

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
 Data File : VX029235.D
 Acq On : 06 Jun 2022 13:37
 Operator : JC/MD
 Sample : N3174-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MID0622

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\82X053122W.M
 Title : SW846 8260

Signal : TIC: VX029235.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	25	29	43	rBV	92784	212329	11.64%	1.941%
2	1.367	43	46	50	rVB	24642	29681	1.63%	0.271%
3	1.752	104	109	115	rVB	81137	108963	5.97%	0.996%
4	2.544	229	239	247	rBV2	9254	23401	1.28%	0.214%
5	2.867	284	292	302	rVV	67967	132813	7.28%	1.214%
6	2.959	302	307	316	rVB2	12803	30883	1.69%	0.282%
7	3.117	325	333	340	rBV4	7871	19998	1.10%	0.183%
8	4.306	518	528	540	rBV3	19385	56460	3.09%	0.516%
9	5.385	693	705	715	rBV	218119	644963	35.35%	5.896%
10	5.556	724	733	748	rVB	338580	954659	52.33%	8.726%
11	5.958	786	799	807	rBV	220908	588914	32.28%	5.383%
12	6.043	807	813	830	rVV2	64603	180540	9.90%	1.650%
13	6.239	830	845	858	rVV3	29239	93673	5.13%	0.856%
14	6.763	921	931	951	rBV	561799	1333922	73.12%	12.193%
15	8.427	1198	1204	1211	rBV2	19428	33023	1.81%	0.302%
16	8.653	1233	1241	1249	rBV	1164761	1824313	100.00%	16.676%
17	8.842	1262	1272	1279	rVB3	12674	23195	1.27%	0.212%
18	9.567	1386	1391	1398	rVB	13027	20021	1.10%	0.183%
19	10.055	1461	1471	1483	rBV	1267246	1684578	92.34%	15.398%
20	11.085	1634	1640	1651	rBV	974629	1288890	70.65%	11.782%
21	12.024	1788	1794	1801	rBV	1369778	1654684	90.70%	15.125%

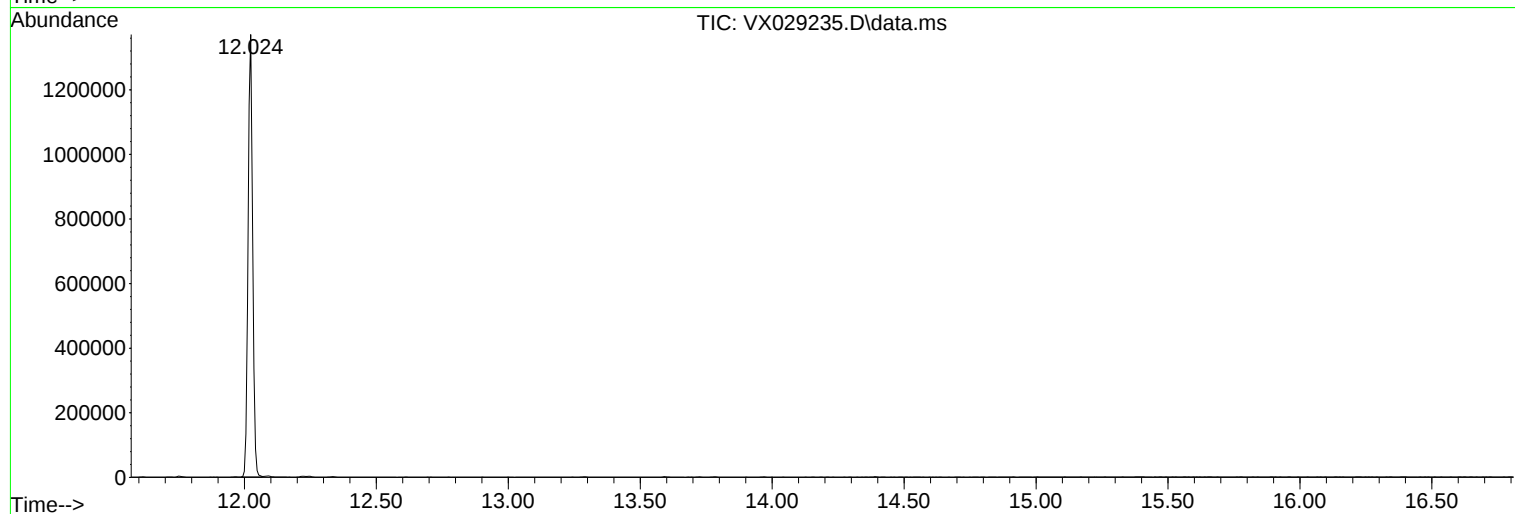
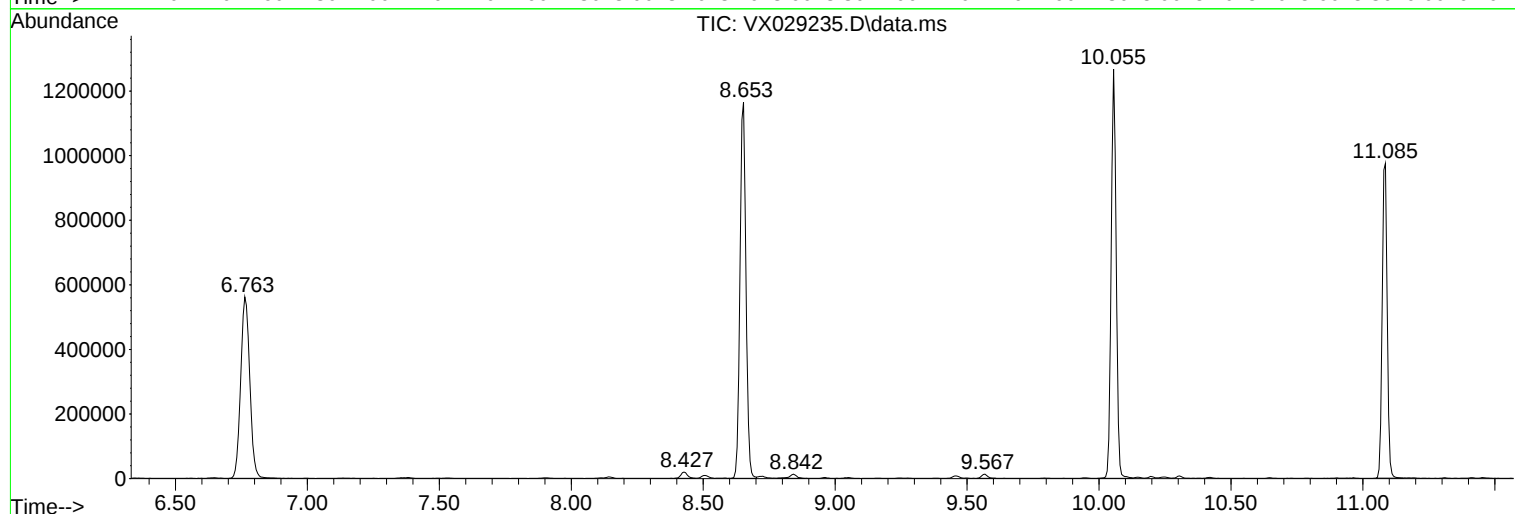
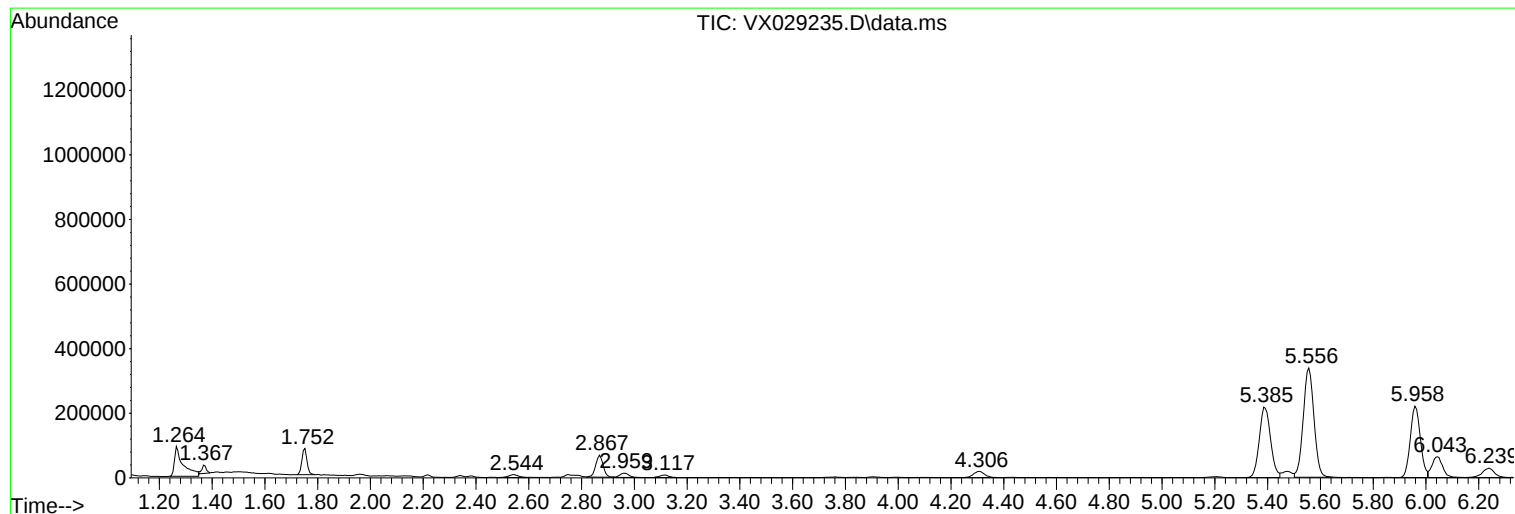
Sum of corrected areas: 10939903

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029235.D
Acq On : 06 Jun 2022 13:37
Operator : JC/MD
Sample : N3174-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MID0622

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029235.D
Acq On : 06 Jun 2022 13:37
Operator : JC/MD
Sample : N3174-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MID0622

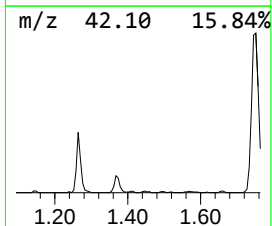
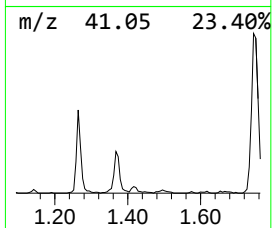
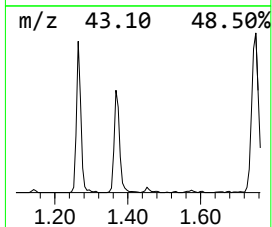
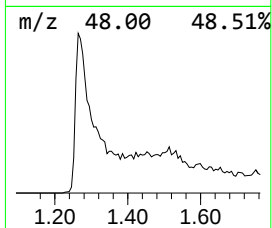
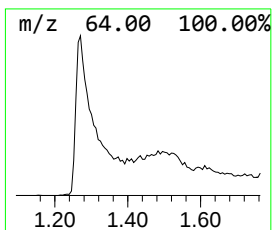
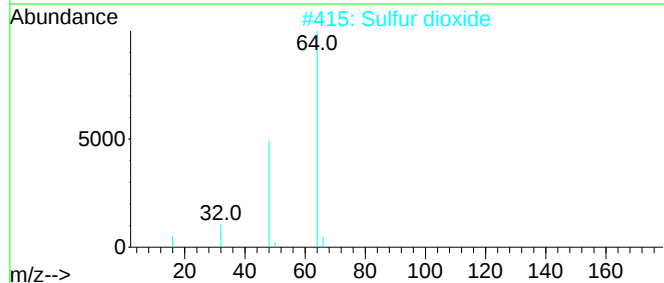
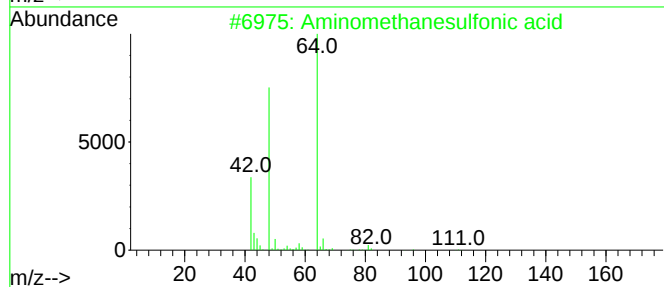
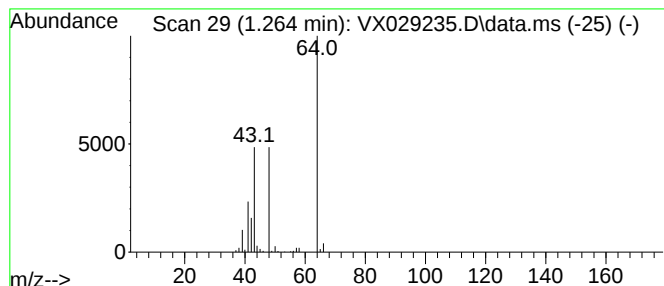
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	11.12 ug/l	212329	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Sulfur dioxide	64	O2S	007446-09-5	78
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029235.D
Acq On : 06 Jun 2022 13:37
Operator : JC/MD
Sample : N3174-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MID0622

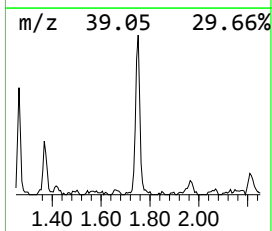
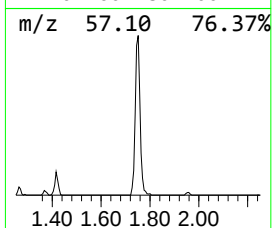
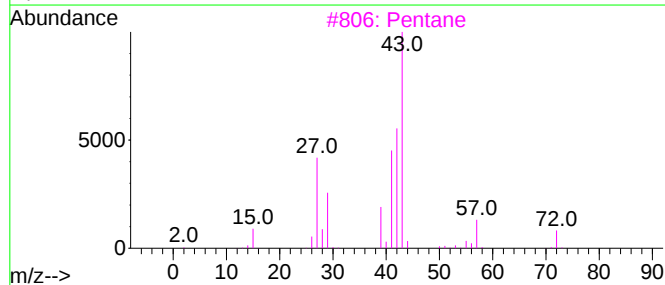
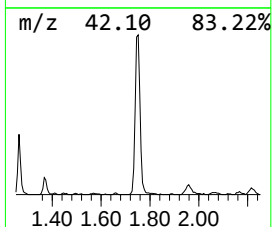
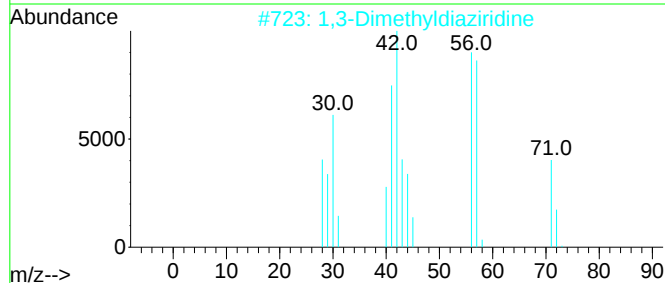
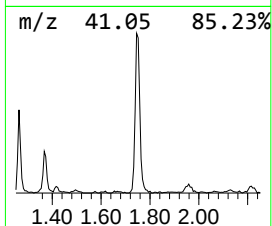
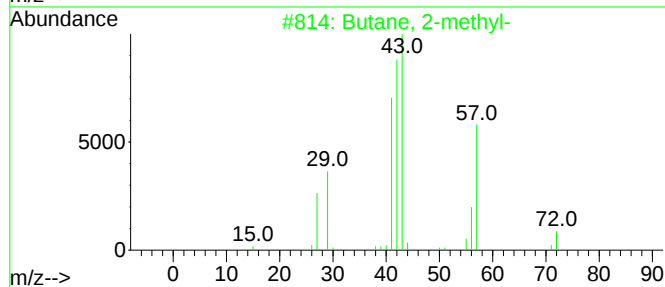
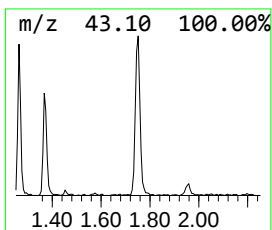
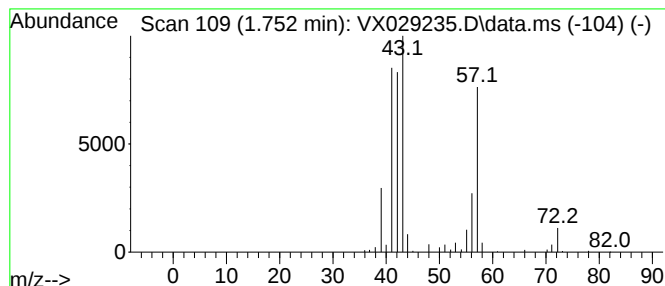
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	5.71 ug/l	108963	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	36
3			Pentane	72	C5H12	000109-66-0	33
4			3-Buten-1-ol	72	C4H8O	000627-27-0	23
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029235.D
Acq On : 06 Jun 2022 13:37
Operator : JC/MD
Sample : N3174-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MID0622

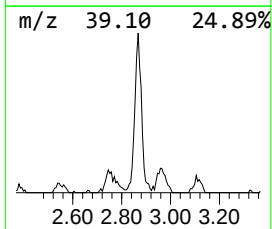
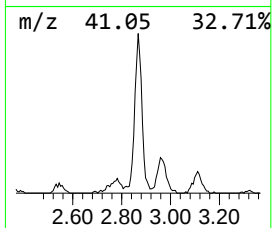
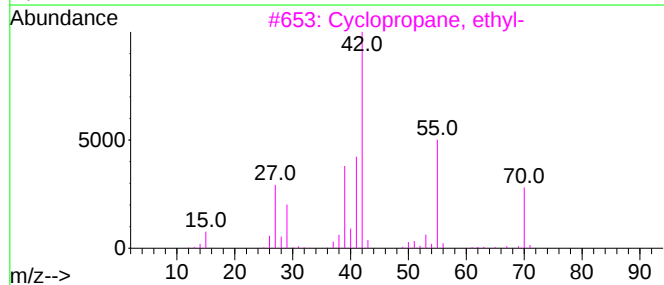
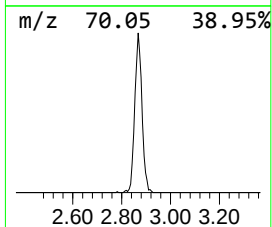
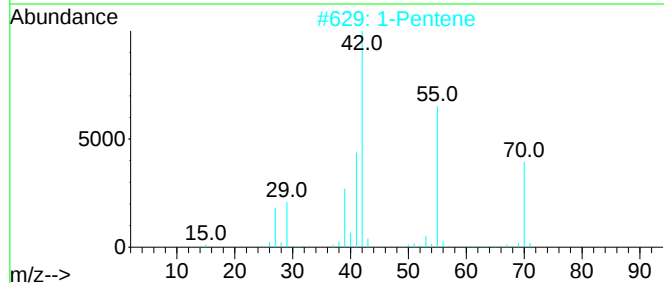
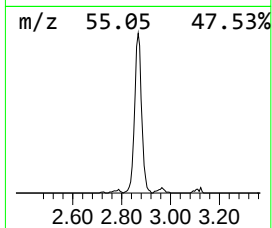
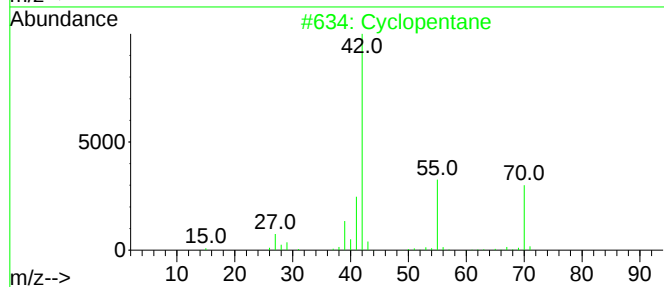
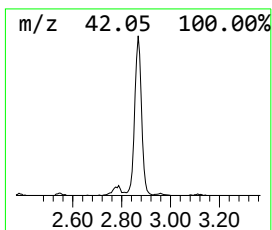
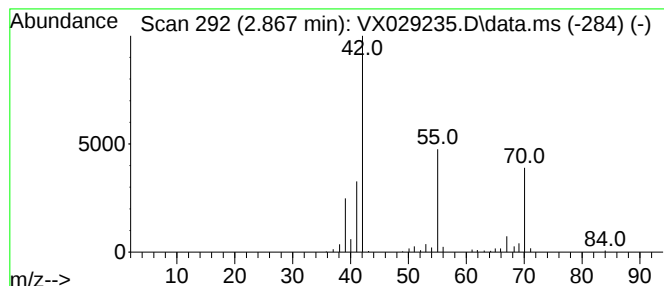
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	6.96 ug/l	132813	Pentafluorobenzene	5.556

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	86
3			Cyclopropane, ethyl-	70	C5H10	001191-96-4	64
4			3-Buten-1-ol	72	C4H8O	000627-27-0	47
5			Cyclobutanone	70	C4H6O	001191-95-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029235.D
Acq On : 06 Jun 2022 13:37
Operator : JC/MD
Sample : N3174-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MID0622

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
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
Aminomethanesul...	1.264	11.1	ug/l	212329	1	5.556	954659	50.0
Butane, 2-methyl-	1.752	5.7	ug/l	108963	1	5.556	954659	50.0
Cyclopentane	2.867	7.0	ug/l	132813	1	5.556	954659	50.0