LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039960.D
Acq On : 25 Jan 2024 17:36
Operator : JC/MD
Sample : P1258-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50236

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: VX039960.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	397171	481748	5.32%	1.416%
2	1.368	41	46	53	rVV	2244717	2911690	32.18%	8.559%
3	1.429	53	56	57	rVV	332813	360657	3.99%	1.060%
4	1.453	57	60	64	rVV	357355	446815	4.94%	1.313%
5	1.496	64	67	84	rVB	260261	303946	3.36%	0.893%
6	1.752	103	109	121	rBV	965683	1266867	14.00%	3.724%
7	1.910	129	135	138	rBV	67914	90641	1.00%	0.266%
8	1.959	138	143	152	rVV3	448004	866927	9.58%	2.548%
9	2.063	152	160	170	rVV2	1724237	2695697	29.79%	7.924%
10	2.166	170	177	180	rVV	148455	240655	2.66%	0.707%
11	2.215	180	185	194	rVB	523095	789373	8.72%	2.320%
12	2.380	208	212	225	rVB	56883	95125	1.05%	0.280%
13	2.745	260	272	280	rBV	156385	356442	3.94%	1.048%
14	2.825	280	285	287	rVV2	69683	129835	1.43%	0.382%
15	2.867	287	292	304	rVB	177676	384885	4.25%	1.131%
16	3.111	321	332	344	rBV3	97202	242088	2.68%	0.712%
17	4.306	518	528	540	rVB2	113231	328929	3.64%	0.967%
18	4.709	584	594	610	rBV	63178	179233	1.98%	0.527%
19	5.196	661	674	690	rVB2	41746	130675	1.44%	0.384%
20	5.385	693	705	712	rBV	57918	168819	1.87%	0.496%
21	5.471	712	719	725	rVV2	67382	204692	2.26%	0.602%
22	5.556	726	733	755	rVB	96428	291684	3.22%	0.857%
23	5.958	789	799	803	rBV	68557	177949	1.97%	0.523%
24	6.038	803	812	828	rVB	2073184	5509227	60.88%	16.194%
25	6.763	922	931	942	rBV	156112	391988	4.33%	1.152%
26	8.647	1234	1240	1245	rBV	306703	497917	5.50%	1.464%
27	8.720	1245	1252	1274	rVB	5762489	9048817	100.00%	26.599%
28	10.055	1465	1471	1488	rVB	353104	494194	5.46%	1.453%
29	10.195	1488	1494	1505	rVV	440957	594073	6.57%	1.746%
30	10.299	1505	1511	1527	rVB	1387823	1838444	20.32%	5.404%
31	10.640	1561	1567	1580	rVB	608882	775042	8.57%	2.278%
32	11.079	1634	1639	1651	rVB	292958	371832	4.11%	1.093%
33	11.378	1682	1688	1696	rBV	141130	235427	2.60%	0.692%
34	11.750	1744	1749	1761	rVB	256493	313882	3.47%	0.923%
35	12.018	1788	1793	1800	rBV	383176	497502	5.50%	1.462%
36	12.085	1800	1804	1816	rVB	84943	108658	1.20%	0.319%

LSC Area Percent Report

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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50236

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	12.244	1822	1830	1838	rBV2	65244	104966	1.16%	0.309%
38	13.774	2077	2081	2088	rVB	71140	91802	1.01%	0.270%

Sum of corrected areas: 34019143

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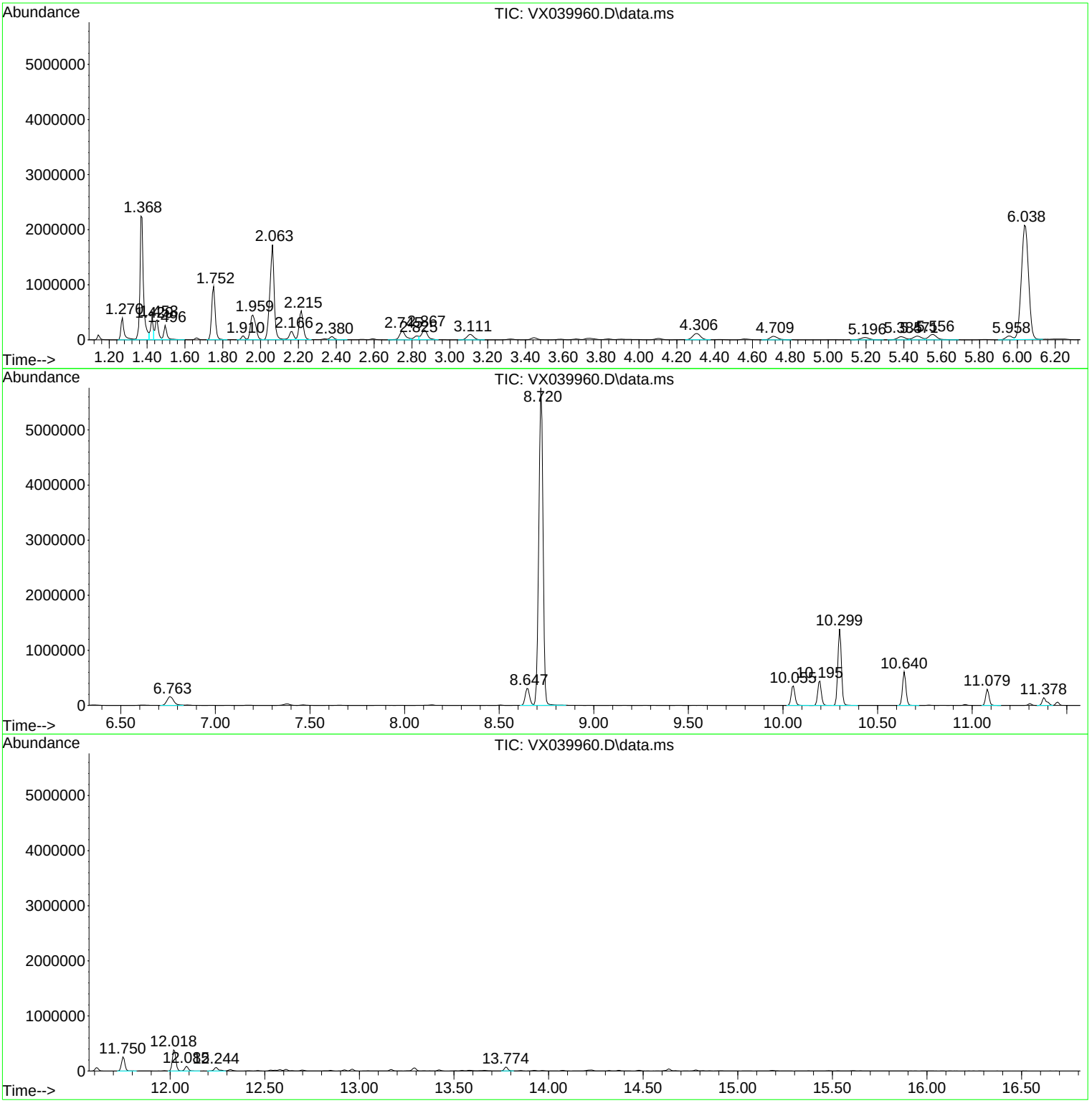
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039960.D
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

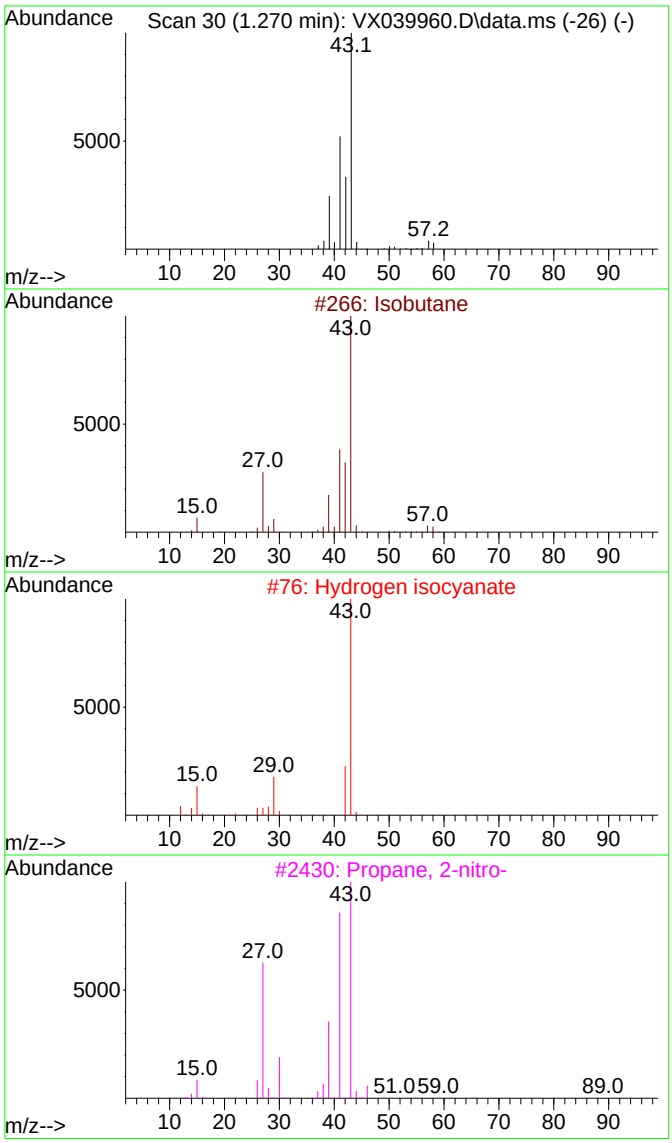
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

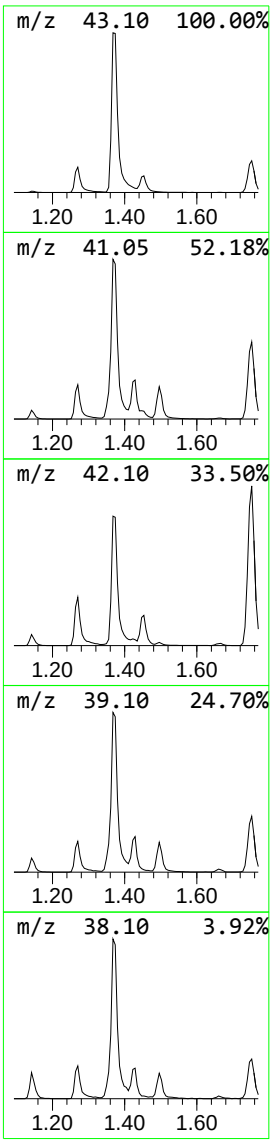
****

Peak Number 1 Isobutane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	82.58 ug/l	481748	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	72
2	Hydrogen isocyanate	43	CHNO	000075-13-8	4
3	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	4
4	Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	4
5	Propene	42	C3H6	000115-07-1	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
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Operator : JC/MD
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50236

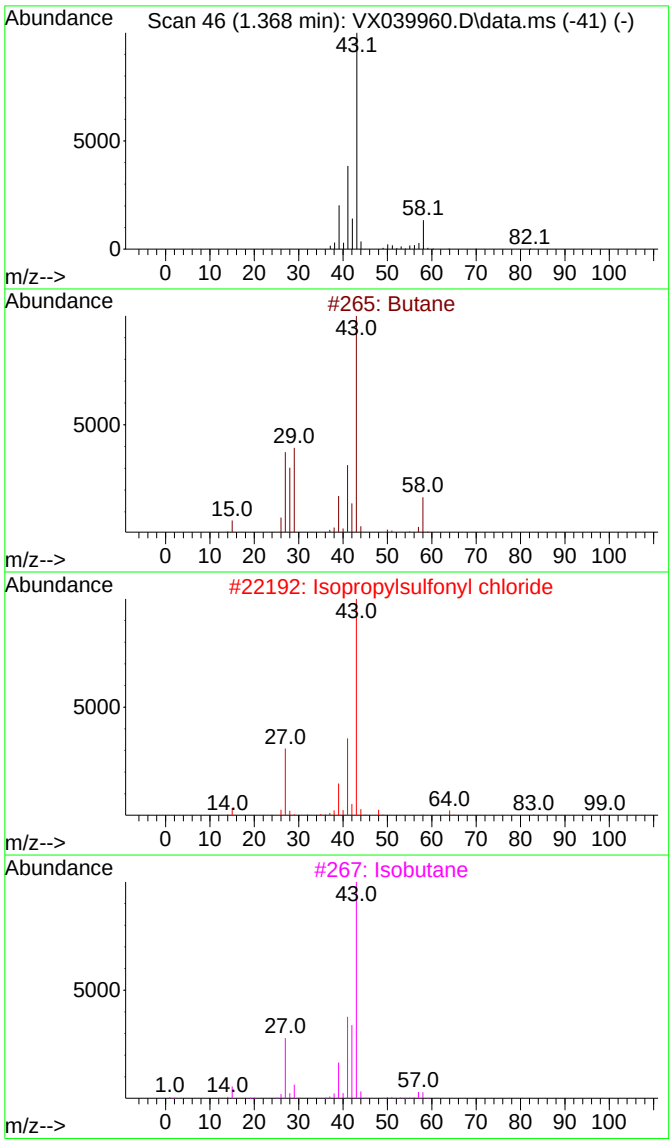
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

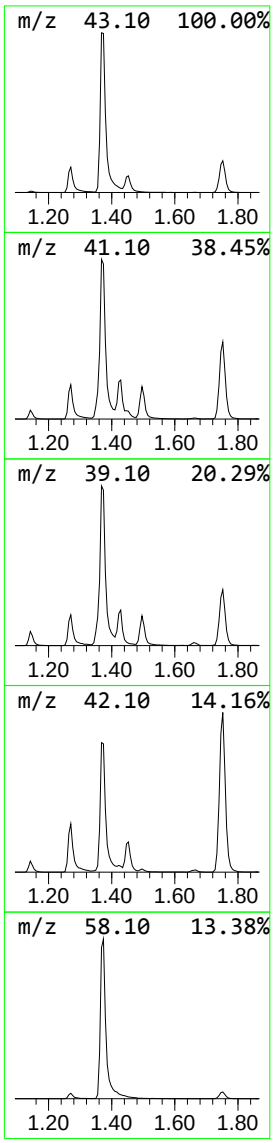
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	499.12 ug/l	2911690	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
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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Data File : VX039960.D
Acq On : 25 Jan 2024 17:36
Operator : JC/MD
Sample : P1258-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50236

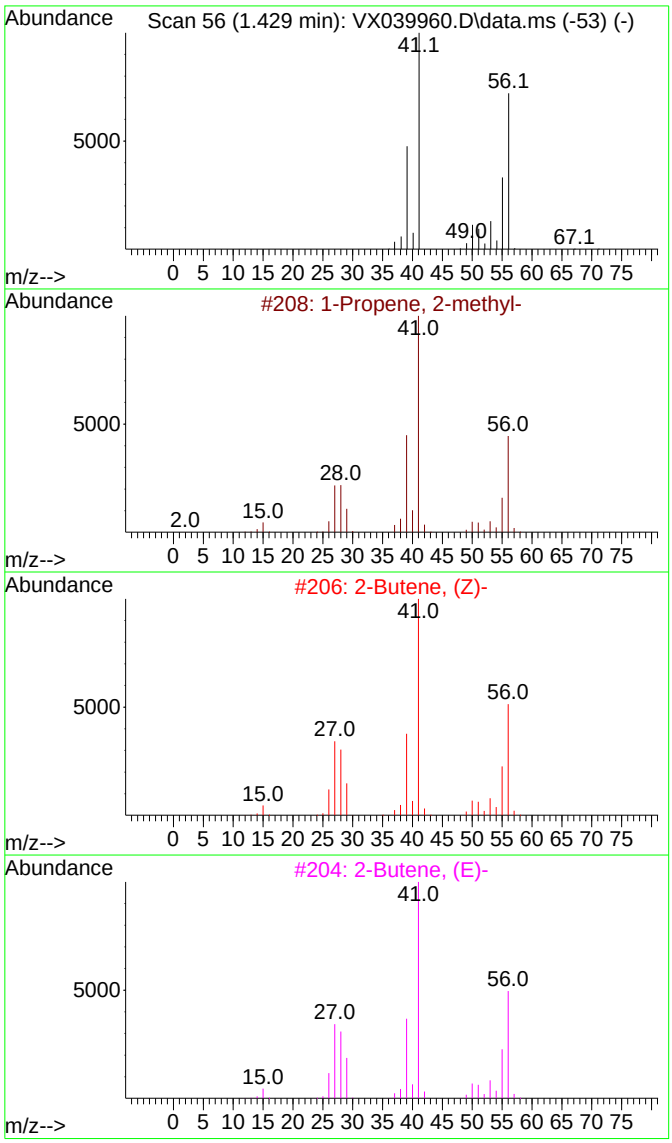
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

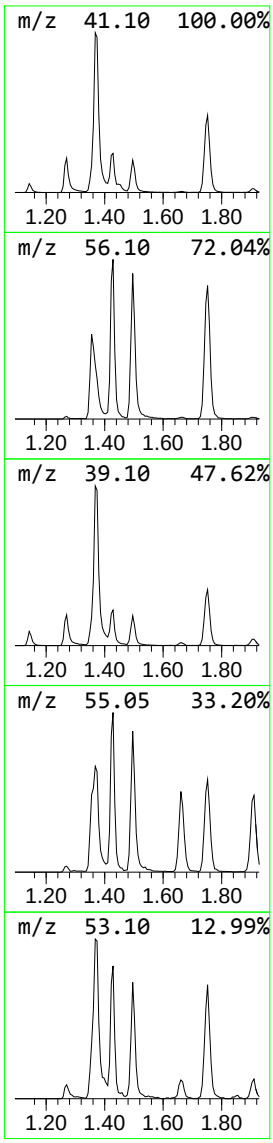
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Propene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.429	61.82 ug/l	360657	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	80
2	2-Butene, (Z)-	56	C4H8	000590-18-1	64
3	2-Butene, (E)-	56	C4H8	000624-64-6	64
4	2-Butene	56	C4H8	000107-01-7	64
5	1-Butene	56	C4H8	000106-98-9	49





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50236

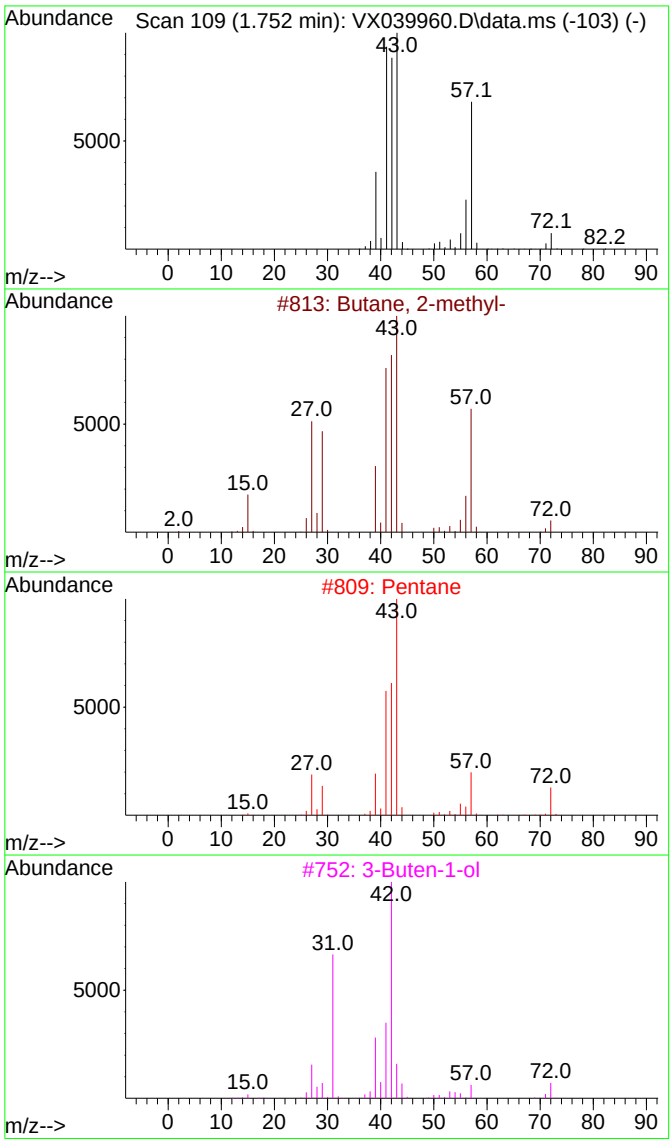
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

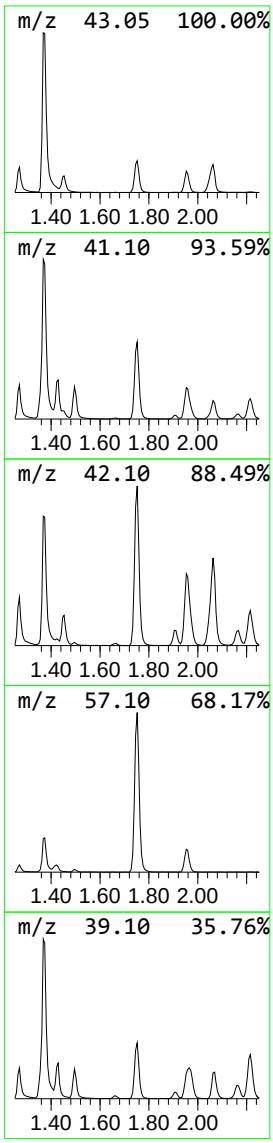
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	217.16 ug/l	1266870	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	Pentane	72	C5H12	000109-66-0	36
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9





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Operator : JC/MD
Sample : P1258-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50236

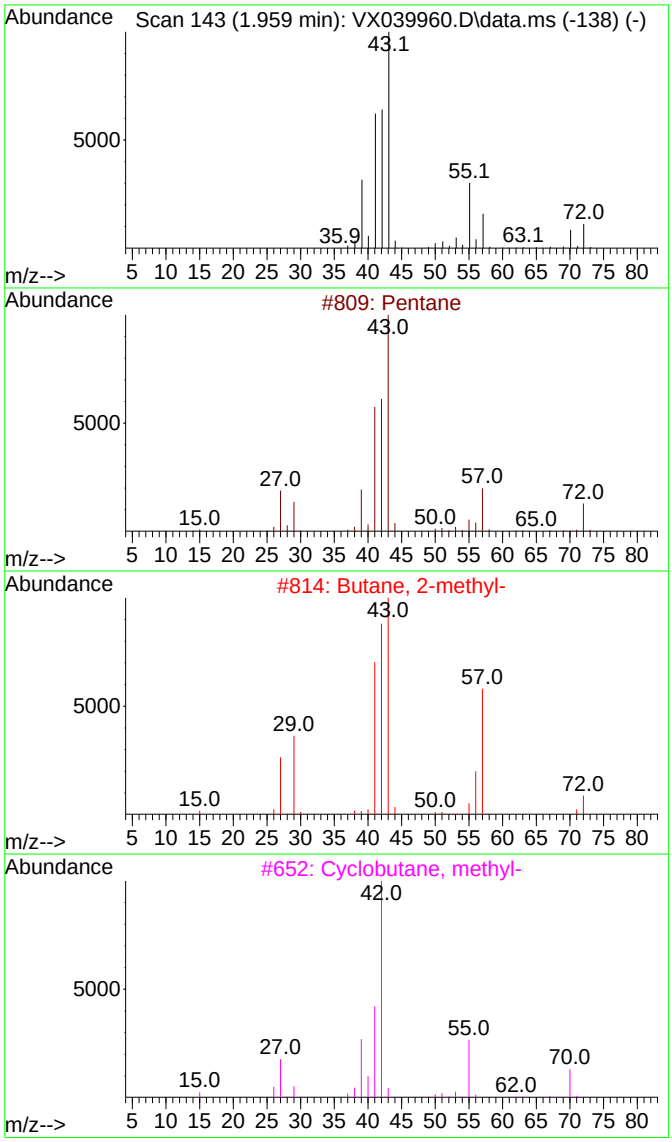
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

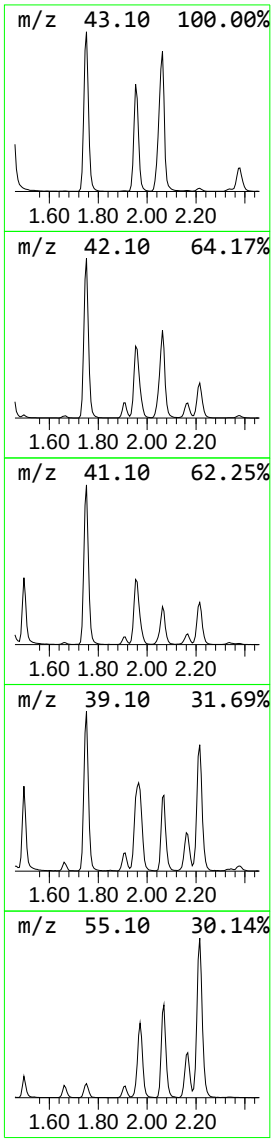
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	148.61 ug/l	866927	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	86
2	Butane, 2-methyl-	72	C5H12	000078-78-4	45
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	43
4	Oxirane, ethyl-	72	C4H8O	000106-88-7	37
5	3-Buten-1-ol	72	C4H8O	000627-27-0	25





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50236

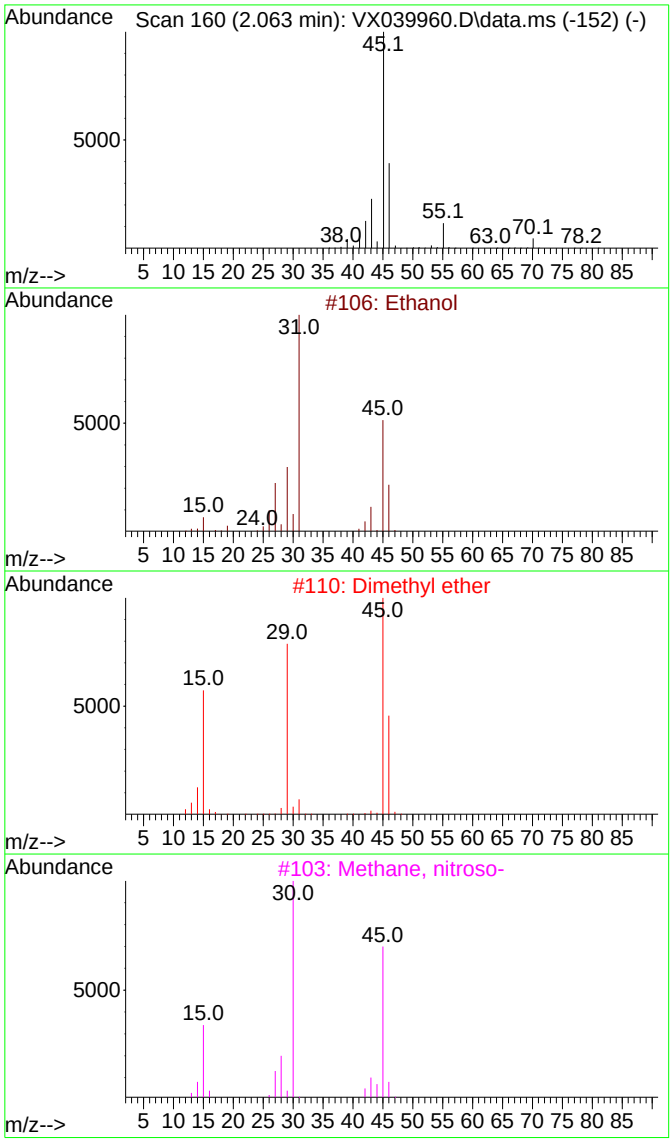
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

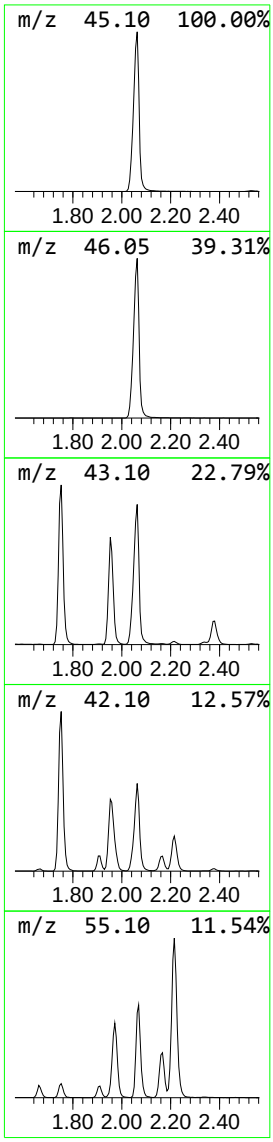
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.063	462.09 ug/l	2695700	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	Formic acid	46	CH2O2	000064-18-6	4
5	Isoamyl lactate	160	C8H16O3	019329-89-6	4





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ALS Vial : 19 Sample Multiplier: 1

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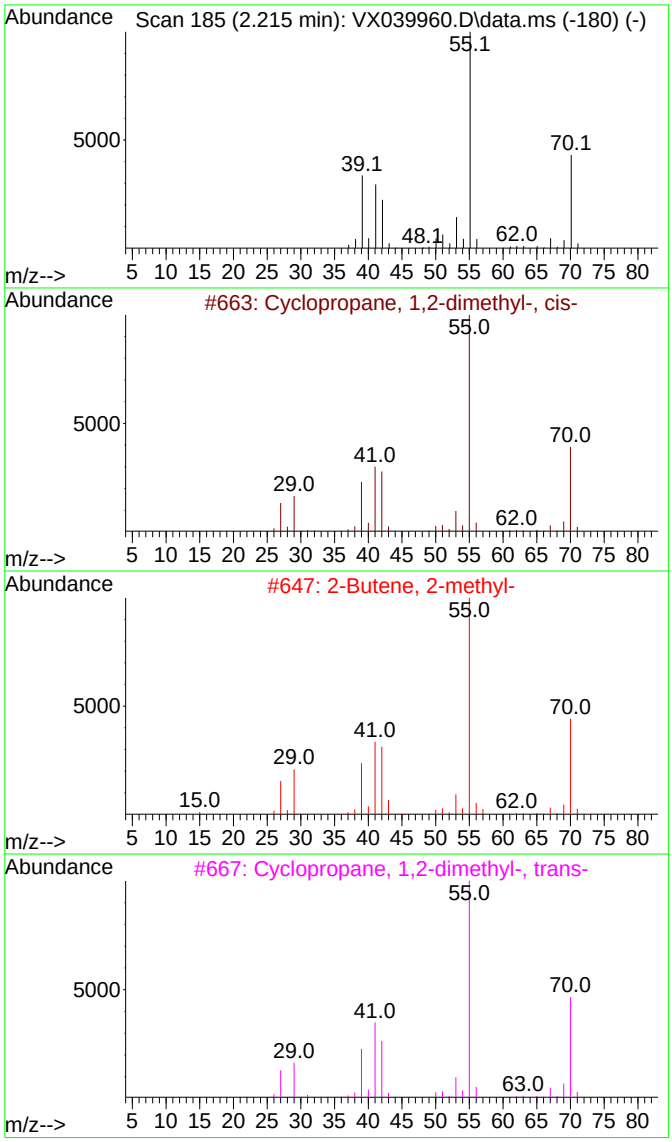
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

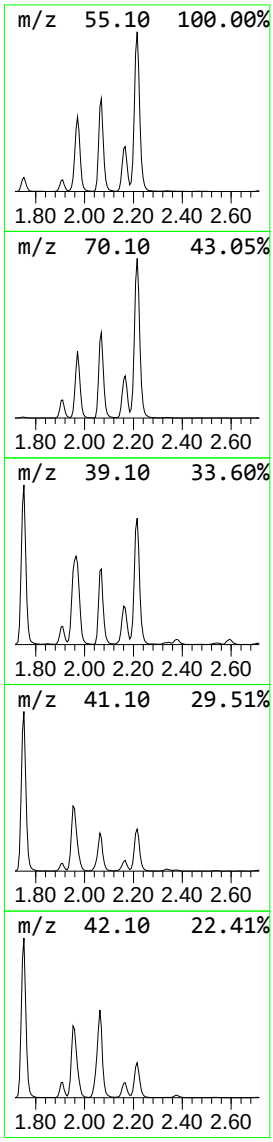
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclopropane, 1,2-dimethyl-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	135.31 ug/l	789373	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	90
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
4	2-Pentene, (E)-	70	C5H10	000646-04-8	87
5	1-Butene, 3-methyl-	70	C5H10	000563-45-1	86





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ALS Vial : 19 Sample Multiplier: 1

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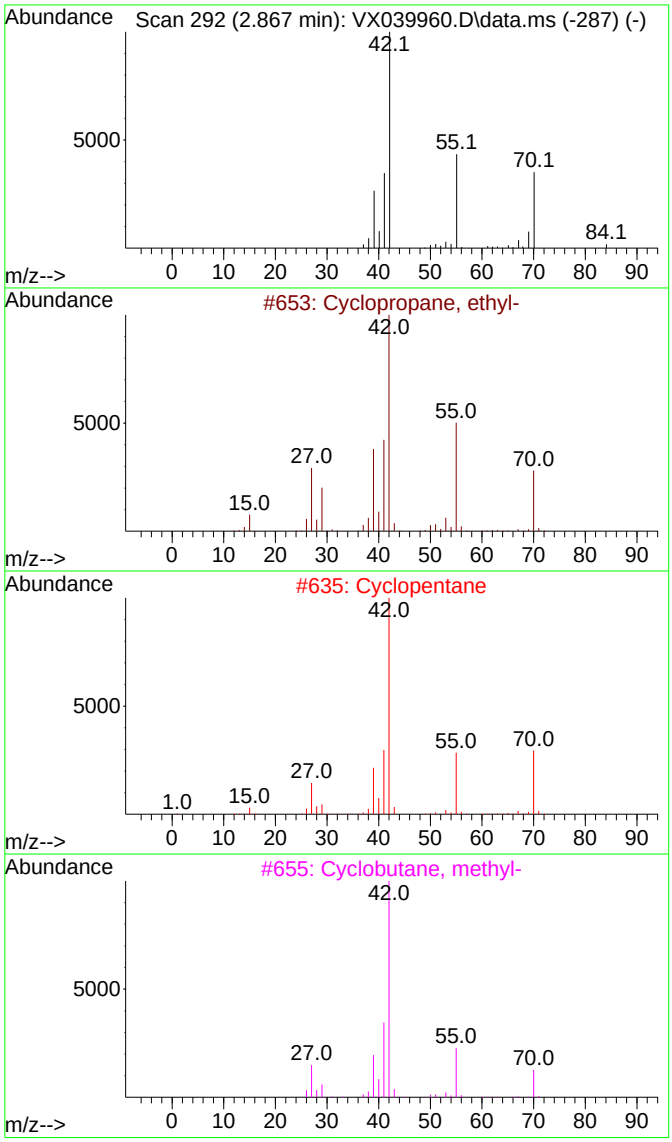
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

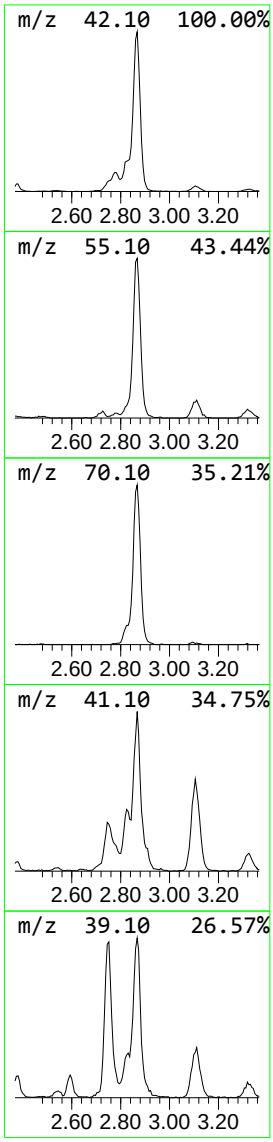
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclopropane, ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	65.98 ug/l	384885	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, ethyl-	70	C5H10	001191-96-4	72
2	Cyclopentane	70	C5H10	000287-92-3	72
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	64
4	1-Pentene	70	C5H10	000109-67-1	64
5	1-Pentanol	88	C5H12O	000071-41-0	40





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50236

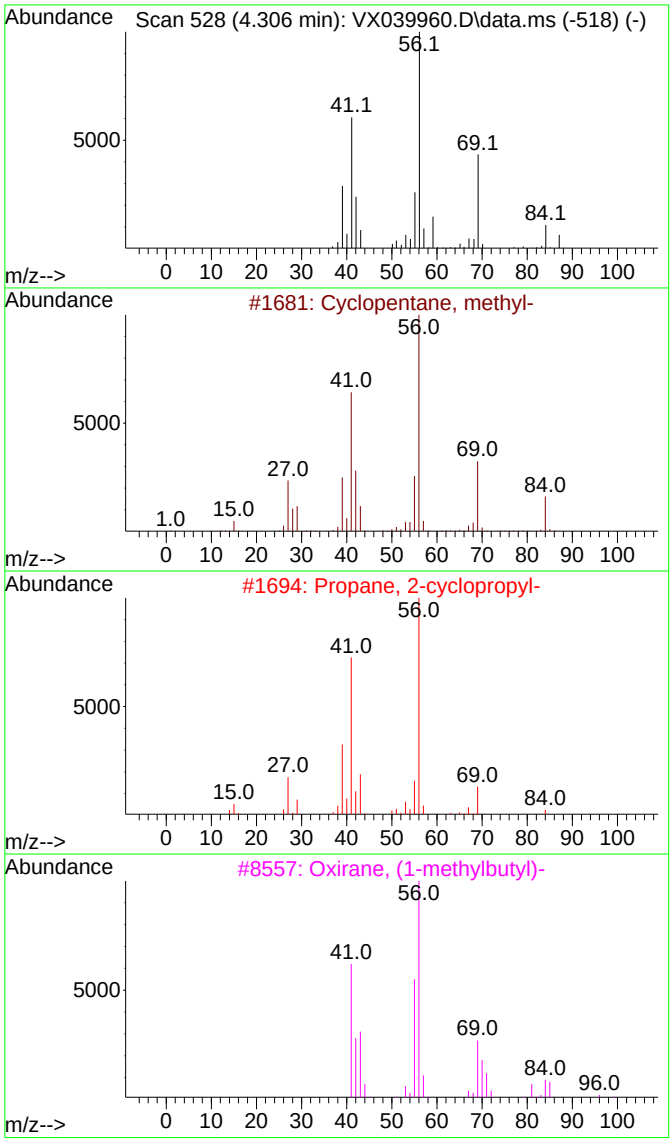
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

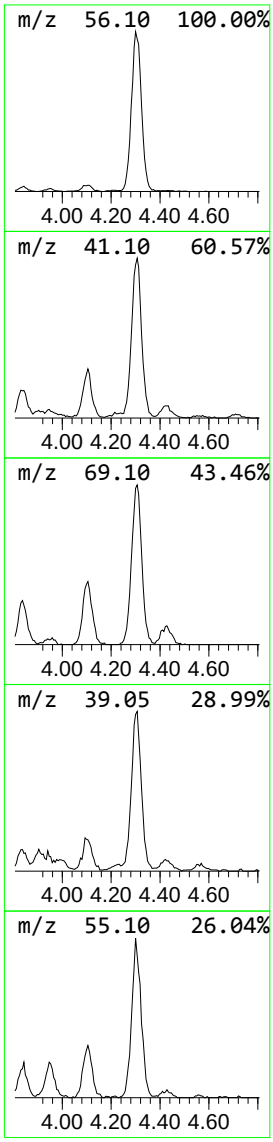
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Cyclopentane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	56.38 ug/l	328929	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	83
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	53
3	Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	50
4	Cyclohexane	84	C6H12	000110-82-7	49
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039960.D
Acq On : 25 Jan 2024 17:36
Operator : JC/MD
Sample : P1258-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50236

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isobutane	1.270	82.6	ug/l	481748	1	5.556	291684	50.0
Butane	1.368	499.1	ug/l	2911690	1	5.556	291684	50.0
1-Propene, 2-me...	1.429	61.8	ug/l	360657	1	5.556	291684	50.0
Butane, 2-methyl-	1.752	217.2	ug/l	1266870	1	5.556	291684	50.0
Pentane	1.959	148.6	ug/l	866927	1	5.556	291684	50.0
Ethanol	2.063	462.1	ug/l	2695700	1	5.556	291684	50.0
Cyclopropane, 1...	2.215	135.3	ug/l	789373	1	5.556	291684	50.0
Cyclopropane, e...	2.867	66.0	ug/l	384885	1	5.556	291684	50.0
Cyclopentane, m...	4.306	56.4	ug/l	328929	1	5.556	291684	50.0