

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
 Data File : VX028766.D
 Acq On : 17 May 2022 18:29
 Operator : JC/MD
 Sample : N2884-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31768

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: VX028766.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.294	192	198	205	rBV	155187	253302	1.04%	0.350%
2	2.373	205	211	229	rVB	2046908	3387056	13.90%	4.675%
3	2.532	230	237	244	rBV	495432	865883	3.55%	1.195%
4	2.958	297	307	325	rBV3	857944	2025157	8.31%	2.795%
5	3.696	416	428	447	rBV	2389805	6434656	26.42%	8.881%
6	4.556	560	569	582	rVB	169137	462314	1.90%	0.638%
7	5.391	695	706	718	rBV2	219559	649850	2.67%	0.897%
8	5.555	723	733	751	rVB	352847	1004078	4.12%	1.386%
9	5.958	788	799	805	rBV2	234756	621568	2.55%	0.858%
10	6.043	805	813	832	rVB	1179910	3319375	13.63%	4.581%
11	6.336	851	861	867	rBV2	89322	253680	1.04%	0.350%
12	6.763	921	931	945	rBV	571254	1352675	5.55%	1.867%
13	7.208	987	1004	1014	rBV	117704	269032	1.10%	0.371%
14	8.573	1222	1228	1235	rBV	686366	1120524	4.60%	1.547%
15	8.652	1235	1241	1246	rVV	1163579	1800675	7.39%	2.485%
16	8.726	1246	1253	1263	rVB	14984199	24359295	100.00%	33.620%
17	9.067	1305	1309	1314	rVB	238554	345535	1.42%	0.477%
18	9.488	1373	1378	1385	rBV	1453326	2128399	8.74%	2.938%
19	9.878	1437	1442	1449	rBV	198065	268228	1.10%	0.370%
20	10.055	1463	1471	1482	rVB	1469156	1962973	8.06%	2.709%
21	10.195	1489	1494	1500	rVB	1835800	2331381	9.57%	3.218%
22	10.299	1507	1511	1522	rVB	3807177	5350372	21.96%	7.384%
23	10.414	1522	1530	1532	rBV2	218620	342059	1.40%	0.472%
24	10.439	1532	1534	1542	rVB4	132540	267825	1.10%	0.370%
25	10.646	1563	1568	1578	rVB2	1752331	2737931	11.24%	3.779%
26	11.079	1634	1639	1648	rBV	1021868	1403283	5.76%	1.937%
27	11.378	1683	1688	1695	rBV	194571	355739	1.46%	0.491%
28	11.756	1745	1750	1754	rVB	270616	335315	1.38%	0.463%
29	12.024	1788	1794	1798	rBV	1412392	1821541	7.48%	2.514%
30	12.243	1822	1830	1834	rBV2	178479	301379	1.24%	0.416%
31	12.414	1853	1858	1864	rBV	2228094	2682573	11.01%	3.702%
32	13.774	2076	2081	2088	rVB	1290721	1640955	6.74%	2.265%

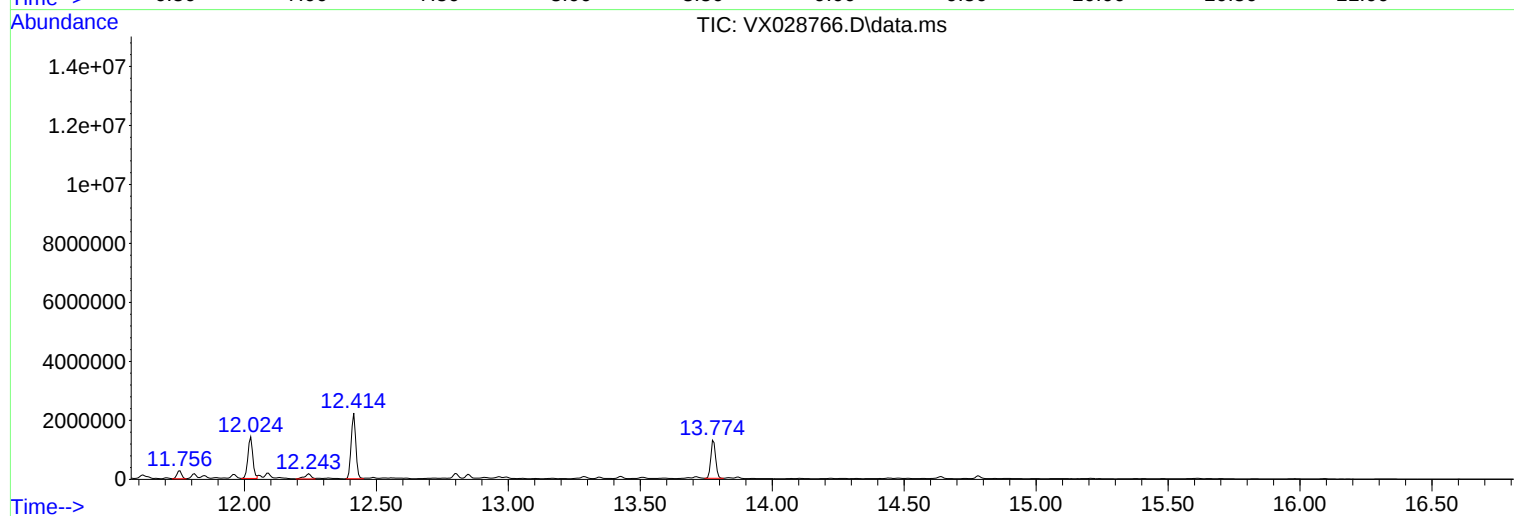
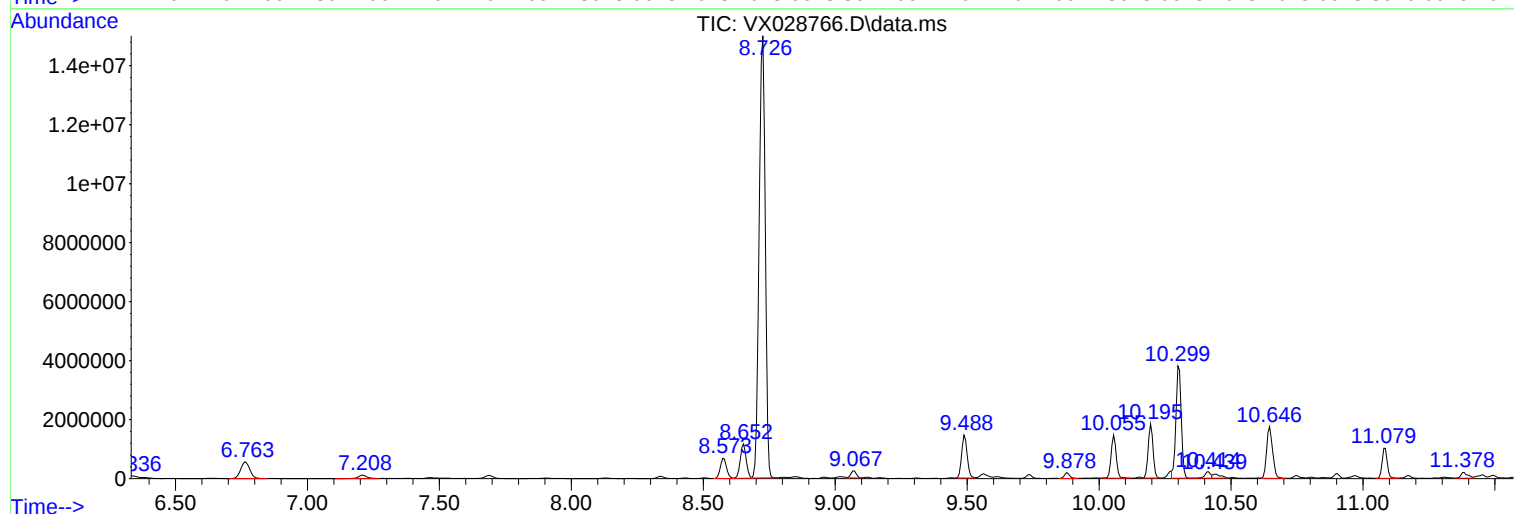
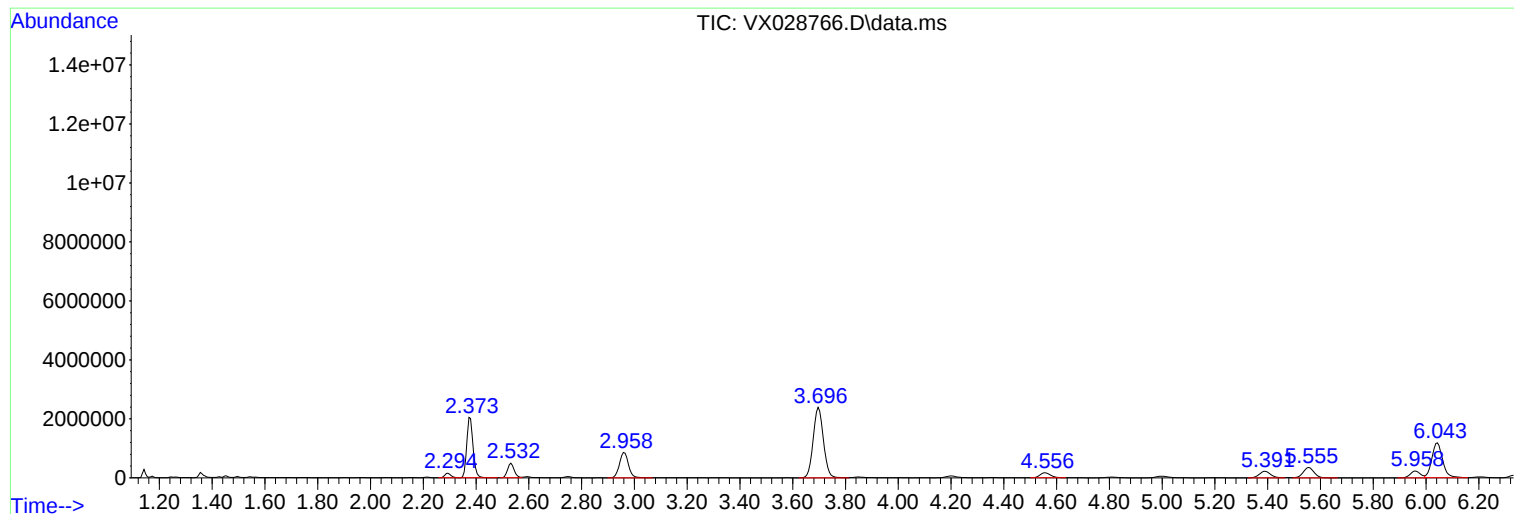
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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



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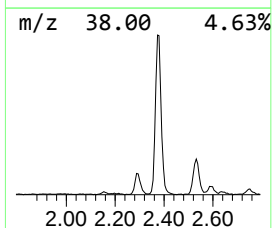
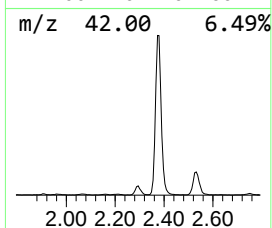
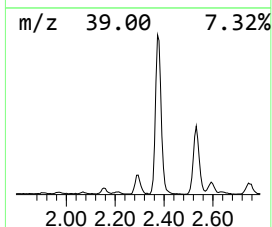
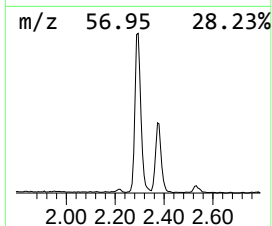
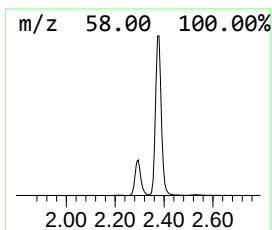
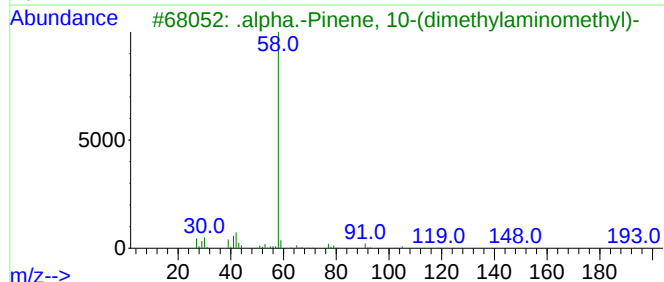
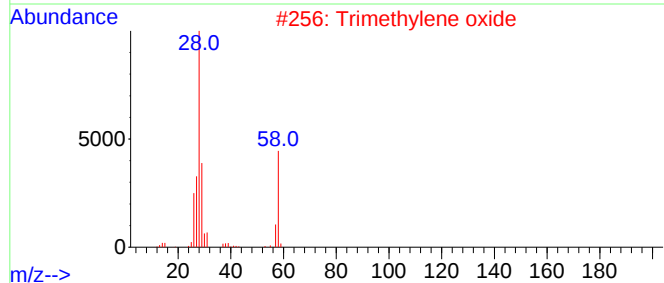
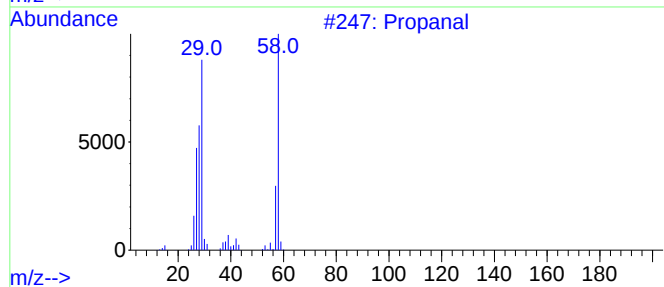
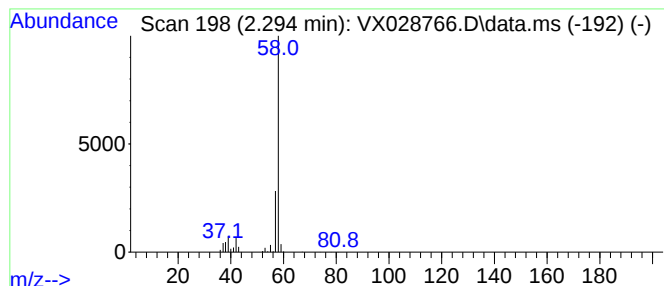
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Quant Title : SW846 8260

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

Peak Number 1 Propanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	12.61 ug/l	253302	Pentafluorobenzene	5.555

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			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
4			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
5			Propylene oxide	58	C3H6O	000075-56-9	7



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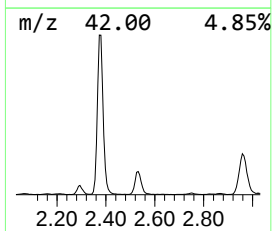
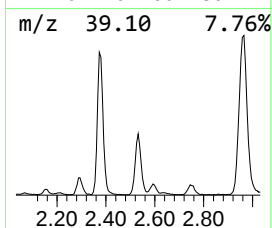
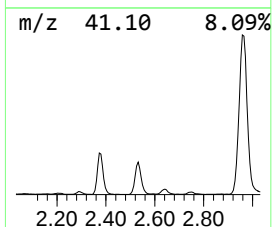
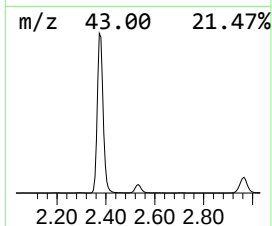
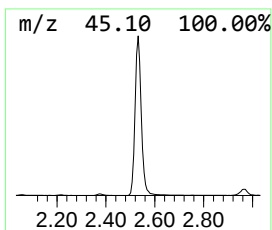
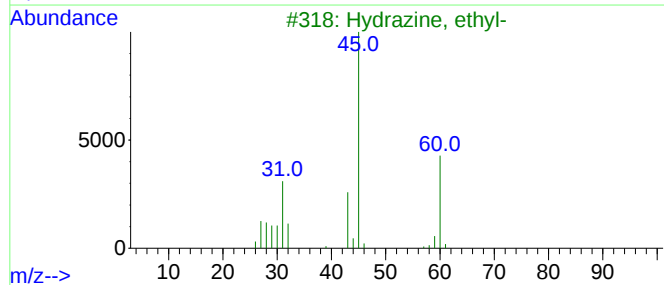
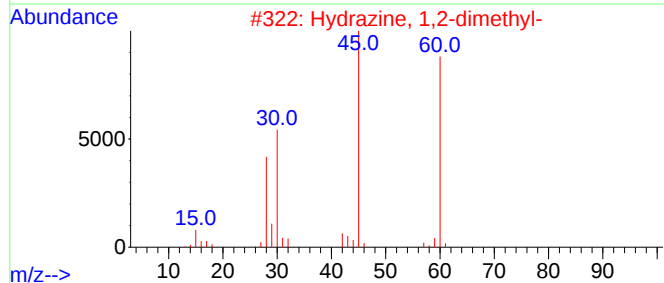
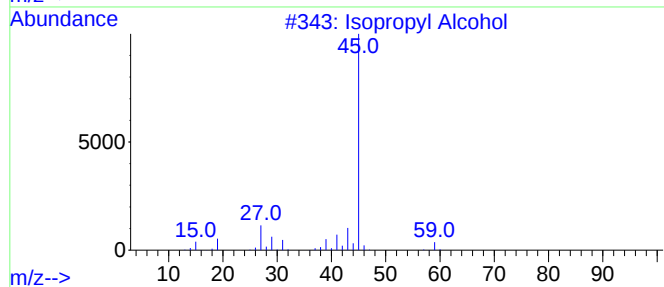
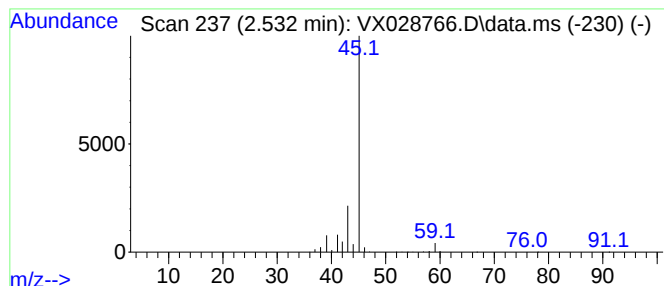
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.532	43.12 ug/l	865883	Pentafluorobenzene	5.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
4			Formamide	45	CH3NO	000075-12-7	5
5			4-Penten-2-ol	86	C5H10O	000625-31-0	4



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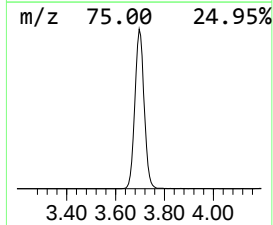
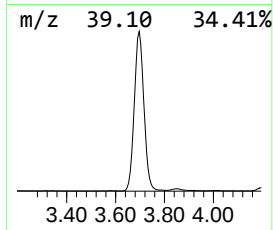
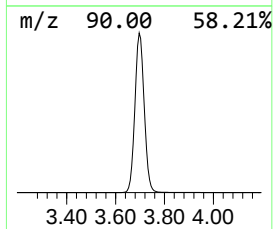
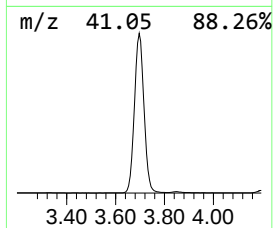
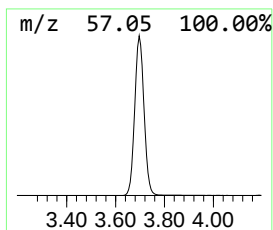
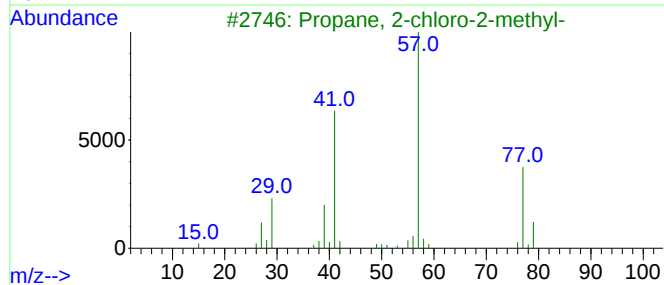
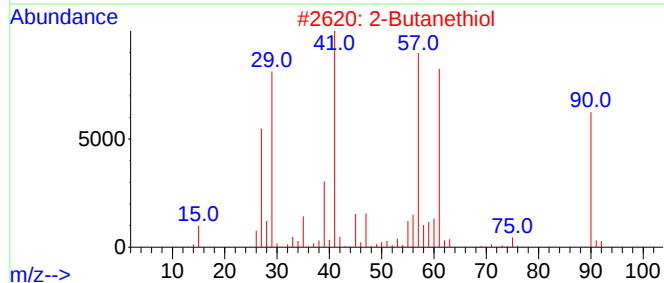
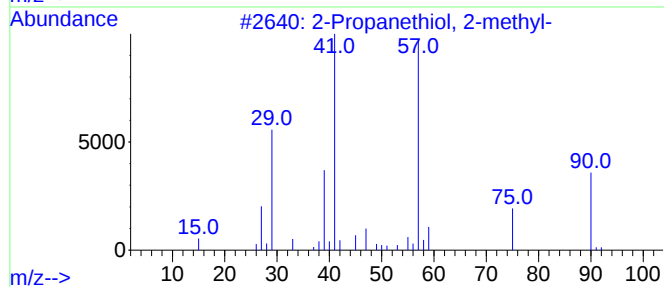
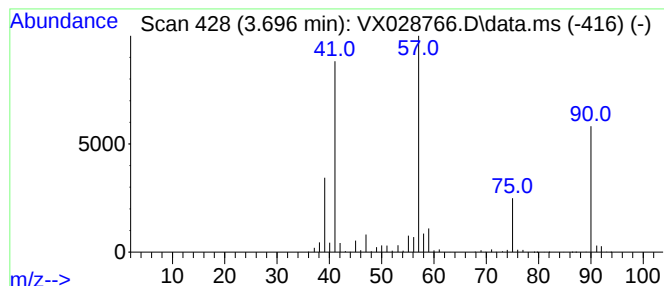
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanethiol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.696	320.43 ug/l	6434660	Pentafluorobenzene	5.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	91
2			2-Butanethiol	90	C4H10S	000513-53-1	42
3			Propane, 2-chloro-2-methyl-	92	C4H9Cl	000507-20-0	22
4			Ethynyl tert-butyl sulfoxide	130	C6H10OS	041463-34-7	16
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	14



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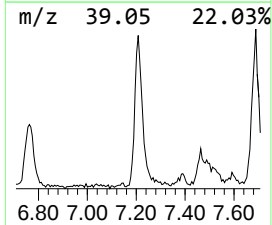
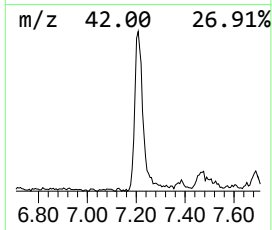
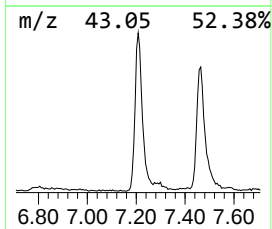
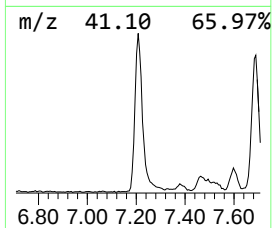
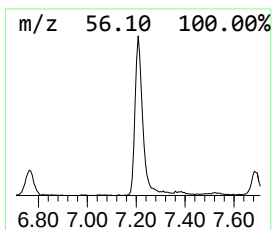
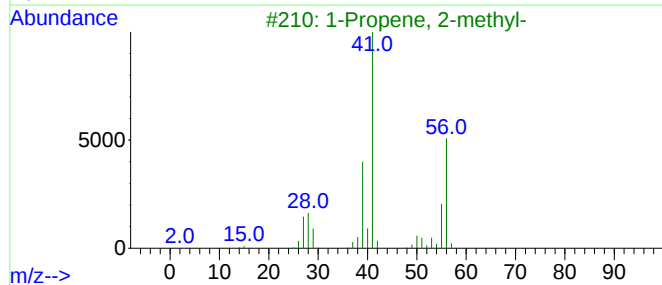
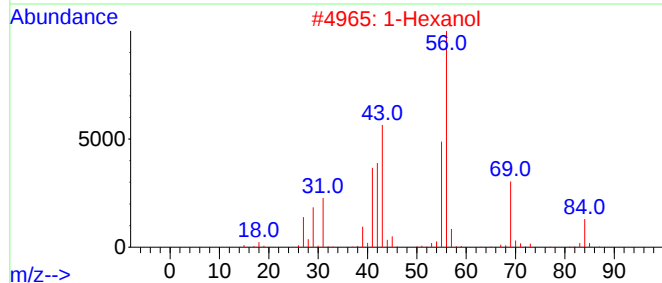
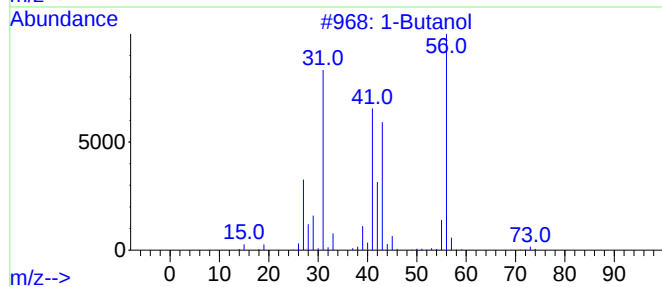
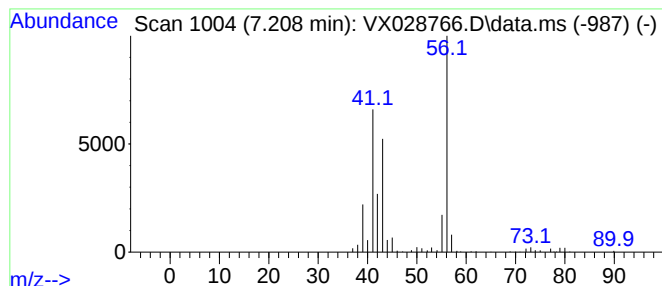
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Peak Number 4 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	9.94 ug/l	269032	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	86
2			1-Hexanol	102	C6H14O	000111-27-3	43
3			1-Propene, 2-methyl-	56	C4H8	000115-11-7	42
4			Cyclopentane, methyl-	84	C6H12	000096-37-7	39
5			2H-Pyran-2-one, tetrahydro-5,6-d...	128	C7H12O2	024405-16-1	36



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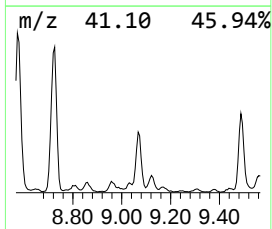
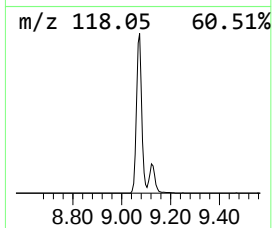
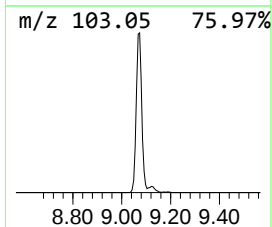
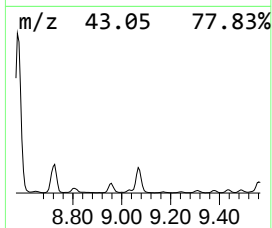
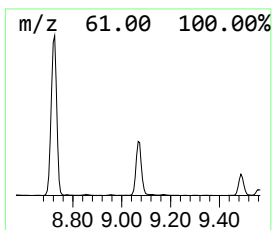
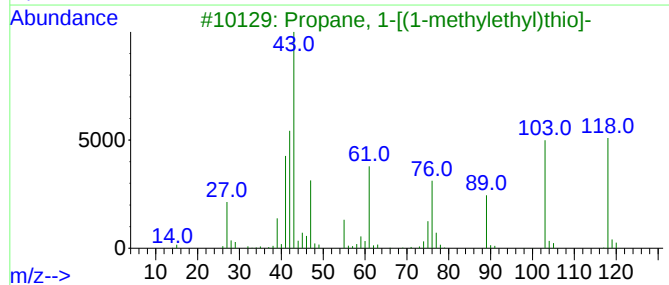
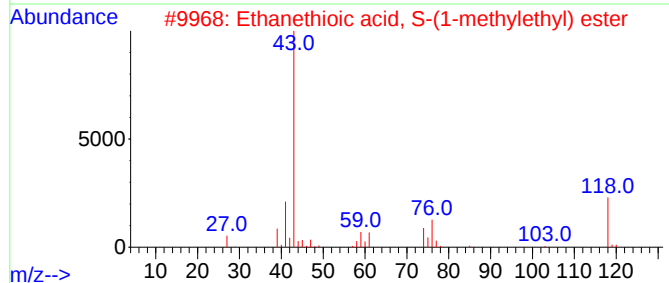
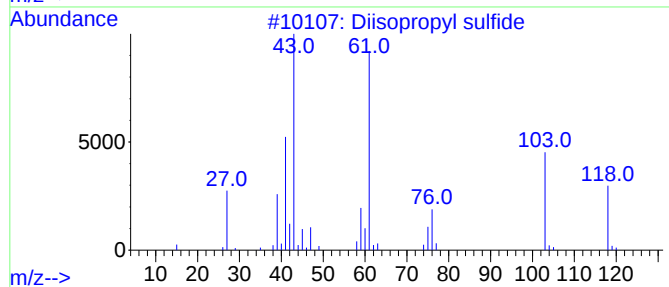
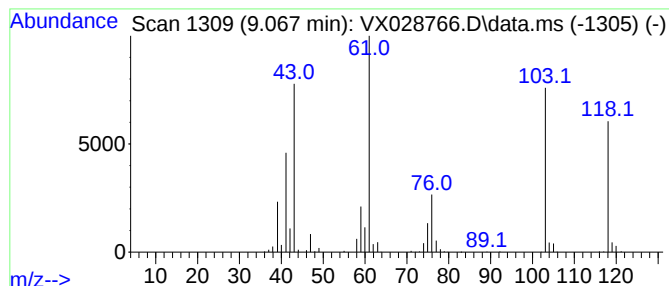
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Quant Title : SW846 8260

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

Peak Number 5 Diisopropyl sulfide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.067	8.80 ug/l	345535	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diisopropyl sulfide	118	C6H14S	000625-80-9	91
2			Ethanethioic acid, S-(1-methylet...	118	C5H10OS	000926-73-8	38
3			Propane, 1-[(1-methylethyl)thio]-	118	C6H14S	005008-73-1	33
4			Tricyclo[3.1.0.0(2,4)]hex-3-ene-...	103	C7H5N	103495-51-8	30
5			Benzonitrile	103	C7H5N	000100-47-0	27



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31768

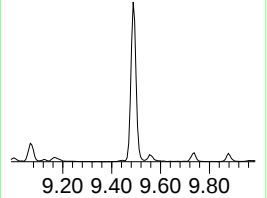
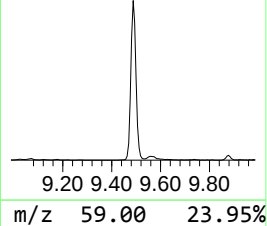
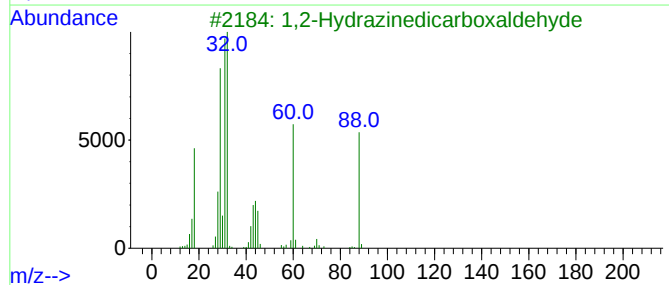
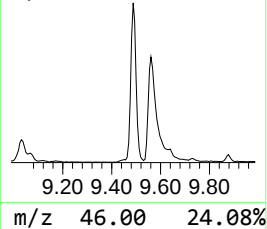
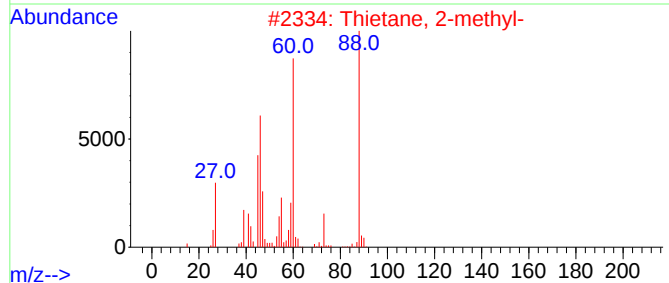
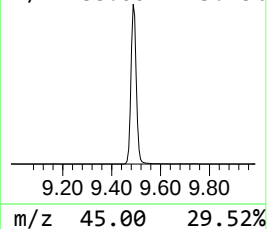
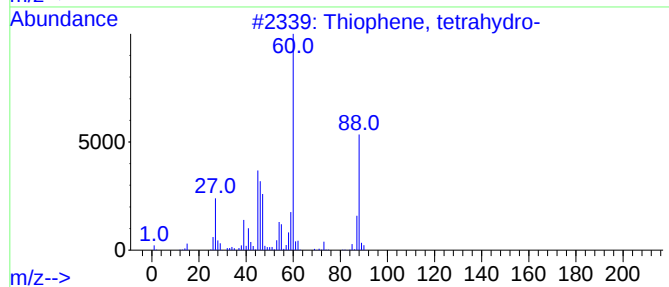
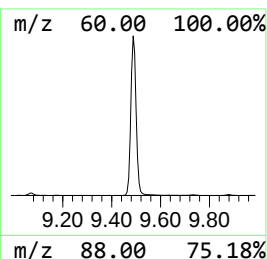
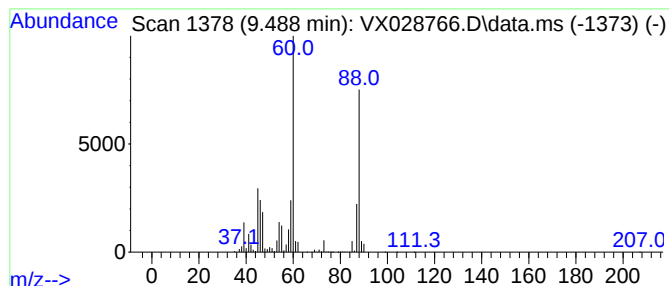
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Quant Title : SW846 8260

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

Peak Number 6 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	54.21 ug/l	2128400	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	95
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	74
3			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	53
4			Ethylvinyl sulfide	88	C4H8S	000627-50-9	42
5			Sulfide, allyl methyl	88	C4H8S	010152-76-8	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028766.D
Acq On : 17 May 2022 18:29
Operator : JC/MD
Sample : N2884-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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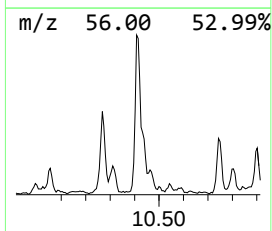
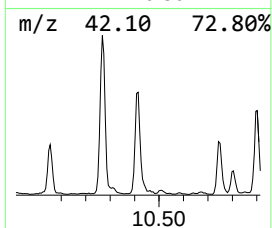
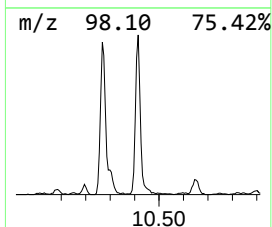
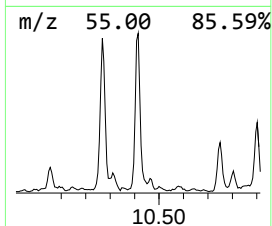
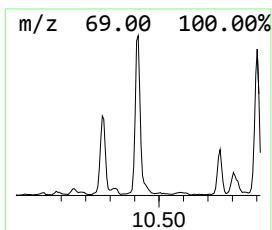
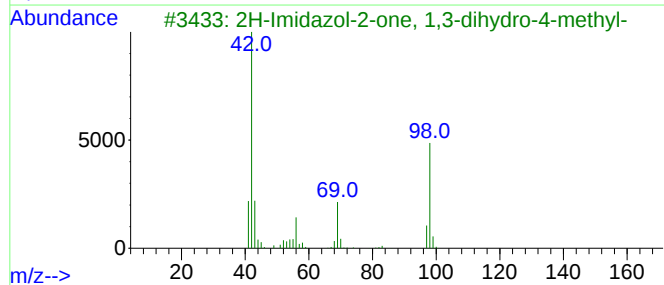
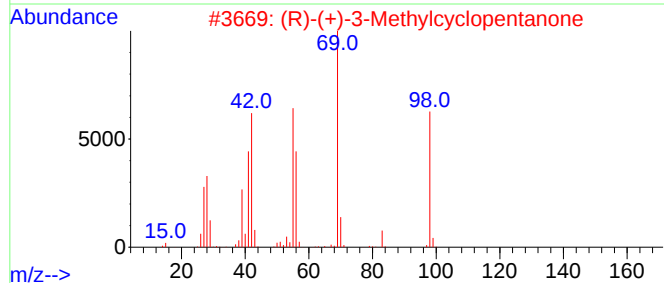
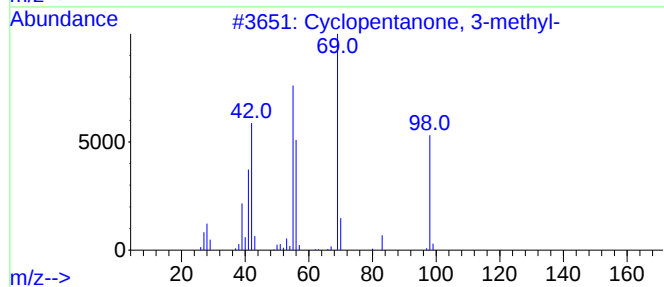
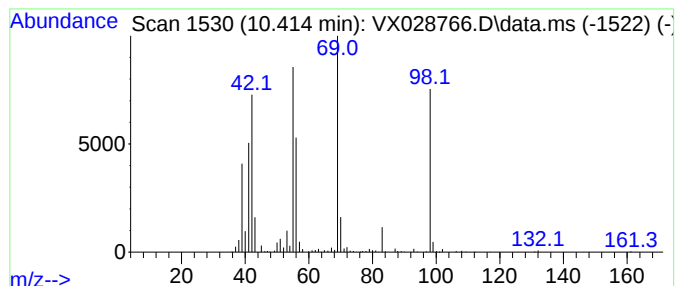
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentanone, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.414	8.71 ug/l	342059	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	94
2			(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	94
3			2H-Imidazol-2-one, 1,3-dihydro-4-methyl-	98	C4H6N2O	001192-34-3	72
4			1H-Tetrazole, 1,5-dimethyl-	98	C3H6N4	005144-11-6	64
5			3-Methyl-3-hexene	98	C7H14	003404-65-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028766.D
Acq On : 17 May 2022 18:29
Operator : JC/MD
Sample : N2884-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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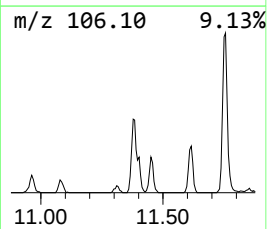
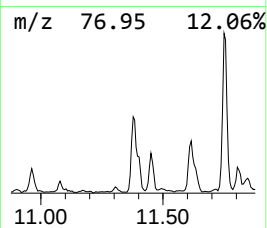
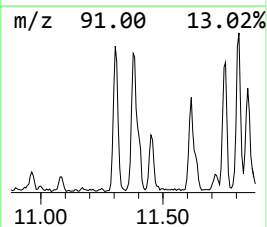
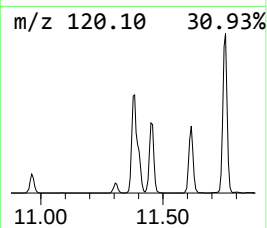
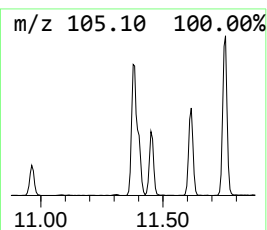
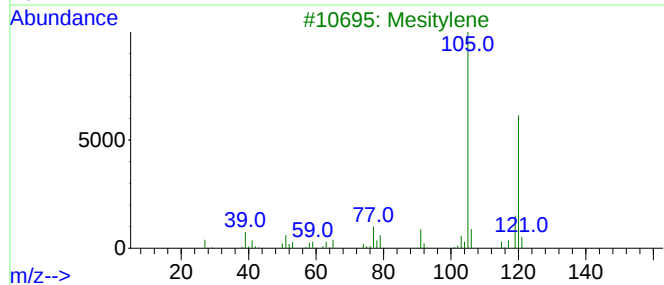
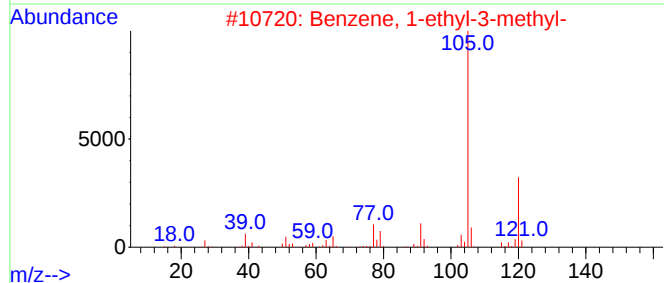
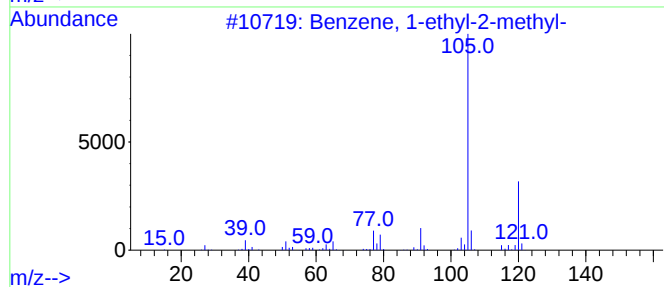
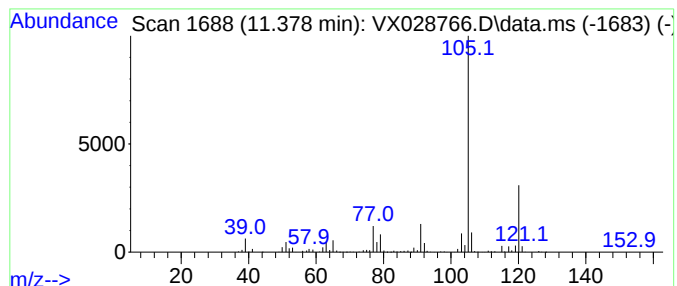
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	9.76 ug/l	355739	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028766.D
Acq On : 17 May 2022 18:29
Operator : JC/MD
Sample : N2884-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31768

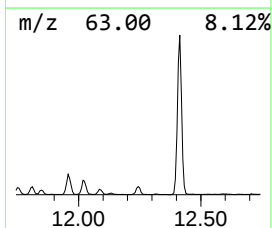
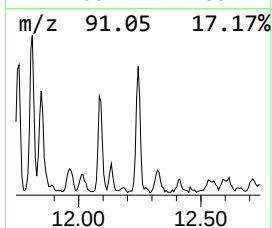
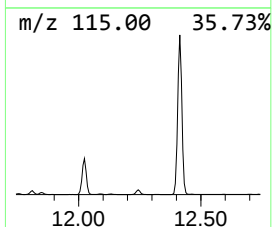
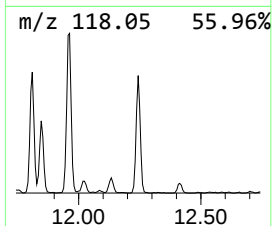
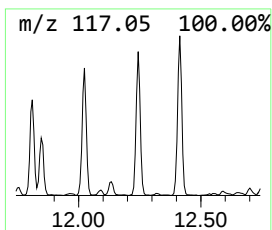
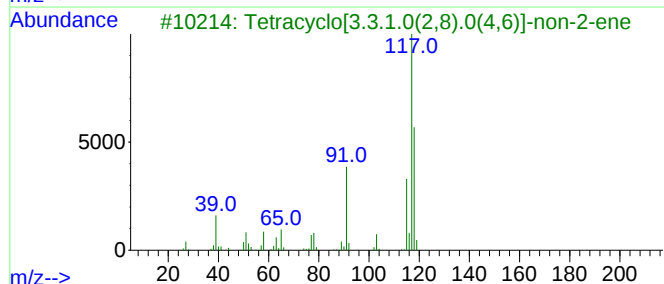
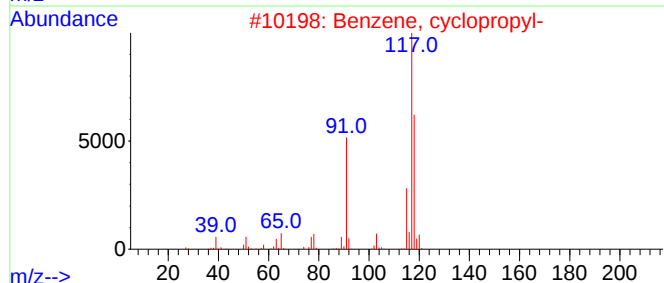
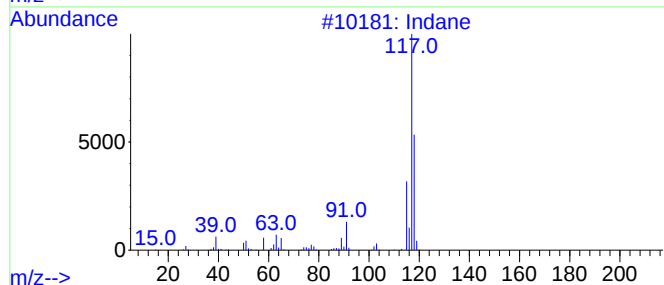
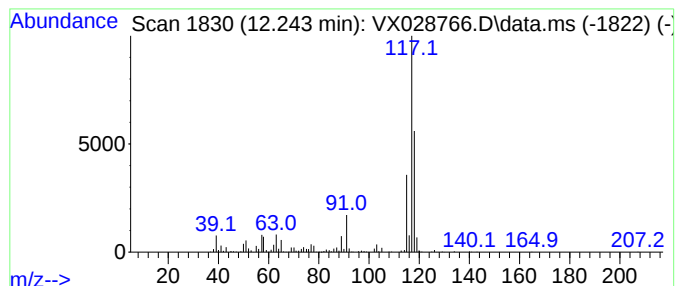
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Quant Title : SW846 8260

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

Peak Number 9 Indane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	8.27 ug/l	301379	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	87
3			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	78
5			Deltacyclene	118	C9H10	007785-10-6	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028766.D
Acq On : 17 May 2022 18:29
Operator : JC/MD
Sample : N2884-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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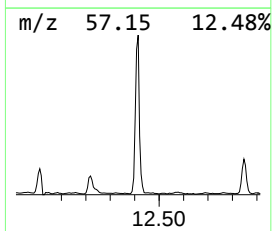
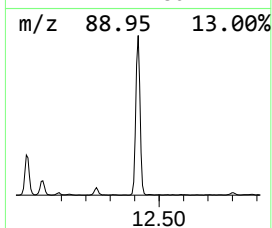
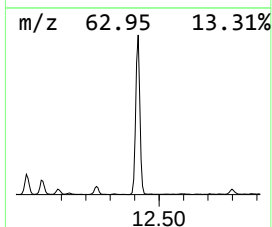
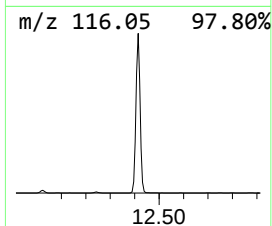
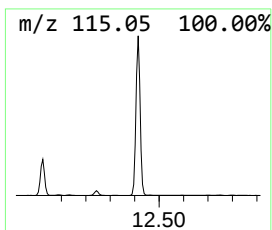
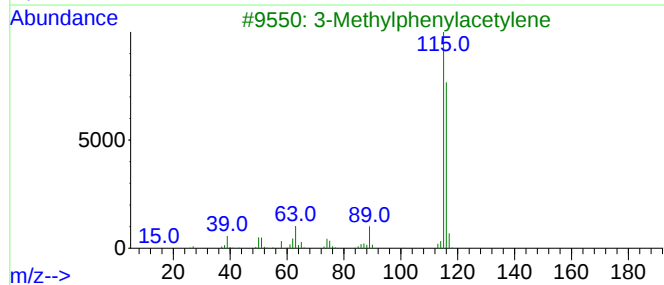
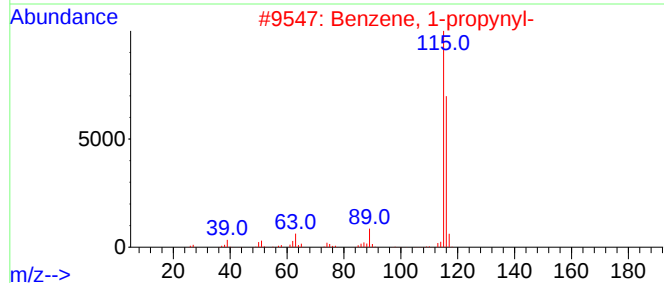
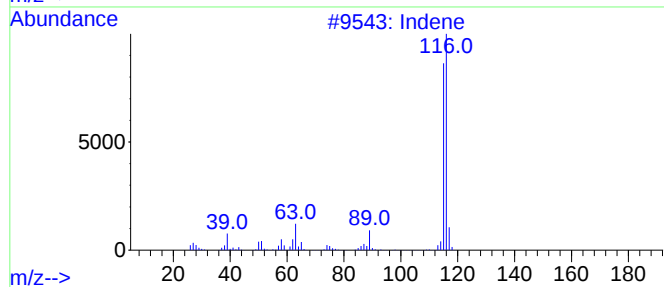
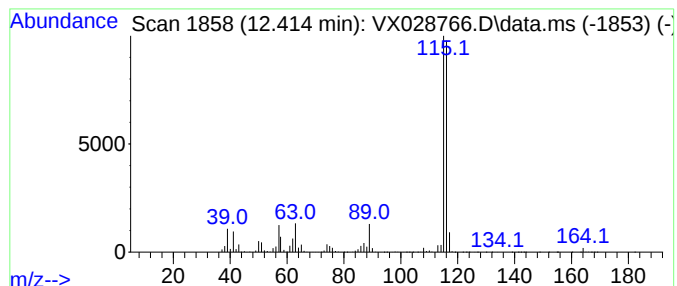
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Quant Title : SW846 8260

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

Peak Number 10 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	73.63 ug/l	2682570	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	95
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	94
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028766.D
Acq On : 17 May 2022 18:29
Operator : JC/MD
Sample : N2884-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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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
Propanal	2.294	12.6	ug/l	253302	1	5.555	1004080	50.0
Isopropyl Alcohol	2.532	43.1	ug/l	865883	1	5.555	1004080	50.0
2-Propanethiol,...	3.696	320.4	ug/l	6434660	1	5.555	1004080	50.0
1-Butanol	7.208	9.9	ug/l	269032	2	6.763	1352680	50.0
Diisopropyl sul...	9.067	8.8	ug/l	345535	3	10.055	1962970	50.0
Thiophene, tetr...	9.488	54.2	ug/l	2128400	3	10.055	1962970	50.0
Cyclopentanone,...	10.414	8.7	ug/l	342059	3	10.055	1962970	50.0
Benzene, 1-ethy...	11.378	9.8	ug/l	355739	4	12.024	1821540	50.0
Indane	12.243	8.3	ug/l	301379	4	12.024	1821540	50.0
Indene	12.414	73.6	ug/l	2682570	4	12.024	1821540	50.0