

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102423\
Data File : VX038460.D
Acq On : 24 Oct 2023 17:04
Operator : JC/MD
Sample : 04975-03
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
61

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_X\Method\82X100523W.M

Title : SW846 8260

Signal : TIC: VX038460.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.763	921	931	950	rVB	251504	632188	1.15%	0.885%
2	8.647	1234	1240	1246	rBV	550339	851624	1.55%	1.192%
3	8.714	1246	1251	1266	rVB	1087577	1788992	3.25%	2.505%
4	10.055	1466	1471	1486	rVB	582389	830025	1.51%	1.162%
5	11.085	1634	1640	1651	rVB	525774	757615	1.38%	1.061%
6	12.024	1789	1794	1799	rBV	806215	1004480	1.83%	1.406%
7	12.994	1945	1953	1958	rBV	6728283	7968265	14.48%	11.157%
8	13.262	1992	1997	2000	rBV2	935125	1304128	2.37%	1.826%
9	14.457	2185	2193	2197	rBV	36879331	55015933	100.00%	77.029%
10	14.981	2274	2279	2285	rBV	1033653	1269066	2.31%	1.777%

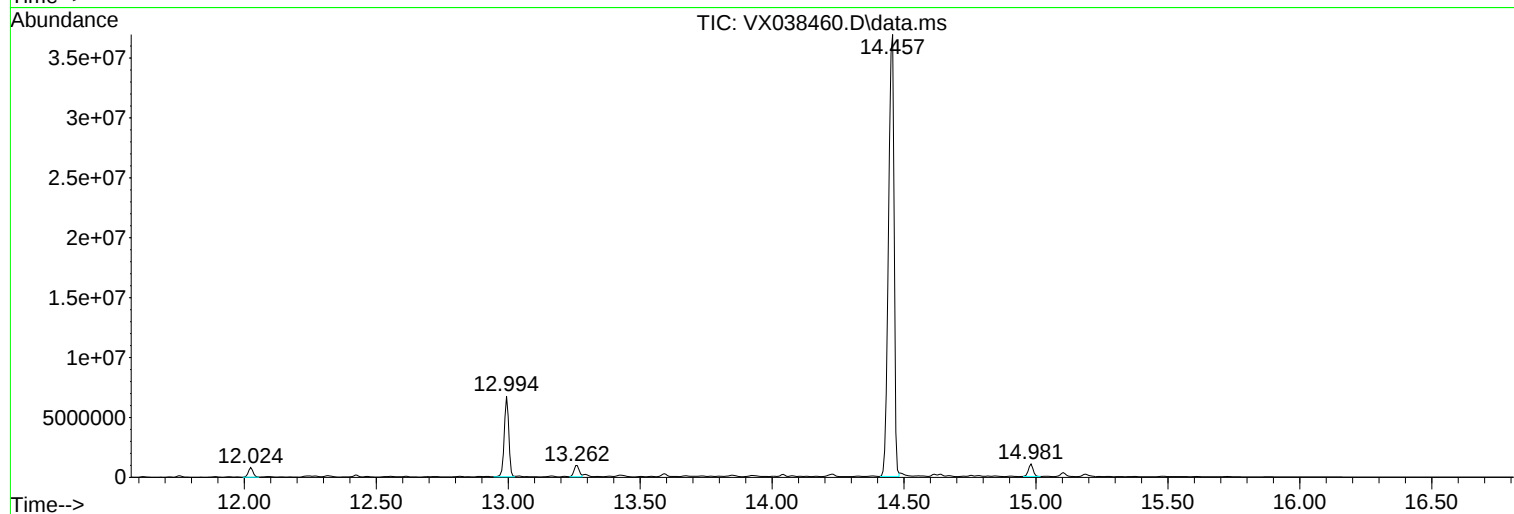
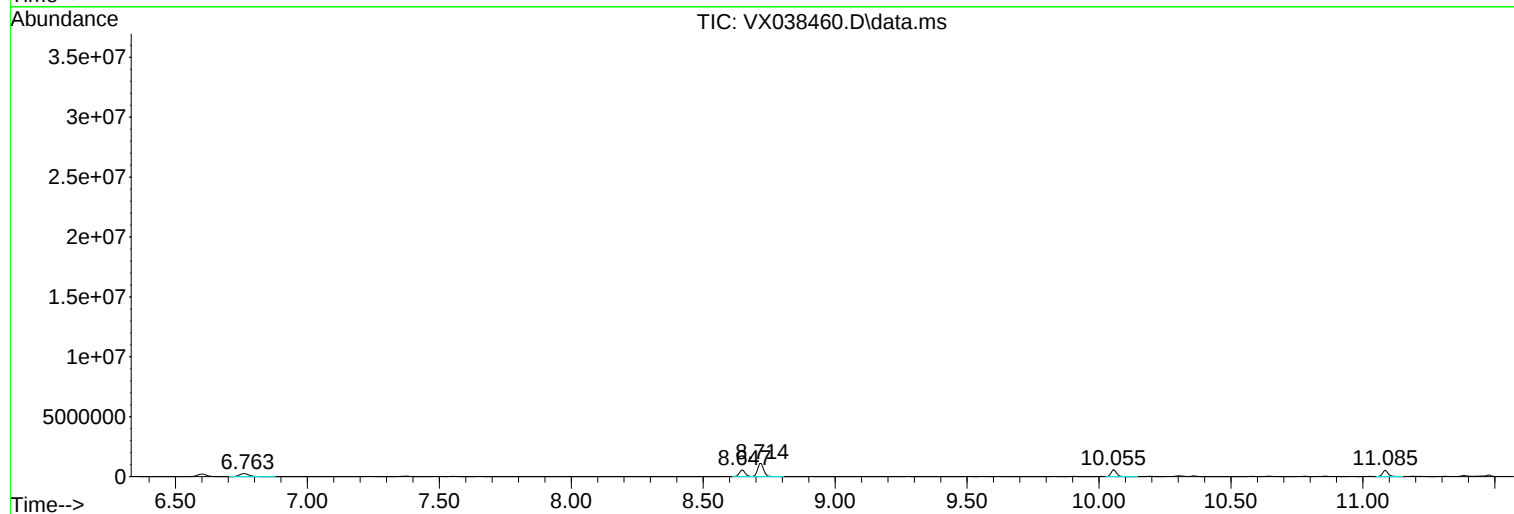
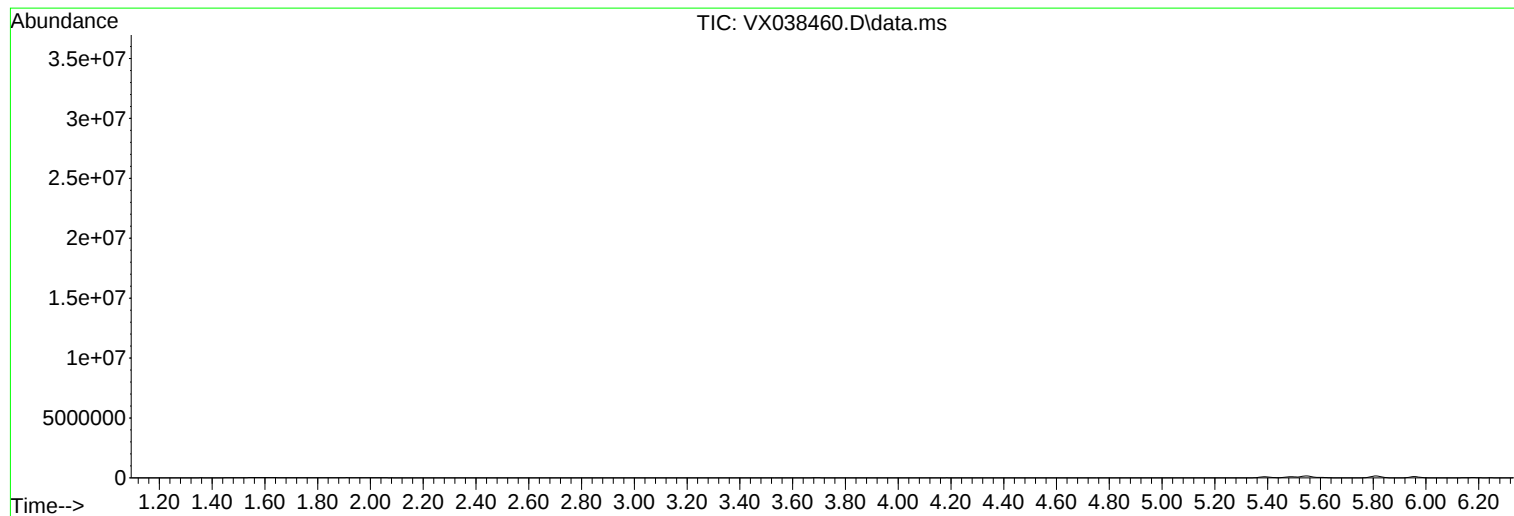
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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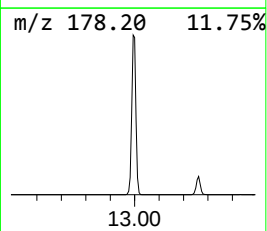
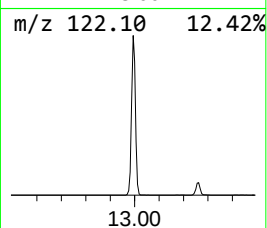
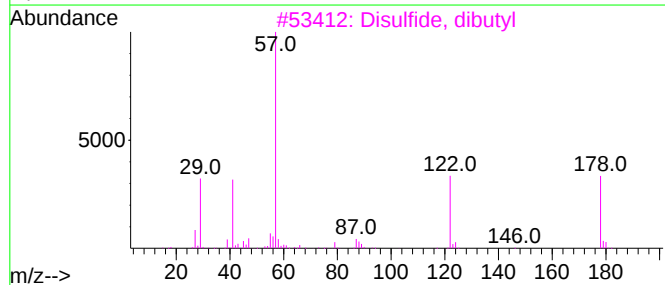
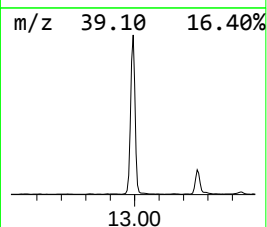
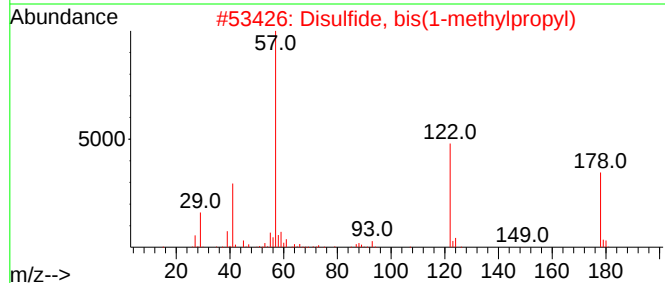
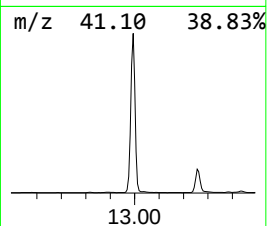
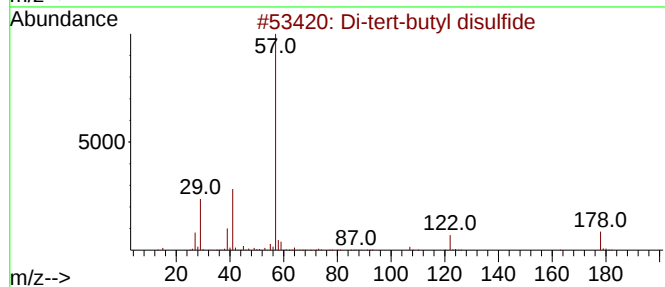
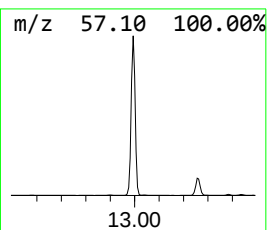
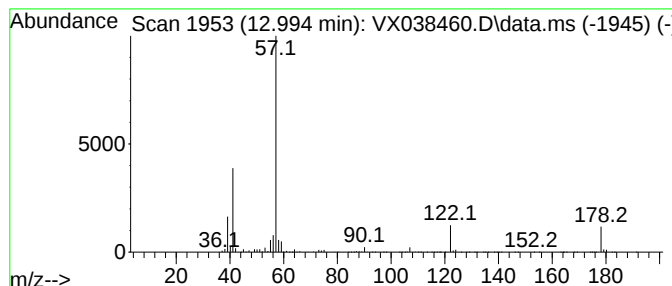
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Di-tert-butyl disulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.994	396.64 ug/l	7968270	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	81
2		Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	72
3		Disulfide, dibutyl	178	C8H18S2	000629-45-8	64
4		Disulfide, bis(2-methylpropyl)	178	C8H18S2	001518-72-5	64
5		Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	38



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Instrument :
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ClientSampleId :
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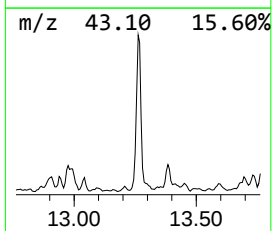
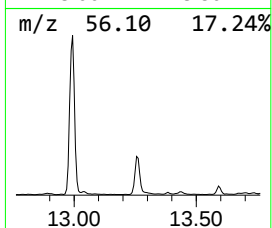
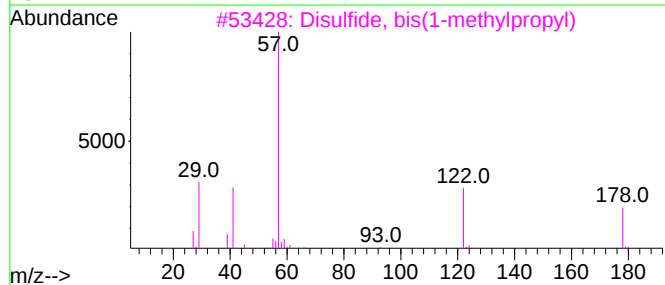
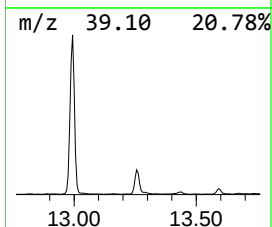
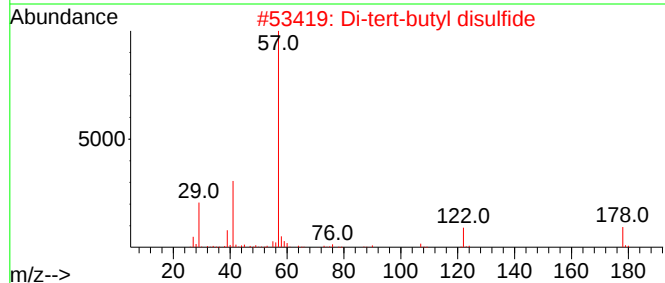
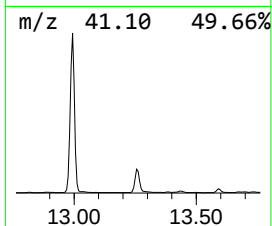
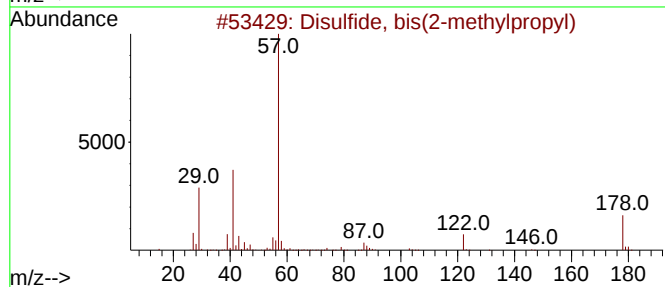
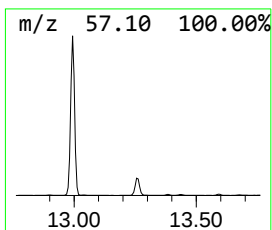
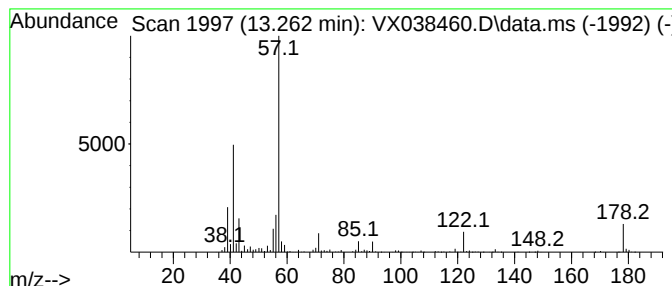
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Disulfide, bis(2-methylpropyl) Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.262	64.92 ug/l	1304130	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, bis(2-methylpropyl)	178	C8H18S2	001518-72-5	53
2			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	52
3			Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	50
4			Disulfide, dibutyl	178	C8H18S2	000629-45-8	38
5			Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	38



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MSVOA_X
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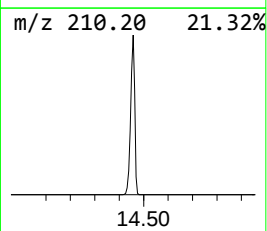
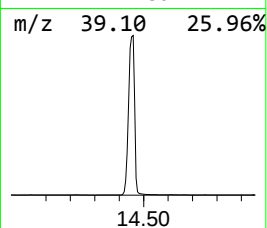
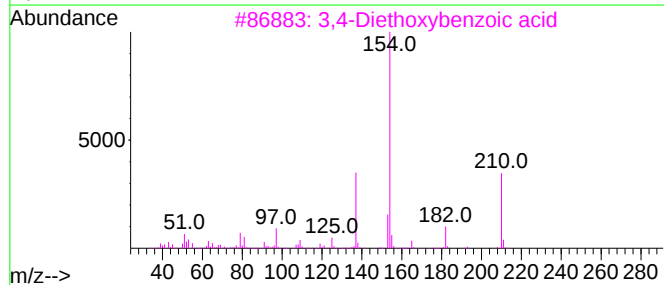
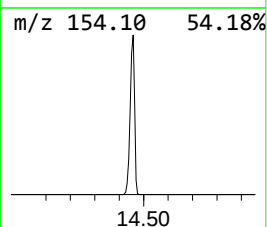
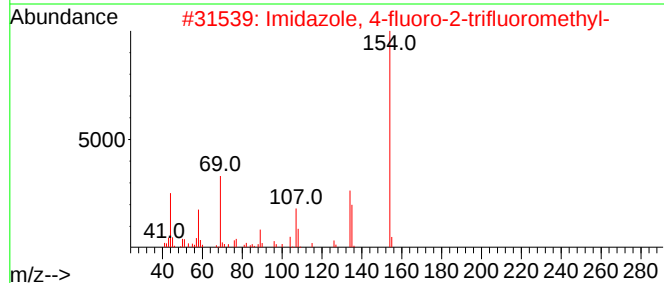
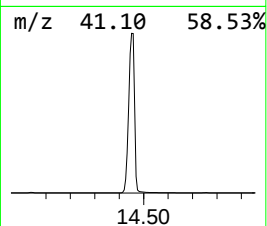
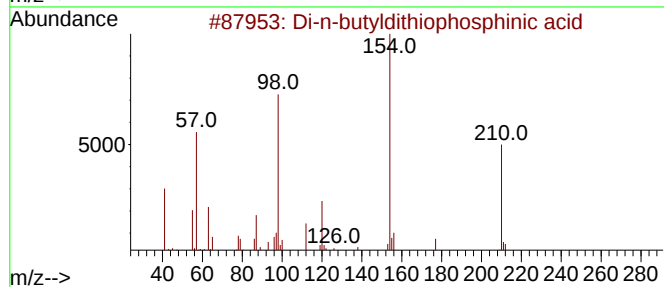
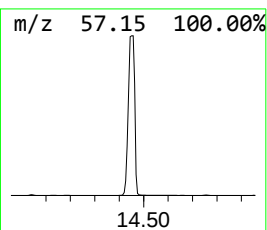
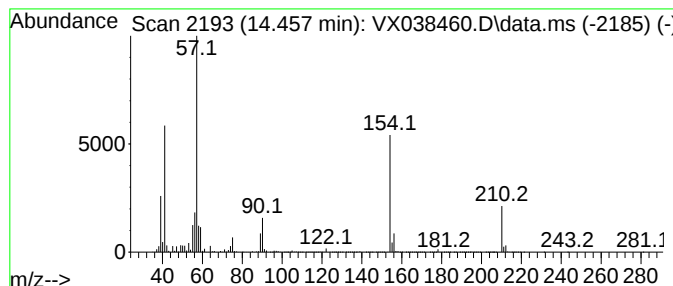
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown14.457 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	2738.53 ug/l	55015900	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-n-butylidithiophosphinic acid	210	C8H19PS2	032435-35-1	43
2			Imidazole, 4-fluoro-2-trifluoromethyl-	154	C4H2F4N2	219534-90-4	38
3			3,4-Diethoxybenzoic acid	210	C11H14O4	005409-31-4	32
4			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	27
5			DL-Alanine, N-methyl-N-(but-3-yn-1-yl)-	255	C13H21NO4	1000392-70-1	17



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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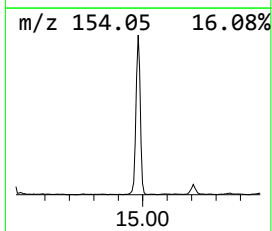
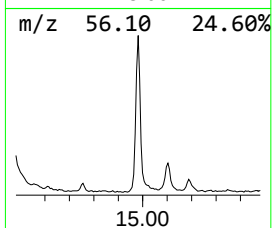
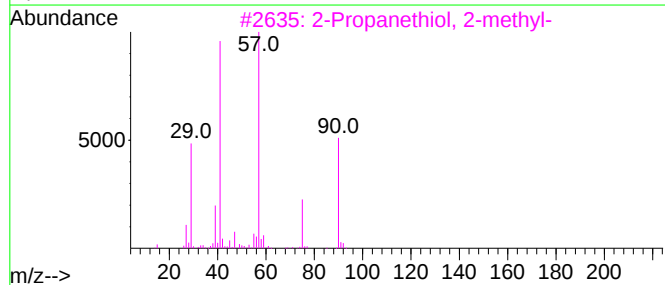
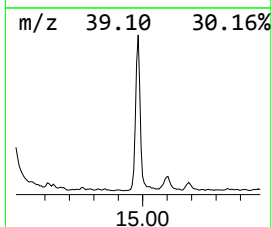
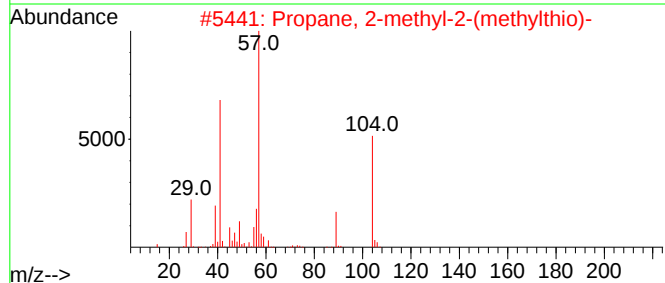
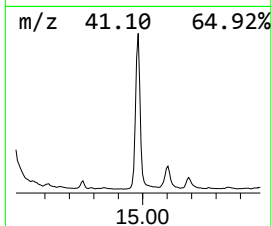
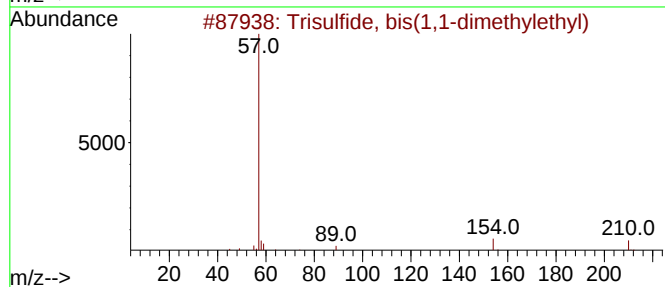
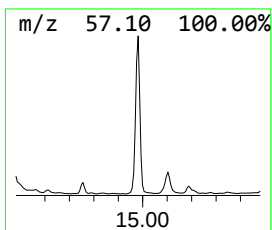
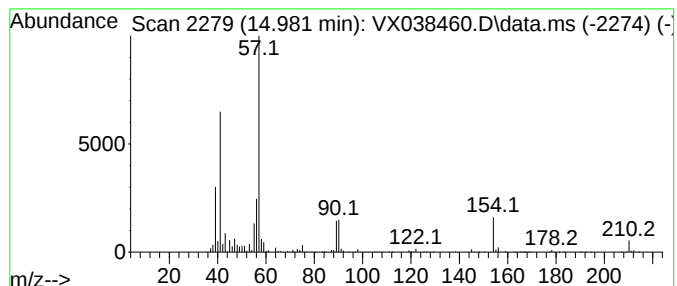
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.981 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.981	63.17 ug/l	1269070	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	46
2			Propane, 2-methyl-2-(methylthio)-	104	C5H12S	006163-64-0	43
3			2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	32
4			Butane, 1-bromo-	136	C4H9Br	000109-65-9	25
5			Hydrazinecarboxylic acid, 1,1-di...	132	C5H12N2O2	000870-46-2	25



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Di-tert-butyl d...	12.994	396.6	ug/l	7968270	4	12.024	1004480	50.0
Disulfide, bis(...	13.262	64.9	ug/l	1304130	4	12.024	1004480	50.0
unknown14.457	14.457	2738.5	ug/l	55015900	4	12.024	1004480	50.0
unknown14.981	14.981	63.2	ug/l	1269070	4	12.024	1004480	50.0