LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_Y\DATA\VY110719\
Data File : VY000581.D
Acq On : 07 Nov 2019 15:27
Operator : SY/MD
Sample : K5723-12
Misc : 6.20G/5ML/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_Y
ClientSampleId : 10-A

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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_Y\METHODS\82Y103019S.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.219	73	79	82	rBV3	16268	28511	2.04%	0.289%
2	4.725	480	490	502	rBV2	18263	58007	4.15%	0.587%
3	5.755	649	659	673	rBV3	29004	92317	6.60%	0.935%
4	7.730	974	983	989	rBV	187690	450871	32.26%	4.566%
5	7.803	989	995	1007	rVB	315618	716661	51.27%	7.258%
6	8.151	1041	1052	1064	rBV	192289	429280	30.71%	4.348%
7	8.699	1131	1142	1156	rBV	522768	1030246	73.71%	10.434%
8	10.181	1375	1385	1392	rBV	823947	1397732	100.00%	14.156%
9	11.492	1593	1600	1611	rVB	742566	1211118	86.65%	12.266%
10	12.479	1755	1762	1771	rVB	586834	917677	65.65%	9.294%
11	13.302	1890	1897	1902	rBV	108513	168619	12.06%	1.708%
12	13.424	1910	1917	1924	rBV	710809	1082243	77.43%	10.961%
13	13.528	1925	1934	1941	rVB2	17115	32164	2.30%	0.326%
14	13.967	2001	2006	2013	rBV2	15542	24870	1.78%	0.252%
15	14.613	2108	2112	2117	rVB	22503	32489	2.32%	0.329%
16	14.674	2117	2122	2128	rBV8	9144	19122	1.37%	0.194%
17	15.265	2204	2219	2224	rBV2	380169	656484	46.97%	6.649%
18	15.332	2224	2230	2237	rVV	300389	521523	37.31%	5.282%
19	15.418	2237	2244	2253	rVV2	453844	821551	58.78%	8.321%
20	15.497	2253	2257	2267	rVV2	7811	19844	1.42%	0.201%
21	15.887	2314	2321	2328	rVB4	20596	42115	3.01%	0.427%
22	16.009	2336	2341	2346	rBV2	21561	45146	3.23%	0.457%
23	16.155	2361	2365	2371	rVB8	7344	14663	1.05%	0.149%
24	16.283	2381	2386	2392	rBV3	18076	34630	2.48%	0.351%
25	16.479	2413	2418	2425	rBV6	11822	25669	1.84%	0.260%

Sum of corrected areas: 9873552

LSC Report - Integrated Chromatogram

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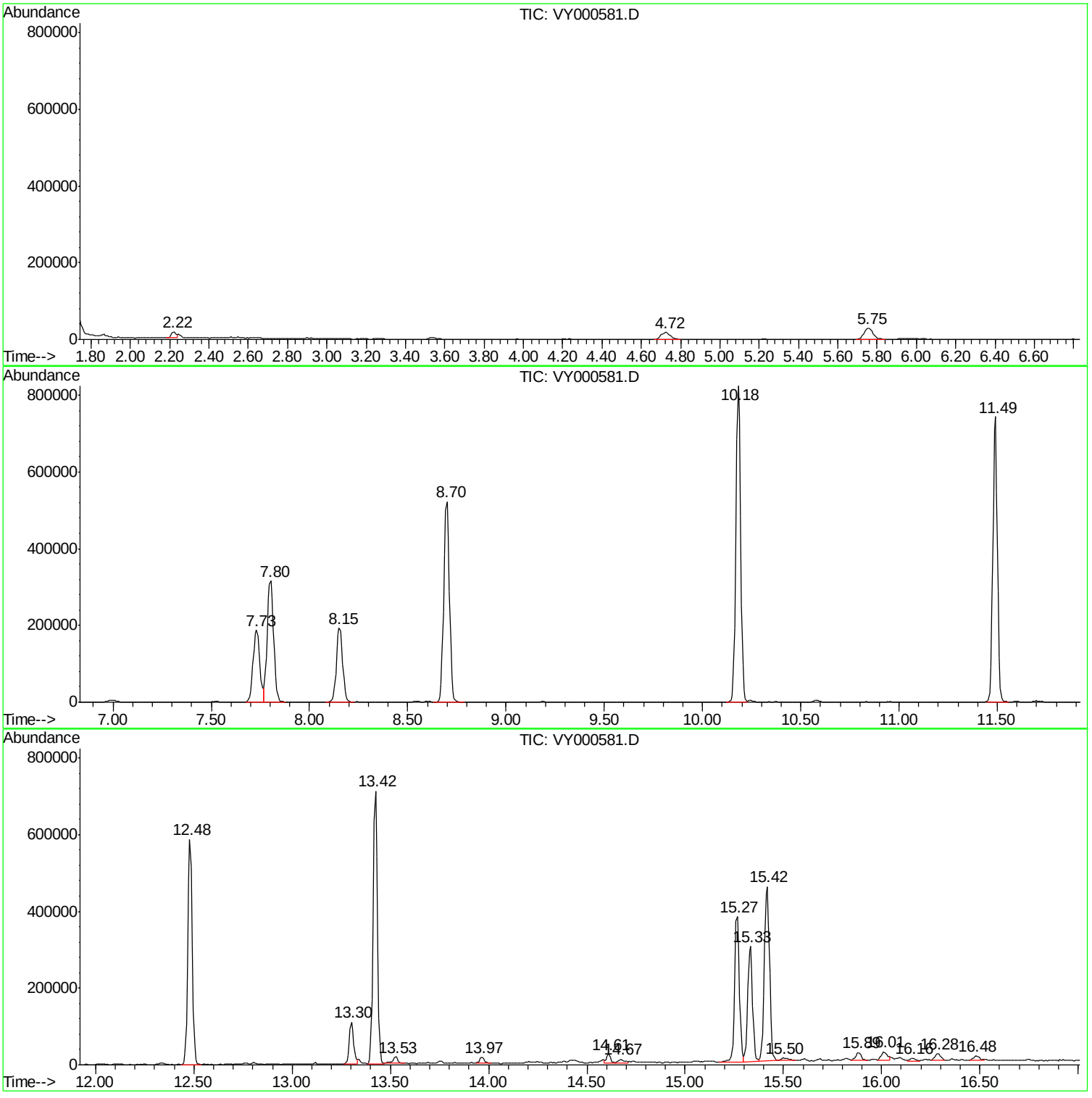
Operator : SY/MD
Sample : K5723-12
Misc : 6.20G/5ML/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
10-A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_Y\DATA\VY110719\
Data File : VY000581.D
Acq On : 07 Nov 2019 15:27
Operator : SY/MD
Sample : K5723-12
Misc : 6.20G/5ML/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_Y
ClientSampleId : 10-A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

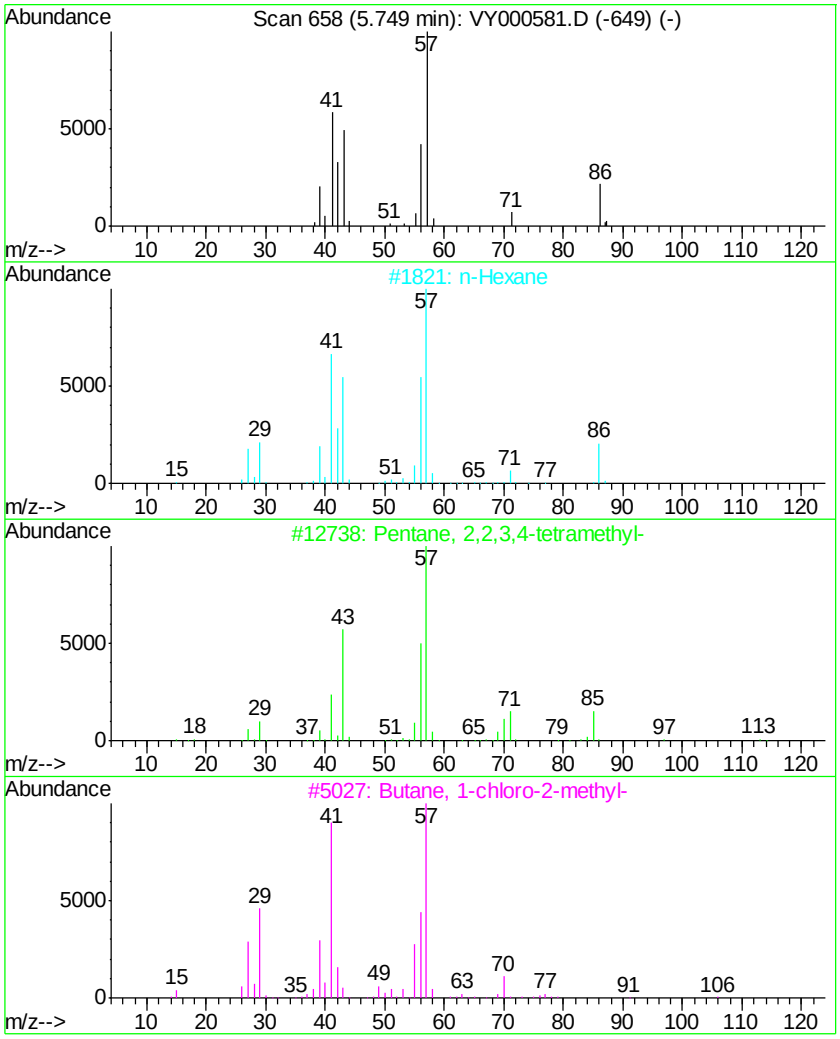
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

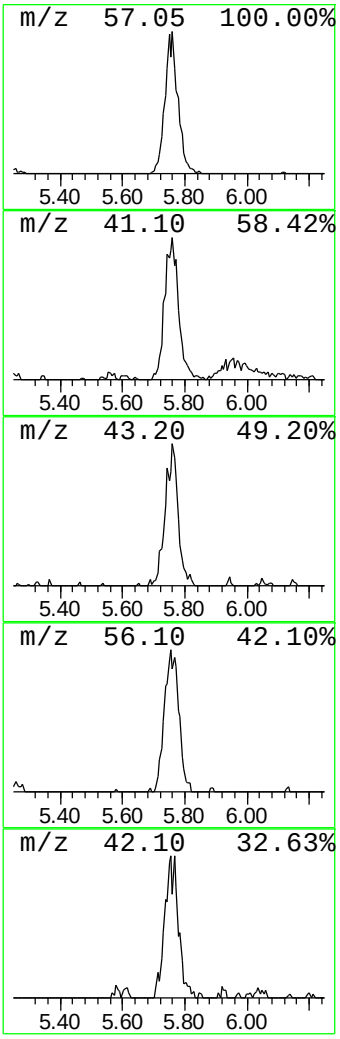
****

Peak Number 1 n-Hexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.75	6.44 ug/l	92317	Pentafluorobenzene	7.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	91
2	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	38
3	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	38
4	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	37
5	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	33





Library Search Compound Report

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Data File : VY000581.D
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Operator : SY/MD
Sample : K5723-12
Misc : 6.20G/5ML/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_Y
ClientSampleId : 10-A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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

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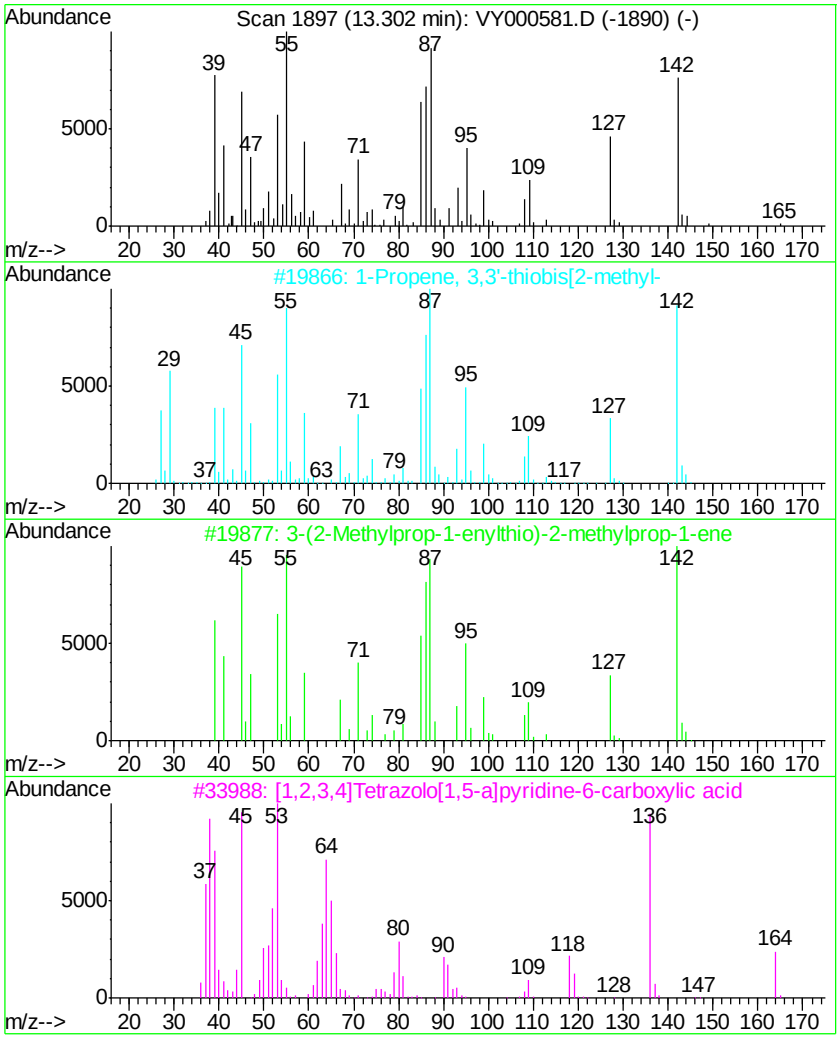
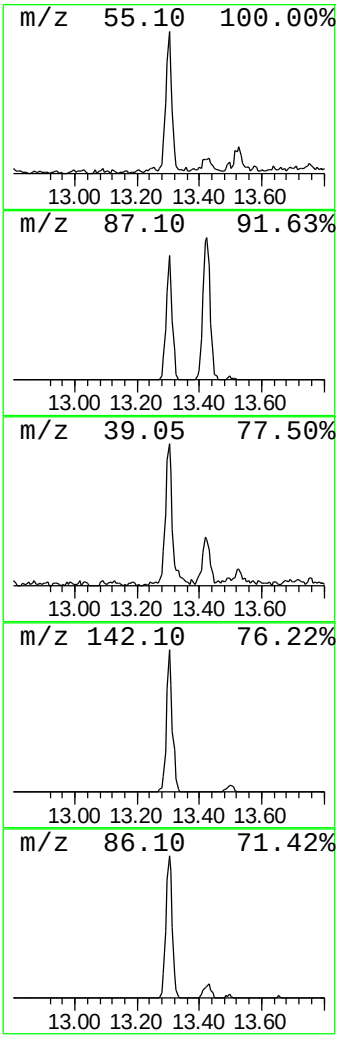
Peak Number 2 1-Propene, 3,3'-thiobis[2-m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	7.79 ug/l	168619	1,4-Dichlorobenzene-d4	13.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 3,3'-thiobis[2-methyl-	142	C8H14S	023973-54-8	95
2	3-(2-Methylprop-1-enylthio)-2-me...	142	C8H14S	1000122-39-8	95
3	[1,2,3,4]Tetrazolo[1,5-a]pyridin...	164	C6H4N4O2	1000362-60-7	53
4	trans-1-Nitro-1-propene	87	C3H5NO2	017082-05-2	35
5	Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	32





Library Search Compound Report

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Data File : VY000581.D
Acq On : 07 Nov 2019 15:27
Operator : SY/MD
Sample : K5723-12
Misc : 6.20G/5ML/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_Y
ClientSampleId : 10-A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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

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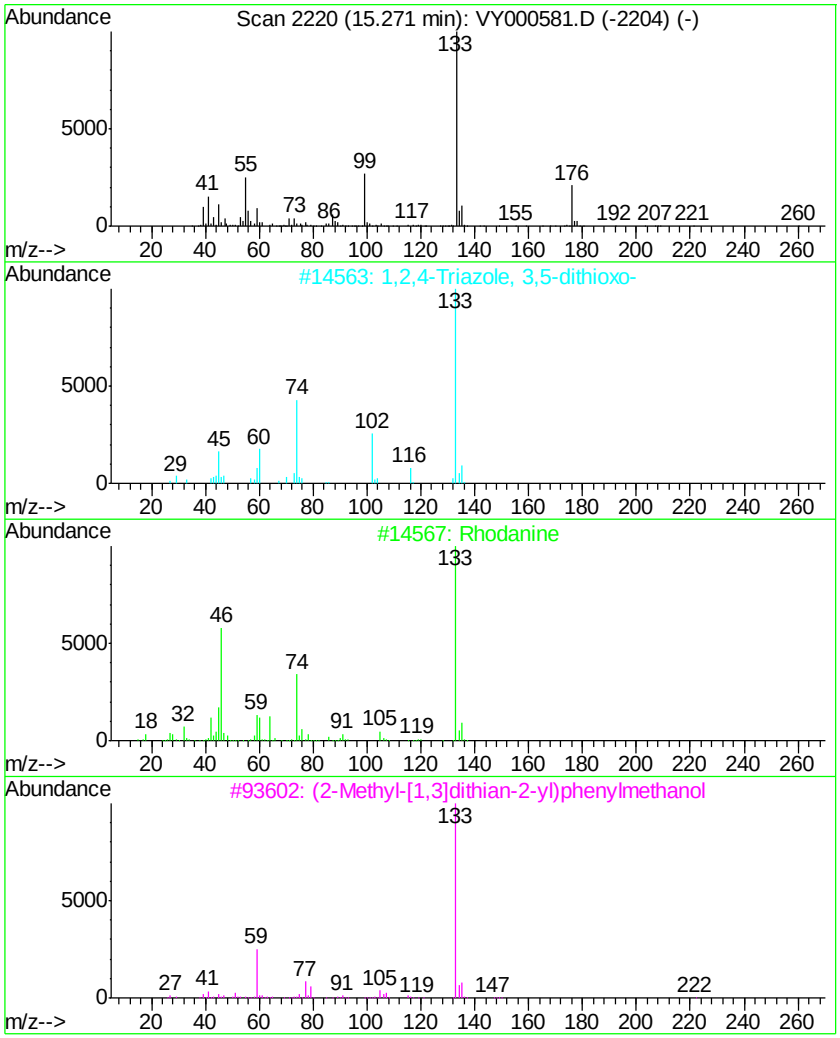
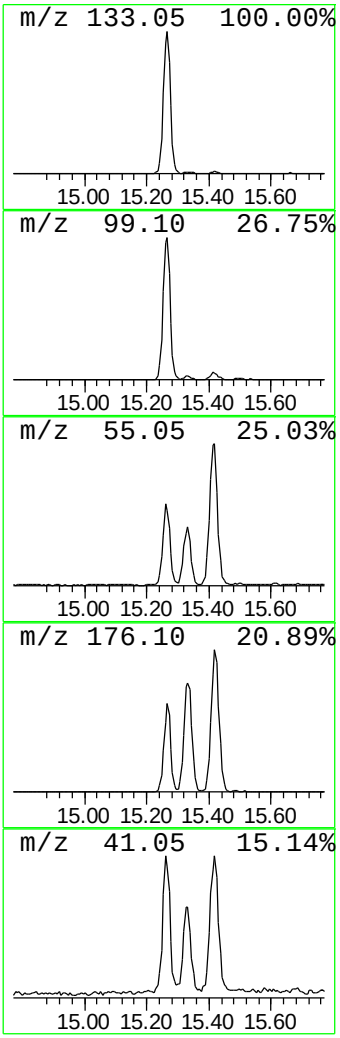
Peak Number 3 1,2,4-Triazole, 3,5-dithioxo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	30.33 ug/l	656484	1,4-Dichlorobenzene-d4	13.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	50
2	Rhodanine	133	C3H3NOS2	000141-84-4	42
3	(2-Methyl-[1,3]dithian-2-yl)phen...	240	C12H16OS2	078349-00-5	40
4	Thiophene, 2,2'-(1,1,2,2,3,3,4,4...	416	C13H6F10S2	024014-44-6	28
5	(2-Methyl[1,3]dithian-2-yl)methanol	164	C6H12OS2	1000191-37-4	12





Library Search Compound Report

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Sample : K5723-12
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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_Y
ClientSampleId : 10-A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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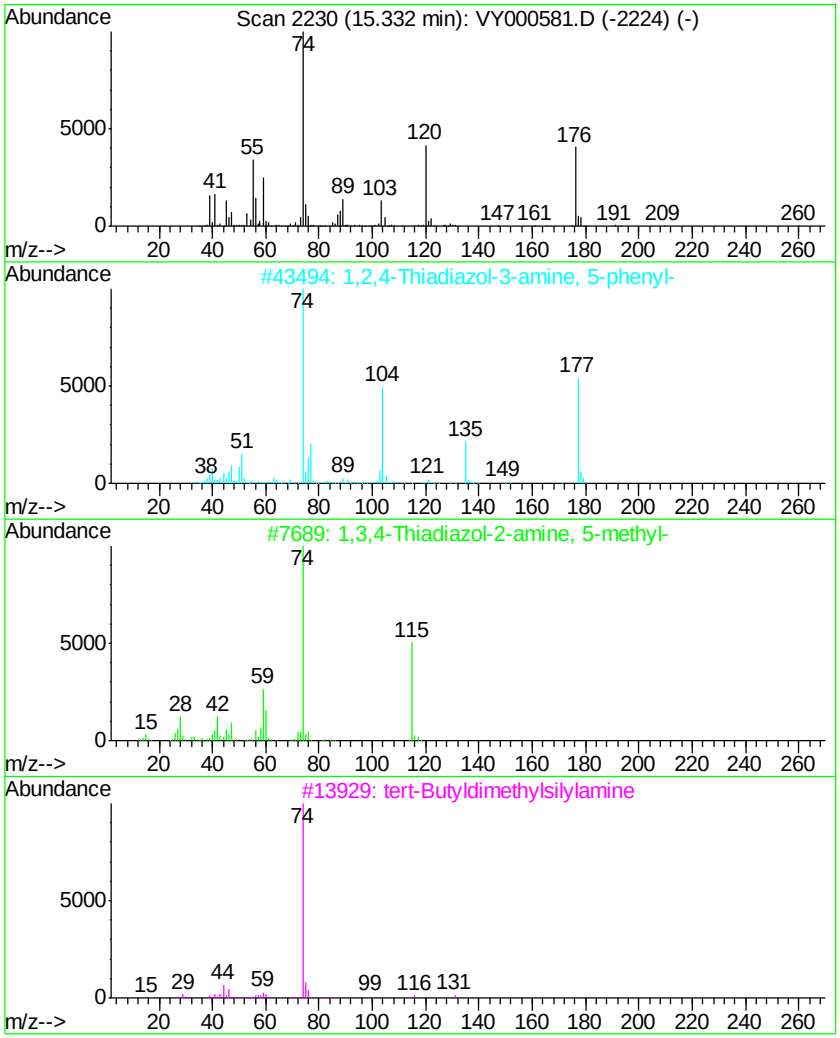
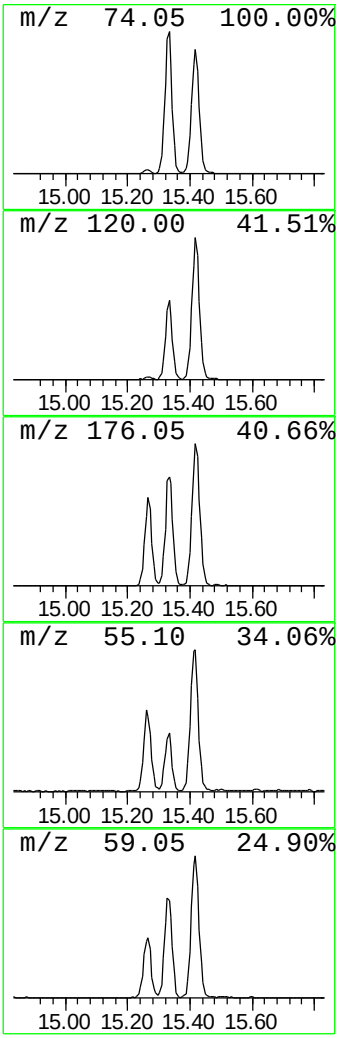
****

Peak Number 4 unknown15.33 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	24.09 ug/l	521523	1,4-Dichlorobenzene-d4	13.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Thiadiazol-3-amine, 5-phenyl-	177	C8H7N3S	027182-54-3	17
2	1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	17
3	tert-Butyldimethylsilylamine	131	C6H17NSi	1000366-62-1	16
4	L-Threonine, ethyl ester	147	C6H13NO3	023926-51-4	16
5	Thiirane, methyl-	74	C3H6S	001072-43-1	16





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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_Y
ClientSampleId : 10-A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

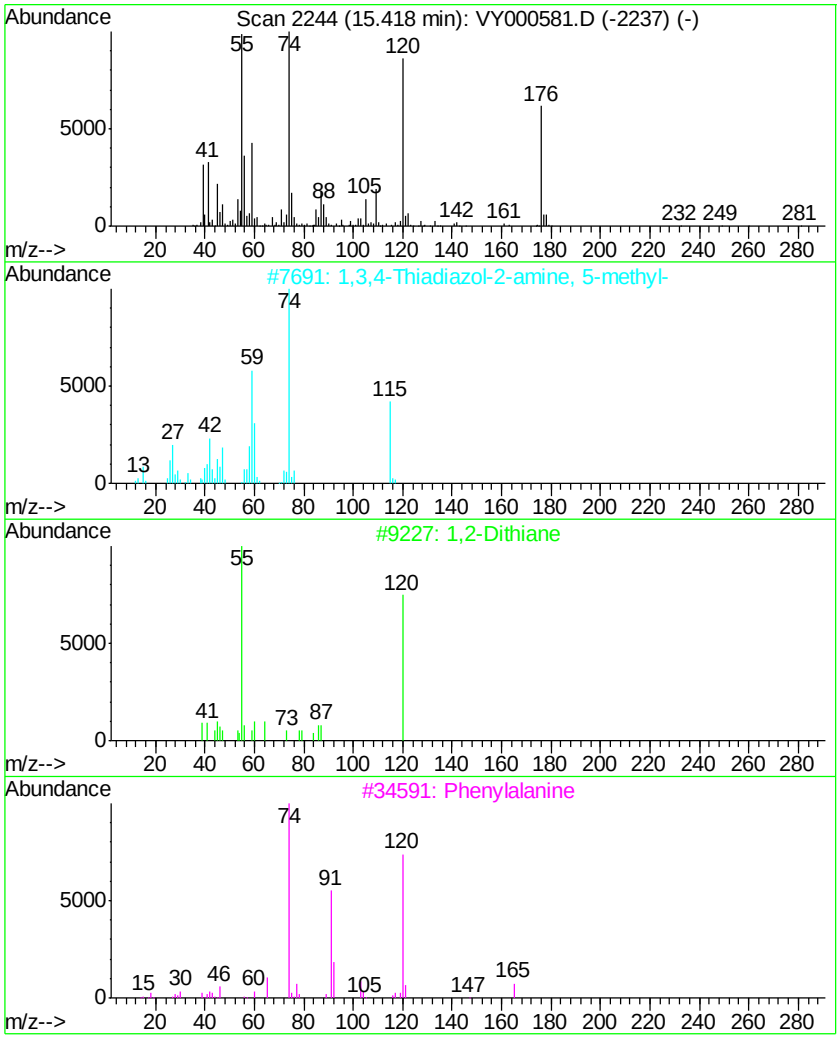
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

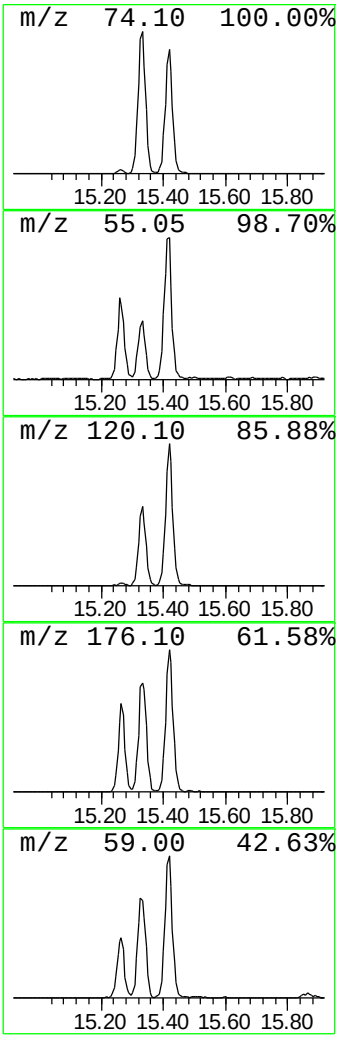
****

Peak Number 5 unknown15.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	37.96 ug/l	821551	1,4-Dichlorobenzene-d4	13.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	27
2	1,2-Dithiane	120	C4H8S2	000505-20-4	22
3	Phenylalanine	165	C9H11NO2	000063-91-2	17
4	dl-Homoserine	119	C4H9NO3	001927-25-9	14
5	5,6-Dihydro-2-methyl-1,4-dithiin...	176	C6H8O2S2	035756-29-7	11





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexane	5.75	6.4	ug/l	92317	1	7.80	716661	50.0
1-Propene, 3,3'-t...	13.30	7.8	ug/l	168619	4	13.42	1082240	50.0
1,2,4-Triazole, 3...	15.27	30.3	ug/l	656484	4	13.42	1082240	50.0
unknown15.33	15.33	24.1	ug/l	521523	4	13.42	1082240	50.0
unknown15.42	15.42	38.0	ug/l	821551	4	13.42	1082240	50.0