

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062922\
 Data File : VX029856.D
 Acq On : 29 Jun 2022 13:00
 Operator : JC/MD
 Sample : N3491-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 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: VX029856.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	25	28	43	rVB	148589	240218	29.49%	4.692%
2	1.453	56	60	71	rVB	99338	117059	14.37%	2.286%
3	2.294	192	198	207	rBV	239841	384371	47.18%	7.507%
4	2.379	207	212	223	rVB	58114	99458	12.21%	1.943%
5	3.855	445	454	474	rBV	328179	814659	100.00%	15.911%
6	5.391	697	706	719	rVB	61628	181045	22.22%	3.536%
7	5.562	722	734	747	rBV	208211	585922	71.92%	11.444%
8	5.964	789	800	809	rBV	53855	142553	17.50%	2.784%
9	6.123	820	826	838	rBV2	13451	37707	4.63%	0.736%
10	6.769	922	932	944	rBV	262161	621982	76.35%	12.148%
11	7.226	1000	1007	1020	rBV3	13039	39387	4.83%	0.769%
12	8.653	1234	1241	1249	rBV	488805	760631	93.37%	14.856%
13	8.775	1257	1261	1272	rVB	22680	45655	5.60%	0.892%
14	9.000	1293	1298	1310	rVB	26150	41589	5.11%	0.812%
15	9.244	1333	1338	1342	rBV2	19415	34708	4.26%	0.678%
16	10.055	1465	1471	1482	rBV	319278	444305	54.54%	8.678%
17	11.085	1635	1640	1646	rVB	183254	230470	28.29%	4.501%
18	11.482	1701	1705	1709	rBV2	14940	18101	2.22%	0.354%
19	12.024	1789	1794	1802	rVB	225628	280208	34.40%	5.473%

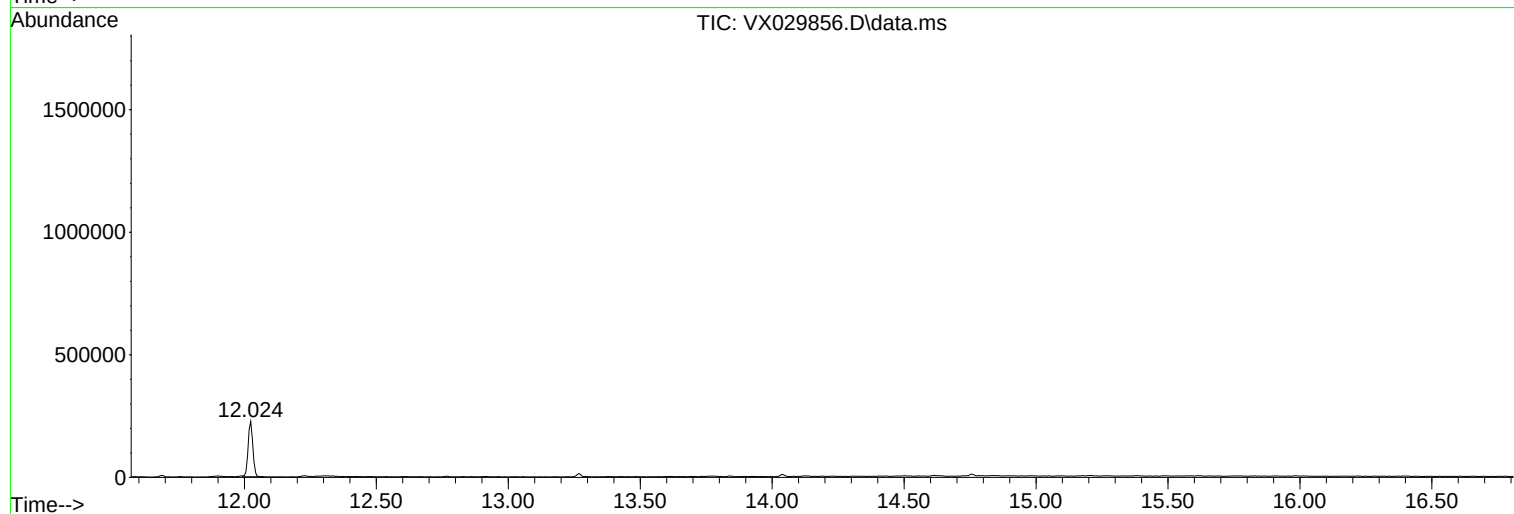
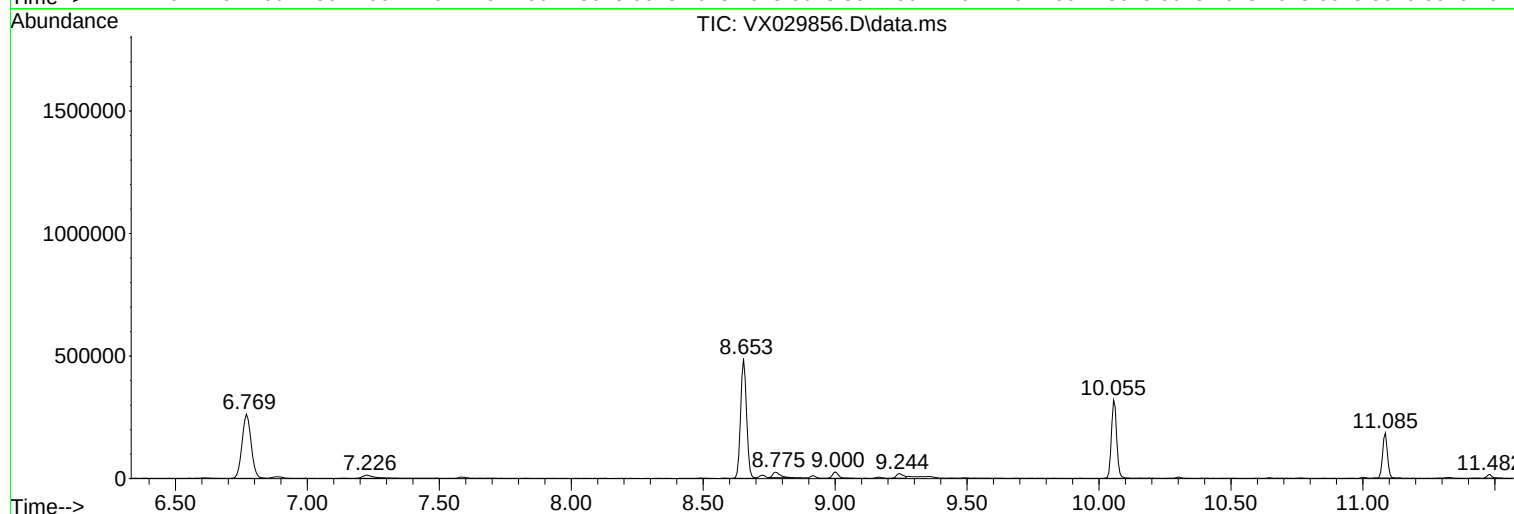
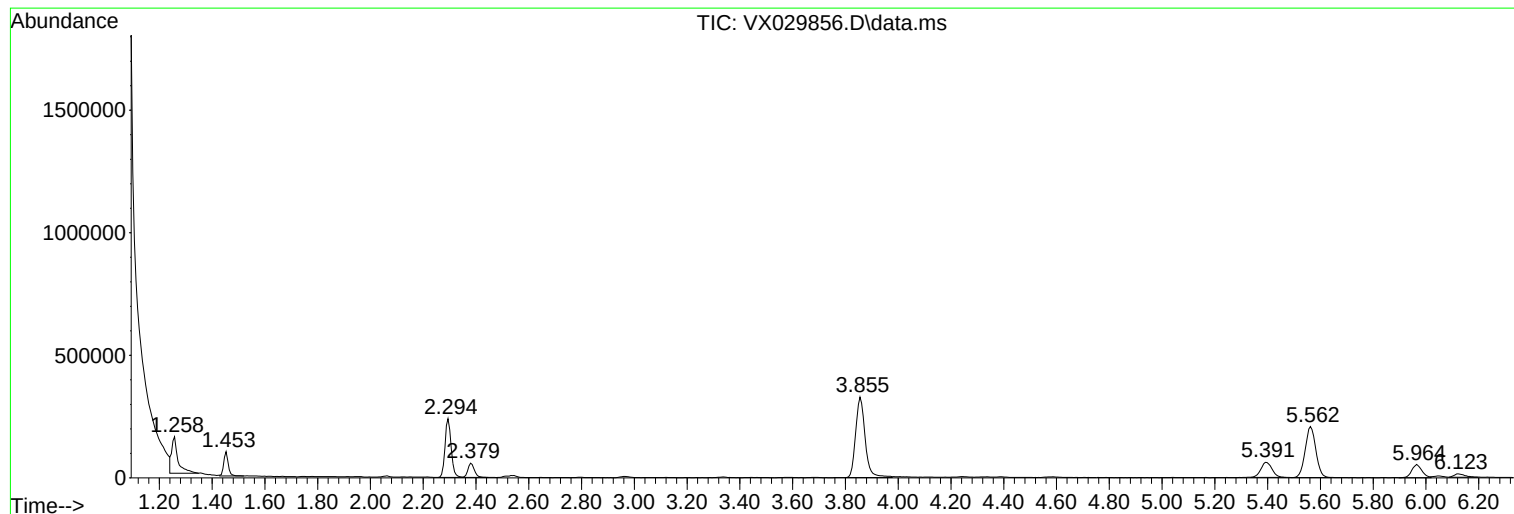
Sum of corrected areas: 5120028

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TIC Library : C:\Database\NIST20.L
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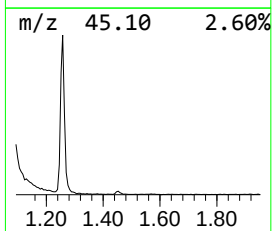
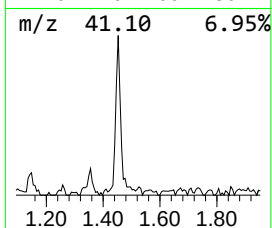
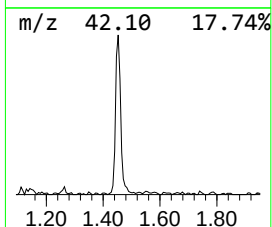
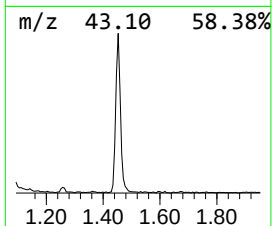
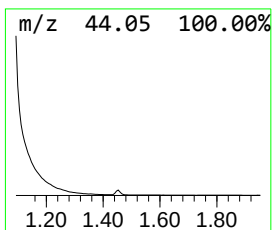
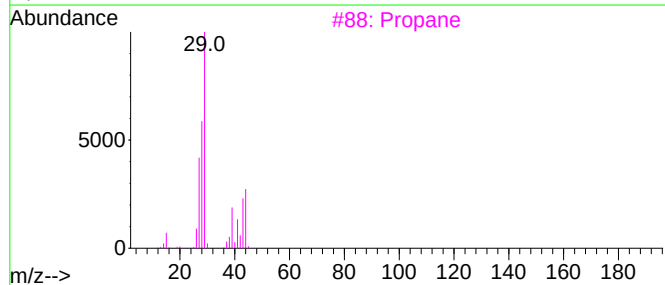
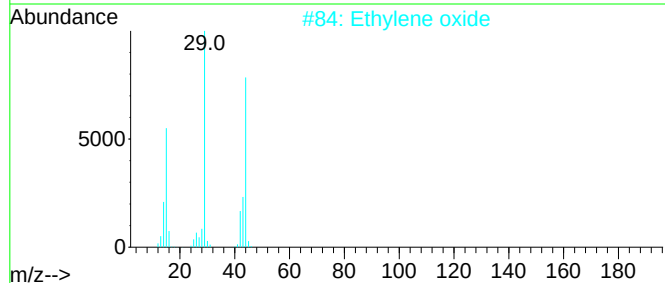
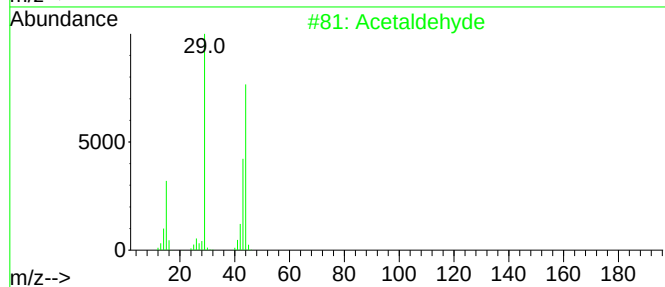
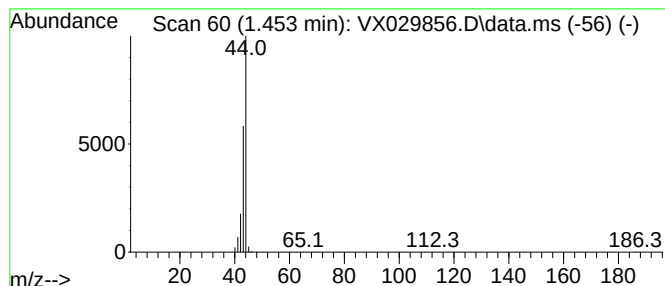
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	9.99 ug/l	117059	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Ethylene oxide	44	C2H4O	000075-21-8	9
3			Propane	44	C3H8	000074-98-6	5
4			Carbon dioxide	44	CO2	000124-38-9	4
5			1,2-Propanediamine	74	C3H10N2	000078-90-0	4



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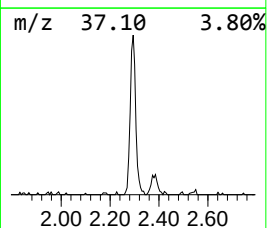
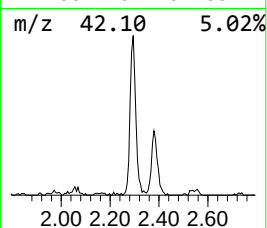
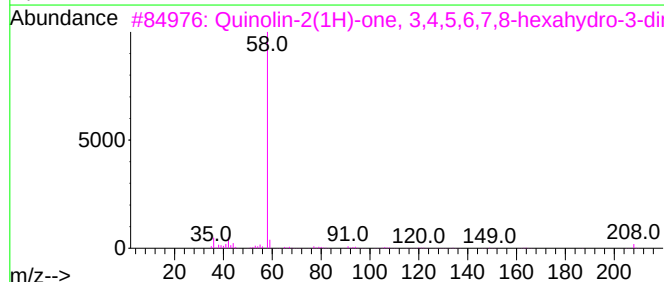
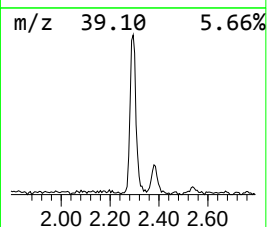
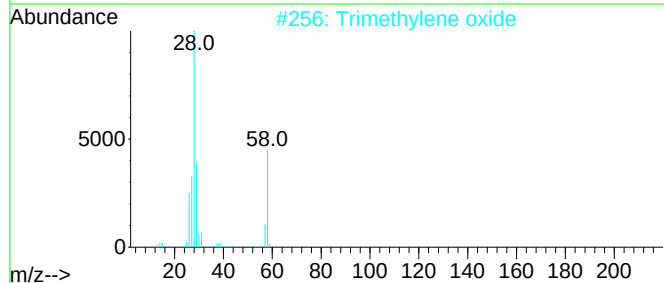
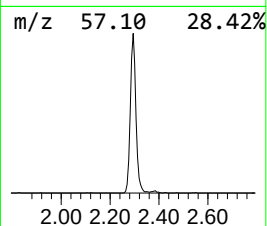
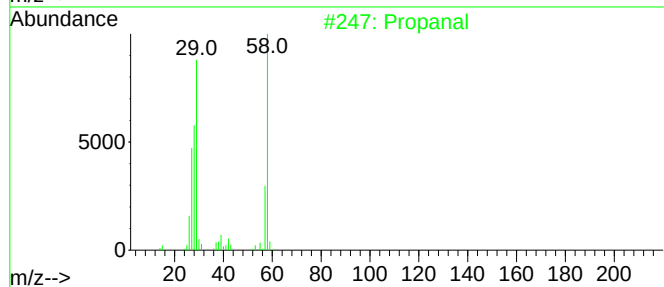
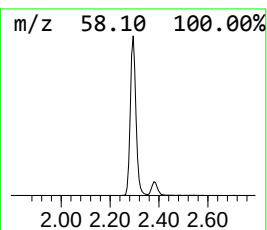
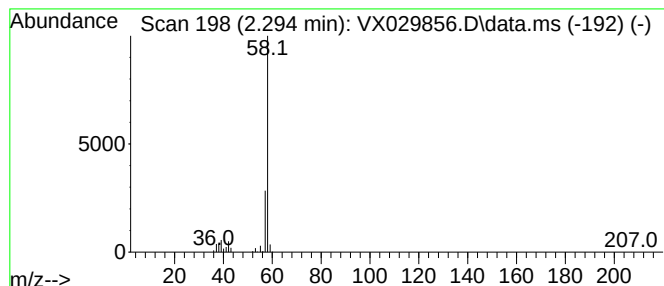
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	32.80 ug/l	384371	Pentafluorobenzene	5.562

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			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
5			Propylene oxide	58	C3H6O	000075-56-9	7



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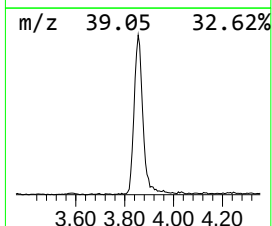
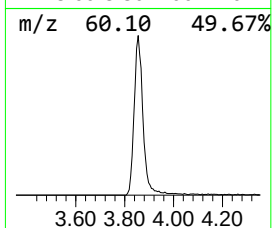
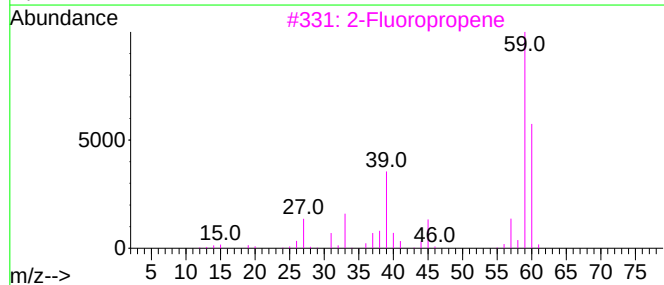
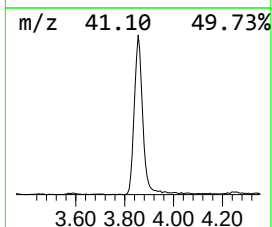
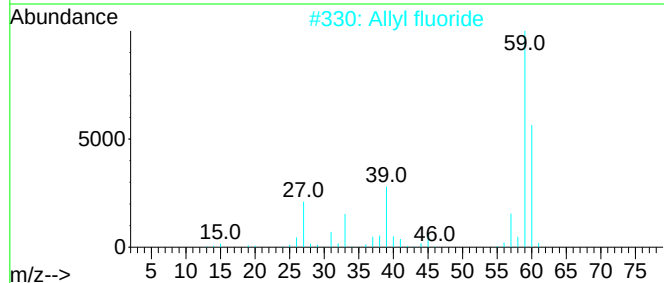
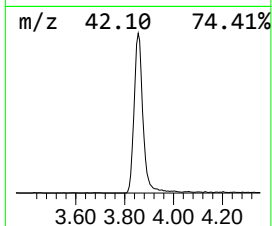
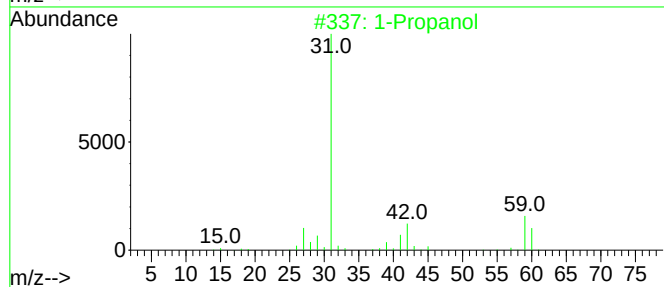
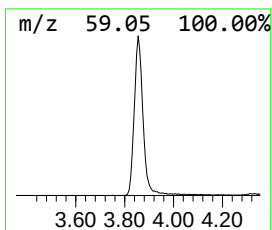
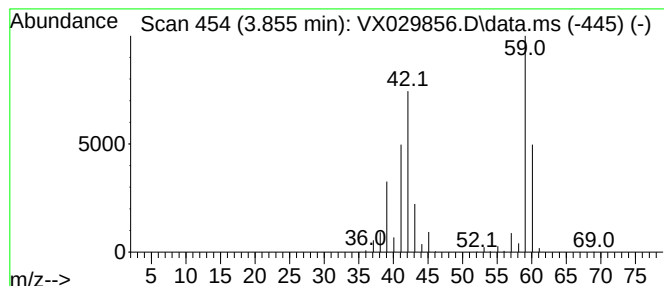
Instrument :
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ClientSampleId :
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Quant Title : SW846 8260

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Peak Number 4 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.855	69.52 ug/l	814659	Pentafluorobenzene	5.562	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	78
2	Allyl fluoride	60	C3H5F	000818-92-8	47
3	2-Fluoropropene	60	C3H5F	001184-60-7	43
4	Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	23
5	Acetaldoxime	59	C2H5NO	000107-29-9	7



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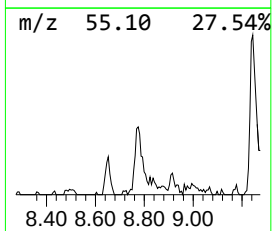
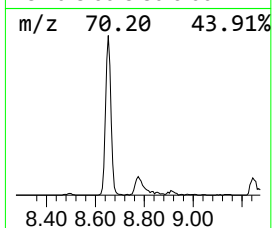
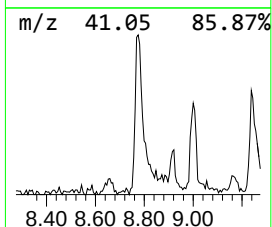
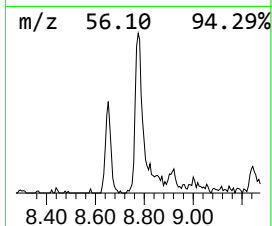
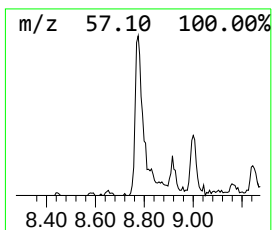
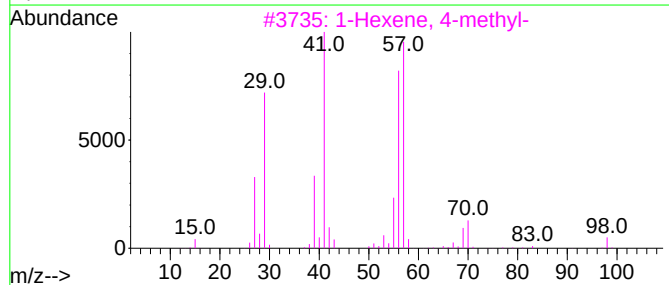
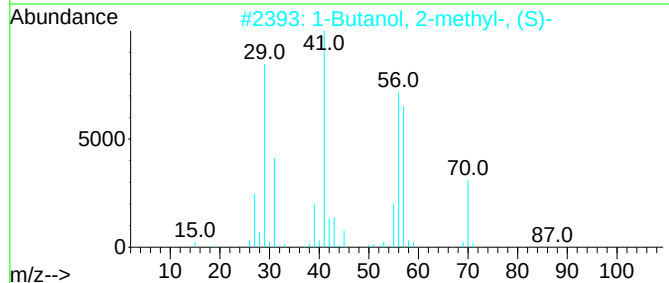
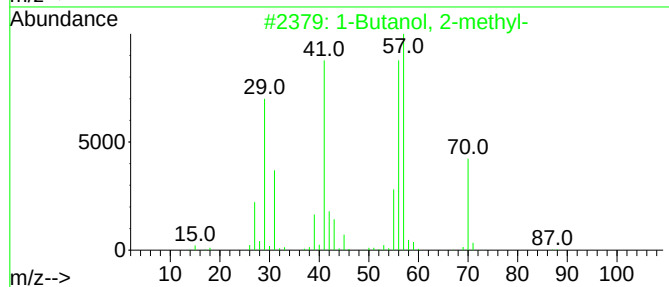
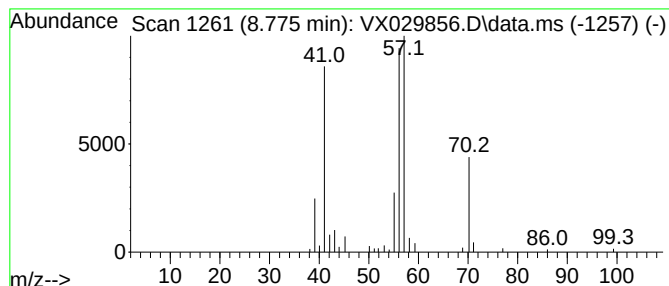
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Peak Number 5 1-Butanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.775	5.14 ug/l	45655	Chlorobenzene-d5	10.055

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	74
2		1-Butanol, 2-methyl-, (S)-	88	C5H12O	001565-80-6	74
3		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	45
4		2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	45
5		Pentane, 3-methyl-	86	C6H14	000096-14-0	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.453	10.0	ug/l	117059	1	5.562	585922	50.0
Propanal	2.294	32.8	ug/l	384371	1	5.562	585922	50.0
1-Propanol	3.855	69.5	ug/l	814659	1	5.562	585922	50.0
1-Butanol, 2-me...	8.775	5.1	ug/l	45655	3	10.055	444305	50.0