

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102423\
 Data File : VX038454.D
 Acq On : 24 Oct 2023 14:45
 Operator : JC/MD
 Sample : 04975-03 10X
 Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 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: VX038454.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	692	705	716	rBV	93384	279568	7.98%	2.450%
2	5.544	717	731	752	rVB	154602	468670	13.39%	4.107%
3	5.952	786	798	814	rBV	106997	279266	7.98%	2.447%
4	6.757	920	930	950	rBV	248498	603502	17.24%	5.289%
5	8.647	1234	1240	1247	rBV	535363	833885	23.82%	7.308%
6	8.720	1247	1252	1266	rVB	101021	164605	4.70%	1.443%
7	10.055	1465	1471	1484	rBV	573387	800464	22.86%	7.015%
8	11.079	1634	1639	1651	rBV	507196	653834	18.67%	5.730%
9	12.024	1788	1794	1800	rBV	704235	916916	26.19%	8.036%
10	12.219	1821	1826	1852	rBV	1429392	2202415	62.90%	19.302%
11	12.420	1856	1859	1863	rVB	33834	45074	1.29%	0.395%
12	12.994	1947	1953	1958	rVB	335378	439489	12.55%	3.852%
13	13.262	1992	1997	2001	rBV2	87821	136210	3.89%	1.194%
14	14.438	2184	2190	2205	rBV	2825230	3501363	100.00%	30.686%
15	14.981	2273	2279	2284	rBV	64105	85051	2.43%	0.745%

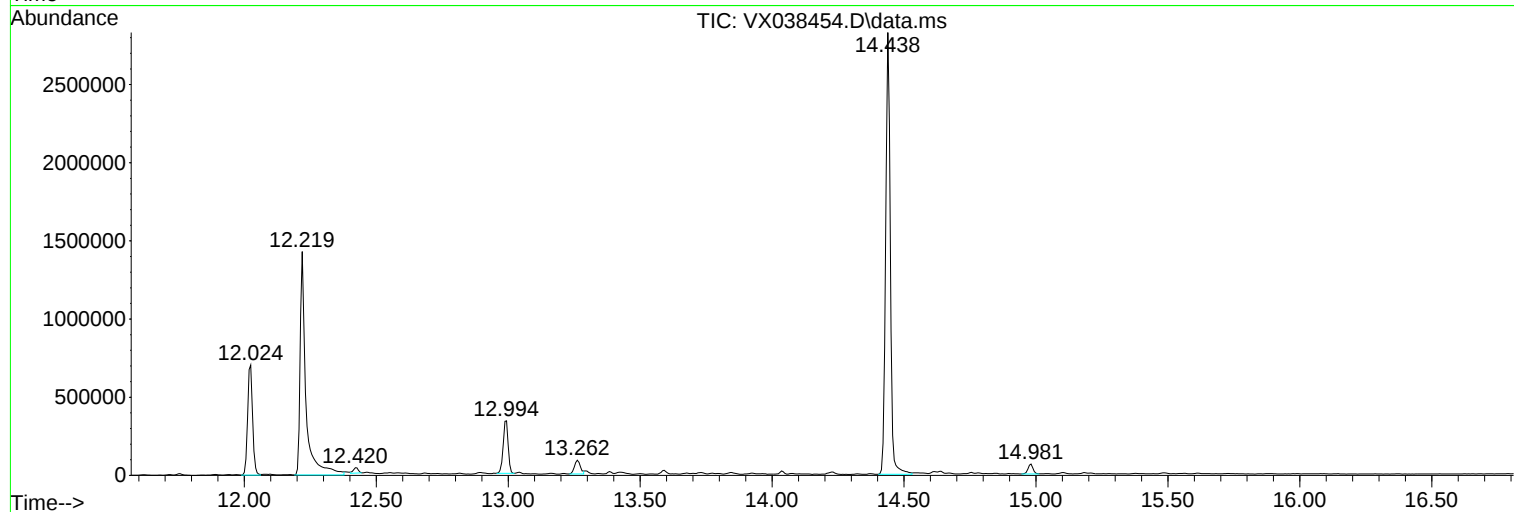
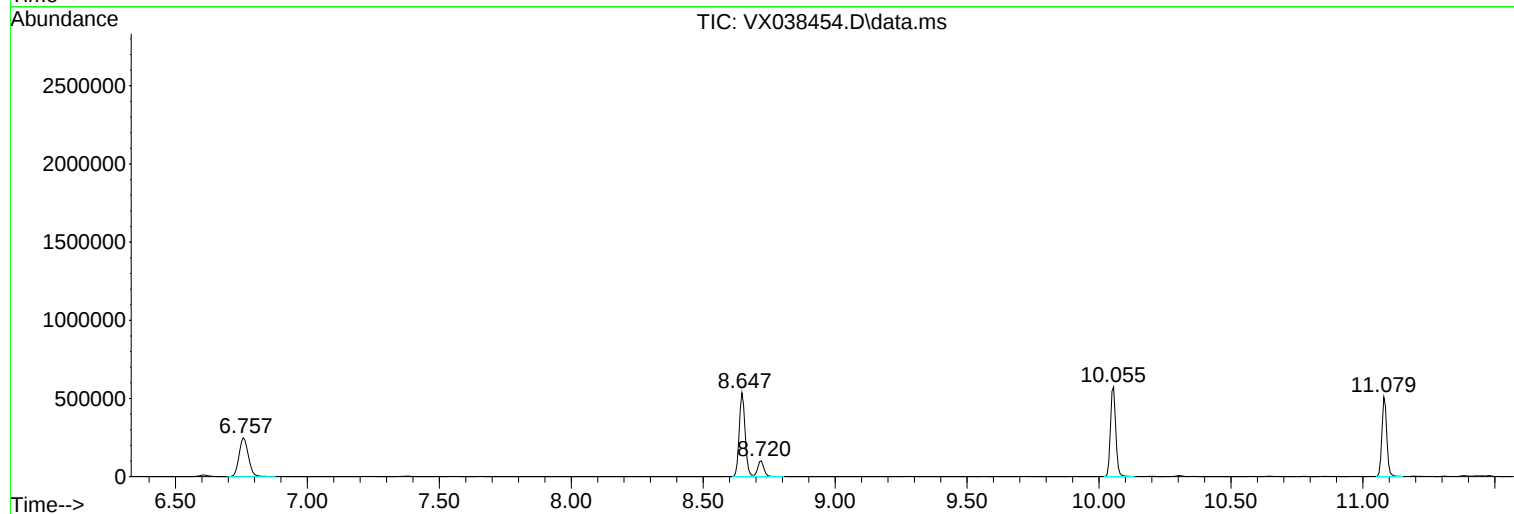
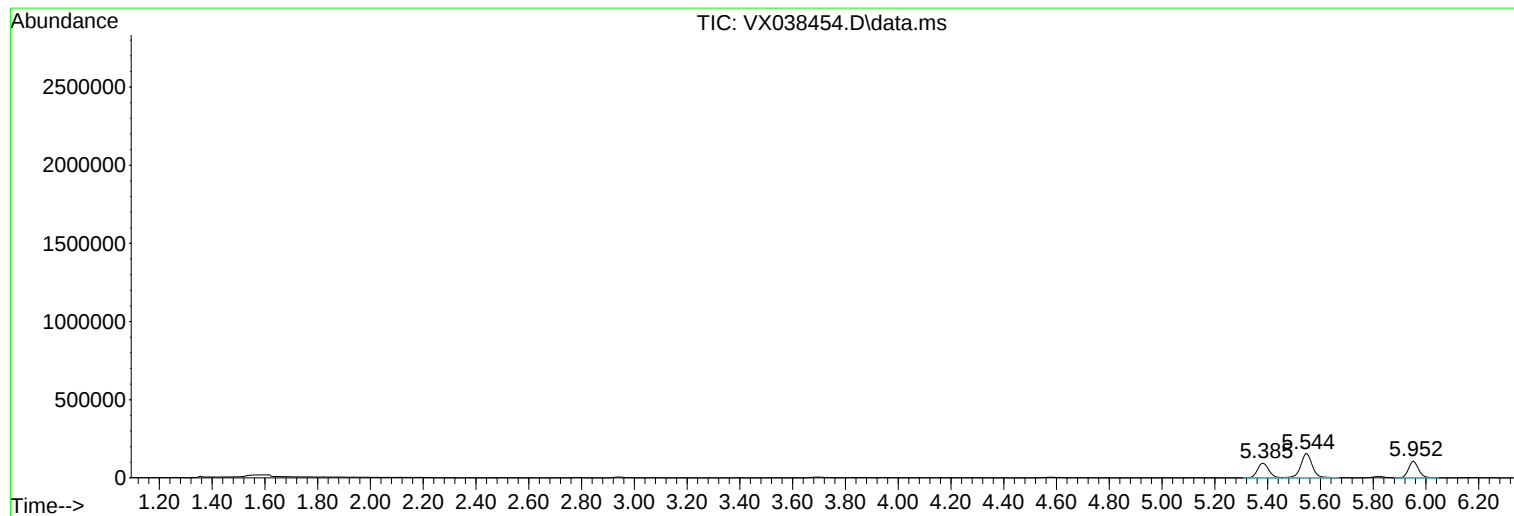
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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



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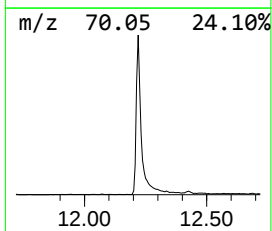
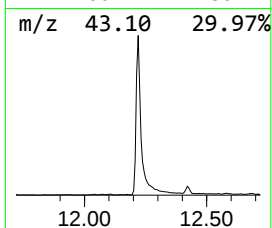
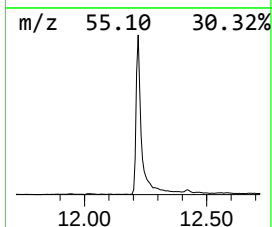
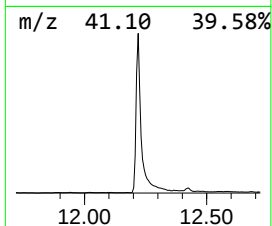
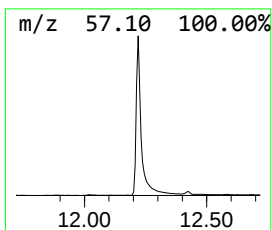
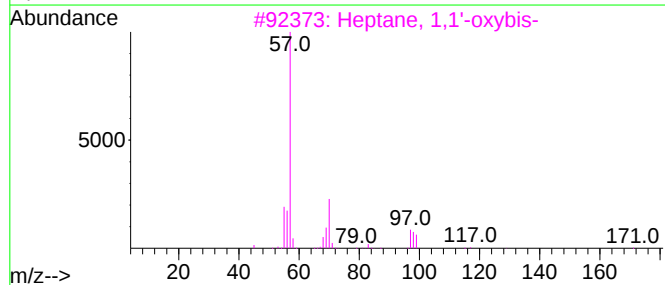
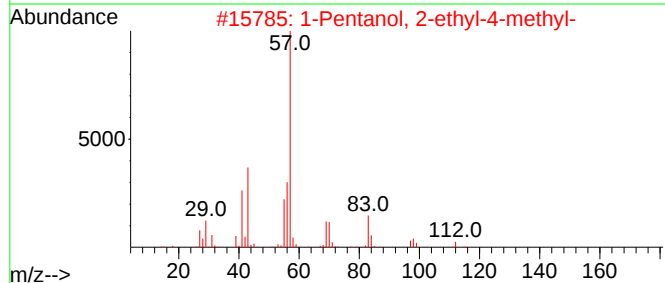
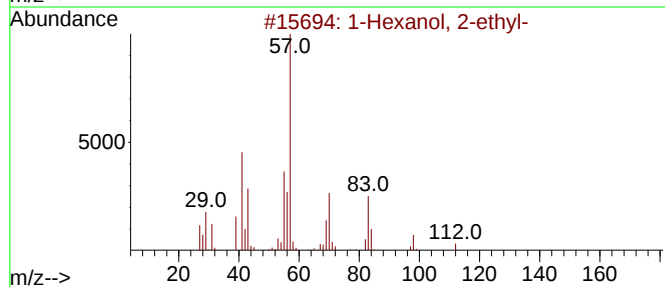
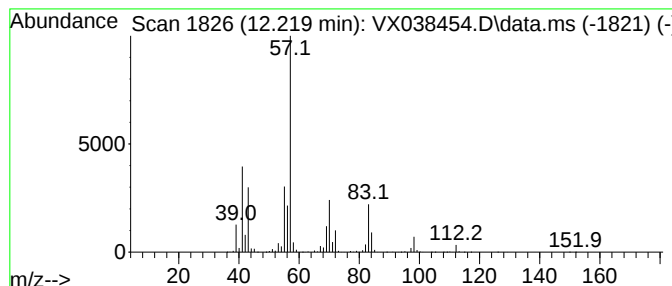
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	120.10 ug/l	2202420	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	43



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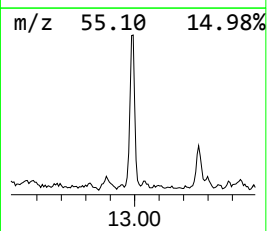
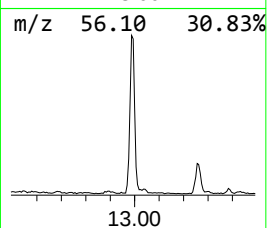
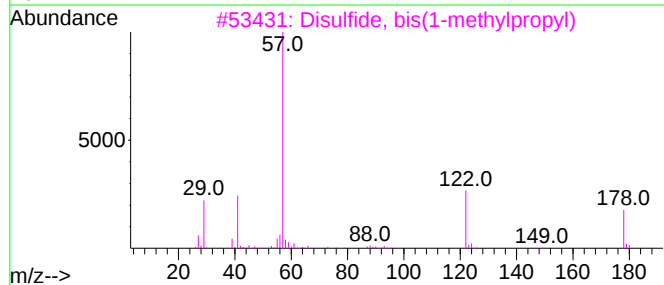
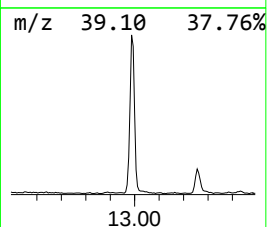
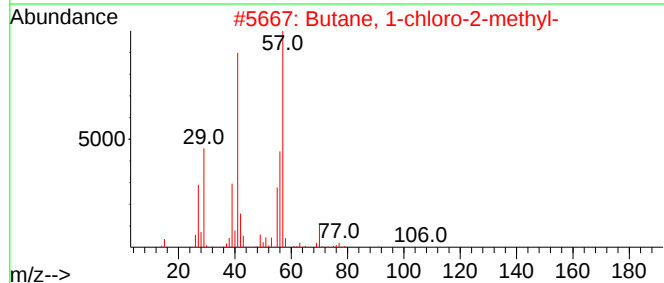
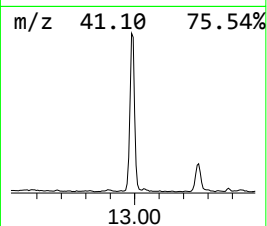
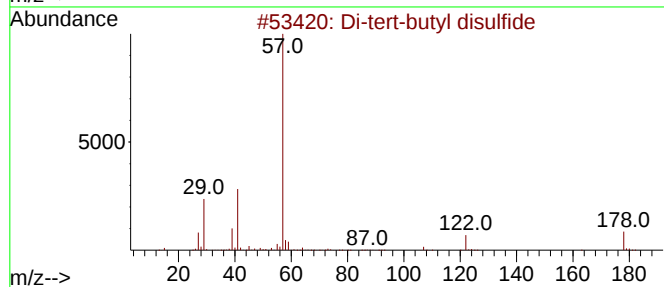
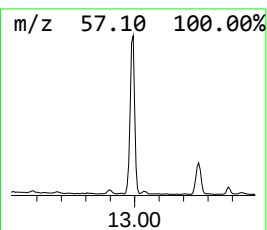
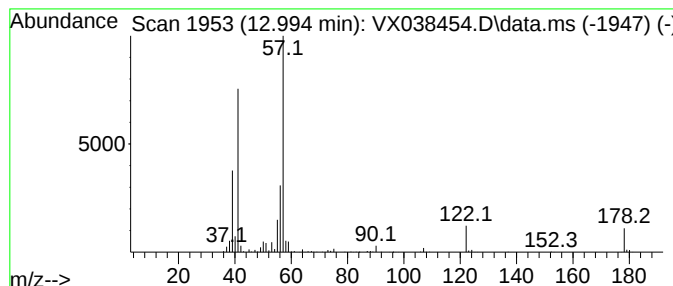
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.993 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.993	23.97 ug/l	439489	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	49
2			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	43
3			Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	43
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	38
5			2-Butene, (Z)-	56	C4H8	000590-18-1	38



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ALS Vial : 8 Sample Multiplier: 1

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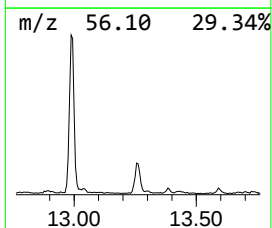
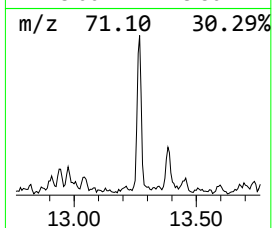
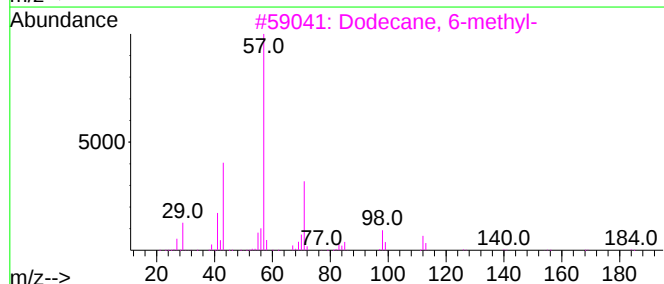
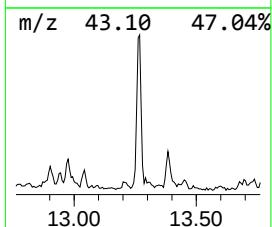
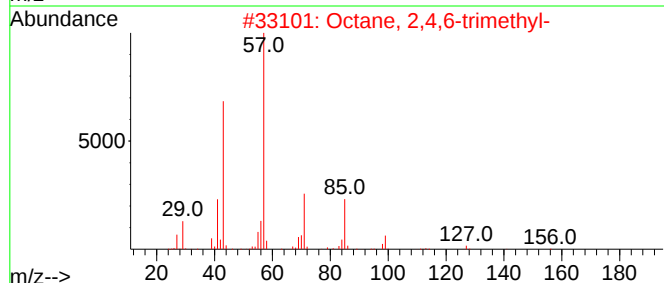
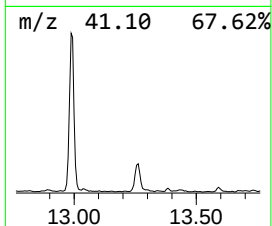
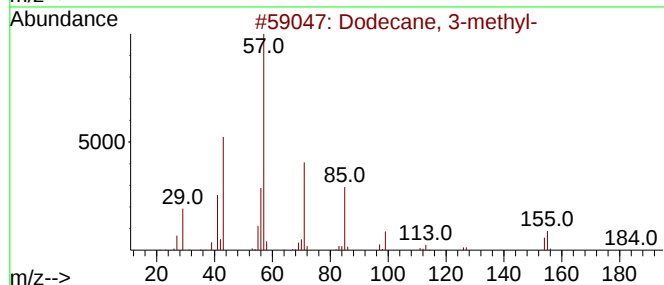
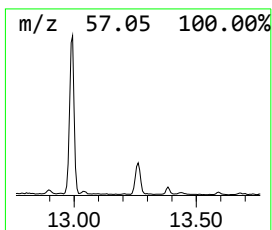
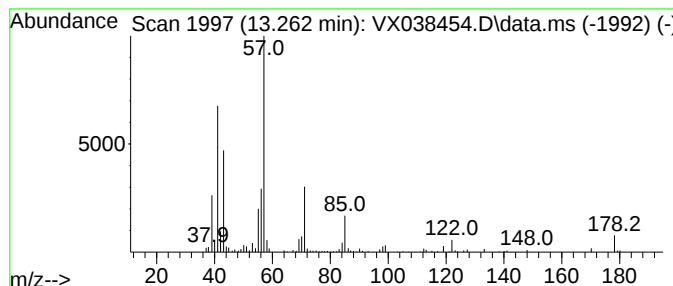
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dodecane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.262	7.43 ug/l	136210	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 3-methyl-	184	C13H28	017312-57-1	59
2			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	53
3			Dodecane, 6-methyl-	184	C13H28	006044-71-9	47
4			Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	47
5			3-Undecanone	170	C11H22O	002216-87-7	46



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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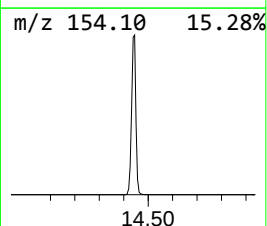
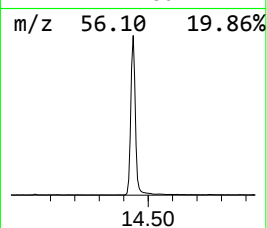
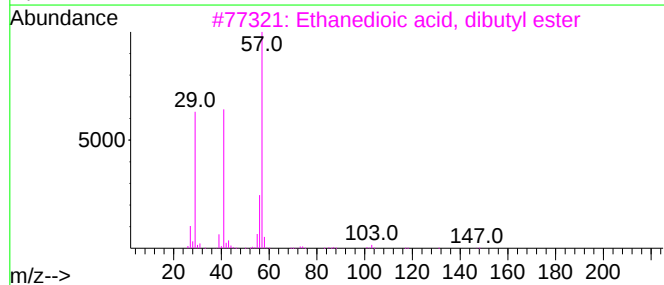
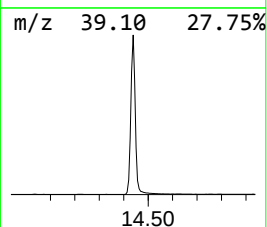
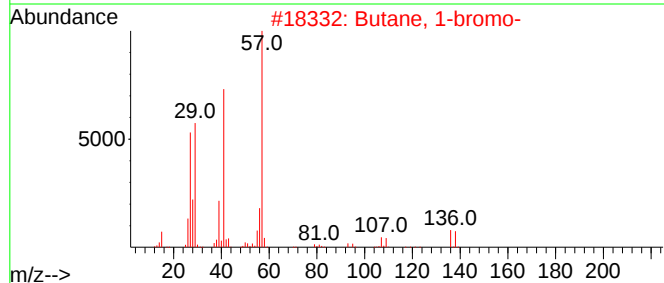
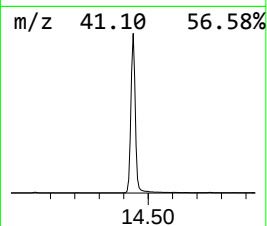
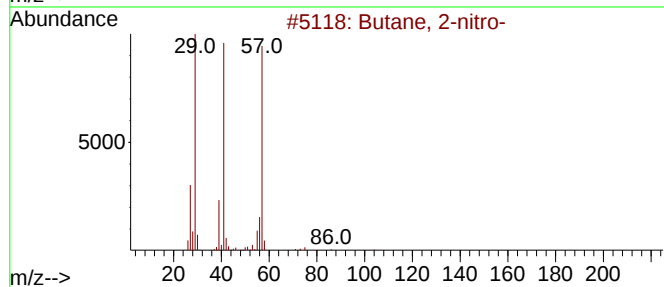
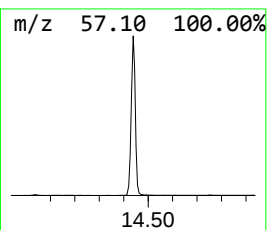
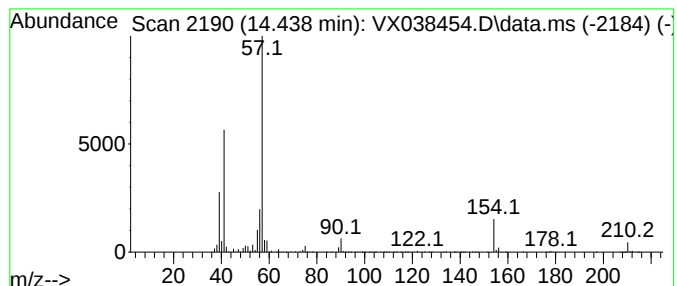
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.438 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.438	190.93 ug/l	3501360	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-nitro-	103	C4H9NO2	000600-24-8	38
2			Butane, 1-bromo-	136	C4H9Br	000109-65-9	32
3			Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	23
4			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	22
5			Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	16



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	12.219	120.1	ug/l	2202420	4	12.024	916916	50.0
unknown12.993	12.993	24.0	ug/l	439489	4	12.024	916916	50.0
Dodecane, 3-met...	13.262	7.4	ug/l	136210	4	12.024	916916	50.0
unknown14.438	14.438	190.9	ug/l	3501360	4	12.024	916916	50.0