LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082120\
Data File : VU039939.D
Acq On : 21 Aug 2020 19:38
Operator : SY/MD
Sample : L3776-17
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y16

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\SOMUTR081920WMA.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	1.363	3	7	16	rVB2	26482	27015	6.74%	0.843%
2	1.607	75	83	92	rVB	41644	46901	11.71%	1.464%
3	1.922	173	181	191	rVB	39458	49460	12.34%	1.544%
4	2.581	374	386	397	rBV	63194	104104	25.98%	3.249%
5	2.658	399	410	433	rVB2	17768	44934	11.21%	1.403%
6	2.842	441	467	469	rBV	58395	157208	39.24%	4.907%
7	4.520	975	989	1004	rBV4	5564	13780	3.44%	0.430%
8	4.652	1013	1030	1051	rBV2	59875	162450	40.54%	5.071%
9	4.825	1071	1084	1100	rBV	42976	96754	24.15%	3.020%
10	5.086	1149	1165	1182	rBV2	66463	146701	36.61%	4.579%
11	5.742	1347	1369	1394	rBV2	125979	329296	82.18%	10.278%
12	6.263	1515	1531	1544	rBV	92508	171586	42.82%	5.356%
13	6.703	1653	1668	1685	rBV3	77425	150364	37.53%	4.693%
14	7.353	1861	1870	1880	rBV4	4308	7041	1.76%	0.220%
15	7.420	1880	1891	1902	rBV3	17789	32984	8.23%	1.030%
16	7.575	1927	1939	1954	rBV2	38793	67530	16.85%	2.108%
17	7.906	2028	2042	2057	rBV2	130804	222564	55.55%	6.947%
18	8.185	2117	2129	2140	rBV3	26551	45528	11.36%	1.421%
19	8.639	2256	2270	2291	rBV	233247	400677	100.00%	12.506%
20	9.420	2501	2513	2527	rBV	141930	230684	57.57%	7.200%
21	9.774	2615	2623	2635	rBV5	4850	7302	1.82%	0.228%
22	10.523	2847	2856	2865	rVB4	3384	5424	1.35%	0.169%
23	10.754	2913	2928	2943	rVB2	62565	102729	25.64%	3.207%
24	11.471	3139	3151	3161	rBV	15811	25151	6.28%	0.785%
25	11.806	3242	3255	3269	rBV	131234	206389	51.51%	6.442%
26	12.050	3321	3331	3347	rBV	46995	74392	18.57%	2.322%
27	12.188	3362	3374	3390	rVB	155296	248264	61.96%	7.749%
28	12.880	3580	3589	3598	rVB5	9320	13596	3.39%	0.424%
29	13.201	3679	3689	3700	rBV3	8830	12946	3.23%	0.404%

Sum of corrected areas: 3203754

LSC Report - Integrated Chromatogram

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Sample : L3776-17
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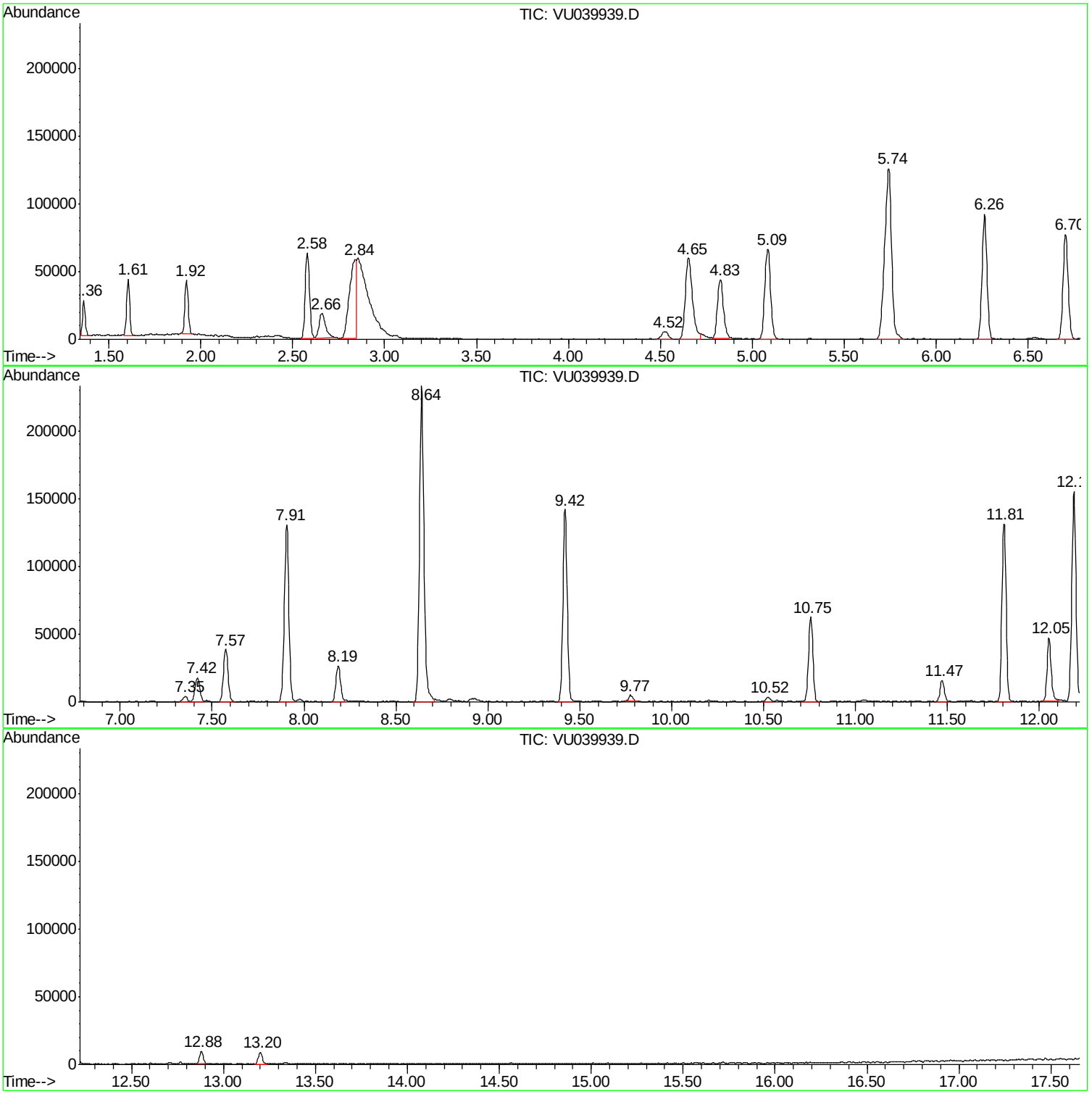
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y16

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

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



Library Search Compound Report

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Acq On : 21 Aug 2020 19:38
Operator : SY/MD
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

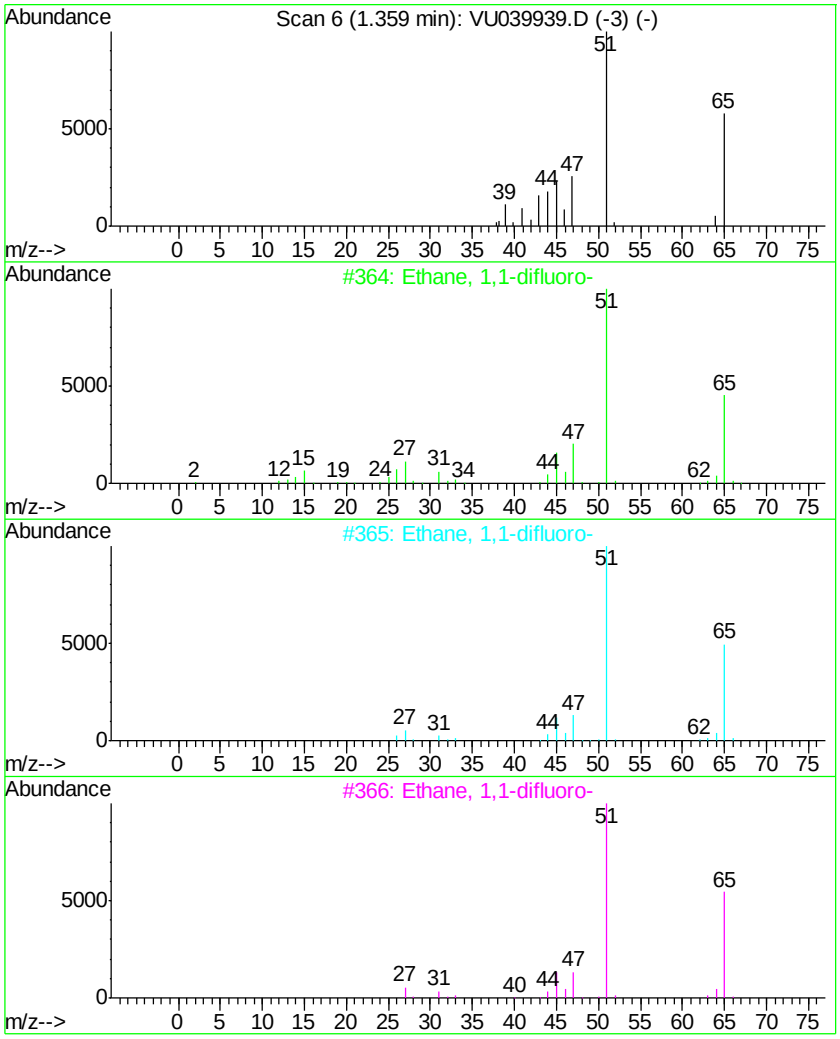
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

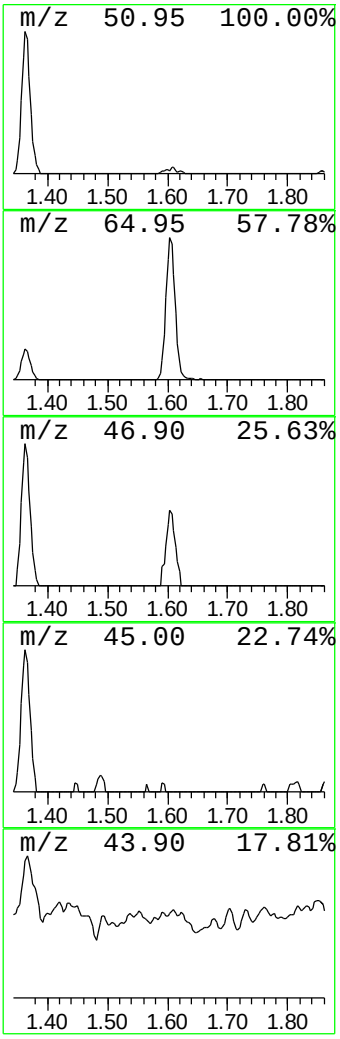
****

Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.36	0.79 ug/L	27015	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	91
2	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	86
3	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	43
4	Propiolonitrile	51	C3HN	001070-71-9	5
5	Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	2





Library Search Compound Report

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Data File : VU039939.D
Acq On : 21 Aug 2020 19:38
Operator : SY/MD
Sample : L3776-17
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y16

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

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

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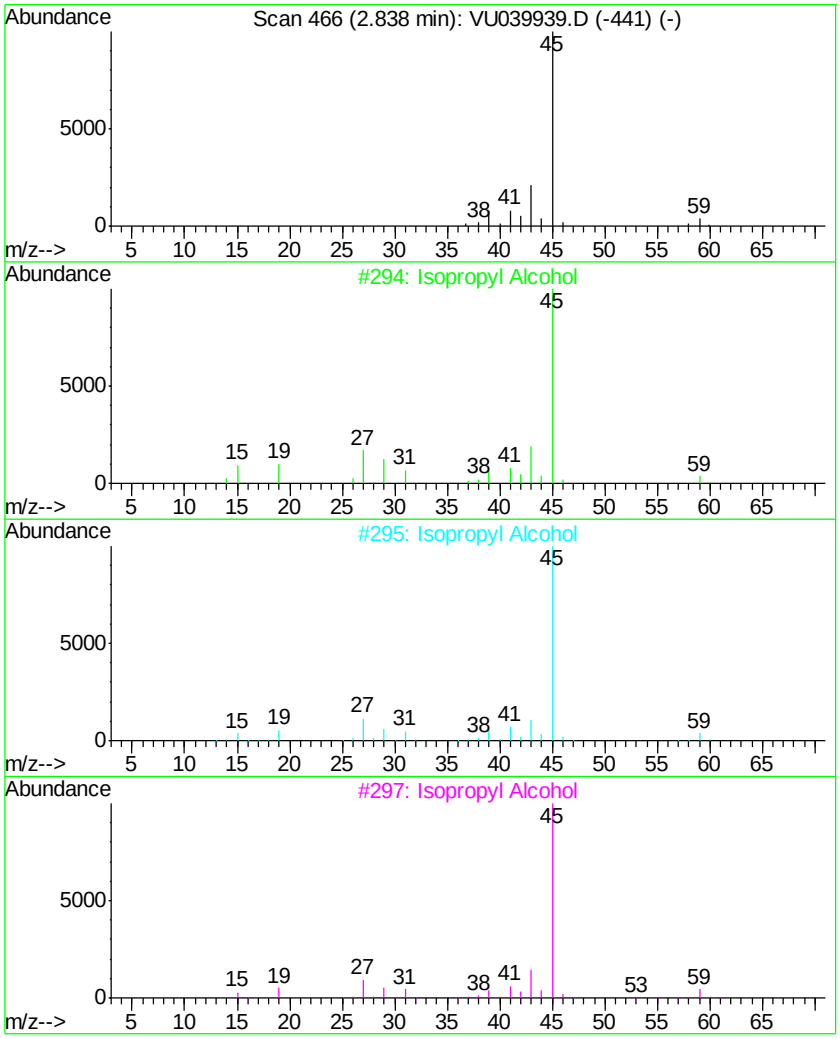
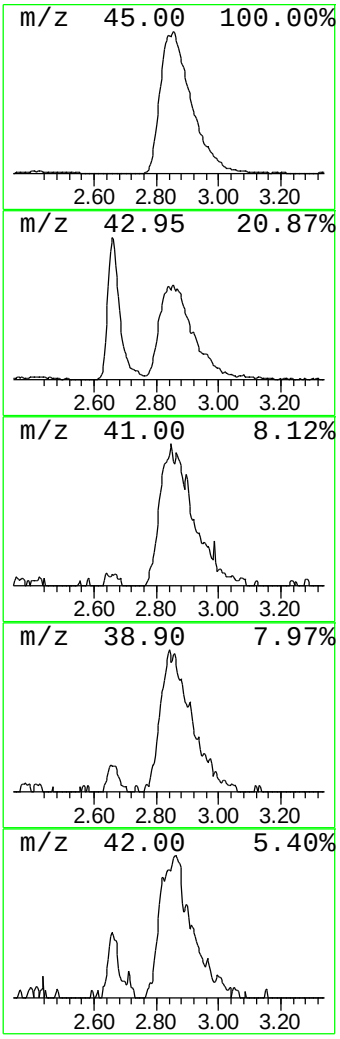
Peak Number 2 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	4.58 ug/L	157208	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	43
5	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU082120\
Data File : VU039939.D
Acq On : 21 Aug 2020 19:38
Operator : SY/MD
Sample : L3776-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y16

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

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

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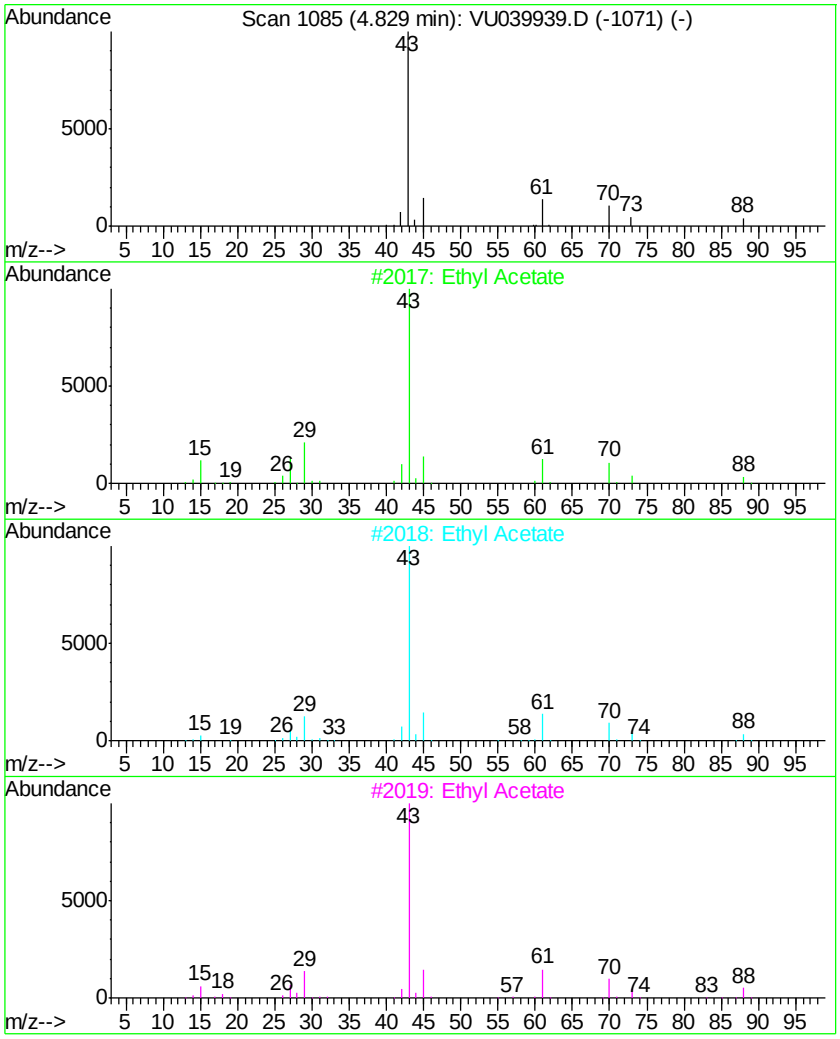
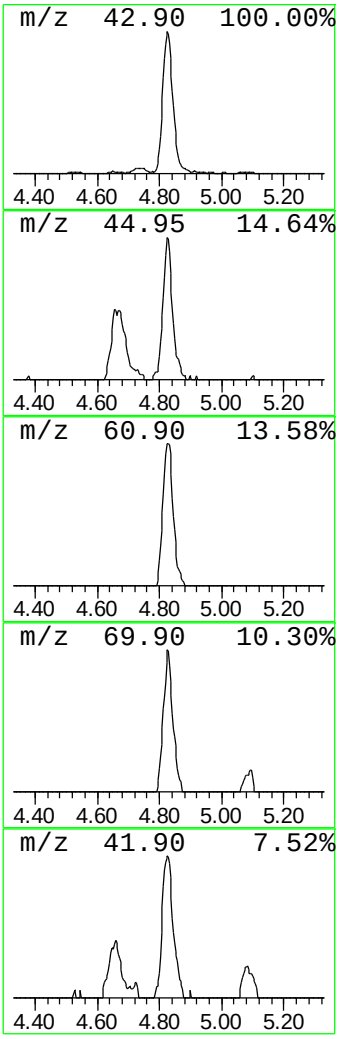
Peak Number 3 Ethyl Acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	2.82 ug/L	96754	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl Acetate	88	C4H8O2	000141-78-6	90
2	Ethyl Acetate	88	C4H8O2	000141-78-6	90
3	Ethyl Acetate	88	C4H8O2	000141-78-6	90
4	Ethyl Acetate	88	C4H8O2	000141-78-6	83
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	42





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Data File : VU039939.D
Acq On : 21 Aug 2020 19:38
Operator : SY/MD
Sample : L3776-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y16

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

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

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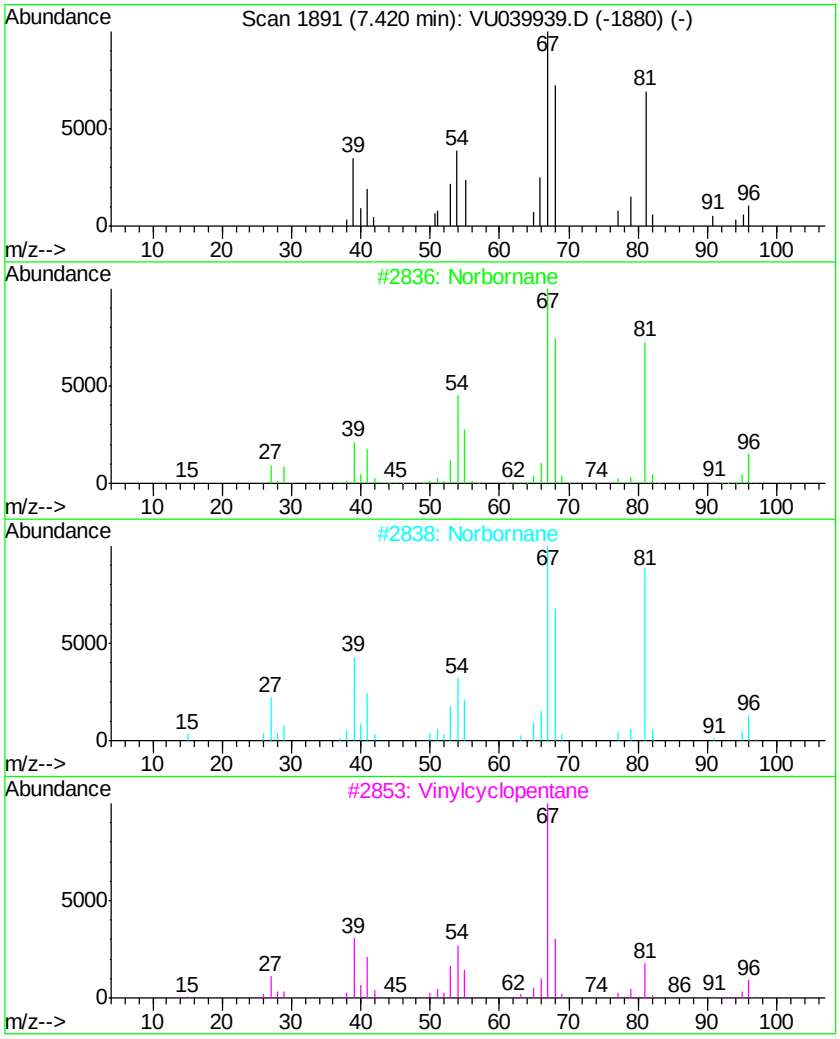
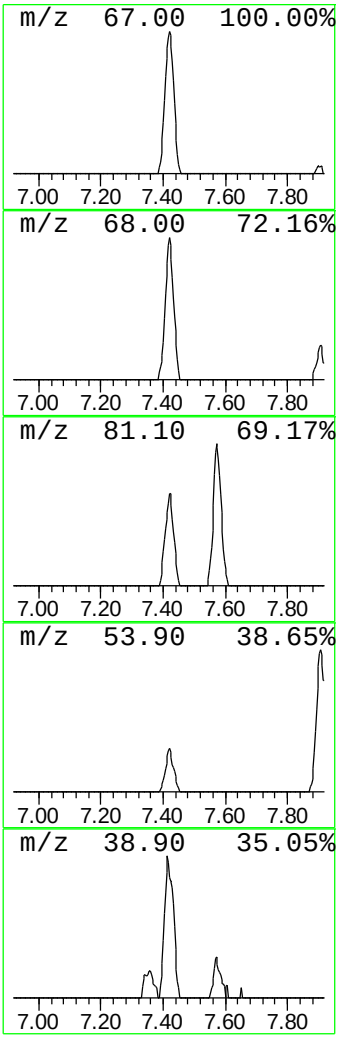
Peak Number 4 Norbornane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	0.96 ug/L	32984	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Norbornane	96	C7H12	000279-23-2	58
2	Norbornane	96	C7H12	000279-23-2	53
3	Vinylcyclopentane	96	C7H12	003742-34-5	52
4	Norbornane	96	C7H12	000279-23-2	50
5	Vinylcyclopentane	96	C7H12	003742-34-5	47





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Operator : SY/MD
Sample : L3776-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y16

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

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

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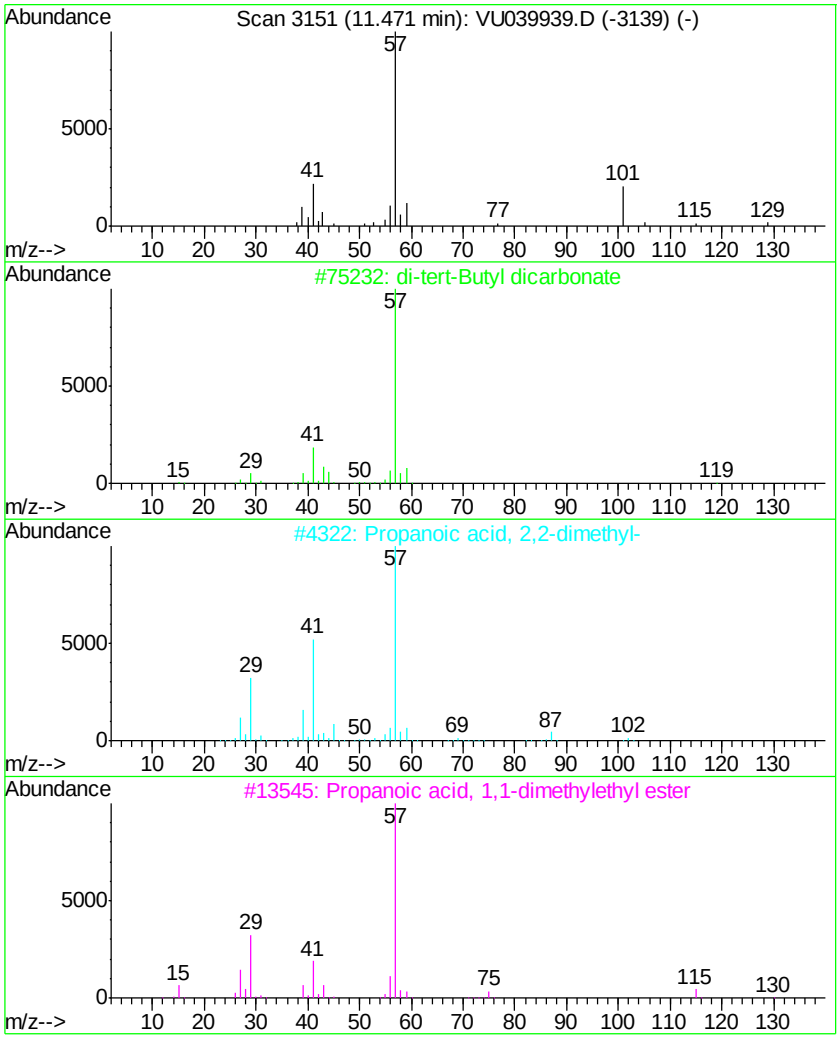
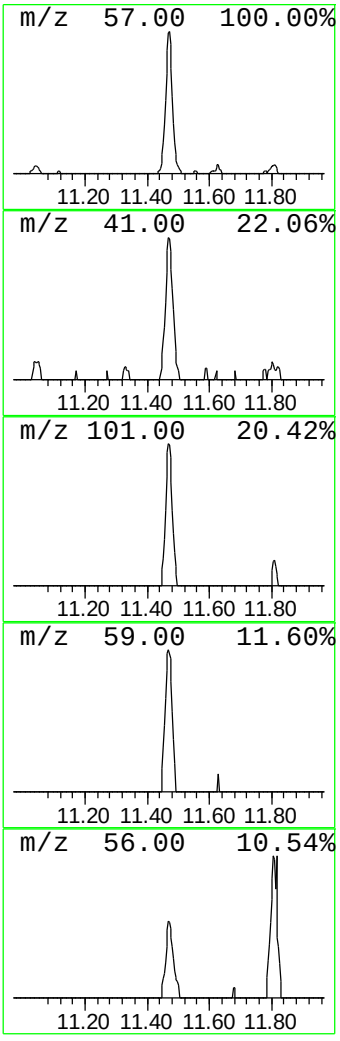
Peak Number 6 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	0.61 ug/L	25151	1,4-Dichlorobenzene-d4	11.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	47
2	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	38
3	Propanoic acid, 1,1-dimethylethy...	130	C7H14O2	020487-40-5	37
4	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	28
5	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	25





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

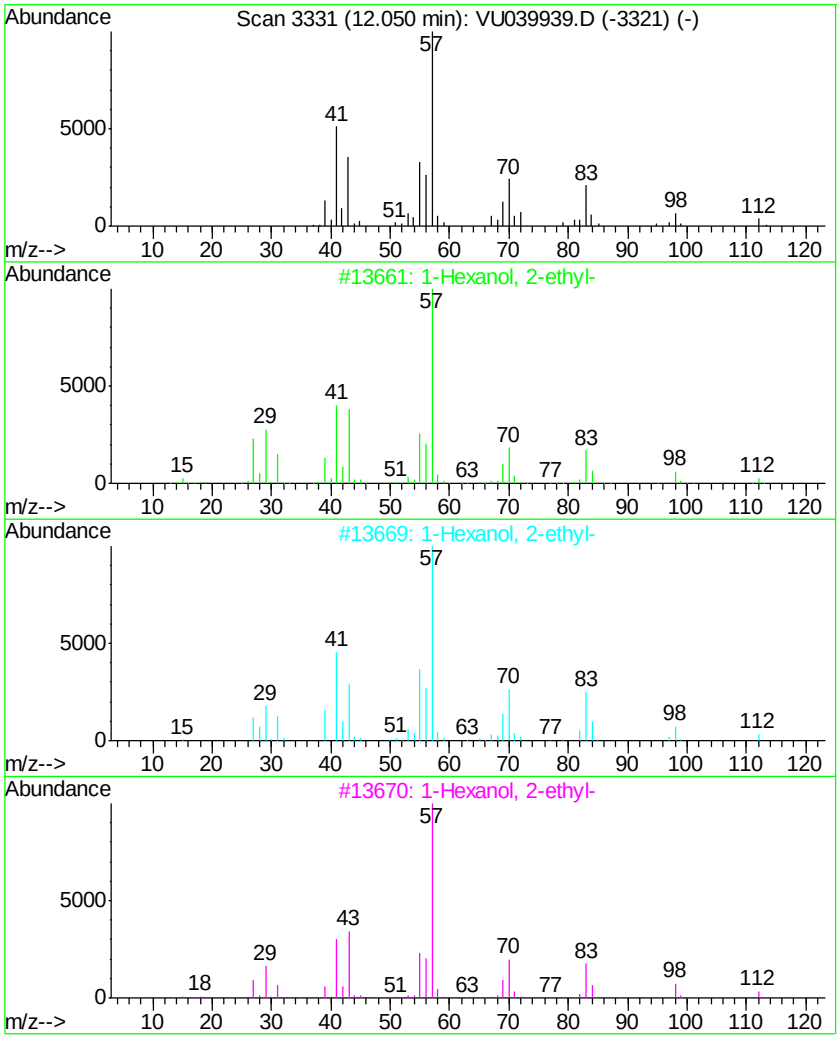
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

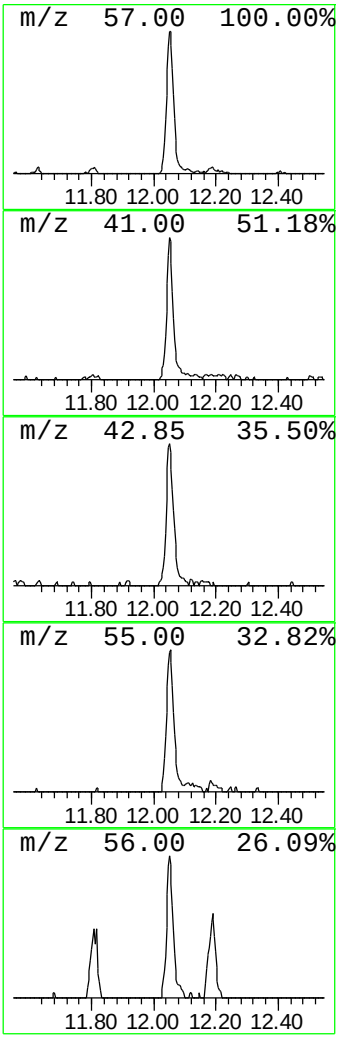
****

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	1.80 ug/L	74392	1,4-Dichlorobenzene-d4	11.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	80
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	50





Tentatively Identified Compound (LSC) summary

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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
Ethane, 1,1-diflu...	1.36	0.8	ug/L	27015	1	6.26	171586	5.0
Isopropyl Alcohol	2.84	4.6	ug/L	157208	1	6.26	171586	5.0
Ethyl Acetate	4.83	2.8	ug/L	96754	1	6.26	171586	5.0
Norbornane	7.42	1.0	ug/L	32984	1	6.26	171586	5.0
unknown-01	11.47	0.6	ug/L	25151	3	11.81	206389	5.0
1-Hexanol, 2-ethyl-	12.05	1.8	ug/L	74392	3	11.81	206389	5.0