LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039959.D
Acq On : 25 Jan 2024 17:13
Operator : JC/MD
Sample : P1258-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50235

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: VX039959.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	344205	415738	2.58%	0.865%
2	1.368	41	46	53	rVV	1970262	2526033	15.67%	5.256%
3	1.429	53	56	57	rVV	303586	334724	2.08%	0.696%
4	1.453	57	60	64	rVV	519082	638064	3.96%	1.328%
5	1.496	64	67	82	rVB	271583	310429	1.93%	0.646%
6	1.752	103	109	121	rVB	845632	1125068	6.98%	2.341%
7	1.959	138	143	152	rVB3	412412	806048	5.00%	1.677%
8	2.063	152	160	170	rBV	1853000	2901935	18.00%	6.038%
9	2.160	170	176	180	rVV	147551	238434	1.48%	0.496%
10	2.215	180	185	194	rVB	561393	845744	5.25%	1.760%
11	2.746	259	272	281	rBV	182332	401511	2.49%	0.835%
12	2.867	287	292	304	rVB	183247	386420	2.40%	0.804%
13	3.111	321	332	345	rBV2	136271	326199	2.02%	0.679%
14	4.306	519	528	540	rVB2	115396	338151	2.10%	0.704%
15	4.709	584	594	613	rVB	117941	332310	2.06%	0.691%
16	5.385	695	705	712	rBV2	59554	176106	1.09%	0.366%
17	5.465	712	718	726	rVV2	68087	221757	1.38%	0.461%
18	5.550	726	732	754	rVB	101315	297730	1.85%	0.619%
19	5.958	789	799	803	rBV	71788	183901	1.14%	0.383%
20	6.044	803	813	829	rVB	3137913	8398404	52.10%	17.475%
21	6.763	922	931	942	rBV	162431	406242	2.52%	0.845%
22	8.647	1234	1240	1245	rBV	330341	540789	3.35%	1.125%
23	8.726	1245	1253	1270	rVB	10063132	16120970	100.00%	33.543%
24	10.055	1458	1471	1481	rBV	369055	511050	3.17%	1.063%
25	10.195	1488	1494	1505	rBV	890663	1201832	7.46%	2.501%
26	10.299	1505	1511	1526	rVB	2664665	3509048	21.77%	7.301%
27	10.640	1560	1567	1583	rVB	1239850	1531329	9.50%	3.186%
28	11.079	1632	1639	1650	rVB	295439	372649	2.31%	0.775%
29	11.378	1683	1688	1696	rBV	264806	453375	2.81%	0.943%
30	11.750	1744	1749	1756	rVB	563659	661066	4.10%	1.375%
31	12.018	1788	1793	1800	rBV	425617	538711	3.34%	1.121%
32	12.085	1800	1804	1815	rVB	198395	254118	1.58%	0.529%
33	12.244	1822	1830	1838	rBV2	137495	234196	1.45%	0.487%
34	12.579	1879	1885	1888	rBV2	261587	325124	2.02%	0.676%
35	13.774	2076	2081	2087	rVB	153137	194982	1.21%	0.406%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039959.D
Acq On : 25 Jan 2024 17:13
Operator : JC/MD
Sample : P1258-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50235

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

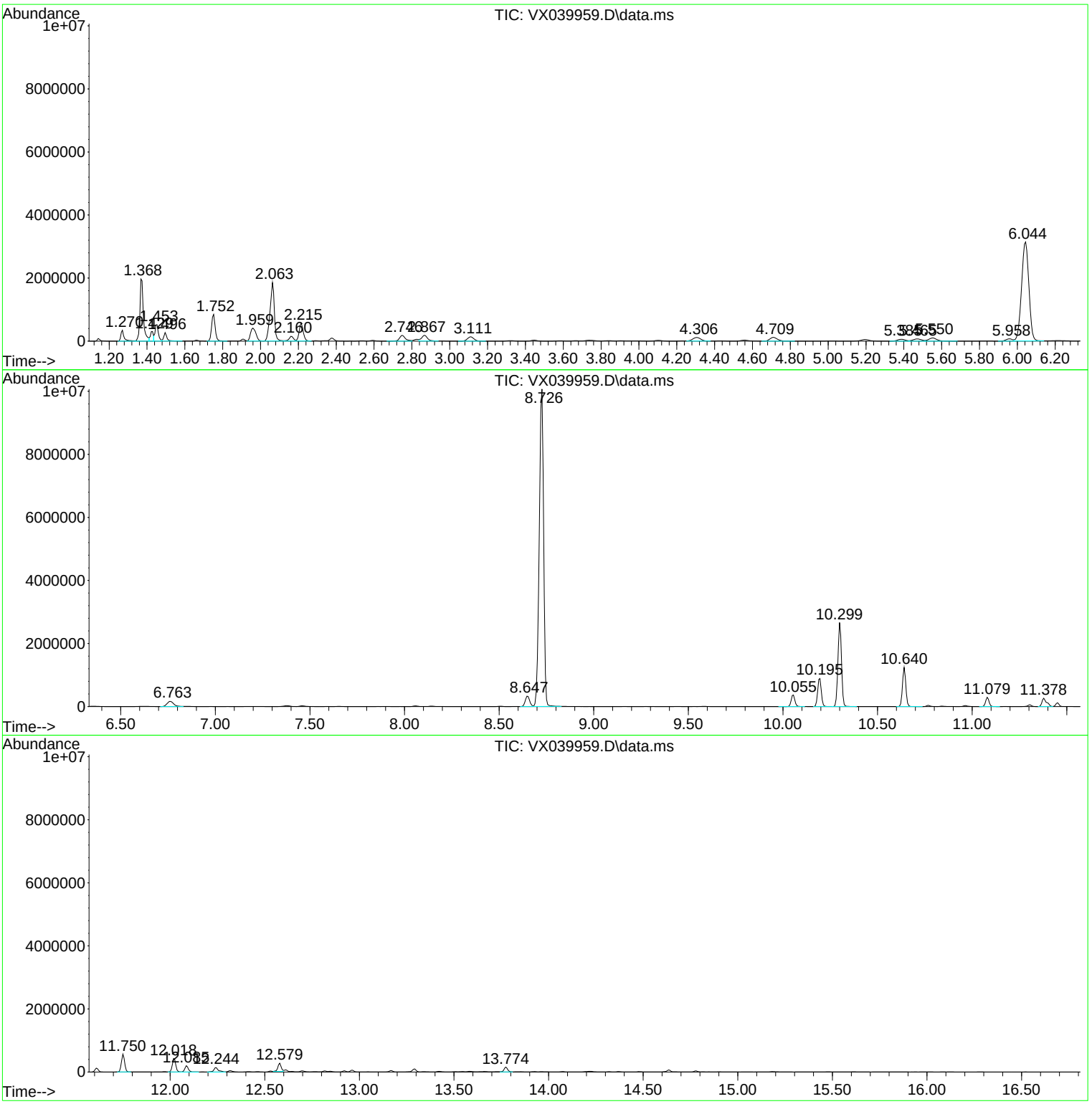
Sum of corrected areas: 48060187

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039959.D
Acq On : 25 Jan 2024 17:13
Operator : JC/MD
Sample : P1258-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50235

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 : VX039959.D
Acq On : 25 Jan 2024 17:13
Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
50235

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

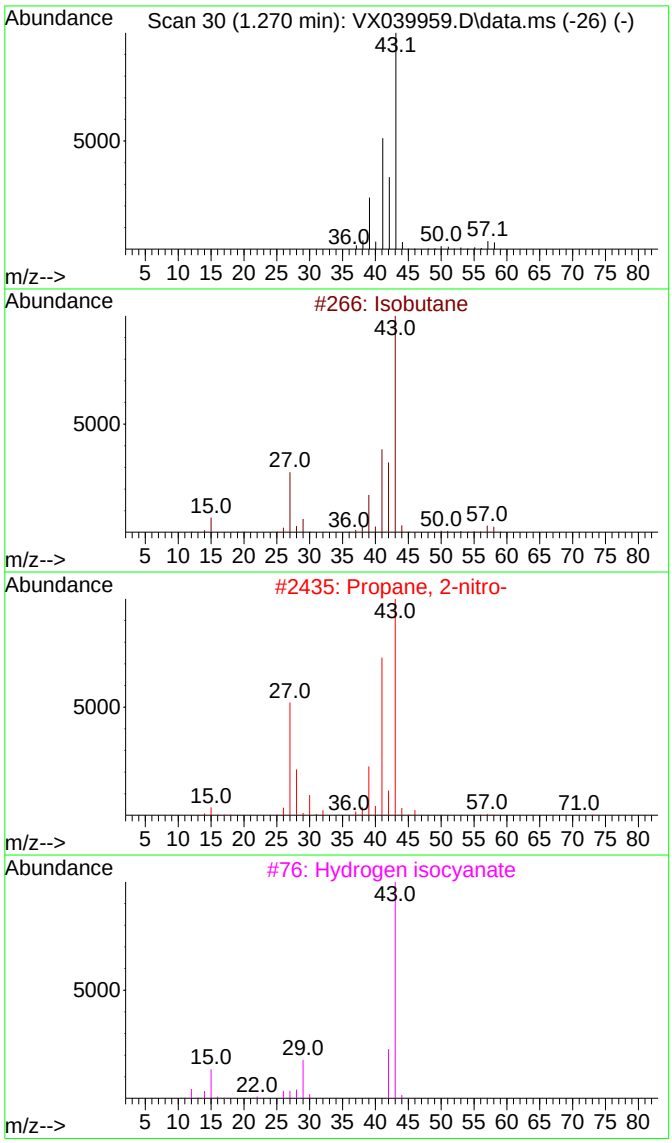
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

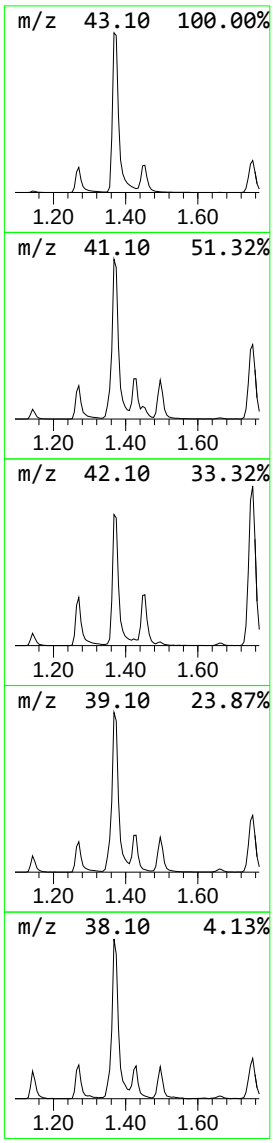
****

Peak Number 1 Isobutane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	69.82 ug/l	415738	Pentafluorobenzene	5.550

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	Hydrogen isocyanate	43	CHNO	000075-13-8	4
4	Propene	42	C3H6	000115-07-1	4
5	Cyclobutylamine	71	C4H9N	002516-34-9	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039959.D
Acq On : 25 Jan 2024 17:13
Operator : JC/MD
Sample : P1258-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50235

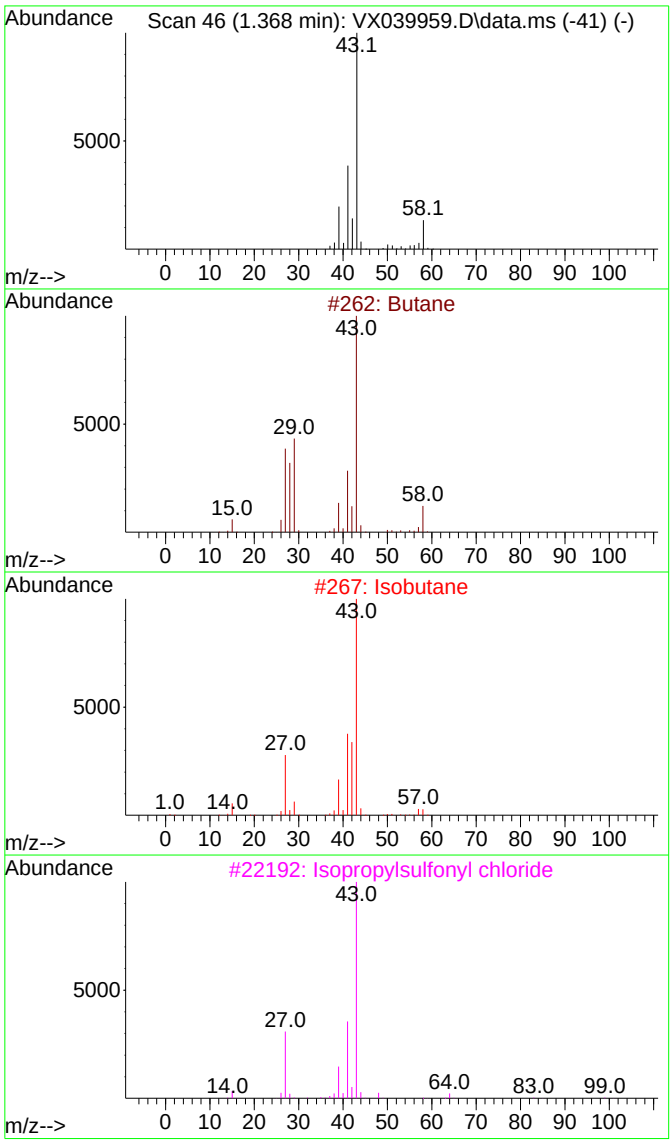
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

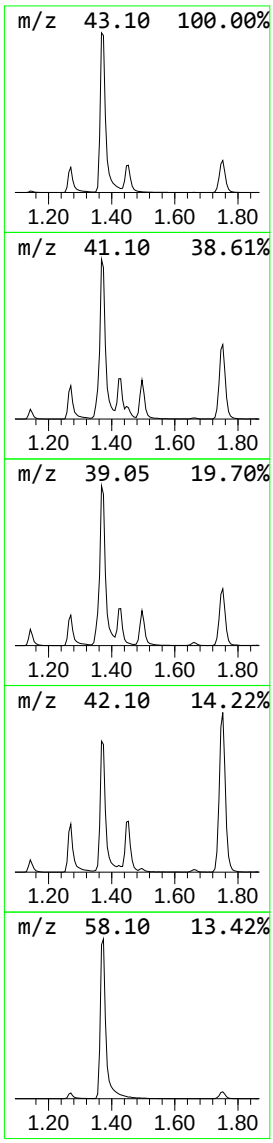
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	424.21 ug/l	2526030	Pentafluorobenzene	5.550

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039959.D
Acq On : 25 Jan 2024 17:13
Operator : JC/MD
Sample : P1258-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50235

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

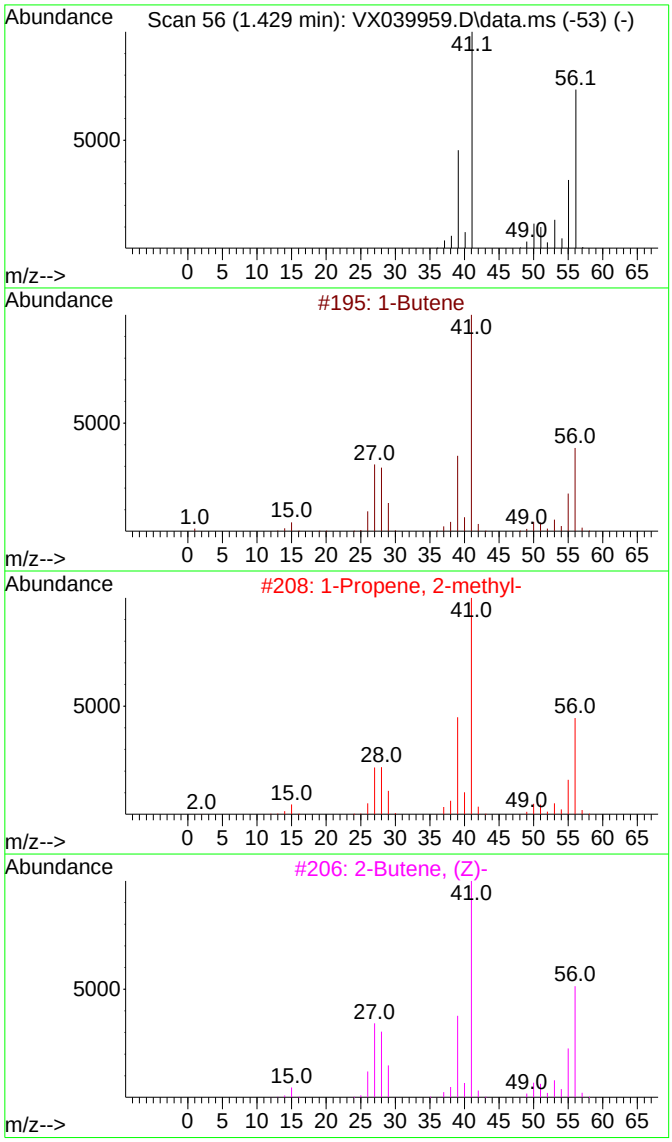
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

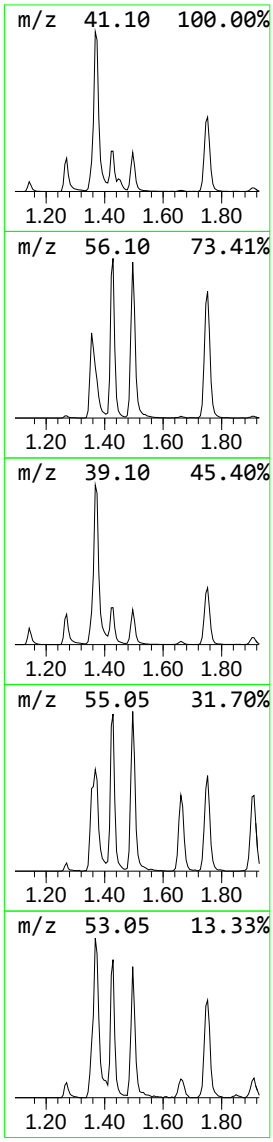
****

Peak Number 3 1-Butene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.429	56.21 ug/l	334724	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene	56	C4H8	000106-98-9	80
2	1-Propene, 2-methyl-	56	C4H8	000115-11-7	80
3	2-Butene, (Z)-	56	C4H8	000590-18-1	72
4	2-Butene	56	C4H8	000107-01-7	72
5	2-Butene, (E)-	56	C4H8	000624-64-6	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039959.D
Acq On : 25 Jan 2024 17:13
Operator : JC/MD
Sample : P1258-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50235

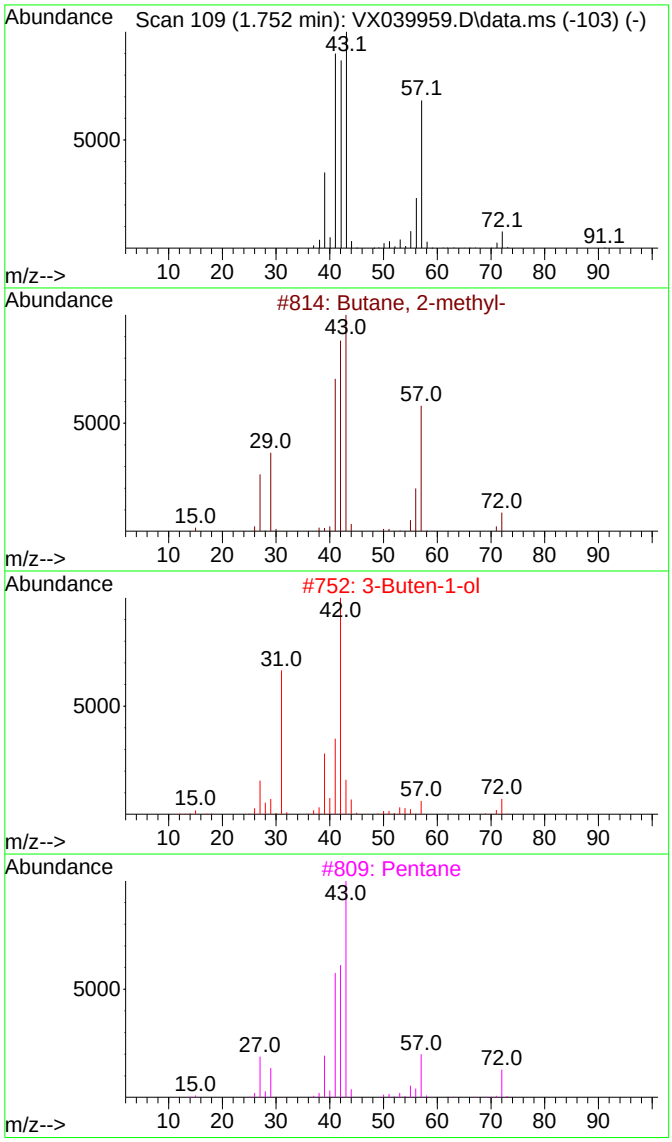
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

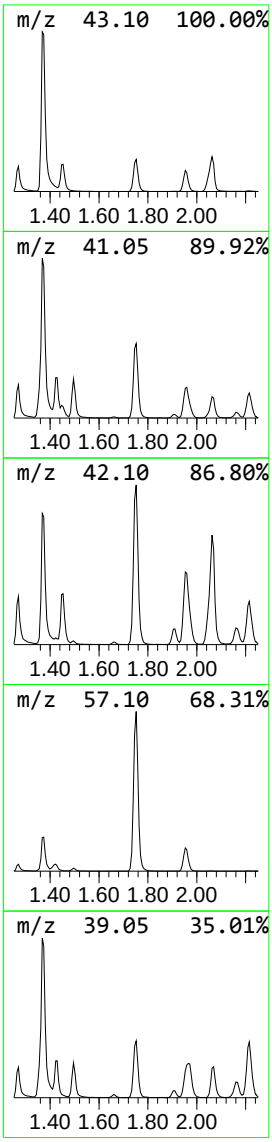
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	188.94 ug/l	1125070	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	Azetidine	57	C3H7N	000503-29-7	9
5	1-Butene	56	C4H8	000106-98-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039959.D
Acq On : 25 Jan 2024 17:13
Operator : JC/MD
Sample : P1258-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50235

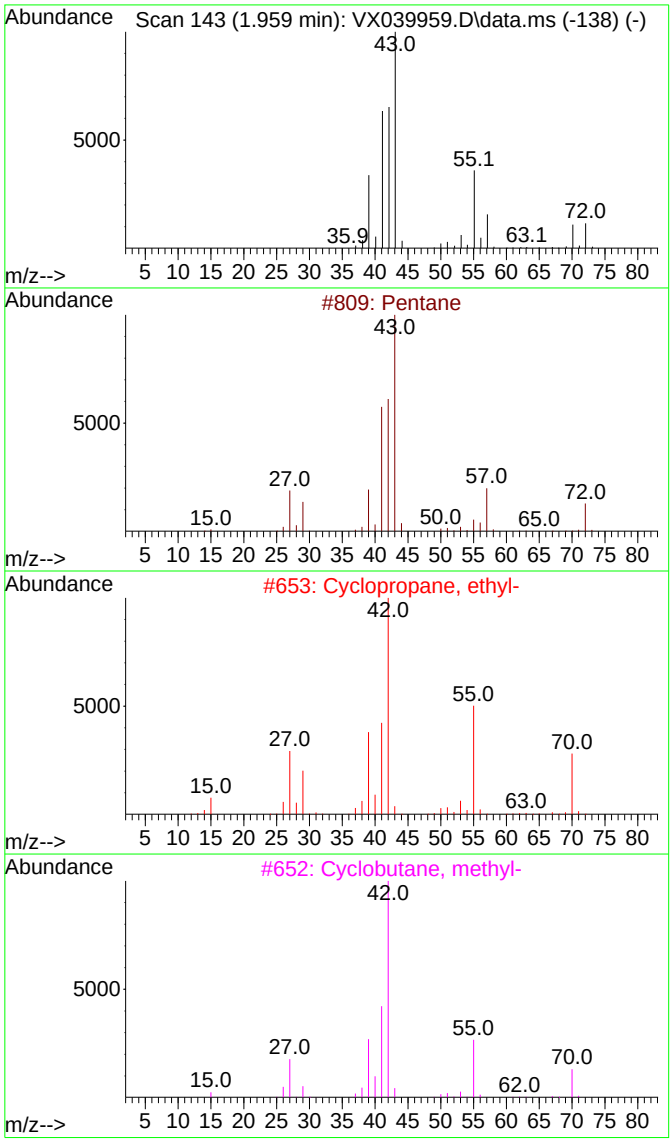
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

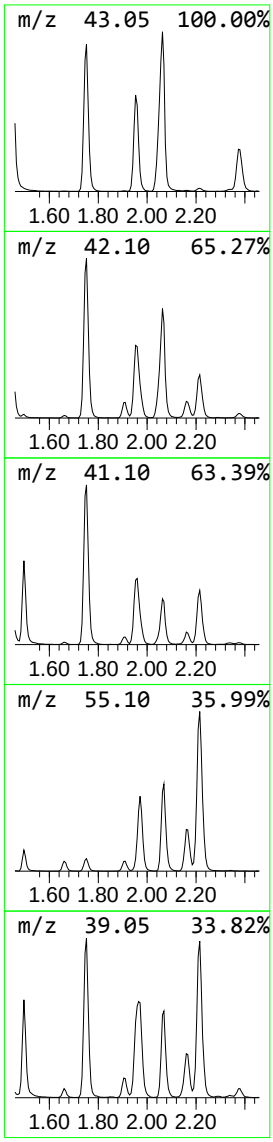
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	135.37 ug/l	806048	Pentafluorobenzene	5.550

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	43
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	43
4	Oxirane, ethyl-	72	C4H8O	000106-88-7	32
5	Isobutyl nitrite	103	C4H9NO2	000542-56-3	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039959.D
Acq On : 25 Jan 2024 17:13
Operator : JC/MD
Sample : P1258-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50235

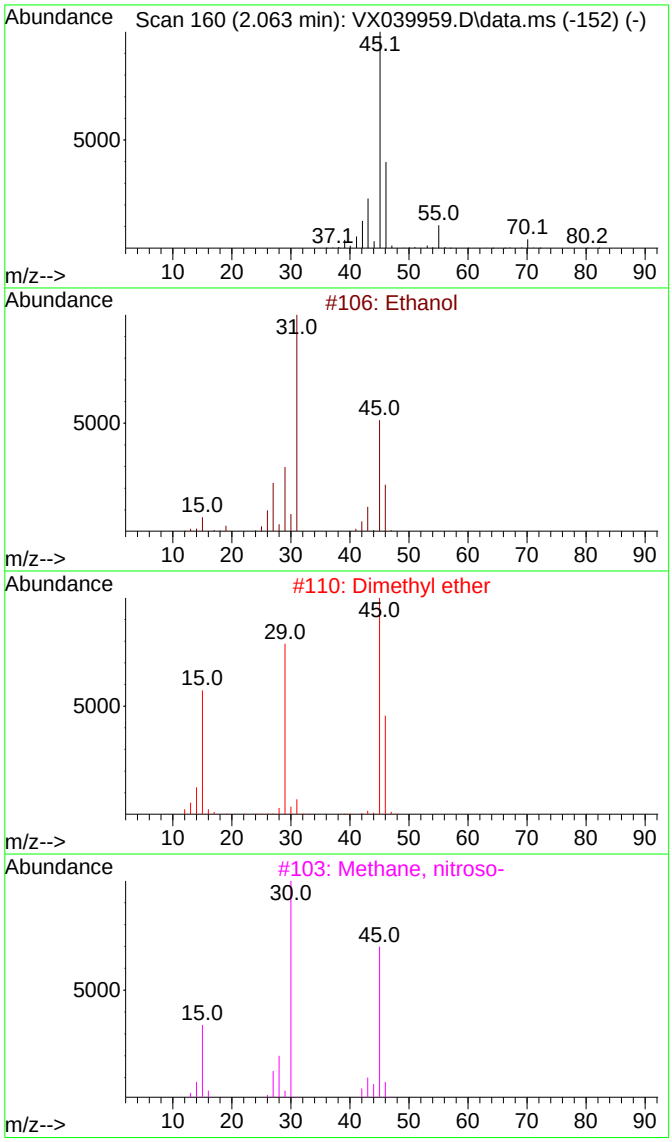
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

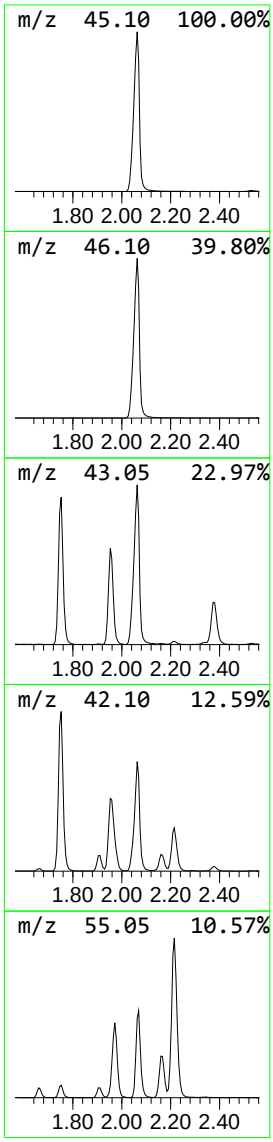
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.063	487.34 ug/l	2901940	Pentafluorobenzene	5.550

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	Oxalic acid	90	C2H2O4	000144-62-7	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039959.D
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Operator : JC/MD
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50235

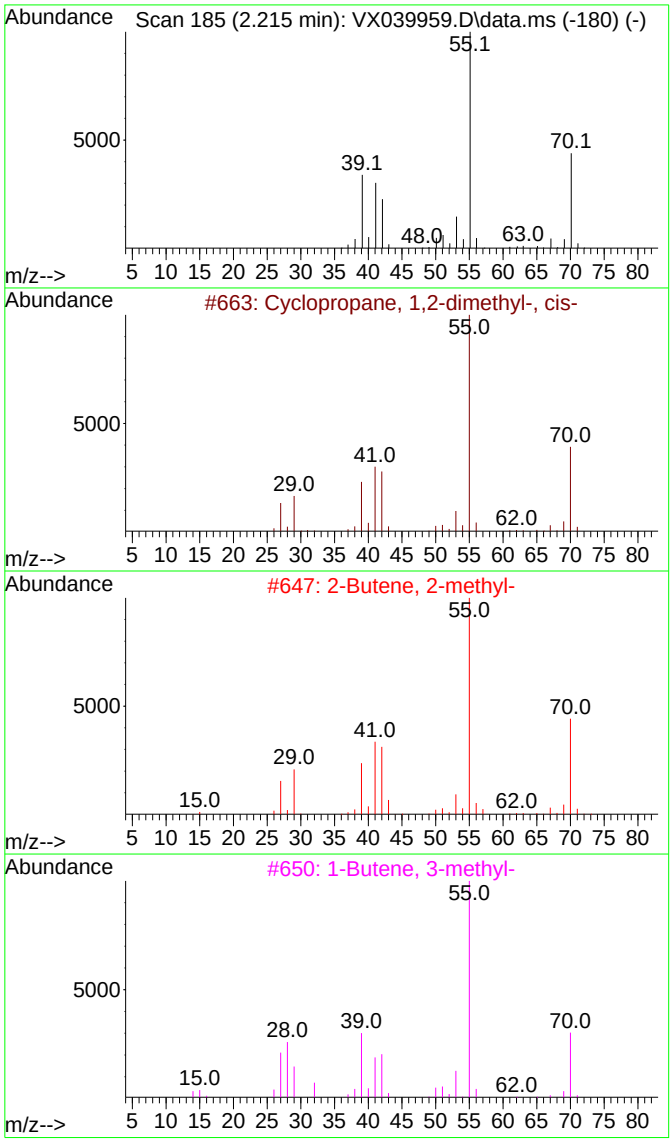
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

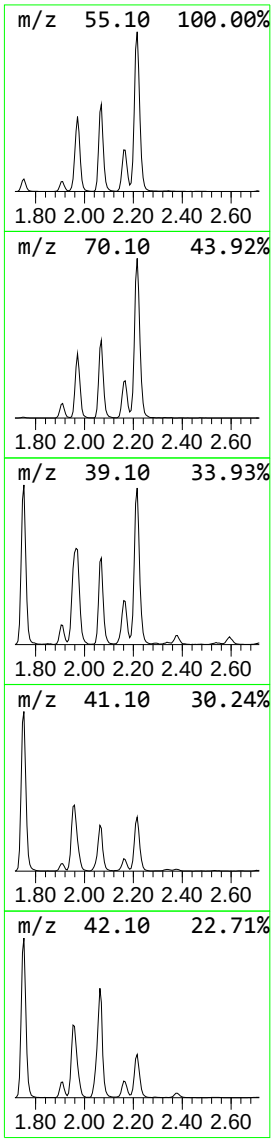
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclopropane, 1,2-dimethyl-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	142.03 ug/l	845744	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	87
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	72





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50235

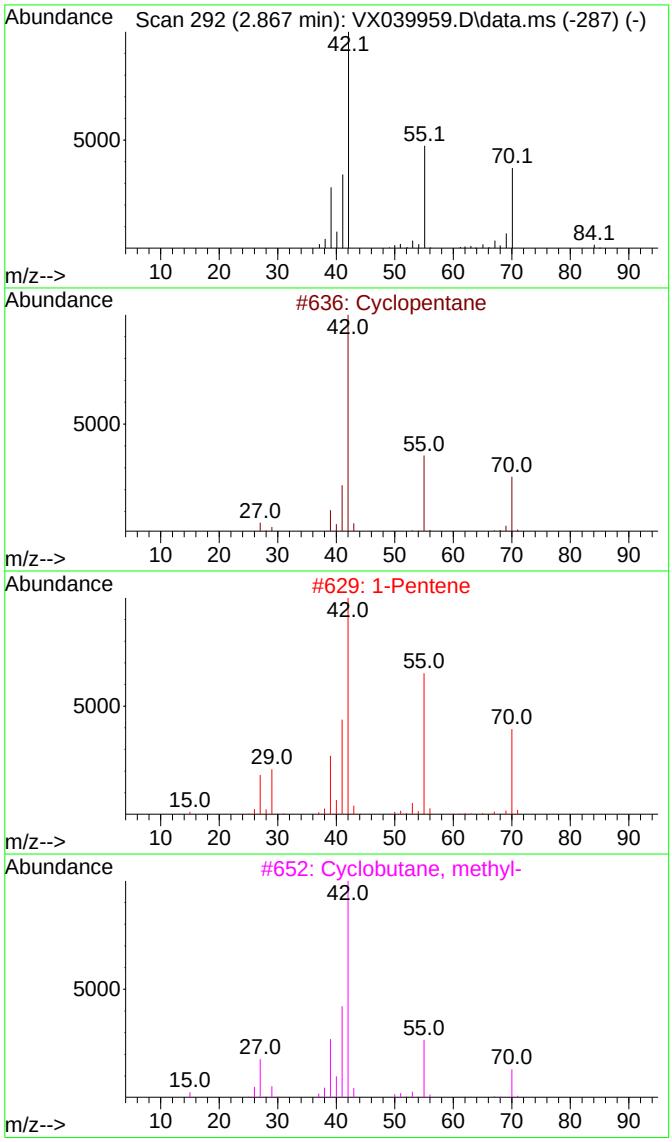
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

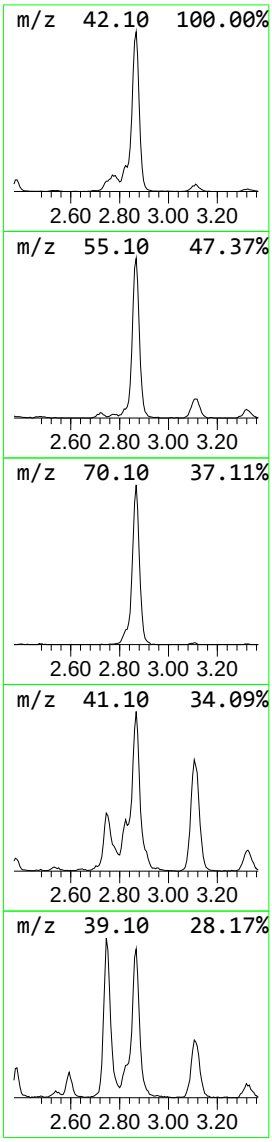
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclopentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	64.89 ug/l	386420	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	78
2	1-Pentene	70	C5H10	000109-67-1	72
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	64
4	1-Pentanol	88	C5H12O	000071-41-0	39
5	Cyclobutanone	70	C4H6O	001191-95-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039959.D
Acq On : 25 Jan 2024 17:13
Operator : JC/MD
Sample : P1258-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50235

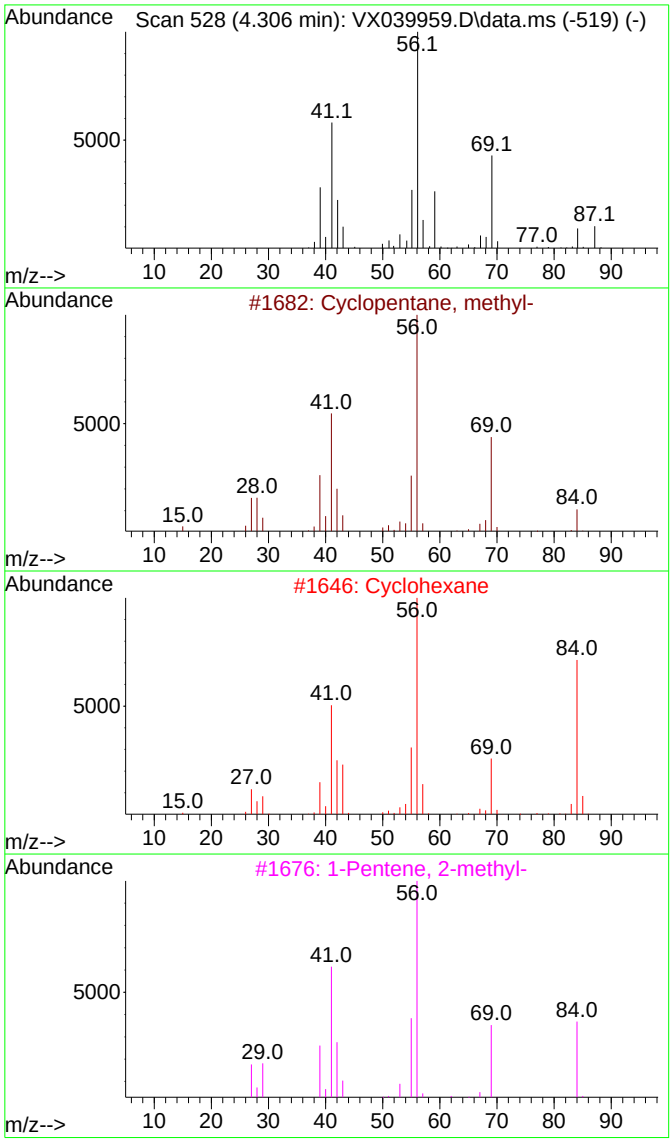
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

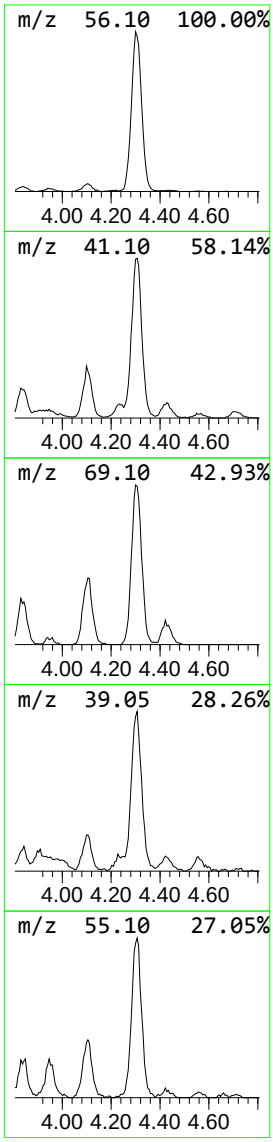
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	56.79 ug/l	338151	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	81
2	Cyclohexane	84	C6H12	000110-82-7	64
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	58
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	50
5	Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039959.D
Acq On : 25 Jan 2024 17:13
Operator : JC/MD
Sample : P1258-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50235

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	69.8	ug/l	415738	1	5.550	297730	50.0
Butane	1.368	424.2	ug/l	2526030	1	5.550	297730	50.0
1-Butene	1.429	56.2	ug/l	334724	1	5.550	297730	50.0
Butane, 2-methyl-	1.752	188.9	ug/l	1125070	1	5.550	297730	50.0
Pentane	1.959	135.4	ug/l	806048	1	5.550	297730	50.0
Ethanol	2.063	487.3	ug/l	2901940	1	5.550	297730	50.0
Cyclopropane, 1...	2.215	142.0	ug/l	845744	1	5.550	297730	50.0
Cyclopentane	2.867	64.9	ug/l	386420	1	5.550	297730	50.0
Cyclopentane, m...	4.306	56.8	ug/l	338151	1	5.550	297730	50.0