

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
 Data File : VX039961.D
 Acq On : 25 Jan 2024 17:59
 Operator : JC/MD
 Sample : P1258-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 50234

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\82X011024W.M
 Title : SW846 8260

Signal : TIC: VX039961.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	26	30	41	rBV	120274	133530	3.60%	0.916%
2	1.368	41	46	53	rVV	766724	835027	22.51%	5.730%
3	1.429	53	56	57	rVV	82900	82099	2.21%	0.563%
4	1.453	57	60	64	rVV	169231	191092	5.15%	1.311%
5	1.496	64	67	73	rVB	86806	82992	2.24%	0.569%
6	1.752	103	109	120	rBV	260178	338084	9.11%	2.320%
7	1.959	138	143	152	rVV2	127212	249607	6.73%	1.713%
8	2.057	152	159	170	rVV	570386	999760	26.95%	6.860%
9	2.166	171	177	180	rVV	46611	73351	1.98%	0.503%
10	2.215	180	185	194	rVB	162644	245238	6.61%	1.683%
11	2.380	207	212	224	rVB	28235	48549	1.31%	0.333%
12	2.752	259	273	281	rBV	55102	124638	3.36%	0.855%
13	2.867	287	292	304	rVB	56039	121203	3.27%	0.832%
14	3.111	322	332	344	rBV2	38905	94128	2.54%	0.646%
15	4.306	518	528	541	rVB3	34853	103399	2.79%	0.709%
16	4.715	587	595	614	rVB	22800	68463	1.85%	0.470%
17	5.196	664	674	686	rBV	13719	40298	1.09%	0.277%
18	5.385	694	705	713	rBV2	56080	160837	4.34%	1.104%
19	5.471	713	719	724	rVV2	20725	59394	1.60%	0.408%
20	5.550	725	732	745	rVB2	92701	263164	7.09%	1.806%
21	5.958	788	799	804	rBV	66917	179453	4.84%	1.231%
22	6.038	804	812	829	rVB	875218	2325550	62.68%	15.957%
23	6.763	921	931	943	rBV	151373	368884	9.94%	2.531%
24	8.647	1234	1240	1246	rBV	304704	473816	12.77%	3.251%
25	8.720	1246	1252	1268	rVB	2450618	3710182	100.00%	25.458%
26	10.055	1465	1471	1487	rBV	331300	459067	12.37%	3.150%
27	10.195	1488	1494	1502	rBV	180407	240266	6.48%	1.649%
28	10.299	1505	1511	1525	rVV	569297	761122	20.51%	5.223%
29	10.640	1561	1567	1583	rVB	253105	338876	9.13%	2.325%
30	11.079	1634	1639	1648	rBV	283440	359121	9.68%	2.464%
31	11.378	1682	1688	1696	rBV	56224	100916	2.72%	0.692%
32	11.451	1696	1700	1709	rVB	30817	38504	1.04%	0.264%
33	11.750	1744	1749	1755	rBV	116424	140059	3.77%	0.961%
34	12.024	1788	1794	1800	rBV	327002	435064	11.73%	2.985%
35	12.085	1800	1804	1812	rVB	48848	65400	1.76%	0.449%
36	12.244	1821	1830	1838	rBV3	36110	59295	1.60%	0.407%

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50234

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\82X011024W.M
Title : SW846 8260

37	13.292	1997	2002	2007	rVB2	43503	58789	1.58%	0.403%
38	13.774	2077	2081	2088	rVB	32790	44532	1.20%	0.306%
39	14.225	2147	2155	2163	rVB4	27842	53827	1.45%	0.369%
40	14.634	2213	2222	2226	rBV2	22005	46103	1.24%	0.316%

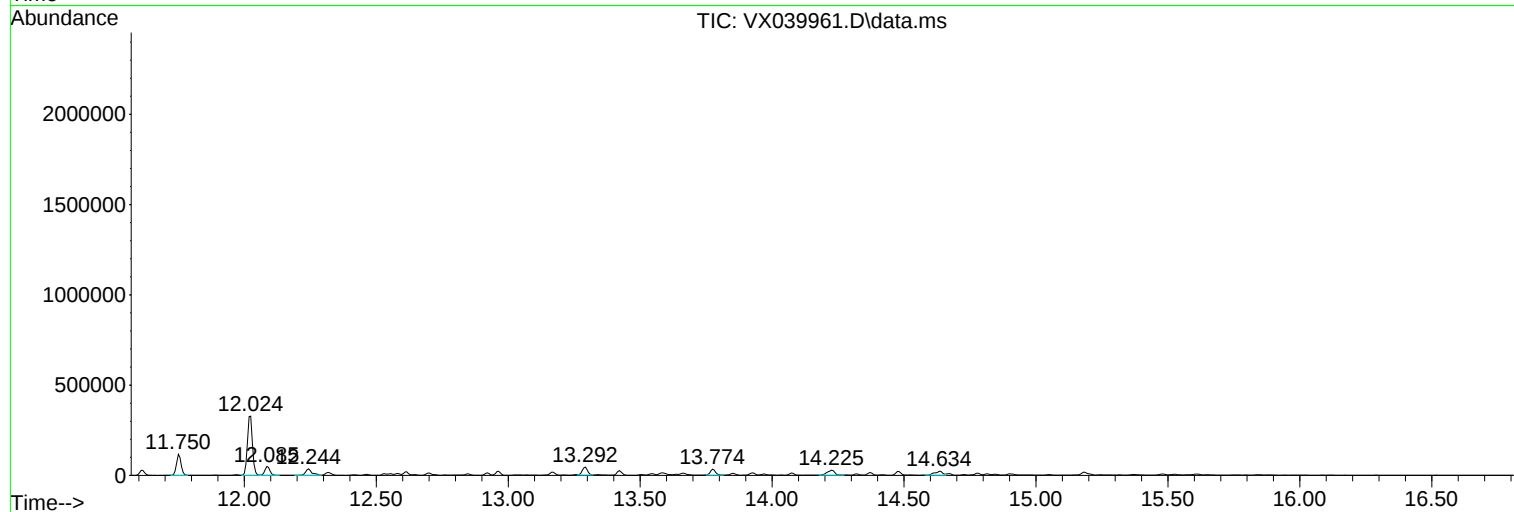
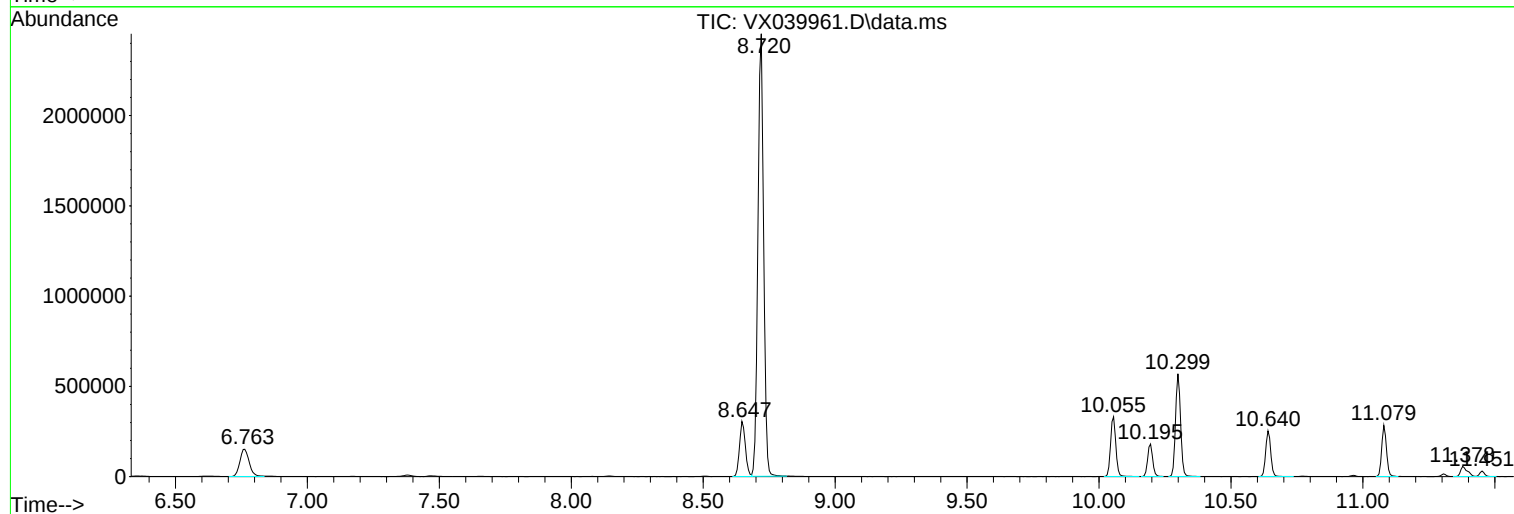
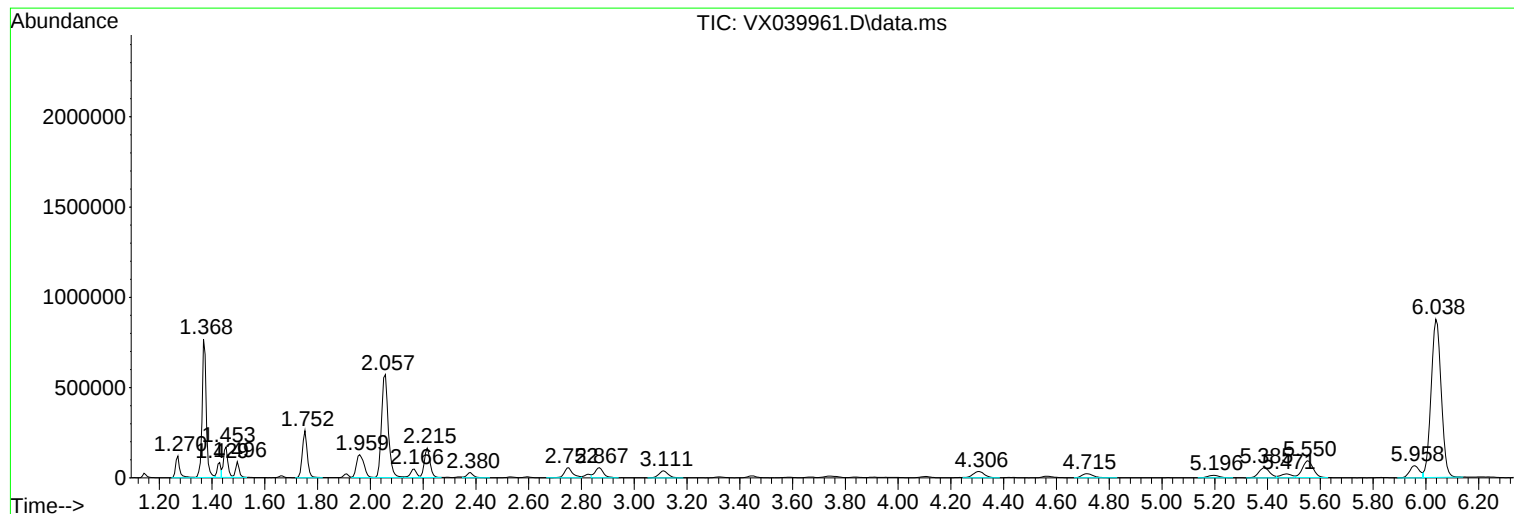
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
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Instrument :
MSVOA_X
ClientSampleId :
50234

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX012524\
Data File : VX039961.D
Acq On : 25 Jan 2024 17:59
Operator : JC/MD
Sample : P1258-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50234

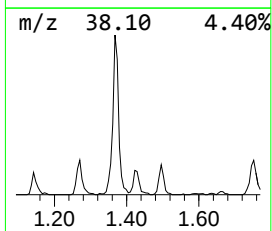
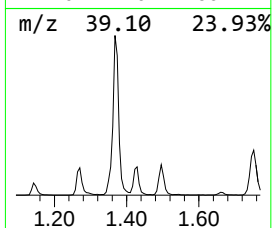
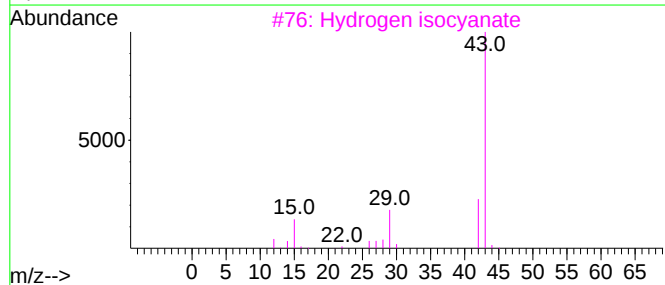
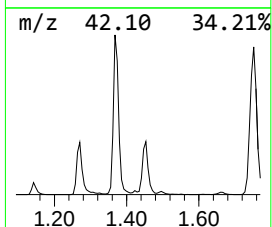
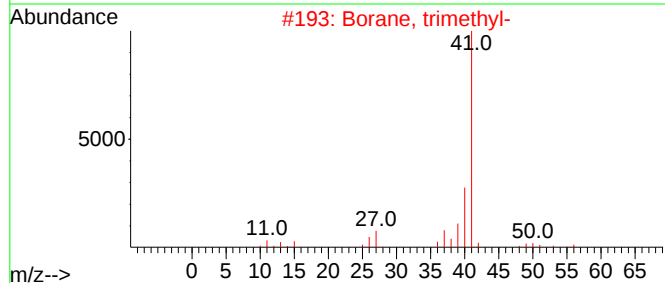
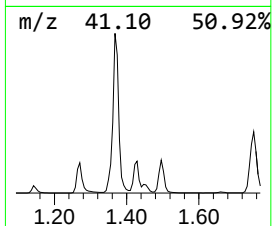
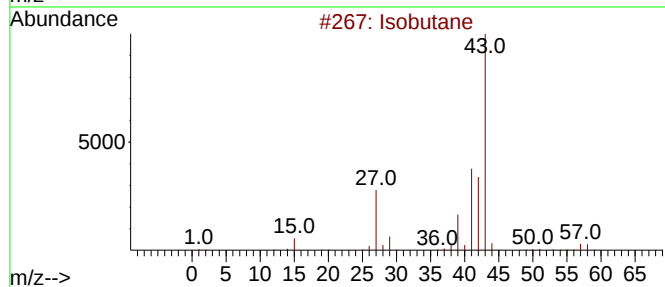
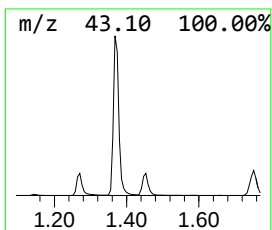
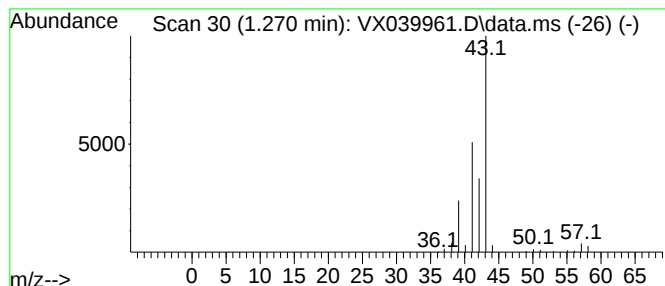
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	25.37 ug/l	133530	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	72
2			Borane, trimethyl-	56	C3H9B	000593-90-8	7
3			Hydrogen isocyanate	43	CHNO	000075-13-8	4
4			Cyclobutylamine	71	C4H9N	002516-34-9	4
5			Propene	42	C3H6	000115-07-1	4



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50234

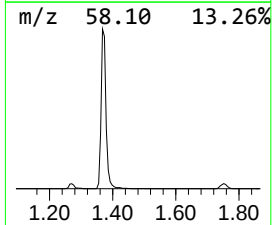
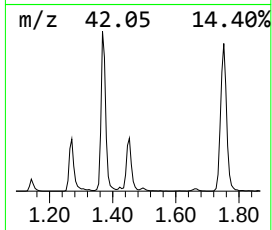
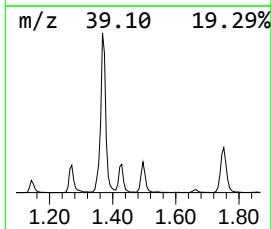
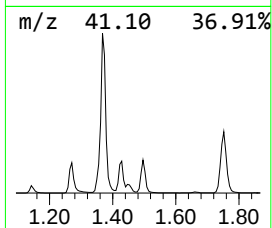
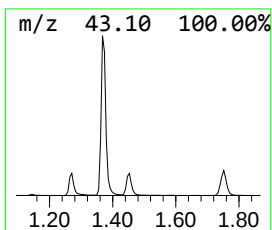
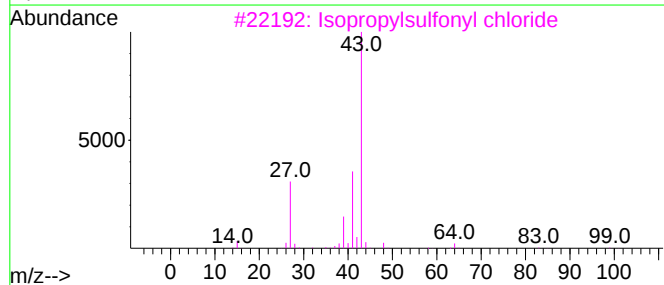
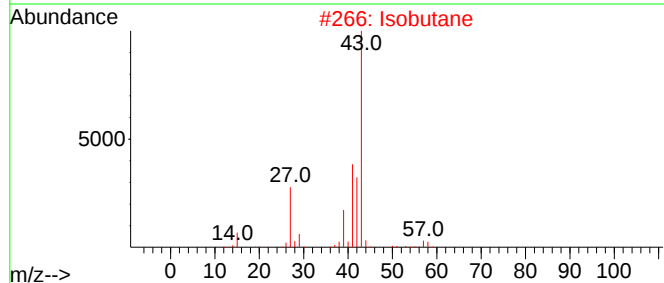
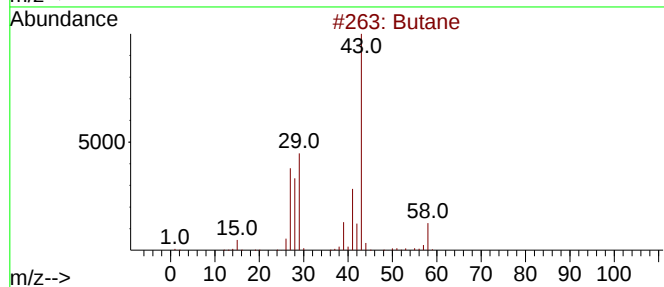
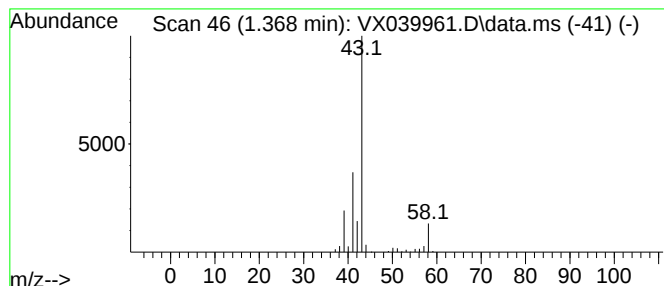
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	158.65 ug/l	835027	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane			58	C4H10	000106-97-8	72
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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Data File : VX039961.D
Acq On : 25 Jan 2024 17:59
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Sample : P1258-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50234

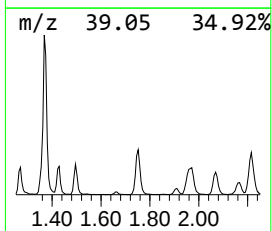
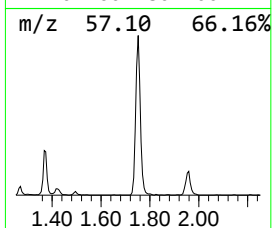
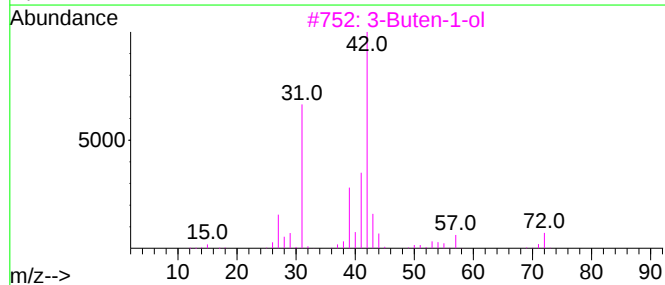
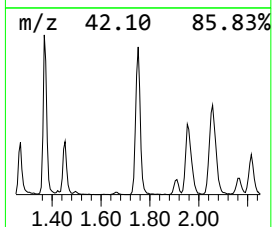
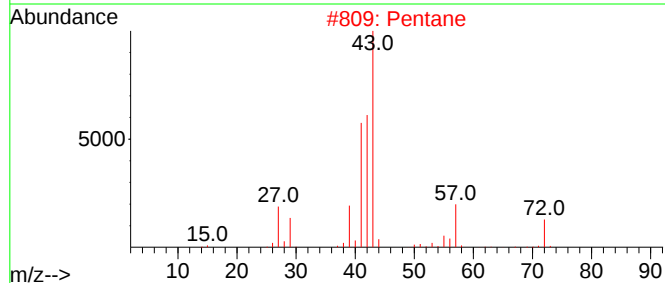
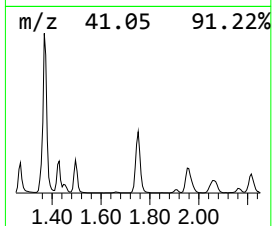
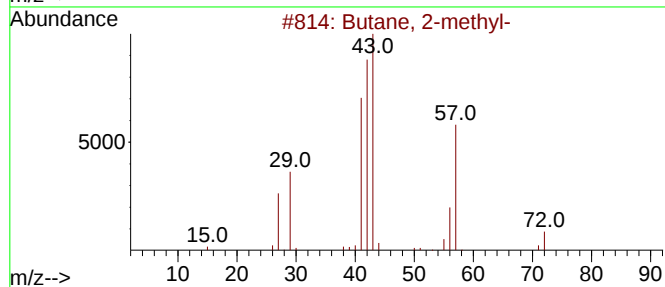
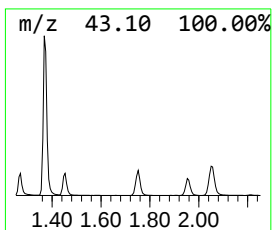
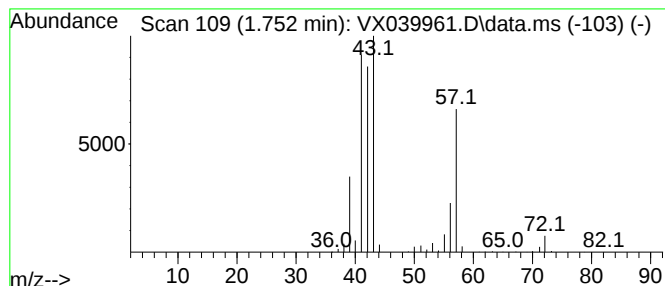
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	64.23 ug/l	338084	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Pentane	72	C5H12	000109-66-0	36
3			3-Buten-1-ol	72	C4H8O	000627-27-0	28
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
5			1-Butene	56	C4H8	000106-98-9	9



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Sample : P1258-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50234

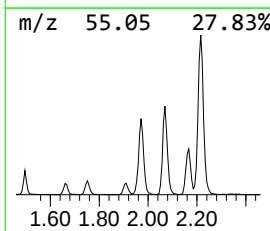
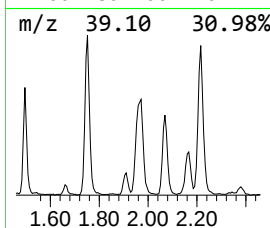
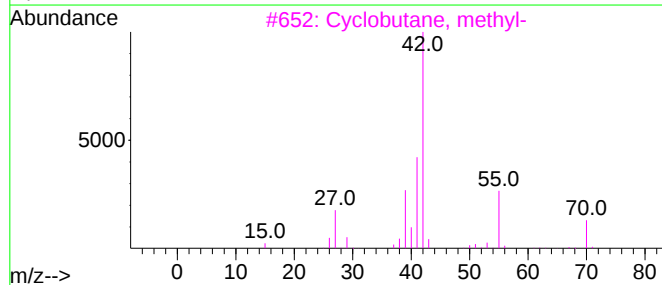
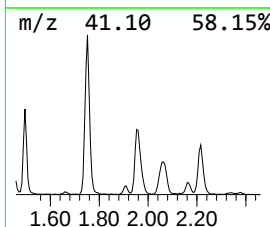
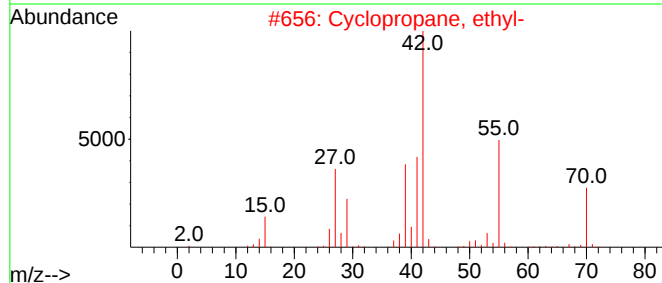
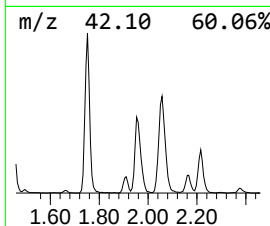
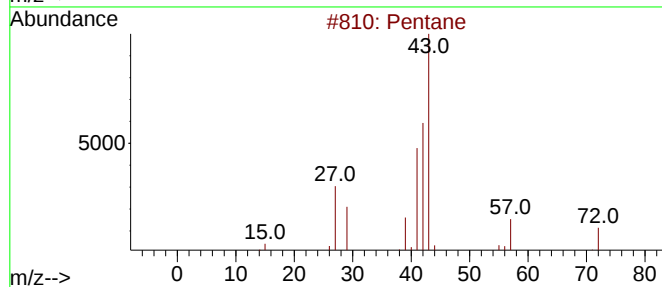
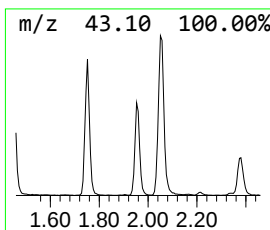
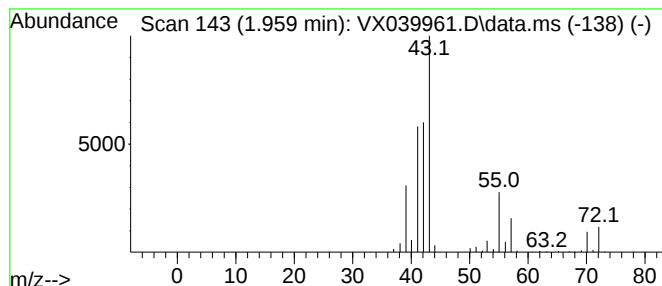
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 5 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	47.42 ug/l	249607	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	80
2			Cyclopropane, ethyl-	70	C5H10	001191-96-4	46
3			Cyclobutane, methyl-	70	C5H10	000598-61-8	43
4			Oxirane, ethyl-	72	C4H8O	000106-88-7	38
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	28



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50234

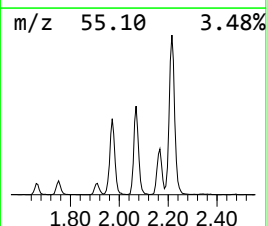
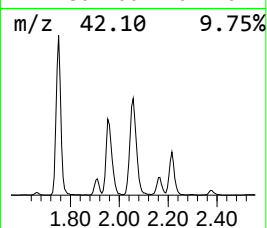
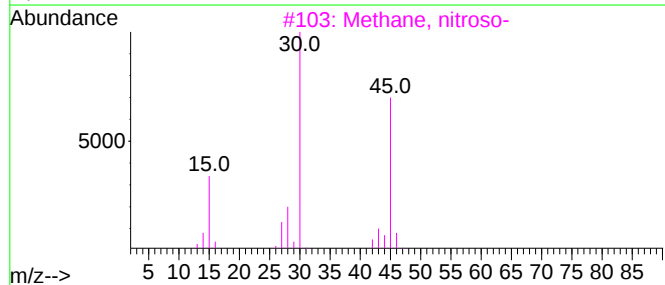
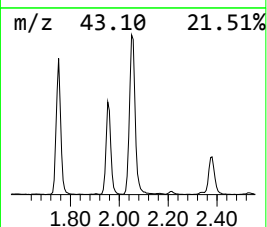
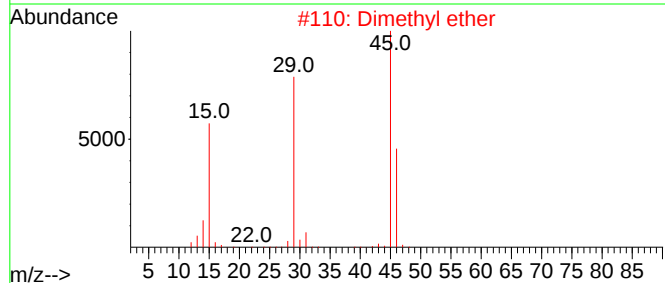
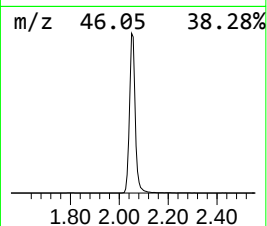
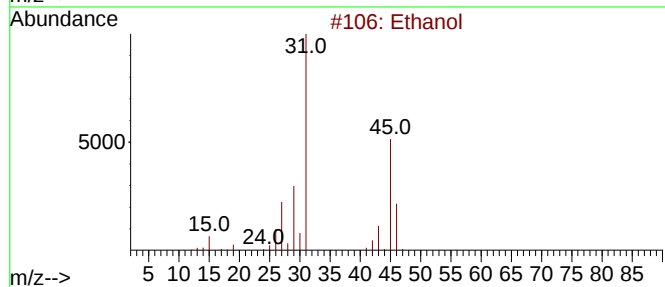
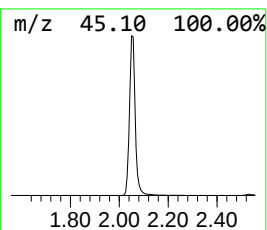
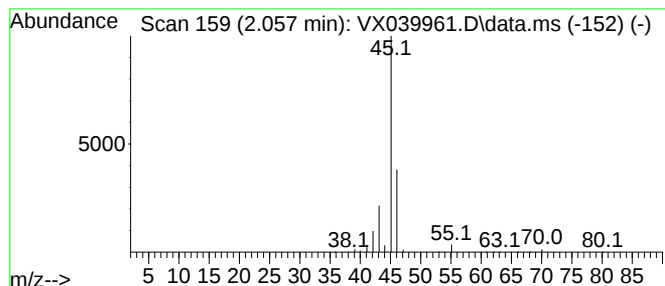
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 6 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.057	189.95 ug/l	999760	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	56
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Methoxyacetyl chloride	108	C3H5ClO2	038870-89-2	4
5	Formic acid	46	CH2O2	000064-18-6	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039961.D
Acq On : 25 Jan 2024 17:59
Operator : JC/MD
Sample : P1258-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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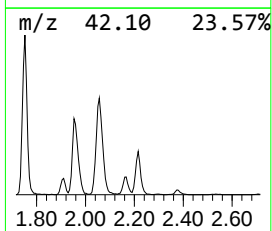
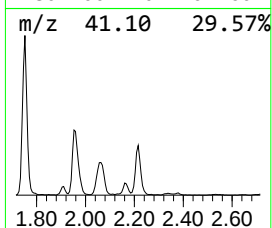
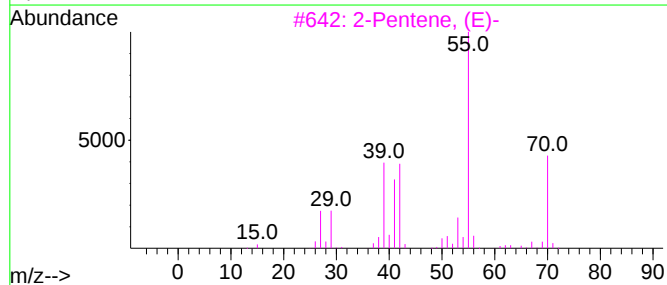
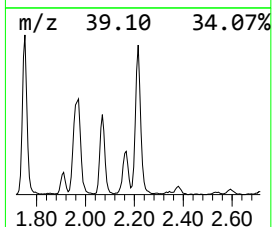
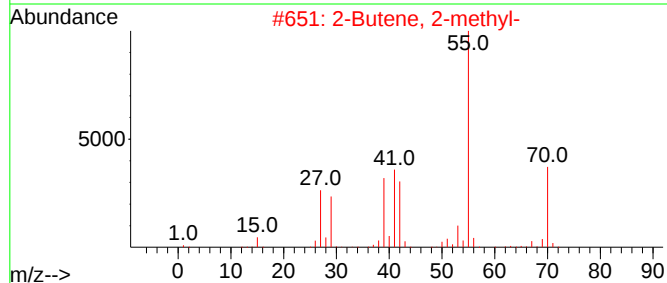
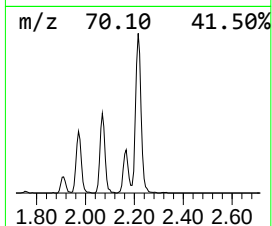
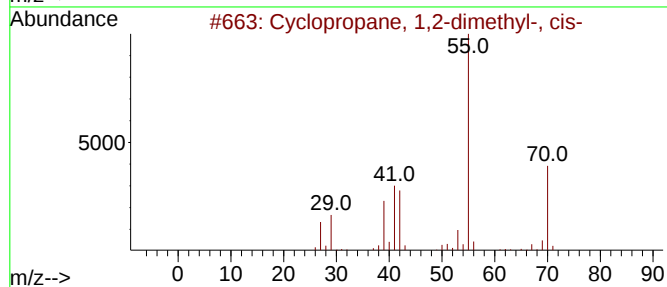
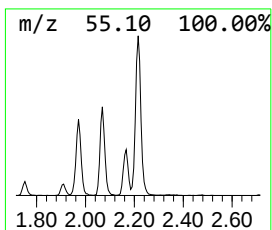
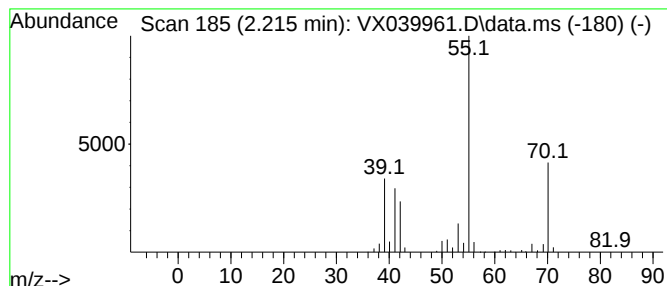
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopropane, 1,2-dimethyl-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	46.59 ug/l	245238	Pentafluorobenzene	5.556

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	91
3			2-Pentene, (E)-	70	C5H10	000646-04-8	87
4			1-Butene, 3-methyl-	70	C5H10	000563-45-1	86
5			2-Pentene, (Z)-	70	C5H10	000627-20-3	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039961.D
Acq On : 25 Jan 2024 17:59
Operator : JC/MD
Sample : P1258-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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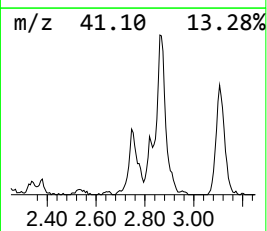
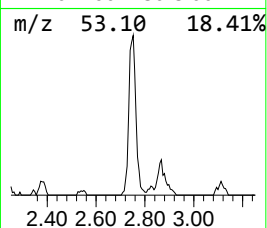
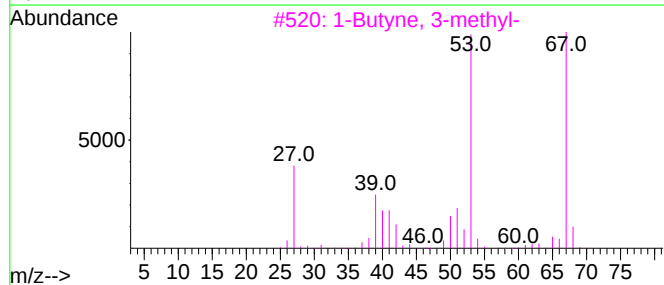
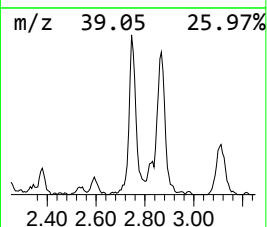
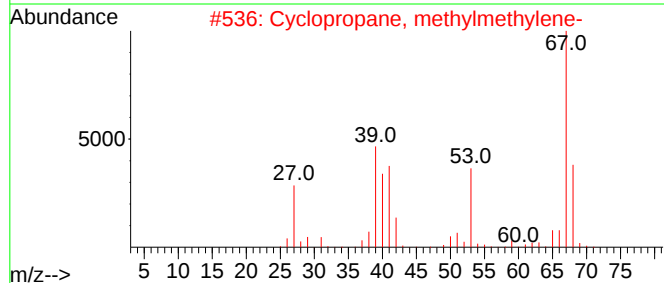
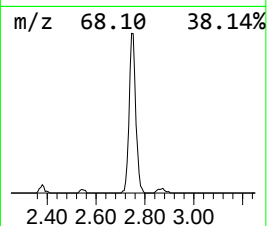
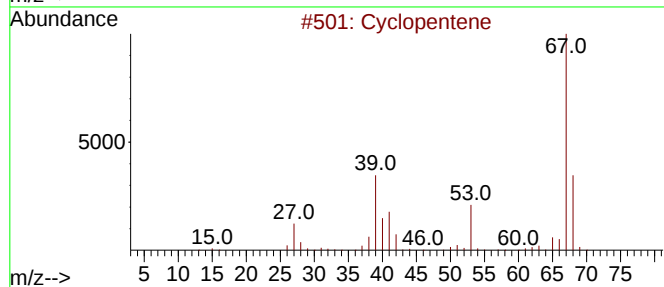
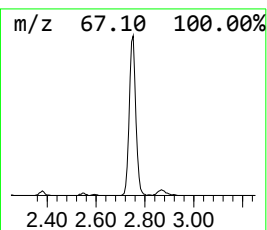
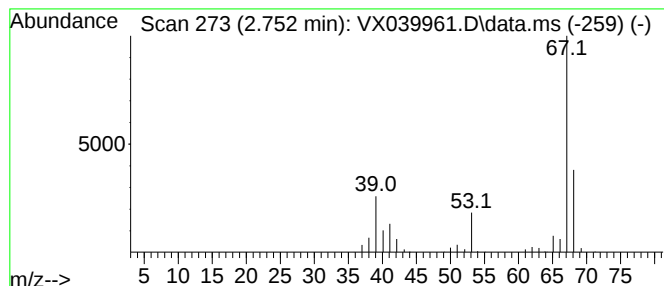
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopentene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.752	23.68 ug/l	124638	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	91
3			1-Butyne, 3-methyl-	68	C5H8	000598-23-2	59
4			Cyclopropane, ethylidene-	68	C5H8	018631-83-9	53
5			Isoprene	68	C5H8	000078-79-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039961.D
Acq On : 25 Jan 2024 17:59
Operator : JC/MD
Sample : P1258-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50234

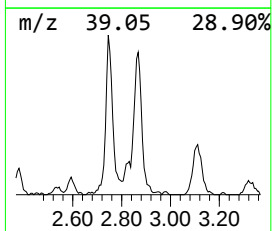
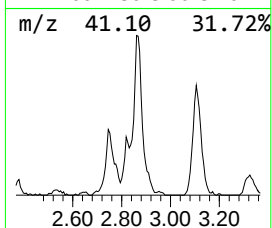
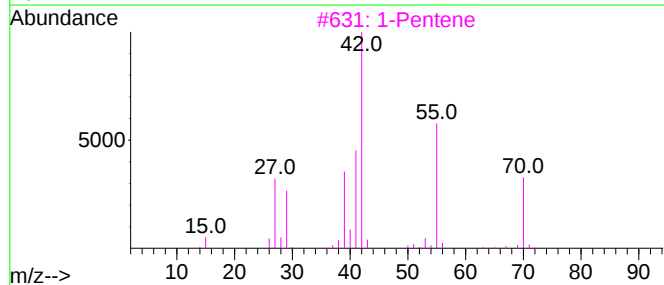
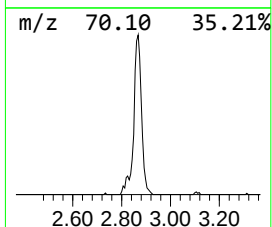
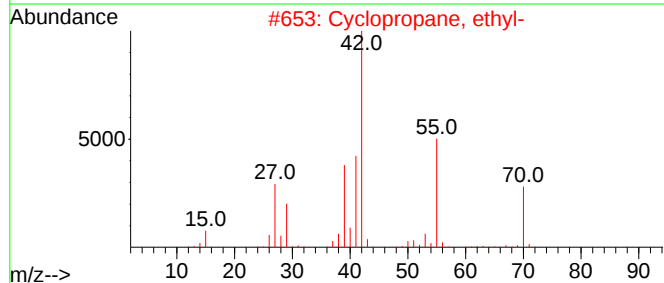
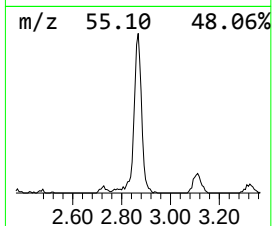
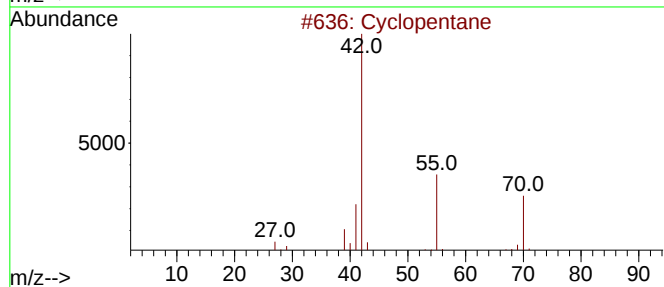
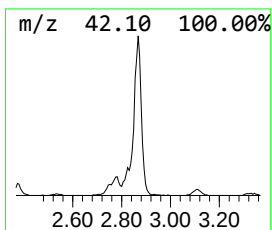
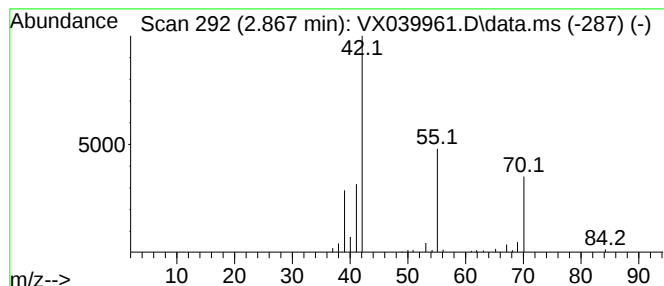
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Quant Title : SW846 8260

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

Peak Number 9 Cyclopropane, ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	23.03 ug/l	121203	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	78
2			Cyclopropane, ethyl-	70	C5H10	001191-96-4	72
3			1-Pentene	70	C5H10	000109-67-1	64
4			Cyclobutane, methyl-	70	C5H10	000598-61-8	50
5			3-Buten-1-ol	72	C4H8O	000627-27-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039961.D
Acq On : 25 Jan 2024 17:59
Operator : JC/MD
Sample : P1258-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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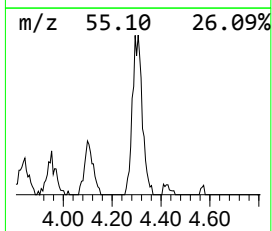
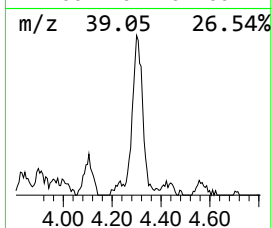
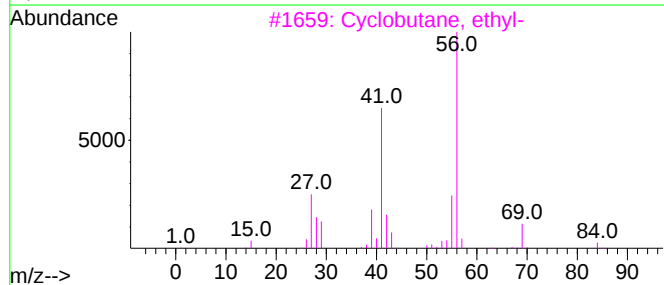
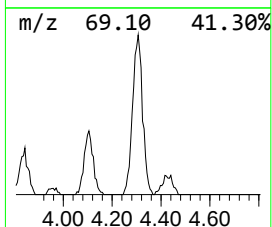
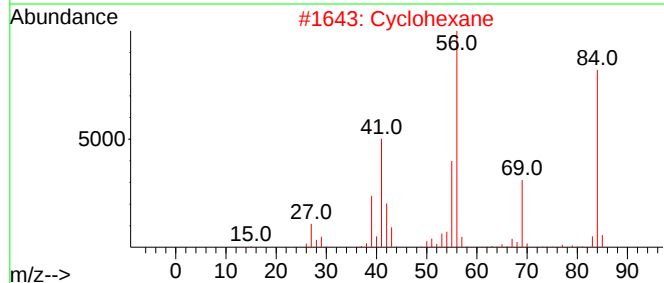
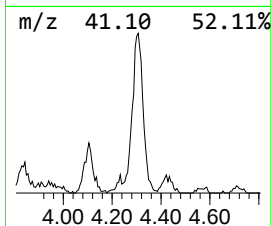
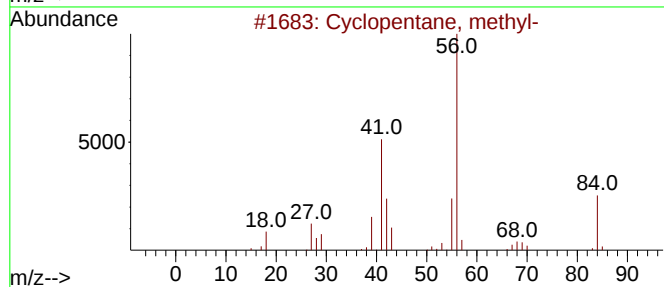
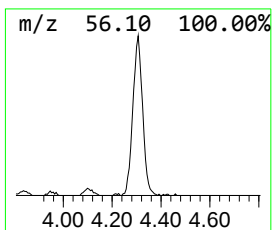
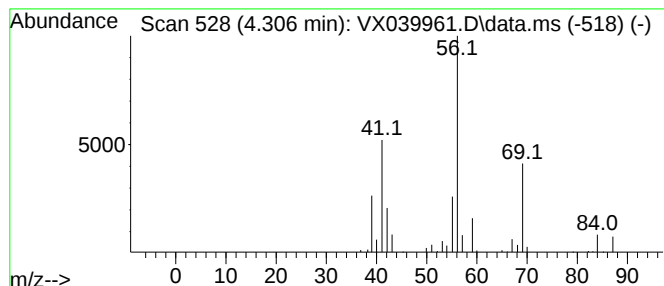
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Quant Title : SW846 8260

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

Peak Number 10 Cyclopentane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	19.65 ug/l	103399	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	72
2		Cyclohexane	84	C6H12	000110-82-7	64
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
4		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	58
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039961.D
Acq On : 25 Jan 2024 17:59
Operator : JC/MD
Sample : P1258-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.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	1.270	25.4	ug/l	133530	1	5.556	263164	50.0
Butane	1.368	158.7	ug/l	835027	1	5.556	263164	50.0
Butane, 2-methyl-	1.752	64.2	ug/l	338084	1	5.556	263164	50.0
Pentane	1.959	47.4	ug/l	249607	1	5.556	263164	50.0
Ethanol	2.057	189.9	ug/l	999760	1	5.556	263164	50.0
Cyclopropane, 1...	2.215	46.6	ug/l	245238	1	5.556	263164	50.0
Cyclopentene	2.752	23.7	ug/l	124638	1	5.556	263164	50.0
Cyclopropane, e...	2.867	23.0	ug/l	121203	1	5.556	263164	50.0
Cyclopentane, m...	4.306	19.6	ug/l	103399	1	5.556	263164	50.0