

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
 Data File : VX039595.D
 Acq On : 03 Jan 2024 12:35
 Operator : JC/MD
 Sample : P1001-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ORA-1207

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\82X121323W.M
 Title : SW846 8260

Signal : TIC: VX039595.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	21	rVB	62616	67043	9.26%	1.152%
2	1.374	41	47	50	rBV	7115	8871	1.23%	0.152%
3	1.453	56	60	68	rVB	14412	16933	2.34%	0.291%
4	1.575	68	80	81	rBV5	7944	23864	3.30%	0.410%
5	2.294	192	198	205	rBV	24328	40201	5.55%	0.690%
6	2.386	205	213	223	rVB	42932	82611	11.41%	1.419%
7	2.587	235	246	254	rBV	7568	22651	3.13%	0.389%
8	3.008	306	315	324	rVB2	4376	13404	1.85%	0.230%
9	4.227	505	515	525	rBV2	24499	69256	9.57%	1.190%
10	4.580	564	573	582	rBV3	2560	8186	1.13%	0.141%
11	5.385	694	705	719	rBV	79632	229406	31.69%	3.940%
12	5.550	721	732	746	rVB	113491	325293	44.93%	5.587%
13	5.952	786	798	810	rBV	91092	245884	33.97%	4.223%
14	6.147	822	830	843	rBV3	8896	27053	3.74%	0.465%
15	6.757	920	930	948	rBV	219539	518190	71.58%	8.900%
16	7.232	999	1008	1025	rBV2	22006	60901	8.41%	1.046%
17	8.647	1234	1240	1249	rBV	460535	723923	100.00%	12.434%
18	8.720	1249	1252	1259	rVV2	5081	10314	1.42%	0.177%
19	10.055	1465	1471	1483	rBV	489657	704032	97.25%	12.092%
20	10.165	1483	1489	1492	rBV4	5638	8994	1.24%	0.154%
21	10.299	1507	1511	1520	rVB	6773	11211	1.55%	0.193%
22	10.646	1560	1568	1571	rBV4	5502	8577	1.18%	0.147%
23	10.689	1571	1575	1581	rVB	11423	15517	2.14%	0.267%
24	10.756	1581	1586	1595	rBV	46034	75396	10.41%	1.295%
25	11.079	1634	1639	1645	rBV	438955	539834	74.57%	9.272%
26	11.134	1645	1648	1656	rVB	9521	13407	1.85%	0.230%
27	11.280	1668	1672	1676	rBV2	7791	10648	1.47%	0.183%
28	11.390	1684	1690	1693	rBV2	14790	21705	3.00%	0.373%
29	11.427	1693	1696	1709	rVB2	9410	16727	2.31%	0.287%
30	11.573	1715	1720	1723	rBV	25455	34730	4.80%	0.597%
31	11.604	1723	1725	1733	rVV2	23602	33922	4.69%	0.583%
32	11.683	1733	1738	1746	rVV	299799	346452	47.86%	5.951%
33	11.756	1746	1750	1754	rVB2	6077	8587	1.19%	0.147%
34	11.835	1759	1763	1768	rVV4	4790	8192	1.13%	0.141%
35	11.896	1768	1773	1779	rVV5	3908	7811	1.08%	0.134%
36	11.988	1779	1788	1790	rVV	158569	194324	26.84%	3.338%

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Integrator: RTE

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37	12.018	1790	1793	1802	rVV	517483	682714	94.31%	11.726%
38	12.219	1820	1826	1836	rBV	222499	344052	47.53%	5.909%
39	12.305	1837	1840	1852	rVB6	13206	33059	4.57%	0.568%
40	13.609	2049	2054	2060	rBV2	11783	16863	2.33%	0.290%
41	13.676	2060	2065	2071	rVB	82026	95263	13.16%	1.636%
42	14.030	2118	2123	2129	rBV	20649	25410	3.51%	0.436%
43	14.140	2135	2141	2147	rBV	27459	36124	4.99%	0.620%
44	14.268	2158	2162	2167	rBV2	16094	20641	2.85%	0.355%
45	14.377	2174	2180	2185	rBV2	10898	13999	1.93%	0.240%

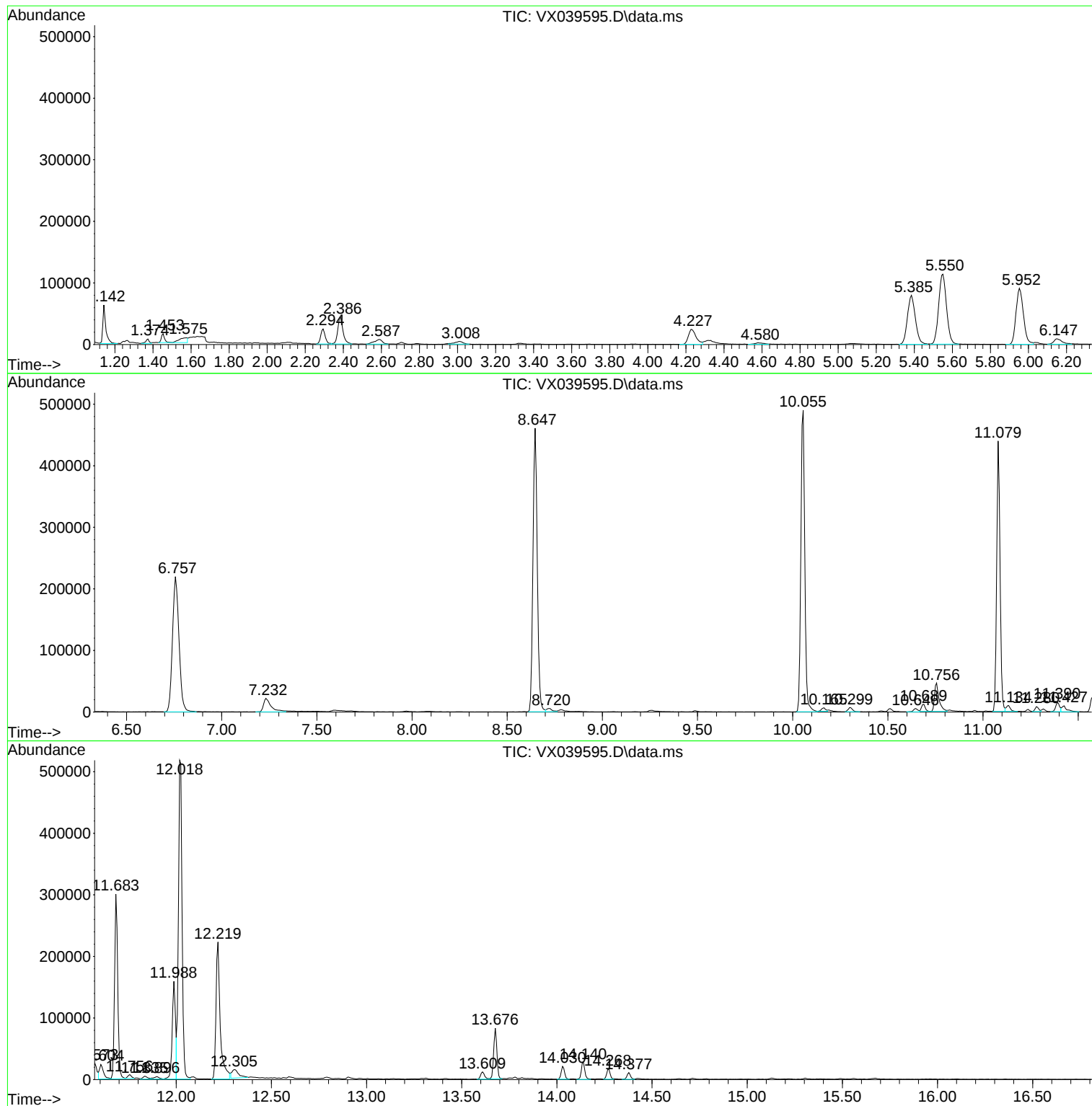
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



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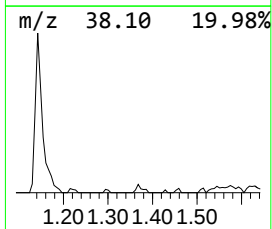
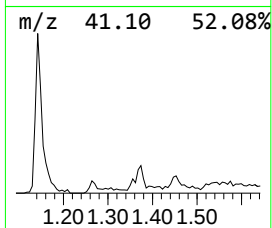
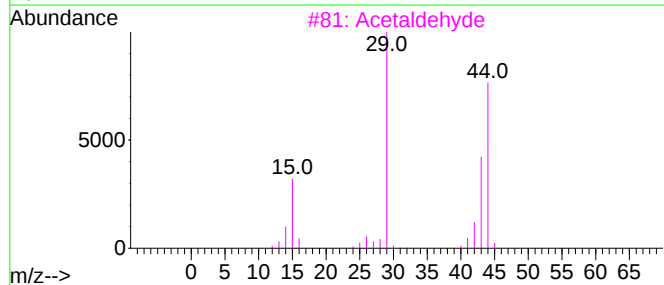
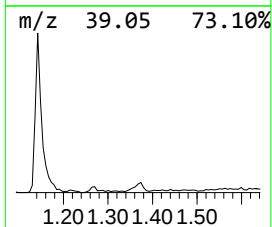
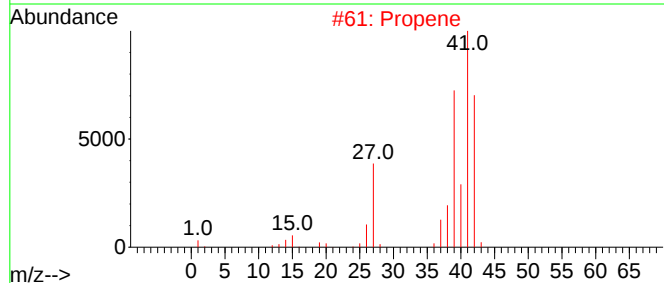
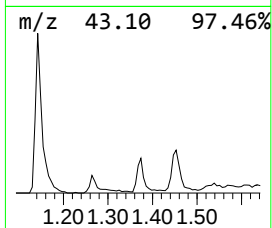
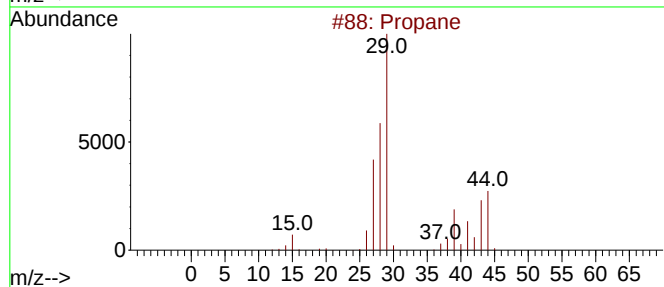
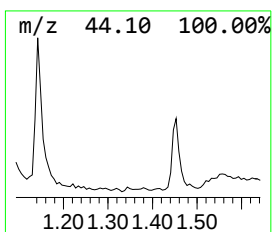
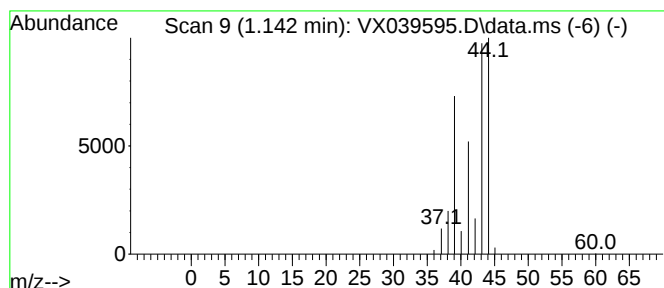
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	10.31 ug/l	67043	Pentafluorobenzene	5.550

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			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Acetonitrile-d3	44	C2D3N	002206-26-0	3



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1207

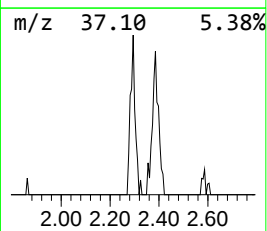
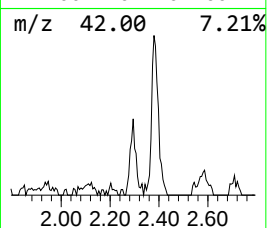
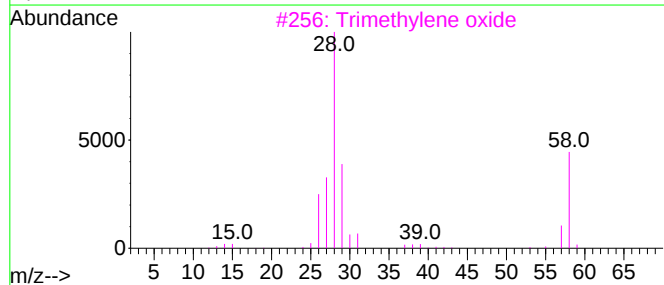
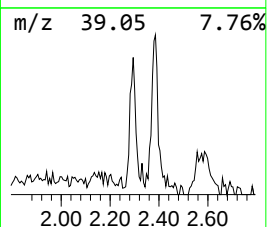
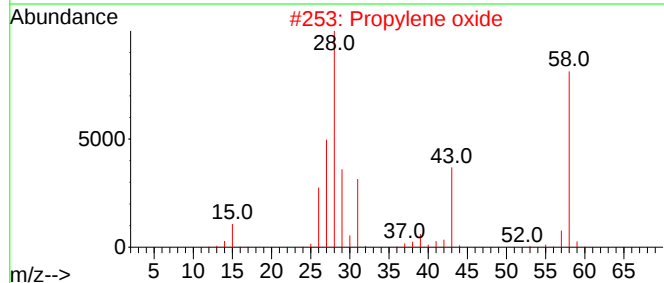
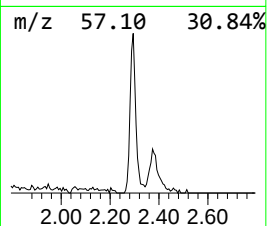
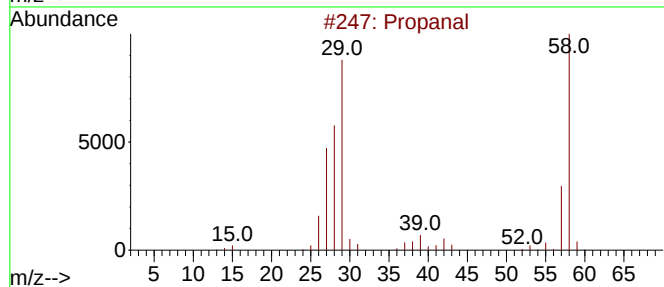
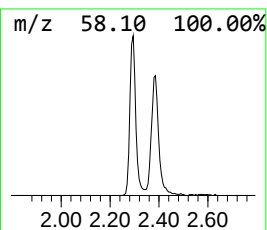
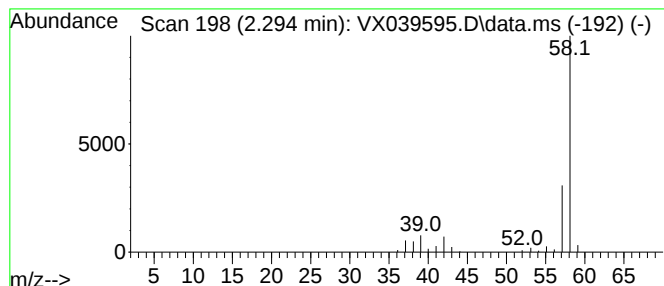
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	6.18 ug/l	40201	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Propylene oxide	58	C3H6O	000075-56-9	9
3			Trimethylene oxide	58	C3H6O	000503-30-0	9
4			2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	9
5			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1207

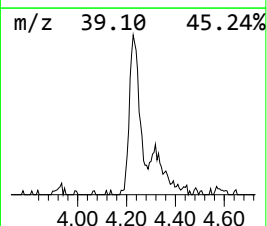
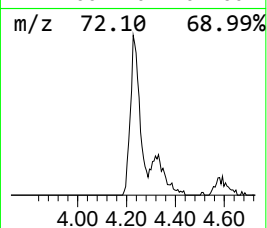
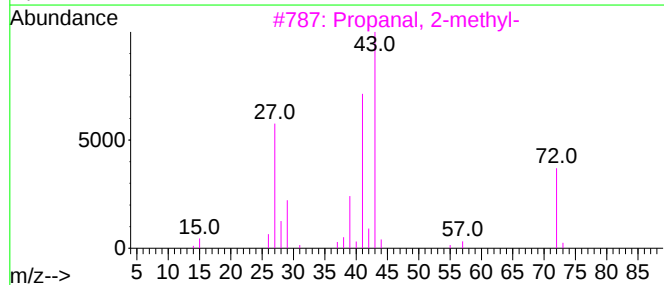
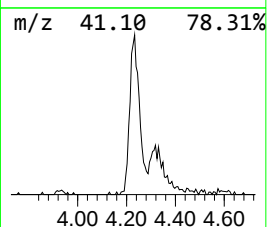
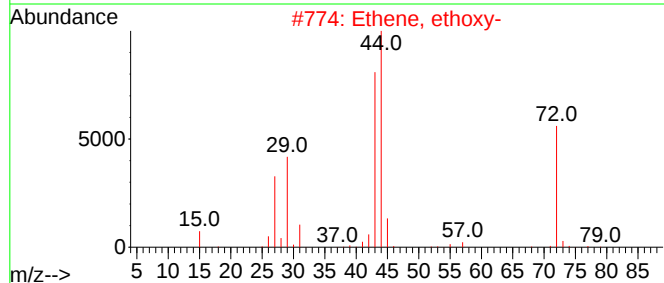
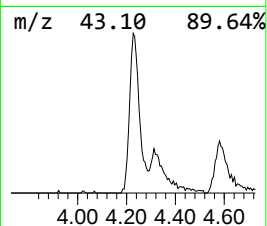
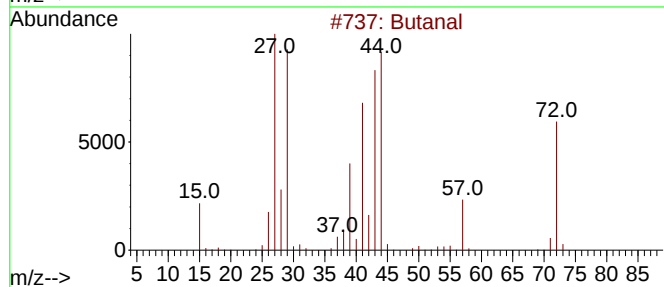
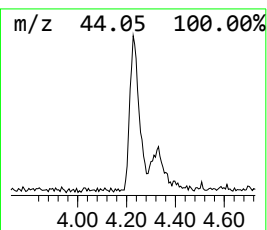
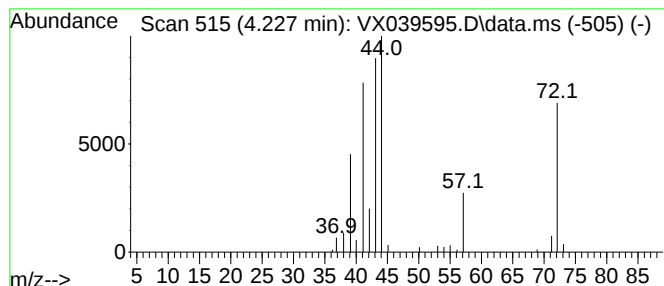
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	10.65 ug/l	69256	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	47
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	27
5			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	25



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ALS Vial : 9 Sample Multiplier: 1

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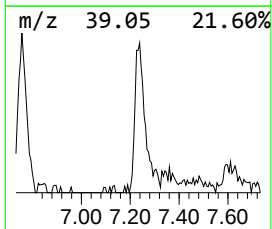
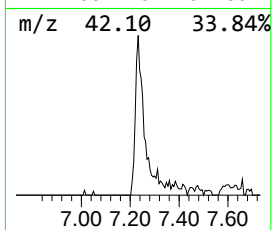
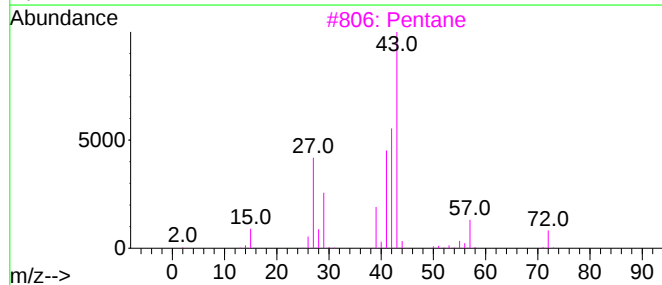
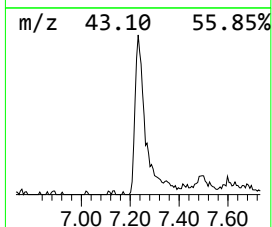
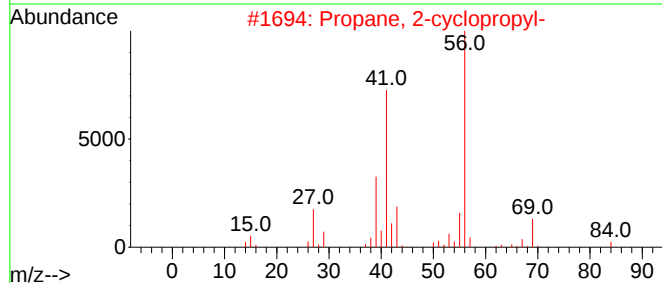
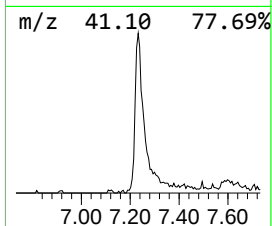
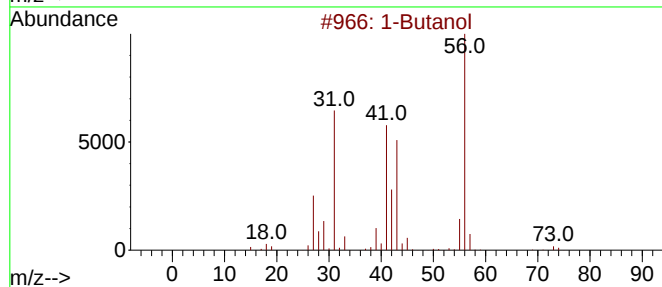
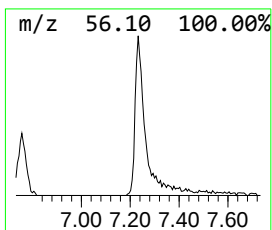
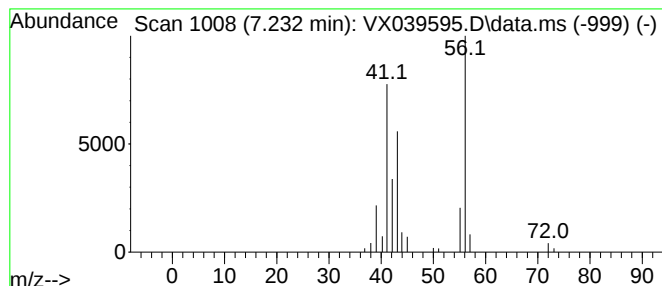
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.232	5.88 ug/l	60901	1,4-Difluorobenzene	6.757

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol		74	C4H10O	000071-36-3	78
2	Propane, 2-cyclopropyl-		84	C6H12	003638-35-5	36
3	Pentane		72	C5H12	000109-66-0	9
4	1-Pentanol, 4-methyl-		102	C6H14O	000626-89-1	9
5	Formic acid, butyl ester		102	C5H10O2	000592-84-7	9



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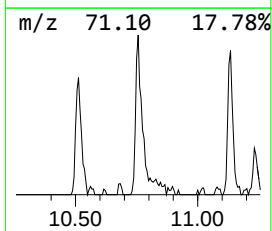
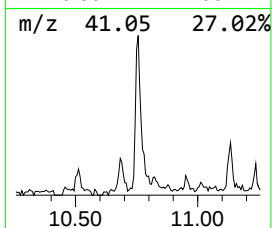
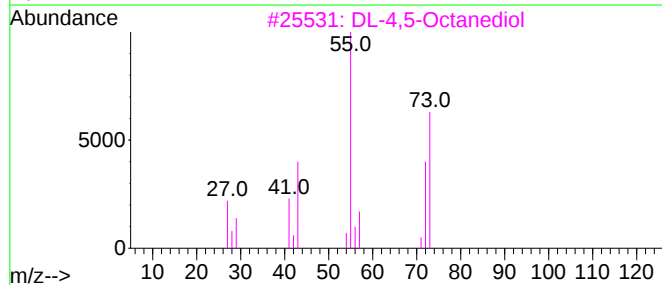
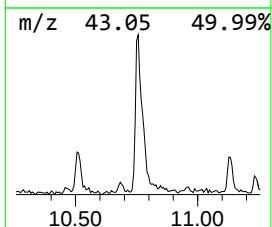
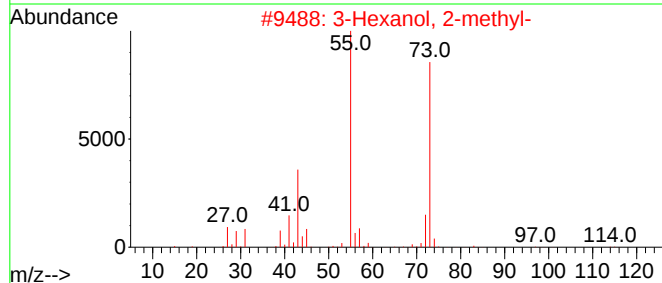
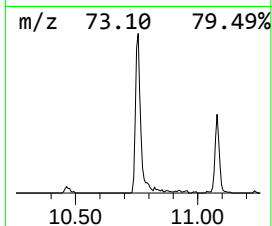
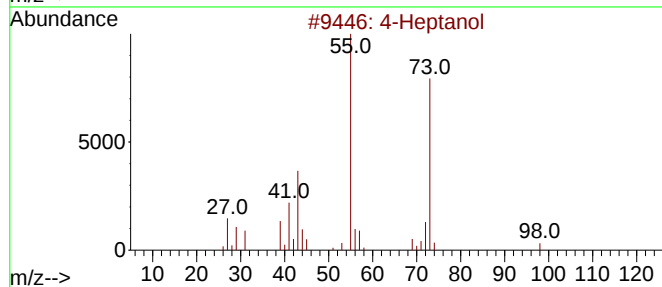
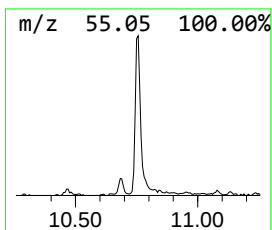
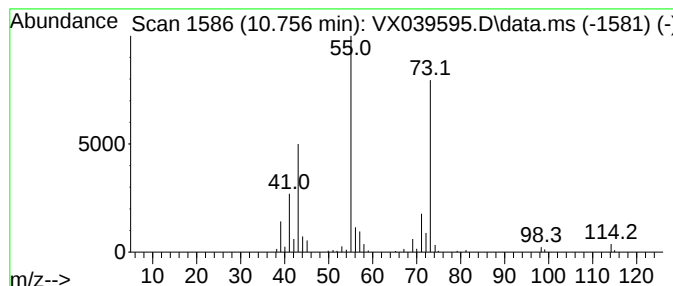
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 5 4-Heptanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.756	5.35 ug/l	75396	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	64
2			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	42
3			DL-4,5-Octanediol	146	C8H18O2	1000099-07-1	28
4			4,5-Octanediol	146	C8H18O2	022607-10-9	28
5			5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039595.D
Acq On : 03 Jan 2024 12:35
Operator : JC/MD
Sample : P1001-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1207

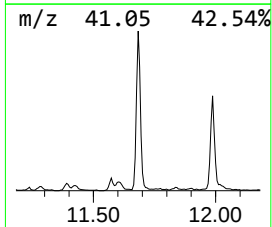
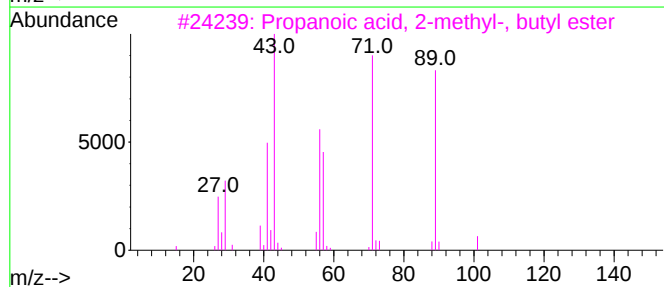
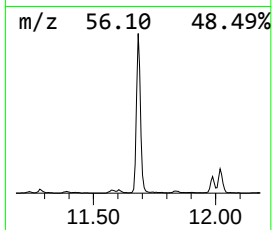
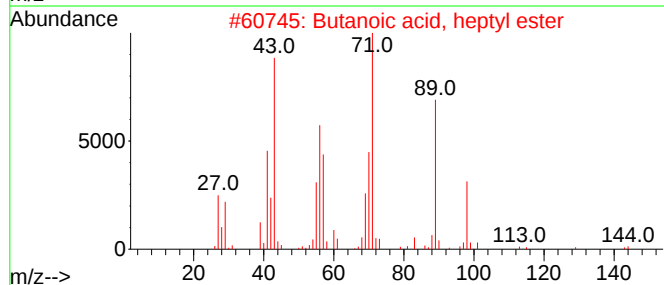
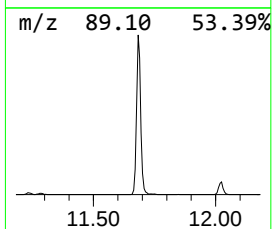
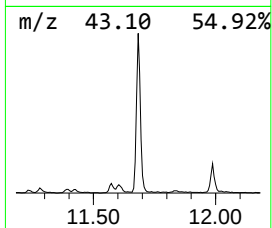
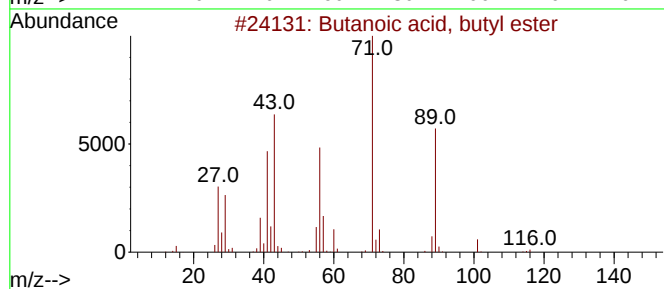
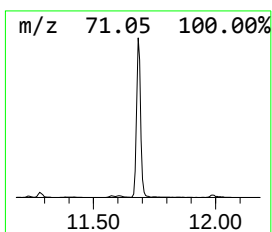
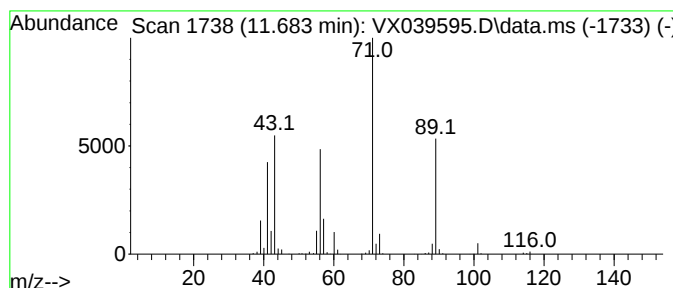
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Quant Title : SW846 8260

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

Peak Number 6 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	25.37 ug/l	346452	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
3			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
4			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	59
5			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039595.D
Acq On : 03 Jan 2024 12:35
Operator : JC/MD
Sample : P1001-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

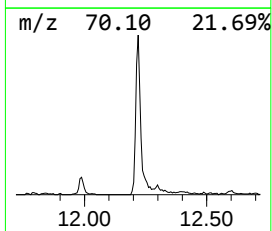
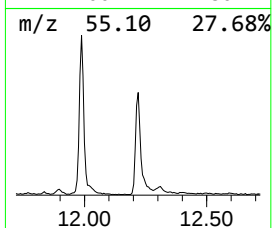
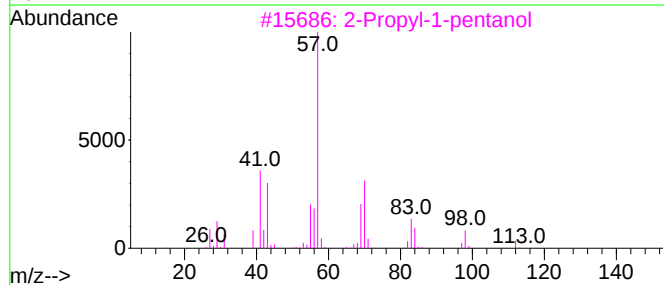
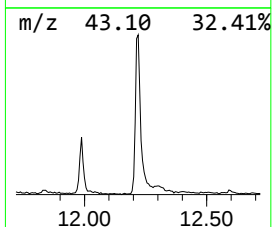
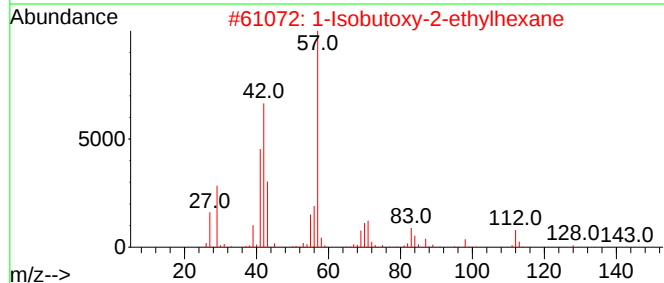
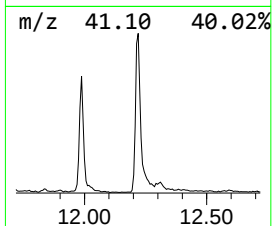
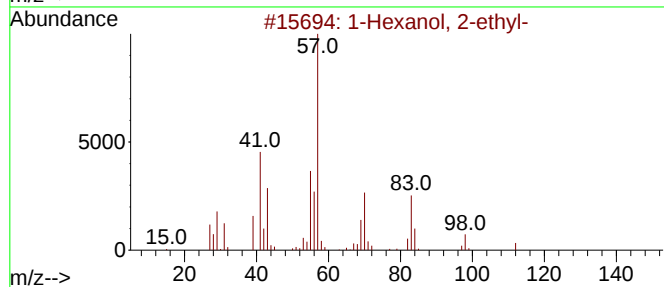
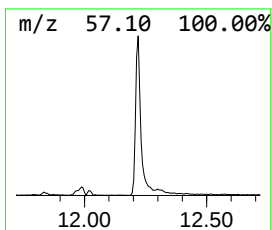
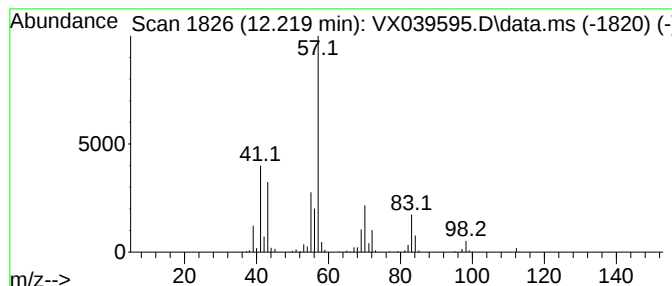
Instrument :
MSVOA_X
ClientSampleId :
ORA-1207

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.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	25.20 ug/l	344052	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	72
2	1-Isobutoxy-2-ethylhexane		186	C12H26O	1000139-90-3	64
3	2-Propyl-1-pentanol		130	C8H18O	058175-57-8	50
4	2-Ethyl-1-hexanol, methyl ether		144	C9H20O	1000365-10-2	50
5	Heptyl isobutyl carbonate		216	C12H24O3	959068-08-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039595.D
Acq On : 03 Jan 2024 12:35
Operator : JC/MD
Sample : P1001-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1207

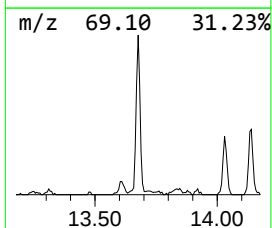
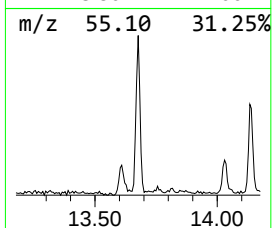
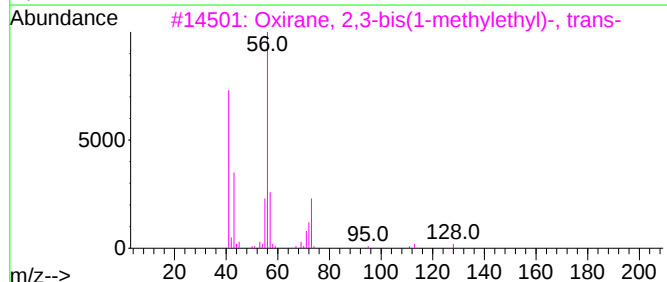
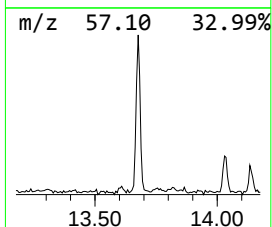
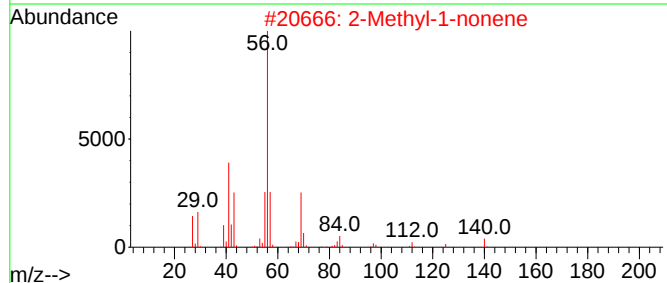
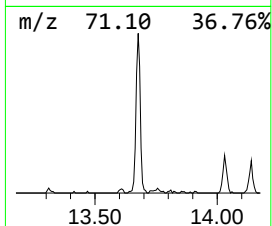
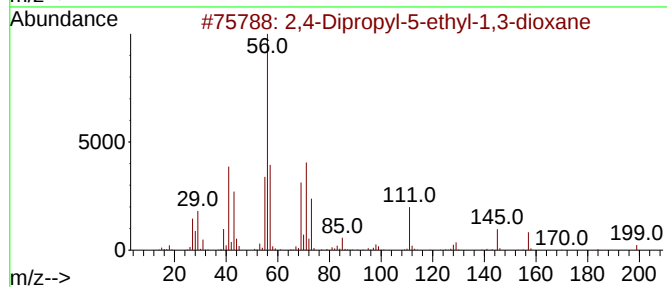
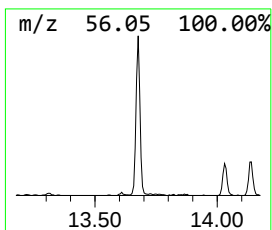
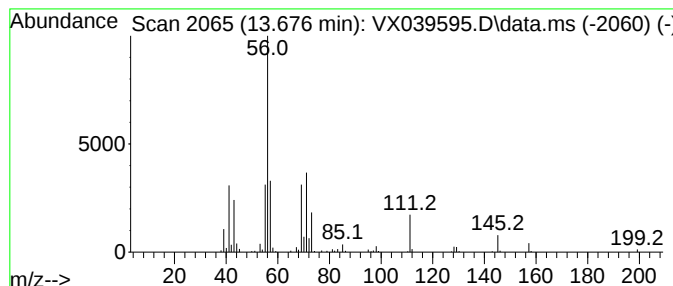
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 8 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	6.98 ug/l	95263	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	53
2			2-Methyl-1-nonene	140	C10H20	002980-71-4	43
3			Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	40
4			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	37
5			1-Octene, 2-methyl-	126	C9H18	004588-18-5	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039595.D
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Sample : P1001-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1207

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.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	10.3	ug/l	67043	1	5.550	325293	50.0
Propanal	2.294	6.2	ug/l	40201	1	5.550	325293	50.0
Butanal	4.227	10.7	ug/l	69256	1	5.550	325293	50.0
1-Butanol	7.232	5.9	ug/l	60901	2	6.757	518190	50.0
4-Heptanol	10.756	5.3	ug/l	75396	3	10.055	704032	50.0
Butanoic acid, ...	11.683	25.4	ug/l	346452	4	12.024	682714	50.0
1-Hexanol, 2-et...	12.219	25.2	ug/l	344052	4	12.024	682714	50.0
2,4-Dipropyl-5-...	13.676	7.0	ug/l	95263	4	12.024	682714	50.0