

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022824\
 Data File : VX040513.D
 Acq On : 28 Feb 2024 16:03
 Operator : JC/MD
 Sample : P1613-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1851

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\82X022624W.M
 Title : SW846 8260

Signal : TIC: VX040513.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	rVB	18032	18427	1.20%	0.205%
2	2.380	205	212	226	rBV	214231	356591	23.13%	3.975%
3	4.233	505	516	530	rBV	26545	70976	4.60%	0.791%
4	5.385	694	705	719	rBV	51444	147119	9.54%	1.640%
5	5.556	722	733	747	rVV	82900	234073	15.18%	2.609%
6	5.958	789	799	814	rBV2	57857	155850	10.11%	1.737%
7	6.763	922	931	943	rBV	129558	310209	20.12%	3.458%
8	7.580	1060	1065	1076	rVB2	9630	19335	1.25%	0.216%
9	8.647	1234	1240	1246	rVV	265966	425303	27.58%	4.741%
10	8.720	1246	1252	1266	rVB	1007572	1541996	100.00%	17.188%
11	9.519	1374	1383	1388	rBV	58058	84420	5.47%	0.941%
12	9.580	1388	1393	1402	rVB	153479	210147	13.63%	2.342%
13	10.055	1465	1471	1481	rBV	293617	417525	27.08%	4.654%
14	10.195	1488	1494	1504	rBV	198533	263706	17.10%	2.939%
15	10.299	1504	1511	1519	rBV	970435	1285444	83.36%	14.328%
16	10.640	1562	1567	1572	rBV	383674	488923	31.71%	5.450%
17	10.762	1581	1587	1596	rBV3	25136	59312	3.85%	0.661%
18	11.079	1633	1639	1644	rBV	255034	325573	21.11%	3.629%
19	11.128	1644	1647	1653	rVB	19736	26250	1.70%	0.293%
20	11.280	1668	1672	1682	rVB2	22150	33066	2.14%	0.369%
21	11.384	1682	1689	1694	rBV3	16269	31084	2.02%	0.346%
22	11.567	1714	1719	1724	rBV	343431	438190	28.42%	4.884%
23	11.610	1724	1726	1733	rVV3	21611	37875	2.46%	0.422%
24	11.683	1733	1738	1746	rVV	1041337	1178152	76.40%	13.132%
25	11.750	1746	1749	1754	rVV	18571	27416	1.78%	0.306%
26	11.823	1757	1761	1767	rVV	33109	45389	2.94%	0.506%
27	11.988	1781	1788	1790	rVV	123454	154588	10.03%	1.723%
28	12.018	1790	1793	1801	rVB	335668	439357	28.49%	4.897%
29	12.232	1823	1828	1836	rBV3	23089	68839	4.46%	0.767%
30	13.609	2047	2054	2060	rBV3	19641	33166	2.15%	0.370%
31	13.676	2060	2065	2070	rVV2	35311	43182	2.80%	0.481%

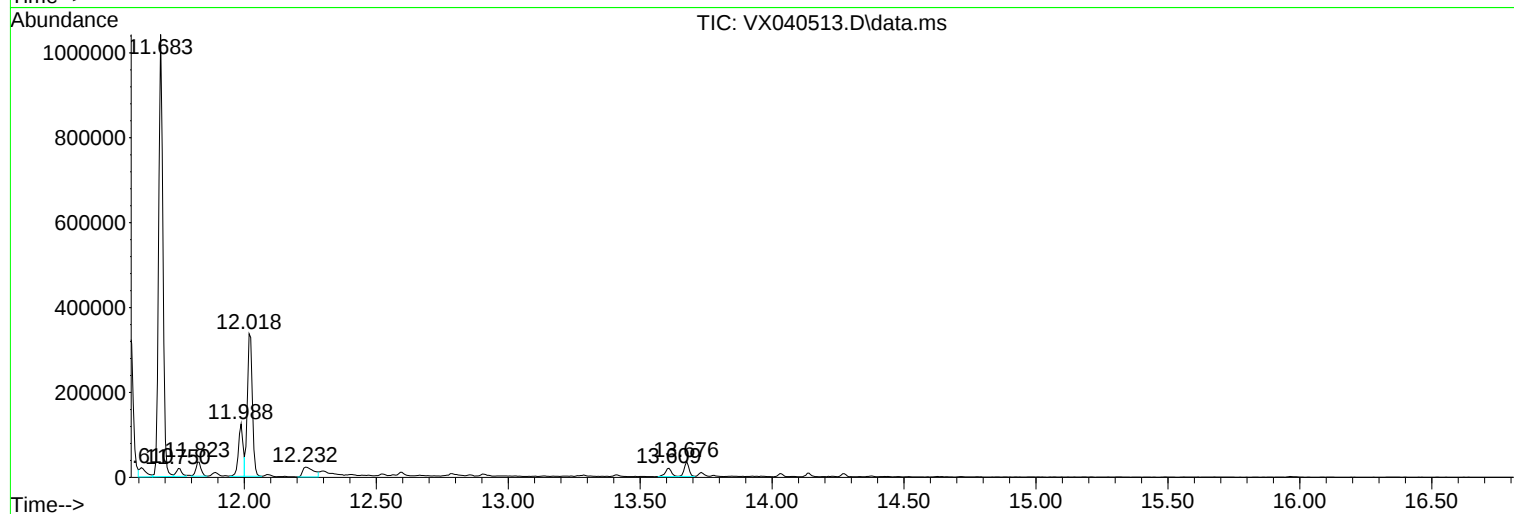
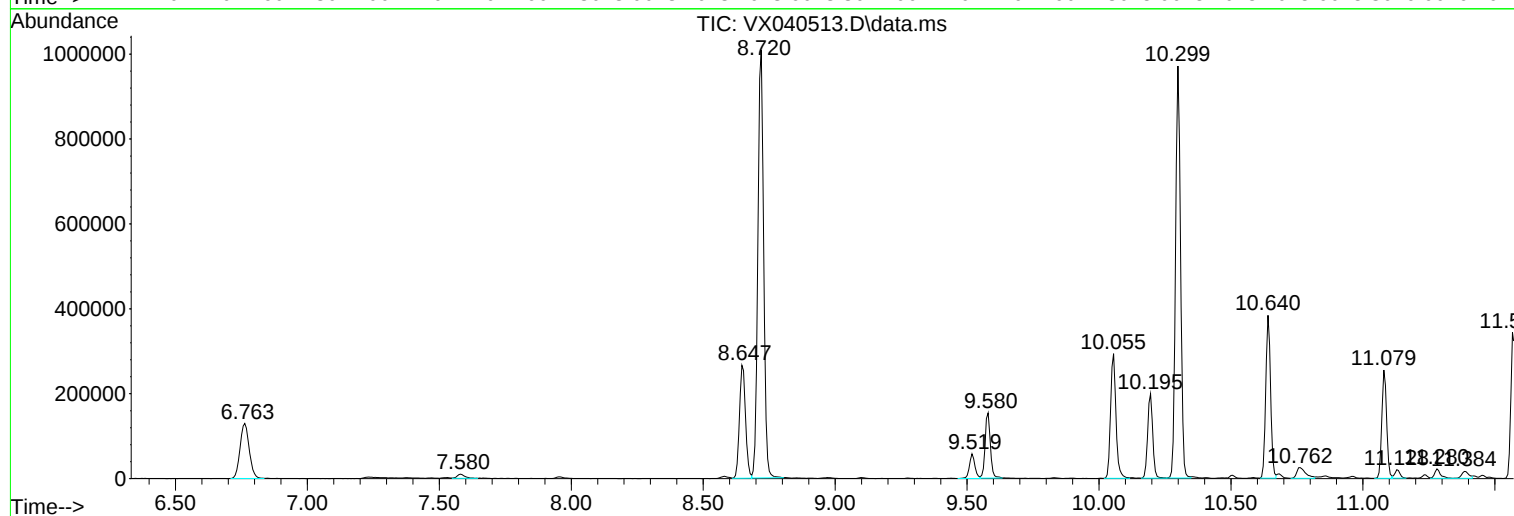
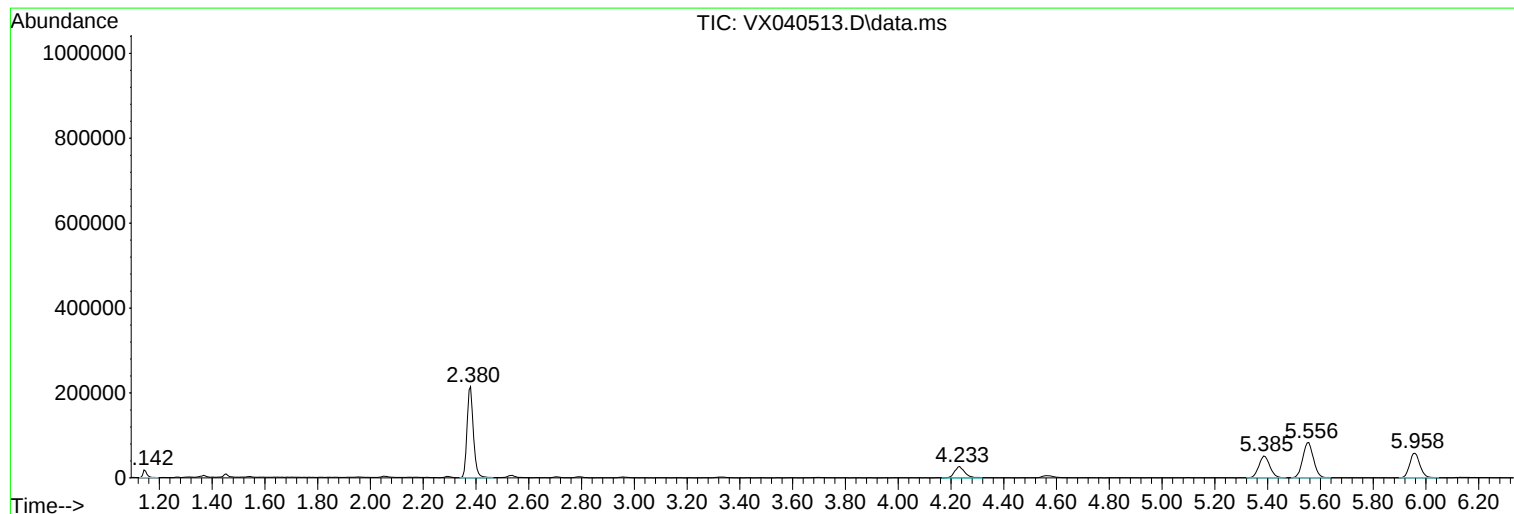
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

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



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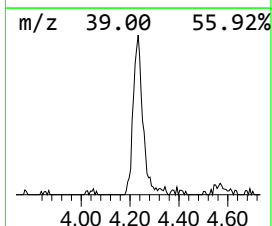
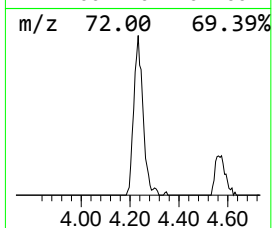
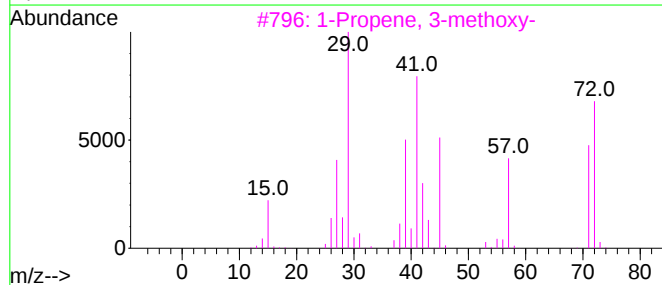
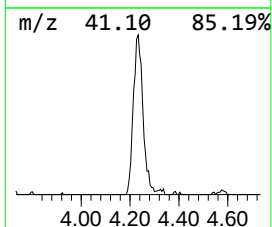
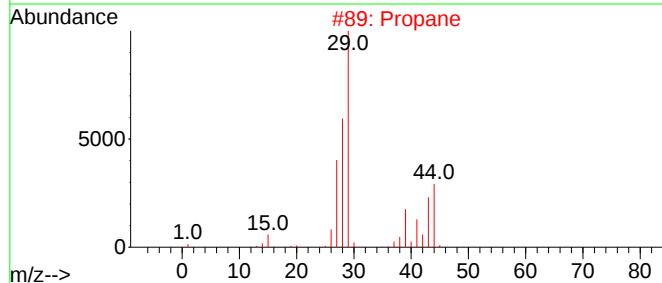
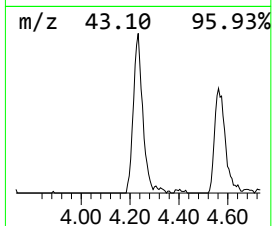
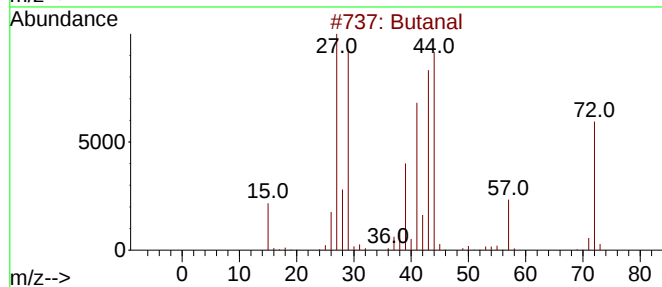
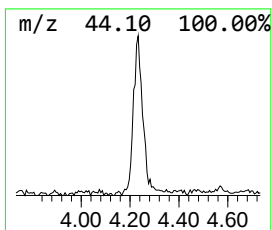
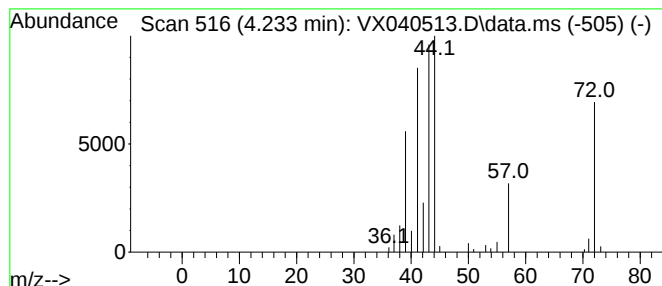
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Quant Title : SW846 8260

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

Peak Number 1 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	15.16 ug/l	70976	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propane	44	C3H8	000074-98-6	47
3			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5			Ethene, ethoxy-	72	C4H8O	000109-92-2	28



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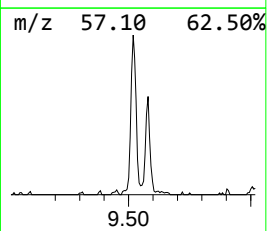
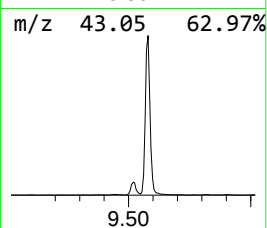
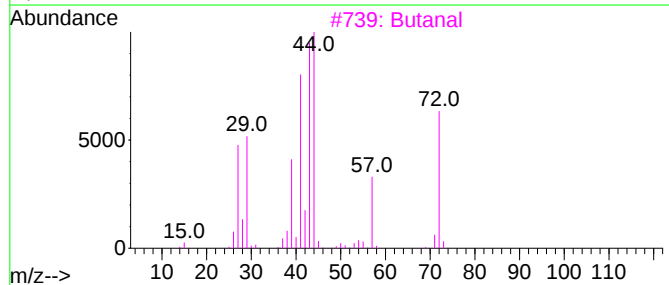
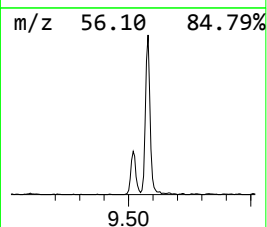
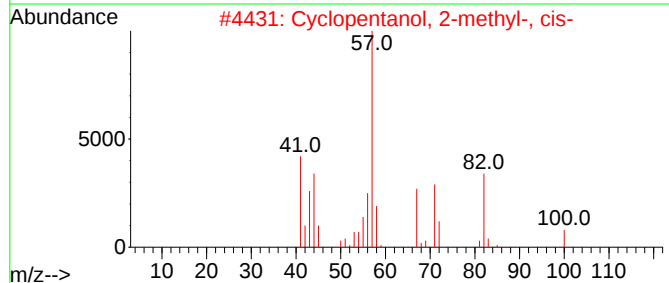
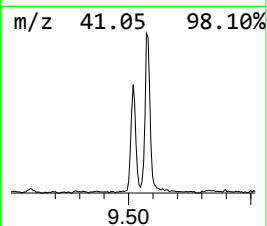
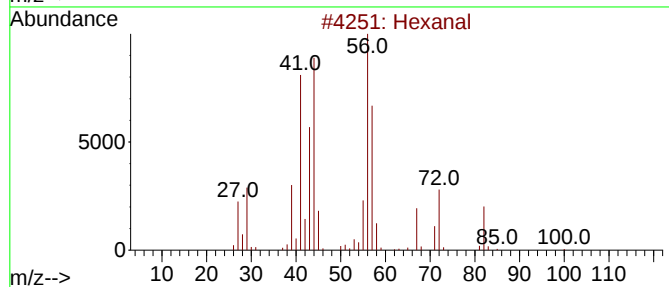
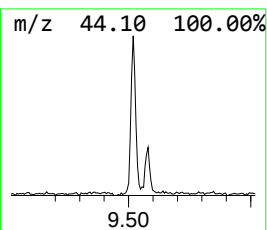
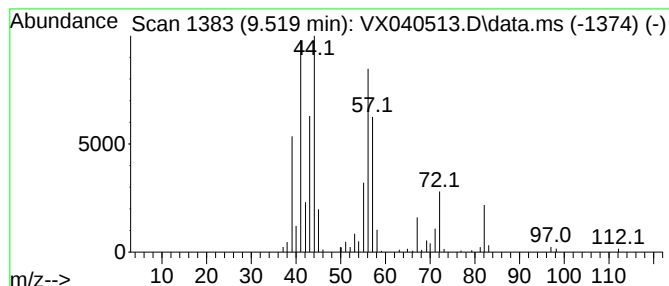
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

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

Peak Number 2 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.519	10.11 ug/l	84420	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	72
2			Cyclopentanol, 2-methyl-, cis-	100	C6H12O	025144-05-2	25
3			Butanal	72	C4H8O	000123-72-8	25
4			Cyclobutane	56	C4H8	000287-23-0	18
5			Glutaraldehyde	100	C5H8O2	000111-30-8	16



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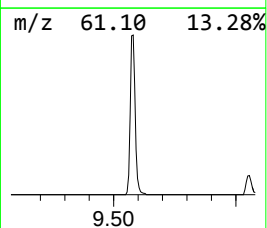
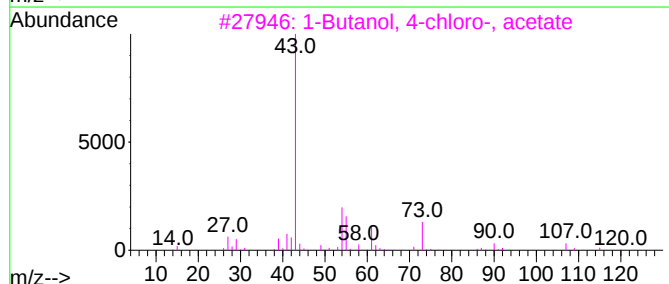
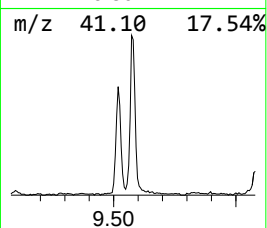
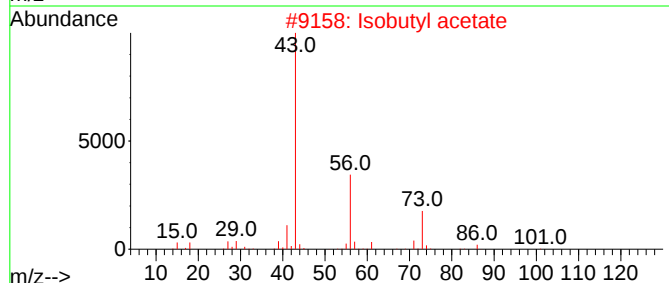
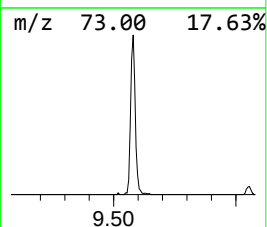
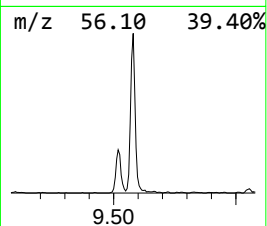
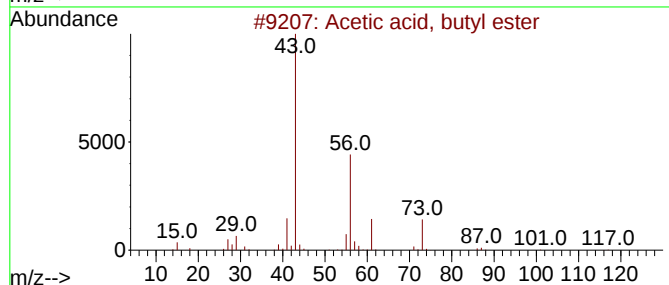
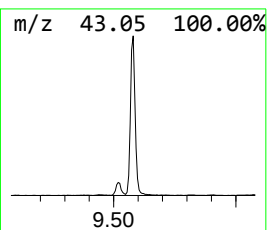
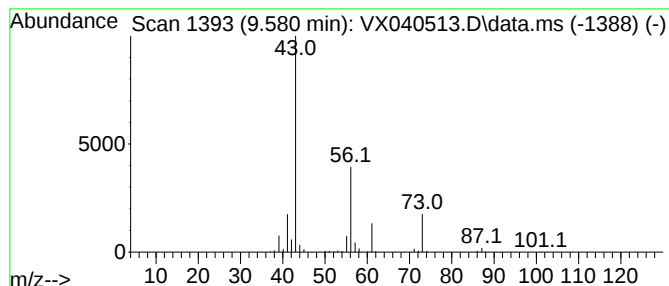
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

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

Peak Number 3 Acetic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	25.17 ug/l	210147	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Isobutyl acetate	116	C6H12O2	000110-19-0	39
3			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	17
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9



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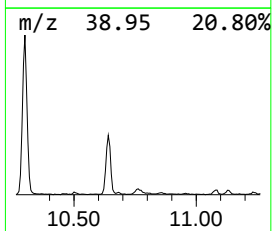
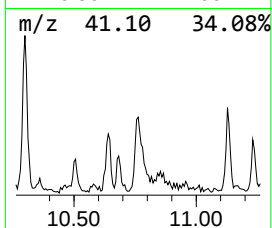
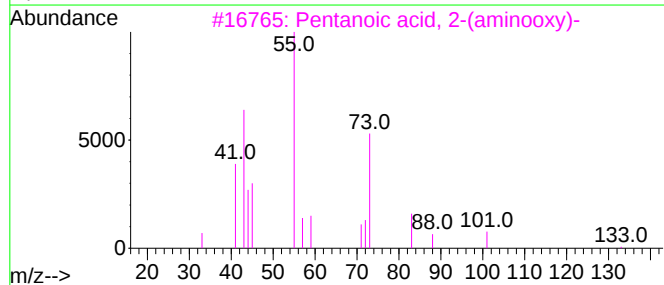
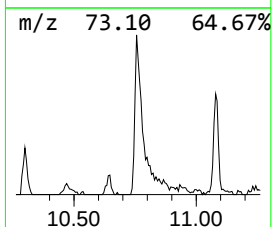
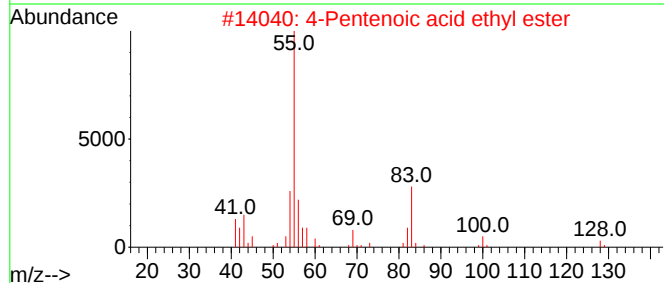
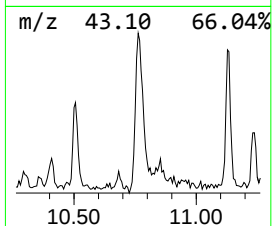
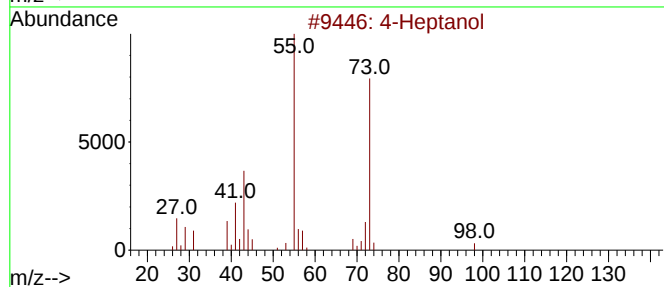
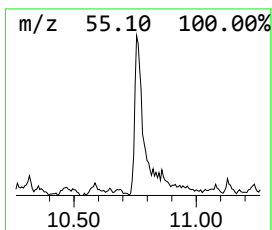
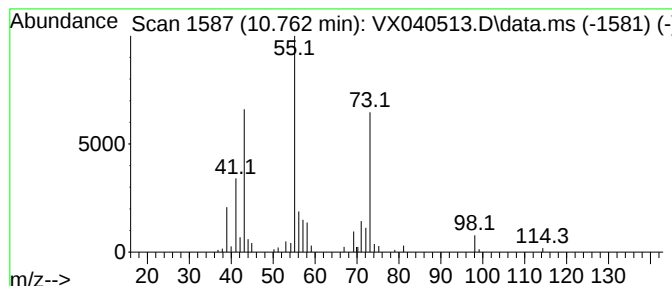
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown10.762 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.762	7.10 ug/l	59312	Chlorobenzene-d5	10.055

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol		116	C7H16O	000589-55-9	45
2	4-Pentenoic acid ethyl ester		128	C7H12O2	001968-40-7	38
3	Pentanoic acid, 2-(aminoxy)-		133	C5H11NO3	005699-55-8	38
4	3-Hexanol, 2-methyl-		116	C7H16O	000617-29-8	37
5	3-Pentanol, 2,4-dimethyl-		116	C7H16O	000600-36-2	33



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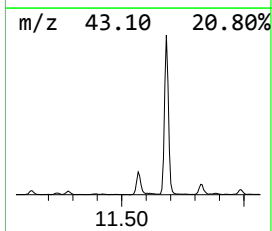
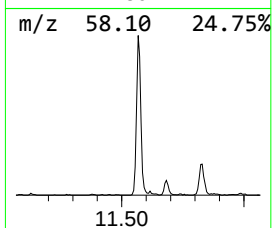
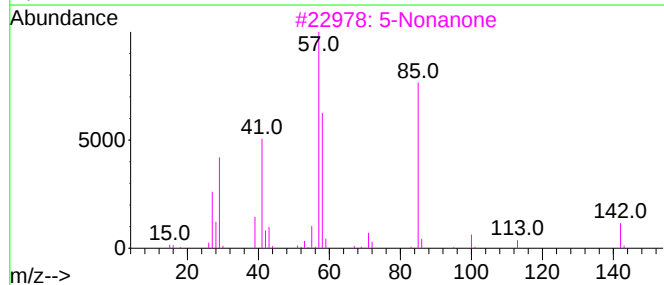
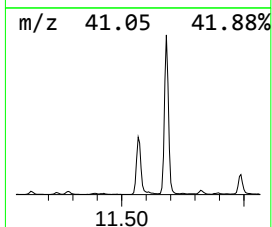
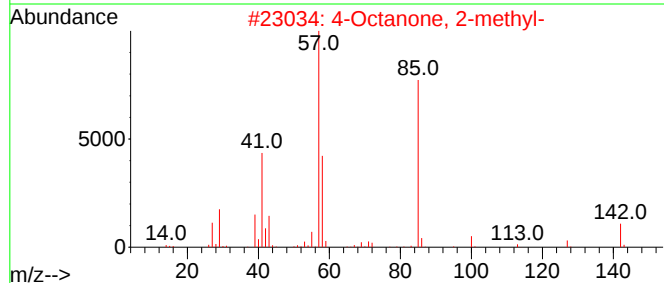
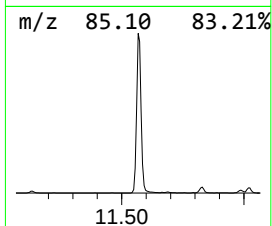
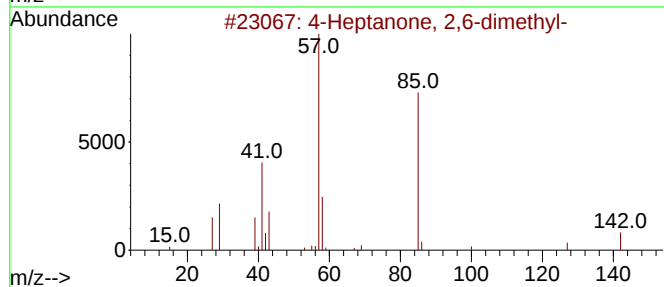
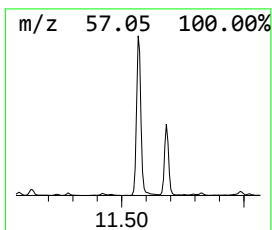
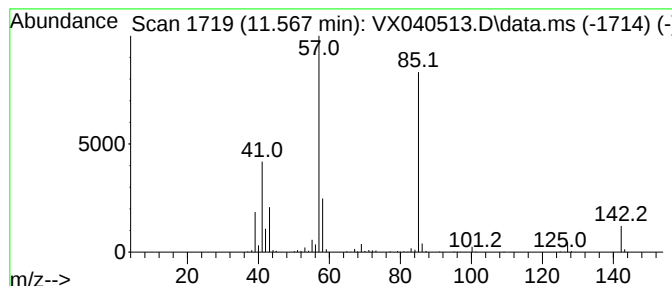
Instrument :
MSVOA_X
ClientSampleId :
1851

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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.567	49.87 ug/l	438190	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	91
2	4-Octanone, 2-methyl-		142	C9H18O	007492-38-8	80
3	5-Nonanone		142	C9H18O	000502-56-7	64
4	t-Butyl isobutyl ketone		142	C9H18O	014705-50-1	53
5	4-Heptanone, 2-methyl-		128	C8H16O	000626-33-5	50



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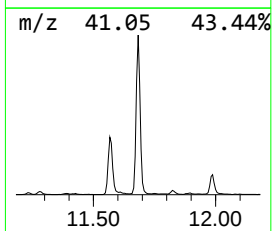
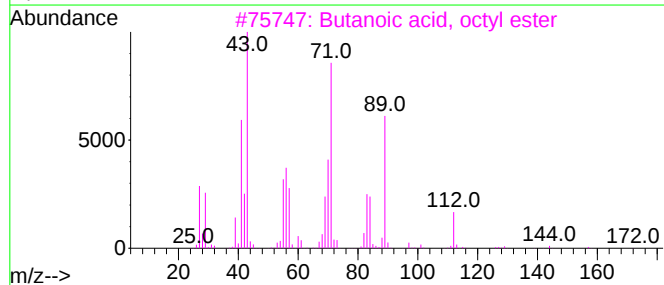
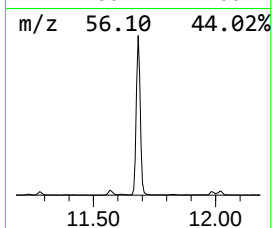
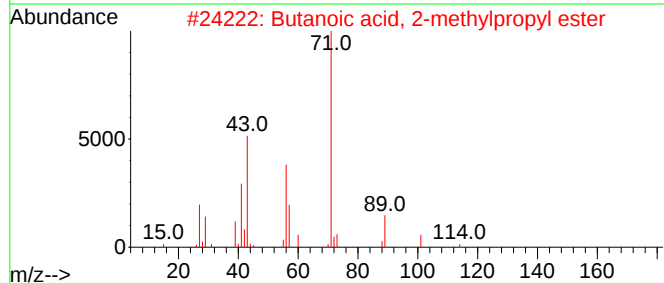
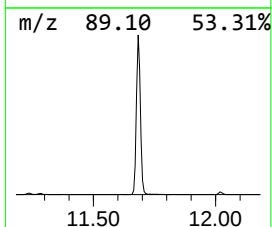
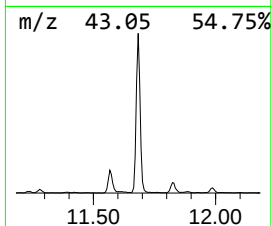
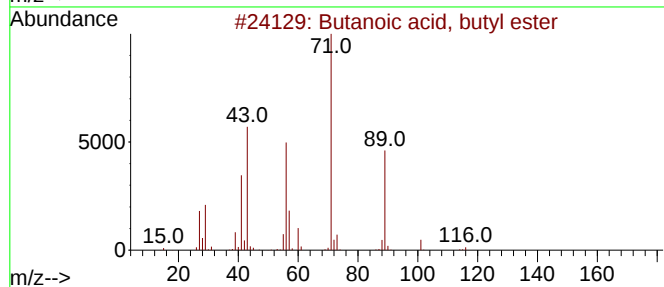
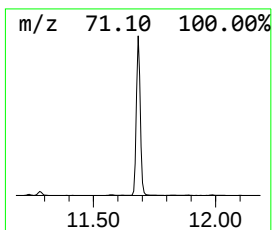
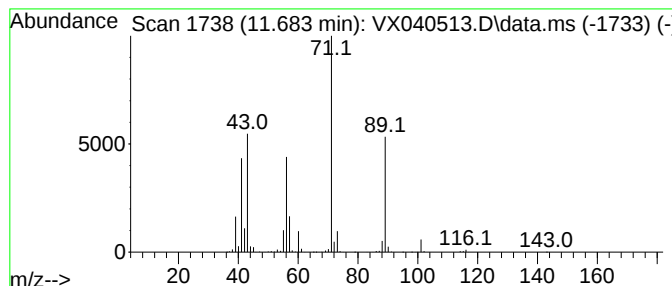
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Quant Title : SW846 8260

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

Peak Number 6 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	134.08 ug/l	1178150	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, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
4			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	59
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022824\
Data File : VX040513.D
Acq On : 28 Feb 2024 16:03
Operator : JC/MD
Sample : P1613-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1851

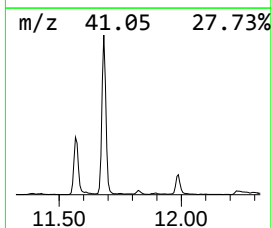
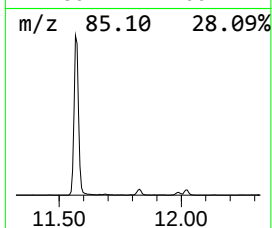
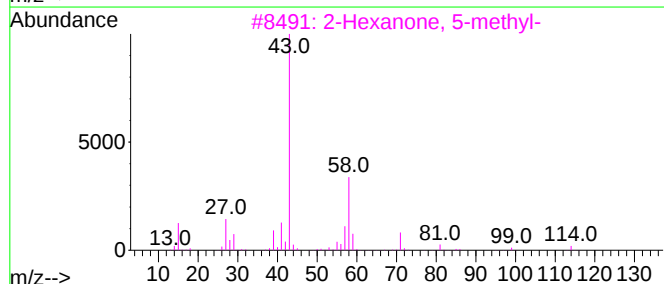
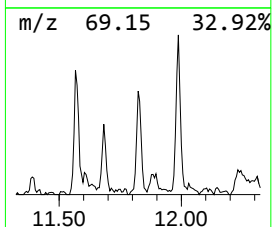
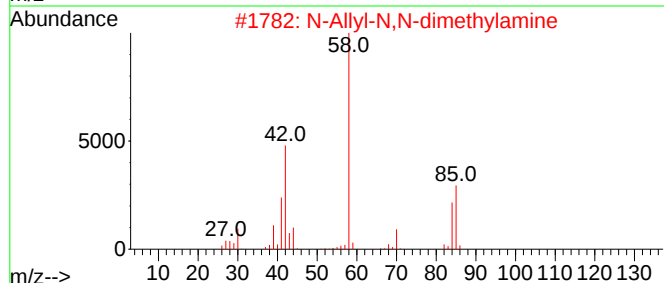
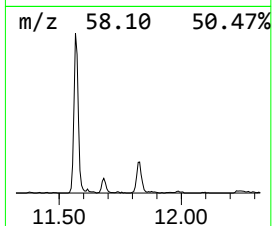
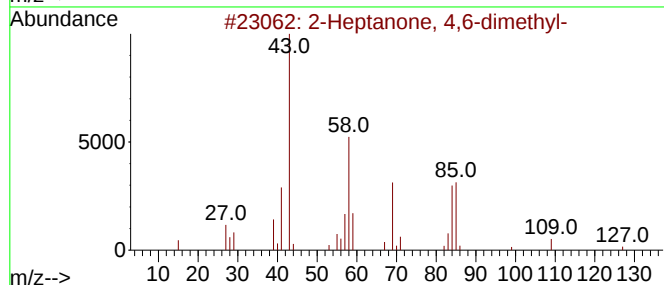
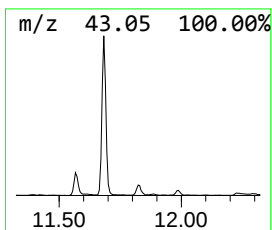
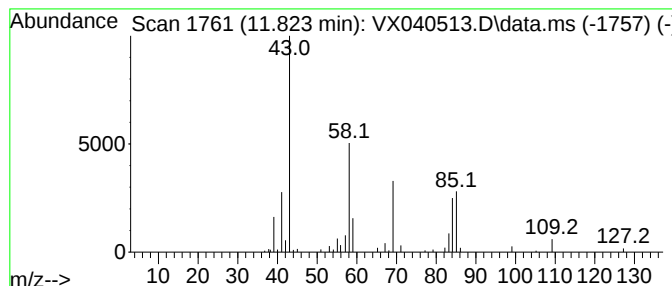
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Quant Title : SW846 8260

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

Peak Number 7 2-Heptanone, 4,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.823	5.17 ug/l	45389	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 4,6-dimethyl-			142	C9H18O	019549-80-5	83
2	N-Allyl-N,N-dimethylamine			85	C5H11N	002155-94-4	40
3	2-Hexanone, 5-methyl-			114	C7H14O	000110-12-3	37
4	2-Hexanone, 4-methyl-			114	C7H14O	000105-42-0	28
5	2-Nonanone, 9-[(tetrahydro-2H-py...			242	C14H26O3	054699-41-1	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022824\
Data File : VX040513.D
Acq On : 28 Feb 2024 16:03
Operator : JC/MD
Sample : P1613-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1851

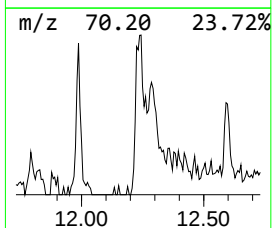
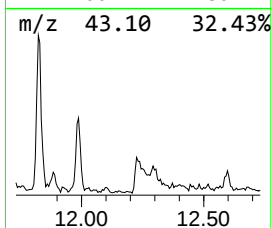
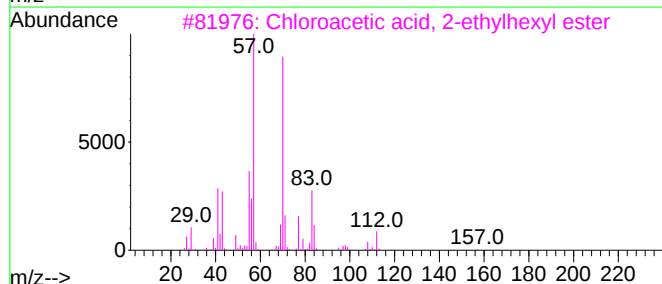
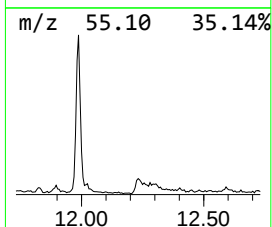
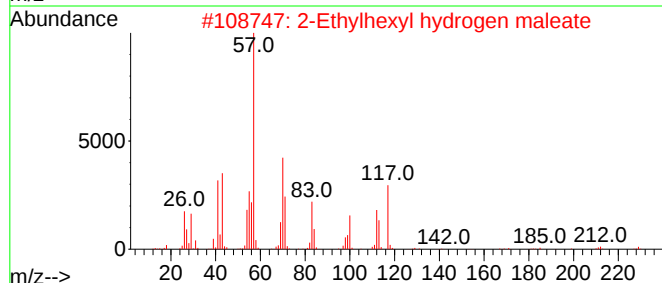
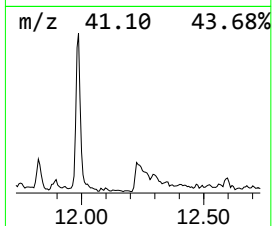
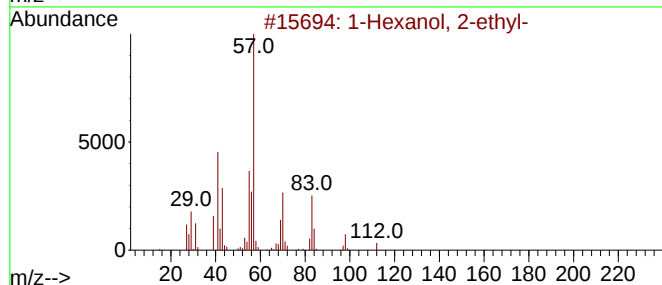
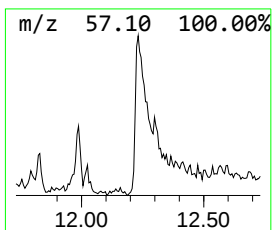
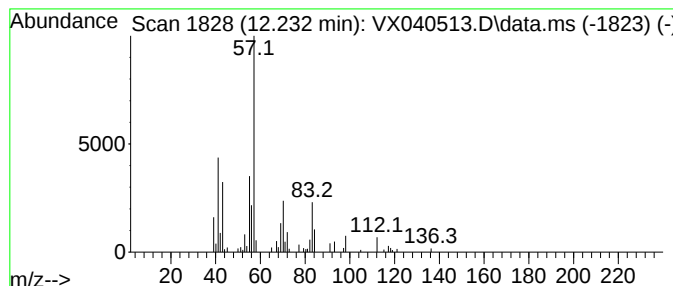
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

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

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.232	7.83 ug/l	68839	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	78
2			2-Ethylhexyl hydrogen maleate	228	C12H20O4	002370-71-0	53
3			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	53
4			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	53
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022824\
Data File : VX040513.D
Acq On : 28 Feb 2024 16:03
Operator : JC/MD
Sample : P1613-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1851

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.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
Butanal	4.233	15.2	ug/l	70976	1	5.556	234073	50.0
Hexanal	9.519	10.1	ug/l	84420	3	10.055	417525	50.0
Acetic acid, bu...	9.580	25.2	ug/l	210147	3	10.055	417525	50.0
unknown10.762	10.762	7.1	ug/l	59312	3	10.055	417525	50.0
4-Heptanone, 2,...	11.567	49.9	ug/l	438190	4	12.024	439357	50.0
Butanoic acid, ...	11.683	134.1	ug/l	1178150	4	12.024	439357	50.0
2-Heptanone, 4,...	11.823	5.2	ug/l	45389	4	12.024	439357	50.0
1-Hexanol, 2-et...	12.232	7.8	ug/l	68839	4	12.024	439357	50.0