

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
 Data File : VX033247.D
 Acq On : 05 Dec 2022 23:31
 Operator : JC/MD
 Sample : N5859-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ORA-0584

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\82X112222W.M
 Title : SW846 8260

Signal : TIC: VX033247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	18	rVB2	46729	50018	3.58%	0.741%
2	1.374	41	47	52	rVB2	10894	15485	1.11%	0.230%
3	1.459	56	61	66	rBV	36192	47016	3.37%	0.697%
4	2.294	191	198	208	rBV	870381	1396703	100.00%	20.703%
5	2.392	208	214	225	rVB	30079	72256	5.17%	1.071%
6	2.599	238	248	260	rBV2	6310	32126	2.30%	0.476%
7	2.703	261	265	273	rVB	9410	18597	1.33%	0.276%
8	2.983	298	311	326	rBV4	7086	36197	2.59%	0.537%
9	3.934	450	467	495	rBV3	11236	82784	5.93%	1.227%
10	4.227	506	515	530	rBV	118685	315680	22.60%	4.679%
11	4.562	561	570	589	rBB	22853	70297	5.03%	1.042%
12	5.391	695	706	719	rBV	58605	171714	12.29%	2.545%
13	5.550	721	732	748	rVB	125401	359180	25.72%	5.324%
14	5.958	789	799	806	rBV	60127	160769	11.51%	2.383%
15	6.037	806	812	823	rVB	49566	131813	9.44%	1.954%
16	6.763	921	931	945	rBV	188807	448037	32.08%	6.641%
17	7.251	1004	1011	1027	rBV4	4733	19729	1.41%	0.292%
18	7.580	1060	1065	1073	rVB2	8854	16782	1.20%	0.249%
19	8.647	1234	1240	1247	rBV	271572	423175	30.30%	6.273%
20	8.720	1247	1252	1258	rVV	96755	149485	10.70%	2.216%
21	10.055	1462	1471	1483	rBV	381677	518375	37.11%	7.684%
22	10.195	1491	1494	1499	rVB	11649	15155	1.09%	0.225%
23	10.299	1507	1511	1519	rVB	53770	74510	5.33%	1.104%
24	10.445	1530	1535	1541	rVB	37162	47725	3.42%	0.707%
25	10.640	1561	1567	1573	rBV2	24995	40818	2.92%	0.605%
26	10.756	1581	1586	1595	rBV3	11476	23232	1.66%	0.344%
27	11.079	1634	1639	1645	rBV	252184	314652	22.53%	4.664%
28	11.152	1645	1651	1660	rVB2	35543	58548	4.19%	0.868%
29	11.378	1682	1688	1693	rBV	10278	18836	1.35%	0.279%
30	11.610	1723	1726	1734	rVB4	10348	20305	1.45%	0.301%
31	11.683	1734	1738	1745	rVB	17908	22175	1.59%	0.329%
32	11.750	1745	1749	1754	rBV	29075	38175	2.73%	0.566%
33	12.024	1789	1794	1801	rVV	392062	510835	36.57%	7.572%
34	12.085	1801	1804	1810	rVB	12566	16477	1.18%	0.244%
35	12.219	1821	1826	1837	rBV	365778	530701	38.00%	7.867%
36	12.311	1837	1841	1854	rVV6	18256	42719	3.06%	0.633%

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37	12.414	1854	1858	1863	rVV	12306	16625	1.19%	0.246%
38	12.798	1918	1921	1926	rVV2	10721	15864	1.14%	0.235%
39	13.286	1997	2001	2007	rVB2	9382	14661	1.05%	0.217%
40	13.774	2074	2081	2086	rBV	87038	139688	10.00%	2.071%
41	13.847	2086	2093	2100	rVV2	32702	55123	3.95%	0.817%
42	13.914	2100	2104	2111	rVB	36833	50784	3.64%	0.753%
43	14.640	2217	2223	2232	rVB	44972	66320	4.75%	0.983%
44	14.780	2240	2246	2251	rBV	30890	39041	2.80%	0.579%
45	15.969	2433	2441	2450	rBV4	17837	37122	2.66%	0.550%

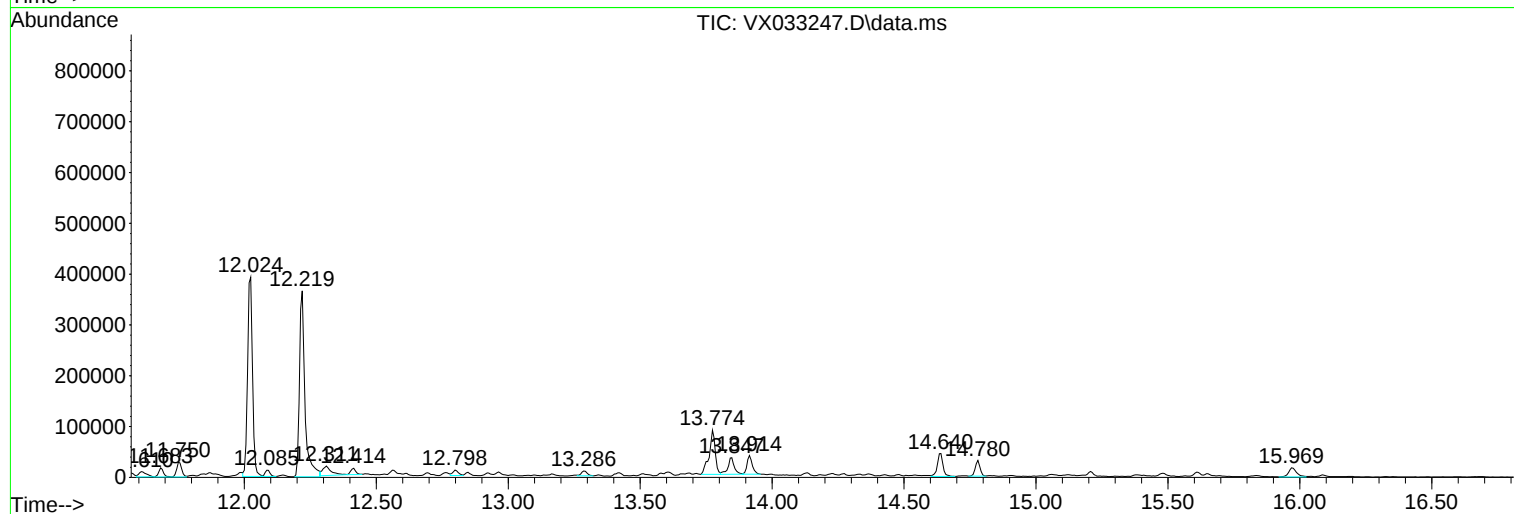
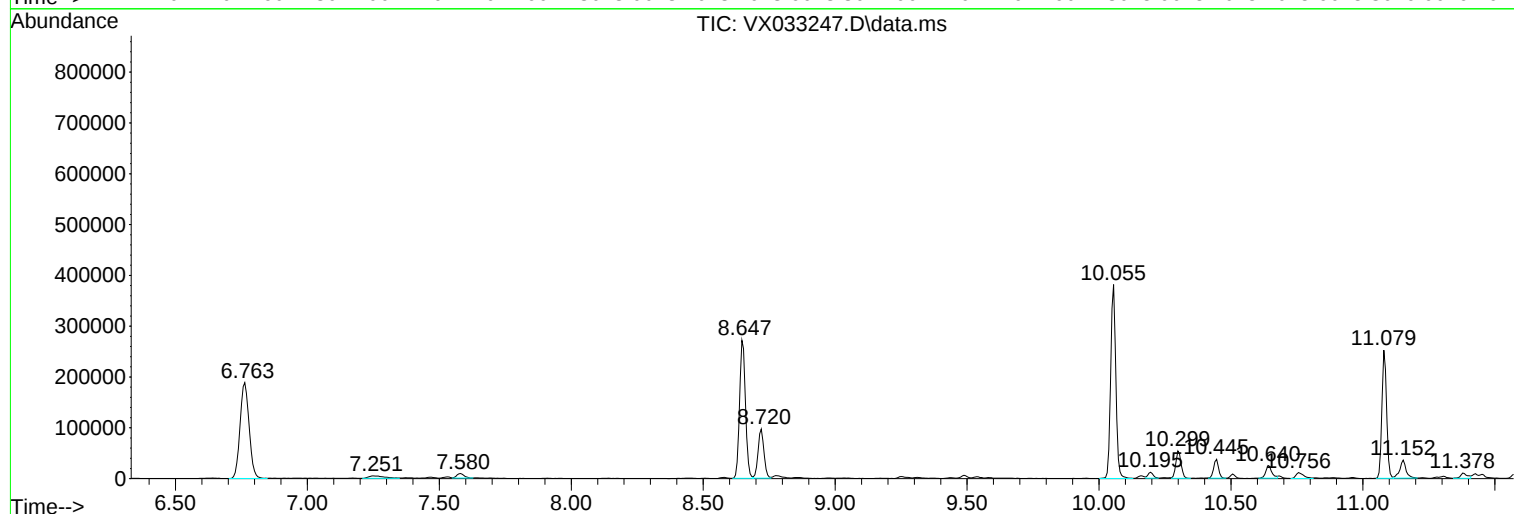
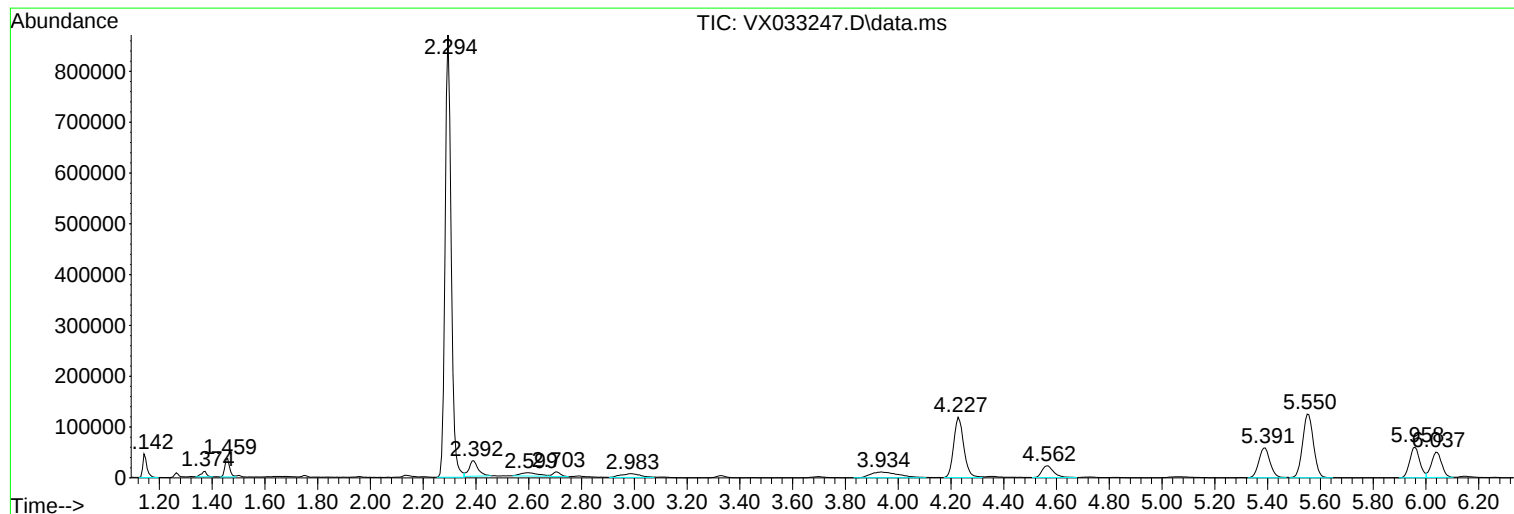
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



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ClientSampleId :
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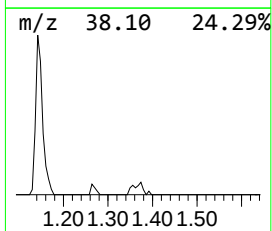
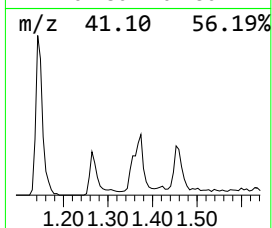
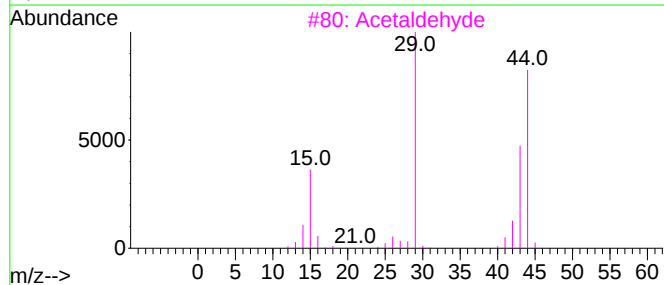
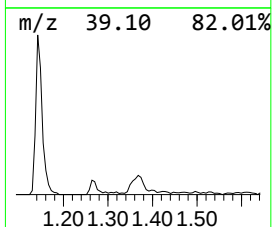
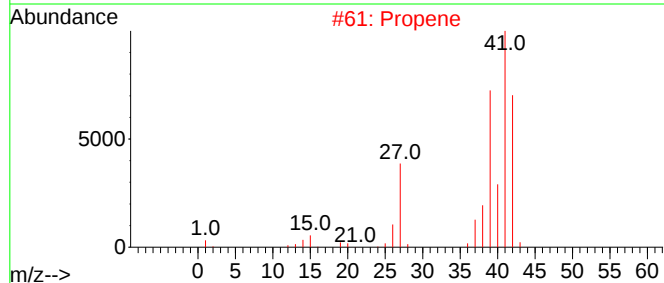
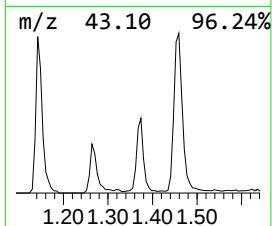
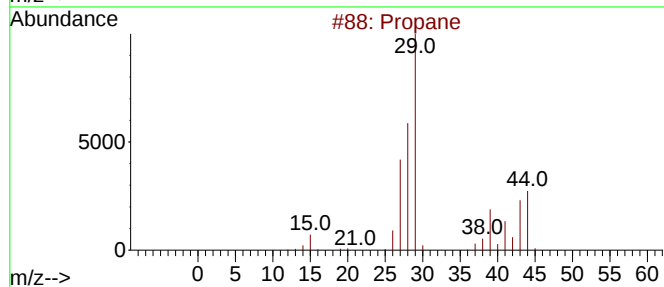
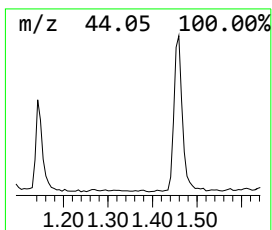
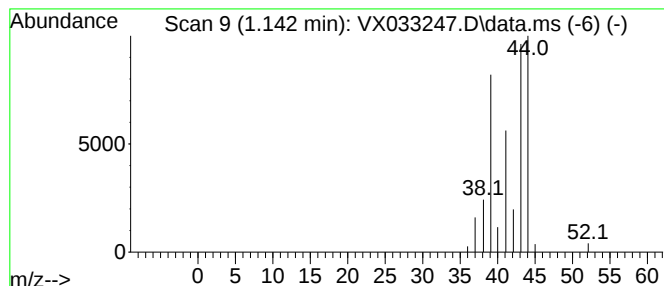
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	6.96 ug/l	50018	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	83
2			Propene	42	C3H6	000115-07-1	9
3			Acetaldehyde	44	C2H4O	000075-07-0	5
4			Cyclopropene	40	C3H4	002781-85-3	4
5			1-(Methylamino)propan-2-ol	89	C4H11NO	1000486-79-1	2



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Instrument :
MSVOA_X
ClientSampleId :
ORA-0584

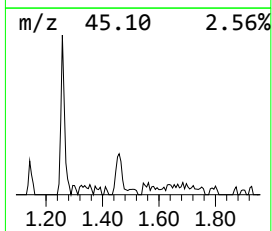
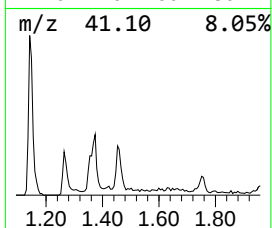
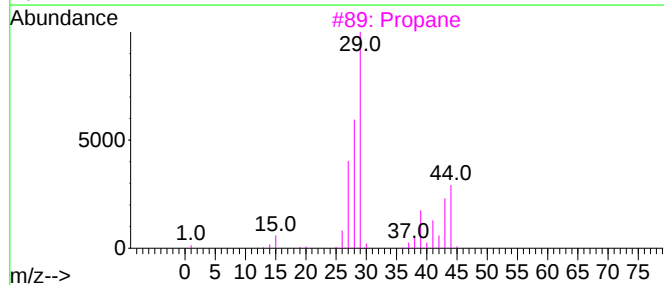
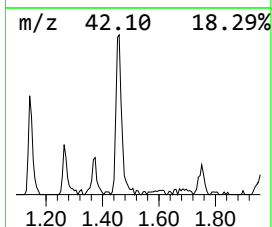
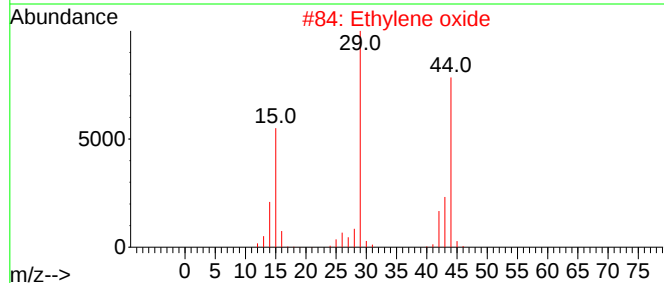
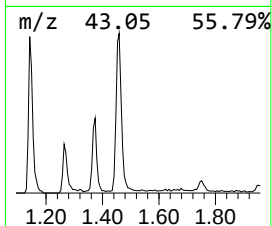
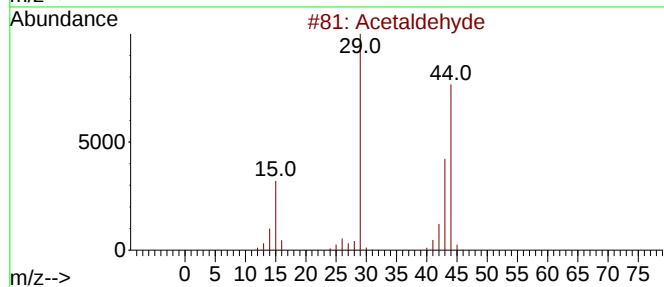
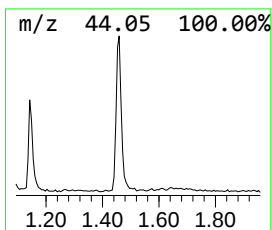
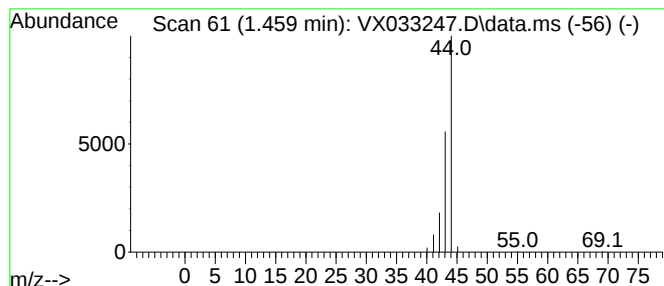
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.459	6.54 ug/l	47016	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			Acetic acid, [(aminocarbonyl)ami...	132	C3H4N2O4	000585-05-7	4
5			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_X
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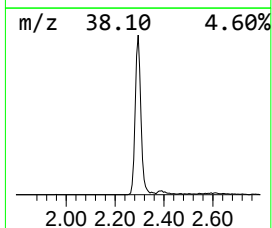
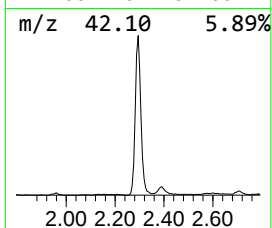
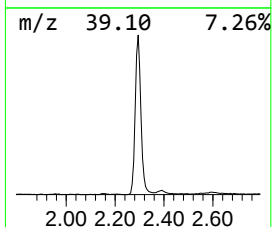
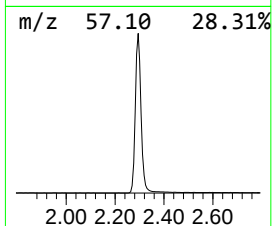
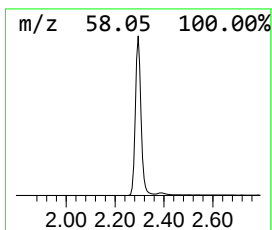
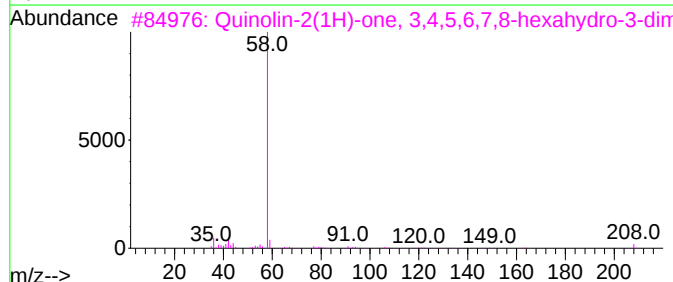
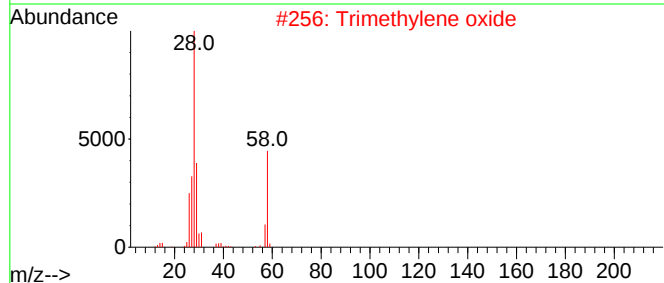
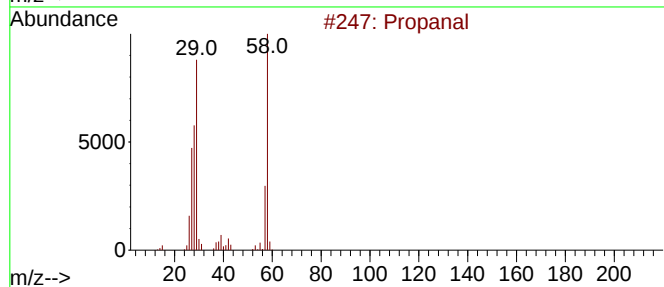
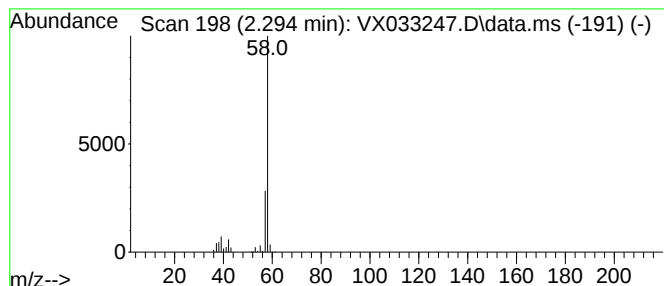
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	194.43 ug/l	1396700	Pentafluorobenzene	5.556

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	9
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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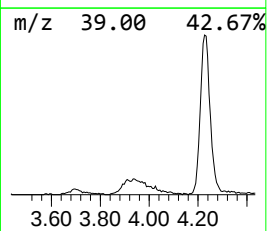
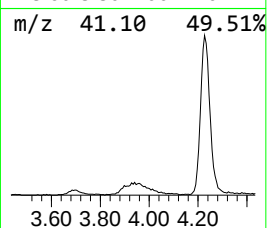
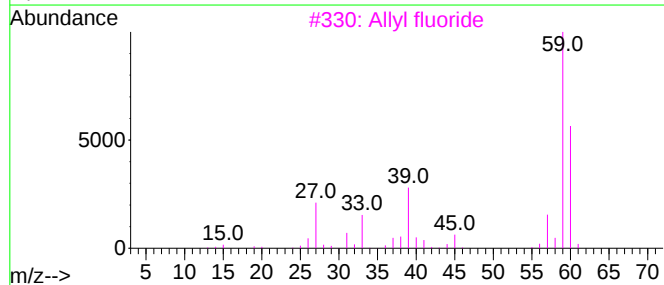
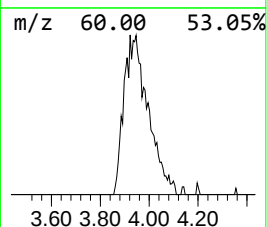
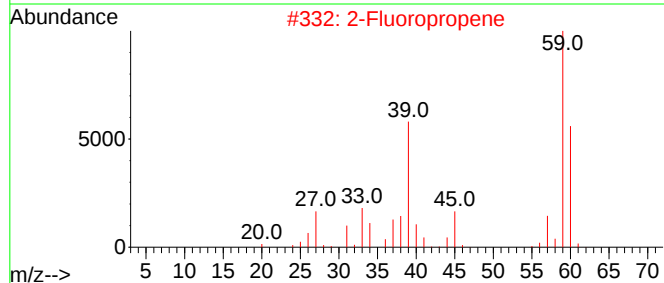
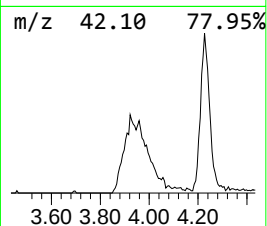
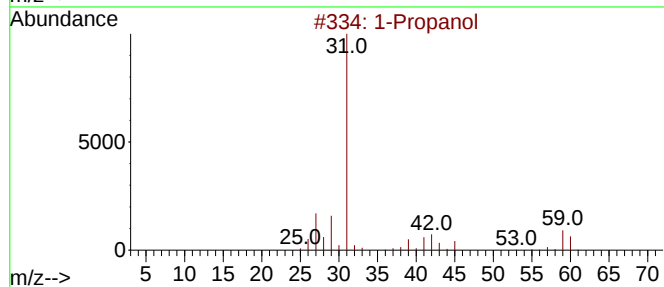
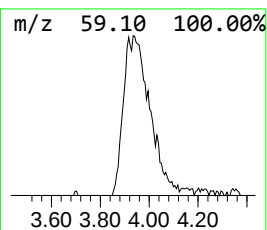
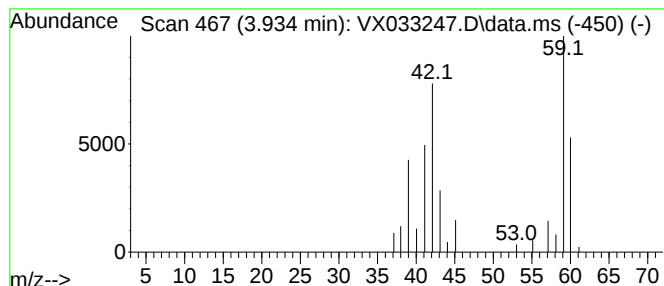
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Quant Title : SW846 8260

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

Peak Number 4 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.934	11.52 ug/l	82784	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	59
2	2-Fluoropropene			60	C3H5F	001184-60-7	58
3	Allyl fluoride			60	C3H5F	000818-92-8	38
4	Cyclopropane			42	C3H6	000075-19-4	35
5	Hydrazine, 1,1-dimethyl-			60	C2H8N2	000057-14-7	5



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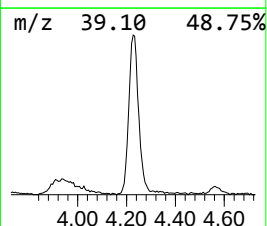
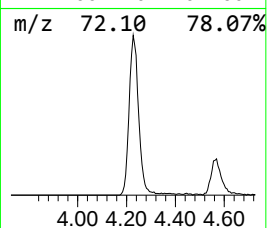
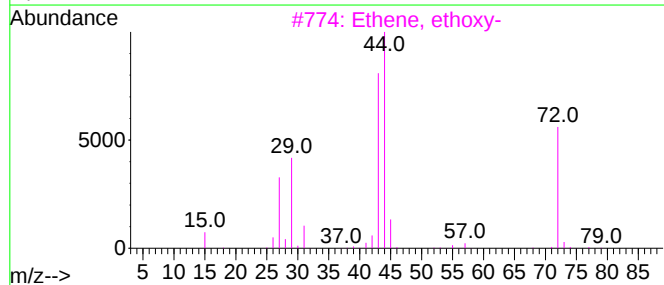
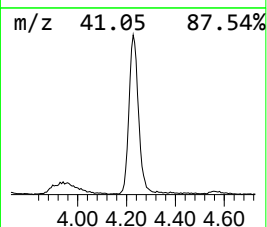
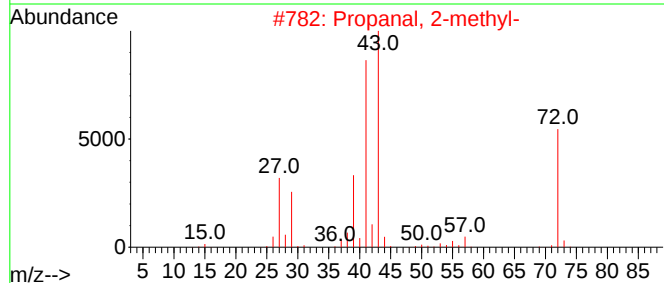
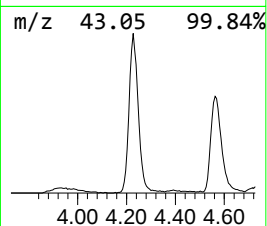
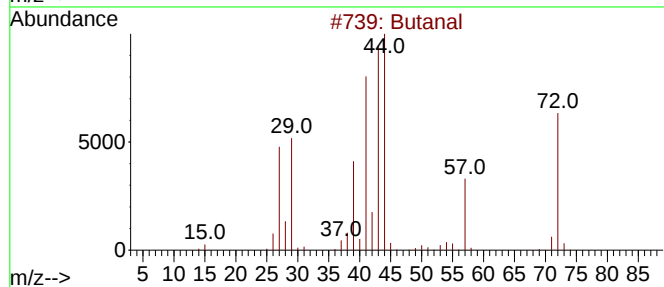
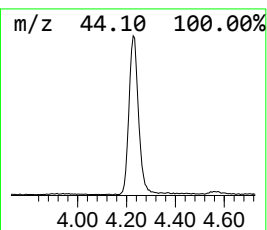
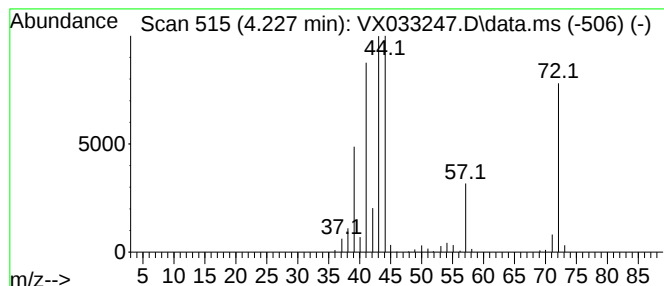
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Quant Title : SW846 8260

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

Peak Number 5 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	43.94 ug/l	315680	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	52
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	52
4			Propane	44	C3H8	000074-98-6	50
5			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033247.D
Acq On : 05 Dec 2022 23:31
Operator : JC/MD
Sample : N5859-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0584

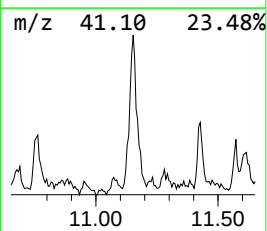
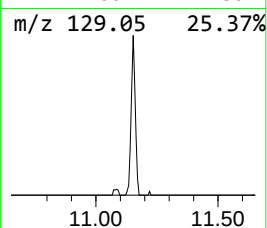
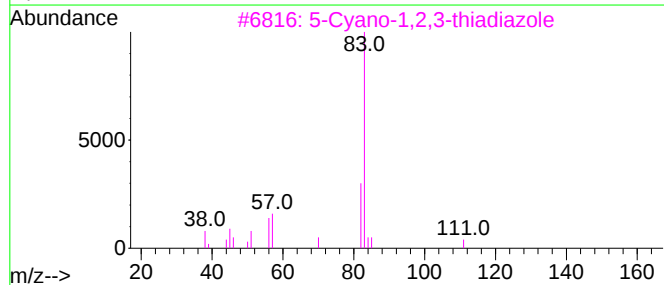
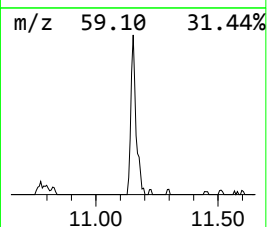
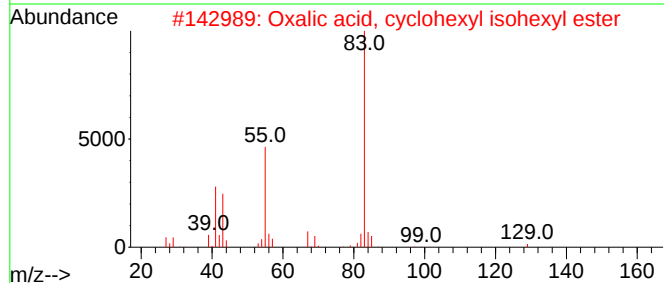
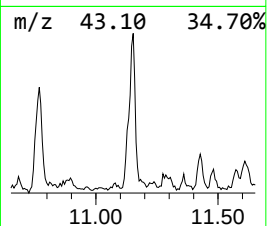
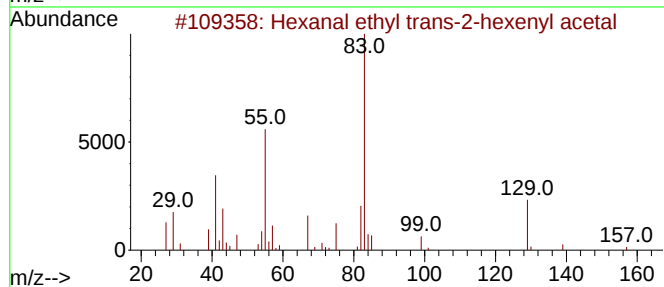
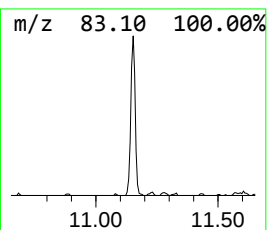
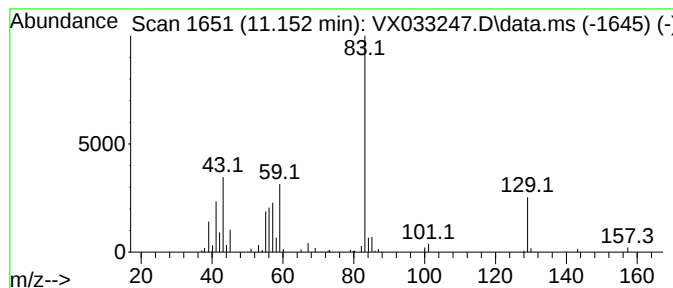
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Quant Title : SW846 8260

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

Peak Number 6 unknown11.152 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.152	5.73 ug/l	58548	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal ethyl trans-2-hexenyl ac...	228	C14H28O2	1000431-42-6	47
2			Oxalic acid, cyclohexyl isohexyl...	256	C14H24O4	1010309-30-7	43
3			5-Cyano-1,2,3-thiadiazole	111	C3HN3S	057352-02-0	40
4			1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	39
5			Oxalic acid, cyclohexyl hexyl ester	256	C14H24O4	1000309-30-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033247.D
Acq On : 05 Dec 2022 23:31
Operator : JC/MD
Sample : N5859-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 32 Sample Multiplier: 1

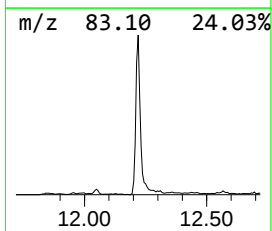
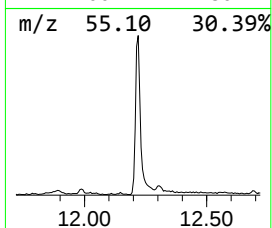
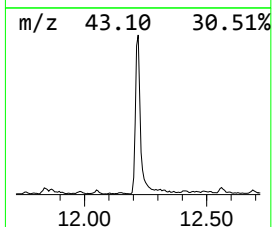
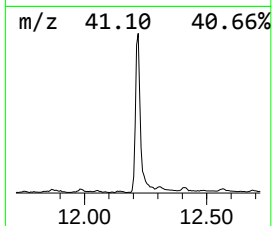
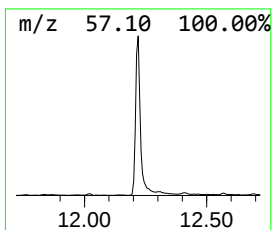
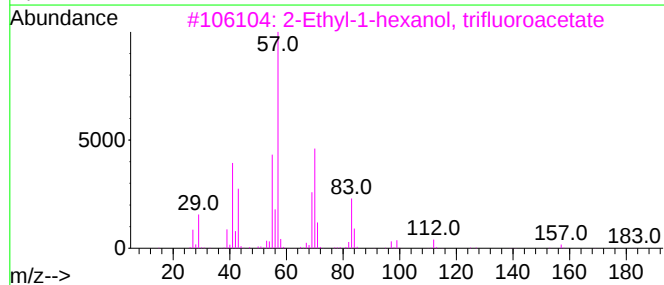
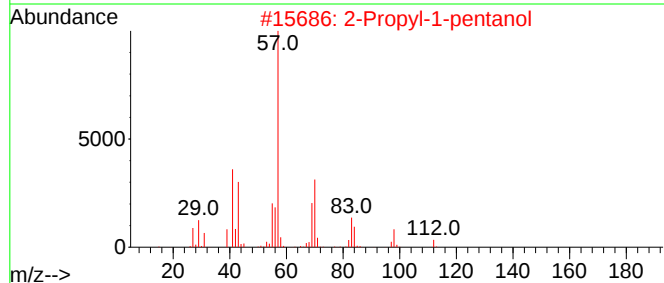
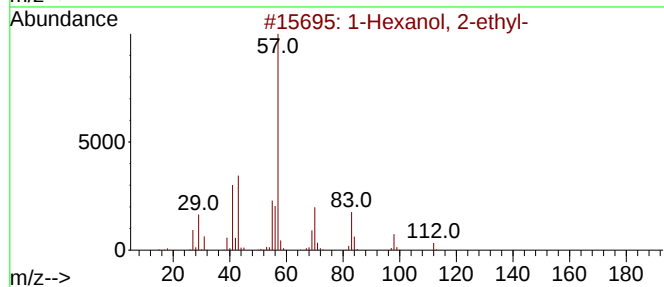
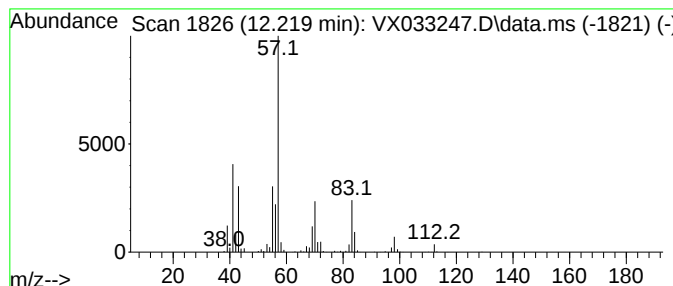
Instrument :
MSVOA_X
ClientSampleId :
ORA-0584

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.219	51.94 ug/l	530701	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	90
2	2-Propyl-1-pentanol		130	C8H18O	058175-57-8	50
3	2-Ethyl-1-hexanol, trifluoroacetate		226	C10H17F3O2	053800-08-1	47
4	2-Propyl-1-pentanol, chlorodiflu...		242	C10H17ClF2O2	1000447-27-3	47
5	Chloroacetic acid, 2-ethylhexyl ...		206	C10H19ClO2	005345-58-4	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033247.D
Acq On : 05 Dec 2022 23:31
Operator : JC/MD
Sample : N5859-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0584

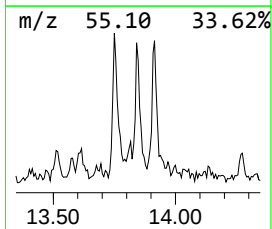
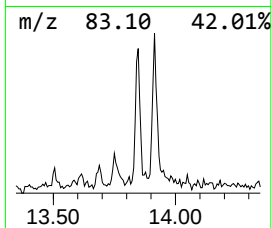
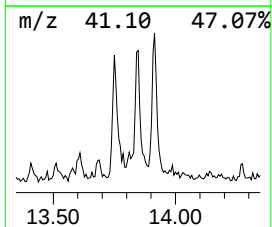
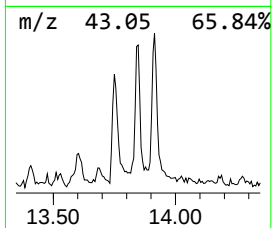
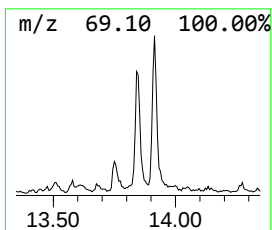
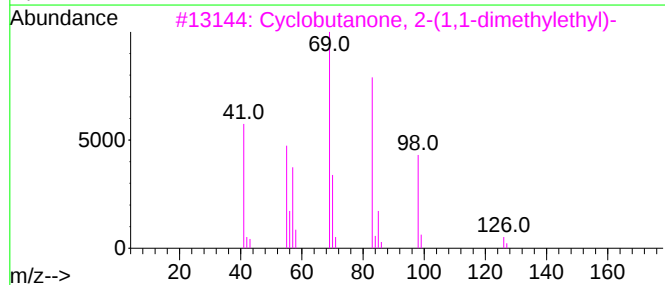
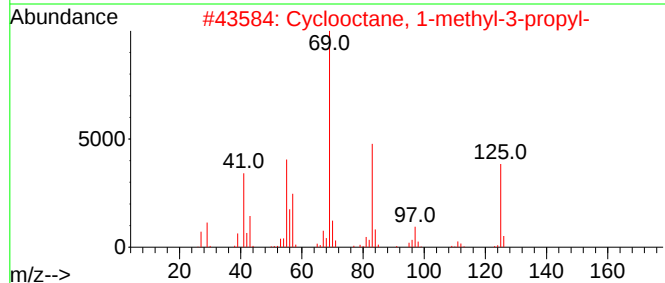
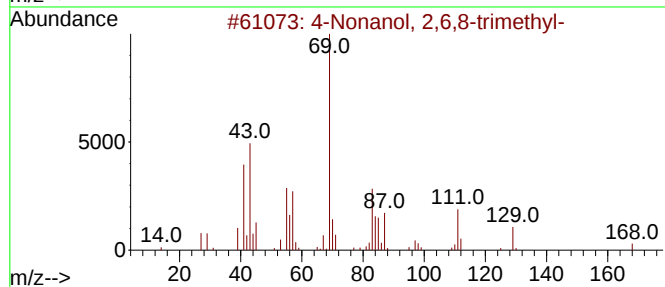
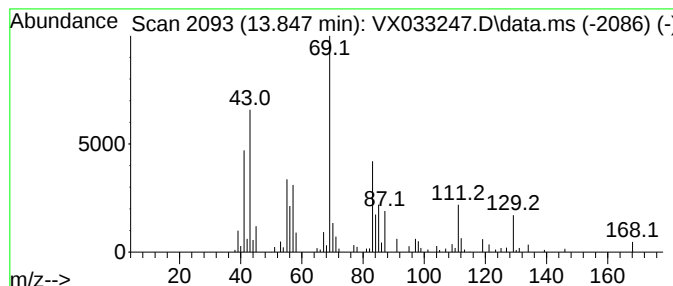
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Quant Title : SW846 8260

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

Peak Number 8 4-Nonanol, 2,6,8-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.847	5.40 ug/l	55123	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Nonanol, 2,6,8-trimethyl-	186	C12H26O	000123-17-1	80
2		Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	47
3		Cyclobutanone, 2-(1,1-dimethylet...	126	C8H14O	004579-31-1	47
4		Cyclopropanecarboxylic acid, isob...	142	C8H14O2	064969-79-5	43
5		Cyclopentane, 1-butyl-2-ethyl-	154	C11H22	072993-32-9	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033247.D
Acq On : 05 Dec 2022 23:31
Operator : JC/MD
Sample : N5859-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0584

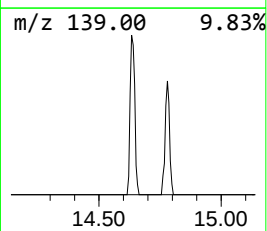
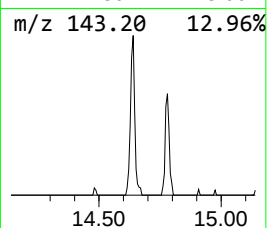
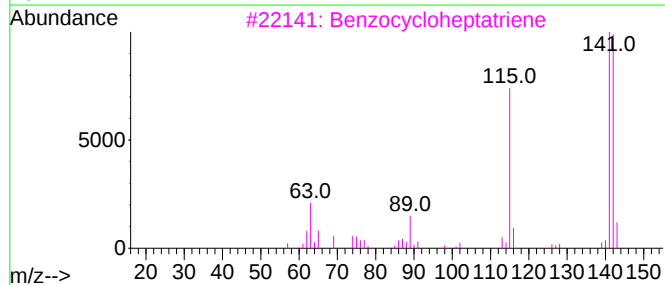
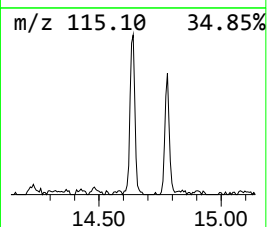
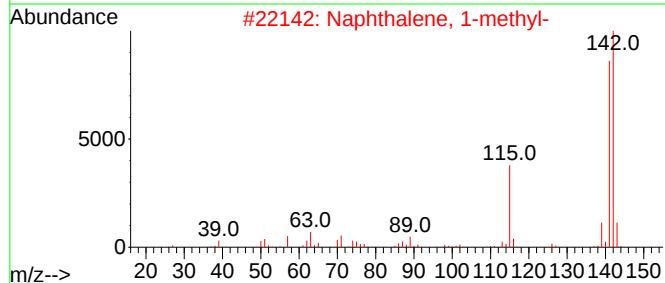
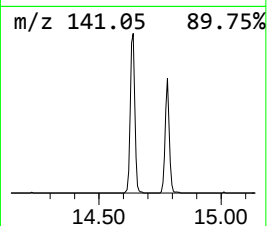
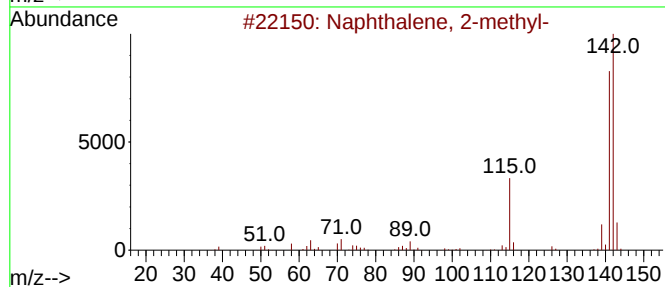
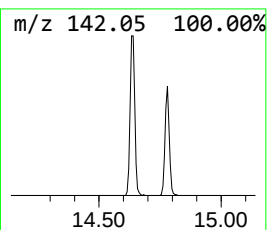
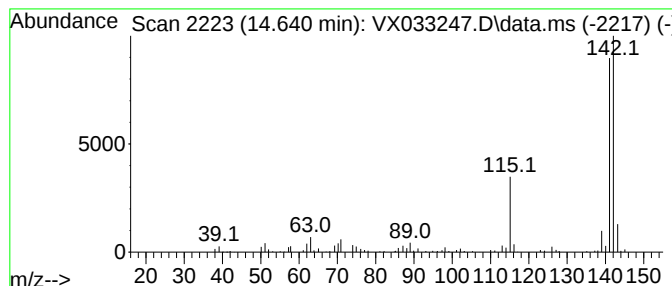
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	6.49 ug/l	66320	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033247.D
Acq On : 05 Dec 2022 23:31
Operator : JC/MD
Sample : N5859-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0584

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.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
Propane	1.142	7.0	ug/l	50018	1	5.556	359180	50.0
Acetaldehyde	1.459	6.5	ug/l	47016	1	5.556	359180	50.0
Propanal	2.294	194.4	ug/l	1396700	1	5.556	359180	50.0
1-Propanol	3.934	11.5	ug/l	82784	1	5.556	359180	50.0
Butanal	4.227	43.9	ug/l	315680	1	5.556	359180	50.0
unknown11.152	11.152	5.7	ug/l	58548	4	12.024	510835	50.0
1-Hexanol, 2-et...	12.219	51.9	ug/l	530701	4	12.024	510835	50.0
4-Nonanol, 2,6,...	13.847	5.4	ug/l	55123	4	12.024	510835	50.0
Naphthalene, 2-...	14.640	6.5	ug/l	66320	4	12.024	510835	50.0