LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
Data File : VN081501.D
Acq On : 20 Mar 2024 18:10
Operator : JC\MD
Sample : P1799-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
50298

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\82N031824W.M
Title : SW846 8260

Signal : TIC: VN081501.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.318	52	62	73	rBV	1863456	2946640	2.71%	0.909%
2	2.512	83	95	108	rBV	11934767	21163505	19.44%	6.529%
3	2.618	108	113	117	rVV	1357056	2348074	2.16%	0.724%
4	2.665	117	121	129	rVV	1124946	1988341	1.83%	0.613%
5	2.748	129	135	143	rVB	1027119	1703695	1.56%	0.526%
6	3.248	210	220	235	rBV	3278587	7389383	6.79%	2.280%
7	3.653	279	289	301	rBV3	1553224	4991212	4.58%	1.540%
8	3.800	301	314	321	rBV	9749821	26744795	24.57%	8.251%
9	4.042	346	355	363	rBV	588279	1537824	1.41%	0.474%
10	4.147	363	373	391	rVB	2214854	6136598	5.64%	1.893%
11	5.159	530	545	556	rBV	785092	2611670	2.40%	0.806%
12	5.389	569	584	612	rVB2	709019	3161528	2.90%	0.975%
13	5.800	638	654	672	rBV2	770692	2787538	2.56%	0.860%
14	6.671	792	802	814	rVB3	438150	1406696	1.29%	0.434%
15	7.330	905	914	924	rVB	595196	1588374	1.46%	0.490%
16	7.559	945	953	973	rVB	963862	2389680	2.19%	0.737%
17	8.230	1061	1067	1081	rVB2	869579	3067621	2.82%	0.946%
18	8.606	1119	1131	1147	rBV2	29145749	68814380	63.21%	21.231%
19	9.100	1206	1215	1237	rBV	1083436	2377137	2.18%	0.733%
20	10.571	1457	1465	1469	rBV	1561533	2997796	2.75%	0.925%
21	10.635	1469	1476	1495	rVB3	55340519	108871660	100.00%	33.590%
22	11.865	1676	1685	1694	rBV	1390036	2501540	2.30%	0.772%
23	11.965	1694	1702	1711	rVV	3967904	6576574	6.04%	2.029%
24	12.070	1711	1720	1731	rBV	10333228	19778971	18.17%	6.102%
25	12.400	1767	1776	1784	rBV	5163754	8716293	8.01%	2.689%
26	12.853	1845	1853	1860	rVB	1083181	1879350	1.73%	0.580%
27	13.100	1889	1895	1899	rBV	1015300	1778375	1.63%	0.549%
28	13.482	1952	1960	1968	rBV	1616477	2691025	2.47%	0.830%
29	13.794	2006	2013	2025	rBV2	1405331	3177700	2.92%	0.980%

Sum of corrected areas: 324123975

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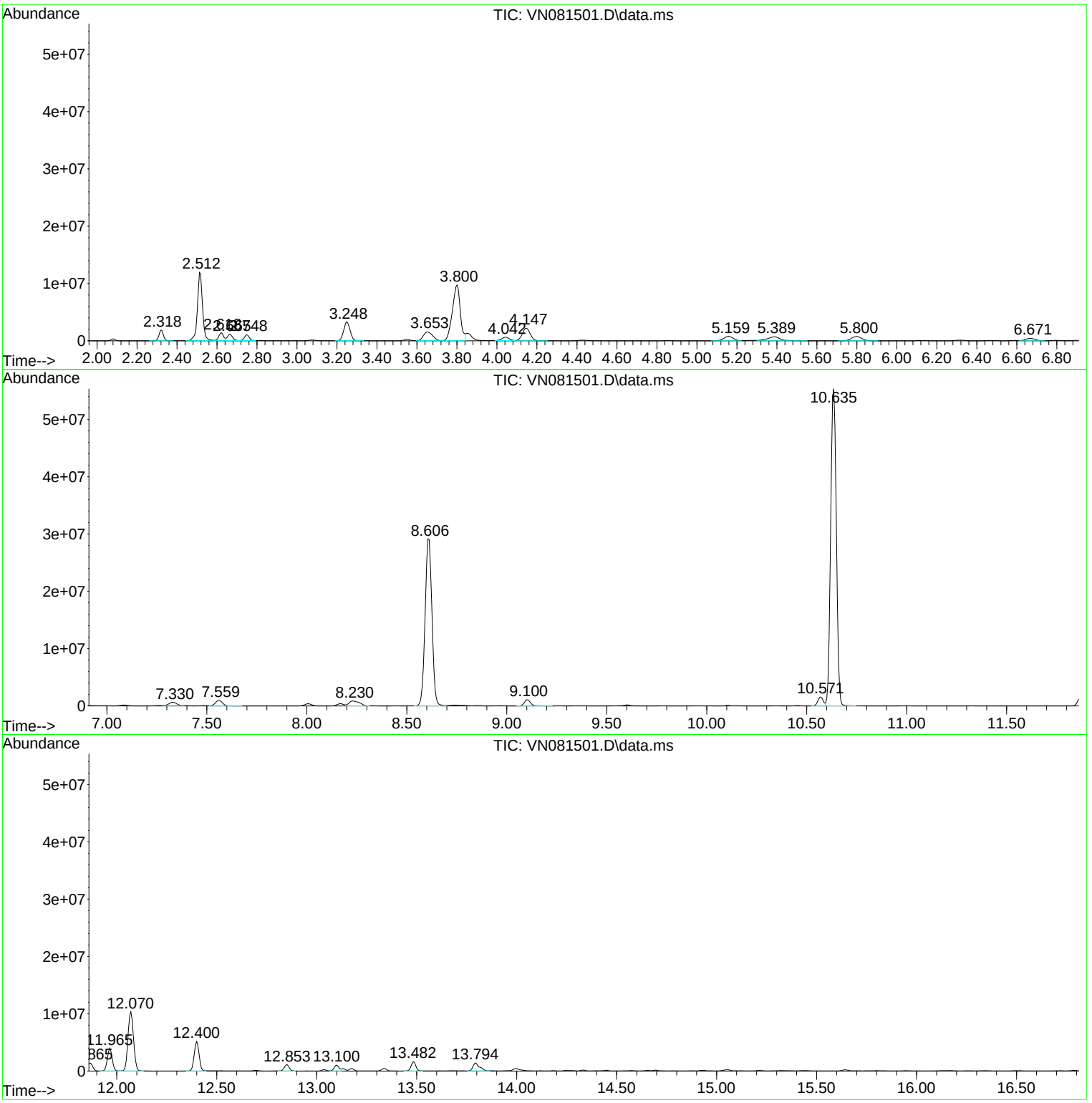
Operator : JC\MD
Sample : P1799-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
50298

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
Data File : VN081501.D
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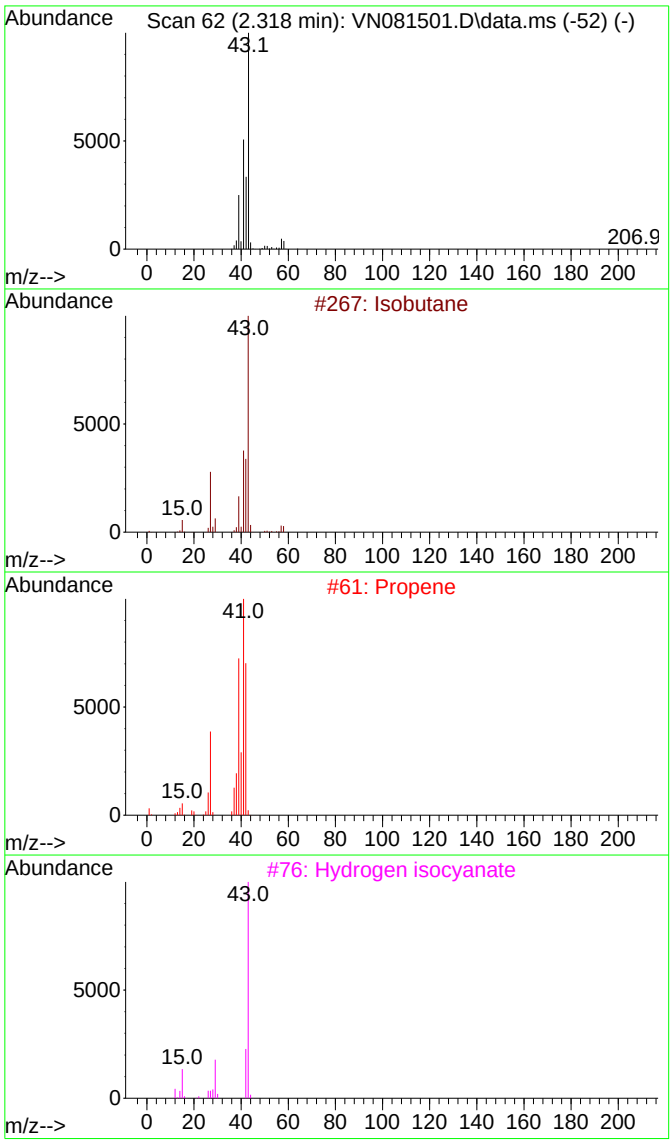
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

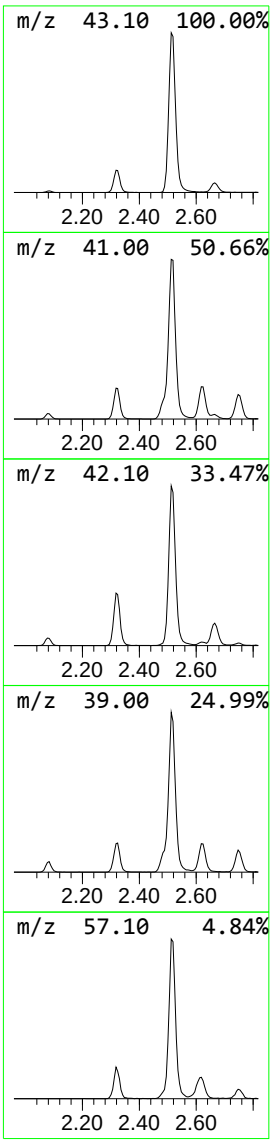
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Isobutane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.318	48.03 ug/l	2946640	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	64
2	Propene	42	C3H6	000115-07-1	5
3	Hydrogen isocyanate	43	CHNO	000075-13-8	4
4	Borane, trimethyl-	56	C3H9B	000593-90-8	4
5	Cyclobutylamine	71	C4H9N	002516-34-9	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
Data File : VN081501.D
Acq On : 20 Mar 2024 18:10
Operator : JC\MD
Sample : P1799-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
50298

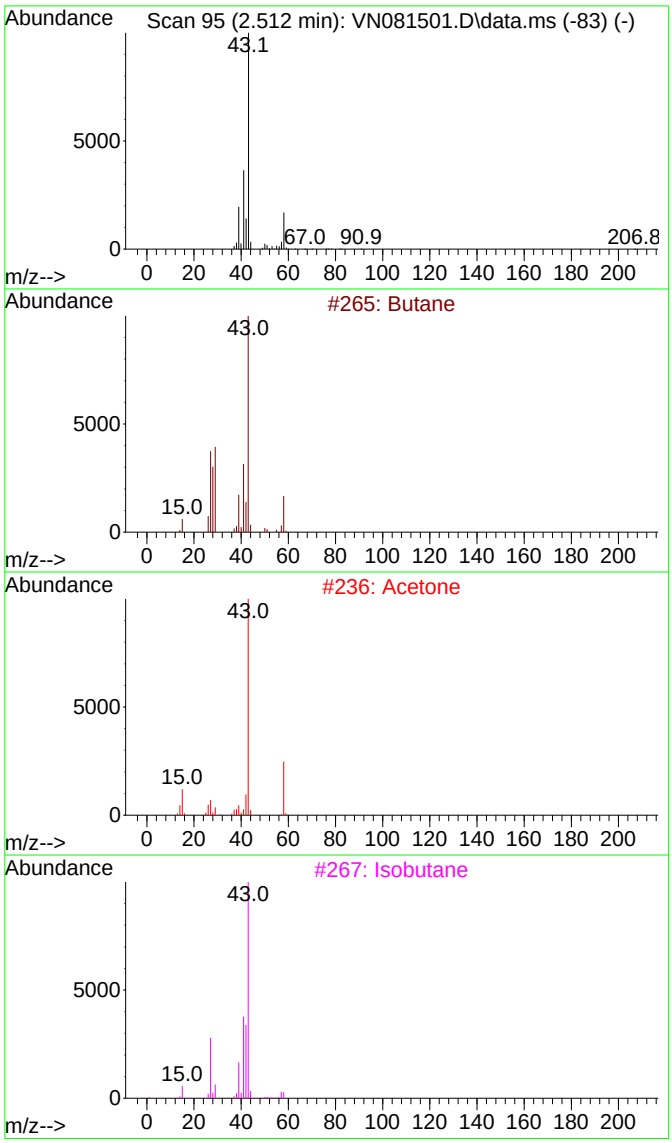
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

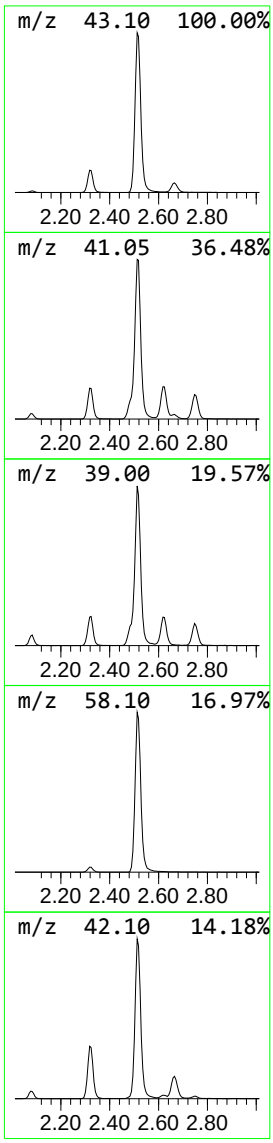
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.512	344.95 ug/l	21163500	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Acetone	58	C3H6O	000067-64-1	9
3	Isobutane	58	C4H10	000075-28-5	9
4	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9





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Data File : VN081501.D
Acq On : 20 Mar 2024 18:10
Operator : JC\MD
Sample : P1799-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
50298

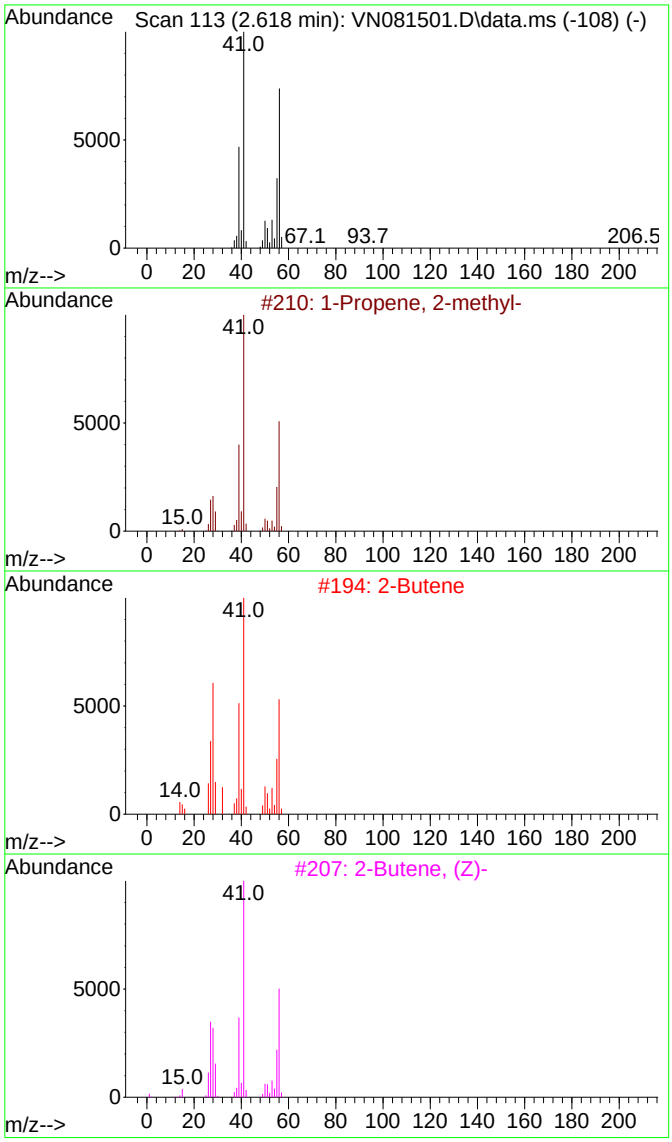
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

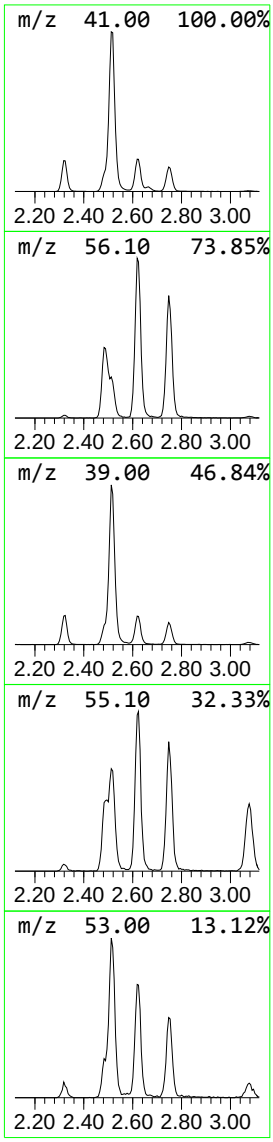
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.618	38.27 ug/l	2348070	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	80
2	2-Butene	56	C4H8	000107-01-7	74
3	2-Butene, (Z)-	56	C4H8	000590-18-1	72
4	2-Butene, (E)-	56	C4H8	000624-64-6	72
5	1-Butene	56	C4H8	000106-98-9	58





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Data File : VN081501.D
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Operator : JC\MD
Sample : P1799-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
50298

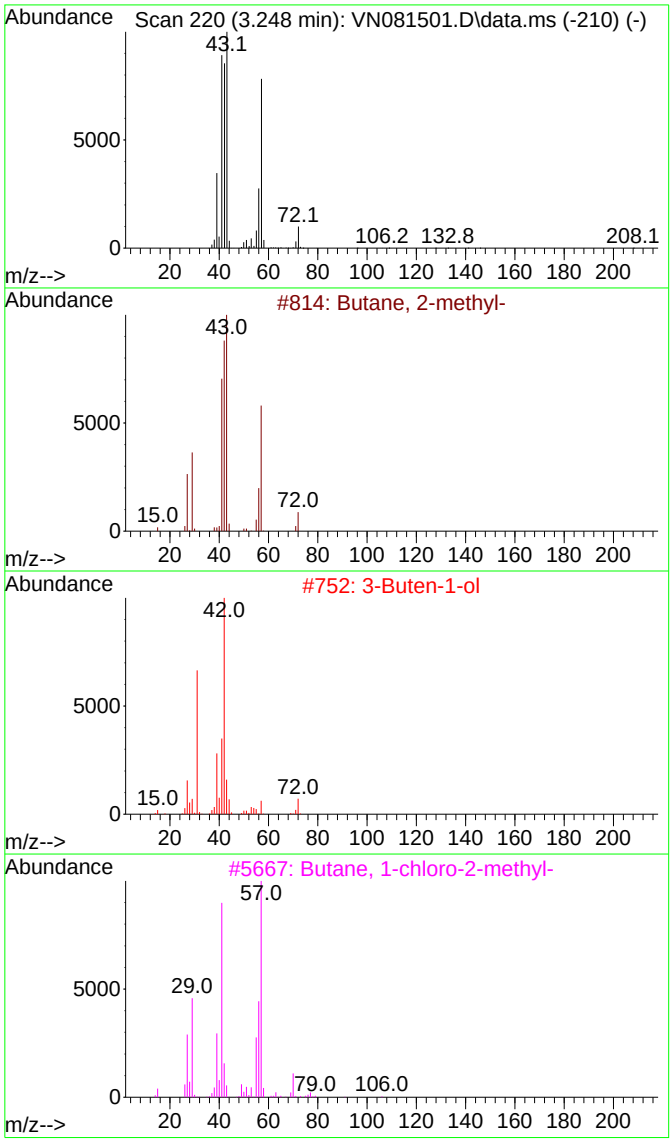
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

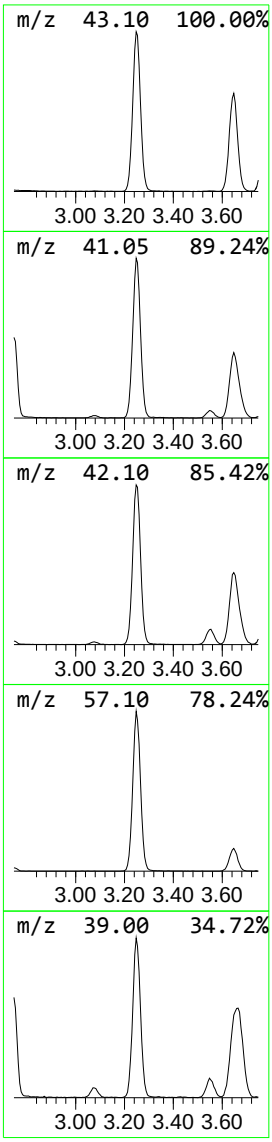
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.248	120.44 ug/l	7389380	Pentafluorobenzene	8.230

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	37
3	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	35
4	Oxirane, trimethyl-	86	C5H10O	005076-19-7	33
5	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
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Operator : JC\MD
Sample : P1799-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
50298

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

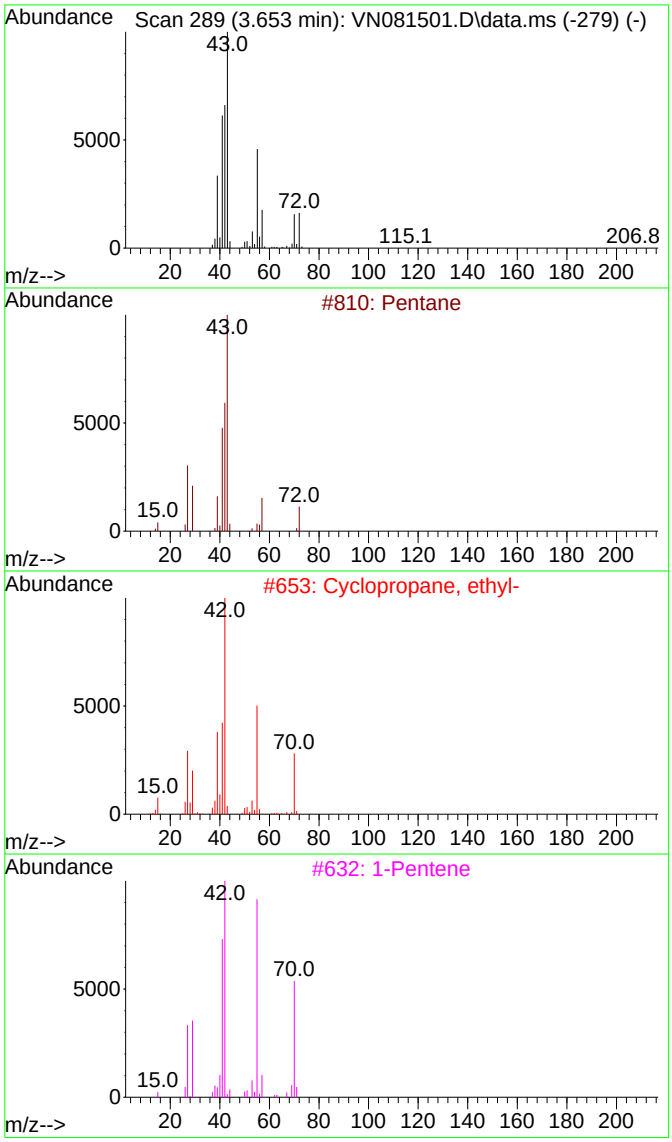
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

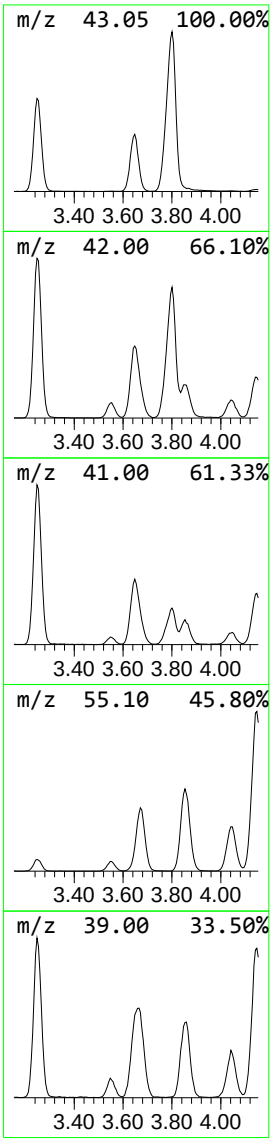
****

Peak Number 6 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.653	81.35 ug/l	4991210	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	64
2	Cyclopropane, ethyl-	70	C5H10	001191-96-4	49
3	1-Pentene	70	C5H10	000109-67-1	49
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	43
5	Cyclopentane	70	C5H10	000287-92-3	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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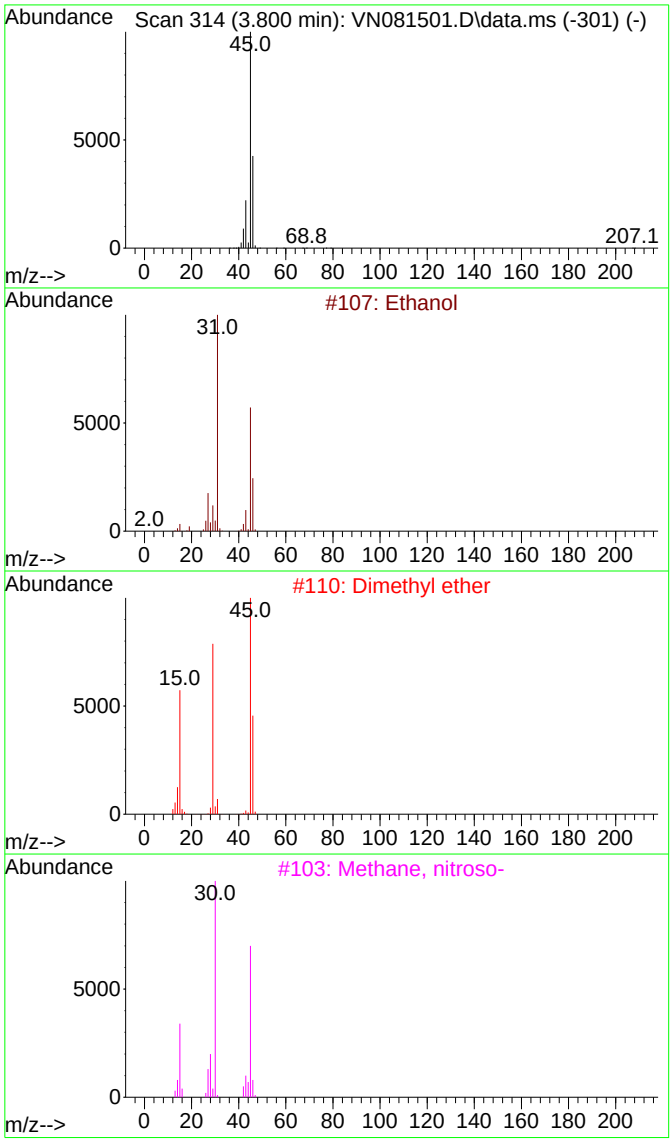
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

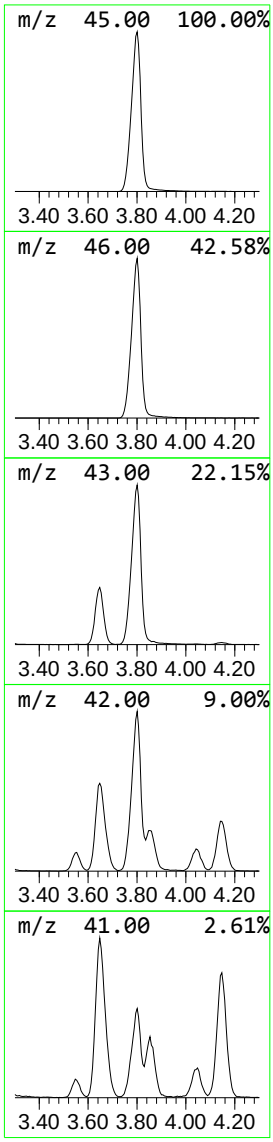
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.800	435.92 ug/l	26744800	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	83
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





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Instrument :
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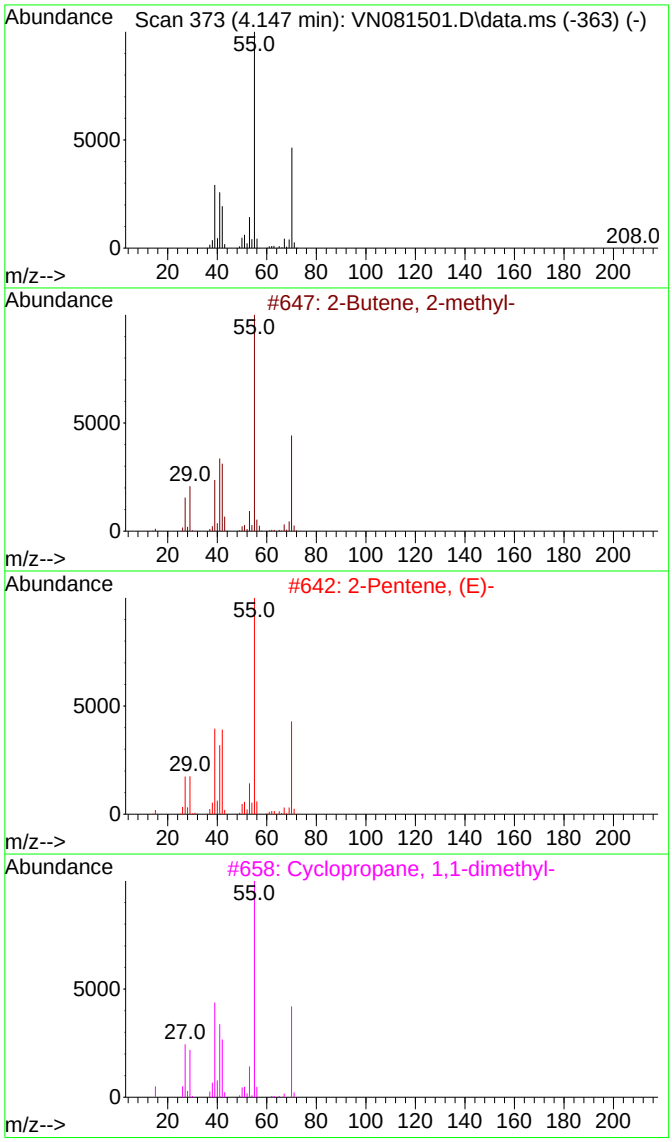
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

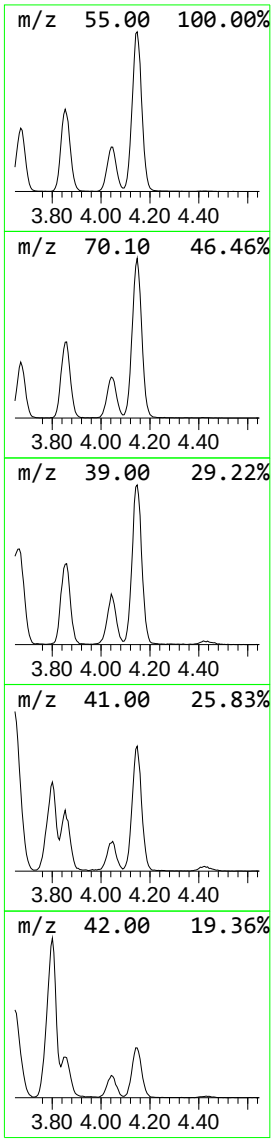
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Butene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.147	100.02 ug/l	6136600	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
2	2-Pentene, (E)-	70	C5H10	000646-04-8	86
3	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
4	1-Butene, 3-methyl-	70	C5H10	000563-45-1	72
5	2-Methyl-1-butene	70	C5H10	000563-46-2	72





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

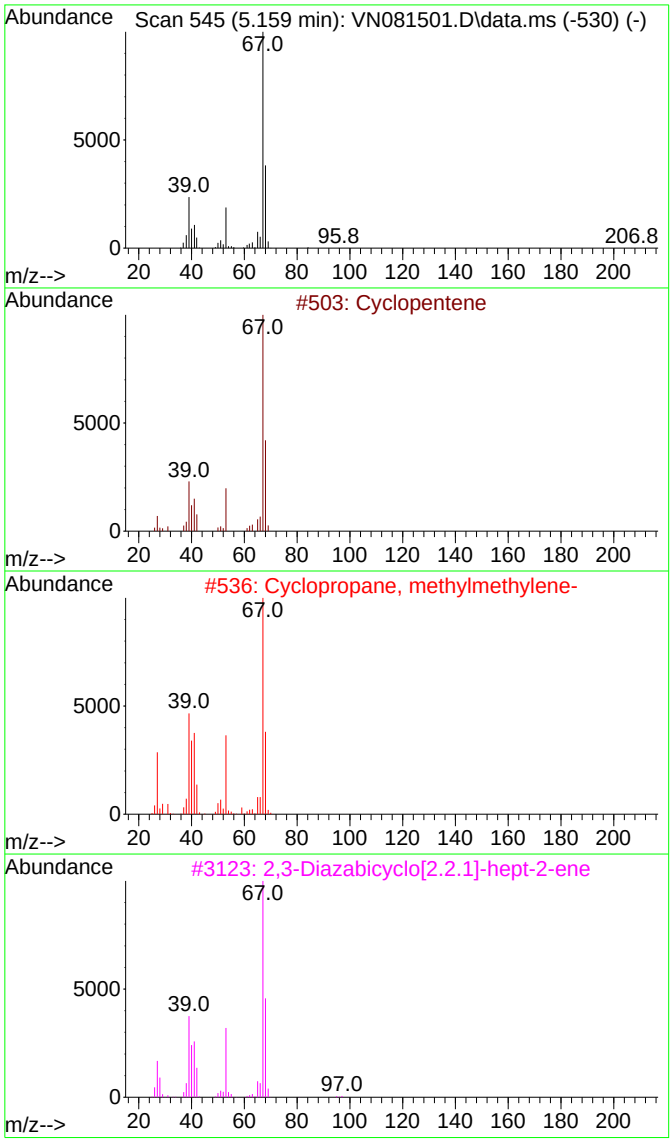
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

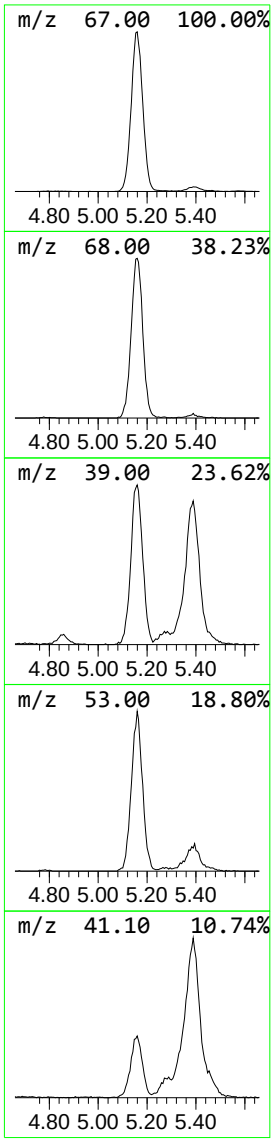
****

Peak Number 9 Cyclopentene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.159	42.57 ug/l	2611670	Pentafluorobenzene	8.230

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	2,3-Diazabicyclo[2.2.1]-hept-2-ene	96	C5H8N2	002721-32-6	78
4	Isoprene	68	C5H8	000078-79-5	59
5	1,4-Pentadiene	68	C5H8	000591-93-5	58





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
50298

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

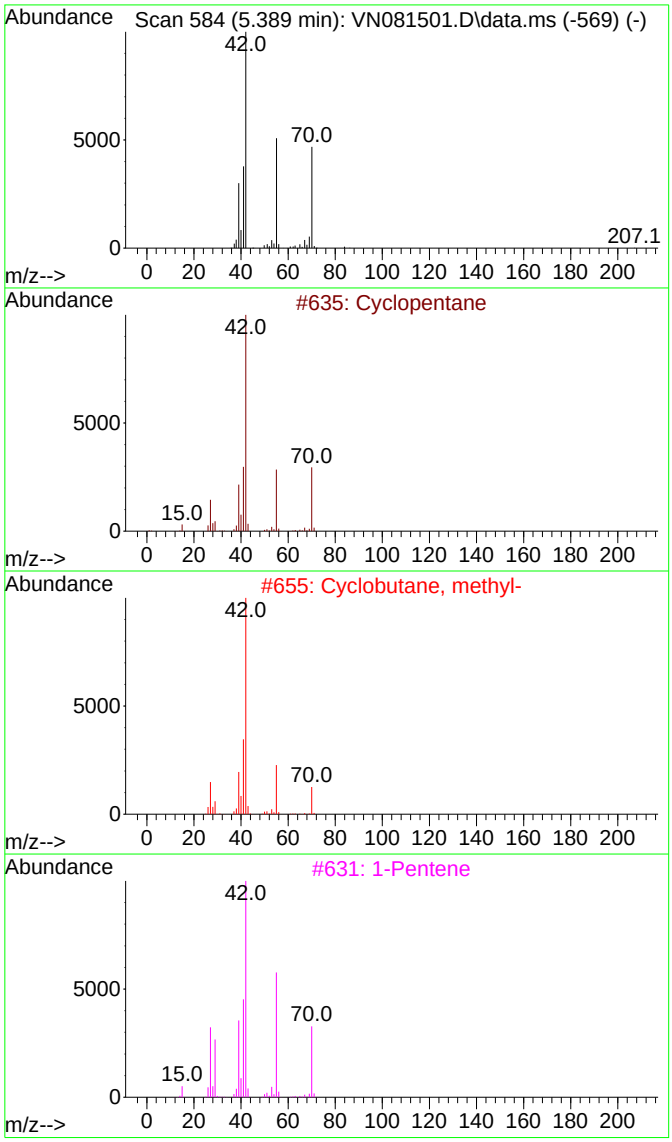
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

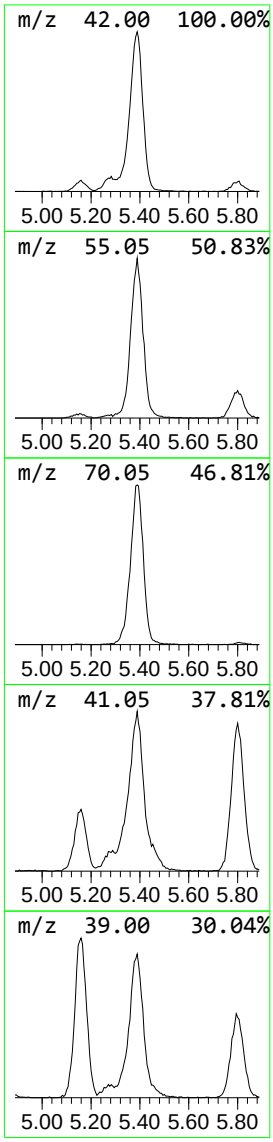
****

Peak Number 10 Cyclobutane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.389	51.53 ug/l	3161530	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	78
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
3	1-Pentene	70	C5H10	000109-67-1	56
4	2-Pentene, (Z)-	70	C5H10	000627-20-3	47
5	2-Pentene	70	C5H10	000109-68-2	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
Data File : VN081501.D
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Sample : P1799-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
50298

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.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	2.318	48.0	ug/l	2946640	1	8.230	3067620	50.0
Butane	2.512	344.9	ug/l	21163500	1	8.230	3067620	50.0
1-Propene, 2-me...	2.618	38.3	ug/l	2348070	1	8.230	3067620	50.0
Butane, 2-methyl-	3.248	120.4	ug/l	7389380	1	8.230	3067620	50.0
Pentane	3.653	81.3	ug/l	4991210	1	8.230	3067620	50.0
Ethanol	3.800	435.9	ug/l	26744800	1	8.230	3067620	50.0
2-Butene, 2-met...	4.147	100.0	ug/l	6136600	1	8.230	3067620	50.0
Cyclopentene	5.159	42.6	ug/l	2611670	1	8.230	3067620	50.0
Cyclobutane, me...	5.389	51.5	ug/l	3161530	1	8.230	3067620	50.0