

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU112118\
 Data File : VU028321.D
 Acq On : 21 Nov 2018 15:50
 Operator : MD/SY
 Sample : J6026-22DL 5X
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 H0FP1DL

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

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_U\METHOD\SOMUTR111718WMA.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	1.302	35	40	52	rVB	45714	44125	6.00%	0.583%
2	1.399	62	70	81	rVB2	196740	213117	28.97%	2.818%
3	1.682	150	158	171	rVB	79840	95018	12.91%	1.256%
4	1.755	172	181	193	rVV	419487	544921	74.06%	7.204%
5	1.948	237	241	253	rVB4	10491	17470	2.37%	0.231%
6	2.273	331	342	356	rBV	151120	236096	32.09%	3.121%
7	2.701	467	475	485	rBV6	12435	21879	2.97%	0.289%
8	2.788	491	502	517	rBV	131743	245985	33.43%	3.252%
9	3.003	554	569	590	rVB2	245092	543091	73.81%	7.180%
10	4.083	891	905	920	rBV5	10024	25859	3.51%	0.342%
11	4.189	920	938	964	rBV	124106	341695	46.44%	4.517%
12	4.646	1060	1080	1101	rBV	121049	277013	37.65%	3.662%
13	4.990	1175	1187	1203	rVB4	5974	13640	1.85%	0.180%
14	5.337	1273	1295	1327	rBV3	236256	694944	94.45%	9.188%
15	5.884	1448	1465	1482	rBV	213031	422269	57.39%	5.583%
16	6.331	1590	1604	1625	rBV	162974	324367	44.09%	4.288%
17	7.228	1870	1883	1899	rBV	89947	161013	21.88%	2.129%
18	7.562	1973	1987	2006	rBV	296629	517964	70.40%	6.848%
19	7.848	2061	2076	2092	rBV	56438	94329	12.82%	1.247%
20	8.311	2209	2220	2254	rBV	411334	735760	100.00%	9.727%
21	8.456	2255	2265	2280	rVB3	66854	117377	15.95%	1.552%
22	9.090	2448	2462	2474	rBV	307101	515221	70.03%	6.812%
23	9.498	2578	2589	2613	rVB	111637	192025	26.10%	2.539%
24	9.700	2641	2652	2656	rBV7	4746	7703	1.05%	0.102%
25	9.954	2722	2731	2739	rBV7	8284	14099	1.92%	0.186%
26	10.038	2746	2757	2768	rBV8	9150	17875	2.43%	0.236%
27	10.099	2768	2776	2784	rVB8	4786	7875	1.07%	0.104%
28	10.430	2867	2879	2898	rBV	113127	196147	26.66%	2.593%
29	11.083	3070	3082	3093	rVB10	5883	10008	1.36%	0.132%
30	11.482	3190	3206	3226	rBV	303697	477693	64.93%	6.316%
31	11.858	3311	3323	3338	rBV	269108	428077	58.18%	5.660%
32	14.279	4061	4076	4085	rBV2	5071	9155	1.24%	0.121%

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ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId :
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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\SOMUTR111718WMA.M
Title : TRACE VOA SOM01.0

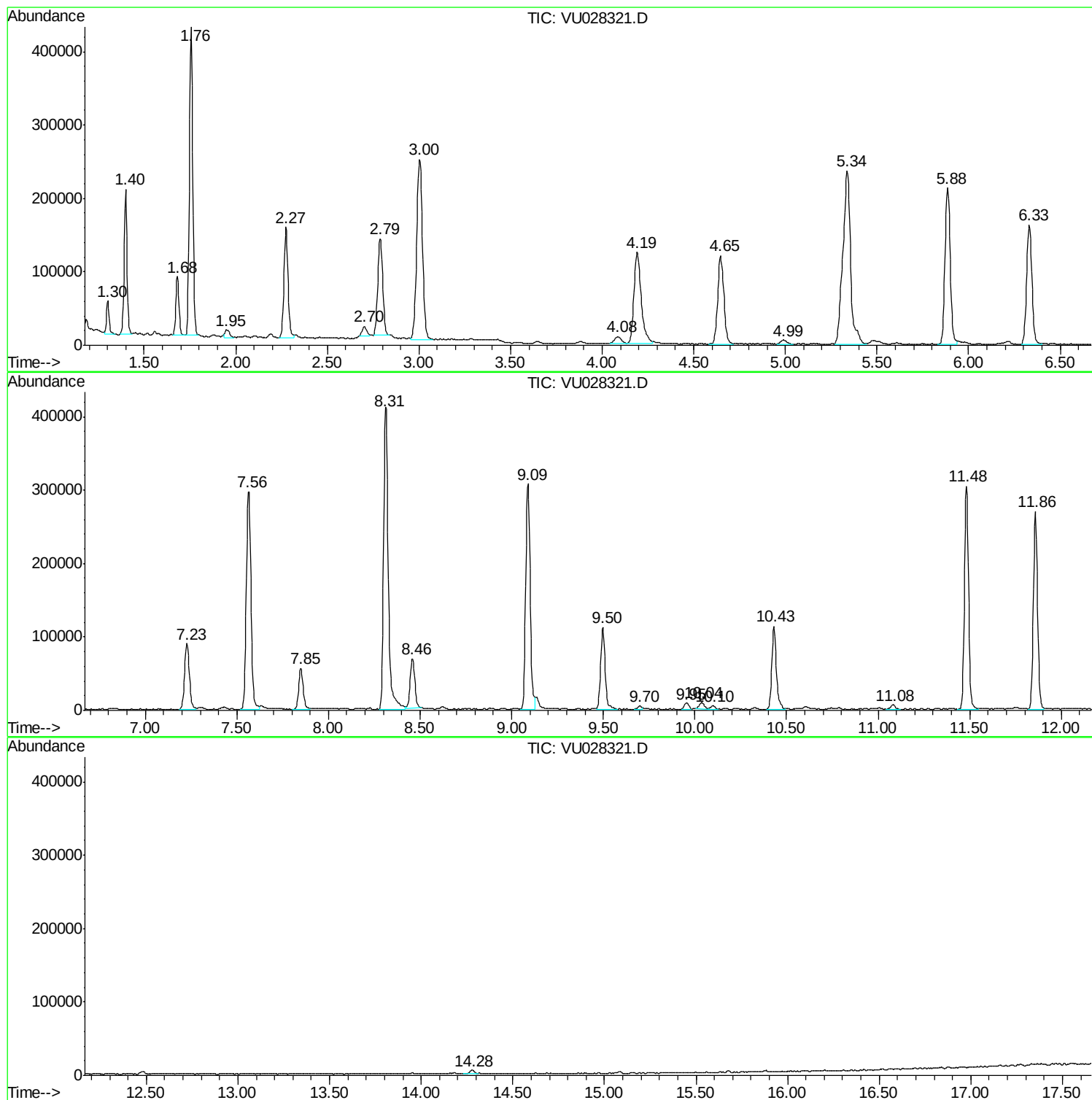
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
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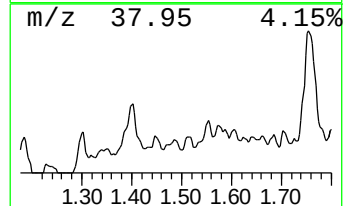
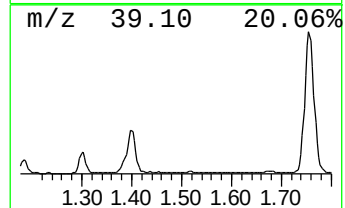
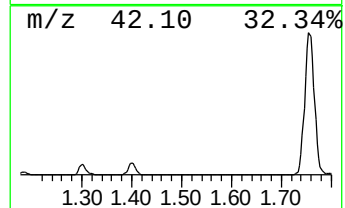
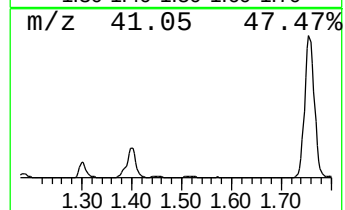
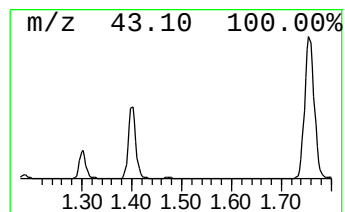
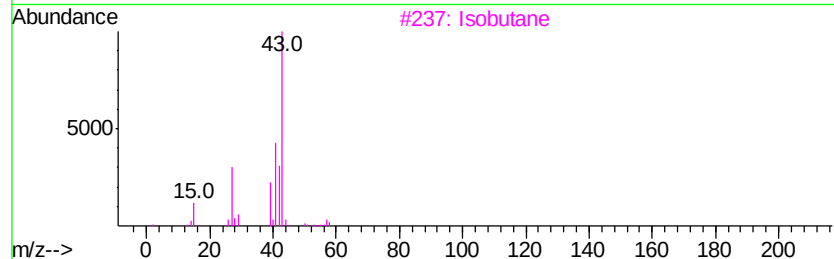
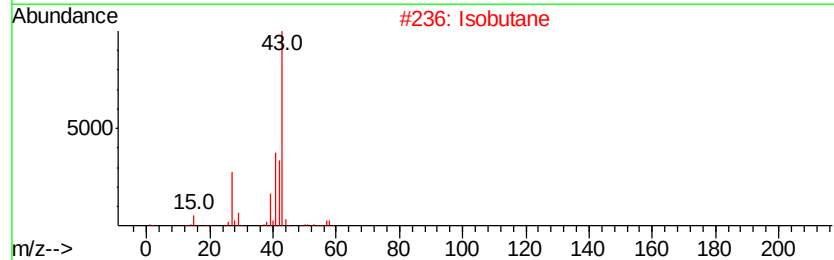
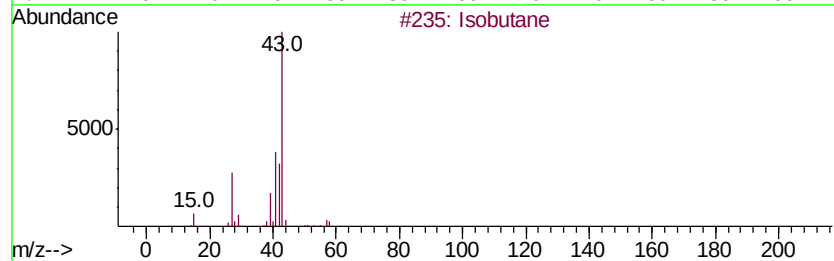
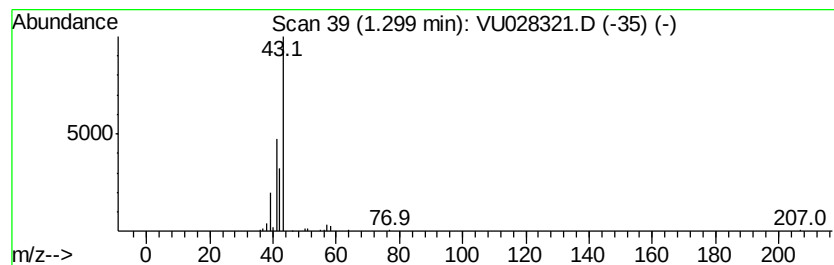
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111718WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.30	0.52 ug/L	44125	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isobutane	58	C4H10	000075-28-5	64
2		Isobutane	58	C4H10	000075-28-5	64
3		Isobutane	58	C4H10	000075-28-5	50
4		Isobutane	58	C4H10	000075-28-5	9
5		Isobutyl nitrite	103	C4H9NO2	000542-56-3	9



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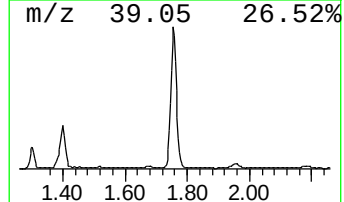
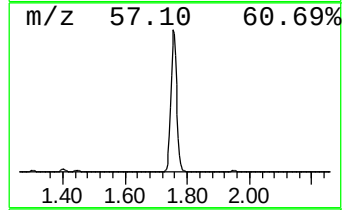
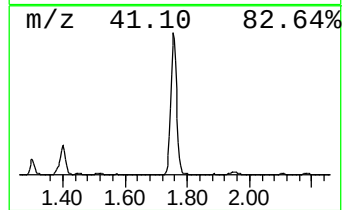
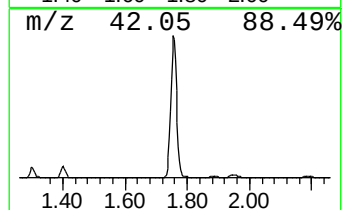
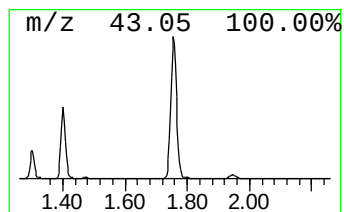
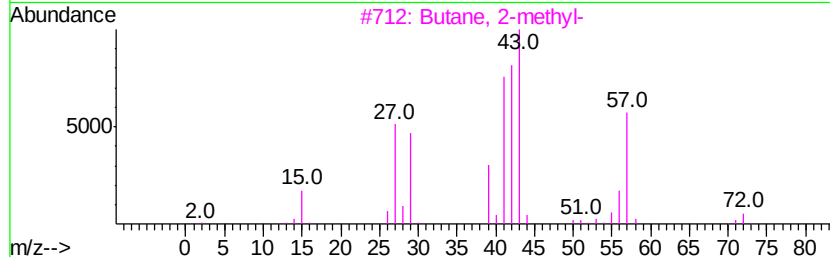
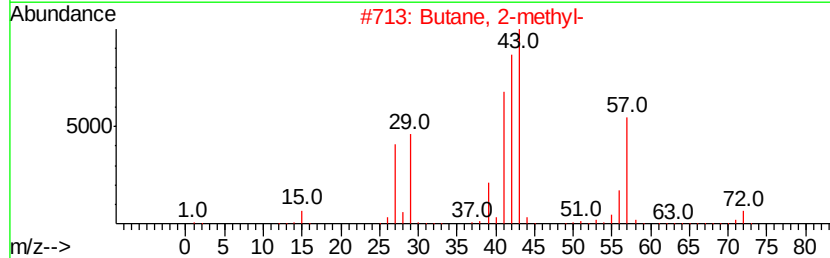
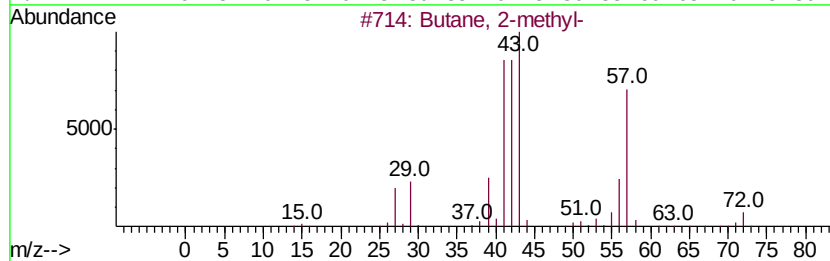
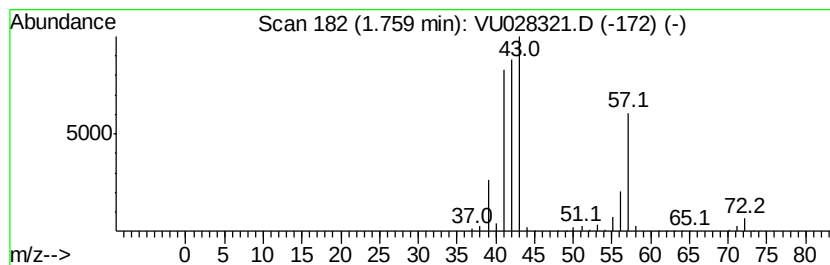
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111718WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.76	6.45 ug/L	544921	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2		Butane, 2-methyl-	72	C5H12	000078-78-4	91
3		Butane, 2-methyl-	72	C5H12	000078-78-4	90
4		Pentane	72	C5H12	000109-66-0	50
5		3-Buten-1-ol	72	C4H8O	000627-27-0	47



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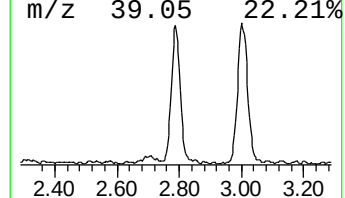
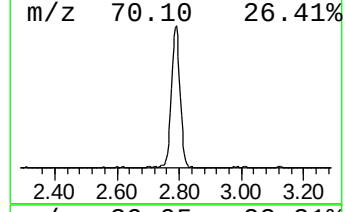
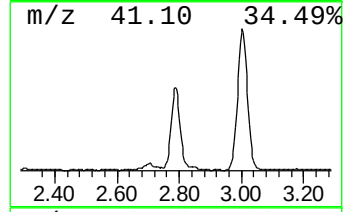
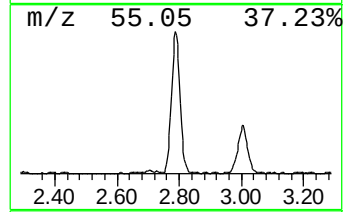
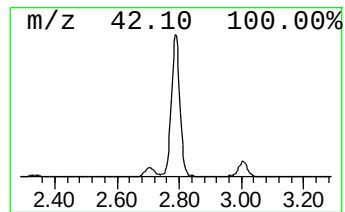
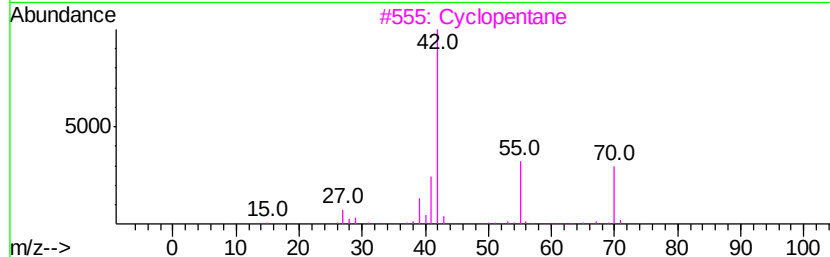
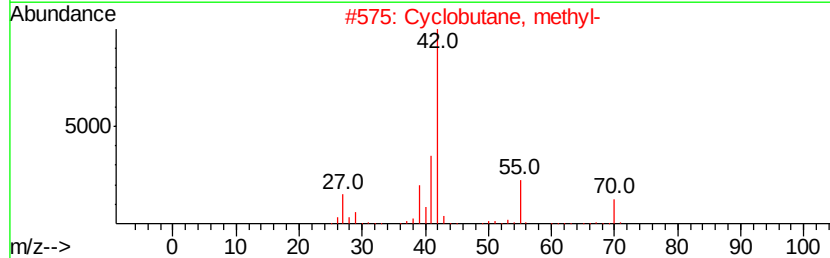
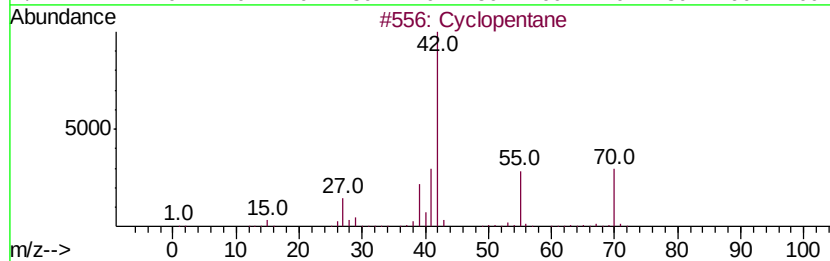
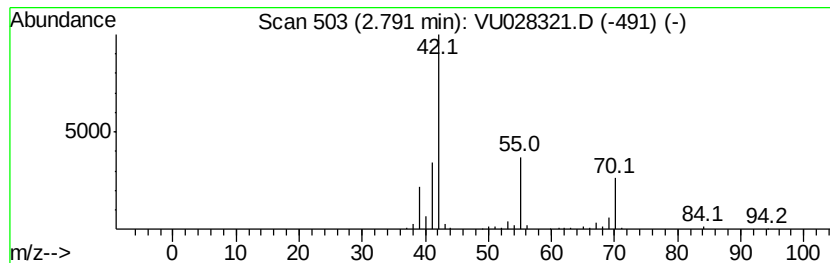
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Cyclic2.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.79	2.91 ug/L	245985	1,4-Difluorobenzene	5.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	86
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3	Cyclopentane	70	C5H10	000287-92-3	72
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	59
5	1-Pentene	70	C5H10	000109-67-1	56



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Instrument :
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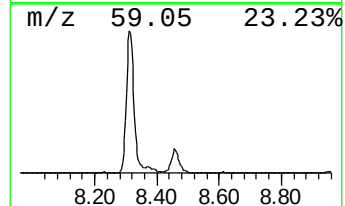
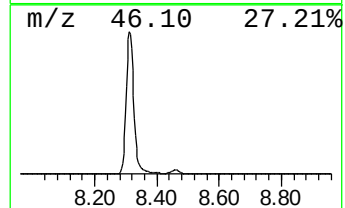
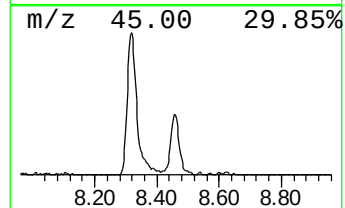
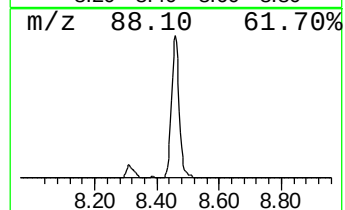
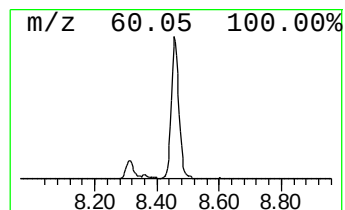
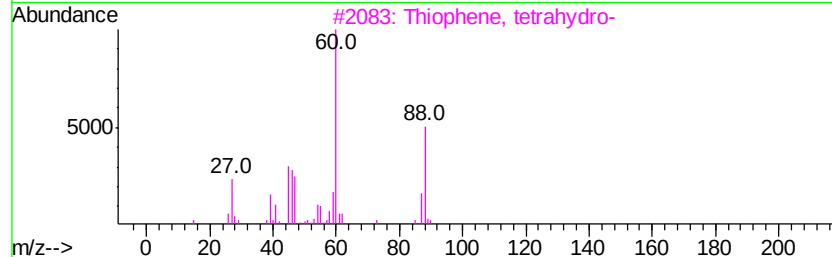
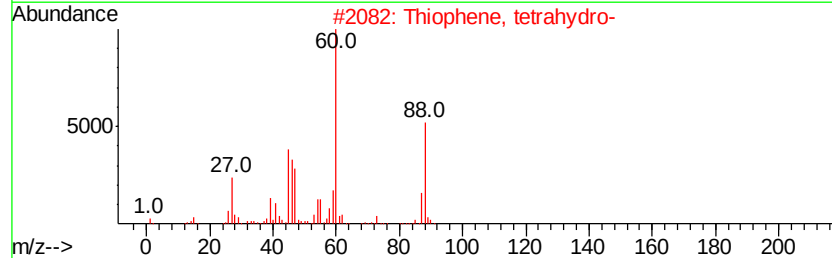
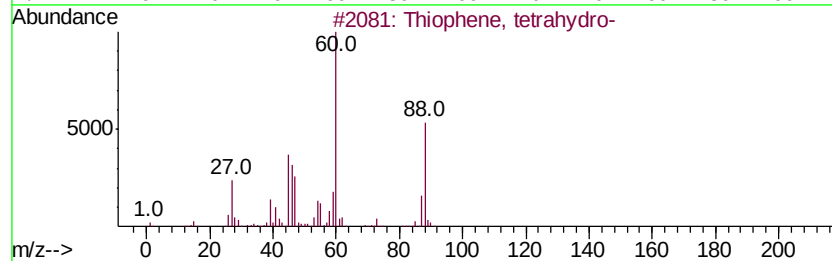
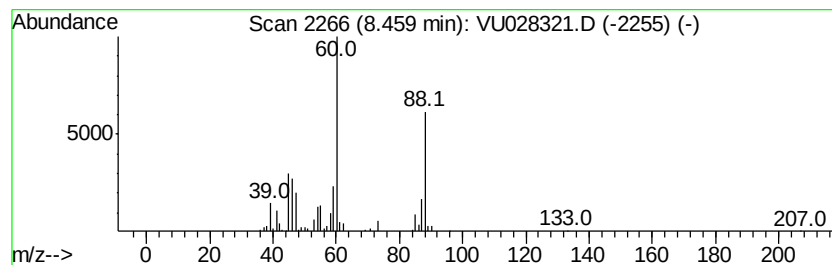
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 Thiophene, tetrahydro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	1.14 ug/L	117377	Chlorobenzene-d5	9.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Thiophene, tetrahydro-	88	C4H8S	000110-01-0	93
2		Thiophene, tetrahydro-	88	C4H8S	000110-01-0	90
3		Thiophene, tetrahydro-	88	C4H8S	000110-01-0	87
4		Thietane, 2-methyl-	88	C4H8S	017837-41-1	81
5		1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	46



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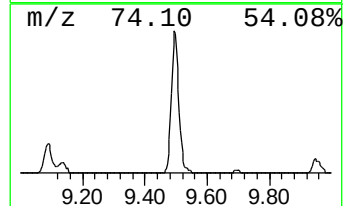
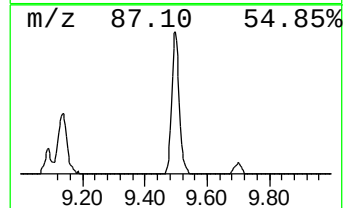
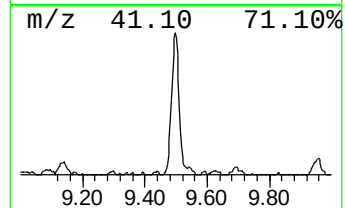
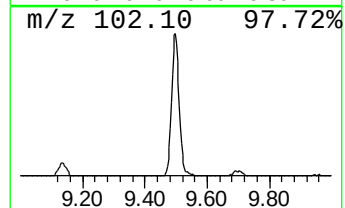
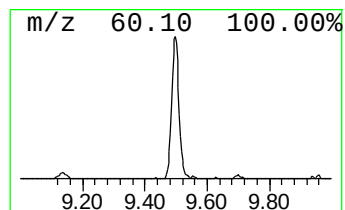
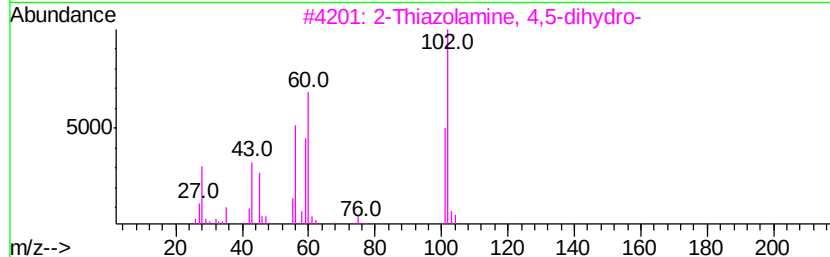
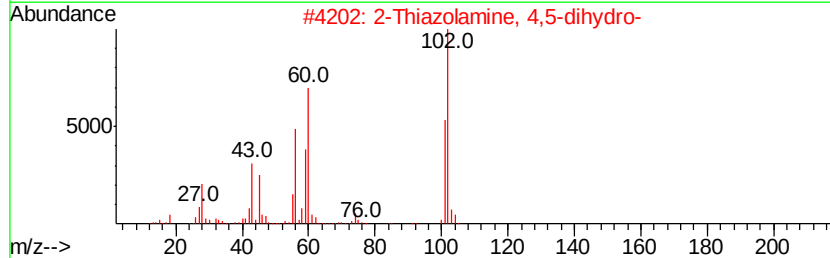
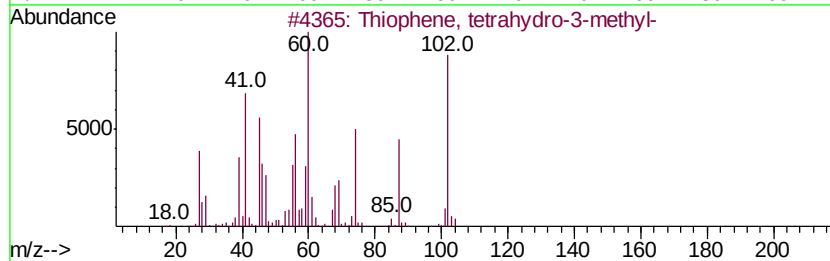
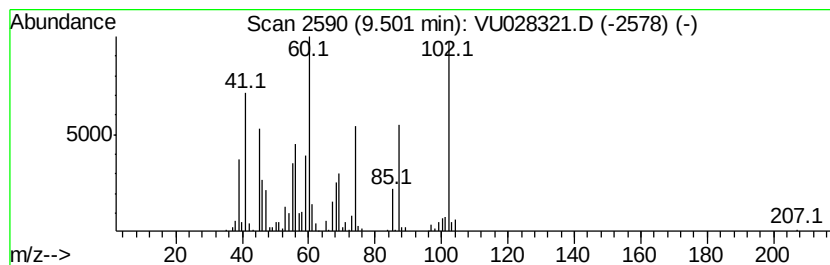
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111718WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Thiophene, tetrahydro-3-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.50	1.86 ug/L	192025	Chlorobenzene-d5	9.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	95
2			2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	50
3			2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	43
4			3-Ethylthio-1-propene	102	C5H10S	005296-62-8	43
5			1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	38



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Quant Title : TRACE VOA SOM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Str...	1.30	0.5	ug/L	44125	1	5.89	422269	5.0
(DEL) Alkane: Str...	1.76	6.5	ug/L	544921	1	5.89	422269	5.0
(DEL) Alkane: Cyc...	2.79	2.9	ug/L	245985	1	5.89	422269	5.0
Thiophene, tetrah...	8.46	1.1	ug/L	117377	2	9.09	515221	5.0
Thiophene, tetrah...	9.50	1.9	ug/L	192025	2	9.09	515221	5.0