

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061320\
 Data File : VU038856.D
 Acq On : 12 Jun 2020 17:04
 Operator : SY/MD
 Sample : L2990-02
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E3YG0

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\SOMUTR061220WMA.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	1.504	44	51	67	rVB	237805	236860	7.66%	1.371%
2	1.613	74	85	94	rBV	141554	158819	5.14%	0.919%
3	1.932	171	184	200	rBV	104686	148676	4.81%	0.860%
4	2.594	378	390	408	rBV	229721	387480	12.54%	2.242%
5	3.620	693	709	729	rBV3	16845	40956	1.32%	0.237%
6	4.678	1020	1038	1078	rBV2	164273	538611	17.42%	3.117%
7	5.102	1152	1170	1185	rBV2	192784	419715	13.58%	2.429%
8	5.423	1255	1270	1282	rBV2	27401	61606	1.99%	0.357%
9	5.494	1282	1292	1311	rVB3	14301	32880	1.06%	0.190%
10	5.671	1327	1347	1357	rBV4	92991	215136	6.96%	1.245%
11	5.761	1357	1375	1383	rVV2	393185	1044105	33.78%	6.043%
12	5.806	1384	1389	1404	rVV	215704	420661	13.61%	2.435%
13	5.880	1405	1412	1424	rVV6	22621	50128	1.62%	0.290%
14	5.951	1425	1434	1447	rVB4	19158	39103	1.27%	0.226%
15	6.279	1522	1536	1567	rBV	364957	717852	23.22%	4.154%
16	6.719	1659	1673	1696	rBV	237006	526713	17.04%	3.048%
17	7.214	1808	1827	1835	rBV2	22006	44286	1.43%	0.256%
18	7.591	1928	1944	1965	rBV	125944	261261	8.45%	1.512%
19	7.922	2026	2047	2062	rBV	464067	825532	26.71%	4.778%
20	8.060	2079	2090	2104	rVB2	36406	68148	2.20%	0.394%
21	8.140	2104	2115	2123	rVV	26662	42140	1.36%	0.244%
22	8.198	2123	2133	2144	rVV2	105781	185034	5.99%	1.071%
23	8.279	2144	2158	2172	rVB6	53974	133965	4.33%	0.775%
24	8.655	2259	2275	2308	rBV	707835	1297820	41.99%	7.511%
25	8.828	2316	2329	2340	rVB8	19286	40976	1.33%	0.237%
26	8.899	2340	2351	2361	rBV2	42787	73539	2.38%	0.426%
27	8.964	2361	2371	2386	rVB	147565	242493	7.85%	1.403%
28	9.436	2503	2518	2537	rBV	538375	924646	29.91%	5.351%
29	9.526	2537	2546	2558	rVV3	58817	106340	3.44%	0.615%
30	9.613	2560	2573	2586	rBV	1480088	2187959	70.78%	12.662%
31	9.690	2586	2597	2615	rVB5	207832	444221	14.37%	2.571%
32	9.822	2626	2638	2648	rVV7	21578	40643	1.31%	0.235%
33	9.893	2651	2660	2671	rVB5	20841	35755	1.16%	0.207%
34	10.500	2836	2849	2862	rBV3	25331	43628	1.41%	0.252%

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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

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Title : TRACE VOA SOM01.0

35	10.771	2922	2933	2948	rVB2	190894	311320	10.07%	1.802%
36	10.938	2977	2985	3001	rVB	106771	161807	5.23%	0.936%
37	11.430	3124	3138	3148	rBV3	28688	55332	1.79%	0.320%
38	11.623	3179	3198	3203	rBV2	25995	55365	1.79%	0.320%
39	11.655	3203	3208	3219	rVB3	20625	33801	1.09%	0.196%
40	11.796	3237	3252	3277	rVB2	1303162	3091046	100.00%	17.889%
41	12.021	3308	3322	3329	rBV2	29895	49732	1.61%	0.288%
42	12.076	3329	3339	3341	rVV	89718	126554	4.09%	0.732%
43	12.105	3341	3348	3360	rVV	212049	353870	11.45%	2.048%
44	12.205	3360	3379	3399	rVB	514853	879963	28.47%	5.093%
45	12.594	3491	3500	3505	rBV2	27438	43198	1.40%	0.250%
46	12.626	3506	3510	3525	rVB2	25291	37206	1.20%	0.215%
47	12.880	3579	3589	3607	rVB3	20585	42233	1.37%	0.244%

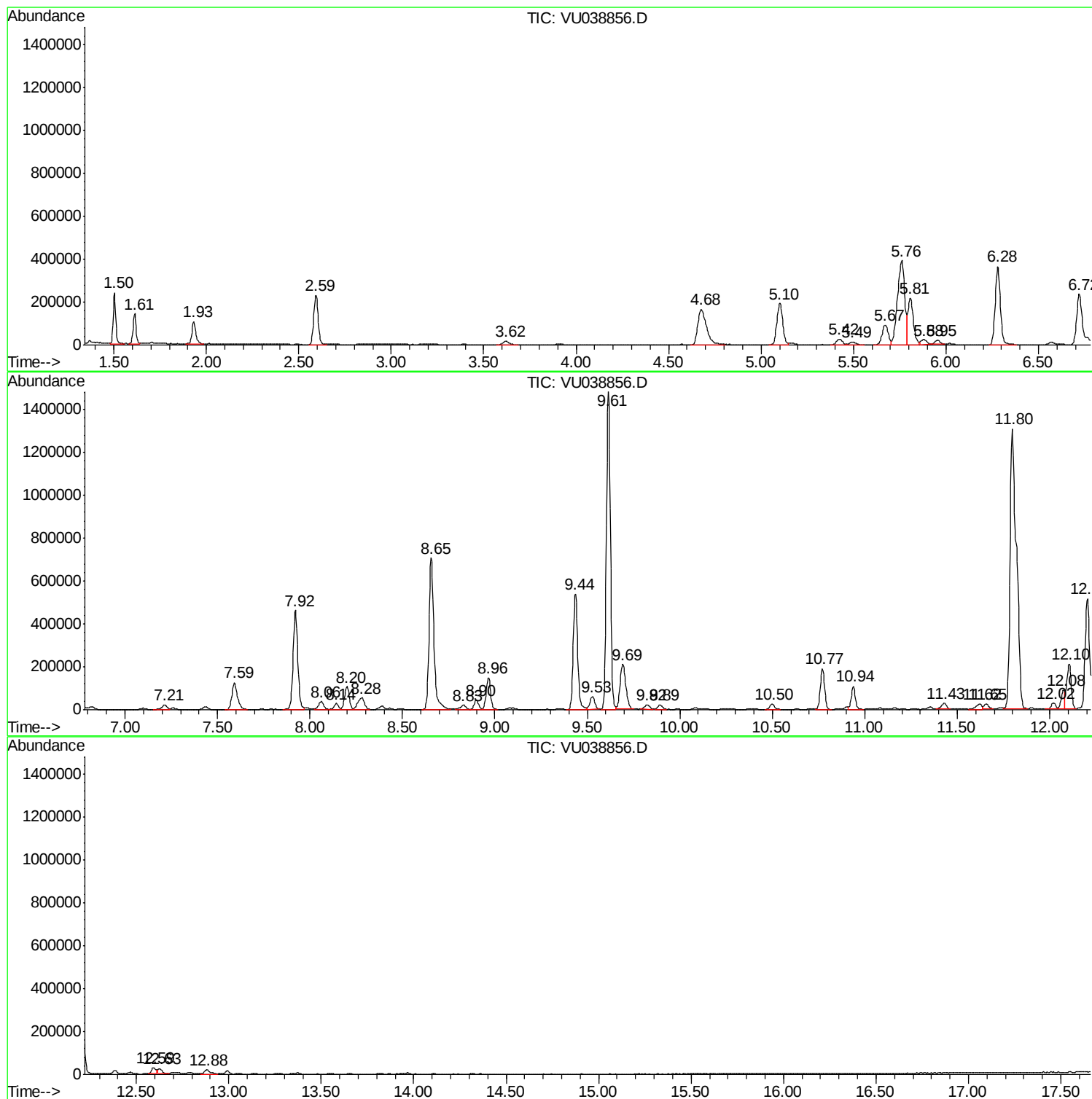
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Quant Title : TRACE VOA SOM01.0

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



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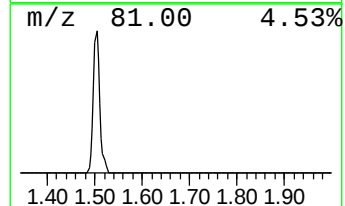
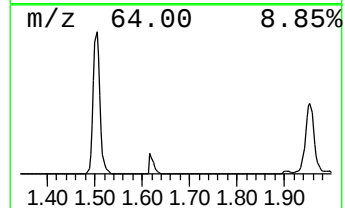
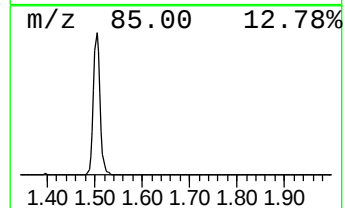
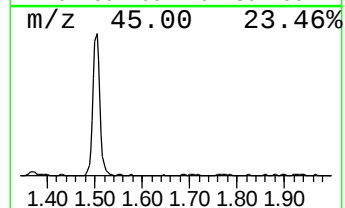
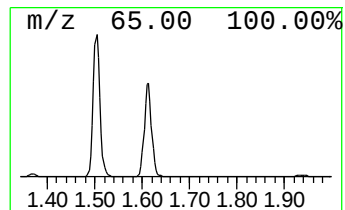
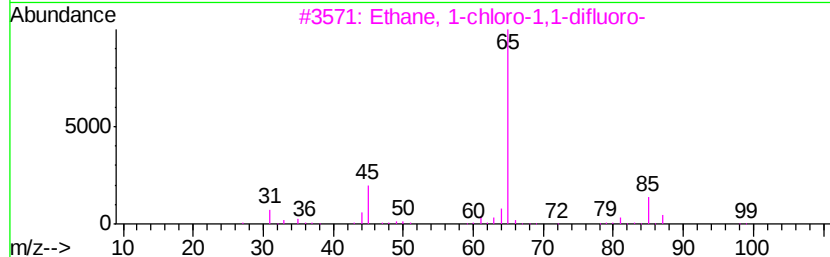
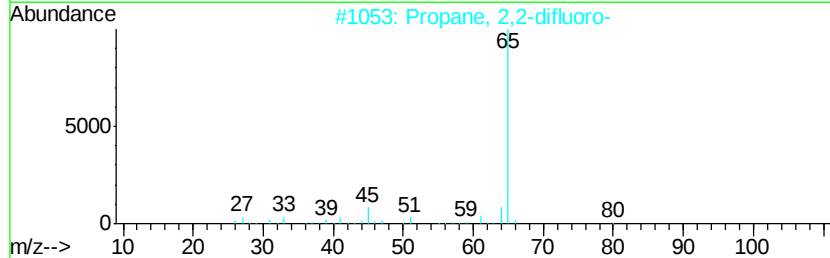
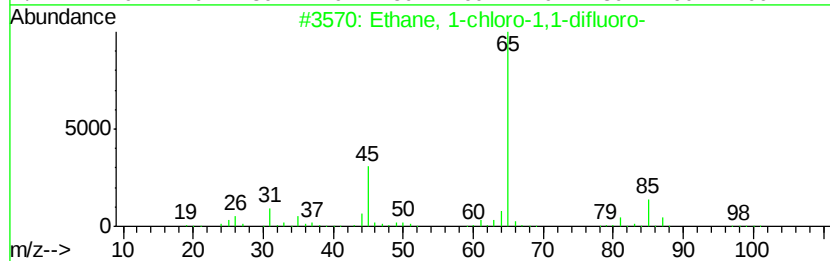
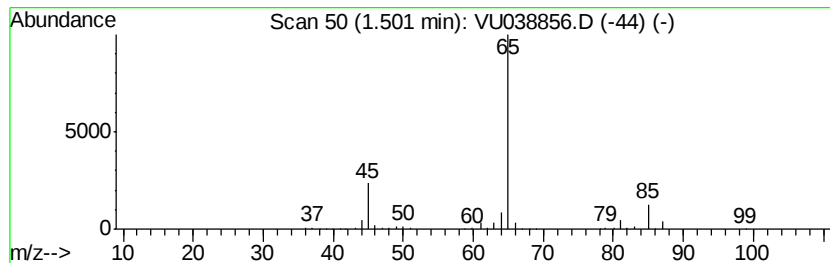
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Ethane, 1-chloro-1,1-difluoro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.50	1.65 ug/L	236860	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	83
2			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	43
3			Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	38
4			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	4
5			Benzene, 1-nitro-2-(p-methylphen...	247	C13H10FN03	028987-57-7	1



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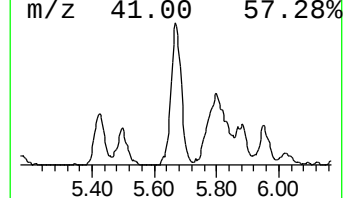
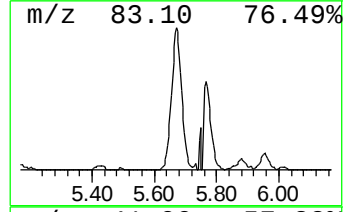
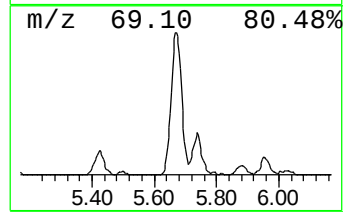
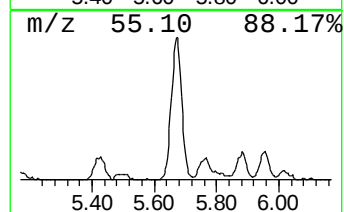
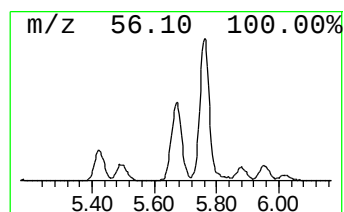
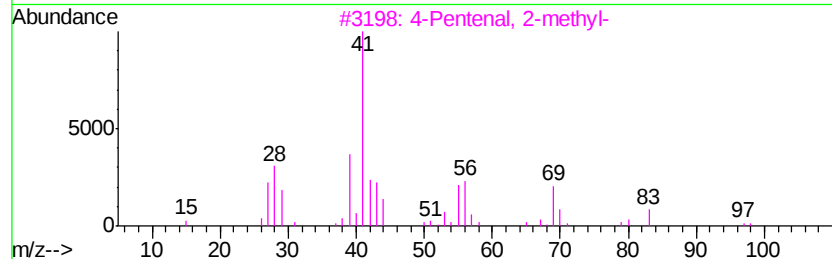
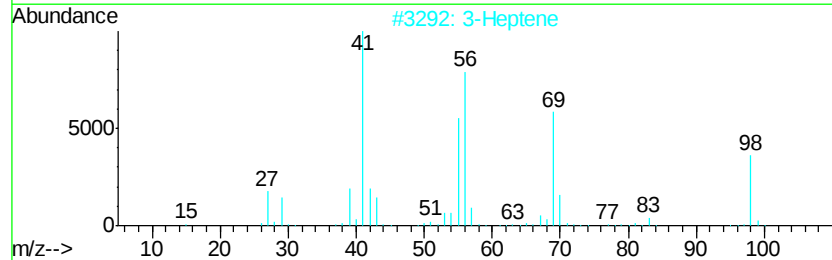
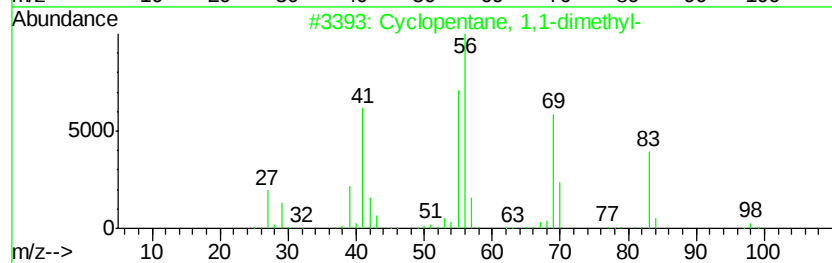
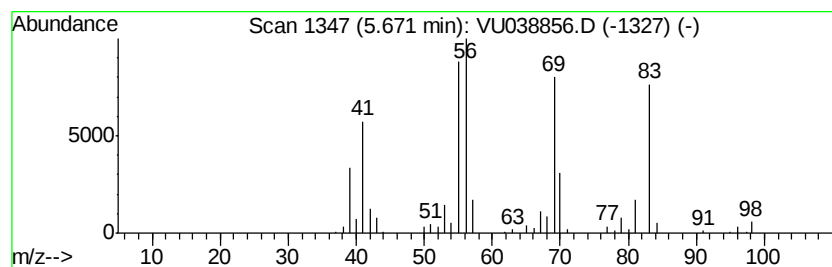
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061220WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 (DEL) Alkane: Cyclic5.67 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.67	1.50 ug/L	215136	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	90
2			3-Heptene	98	C7H14	000592-78-9	70
3			4-Pentenal, 2-methyl-	98	C6H10O	005187-71-3	53
4			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	46
5			3-Hexene, 2-methyl-, (E)-	98	C7H14	000692-24-0	38



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ALS Vial : 1 Sample Multiplier: 1

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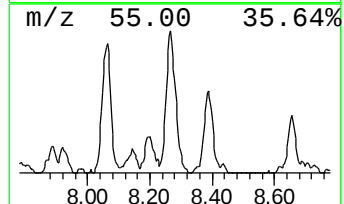
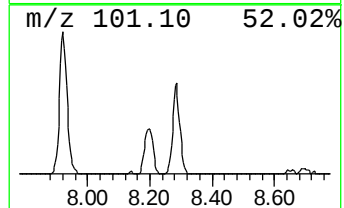
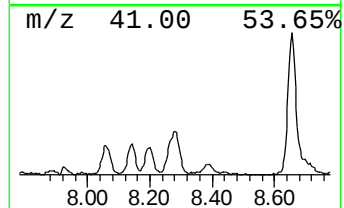
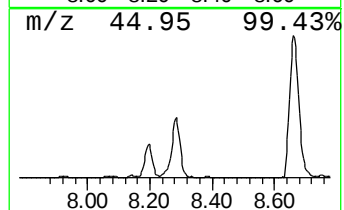
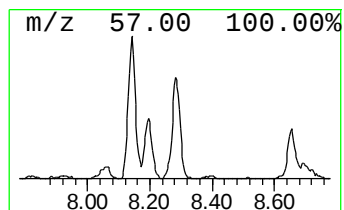
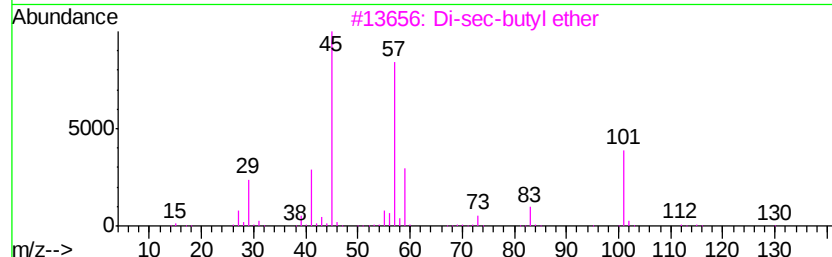
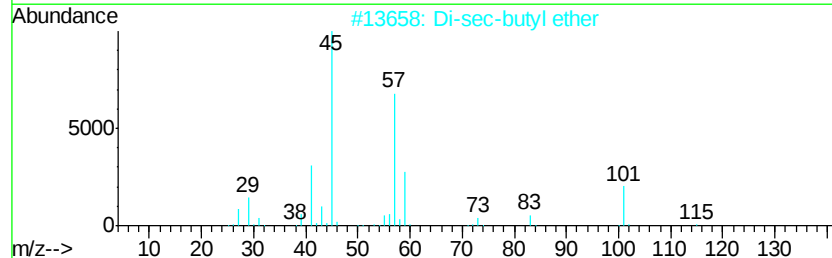
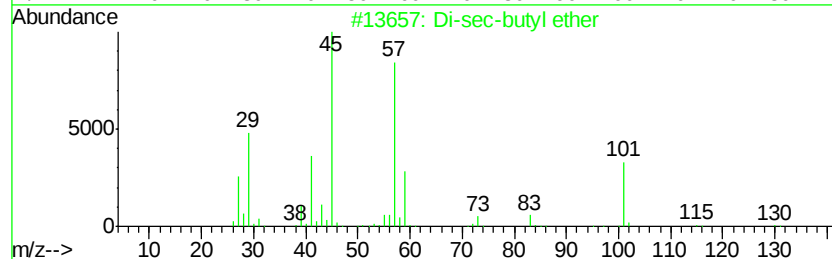
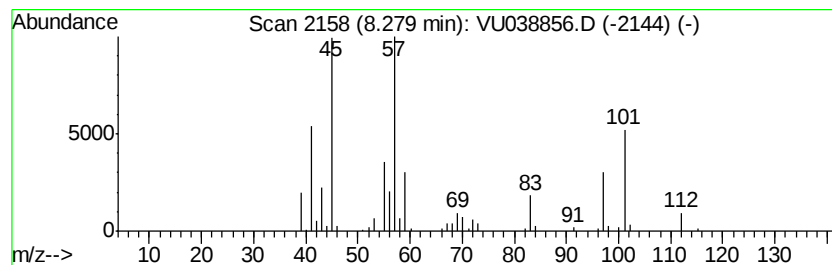
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Di-sec-butyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	0.72 ug/L	133965	Chlorobenzene-d5	9.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Di-sec-butyl ether	130	C8H18O	006863-58-7	50
2		Di-sec-butyl ether	130	C8H18O	006863-58-7	50
3		Di-sec-butyl ether	130	C8H18O	006863-58-7	45
4		2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	38
5		Fructofuranose, 2,6-anhydro-1,3,...	204	C9H16O5	004451-11-0	37



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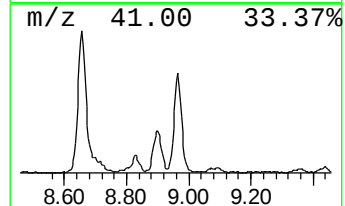
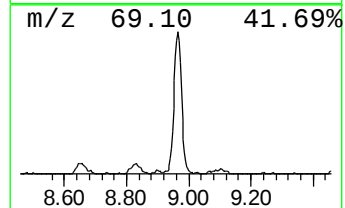
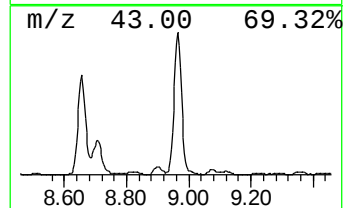
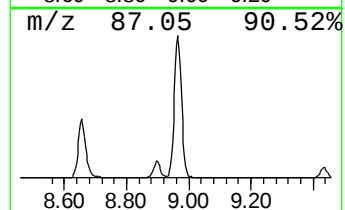
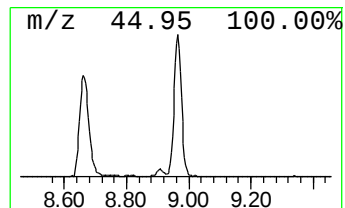
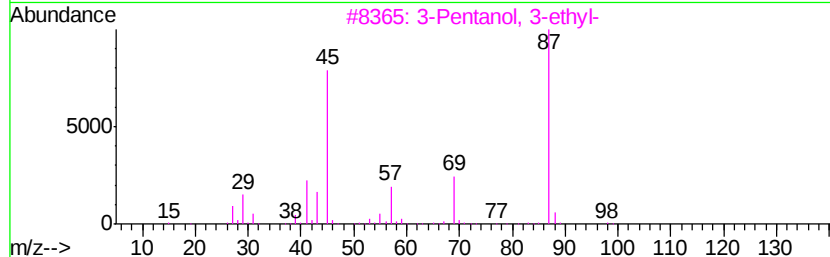
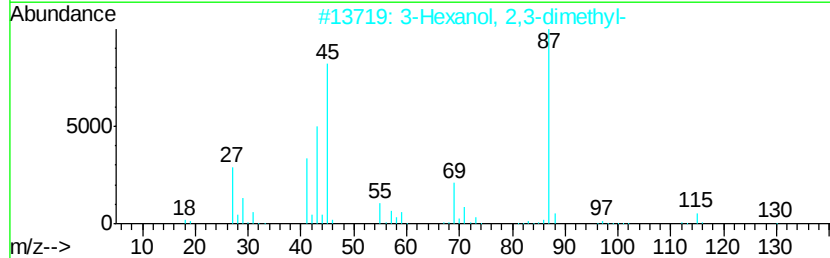
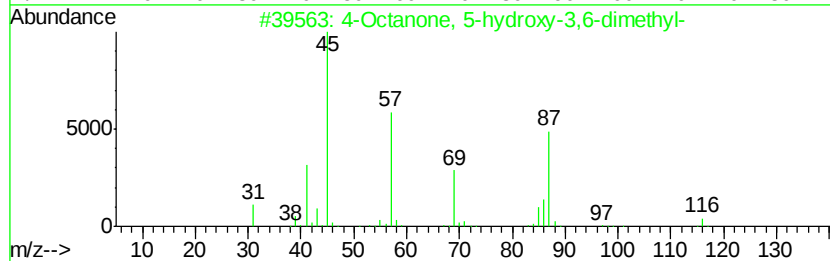
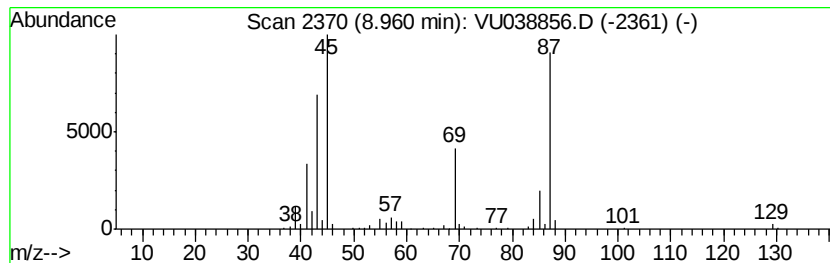
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4-Octanone, 5-hydroxy-3,6-d... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.96	1.31 ug/L	242493	Chlorobenzene-d5	9.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Octanone, 5-hydroxy-3,6-dimethyl-	172	C10H20O2	062759-47-1	72
2		3-Hexanol, 2,3-dimethyl-	130	C8H18O	004166-46-5	64
3		3-Pentanol, 3-ethyl-	116	C7H16O	000597-49-9	64
4		Hydrazine, 1,1-dipropyl-	116	C6H16N2	004986-50-9	64
5		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	64



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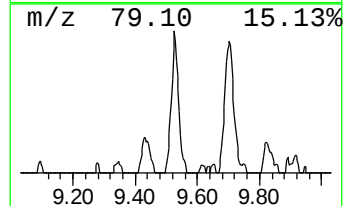
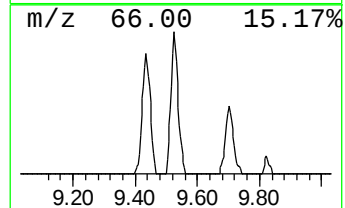
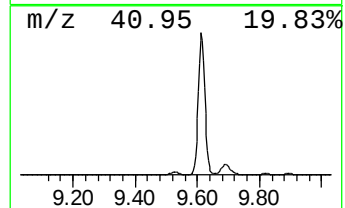
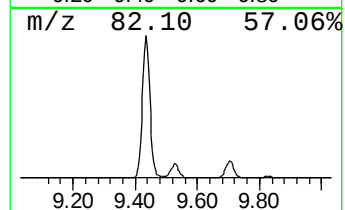
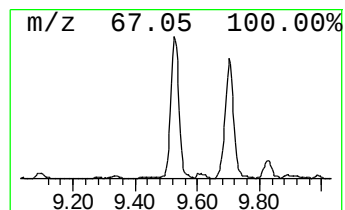
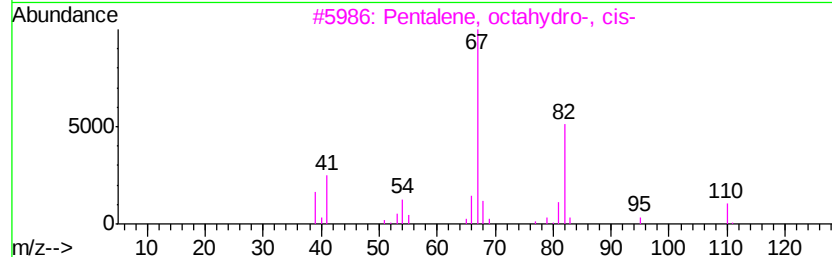
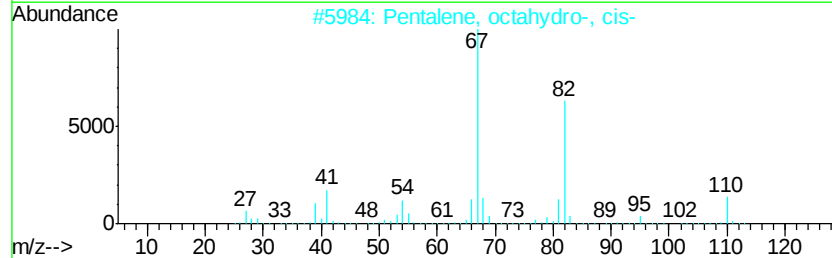
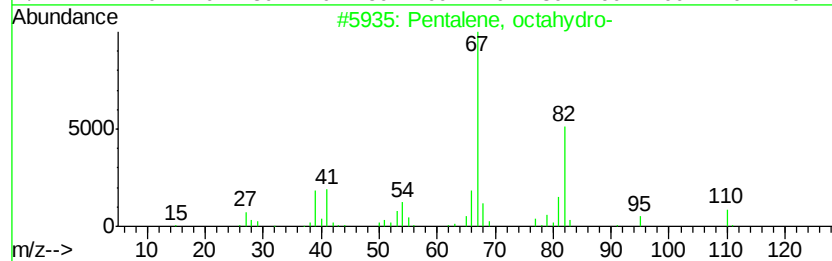
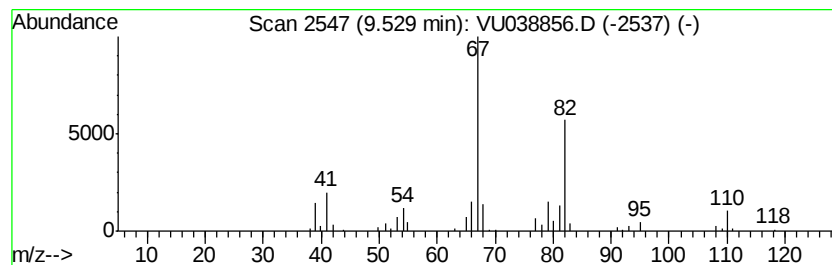
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Pentalene, octahydro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.53	0.58 ug/L	106340	Chlorobenzene-d5	9.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentalene, octahydro-	110	C8H14	000694-72-4	94
2		Pentalene, octahydro-, cis-	110	C8H14	001755-05-1	90
3		Pentalene, octahydro-, cis-	110	C8H14	001755-05-1	90
4		Pentalene, octahydro-	110	C8H14	000694-72-4	87
5		4-Methyl-1,3-pentadiene	82	C6H10	000926-56-7	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061320\
Data File : VU038856.D
Acq On : 12 Jun 2020 17:04
Operator : SY/MD
Sample : L2990-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E3YG0

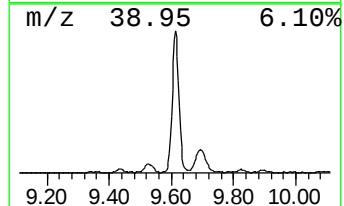
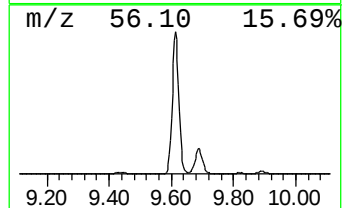
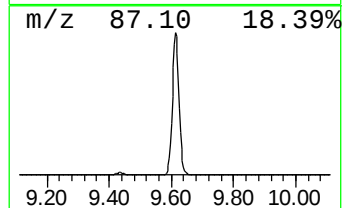
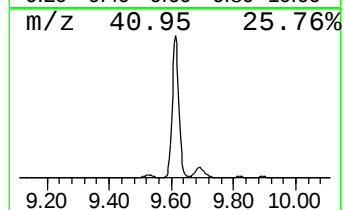
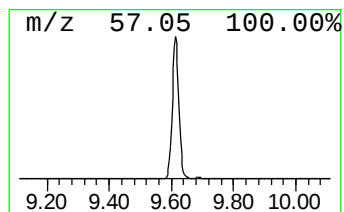
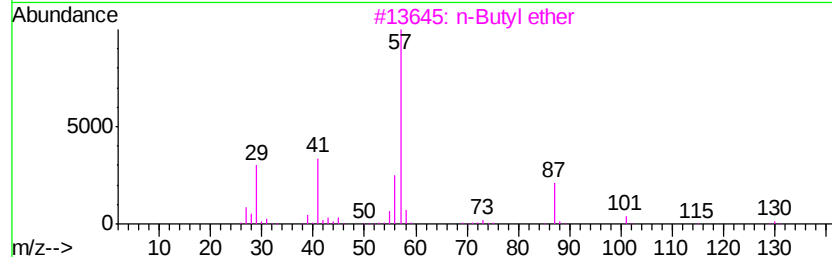
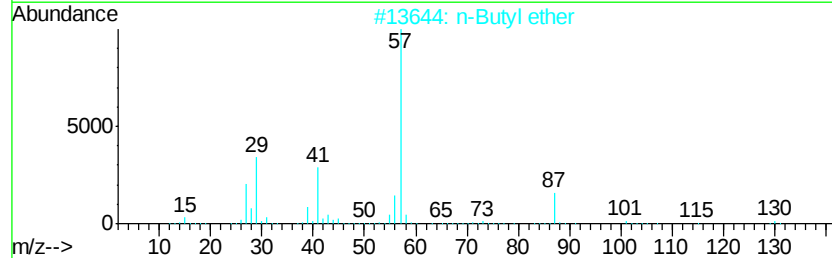
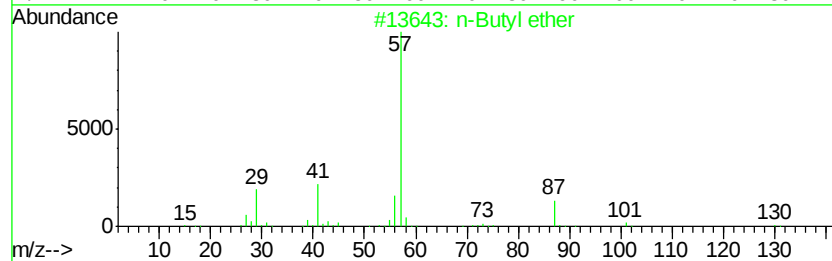
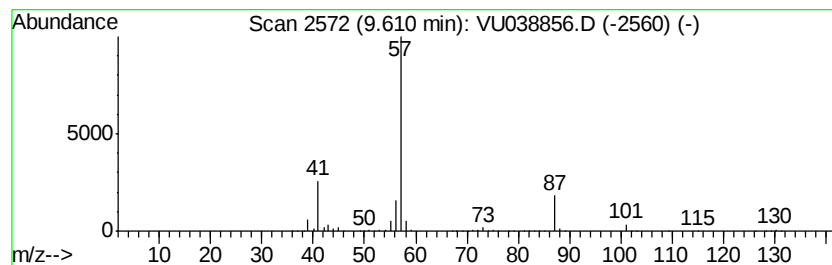
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 n-Butyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.61	11.83 ug/L	2187960	Chlorobenzene-d5	9.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Butyl ether	130	C8H18O	000142-96-1	90
2		n-Butyl ether	130	C8H18O	000142-96-1	72
3		n-Butyl ether	130	C8H18O	000142-96-1	72
4		Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	53
5		Oxalic acid, butyl isobutyl ester	202	C10H18O4	1000309-36-9	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061320\
Data File : VU038856.D
Acq On : 12 Jun 2020 17:04
Operator : SY/MD
Sample : L2990-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E3YG0

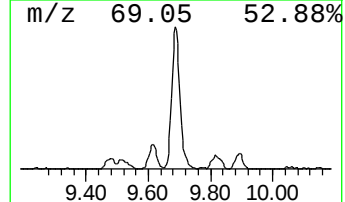
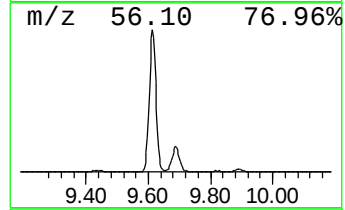
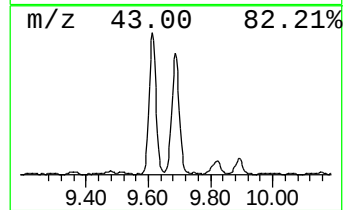
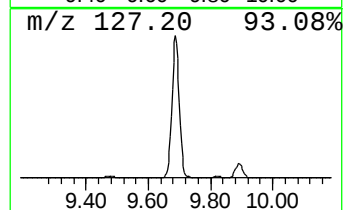
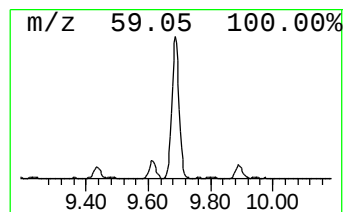
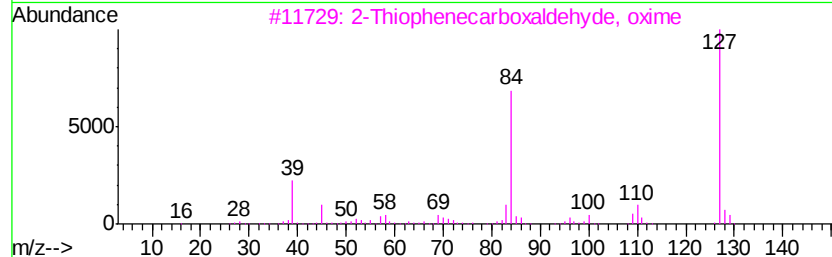
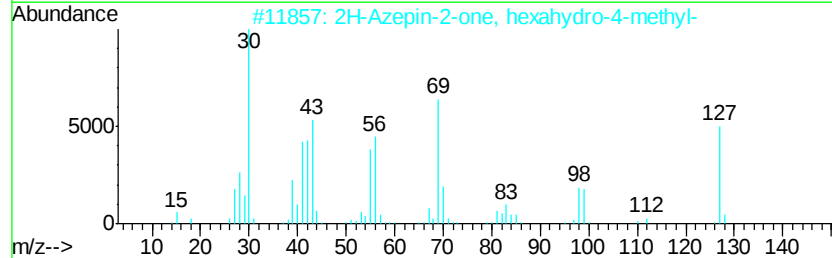
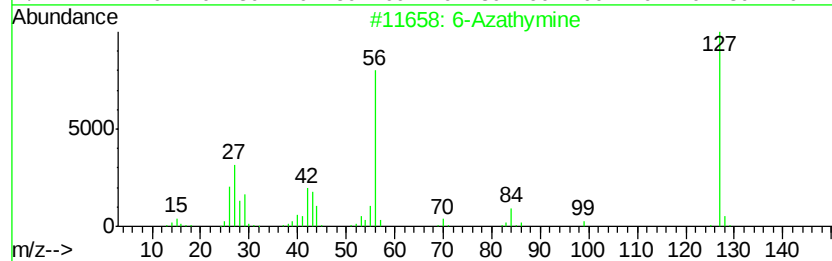
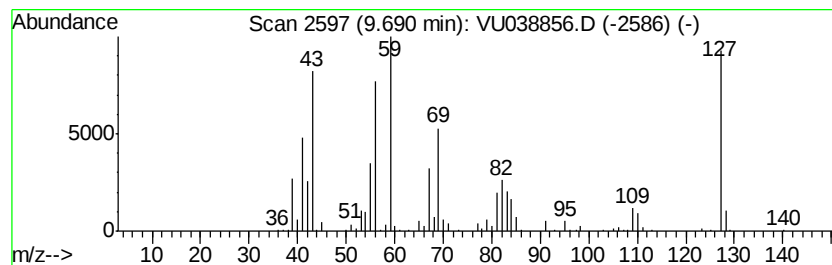
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	2.40 ug/L	444221	Chlorobenzene-d5	9.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6-Azathymine	127	C4H5N3O2	000932-53-6	43
2		2H-Azepin-2-one, hexahydro-4-met...	127	C7H13NO	003623-05-0	37
3		2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	14
4		2(1H)-Pyridinethione, 3-hydroxy-	127	C5H5NOS	023003-22-7	14
5		2(1H)-Pyridinethione, 3-hydroxy-	127	C5H5NOS	023003-22-7	14



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061320\
Data File : VU038856.D
Acq On : 12 Jun 2020 17:04
Operator : SY/MD
Sample : L2990-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E3YG0

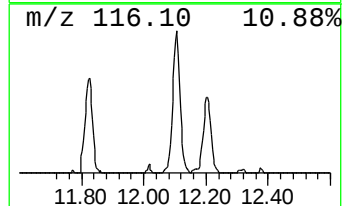
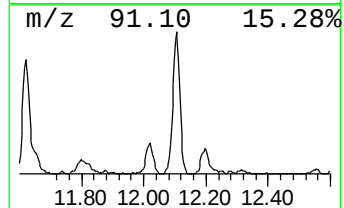
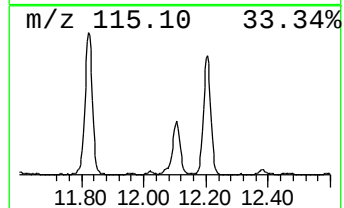
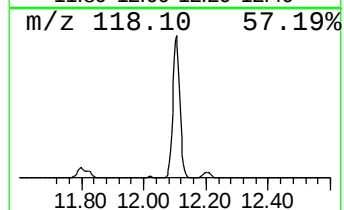
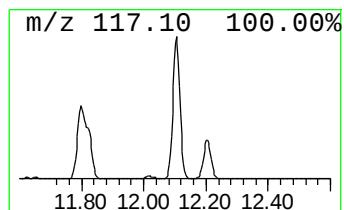
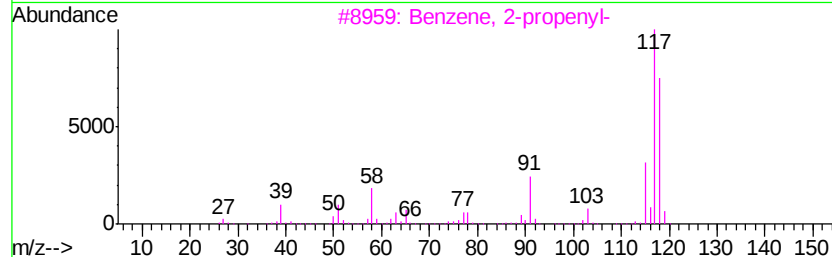
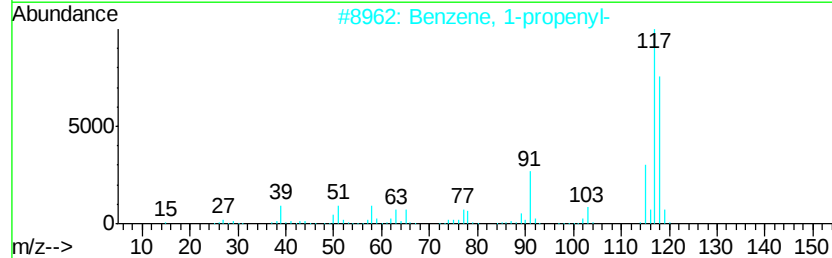
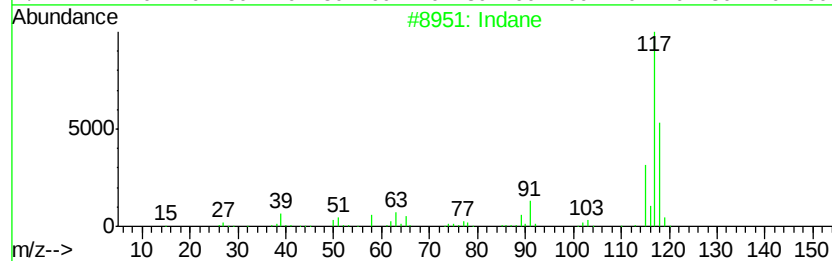
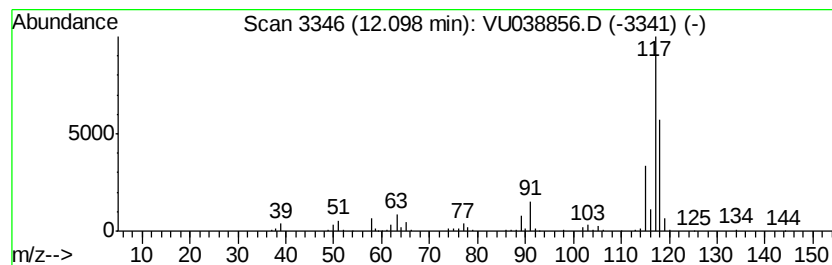
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061220WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 Indane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.10	0.57 ug/L	353870	1,4-Dichlorobenzene-d4	11.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane		118	C9H10	000496-11-7	95
2	Benzene, 1-propenyl-		118	C9H10	000637-50-3	83
3	Benzene, 2-propenyl-		118	C9H10	000300-57-2	83
4	(Z)-1-Phenylpropene		118	C9H10	000766-90-5	81
5	Benzene, cyclopropyl-		118	C9H10	000873-49-4	81



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061320\
Data File : VU038856.D
Acq On : 12 Jun 2020 17:04
Operator : SY/MD
Sample : L2990-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E3YG0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061220WMA.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
Ethane, 1-chloro-...	1.50	1.6	ug/L	236860	1	6.28	717852	5.0
(DEL) Alkane: Cyc...	5.67	1.5	ug/L	215136	1	6.28	717852	5.0
Di-sec-butyl ether	8.28	0.7	ug/L	133965	2	9.44	924646	5.0
4-Octanone, 5-hyd...	8.96	1.3	ug/L	242493	2	9.44	924646	5.0
Pentalene, octahy...	9.53	0.6	ug/L	106340	2	9.44	924646	5.0
n-Butyl ether	9.61	11.8	ug/L	2187960	2	9.44	924646	5.0
unknown-01	9.69	2.4	ug/L	444221	2	9.44	924646	5.0
Indane	12.10	0.6	ug/L	353870	3	11.82	3091050	5.0