LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082520\
Data File : VU039968.D
Acq On : 25 Aug 2020 15:20
Operator : SY/MD
Sample : L3777-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y24

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	1.366	3	8	14	rBV	21045	20732	5.56%	0.554%
2	1.498	45	49	57	rVB2	4930	5410	1.45%	0.145%
3	1.604	73	82	90	rBV	43052	53979	14.47%	1.443%
4	1.922	173	181	192	rBV	34341	44324	11.88%	1.185%
5	2.581	376	386	398	rVV	65491	104838	28.10%	2.803%
6	2.658	398	410	429	rVV	22636	49796	13.35%	1.331%
7	2.838	442	466	523	rBV2	58434	373072	100.00%	9.974%
8	3.388	622	637	653	rVB2	8987	19930	5.34%	0.533%
9	3.893	777	794	815	rBV	123605	293757	78.74%	7.853%
10	4.022	819	834	847	rVB3	3398	8170	2.19%	0.218%
11	4.526	969	991	1013	rVB	45741	116753	31.30%	3.121%
12	4.655	1013	1031	1053	rBV	50131	131054	35.13%	3.504%
13	4.829	1073	1085	1104	rVB2	13412	31241	8.37%	0.835%
14	5.086	1149	1165	1181	rBV	60814	132832	35.60%	3.551%
15	5.600	1310	1325	1341	rBV2	23803	52319	14.02%	1.399%
16	5.742	1348	1369	1384	rBV2	119218	304869	81.72%	8.151%
17	6.266	1518	1532	1552	rBV	102326	196599	52.70%	5.256%
18	6.510	1594	1608	1623	rBV2	41090	79781	21.38%	2.133%
19	6.703	1654	1668	1684	rBV2	75652	147693	39.59%	3.949%
20	7.169	1805	1813	1823	rBV6	2199	3936	1.06%	0.105%
21	7.308	1849	1856	1867	rVB4	2506	4027	1.08%	0.108%
22	7.472	1896	1907	1922	rBV3	6239	12220	3.28%	0.327%
23	7.575	1928	1939	1953	rBV2	38845	66264	17.76%	1.772%
24	7.726	1979	1986	1996	rVB6	2641	4500	1.21%	0.120%
25	7.906	2022	2042	2057	rBV	143311	245046	65.68%	6.551%
26	8.189	2119	2130	2143	rBV	24806	41806	11.21%	1.118%
27	8.639	2258	2270	2298	rBV	178992	316563	84.85%	8.463%
28	8.931	2349	2361	2371	rBV4	2132	4125	1.11%	0.110%
29	9.420	2500	2513	2527	rBV	147685	242362	64.96%	6.479%
30	10.754	2915	2928	2943	rVB	53175	86993	23.32%	2.326%
31	11.471	3137	3151	3166	rBV	29804	47090	12.62%	1.259%
32	11.806	3244	3255	3270	rVB	149293	232275	62.26%	6.210%
33	12.053	3322	3332	3348	rBV3	24887	40356	10.82%	1.079%
34	12.188	3362	3374	3390	rVB	142883	225749	60.51%	6.035%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082520\
Data File : VU039968.D
Acq On : 25 Aug 2020 15:20
Operator : SY/MD
Sample : L3777-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y24

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

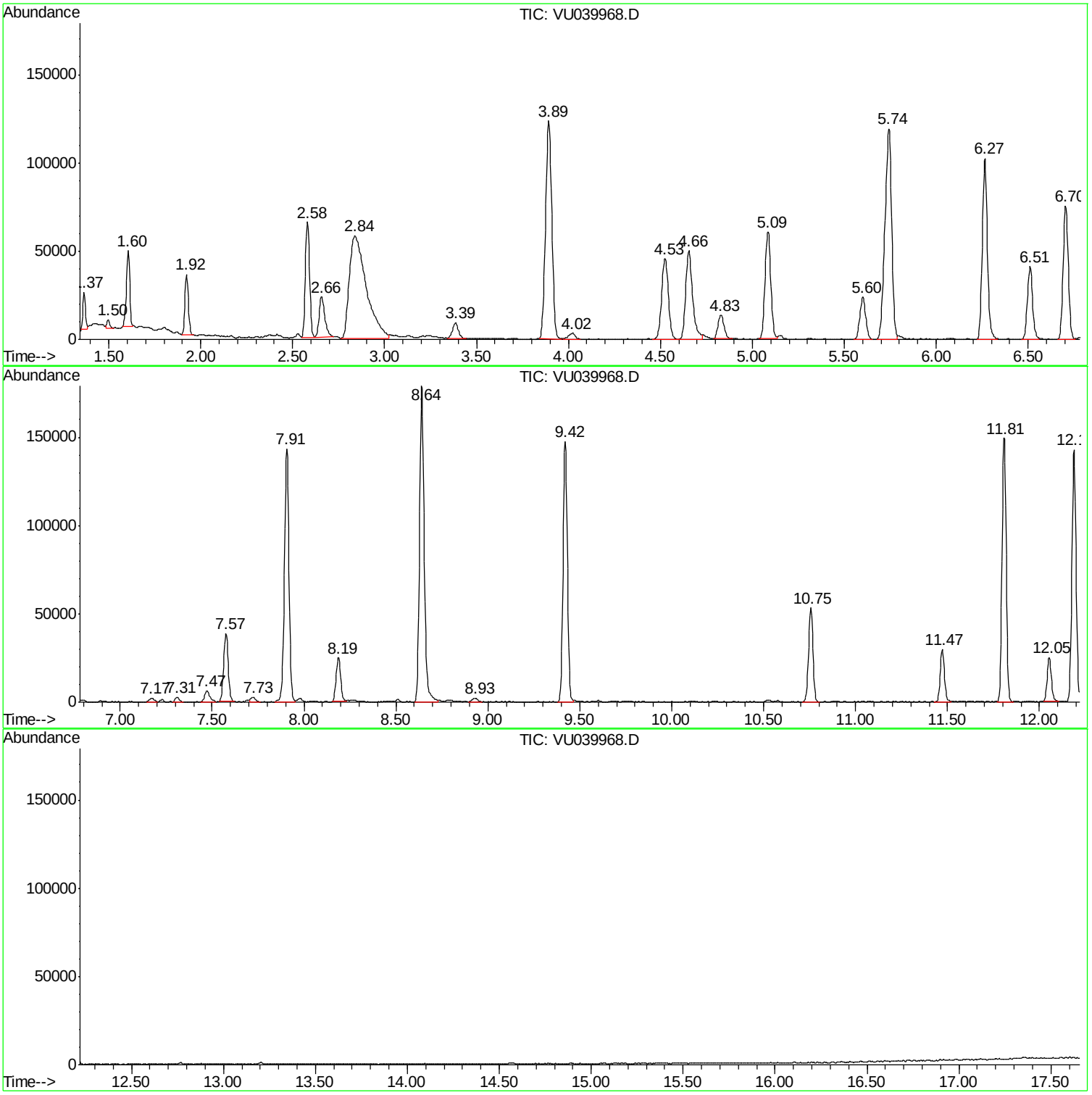
Sum of corrected areas: 3740461

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082520\
Data File : VU039968.D
Acq On : 25 Aug 2020 15:20
Operator : SY/MD
Sample : L3777-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y24

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

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082520\
Data File : VU039968.D
Acq On : 25 Aug 2020 15:20
Operator : SY/MD
Sample : L3777-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y24

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

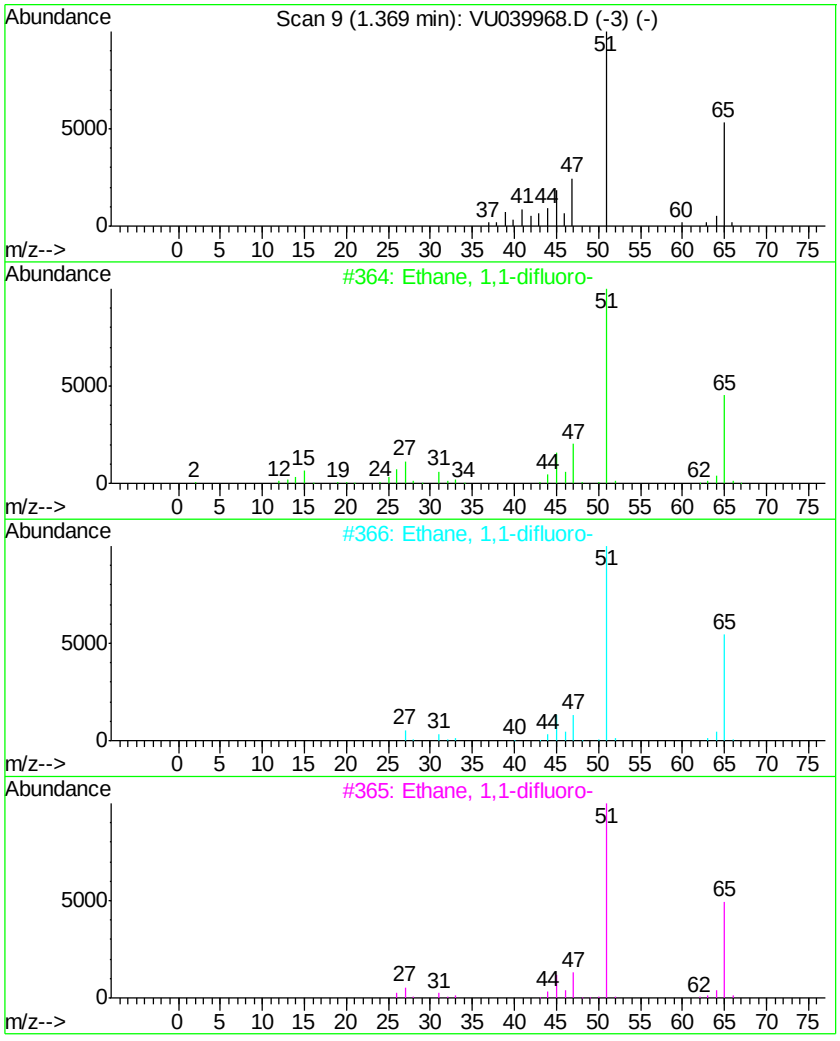
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

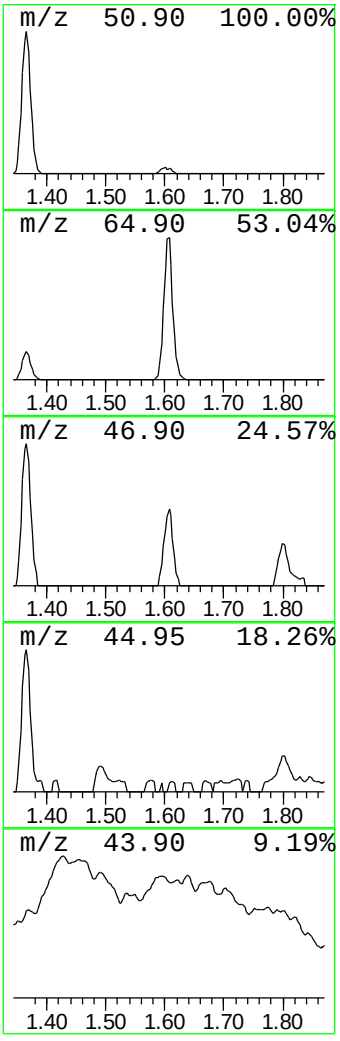
****

Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	0.53 ug/L	20732	1,4-Difluorobenzene	6.27

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	90
3	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	90
4	Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	4
5	Propiolonitrile	51	C3HN	001070-71-9	3





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082520\
Data File : VU039968.D
Acq On : 25 Aug 2020 15:20
Operator : SY/MD
Sample : L3777-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y24

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

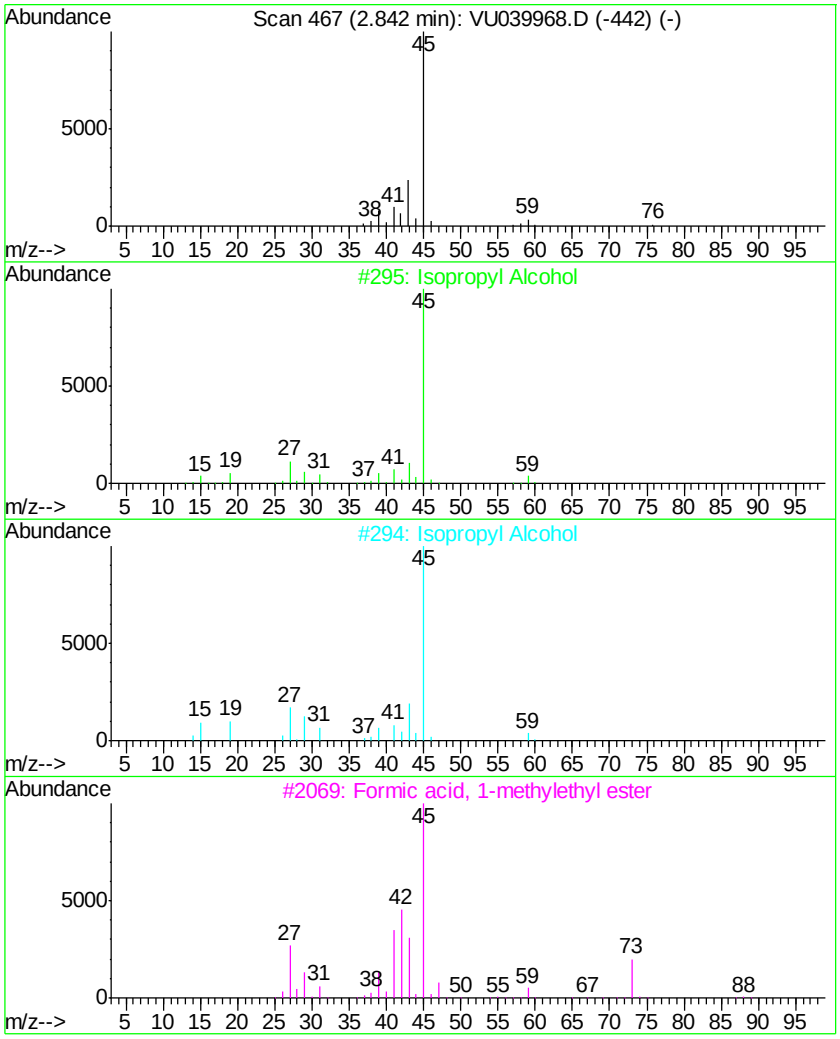
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

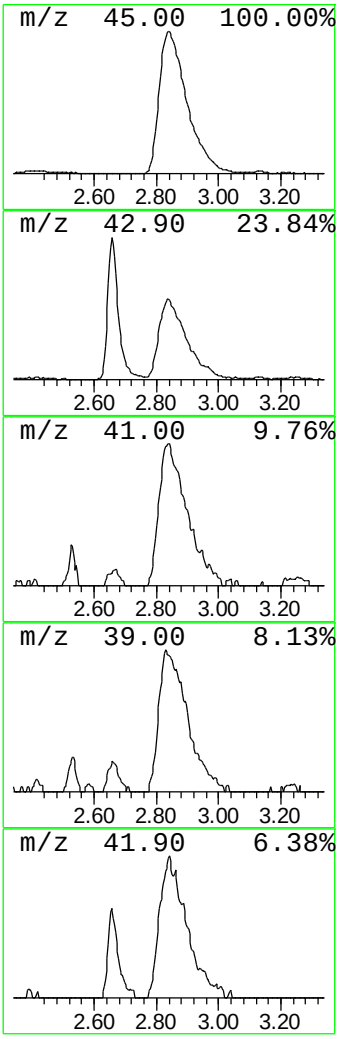
****

Peak Number 2 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	9.49 ug/L	373072	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3	Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	Propylene Glycol	76	C3H8O2	000057-55-6	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082520\
Data File : VU039968.D
Acq On : 25 Aug 2020 15:20
Operator : SY/MD
Sample : L3777-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y24

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

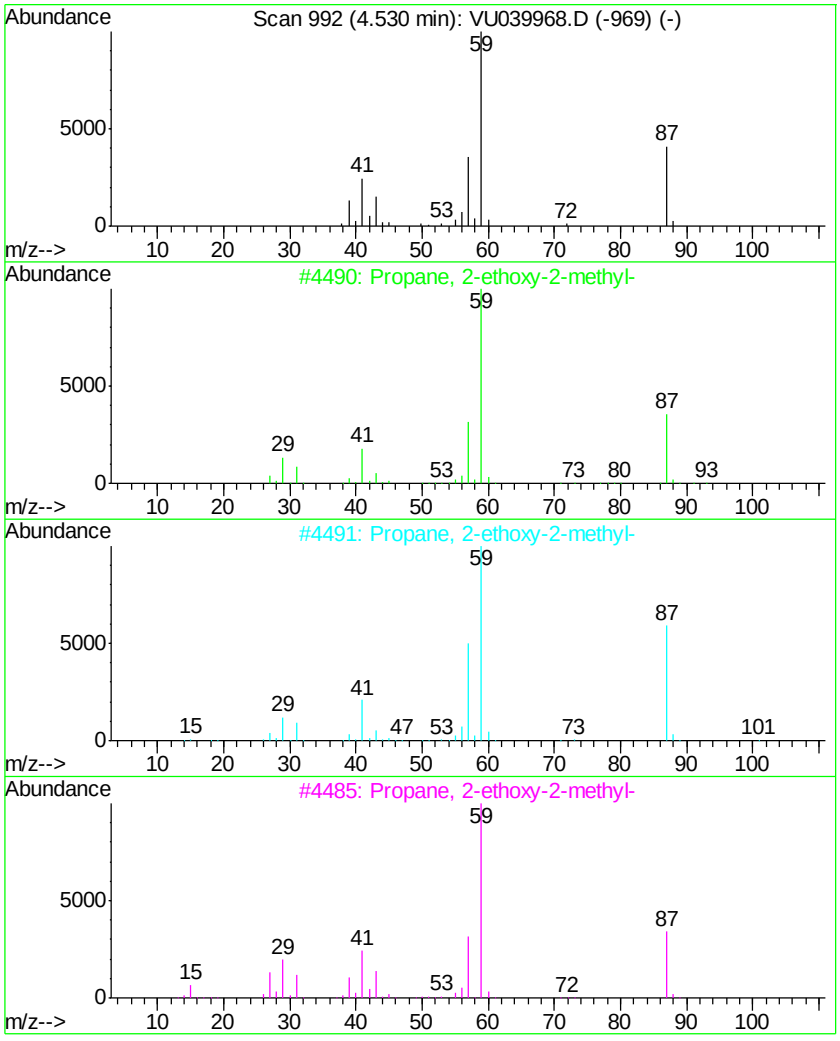
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

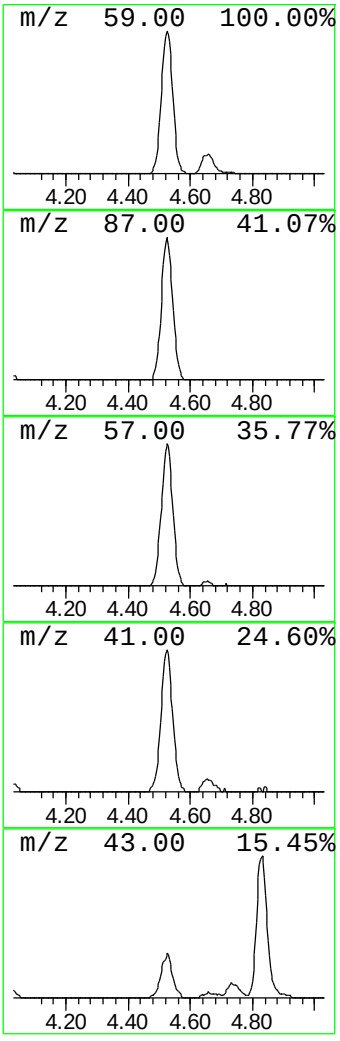
****

Peak Number 3 Propane, 2-ethoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	2.97 ug/L	116753	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	83
2	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	83
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	83
4	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	43
5	Propanamide, 2-methoxy-N-methyl-	117	C5H11NO2	1000196-12-6	40





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082520\
Data File : VU039968.D
Acq On : 25 Aug 2020 15:20
Operator : SY/MD
Sample : L3777-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y24

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

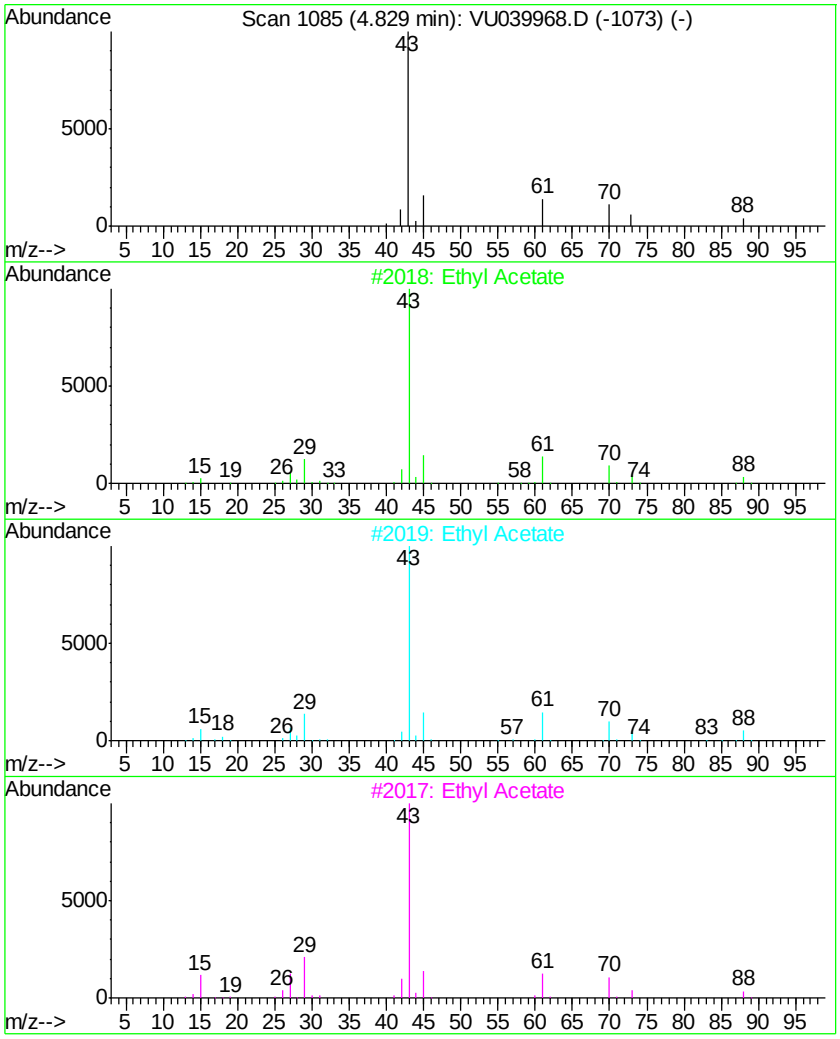
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

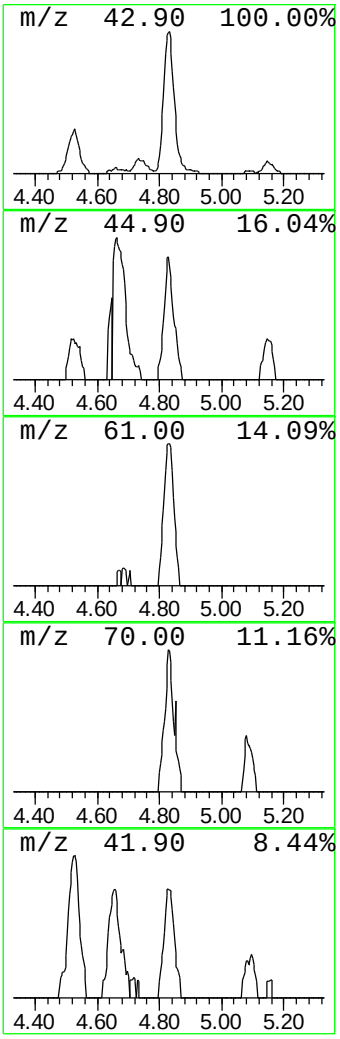
****

Peak Number 4 Ethyl Acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	0.79 ug/L	31241	1,4-Difluorobenzene	6.27

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	64





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082520\
Data File : VU039968.D
Acq On : 25 Aug 2020 15:20
Operator : SY/MD
Sample : L3777-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y24

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

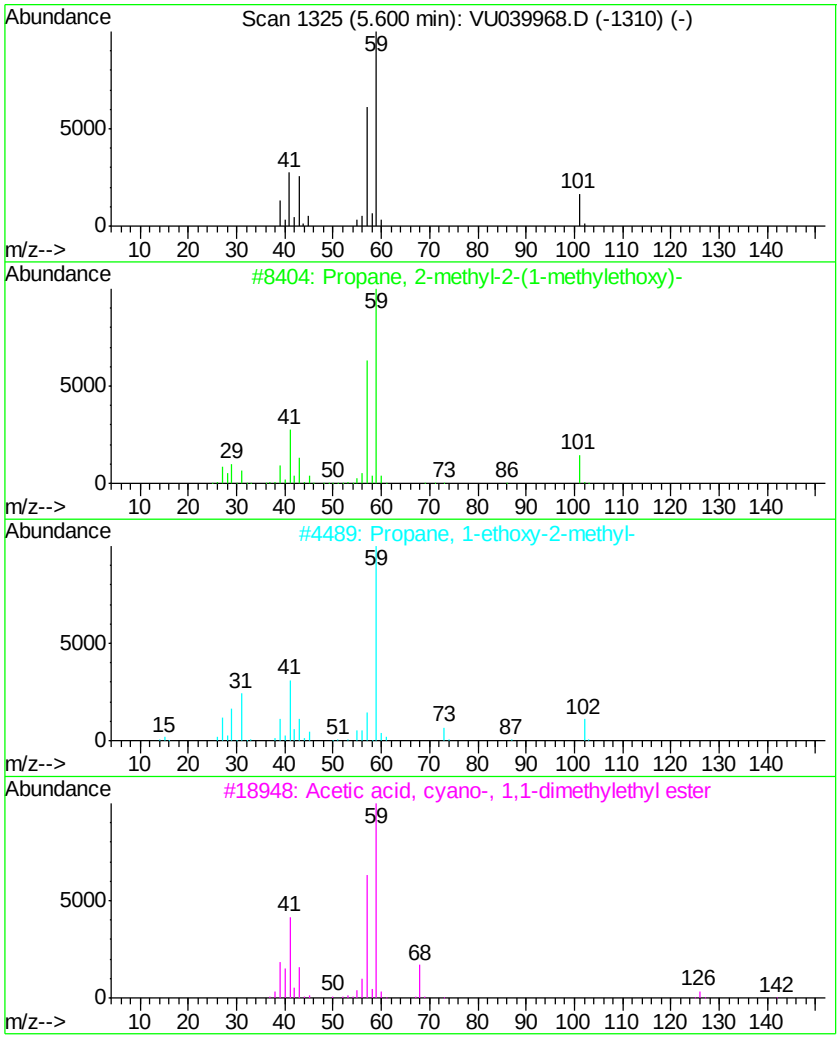
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

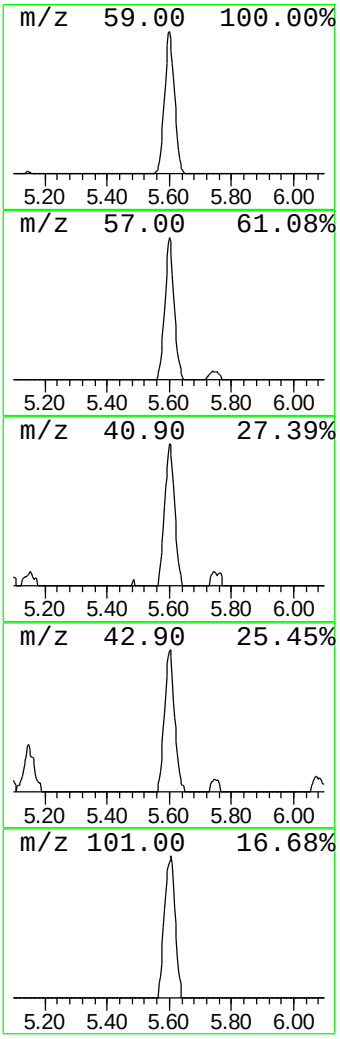
****

Peak Number 5 Propane, 2-methyl-2-(1-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	1.33 ug/L	52319	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	83
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	56
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	56
4	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	40
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	40





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082520\
Data File : VU039968.D
Acq On : 25 Aug 2020 15:20
Operator : SY/MD
Sample : L3777-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y24

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

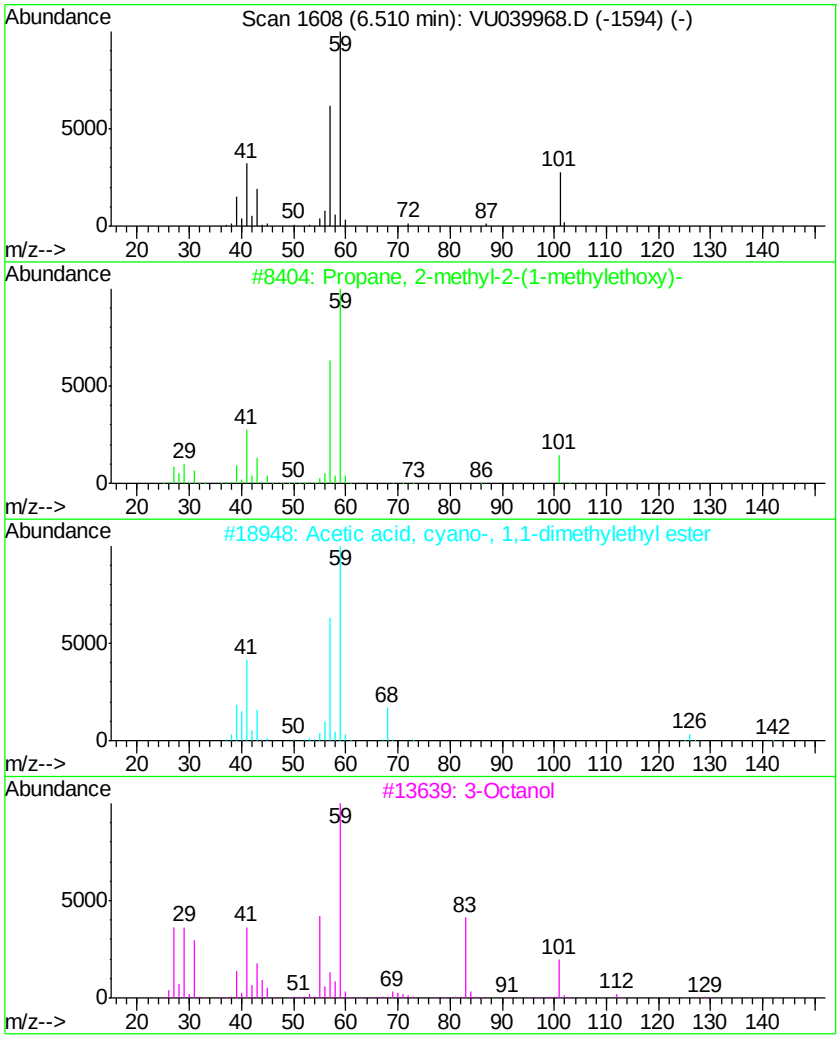
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

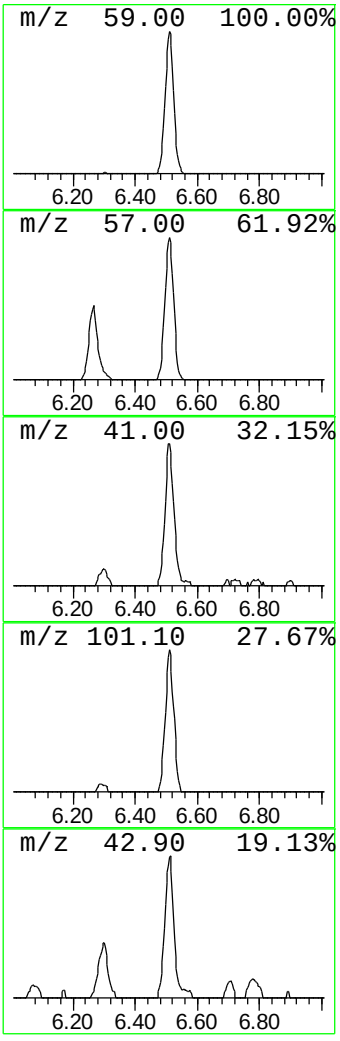
****

Peak Number 6 Acetic acid, cyano-, 1,1-di... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	2.03 ug/L	79781	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	78
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	64
3	3-Octanol	130	C8H18O	000589-98-0	64
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	36





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU082520\
Data File : VU039968.D
Acq On : 25 Aug 2020 15:20
Operator : SY/MD
Sample : L3777-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y24

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

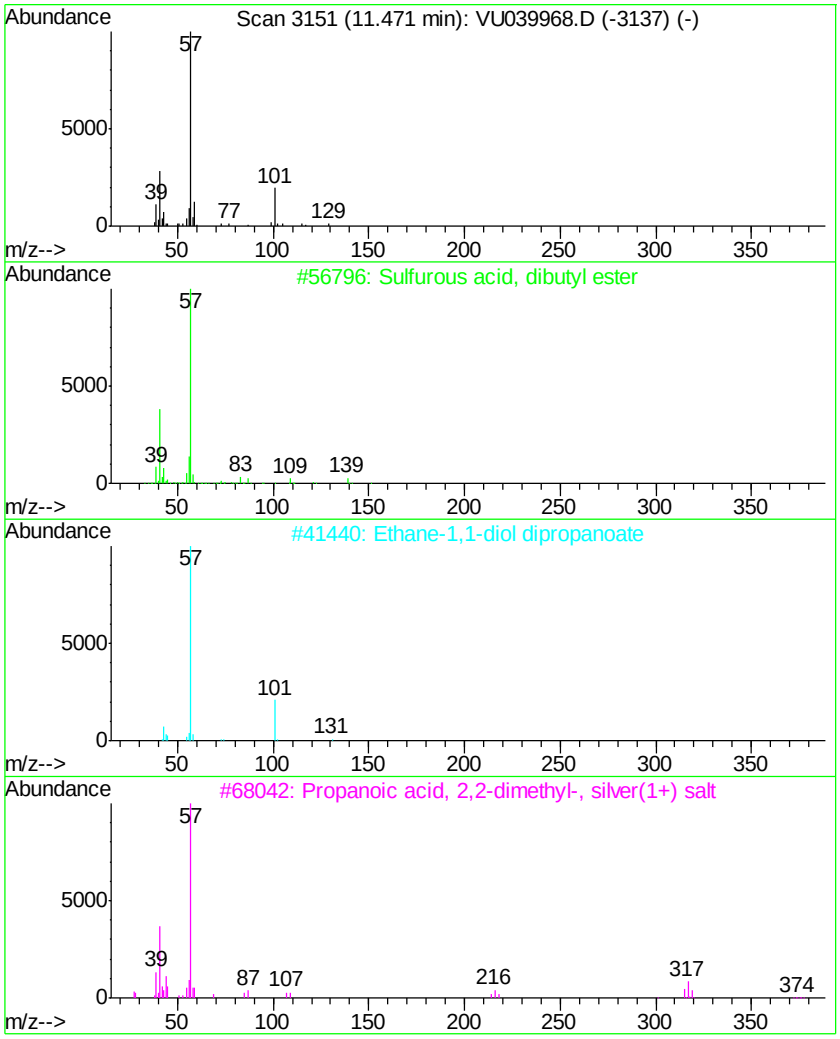
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

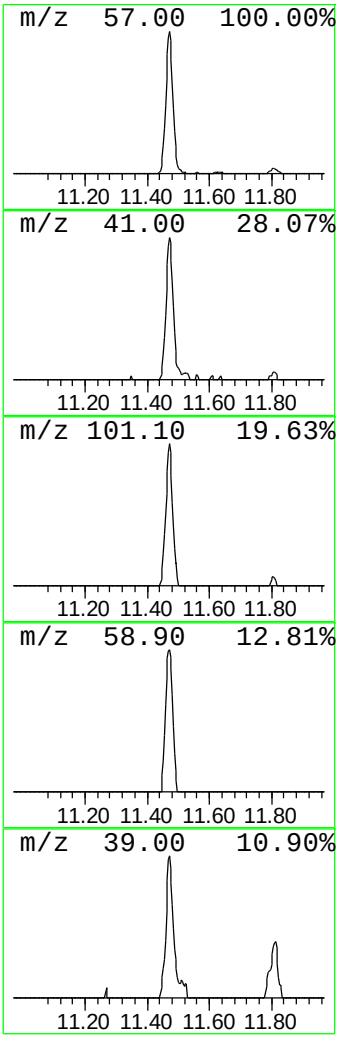
****

Peak Number 8 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	1.01 ug/L	47090	1,4-Dichlorobenzene-d4	11.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	38
2	Ethane-1,1-diol dipropanoate	174	C8H14O4	026880-30-8	38
3	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	37
4	Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	32
5	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	28





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082520\
Data File : VU039968.D
Acq On : 25 Aug 2020 15:20
Operator : SY/MD
Sample : L3777-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y24

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

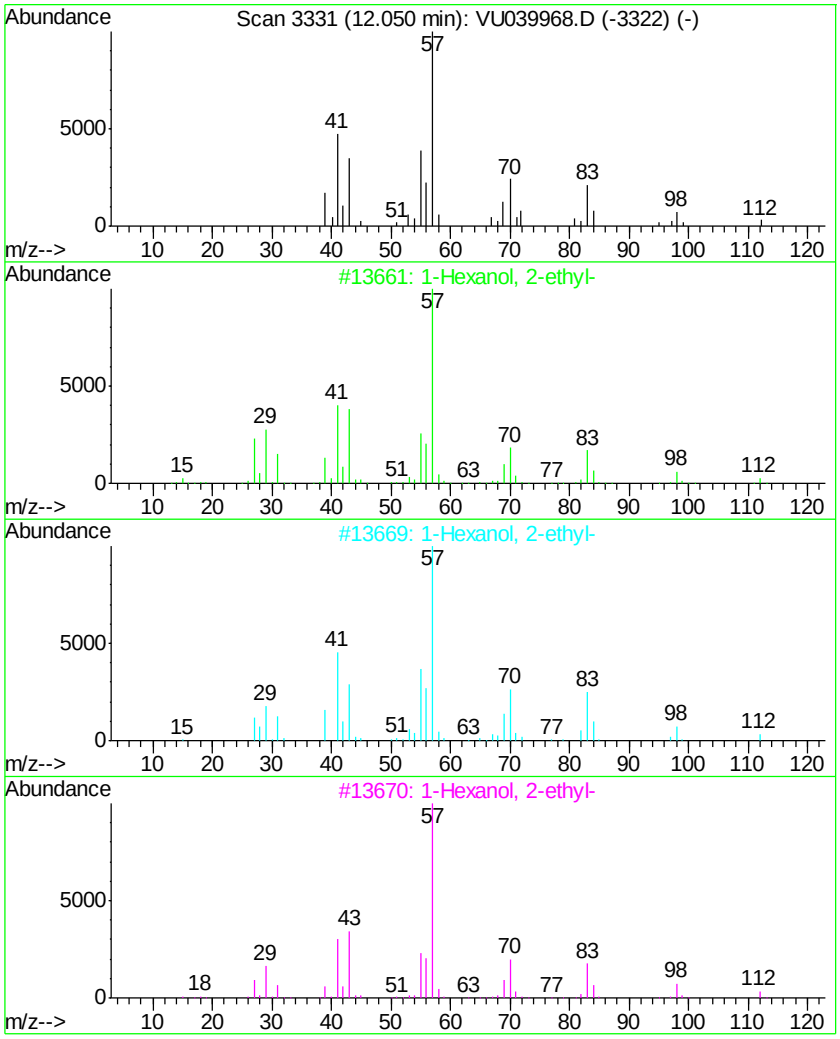
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

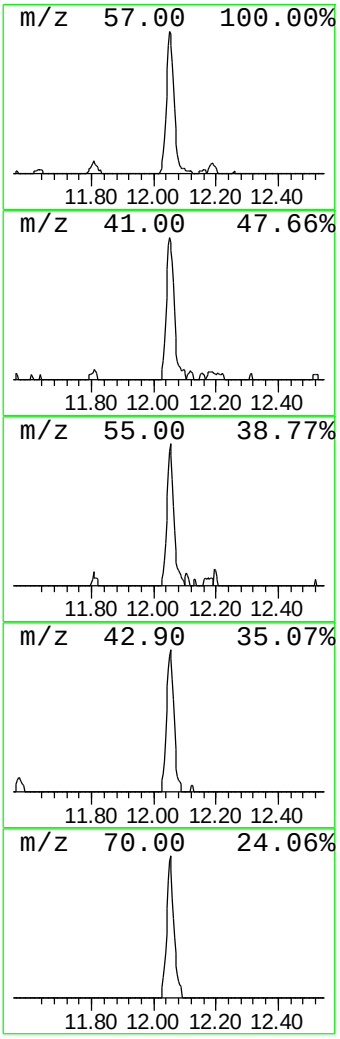
****

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	0.87 ug/L	40356	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	78
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU082520\
Data File : VU039968.D
Acq On : 25 Aug 2020 15:20
Operator : SY/MD
Sample : L3777-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y24

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethane, 1,1-diflu...	1.37	0.5	ug/L	20732	1	6.27	196599	5.0
Isopropyl Alcohol	2.84	9.5	ug/L	373072	1	6.27	196599	5.0
Propane, 2-ethoxy...	4.53	3.0	ug/L	116753	1	6.27	196599	5.0
Ethyl Acetate	4.83	0.8	ug/L	31241	1	6.27	196599	5.0
Propane, 2-methyl...	5.60	1.3	ug/L	52319	1	6.27	196599	5.0
Acetic acid, cyan...	6.51	2.0	ug/L	79781	1	6.27	196599	5.0
unknown-01	11.47	1.0	ug/L	47090	3	11.81	232275	5.0
1-Hexanol, 2-ethyl-	12.05	0.9	ug/L	40356	3	11.81	232275	5.0