

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX040620\
 Data File : VX015525.D
 Acq On : 06 Apr 2020 19:57
 Operator : JC/SP
 Sample : L2097-15 10X
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 40788

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.064	25	29	42	rBV	2557707	3066546	25.69%	4.052%
2	1.472	92	96	107	rBV	3320200	3525454	29.53%	4.658%
3	2.088	193	197	206	rVB	133334	207813	1.74%	0.275%
4	2.332	231	237	245	rVB	94439	147913	1.24%	0.195%
5	2.417	245	251	266	rVB	964348	1535755	12.87%	2.029%
6	2.576	271	277	288	rVB	281898	505681	4.24%	0.668%
7	3.003	337	347	356	rVB3	57164	154140	1.29%	0.204%
8	3.917	490	497	506	rBV	163082	406035	3.40%	0.536%
9	4.649	607	617	630	rBV2	123388	389124	3.26%	0.514%
10	5.472	737	752	765	rBV2	680033	1967618	16.48%	2.600%
11	5.636	768	779	792	rVV	1175526	3243759	27.17%	4.286%
12	6.032	834	844	859	rBV	770323	2003117	16.78%	2.647%
13	6.837	964	976	985	rBV	1848380	4535561	38.00%	5.993%
14	6.941	985	993	1005	rVB	4495595	10191861	85.38%	13.466%
15	7.270	1039	1047	1056	rBV	3599715	7414977	62.12%	9.797%
16	7.349	1056	1060	1069	rVB	71398	147798	1.24%	0.195%
17	8.697	1273	1281	1298	rBV	3814715	6141015	51.45%	8.114%
18	9.044	1332	1338	1344	rBV	125801	200129	1.68%	0.264%
19	9.203	1360	1364	1372	rVB	107328	156423	1.31%	0.207%
20	10.099	1505	1511	1522	rVB	4078994	5599609	46.91%	7.398%
21	10.355	1547	1553	1563	rBV	8700178	11936691	100.00%	15.771%
22	11.123	1673	1679	1686	rBV	3847032	4854863	40.67%	6.414%
23	11.190	1686	1690	1695	rVB	189439	244897	2.05%	0.324%
24	12.062	1828	1833	1841	rVB	5125315	6374308	53.40%	8.422%
25	12.257	1861	1865	1870	rBV	108730	173287	1.45%	0.229%
26	15.153	2335	2340	2343	rBV	82776	129217	1.08%	0.171%
27	15.256	2350	2357	2361	rVV3	108854	173892	1.46%	0.230%
28	16.147	2498	2503	2509	rBV	139343	259324	2.17%	0.343%

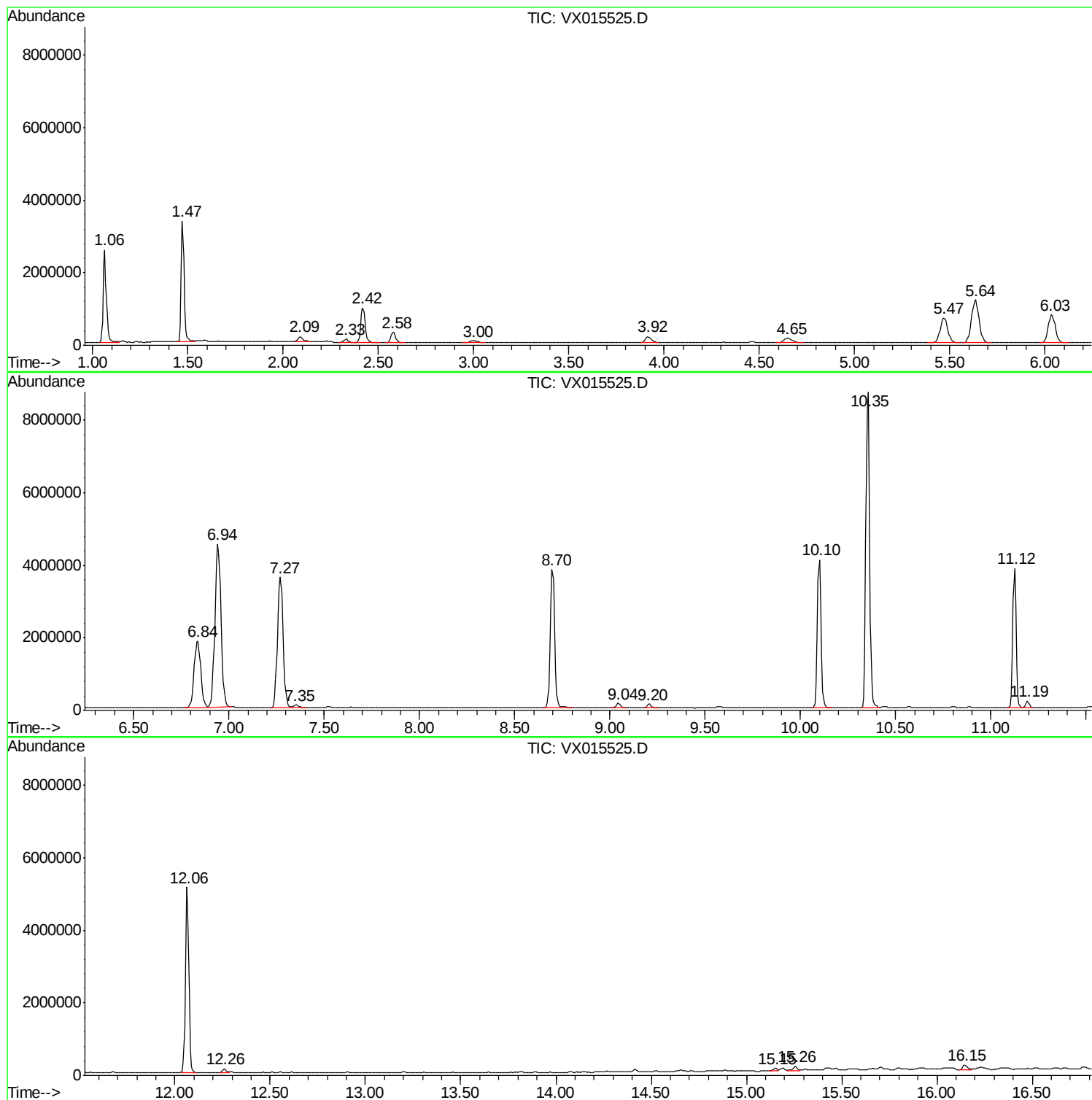
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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



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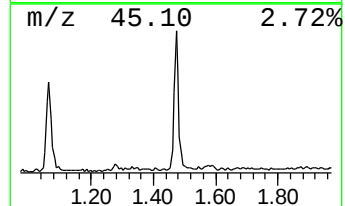
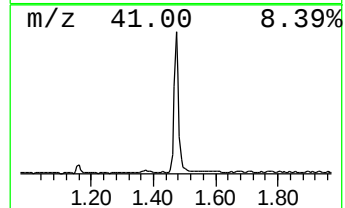
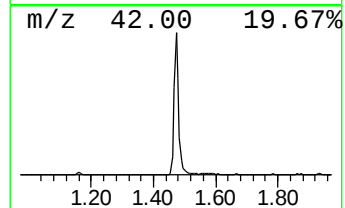
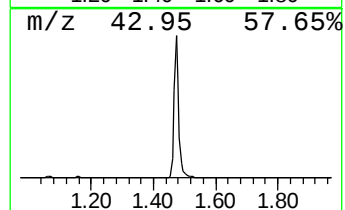
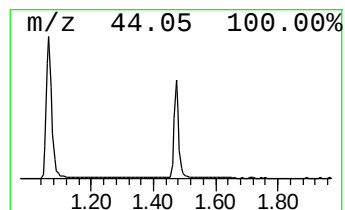
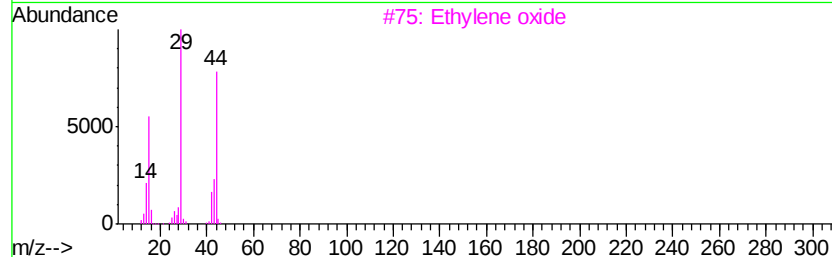
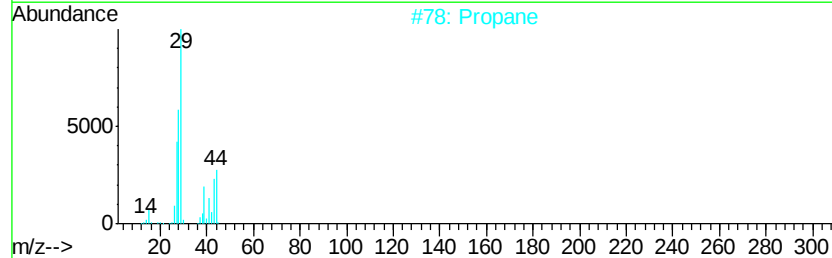
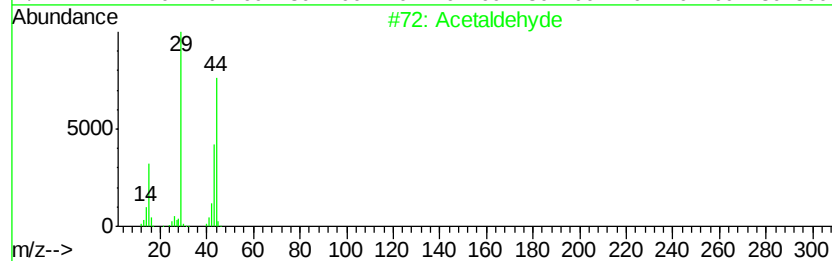
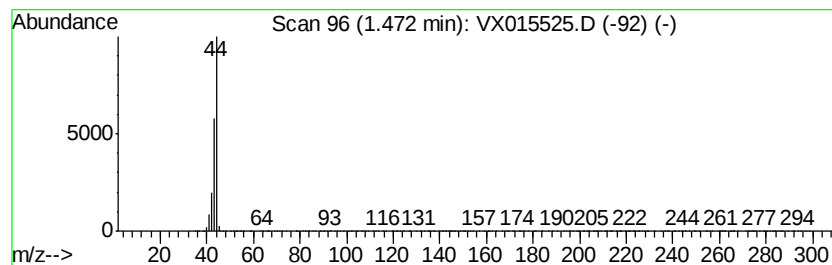
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	54.34 ug/l	3525450	Pentafluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetaldehydve	44	C2H4O	000075-07-0	64
2		Propane	44	C3H8	000074-98-6	5
3		Ethylene oxide	44	C2H4O	000075-21-8	5
4		Alanine	89	C3H7NO2	000056-41-7	4
5		Ethyne, fluoro-	44	C2HF	002713-09-9	3



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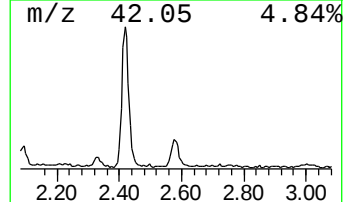
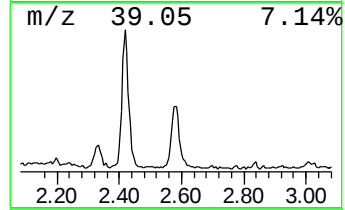
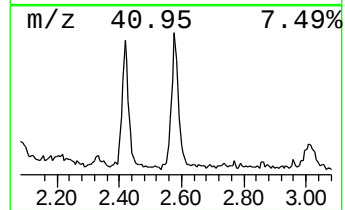
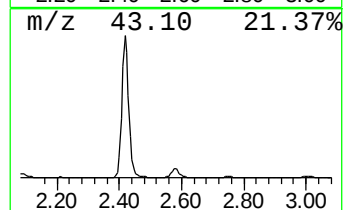
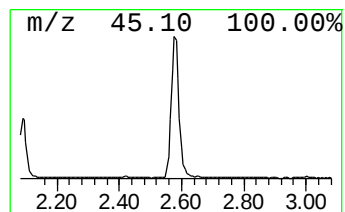
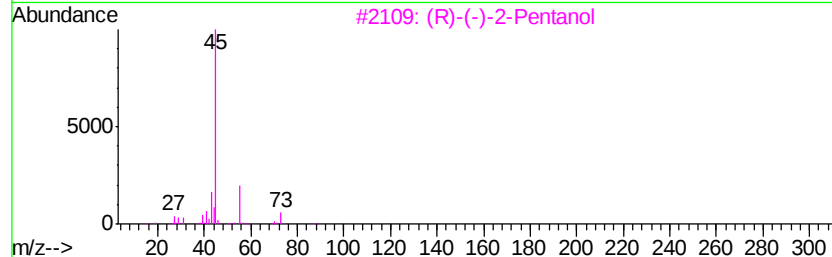
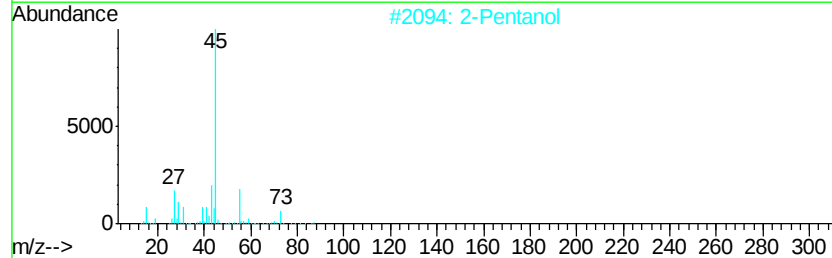
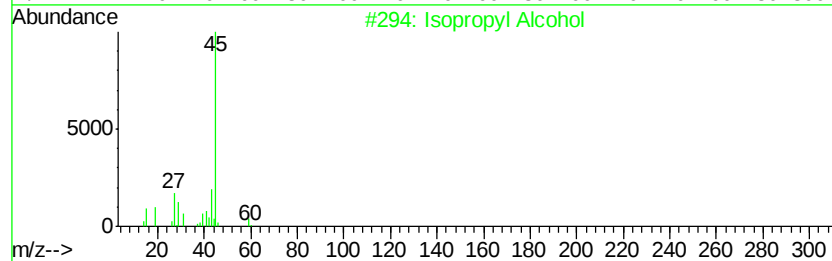
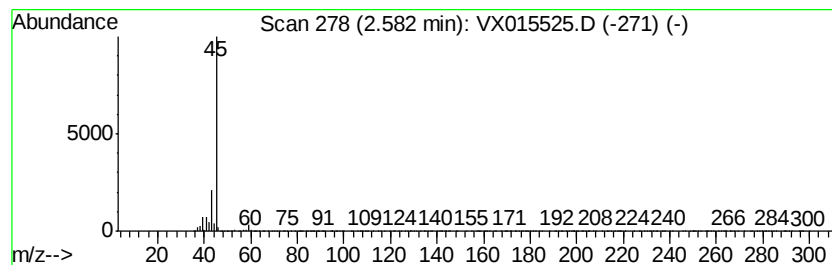
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Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.58	7.79 ug/l	505681	Pentafluorobenzene	5.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2		2-Pentanol	88	C5H12O	006032-29-7	9
3		(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	9
4		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
5		(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	9



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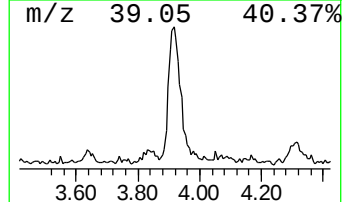
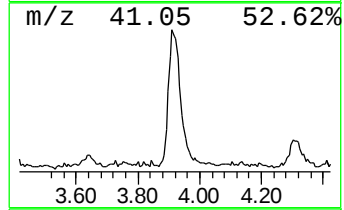
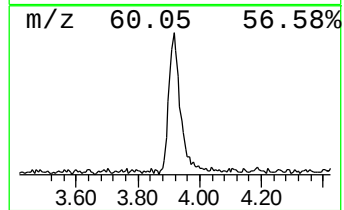
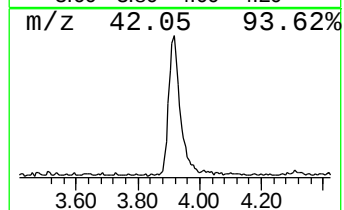
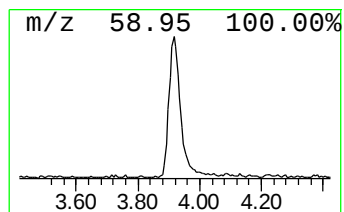
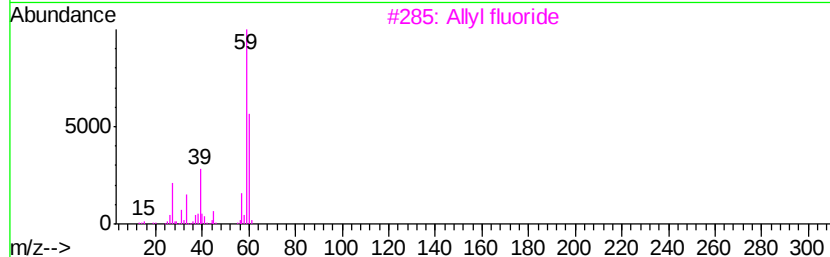
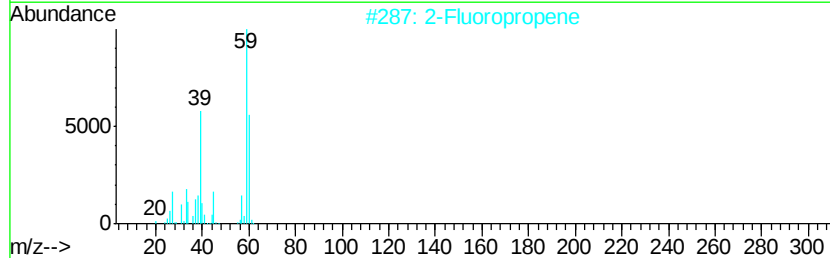
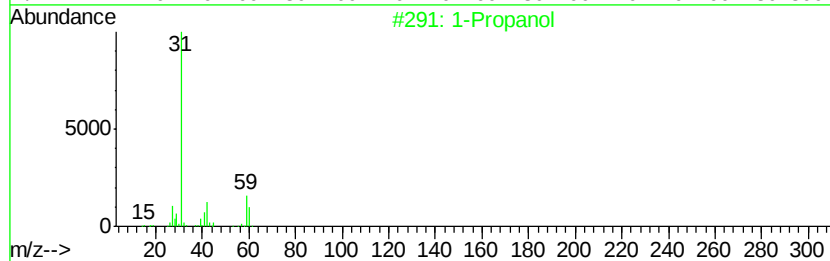
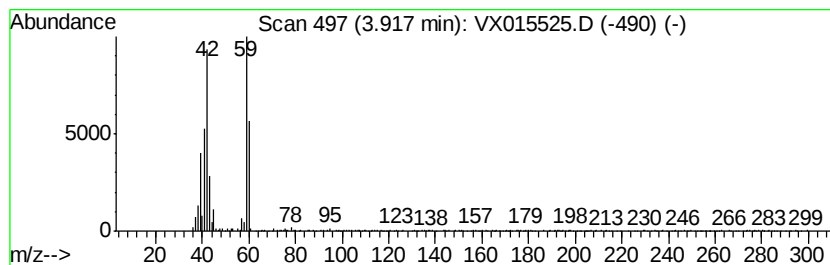
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Peak Number 4 1-Propanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.92	6.26 ug/l	406035	Pentafluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	59
2		2-Fluoropropene	60	C3H5F	001184-60-7	58
3		Allyl fluoride	60	C3H5F	000818-92-8	38
4		Erythro-2-bromo-3-pentanol	166	C5H11BrO	1000288-18-2	33
5		1-Bromo-2-methyl-2-propanol	152	C4H9BrO	038254-49-8	28



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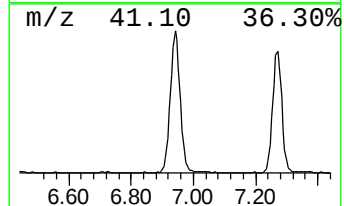
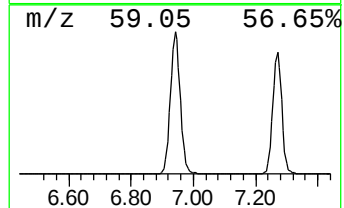
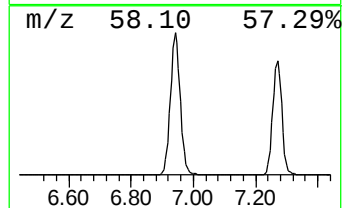
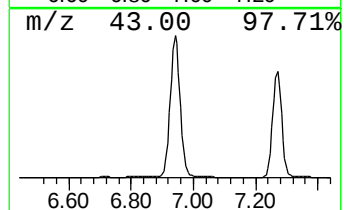
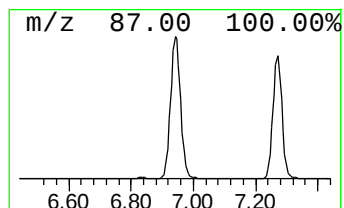
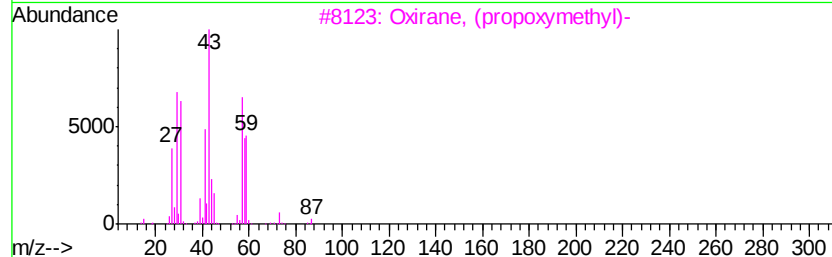
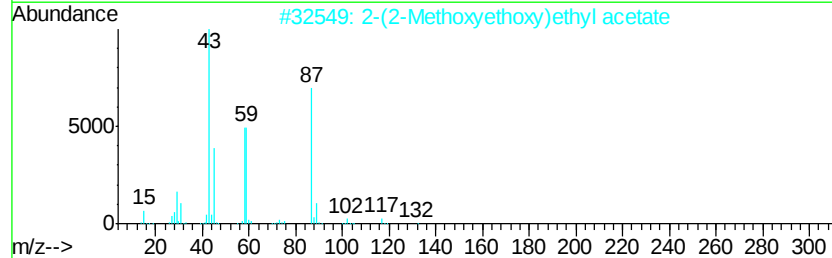
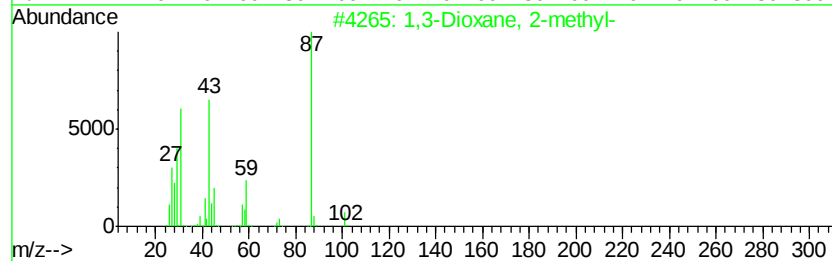
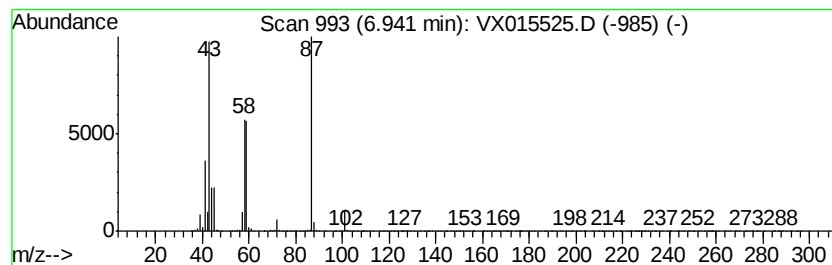
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1,3-Dioxane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	112.36 ug/l	10191900	1,4-Difluorobenzene	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	53
2		2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	45
3		Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	43
4		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	32
5		1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	23



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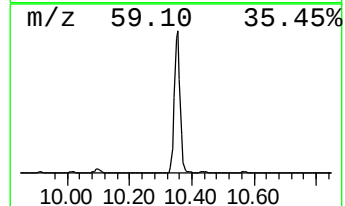
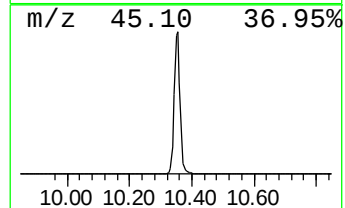
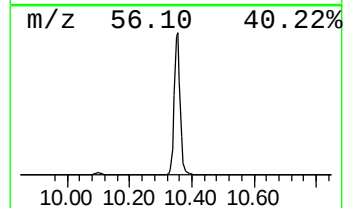
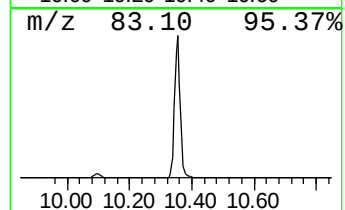
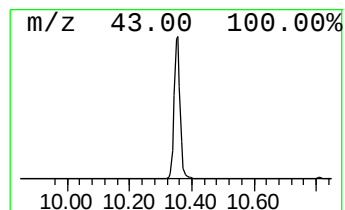
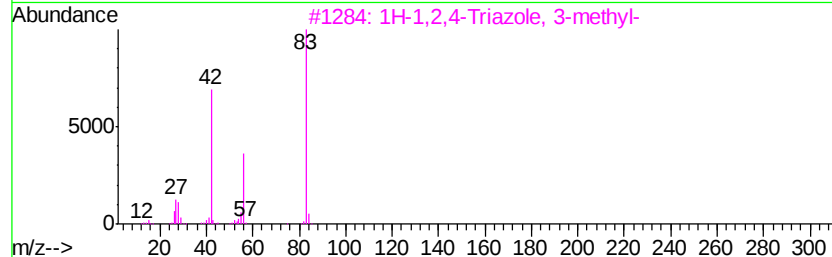
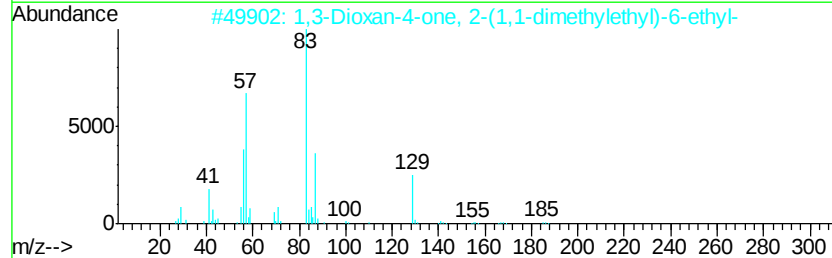
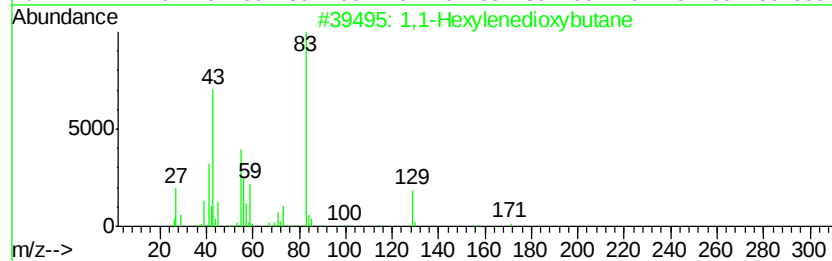
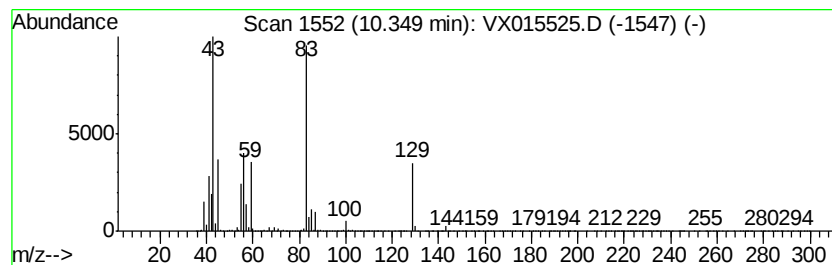
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Peak Number 7 unknown10.35 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	106.59 ug/l	11936700	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	38
2		1,3-Dioxan-4-one, 2-(1,1-dimethyl-...	186	C10H18O3	113505-80-9	33
3		1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	32
4		Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	25
5		Oxalic acid, cyclohexyl butyl ester	228	C12H20O4	1000309-30-5	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.47	54.3	ug/l	3525450	1	5.64	3243760	50.0
Isopropyl Alcohol	2.58	7.8	ug/l	505681	1	5.64	3243760	50.0
1-Propanol	3.92	6.3	ug/l	406035	1	5.64	3243760	50.0
1,3-Dioxane, 2-me...	6.94	112.4	ug/l	10191900	2	6.84	4535560	50.0
unknown10.35	10.35	106.6	ug/l	11936700	3	10.10	5599610	50.0