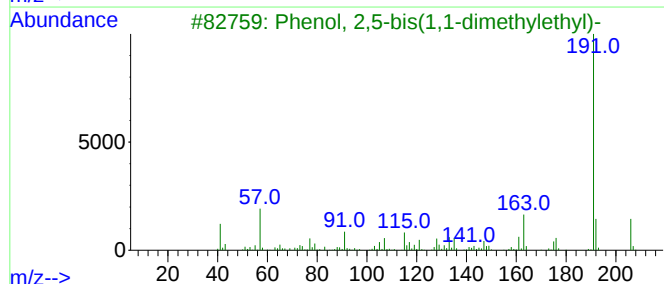
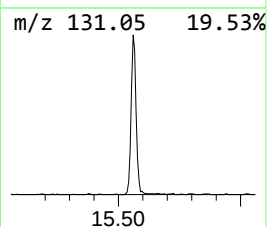
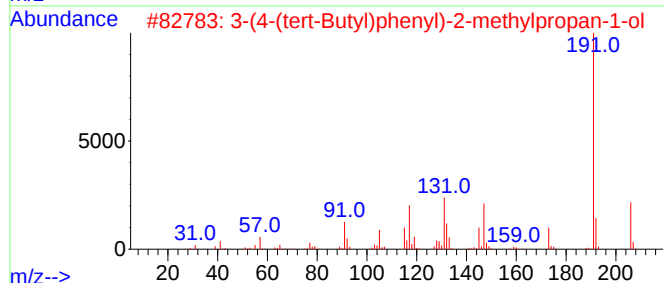
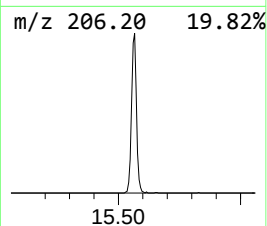
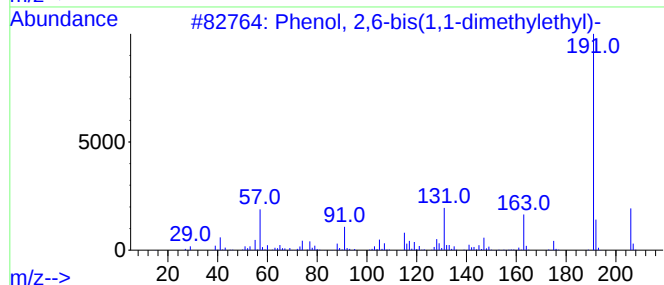
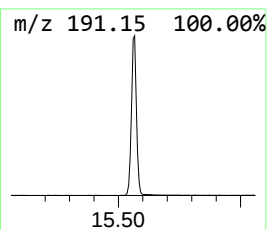
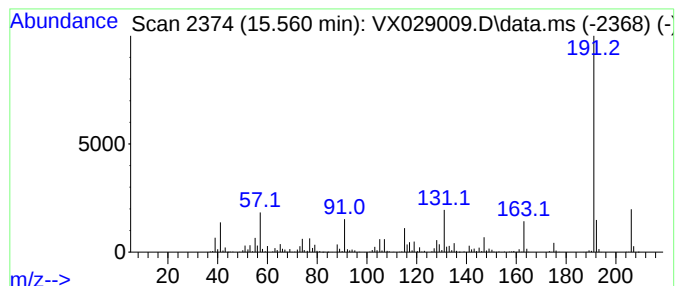
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	18.54 ug/l	618837	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	98
2			3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	87
3			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	81
4			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	76
5			Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052622\
Data File : VX029009.D
Acq On : 26 May 2022 19:09
Operator : JC/MD
Sample : N3053-05 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
52322-G

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.453	12.3	ug/l	242487	1	5.556	984350	50.0
Ethanol	2.081	417.6	ug/l	8222000	1	5.556	984350	50.0
1-Propanol	3.855	11.1	ug/l	218774	1	5.556	984350	50.0
1,3-Dioxolane, ...	5.830	5.2	ug/l	101701	1	5.556	984350	50.0
1-Butanol	7.214	17.8	ug/l	475336	2	6.763	1334540	50.0
Phenol, 2,6-bis...	15.560	18.5	ug/l	618837	4	12.024	1668760	50.0