

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
 Data File : VX022280.D
 Acq On : 29 May 2021 03:04
 Operator : JC/MD
 Sample : M2529-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 36 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: VX022280.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	188801	162594	4.67%	1.451%
2	1.374	41	47	53	rBV	53748	63840	1.83%	0.570%
3	1.453	56	60	76	rBV	3061810	3484775	100.00%	31.102%
4	2.069	155	161	173	rBV	116322	172623	4.95%	1.541%
5	2.300	192	199	208	rVV	236296	376162	10.79%	3.357%
6	2.386	208	213	224	rVB	194184	307853	8.83%	2.748%
7	2.550	231	240	251	rBV	49671	90061	2.58%	0.804%
8	3.581	400	409	421	rBV	24207	57578	1.65%	0.514%
9	3.885	447	459	473	rVB	551321	1423647	40.85%	12.706%
10	4.245	509	518	526	rBV2	15088	43749	1.26%	0.390%
11	4.391	532	542	552	rBV	62036	168586	4.84%	1.505%
12	5.397	695	707	716	rBV2	40745	117443	3.37%	1.048%
13	5.562	725	734	751	rVB	71336	207006	5.94%	1.848%
14	5.970	789	801	806	rBV	45903	121768	3.49%	1.087%
15	6.044	806	813	823	rVB	105060	272410	7.82%	2.431%
16	6.769	918	932	942	rBV	124011	293851	8.43%	2.623%
17	6.879	942	950	961	rVB3	55842	130148	3.73%	1.162%
18	7.129	984	991	1000	rBV	30692	67727	1.94%	0.604%
19	7.220	1000	1006	1023	rVB	42145	99393	2.85%	0.887%
20	8.653	1234	1241	1247	rBV	262310	406195	11.66%	3.625%
21	8.720	1247	1252	1259	rVB	463230	725111	20.81%	6.472%
22	10.055	1466	1471	1481	rVB	179831	257480	7.39%	2.298%
23	10.159	1482	1488	1491	rBV	36869	50285	1.44%	0.449%
24	10.195	1491	1494	1499	rVB	31991	41976	1.20%	0.375%
25	10.305	1506	1512	1518	rVB	143217	200423	5.75%	1.789%
26	10.646	1563	1568	1577	rVB	59781	83213	2.39%	0.743%
27	11.085	1634	1640	1645	rBV	100802	124941	3.59%	1.115%
28	11.689	1733	1739	1745	rBV	70322	84397	2.42%	0.753%
29	11.975	1776	1786	1790	rBV5	21660	48220	1.38%	0.430%
30	12.024	1790	1794	1798	rVB	95782	116704	3.35%	1.042%
31	13.292	1993	2002	2008	rBV4	14556	36890	1.06%	0.329%
32	14.621	2216	2220	2226	rBV2	55322	104034	2.99%	0.929%
33	14.755	2239	2242	2245	rBV2	29848	35914	1.03%	0.321%
34	14.847	2254	2257	2261	rVB4	37166	44633	1.28%	0.398%
35	15.036	2285	2288	2293	rBV3	20775	35213	1.01%	0.314%
36	15.188	2307	2313	2314	rBV4	38521	63750	1.83%	0.569%

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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

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Title : SW846 8260

37	15.219	2315	2318	2321	rVB3	45986	60966	1.75%	0.544%
38	15.426	2347	2352	2357	rVB	127155	190211	5.46%	1.698%
39	15.493	2358	2363	2365	rBV4	50521	91826	2.64%	0.820%
40	15.615	2380	2383	2387	rBV2	47558	56863	1.63%	0.508%
41	15.688	2392	2395	2399	rVV6	48615	64512	1.85%	0.576%
42	15.749	2401	2405	2410	rVB3	164666	250996	7.20%	2.240%
43	15.822	2413	2417	2419	rBV4	33160	53129	1.52%	0.474%
44	16.097	2458	2462	2467	rBV8	36138	74288	2.13%	0.663%
45	16.615	2543	2547	2553	rVB8	30678	58397	1.68%	0.521%
46	16.712	2559	2563	2570	rVB2	97656	182409	5.23%	1.628%

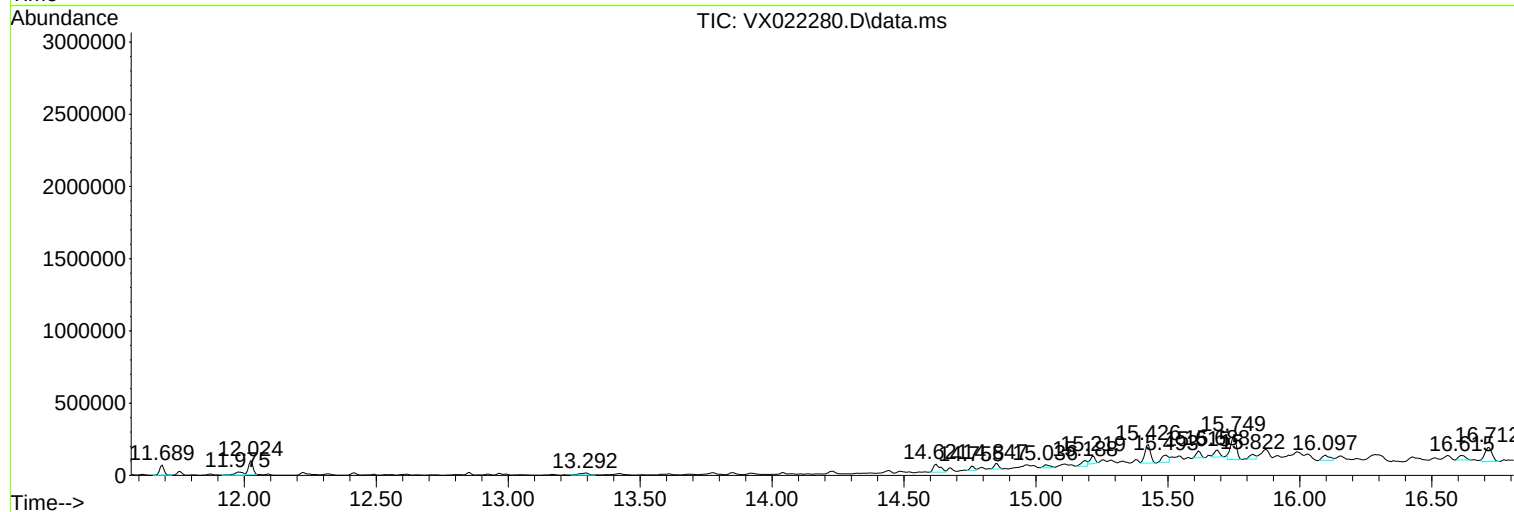
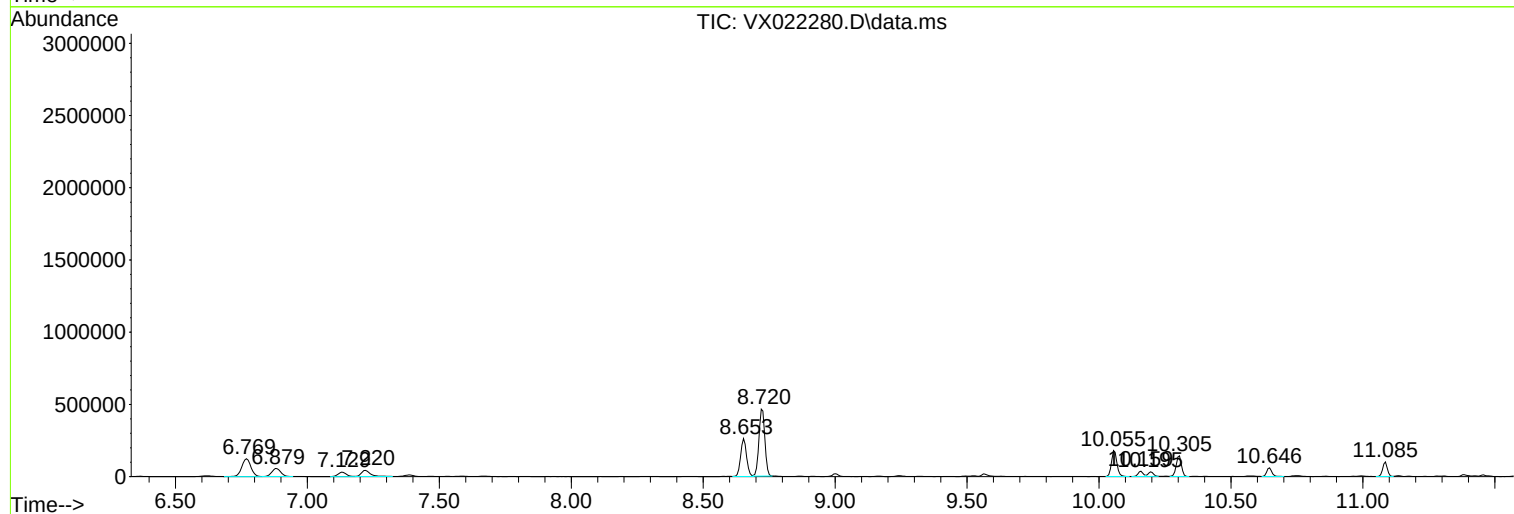
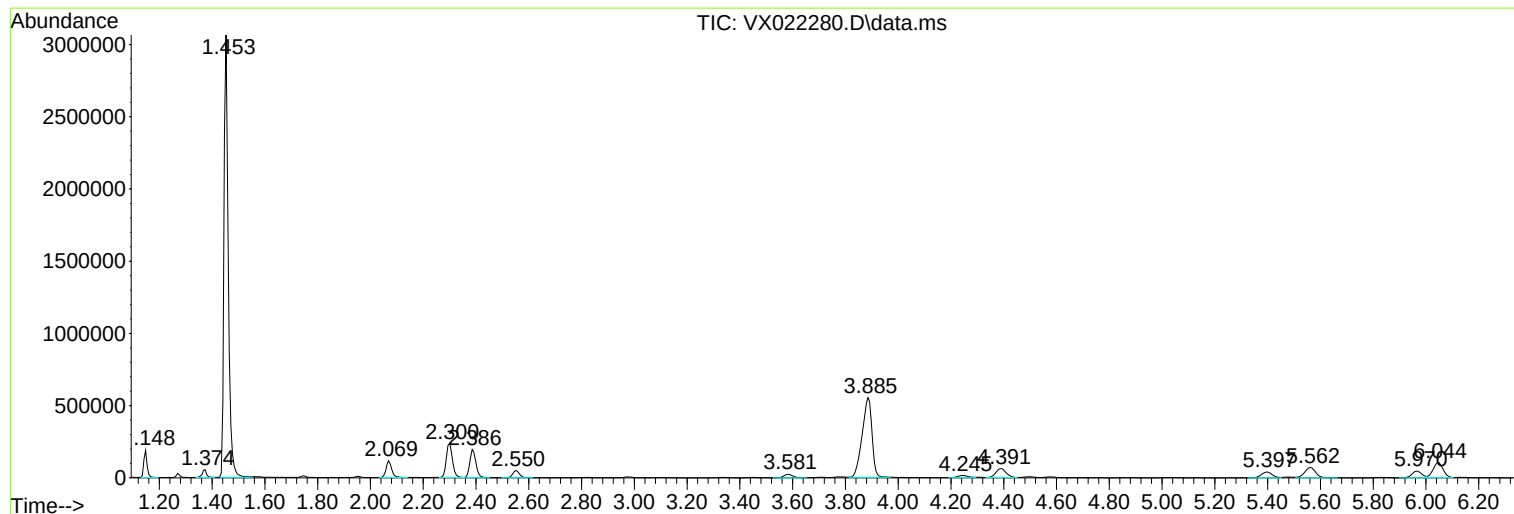
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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



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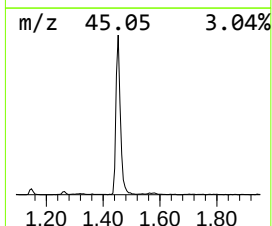
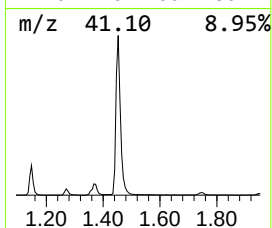
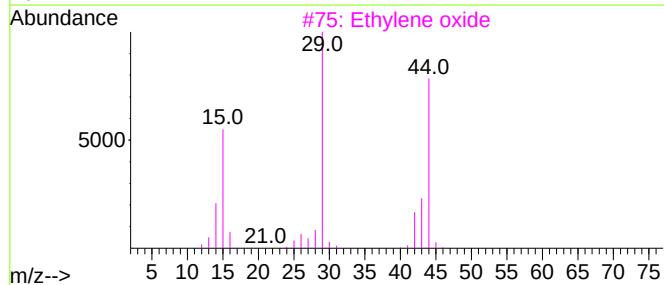
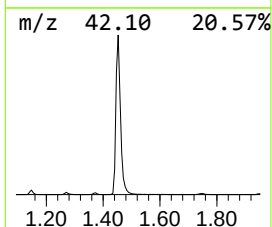
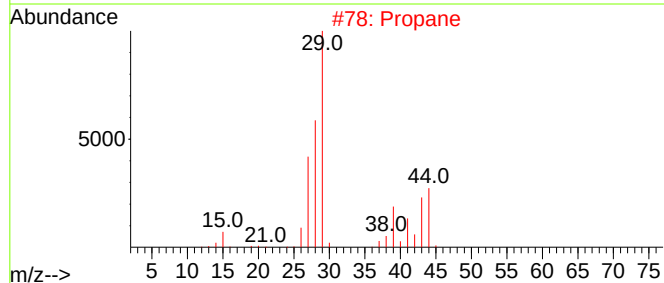
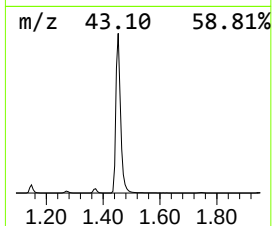
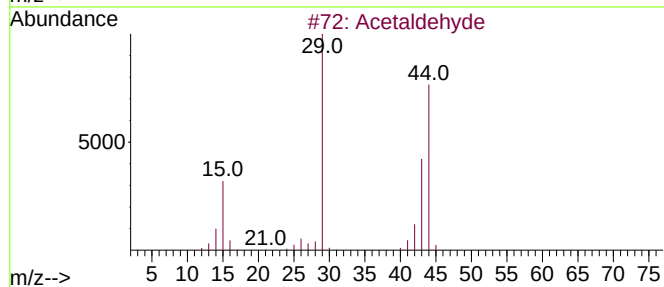
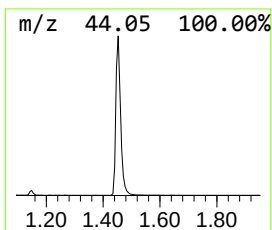
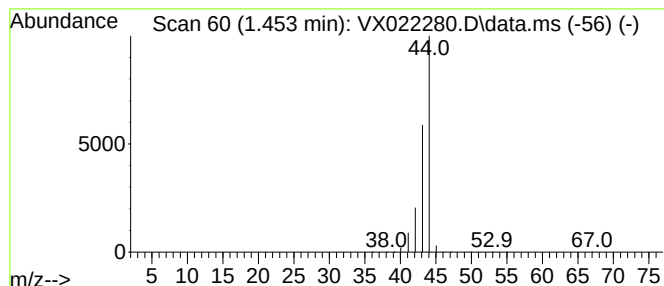
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	841.71 ug/l	3484780	Pentafluorobenzene	5.562

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



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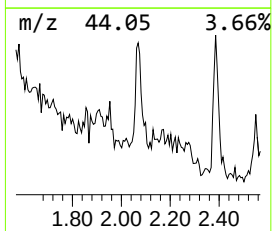
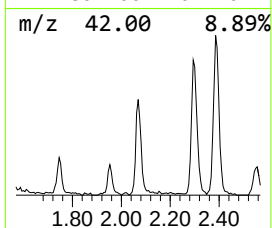
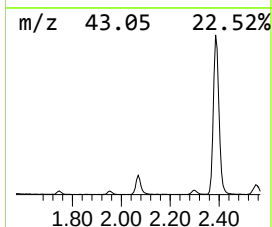
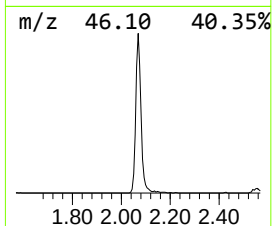
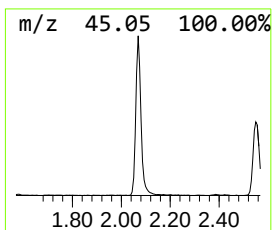
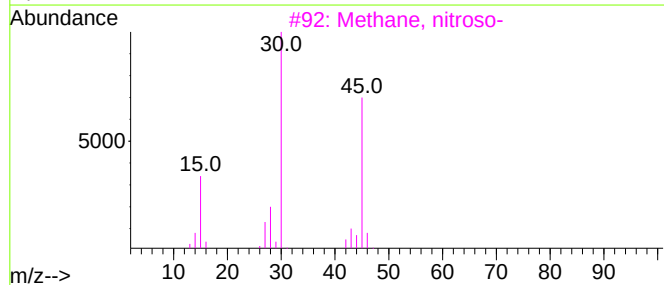
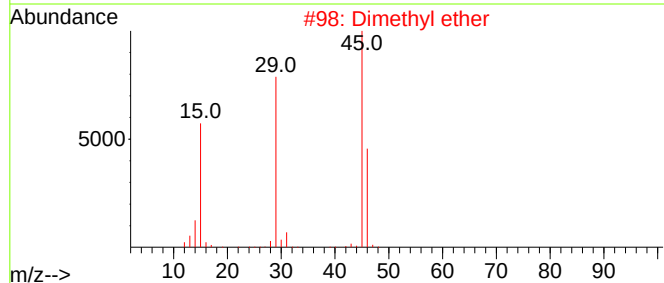
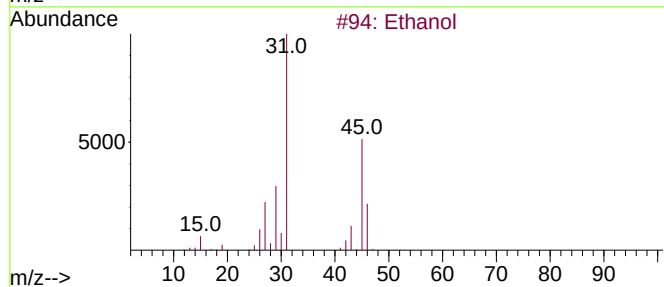
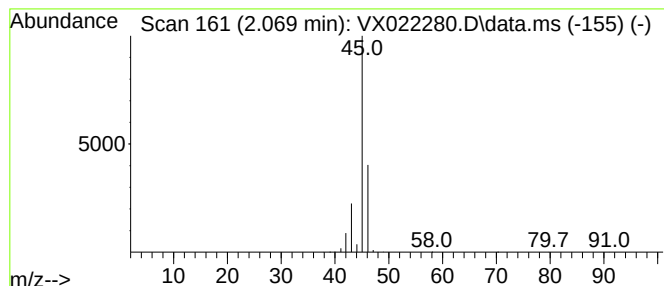
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	41.70 ug/l	172623	Pentafluorobenzene	5.562

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



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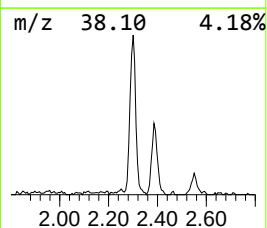
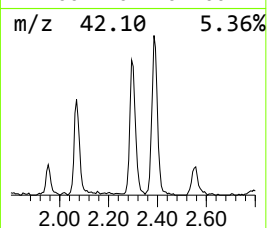
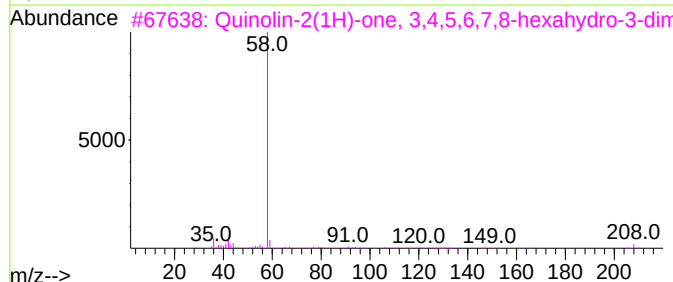
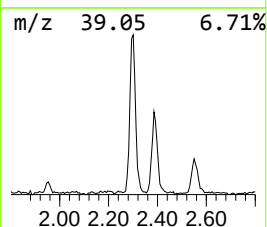
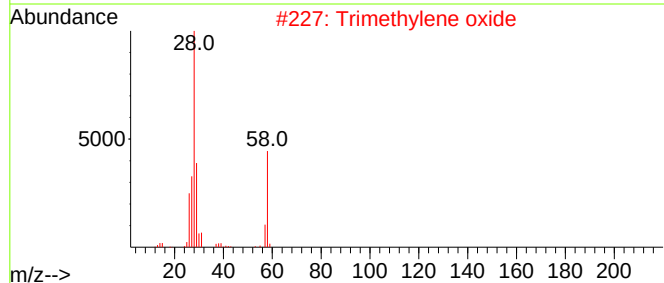
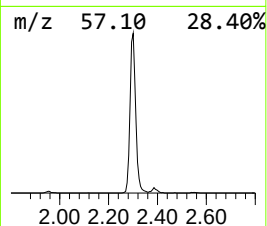
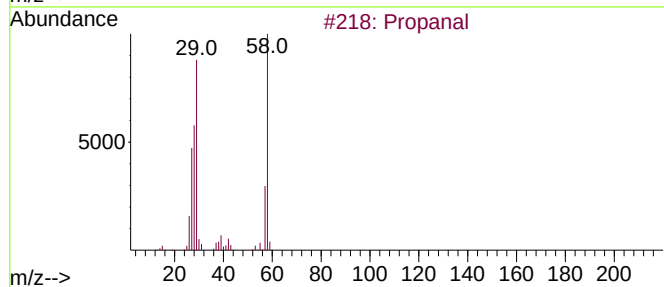
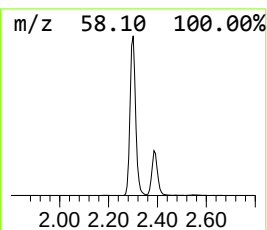
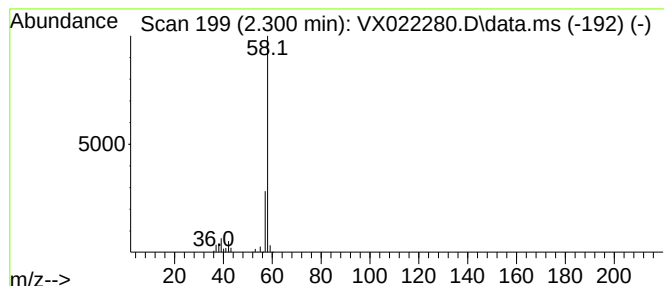
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.300	90.86 ug/l	376162	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Trimethylene oxide	58	C3H6O	000503-30-0	56
3			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4			Propylene oxide	58	C3H6O	000075-56-9	7
5			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7



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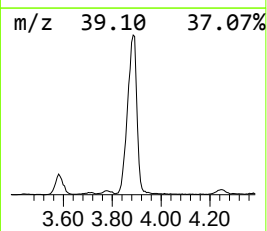
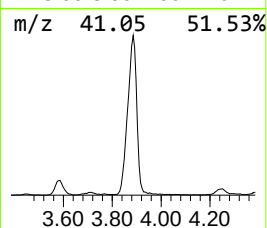
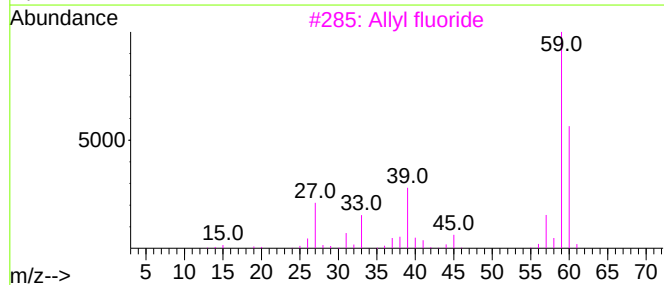
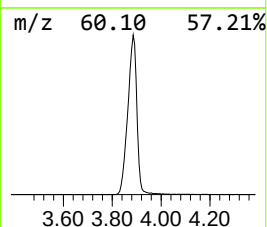
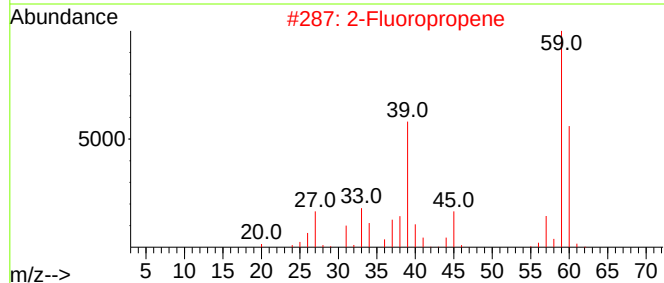
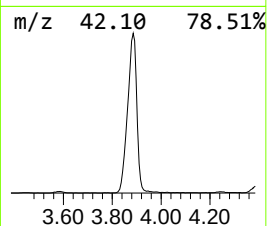
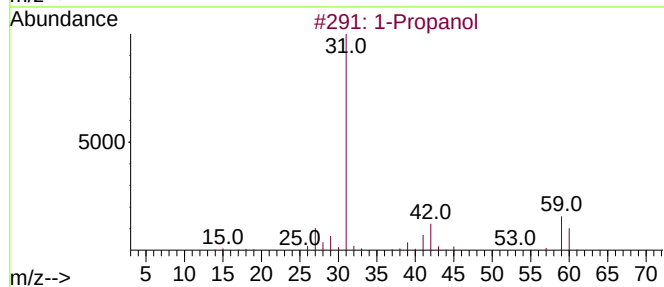
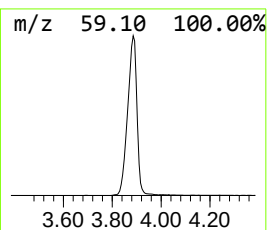
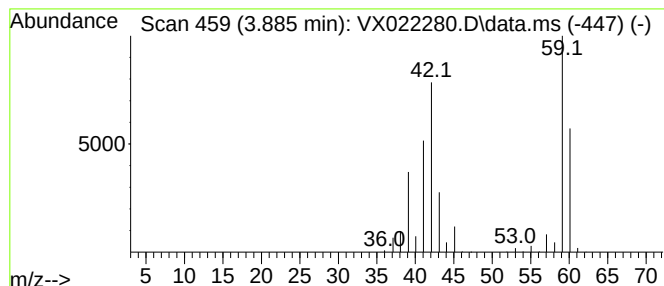
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Quant Title : SW846 8260

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	343.87 ug/l	1423650	Pentafluorobenzene	5.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol		60	C3H8O	000071-23-8	78
2	2-Fluoropropene		60	C3H5F	001184-60-7	47
3	Allyl fluoride		60	C3H5F	000818-92-8	43
4	Cyclopropane		42	C3H6	000075-19-4	16
5	2-Butanol, 3-methoxy-		104	C5H12O2	053778-72-6	12



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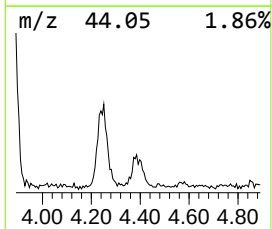
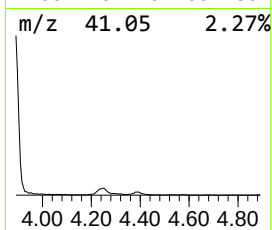
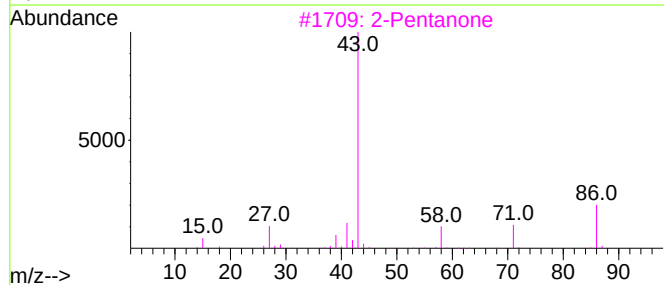
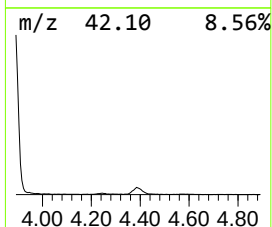
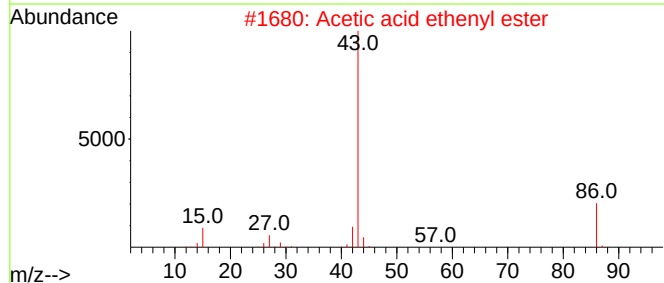
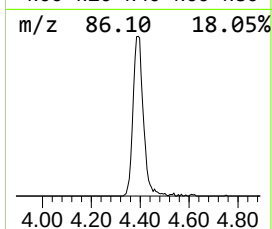
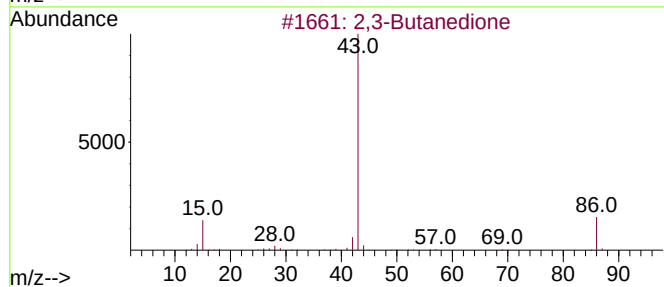
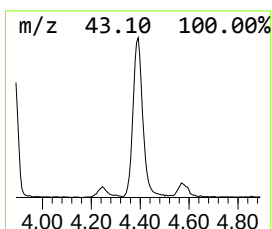
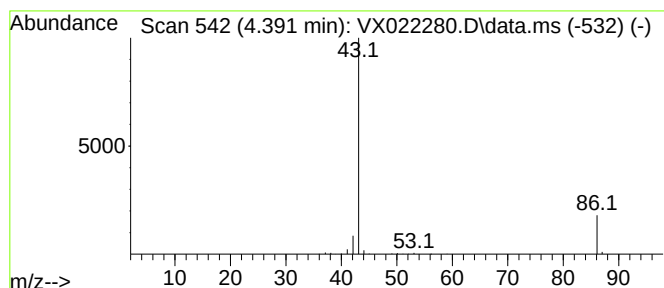
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Quant Title : SW846 8260

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

Peak Number 5 2,3-Butanedione Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.391	40.72 ug/l	168586	Pentafluorobenzene	5.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione		86	C4H6O2	000431-03-8	64
2	Acetic acid ethenyl ester		86	C4H6O2	000108-05-4	9
3	2-Pentanone		86	C5H10O	000107-87-9	9
4	2-Butanone, 3-methyl-		86	C5H10O	000563-80-4	7
5	Ethanone, 1-oxiranyl-		86	C4H6O2	004401-11-0	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
Data File : VX022280.D
Acq On : 29 May 2021 03:04
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

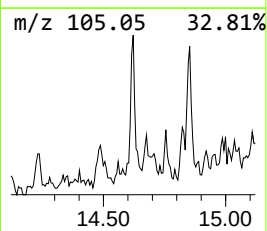
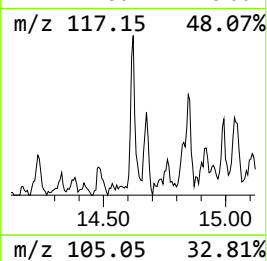
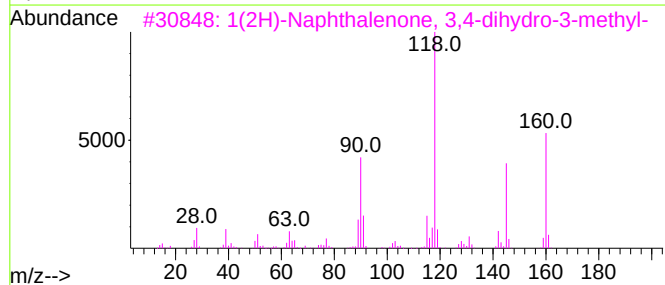
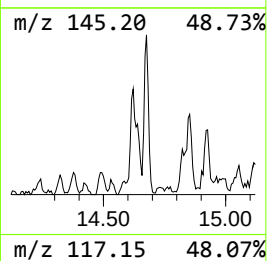
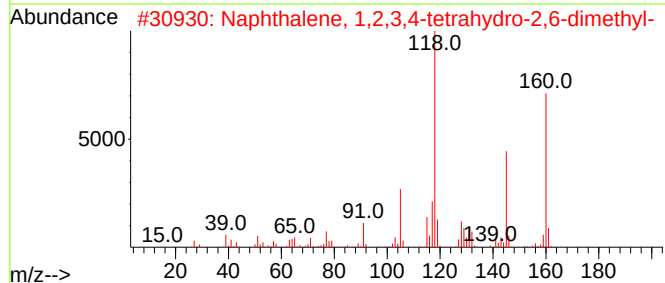
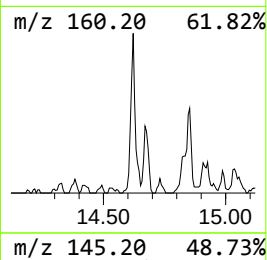
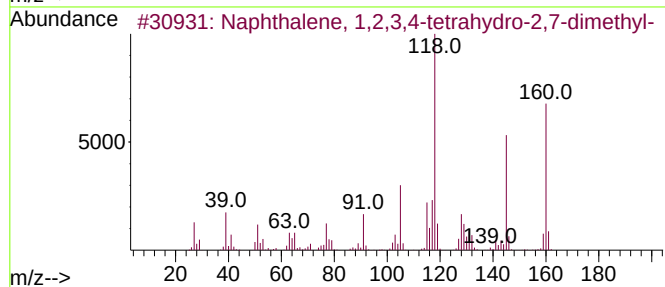
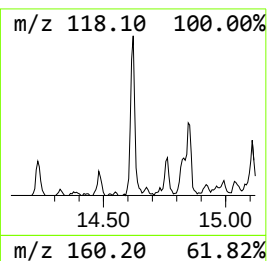
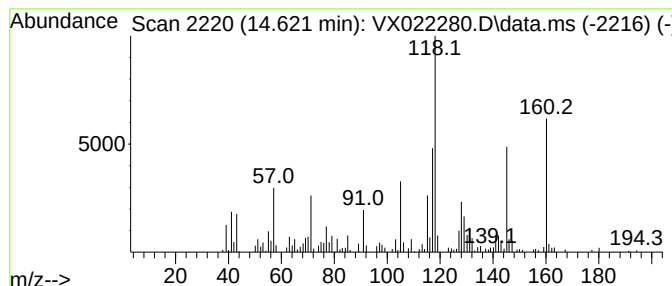
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	44.57 ug/l	104034	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	87
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	62
3			1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	53
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	50
5			Acetonitrile, 2-[4-(cyanomethyl)]...	145	C8H7N3	1000197-65-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
Data File : VX022280.D
Acq On : 29 May 2021 03:04
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

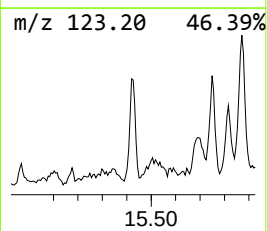
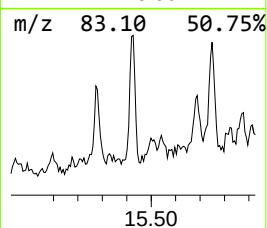
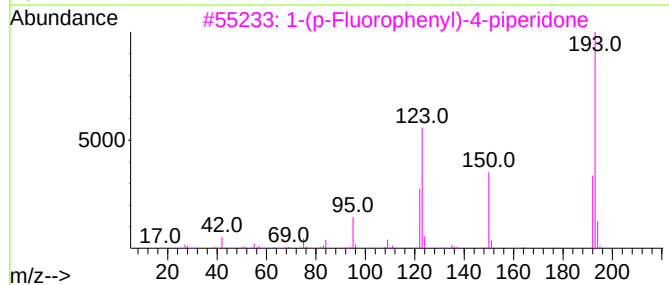
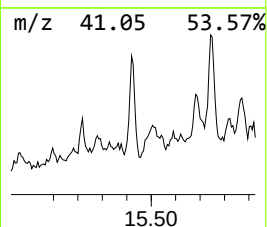
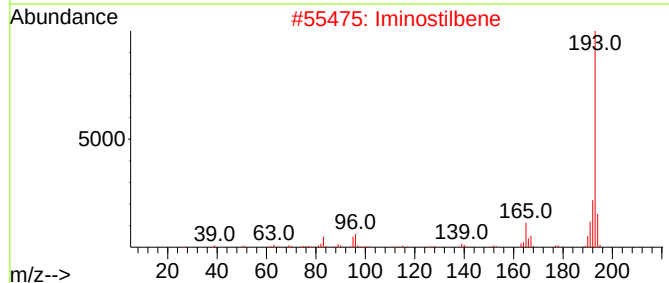
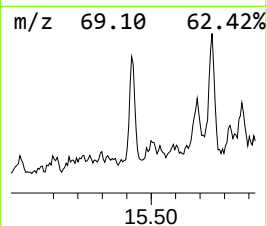
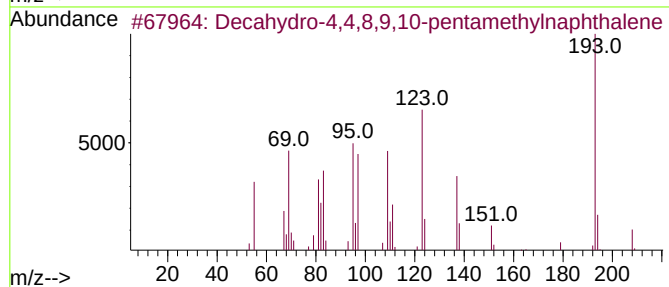
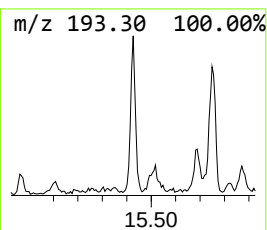
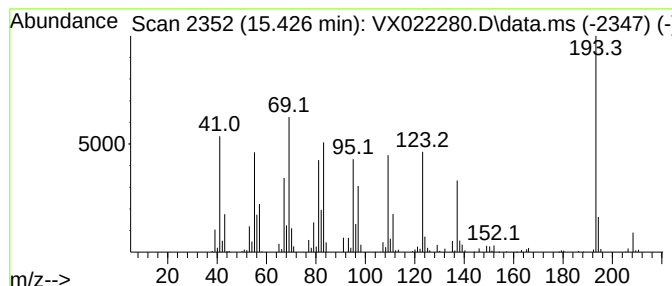
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 7 Decahydro-4,4,8,9,10-pentam... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.426	81.49 ug/l	190211	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	93
2			Iminostilbene	193	C14H11N	000256-96-2	37
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
4			2-Butenamide, N-(4-fluorophenyl)...	193	C11H12FNO	1000307-26-7	35
5			Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
Data File : VX022280.D
Acq On : 29 May 2021 03:04
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

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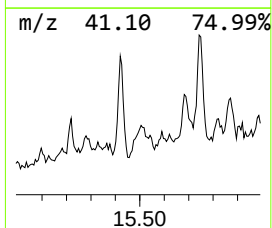
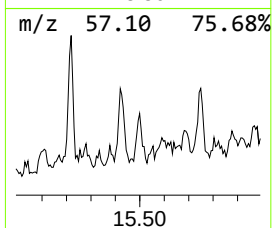
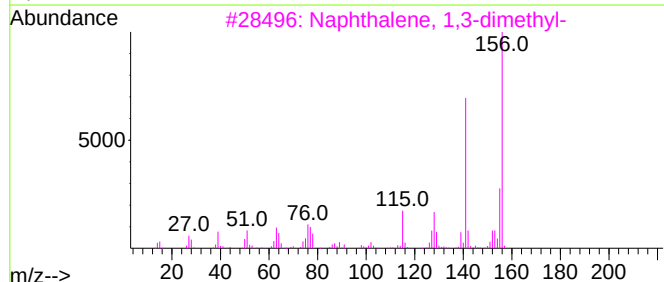
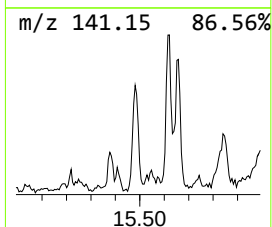
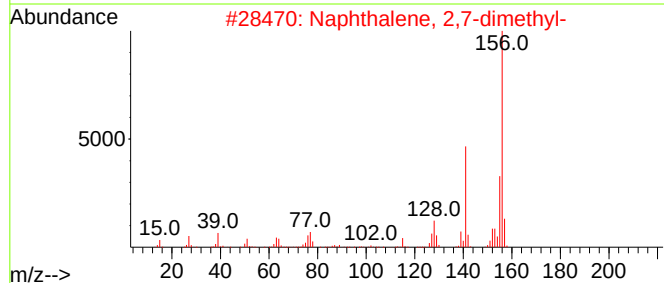
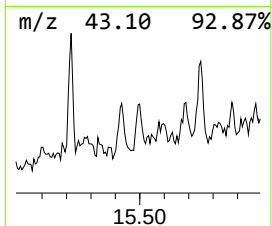
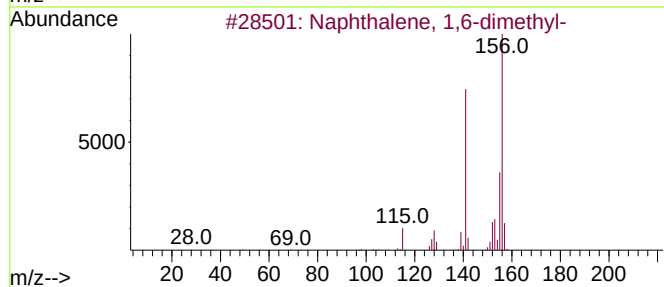
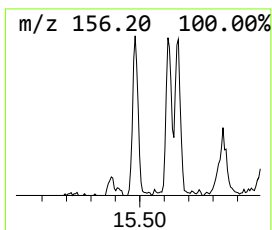
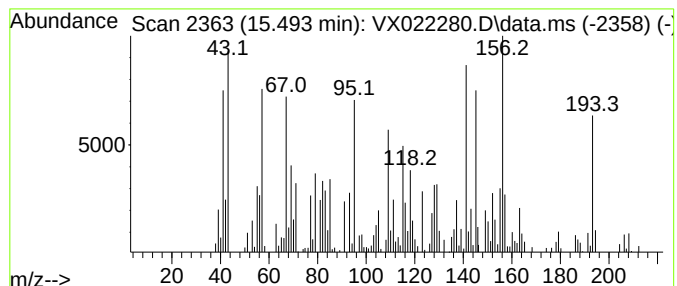
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 8 unknown15.493 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.493	39.34 ug/l	91826	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	42
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	38
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	38
4			Butanenitrile, 2-(amino)(methylt...	156	C6H8N2OS	058955-39-8	38
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
Data File : VX022280.D
Acq On : 29 May 2021 03:04
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

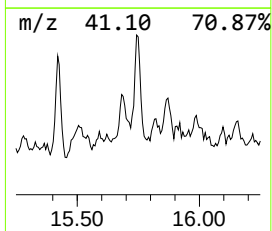
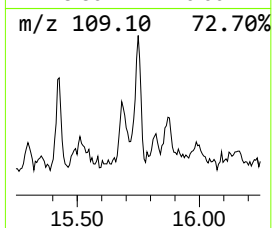
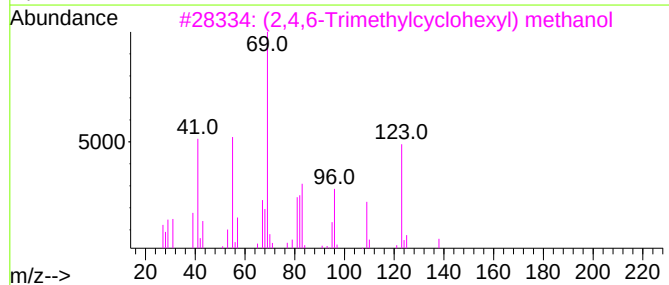
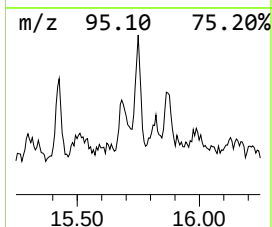
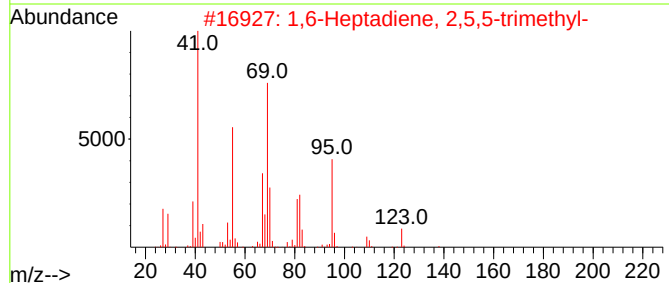
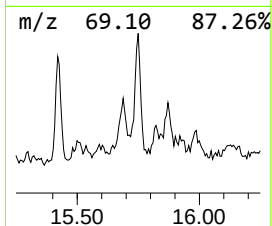
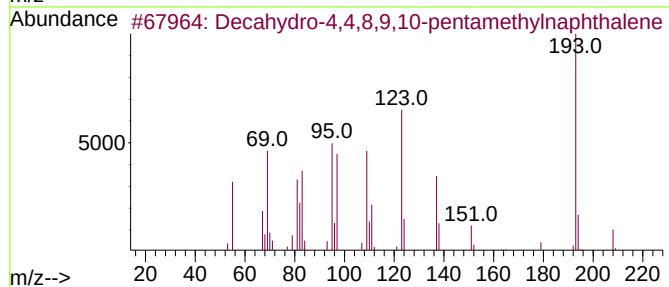
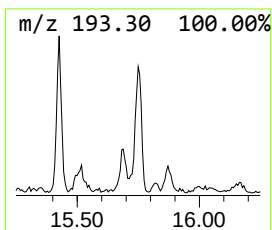
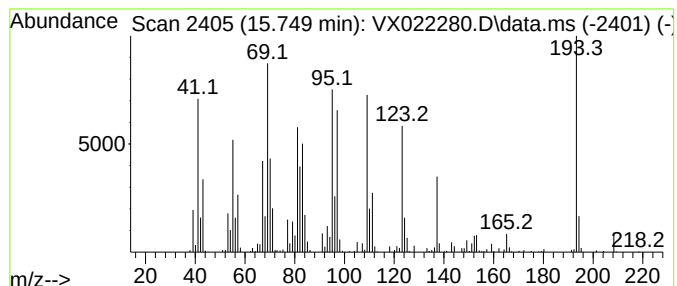
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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	107.54 ug/l	250996	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	90
2			1,6-Heptadiene, 2,5,5-trimethyl-	138	C10H18	062238-28-2	38
3			(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	22
4			Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	069147-03-1	18
5			1,2-Cyclohexanediol, cyclic sulf...	162	C6H10O3S	019456-18-9	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
Data File : VX022280.D
Acq On : 29 May 2021 03:04
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41815

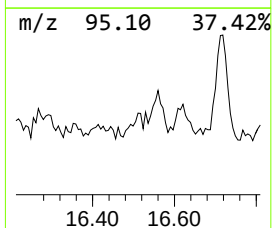
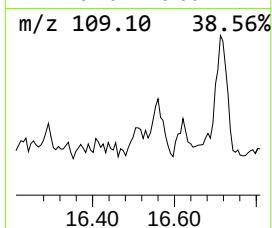
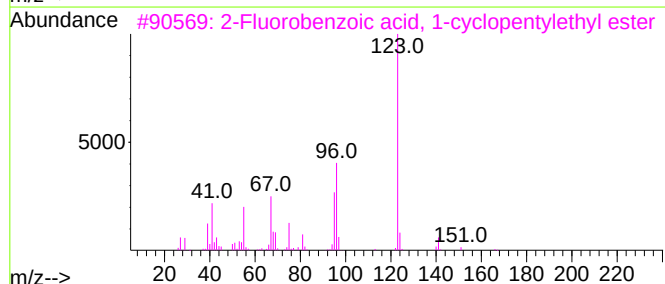
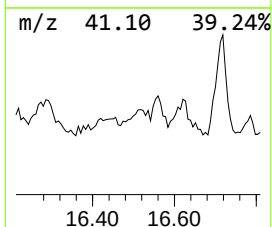
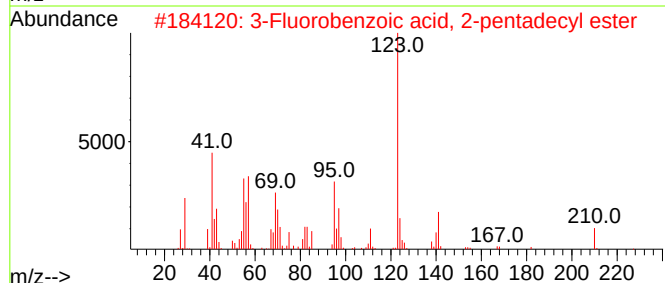
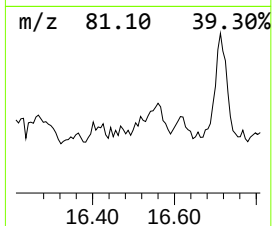
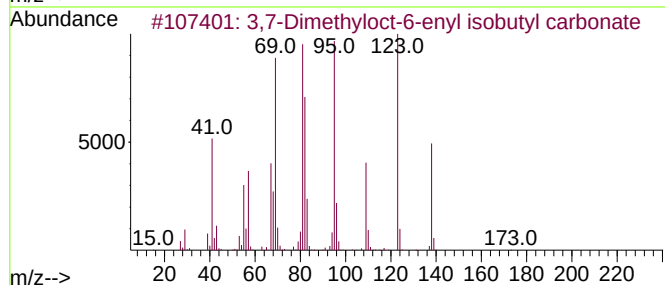
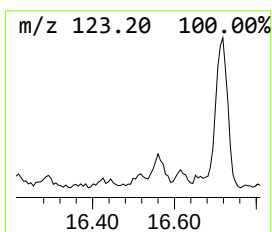
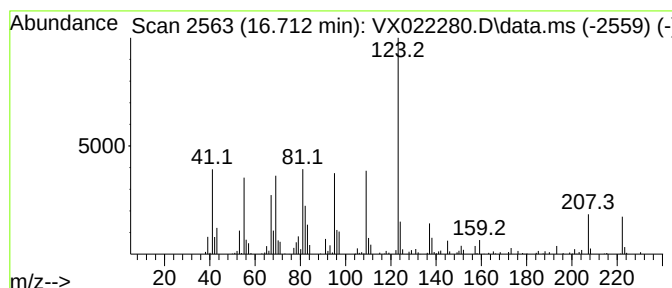
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 10 3,7-Dimethyloct-6-enyl isob... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.712	78.15 ug/l	182409	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,7-Dimethyloct-6-enyl isobutyl ...	256	C15H28O3	1000372-79-6	53
2			3-Fluorobenzoic acid, 2-pentadec...	350	C22H35FO2	1000280-60-7	47
3			2-Fluorobenzoic acid, 1-cyclopen...	236	C14H17FO2	1000278-98-2	43
4			3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	43
5			3-Fluorobenzoic acid, 1-cyclopen...	236	C14H17FO2	1000279-04-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
Data File : VX022280.D
Acq On : 29 May 2021 03:04
Operator : JC/MD
Sample : M2529-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 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
Acetaldehyde	1.453	841.7	ug/l	3484780	1	5.562	207006	50.0
Ethanol	2.069	41.7	ug/l	172623	1	5.562	207006	50.0
Propanal	2.300	90.9	ug/l	376162	1	5.562	207006	50.0
1-Propanol	3.885	343.9	ug/l	1423650	1	5.562	207006	50.0
2,3-Butanedione	4.391	40.7	ug/l	168586	1	5.562	207006	50.0
Naphthalene, 1,...	14.621	44.6	ug/l	104034	4	12.024	116704	50.0
Decahydro-4,4,8...	15.426	81.5	ug/l	190211	4	12.024	116704	50.0
unknown15.493	15.493	39.3	ug/l	91826	4	12.024	116704	50.0
unknown15.749	15.749	107.5	ug/l	250996	4	12.024	116704	50.0
3,7-Dimethyloct...	16.712	78.2	ug/l	182409	4	12.024	116704	50.0