LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN110223\
Data File : VN079827.D
Acq On : 03 Nov 2023 05:57
Operator : JC\MD
Sample : 05222-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FSND-MW-30-20231101

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\82N110123W.M
Title : SW846 8260

Signal : TIC: VN079827.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	16	22	30	rBV	505005	694011	44.20%	6.337%
2	2.289	51	57	58	rBV	38200	48007	3.06%	0.438%
3	2.318	59	62	78	rVB	65438	138571	8.82%	1.265%
4	2.483	83	90	92	rVV	215458	344272	21.92%	3.143%
5	2.512	92	95	107	rVV	321492	502172	31.98%	4.585%
6	2.618	108	113	119	rVB2	37136	62730	3.99%	0.573%
7	2.748	129	135	140	rVV	59272	97835	6.23%	0.893%
8	2.812	144	146	156	rVB3	14658	26767	1.70%	0.244%
9	3.065	183	189	198	rVB2	29696	63937	4.07%	0.584%
10	3.248	210	220	236	rVB2	81692	220071	14.01%	2.009%
11	3.553	262	272	279	rBV2	46609	111930	7.13%	1.022%
12	3.648	279	288	302	rVB4	86228	247639	15.77%	2.261%
13	3.859	317	324	334	rVB2	11922	29584	1.88%	0.270%
14	4.042	346	355	364	rBV3	16872	43185	2.75%	0.394%
15	5.159	530	545	556	rVB6	16277	63948	4.07%	0.584%
16	5.347	569	577	579	rBV5	7707	17710	1.13%	0.162%
17	5.812	646	656	667	rBV4	11751	37863	2.41%	0.346%
18	6.153	701	714	726	rVB6	14111	52583	3.35%	0.480%
19	6.924	833	845	854	rBV9	6920	25451	1.62%	0.232%
20	8.165	1047	1056	1061	rBV	234613	555769	35.39%	5.074%
21	8.224	1061	1066	1077	rVB	319175	716998	45.66%	6.546%
22	8.582	1117	1127	1137	rBV	243581	560684	35.71%	5.119%
23	9.106	1205	1216	1228	rBV	535257	1081171	68.85%	9.871%
24	9.353	1251	1258	1267	rVB3	39367	80132	5.10%	0.732%
25	10.571	1456	1465	1473	rBV	867901	1570314	100.00%	14.337%
26	11.865	1677	1685	1698	rBV	783601	1423562	90.65%	12.998%
27	12.853	1845	1853	1867	rBV	573741	984986	62.73%	8.993%
28	13.794	2006	2013	2026	rBV	683043	1150624	73.27%	10.506%

Sum of corrected areas: 10952506

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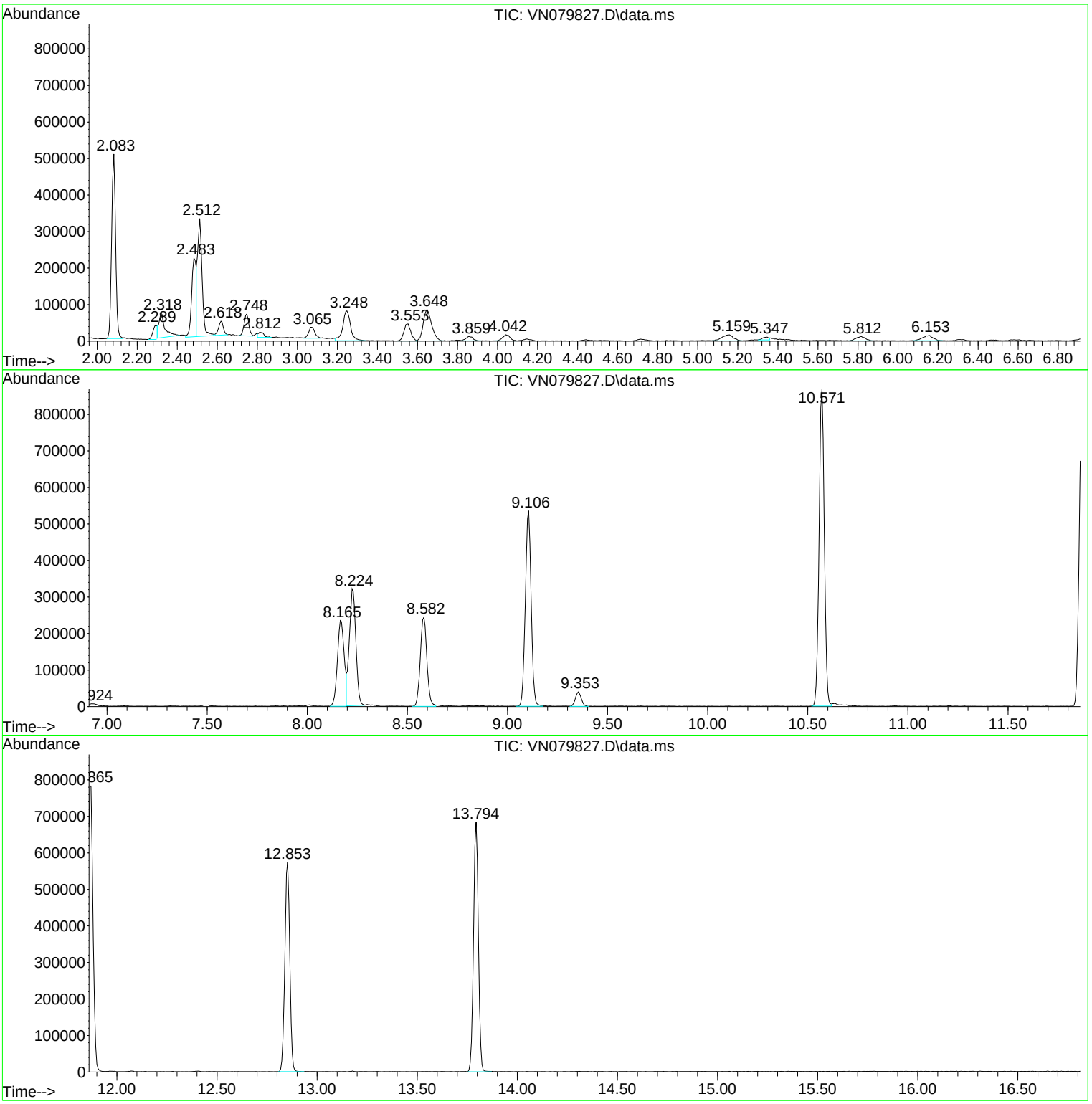
ClientSampleId :
FSND-MW-30-20231101

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

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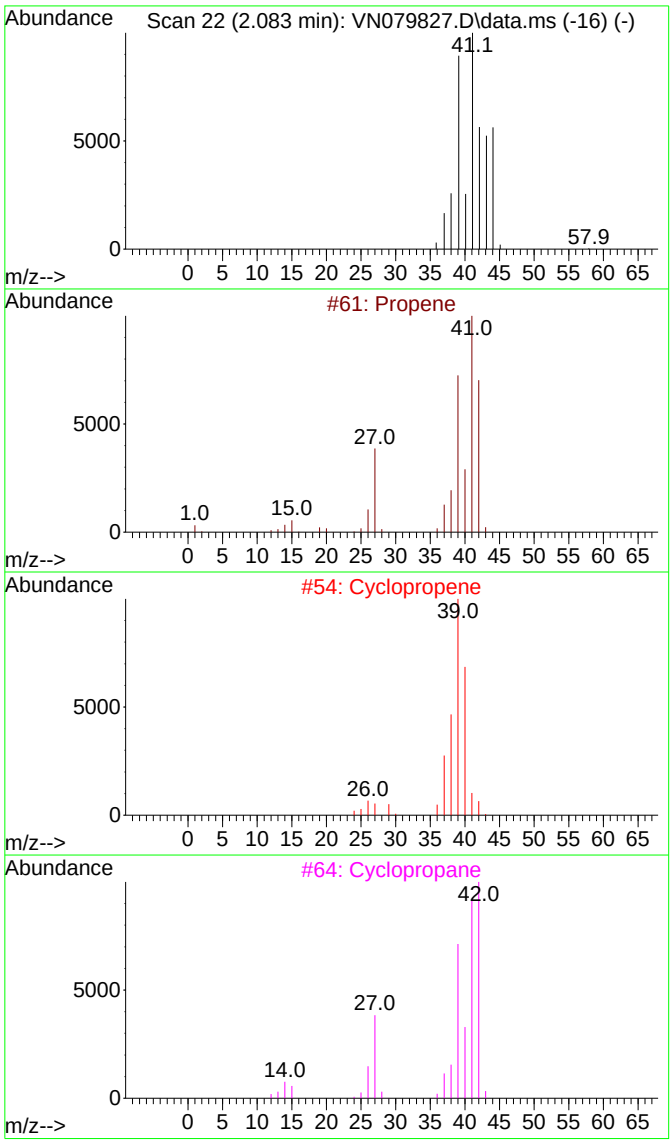
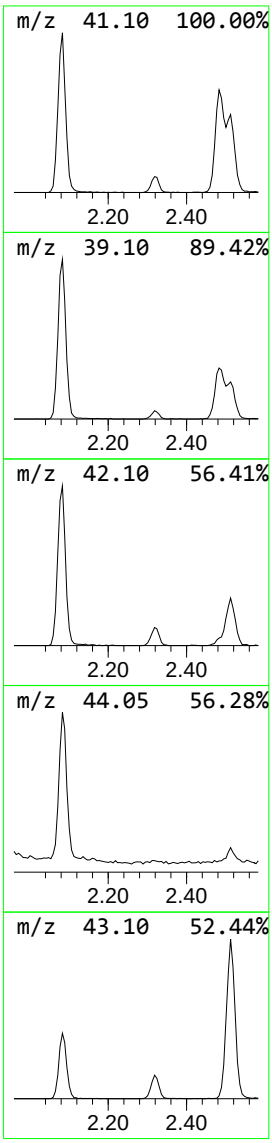
Peak Number 1 Propene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	48.40 ug/l	694011	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	86
2	Cyclopropene	40	C3H4	002781-85-3	5
3	Cyclopropane	42	C3H6	000075-19-4	4
4	Propane	44	C3H8	000074-98-6	4
5	Cyclobutylamine	71	C4H9N	002516-34-9	2





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ALS Vial : 48 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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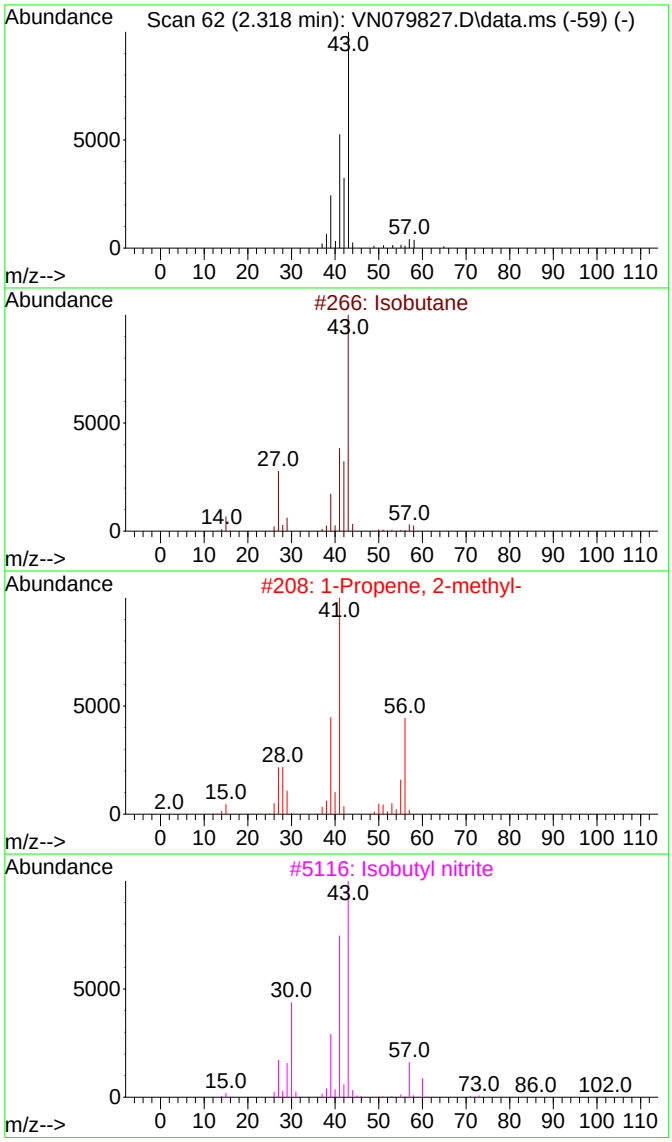
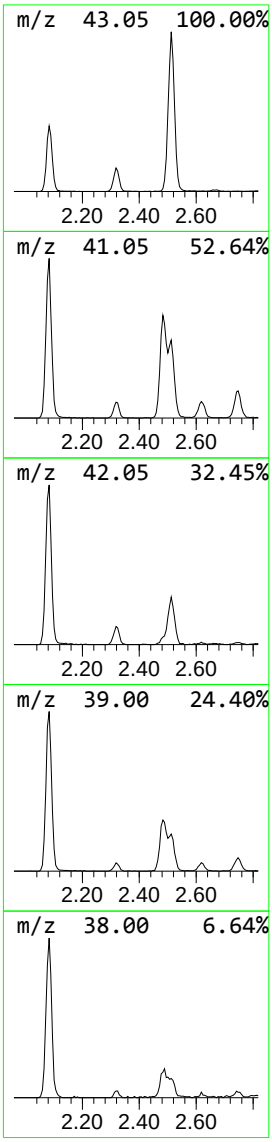
Peak Number 2 Isobutane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.318	9.66 ug/l	138571	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	64
2	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
3	Isobutyl nitrite	103	C4H9NO2	000542-56-3	9
4	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
5	Propene	42	C3H6	000115-07-1	7





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ClientSampleId :
FSND-MW-30-20231101

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

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

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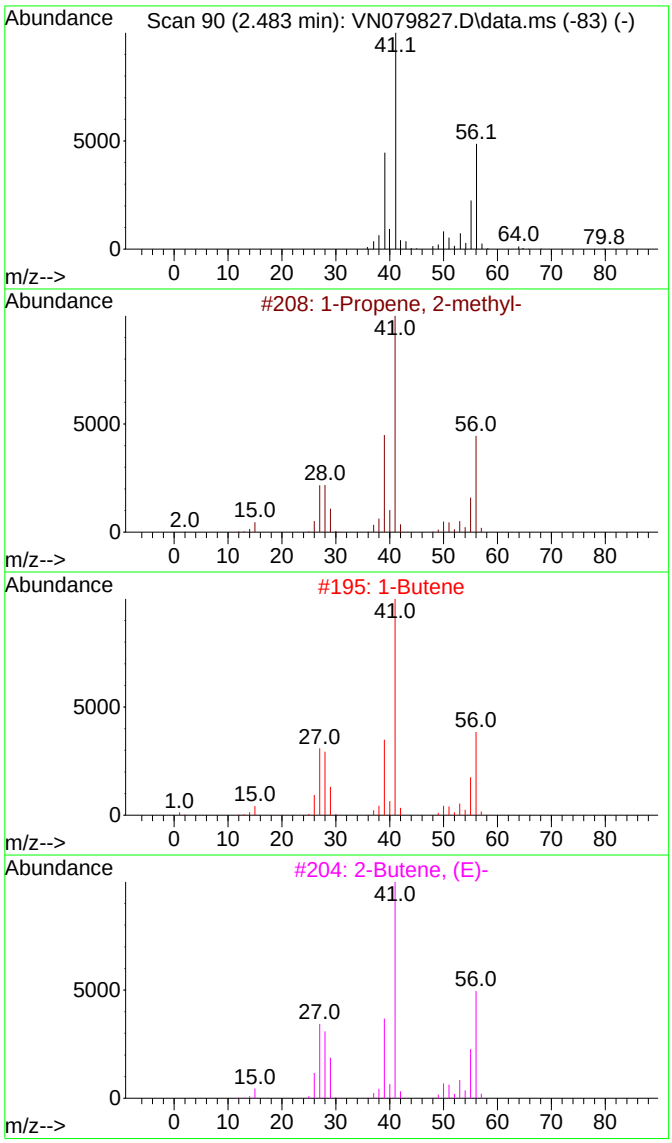
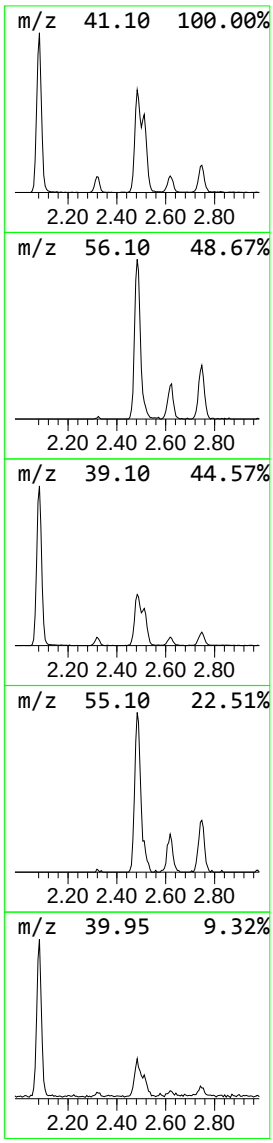
Peak Number 3 1-Propene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.483	24.01 ug/l	344272	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	90
2	1-Butene	56	C4H8	000106-98-9	87
3	2-Butene, (E)-	56	C4H8	000624-64-6	80
4	2-Butene, (Z)-	56	C4H8	000590-18-1	80
5	2-Butene	56	C4H8	000107-01-7	72





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Instrument :
MSVOA_N
ClientSampleId :
FSND-MW-30-20231101

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

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

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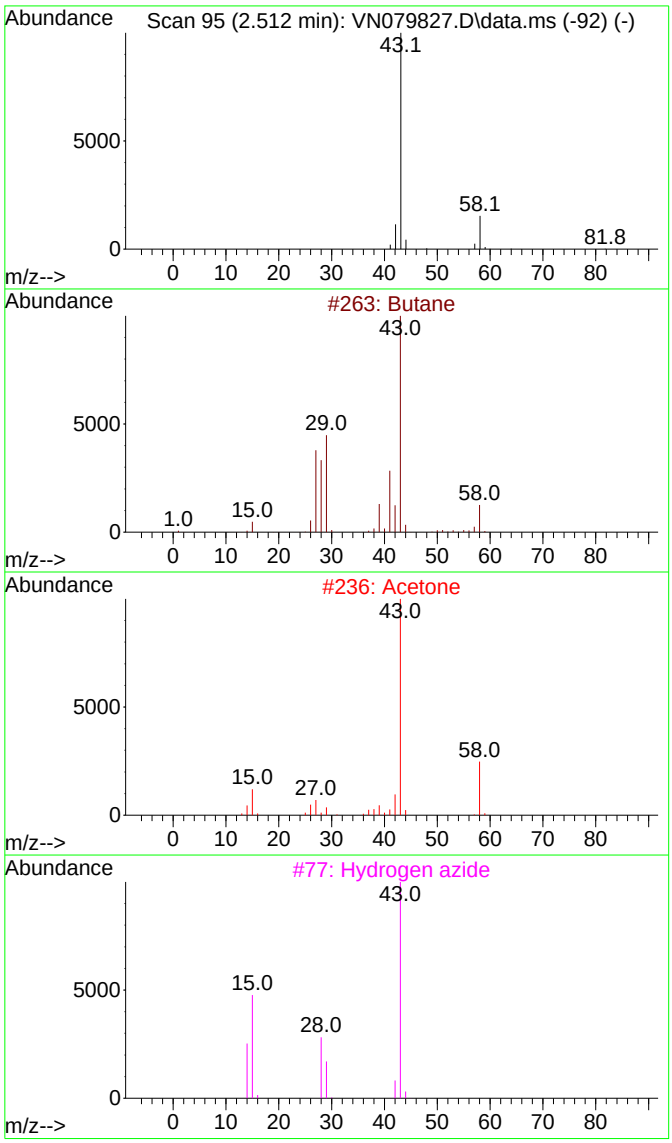
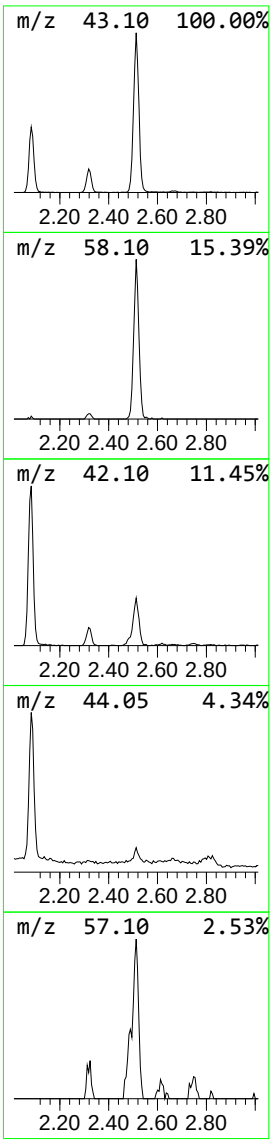
Peak Number 4 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.512	35.02 ug/l	502172	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	64
2	Acetone	58	C3H6O	000067-64-1	5
3	Hydrogen azide	43	HN3	007782-79-8	4
4	Diazene, dimethyl-	58	C2H6N2	000503-28-6	4
5	Propylene oxide	58	C3H6O	000075-56-9	3





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ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

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

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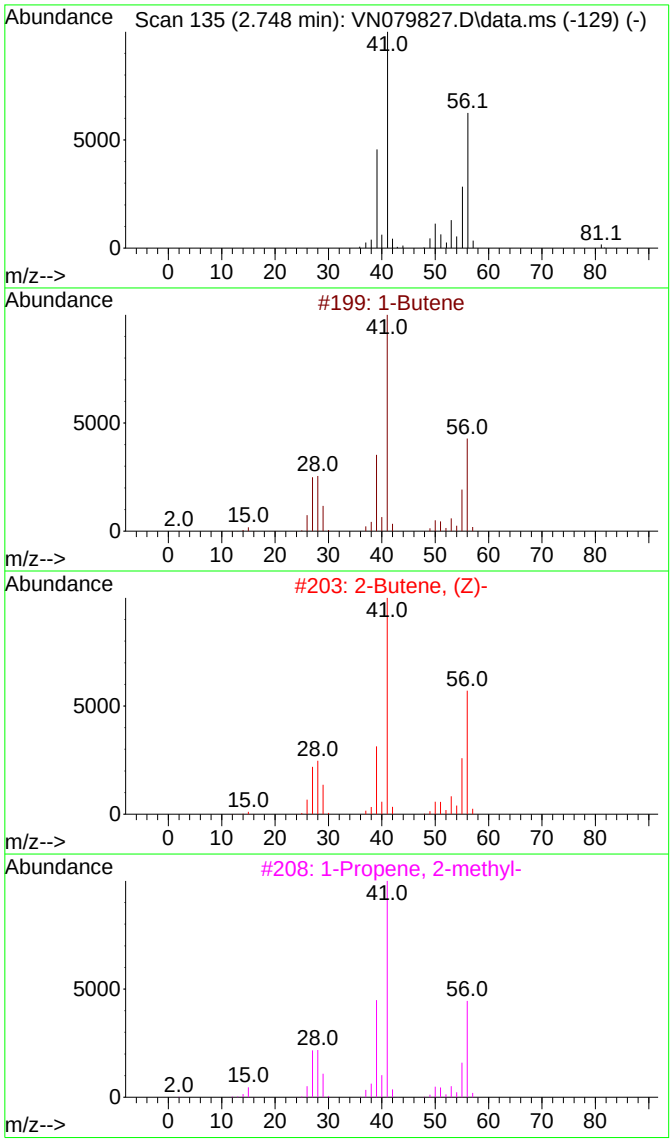
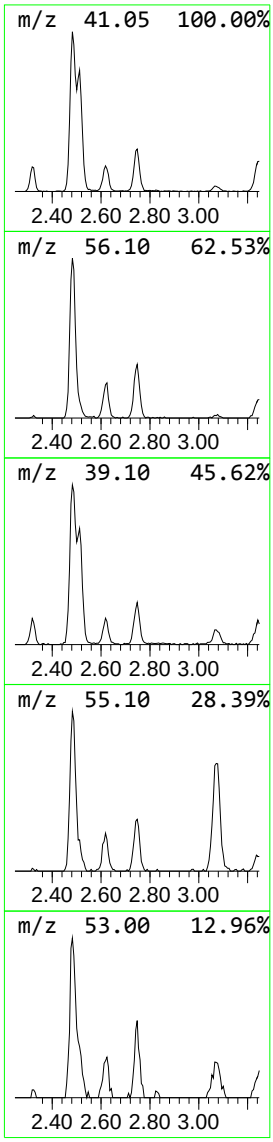
Peak Number 5 1-Butene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.748	6.82 ug/l	97835	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene	56	C4H8	000106-98-9	86
2	2-Butene, (Z)-	56	C4H8	000590-18-1	86
3	1-Propene, 2-methyl-	56	C4H8	000115-11-7	86
4	2-Butene	56	C4H8	000107-01-7	72
5	2-Butene, (E)-	56	C4H8	000624-64-6	72





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MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

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

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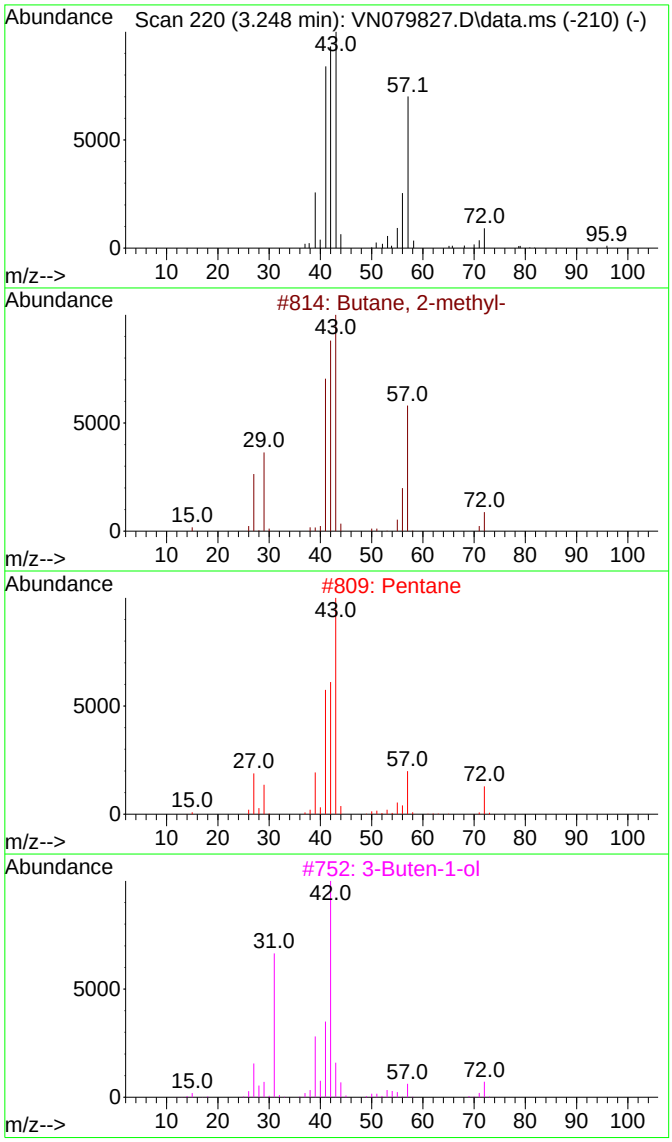
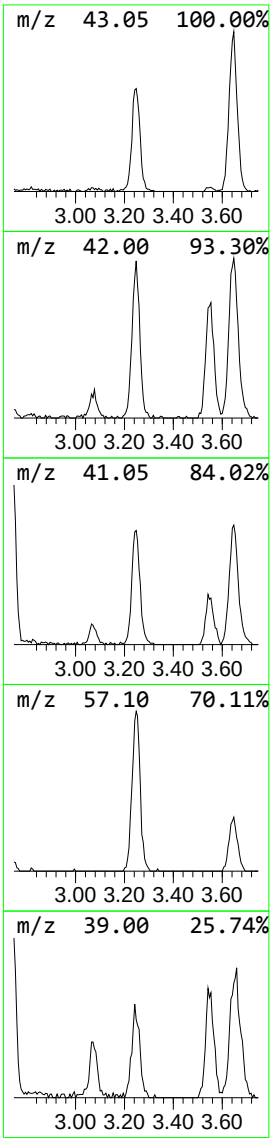
Peak Number 6 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.248	15.35 ug/l	220071	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Pentane	72	C5H12	000109-66-0	50
3	3-Buten-1-ol	72	C4H8O	000627-27-0	47
4	Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	33





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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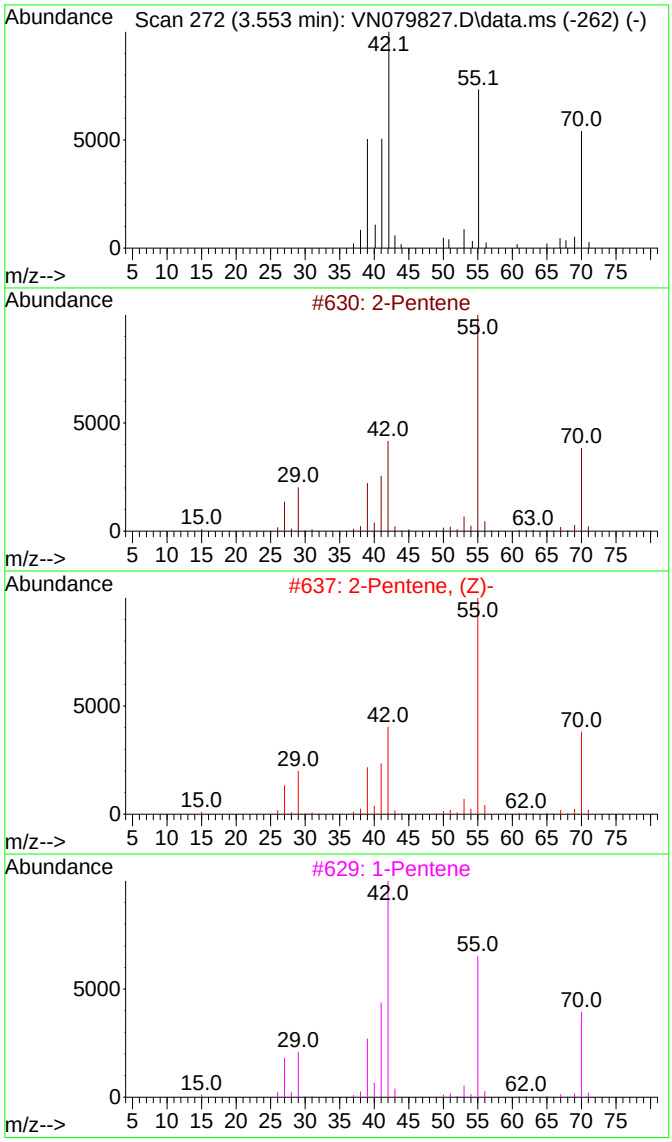
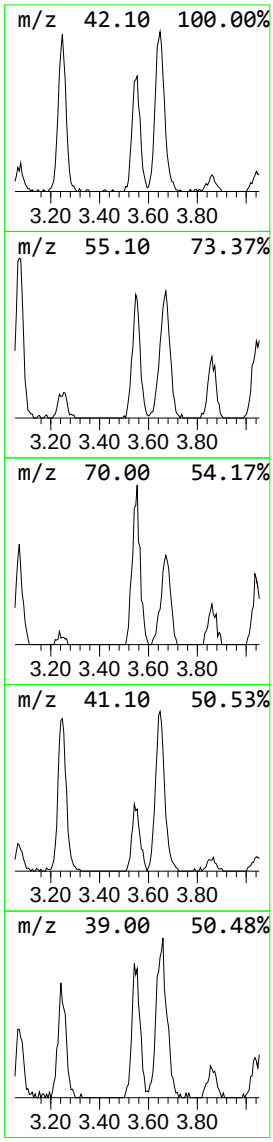
Peak Number 7 2-Pentene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.553	7.81 ug/l	111930	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene	70	C5H10	000109-68-2	80
2	2-Pentene, (Z)-	70	C5H10	000627-20-3	80
3	1-Pentene	70	C5H10	000109-67-1	64
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	64
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	64





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TIC Library : C:\Database\NIST20.L
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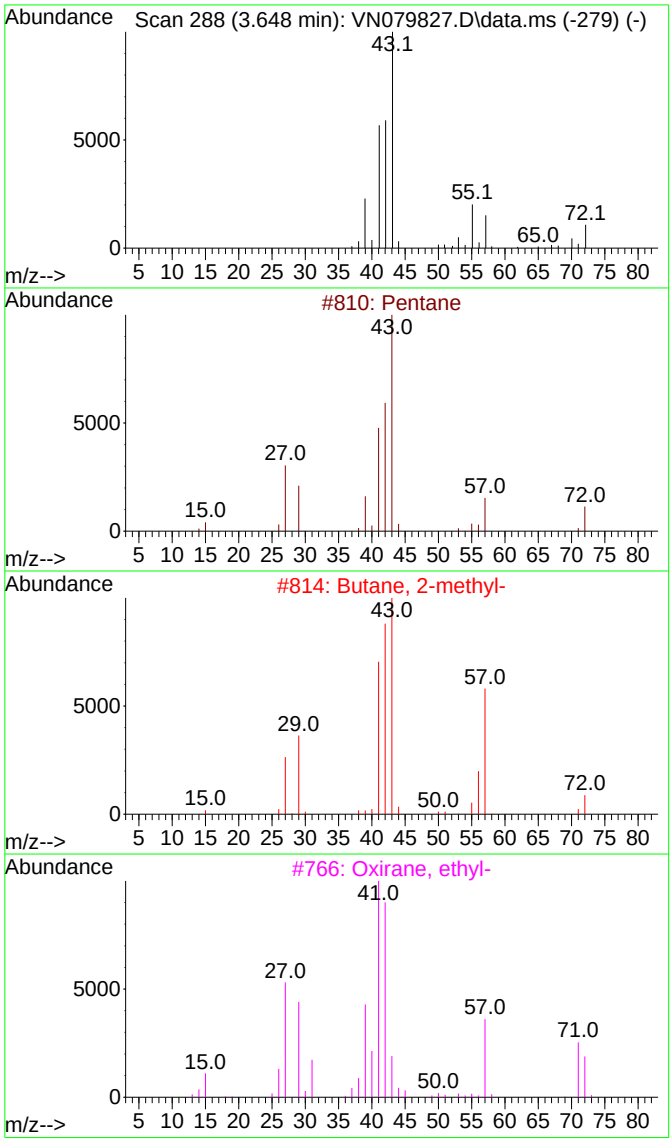
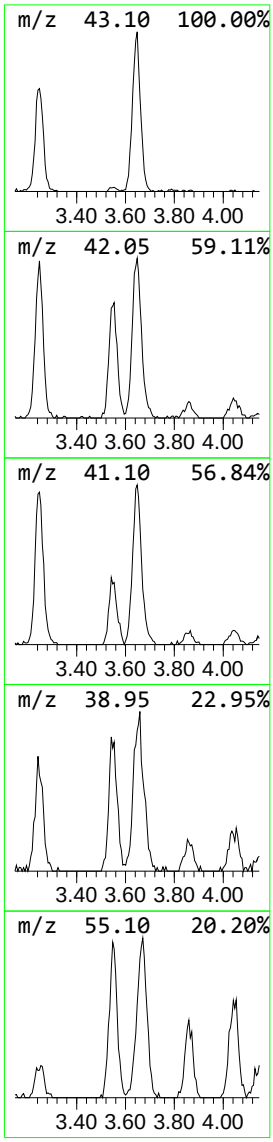
Peak Number 8 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.648	17.27 ug/l	247639	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	80
2	Butane, 2-methyl-	72	C5H12	000078-78-4	64
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	43
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	32
5	1-Pentene	70	C5H10	000109-67-1	23





Tentatively Identified Compound (LSC) summary

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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
Propene	2.083	48.4	ug/l	694011	1	8.224	716998	50.0
Isobutane	2.318	9.7	ug/l	138571	1	8.224	716998	50.0
1-Propene, 2-me...	2.483	24.0	ug/l	344272	1	8.224	716998	50.0
Butane	2.512	35.0	ug/l	502172	1	8.224	716998	50.0
1-Butene	2.748	6.8	ug/l	97835	1	8.224	716998	50.0
Butane, 2-methyl-	3.248	15.4	ug/l	220071	1	8.224	716998	50.0
2-Pentene	3.553	7.8	ug/l	111930	1	8.224	716998	50.0
Pentane	3.648	17.3	ug/l	247639	1	8.224	716998	50.0