

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
 Data File : VX031417.D
 Acq On : 16 Sep 2022 17:59
 Operator : JC/MD
 Sample : N4526-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MID-0907

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\82X091422W.M
 Title : SW846 8260

Signal : TIC: VX031417.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	21	29	31	rBV	23044	33516	4.60%	1.036%
2	1.746	104	108	117	rVB	23068	32471	4.46%	1.004%
3	2.867	282	292	299	rBV	22033	43608	5.98%	1.349%
4	2.947	299	305	318	rVB	10124	29757	4.08%	0.920%
5	5.385	692	705	717	rBV	86719	252702	34.68%	7.815%
6	5.556	724	733	746	rVB2	88059	242781	33.32%	7.508%
7	5.964	789	800	809	rBV	97703	256560	35.21%	7.934%
8	6.044	809	813	831	rVB3	7507	20651	2.83%	0.639%
9	6.239	837	845	859	rVB2	11494	35031	4.81%	1.083%
10	6.763	921	931	944	rBV	135781	316850	43.48%	9.798%
11	8.427	1198	1204	1212	rBV2	6970	13056	1.79%	0.404%
12	8.653	1234	1241	1251	rBV	460123	728695	100.00%	22.534%
13	9.567	1386	1391	1397	rBV3	5651	7795	1.07%	0.241%
14	10.055	1465	1471	1480	rBV	290663	381329	52.33%	11.792%
15	11.079	1634	1639	1649	rBV	386693	488708	67.07%	15.113%
16	12.024	1789	1794	1808	rVB	291625	350221	48.06%	10.830%

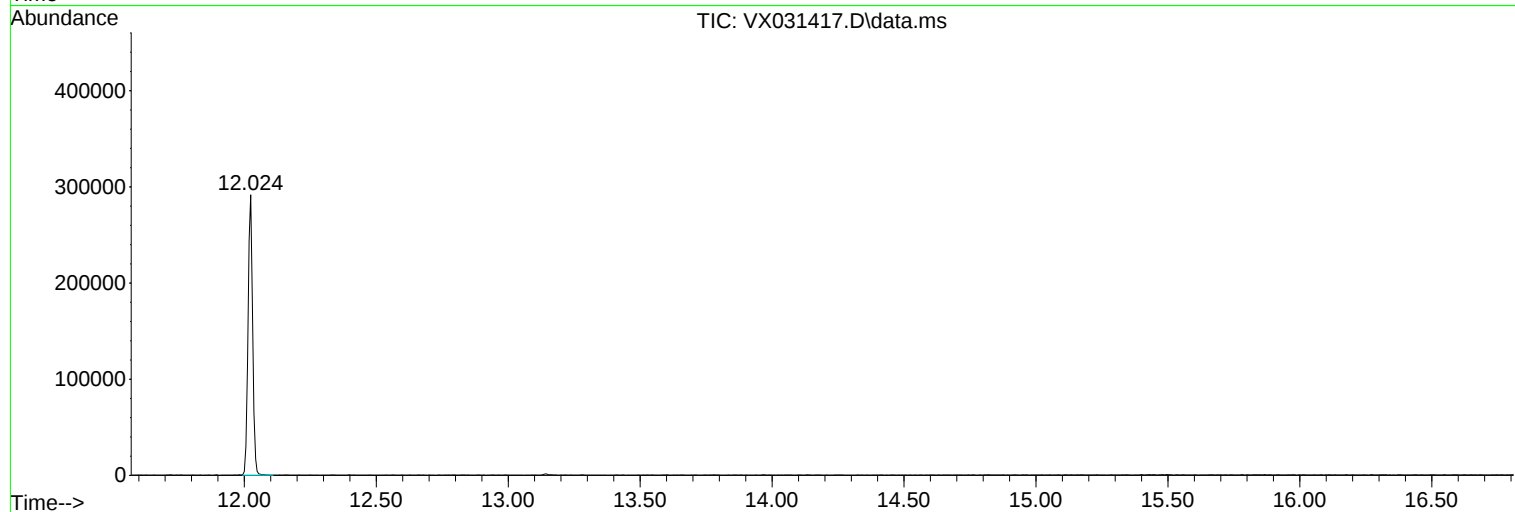
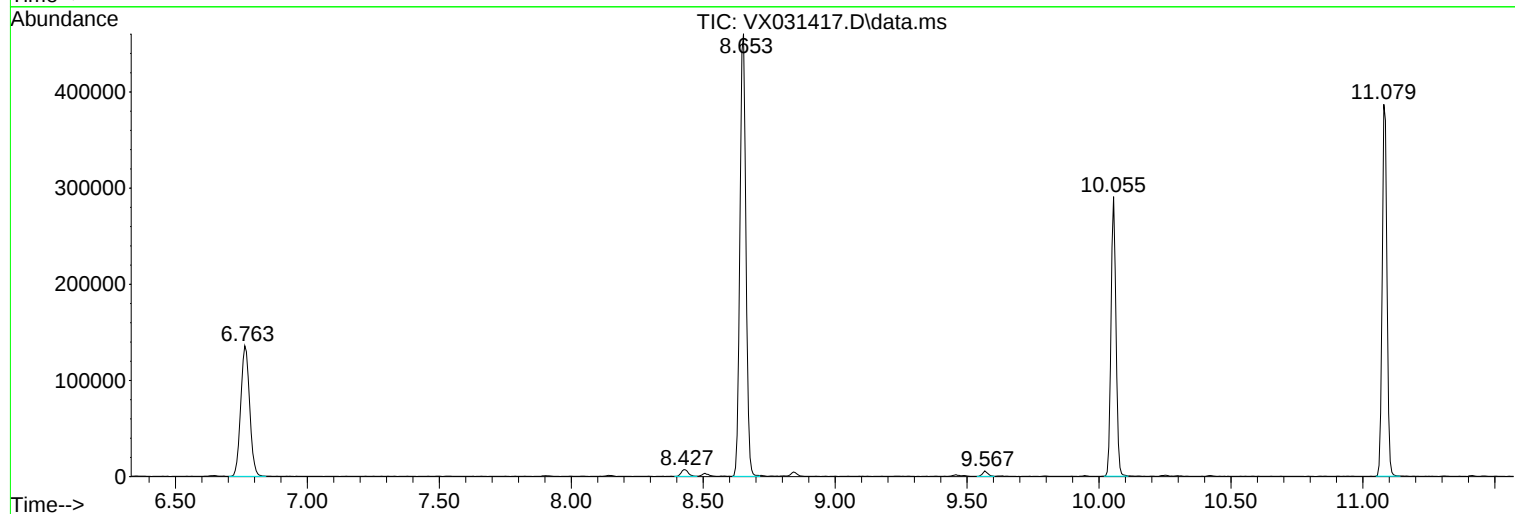
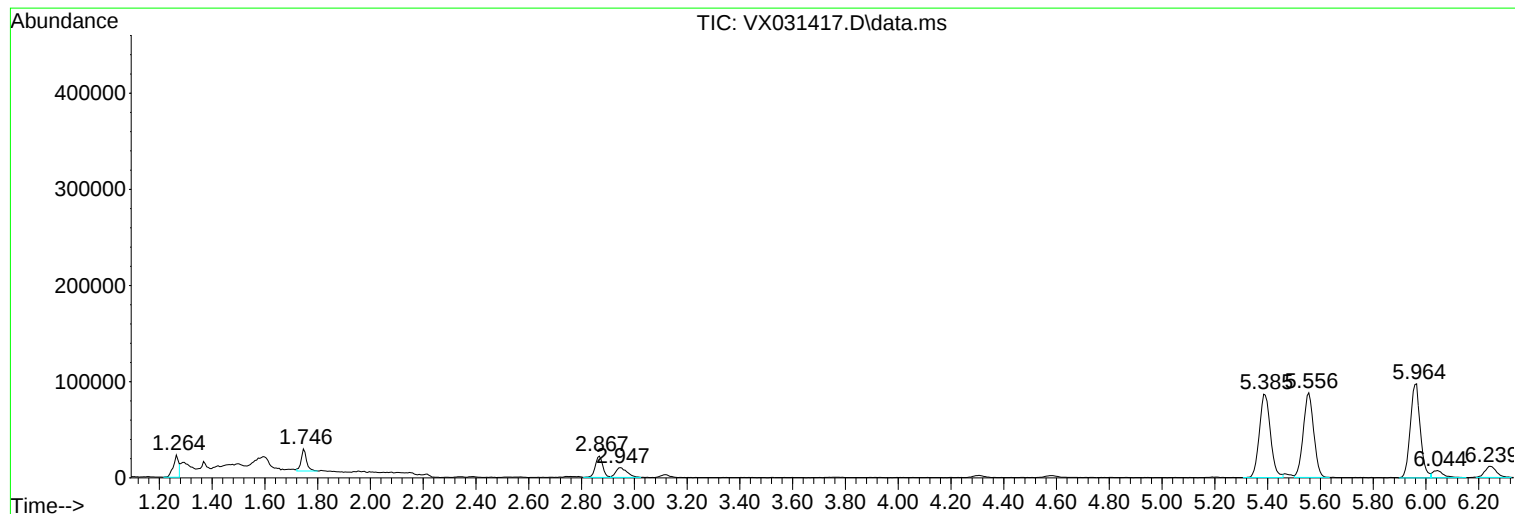
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Quant Title : SW846 8260

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



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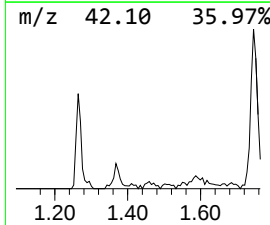
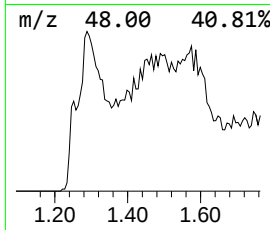
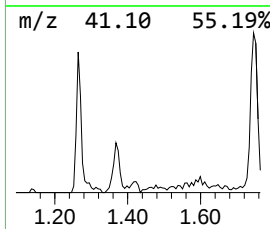
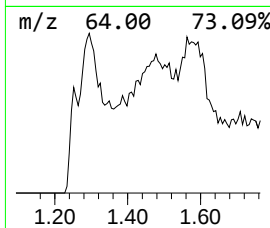
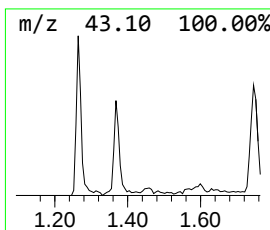
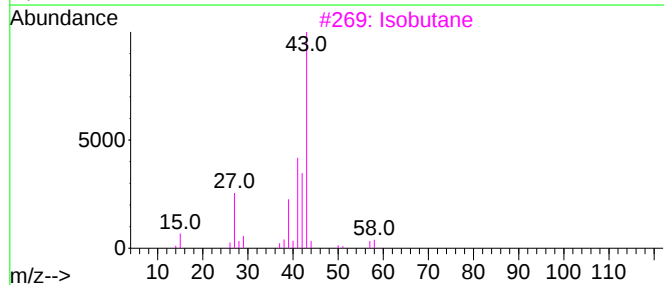
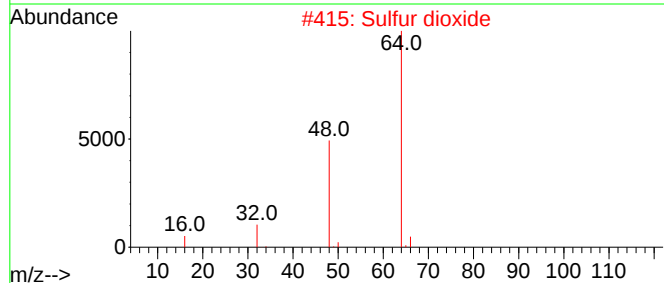
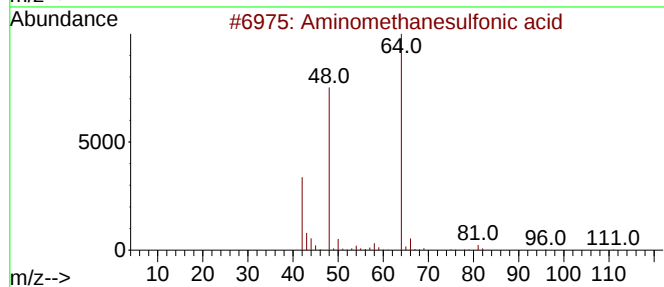
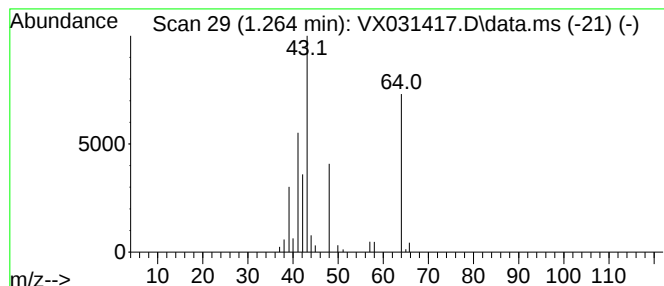
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	6.90 ug/l	33516	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	78
2			Sulfur dioxide	64	O2S	007446-09-5	64
3			Isobutane	58	C4H10	000075-28-5	10
4			5-Methyloxazolidine	87	C4H9NO	058328-22-6	9
5			Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	9



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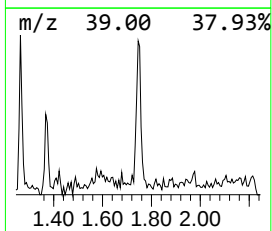
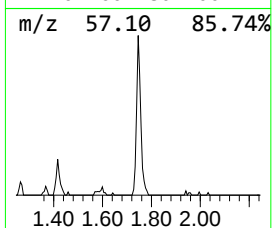
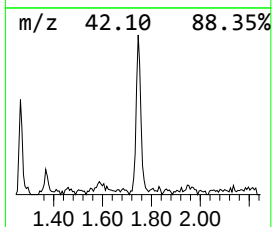
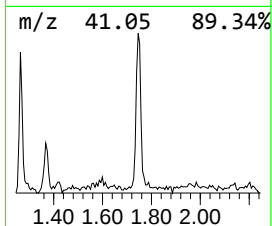
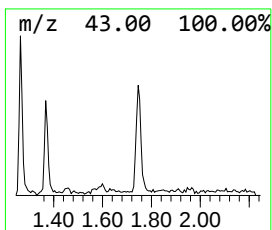
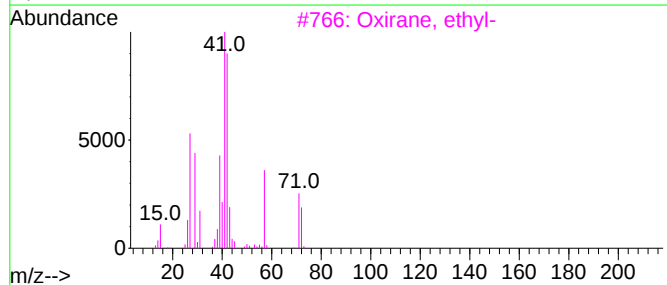
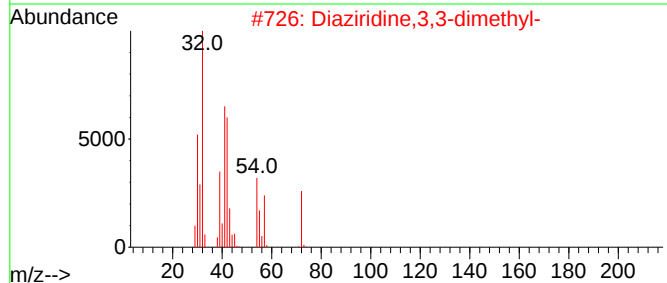
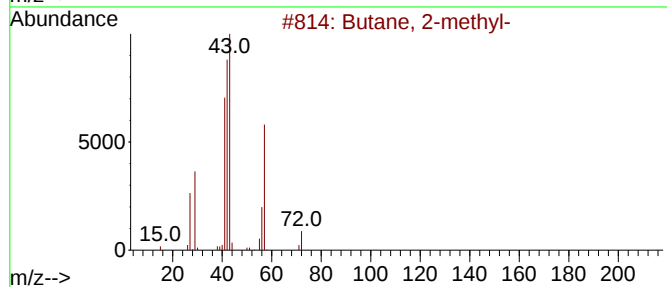
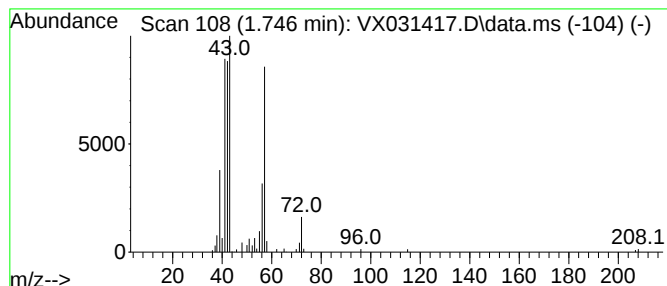
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	6.69 ug/l	32471	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	53
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	47
4			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	42
5			Pentane	72	C5H12	000109-66-0	33



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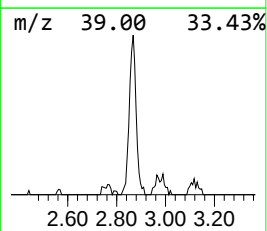
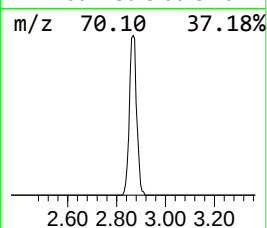
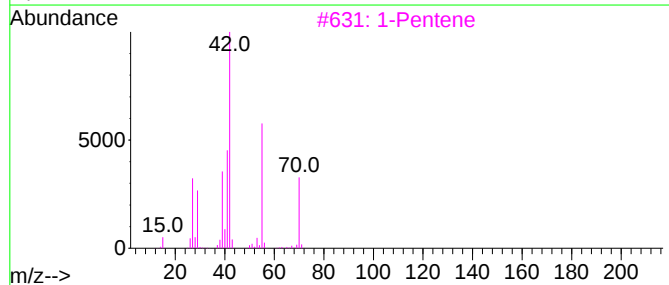
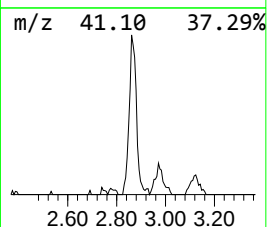
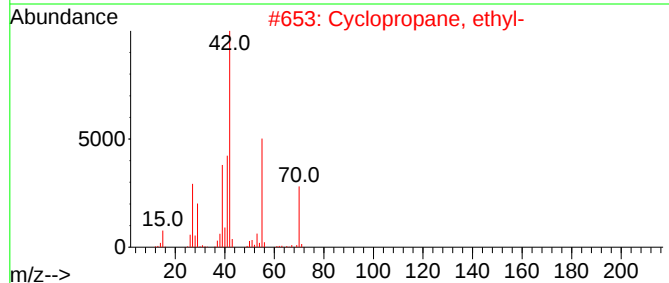
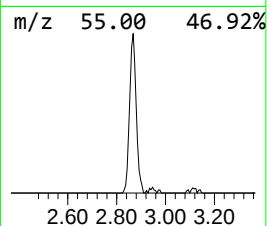
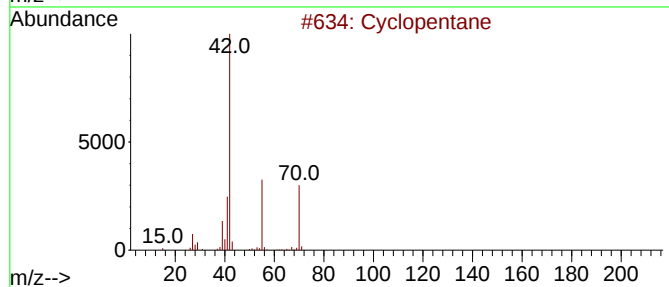
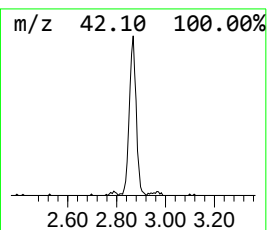
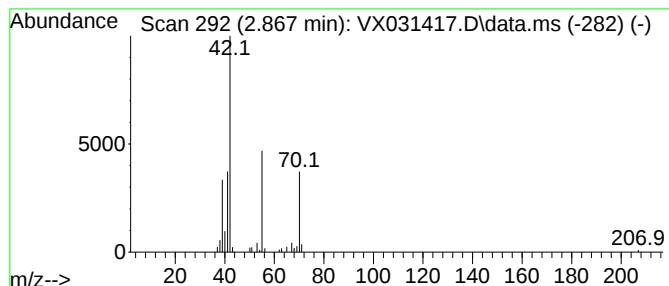
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Peak Number 3 Cyclopentane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	8.98 ug/l	43608	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	86
2			Cyclopropane, ethyl-	70	C5H10	001191-96-4	64
3			1-Pentene	70	C5H10	000109-67-1	64
4			Cyclobutane, methyl-	70	C5H10	000598-61-8	59
5			1-Pentanol	88	C5H12O	000071-41-0	50



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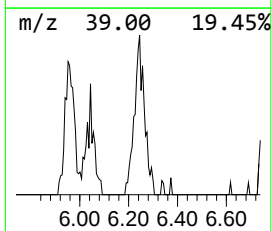
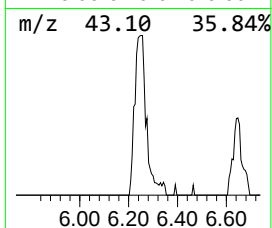
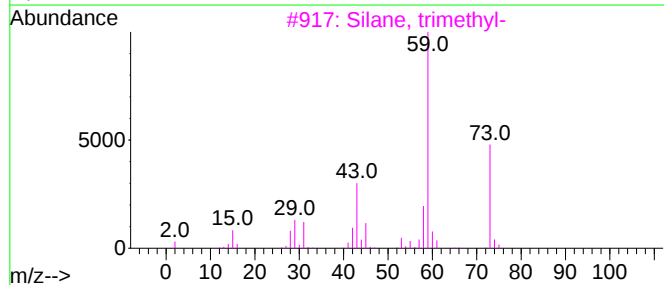
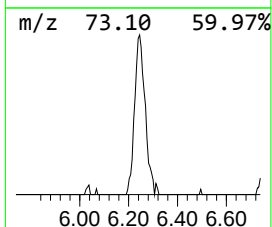
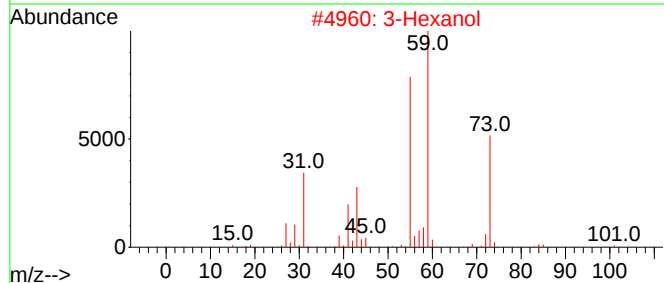
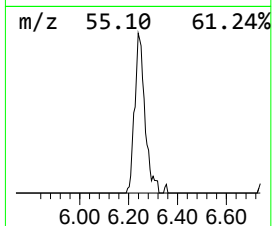
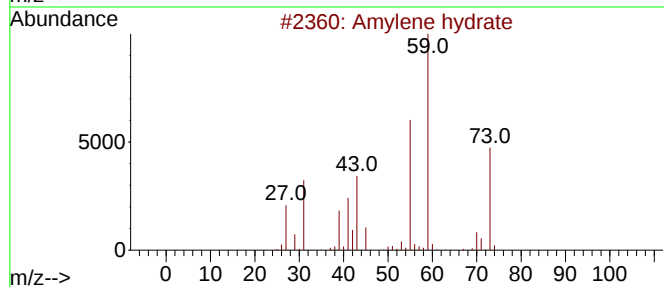
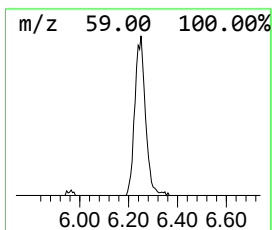
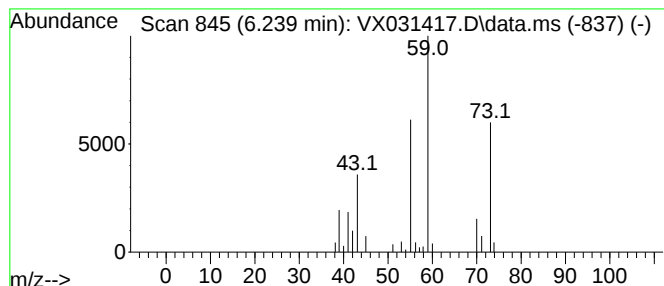
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Peak Number 5 Amylene hydrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.239	5.53 ug/l	35031	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	83
2			3-Hexanol	102	C6H14O	000623-37-0	50
3			Silane, trimethyl-	74	C3H10Si	000993-07-7	36
4			Butanamide	87	C4H9NO	000541-35-5	36
5			1-Butene, 3-methyl-	70	C5H10	000563-45-1	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aminomethanesul...	1.264	6.9	ug/l	33516	1	5.556	242781	50.0
Butane, 2-methyl-	1.746	6.7	ug/l	32471	1	5.556	242781	50.0
Cyclopentane	2.867	9.0	ug/l	43608	1	5.556	242781	50.0
Amylene hydrate	6.239	5.5	ug/l	35031	2	6.763	316850	50.0