

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072922\
 Data File : VX030296.D
 Acq On : 29 Jul 2022 12:38
 Operator : JC/MD
 Sample : N3861-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-14R

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\82X072522W.M
 Title : SW846 8260

Signal : TIC: VX030296.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.282	22	32	44	rBV	156823	527502	38.67%	7.291%
2	1.368	44	46	49	rVB	26137	30415	2.23%	0.420%
3	1.746	104	108	114	rVB	42517	57360	4.20%	0.793%
4	2.215	179	185	193	rVB2	13524	23817	1.75%	0.329%
5	2.538	229	238	246	rBV2	22892	54925	4.03%	0.759%
6	2.782	268	278	285	rBV2	23536	58427	4.28%	0.808%
7	2.867	286	292	300	rVV2	47994	99034	7.26%	1.369%
8	3.105	325	331	339	rVB5	5305	15226	1.12%	0.210%
9	4.306	518	528	538	rVB2	35066	95352	6.99%	1.318%
10	5.391	695	706	714	rBV	151494	439406	32.21%	6.073%
11	5.477	714	720	725	rVV3	33496	101903	7.47%	1.408%
12	5.556	725	733	753	rVB	166541	490092	35.92%	6.774%
13	5.958	789	799	817	rVB	182562	486597	35.67%	6.725%
14	6.361	857	865	874	rVB6	6387	18367	1.35%	0.254%
15	6.763	922	931	945	rBV	258141	638743	46.82%	8.828%
16	7.373	1022	1031	1042	rVB6	13567	40031	2.93%	0.553%
17	8.147	1154	1158	1163	rVB2	13001	24085	1.77%	0.333%
18	8.653	1234	1241	1252	rBV	869803	1364242	100.00%	18.856%
19	9.165	1319	1325	1333	rVB3	10873	18957	1.39%	0.262%
20	10.055	1461	1471	1481	rBV	612547	844611	61.91%	11.674%
21	11.085	1634	1640	1651	rVB	665172	837069	61.36%	11.569%
22	12.024	1789	1794	1803	rBV	814335	968990	71.03%	13.393%

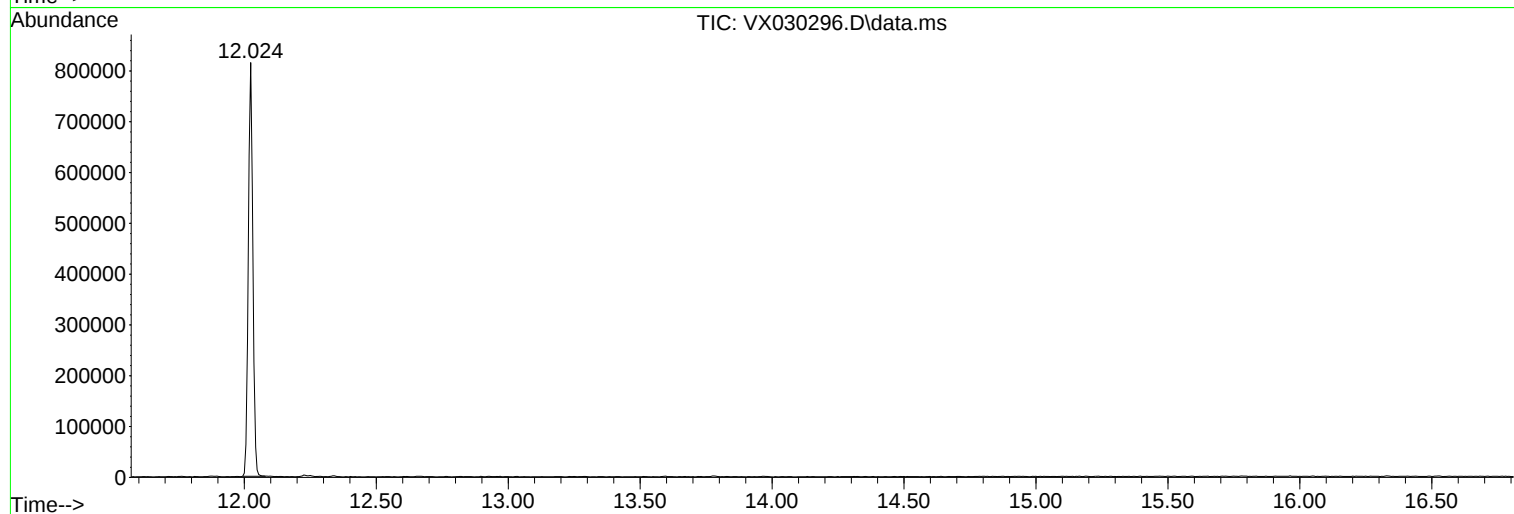
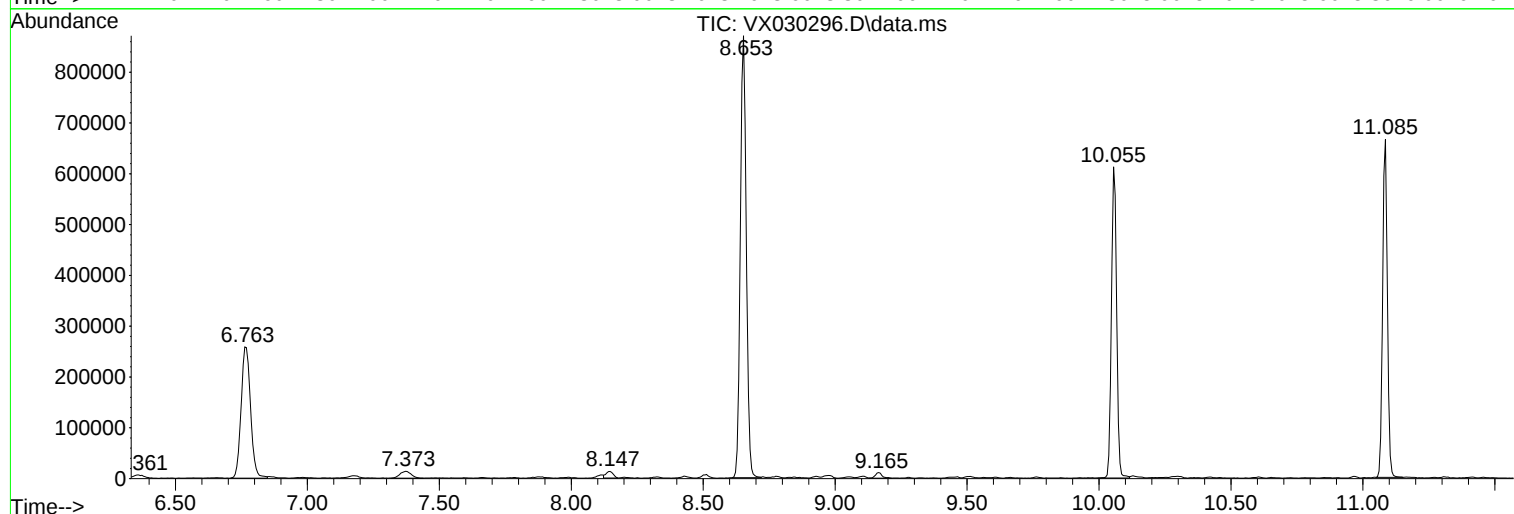
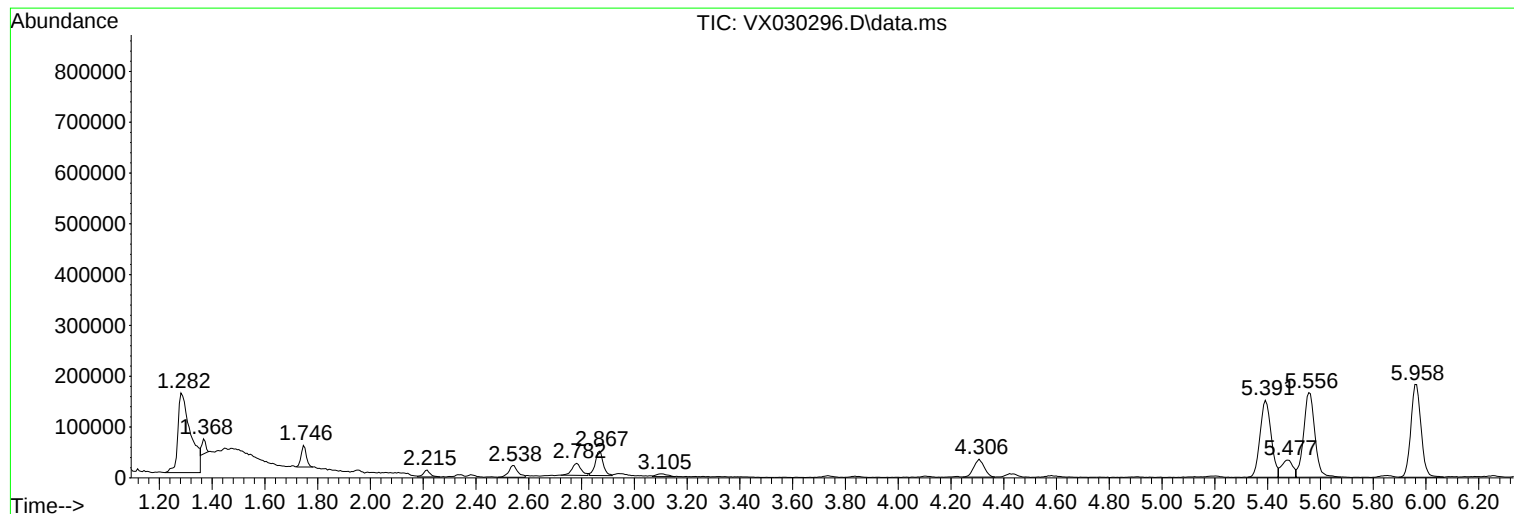
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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



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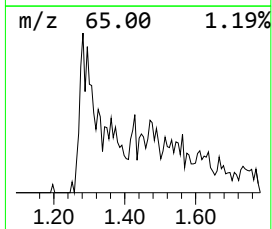
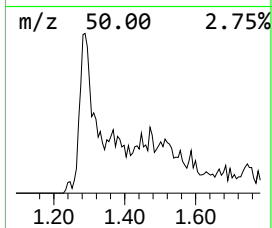
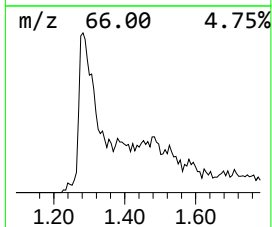
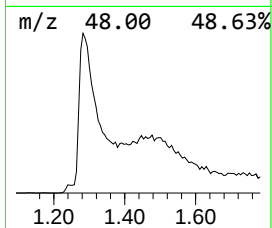
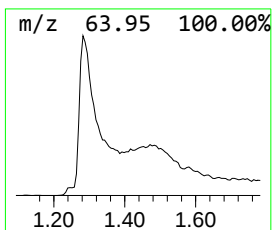
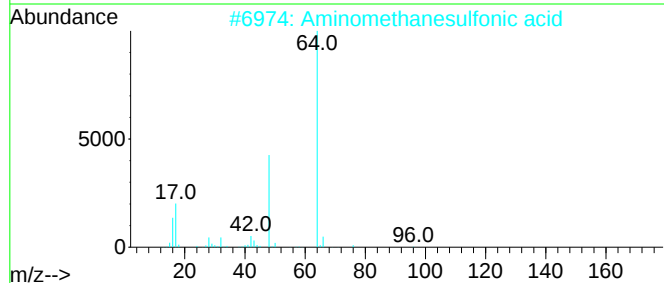
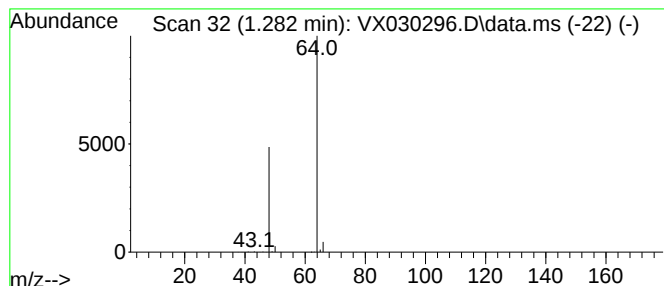
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Quant Title : SW846 8260

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Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.282	53.82 ug/l	527502	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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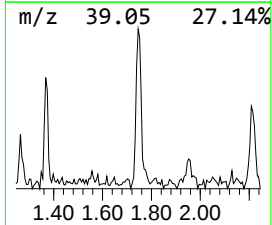
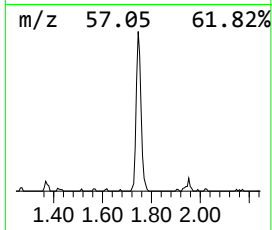
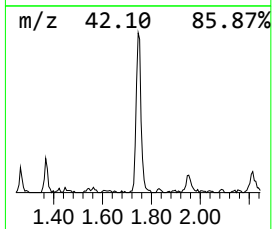
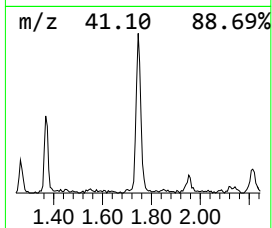
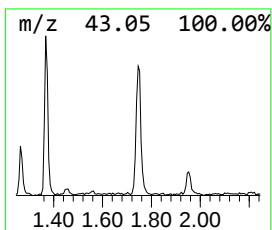
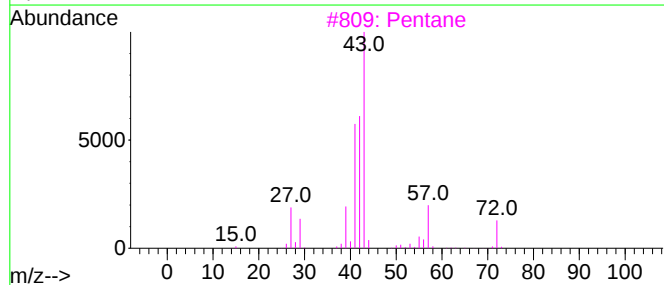
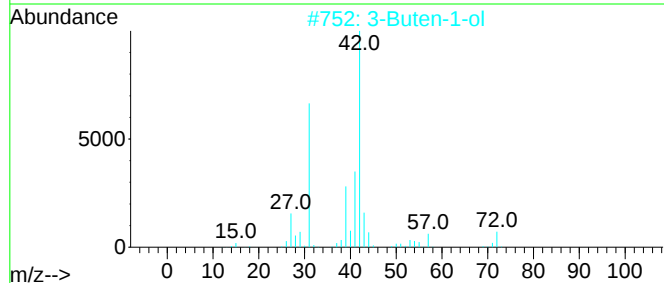
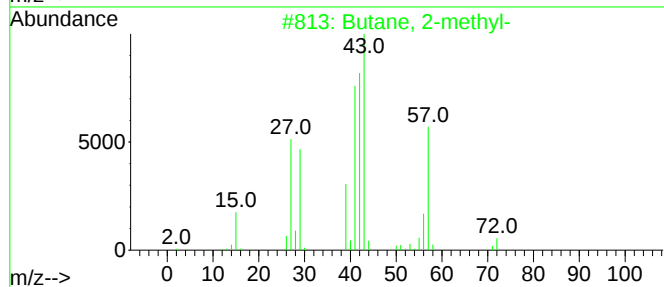
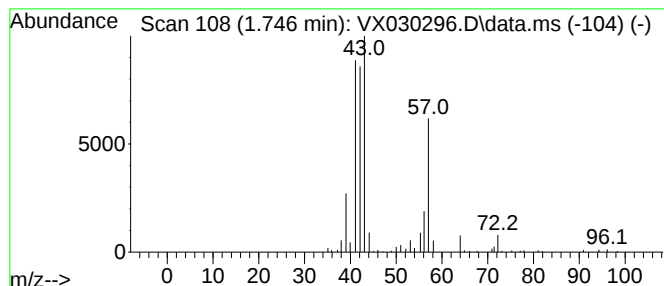
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	5.85 ug/l	57360	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	42
4			2-Carbomethoxyaziridine	101	C4H7N02	005950-34-5	28
5			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	12



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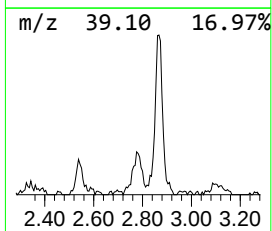
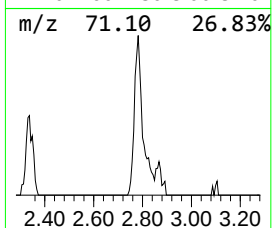
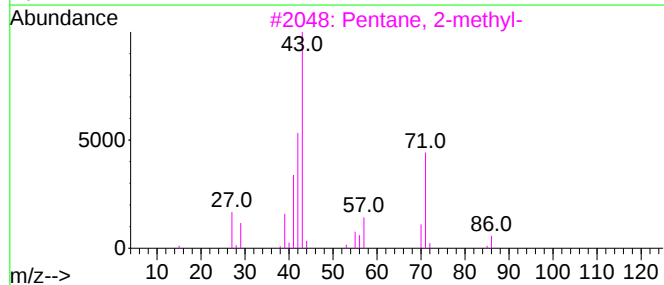
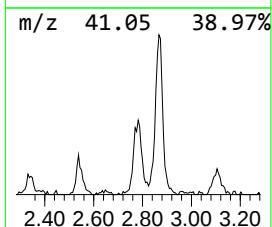
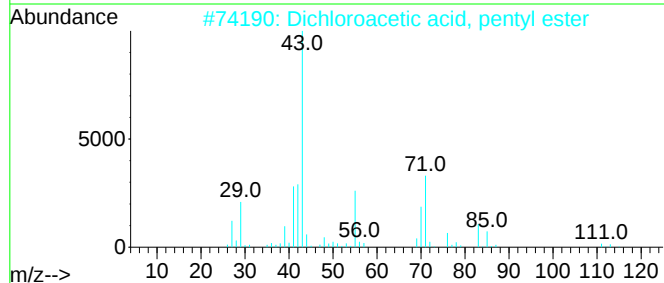
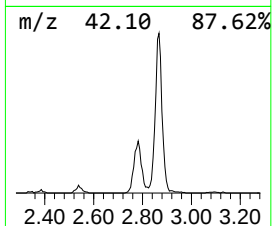
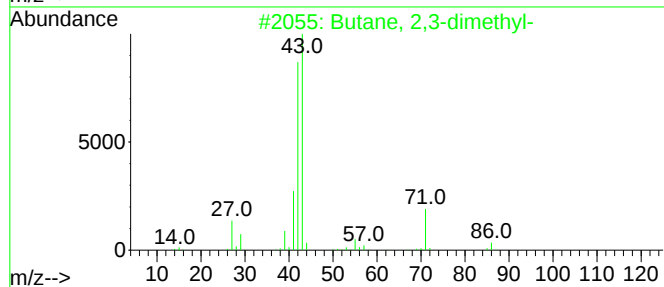
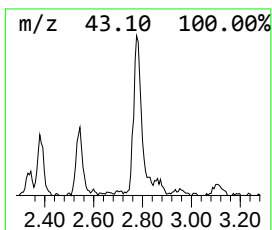
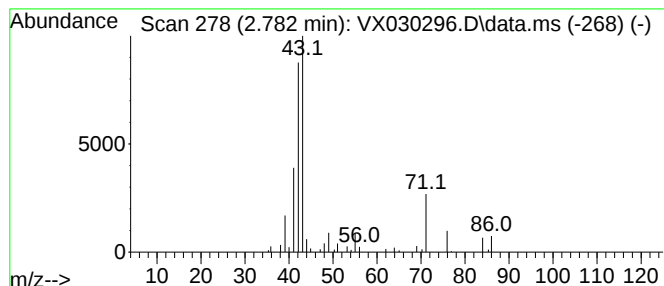
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	5.96 ug/l	58427	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	74
2			Dichloroacetic acid, pentyl ester	198	C7H12Cl2O2	037079-03-1	38
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	27
4			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	10
5			4-Penten-2-one	84	C5H8O	013891-87-7	9



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Instrument :
MSVOA_X
ClientSampleId :
MW-14R

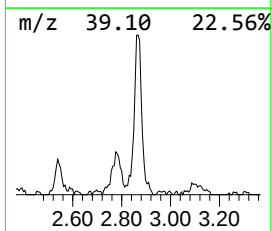
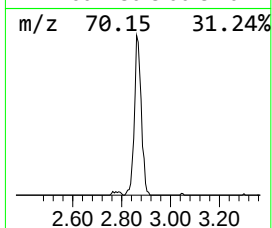
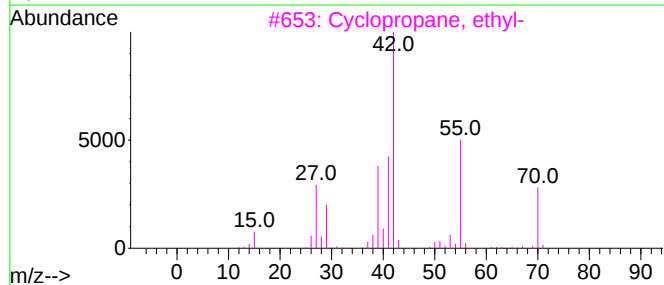
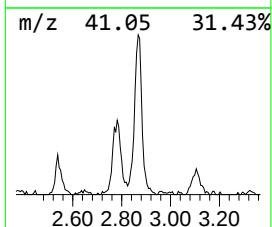
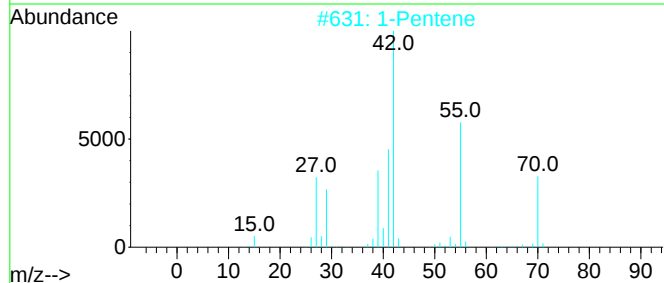
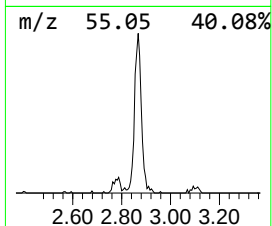
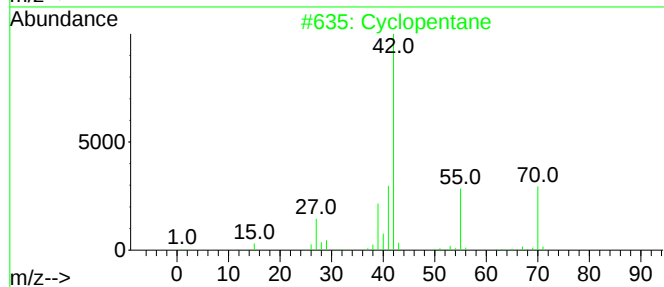
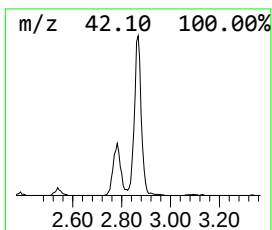
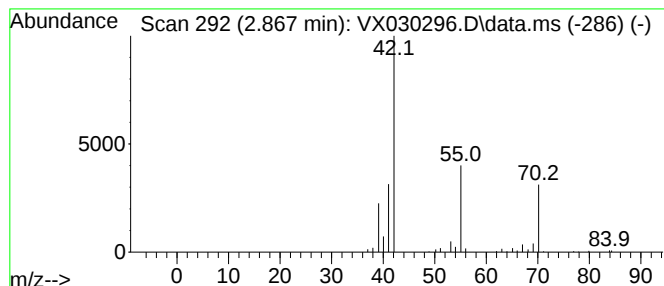
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	10.10 ug/l	99034	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	86
2			1-Pentene	70	C5H10	000109-67-1	64
3			Cyclopropane, ethyl-	70	C5H10	001191-96-4	56
4			Cyclobutane, methyl-	70	C5H10	000598-61-8	45
5			Cyclobutanone	70	C4H6O	001191-95-3	5



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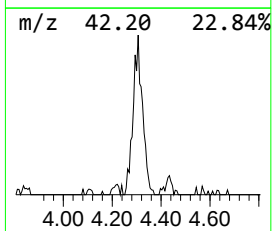
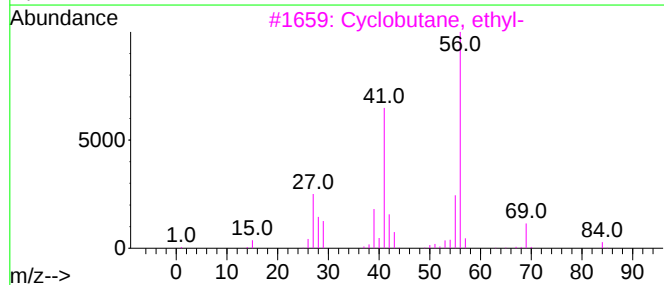
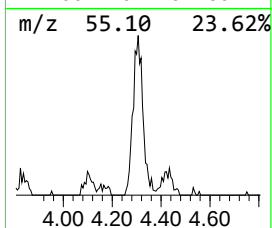
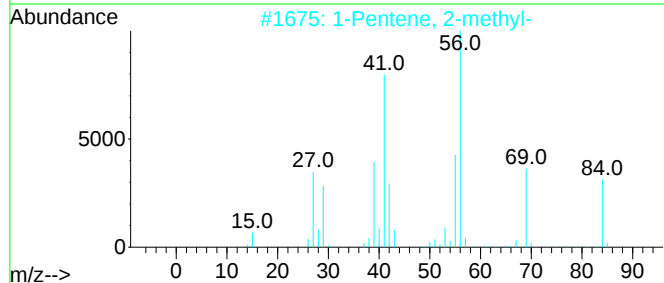
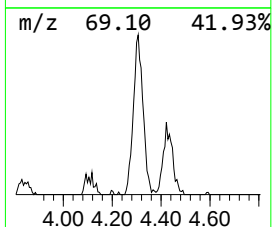
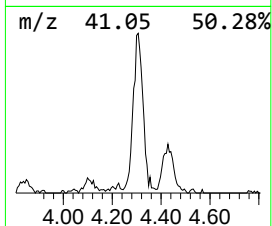
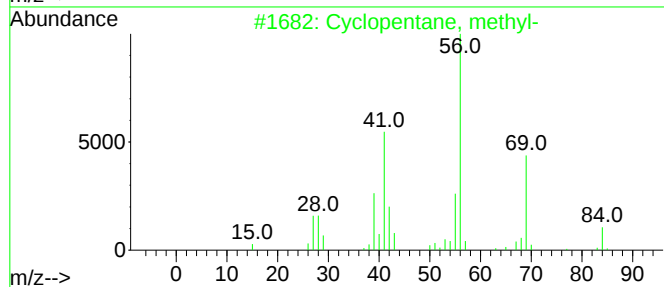
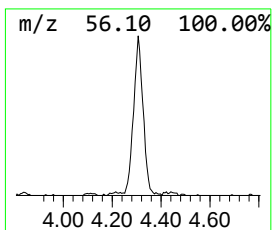
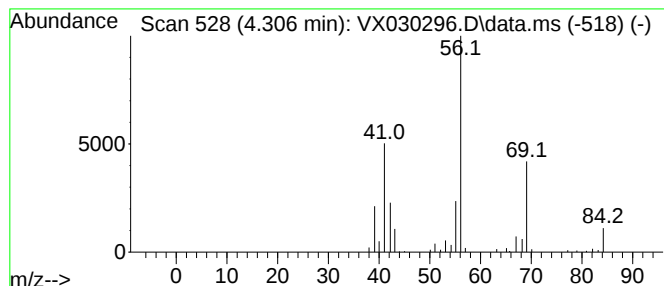
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	9.73 ug/l	95352	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50
5			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	39



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.282	53.8	ug/l	527502	1	5.562	490092	50.0
Butane, 2-methyl-	1.746	5.8	ug/l	57360	1	5.562	490092	50.0
Butane, 2,3-dim...	2.782	6.0	ug/l	58427	1	5.562	490092	50.0
Cyclopentane	2.867	10.1	ug/l	99034	1	5.562	490092	50.0
Cyclopentane, m...	4.306	9.7	ug/l	95352	1	5.562	490092	50.0