

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU052319\
 Data File : VU032276.D
 Acq On : 23 May 2019 18:14
 Operator : JC/SP
 Sample : K3001-02DL 5X
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E3YE9DL

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\SOMUTR052219WMA.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	1.283	54	60	64	rBV	98303	98063	5.01%	0.630%
2	1.396	85	95	108	rBV	167331	184049	9.40%	1.183%
3	1.672	173	181	194	rVB	130739	166547	8.51%	1.070%
4	2.270	355	367	379	rBV	301206	461950	23.60%	2.968%
5	2.450	415	423	440	rVB3	13111	28020	1.43%	0.180%
6	2.833	526	542	557	rBV	87065	190044	9.71%	1.221%
7	4.190	946	964	1003	rBV2	157776	520976	26.62%	3.347%
8	4.643	1087	1105	1126	rBV3	211025	492458	25.16%	3.164%
9	5.244	1277	1292	1301	rBV5	40414	96872	4.95%	0.622%
10	5.331	1301	1319	1331	rBV3	404659	1068697	54.60%	6.867%
11	5.469	1351	1362	1375	rVB7	23671	51593	2.64%	0.332%
12	5.550	1375	1387	1402	rVB9	18840	47235	2.41%	0.304%
13	5.881	1477	1490	1514	rBV	392343	778281	39.77%	5.001%
14	6.328	1613	1629	1642	rBV2	254992	516595	26.39%	3.319%
15	6.428	1654	1660	1676	rVB7	16954	35323	1.80%	0.227%
16	6.865	1784	1796	1812	rBV4	32052	63913	3.27%	0.411%
17	7.225	1896	1908	1927	rBV	110506	220086	11.25%	1.414%
18	7.559	2000	2012	2045	rBV	509094	929467	47.49%	5.972%
19	7.701	2048	2056	2068	rVB5	13410	27804	1.42%	0.179%
20	7.849	2089	2102	2116	rBV3	76278	149984	7.66%	0.964%
21	7.952	2127	2134	2149	rVB5	24172	44098	2.25%	0.283%
22	8.312	2230	2246	2277	rBV	602249	1127571	57.61%	7.245%
23	8.643	2337	2349	2366	rVB	127349	208731	10.66%	1.341%
24	9.087	2474	2487	2509	rBV	591077	1007607	51.48%	6.474%
25	9.183	2509	2517	2529	rVB2	32706	60016	3.07%	0.386%
26	9.292	2535	2551	2563	rBV	1294989	1957187	100.00%	12.576%
27	9.360	2563	2572	2588	rVB2	312987	536208	27.40%	3.445%
28	9.489	2602	2612	2623	rVB8	15190	30459	1.56%	0.196%
29	9.566	2624	2636	2647	rVB5	22109	39402	2.01%	0.253%
30	10.161	2808	2821	2835	rBV	555578	892453	45.60%	5.734%
31	10.427	2893	2904	2922	rBV2	210972	344357	17.59%	2.213%
32	10.588	2944	2954	2964	rBV2	14765	28362	1.45%	0.182%
33	11.099	3097	3113	3120	rBV6	11806	24460	1.25%	0.157%
34	11.292	3158	3173	3175	rBV3	16176	24323	1.24%	0.156%

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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	11.321	3175	3182	3197	rVB	50672	79935	4.08%	0.514%
36	11.479	3216	3231	3253	rBV2	644544	1207766	61.71%	7.760%
37	11.685	3284	3295	3303	rBV2	26881	41946	2.14%	0.270%
38	11.762	3303	3319	3336	rVV	374852	657190	33.58%	4.223%
39	11.855	3337	3348	3374	rVB	537799	943165	48.19%	6.060%
40	12.283	3467	3481	3491	rBV2	42299	73142	3.74%	0.470%
41	12.350	3492	3502	3522	rVB2	44045	83759	4.28%	0.538%
42	12.537	3549	3560	3571	rVB3	14489	23097	1.18%	0.148%

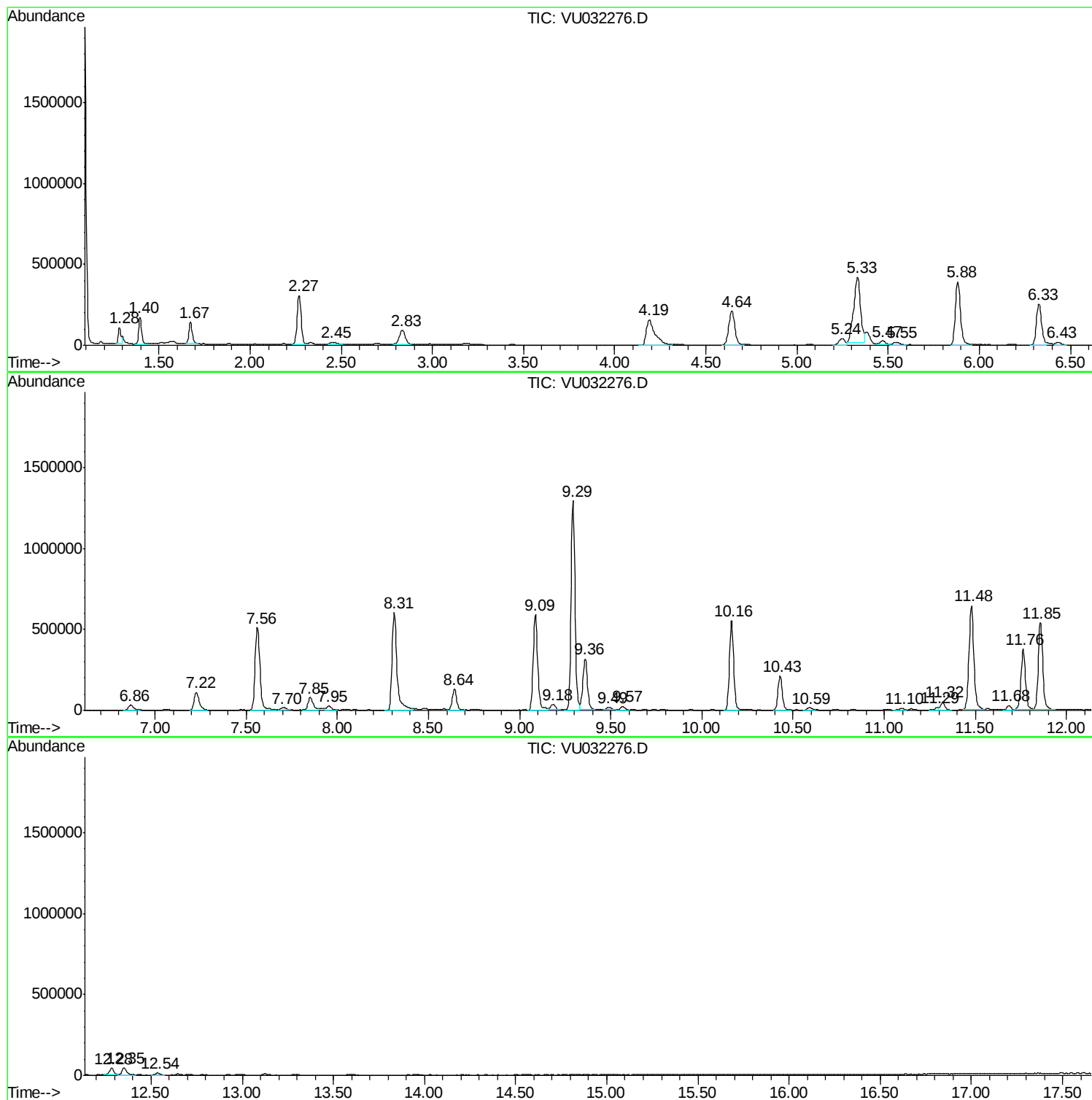
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR052219WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Instrument :
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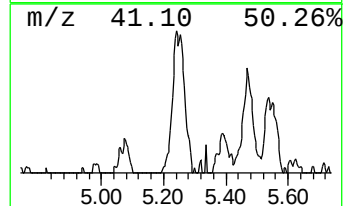
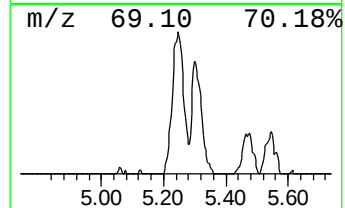
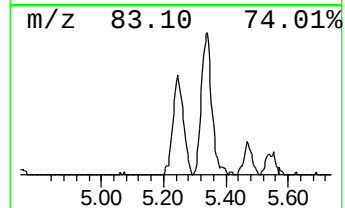
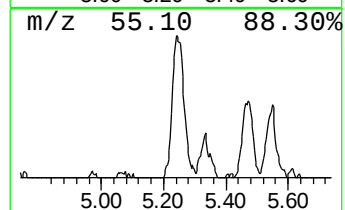
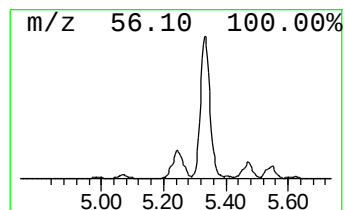
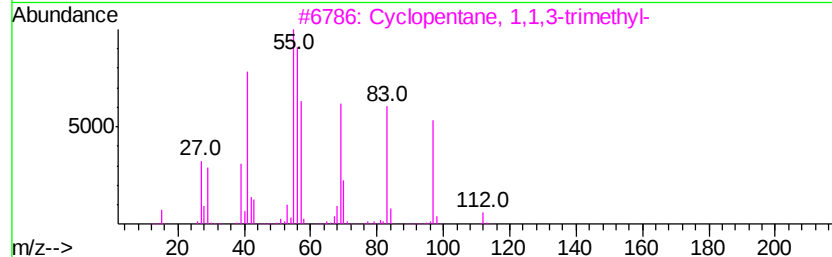
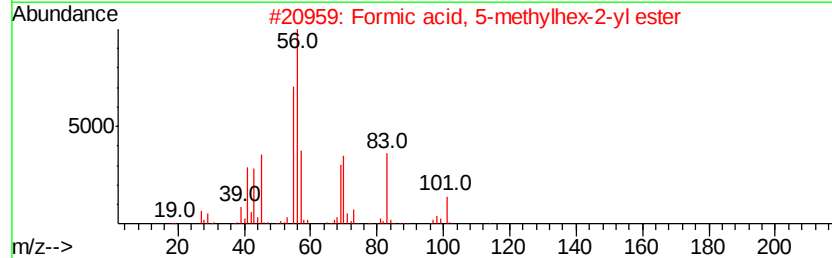
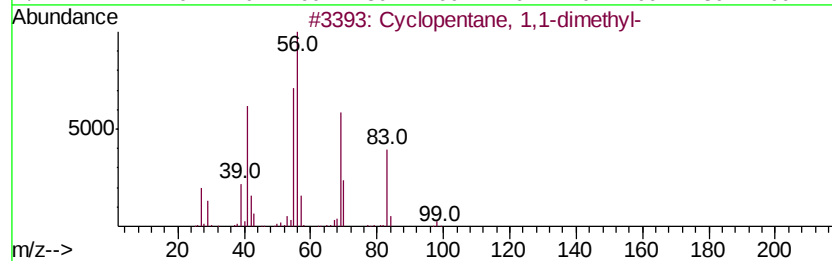
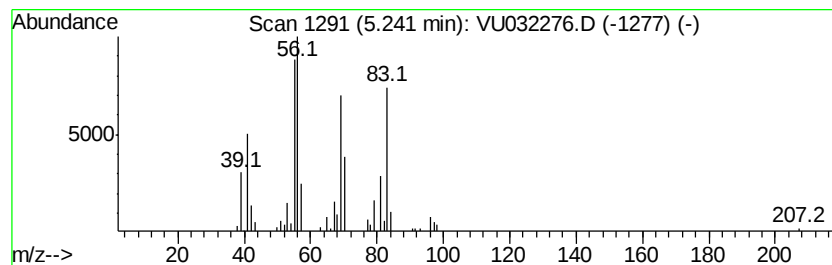
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 (DEL) Alkane: Cyclic5.24 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	0.62 ug/L	96872	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	72
2		Formic acid, 5-methylhex-2-yl ester	144	C8H16O2	1000368-88-7	64
3		Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	56
4		Pentane, 2-cyclopropyl-	112	C8H16	005458-16-2	53
5		4-Decene, 5-methyl-, (E)-	154	C11H22	062338-51-6	50



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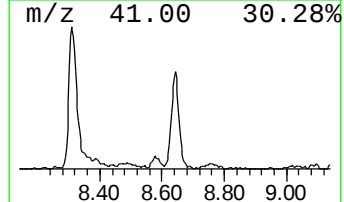
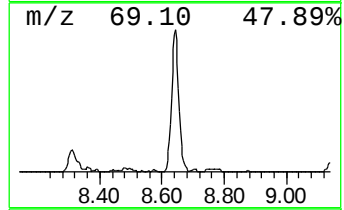
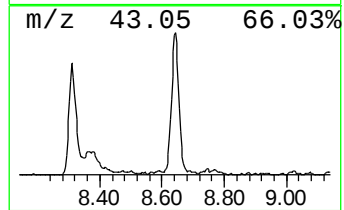
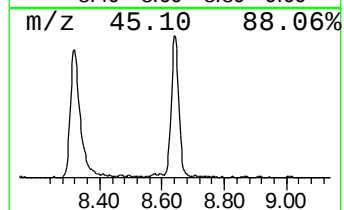
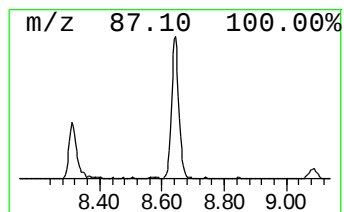
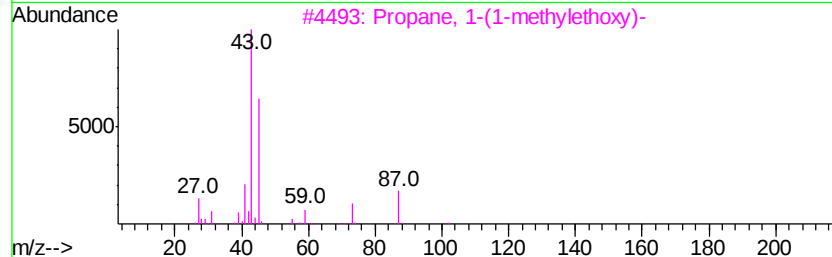
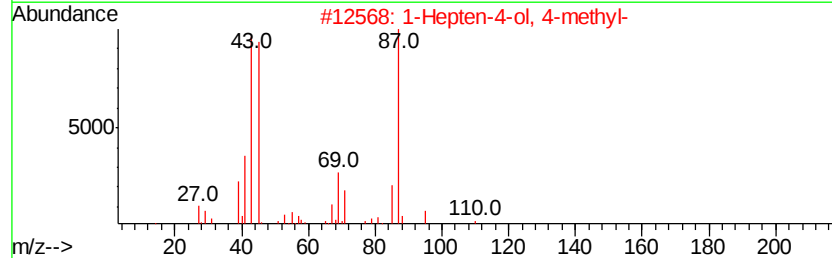
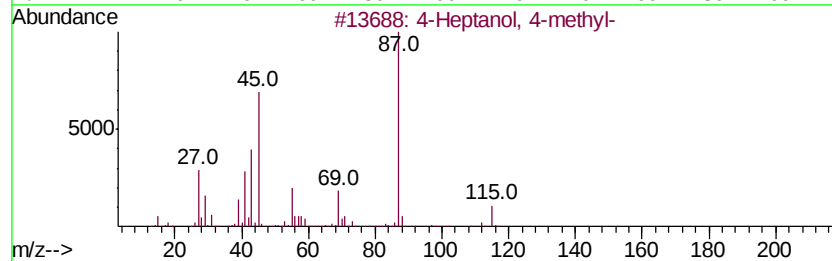
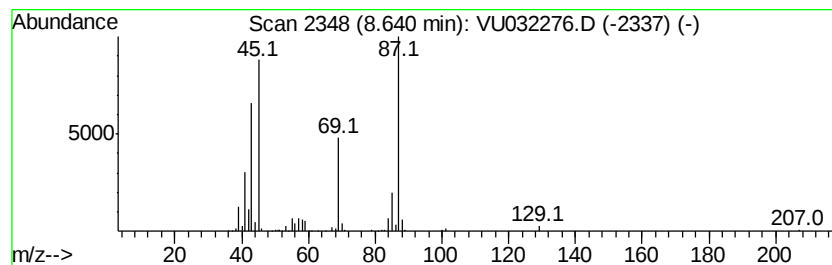
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4-Heptanol, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.64	1.04 ug/L	208731	Chlorobenzene-d5	9.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol, 4-methyl-	130	C8H18O	000598-01-6	72
2			1-Hepten-4-ol, 4-methyl-	128	C8H16O	001186-31-8	72
3			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	64
4			Hydrazine, 1,1-dipropyl-	116	C6H16N2	004986-50-9	64
5			4-Heptanol, 4-methyl-	130	C8H18O	000598-01-6	64



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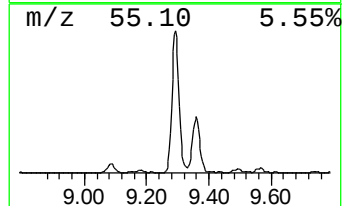
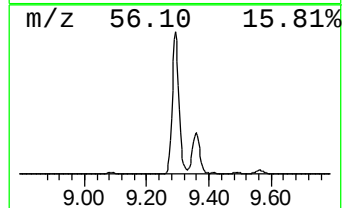
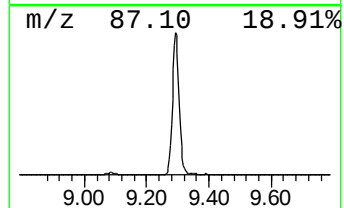
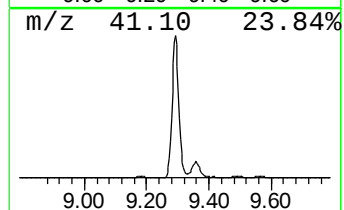
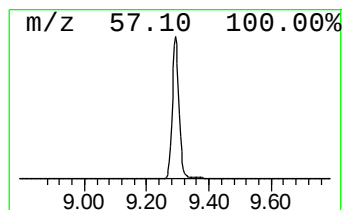
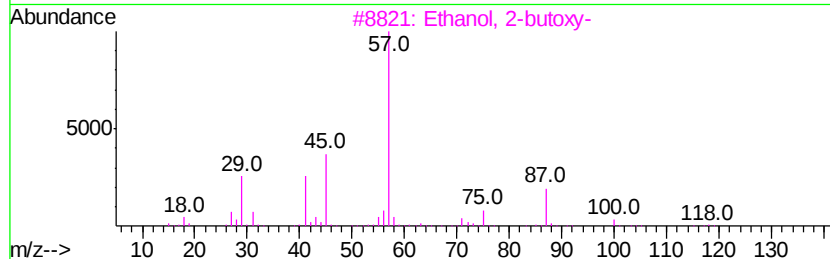
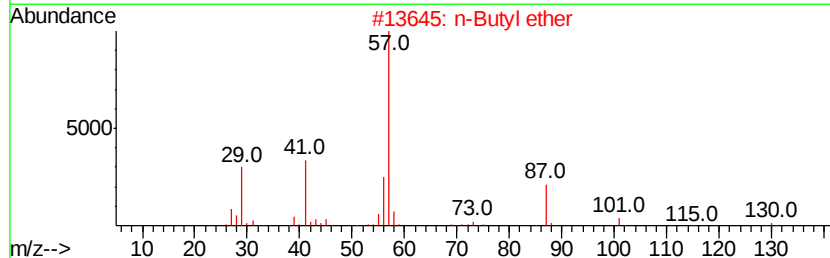
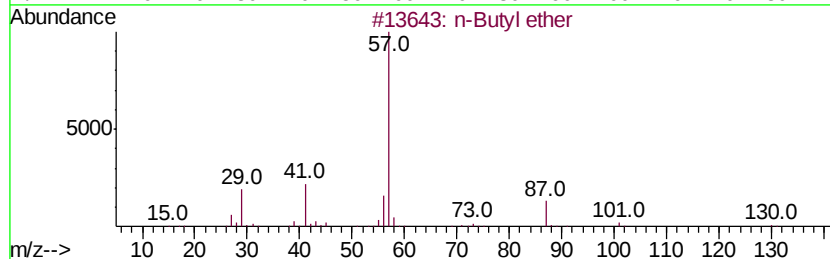
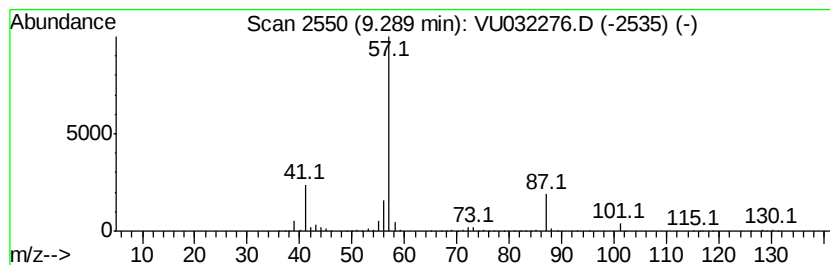
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR052219WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 n-Butyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.29	9.71 ug/L	1957190	Chlorobenzene-d5	9.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Butyl ether	130 C8H18O	000142-96-1	72
2	n-Butyl ether	130 C8H18O	000142-96-1	53
3	Ethanol, 2-butoxy-	118 C6H14O2	000111-76-2	50
4	n-Butyl ether	130 C8H18O	000142-96-1	38
5	Octane, 3-methyl-	128 C9H20	002216-33-3	38



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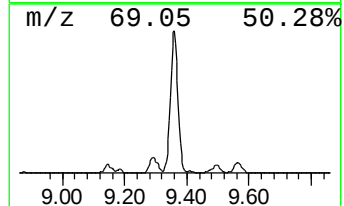
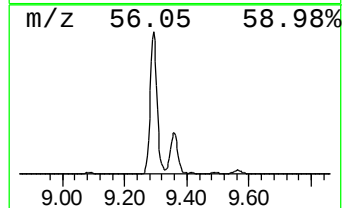
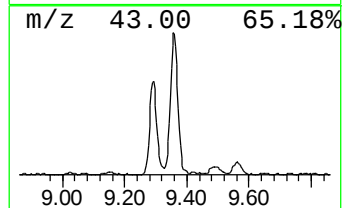
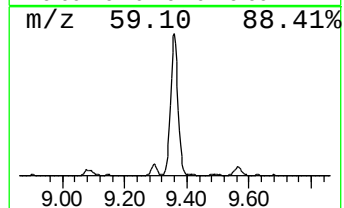
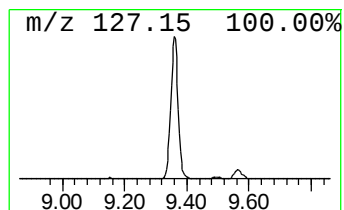
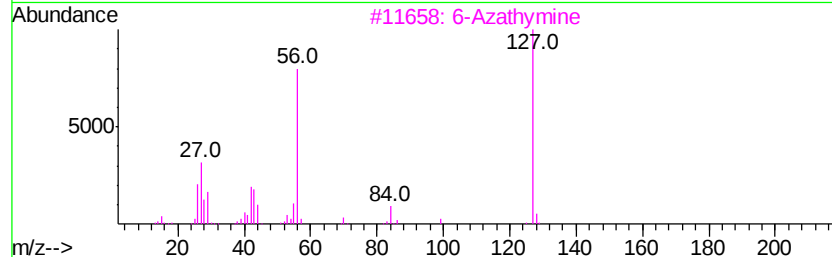
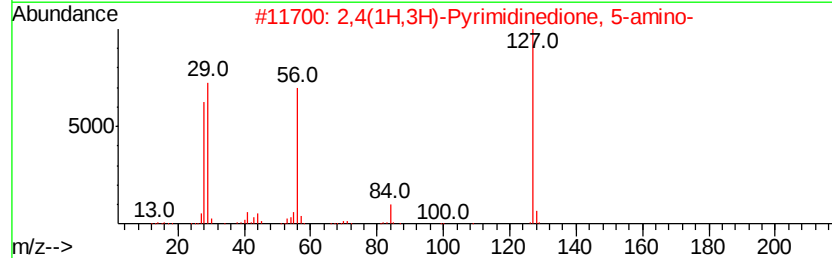
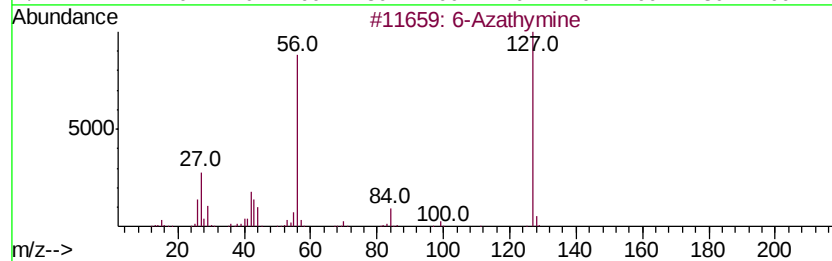
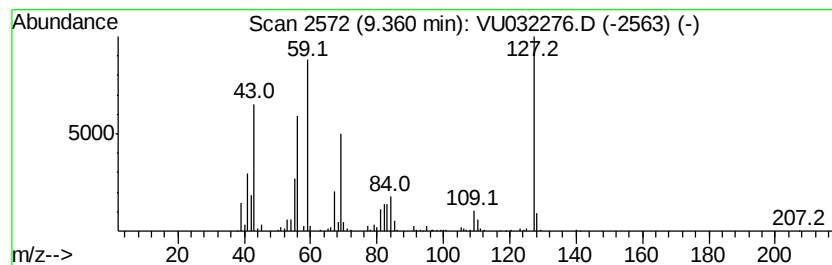
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TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.36	2.66 ug/L	536208	Chlorobenzene-d5	9.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Azathymine	127	C4H5N3O2	000932-53-6	43
2			2,4(1H,3H)-Pyrimidinedione, 5-am...	127	C4H5N3O2	000932-52-5	38
3			6-Azathymine	127	C4H5N3O2	000932-53-6	38
4			2-Thiazoleamine, 4-(2-acetylfura...	196	C8H8N2O2S	115154-38-6	38
5			4-Amino-2,6-dihydroxypyrimidine	127	C4H5N3O2	000873-83-6	30



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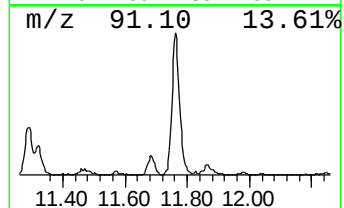
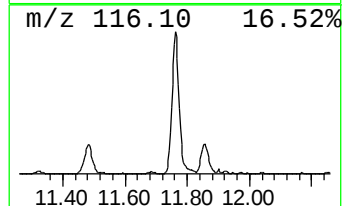
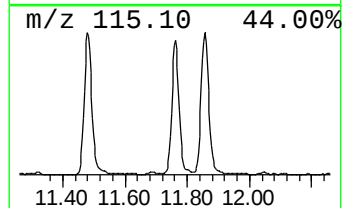
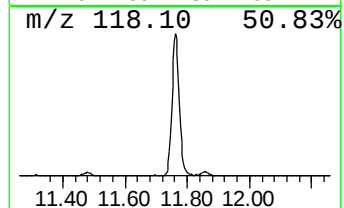
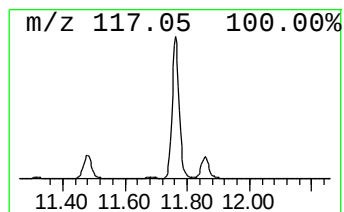
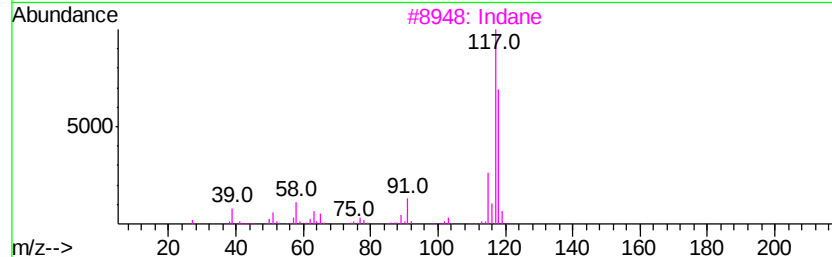
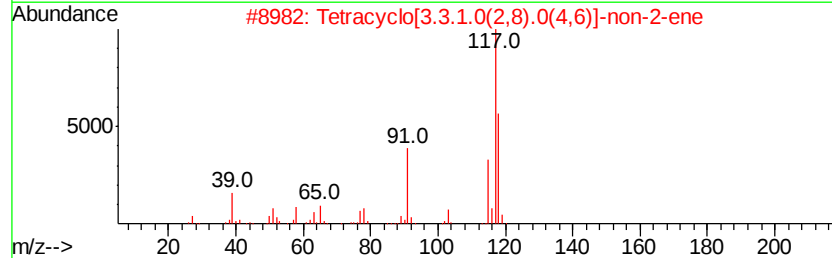
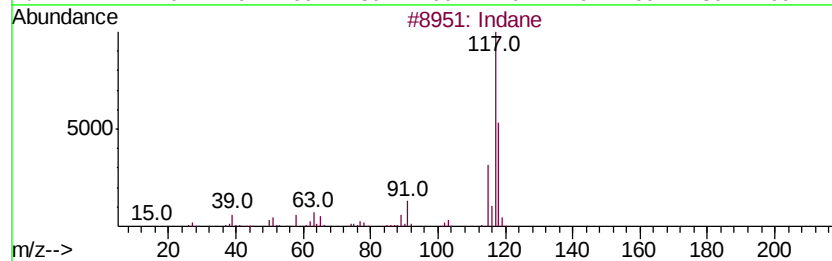
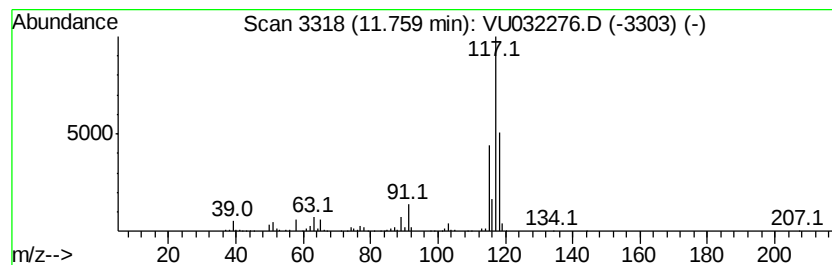
Instrument :
MSVOA_U
ClientSampleId :
E3YE9DL

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR052219WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	2.72 ug/L	657190	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Indane		118 C9H10	000496-11-7 93
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-	...	118 C9H10	1000191-13-7 58
3	Indane		118 C9H10	000496-11-7 55
4	Benzene, (2-bromocyclopropyl)-		196 C9H9Br	036617-02-4 53
5	1,3-Methanopentalene, 1,2,3,5-te...		118 C9H10	128600-88-4 53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU052319\
Data File : VU032276.D
Acq On : 23 May 2019 18:14
Operator : JC/SP
Sample : K3001-02DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E3YE9DL

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR052219WMA.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: Cyc...	5.24	0.6	ug/L	96872	1	5.88	778281	5.0
4-Heptanol, 4-met...	8.64	1.0	ug/L	208731	2	9.09	1007610	5.0
n-Butyl ether	9.29	9.7	ug/L	1957190	2	9.09	1007610	5.0
unknown-01	9.36	2.7	ug/L	536208	2	9.09	1007610	5.0
Indane	11.76	2.7	ug/L	657190	3	11.48	1207770	5.0