

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
 Data File : VU042938.D
 Acq On : 05 Apr 2021 18:06
 Operator : SY/MD
 Sample : M1903-09
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 31031

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_U\Method\82U032421W.M
 Title : SW846 8260

Signal : TIC: VU042938.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.552	351	377	394	rBV2	19107141	37036615	100.00%	65.929%
2	2.633	395	402	439	rVB	1329018	2773918	7.49%	4.938%
3	4.089	829	855	891	rBV2	656934	2556057	6.90%	4.550%
4	5.382	1244	1257	1276	rVB	209667	424776	1.15%	0.756%
5	6.256	1514	1529	1550	rBV2	431406	813412	2.20%	1.448%
6	7.906	2028	2042	2053	rBV	472564	812907	2.19%	1.447%
7	9.423	2501	2514	2525	rBV	454391	753693	2.03%	1.342%
8	9.491	2525	2535	2567	rVB	567697	981953	2.65%	1.748%
9	10.639	2879	2892	2902	rBV	378591	593698	1.60%	1.057%
10	10.710	2902	2914	2933	rVB	1266937	2032435	5.49%	3.618%
11	11.613	3186	3195	3218	rVB	374318	639099	1.73%	1.138%
12	11.819	3250	3259	3277	rVB	489015	766776	2.07%	1.365%
13	12.066	3322	3336	3364	rBV	3764395	5991541	16.18%	10.665%

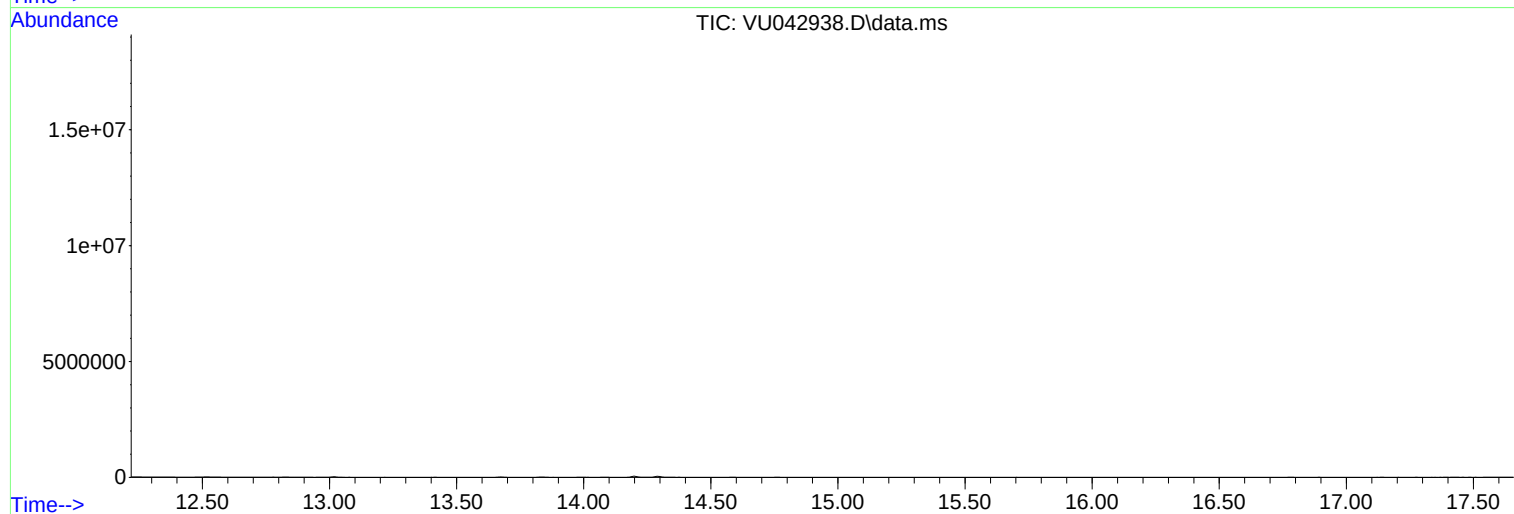
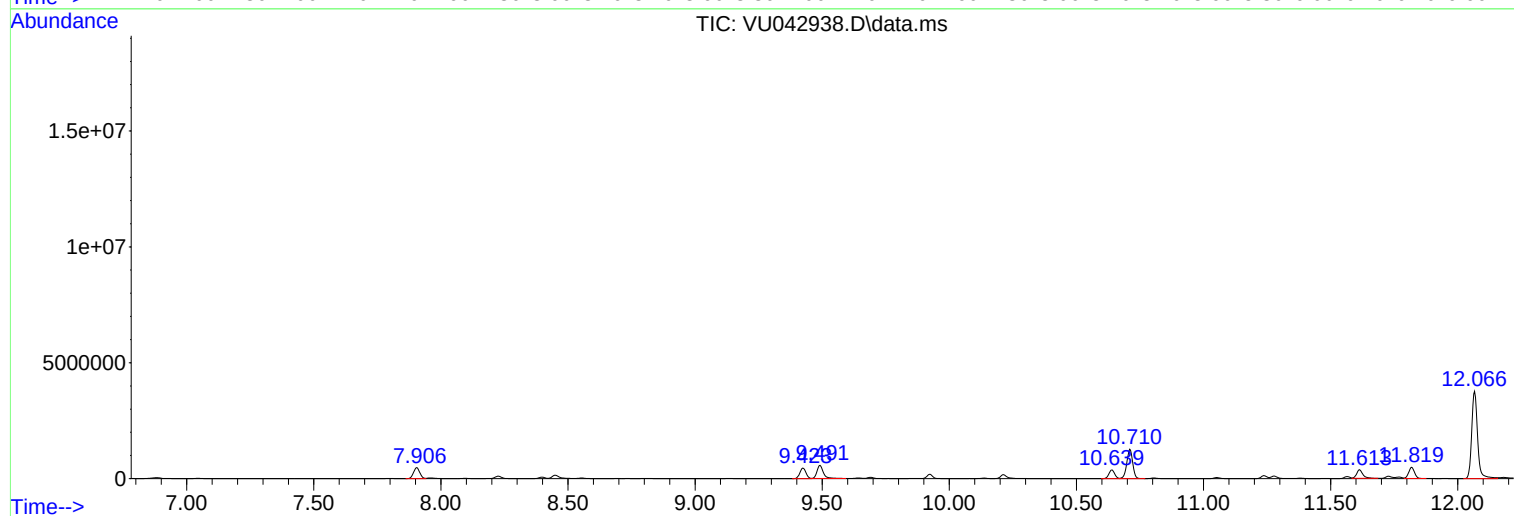
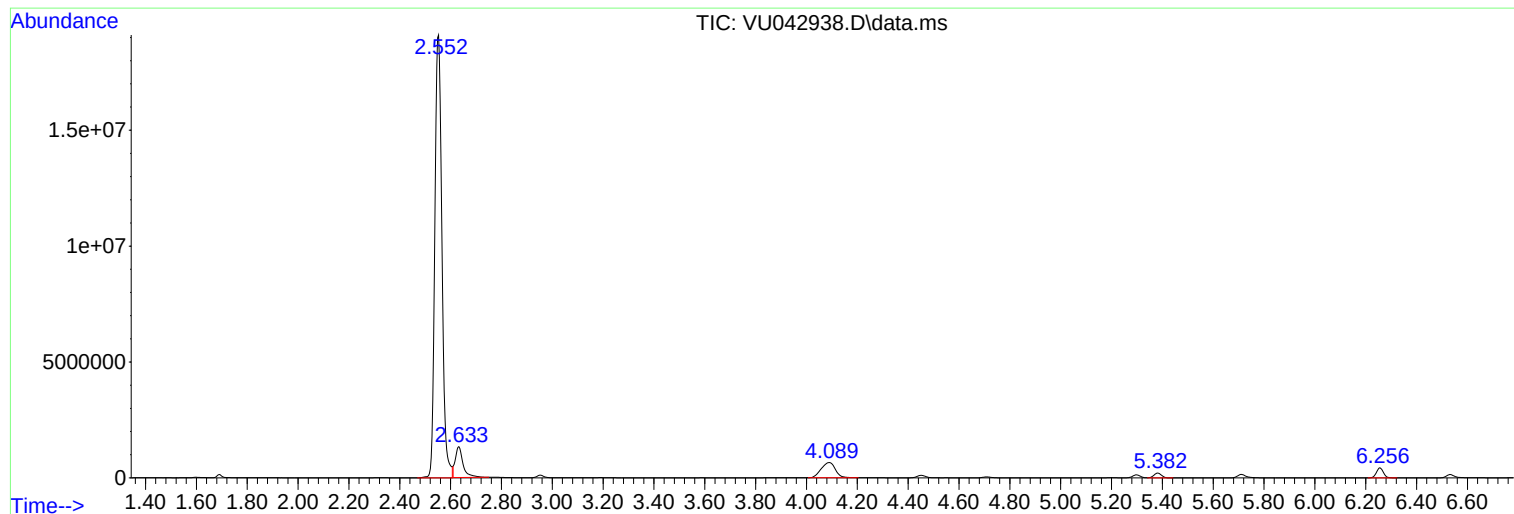
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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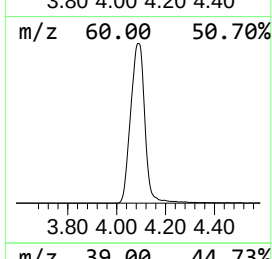
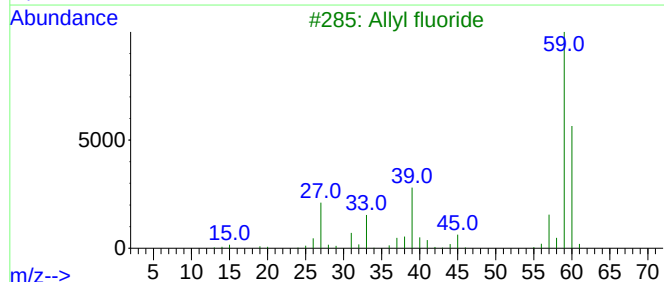
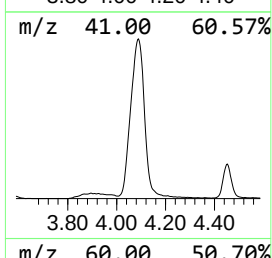
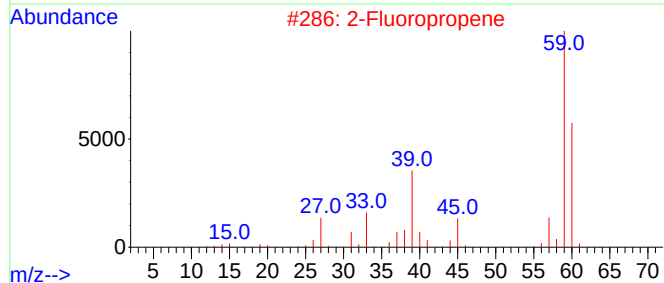
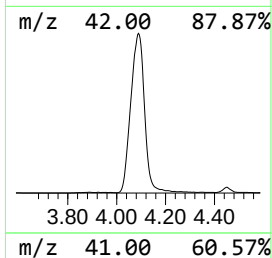
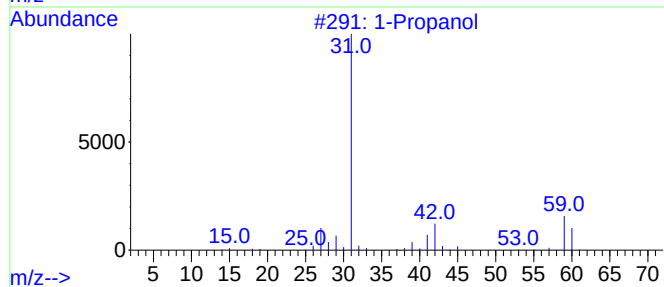
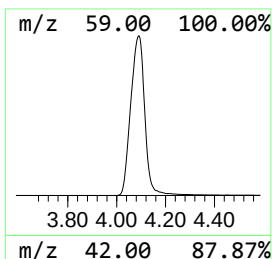
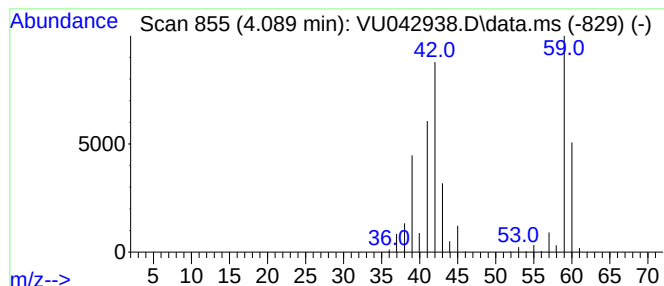
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Peak Number 1 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.089	300.87 ug/l	2556060	Pentafluorobenzene	5.382

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	64
2			2-Fluoropropene	60	C3H5F	001184-60-7	52
3			Allyl fluoride	60	C3H5F	000818-92-8	32
4			Cyclopropane	42	C3H6	000075-19-4	25
5			Propene	42	C3H6	000115-07-1	8



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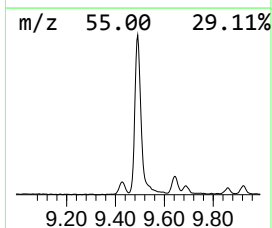
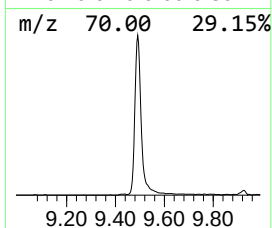
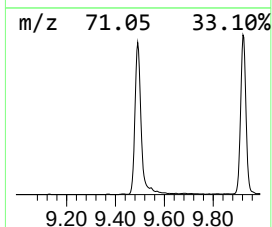
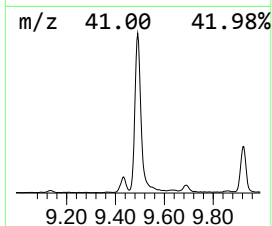
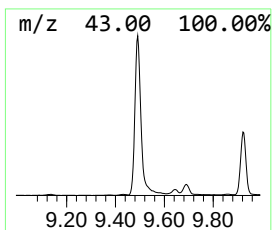
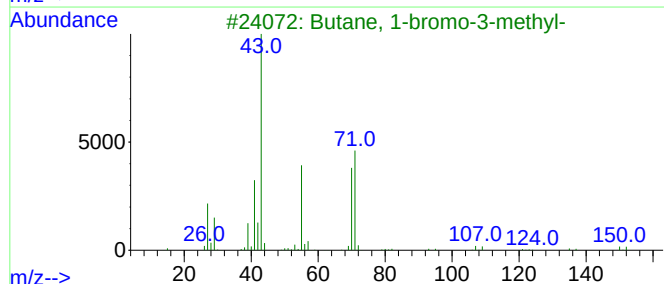
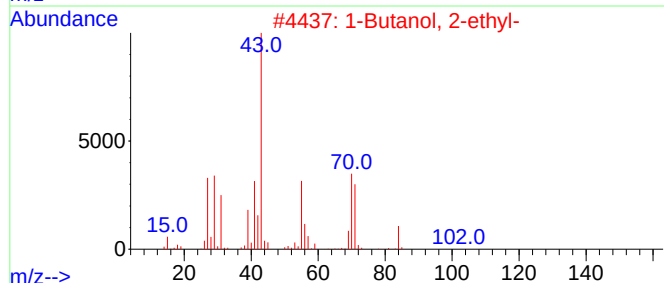
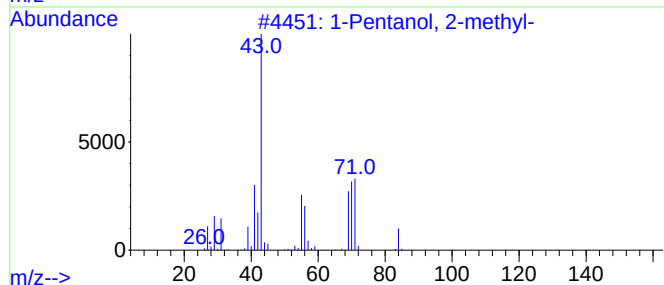
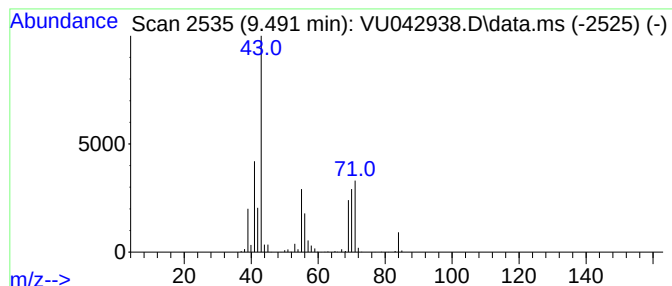
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Pentanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.491	65.14 ug/l	981953	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	90
2			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	64
3			Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	42
4			Pyrrolidine	71	C4H9N	000123-75-1	42
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38



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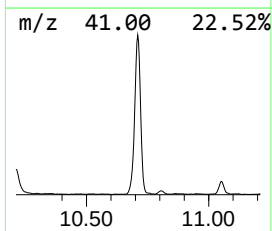
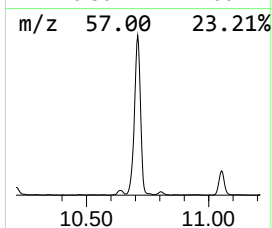
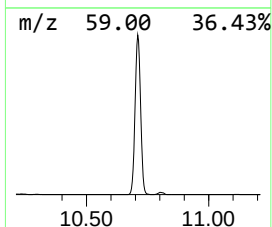
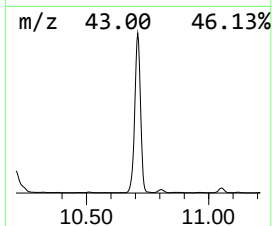
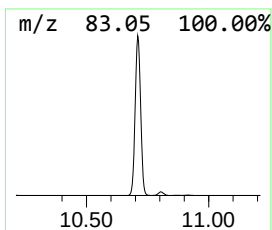
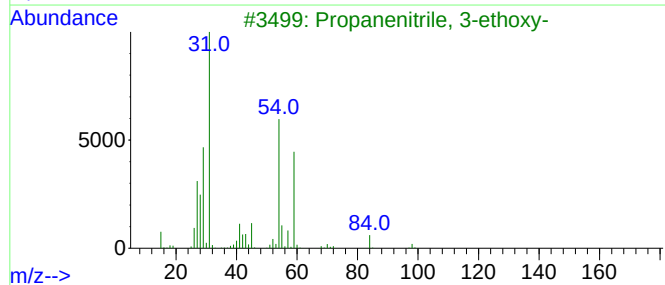
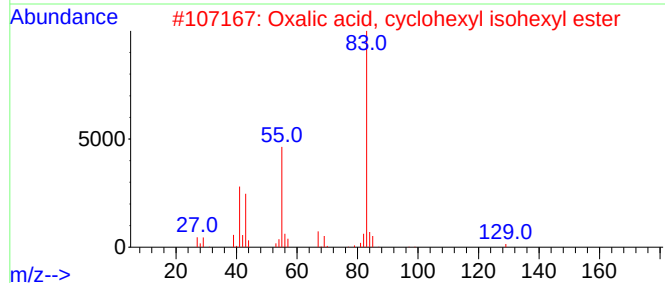
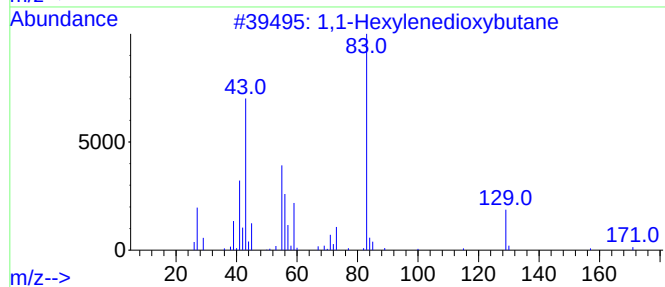
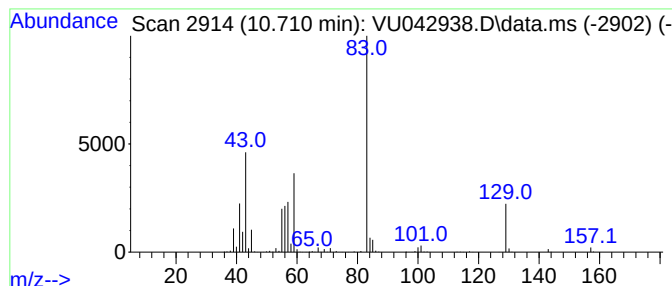
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,1-Hexylenedioxybutane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.710	132.53 ug/l	2032440	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	78
2			Oxalic acid, cyclohexyl isohexyl...	256	C14H24O4	1000309-30-7	28
3			Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	10
4			1H-Imidazol-2-amine	83	C3H5N3	007720-39-0	9
5			.alpha.-Amino-2,5-dihydro-5-meth...	157	C7H11NO3	018455-25-9	9



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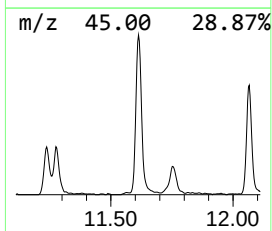
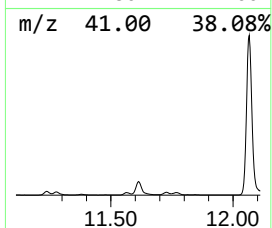
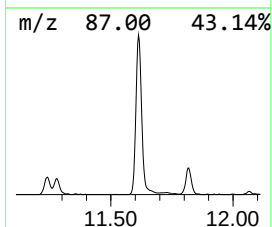
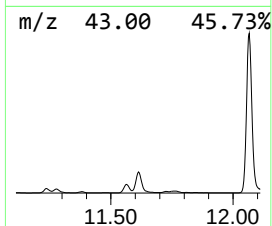
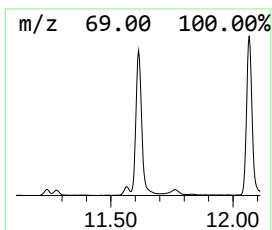
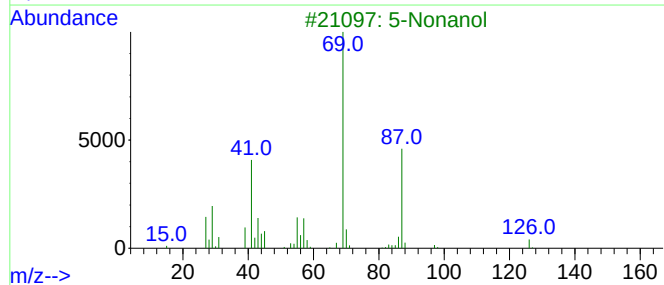
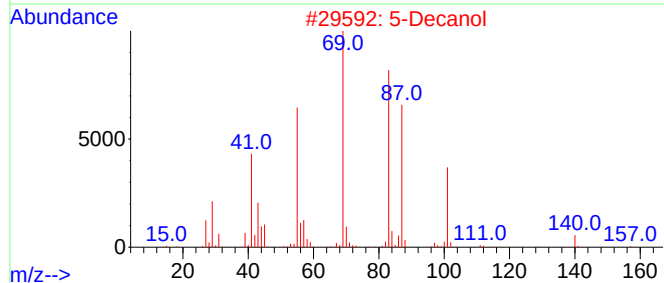
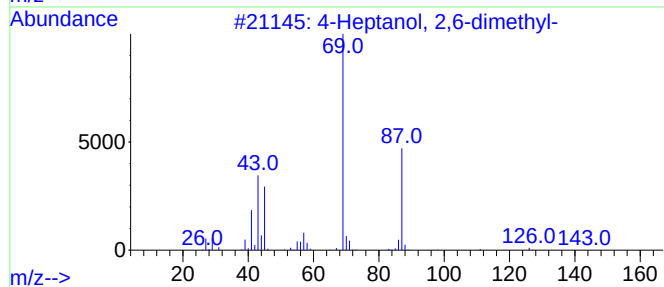
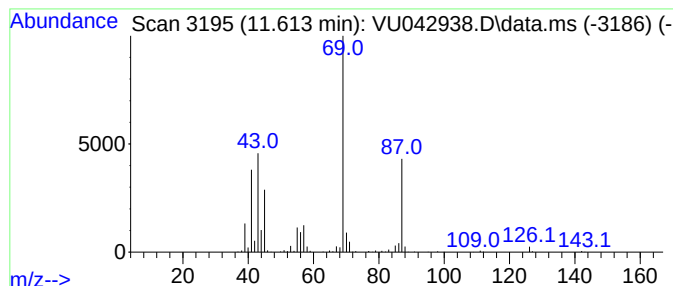
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Peak Number 4 4-Heptanol, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.613	41.67 ug/l	639099	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	83
2			5-Decanol	158	C10H22O	005205-34-5	78
3			5-Nonanol	144	C9H20O	000623-93-8	72
4			1,2-Hexanediol	118	C6H14O2	006920-22-5	72
5			4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	72



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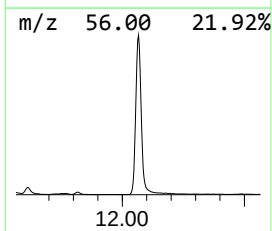
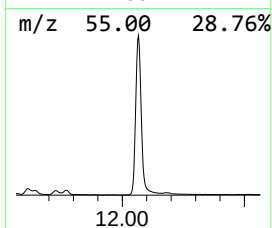
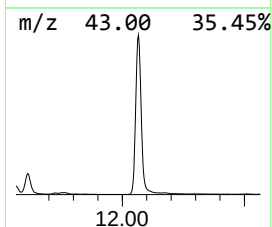
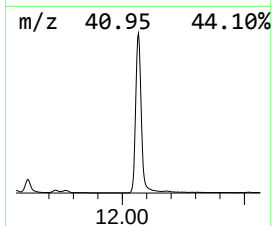
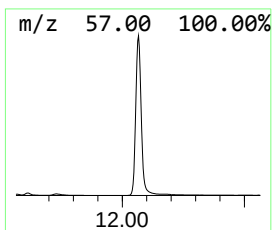
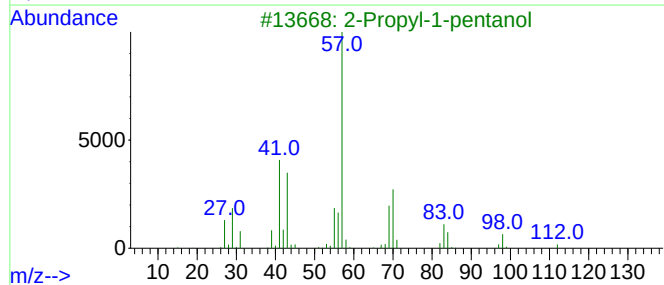
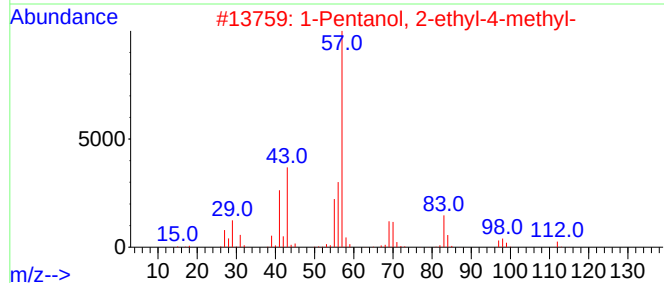
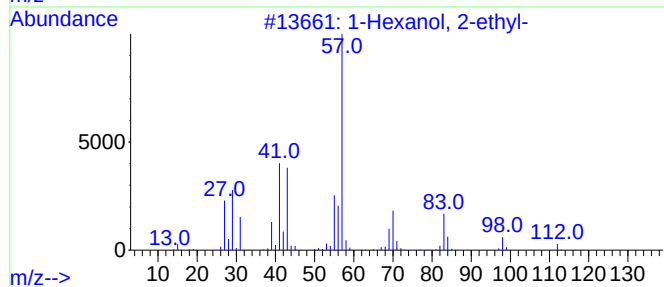
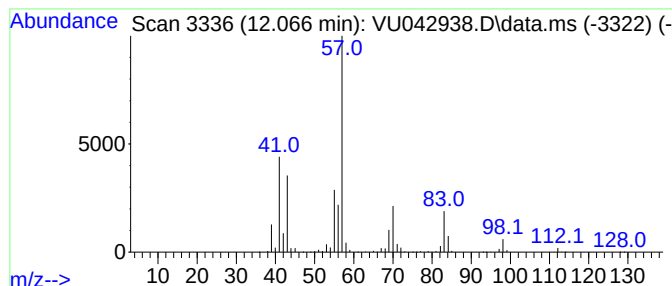
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.066	390.70 ug/l	5991540	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	45
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propanol	4.089	300.9	ug/l	2556060	1	5.382	424776	50.0
1-Pentanol, 2-m...	9.491	65.1	ug/l	981953	3	9.423	753693	50.0
1,1-Hexylenedio...	10.710	132.5	ug/l	2032440	4	11.819	766776	50.0
4-Heptanol, 2,6...	11.613	41.7	ug/l	639099	4	11.819	766776	50.0
1-Hexanol, 2-et...	12.066	390.7	ug/l	5991540	4	11.819	766776	50.0