LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111020\
Data File : VU041172.D
Acq On : 10 Nov 2020 12:50
Operator : SY/MD
Sample : L4646-13DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB0T7DL

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\SOMUTR102620WMA.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	1.494	41	48	58	rVB	12846	12423	1.91%	0.387%
2	1.607	74	83	94	rVB2	91419	98635	15.14%	3.069%
3	1.922	172	181	193	rVB	21215	27272	4.18%	0.849%
4	2.006	196	207	220	rBV	99265	137557	21.11%	4.280%
5	2.218	263	273	287	rVB3	18987	36589	5.61%	1.139%
6	2.327	299	307	318	rVB	12382	17638	2.71%	0.549%
7	2.427	330	338	345	rBV3	5479	7748	1.19%	0.241%
8	2.478	345	354	367	rVB	24070	36680	5.63%	1.141%
9	2.578	372	385	404	rBV	38864	65002	9.97%	2.023%
10	3.057	518	534	541	rBV7	11034	28883	4.43%	0.899%
11	3.154	555	564	578	rVB3	11926	23591	3.62%	0.734%
12	3.375	622	633	646	rBB3	6934	14758	2.26%	0.459%
13	3.999	814	827	837	rBV5	2941	6932	1.06%	0.216%
14	4.549	981	998	1013	rBB2	15693	36715	5.63%	1.142%
15	4.652	1014	1030	1076	rBV2	46557	150285	23.06%	4.676%
16	5.083	1149	1164	1182	rBV	44199	99020	15.19%	3.081%
17	5.404	1250	1264	1277	rBV4	13287	29152	4.47%	0.907%
18	5.739	1348	1368	1374	rBV2	81673	208585	32.01%	6.490%
19	5.790	1374	1384	1400	rVB	318093	651693	100.00%	20.278%
20	5.912	1414	1422	1438	rVB9	4480	10826	1.66%	0.337%
21	6.263	1516	1531	1552	rBV	76712	144642	22.19%	4.501%
22	6.703	1655	1668	1681	rBV	56789	107029	16.42%	3.330%
23	7.575	1927	1939	1952	rVB2	26317	45326	6.96%	1.410%
24	7.906	2029	2042	2056	rBV	88718	150842	23.15%	4.694%
25	8.185	2117	2129	2144	rBV	17308	28750	4.41%	0.895%
26	8.639	2257	2270	2293	rBV	183907	329299	50.53%	10.247%
27	8.919	2346	2357	2377	rBB3	4437	8504	1.30%	0.265%
28	9.420	2501	2513	2527	rBV	110293	179683	27.57%	5.591%
29	9.697	2587	2599	2614	rVB	32457	51937	7.97%	1.616%
30	10.755	2918	2928	2944	rVB	49473	77337	11.87%	2.406%
31	10.902	2964	2974	2990	rVB	4996	7996	1.23%	0.249%
32	11.288	3085	3094	3104	rVB	8742	11600	1.78%	0.361%
33	11.465	3139	3149	3158	rVB3	5185	7183	1.10%	0.224%
34	11.806	3243	3255	3268	rBV	106800	169640	26.03%	5.279%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111020\
Data File : VU041172.D
Acq On : 10 Nov 2020 12:50
Operator : SY/MD
Sample : L4646-13DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB0T7DL

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\SOMUTR102620WMA.M
Title : TRACE VOA SOM01.0

35	12.089	3334	3343	3358	rBV	13619	21599	3.31%	0.672%
36	12.189	3362	3374	3387	rVB	106814	172401	26.45%	5.364%

Sum of corrected areas: 3213752

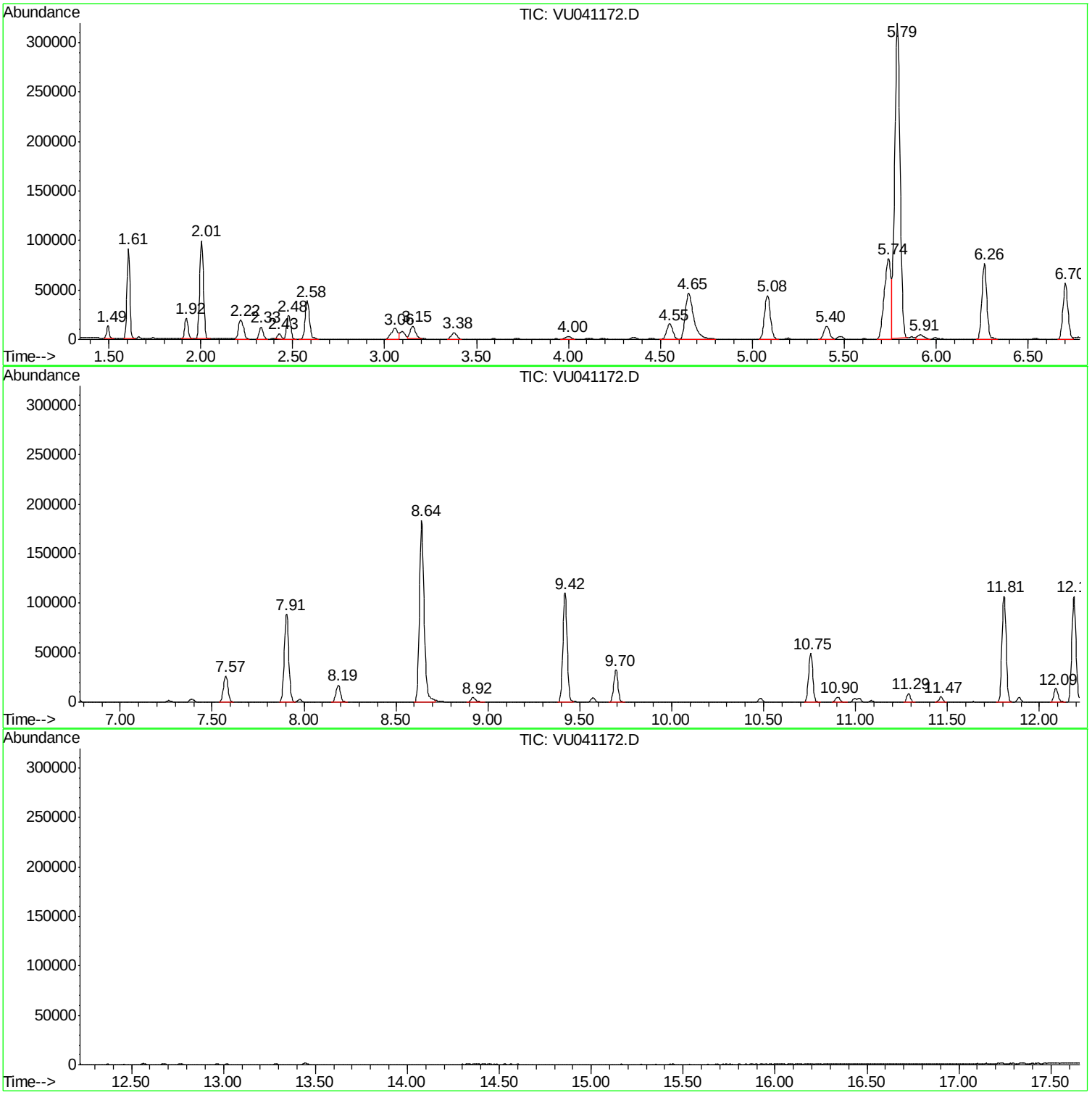
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111020\
Data File : VU041172.D
Acq On : 10 Nov 2020 12:50
Operator : SY/MD
Sample : L4646-13DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB0T7DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.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\VU111020\
Data File : VU041172.D
Acq On : 10 Nov 2020 12:50
Operator : SY/MD
Sample : L4646-13DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB0T7DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

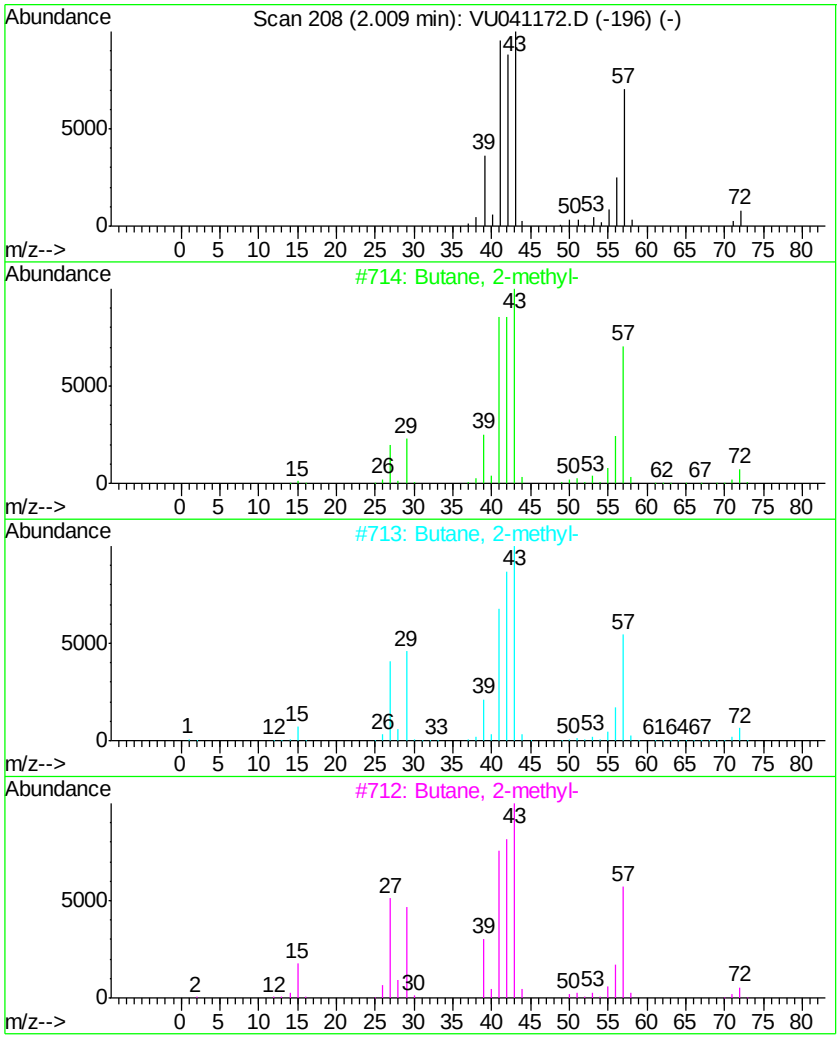
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

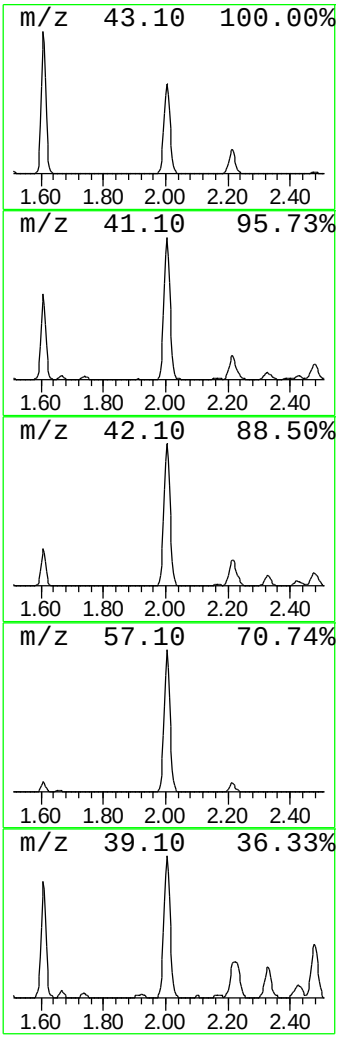
****

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.01	4.76 ug/L	137557	1,4-Difluorobenzene	6.26

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	90
3	Butane, 2-methyl-	72	C5H12	000078-78-4	86
4	3-Buten-1-ol	72	C4H8O	000627-27-0	47
5	Pentane	72	C5H12	000109-66-0	36





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111020\
Data File : VU041172.D
Acq On : 10 Nov 2020 12:50
Operator : SY/MD
Sample : L4646-13DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB0T7DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

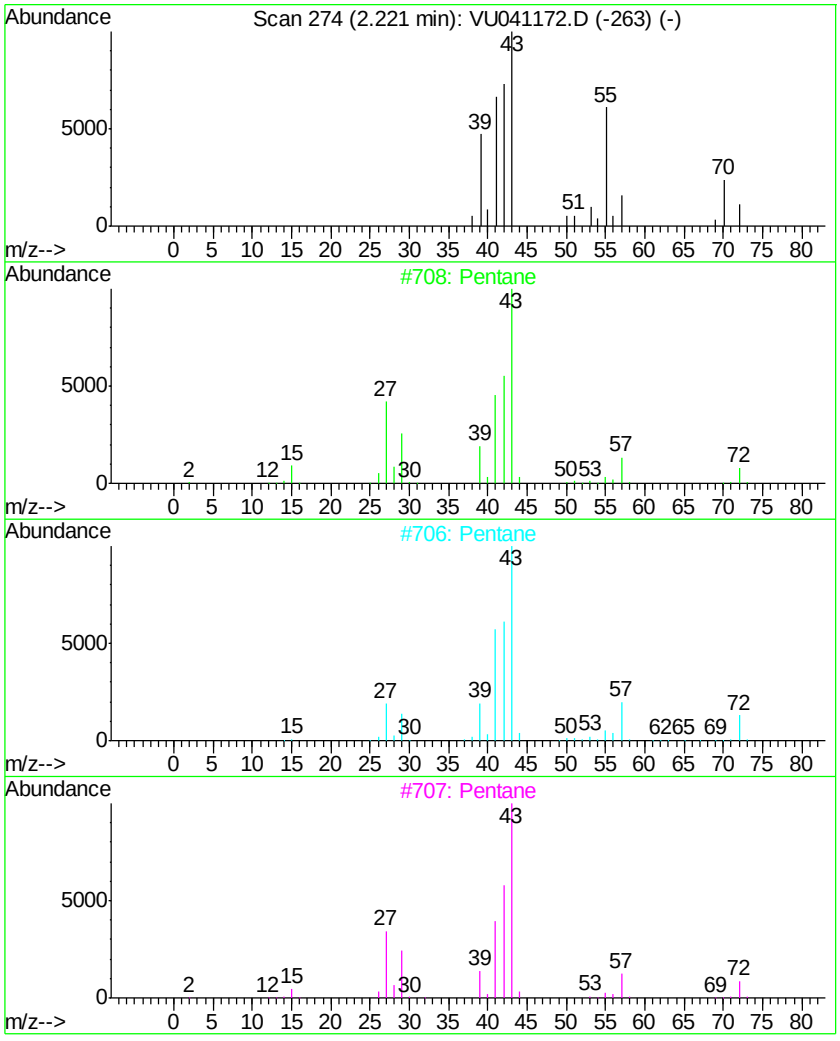
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

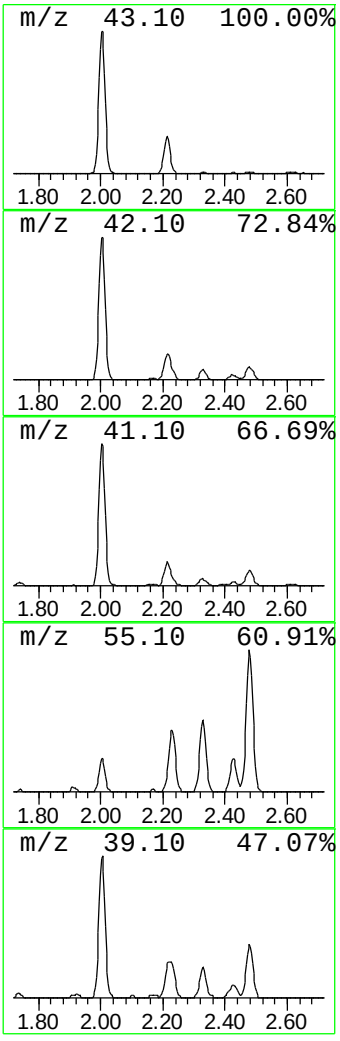
****

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	1.26 ug/L	36589	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	64
2	Pentane	72	C5H12	000109-66-0	64
3	Pentane	72	C5H12	000109-66-0	59
4	Butane, 2-methyl-	72	C5H12	000078-78-4	33
5	Pentane	72	C5H12	000109-66-0	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111020\
Data File : VU041172.D
Acq On : 10 Nov 2020 12:50
Operator : SY/MD
Sample : L4646-13DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB0T7DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

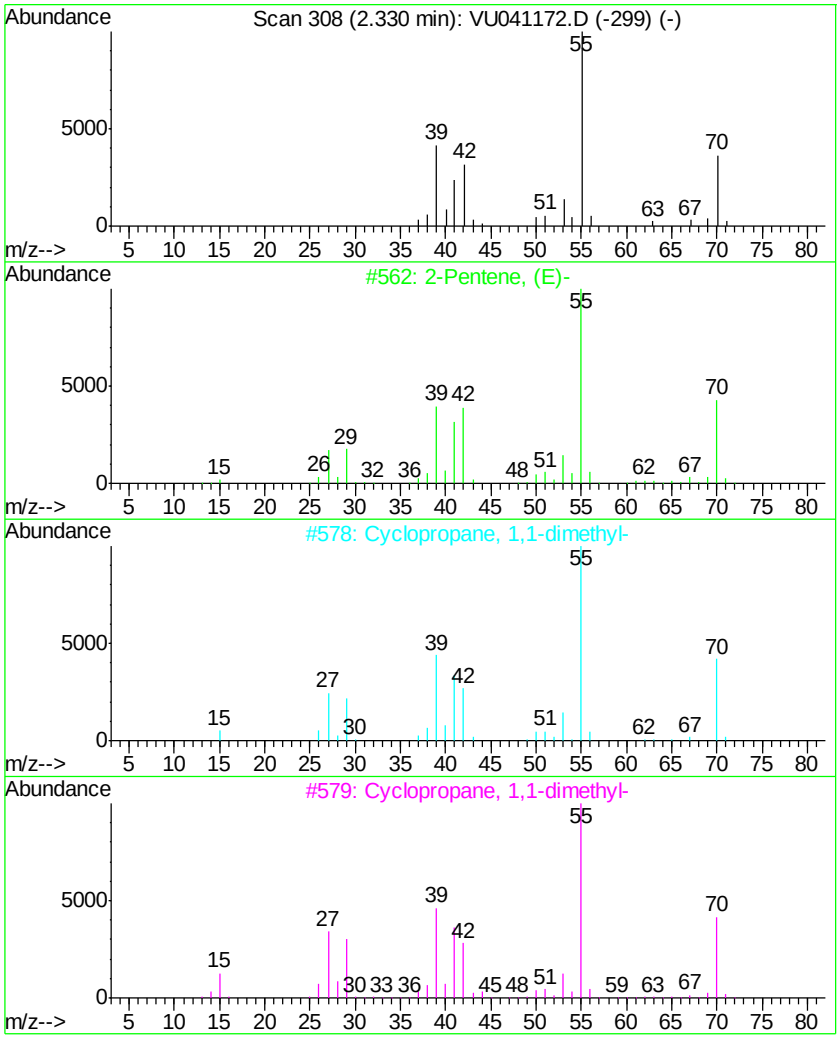
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

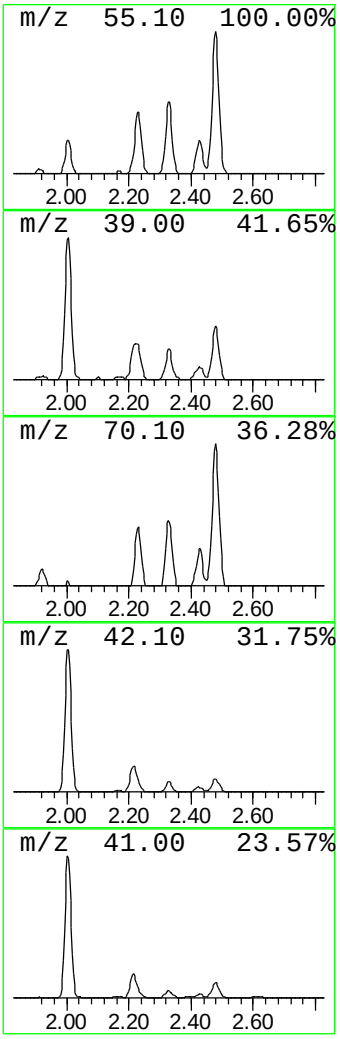
****

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	0.61 ug/L	17638	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-	70	C5H10	000646-04-8	91
2	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	90
3	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	87
4	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	83
5	2-Pentene, (Z)-	70	C5H10	000627-20-3	81





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU111020\
Data File : VU041172.D
Acq On : 10 Nov 2020 12:50
Operator : SY/MD
Sample : L4646-13DL 100X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB0T7DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

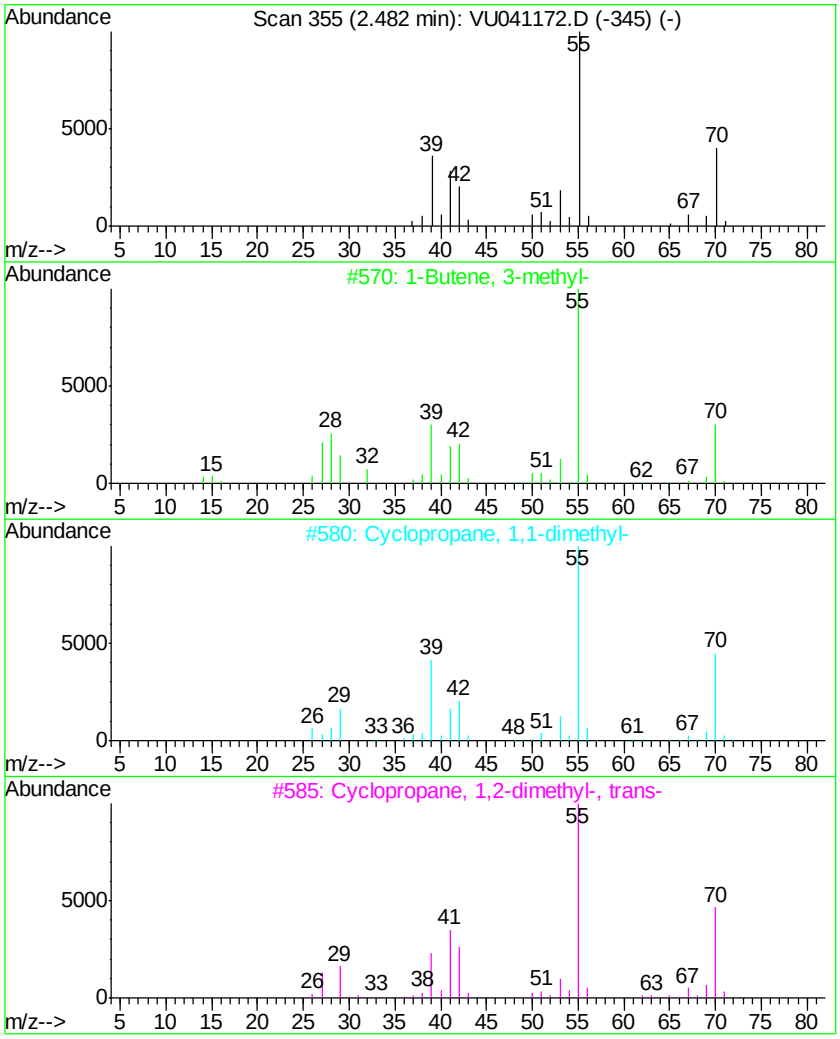
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

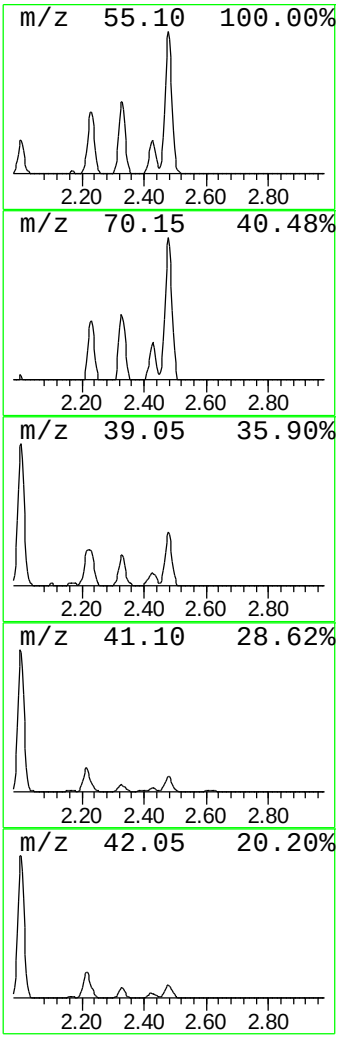
****

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.48	1.27 ug/L	36680	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 3-methyl-	70	C5H10	000563-45-1	87
2	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	87
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	86
4	2-Butene, 2-methyl-	70	C5H10	000513-35-9	83
5	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111020\
Data File : VU041172.D
Acq On : 10 Nov 2020 12:50
Operator : SY/MD
Sample : L4646-13DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB0T7DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

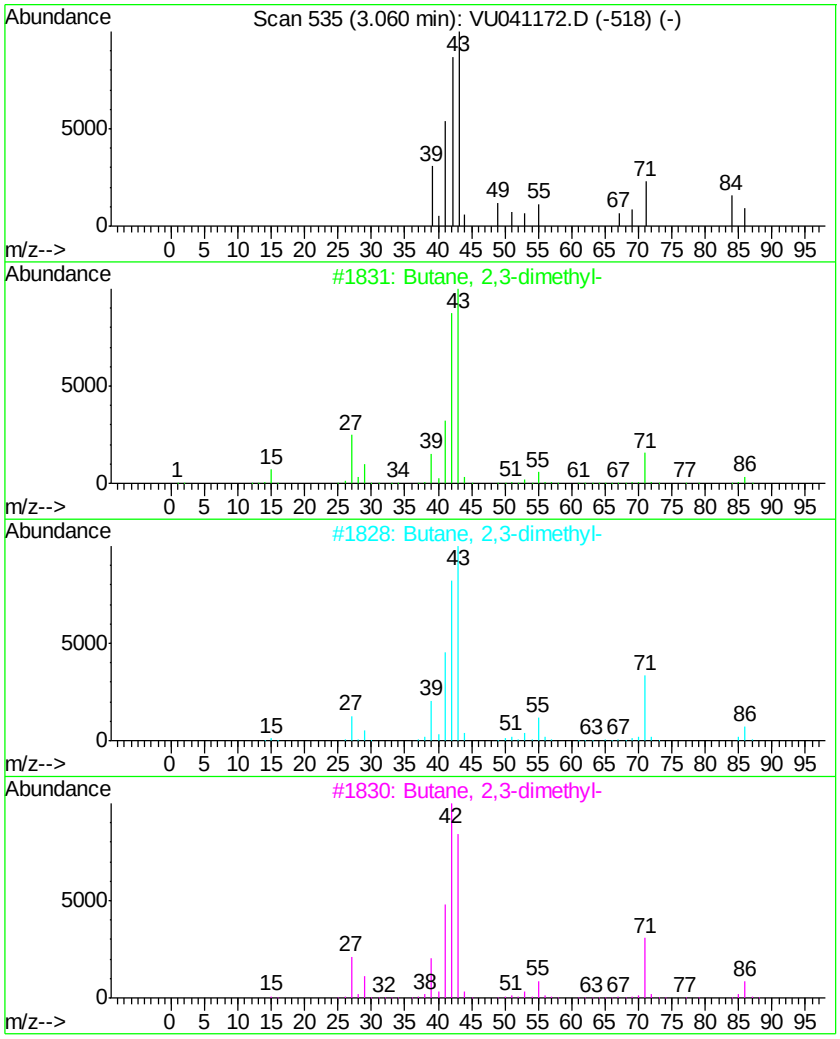
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

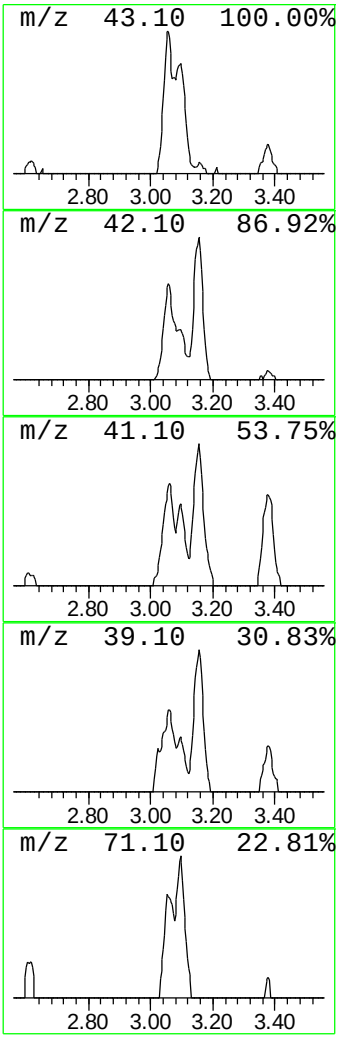
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	1.00 ug/L	28883	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	59
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	45
3	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	42
4	Butane, 2-methyl-	72	C5H12	000078-78-4	28
5	Pentane, 2-methyl-	86	C6H14	000107-83-5	23





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111020\
Data File : VU041172.D
Acq On : 10 Nov 2020 12:50
Operator : SY/MD
Sample : L4646-13DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB0T7DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

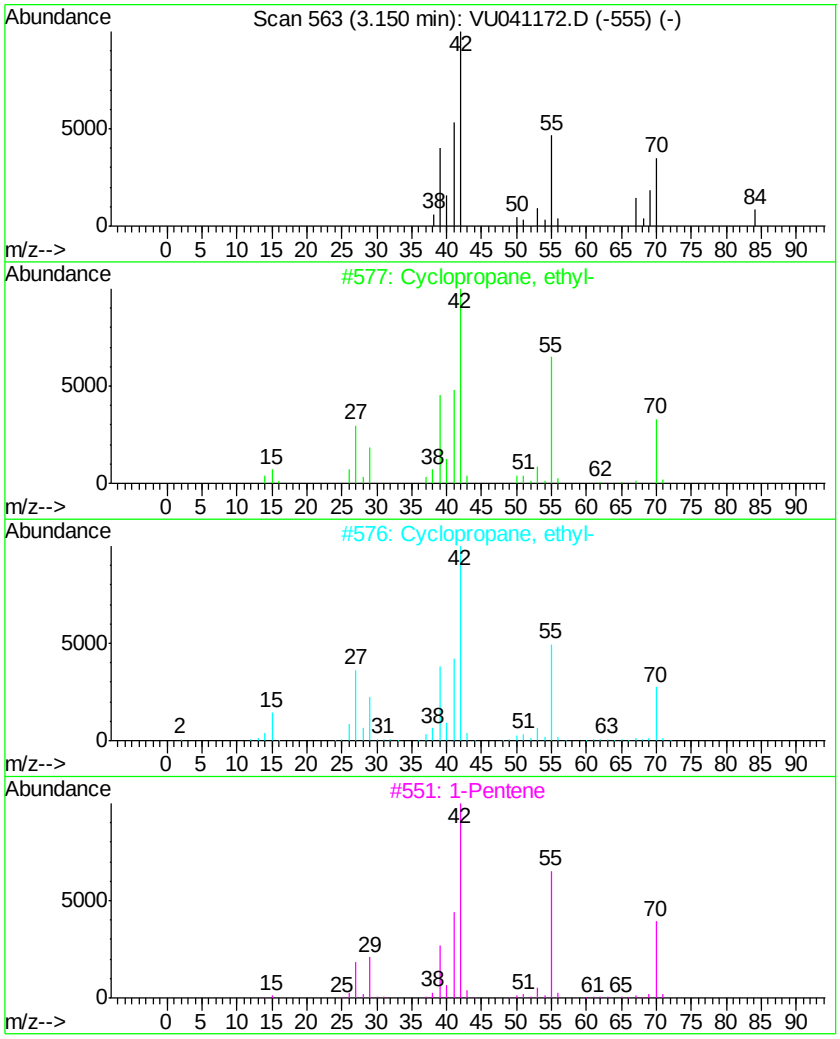
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

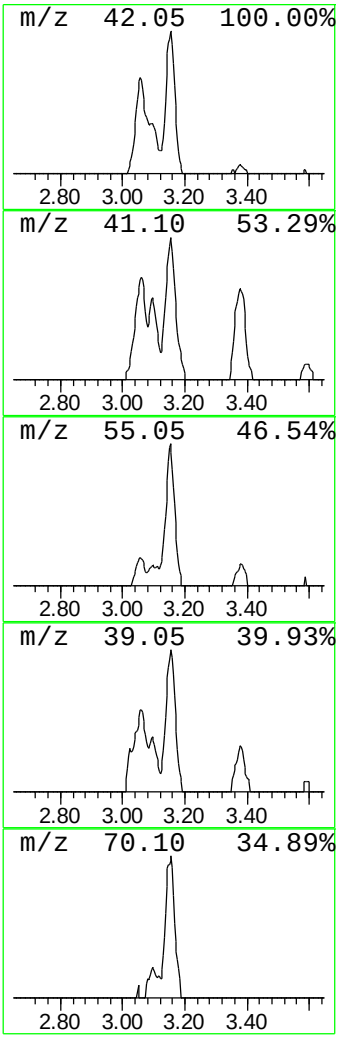
****

Peak Number 6 (DEL) Alkane: Cyclic3.15 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	0.82 ug/L	23591	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, ethyl-	70	C5H10	001191-96-4	72
2	Cyclopropane, ethyl-	70	C5H10	001191-96-4	59
3	1-Pentene	70	C5H10	000109-67-1	50
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	50
5	1-Pentene	70	C5H10	000109-67-1	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111020\
Data File : VU041172.D
Acq On : 10 Nov 2020 12:50
Operator : SY/MD
Sample : L4646-13DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB0T7DL

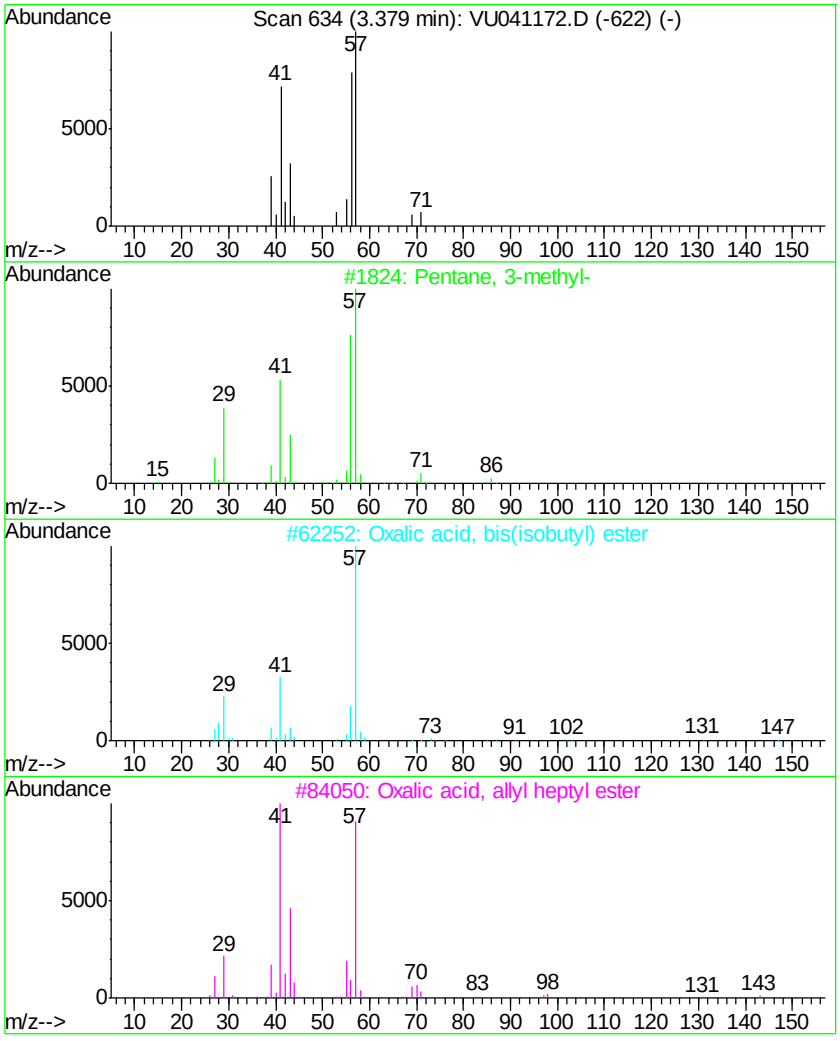
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

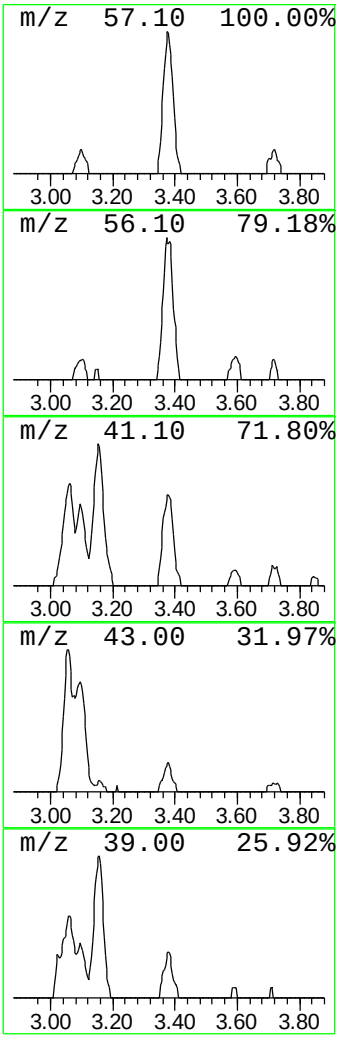
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.38	0.51 ug/L	14758	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	40
2	Oxalic acid, bis(isobutyl) ester	202	C10H18O4	1000309-36-8	9
3	Oxalic acid, allyl heptyl ester	228	C12H20O4	1000309-23-5	9
4	Pentane, 3-methyl-	86	C6H14	000096-14-0	9
5	Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111020\
Data File : VU041172.D
Acq On : 10 Nov 2020 12:50
Operator : SY/MD
Sample : L4646-13DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB0T7DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

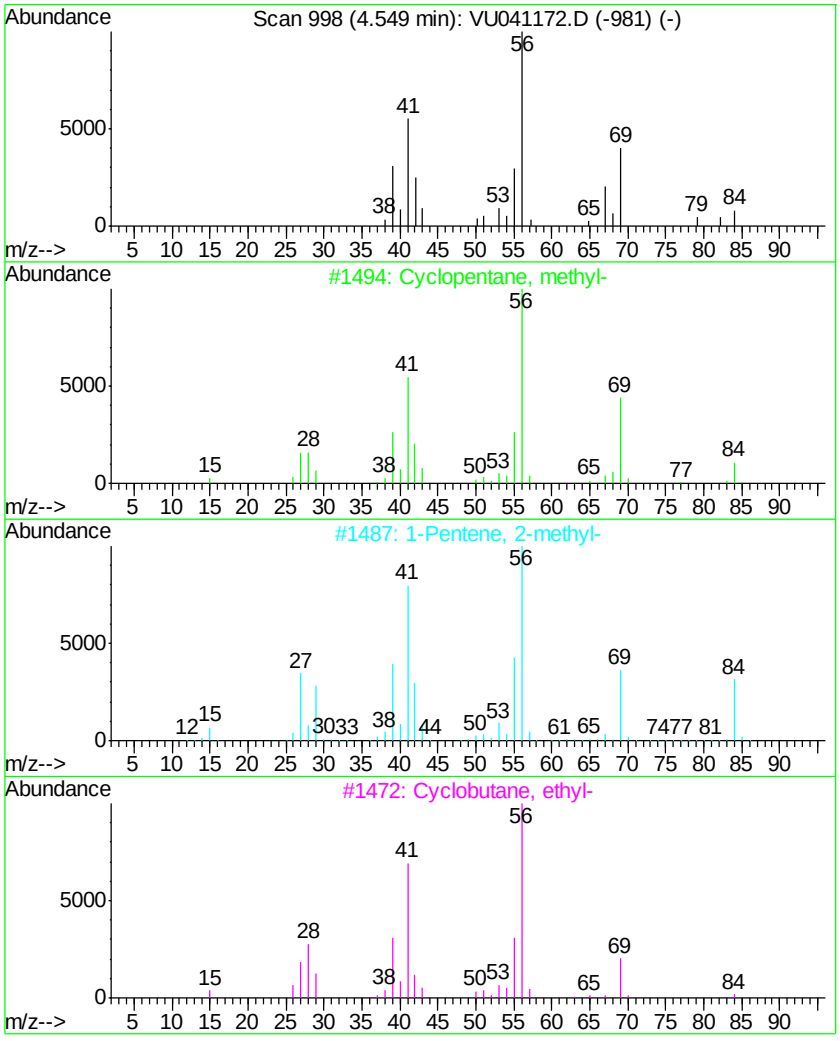
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

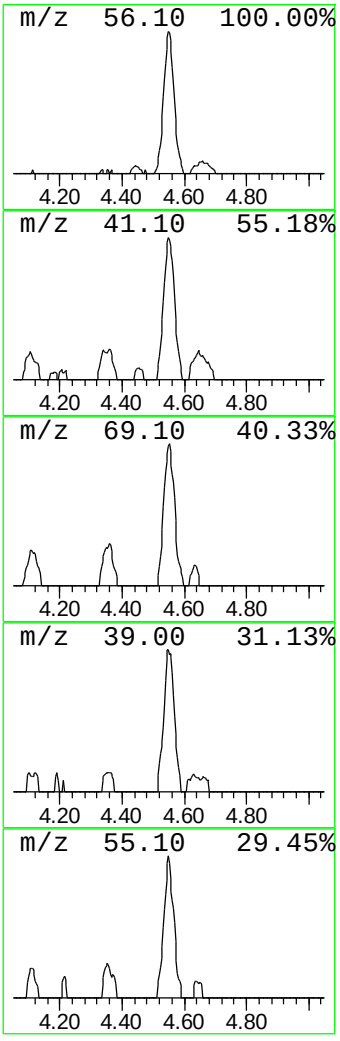
****

Peak Number 8 (DEL) Alkane: Cyclic4.55 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	1.27 ug/L	36715	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	64
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	53
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	50
4	Cyclobutane	56	C4H8	000287-23-0	49
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	45





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111020\
Data File : VU041172.D
Acq On : 10 Nov 2020 12:50
Operator : SY/MD
Sample : L4646-13DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB0T7DL

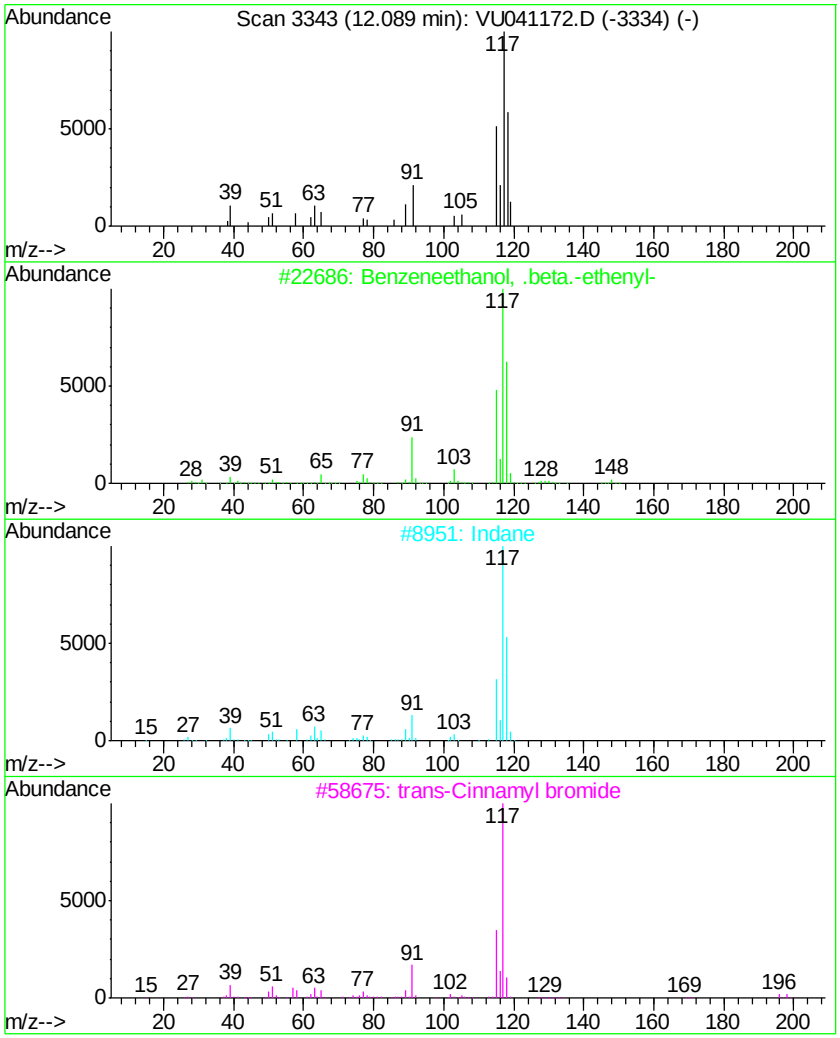
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

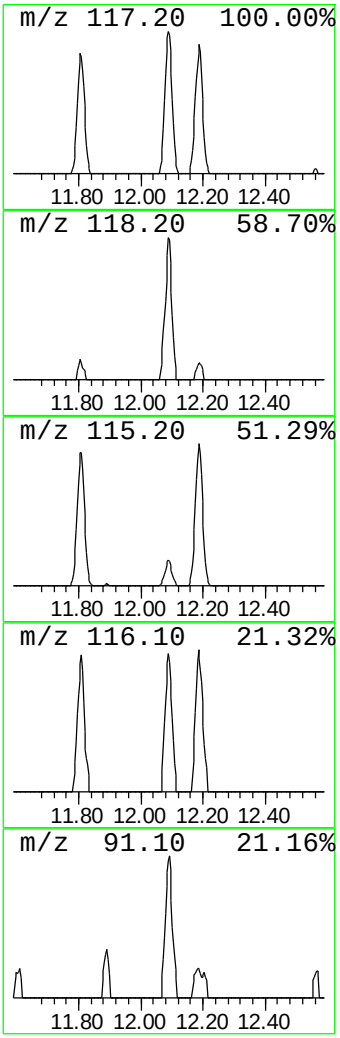
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzeneethanol, .beta.-ethe... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.09	0.64 ug/L	21599	1,4-Dichlorobenzene-d4	11.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	64
2	Indane	118	C9H10	000496-11-7	58
3	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53
4	Indane	118	C9H10	000496-11-7	52
5	3-Phenyl-1-propanol, acetate	178	C11H14O2	000122-72-5	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU111020\
Data File : VU041172.D
Acq On : 10 Nov 2020 12:50
Operator : SY/MD
Sample : L4646-13DL 100X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB0T7DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.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: Str...	2.01	4.8	ug/L	137557	1	6.26	144642	5.0
(DEL) Alkane: Str...	2.22	1.3	ug/L	36589	1	6.26	144642	5.0
(DEL) Alkane: Str...	2.33	0.6	ug/L	17638	1	6.26	144642	5.0
(DEL) Alkane: Str...	2.48	1.3	ug/L	36680	1	6.26	144642	5.0
(DEL) Alkane: Str...	3.06	1.0	ug/L	28883	1	6.26	144642	5.0
(DEL) Alkane: Cyc...	3.15	0.8	ug/L	23591	1	6.26	144642	5.0
(DEL) Alkane: Str...	3.38	0.5	ug/L	14758	1	6.26	144642	5.0
(DEL) Alkane: Cyc...	4.55	1.3	ug/L	36715	1	6.26	144642	5.0
Benzeneethanol, ...	12.09	0.6	ug/L	21599	3	11.81	169640	5.0