

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
 Data File : VN073030.D
 Acq On : 22 Jun 2022 17:18
 Operator : JC\MD
 Sample : N3381-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-1

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\82N061722W.M
 Title : SW846 8260

Signal : TIC: VN073030.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	48	58	69	rBV	427526	625743	1.15%	0.581%
2	2.405	78	88	97	rBV	1299704	2068761	3.80%	1.922%
3	3.087	193	204	220	rBV	744430	1675613	3.08%	1.557%
4	3.457	258	267	281	rVB3	315893	852792	1.57%	0.792%
5	3.663	290	302	315	rBV	260172	642348	1.18%	0.597%
6	3.934	339	348	361	rVB	569860	1526514	2.81%	1.418%
7	4.881	494	509	521	rBV2	379486	1260748	2.32%	1.171%
8	5.104	533	547	571	rVB	362050	1463660	2.69%	1.360%
9	7.069	868	881	891	rBV	235345	701134	1.29%	0.651%
10	7.951	1021	1031	1036	rBV	231609	550065	1.01%	0.511%
11	8.016	1036	1042	1053	rVB2	525362	1273638	2.34%	1.183%
12	8.392	1092	1106	1124	rBV	21972367	54385595	100.00%	50.535%
13	8.904	1183	1193	1206	rBV	608222	1274637	2.34%	1.184%
14	10.375	1436	1443	1448	rBV	818885	1511230	2.78%	1.404%
15	10.439	1448	1454	1471	rVB	6500023	11964882	22.00%	11.118%
16	11.680	1656	1665	1675	rBV	899189	1595111	2.93%	1.482%
17	11.780	1675	1682	1691	rVB	1201918	2026879	3.73%	1.883%
18	11.886	1691	1700	1712	rBV	5724688	11197494	20.59%	10.405%
19	12.216	1743	1756	1768	rBV	3594669	6007868	11.05%	5.583%
20	12.669	1825	1833	1845	rBV	734960	1256676	2.31%	1.168%
21	12.921	1869	1876	1879	rBV	377849	651699	1.20%	0.606%
22	13.304	1929	1941	1948	rBV	659113	1064220	1.96%	0.989%
23	13.610	1985	1993	2005	rBV2	954193	2041593	3.75%	1.897%

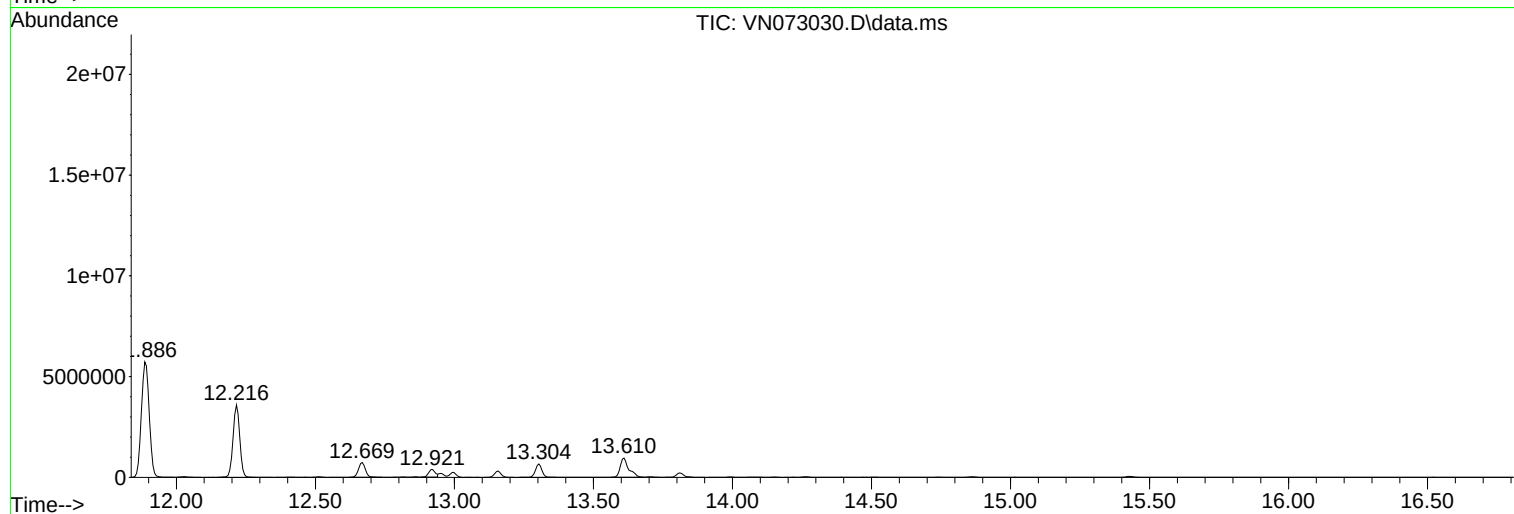
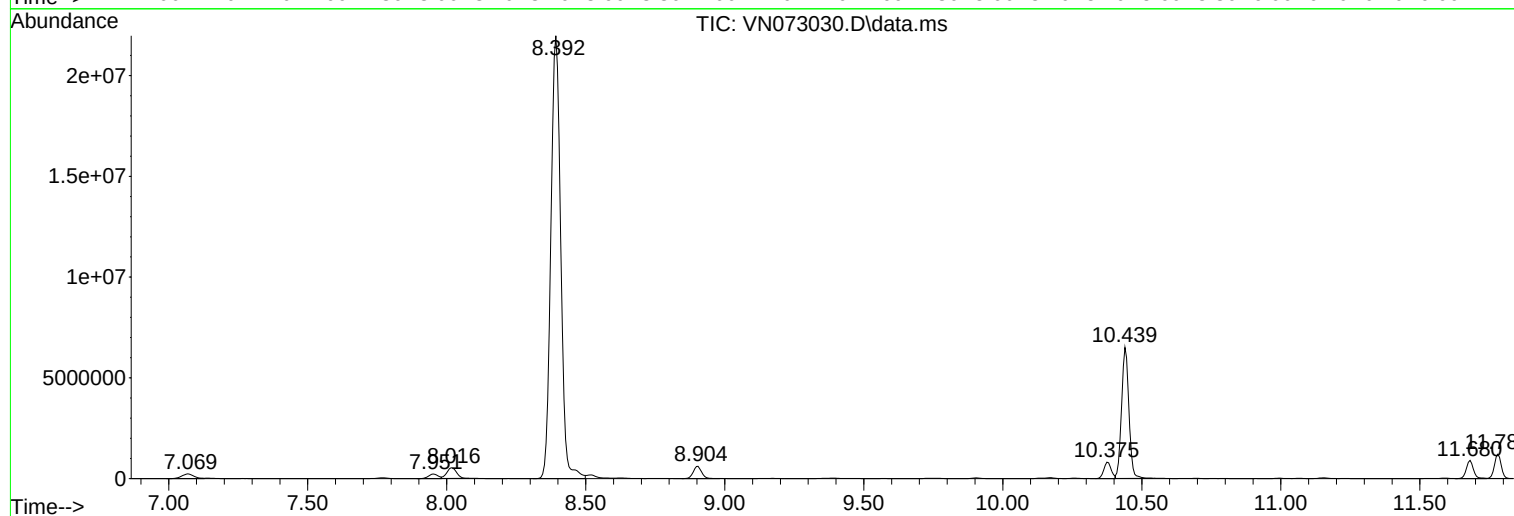
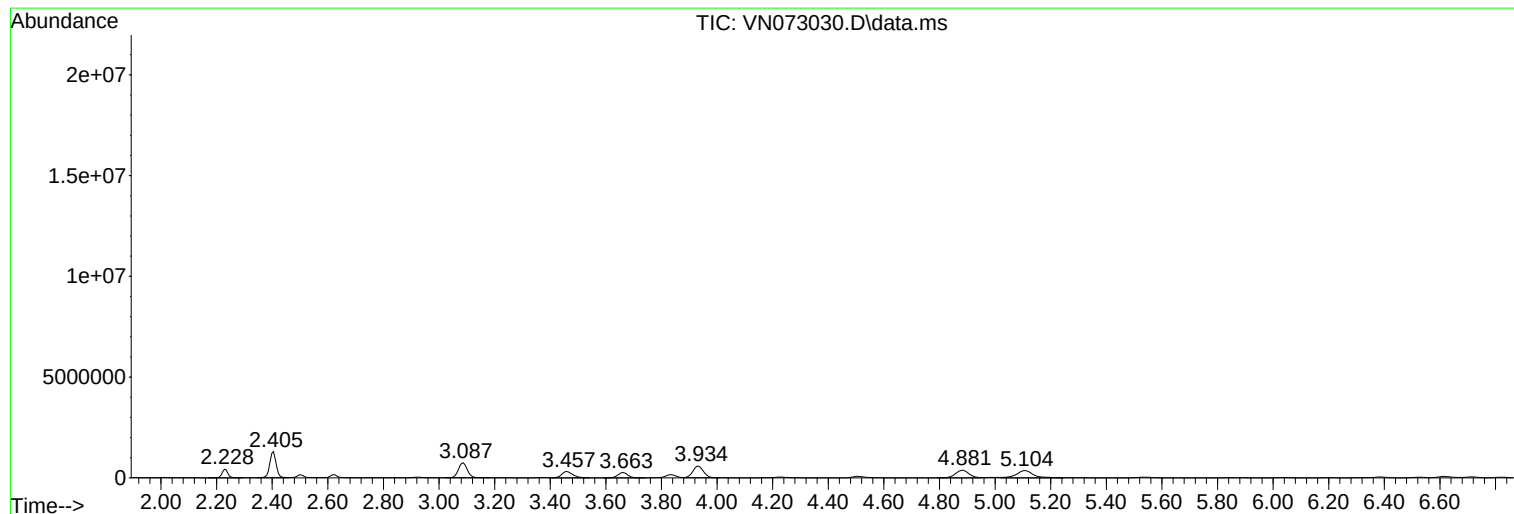
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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



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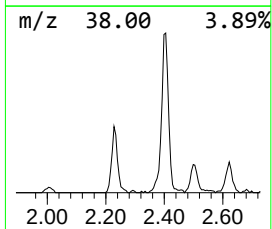
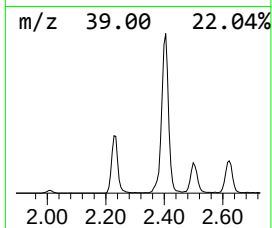
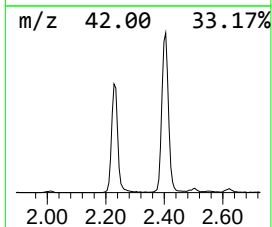
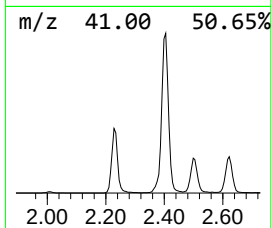
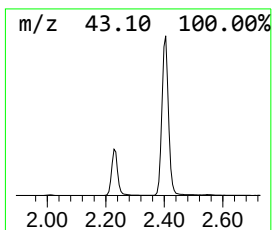
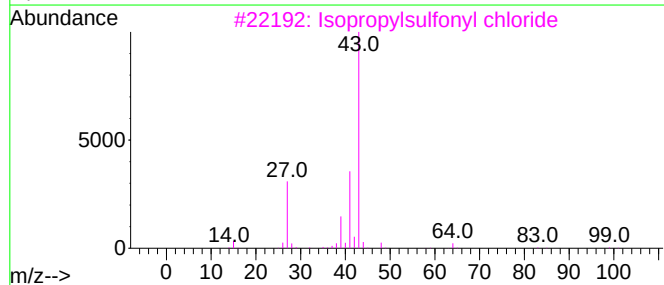
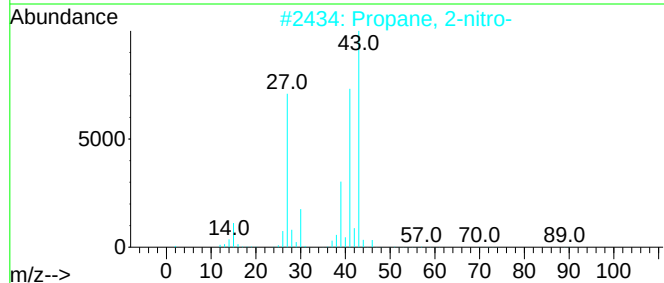
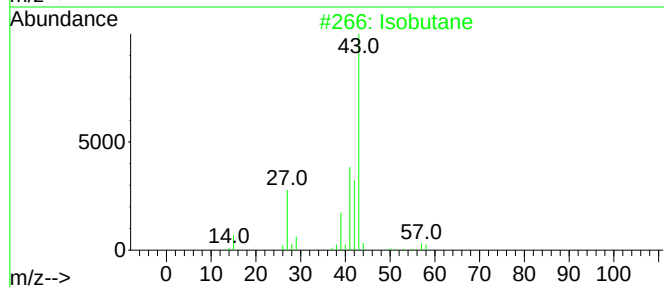
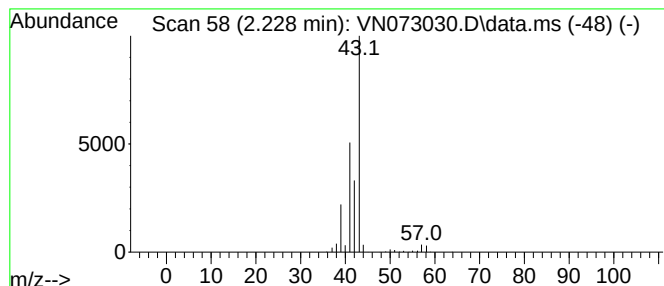
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	24.57 ug/l	625743	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	72
2			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4			Borane, trimethyl-	56	C3H9B	000593-90-8	4
5			Hydrogen isocyanate	43	CHNO	000075-13-8	4



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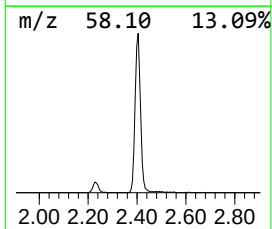
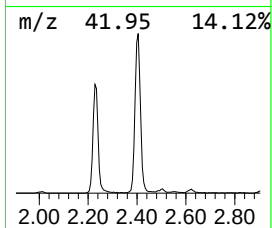
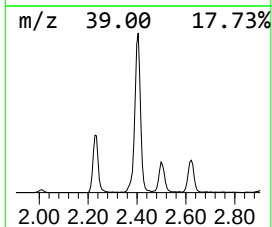
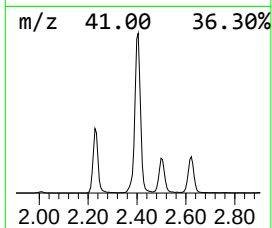
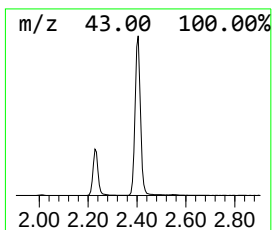
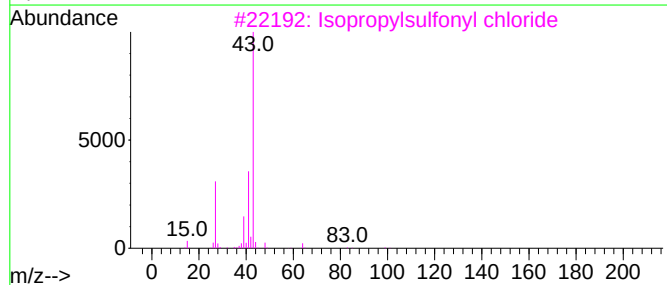
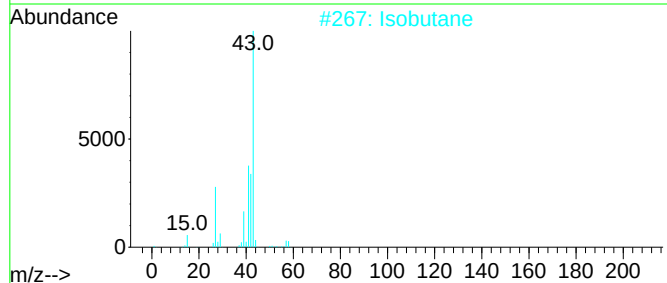
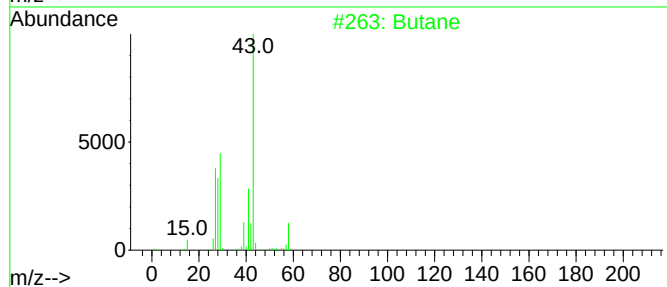
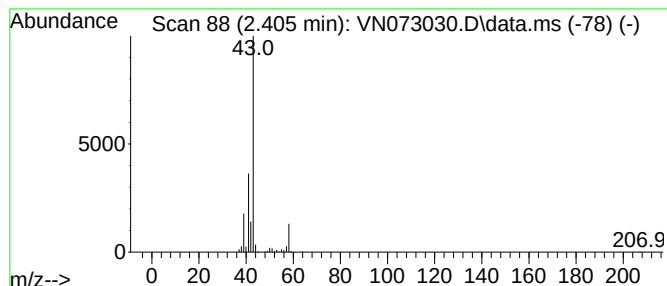
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.405	81.21 ug/l	2068760	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane			58	C4H10	000106-97-8	80
2	Isobutane			58	C4H10	000075-28-5	9
3	Isopropylsulfonyl chloride			142	C3H7ClO2S	010147-37-2	9
4	Propane, 1-nitro-			89	C3H7NO2	000108-03-2	9
5	Diazene, dimethyl-			58	C2H6N2	000503-28-6	5



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Instrument :
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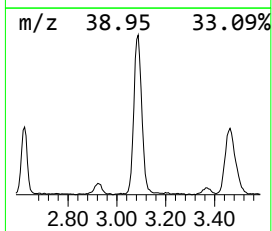
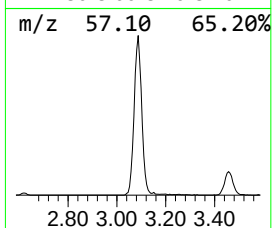
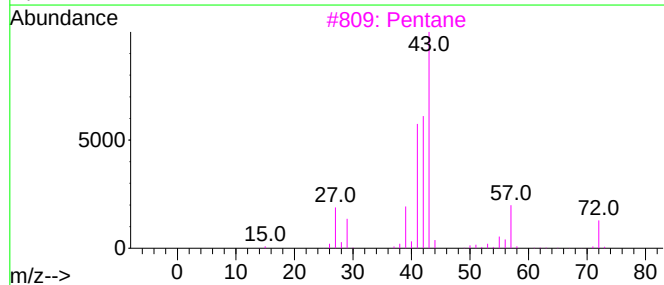
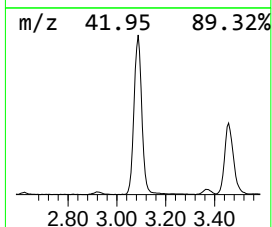
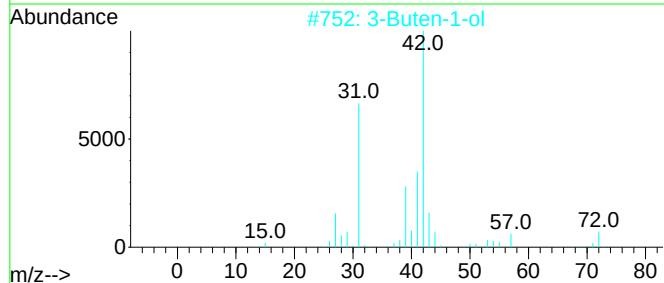
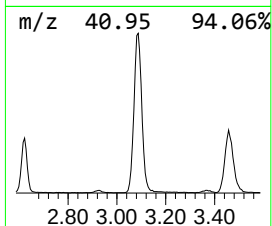
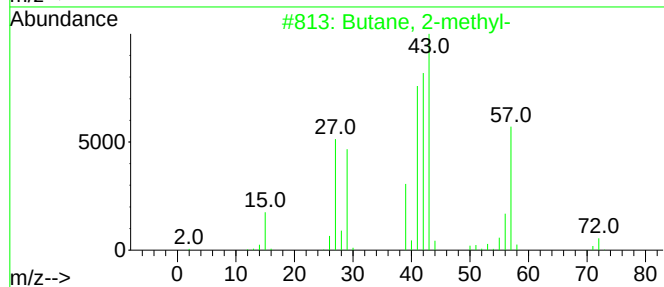
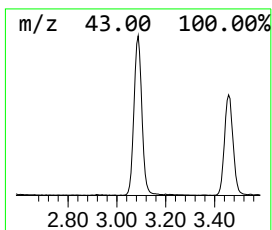
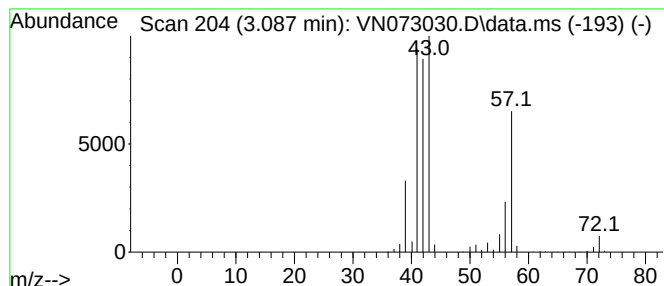
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	65.78 ug/l	1675610	Pentafluorobenzene	8.016

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	36
4			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	12
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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ALS Vial : 11 Sample Multiplier: 1

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ClientSampleId :
MW-1

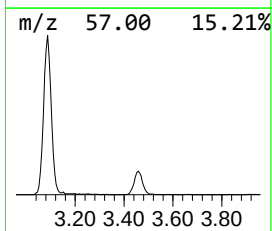
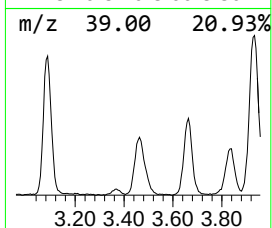
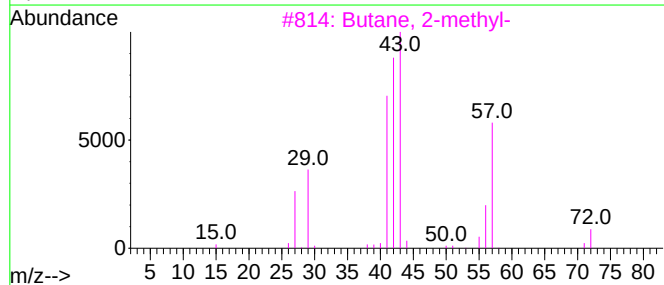
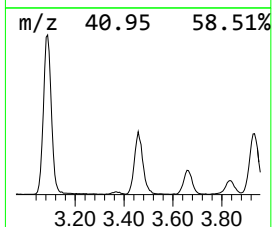
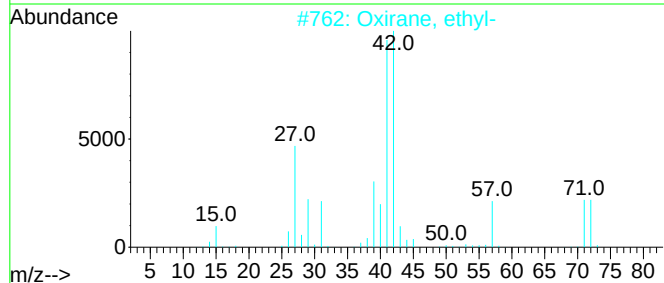
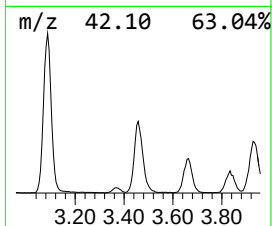
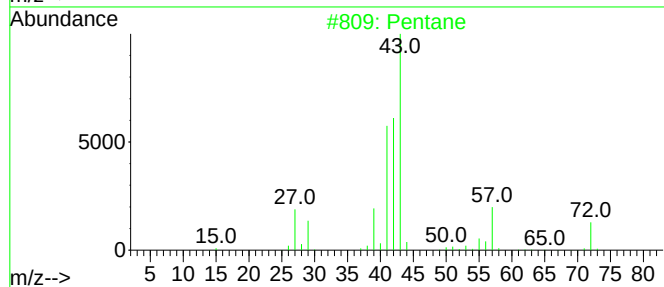
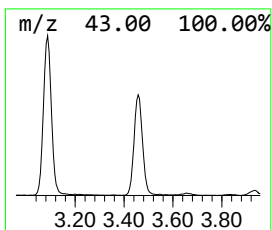
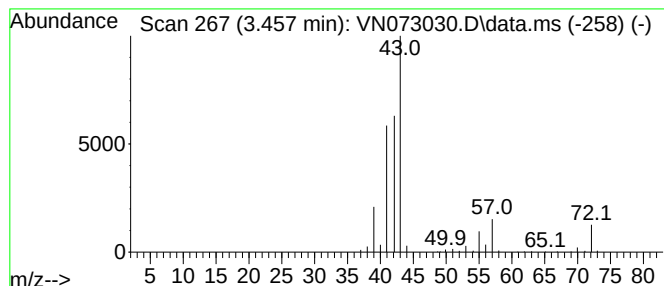
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Quant Title : SW846 8260

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

Peak Number 4 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.457	33.48 ug/l	852792	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	53
3			Butane, 2-methyl-	72	C5H12	000078-78-4	45
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5			Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	12



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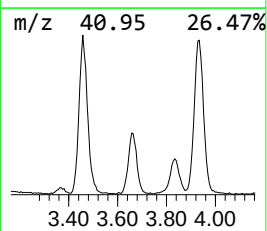
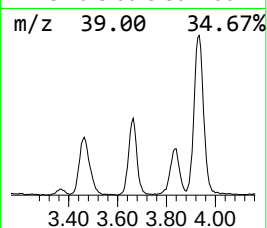
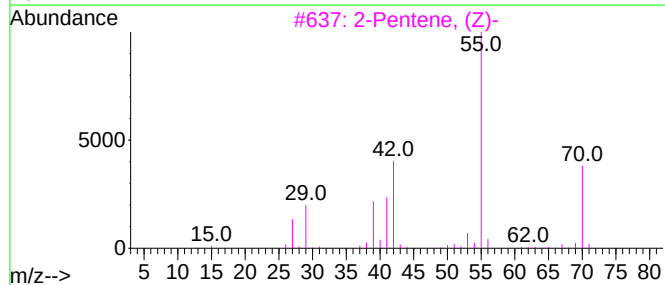
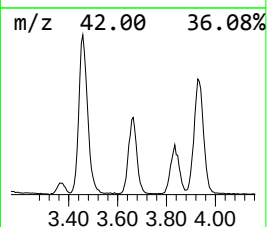
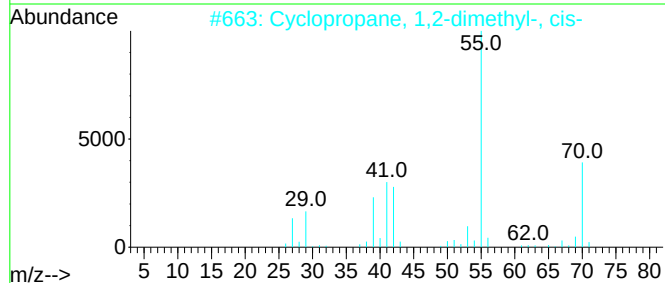
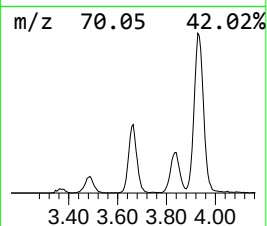
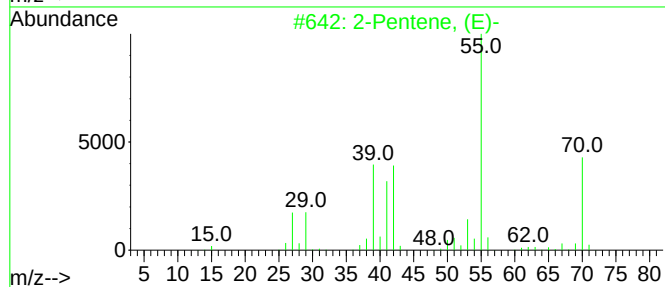
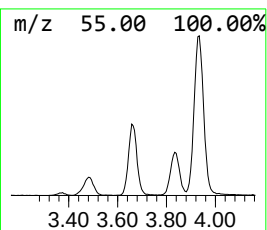
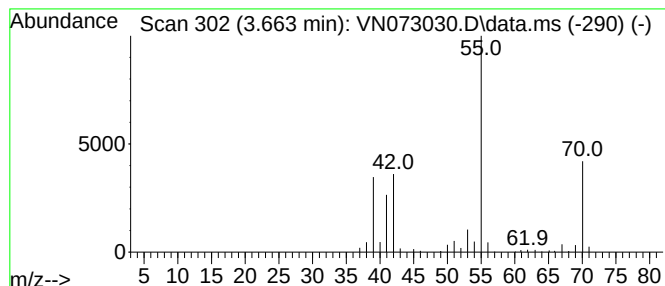
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 5 2-Pentene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.663	25.22 ug/l	642348	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentene, (E)-	70	C5H10	000646-04-8	93
2			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
3			2-Pentene, (Z)-	70	C5H10	000627-20-3	90
4			2-Butene, 2-methyl-	70	C5H10	000513-35-9	87
5			2-Pentene	70	C5H10	000109-68-2	87



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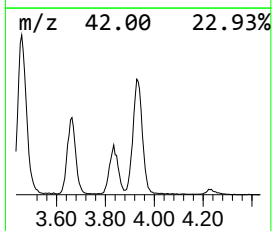
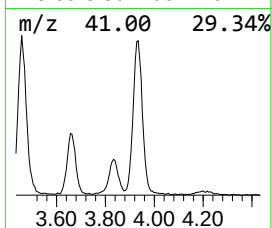
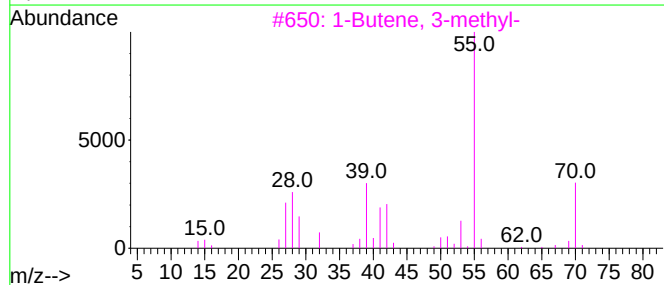
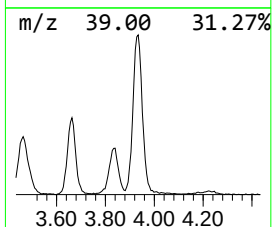
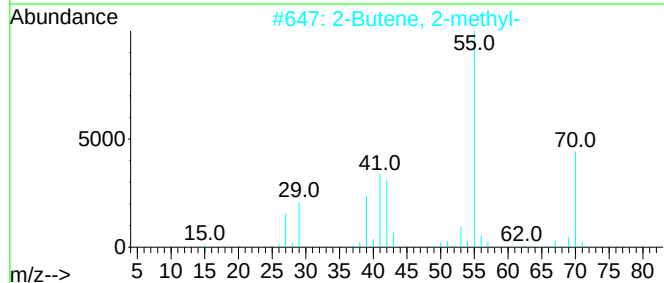
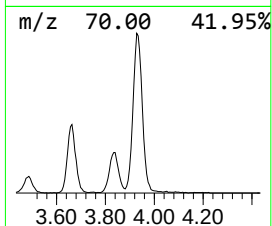
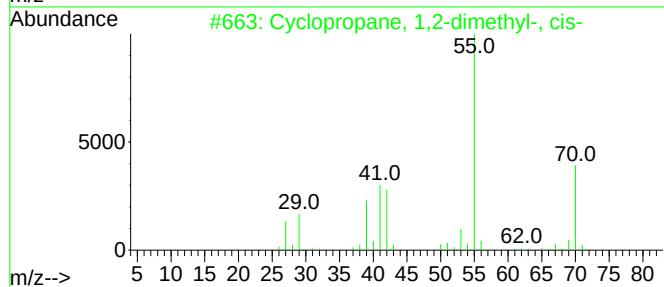
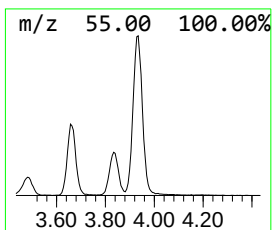
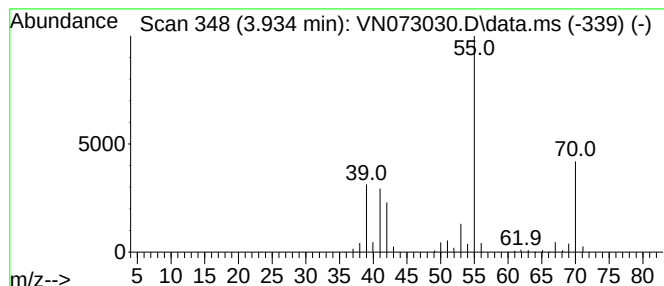
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopropane, 1,2-dimethyl-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.934	59.93 ug/l	1526510	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3			1-Butene, 3-methyl-	70	C5H10	000563-45-1	86
4			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
5			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073030.D
Acq On : 22 Jun 2022 17:18
Operator : JC\MD
Sample : N3381-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

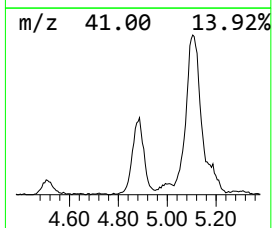
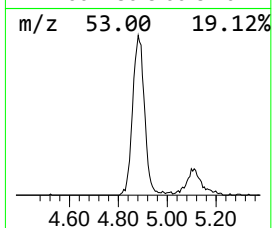
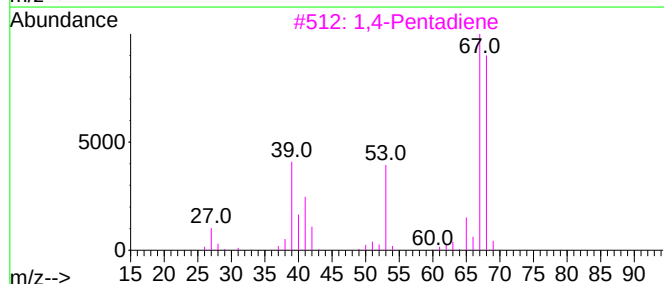
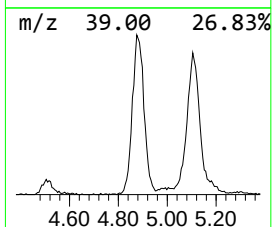
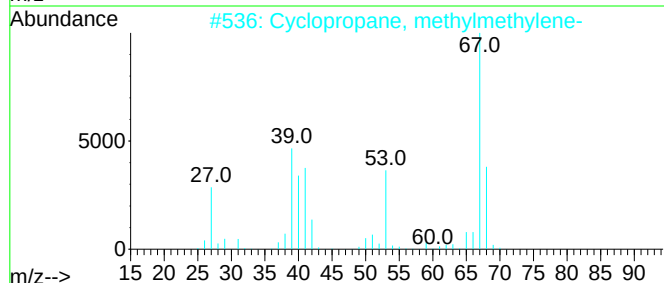
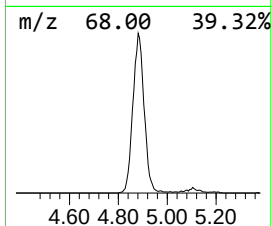
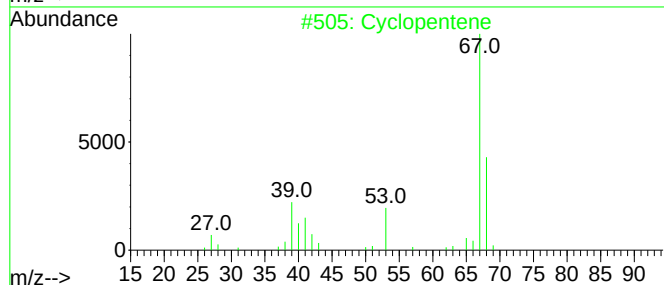
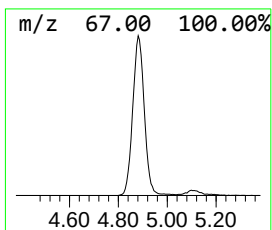
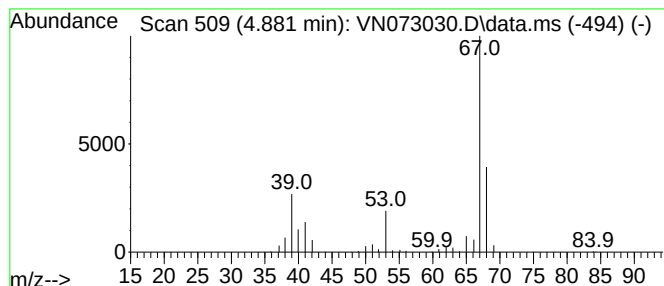
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.881	49.49 ug/l	1260750	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene	68	C5H8	000142-29-0	91
2	Cyclopropane, methylnmethylene-	68	C5H8	018631-84-0	91
3	1,4-Pentadiene	68	C5H8	000591-93-5	64
4	1-Butyne, 3-methyl-	68	C5H8	000598-23-2	59
5	Isoprene	68	C5H8	000078-79-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073030.D
Acq On : 22 Jun 2022 17:18
Operator : JC\MD
Sample : N3381-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

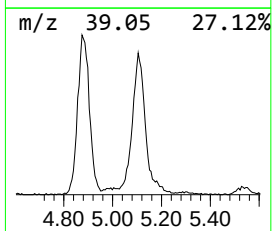
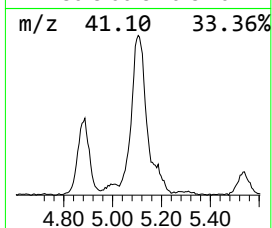
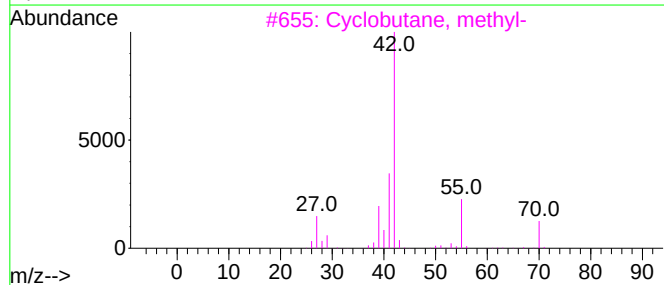
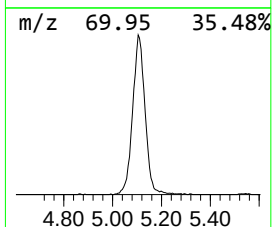
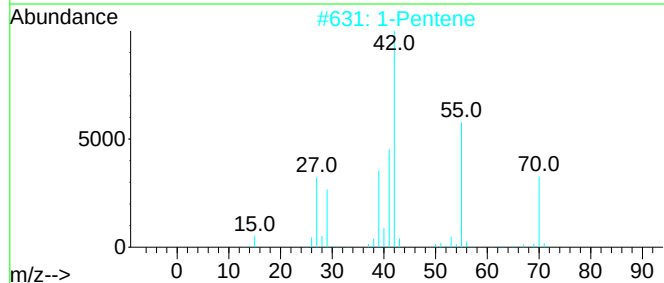
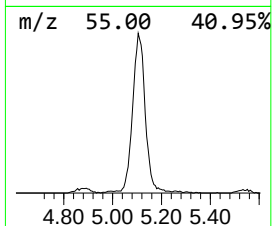
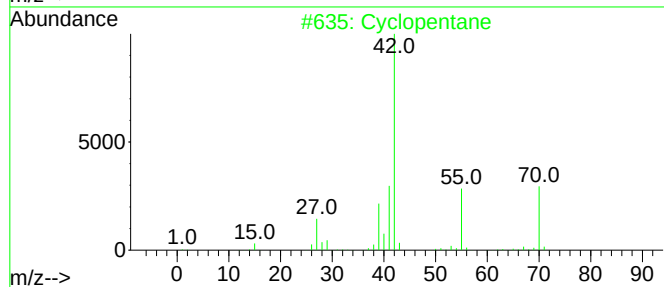
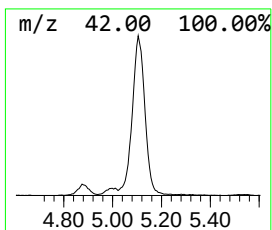
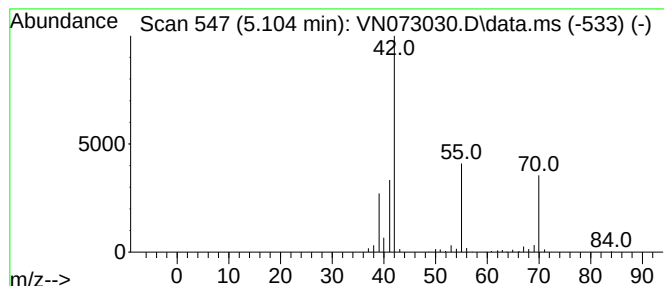
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	57.46 ug/l	1463660	Pentafluorobenzene	8.016

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			Cyclobutane, methyl-	70	C5H10	000598-61-8	56
4			2H-Pyran-2,6(3H)-dione, dihydro-	114	C5H6O3	000108-55-4	9
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073030.D
Acq On : 22 Jun 2022 17:18
Operator : JC\MD
Sample : N3381-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

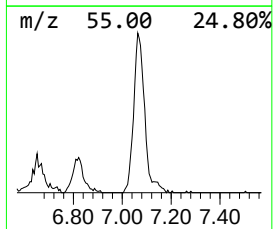
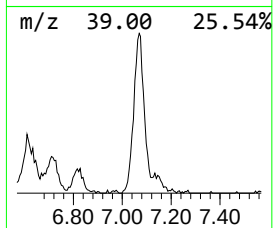
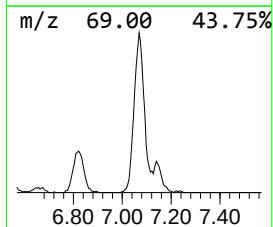
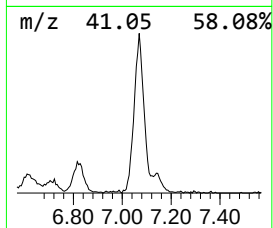
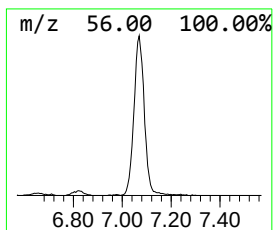
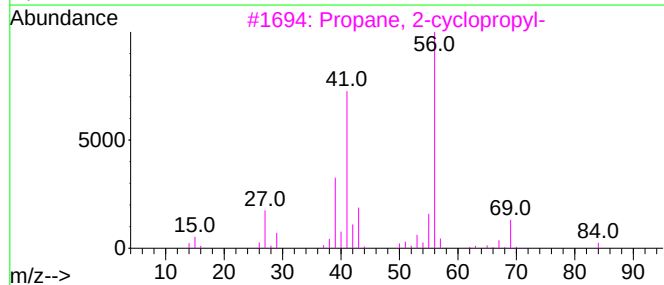
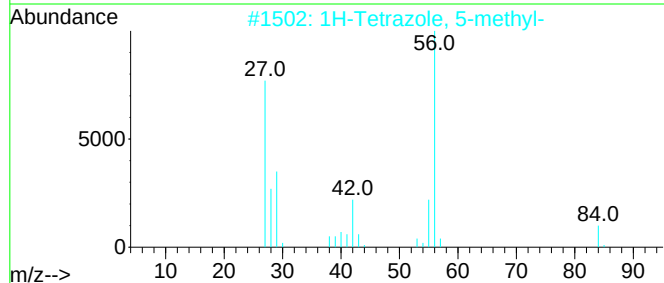
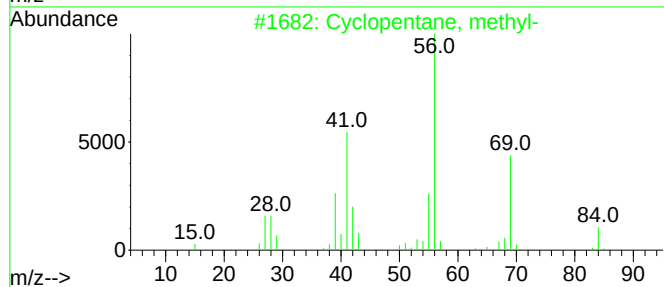
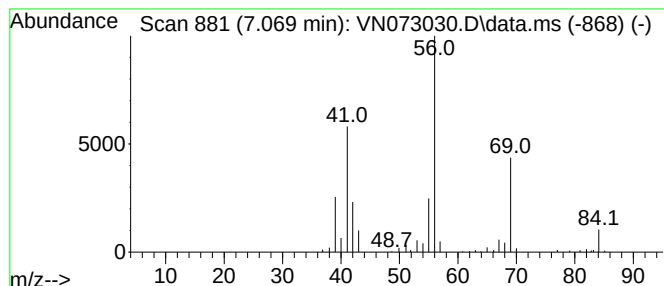
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Quant Title : SW846 8260

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

Peak Number 9 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	27.52 ug/l	701134	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	72
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073030.D
Acq On : 22 Jun 2022 17:18
Operator : JC\MD
Sample : N3381-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

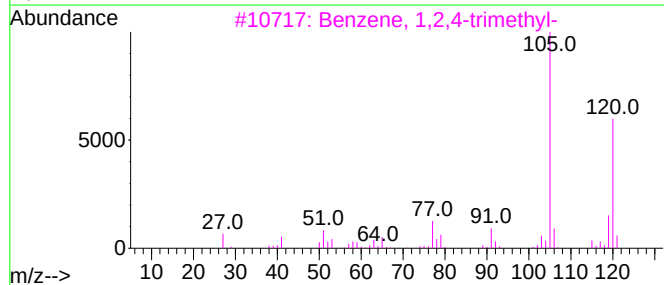
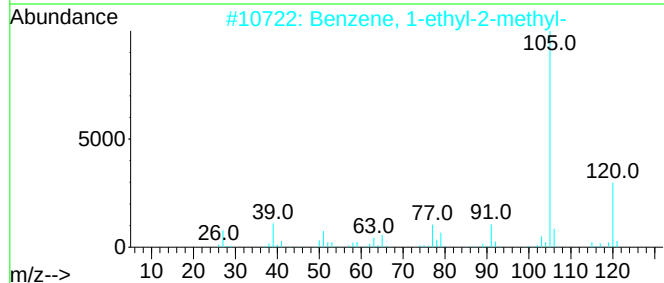
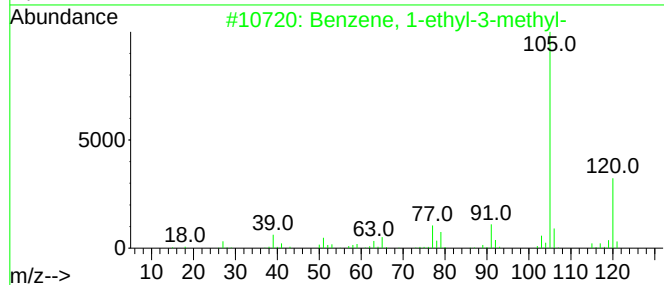
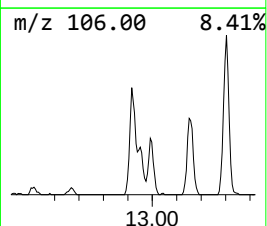
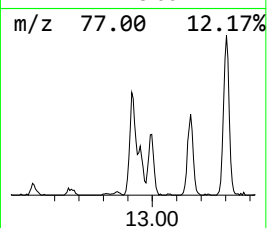
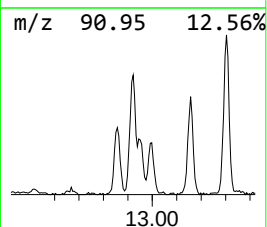
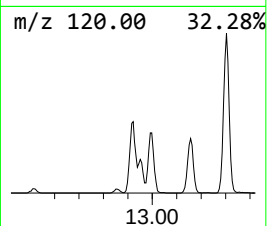
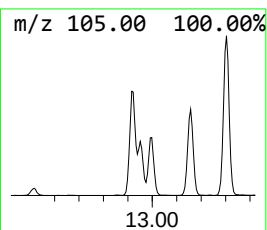
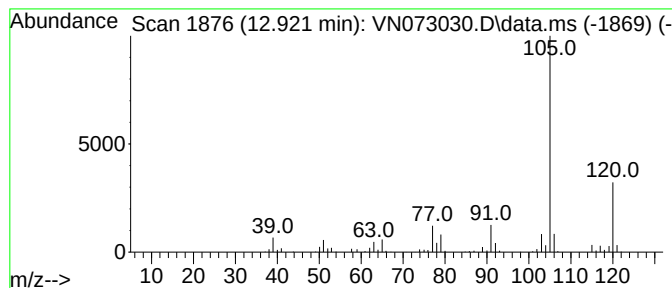
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethyl-3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.922	15.96 ug/l	651699	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Mesitylene	120	C9H12	000108-67-8	90
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073030.D
Acq On : 22 Jun 2022 17:18
Operator : JC\MD
Sample : N3381-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isobutane	2.228	24.6	ug/l	625743	1	8.016	1273640	50.0
Butane	2.405	81.2	ug/l	2068760	1	8.016	1273640	50.0
Butane, 2-methyl-	3.087	65.8	ug/l	1675610	1	8.016	1273640	50.0
Pentane	3.457	33.5	ug/l	852792	1	8.016	1273640	50.0
2-Pentene, (E)-	3.663	25.2	ug/l	642348	1	8.016	1273640	50.0
Cyclopropane, 1...	3.934	59.9	ug/l	1526510	1	8.016	1273640	50.0
Cyclopentene	4.881	49.5	ug/l	1260750	1	8.016	1273640	50.0
Cyclopentane	5.104	57.5	ug/l	1463660	1	8.016	1273640	50.0
Cyclopentane, m...	7.069	27.5	ug/l	701134	1	8.016	1273640	50.0
Benzene, 1-ethy...	12.922	16.0	ug/l	651699	4	13.610	2041590	50.0