LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU022019\
Data File : VU029584.D
Acq On : 20 Feb 2019 16:37
Operator : JC/SP
Sample : K1488-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXE8

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\SOMUTR021219WMA.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	1.183	22	29	42	rBV2	179769	191337	2.94%	1.270%
2	1.331	60	75	87	rBV2	202546	768516	11.81%	5.100%
3	1.402	88	97	107	rVV	1264575	1488258	22.88%	9.876%
4	1.453	109	113	118	rVV	63784	73383	1.13%	0.487%
5	1.679	178	183	196	rVB2	87337	116884	1.80%	0.776%
6	2.273	359	368	381	rVB	153611	238345	3.66%	1.582%
7	2.981	580	588	603	rVB	51047	94394	1.45%	0.626%
8	4.222	952	974	1013	rBV	2647727	6504619	100.00%	43.166%
9	4.646	1089	1106	1129	rVB	108911	259308	3.99%	1.721%
10	5.334	1295	1320	1349	rBV2	213187	605292	9.31%	4.017%
11	5.884	1477	1491	1518	rBV	220879	437425	6.72%	2.903%
12	6.328	1612	1629	1647	rBV2	142091	284070	4.37%	1.885%
13	7.225	1896	1908	1929	rBV	71256	133765	2.06%	0.888%
14	7.563	1997	2013	2030	rBV	291929	517352	7.95%	3.433%
15	7.849	2092	2102	2119	rBV2	41998	74290	1.14%	0.493%
16	8.177	2188	2204	2211	rBV	68546	126669	1.95%	0.841%
17	8.225	2211	2219	2235	rVB	88208	151602	2.33%	1.006%
18	8.312	2235	2246	2278	rBV	415602	739873	11.37%	4.910%
19	9.087	2475	2487	2512	rBV	323146	541612	8.33%	3.594%
20	10.431	2892	2905	2919	rBV	132873	215018	3.31%	1.427%
21	10.604	2947	2959	2982	rVB	104945	179364	2.76%	1.190%
22	11.482	3221	3232	3256	rBV	361784	588559	9.05%	3.906%
23	11.746	3304	3314	3336	rBV3	39614	89377	1.37%	0.593%
24	11.858	3336	3349	3371	rVB	333411	550491	8.46%	3.653%
25	12.476	3528	3541	3556	rBV2	58335	98879	1.52%	0.656%

Sum of corrected areas: 15068682

LSC Report - Integrated Chromatogram

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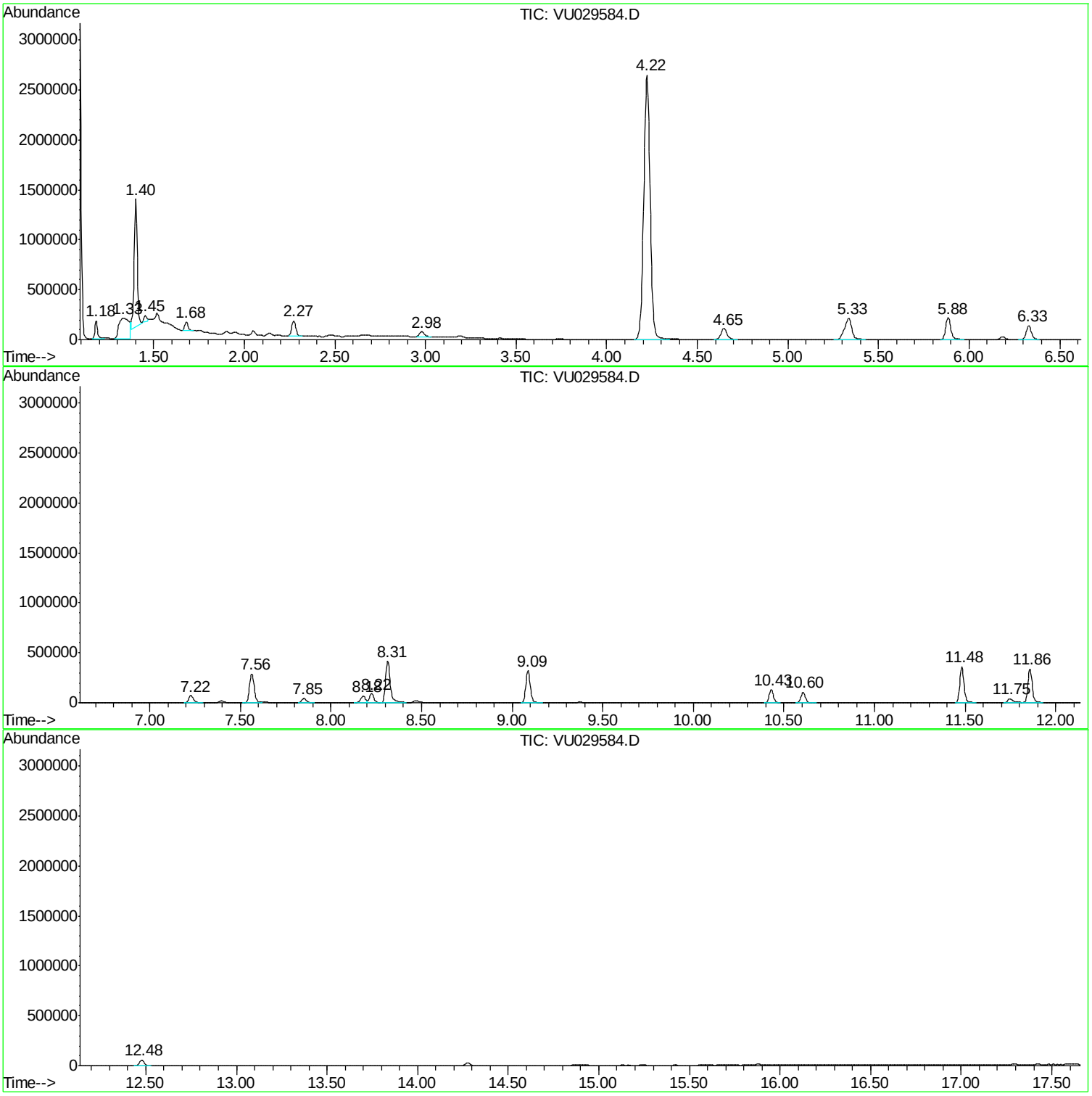
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ESXE8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Acq On : 20 Feb 2019 16:37
Operator : JC/SP
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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXE8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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

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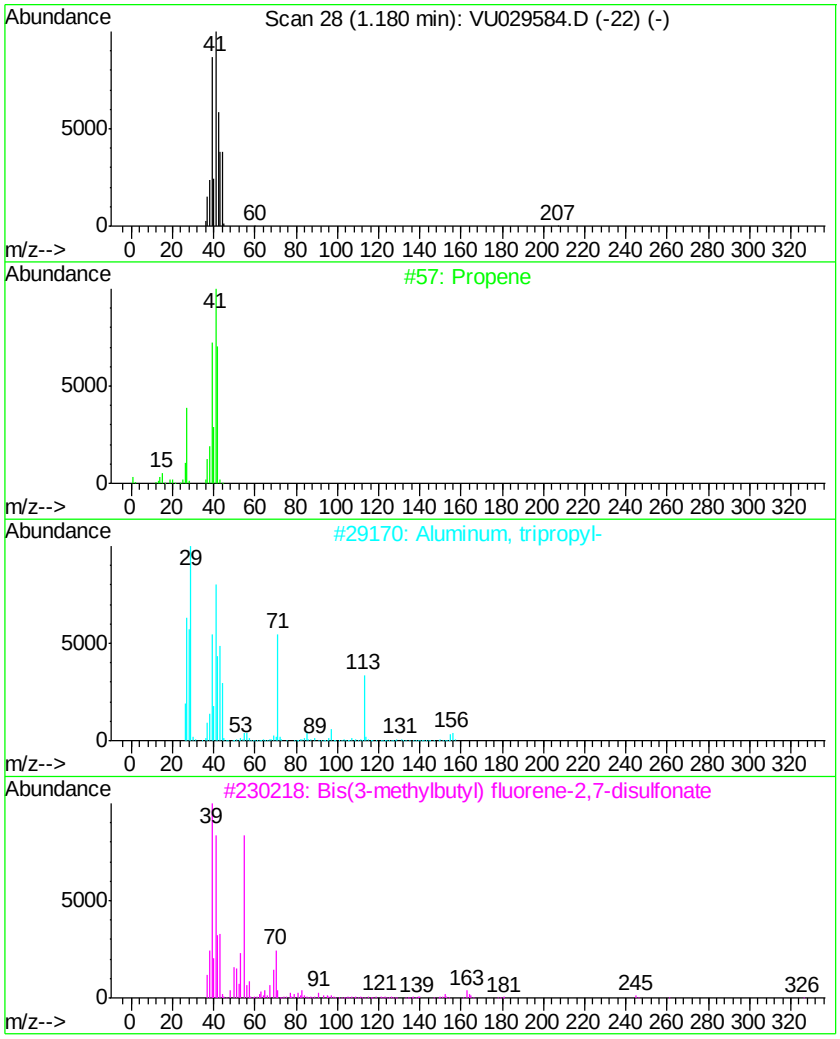
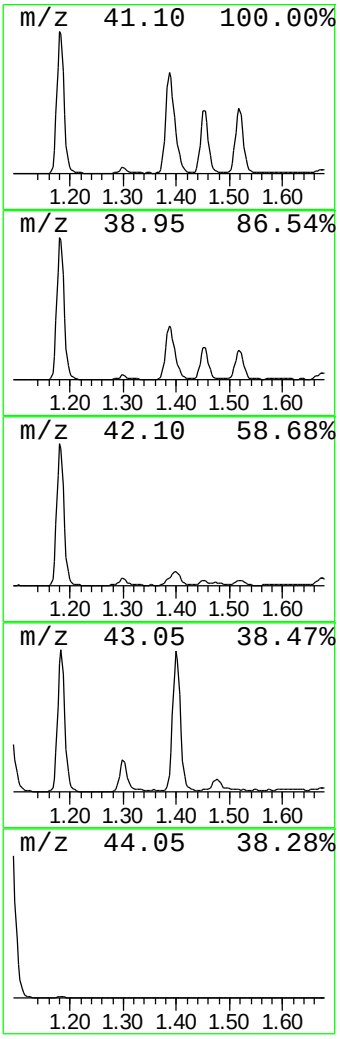
Peak Number 1 (DEL) Alkane: Cyclic1.18 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.18	2.19 ug/L	191337	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	86
2	Aluminum, tripropyl-	156	C9H21Al	000102-67-0	83
3	Bis(3-methylbutyl) fluorene-2,7-...	466	C23H30O6S2	253664-95-8	72
4	2-Butenal, (E)-	70	C4H6O	000123-73-9	72
5	Cyclopropanecarboxylic acid	86	C4H6O2	001759-53-1	64





Library Search Compound Report

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Operator : JC/SP
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Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXE8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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

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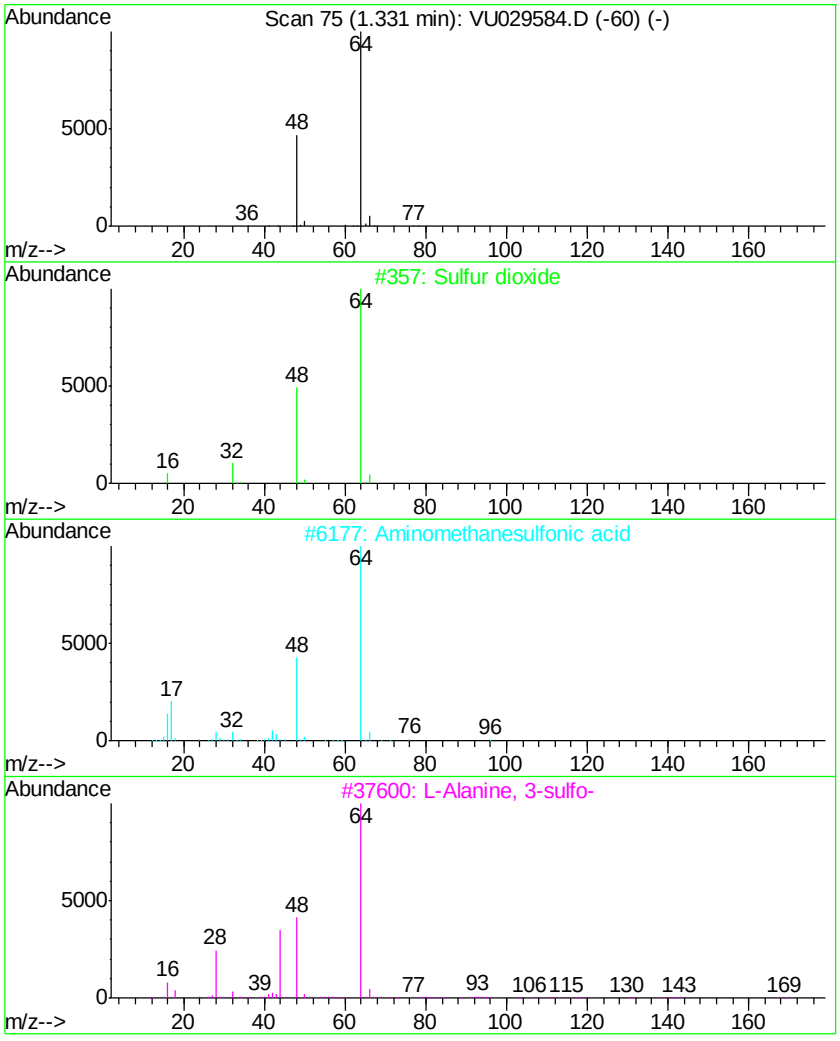
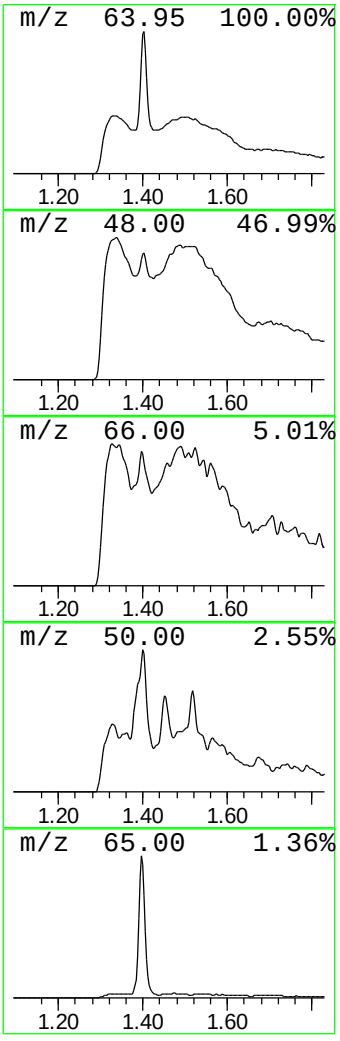
Peak Number 2 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.33	8.78 ug/L	768516	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Sulfur dioxide	64	O2S	007446-09-5	5





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Acq On : 20 Feb 2019 16:37
Operator : JC/SP
Sample : K1488-12
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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXE8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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TIC Integration Parameters: LSCINT.P

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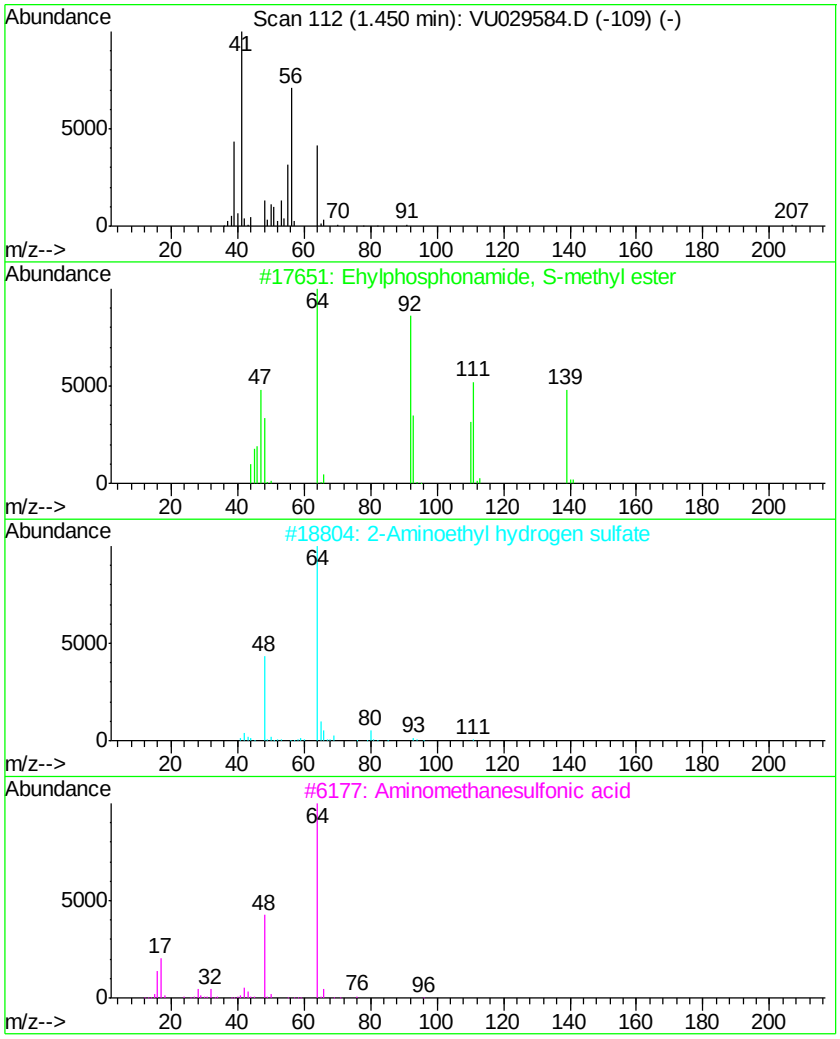
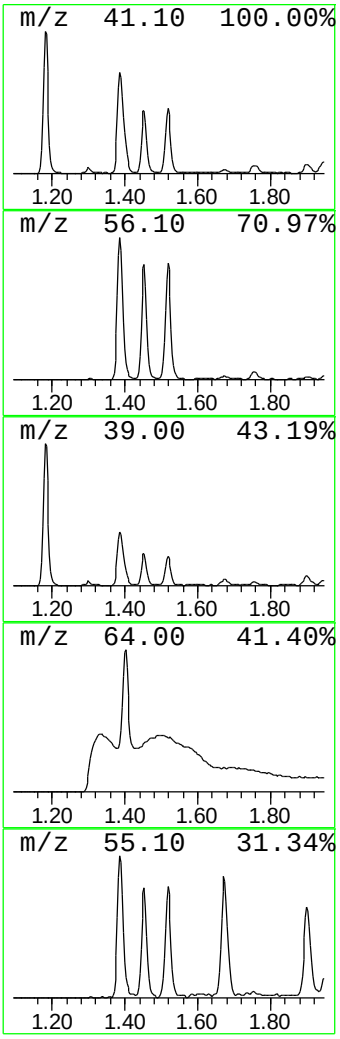
Peak Number 3 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.45	0.84 ug/L	73383	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ehylphosphonamide, S-methyl ester	139	C3H10NOPS	1000306-03-8	36
2	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	33
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	28
4	Benzenesulfonic acid, 2,5-diamino-	188	C6H8N2O3S	000088-45-9	28
5	2-Butene, (E)-	56	C4H8	000624-64-6	20





Library Search Compound Report

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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXE8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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

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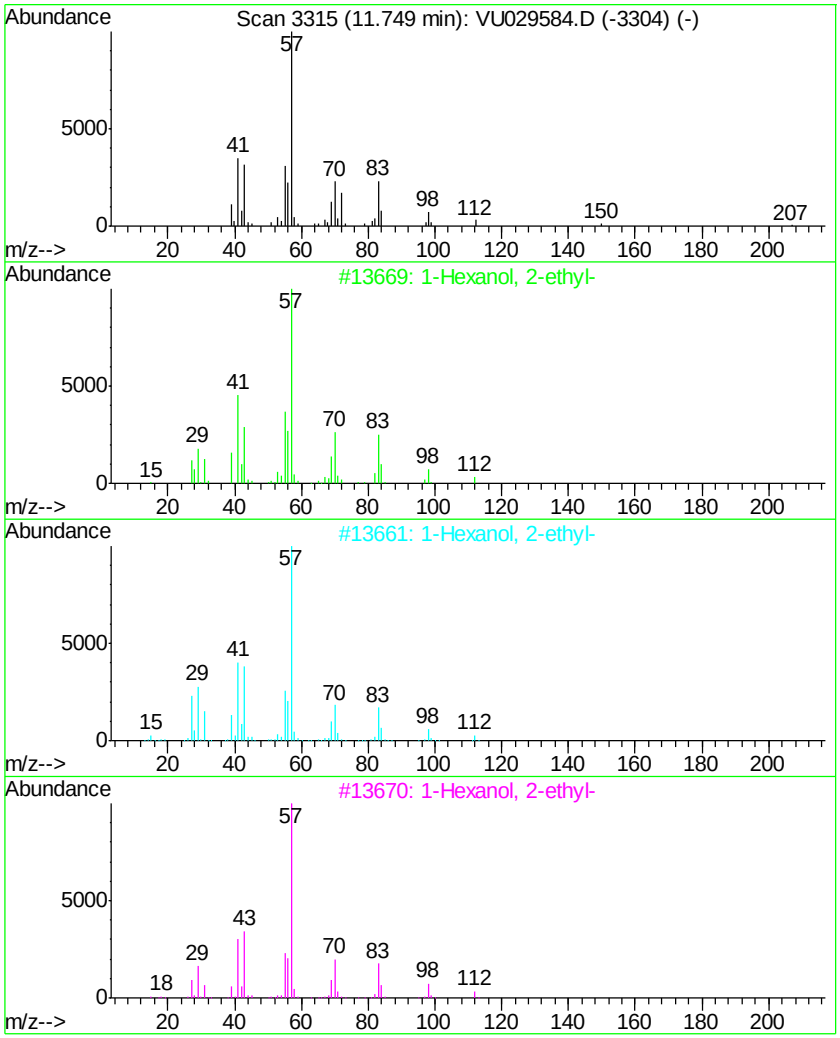
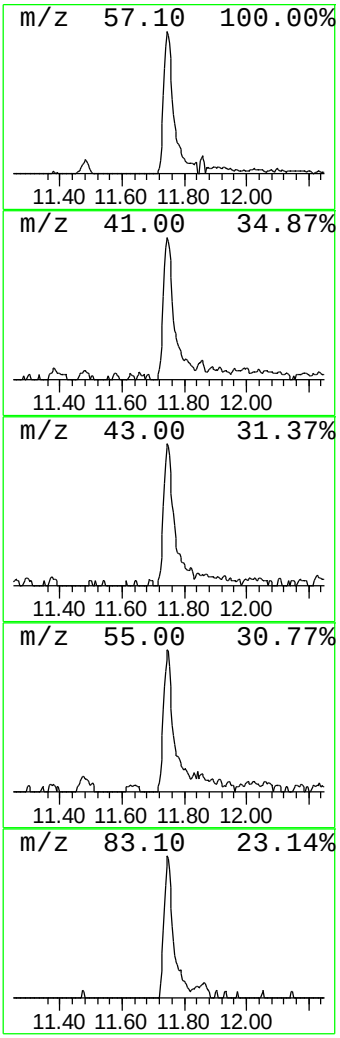
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	0.76 ug/L	89377	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50





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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXE8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

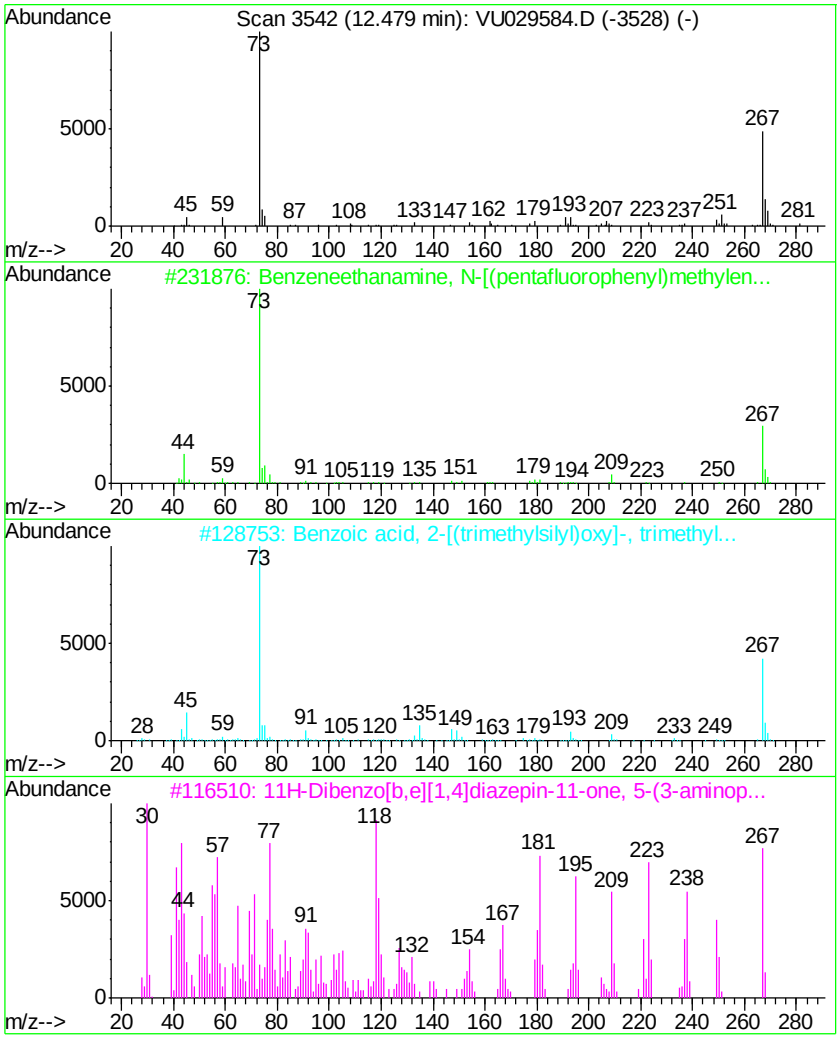
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

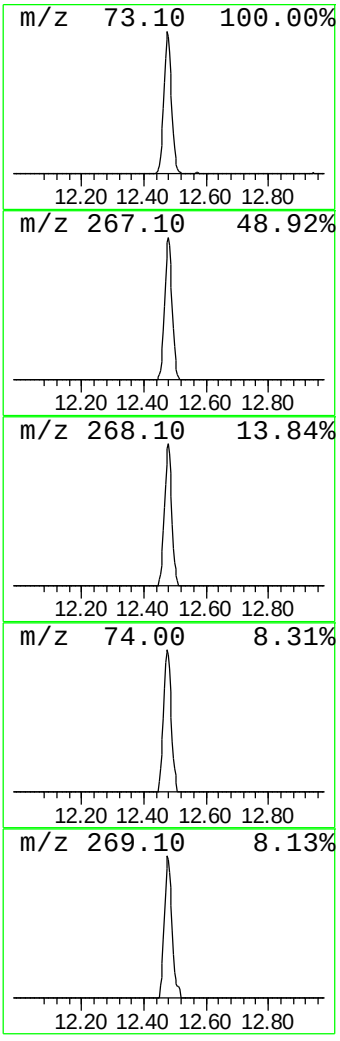
****

Peak Number 7 Benzeneethanamine, N-[(pent... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	0.84 ug/L	98879	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneethanamine, N-[(pentafluo...	475	C21H26F5NO2Si2	055429-85-1	72
2	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	50
3	11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	43
4	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	38
5	1-(3-Chlorophenyl)piperazine, 4-...	268	C13H21ClN2Si	1000373-99-3	10





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: Cyc...	1.18	2.2	ug/L	191337	1	5.88	437425	5.0
Sulfur dioxide	1.33	8.8	ug/L	768516	1	5.88	437425	5.0
unknown-01	1.45	0.8	ug/L	73383	1	5.88	437425	5.0
1-Hexanol, 2-ethyl-	11.75	0.8	ug/L	89377	3	11.48	588559	5.0
Benzeneethanamine...	12.48	0.8	ug/L	98879	3	11.48	588559	5.0