

Data Path : Z:\VOASRV\HPCHEM1\MSVOA Y\DATA\VY110819\
 Data File : VY000625.D
 Acq On : 08 Nov 2019 18:10
 Operator : SY/MD
 Sample : K5723-12
 Misc : 6.61G/5ML/MSVOA Y/SOIL
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 10-A

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	1.865	16	21	27	rVB3	6754	12480	1.00%	0.155%
2	2.225	75	80	84	rBV	15552	24161	1.94%	0.300%
3	4.724	481	490	501	rBV4	12588	38714	3.11%	0.481%
4	5.767	650	661	669	rBV4	23224	72652	5.84%	0.903%
5	7.730	972	983	989	rBV	168752	398374	32.03%	4.952%
6	7.803	989	995	1008	rVB	276897	639380	51.41%	7.948%
7	8.151	1043	1052	1063	rBV	171834	381325	30.66%	4.740%
8	8.699	1132	1142	1153	rBV	466112	916739	73.72%	11.395%
9	10.181	1378	1385	1393	rBV	717786	1243626	100.00%	15.459%
10	11.491	1593	1600	1609	rBV	668717	1092639	87.86%	13.582%
11	12.479	1755	1762	1772	rVB	523237	831654	66.87%	10.338%
12	13.302	1892	1897	1908	rBV3	56651	92299	7.42%	1.147%
13	13.424	1910	1917	1924	rBV	667532	1015336	81.64%	12.621%
14	13.528	1929	1934	1941	rVB2	12952	22318	1.79%	0.277%
15	13.967	2000	2006	2012	rVB2	10526	19369	1.56%	0.241%
16	14.210	2041	2046	2053	rVB10	8073	18122	1.46%	0.225%
17	15.265	2212	2219	2224	rBV	242715	396011	31.84%	4.923%
18	15.332	2224	2230	2237	rVV2	183450	310703	24.98%	3.862%
19	15.418	2237	2244	2252	rVV2	262984	482343	38.79%	5.996%
20	15.881	2315	2320	2326	rVB8	8125	16407	1.32%	0.204%
21	16.015	2336	2342	2347	rBV2	9459	20221	1.63%	0.251%

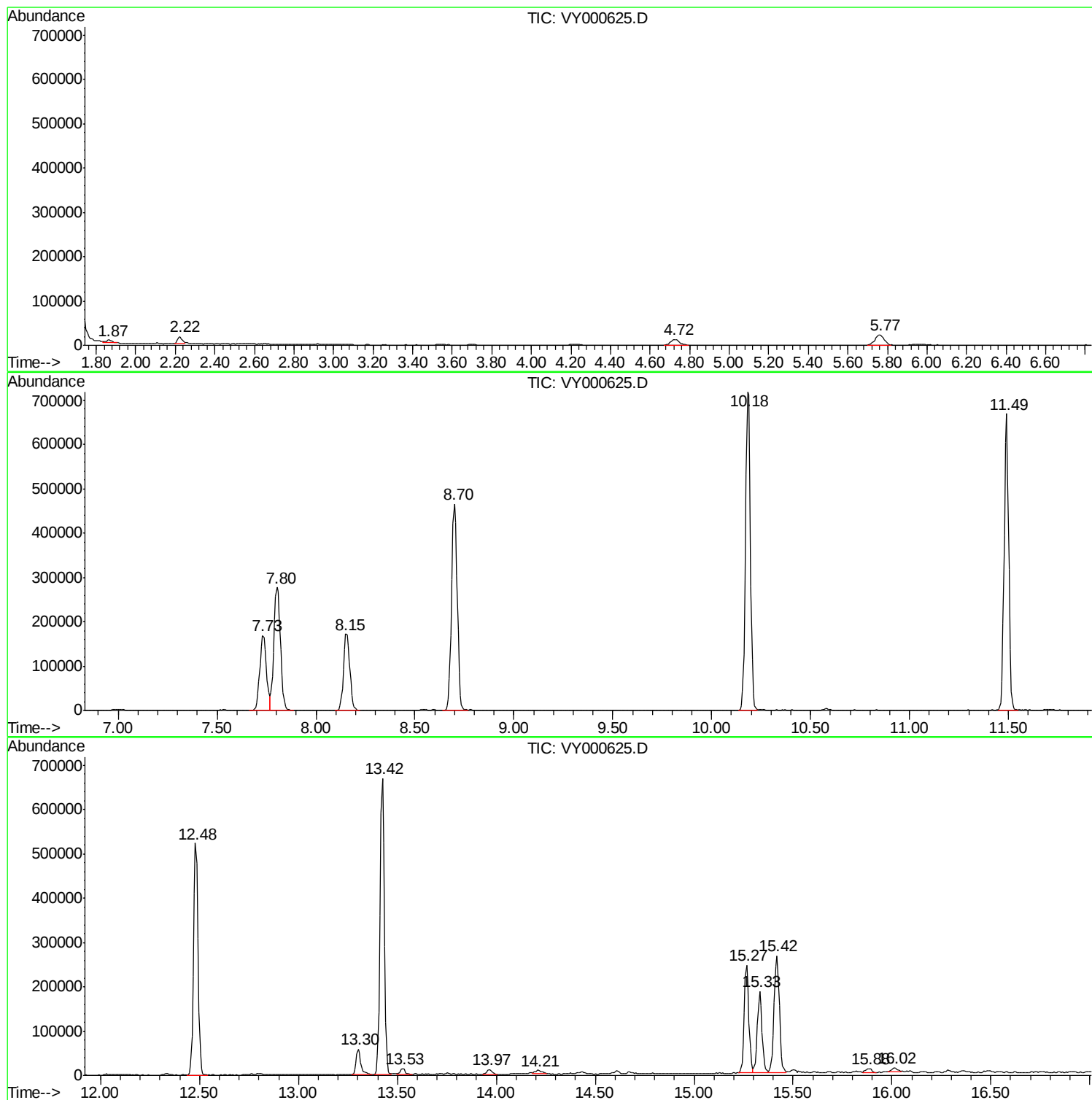
Sum of corrected areas: 8044873

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Quant Method : Z:\V0ASRV\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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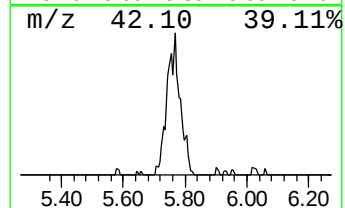
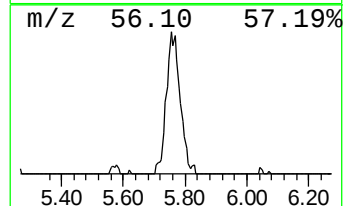
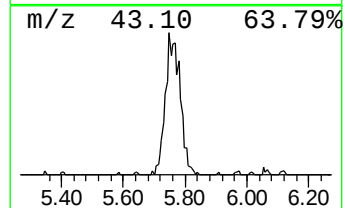
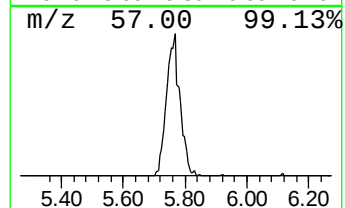
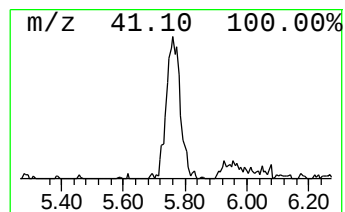
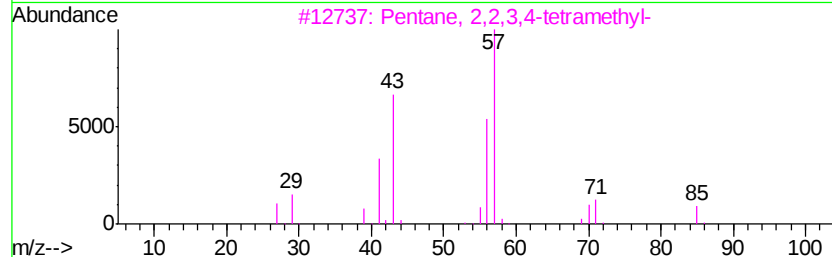
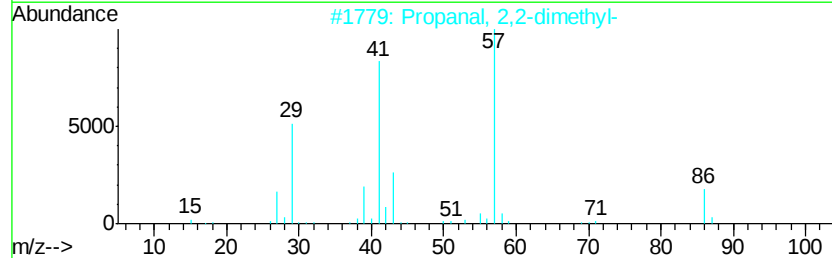
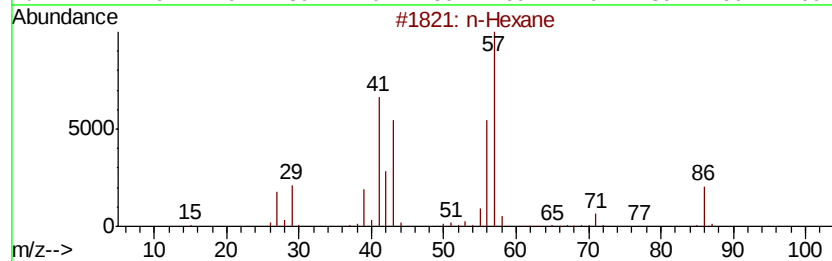
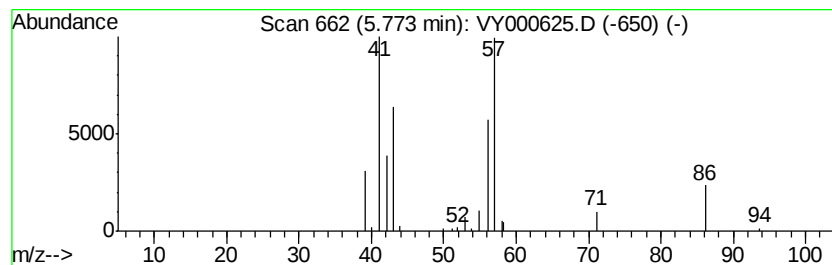
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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

Peak Number 1 n-Hexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	5.68 ug/l	72652	Pentafluorobenzene	7.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	87
2		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	38
3		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	36
4		1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	33
5		Decane, 2,2,7-trimethyl-	184	C13H28	062237-99-4	33



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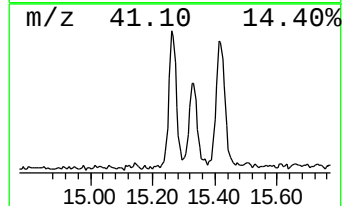
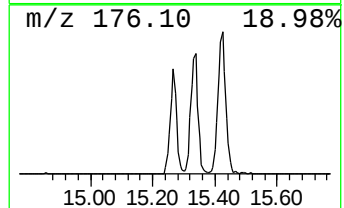
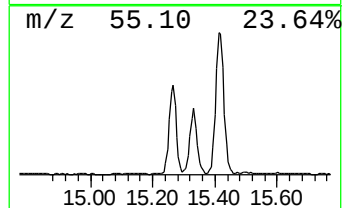
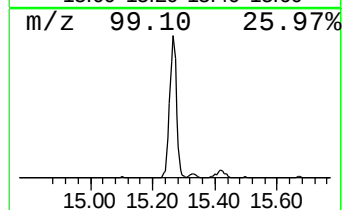
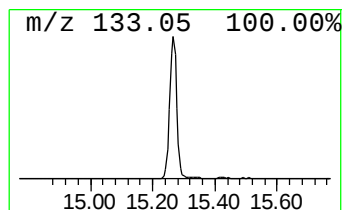
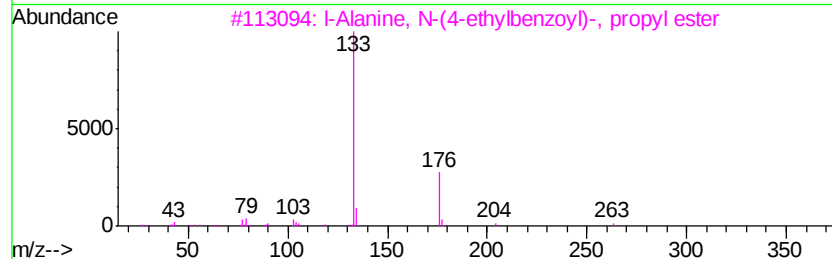
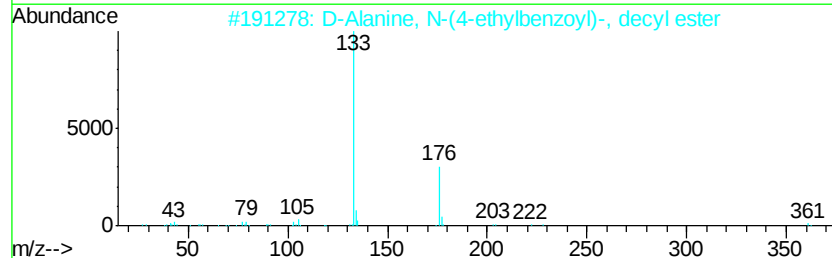
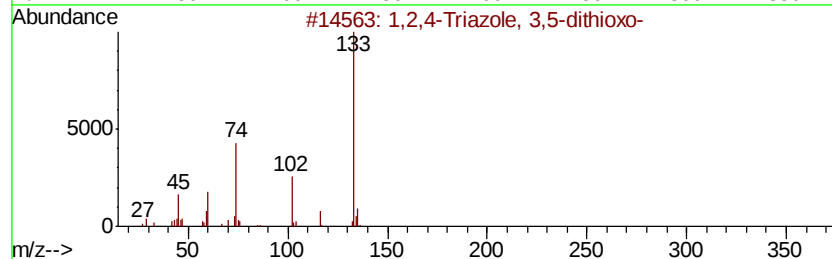
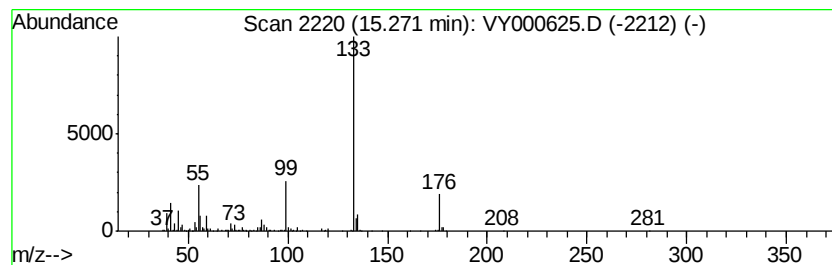
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Quant Title : SW846 8260

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

Peak Number 2 unknown15.27 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	19.50 ug/l	396011	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	47
2		D-Alanine, N-(4-ethylbenzoyl)-, ...	361	C22H35NO3	1000354-09-1	40
3		L-Alanine, N-(4-ethylbenzoyl)-, ...	263	C15H21NO3	1000314-15-9	33
4		L-Alanine, N-(4-ethylbenzoyl)-, ...	361	C22H35NO3	1000314-16-5	33
5		Silane, diethoxydimethyl-	148	C6H16O2Si	000078-62-6	28



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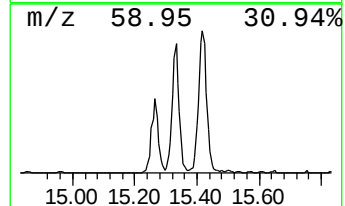
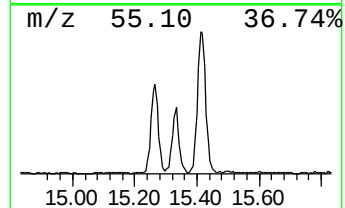
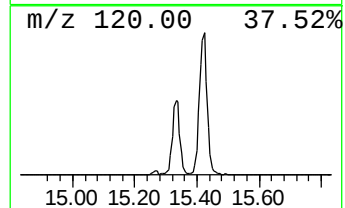
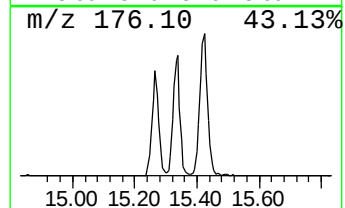
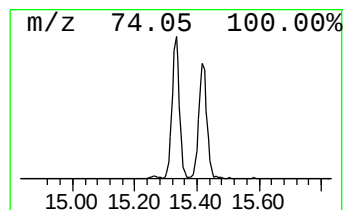
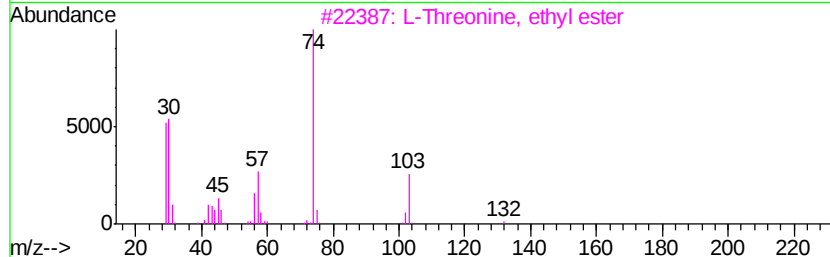
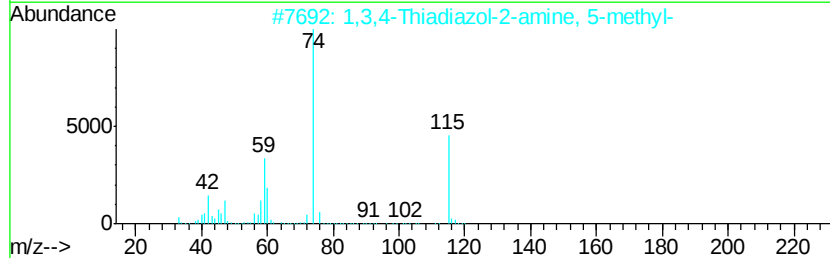
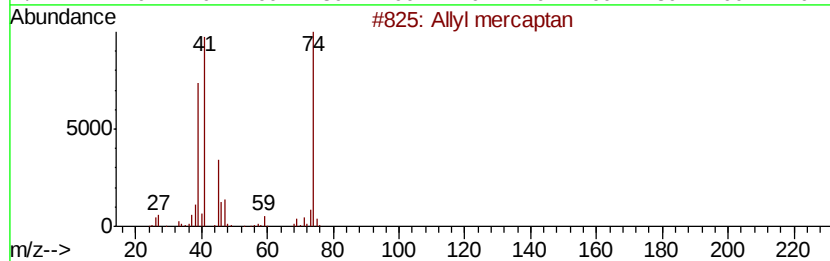
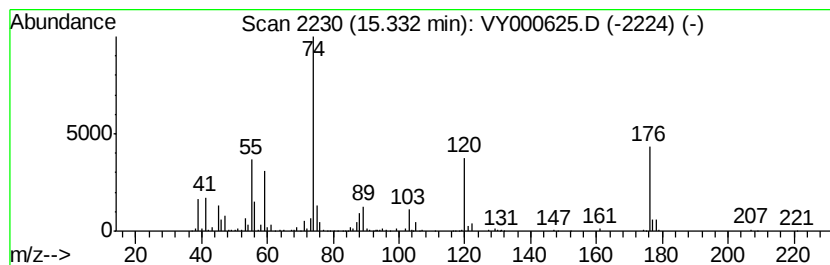
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Peak Number 3 unknown15.33 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	15.30 ug/l	310703	1,4-Dichlorobenzene-d4	13.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Allvl mercaptan	74 C3H6S	000870-23-5	35
2	1,3,4-Thiadiazol-2-amine, 5-methyl-	115 C3H5N3S	000108-33-8	32
3	L-Threonine, ethyl ester	147 C6H13NO3	023926-51-4	25
4	1,3,2-Oxathioborolane, 2-ethyl-5...	130 C5H11BOS	1000163-05-5	25
5	Hexanoic acid, methyl ester	130 C7H14O2	000106-70-7	23



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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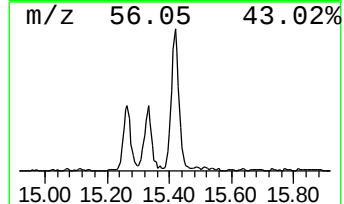
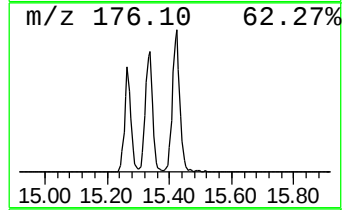
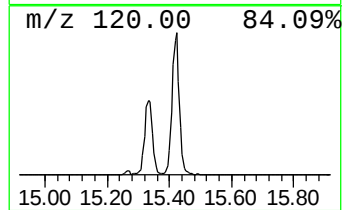
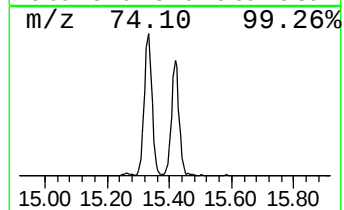
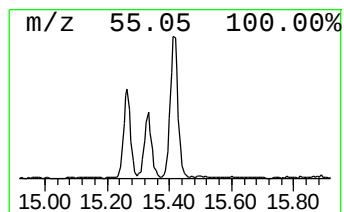
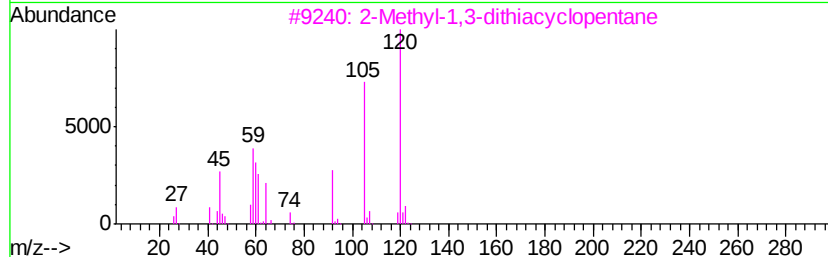
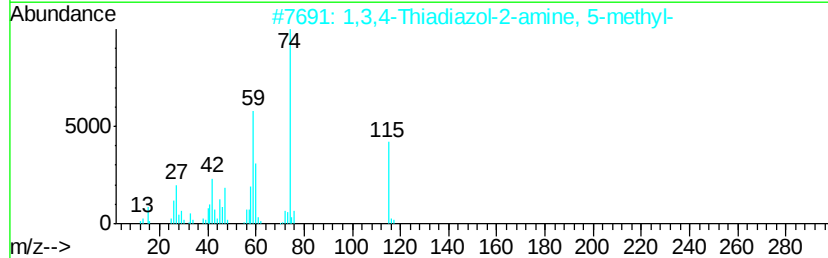
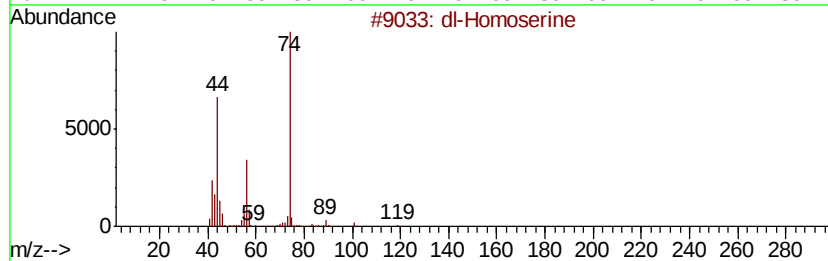
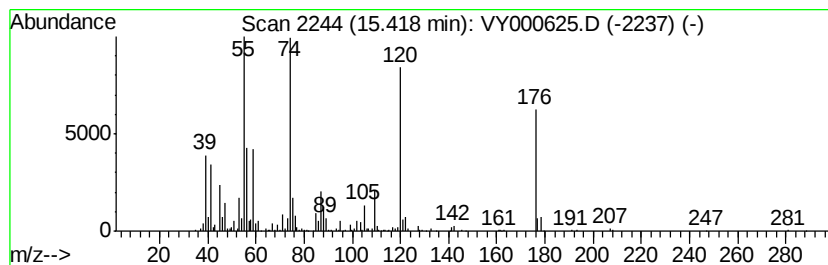
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Peak Number 4 unknown15.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	23.75 ug/l	482343	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	dl-Homoserine	119	C4H9NO3	001927-25-9	25
2		1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	22
3		2-Methyl-1,3-dithiacyclopentane	120	C4H8S2	005616-51-3	14
4		7-Methoxy-1-tetralone	176	C11H12O2	006836-19-7	12
5		5,6-Dihydro-2-methyl-1,4-dithiin...	176	C6H8O2S2	035756-29-7	11



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexane	5.77	5.7	ug/l	72652	1	7.80	639380	50.0
unknown15.27	15.27	19.5	ug/l	396011	4	13.42	1015340	50.0
unknown15.33	15.33	15.3	ug/l	310703	4	13.42	1015340	50.0
unknown15.42	15.42	23.8	ug/l	482343	4	13.42	1015340	50.0