LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038382.D
Acq On : 29 May 2020 17:42
Operator : JC/MD
Sample : L2749-08DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X3DL

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\SOMUTR050720WMA.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	1.514	43	54	69	rBV3	28516	88658	4.54%	0.493%
2	1.613	77	85	95	rVB	142957	158869	8.13%	0.884%
3	1.932	176	184	202	rVB	124030	165364	8.46%	0.920%
4	2.401	318	330	349	rVB	413282	618259	31.65%	3.440%
5	2.591	377	389	405	rBV	240241	392614	20.10%	2.185%
6	2.671	405	414	432	rVB2	13505	28695	1.47%	0.160%
7	3.218	570	584	595	rBV2	17849	40297	2.06%	0.224%
8	3.395	625	639	655	rVB5	29887	66095	3.38%	0.368%
9	3.735	730	745	763	rBV4	21728	49114	2.51%	0.273%
10	4.035	817	838	866	rBV	754253	1953626	100.00%	10.871%
11	4.571	987	1005	1021	rBV3	74816	180640	9.25%	1.005%
12	4.674	1021	1037	1082	rVB3	231228	665178	34.05%	3.701%
13	5.102	1154	1170	1194	rBV	217927	481548	24.65%	2.680%
14	5.424	1252	1270	1284	rBV5	21997	50736	2.60%	0.282%
15	5.761	1354	1375	1402	rBV2	440604	1211082	61.99%	6.739%
16	5.887	1402	1414	1427	rBV7	12721	31669	1.62%	0.176%
17	6.282	1520	1537	1563	rBV	404508	789444	40.41%	4.393%
18	6.723	1659	1674	1688	rBV	281756	549469	28.13%	3.057%
19	6.790	1689	1695	1705	rVB5	12710	24638	1.26%	0.137%
20	7.591	1930	1944	1962	rBV2	143242	249764	12.78%	1.390%
21	7.742	1978	1991	2006	rVB3	11523	22722	1.16%	0.126%
22	7.922	2025	2047	2065	rBV	531197	985961	50.47%	5.486%
23	8.202	2120	2134	2149	rBV	93088	153722	7.87%	0.855%
24	8.655	2262	2275	2307	rBV	802304	1452333	74.34%	8.081%
25	9.439	2504	2519	2521	rBV	598627	868807	44.47%	4.834%
26	9.465	2522	2527	2558	rVB	946901	1561966	79.95%	8.691%
27	10.124	2714	2732	2746	rVB6	18141	37254	1.91%	0.207%
28	10.500	2834	2849	2863	rBV	1021944	1632897	83.58%	9.086%
29	10.771	2913	2933	2958	rVB	222674	383894	19.65%	2.136%
30	10.906	2961	2975	2990	rBV4	91551	168684	8.63%	0.939%
31	11.002	2997	3005	3013	rBV3	12555	23014	1.18%	0.128%
32	11.304	3089	3099	3120	rVB	34228	63828	3.27%	0.355%
33	11.433	3123	3139	3148	rBV	45387	75584	3.87%	0.421%
34	11.652	3201	3207	3230	rVB5	16073	29583	1.51%	0.165%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038382.D
Acq On : 29 May 2020 17:42
Operator : JC/MD
Sample : L2749-08DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X3DL

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\SOMUTR050720WMA.M
Title : TRACE VOA SOM01.0

35	11.825	3246	3261	3276	rBV	658511	1141351	58.42%	6.351%
36	11.899	3276	3284	3295	rVB4	89022	139072	7.12%	0.774%
37	12.105	3335	3348	3359	rVB2	40468	64711	3.31%	0.360%
38	12.205	3365	3379	3398	rBV	605665	1038446	53.15%	5.778%
39	12.584	3477	3497	3506	rBV2	38824	66044	3.38%	0.367%
40	12.796	3553	3563	3568	rBV3	21839	35331	1.81%	0.197%
41	12.838	3568	3576	3585	rVV	66589	109155	5.59%	0.607%
42	12.889	3585	3592	3603	rVB4	12552	21155	1.08%	0.118%
43	12.992	3614	3624	3632	rBV2	22770	34379	1.76%	0.191%
44	13.880	3886	3900	3912	rBV2	9623	21233	1.09%	0.118%
45	14.028	3937	3946	3960	rVB6	22495	44426	2.27%	0.247%

Sum of corrected areas: 17971311

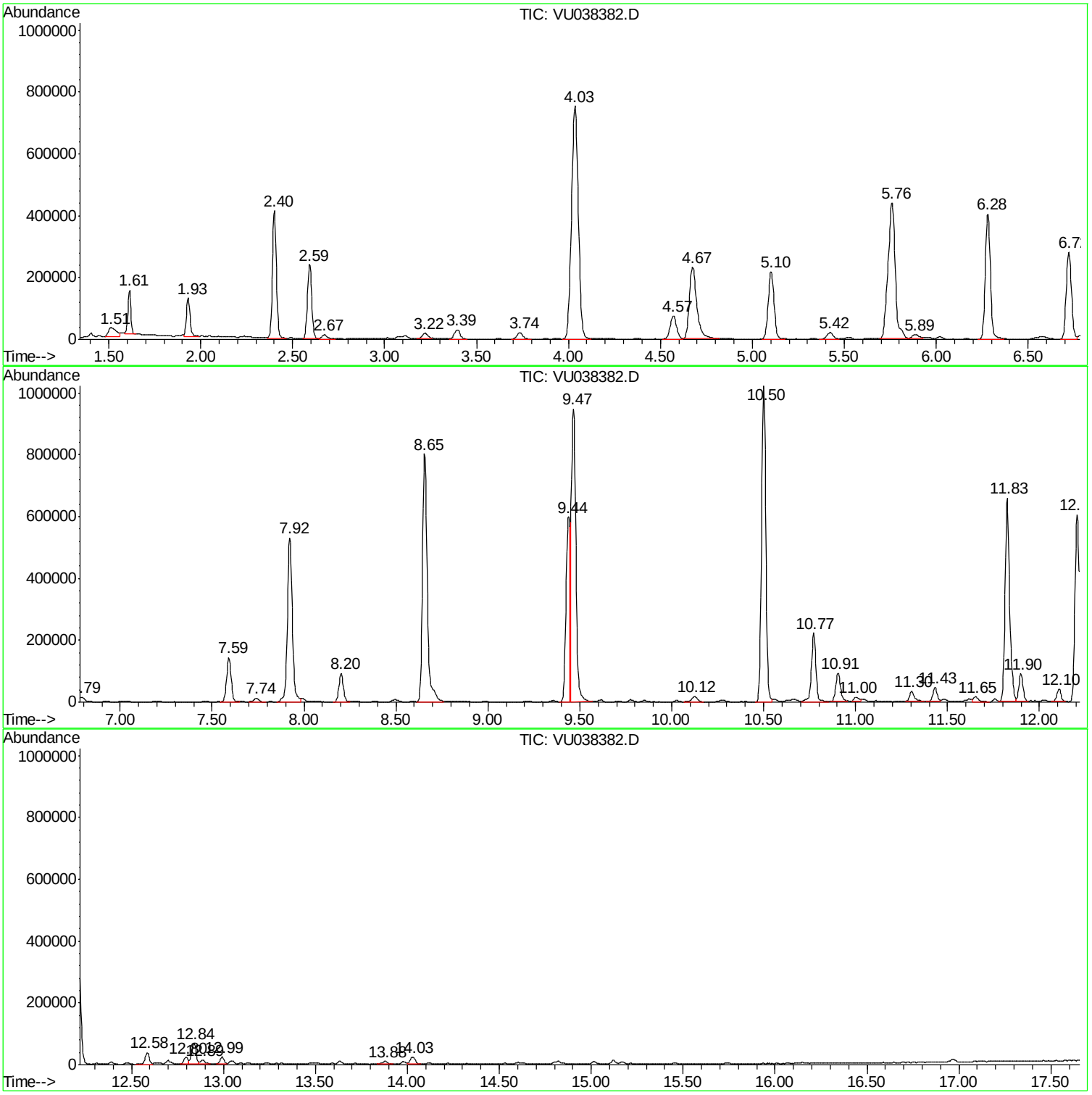
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038382.D
Acq On : 29 May 2020 17:42
Operator : JC/MD
Sample : L2749-08DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.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\VU053020\
Data File : VU038382.D
Acq On : 29 May 2020 17:42
Operator : JC/MD
Sample : L2749-08DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

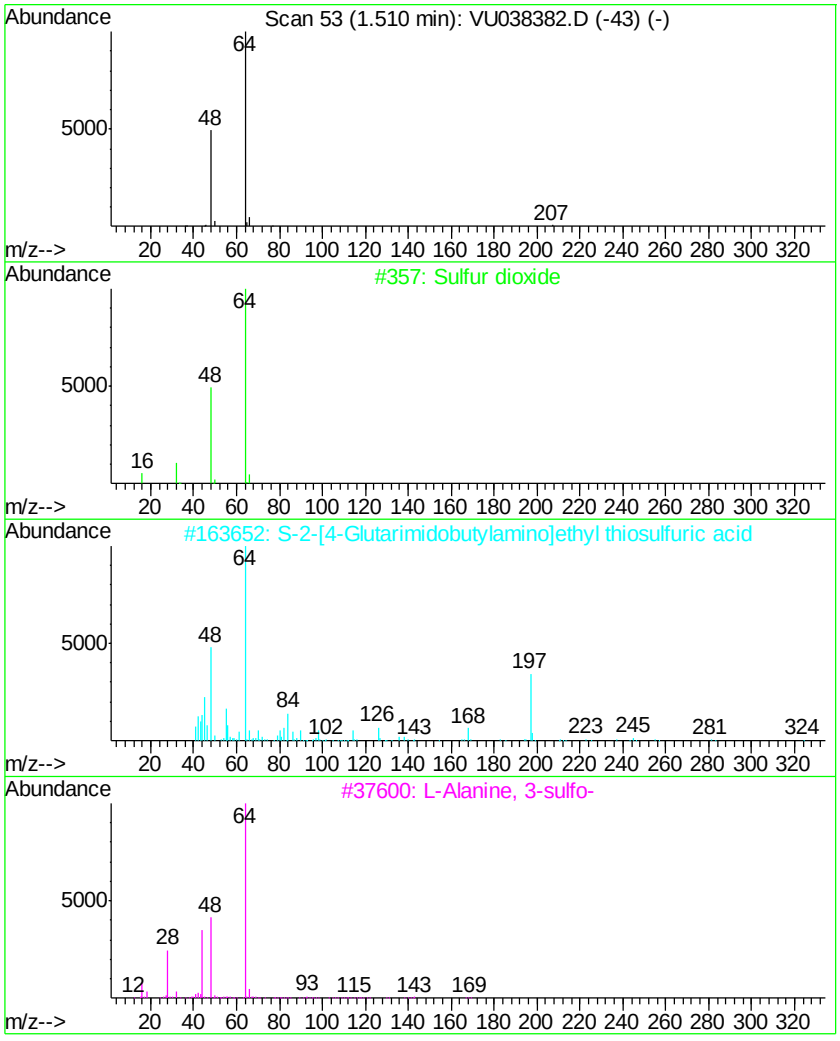
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

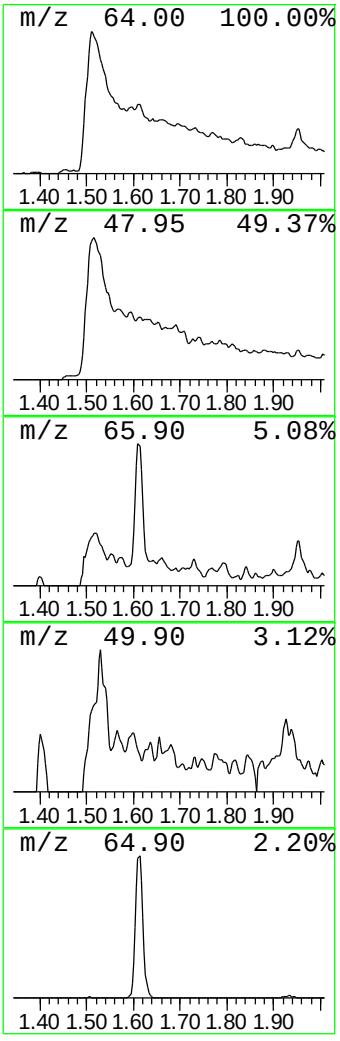
****

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.51	0.56 ug/L	88658	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	74
2	S-2-[4-Glutarimidobutylamino]eth...	324	C11H20N2O5S2	031701-78-7	9
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038382.D
Acq On : 29 May 2020 17:42
Operator : JC/MD
Sample : L2749-08DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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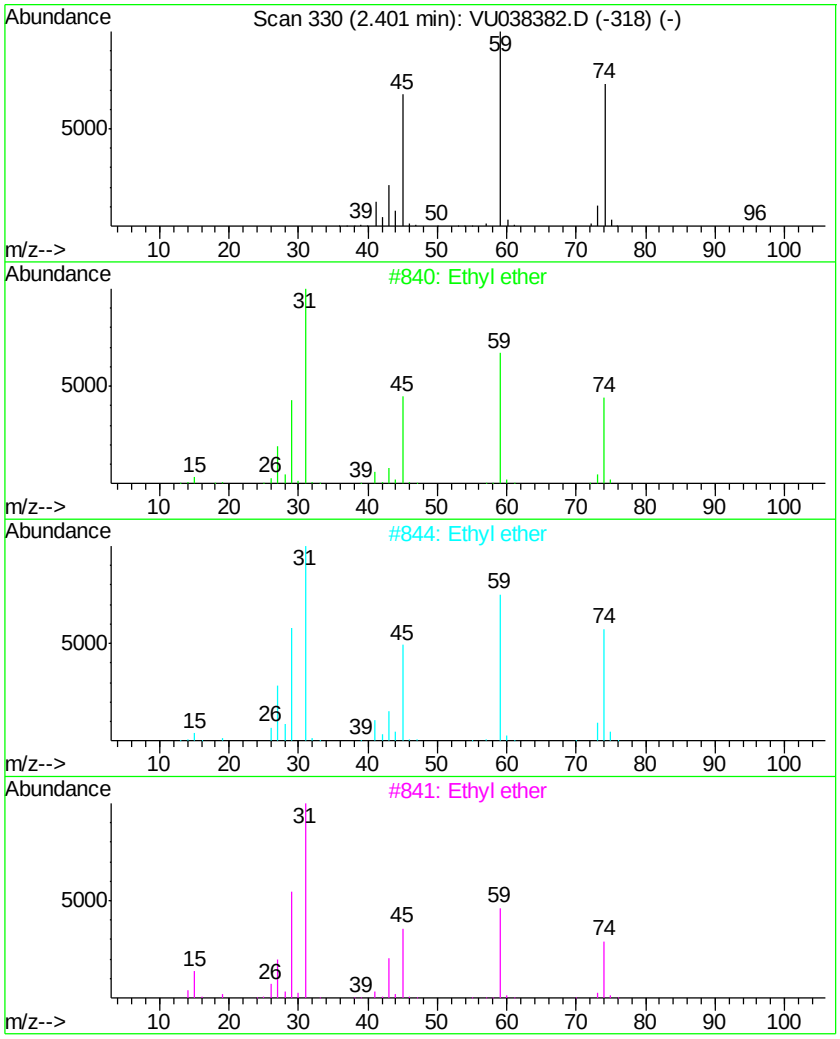
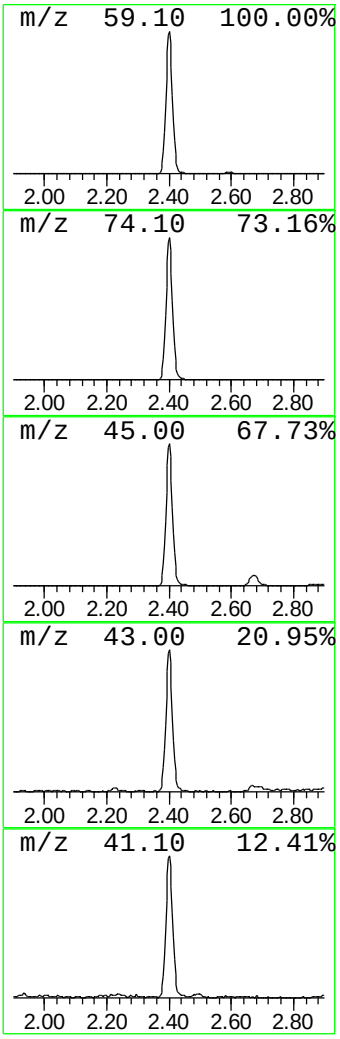
Peak Number 2 Ethyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.40	3.92 ug/L	618259	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl ether	74	C4H10O	000060-29-7	90
2	Ethyl ether	74	C4H10O	000060-29-7	90
3	Ethyl ether	74	C4H10O	000060-29-7	83
4	Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	78
5	Ethyl ether	74	C4H10O	000060-29-7	56





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038382.D
Acq On : 29 May 2020 17:42
Operator : JC/MD
Sample : L2749-08DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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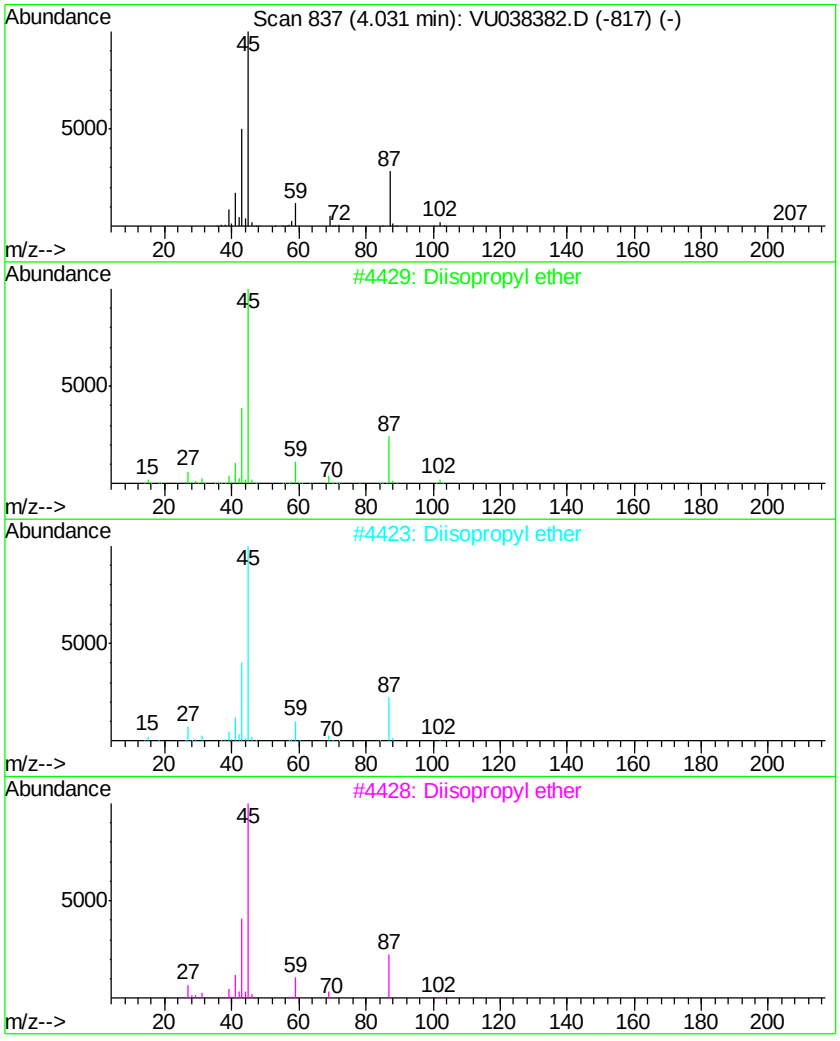
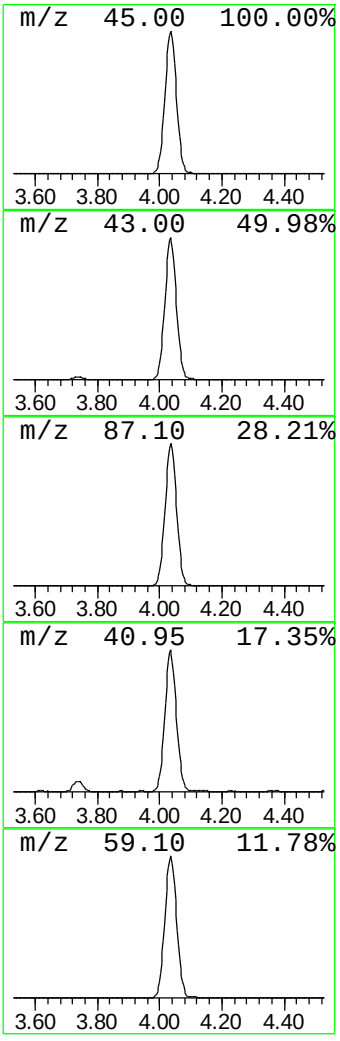
Peak Number 3 Diisopropyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.03	12.37 ug/L	1953630	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisopropyl ether	102	C6H14O	000108-20-3	90
2	Diisopropyl ether	102	C6H14O	000108-20-3	83
3	Diisopropyl ether	102	C6H14O	000108-20-3	83
4	Ether, 2-chloro-1-methylethyl is...	136	C6H13ClO	098277-76-0	64
5	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	56





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038382.D
Acq On : 29 May 2020 17:42
Operator : JC/MD
Sample : L2749-08DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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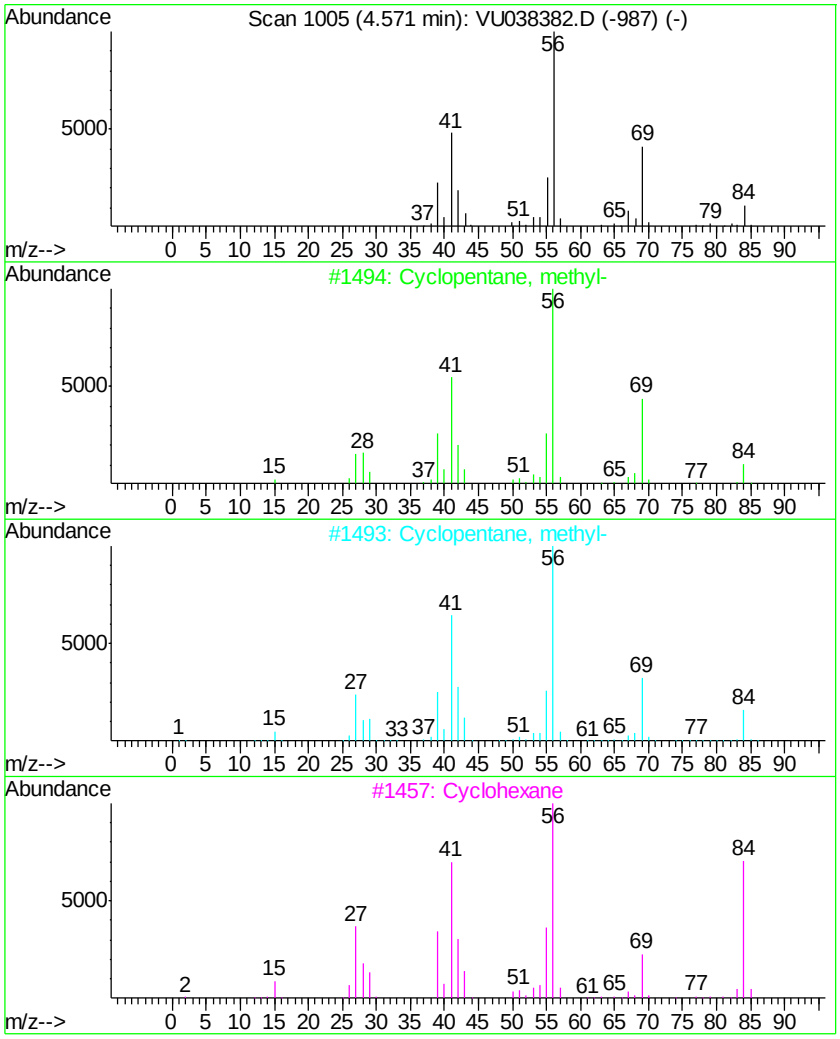
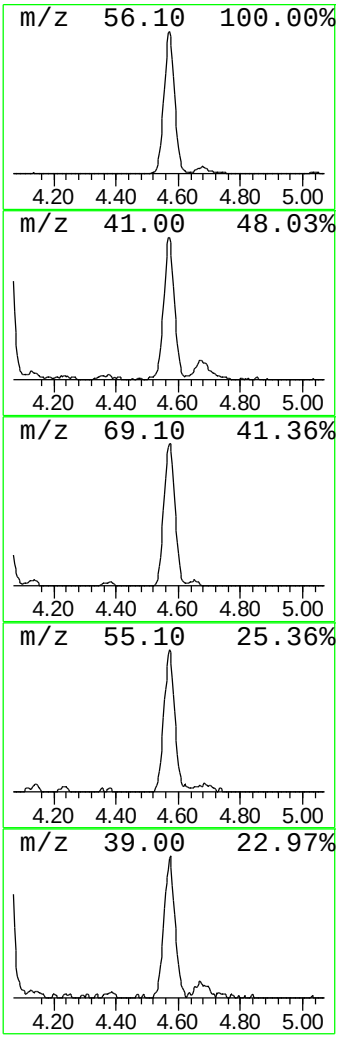
Peak Number 4 (DEL) Alkane: Cyclic4.57 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	1.14 ug/L	180640	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
3	Cyclohexane	84	C6H12	000110-82-7	87
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	83
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	78





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038382.D
Acq On : 29 May 2020 17:42
Operator : JC/MD
Sample : L2749-08DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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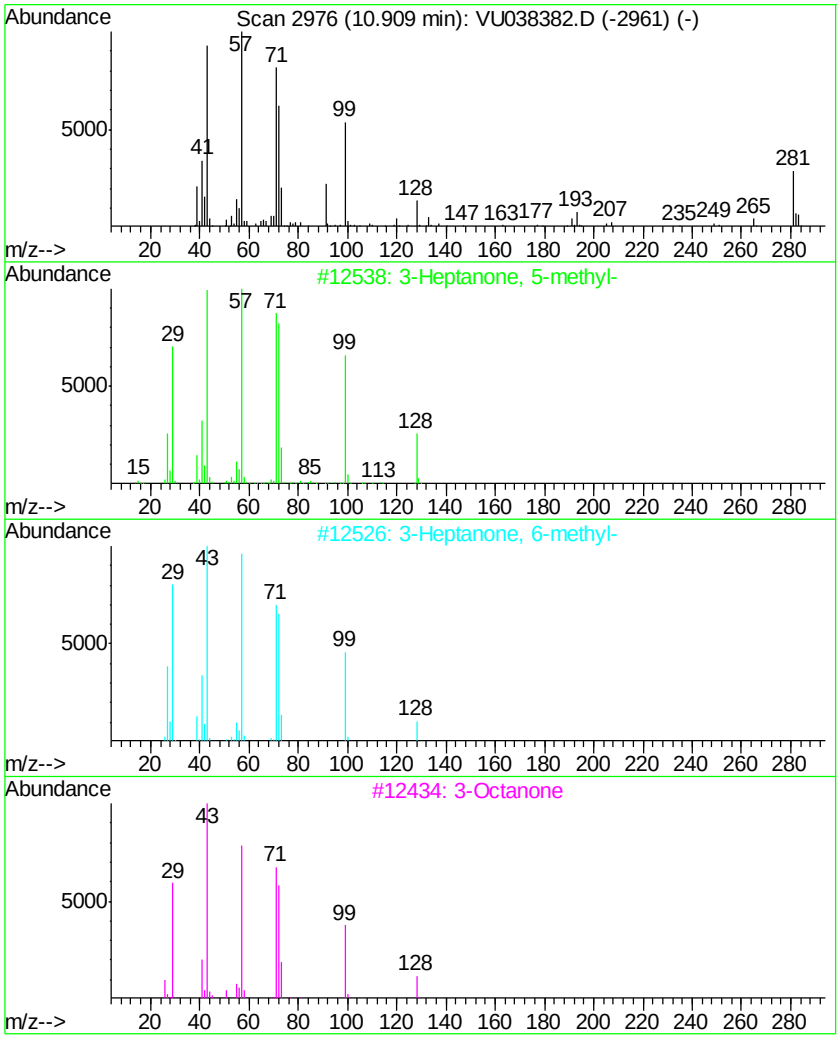
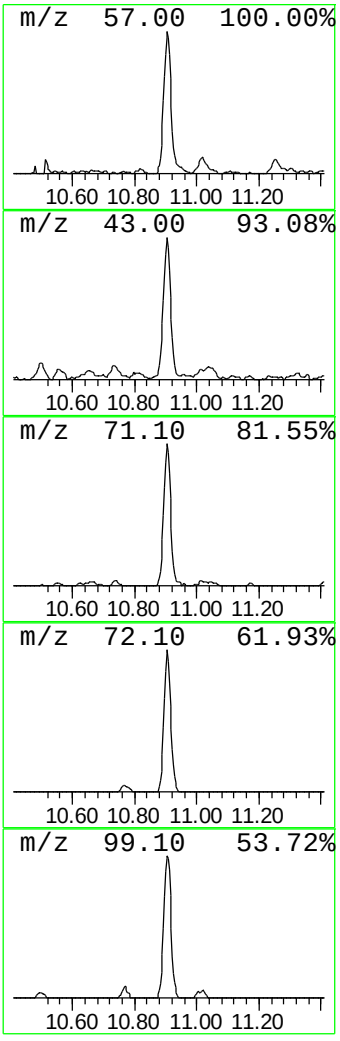
Peak Number 6 3-Heptanone, 5-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	0.74 ug/L	168684	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	81
2	3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	81
3	3-Octanone	128	C8H16O	000106-68-3	81
4	3-Octanone	128	C8H16O	000106-68-3	74
5	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	60





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038382.D
Acq On : 29 May 2020 17:42
Operator : JC/MD
Sample : L2749-08DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

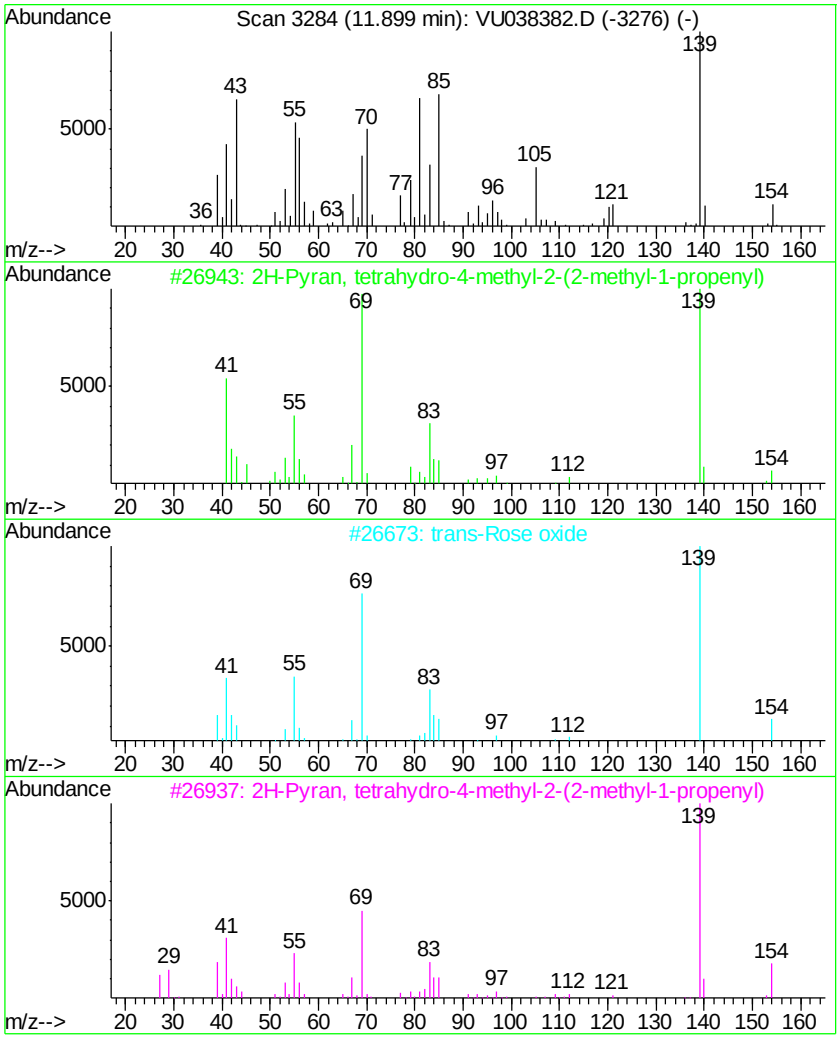
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

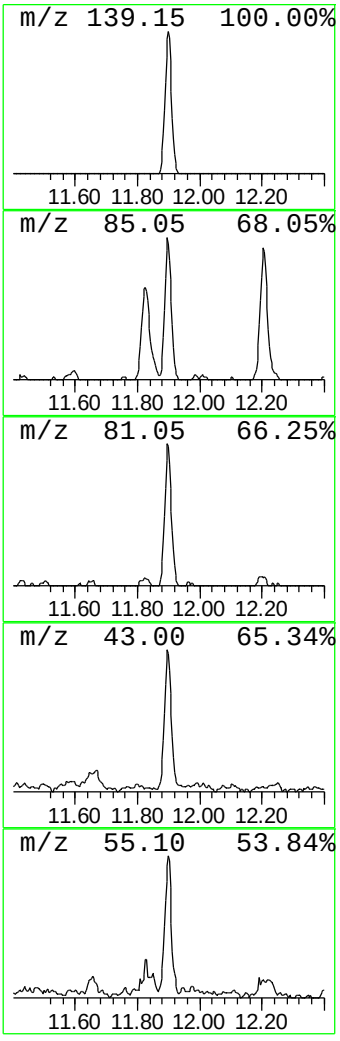
****

Peak Number 7 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	0.61 ug/L	139072	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran, tetrahydro-4-methyl-2-...	154	C10H18O	016409-43-1	38
2	trans-Rose oxide	154	C10H18O	000876-18-6	30
3	2H-Pyran, tetrahydro-4-methyl-2-...	154	C10H18O	016409-43-1	27
4	Silane, (cyclopentylidenemethyl)...	154	C9H18Si	094012-70-1	25
5	Cyclodecane	140	C10H20	000293-96-9	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053020\
Data File : VU038382.D
Acq On : 29 May 2020 17:42
Operator : JC/MD
Sample : L2749-08DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BE4X3DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.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
Sulfur dioxide	1.51	0.6	ug/L	88658	1	6.28	789444	5.0
Ethyl ether	2.40	3.9	ug/L	618259	1	6.28	789444	5.0
Diisopropyl ether	4.03	12.4	ug/L	1953630	1	6.28	789444	5.0
(DEL) Alkane: Cyc...	4.57	1.1	ug/L	180640	1	6.28	789444	5.0
3-Heptanone, 5-me...	10.91	0.7	ug/L	168684	3	11.83	1141350	5.0
unknown-01	11.90	0.6	ug/L	139072	3	11.83	1141350	5.0