

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050222\
 Data File : VX028487.D
 Acq On : 02 May 2022 20:42
 Operator : JC/MD
 Sample : N2642-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 30989

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\82X041922W.M
 Title : SW846 8260

Signal : TIC: VX028487.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	70	rBV	1547511	1954629	80.76%	6.914%
2	1.569	72	79	83	rVB9	21200	58620	2.42%	0.207%
3	2.056	152	159	169	rBV	306480	471171	19.47%	1.667%
4	2.380	205	212	223	rBV	1206993	1985591	82.04%	7.023%
5	2.532	228	237	252	rBV	845928	1541774	63.70%	5.453%
6	2.953	297	306	316	rVB3	20822	54376	2.25%	0.192%
7	4.233	507	516	529	rBV2	24407	71731	2.96%	0.254%
8	4.556	558	569	585	rBV	272530	754671	31.18%	2.669%
9	5.007	631	643	668	rBV	340632	1065280	44.02%	3.768%
10	5.391	693	706	720	rBV	283452	824815	34.08%	2.917%
11	5.556	721	733	752	rVB	394935	1107658	45.77%	3.918%
12	5.830	770	778	789	rBV2	39369	109042	4.51%	0.386%
13	5.958	789	799	810	rBV	280860	744918	30.78%	2.635%
14	6.647	900	912	919	rBV2	9735	26889	1.11%	0.095%
15	6.763	921	931	945	rVV	616549	1478401	61.09%	5.229%
16	7.104	980	987	996	rBV2	15839	37301	1.54%	0.132%
17	7.214	996	1005	1018	rBV	141672	323032	13.35%	1.143%
18	7.464	1039	1046	1055	rVB2	24680	52646	2.18%	0.186%
19	8.574	1222	1228	1235	rBV	248447	404530	16.71%	1.431%
20	8.653	1235	1241	1247	rVV	1547832	2420208	100.00%	8.561%
21	8.720	1247	1252	1264	rVB	977667	1473661	60.89%	5.212%
22	9.195	1323	1330	1334	rBV	31635	48292	2.00%	0.171%
23	9.433	1365	1369	1376	rBV2	21030	33025	1.36%	0.117%
24	10.055	1463	1471	1485	rBV	1451864	1939801	80.15%	6.861%
25	10.195	1489	1494	1499	rBV	28841	42629	1.76%	0.151%
26	10.299	1506	1511	1520	rVB	125466	182186	7.53%	0.644%
27	10.646	1562	1568	1572	rBV	144241	205316	8.48%	0.726%
28	10.683	1572	1574	1581	rVB	22876	27363	1.13%	0.097%
29	10.774	1585	1589	1598	rVV	36480	50803	2.10%	0.180%
30	11.085	1634	1640	1652	rVB	1402378	1816754	75.07%	6.426%
31	11.384	1684	1689	1691	rBV	36523	48921	2.02%	0.173%
32	11.482	1702	1705	1714	rVB	46715	69386	2.87%	0.245%
33	11.573	1715	1720	1724	rBV	336028	411426	17.00%	1.455%
34	11.634	1724	1730	1741	rVB2	207261	325846	13.46%	1.153%
35	11.756	1745	1750	1758	rVB	163821	209635	8.66%	0.742%
36	11.835	1758	1763	1767	rBV3	62738	108586	4.49%	0.384%

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37	11.975	1782	1786	1789	rBV	22744	26338	1.09%	0.093%
38	12.024	1789	1794	1800	rVV	1670014	2029199	83.84%	7.177%
39	12.091	1800	1805	1809	rVB	128786	159928	6.61%	0.566%
40	12.219	1821	1826	1839	rBV	565612	852056	35.21%	3.014%
41	12.323	1839	1843	1854	rVB6	29591	63448	2.62%	0.224%
42	12.420	1854	1859	1862	rBV3	23455	37362	1.54%	0.132%
43	12.463	1862	1866	1872	rVB2	21431	34293	1.42%	0.121%
44	12.530	1872	1877	1879	rBV2	23692	38042	1.57%	0.135%
45	12.719	1901	1908	1913	rBV	431352	567788	23.46%	2.008%
46	12.798	1917	1921	1927	rVV	276110	380474	15.72%	1.346%
47	12.847	1927	1929	1934	rVB3	24658	29171	1.21%	0.103%
48	12.920	1937	1941	1943	rBV	28183	35412	1.46%	0.125%
49	12.957	1943	1947	1954	rVB2	638330	797673	32.96%	2.821%
50	13.164	1977	1981	1987	rBV2	28815	40416	1.67%	0.143%
51	13.292	1991	2002	2007	rBV2	82223	132614	5.48%	0.469%
52	13.426	2019	2024	2029	rBV	45650	60670	2.51%	0.215%
53	13.603	2046	2053	2057	rBV6	13119	33084	1.37%	0.117%
54	13.780	2075	2082	2088	rBV	229048	307911	12.72%	1.089%
55	14.640	2215	2223	2227	rBV	64289	83751	3.46%	0.296%
56	14.780	2239	2246	2251	rBV	60741	81185	3.35%	0.287%

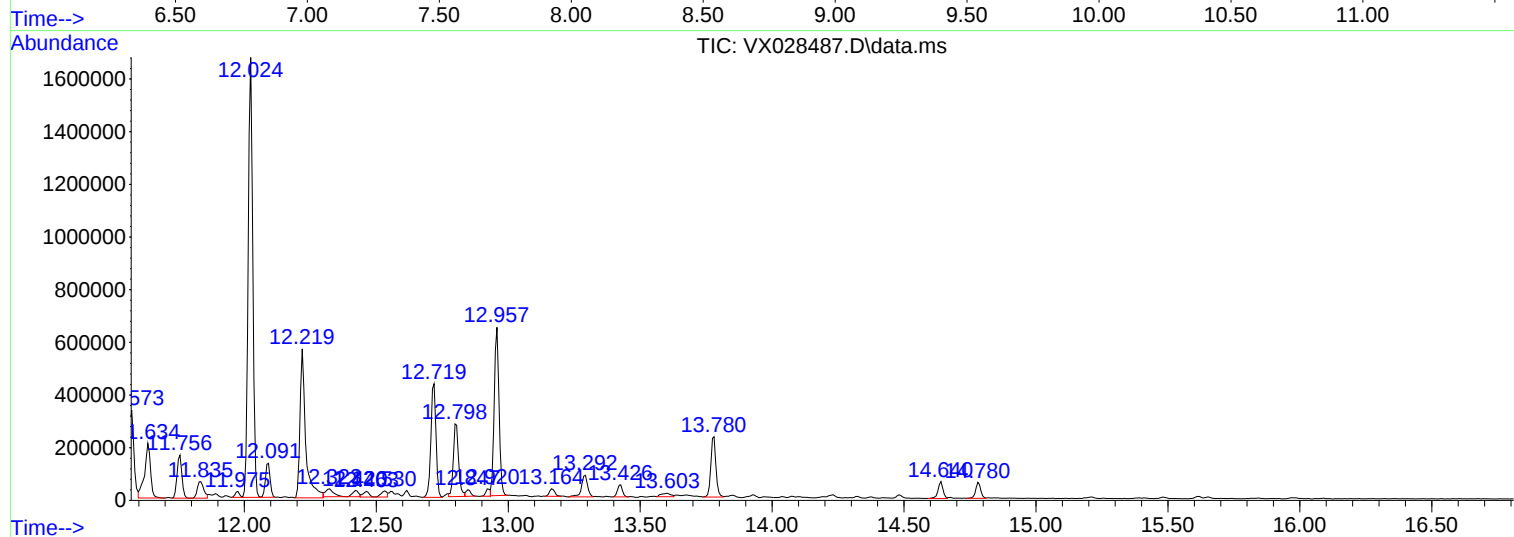
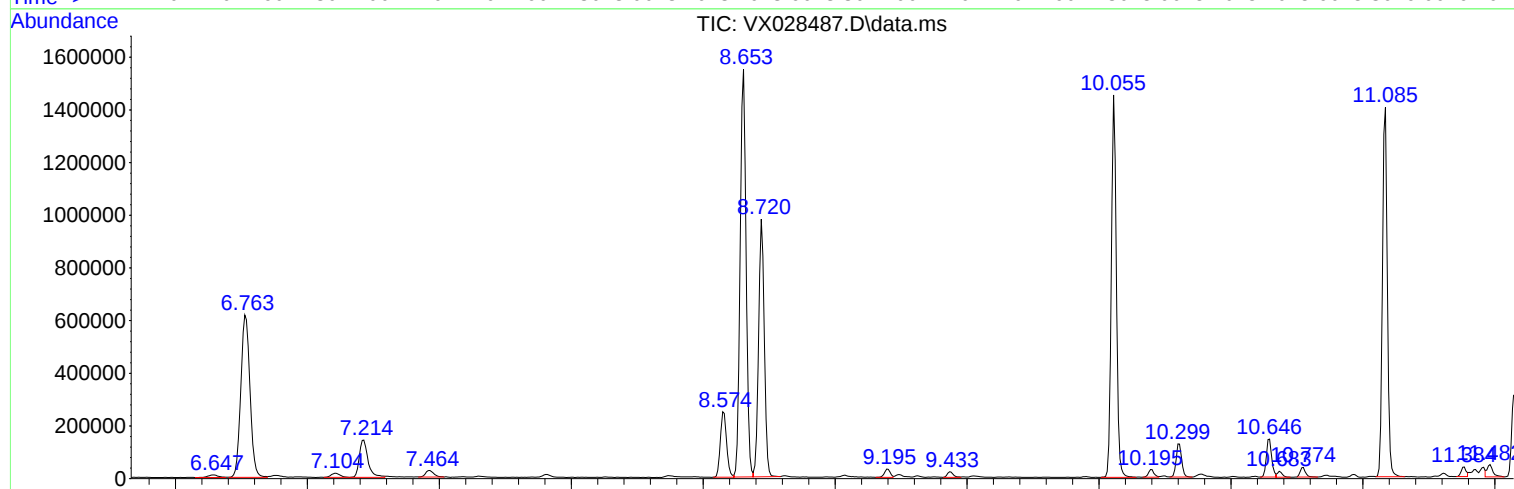
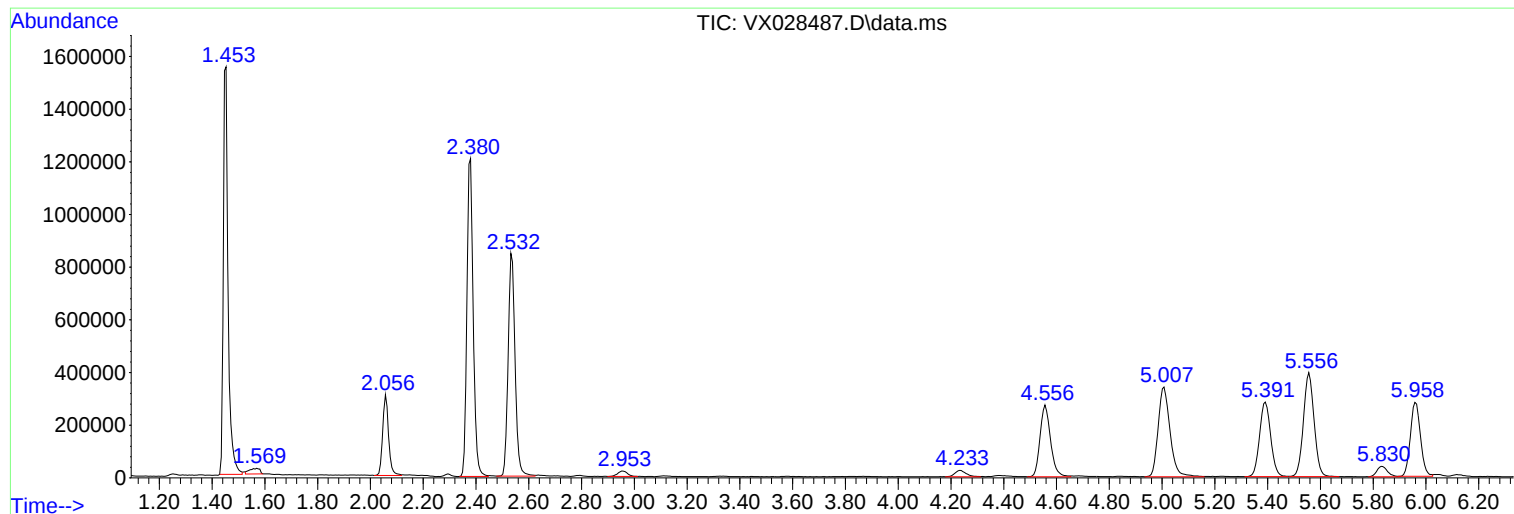
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TIC Library : C:\Database\NIST20.L
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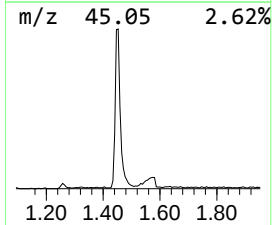
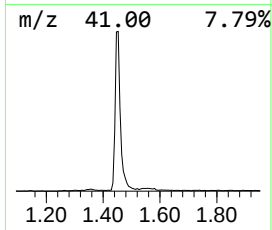
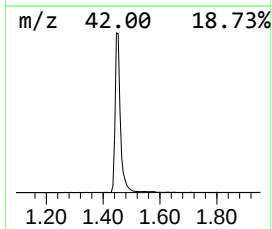
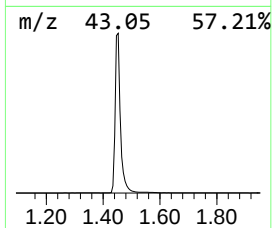
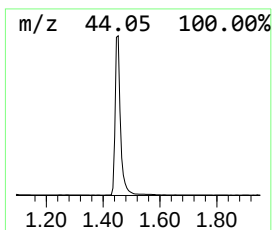
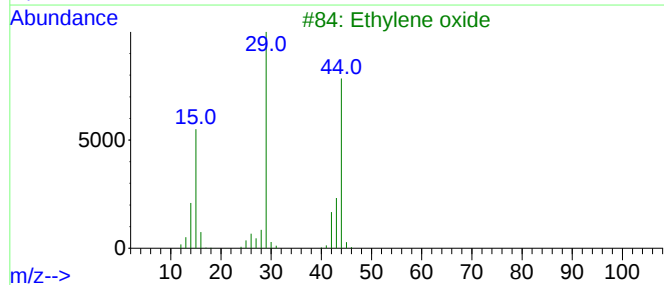
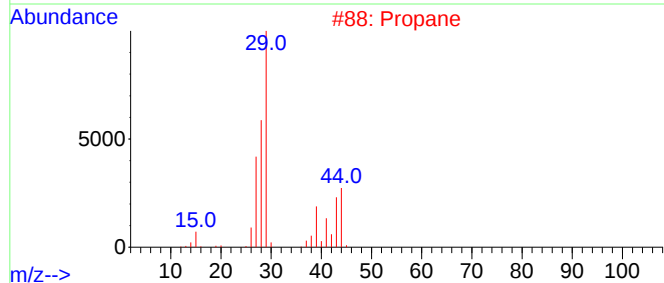
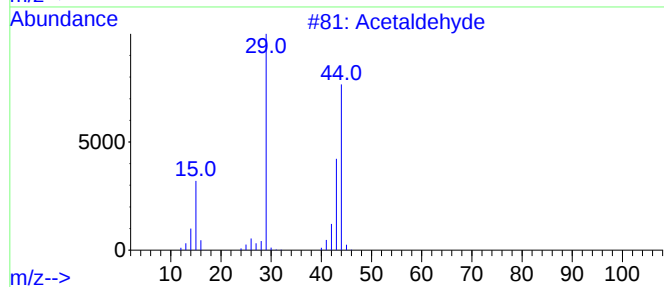
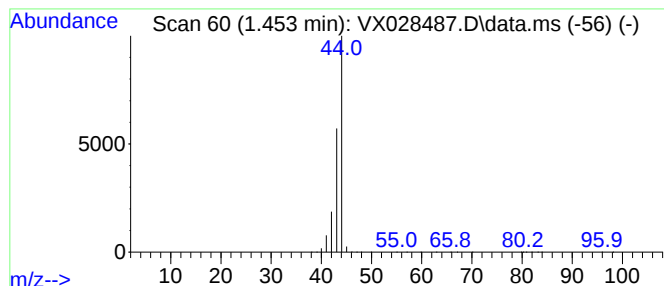
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	88.23 ug/l	1954630	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			Carbon dioxide	44	CO2	000124-38-9	3



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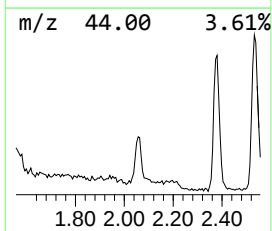
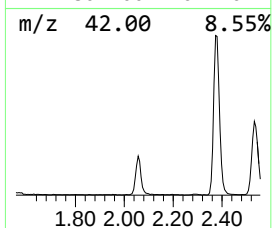
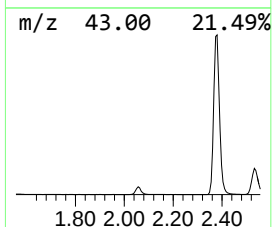
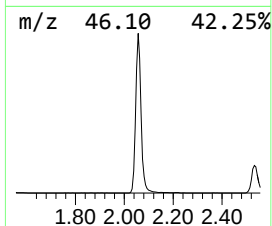
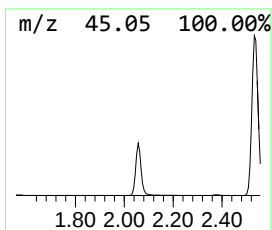
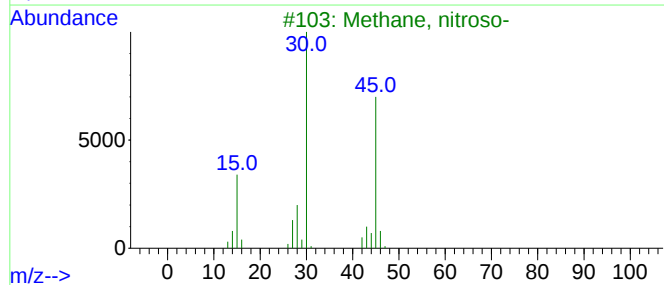
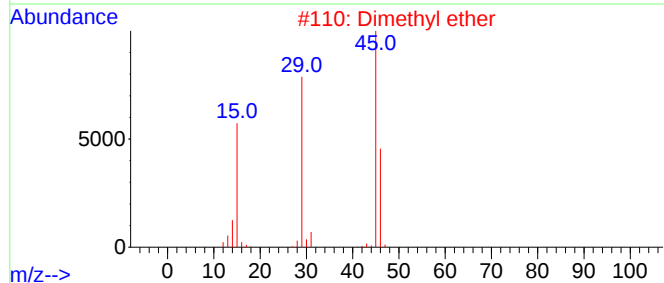
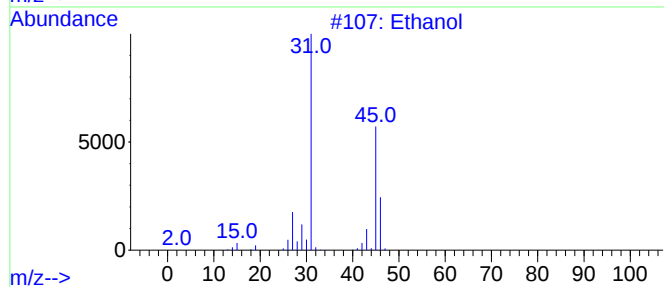
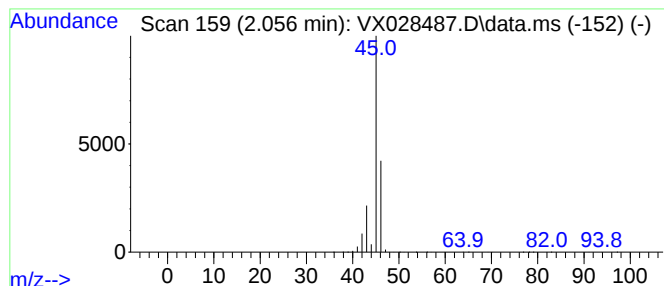
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.056	21.27 ug/l	471171	Pentafluorobenzene	5.556

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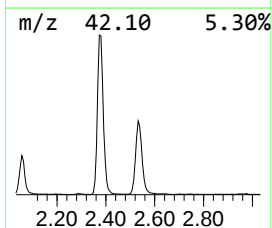
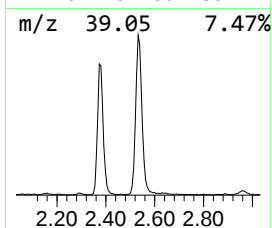
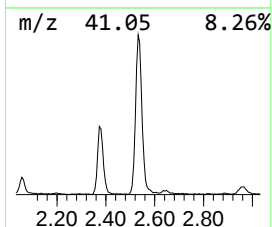
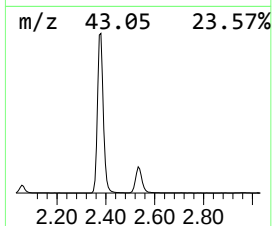
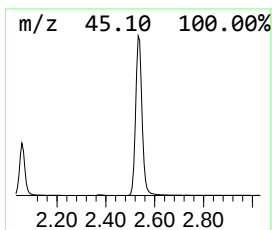
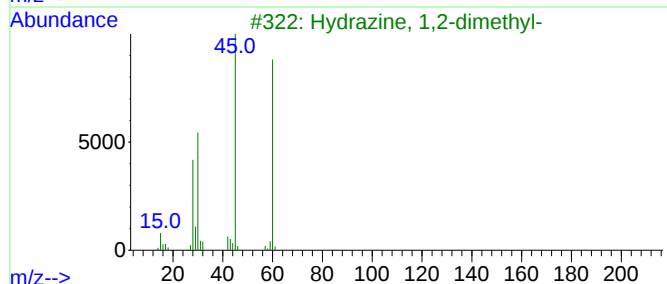
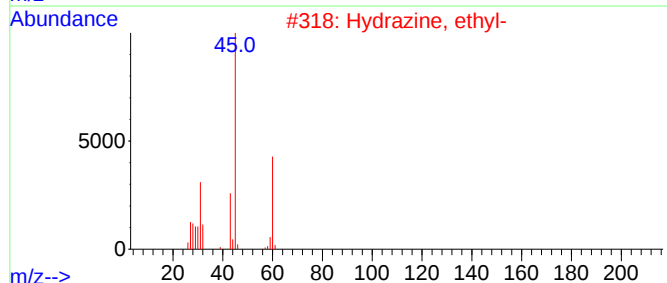
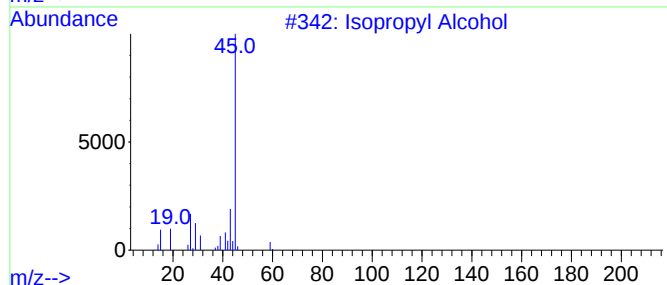
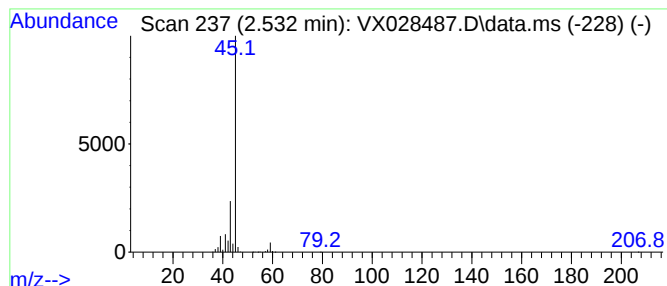
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.532	69.60 ug/l	1541770	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4
5			Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4



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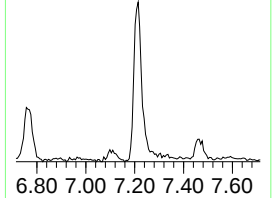
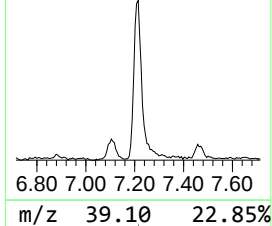
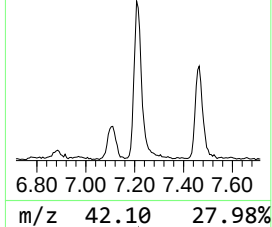
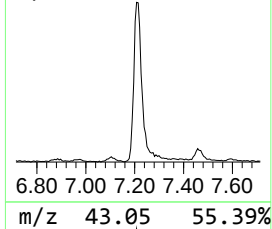
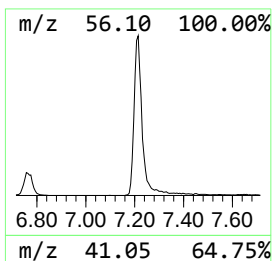
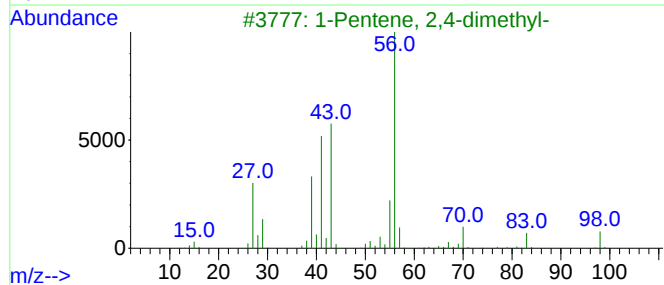
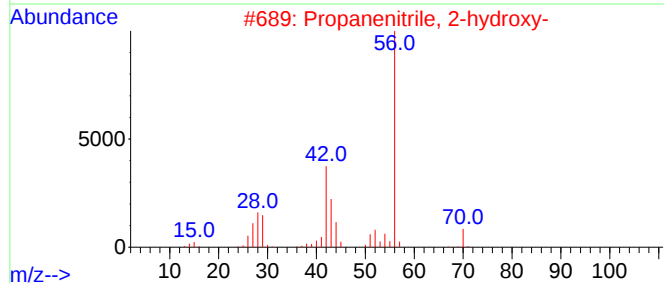
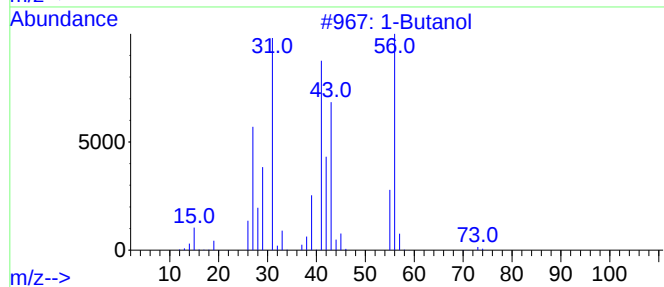
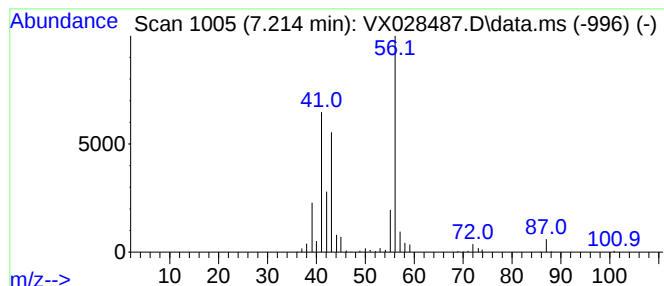
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	10.93 ug/l	323032	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol		74	C4H10O	000071-36-3	72
2	Propanenitrile, 2-hydroxy-		71	C3H5NO	000078-97-7	45
3	1-Pentene, 2,4-dimethyl-		98	C7H14	002213-32-3	42
4	3-Butenoic acid, 2-amino-		101	C4H7NO2	056512-51-7	42
5	2,3-Dimethylsuccinic acid		146	C6H10O4	013545-04-5	40



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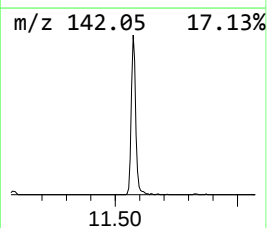
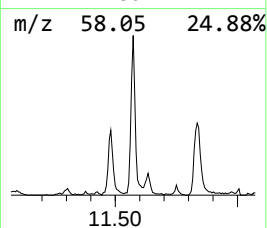
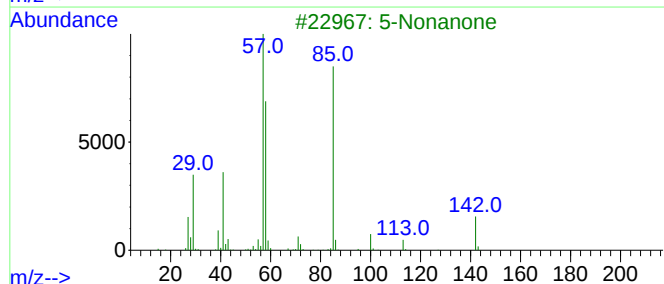
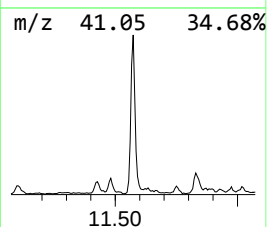
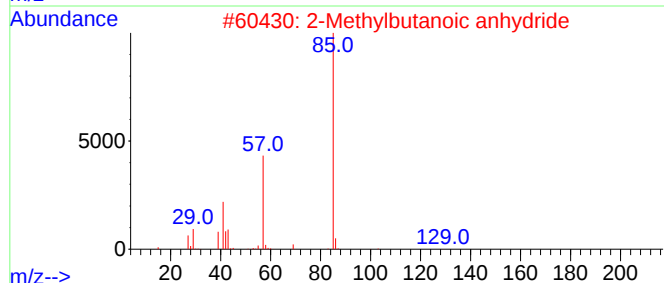
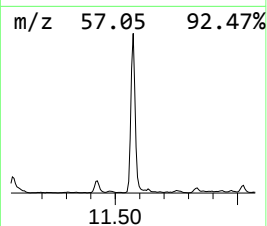
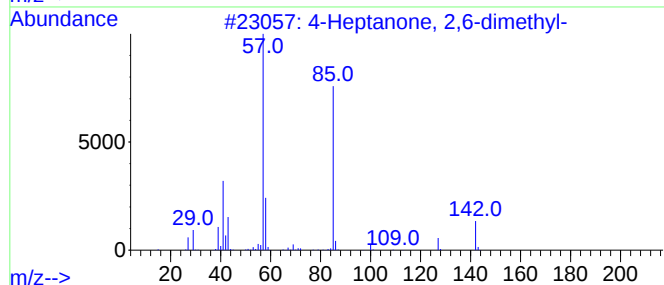
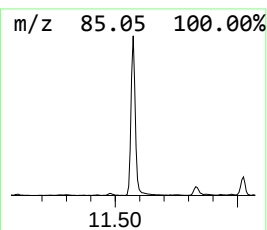
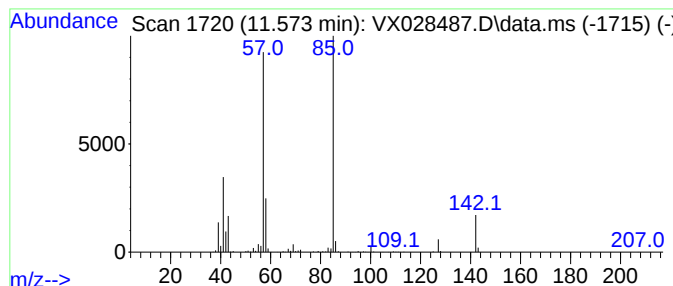
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Quant Title : SW846 8260

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

Peak Number 5 4-Heptanone, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.573	10.14 ug/l	411426	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2			2-Methylbutanoic anhydride	186	C10H18O3	001468-39-9	59
3			5-Nonanone	142	C9H18O	000502-56-7	59
4			4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	50
5			2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050222\
Data File : VX028487.D
Acq On : 02 May 2022 20:42
Operator : JC/MD
Sample : N2642-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30989

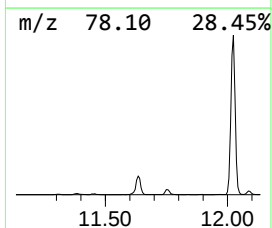
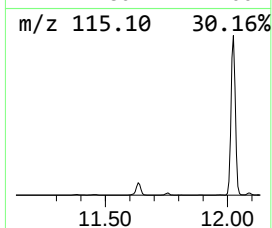
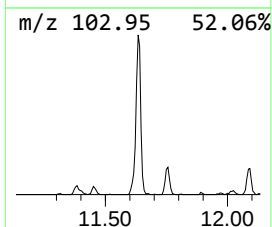
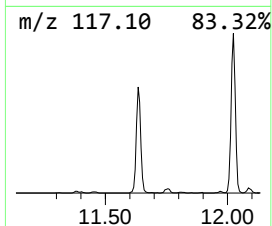
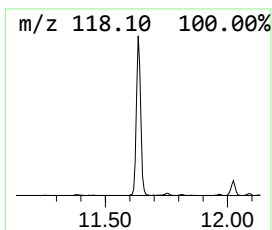
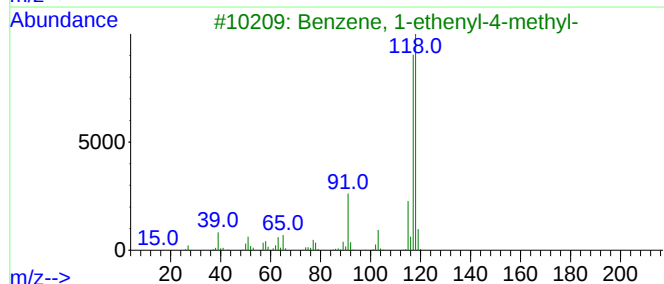
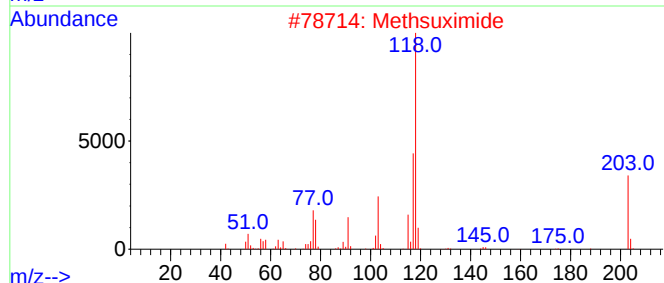
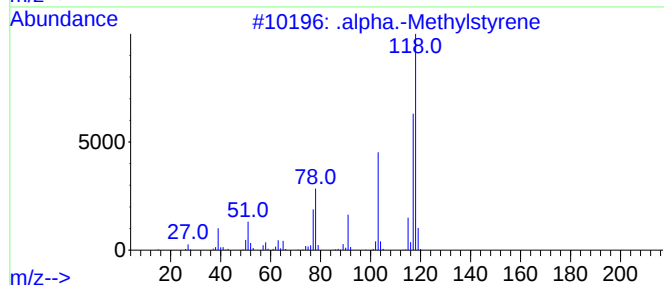
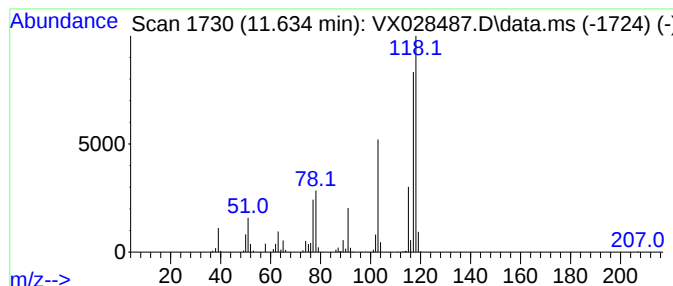
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Quant Title : SW846 8260

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

Peak Number 6 .alpha.-Methylstyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.634	8.03 ug/l	325846	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.alpha.-Methylstyrene	118	C9H10	000098-83-9	96
2		Methsuximide	203	C12H13NO2	000077-41-8	53
3		Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	52
4		Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	52
5		3-Phenylpropyl benzoate	240	C16H16O2	060045-26-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050222\
Data File : VX028487.D
Acq On : 02 May 2022 20:42
Operator : JC/MD
Sample : N2642-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30989

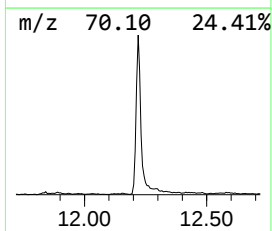
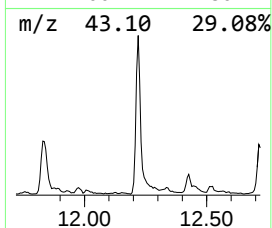
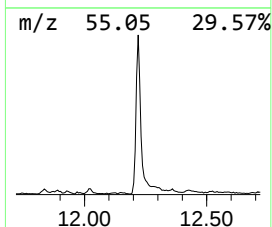
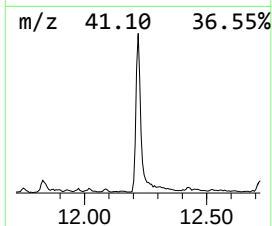
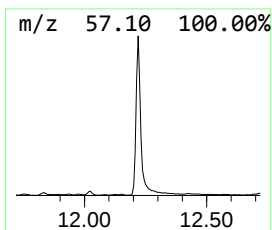
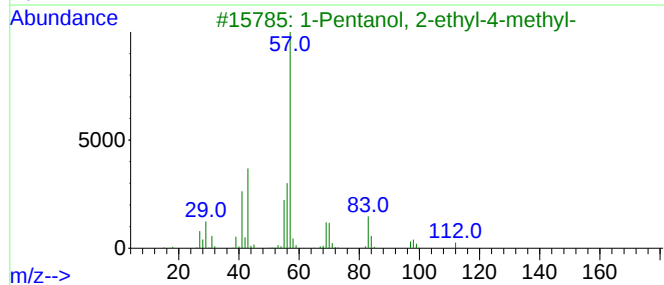
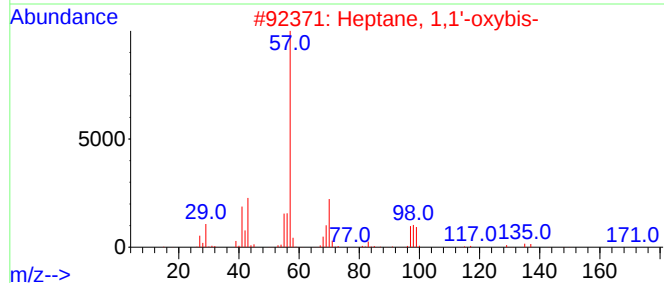
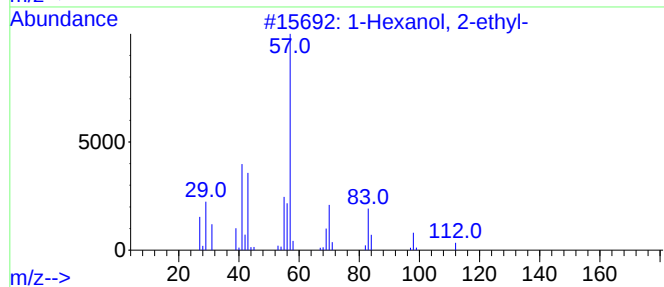
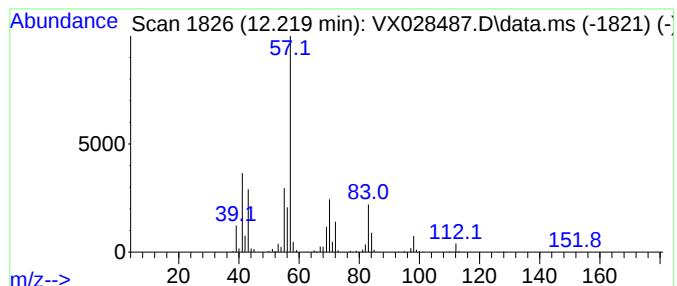
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Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	20.99 ug/l	852056	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050222\
Data File : VX028487.D
Acq On : 02 May 2022 20:42
Operator : JC/MD
Sample : N2642-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30989

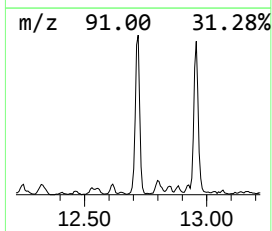
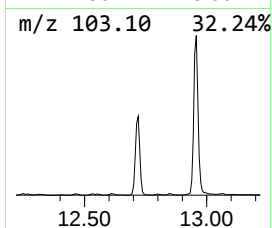
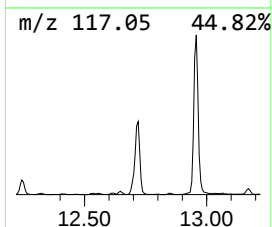
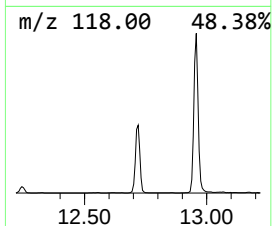
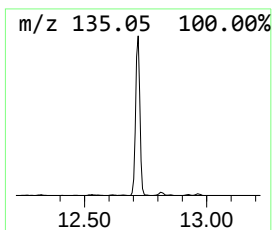
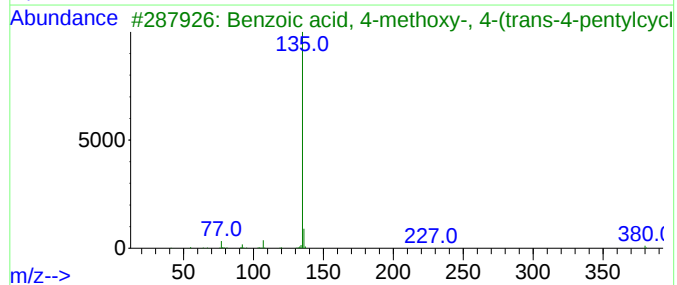
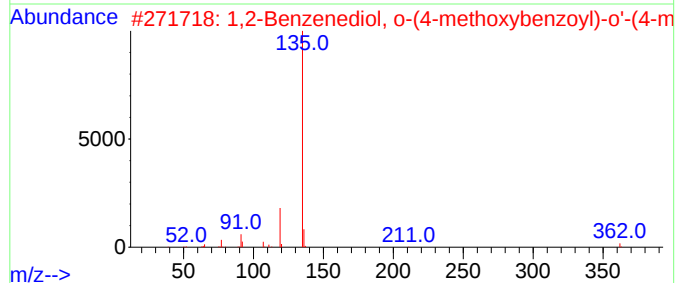
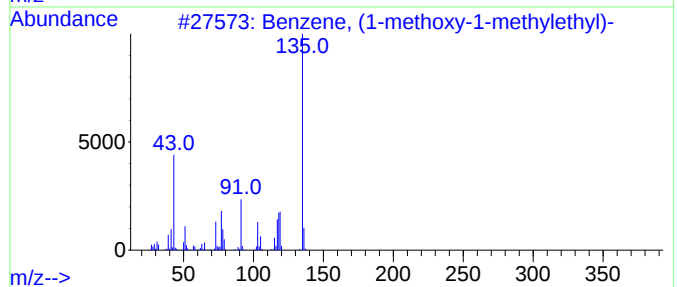
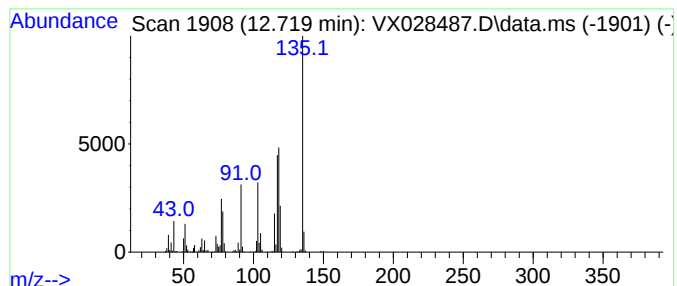
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, (1-methoxy-1-methy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.719	13.99 ug/l	567788	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methoxy-1-methylethyl)-	150	C10H14O	000935-67-1	50
2			1,2-Benzenediol, o-(4-methoxyben...	362	C22H18O5	1000325-99-0	35
3			Benzoic acid, 4-methoxy-, 4-(tra...	380	C25H32O3	1229648-08-1	35
4			Formamide, N-methyl-N-phenyl-	135	C8H9NO	000093-61-8	35
5			Ethanedione, (4-methoxyphenyl)ph...	240	C15H12O3	022711-21-3	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050222\
Data File : VX028487.D
Acq On : 02 May 2022 20:42
Operator : JC/MD
Sample : N2642-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30989

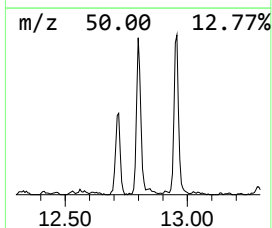
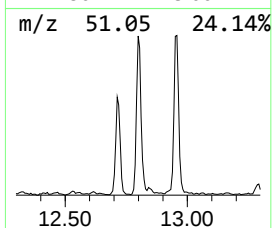
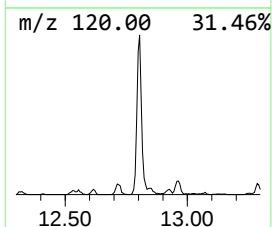
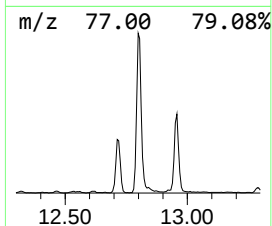
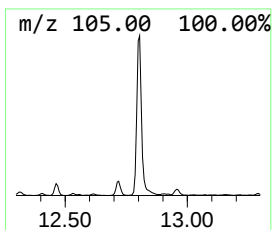
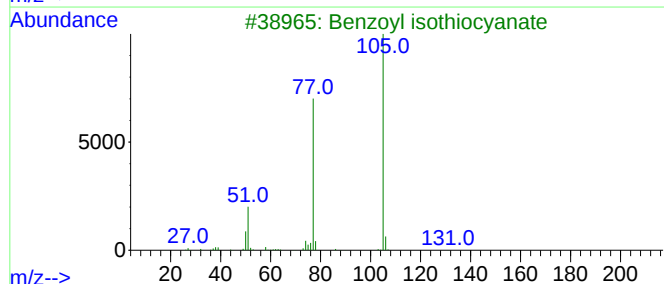
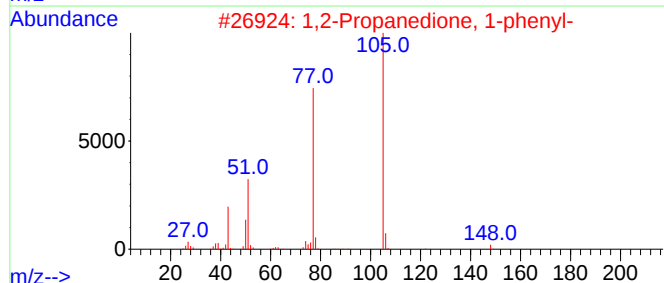
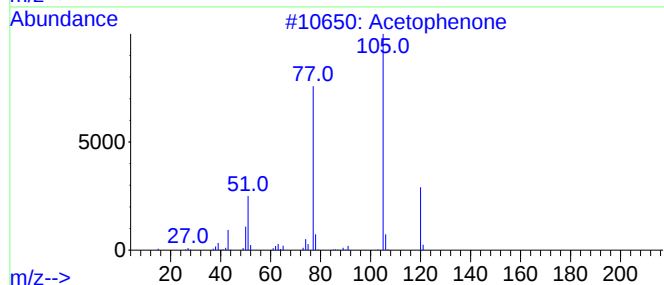
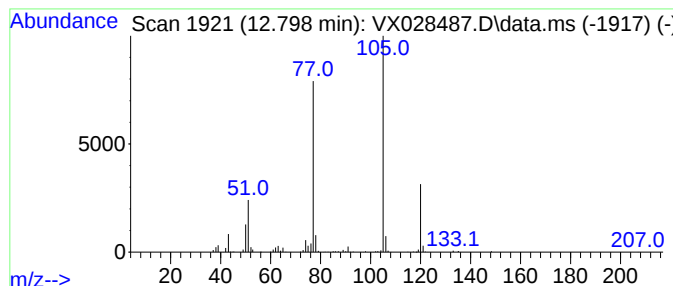
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 9 Acetophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.798	9.37 ug/l	380474	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetophenone	120	C8H8O	000098-86-2	97
2			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	72
3			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	72
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	72
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050222\
Data File : VX028487.D
Acq On : 02 May 2022 20:42
Operator : JC/MD
Sample : N2642-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30989

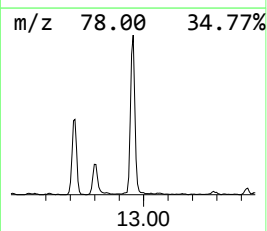
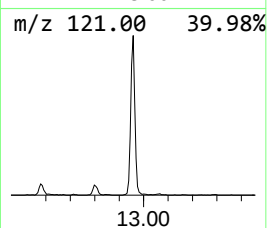
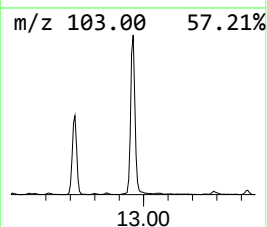
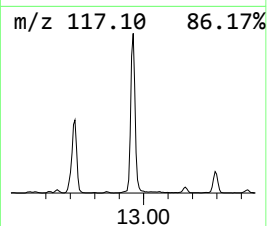
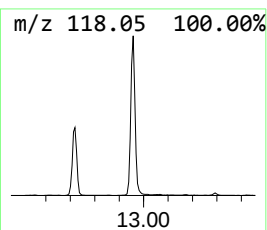
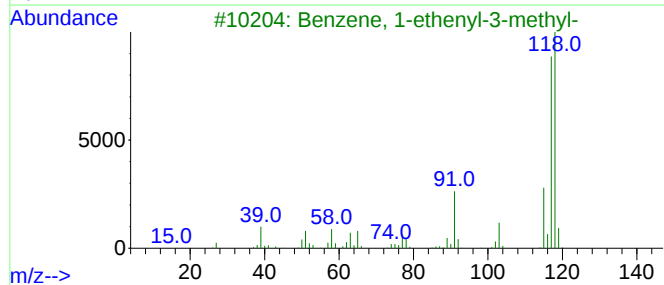
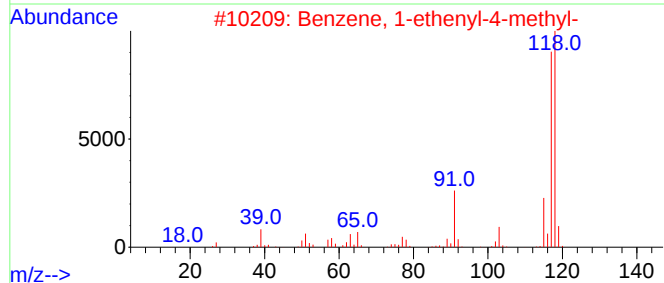
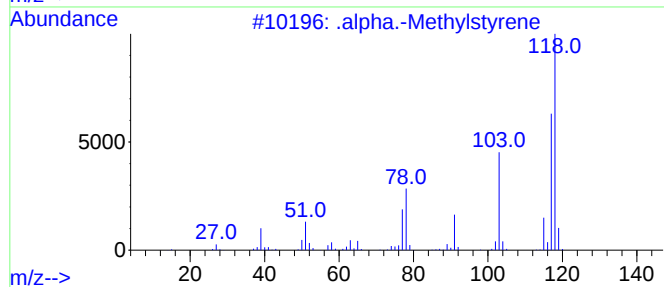
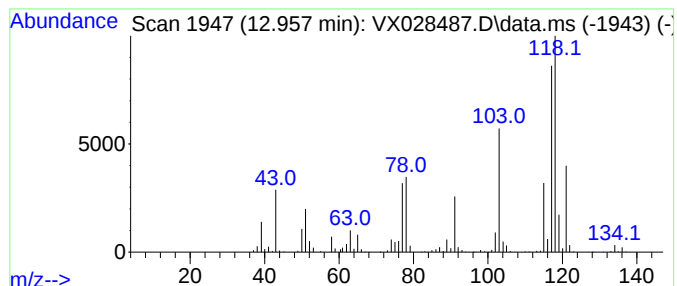
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethenyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.957	19.65 ug/l	797673	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-Methylstyrene	118	C9H10	000098-83-9	93
2			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	49
3			Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	49
4			Butanoic acid, 3-phenylpropyl ester	206	C13H18O2	007402-29-1	43
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050222\
Data File : VX028487.D
Acq On : 02 May 2022 20:42
Operator : JC/MD
Sample : N2642-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30989

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.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	88.2	ug/l	1954630	1	5.556	1107660	50.0
Ethanol	2.056	21.3	ug/l	471171	1	5.556	1107660	50.0
Isopropyl Alcohol	2.532	69.6	ug/l	1541770	1	5.556	1107660	50.0
1-Butanol	7.214	10.9	ug/l	323032	2	6.763	1478400	50.0
4-Heptanone, 2,...	11.573	10.1	ug/l	411426	4	12.024	2029200	50.0
.alpha.-Methyls...	11.634	8.0	ug/l	325846	4	12.024	2029200	50.0
1-Hexanol, 2-et...	12.219	21.0	ug/l	852056	4	12.024	2029200	50.0
Benzene, (1-met...	12.719	14.0	ug/l	567788	4	12.024	2029200	50.0
Acetophenone	12.798	9.4	ug/l	380474	4	12.024	2029200	50.0
Benzene, 1-ethe...	12.957	19.6	ug/l	797673	4	12.024	2029200	50.0