

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
 Data File : VN074245.D
 Acq On : 01 Sep 2022 16:19
 Operator : JC\MD
 Sample : N4329-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-3R

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\82N083022W.M
 Title : SW846 8260

Signal : TIC: VN074245.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.399	80	87	94	rBV	49029	83865	2.25%	0.521%
2	3.087	195	204	213	rBV	141450	305956	8.21%	1.901%
3	3.451	259	266	278	rVB3	40947	94940	2.55%	0.590%
4	5.087	533	544	559	rVB6	36179	181530	4.87%	1.128%
5	5.534	605	620	637	rBV2	817308	2880727	77.27%	17.901%
6	6.410	759	769	782	rVB4	47674	150437	4.04%	0.935%
7	7.063	870	880	890	rBV2	47498	138560	3.72%	0.861%
8	7.251	902	912	924	rBV2	62128	179351	4.81%	1.114%
9	7.951	1020	1031	1037	rBV	223467	543334	14.57%	3.376%
10	8.022	1037	1043	1052	rVB	352844	802874	21.53%	4.989%
11	8.392	1093	1106	1117	rBV2	1477637	3728241	100.00%	23.167%
12	8.569	1134	1136	1142	rVB4	33170	53220	1.43%	0.331%
13	8.904	1183	1193	1206	rBV	587954	1177884	31.59%	7.319%
14	9.957	1366	1372	1381	rVB5	17096	38199	1.02%	0.237%
15	10.380	1436	1444	1453	rBV	868506	1592825	42.72%	9.898%
16	11.686	1656	1666	1673	rBV	828954	1497002	40.15%	9.302%
17	11.786	1678	1683	1690	rVB2	33880	62636	1.68%	0.389%
18	12.668	1827	1833	1843	rBV	680431	1161043	31.14%	7.215%
19	13.615	1984	1994	2003	rBV	816383	1420323	38.10%	8.826%

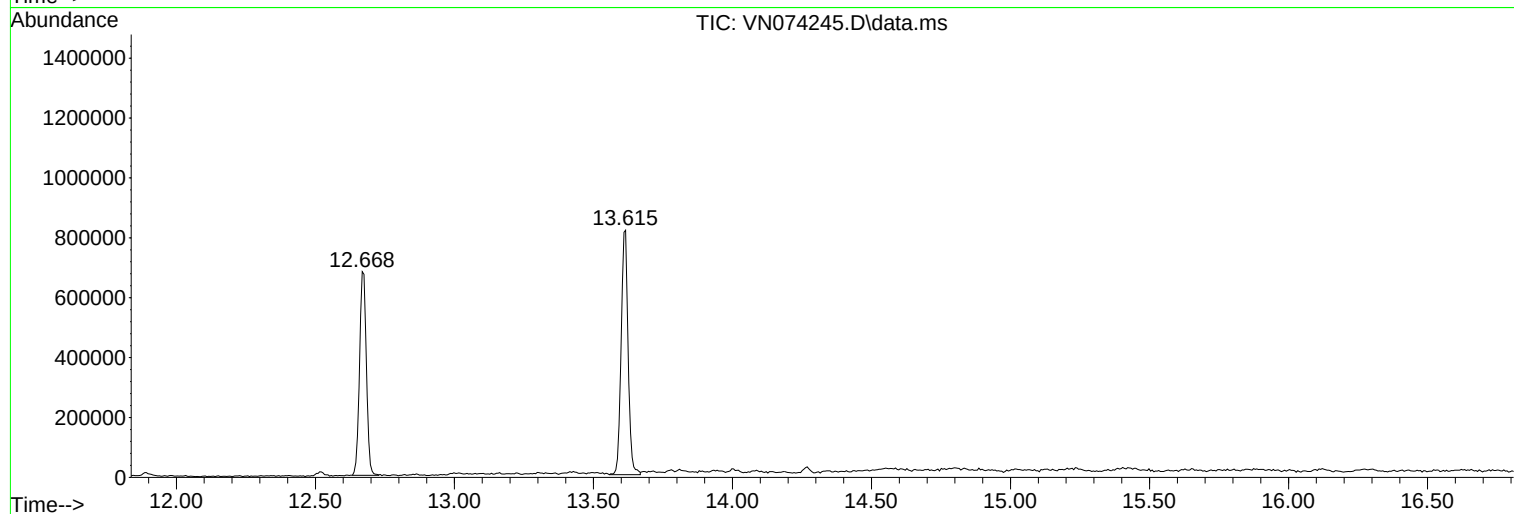
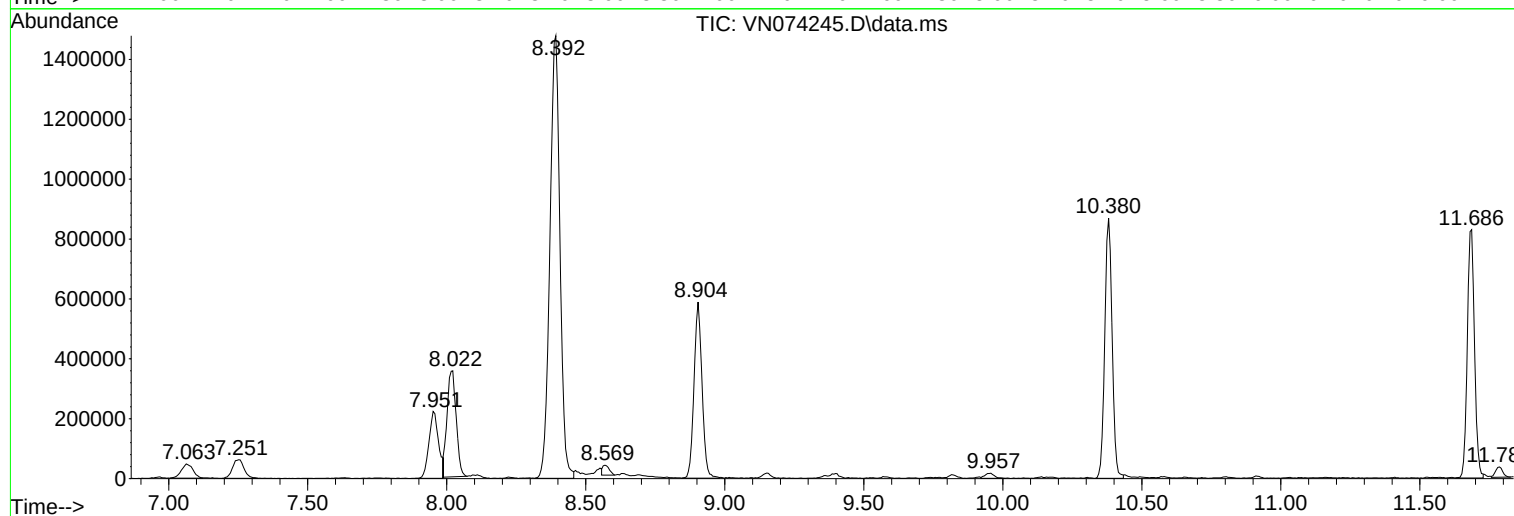
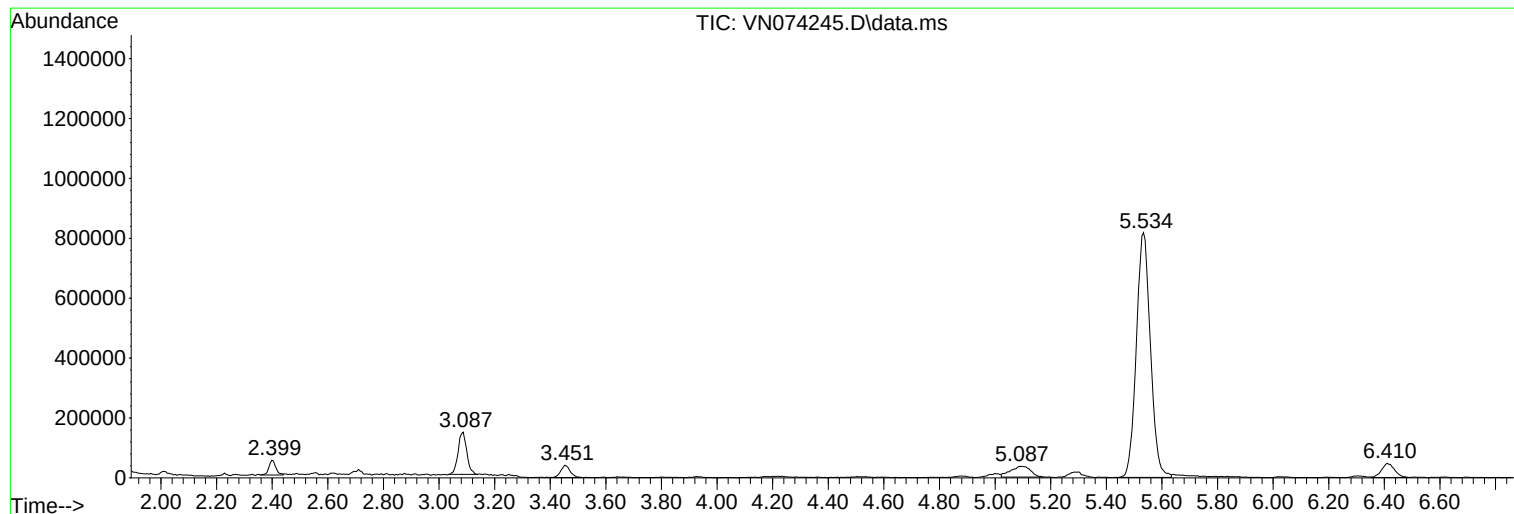
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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



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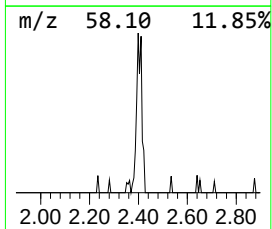
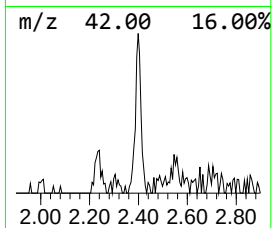
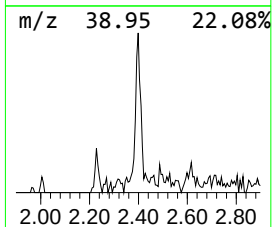
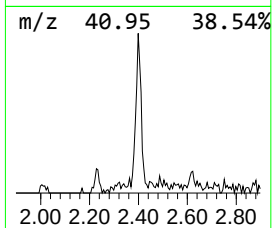
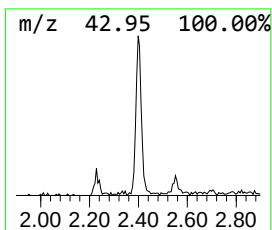
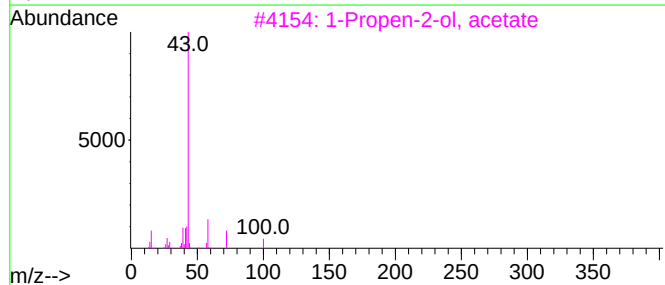
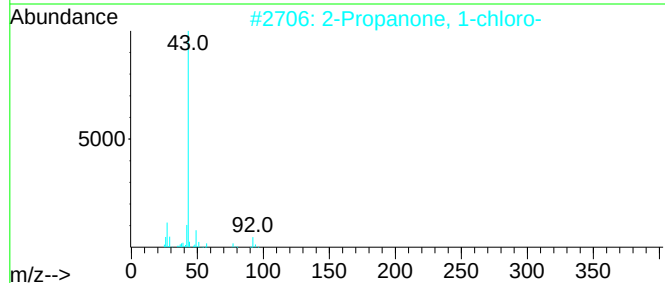
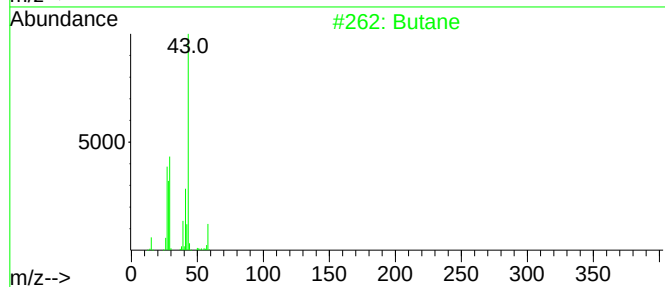
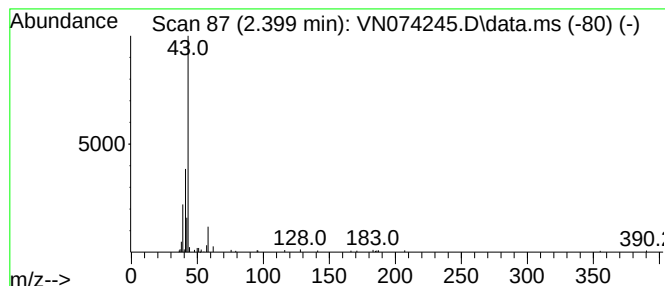
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.399 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.399	5.22 ug/l	83865	Pentafluorobenzene	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	42
2			2-Propanone, 1-chloro-	92	C3H5ClO	000078-95-5	9
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4			Hydrogen isocyanate	43	CHNO	000075-13-8	4
5			2-Furanol, tetrahydro-2,3-dimeth...	116	C6H12O2	061142-77-6	4



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ALS Vial : 18 Sample Multiplier: 1

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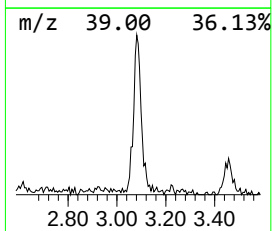
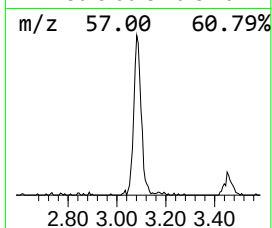
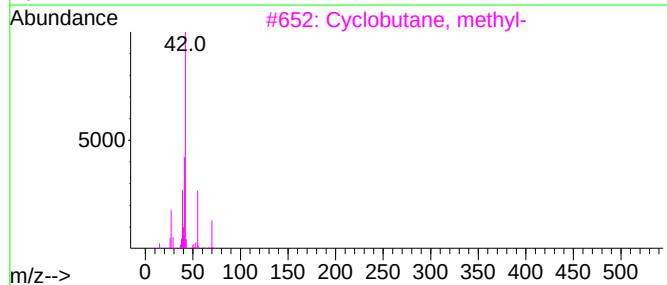
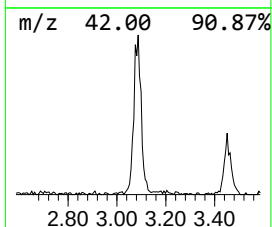
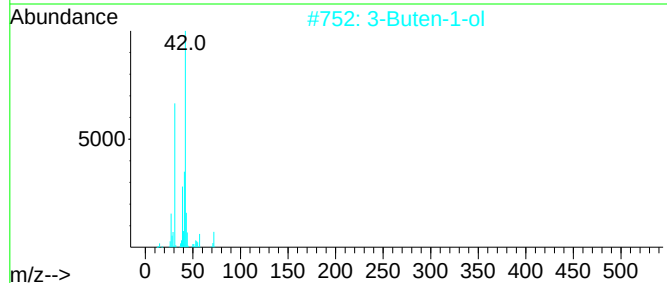
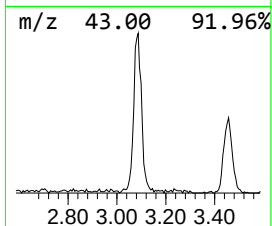
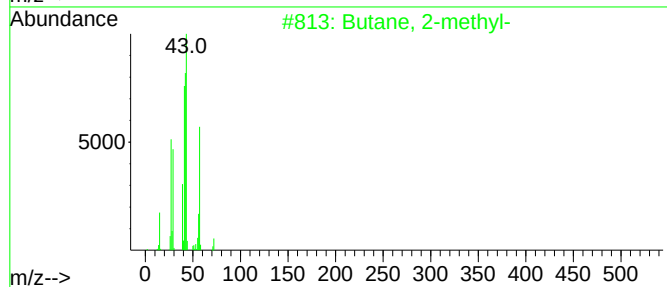
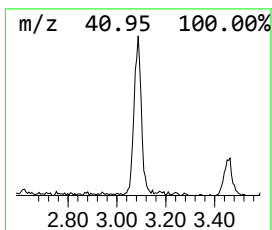
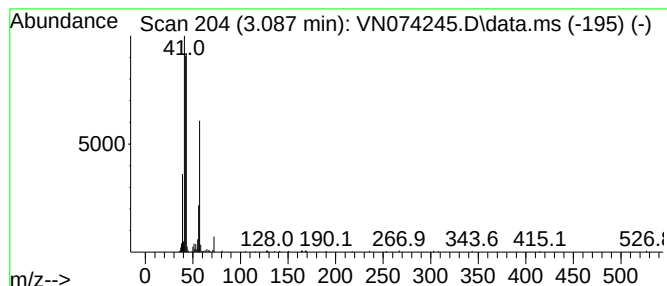
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	19.05 ug/l	305956	Pentafluorobenzene	8.022

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	43
3			Cyclobutane, methyl-	70	C5H10	000598-61-8	28
4			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28
5			1-Butene	56	C4H8	000106-98-9	10



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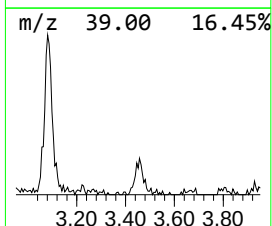
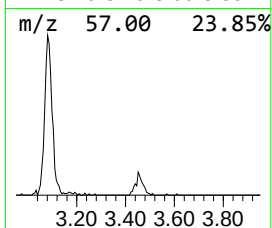
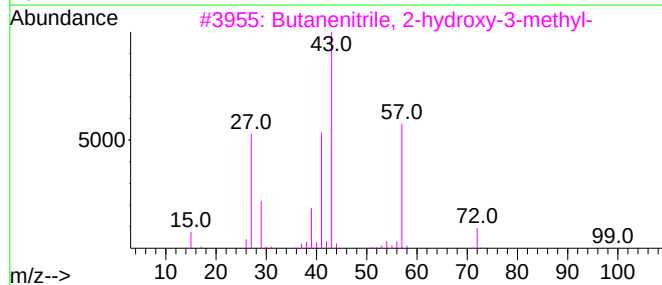
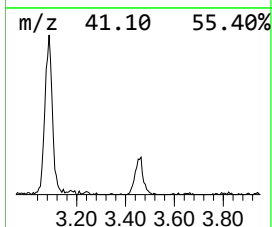
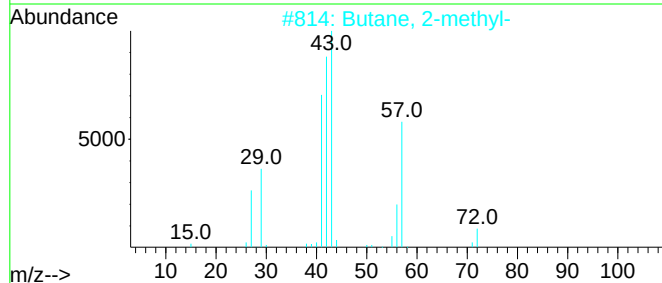
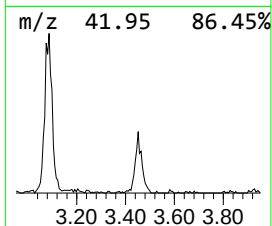
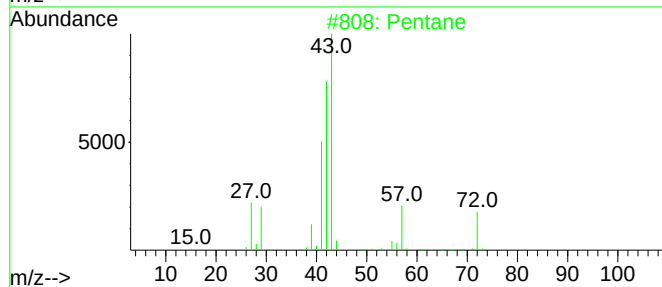
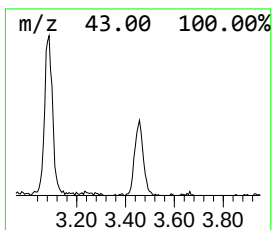
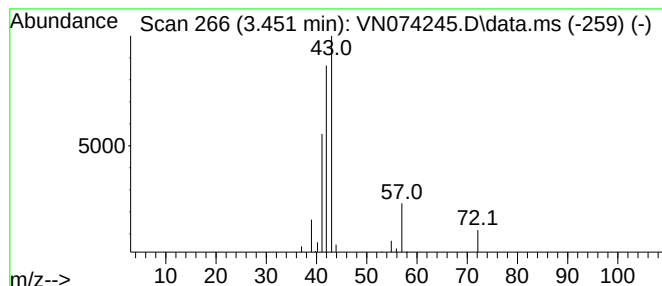
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.451	5.91 ug/l	94940	Pentafluorobenzene	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	90
2			Butane, 2-methyl-	72	C5H12	000078-78-4	78
3			Butanenitrile, 2-hydroxy-3-methyl-	99	C5H9NO	010021-64-4	10
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5			Butane, 2-chloro-3-methyl-	106	C5H11Cl	000631-65-2	9



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3R

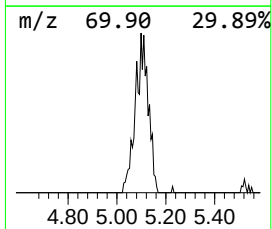
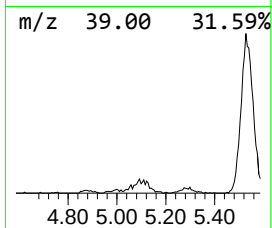
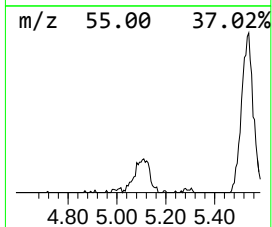
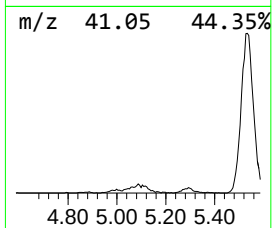
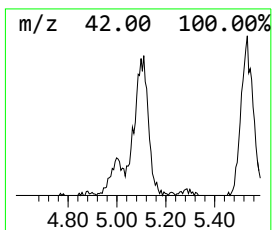
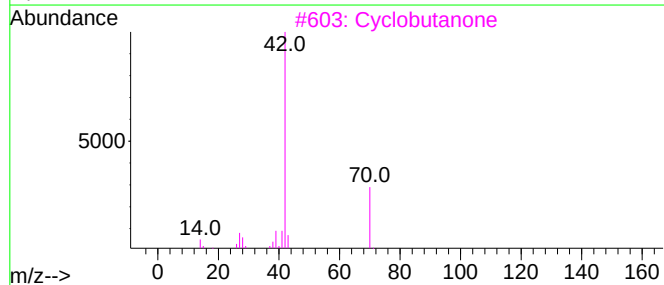
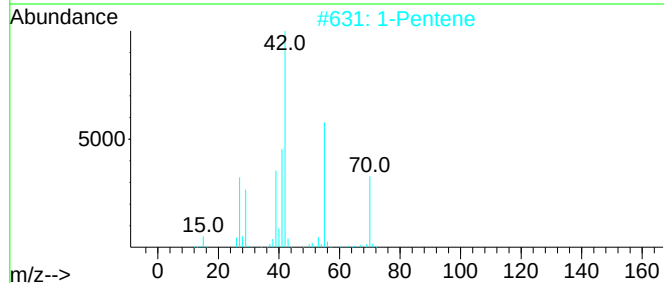
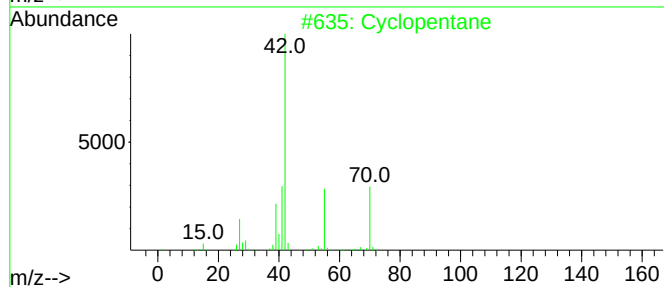
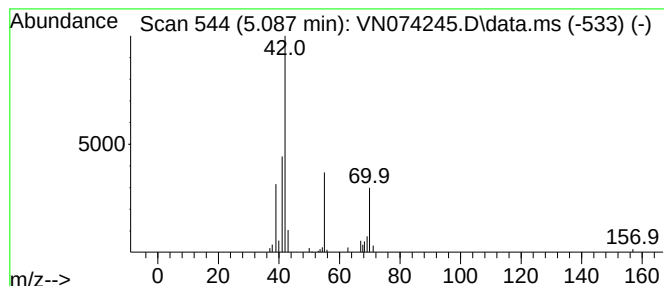
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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.
5.087	11.31 ug/l	181530	Pentafluorobenzene	8.022

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	56
3			Cyclobutanone	70	C4H6O	001191-95-3	50
4			Cyclopropane, ethyl-	70	C5H10	001191-96-4	45
5			2-Butene-1,4-diol, (Z)-	88	C4H8O2	006117-80-2	39



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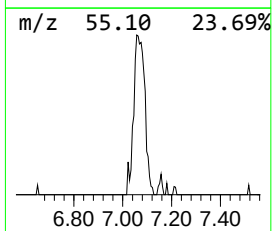
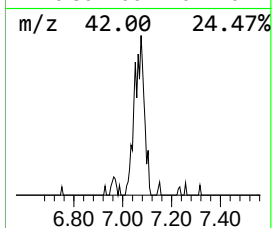
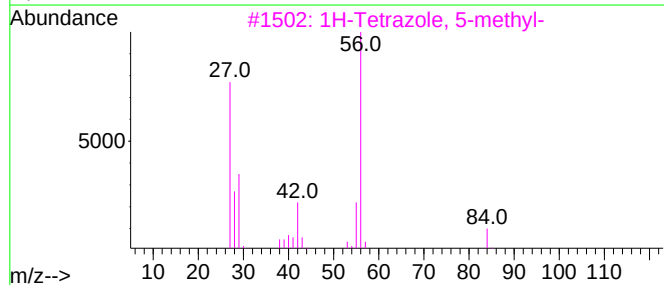
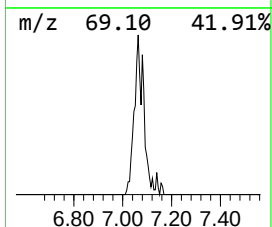
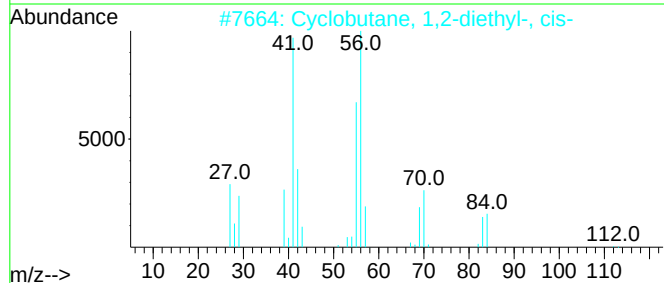
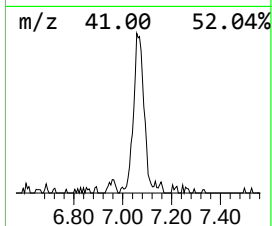
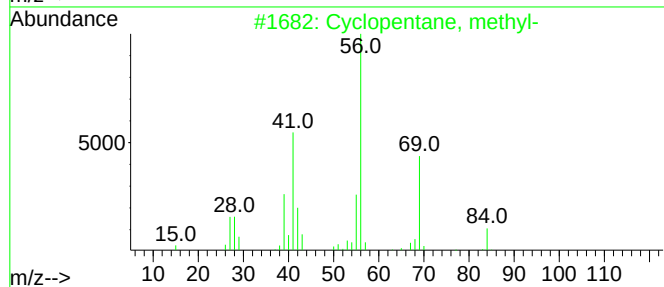
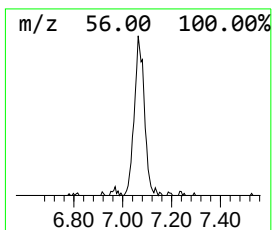
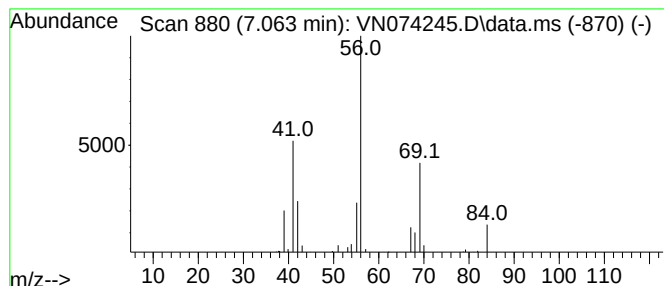
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.063	8.63 ug/l	138560	Pentafluorobenzene	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	86
2			Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	45
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	36
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	33
5			Cyclobutane, butyl-	112	C8H16	013152-44-8	23



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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
unknown2.399	2.399	5.2	ug/l	83865	1	8.022	802874	50.0
Butane, 2-methyl-	3.087	19.1	ug/l	305956	1	8.022	802874	50.0
Pentane	3.451	5.9	ug/l	94940	1	8.022	802874	50.0
Cyclopentane	5.087	11.3	ug/l	181530	1	8.022	802874	50.0
Cyclopentane, m...	7.063	8.6	ug/l	138560	1	8.022	802874	50.0