

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091521\
 Data File : VN068487.D
 Acq On : 15 Sep 2021 16:34
 Operator : JC/MD
 Sample : M3759-05
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31201

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_N\methods\82N090721W.M

Title : SW846 8260

Signal : TIC: VN068487.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.588	210	223	241	rBV	200970	349073	4.60%	1.622%
2	4.146	780	804	847	rBV	2682379	7582851	100.00%	35.244%
3	6.578	1688	1711	1772	rBV2	437481	1455021	19.19%	6.763%
4	7.069	1873	1894	1918	rBV5	56105	165483	2.18%	0.769%
5	8.024	2223	2250	2261	rBV2	318646	767726	10.12%	3.568%
6	8.088	2262	2274	2297	rVB	617599	1392602	18.37%	6.473%
7	8.440	2379	2405	2429	rBV	301115	708950	9.35%	3.295%
8	8.971	2583	2603	2633	rBV	776086	1617749	21.33%	7.519%
9	10.446	3134	3153	3171	rBV	1151049	2180091	28.75%	10.133%
10	10.687	3229	3243	3265	rBV3	93586	175945	2.32%	0.818%
11	10.832	3284	3297	3311	rBV2	61365	113271	1.49%	0.526%
12	11.747	3617	3638	3667	rBV	996731	1858148	24.50%	8.636%
13	12.736	3990	4007	4027	rBV	760324	1352045	17.83%	6.284%
14	13.678	4341	4358	4380	rBV	878122	1534886	20.24%	7.134%
15	13.774	4380	4394	4412	rBV2	143626	261275	3.45%	1.214%

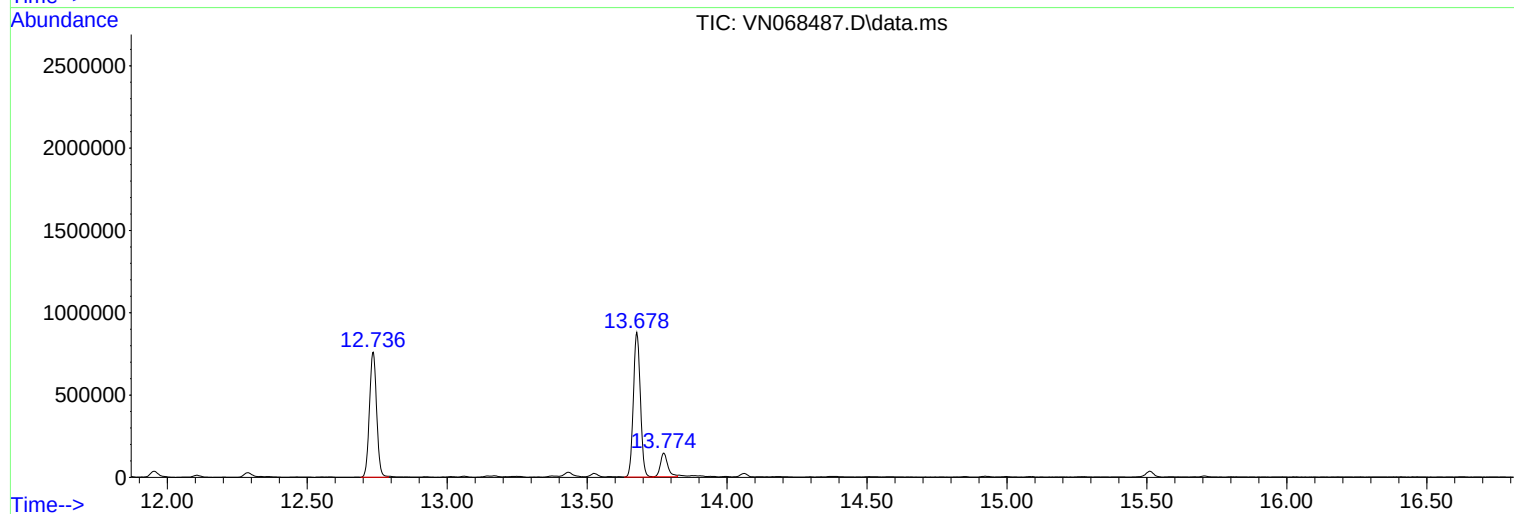
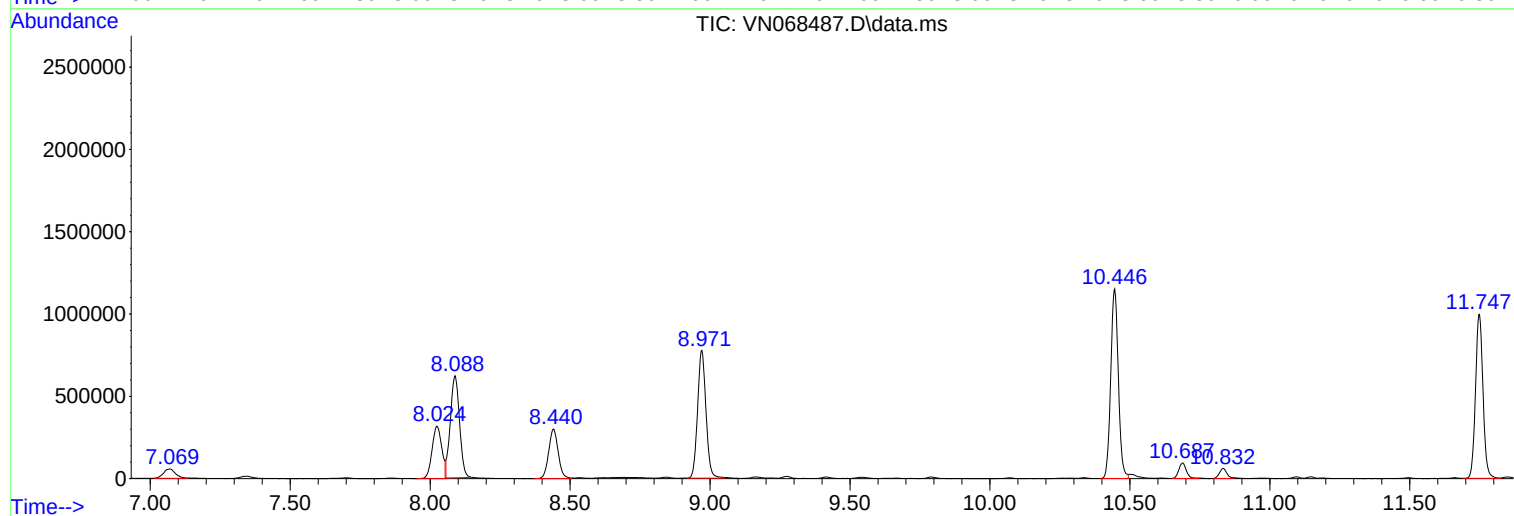
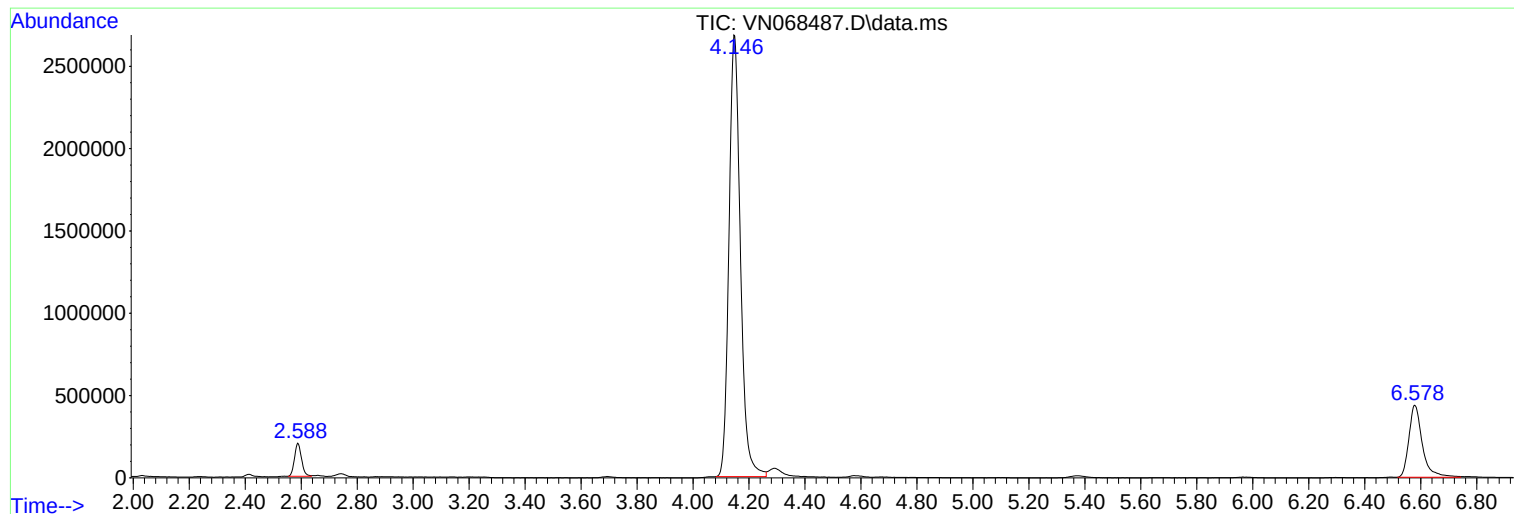
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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



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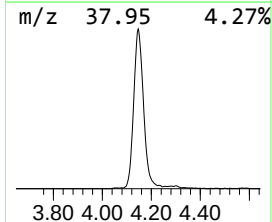
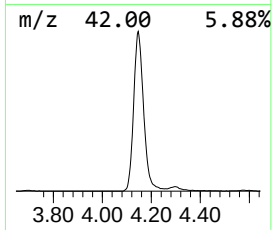
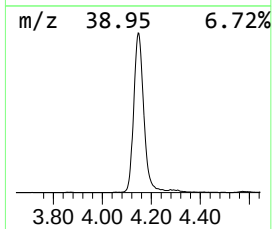
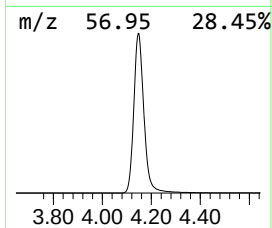
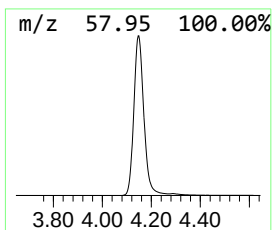
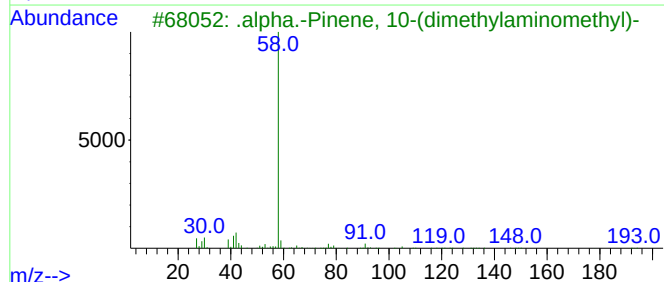
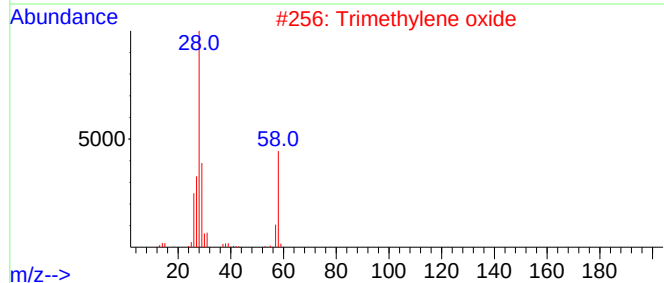
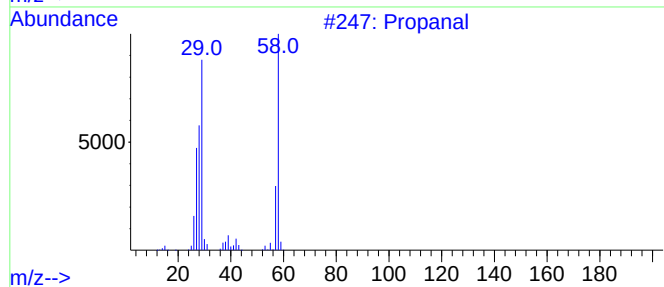
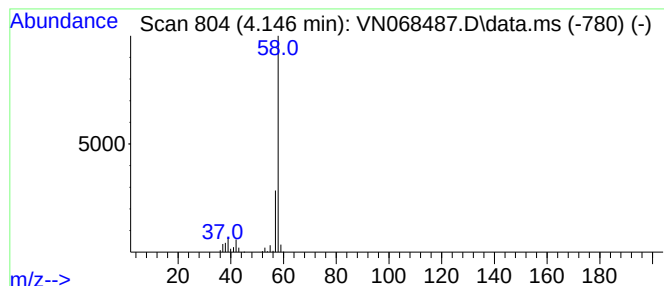
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 2 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.146	272.26 ug/l	7582850	Pentafluorobenzene	8.088

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			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
4			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
5			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7



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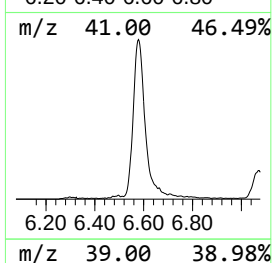
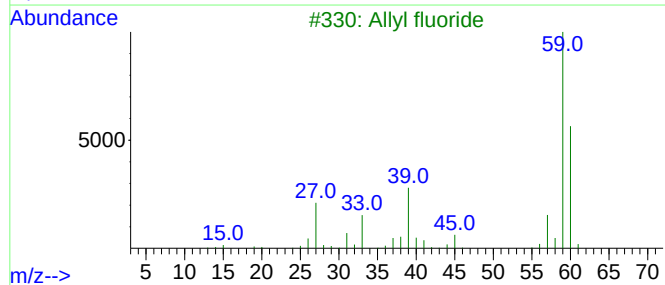
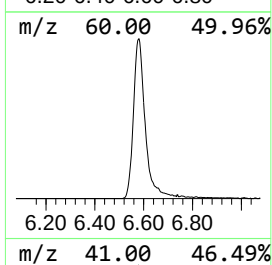
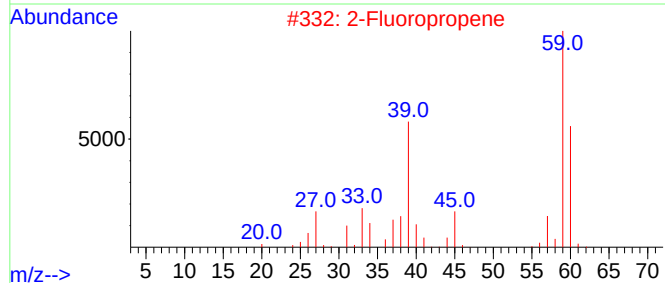
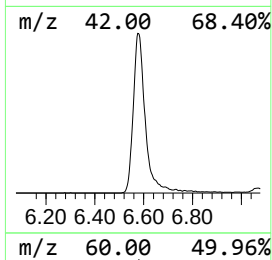
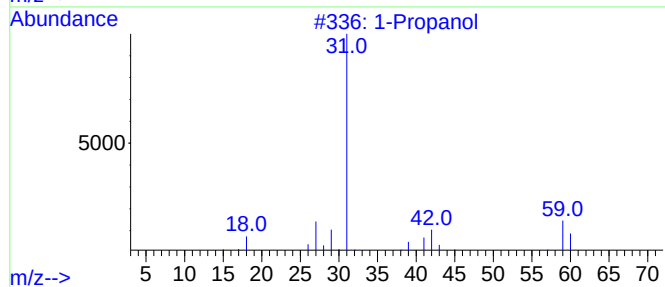
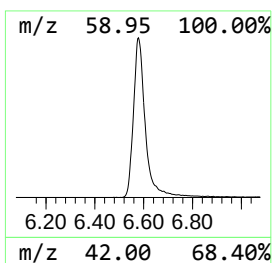
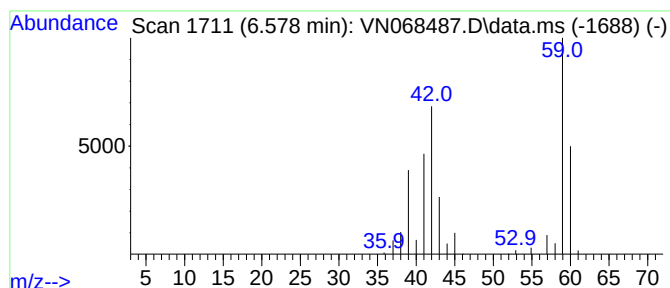
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.578	52.24 ug/l	1455020	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	59
2			2-Fluoropropene	60	C3H5F	001184-60-7	49
3			Allyl fluoride	60	C3H5F	000818-92-8	47
4			Cyclopropane	42	C3H6	000075-19-4	16
5			Acetaldoxime	59	C2H5NO	000107-29-9	7



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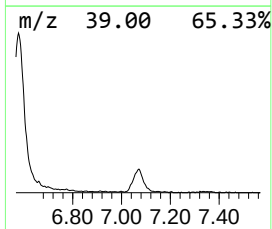
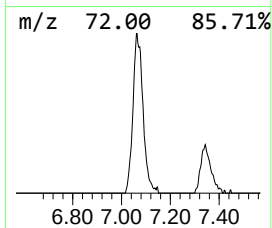
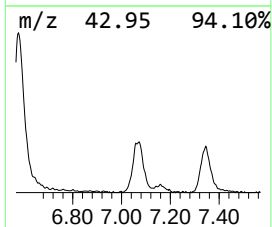
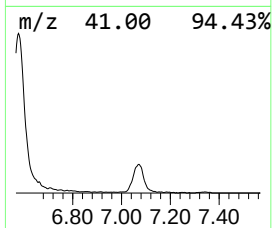
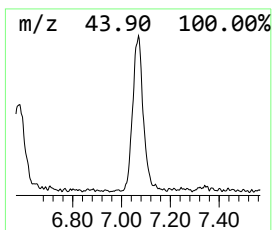
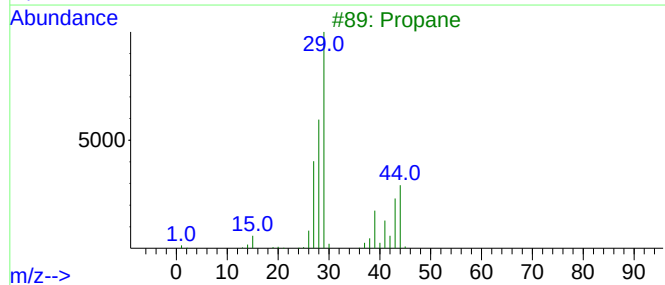
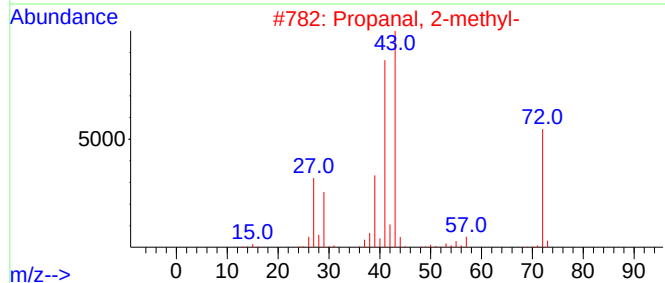
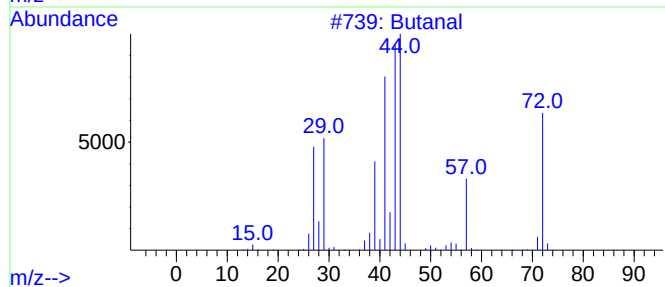
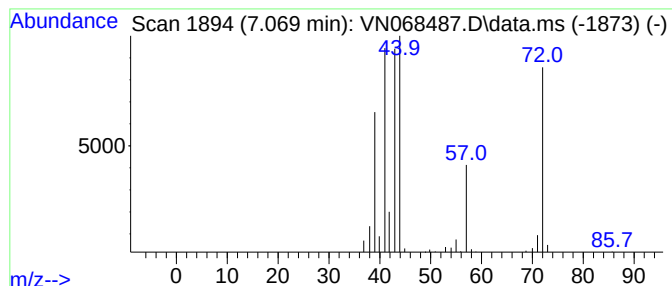
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Peak Number 4 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	5.94 ug/l	165483	Pentafluorobenzene	8.088

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	91
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3		Propane	44	C3H8	000074-98-6	35
4		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32
5		2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	28



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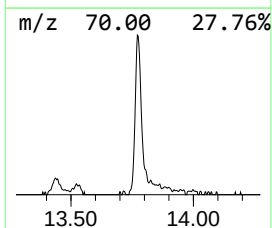
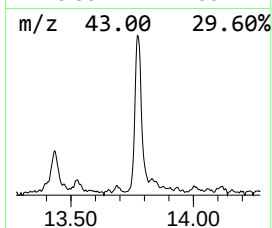
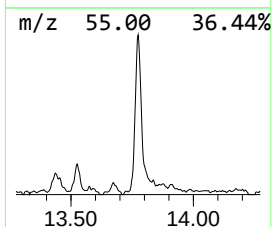
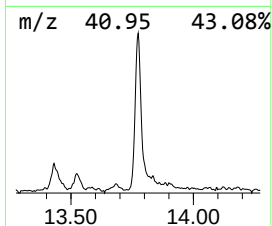
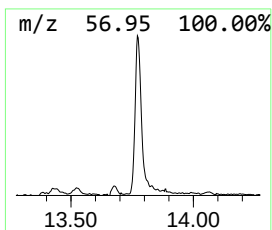
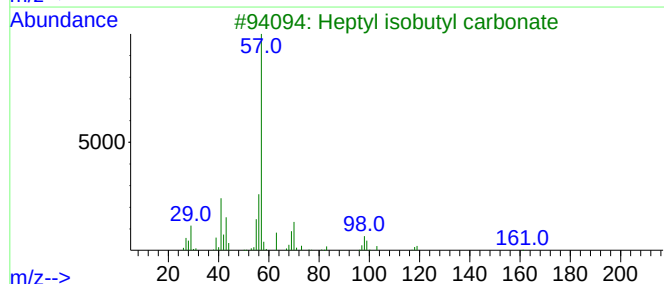
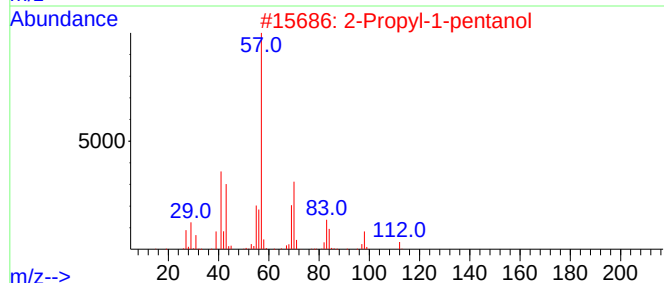
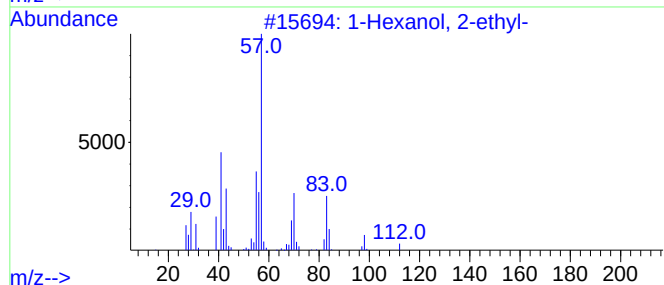
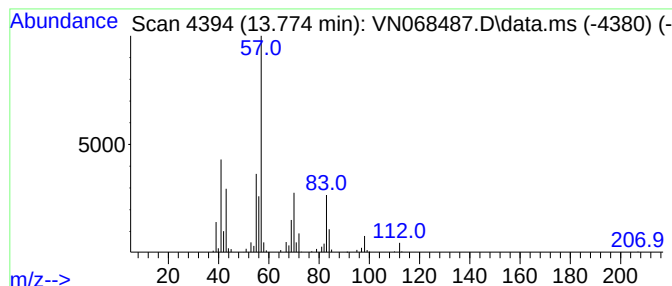
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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	8.51 ug/l	261275	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	45



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal	4.146	272.3	ug/l	7582850	1	8.088	1392600	50.0
1-Propanol	6.578	52.2	ug/l	1455020	1	8.088	1392600	50.0
Butanal	7.069	5.9	ug/l	165483	1	8.088	1392600	50.0
1-Hexanol, 2-et...	13.774	8.5	ug/l	261275	4	13.678	1534890	50.0