

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101823\
 Data File : VX038367.D
 Acq On : 18 Oct 2023 16:58
 Operator : JC/MD
 Sample : 04936-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1026

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\82X100523W.M
 Title : SW846 8260

Signal : TIC: VX038367.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.379	205	212	221	rBV	35063	59910	4.71%	0.843%
2	3.331	361	368	379	rBV3	6310	14980	1.18%	0.211%
3	4.227	505	515	537	rBV	483403	1272616	100.00%	17.913%
4	4.550	559	568	590	rBV	209147	579294	45.52%	8.154%
5	4.995	629	641	658	rBV2	16340	59365	4.66%	0.836%
6	5.385	694	705	718	rBV	77060	225512	17.72%	3.174%
7	5.550	722	732	750	rVV	122422	349067	27.43%	4.913%
8	5.958	789	799	809	rBV	90714	233090	18.32%	3.281%
9	6.117	818	825	839	rVB4	4926	15652	1.23%	0.220%
10	6.763	921	931	952	rBV	202535	482035	37.88%	6.785%
11	7.208	995	1004	1025	rBV	49166	131793	10.36%	1.855%
12	7.580	1059	1065	1073	rBV2	20965	41208	3.24%	0.580%
13	8.647	1233	1240	1248	rBV	430064	691017	54.30%	9.727%
14	8.720	1248	1252	1257	rVB	10207	16439	1.29%	0.231%
15	10.055	1465	1471	1482	rBV	467911	657717	51.68%	9.258%
16	10.305	1505	1512	1520	rVB	10596	16771	1.32%	0.236%
17	10.506	1541	1545	1557	rVB	14162	20179	1.59%	0.284%
18	10.683	1571	1574	1580	rVB	13883	17553	1.38%	0.247%
19	10.756	1580	1586	1607	rBV	53877	103221	8.11%	1.453%
20	11.079	1634	1639	1645	rBV	431205	538757	42.33%	7.584%
21	11.134	1645	1648	1655	rVB	14732	20818	1.64%	0.293%
22	11.573	1715	1720	1723	rBV2	26194	38069	2.99%	0.536%
23	11.603	1723	1725	1735	rVV2	25632	42205	3.32%	0.594%
24	11.872	1765	1769	1777	rVB	15584	27744	2.18%	0.391%
25	12.024	1789	1794	1802	rVB	575574	732503	57.56%	10.311%
26	12.219	1821	1826	1839	rBV	414045	664537	52.22%	9.354%
27	13.755	2073	2078	2086	rBV4	15215	38174	3.00%	0.537%
28	13.847	2090	2093	2100	rVV3	7962	14053	1.10%	0.198%

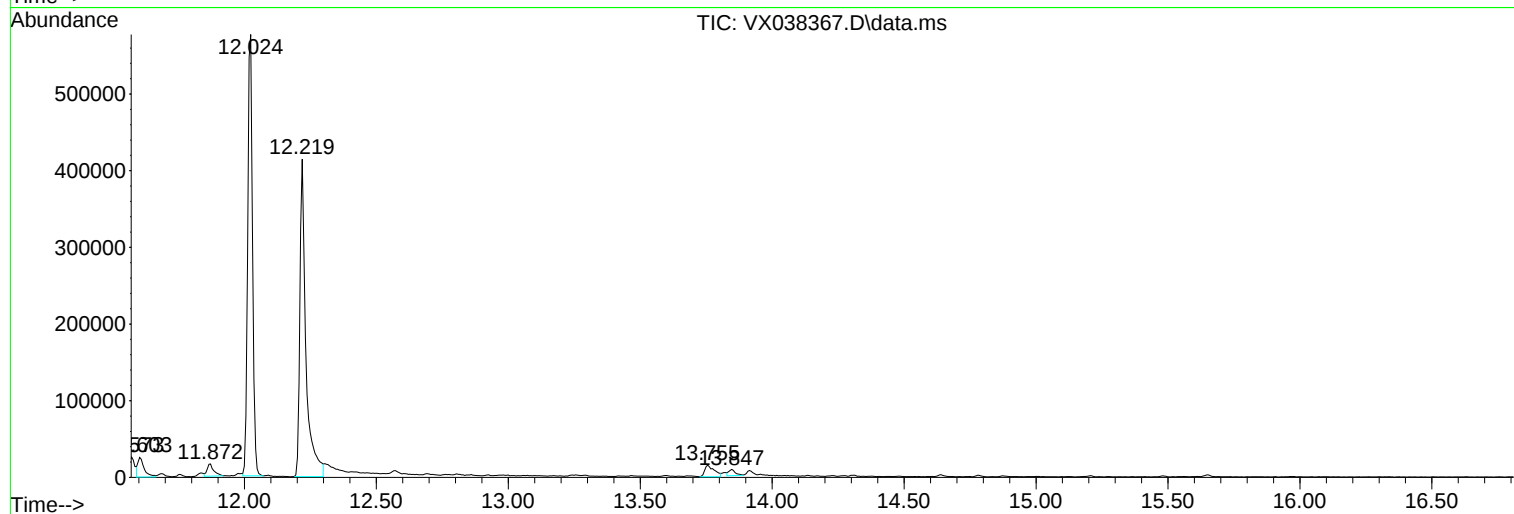
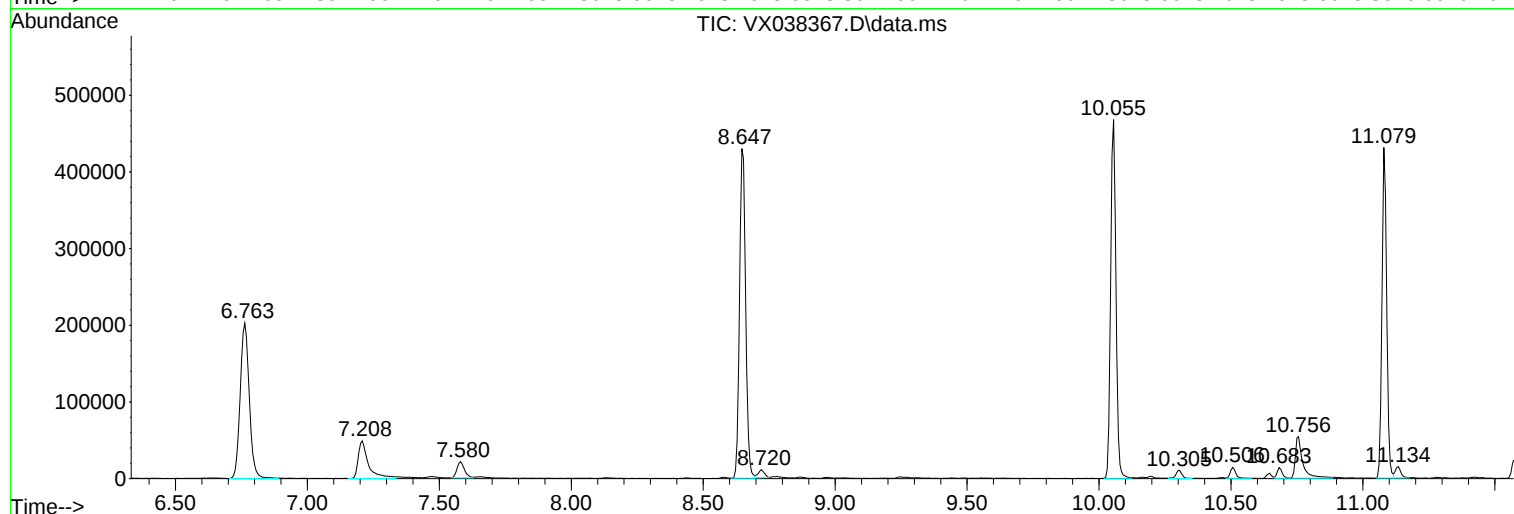
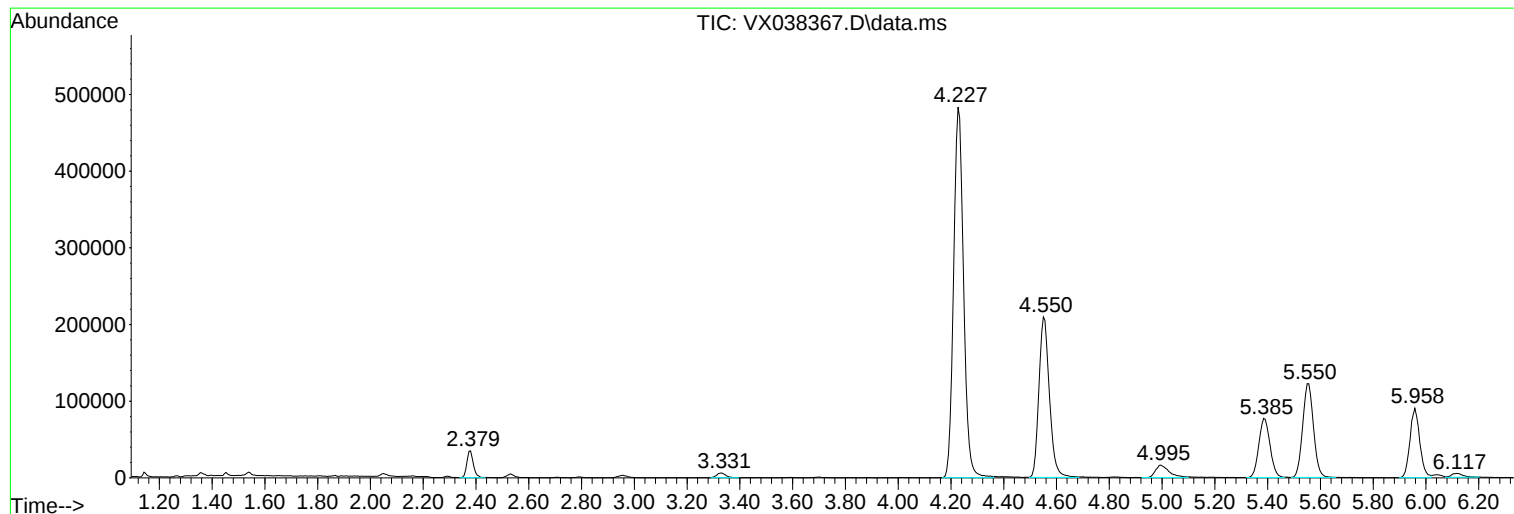
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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



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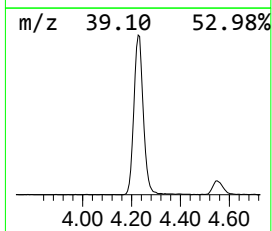
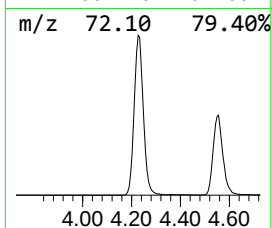
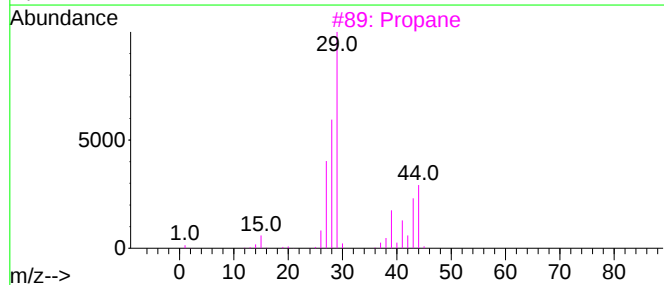
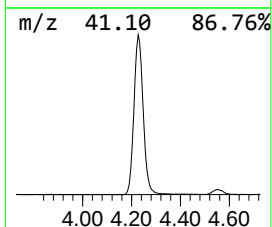
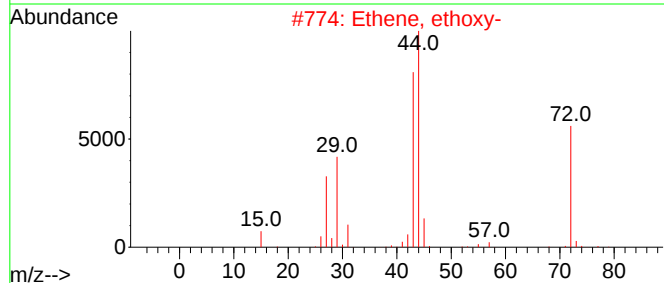
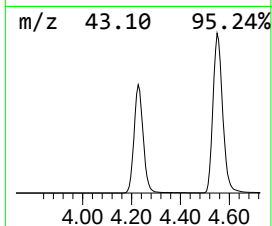
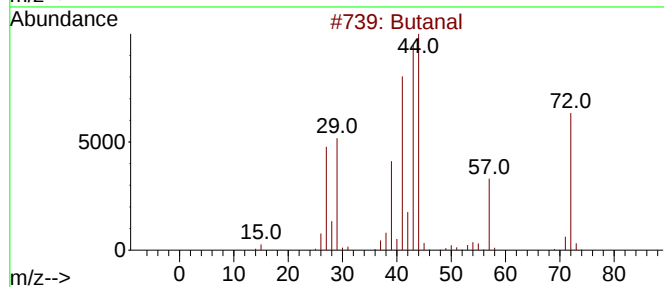
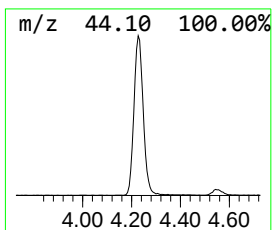
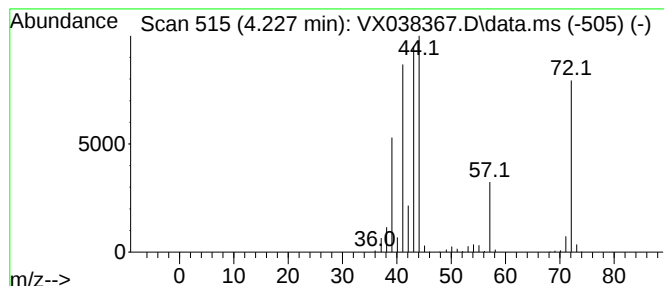
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Quant Title : SW846 8260

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

Peak Number 1 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	182.29 ug/l	1272620	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3			Propane	44	C3H8	000074-98-6	47
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
5			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38



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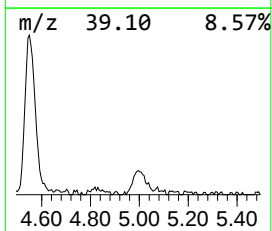
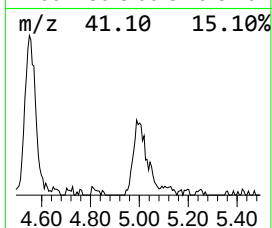
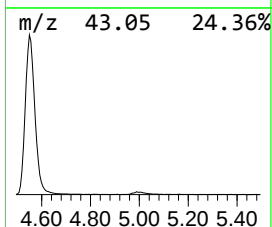
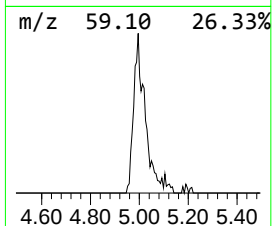
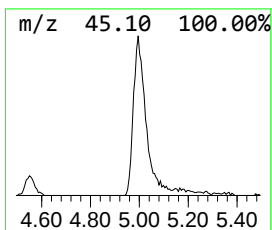
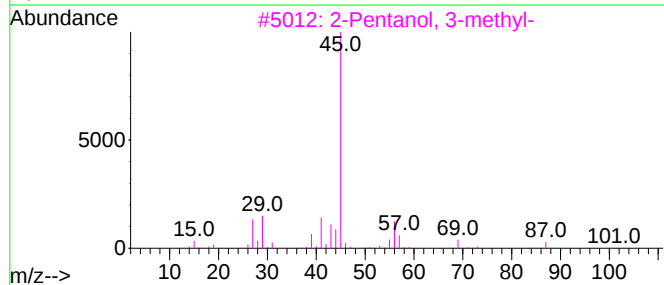
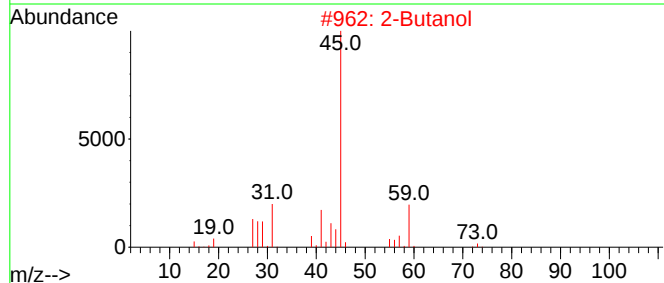
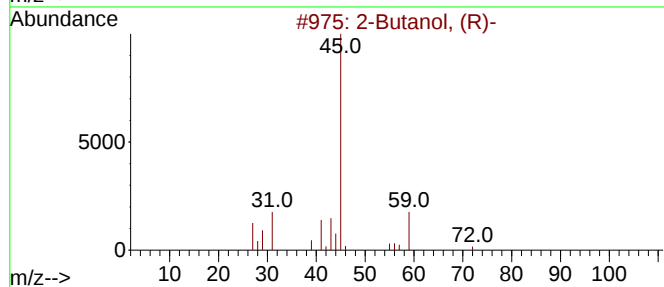
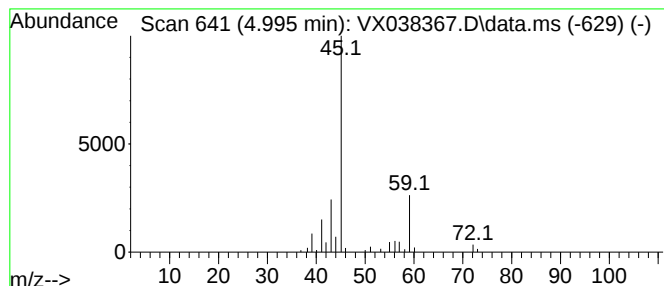
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Butanol, (R)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.995	8.50 ug/l	59365	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, (R)-			74	C4H10O	014898-79-4	74
2	2-Butanol			74	C4H10O	000078-92-2	72
3	2-Pentanol, 3-methyl-			102	C6H14O	000565-60-6	36
4	Propane, 2-ethoxy-			88	C5H12O	000625-54-7	9
5	2-Hexanol			102	C6H14O	000626-93-7	9



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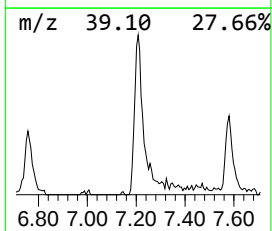
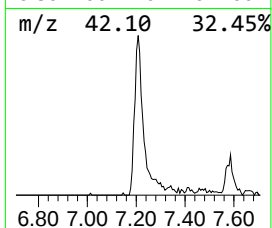
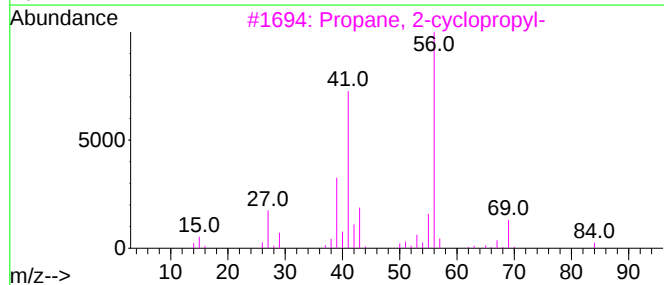
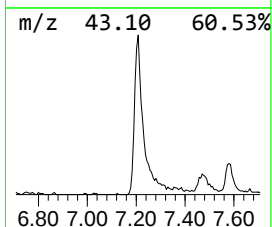
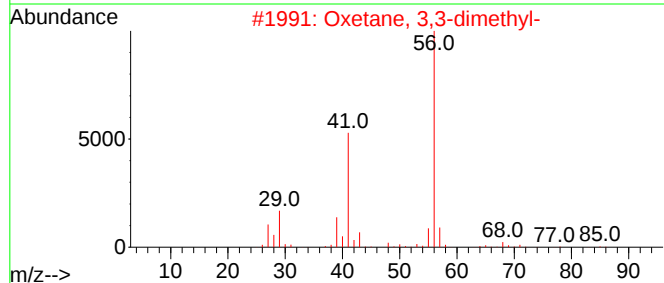
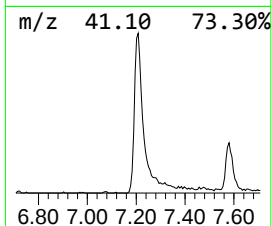
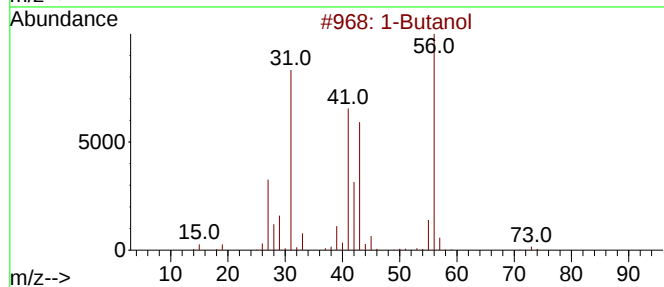
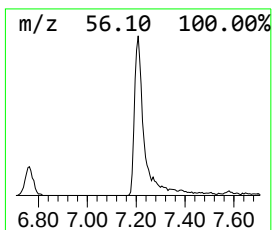
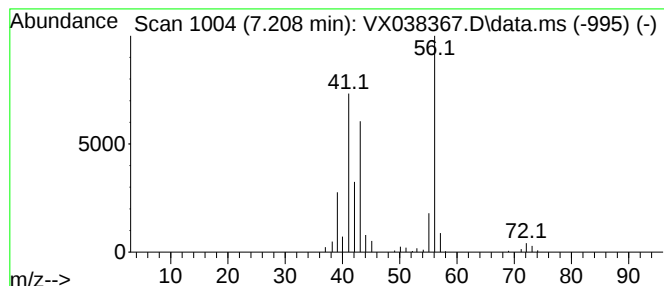
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	13.67 ug/l	131793	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	86
2			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	45
3			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
4			Pentane	72	C5H12	000109-66-0	9
5			Isobutane	58	C4H10	000075-28-5	9



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Instrument :
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ClientSampleId :
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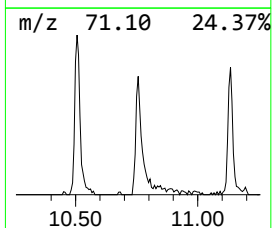
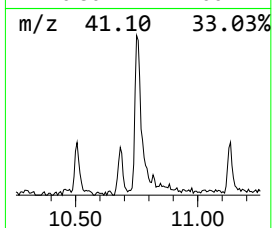
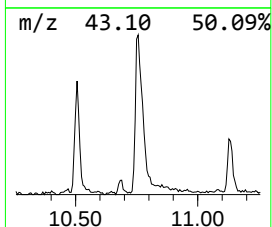
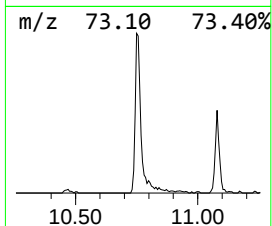
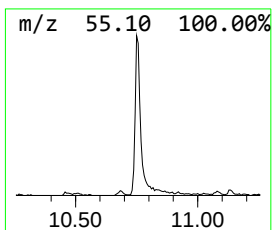
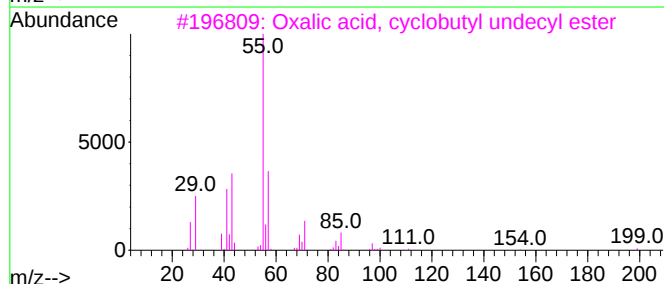
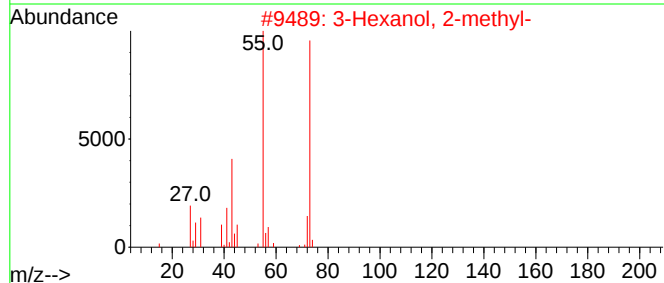
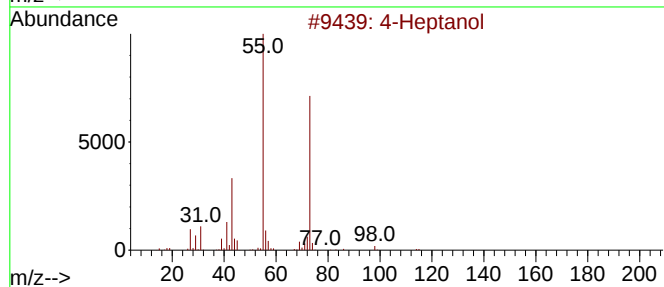
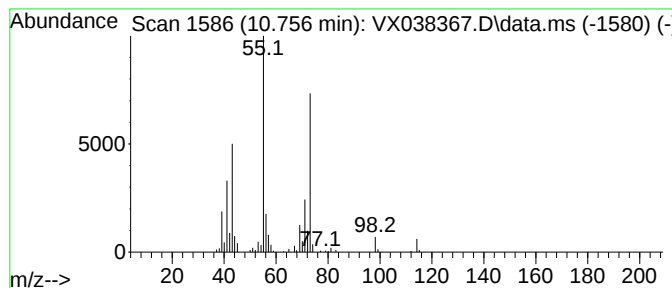
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 4 4-Heptanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.756	7.85 ug/l	103221	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	53
2			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	37
3			Oxalic acid, cyclobutyl undecyl ...	298	C17H30O4	1000309-70-2	35
4			1-Hepten-4-ol	114	C7H14O	003521-91-3	35
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	32



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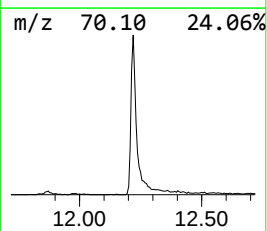
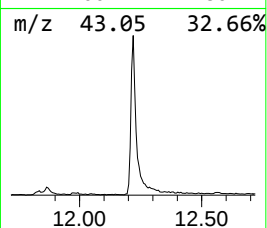
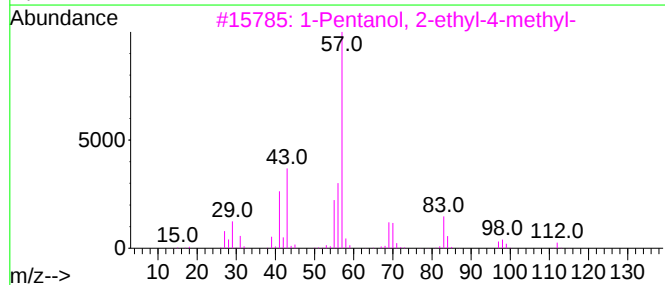
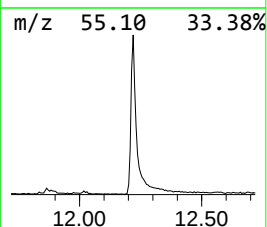
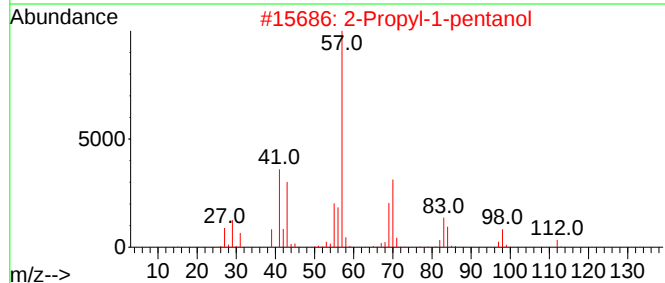
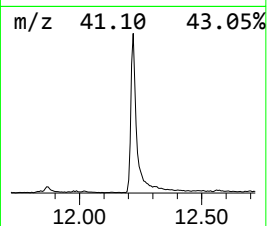
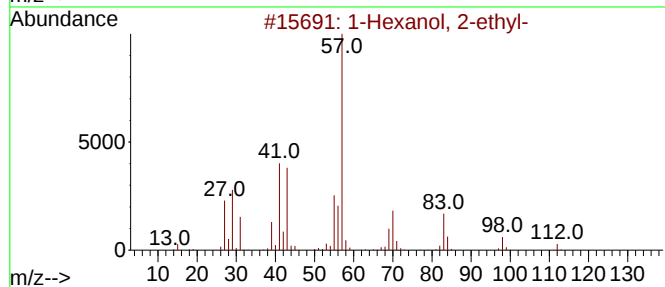
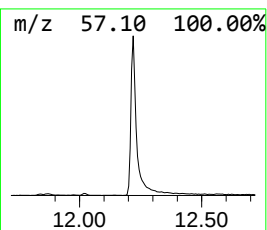
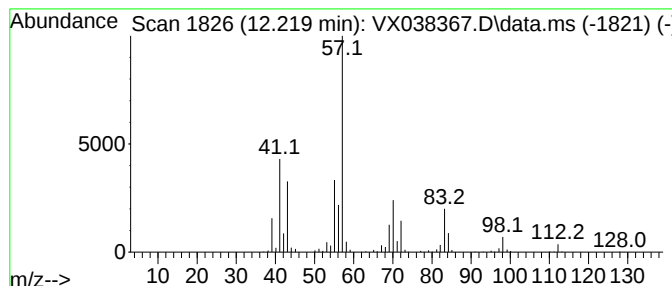
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	45.36 ug/l	664537	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			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
4			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	42
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	40



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	4.227	182.3	ug/l	1272620	1	5.556	349067	50.0
2-Butanol, (R)-	4.995	8.5	ug/l	59365	1	5.556	349067	50.0
1-Butanol	7.208	13.7	ug/l	131793	2	6.763	482035	50.0
4-Heptanol	10.756	7.8	ug/l	103221	3	10.055	657717	50.0
1-Hexanol, 2-et...	12.219	45.4	ug/l	664537	4	12.024	732503	50.0