LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111819\
Data File : VU035748.D
Acq On : 18 Nov 2019 17:10
Operator : JC/SP
Sample : K5911-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAQK7

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\METHOD\SOMUTR110419WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.372	3	10	28	rVB	828413	841675	38.36%	6.749%
2	1.459	31	37	42	rBV	26713	27504	1.25%	0.221%
3	1.507	44	52	58	rBV	73764	82390	3.75%	0.661%
4	1.617	75	86	95	rBV3	381534	644085	29.35%	5.164%
5	1.752	121	128	151	rVB3	55115	79218	3.61%	0.635%
6	1.935	176	185	201	rVB	121672	172451	7.86%	1.383%
7	2.015	202	210	222	rVB	69324	94880	4.32%	0.761%
8	2.179	252	261	268	rBV	67037	92888	4.23%	0.745%
9	2.231	269	277	298	rVB3	74181	156435	7.13%	1.254%
10	2.443	336	343	352	rVB	25474	38464	1.75%	0.308%
11	2.597	380	391	405	rBV	186602	311720	14.21%	2.499%
12	2.822	453	461	473	rBV	22502	38174	1.74%	0.306%
13	3.362	613	629	658	rBV	79352	194908	8.88%	1.563%
14	3.623	697	710	729	rVB6	17358	44566	2.03%	0.357%
15	4.700	1030	1045	1066	rBV	145141	380801	17.35%	3.053%
16	5.115	1157	1174	1197	rBV2	159176	388827	17.72%	3.118%
17	5.771	1358	1378	1405	rBV2	340275	915246	41.71%	7.339%
18	6.295	1526	1541	1562	rBV	231068	476608	21.72%	3.822%
19	6.735	1664	1678	1697	rBV2	213253	432645	19.72%	3.469%
20	7.603	1933	1948	1967	rBV	94659	183509	8.36%	1.471%
21	7.935	2032	2051	2065	rBV	347785	640455	29.19%	5.135%
22	8.005	2066	2073	2085	rVV	48733	95609	4.36%	0.767%
23	8.073	2087	2094	2107	rVV5	20014	36232	1.65%	0.291%
24	8.160	2110	2121	2129	rVV3	39007	66941	3.05%	0.537%
25	8.218	2130	2139	2164	rVB2	54942	110616	5.04%	0.887%
26	8.697	2267	2288	2319	rBV2	303241	981506	44.73%	7.870%
27	8.835	2321	2331	2367	rVB2	125705	322727	14.71%	2.588%
28	9.452	2503	2523	2549	rBV	331524	681221	31.05%	5.462%
29	9.603	2562	2570	2578	rVB2	15260	25681	1.17%	0.206%
30	9.722	2597	2607	2620	rBV2	16695	32062	1.46%	0.257%
31	10.388	2801	2814	2837	rBV3	41250	86431	3.94%	0.693%
32	10.790	2926	2939	2961	rVB	177575	319572	14.56%	2.562%
33	11.722	3217	3229	3244	rBV3	75839	132692	6.05%	1.064%
34	11.841	3254	3266	3285	rVB	320830	596394	27.18%	4.782%

LSC Area Percent Report

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Data File : VU035748.D
Acq On : 18 Nov 2019 17:10
Operator : JC/SP
Sample : K5911-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAQK7

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\METHOD\SOMUTR110419WMA.M
Title : TRACE VOA SOM01.0

35	12.224	3370	3385	3403	rBV	303654	552162	25.16%	4.427%
36	12.918	3587	3601	3635	rBV	1479055	2194246	100.00%	17.594%

Sum of corrected areas: 12471541

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111819\
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Acq On : 18 Nov 2019 17:10
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ALS Vial : 19 Sample Multiplier: 1

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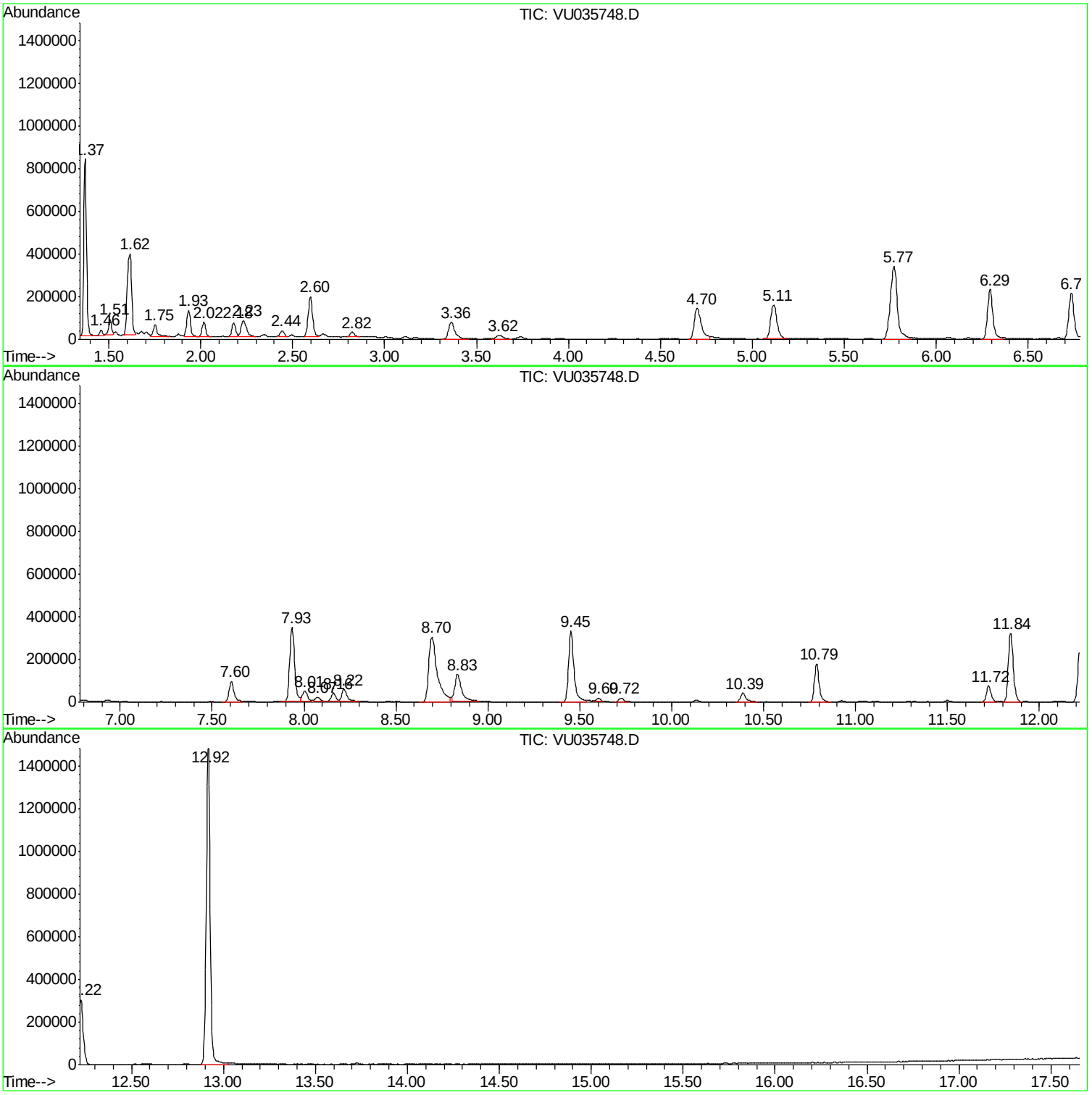
ClientSampleId : GAQK7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111819\
Data File : VU035748.D
Acq On : 18 Nov 2019 17:10
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

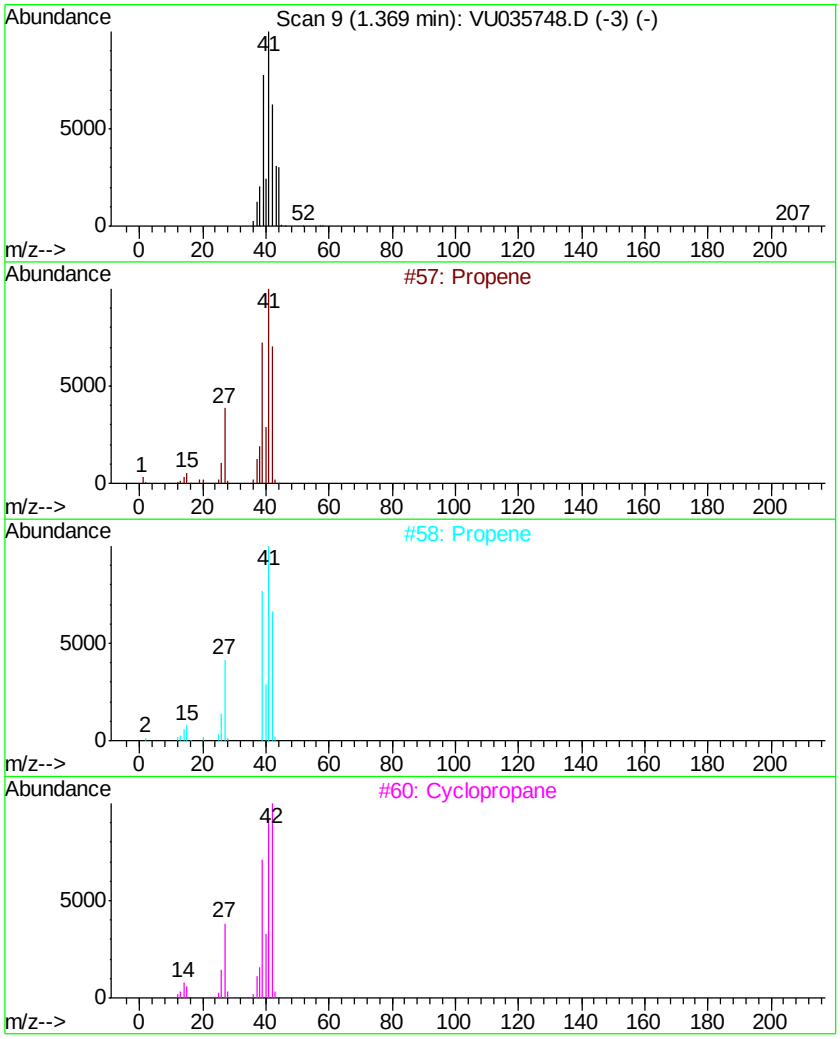
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

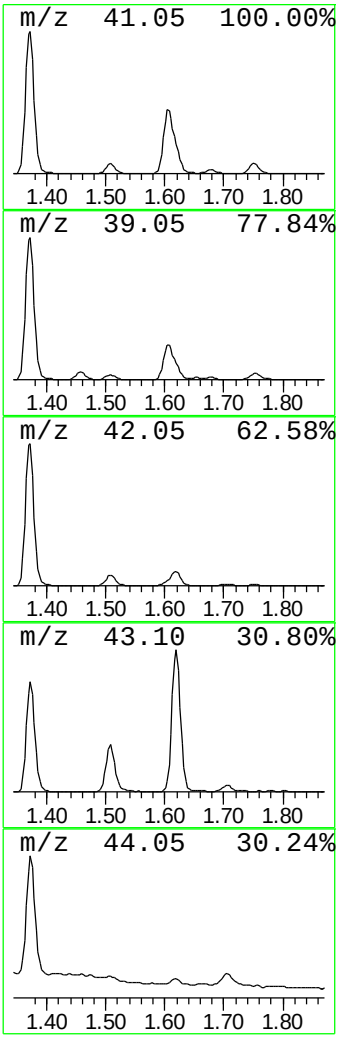
****

Peak Number 1 (DEL) Alkane: Cyclic1.37 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	8.83 ug/L	841675	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Propene	42	C3H6	000115-07-1	42
3	Cyclopropane	42	C3H6	000075-19-4	9
4	Cyclopropene	40	C3H4	002781-85-3	9
5	Cyclopropane	42	C3H6	000075-19-4	7





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Data File : VU035748.D
Acq On : 18 Nov 2019 17:10
Operator : JC/SP
Sample : K5911-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAQK7

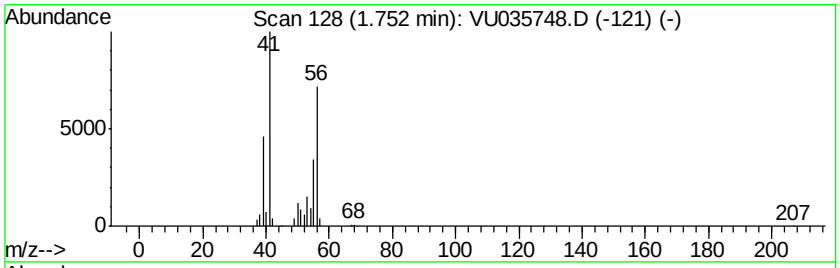
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

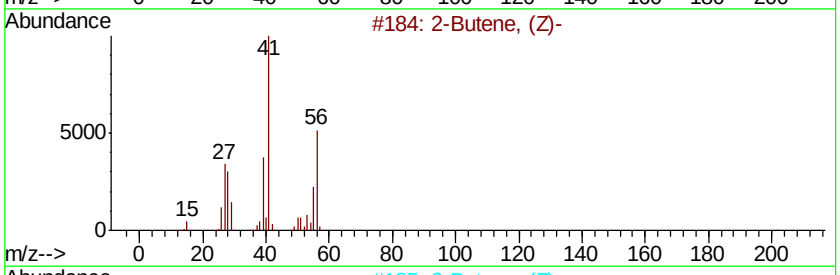
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

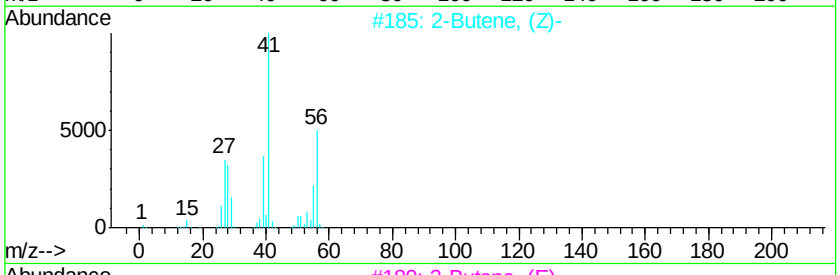
****
Peak Number 2 (DEL) Alkane: Cyclic1.75 Concentration Rank 10

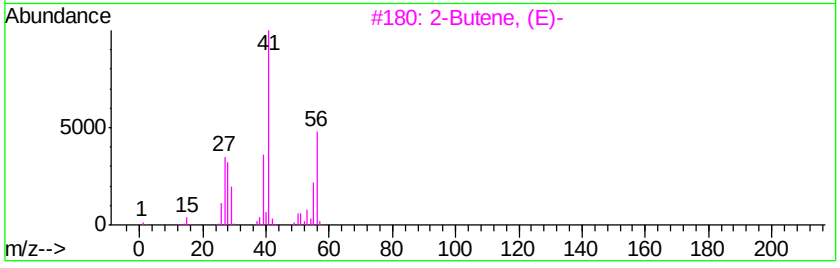
R.T.	EstConc	Area	Relative to ISTD	R.T.
1.75	0.83 ug/L	79218	1,4-Difluorobenzene	6.29

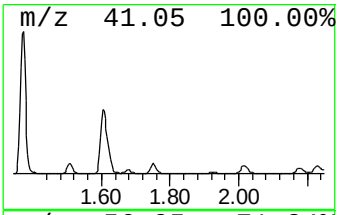
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, (Z)-	56	C4H8	000590-18-1	83
2	2-Butene, (Z)-	56	C4H8	000590-18-1	83
3	2-Butene, (E)-	56	C4H8	000624-64-6	83
4	2-Butene, (E)-	56	C4H8	000624-64-6	80
5	1-Butene	56	C4H8	000106-98-9	72

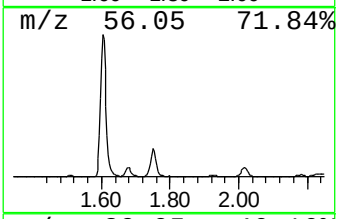


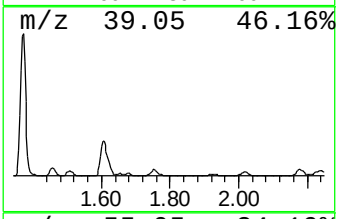


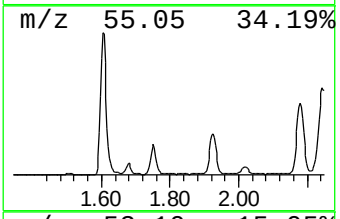


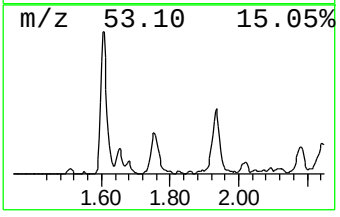












Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111819\
Data File : VU035748.D
Acq On : 18 Nov 2019 17:10
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Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAQK7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

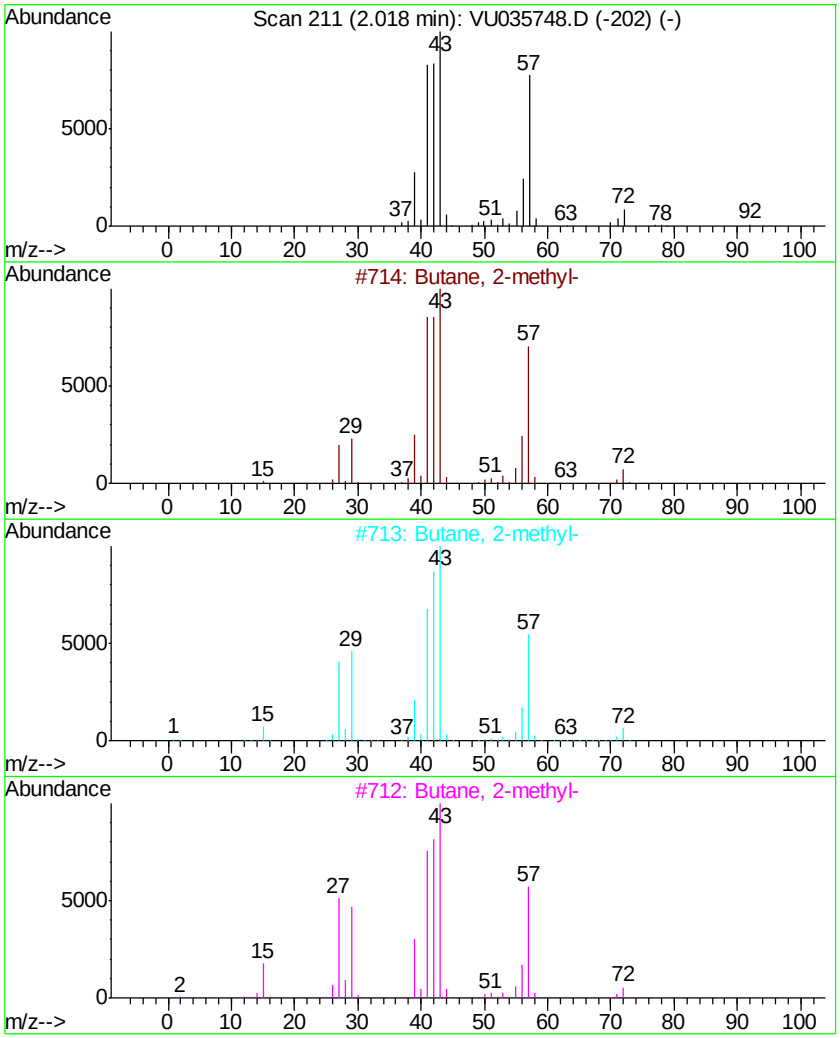
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

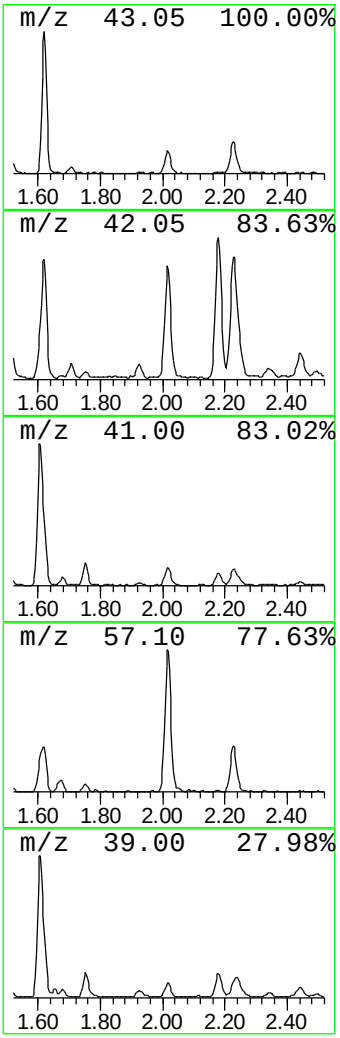
****

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	1.00 ug/L	94880	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	91
3	Butane, 2-methyl-	72	C5H12	000078-78-4	90
4	3-Buten-1-ol	72	C4H8O	000627-27-0	43
5	Pentane	72	C5H12	000109-66-0	42





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111819\
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Operator : JC/SP
Sample : K5911-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAQK7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

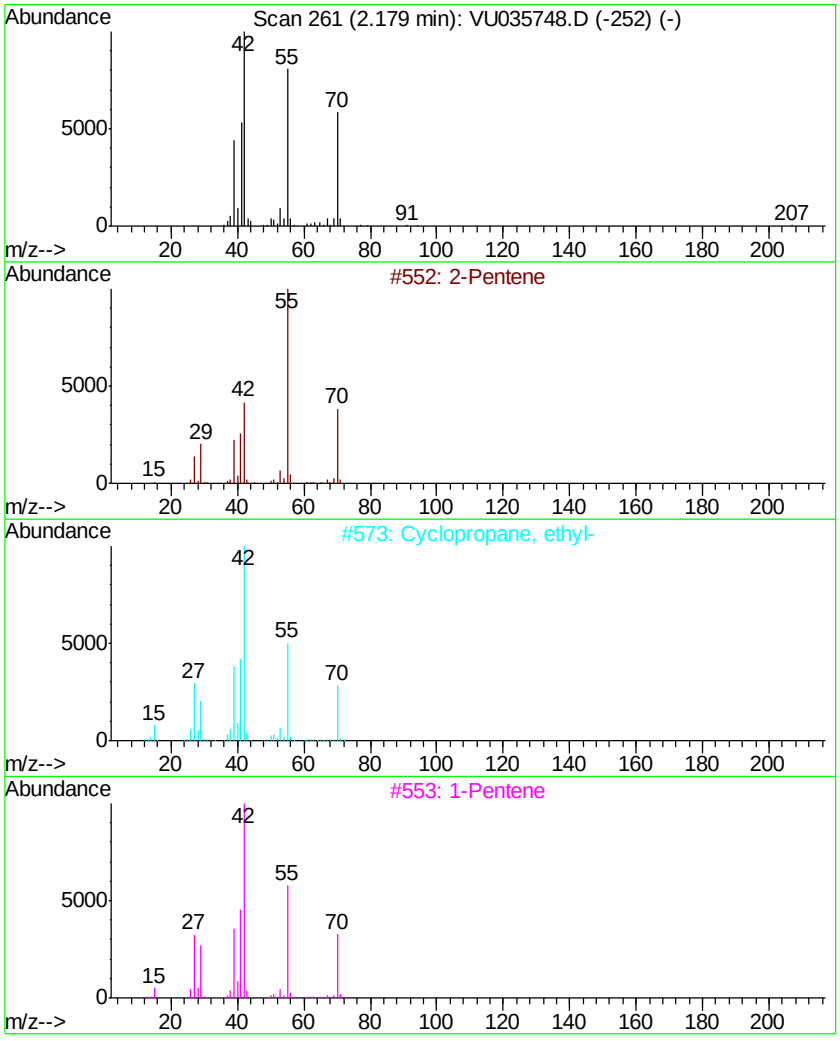
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

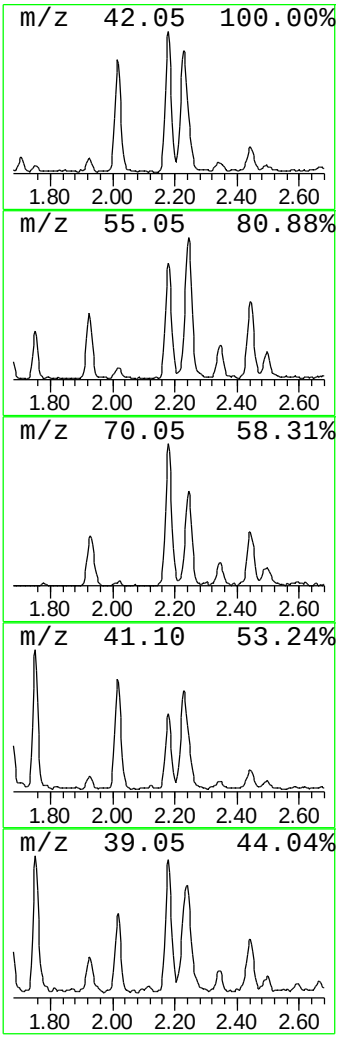
****

Peak Number 4 (DEL) Alkane: Cyclic2.18 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	0.97 ug/L	92888	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene	70	C5H10	000109-68-2	83
2	Cyclopropane, ethyl-	70	C5H10	001191-96-4	70
3	1-Pentene	70	C5H10	000109-67-1	68
4	1-Pentene	70	C5H10	000109-67-1	64
5	Cyclopentane	70	C5H10	000287-92-3	59





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Data File : VU035748.D
Acq On : 18 Nov 2019 17:10
Operator : JC/SP
Sample : K5911-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAQK7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

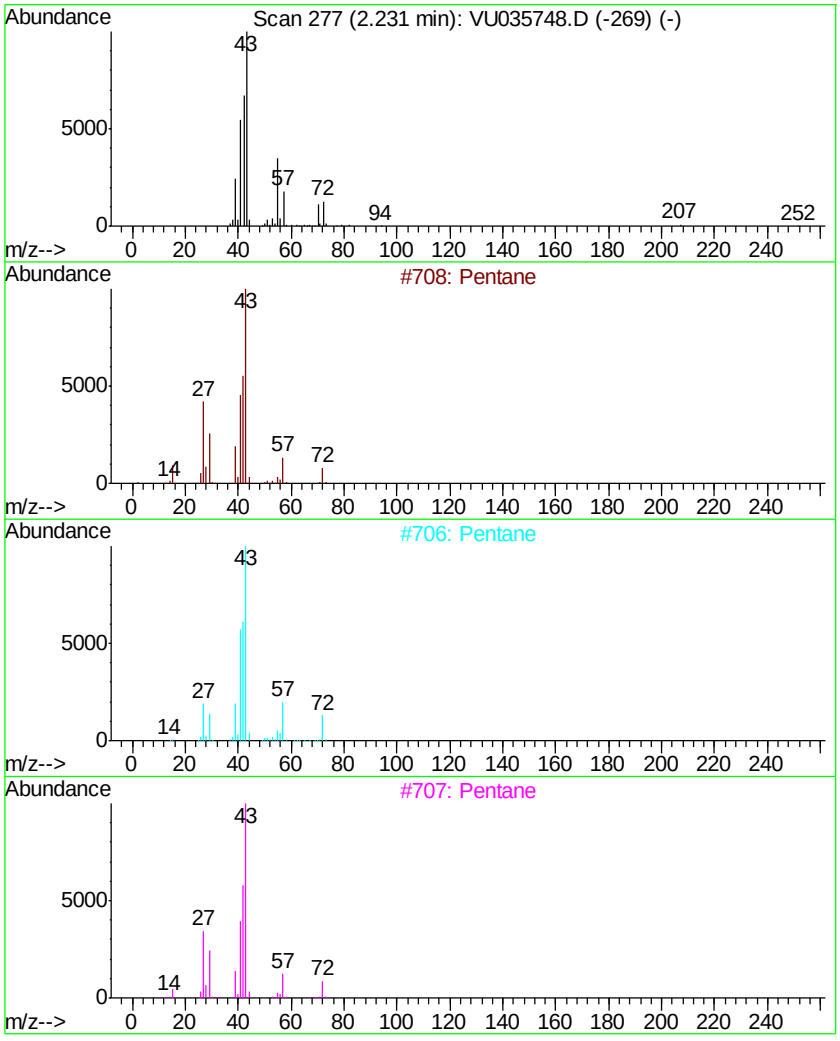
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

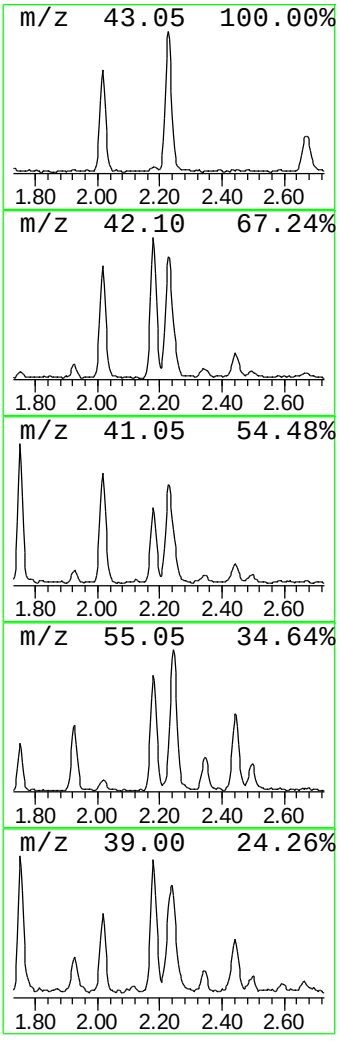
****

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	1.64 ug/L	156435	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	72
2	Pentane	72	C5H12	000109-66-0	72
3	Pentane	72	C5H12	000109-66-0	64
4	Pentane	72	C5H12	000109-66-0	64
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	47





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Data File : VU035748.D
Acq On : 18 Nov 2019 17:10
Operator : JC/SP
Sample : K5911-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAQK7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

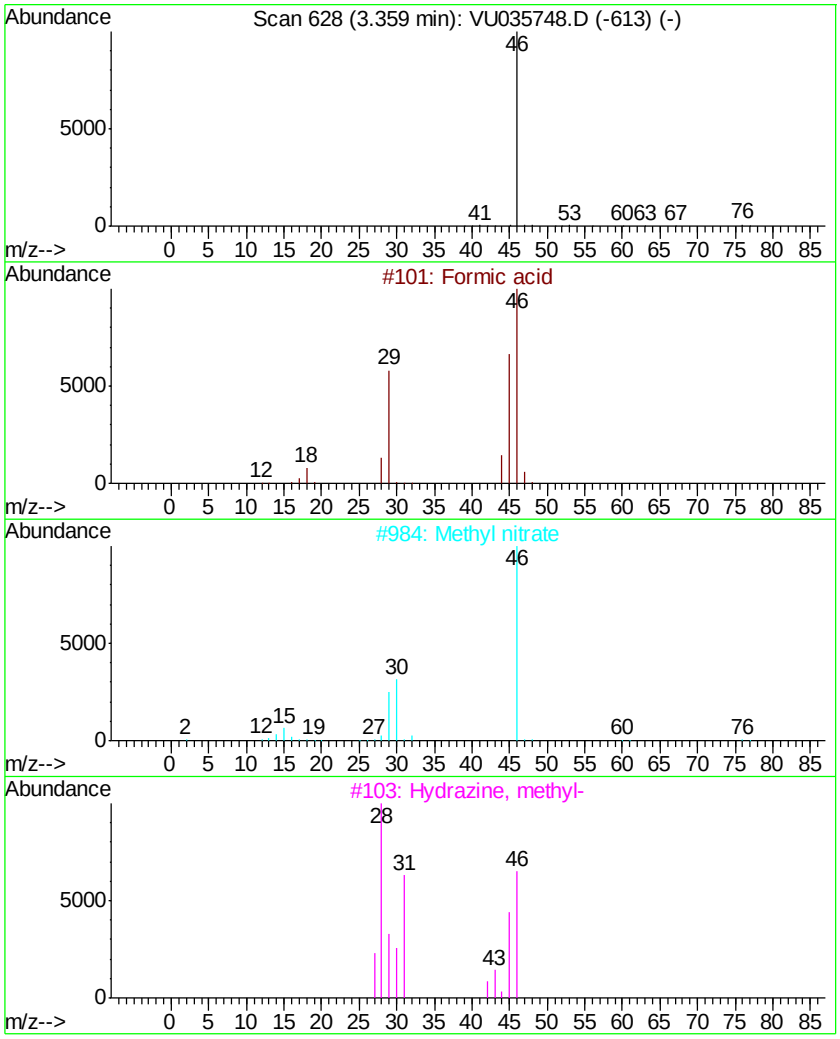
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

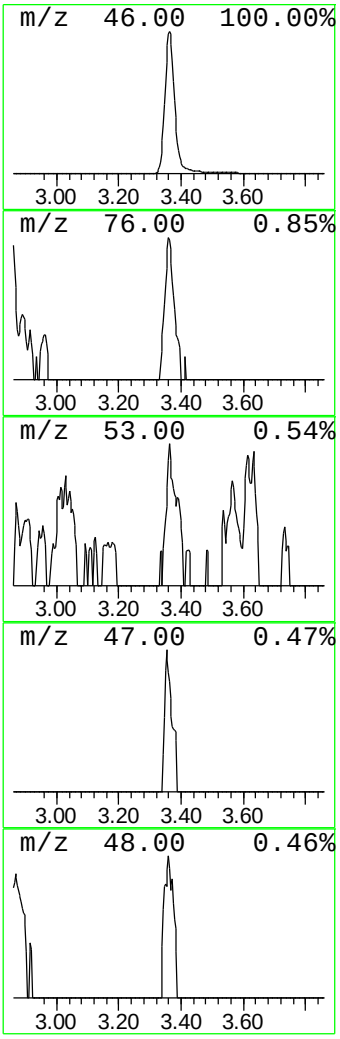
****

Peak Number 6 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.36	2.04 ug/L	194908	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formic acid	46	CH2O2	000064-18-6	4
2	Methyl nitrate	77	CH3NO3	000598-58-3	4
3	Hydrazine, methyl-	46	CH6N2	000060-34-4	3
4	Hydrazine, methyl-	46	CH6N2	000060-34-4	3
5	Hydrazine, methyl-	46	CH6N2	000060-34-4	3





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Instrument : MSVOA_U
ClientSampleId : GAQK7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

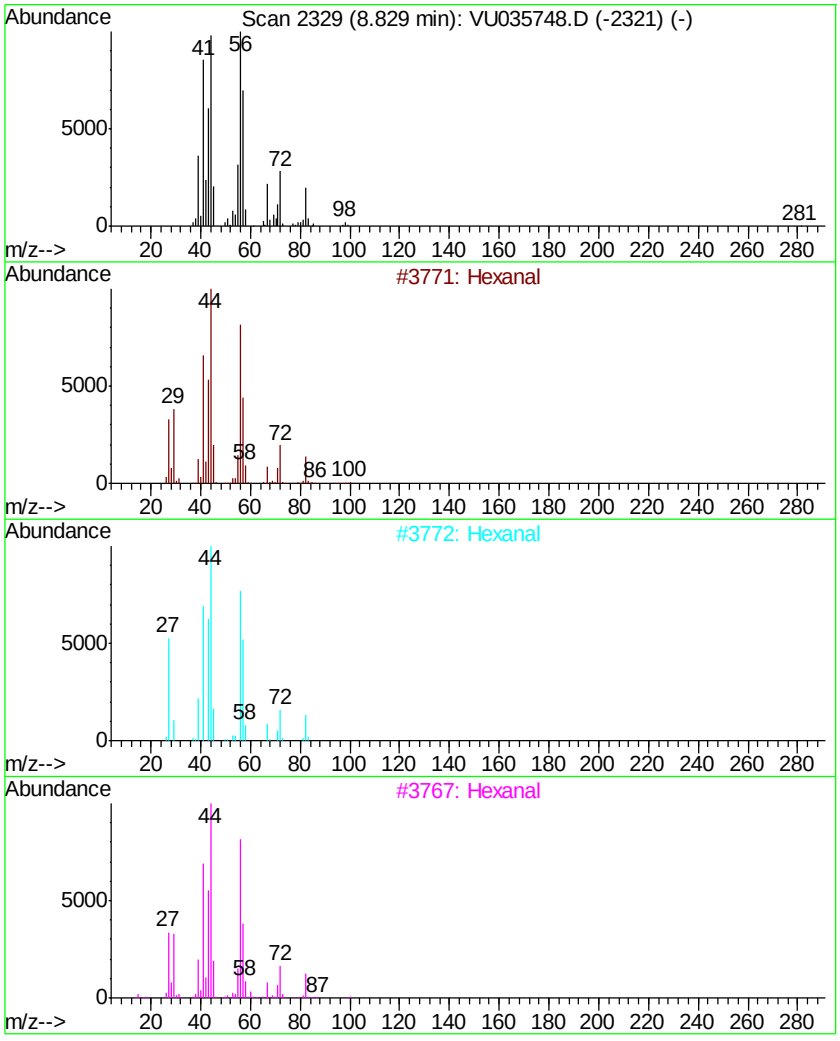
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

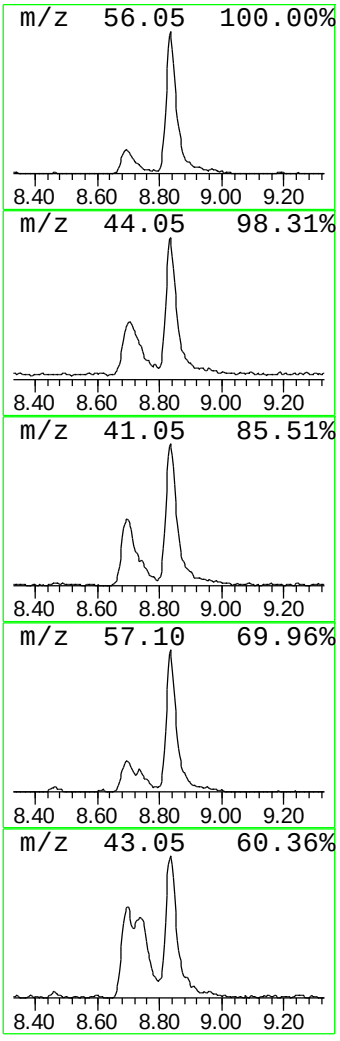
****

Peak Number 8 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.83	2.37 ug/L	322727	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	87
2	Hexanal	100	C6H12O	000066-25-1	64
3	Hexanal	100	C6H12O	000066-25-1	64
4	Hexanal	100	C6H12O	000066-25-1	56
5	Glutaraldehyde	100	C5H8O2	000111-30-8	38





Library Search Compound Report

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Data File : VU035748.D
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

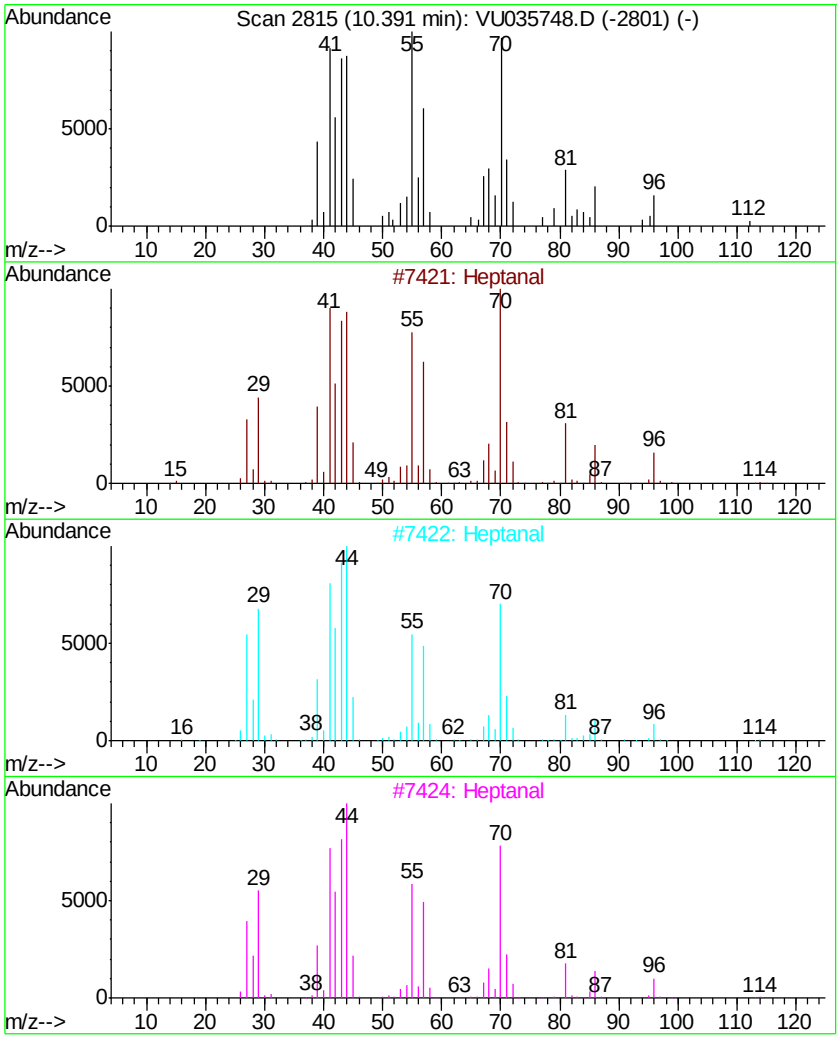
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

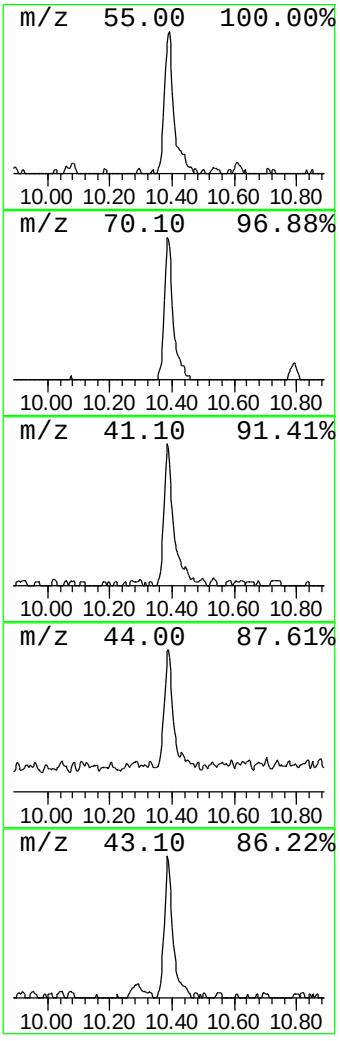
****

Peak Number 9 Heptanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.39	0.63 ug/L	86431	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	87
2	Heptanal	114	C7H14O	000111-71-7	72
3	Heptanal	114	C7H14O	000111-71-7	72
4	Heptanal	114	C7H14O	000111-71-7	64
5	Heptanal	114	C7H14O	000111-71-7	64





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU111819\
Data File : VU035748.D
Acq On : 18 Nov 2019 17:10
Operator : JC/SP
Sample : K5911-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAQK7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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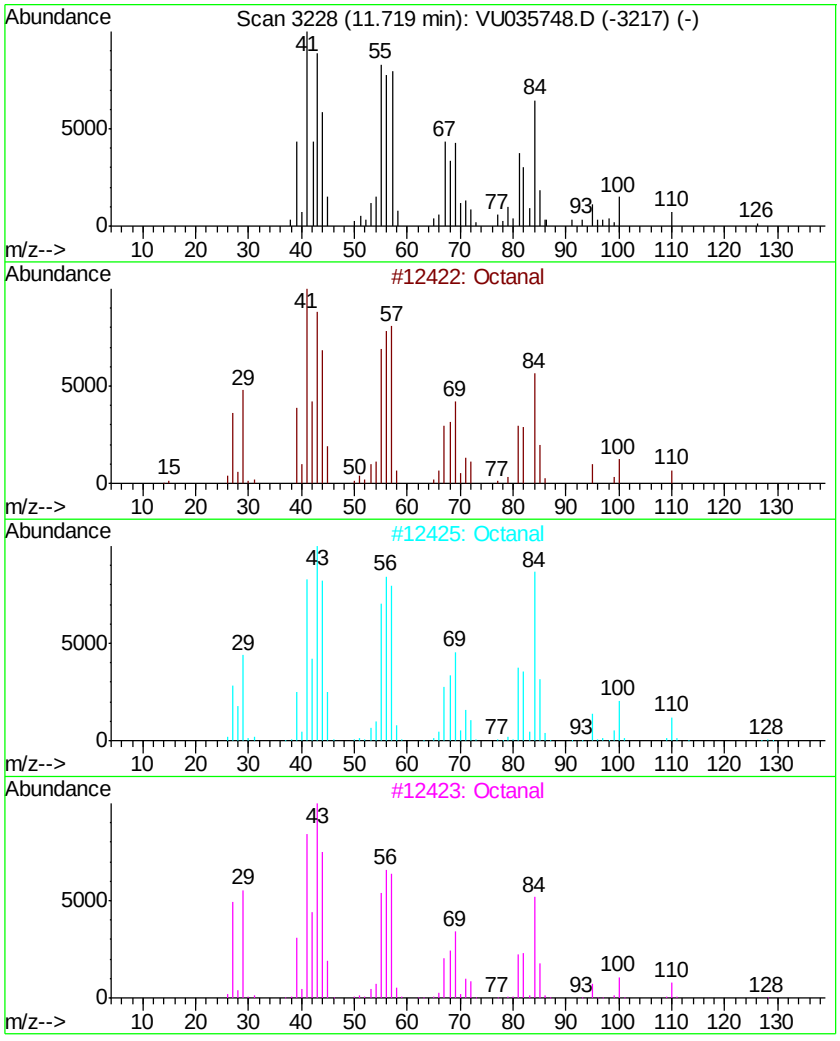
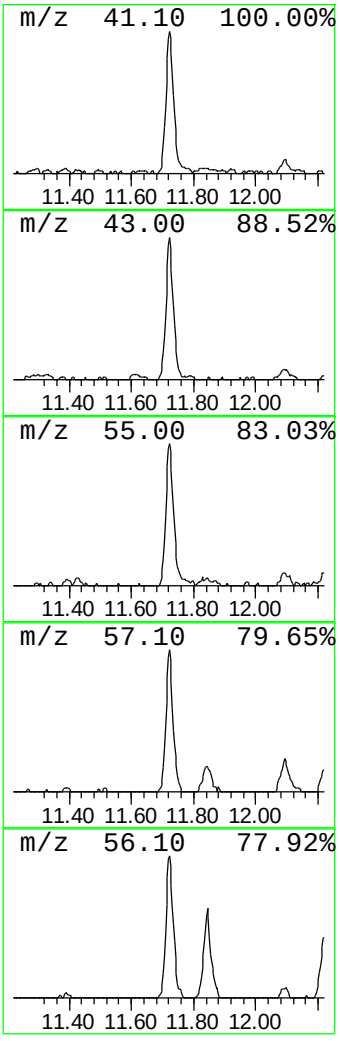
Peak Number 10 Octanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	1.11 ug/L	132692	1,4-Dichlorobenzene-d4	11.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal	128	C8H16O	000124-13-0	87
2	Octanal	128	C8H16O	000124-13-0	64
3	Octanal	128	C8H16O	000124-13-0	64
4	1-Pentene, 3-methyl-	84	C6H12	000760-20-3	46
5	3-Chlorohexane	120	C6H13Cl	002346-81-8	43





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111819\
Data File : VU035748.D
Acq On : 18 Nov 2019 17:10
Operator : JC/SP
Sample : K5911-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAQK7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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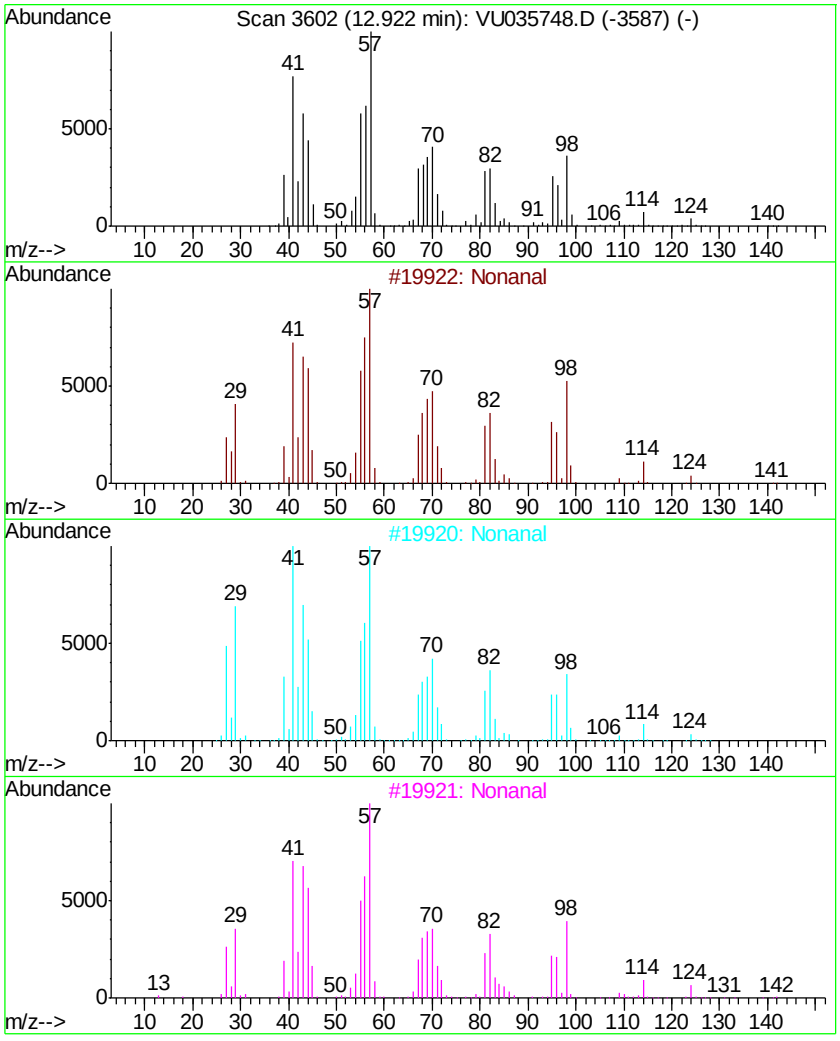
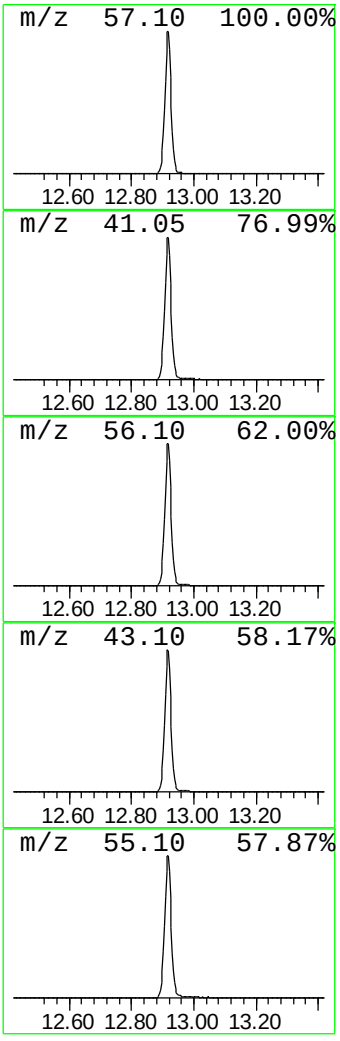
Peak Number 11 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.92	18.40 ug/L	2194250	1,4-Dichlorobenzene-d4	11.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	91
2	Nonanal	142	C9H18O	000124-19-6	91
3	Nonanal	142	C9H18O	000124-19-6	91
4	Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	27
5	Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU111819\
Data File : VU035748.D
Acq On : 18 Nov 2019 17:10
Operator : JC/SP
Sample : K5911-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAQK7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: Cyc...	1.37	8.8	ug/L	841675	1	6.29	476608	5.0
(DEL) Alkane: Cyc...	1.75	0.8	ug/L	79218	1	6.29	476608	5.0
(DEL) Alkane: Str...	2.02	1.0	ug/L	94880	1	6.29	476608	5.0
(DEL) Alkane: Cyc...	2.18	1.0	ug/L	92888	1	6.29	476608	5.0
(DEL) Alkane: Str...	2.23	1.6	ug/L	156435	1	6.29	476608	5.0
unknown-01	3.36	2.0	ug/L	194908	1	6.29	476608	5.0
Hexanal	8.83	2.4	ug/L	322727	2	9.45	681221	5.0
Heptanal	10.39	0.6	ug/L	86431	2	9.45	681221	5.0
Octanal	11.72	1.1	ug/L	132692	3	11.84	596394	5.0
Nonanal	12.92	18.4	ug/L	2194250	3	11.84	596394	5.0