

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU112118\
 Data File : VU028309.D
 Acq On : 21 Nov 2018 11:05
 Operator : MD/SY
 Sample : J5997-13DL 4X
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E3YA9DL

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	1.283	29	34	44	rBV	167700	160537	8.03%	1.537%
2	1.398	63	70	79	rVB	94605	99767	4.99%	0.955%
3	1.681	151	158	174	rVB	78777	110679	5.54%	1.059%
4	2.273	333	342	353	rBV	153875	226349	11.33%	2.167%
5	4.196	923	940	974	rBV	110460	317574	15.89%	3.040%
6	4.646	1063	1080	1097	rBV2	112477	270560	13.54%	2.590%
7	5.250	1252	1268	1277	rBV3	42442	100833	5.05%	0.965%
8	5.337	1278	1295	1307	rVV2	218589	560506	28.05%	5.365%
9	5.472	1325	1337	1349	rBV2	23913	50125	2.51%	0.480%
10	5.549	1350	1361	1374	rVB3	17802	37774	1.89%	0.362%
11	5.884	1449	1465	1481	rBV	218492	428323	21.43%	4.100%
12	6.331	1590	1604	1617	rBV2	160395	314635	15.75%	3.012%
13	7.228	1870	1883	1902	rBV	88150	166862	8.35%	1.597%
14	7.562	1973	1987	2005	rBV	298196	523048	26.17%	5.007%
15	7.710	2022	2033	2043	rBV2	12313	23052	1.15%	0.221%
16	7.851	2066	2077	2090	rBV	57350	102553	5.13%	0.982%
17	7.958	2103	2110	2120	rVB4	13521	22282	1.12%	0.213%
18	8.314	2204	2221	2247	rBV	381294	670424	33.55%	6.417%
19	8.646	2312	2324	2342	rVB	154160	257354	12.88%	2.463%
20	9.089	2448	2462	2477	rBV	318767	526538	26.35%	5.040%
21	9.186	2483	2492	2506	rVB2	23855	42662	2.13%	0.408%
22	9.295	2511	2526	2538	rBV	1351817	1998311	100.00%	19.128%
23	9.363	2538	2547	2564	rVB2	180172	309832	15.50%	2.966%
24	9.568	2601	2611	2622	rBV3	20135	33830	1.69%	0.324%
25	10.166	2780	2797	2820	rBV	474742	760783	38.07%	7.282%
26	10.430	2865	2879	2895	rBV	106143	169608	8.49%	1.623%
27	10.585	2917	2927	2935	rBV2	49434	81485	4.08%	0.780%
28	11.099	3072	3087	3093	rBV3	12414	21536	1.08%	0.206%
29	11.147	3093	3102	3114	rVB	66838	96962	4.85%	0.928%
30	11.292	3133	3147	3149	rBV2	17697	25102	1.26%	0.240%
31	11.324	3150	3157	3168	rVB2	53712	85527	4.28%	0.819%
32	11.482	3192	3206	3222	rBV2	356123	610368	30.54%	5.842%
33	11.687	3260	3270	3279	rBV	27379	40713	2.04%	0.390%
34	11.765	3279	3294	3311	rVV2	235488	424917	21.26%	4.067%

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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	11.858	3311	3323	3343	rVB	276903	458024	22.92%	4.384%
36	12.285	3447	3456	3466	rVB3	35271	55134	2.76%	0.528%
37	12.353	3466	3477	3496	rVB2	86697	164903	8.25%	1.578%
38	13.125	3709	3717	3730	rVB3	27260	44919	2.25%	0.430%
39	13.289	3755	3768	3780	rBV3	33647	52906	2.65%	0.506%

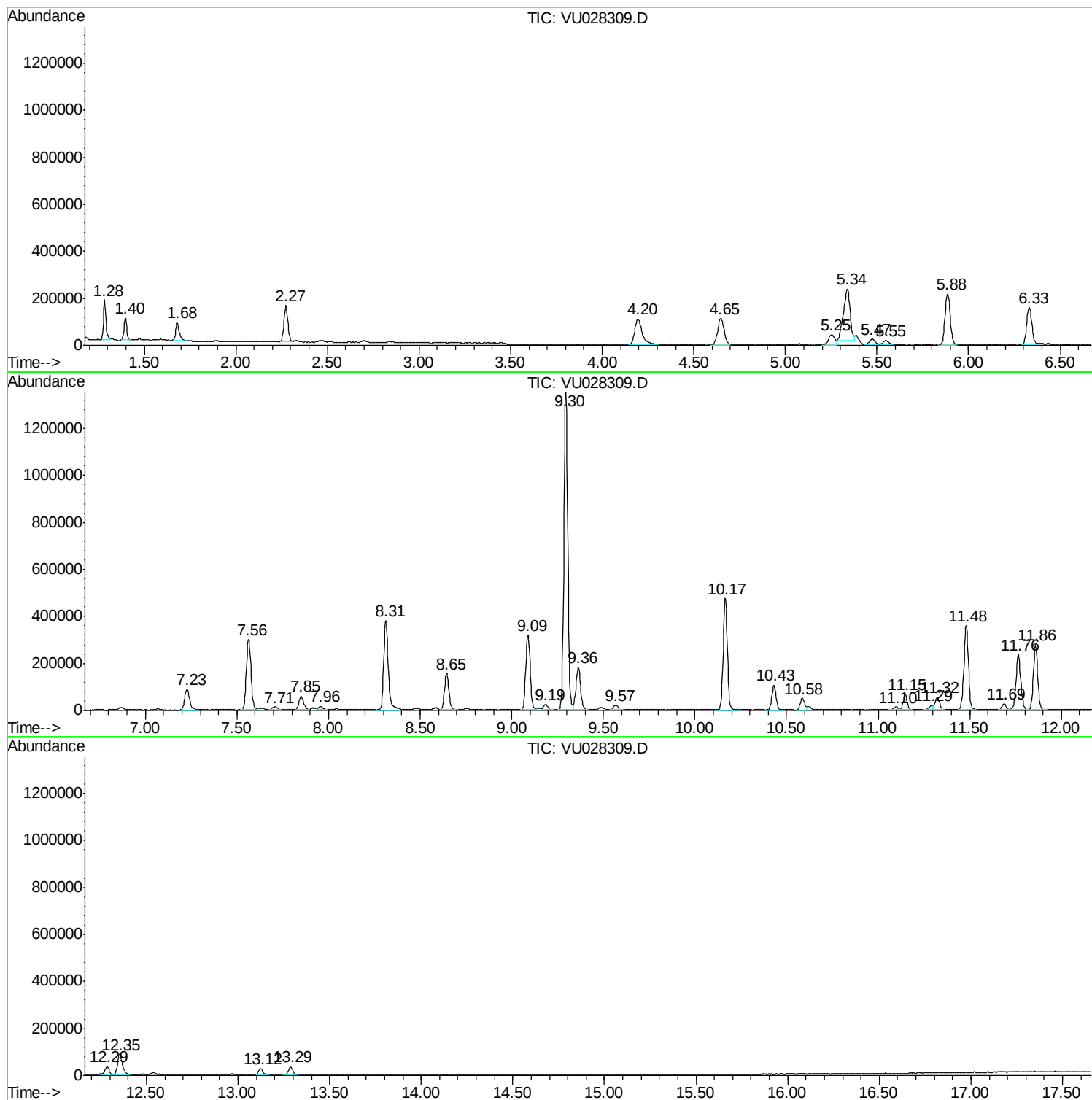
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111718WMA.M
Quant Title : TRACE VOA SOM01.0

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



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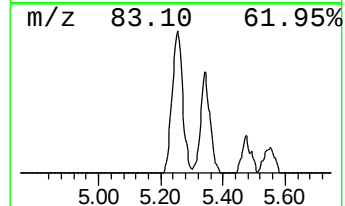
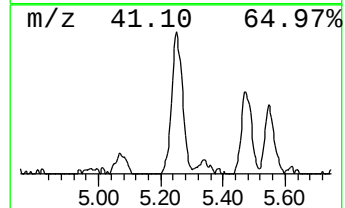
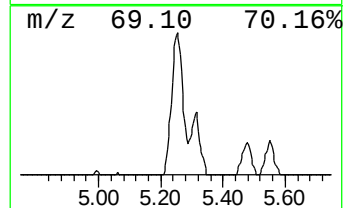
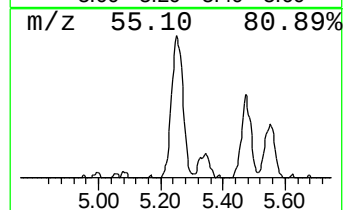
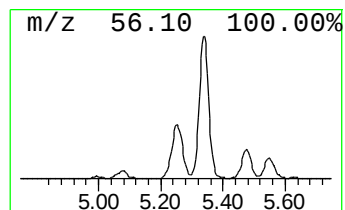
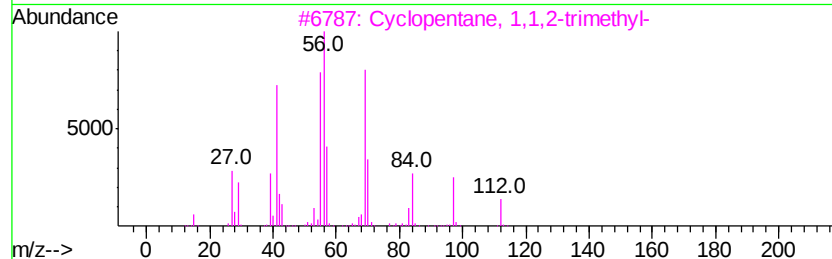
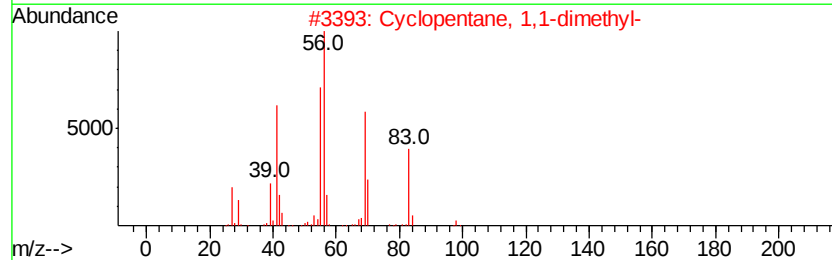
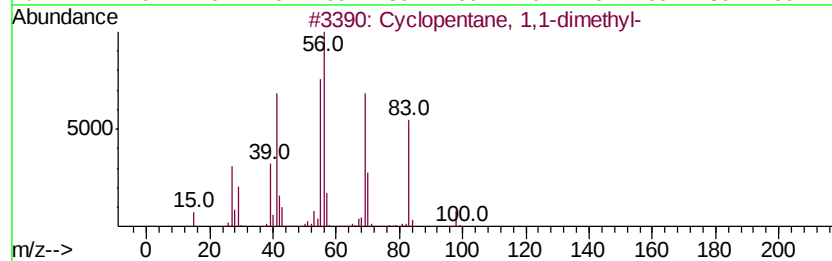
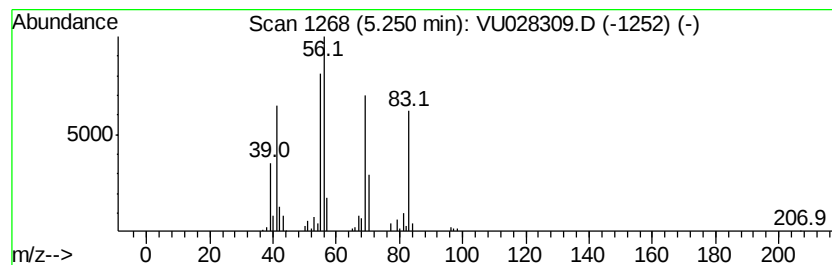
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111718WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 (DEL) Alkane: Cyclic5.25 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	1.18 ug/L	100833	1,4-Difluorobenzene	5.88

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	86
2		Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	72
3		Cyclopentane, 1,1,2-trimethyl-	112	C8H16	004259-00-1	53
4		1-Heptene, 2,6-dimethyl-	126	C9H18	003074-78-0	53
5		1-Hexene, 5-methyl-	98	C7H14	003524-73-0	49



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Instrument :
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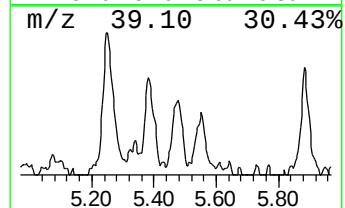
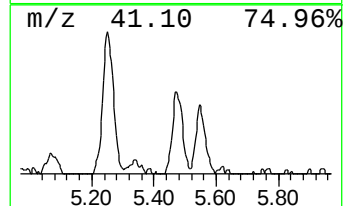
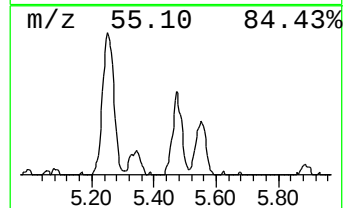
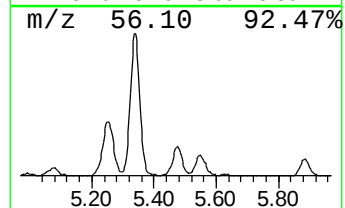
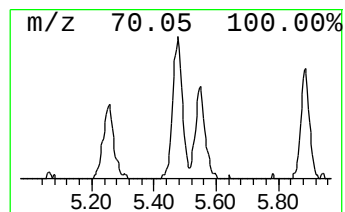
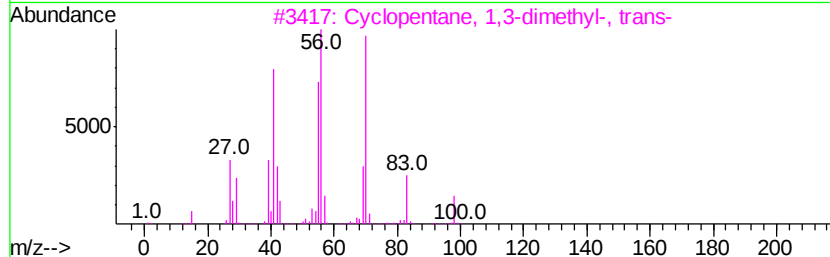
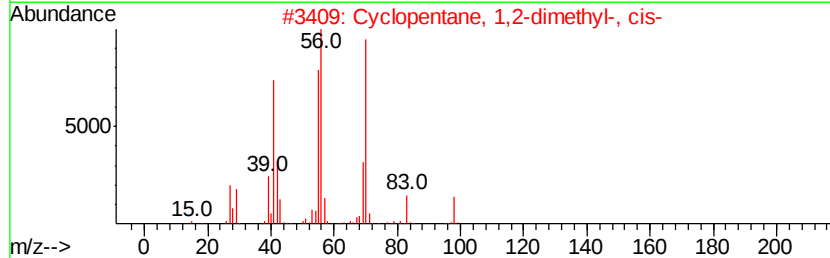
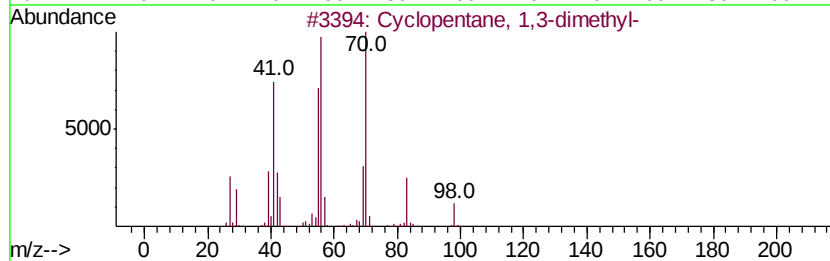
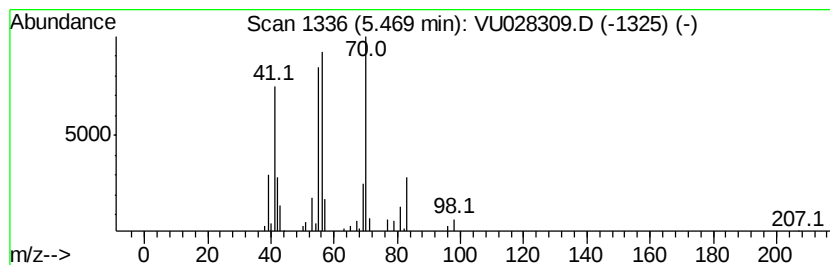
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 (DEL) Alkane: Cyclic5.47 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.47	0.59 ug/L	50125	1,4-Difluorobenzene	5.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	87
2			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	87
3			Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	86
4			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	78
5			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	78



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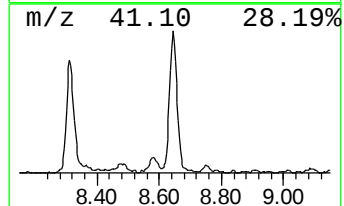
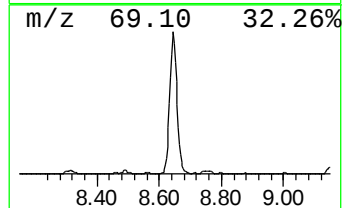
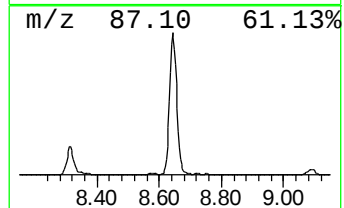
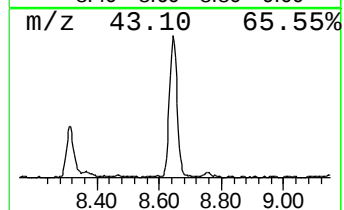
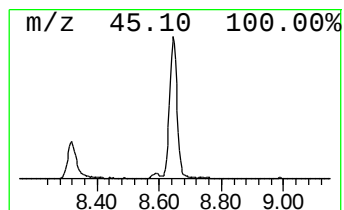
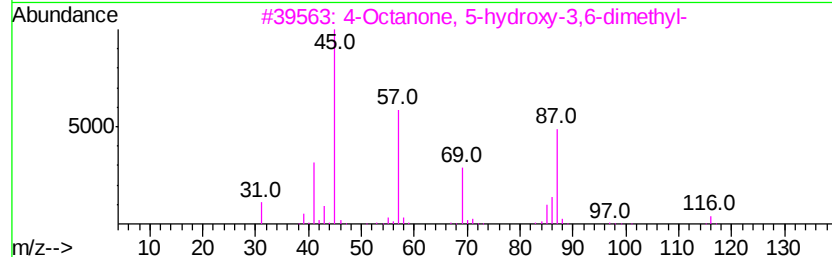
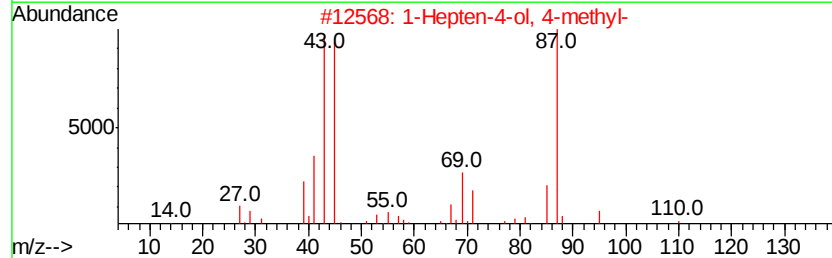
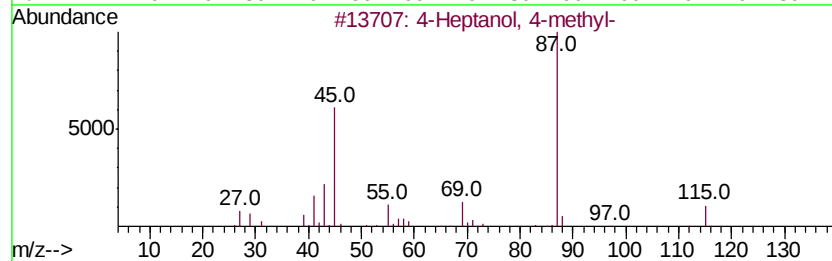
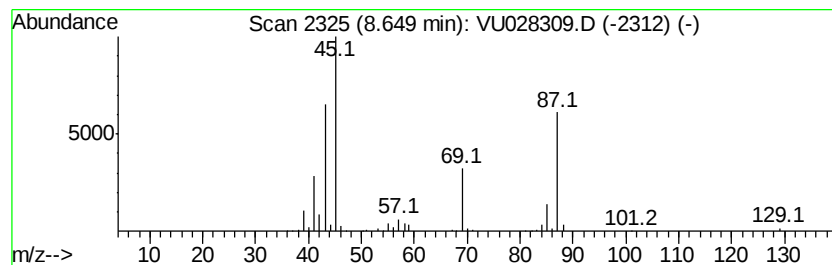
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.65	2.44 ug/L	257354	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Heptanol, 4-methyl-	130	C8H18O	000598-01-6	78
2		1-Hepten-4-ol, 4-methyl-	128	C8H16O	001186-31-8	78
3		4-Octanone, 5-hydroxy-3,6-dimethyl-	172	C10H20O2	062759-47-1	78
4		3-Bromobutyric acid	166	C4H7BrO2	1000131-80-6	56
5		3-Hexanol, 2,3-dimethyl-	130	C8H18O	004166-46-5	56



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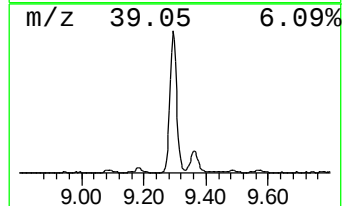
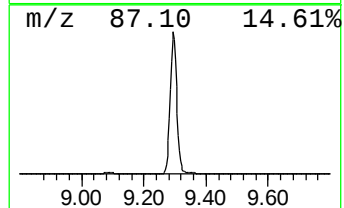
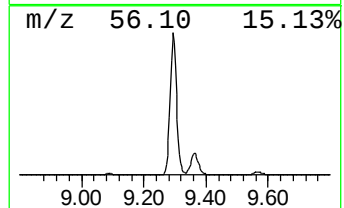
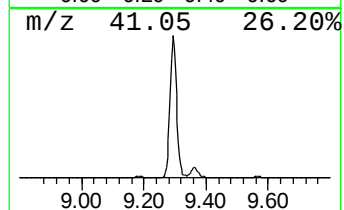
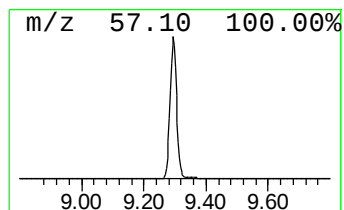
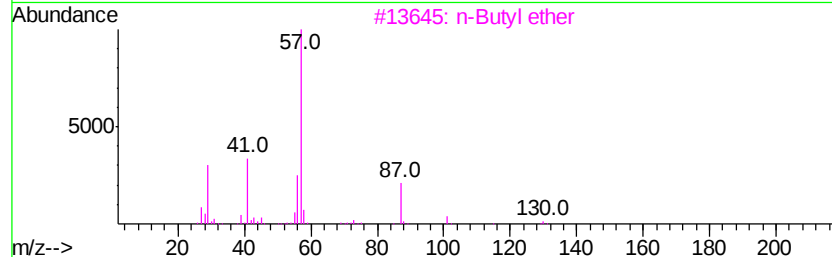
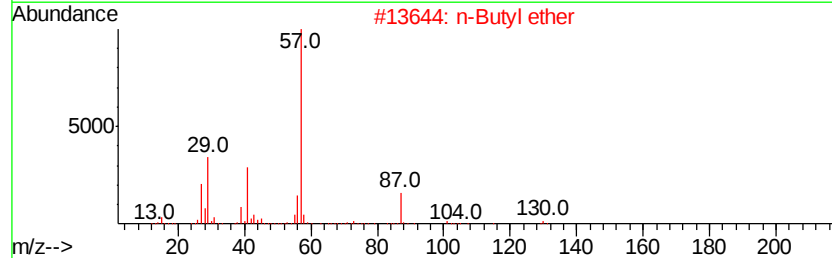
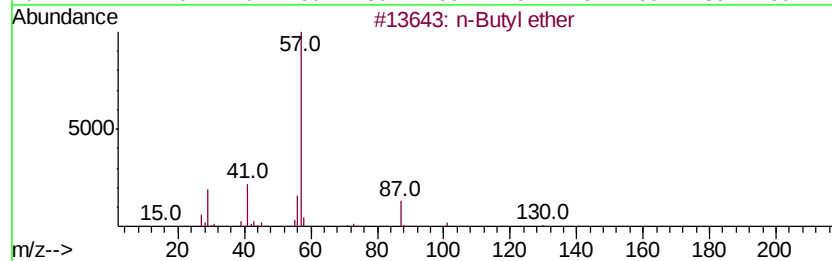
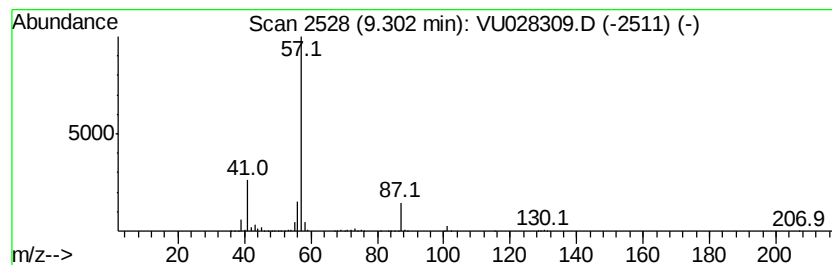
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Peak Number 6 n-Butyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
9.30	18.98 ug/L	1998310	Chlorobenzene-d5	9.09		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Butyl ether		130	C8H18O	000142-96-1	78
2	n-Butyl ether		130	C8H18O	000142-96-1	78
3	n-Butyl ether		130	C8H18O	000142-96-1	59
4	Sulfurous acid, dibutyl ester		194	C8H18O3S	000626-85-7	53
5	Isobutyl ether		130	C8H18O	000628-55-7	42



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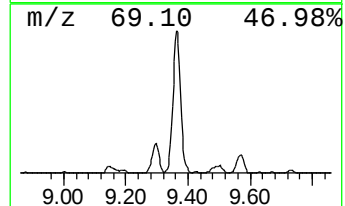
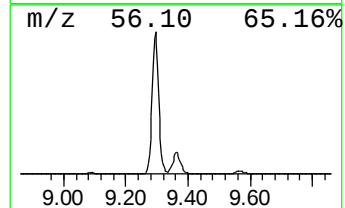
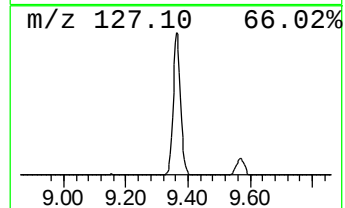
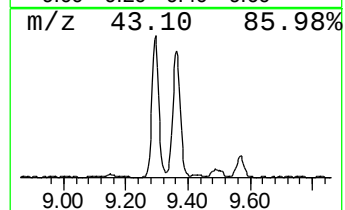
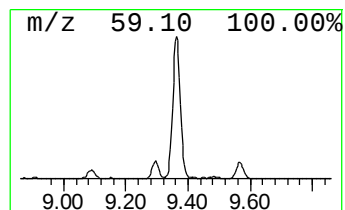
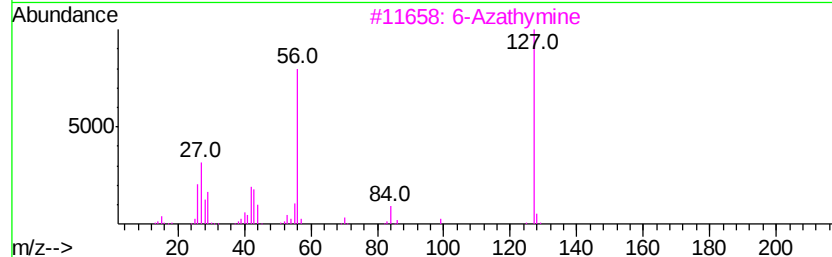
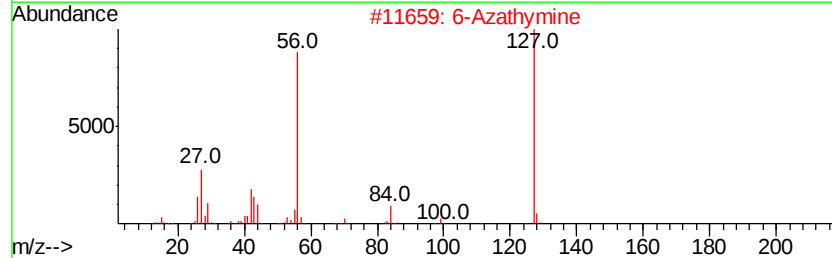
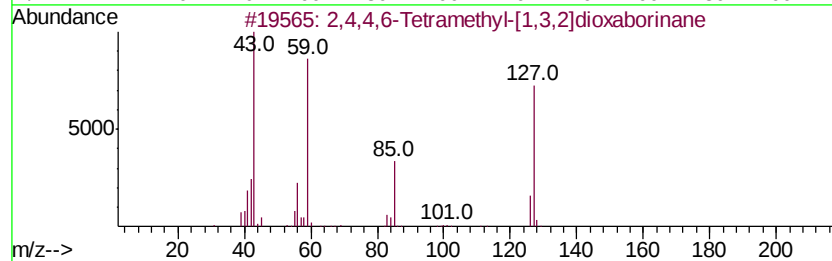
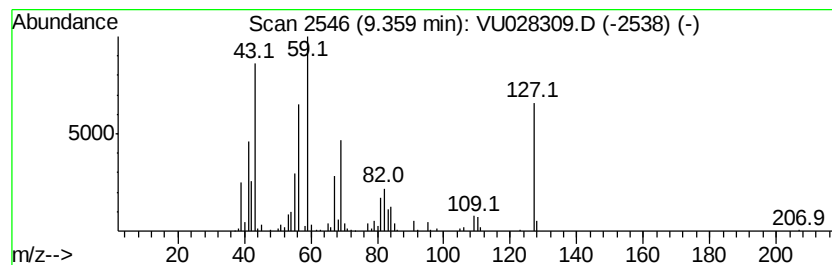
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 2,4,4,6-Tetramethyl-[1,3,2]... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.36	2.94 ug/L	309832	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4,4,6-Tetramethyl-[1,3,2]dioxab...	142	C7H15B02	211613-23-9	53
2		6-Azathymine	127	C4H5N3O2	000932-53-6	30
3		6-Azathymine	127	C4H5N3O2	000932-53-6	27
4		Guanidine	59	CH5N3	000113-00-8	27
5		2,4(1H,3H)-Pyrimidinedione, 5-am...	127	C4H5N3O2	000932-52-5	25



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU112118\
Data File : VU028309.D
Acq On : 21 Nov 2018 11:05
Operator : MD/SY
Sample : J5997-13DL 4X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

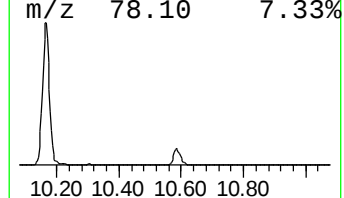
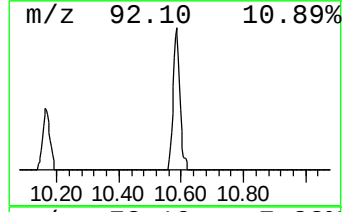
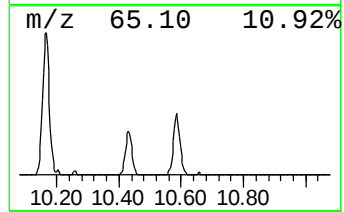
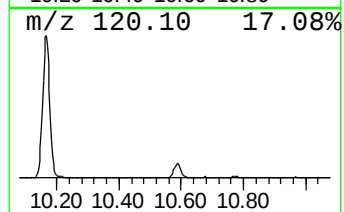
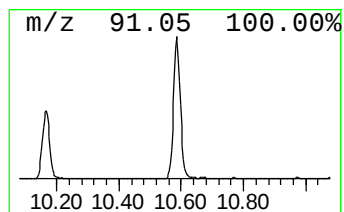
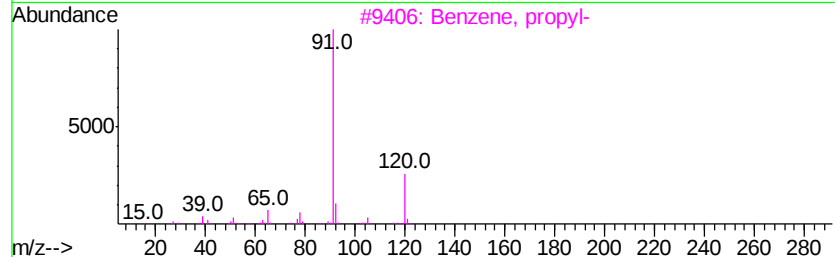
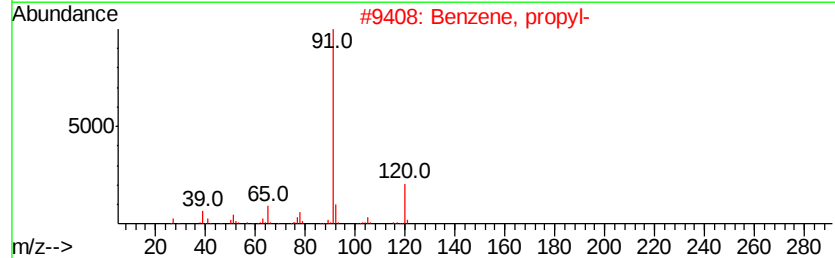
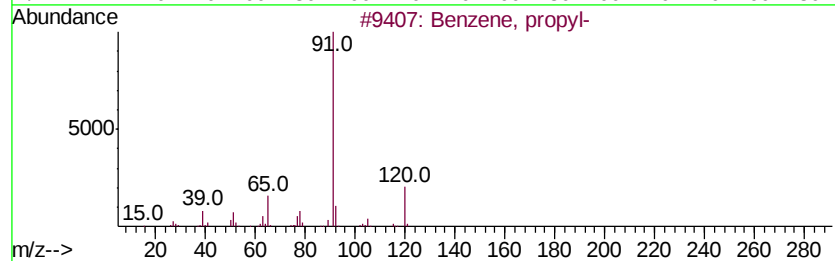
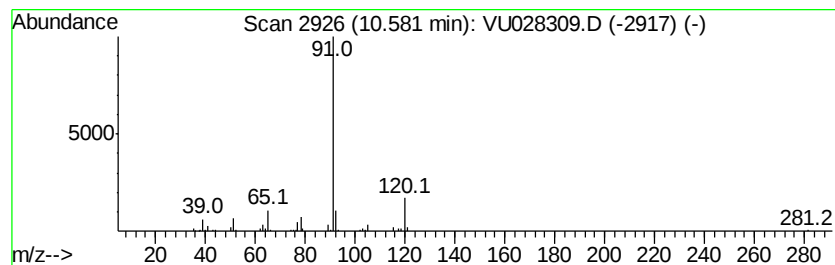
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ClientSampleId :
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Benzene, propyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	0.67 ug/L	81485	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, propyl-	120 C9H12	000103-65-1 87
2		Benzene, propyl-	120 C9H12	000103-65-1 87
3		Benzene, propyl-	120 C9H12	000103-65-1 80
4		N-Benzyl-2-phenethylamine	211 C15H17N	003647-71-0 72
5		Benzene, (4-bromobutyl)-	212 C10H13Br	013633-25-5 53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU112118\
Data File : VU028309.D
Acq On : 21 Nov 2018 11:05
Operator : MD/SY
Sample : J5997-13DL 4X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

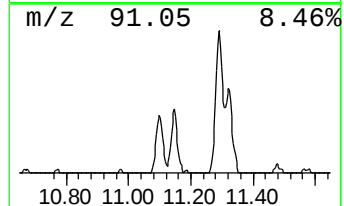
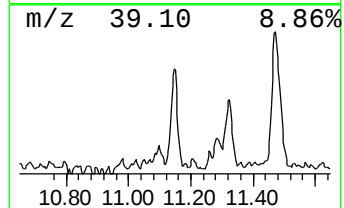
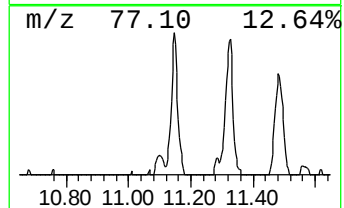
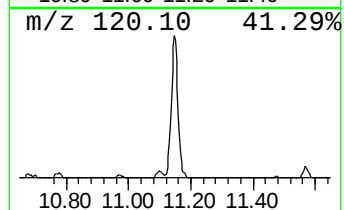
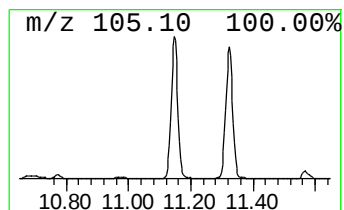
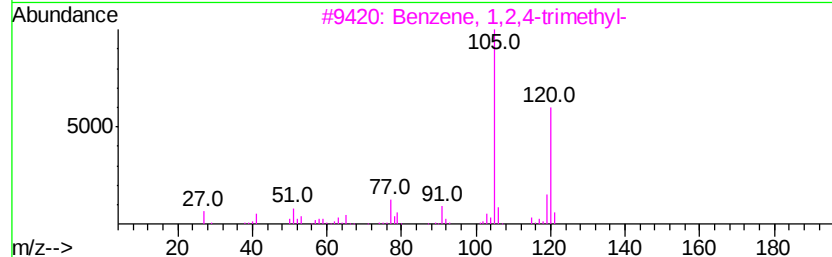
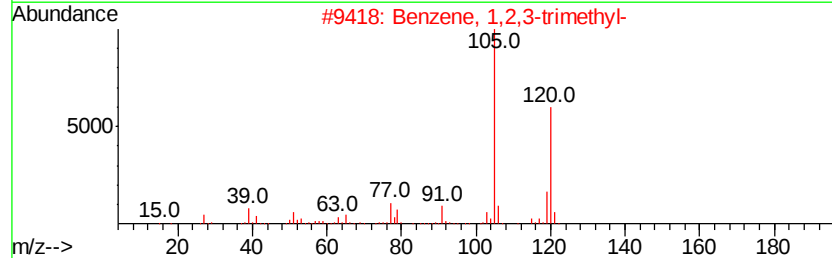
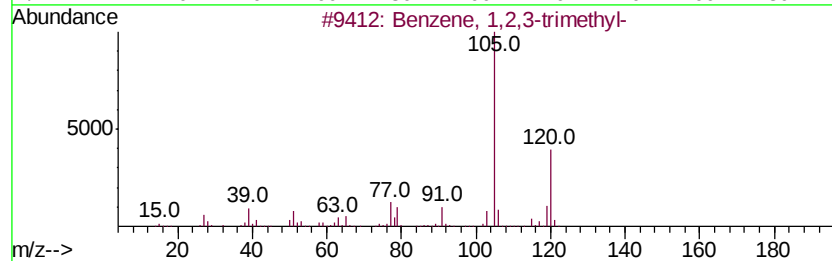
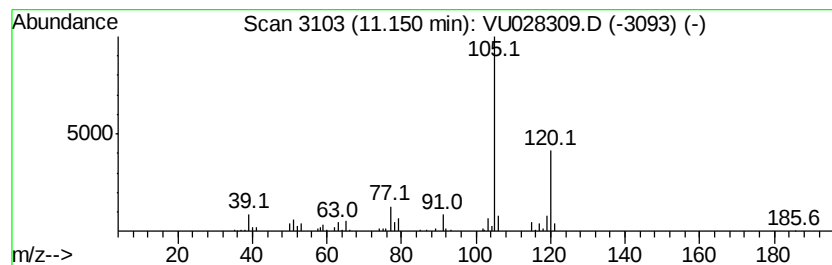
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ClientSampleId :
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.15	0.79 ug/L	96962	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1,2,3-trimethyl-	120 C9H12	000526-73-8 95
2		Benzene, 1,2,3-trimethyl-	120 C9H12	000526-73-8 94
3		Benzene, 1,2,4-trimethyl-	120 C9H12	000095-63-6 93
4		Mesitylene	120 C9H12	000108-67-8 93
5		Benzene, 1-ethyl-3-methyl-	120 C9H12	000620-14-4 91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU112118\
Data File : VU028309.D
Acq On : 21 Nov 2018 11:05
Operator : MD/SY
Sample : J5997-13DL 4X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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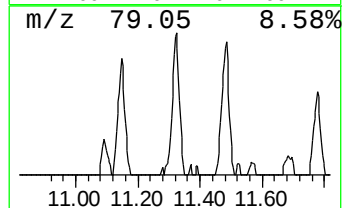
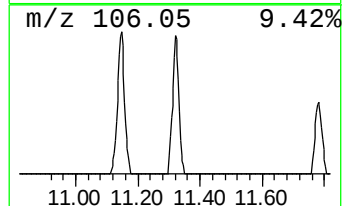
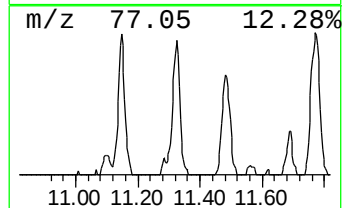
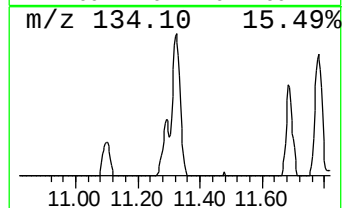
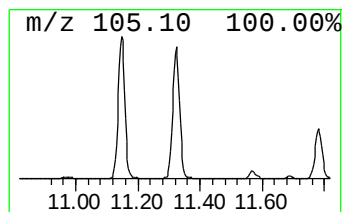
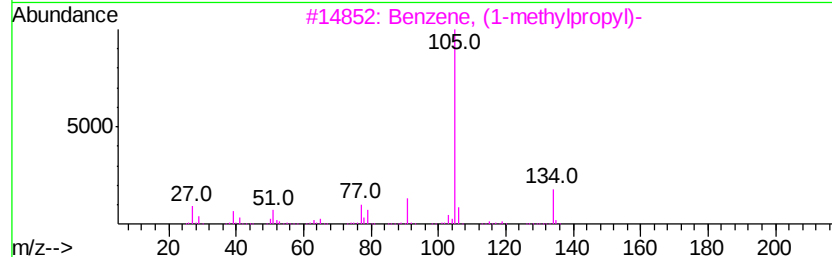
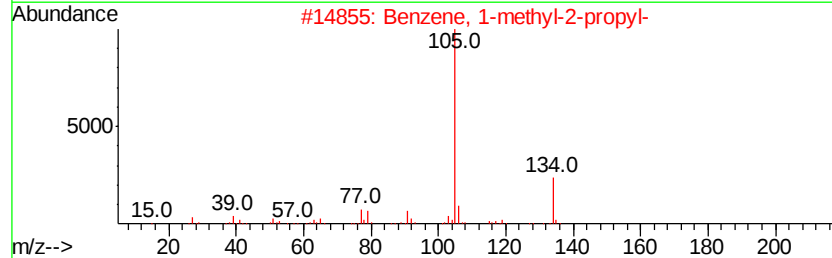
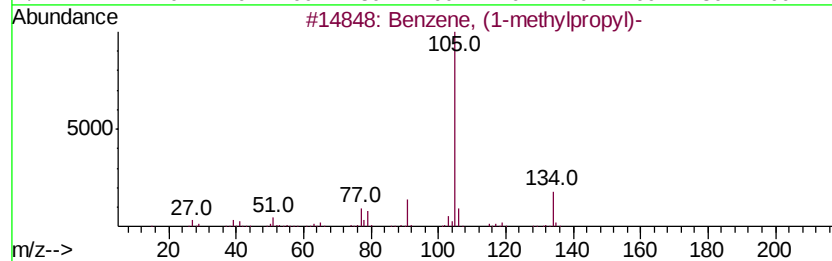
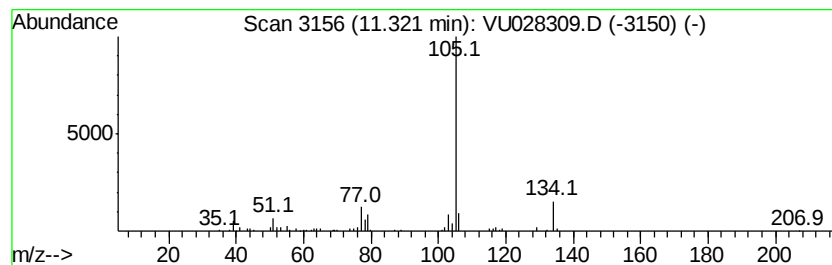
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 Benzene, (1-methylpropyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.32	0.70 ug/L	85527	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	90
2		Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	86
3		Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	83
4		Benzeneacetaldehyde, .alpha.-met...	134	C9H10O	000093-53-8	83
5		Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	83



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU112118\
Data File : VU028309.D
Acq On : 21 Nov 2018 11:05
Operator : MD/SY
Sample : J5997-13DL 4X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E3YA9DL

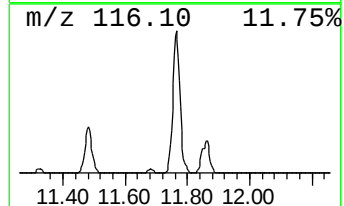
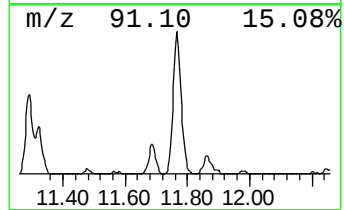
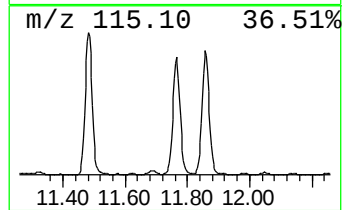
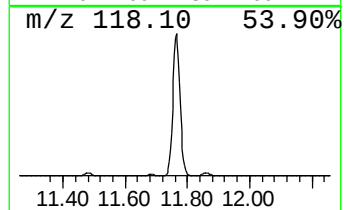
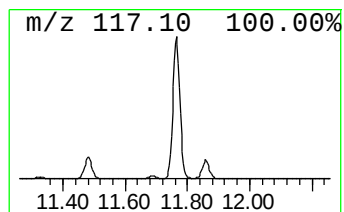
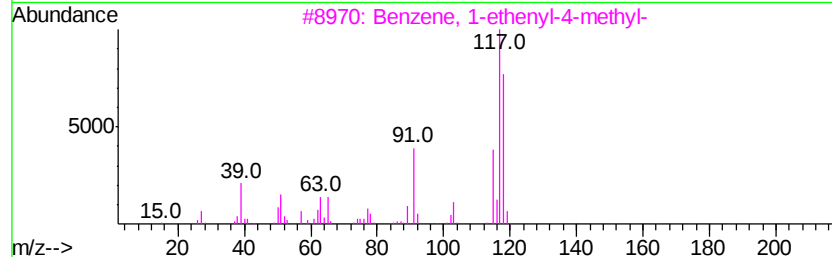
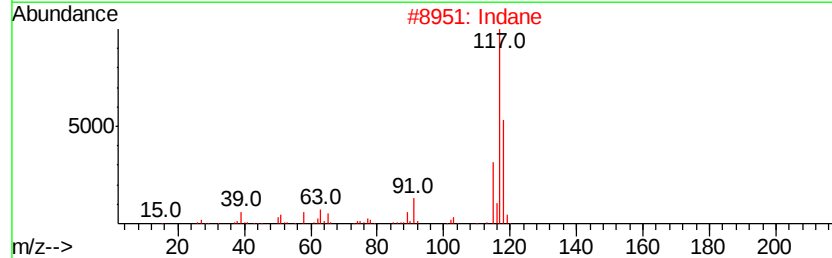
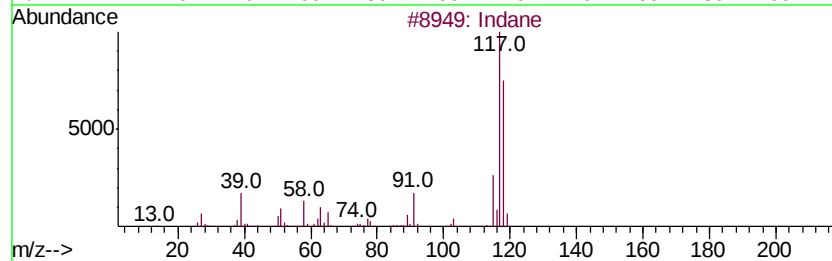
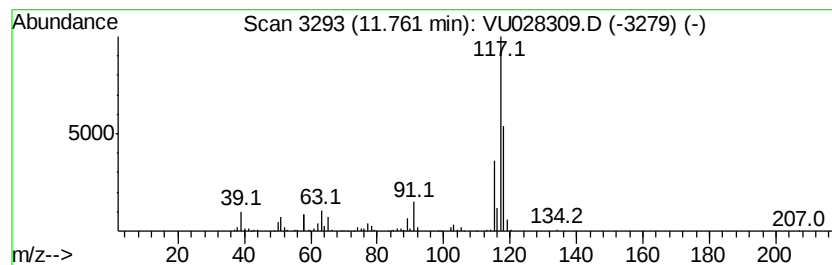
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 11 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	3.48 ug/L	424917	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indane	118	C9H10	000496-11-7	95
2		Indane	118	C9H10	000496-11-7	93
3		Benzene, 1-ethenvl-4-methvl-	118	C9H10	000622-97-9	83
4		Indane	118	C9H10	000496-11-7	81
5		Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU112118\
Data File : VU028309.D
Acq On : 21 Nov 2018 11:05
Operator : MD/SY
Sample : J5997-13DL 4X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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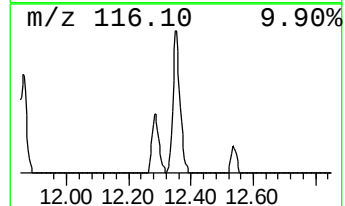
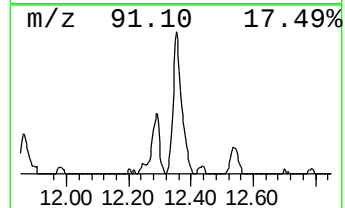
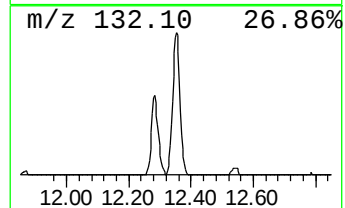
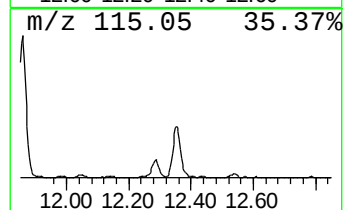
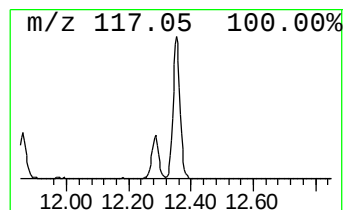
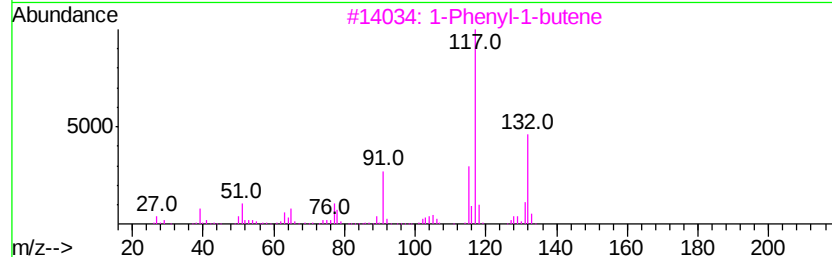
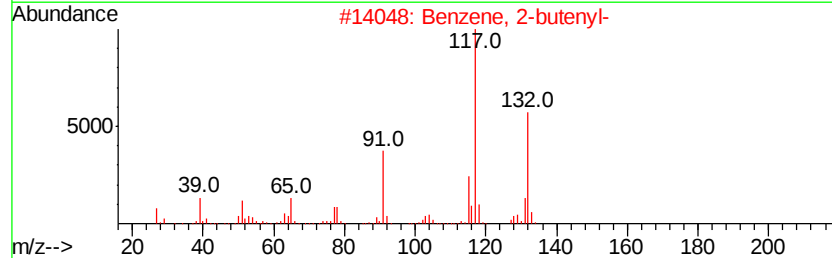
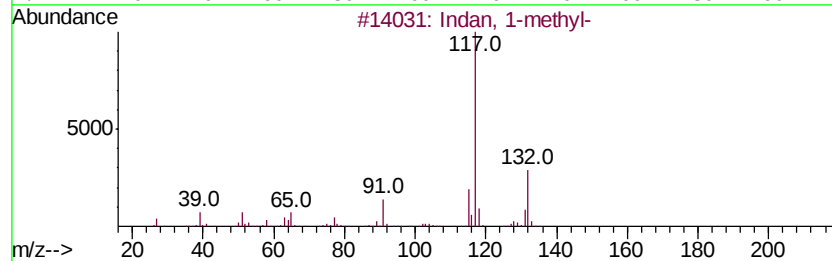
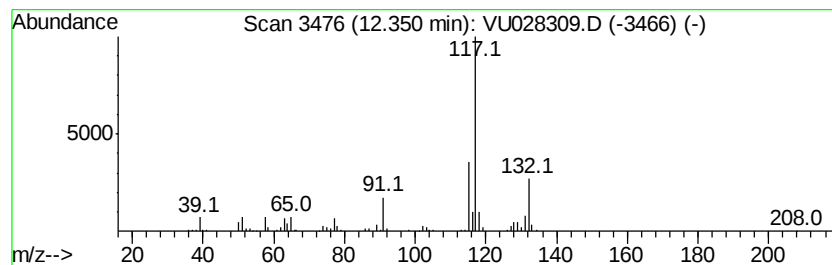
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 12 Indan, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.35	1.35 ug/L	164903	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indan, 1-methyl-	132	C10H12	000767-58-8	87
2		Benzene, 2-butenyl-	132	C10H12	001560-06-1	86
3		1-Phenyl-1-butene	132	C10H12	000824-90-8	86
4		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86
5		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	83



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU112118\
Data File : VU028309.D
Acq On : 21 Nov 2018 11:05
Operator : MD/SY
Sample : J5997-13DL 4X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E3YA9DL

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Cyc...	5.25	1.2	ug/L	100833	1	5.88	428323	5.0
(DEL) Alkane: Cyc...	5.47	0.6	ug/L	50125	1	5.88	428323	5.0
4-Heptanol, 4-met...	8.65	2.4	ug/L	257354	2	9.09	526538	5.0
n-Butyl ether	9.30	19.0	ug/L	1998310	2	9.09	526538	5.0
2,4,4,6-Tetrameth...	9.36	2.9	ug/L	309832	2	9.09	526538	5.0
Benzene, propyl-	10.58	0.7	ug/L	81485	3	11.48	610368	5.0
Benzene, 1,2,3-tr...	11.15	0.8	ug/L	96962	3	11.48	610368	5.0
Benzene, (1-methy...	11.32	0.7	ug/L	85527	3	11.48	610368	5.0
Indane	11.76	3.5	ug/L	424917	3	11.48	610368	5.0
Indan, 1-methyl-	12.35	1.4	ug/L	164903	3	11.48	610368	5.0