

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
 Data File : VX036240.D
 Acq On : 20 Jun 2023 14:07
 Operator : JC/MD
 Sample : 03291-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-6A

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\82X061623W.M
 Title : SW846 8260

Signal : TIC: VX036240.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	42	46	53	rVV	5593326	6862521	3.87%	1.488%
2	1.746	103	108	123	rBV	7449183	10487149	5.91%	2.274%
3	1.959	138	143	155	rVV3	3914615	8127758	4.58%	1.763%
4	2.069	155	161	171	rVV	2558083	3540463	1.99%	0.768%
5	2.166	171	177	180	rVV	1661548	2475396	1.39%	0.537%
6	2.215	180	185	199	rVB	6407683	9986102	5.63%	2.166%
7	2.745	256	272	281	rBV	2377152	5564892	3.14%	1.207%
8	2.867	287	292	316	rVV	3002193	6740854	3.80%	1.462%
9	4.306	517	528	540	rBV	1521634	4366924	2.46%	0.947%
10	5.196	661	674	691	rVB	1059613	3211625	1.81%	0.696%
11	5.477	711	720	729	rBV2	589684	1887882	1.06%	0.409%
12	6.056	802	815	827	rVB	14710698	42035804	23.69%	9.116%
13	6.202	827	839	857	rVB4	447919	1857869	1.05%	0.403%
14	8.775	1246	1261	1267	rVV5	40462773	177471820	100.00%	38.487%
15	10.201	1488	1495	1501	rBV	19212217	26731533	15.06%	5.797%
16	10.317	1504	1514	1519	rBV	37312612	66440272	37.44%	14.408%
17	10.646	1562	1568	1574	rVB	21051803	29668306	16.72%	6.434%
18	11.305	1671	1676	1681	rBV	1639956	2043647	1.15%	0.443%
19	11.378	1681	1688	1696	rVV	6940245	12351202	6.96%	2.678%
20	11.451	1696	1700	1707	rVB	3463918	4030949	2.27%	0.874%
21	11.616	1721	1727	1737	rVB	3227079	4272025	2.41%	0.926%
22	11.756	1744	1750	1755	rBV	12619606	15442876	8.70%	3.349%
23	12.085	1799	1804	1809	rBV	3782849	4568106	2.57%	0.991%
24	12.244	1824	1830	1838	rBV2	4241710	5688009	3.21%	1.234%
25	13.774	2075	2081	2091	rBV	4351616	5270703	2.97%	1.143%

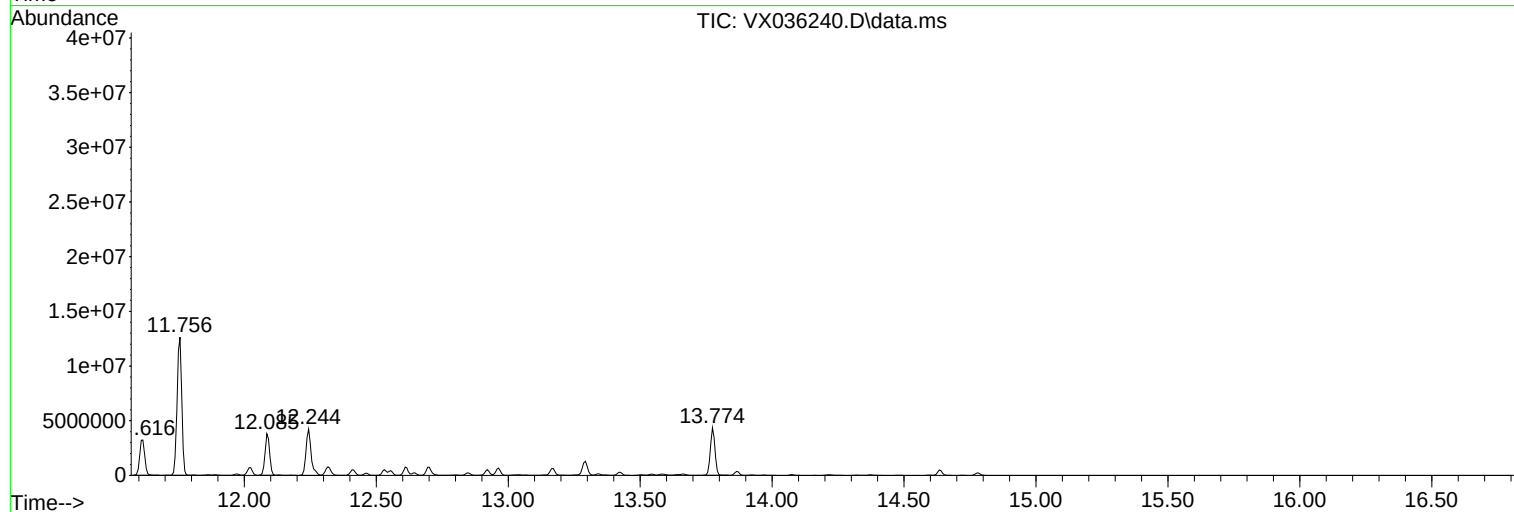
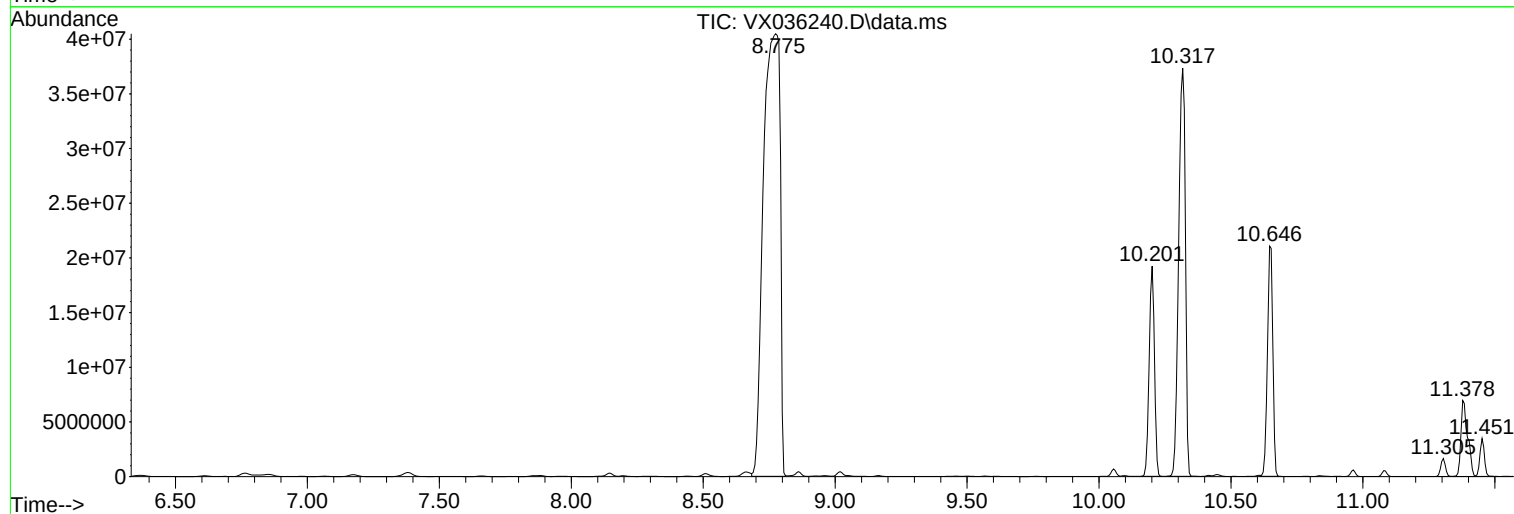
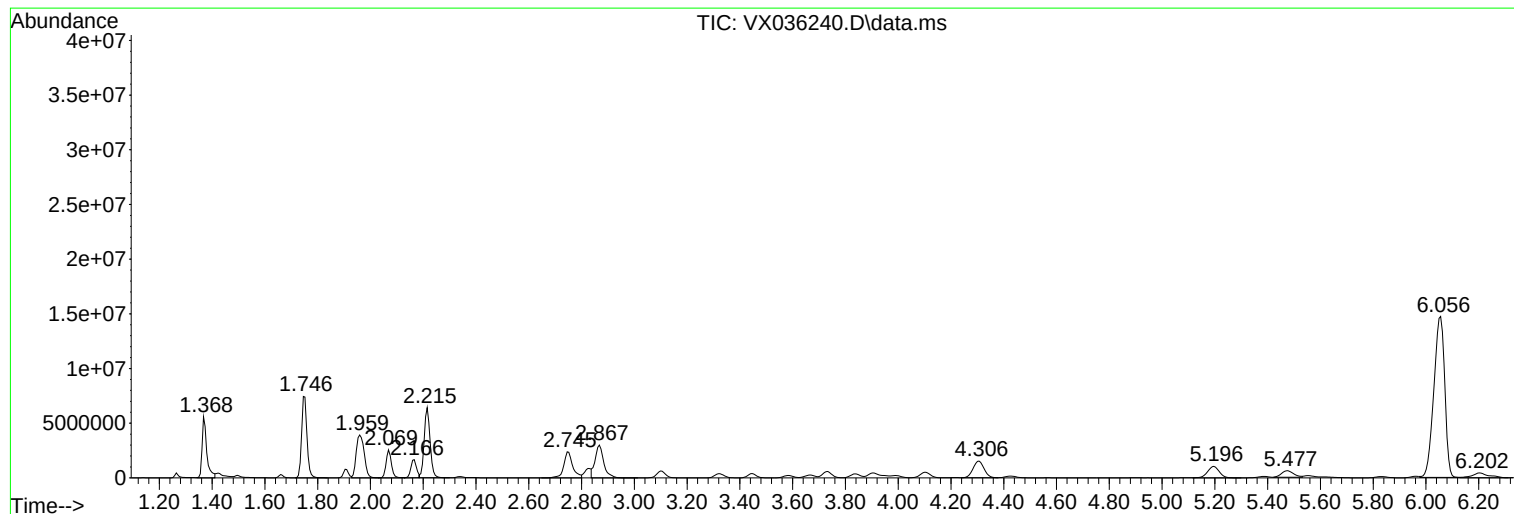
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Instrument :
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ClientSampleId :
MW-6A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

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



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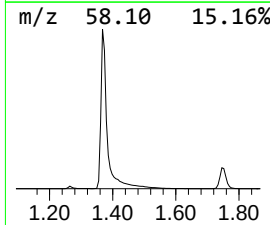
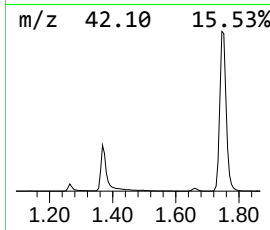
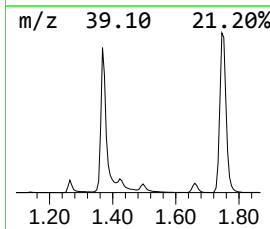
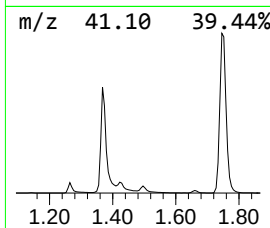
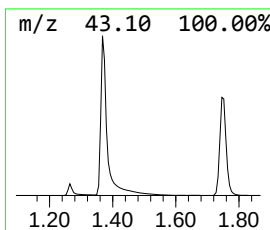
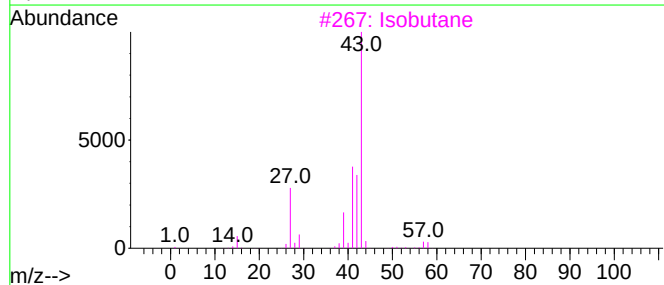
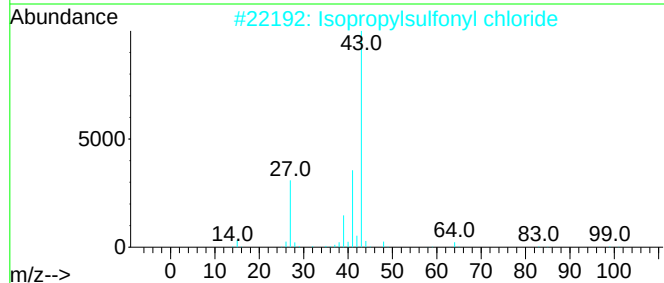
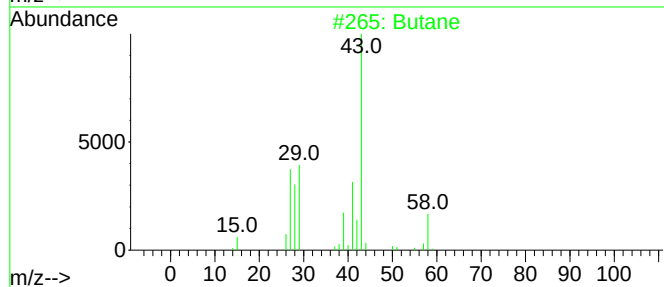
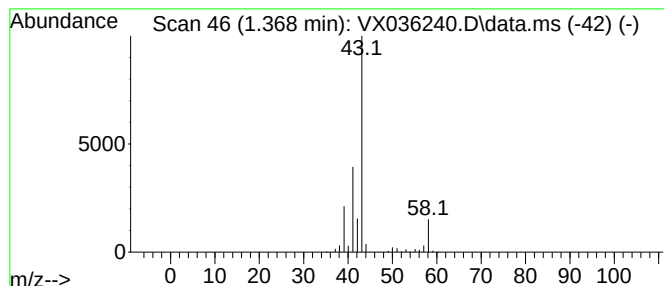
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	181.75 ug/l	6862520	Pentafluorobenzene	5.556

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



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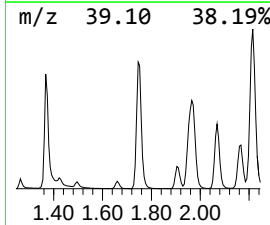
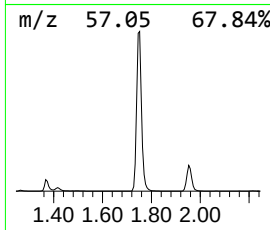
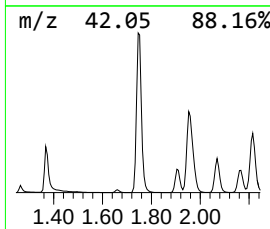
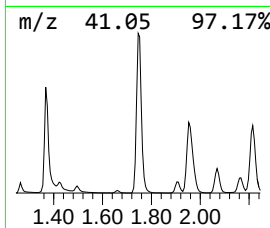
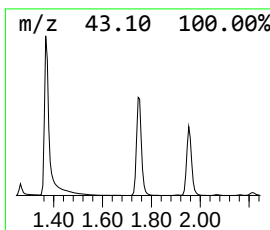
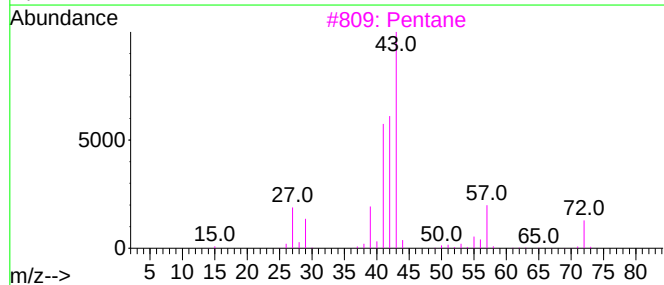
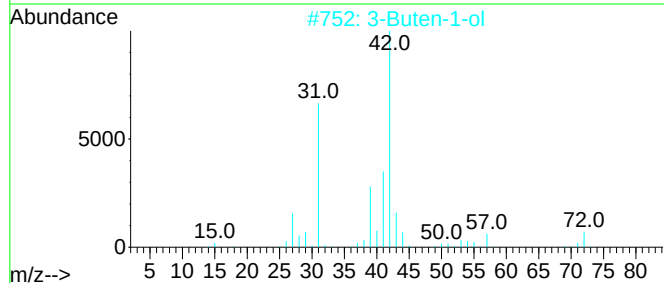
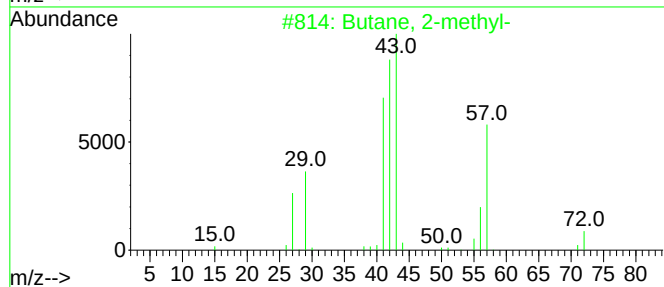
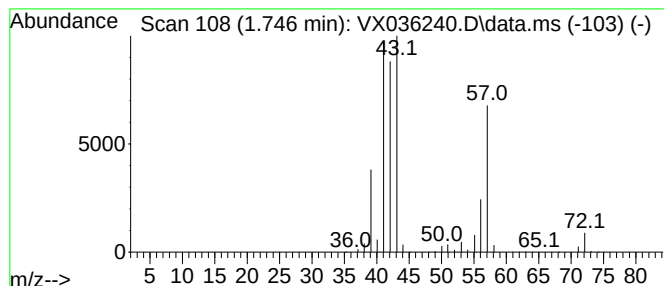
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

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.
1.746	277.75 ug/l	10487100	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	64
2			3-Buten-1-ol	72	C4H8O	000627-27-0	38
3			Pentane	72	C5H12	000109-66-0	38
4			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10
5			1-Butene	56	C4H8	000106-98-9	9



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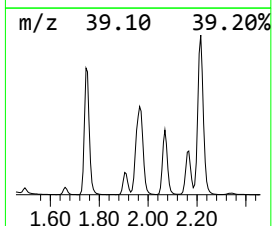
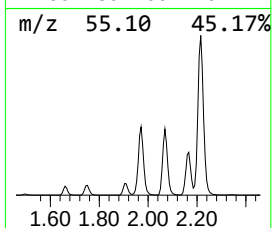
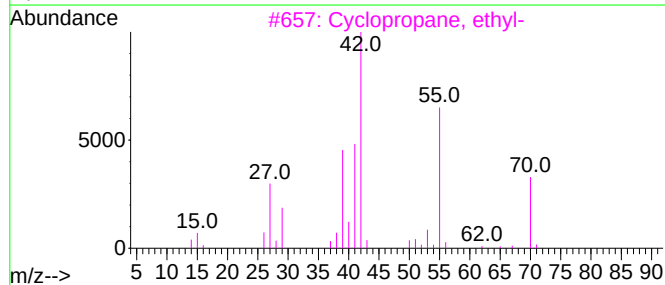
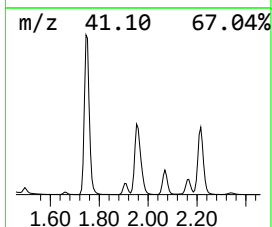
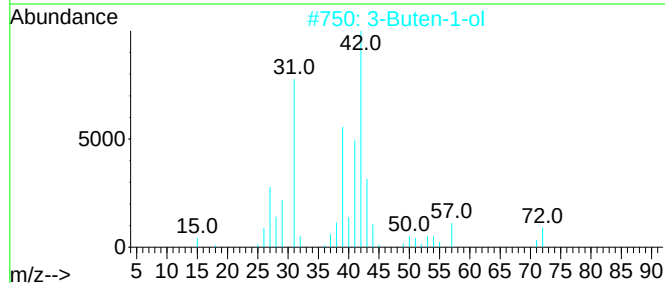
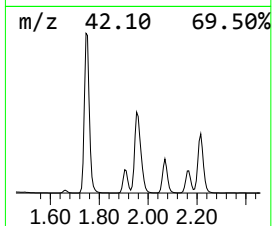
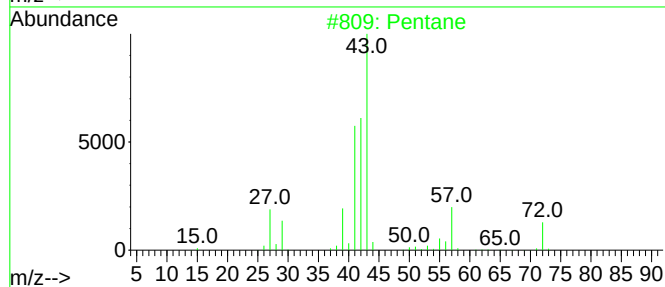
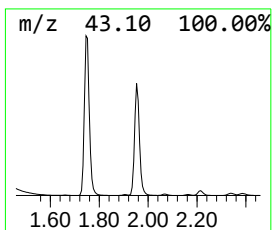
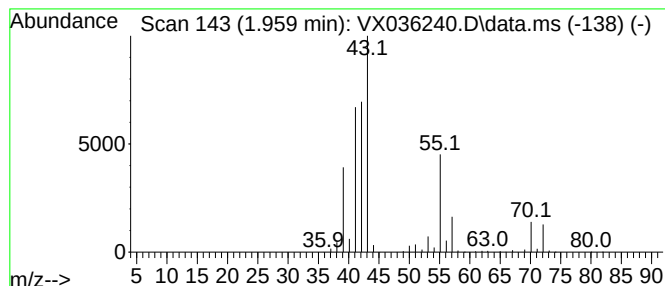
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

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

Peak Number 3 unknown1.959 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	215.26 ug/l	8127760	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	49
2			3-Buten-1-ol	72	C4H8O	000627-27-0	40
3			Cyclopropane, ethyl-	70	C5H10	001191-96-4	35
4			Cyclobutane, methyl-	70	C5H10	000598-61-8	35
5			1-Pentene	70	C5H10	000109-67-1	30



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

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ClientSampleId :
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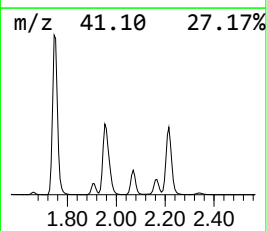
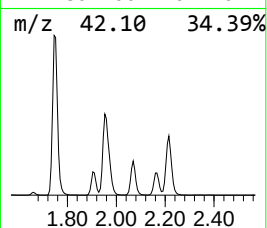
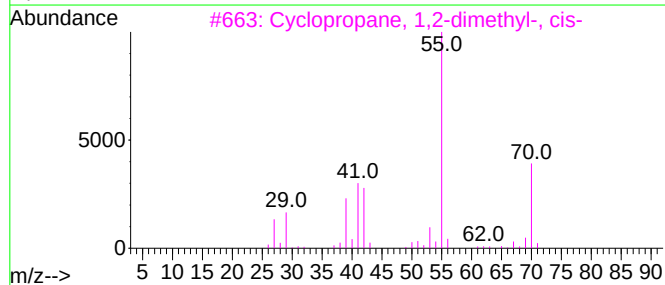
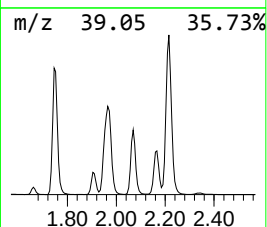
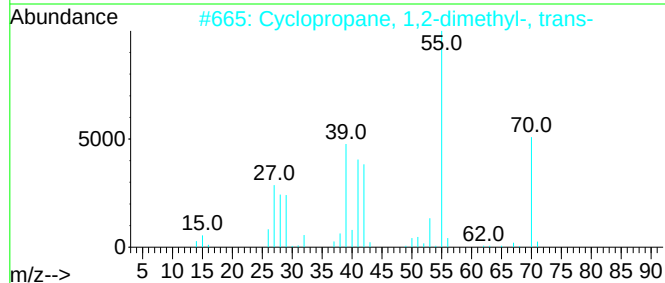
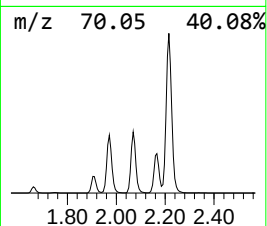
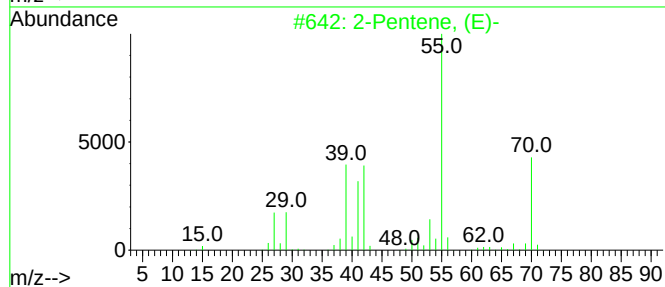
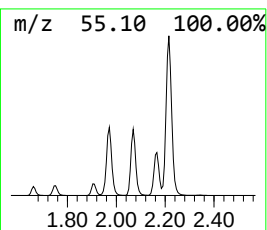
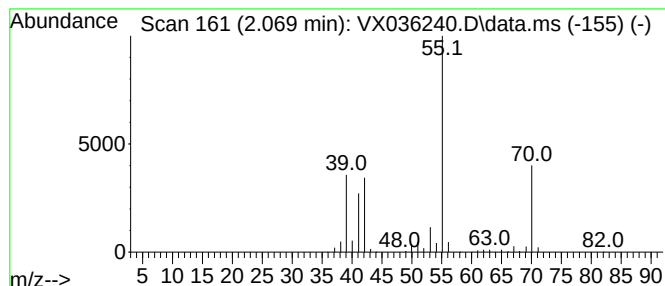
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Quant Title : SW846 8260

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

Peak Number 4 2-Pentene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	93.77 ug/l	3540460	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-			70	C5H10	000646-04-8	93
2	Cyclopropane, 1,2-dimethyl-, trans-			70	C5H10	002402-06-4	90
3	Cyclopropane, 1,2-dimethyl-, cis-			70	C5H10	000930-18-7	90
4	2-Pentene, (Z)-			70	C5H10	000627-20-3	90
5	2-Butene, 2-methyl-			70	C5H10	000513-35-9	87



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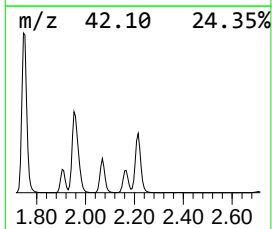
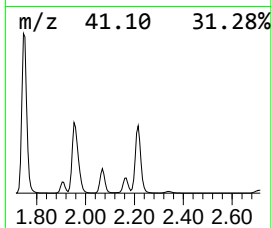
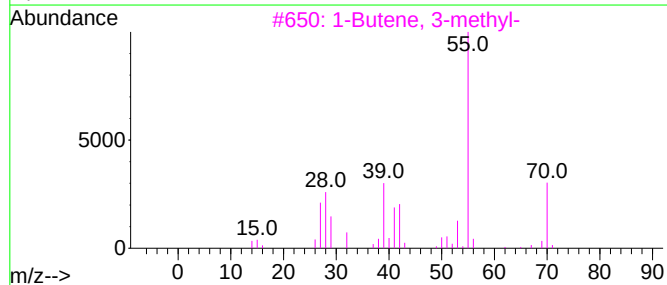
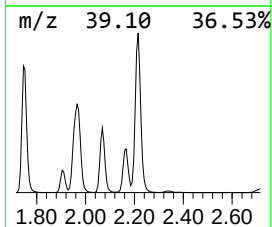
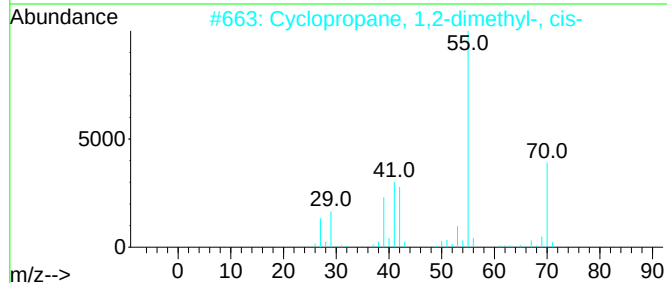
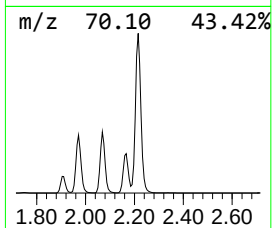
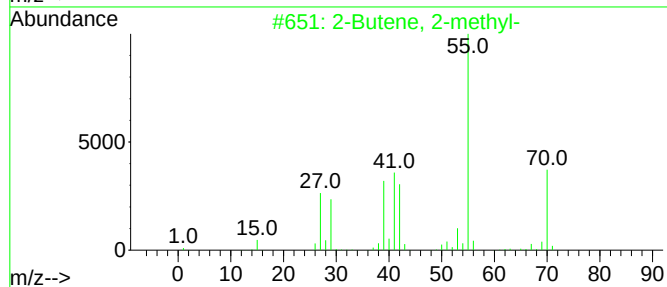
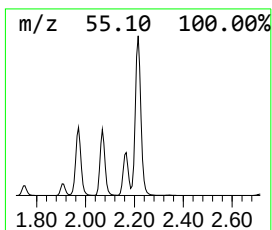
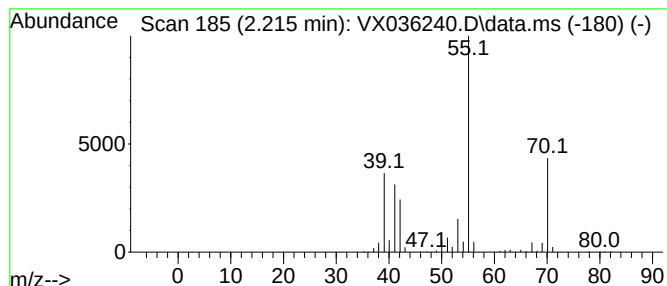
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	264.48 ug/l	9986100	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
2			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
3			1-Butene, 3-methyl-	70	C5H10	000563-45-1	86
4			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	83
5			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80



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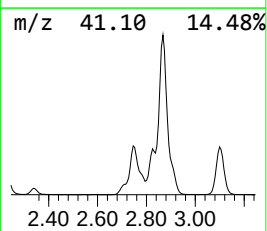
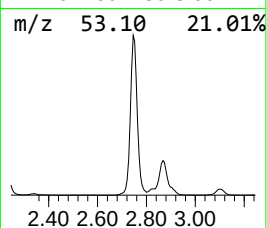
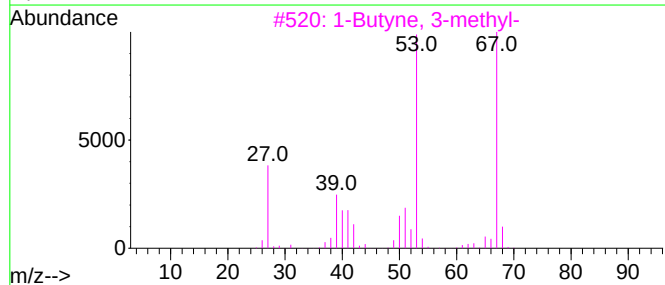
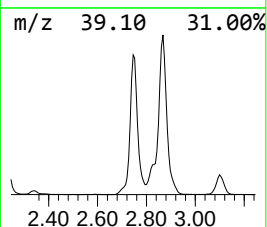
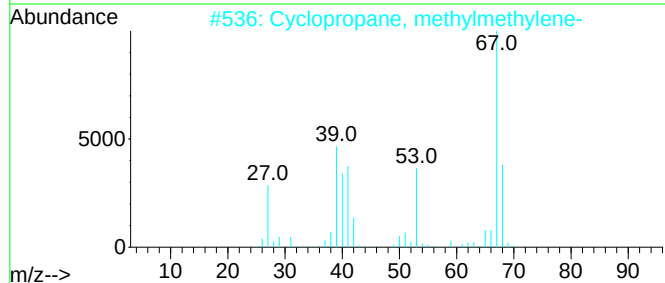
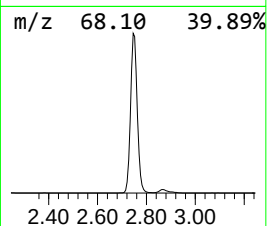
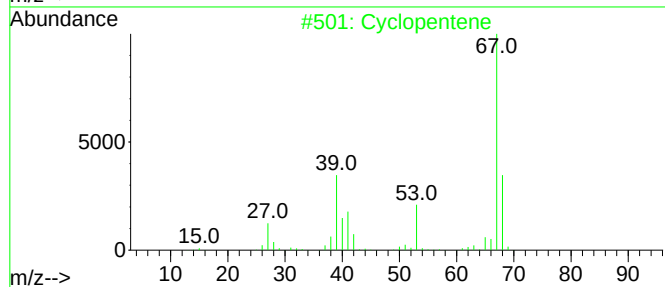
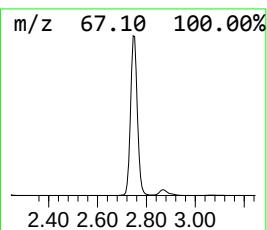
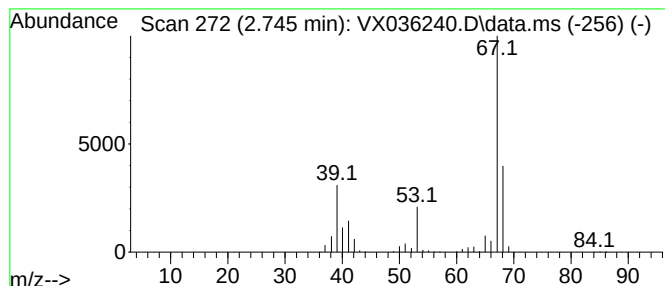
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.745	147.38 ug/l	5564890	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene	68	C5H8	000142-29-0	91
2			Cyclopropane, methylmethylene-	68	C5H8	018631-84-0	64
3			1-Butyne, 3-methyl-	68	C5H8	000598-23-2	64
4			Isoprene	68	C5H8	000078-79-5	59
5			1,4-Pentadiene	68	C5H8	000591-93-5	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
Data File : VX036240.D
Acq On : 20 Jun 2023 14:07
Operator : JC/MD
Sample : 03291-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

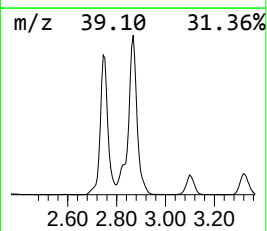
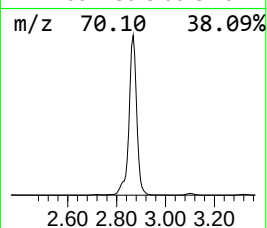
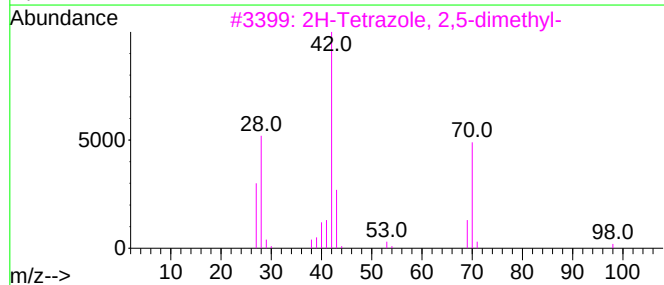
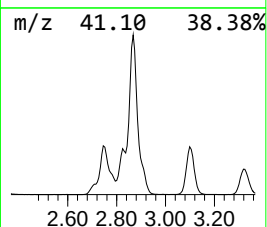
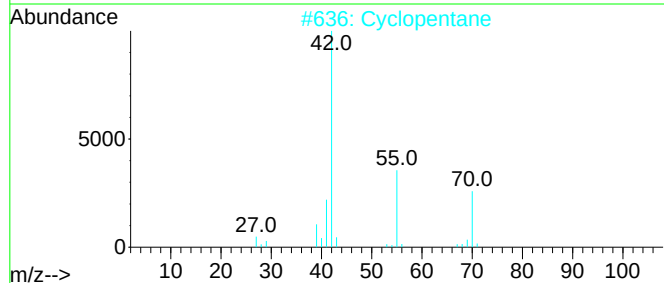
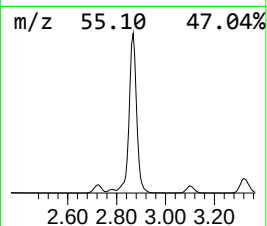
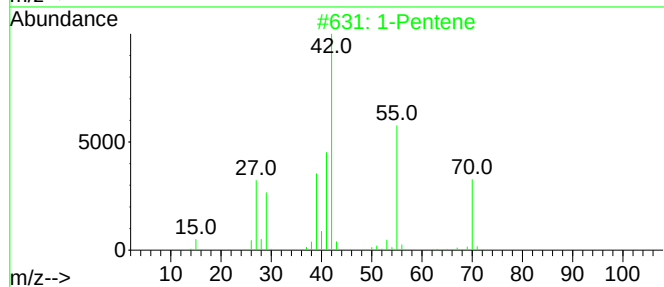
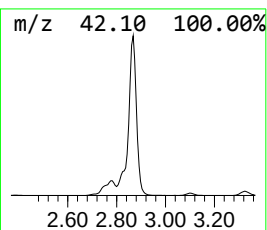
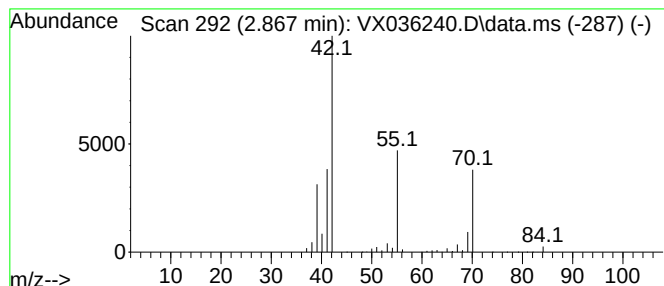
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Quant Title : SW846 8260

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

Peak Number 7 1-Pentene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	178.53 ug/l	6740850	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene			70	C5H10	000109-67-1	86
2	Cyclopentane			70	C5H10	000287-92-3	78
3	2H-Tetrazole, 2,5-dimethyl-			98	C3H6N4	004135-93-7	39
4	Cyclobutanone			70	C4H6O	001191-95-3	9
5	Cyclopropane, ethyl-			70	C5H10	001191-96-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
Data File : VX036240.D
Acq On : 20 Jun 2023 14:07
Operator : JC/MD
Sample : 03291-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

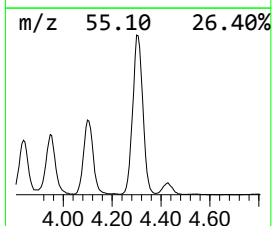
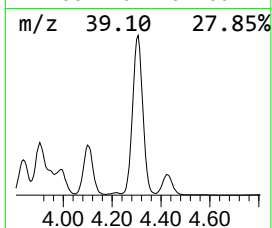
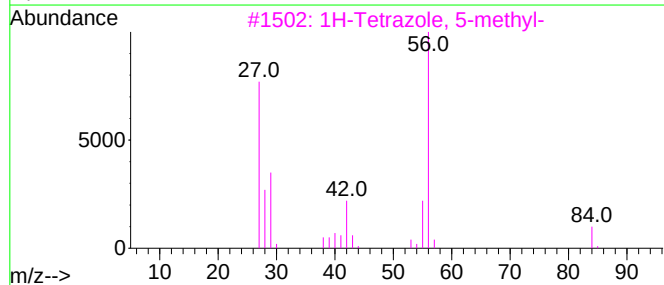
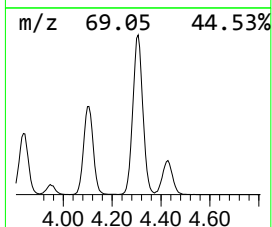
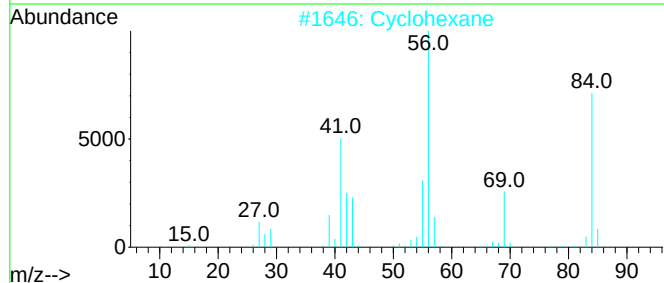
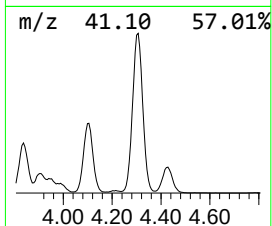
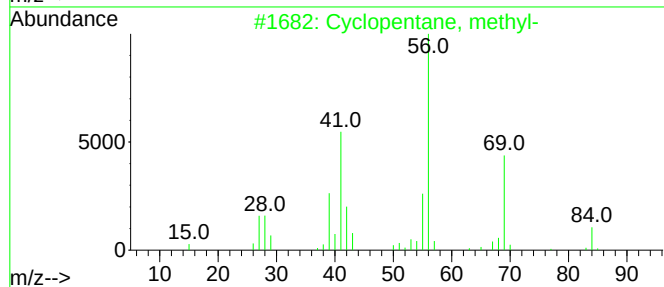
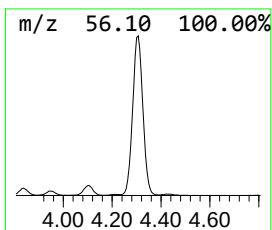
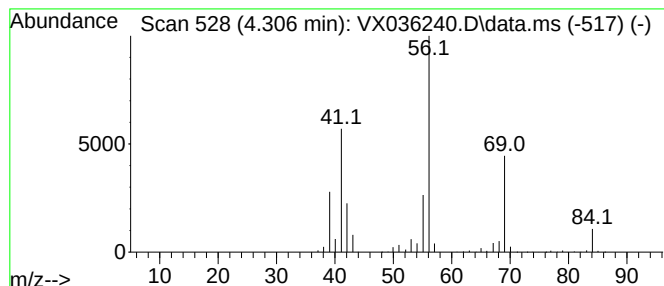
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	115.66 ug/l	4366920	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclohexane	84	C6H12	000110-82-7	78
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
Data File : VX036240.D
Acq On : 20 Jun 2023 14:07
Operator : JC/MD
Sample : 03291-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

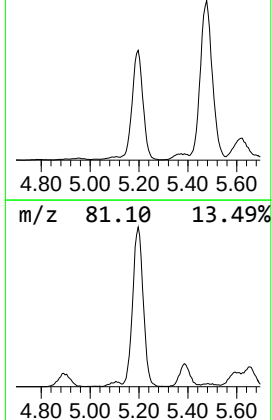
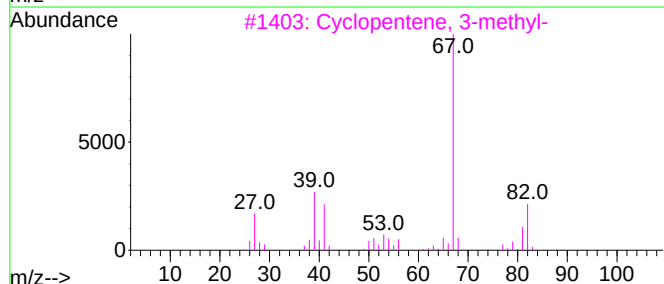
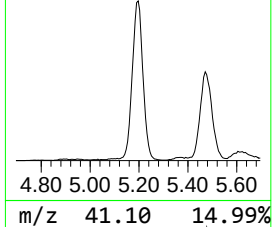
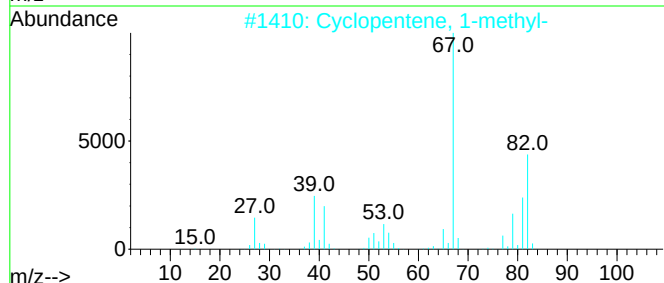
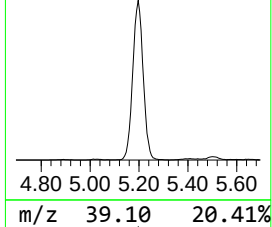
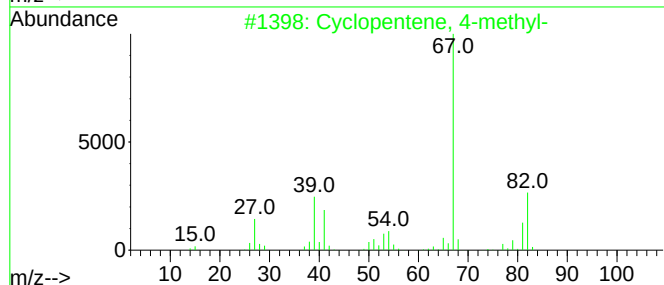
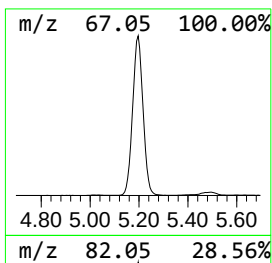
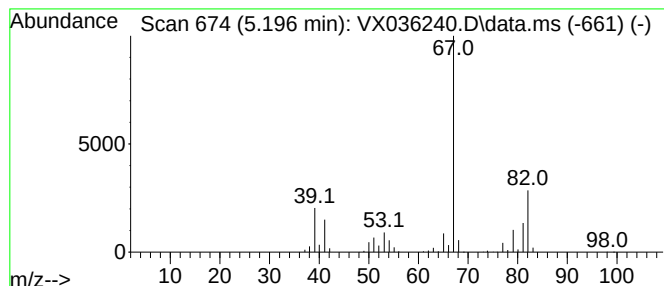
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Quant Title : SW846 8260

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

Peak Number 9 Cyclopentene, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.196	85.06 ug/l	3211630	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	91
2			Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	90
3			Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	86
4			1,4-Hexadiene	82	C6H10	000592-45-0	86
5			Cyclohexene	82	C6H10	000110-83-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
Data File : VX036240.D
Acq On : 20 Jun 2023 14:07
Operator : JC/MD
Sample : 03291-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

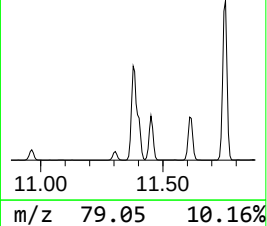
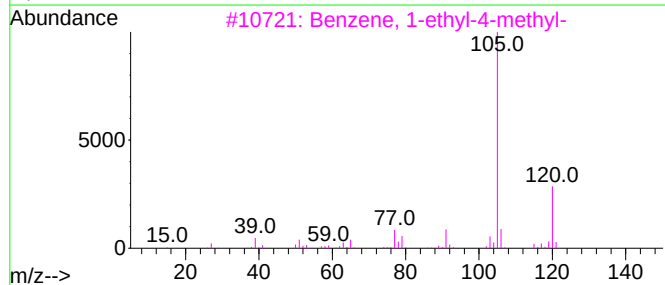
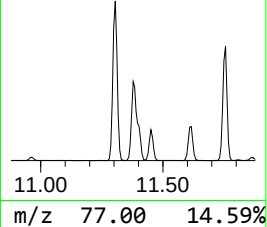
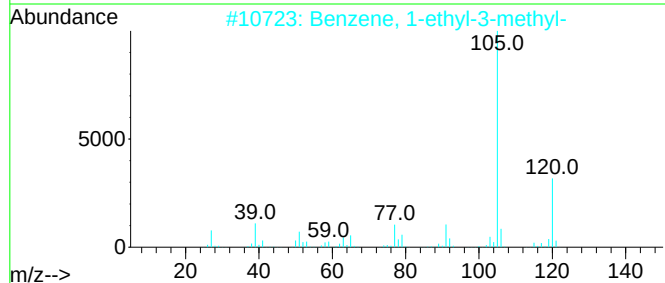
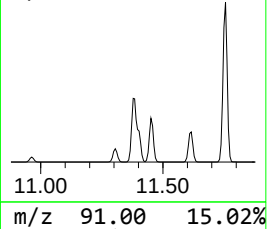
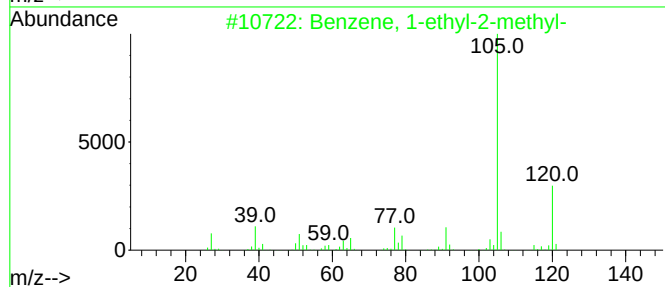
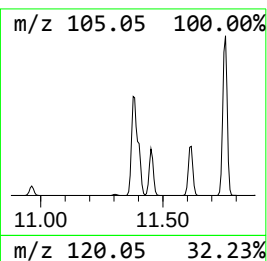
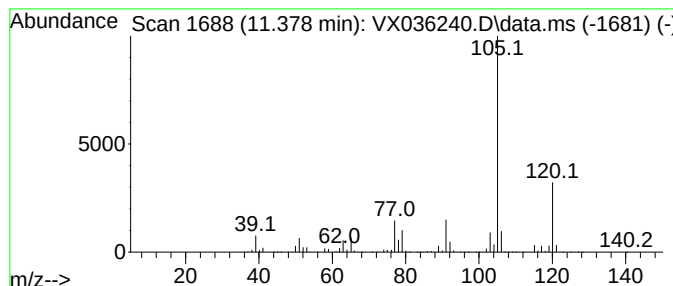
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	135.19 ug/l	12351200	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
Data File : VX036240.D
Acq On : 20 Jun 2023 14:07
Operator : JC/MD
Sample : 03291-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.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
Butane	1.368	181.8	ug/l	6862520	1	5.556	1887880	50.0
Butane, 2-methyl-	1.746	277.8	ug/l	10487100	1	5.556	1887880	50.0
unknown1.959	1.959	215.3	ug/l	8127760	1	5.556	1887880	50.0
2-Pentene, (E)-	2.069	93.8	ug/l	3540460	1	5.556	1887880	50.0
2-Butene, 2-met...	2.215	264.5	ug/l	9986100	1	5.556	1887880	50.0
Cyclopentene	2.745	147.4	ug/l	5564890	1	5.556	1887880	50.0
1-Pentene	2.867	178.5	ug/l	6740850	1	5.556	1887880	50.0
Cyclopentane, m...	4.306	115.7	ug/l	4366920	1	5.556	1887880	50.0
Cyclopentene, 4...	5.196	85.1	ug/l	3211630	1	5.556	1887880	50.0
Benzene, 1-ethy...	11.378	135.2	ug/l	12351200	4	12.024	4568110	50.0