LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074597.D
Acq On : 19 Sep 2022 19:44
Operator : JC\MD
Sample : N4566-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-GR

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\82N091522W.M
Title : SW846 8260

Signal : TIC: VN074597.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	% max.	% of total
1	2.228	47	58	78	rBV	4617190	7884289	1.12%	0.332%
2	2.399	78	87	99	rBV2	31415733	50436367	7.16%	2.125%
3	3.075	192	202	220	rBV	11159862	24867779	3.53%	1.048%
4	3.357	241	250	258	rBV	3889204	8814937	1.25%	0.371%
5	3.651	289	300	316	rBV	13007972	31324915	4.45%	1.320%
6	3.822	318	329	353	rVB	10049608	25584008	3.63%	1.078%
7	4.875	489	508	520	rBV	2519451	8554904	1.21%	0.360%
8	5.098	532	546	573	rVB	5523605	21329005	3.03%	0.899%
9	7.063	868	880	899	rVB	2939020	8634089	1.23%	0.364%
10	10.457	1448	1457	1458	rBV5	166113530	292021415	41.47%	12.306%
11	11.704	1659	1669	1676	rBV2	3961927	9293416	1.32%	0.392%
12	11.792	1676	1684	1694	rBV2	99404458	162299777	23.05%	6.839%
13	11.910	1694	1704	1716	rBV7	218780045	704208845	100.00%	29.675%
14	12.233	1749	1759	1767	rBV3	202672383	465013007	66.03%	19.595%
15	12.674	1825	1834	1845	rVB3	4378718	8008362	1.14%	0.337%
16	12.863	1858	1866	1871	rVV	4745303	7882788	1.12%	0.332%
17	12.927	1871	1877	1881	rVV2	63340084	102438055	14.55%	4.317%
18	12.963	1881	1883	1886	rVV	22208717	26291076	3.73%	1.108%
19	13.004	1886	1890	1909	rVB	28518969	42526313	6.04%	1.792%
20	13.163	1909	1917	1932	rBV	23069591	36651025	5.20%	1.544%
21	13.316	1932	1943	1950	rBV3	123024987	193711980	27.51%	8.163%
22	13.651	1988	2000	2008	rBV	30175764	51922749	7.37%	2.188%
23	13.821	2019	2029	2044	rVB2	22343689	43902424	6.23%	1.850%
24	14.868	2199	2207	2213	rBV3	3813966	7959925	1.13%	0.335%
25	15.439	2290	2304	2316	rVB	17322689	31534307	4.48%	1.329%

Sum of corrected areas: 2373095757

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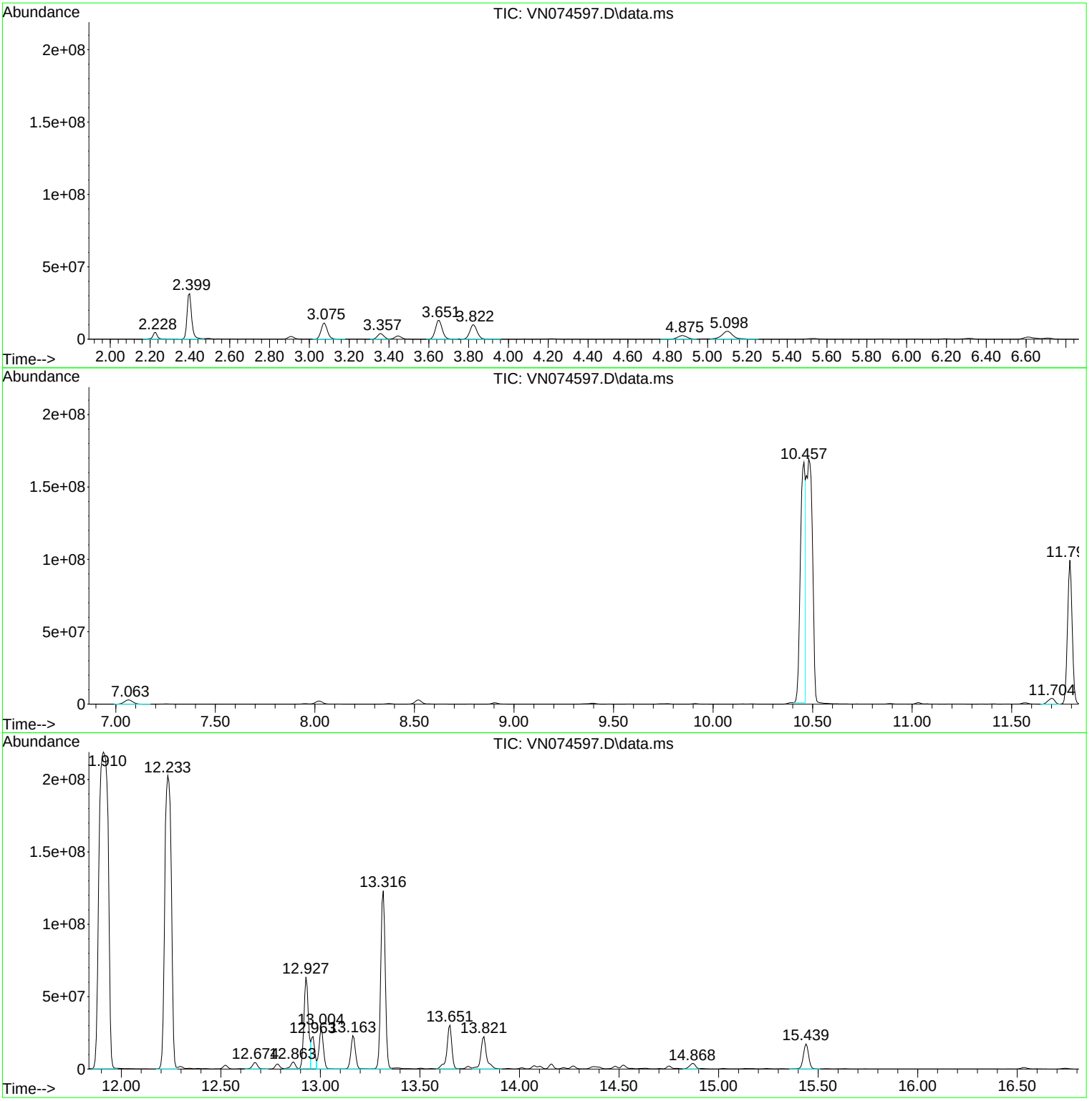
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



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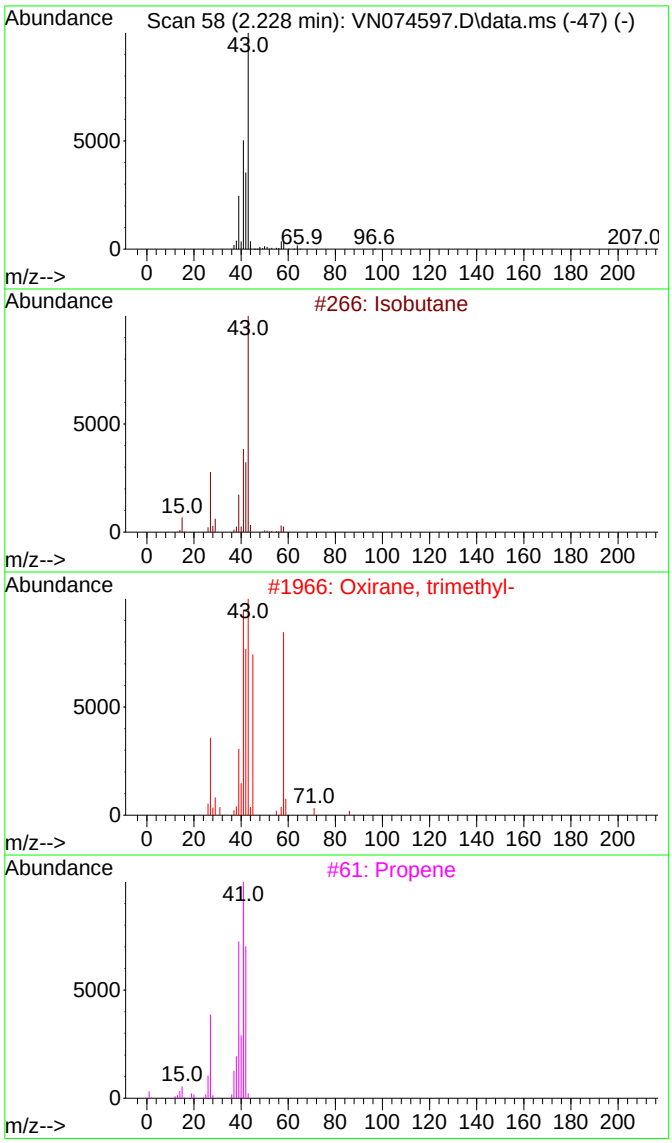
Quant Title : SW846 8260

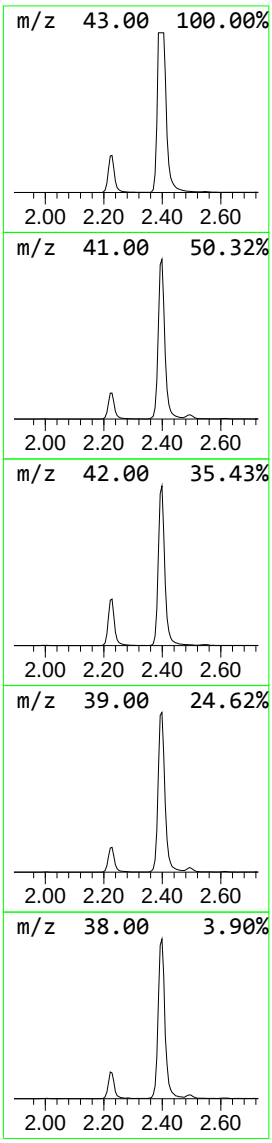
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Isobutane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	45.66 ug/l	7884290	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	72
2	Oxirane, trimethyl-	86	C5H10O	005076-19-7	9
3	Propene	42	C3H6	000115-07-1	5
4	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	4
5	Cyclobutylamine	71	C4H9N	002516-34-9	4





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Operator : JC\MD
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-GR

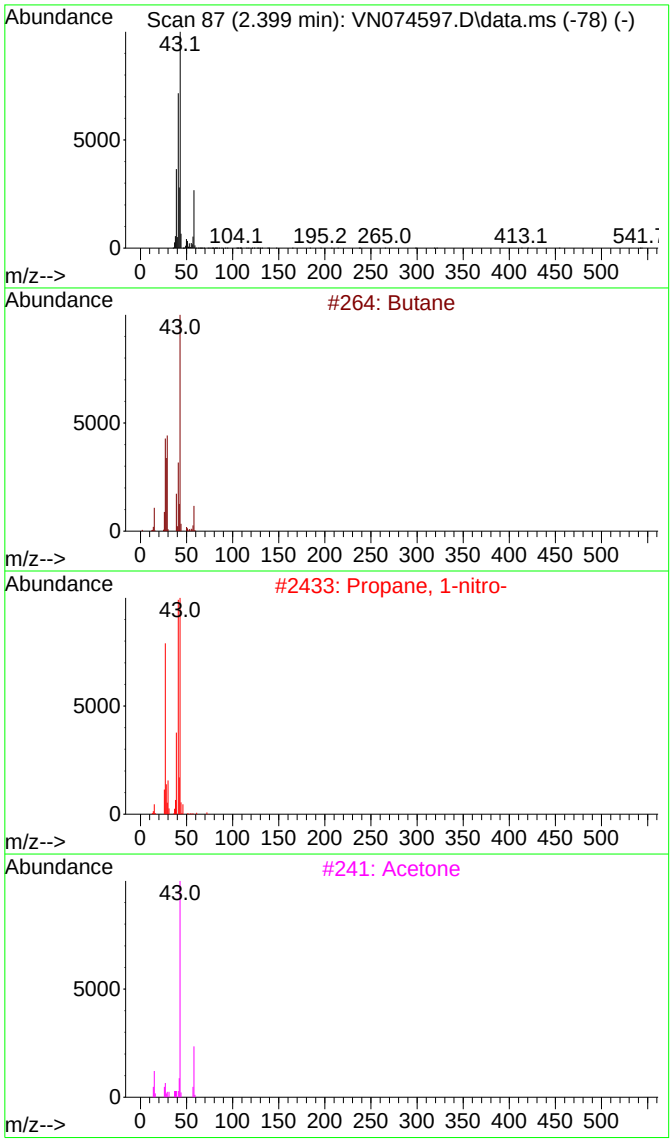
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

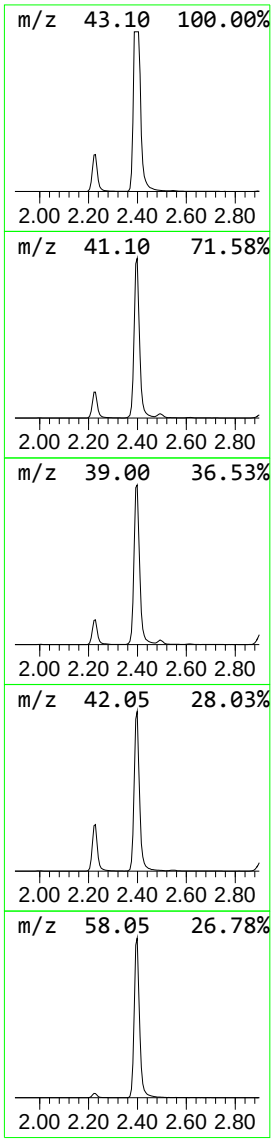
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.399	292.08 ug/l	50436400	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	50
2	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
3	Acetone	58	C3H6O	000067-64-1	7
4	Borane, trimethyl-	56	C3H9B	000593-90-8	5
5	Diazene, dimethyl-	58	C2H6N2	000503-28-6	5





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ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-GR

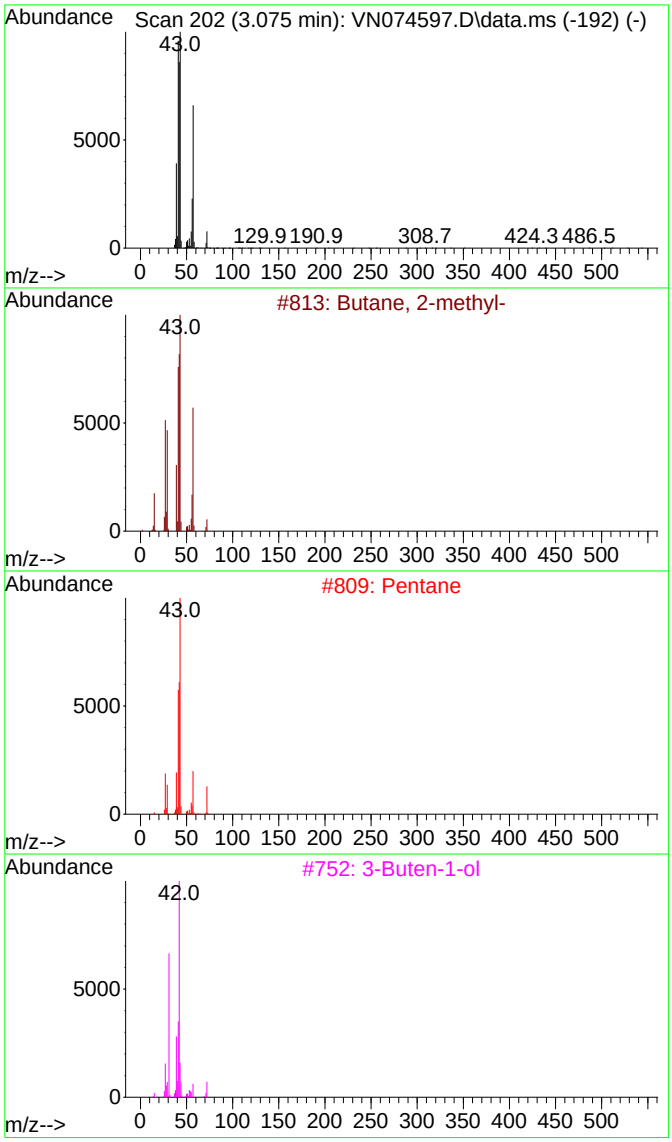
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

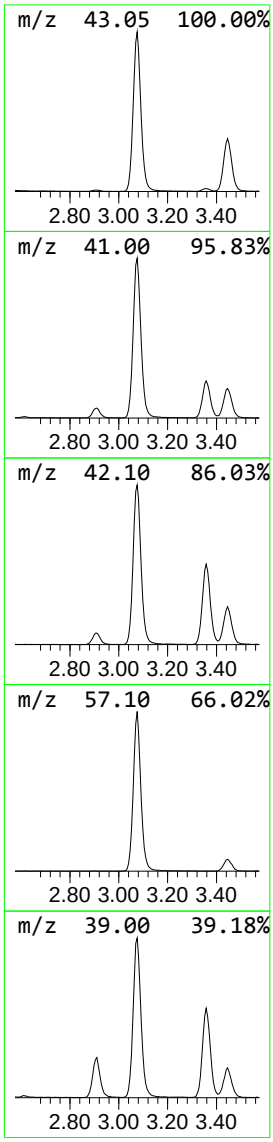
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.075	144.01 ug/l	24867800	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	64
2	Pentane	72	C5H12	000109-66-0	38
3	3-Buten-1-ol	72	C4H8O	000627-27-0	38
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10
5	1-Butene	56	C4H8	000106-98-9	9





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Instrument :
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ClientSampleId :
MW-GR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

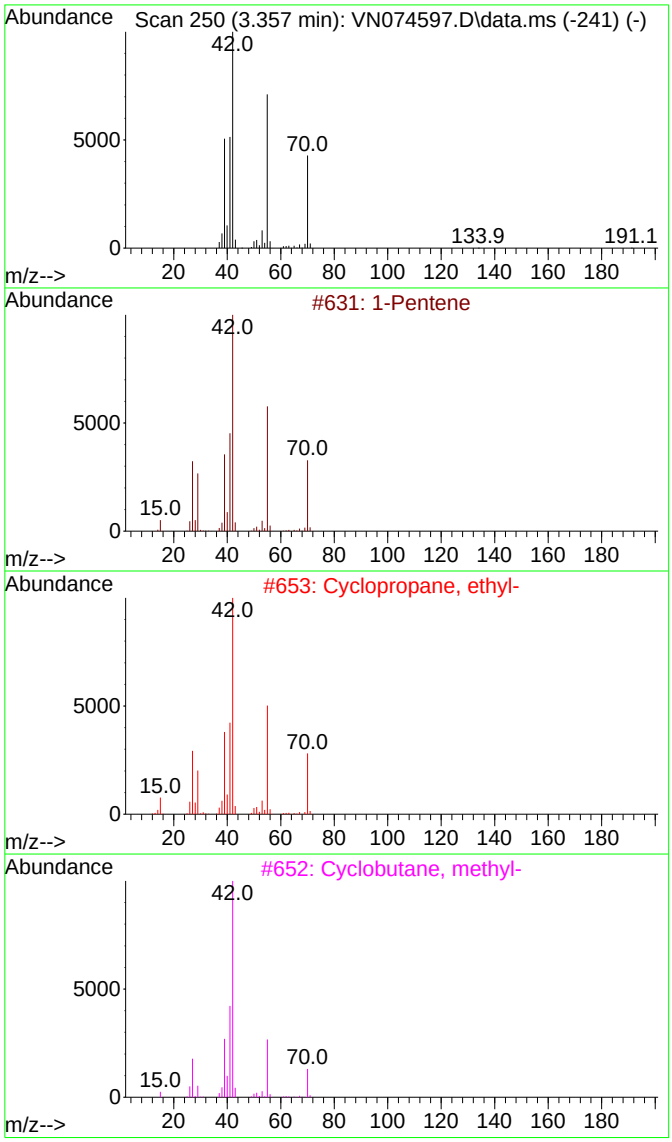
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

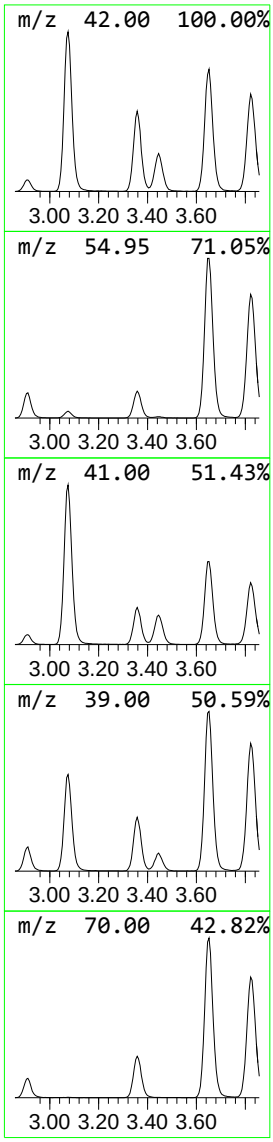
****

Peak Number 4 1-Pentene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.357	51.05 ug/l	8814940	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	76
2	Cyclopropane, ethyl-	70	C5H10	001191-96-4	68
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	64
4	Cyclopentane	70	C5H10	000287-92-3	52
5	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	43





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Operator : JC\MD
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-GR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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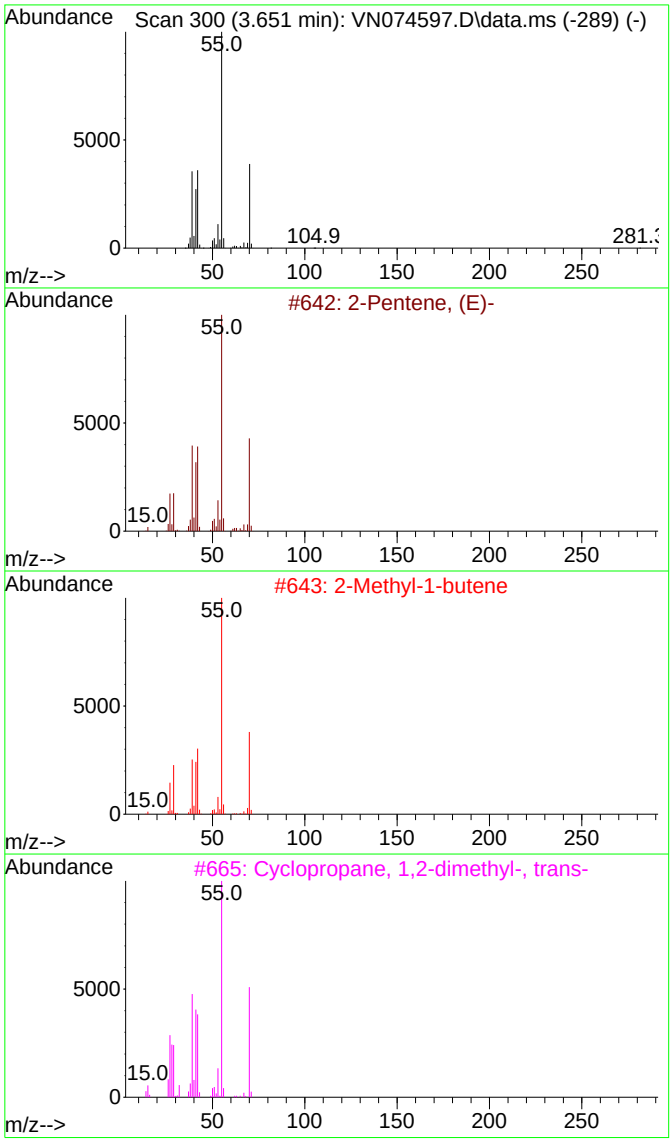
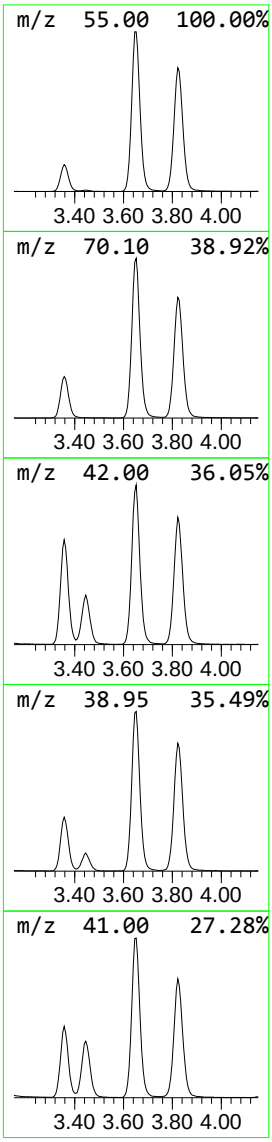
****
Peak Number 5 2-Pentene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.651	181.40 ug/l	31324900	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-	70	C5H10	000646-04-8	93
2	2-Methyl-1-butene	70	C5H10	000563-46-2	90
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	90
4	2-Pentene, (Z)-	70	C5H10	000627-20-3	90
5	2-Pentene	70	C5H10	000109-68-2	87





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ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-GR

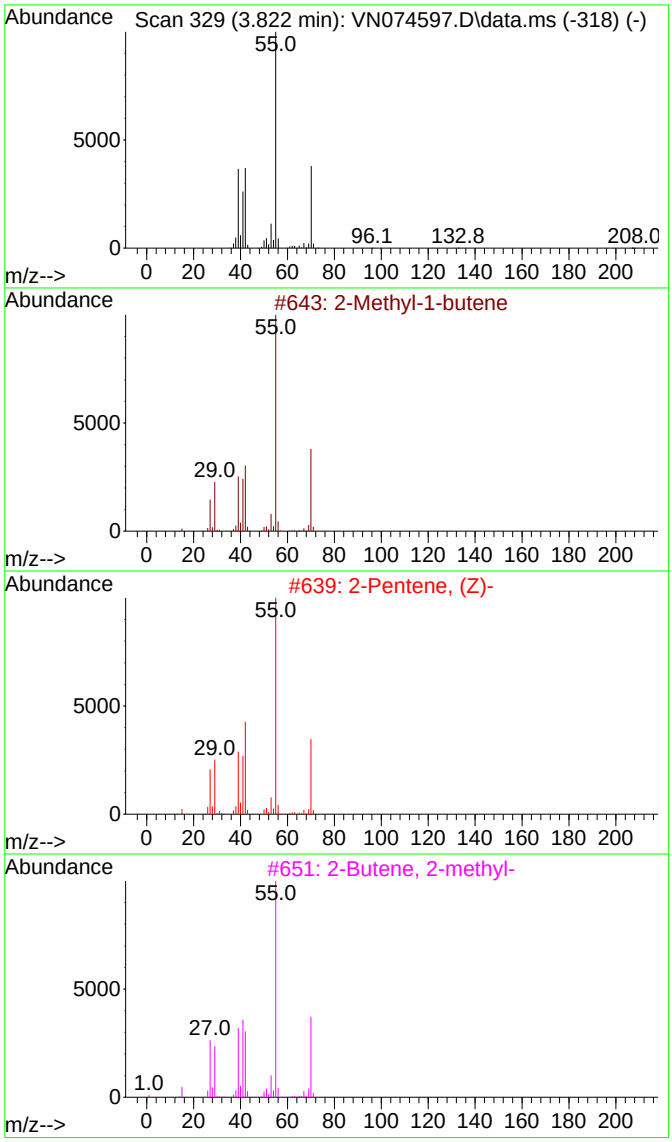
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

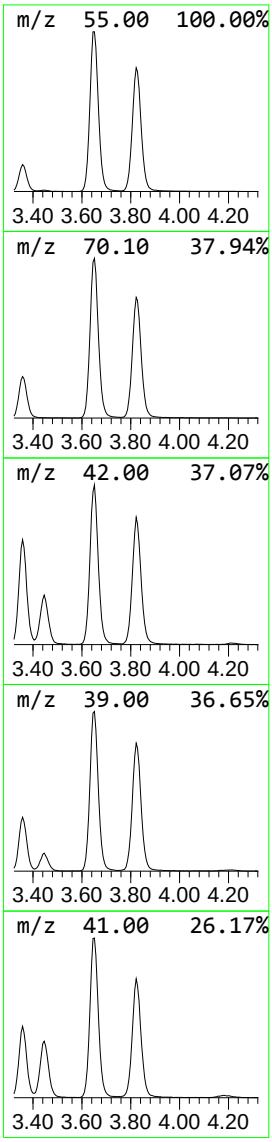
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Methyl-1-butene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.822	148.16 ug/l	25584000	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-1-butene	70	C5H10	000563-46-2	90
2	2-Pentene, (Z)-	70	C5H10	000627-20-3	90
3	2-Butene, 2-methyl-	70	C5H10	000513-35-9	87
4	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	87
5	2-Pentene	70	C5H10	000109-68-2	87





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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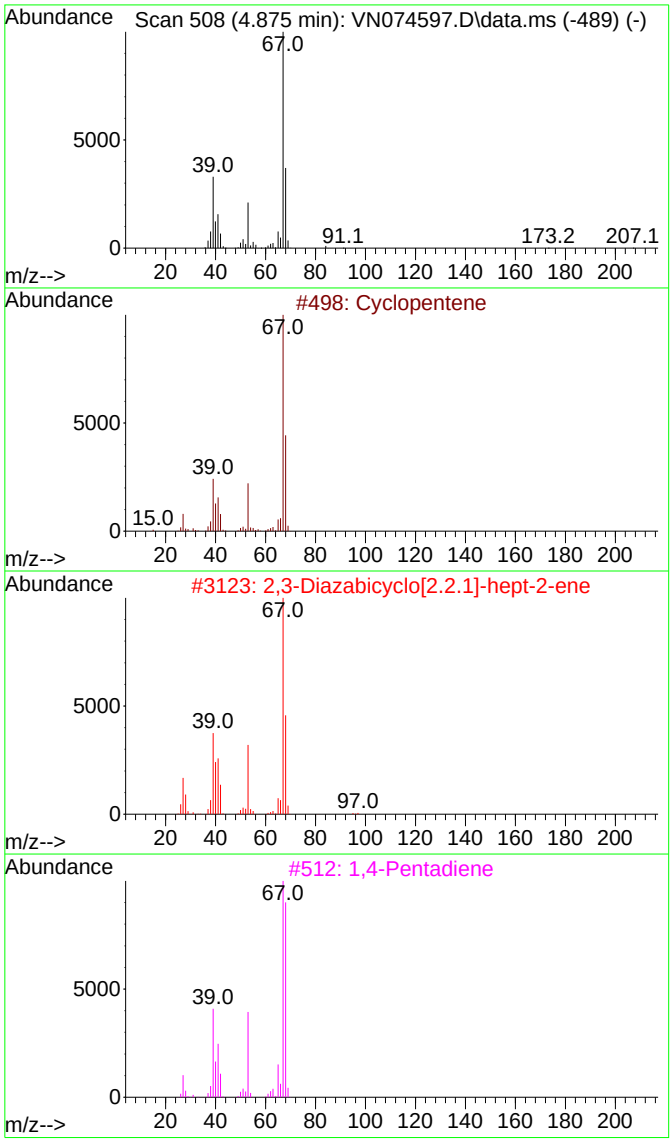
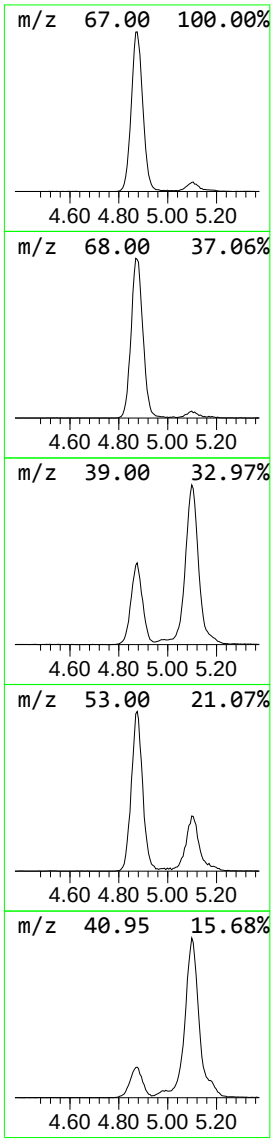
****

Peak Number 7 Cyclopentene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	49.54 ug/l	8554900	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene	68	C5H8	000142-29-0	91
2	2,3-Diazabicyclo[2.2.1]-hept-2-ene	96	C5H8N2	002721-32-6	64
3	1,4-Pentadiene	68	C5H8	000591-93-5	52
4	1,3-Pentadiene, (Z)-	68	C5H8	001574-41-0	50
5	1,3-Pentadiene, (E)-	68	C5H8	002004-70-8	50





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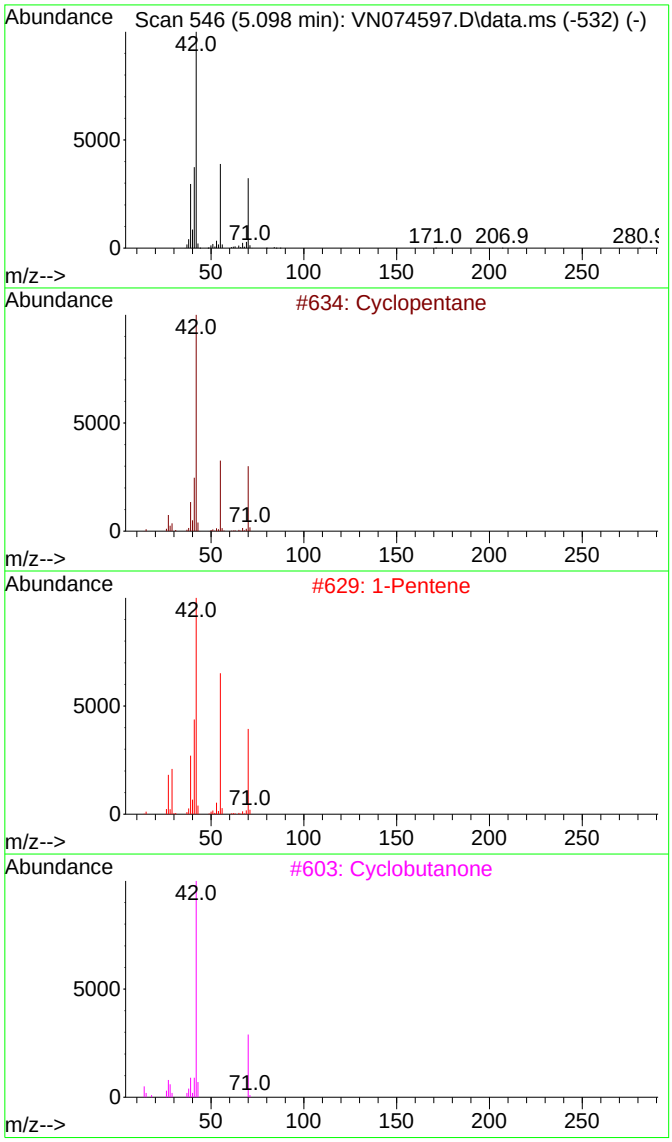
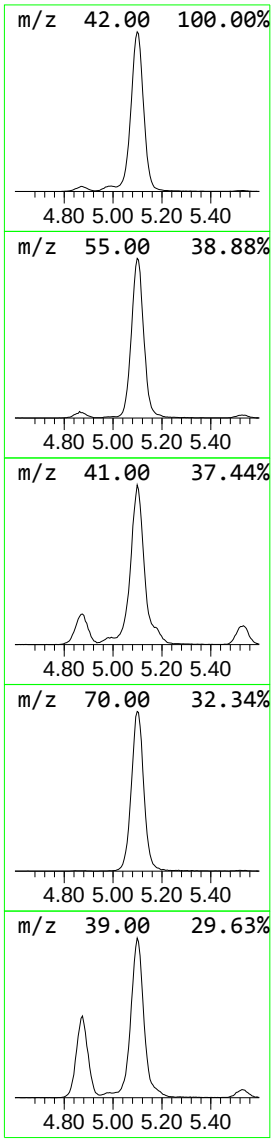
****

Peak Number 8 Cyclobutanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	123.52 ug/l	21329000	Pentafluorobenzene	8.016

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	Cyclobutanone	70	C4H6O	001191-95-3	56
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	45
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	23





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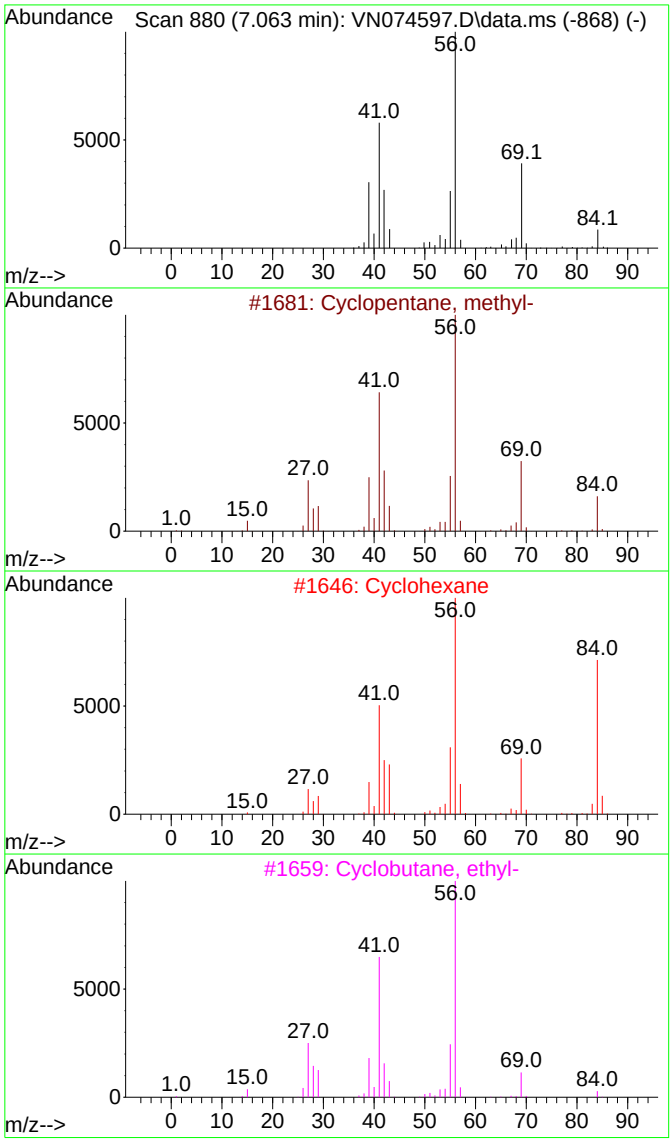
Quant Title : SW846 8260

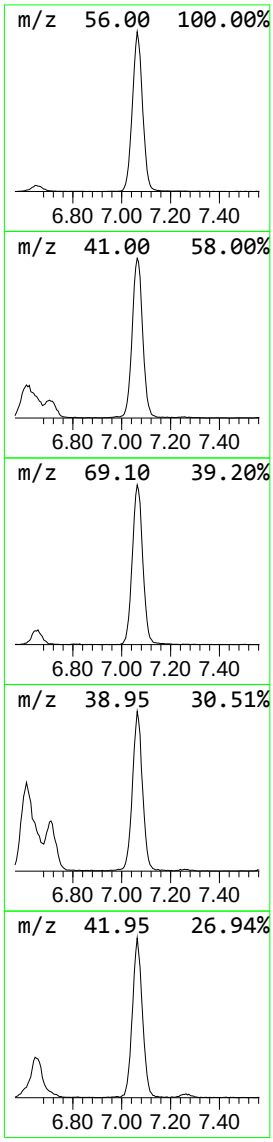
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.063	50.00 ug/l	8634090	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclohexane	84	C6H12	000110-82-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	Cyclobutane, butyl-	112	C8H16	013152-44-8	64
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56





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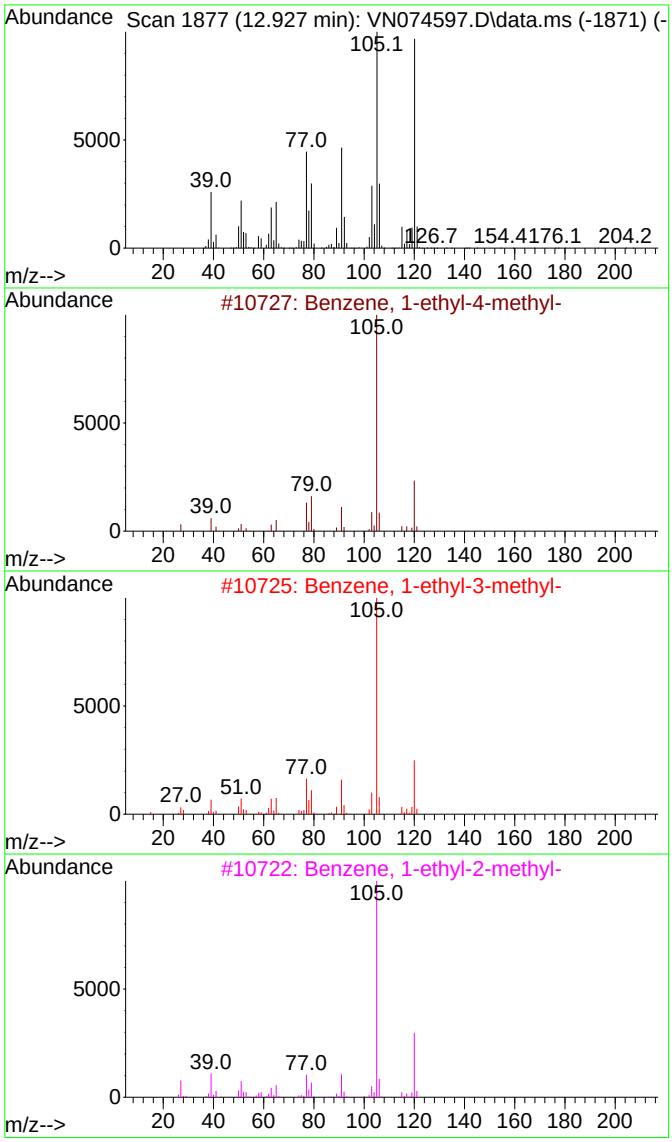
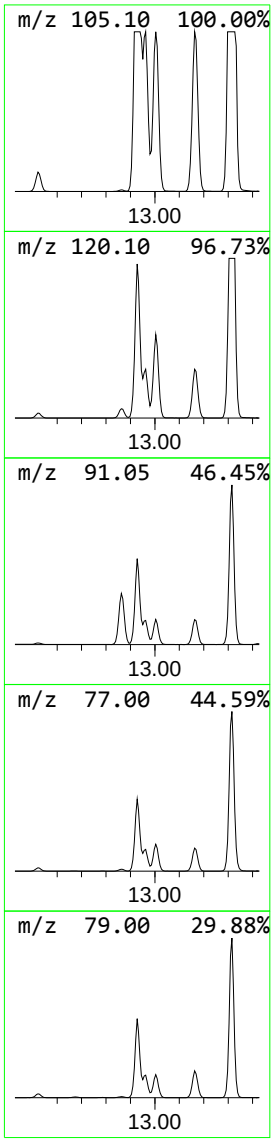
****
Peak Number 10 Benzene, 1-ethyl-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.927	98.64 ug/l	102438000	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	87
3	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87
4	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	64
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074597.D
Acq On : 19 Sep 2022 19:44
Operator : JC\MD
Sample : N4566-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-GR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.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	2.228	45.7	ug/l	7884290	1	8.016	8634090	50.0
Butane	2.399	292.1	ug/l	50436400	1	8.016	8634090	50.0
Butane, 2-methyl-	3.075	144.0	ug/l	24867800	1	8.016	8634090	50.0
1-Pentene	3.357	51.0	ug/l	8814940	1	8.016	8634090	50.0
2-Pentene, (E)-	3.651	181.4	ug/l	31324900	1	8.016	8634090	50.0
2-Methyl-1-butene	3.822	148.2	ug/l	25584000	1	8.016	8634090	50.0
Cyclopentene	4.875	49.5	ug/l	8554900	1	8.016	8634090	50.0
Cyclobutanone	5.098	123.5	ug/l	21329000	1	8.016	8634090	50.0
Cyclopentane, m...	7.063	50.0	ug/l	8634090	1	8.016	8634090	50.0
Benzene, 1-ethy...	12.927	98.6	ug/l	102438000	4	13.616	51922700	50.0