

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100820\
 Data File : VU040566.D
 Acq On : 08 Oct 2020 17:10
 Operator : SY/MD
 Sample : L4240-08DL 20X
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BG3S5DL

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\SOMUTR100820WMA.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	2.581	374	386	408	rBV	137977	242775	1.32%	0.503%
2	3.099	518	547	570	rBV	2525582	5781979	31.37%	11.969%
3	3.382	613	635	664	rBV	4109804	9067522	49.19%	18.770%
4	3.723	720	741	767	rBV	8323819	18432395	100.00%	38.156%
5	4.317	909	926	947	rBV2	102152	289012	1.57%	0.598%
6	4.552	981	999	1019	rVV	3306396	7904624	42.88%	16.363%
7	4.661	1019	1033	1081	rVB	97464	363826	1.97%	0.753%
8	5.083	1149	1164	1179	rBV	112136	242667	1.32%	0.502%
9	5.407	1248	1265	1281	rVB	191090	422393	2.29%	0.874%
10	5.742	1348	1369	1392	rBV2	224727	588642	3.19%	1.219%
11	6.263	1514	1531	1549	rBV	187997	357009	1.94%	0.739%
12	6.703	1653	1668	1683	rBV2	143273	279148	1.51%	0.578%
13	7.906	2025	2042	2055	rBV	264056	449241	2.44%	0.930%
14	8.642	2257	2271	2304	rBV	412002	775460	4.21%	1.605%
15	9.420	2498	2513	2533	rBV	270714	451570	2.45%	0.935%
16	10.902	2961	2974	2989	rVB	121217	187665	1.02%	0.388%
17	10.996	2989	3003	3009	rBV	297387	522920	2.84%	1.082%
18	11.086	3021	3031	3048	rVB	221500	344980	1.87%	0.714%
19	11.465	3135	3149	3162	rBV	337640	520148	2.82%	1.077%
20	11.806	3242	3255	3271	rVB	297775	486898	2.64%	1.008%
21	12.185	3361	3373	3390	rVB2	351332	597182	3.24%	1.236%

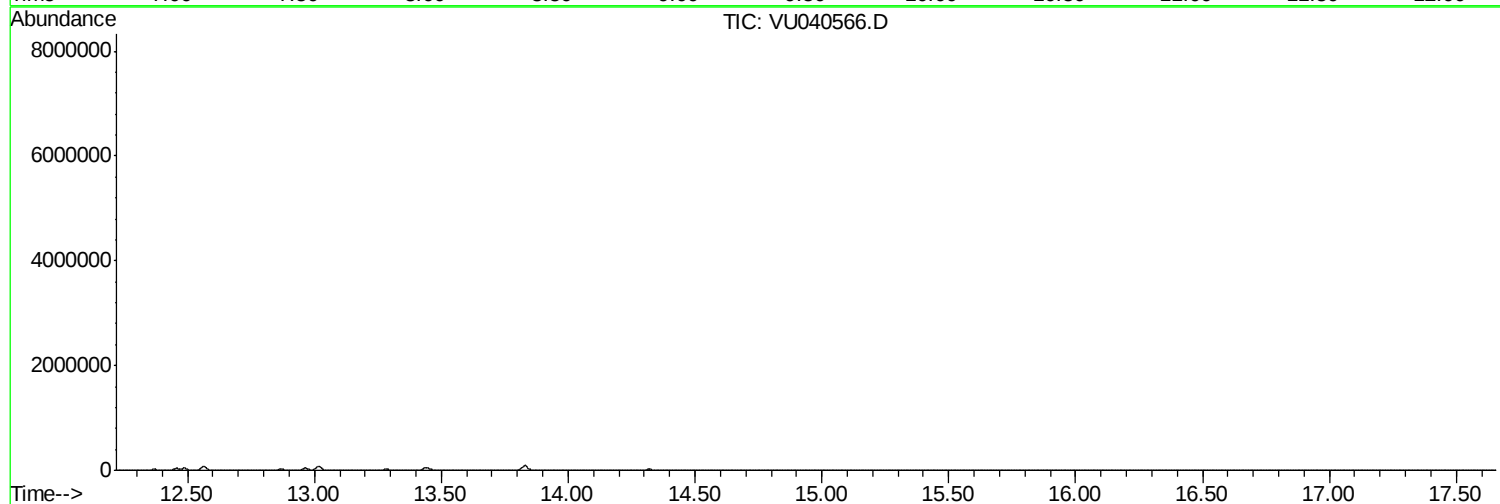
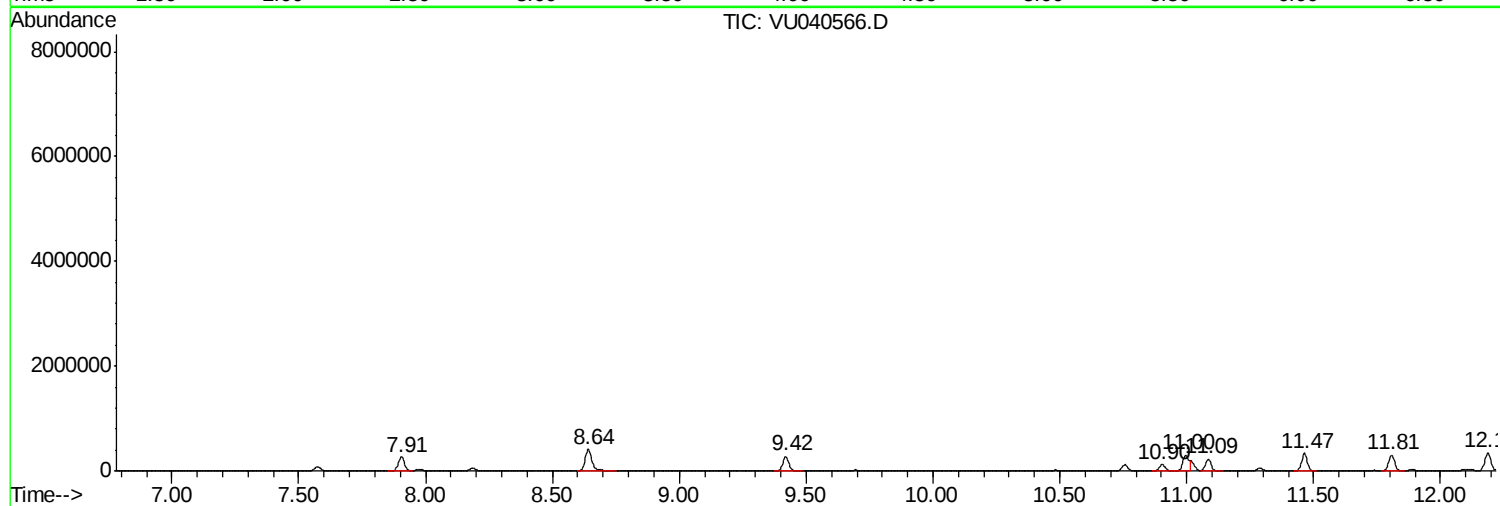
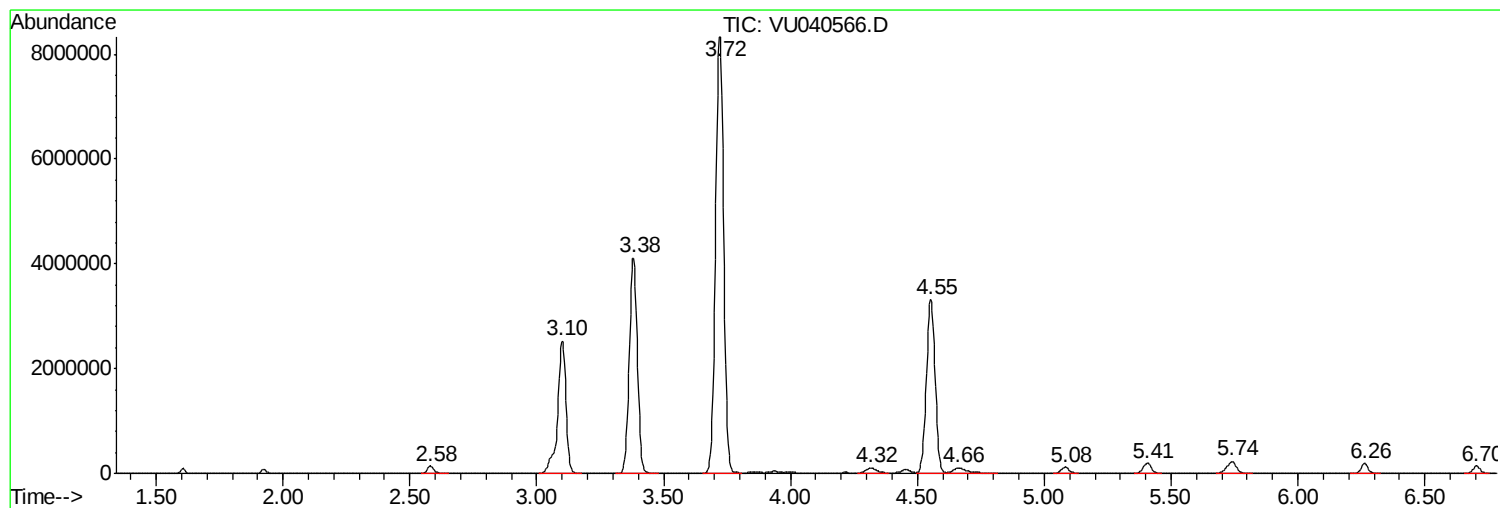
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR100820WMA.M
Quant Title : TRACE VOA SOM01.0

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



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ClientSampleId :
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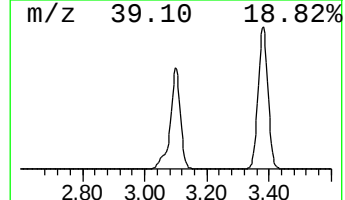
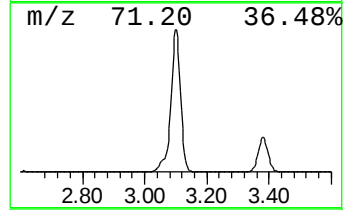
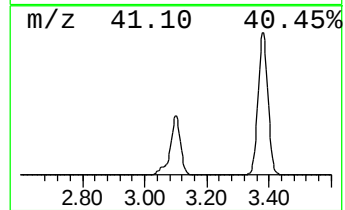
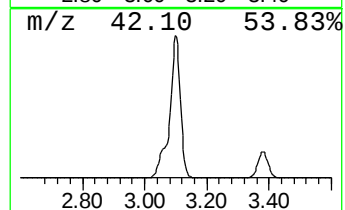
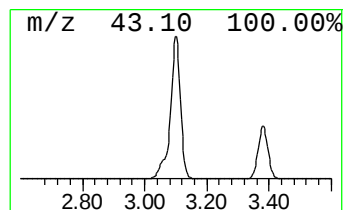
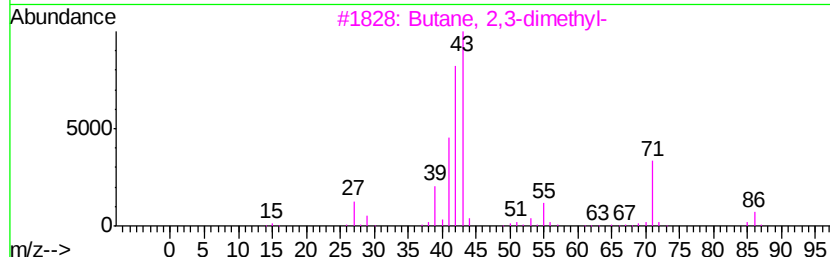
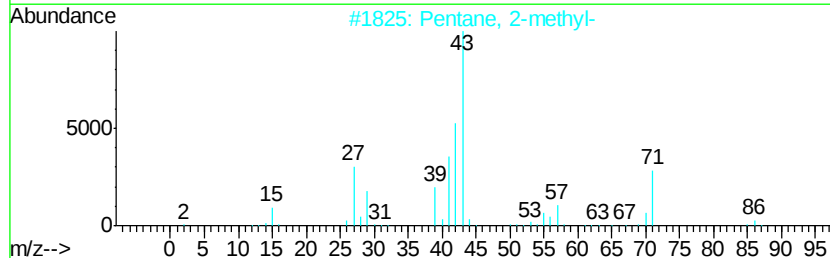
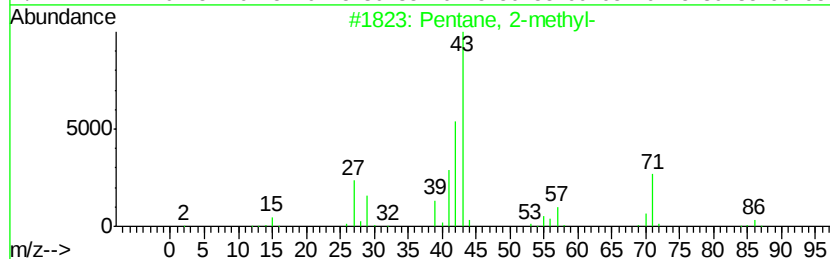
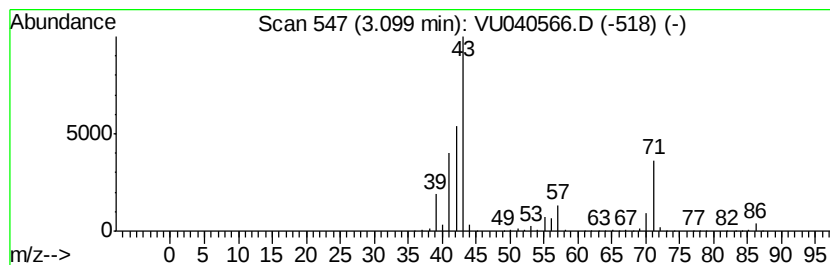
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.10	80.98 ug/L	5781980	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	91
3		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	49
4		Pentane	72	C5H12	000109-66-0	37
5		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	33



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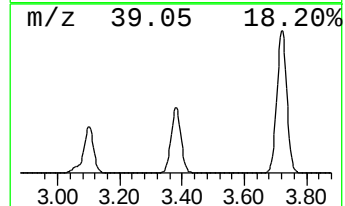
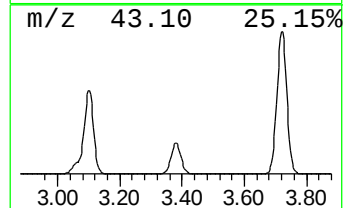
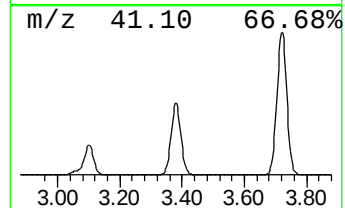
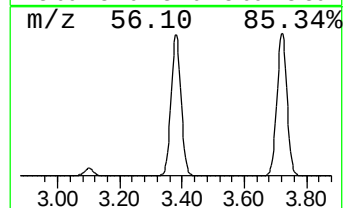
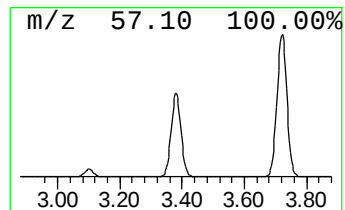
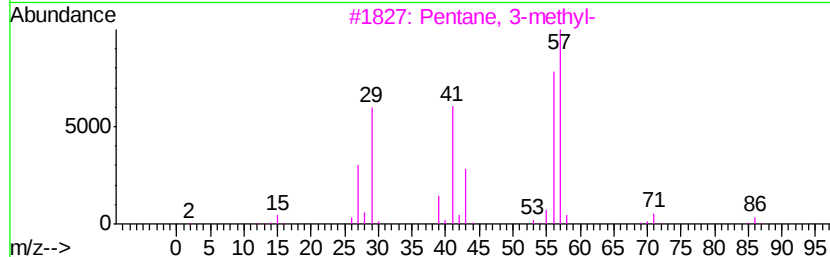
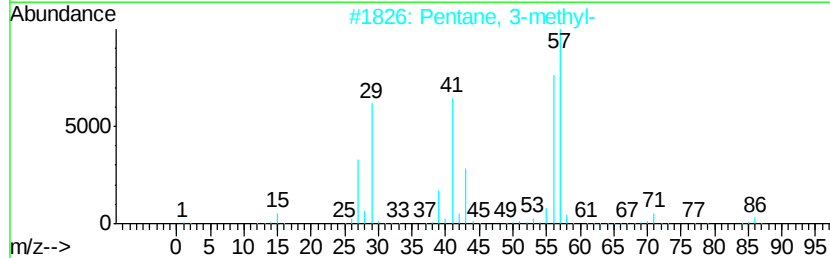
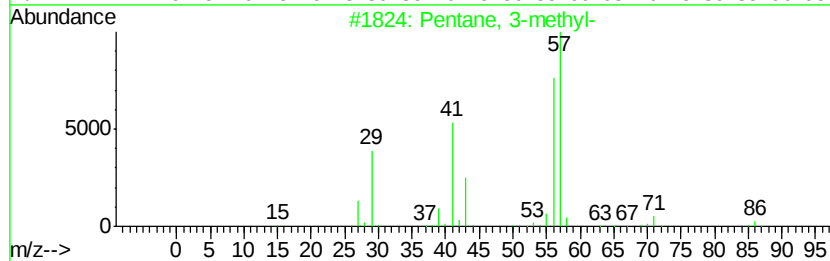
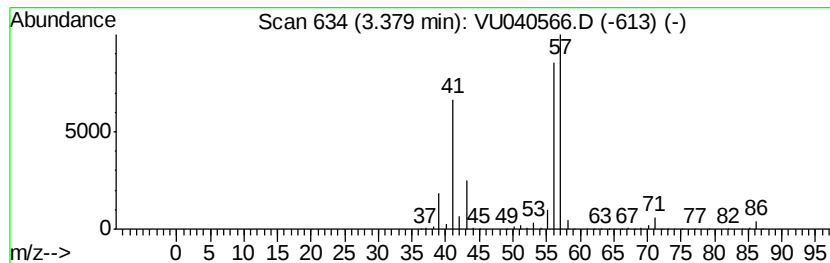
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.38	126.99 ug/L	9067520	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2		Pentane, 3-methyl-	86	C6H14	000096-14-0	91
3		Pentane, 3-methyl-	86	C6H14	000096-14-0	91
4		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
5		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64



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Instrument :
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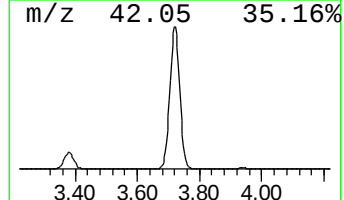
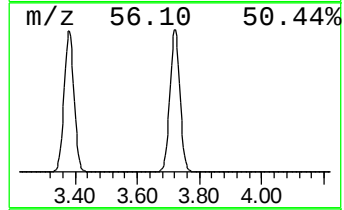
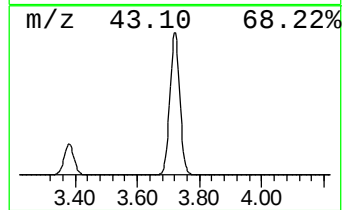
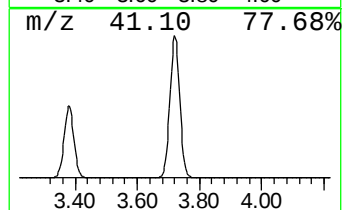
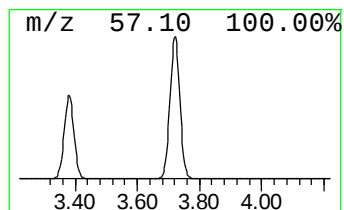
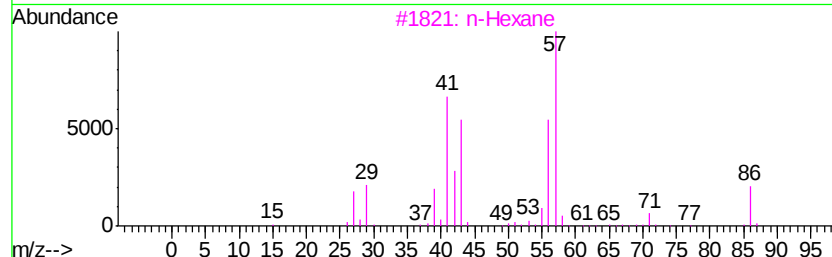
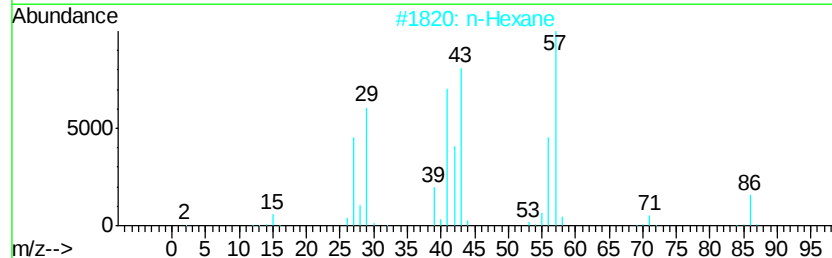
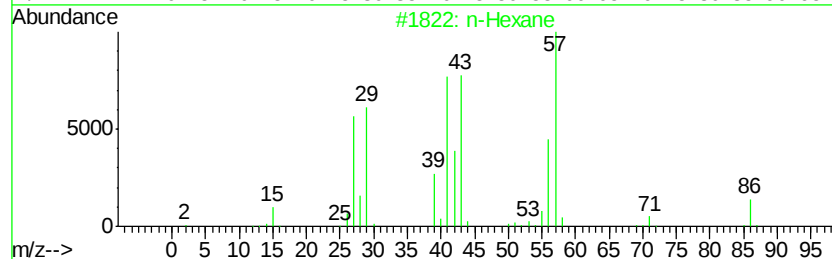
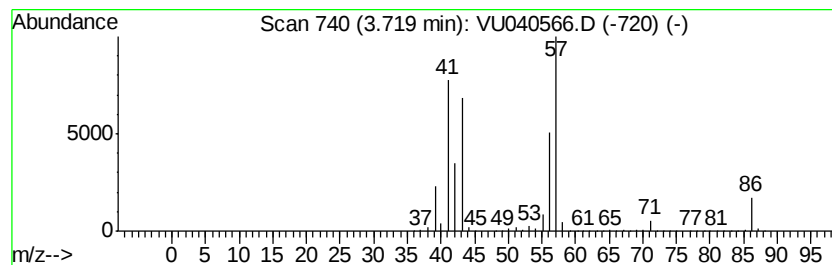
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.72	258.15 ug/L	18432400	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	91
2		n-Hexane	86	C6H14	000110-54-3	91
3		n-Hexane	86	C6H14	000110-54-3	91
4		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	40
5		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	38



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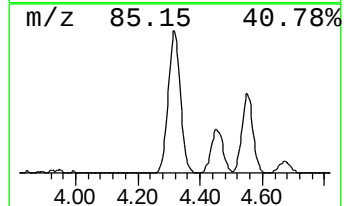
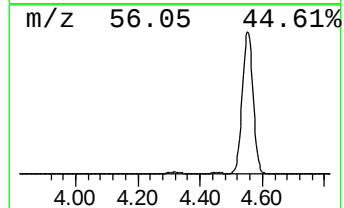
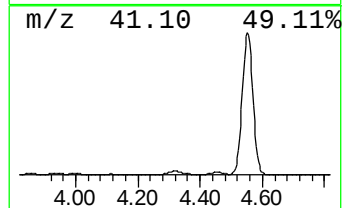
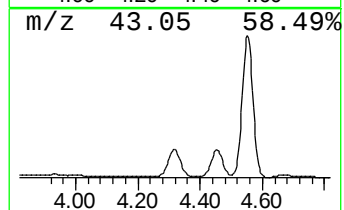
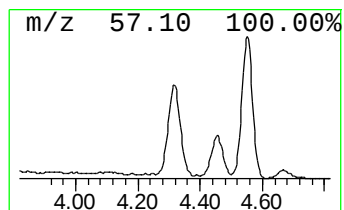
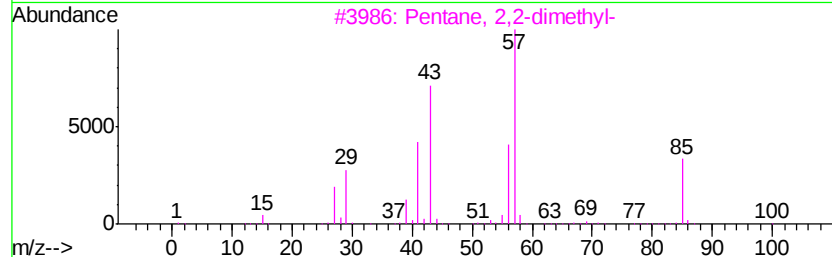
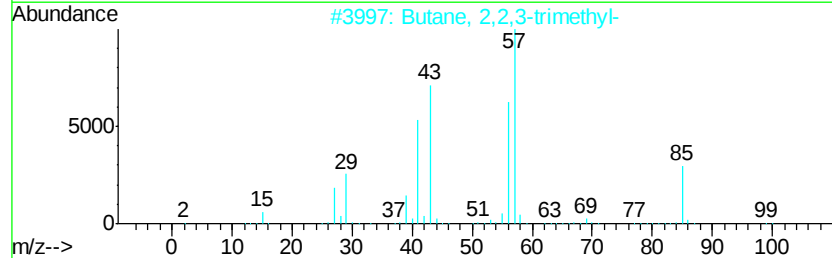
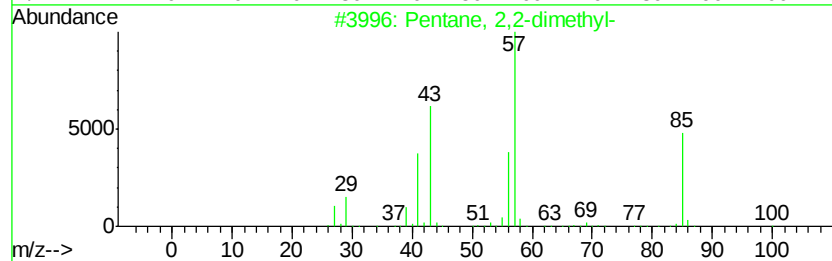
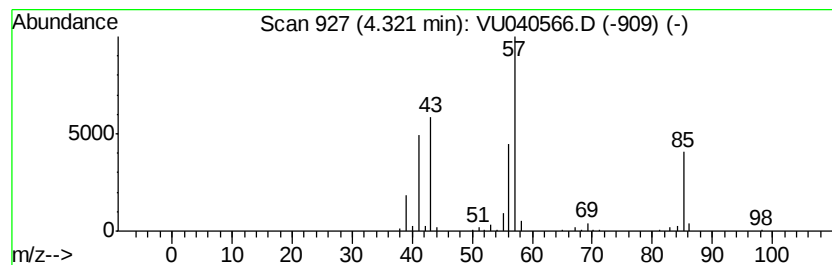
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Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.32	4.05 ug/L	289012	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	83
2		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	83
3		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	78
4		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
5		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	72



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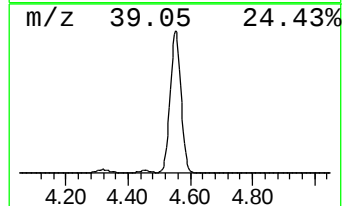
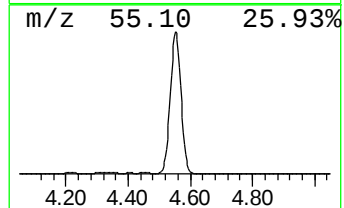
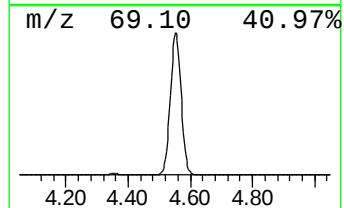
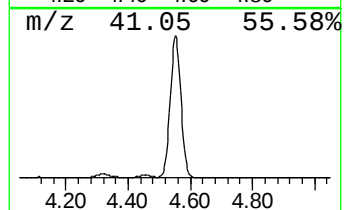
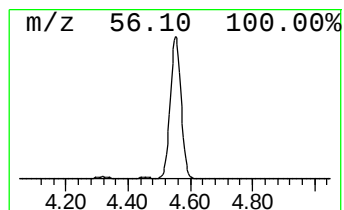
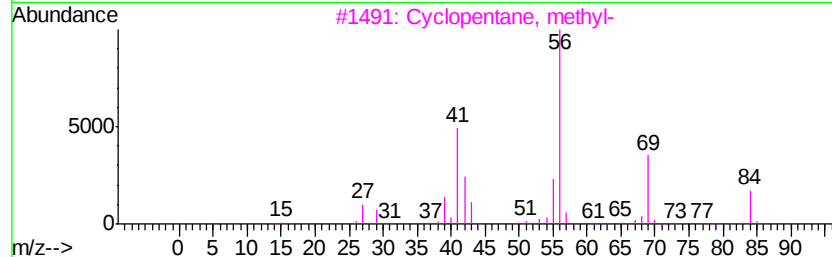
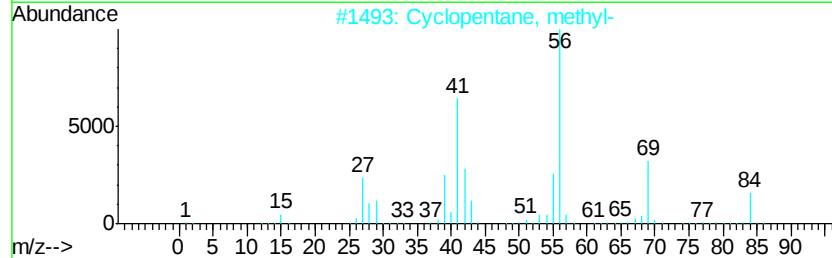
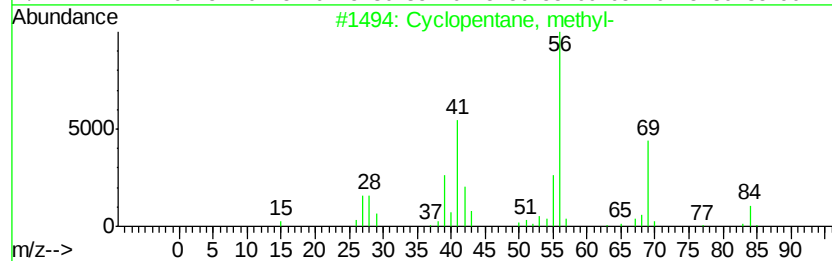
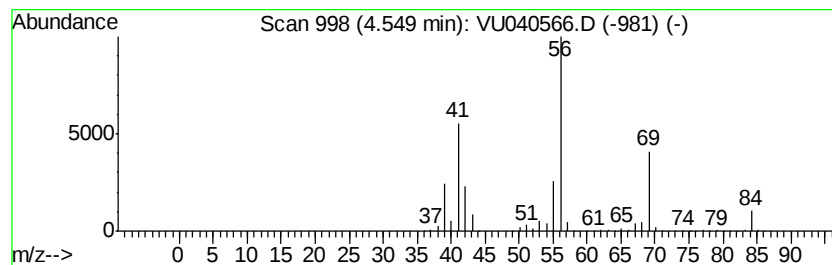
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 (DEL) Alkane: Cyclic4.55 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	110.71 ug/L	7904620	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	78
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72



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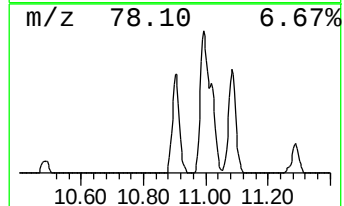
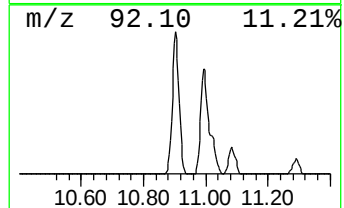
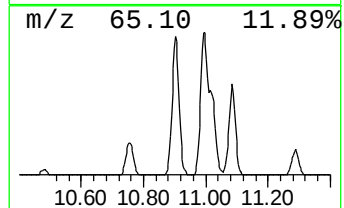
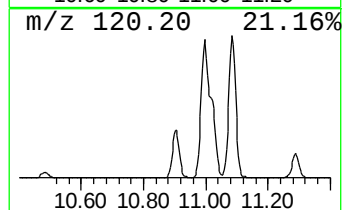
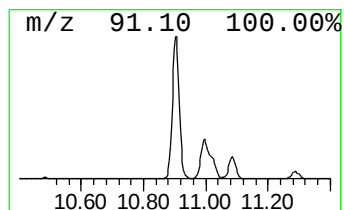
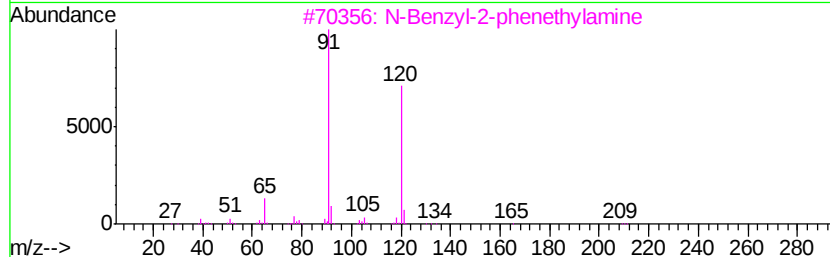
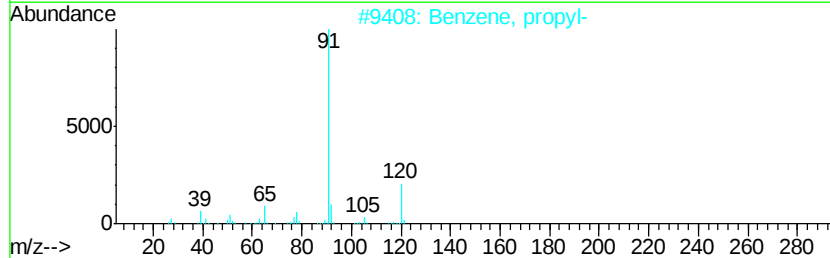
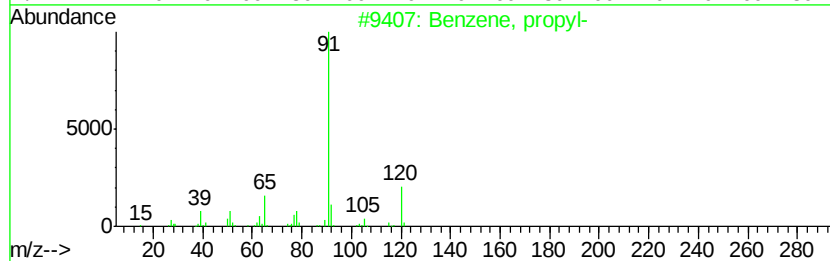
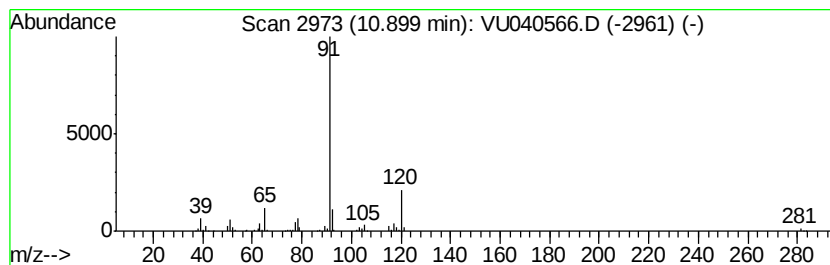
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MSVOA_U
ClientSampleId :
BG3S5DL

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR100820WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Benzene, propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.90	1.93 ug/L	187665	1,4-Dichlorobenzene-d4	11.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, propyl-	120	C9H12	000103-65-1	81
2	Benzene, propyl-	120	C9H12	000103-65-1	81
3	N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	78
4	Phenethylamine, N-benzyl-p-chloro-	245	C15H16ClN	013622-43-0	72
5	Ethanol, 2-[(phenylmethyl)amino]-	151	C9H13NO	000104-63-2	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU100820\
Data File : VU040566.D
Acq On : 08 Oct 2020 17:10
Operator : SY/MD
Sample : L4240-08DL 20X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG3S5DL

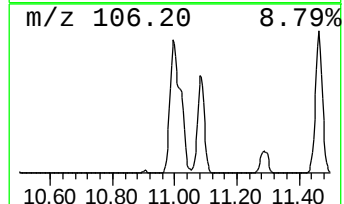
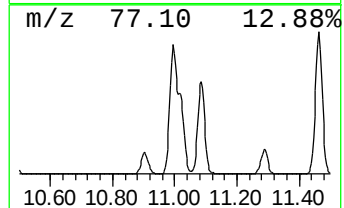
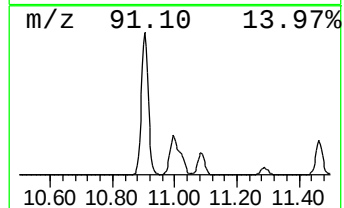
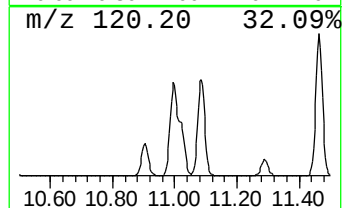
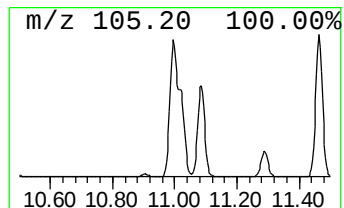
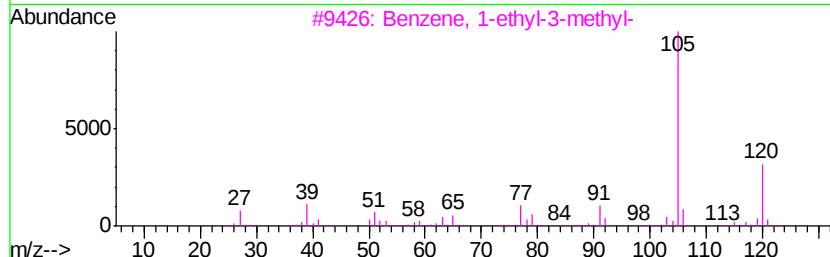
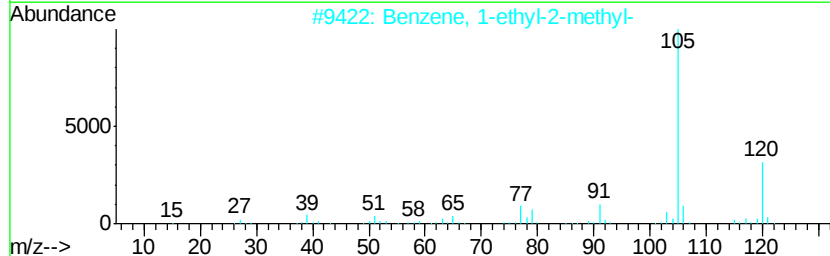
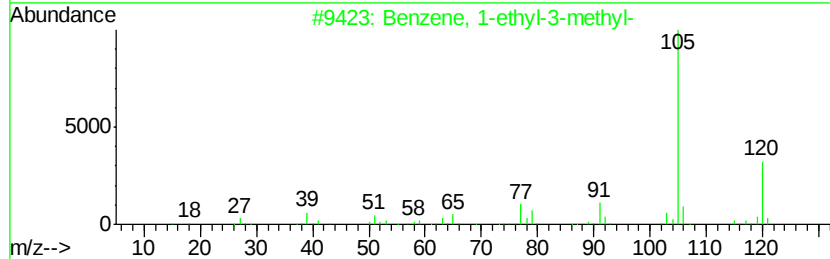
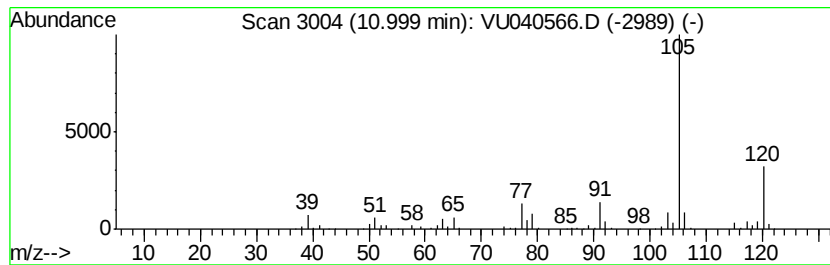
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	5.37 ug/L	522920	1,4-Dichlorobenzene-d4	11.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU100820\
Data File : VU040566.D
Acq On : 08 Oct 2020 17:10
Operator : SY/MD
Sample : L4240-08DL 20X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG3S5DL

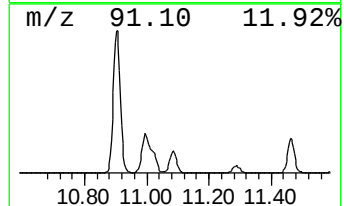
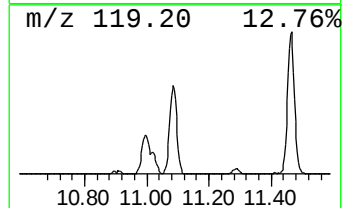
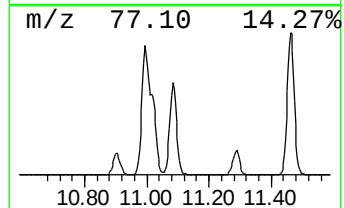
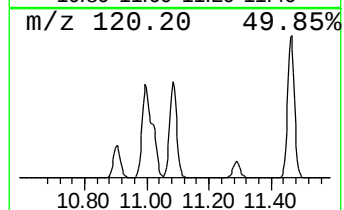
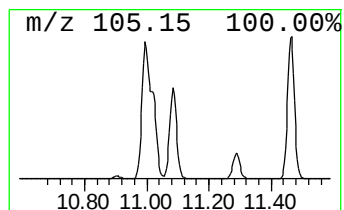
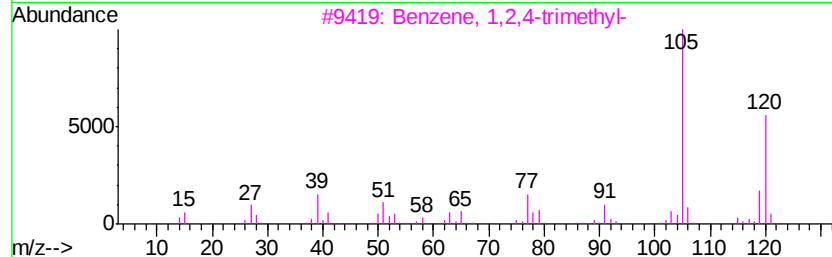
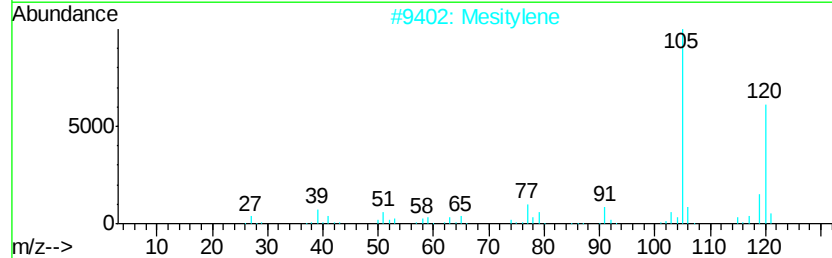
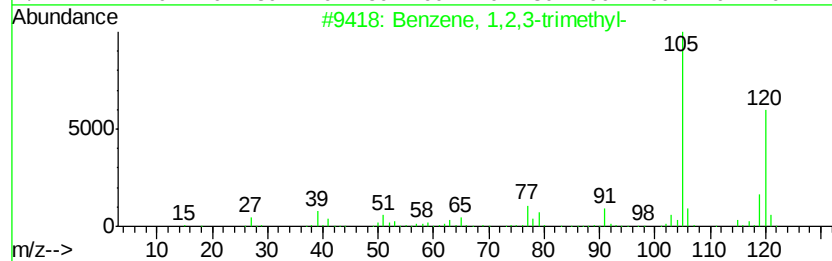
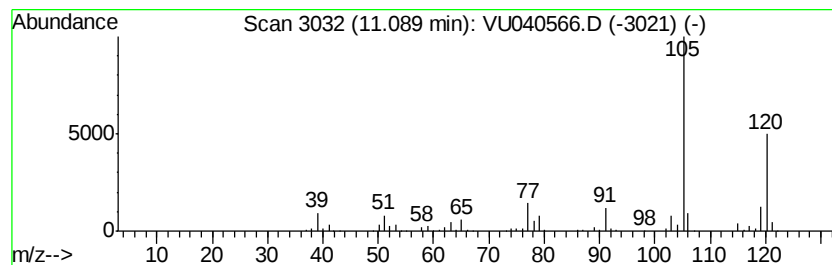
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.09	3.54 ug/L	344980	1,4-Dichlorobenzene-d4	11.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2		Mesitylene	120	C9H12	000108-67-8	95
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
4		Mesitylene	120	C9H12	000108-67-8	95
5		Mesitylene	120	C9H12	000108-67-8	94



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU100820\
Data File : VU040566.D
Acq On : 08 Oct 2020 17:10
Operator : SY/MD
Sample : L4240-08DL 20X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

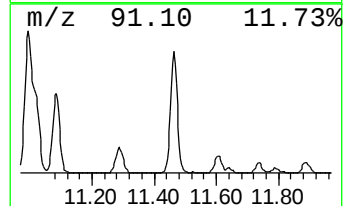
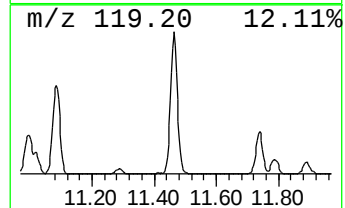
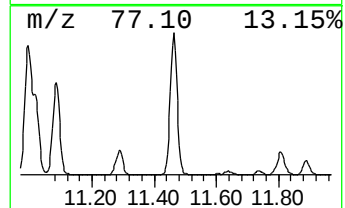
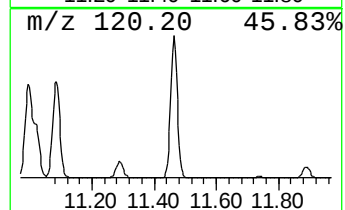
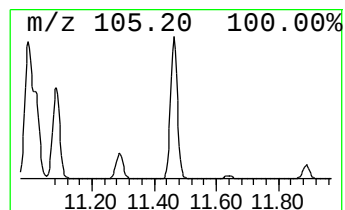
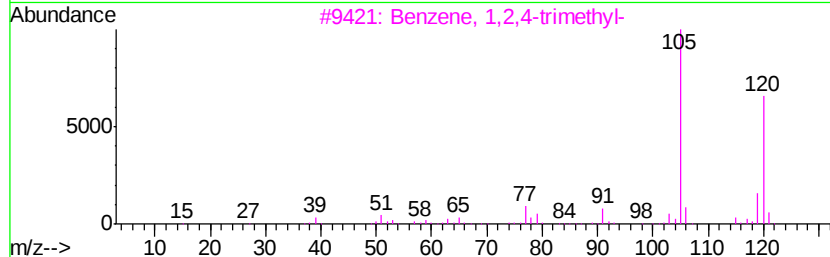
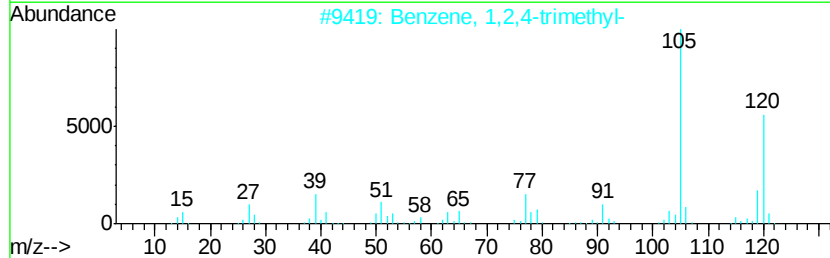
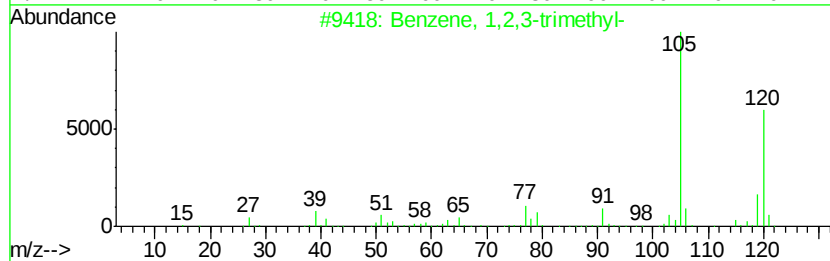
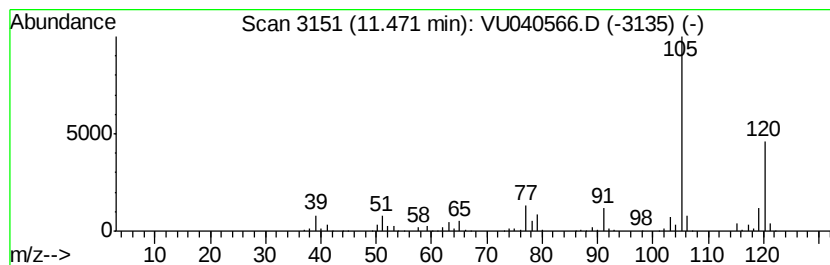
Instrument :
MSVOA_U
ClientSampleId :
BG3S5DL

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR100820WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 Benzene, 1,2,4-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.47	5.34 ug/L	520148	1,4-Dichlorobenzene-d4	11.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
4	Mesitylene	120	C9H12	000108-67-8	94
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU100820\
Data File : VU040566.D
Acq On : 08 Oct 2020 17:10
Operator : SY/MD
Sample : L4240-08DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG3S5DL

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR100820WMA.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...	3.10	81.0	ug/L	5781980	1	6.26	357009	5.0
(DEL) Alkane: Str...	3.38	127.0	ug/L	9067520	1	6.26	357009	5.0
(DEL) Alkane: Str...	3.72	258.1	ug/L	18432400	1	6.26	357009	5.0
(DEL) Alkane: Str...	4.32	4.0	ug/L	289012	1	6.26	357009	5.0
(DEL) Alkane: Cyc...	4.55	110.7	ug/L	7904620	1	6.26	357009	5.0
Benzene, propyl-	10.90	1.9	ug/L	187665	3	11.81	486898	5.0
Benzene, 1-ethyl-...	11.00	5.4	ug/L	522920	3	11.81	486898	5.0
Benzene, 1,2,3-tr...	11.09	3.5	ug/L	344980	3	11.81	486898	5.0
Benzene, 1,2,4-tr...	11.47	5.3	ug/L	520148	3	11.81	486898	5.0