

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062922\
 Data File : VX029859.D
 Acq On : 29 Jun 2022 14:10
 Operator : JC/MD
 Sample : N3491-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 AUD-1728

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\82X062822W.M

Title : SW846 8260

Signal : TIC: VX029859.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.300	192	199	211	rBV	139030	261883	2.23%	1.385%
2	3.995	456	477	478	rBV	35923	129440	1.10%	0.685%
3	5.391	693	706	722	rBV	133860	392368	3.34%	2.075%
4	5.556	722	733	747	rVB2	247533	693397	5.90%	3.667%
5	5.964	788	800	818	rBV	151595	407451	3.47%	2.155%
6	6.769	921	932	945	rBV	384832	930430	7.92%	4.921%
7	8.653	1233	1241	1249	rBV	791365	1232504	10.49%	6.518%
8	9.610	1384	1398	1427	rBV	2765644	11754364	100.00%	62.163%
9	10.055	1466	1471	1480	rVB	813384	1089603	9.27%	5.762%
10	11.086	1634	1640	1647	rVV	590013	767410	6.53%	4.058%
11	11.890	1765	1772	1781	rBV	61538	127649	1.09%	0.675%
12	12.024	1789	1794	1802	rVB	828636	999751	8.51%	5.287%
13	12.219	1821	1826	1831	rBV	86062	122803	1.04%	0.649%

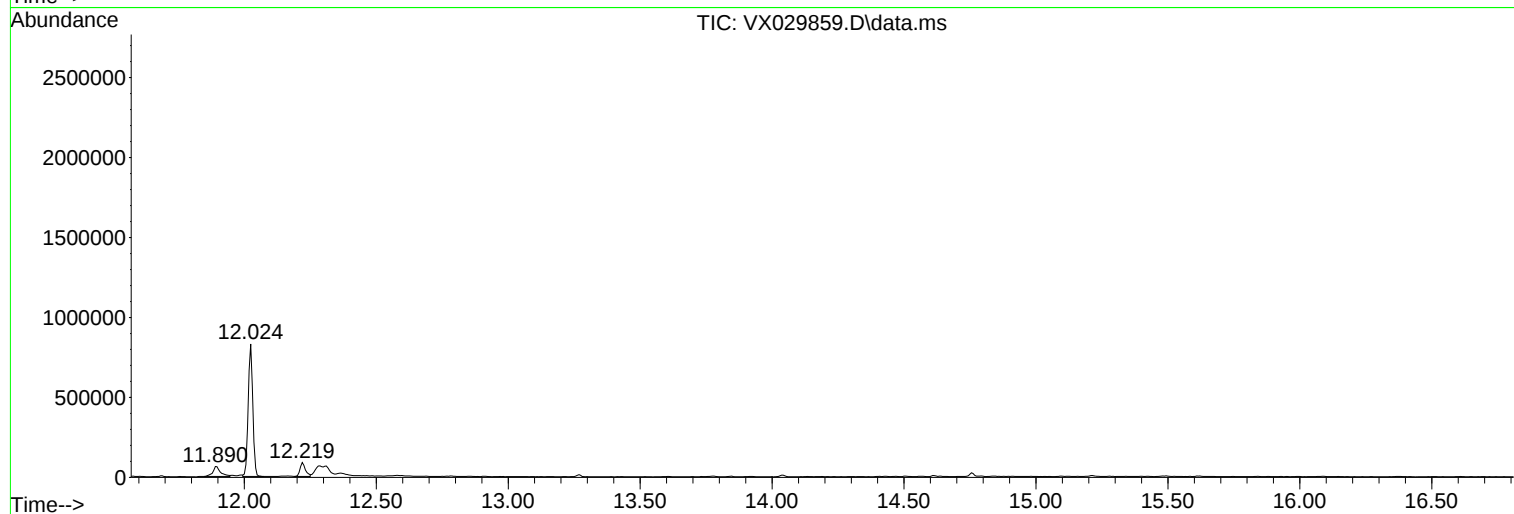
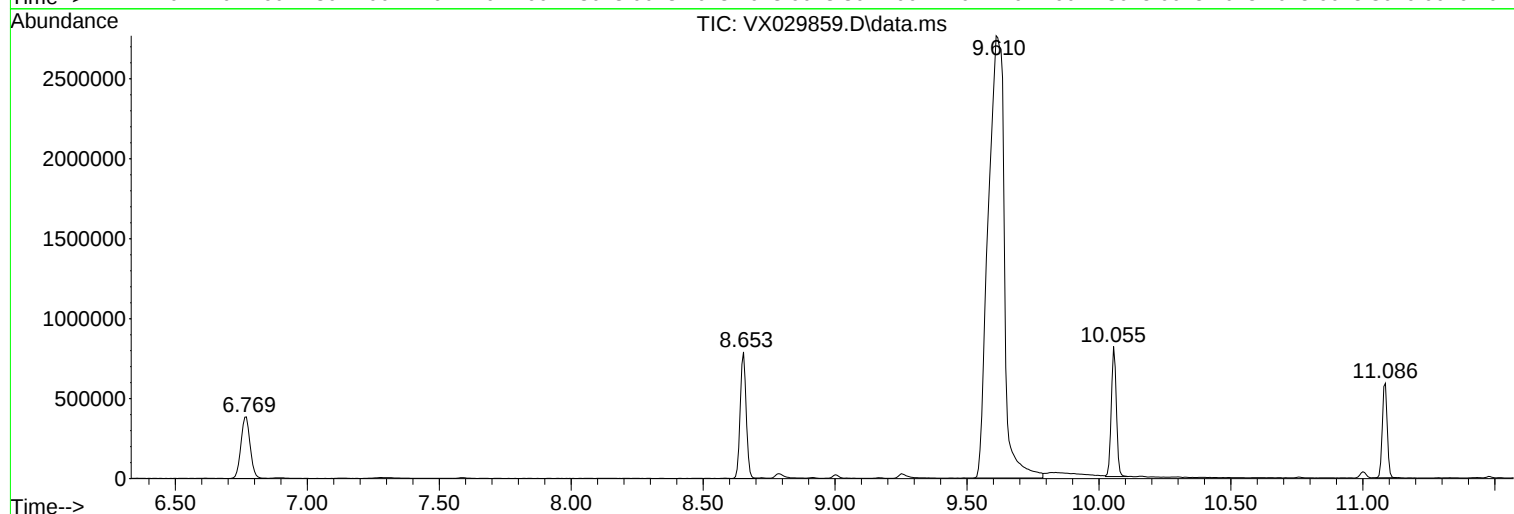
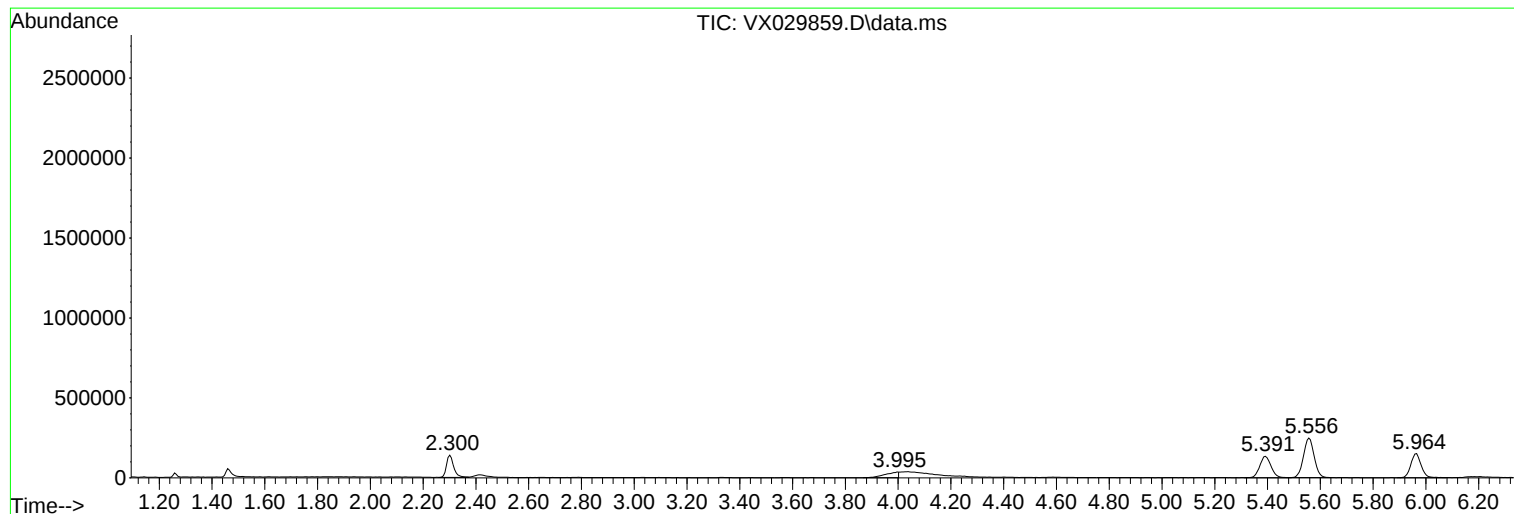
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Instrument :
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ClientSampleId :
AUD-1728

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

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



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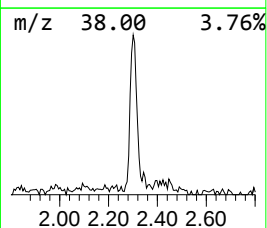
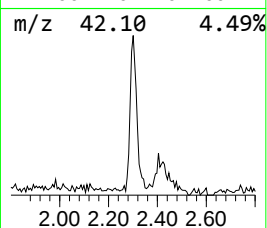
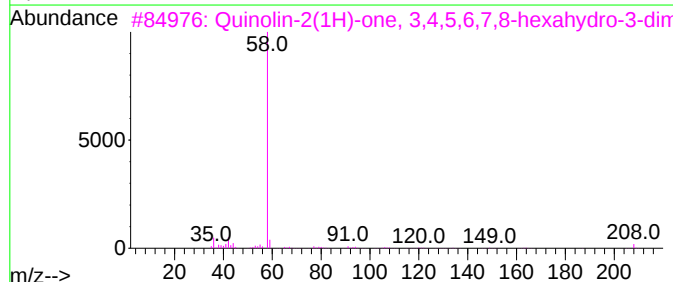
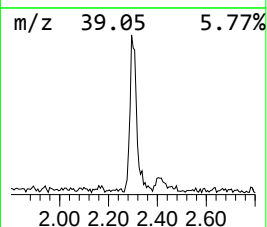
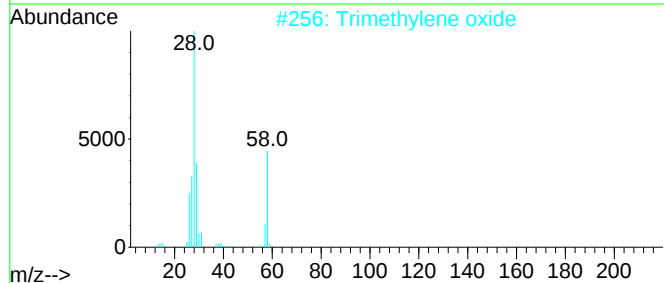
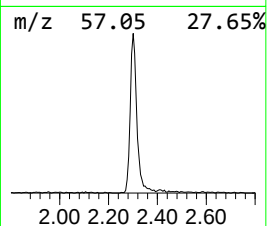
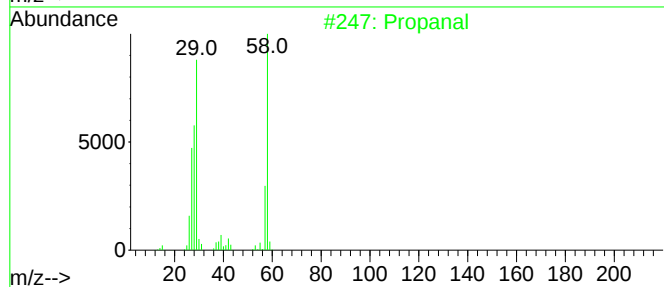
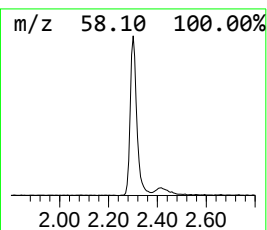
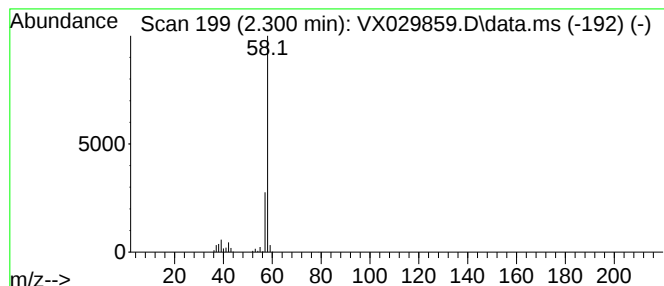
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.300	18.88 ug/l	261883	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	56
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	4



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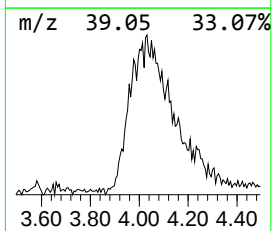
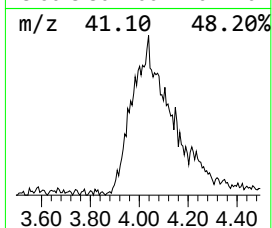
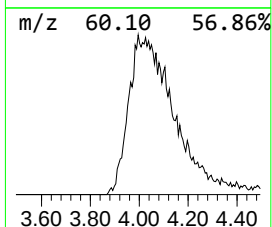
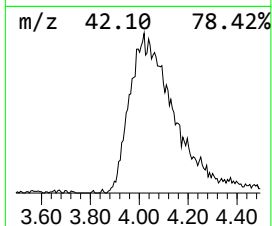
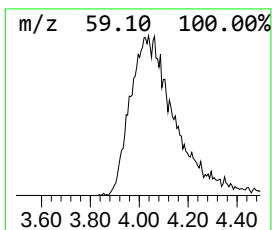
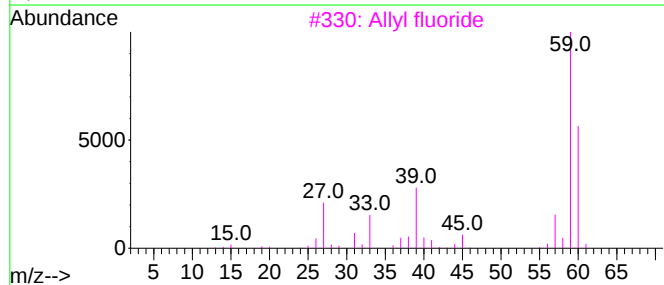
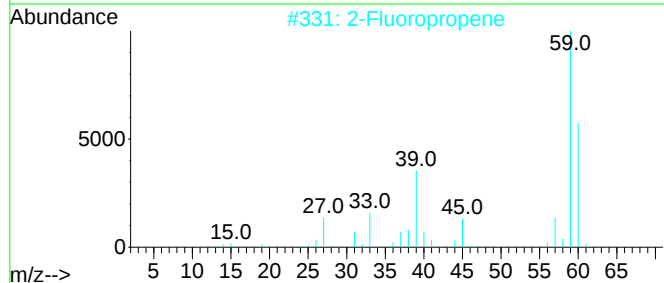
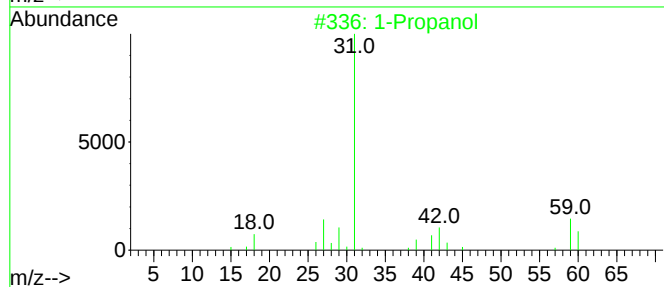
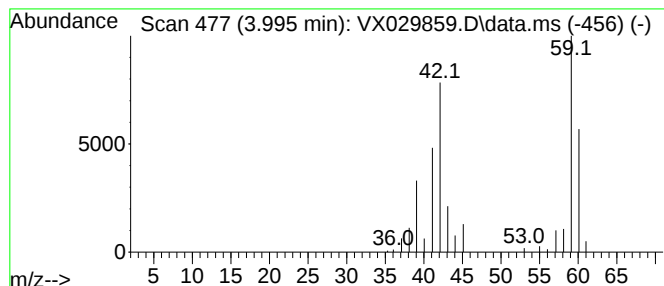
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Quant Title : SW846 8260

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

Peak Number 2 1-Propanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.995	9.33 ug/l	129440	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	72
2		2-Fluoropropene	60	C3H5F	001184-60-7	49
3		Allyl fluoride	60	C3H5F	000818-92-8	47
4		1,2-Butanediol	90	C4H10O2	000584-03-2	9
5		Butanoic acid, 2-hydroxy-, methy...	118	C5H10O3	029674-47-3	9



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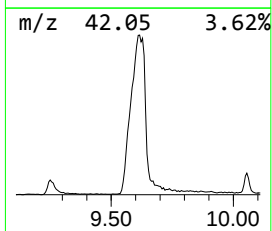
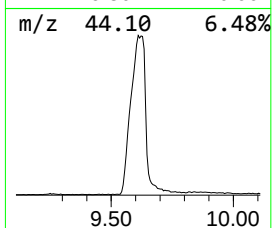
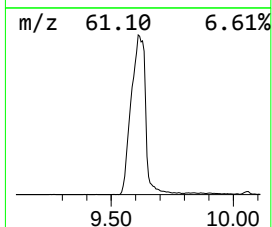
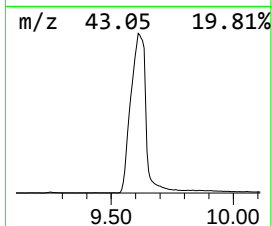
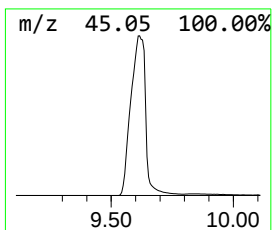
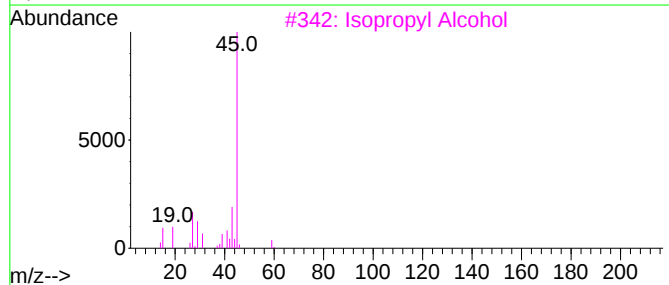
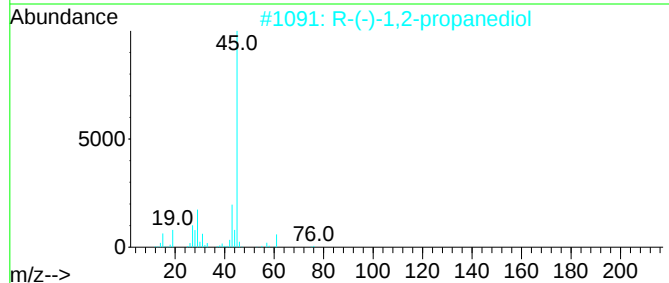
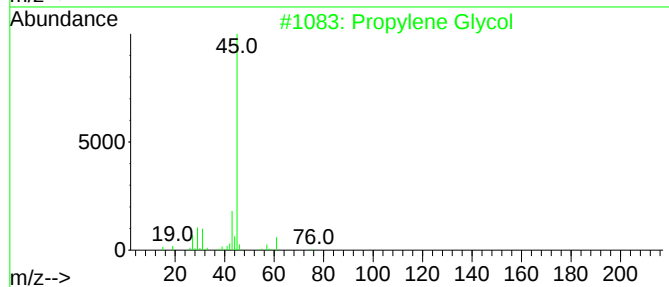
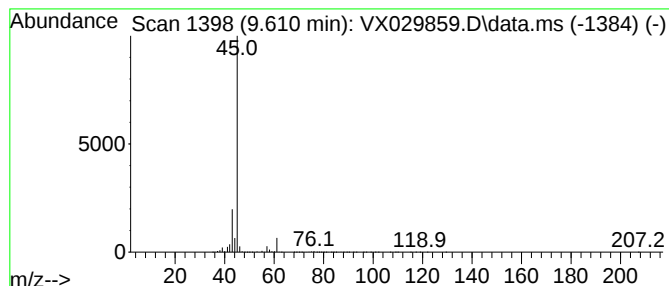
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Peak Number 3 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.610	539.39 ug/l	11754400	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40



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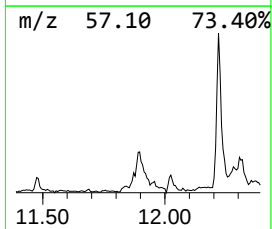
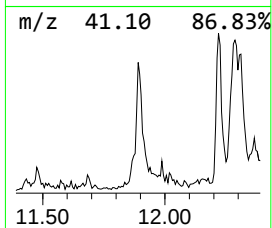
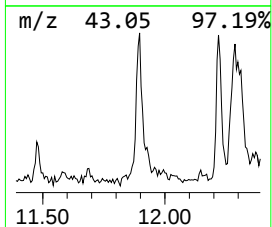
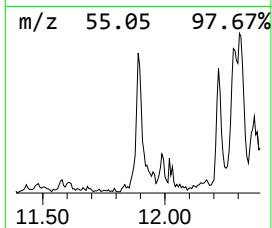
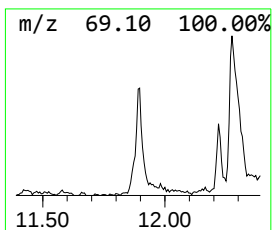
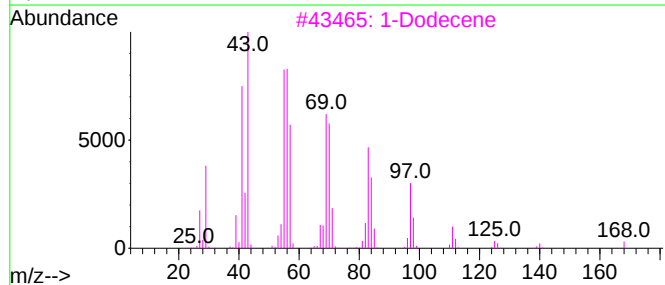
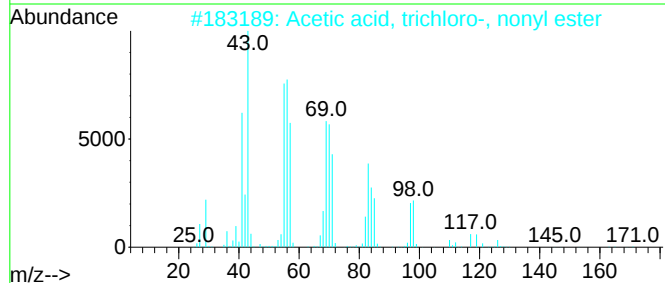
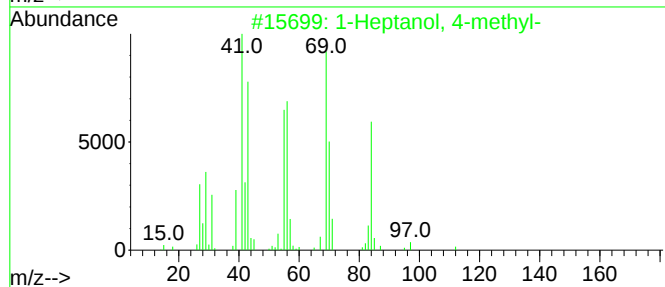
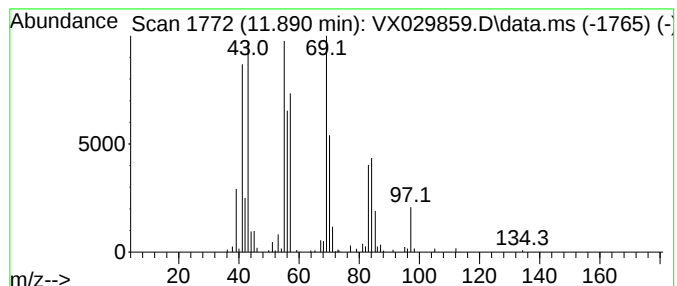
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TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heptanol, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.890	6.38 ug/l	127649	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	53
2			Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	50
3			1-Dodecene	168	C12H24	000112-41-4	47
4			1-Pentene, 3-methyl-	84	C6H12	000760-20-3	47
5			Pentane, 3-methylene-	84	C6H12	000760-21-4	43



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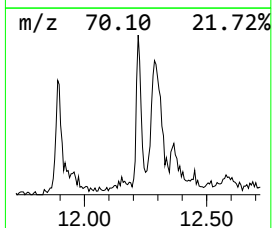
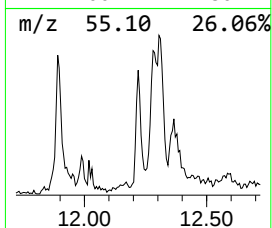
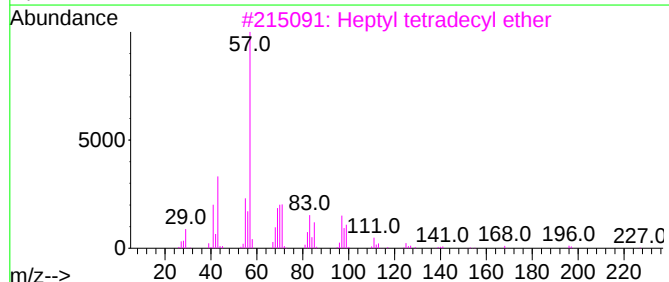
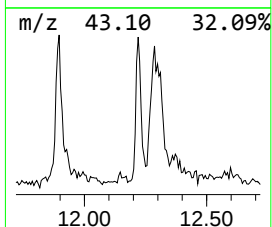
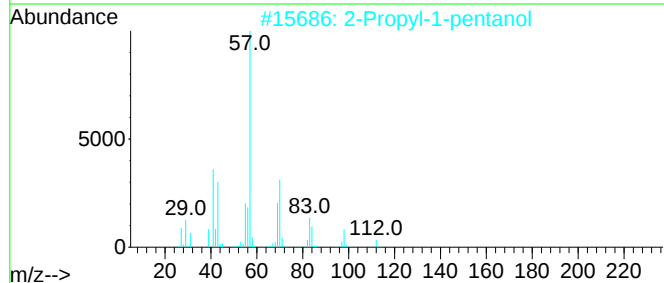
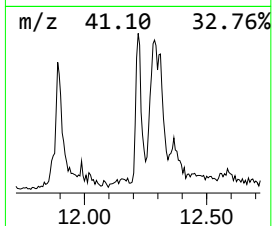
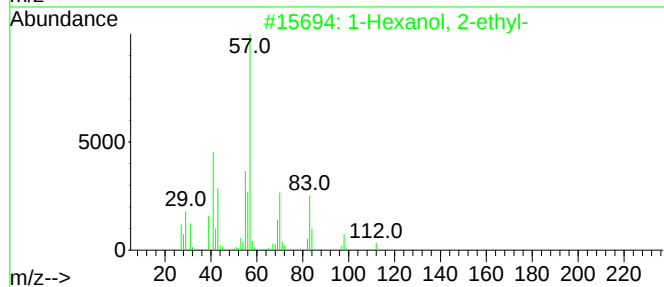
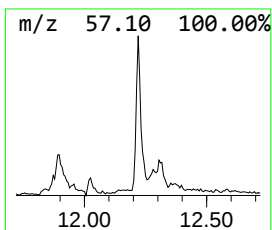
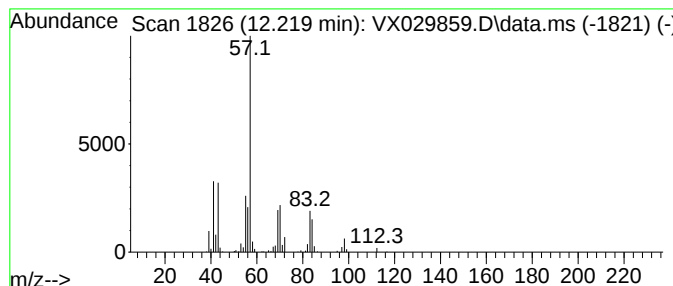
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	6.14 ug/l	122803	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	64
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	50
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal	2.300	18.9	ug/l	261883	1	5.556	693397	50.0
1-Propanol	3.995	9.3	ug/l	129440	1	5.556	693397	50.0
Propylene Glycol	9.610	539.4	ug/l	11754400	3	10.055	1089600	50.0
1-Heptanol, 4-m...	11.890	6.4	ug/l	127649	4	12.024	999751	50.0
1-Hexanol, 2-et...	12.219	6.1	ug/l	122803	4	12.024	999751	50.0