

Data Path : Z:\voasrv\HPCHEM1\MSVOA U\Data\VU040120\
 Data File : VU037537.D
 Acq On : 01 Apr 2020 22:04
 Operator : JC/MD
 Sample : L2065-16
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBF12

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\SOMUTR040120WMA.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	1.369	3	9	23	rVB	137276	134322	34.89%	4.117%
2	1.485	39	45	60	rVB2	44104	51681	13.43%	1.584%
3	1.610	74	84	94	rBV2	80413	123884	32.18%	3.797%
4	1.745	120	126	135	rVB4	6611	8860	2.30%	0.272%
5	1.929	173	183	194	rVB	32182	44343	11.52%	1.359%
6	2.009	201	208	218	rBV2	10217	13567	3.52%	0.416%
7	2.173	250	259	267	rBV	18665	25374	6.59%	0.778%
8	2.221	267	274	283	rVV2	15931	22284	5.79%	0.683%
9	2.434	333	340	350	rVB5	5243	8475	2.20%	0.260%
10	2.591	377	389	402	rVB	51331	82445	21.42%	2.527%
11	2.662	402	411	422	rBV2	3358	6219	1.62%	0.191%
12	2.819	449	460	473	rVB	25152	40688	10.57%	1.247%
13	3.398	634	640	652	rVB4	2178	4115	1.07%	0.126%
14	3.630	695	712	725	rVB9	4390	11348	2.95%	0.348%
15	3.733	736	744	758	rVB5	2479	5205	1.35%	0.160%
16	4.671	1018	1036	1060	rBV	61169	147744	38.38%	4.529%
17	5.105	1151	1171	1189	rBV	54364	126642	32.90%	3.882%
18	5.758	1355	1374	1398	rVB2	101848	266792	69.31%	8.178%
19	6.054	1454	1466	1473	rBV5	2236	4083	1.06%	0.125%
20	6.282	1523	1537	1553	rVB	110899	204814	53.21%	6.278%
21	6.723	1661	1674	1690	rBV2	68294	130215	33.83%	3.991%
22	7.591	1931	1944	1958	rBV	36432	63750	16.56%	1.954%
23	7.922	2035	2047	2061	rBV	121262	208395	54.14%	6.388%
24	7.996	2062	2070	2077	rVB3	3491	5371	1.40%	0.165%
25	8.205	2124	2135	2148	rBV3	23557	38779	10.07%	1.189%
26	8.658	2259	2276	2302	rBV	222277	384939	100.00%	11.799%
27	9.436	2506	2518	2533	rBV	157476	256656	66.67%	7.867%
28	10.774	2920	2934	2945	rBV	58950	92169	23.94%	2.825%
29	11.825	3249	3261	3276	rVB	169135	263532	68.46%	8.078%
30	12.073	3332	3338	3355	rVV4	7365	14292	3.71%	0.438%
31	12.153	3355	3363	3368	rVV7	4445	6283	1.63%	0.193%
32	12.205	3368	3379	3391	rVB	142741	237479	61.69%	7.279%
33	12.768	3548	3554	3557	rBV3	3664	3923	1.02%	0.120%
34	12.854	3571	3581	3594	rBV7	16618	29398	7.64%	0.901%

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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\SOMUTR040120WMA.M
Title : TRACE VOA SOM01.0

35	12.912	3594	3599	3608	rVB6	4169	5301	1.38%	0.162%
36	13.070	3639	3648	3662	rVB5	12646	20739	5.39%	0.636%
37	13.147	3662	3672	3683	rBV9	8571	17021	4.42%	0.522%
38	13.327	3717	3728	3737	rVV8	4003	6795	1.77%	0.208%
39	13.404	3741	3752	3761	rVB8	4154	6880	1.79%	0.211%
40	13.475	3761	3774	3784	rBV8	6364	11301	2.94%	0.346%
41	13.555	3791	3799	3806	rBV6	3578	5551	1.44%	0.170%
42	13.632	3810	3823	3830	rBV6	4554	9255	2.40%	0.284%
43	14.115	3963	3973	3982	rBV	26998	41856	10.87%	1.283%
44	15.263	4322	4330	4338	rVB2	6599	9764	2.54%	0.299%
45	15.449	4380	4388	4397	rBV2	3820	6610	1.72%	0.203%
46	17.160	4909	4920	4929	rBV3	13295	23744	6.17%	0.728%
47	17.478	5011	5019	5030	rVB2	15972	29552	7.68%	0.906%

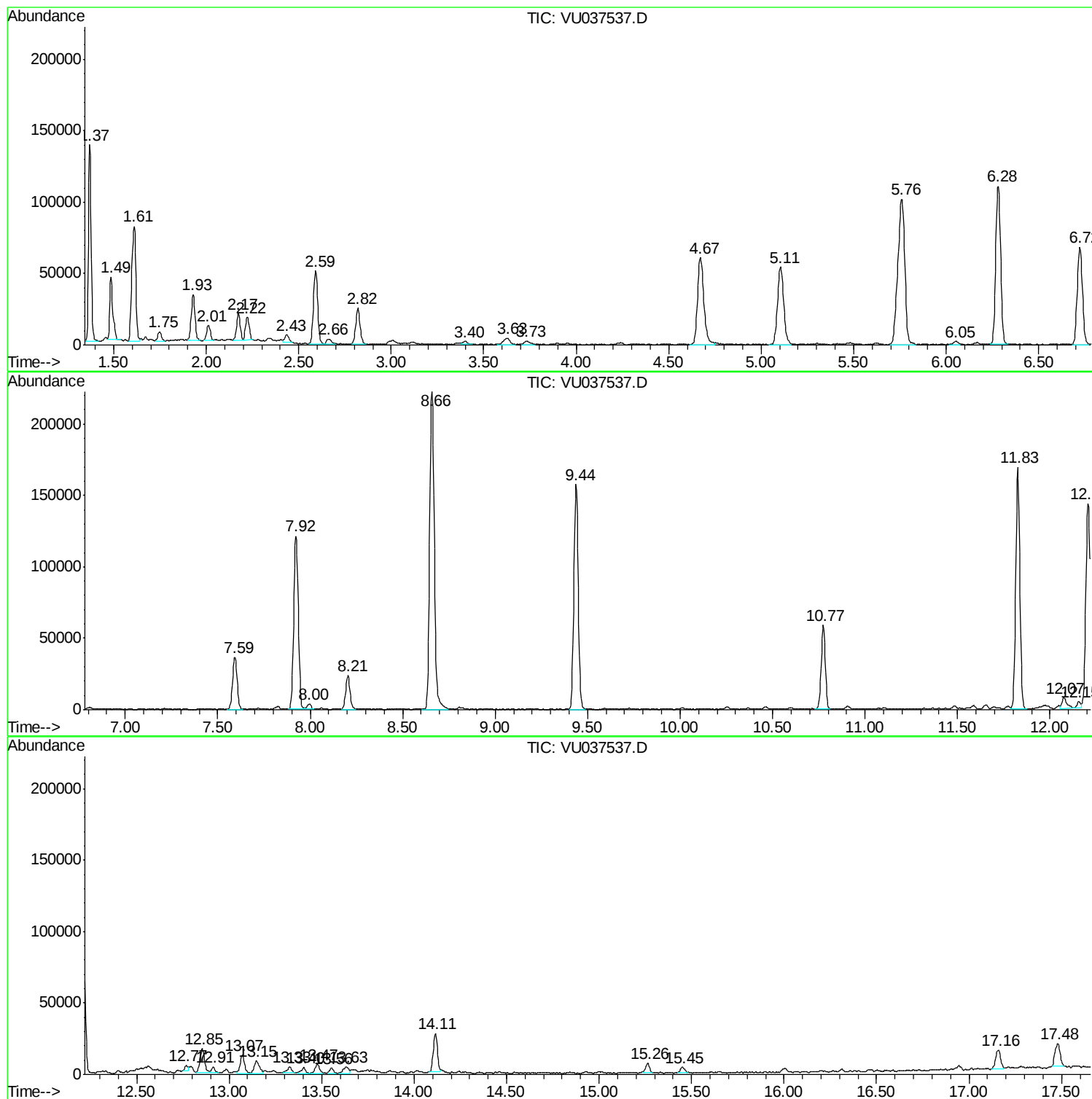
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR040120WMA.M
Quant Title : TRACE VOA SOM01.0

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



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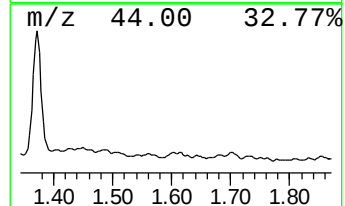
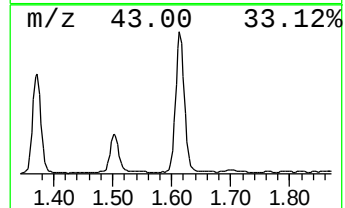
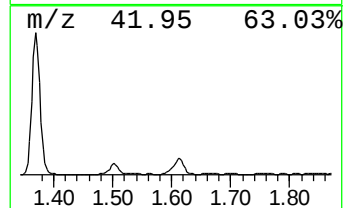
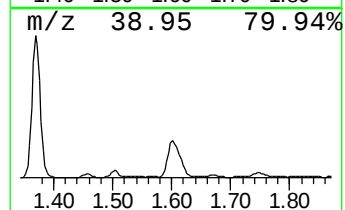
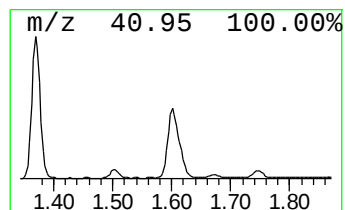
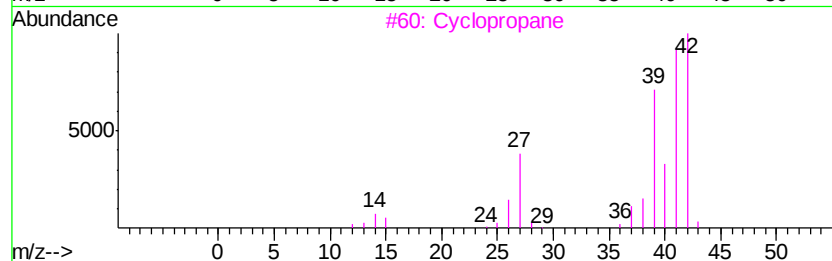
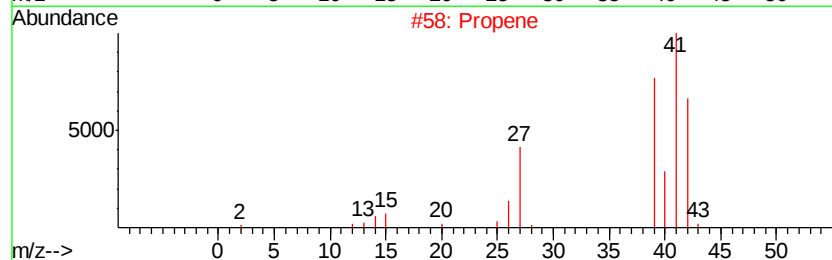
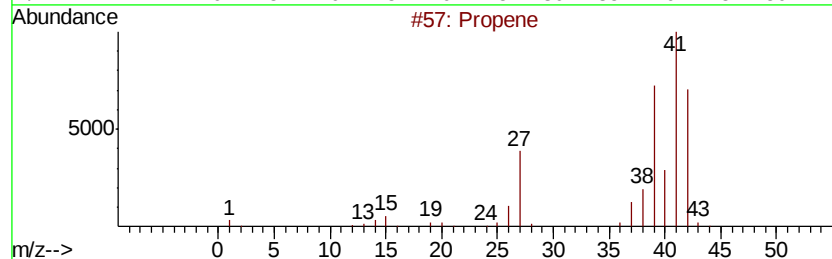
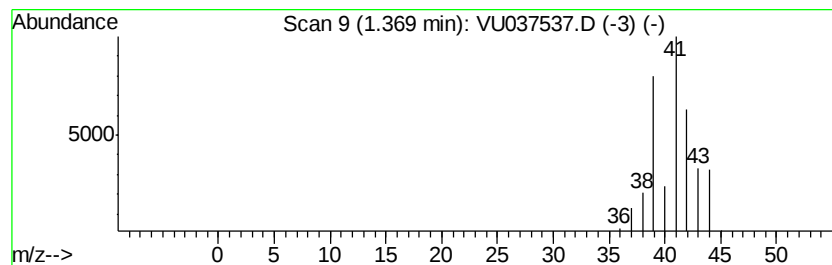
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	3.28 ug/L	134322	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene			42	C3H6	000115-07-1	90
2	Propene			42	C3H6	000115-07-1	42
3	Cyclopropane			42	C3H6	000075-19-4	9
4	Cyclopropene			40	C3H4	002781-85-3	9
5	Cyclopropane			42	C3H6	000075-19-4	7



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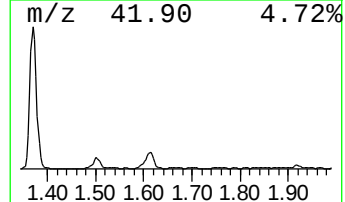
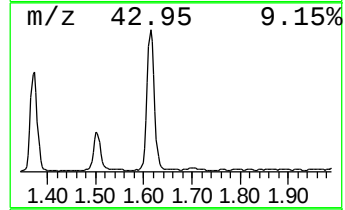
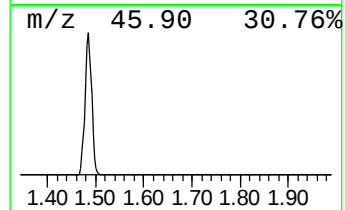
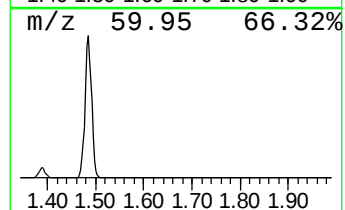
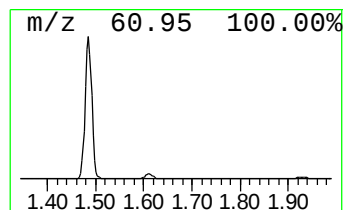
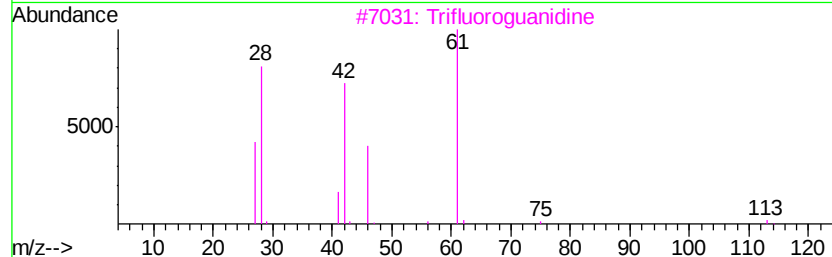
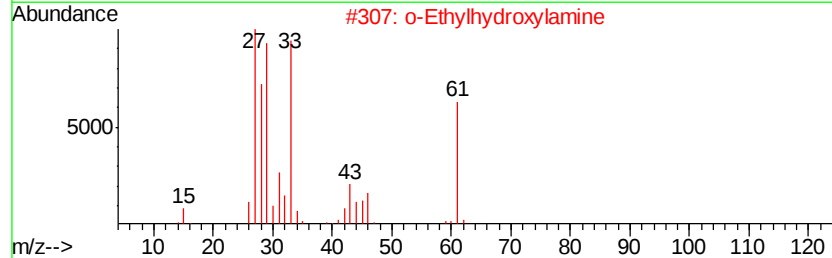
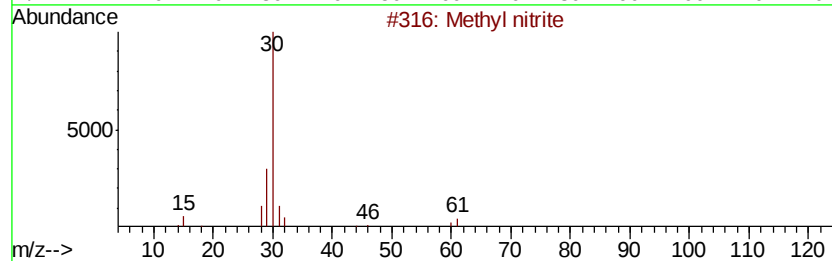
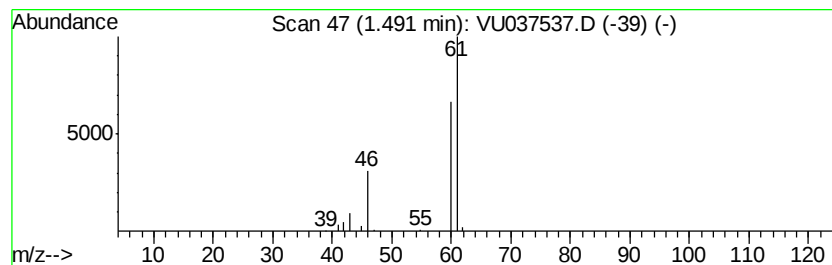
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR040120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	1.26 ug/L	51681	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl nitrite	61	CH3NO2	000624-91-9	5
2		o-Ethylhydroxylamine	61	C2H7NO	1000322-42-5	4
3		Trifluoroquinidine	113	CH2F3N3	037950-72-4	4
4		Urea	60	CH4N2O	000057-13-6	3
5		Methyl formate	60	C2H4O2	000107-31-3	3



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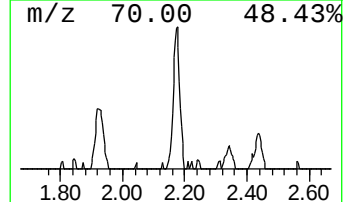
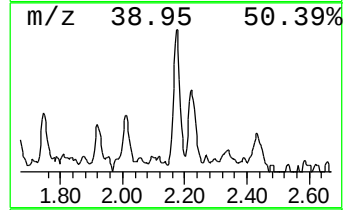
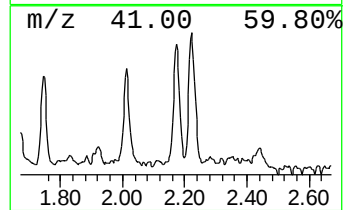
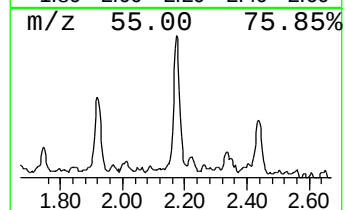
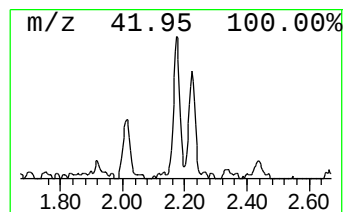
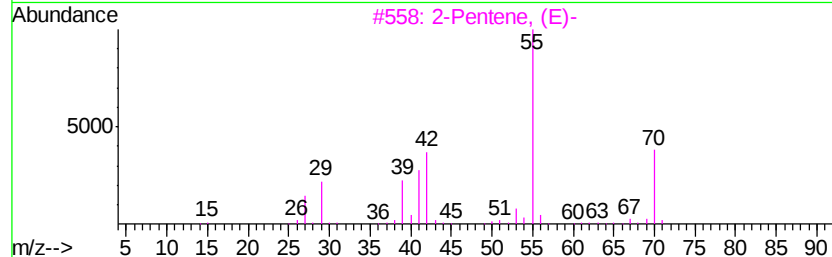
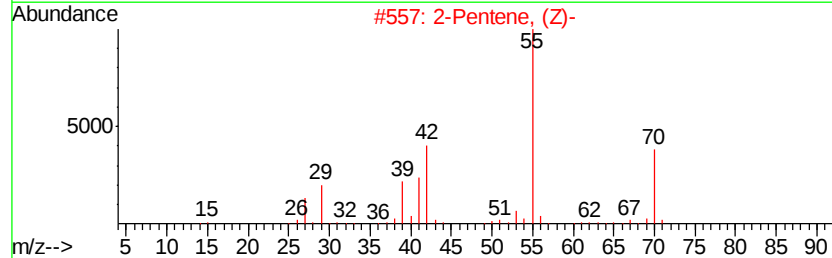
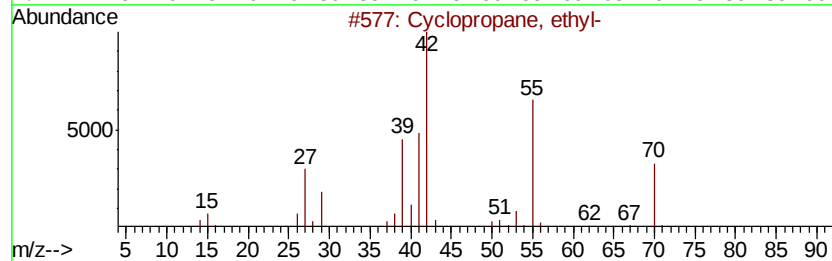
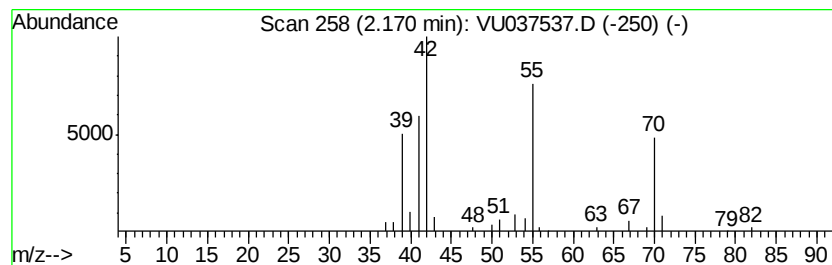
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR040120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 (DEL) Alkane: Cyclic2.17 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	0.62 ug/L	25374	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	90
2		2-Pentene, (Z)-	70	C5H10	000627-20-3	72
3		2-Pentene, (E)-	70	C5H10	000646-04-8	64
4		1-Pentene	70	C5H10	000109-67-1	64
5		1-Pentene	70	C5H10	000109-67-1	64



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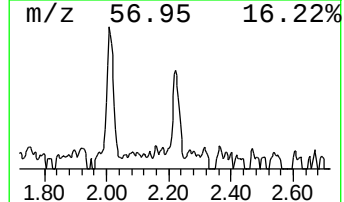
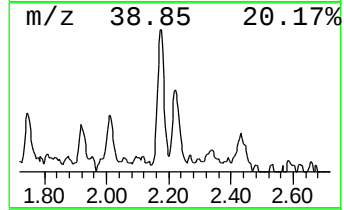
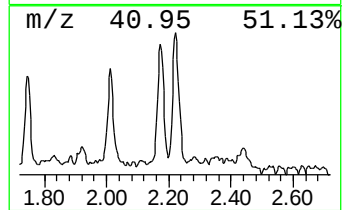
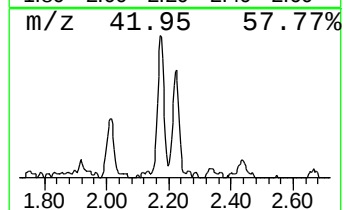
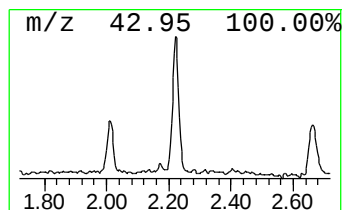
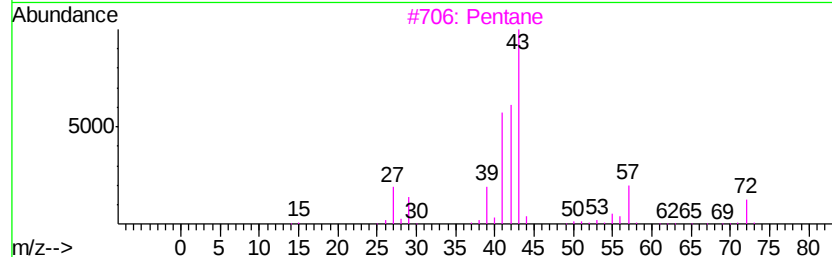
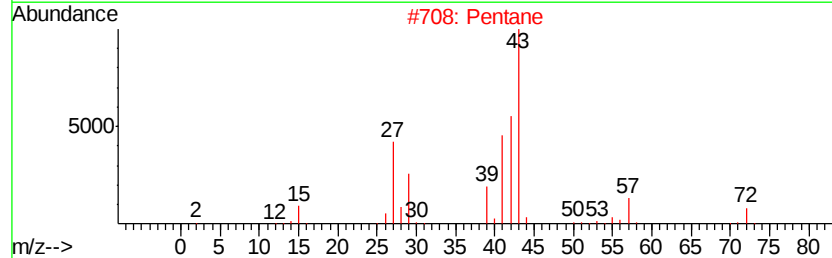
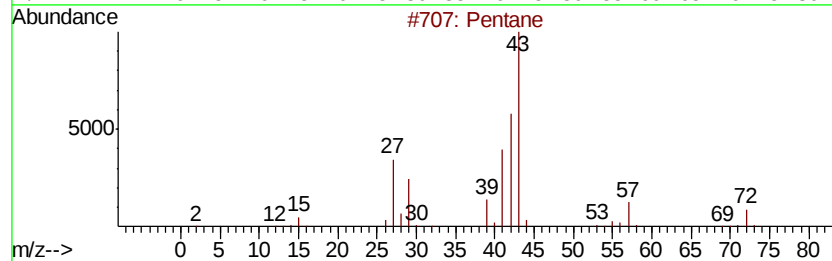
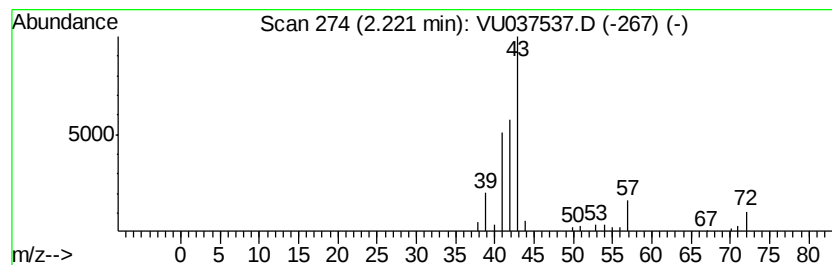
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	0.54 ug/L	22284	1,4-Difluorobenzene	6.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane		72	C5H12	000109-66-0	80
2	Pentane		72	C5H12	000109-66-0	80
3	Pentane		72	C5H12	000109-66-0	64
4	3-Buten-1-ol		72	C4H8O	000627-27-0	59
5	Pentane		72	C5H12	000109-66-0	53



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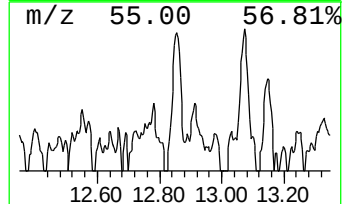
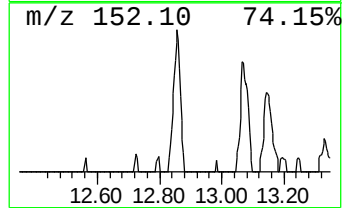
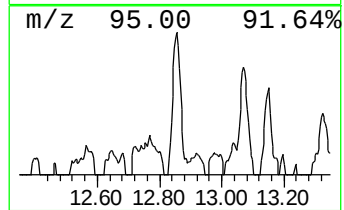
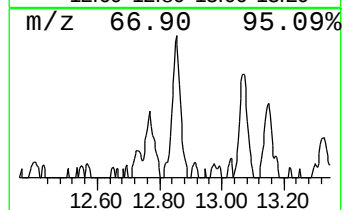
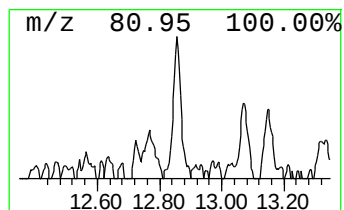
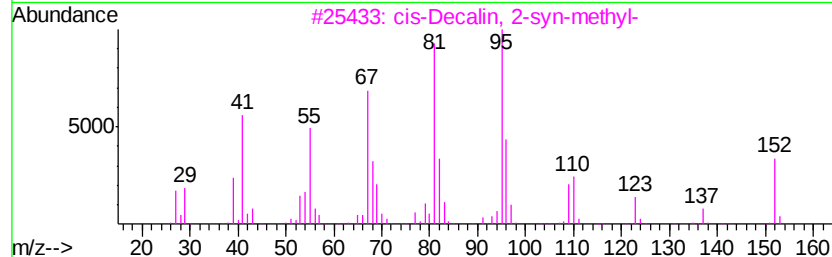
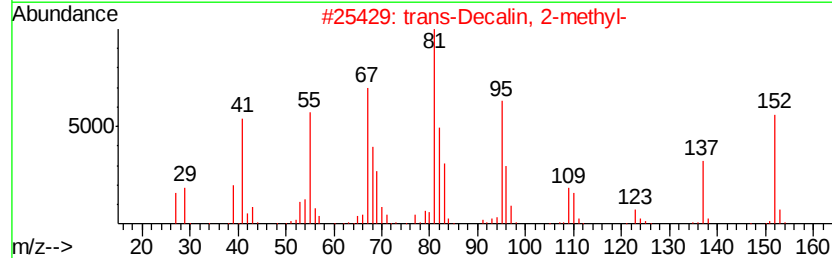
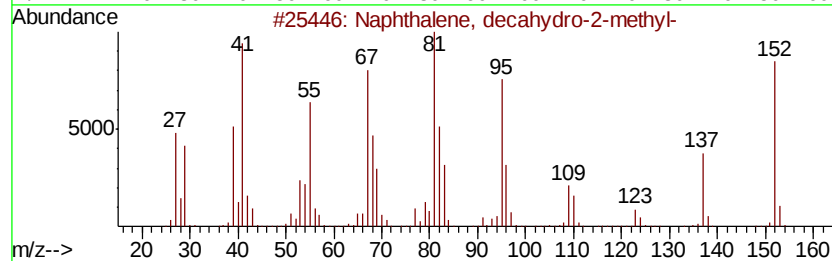
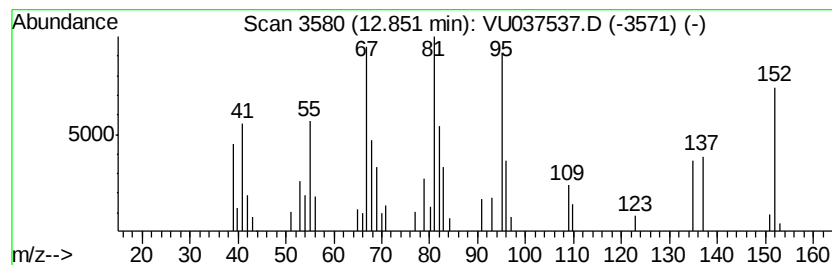
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR040120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Naphthalene, decahydro-2-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	0.56 ug/L	29398	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	95
2		trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	93
3		cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	83
4		Bicyclo[3.3.2]decan-9-one	152	C10H16O	028054-91-3	68
5		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040120\
Data File : VU037537.D
Acq On : 01 Apr 2020 22:04
Operator : JC/MD
Sample : L2065-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBF12

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR040120WMA.M
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...	1.37	3.3	ug/L	134322	1	6.28	204814	5.0
unknown-01	1.49	1.3	ug/L	51681	1	6.28	204814	5.0
(DEL) Alkane: Cyc...	2.17	0.6	ug/L	25374	1	6.28	204814	5.0
(DEL) Alkane: Str...	2.22	0.5	ug/L	22284	1	6.28	204814	5.0
Naphthalene, deca...	12.85	0.6	ug/L	29398	3	11.83	263532	5.0