

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100620\
 Data File : VX018792.D
 Acq On : 06 Oct 2020 12:08
 Operator : JC/SP
 Sample : L4240-02
 Misc : 25.0mL/MSVOA X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BG3Q9

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_X\METHOD\SOMXTR100220WMA.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	2.831	276	286	287	rBV	2890559	5315752	3.75%	1.235%
2	2.873	287	293	324	rVB	20838977	45056448	31.82%	10.472%
3	3.160	327	340	367	rBV	30429296	72817266	51.43%	16.924%
4	3.538	386	402	414	rBV3	52512160	141583870	100.00%	32.906%
5	4.123	487	498	513	rVV	1369124	4475770	3.16%	1.040%
6	4.288	513	525	530	rVV	877720	2780260	1.96%	0.646%
7	4.397	530	543	555	rVV	27524332	84769999	59.87%	19.702%
8	5.550	721	732	747	rVB	2738055	8399421	5.93%	1.952%
9	8.763	1253	1259	1266	rBV	5181725	8057266	5.69%	1.873%
10	10.342	1511	1518	1524	rBV	2799326	3734441	2.64%	0.868%
11	11.341	1677	1682	1689	rBV	1844210	2249341	1.59%	0.523%
12	11.421	1689	1695	1702	rVV	6321698	10725680	7.58%	2.493%
13	11.494	1702	1707	1714	rVB	3105835	3918287	2.77%	0.911%
14	11.610	1721	1726	1729	rBV	1477809	1755616	1.24%	0.408%
15	11.652	1729	1733	1742	rVB	2329708	2803033	1.98%	0.651%
16	11.792	1751	1756	1761	rBV	9346066	10852896	7.67%	2.522%
17	12.079	1795	1803	1807	rBV2	945750	1456609	1.03%	0.339%
18	12.128	1807	1811	1816	rVB	1976030	2383533	1.68%	0.554%
19	12.359	1844	1849	1858	rVB3	953599	1843068	1.30%	0.428%
20	13.628	2051	2057	2063	rBV	9302378	11763133	8.31%	2.734%
21	13.999	2113	2118	2126	rVB	2762259	3529282	2.49%	0.820%

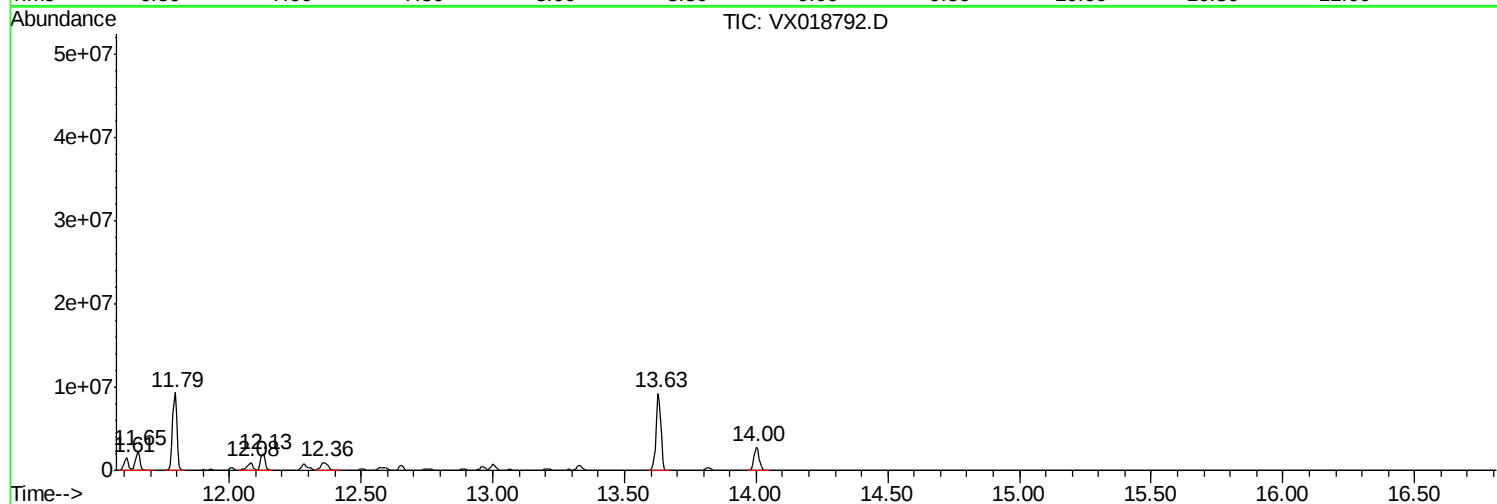
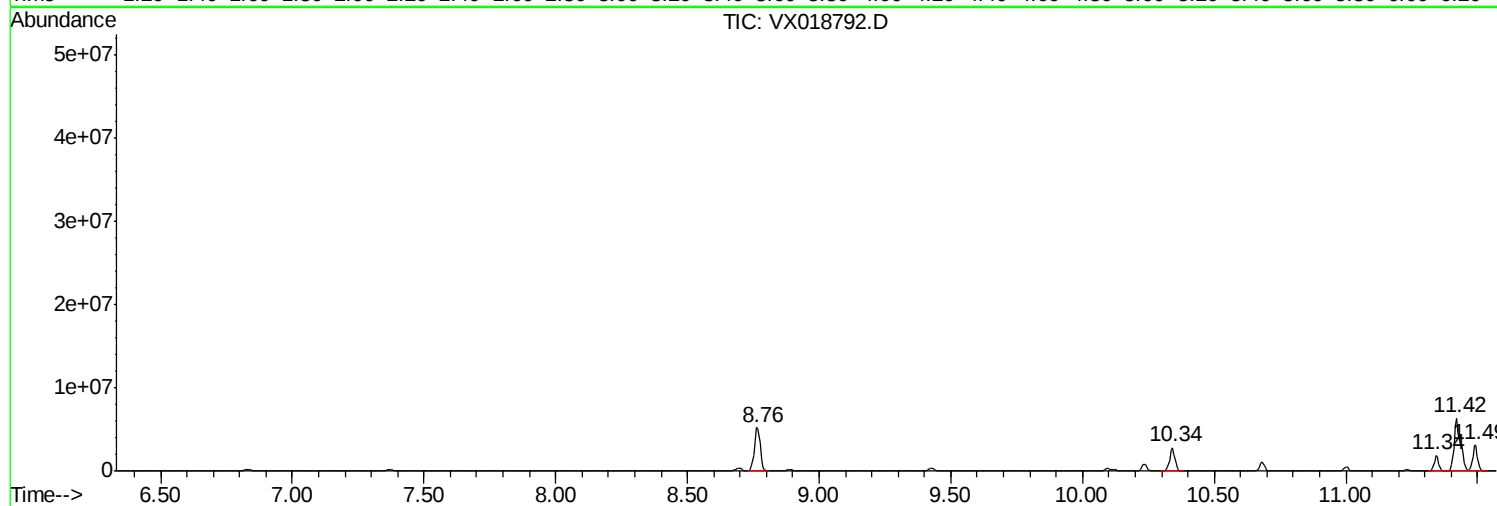
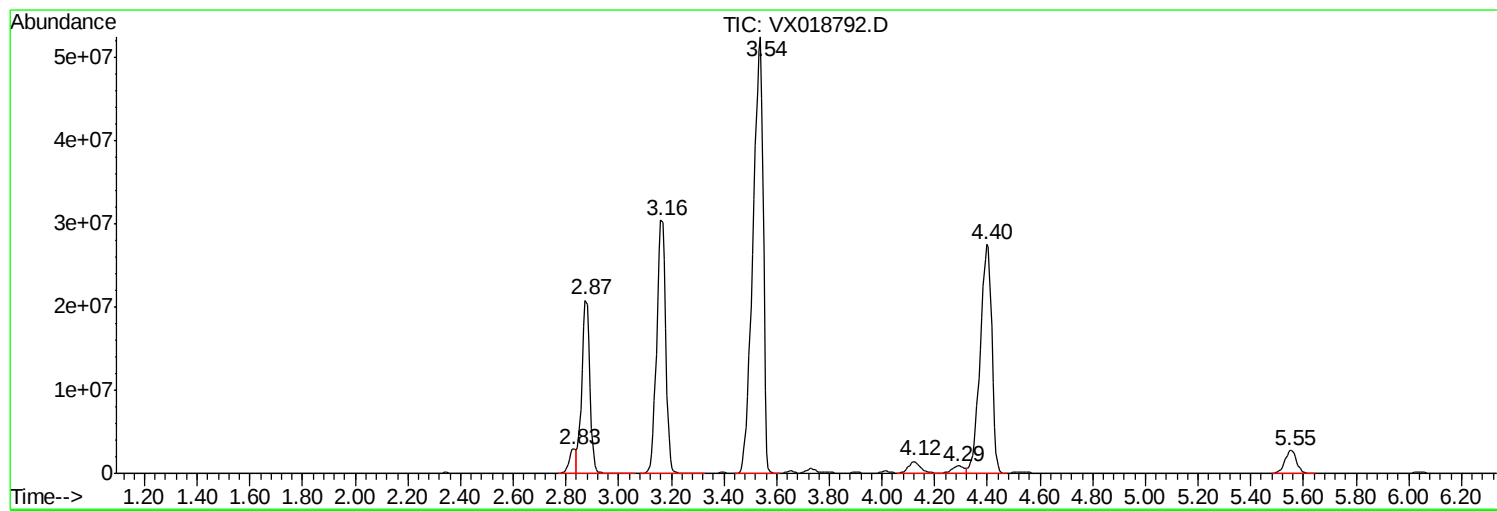
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Quant Title : TRACE VOA SOM01.0

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



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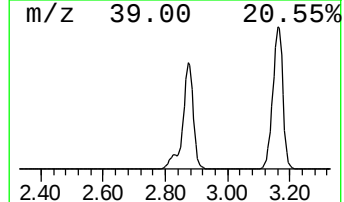
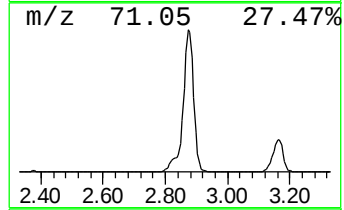
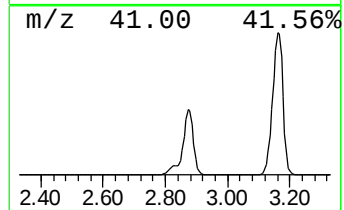
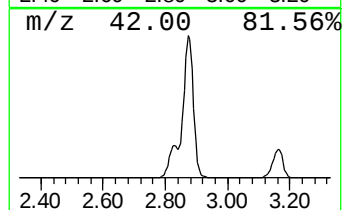
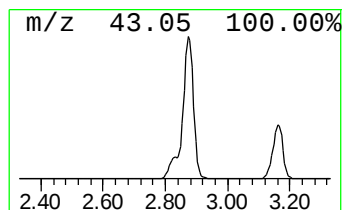
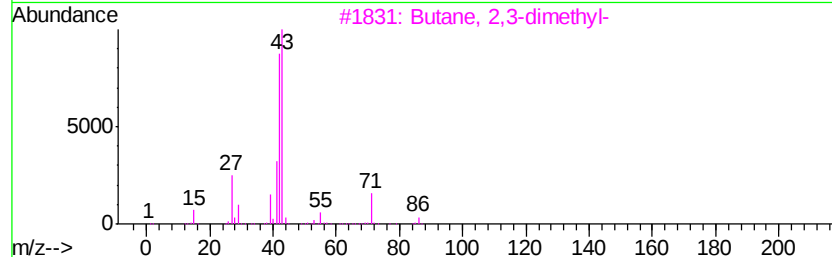
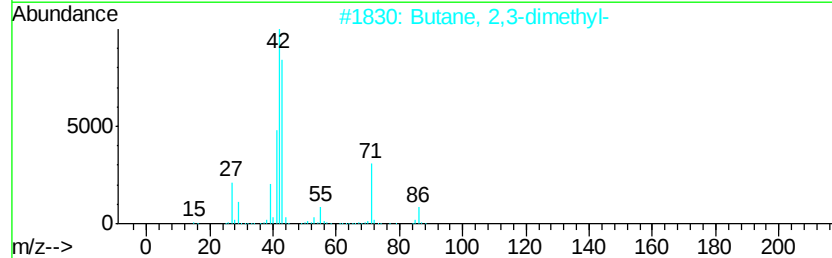
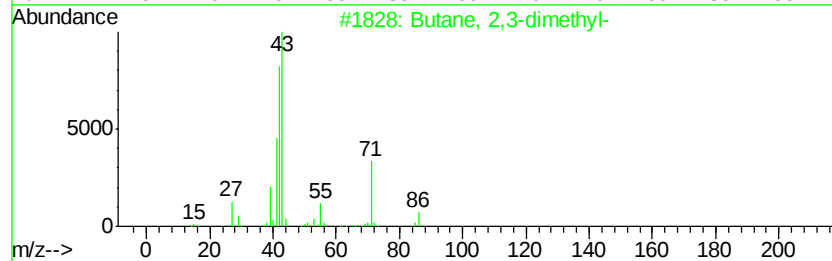
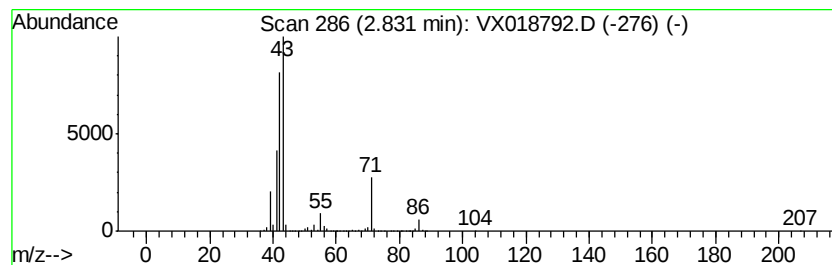
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.83	3.16 ug/L	5315750	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
3		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
4		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64
5		Pentane, 2-methyl-	86	C6H14	000107-83-5	50



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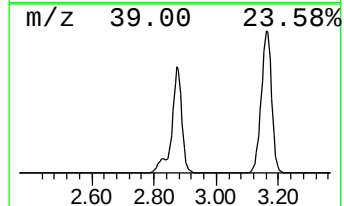
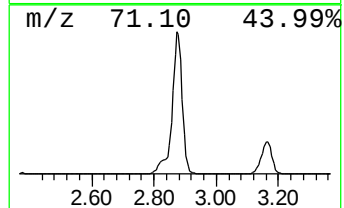
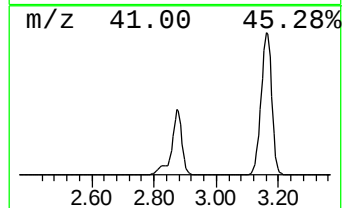
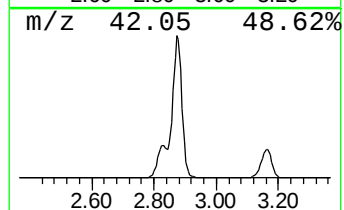
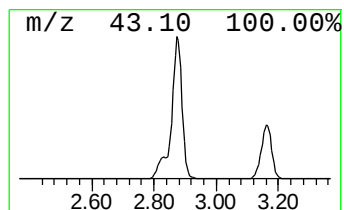
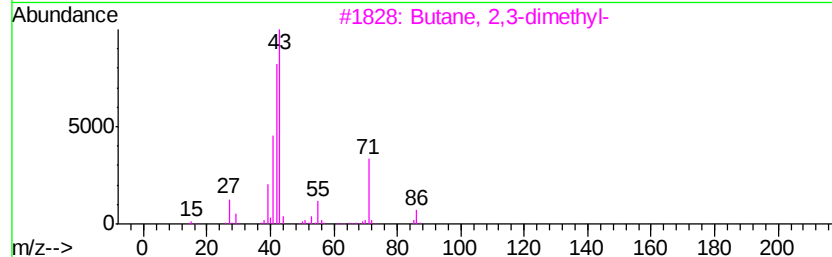
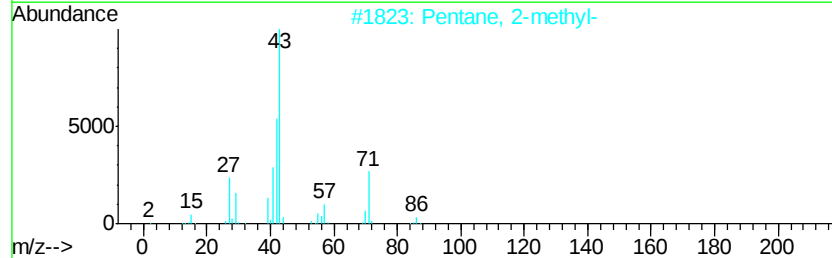
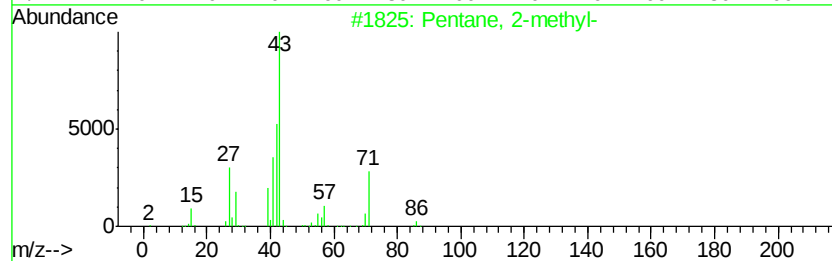
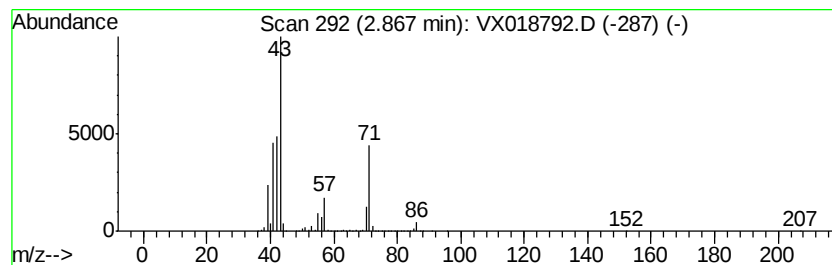
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 Quant Title : TRACE VOA SOM01.0

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

 Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.87	26.82 ug/L	45056400	1,4-Difluorobenzene	6.83

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	90
3		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	52
4		Pentane	72	C5H12	000109-66-0	46
5		1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45



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Instrument :
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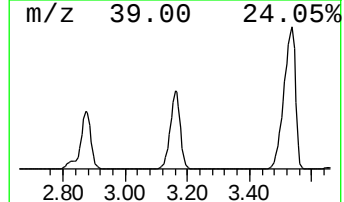
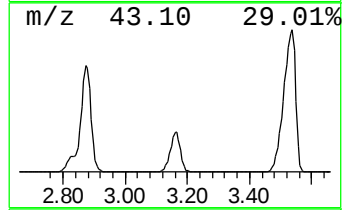
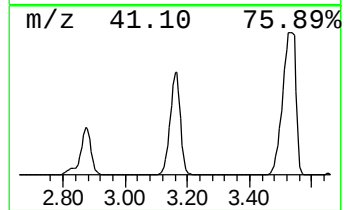
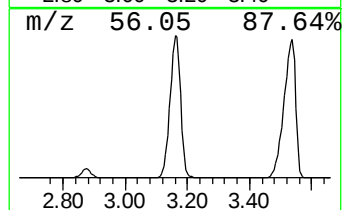
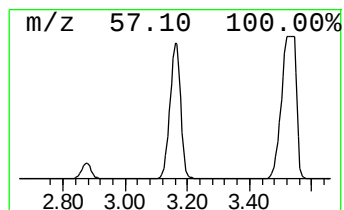
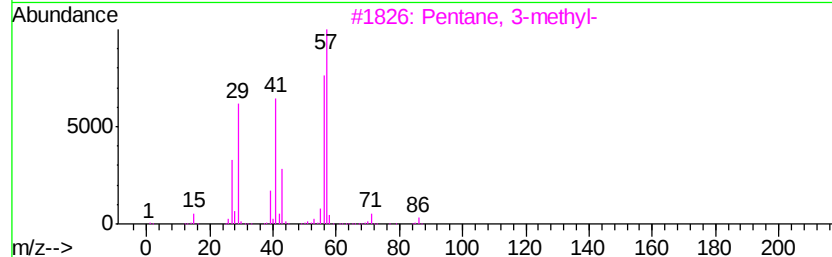
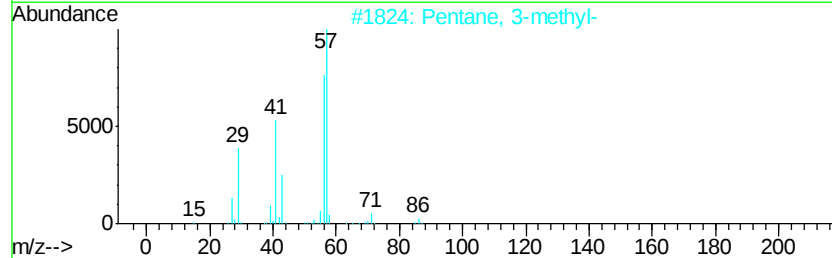
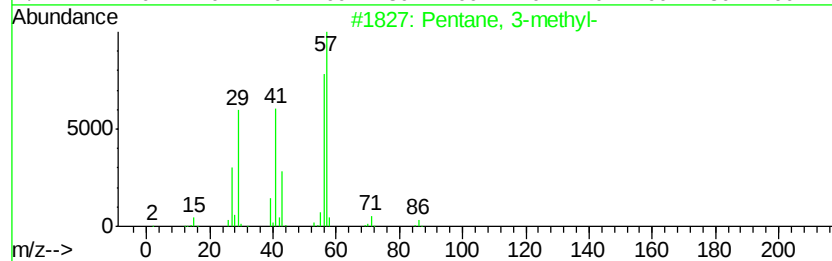
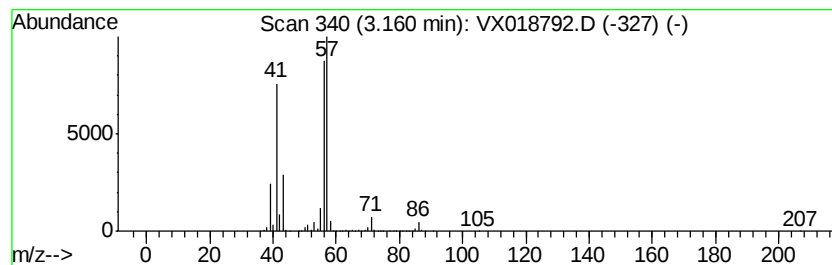
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.16	43.35 ug/L	72817300	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2		Pentane, 3-methyl-	86	C6H14	000096-14-0	90
3		Pentane, 3-methyl-	86	C6H14	000096-14-0	90
4		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
5		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43



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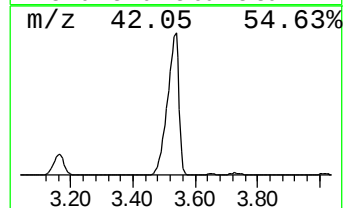
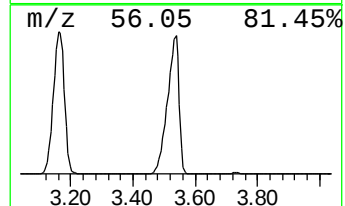
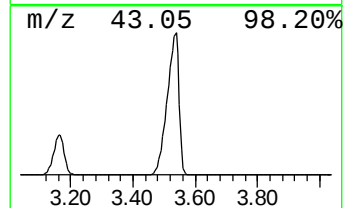
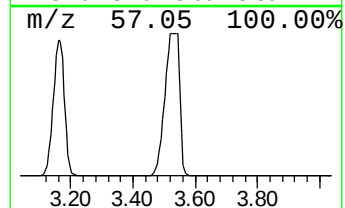
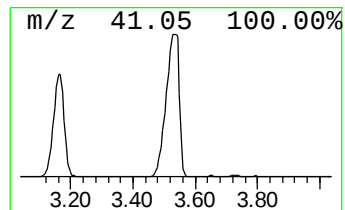
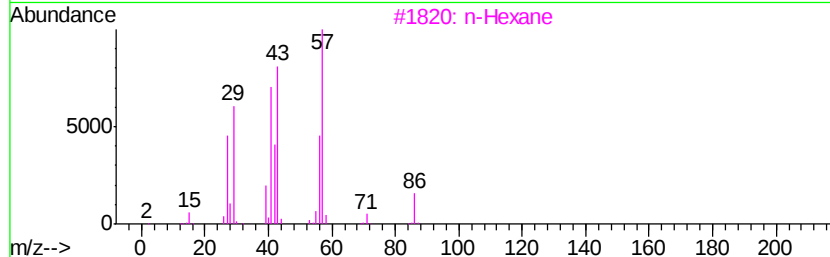
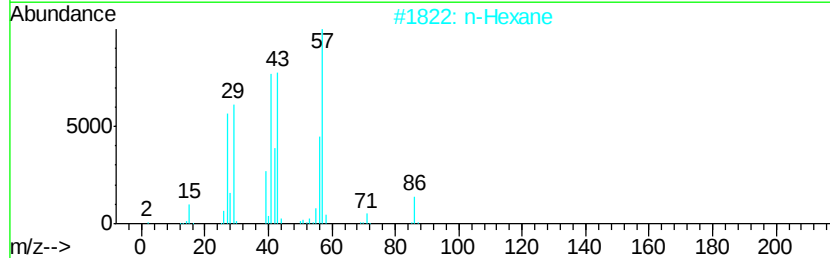
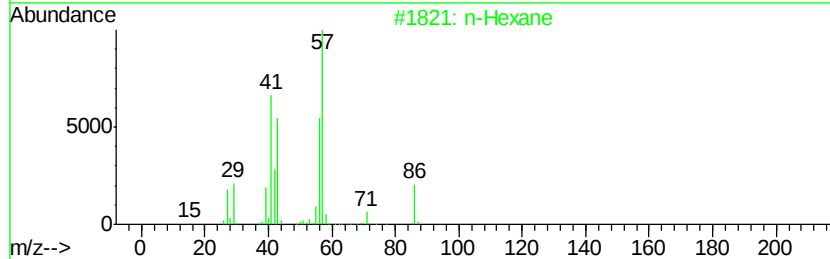
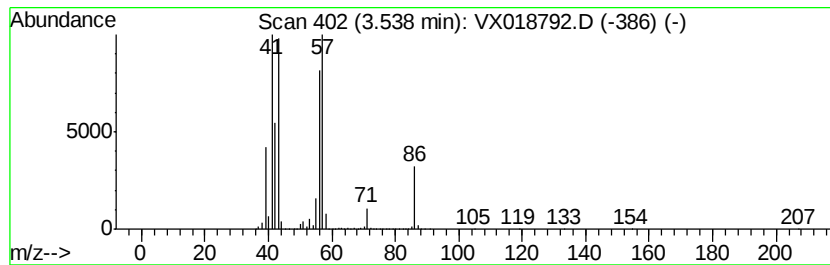
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.54	84.28 ug/L	141584000	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	76
2		n-Hexane	86	C6H14	000110-54-3	47
3		n-Hexane	86	C6H14	000110-54-3	47
4		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	42
5		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	42



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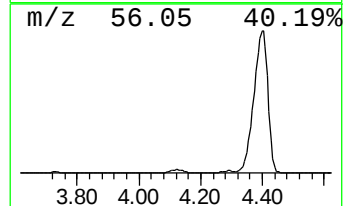
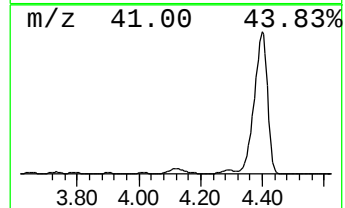
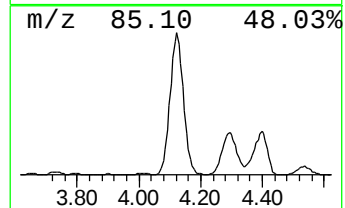
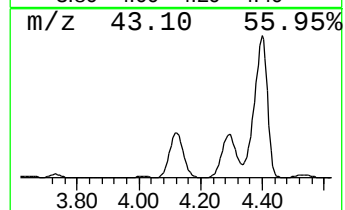
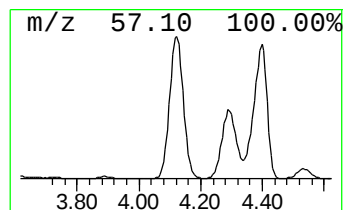
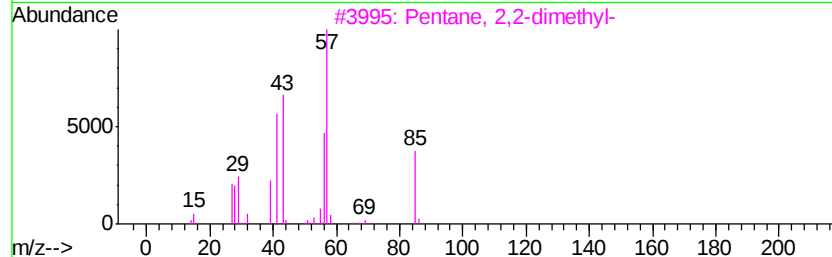
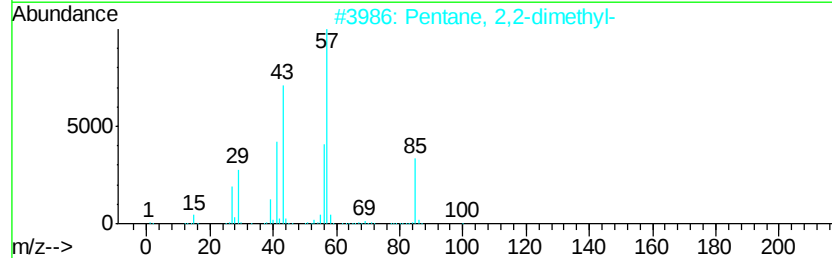
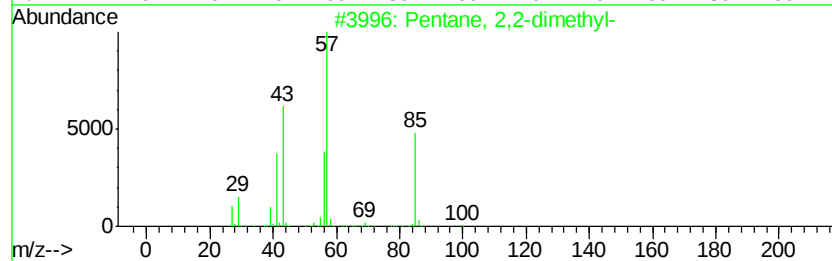
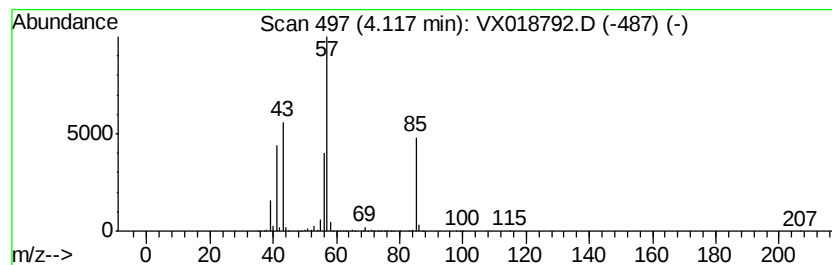
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.12	2.66 ug/L	4475770	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	90
2		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	64
3		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	64
4		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	64
5		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	59



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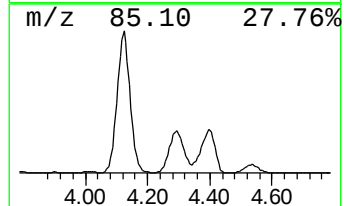
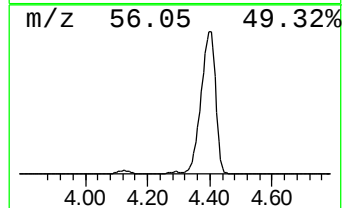
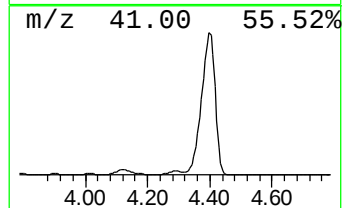
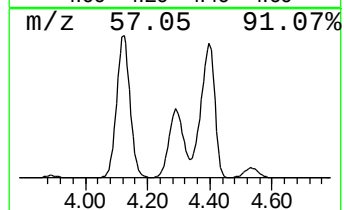
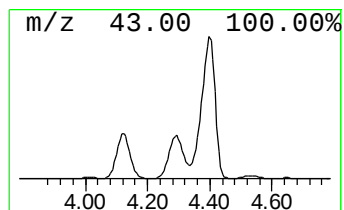
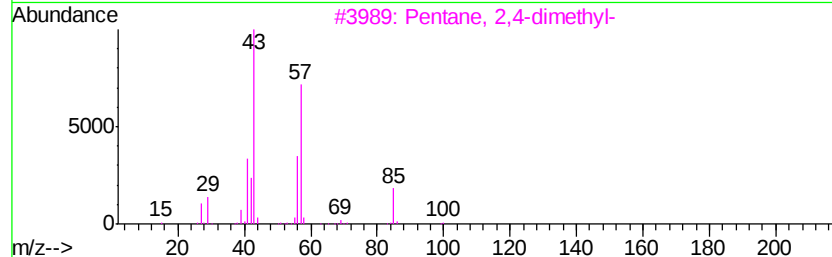
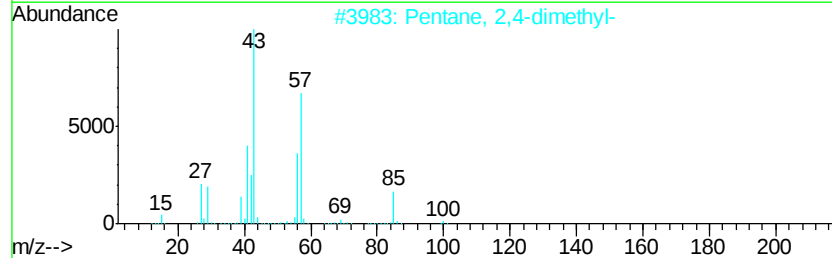
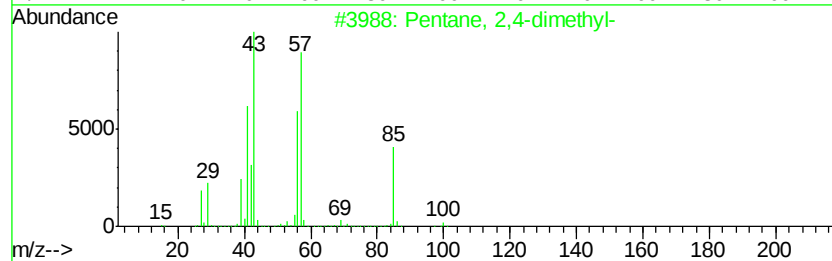
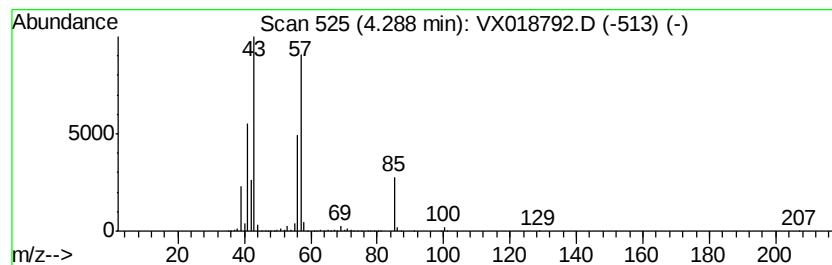
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	1.66 ug/L	2780260	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	90
2		Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	90
3		Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	74
4		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
5		Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX100620\
Data File : VX018792.D
Acq On : 06 Oct 2020 12:08
Operator : JC/SP
Sample : L4240-02
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3Q9

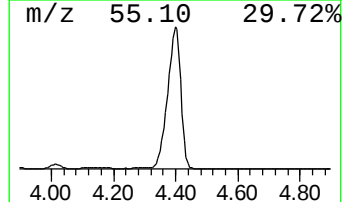
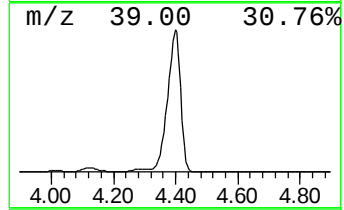
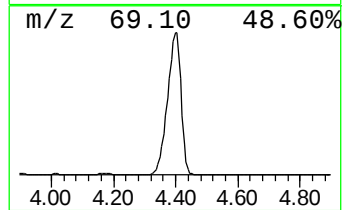
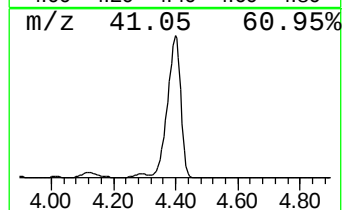
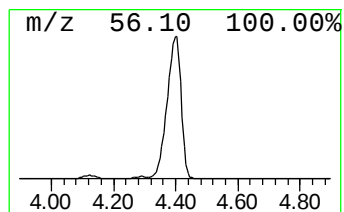
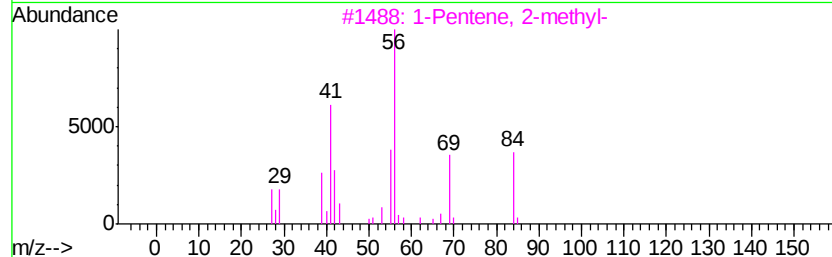
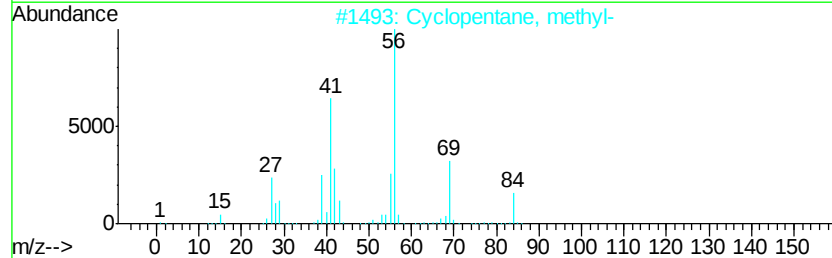
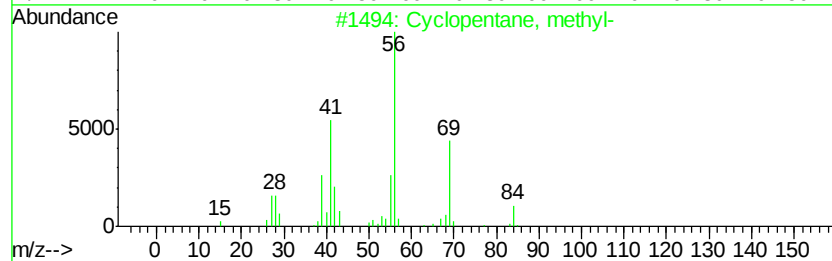
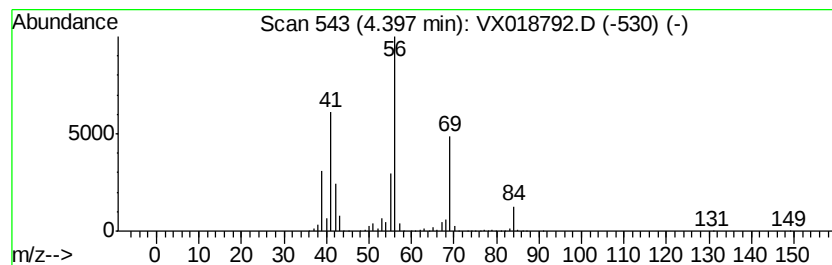
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 (DEL) Alkane: Cyclic4.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	50.46 ug/L	84770000	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	91
3		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	86
4		Cyclohexane	84	C6H12	000110-82-7	78
5		Cyclohexane	84	C6H12	000110-82-7	78



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100620\
Data File : VX018792.D
Acq On : 06 Oct 2020 12:08
Operator : JC/SP
Sample : L4240-02
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3Q9

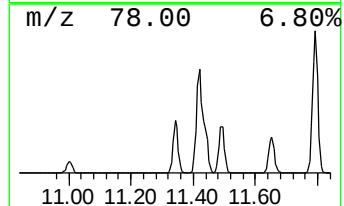
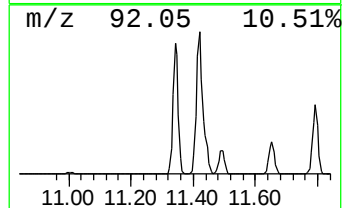
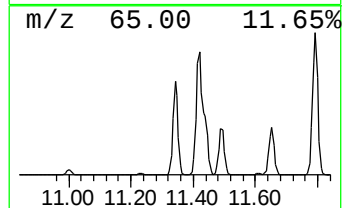
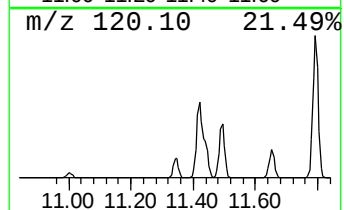
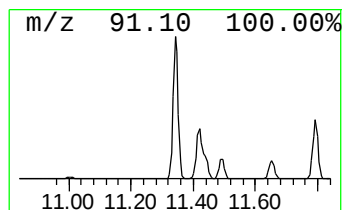
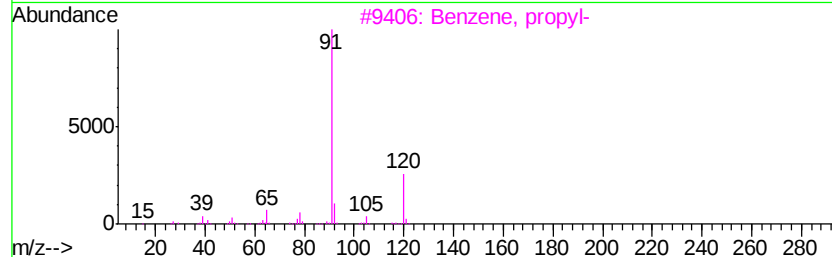
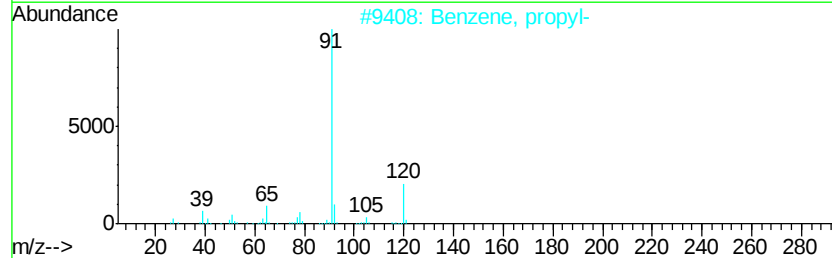
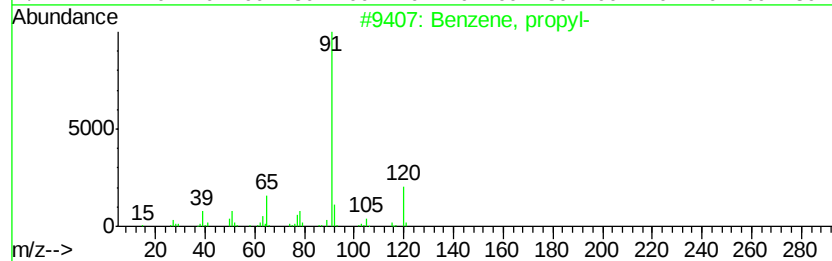
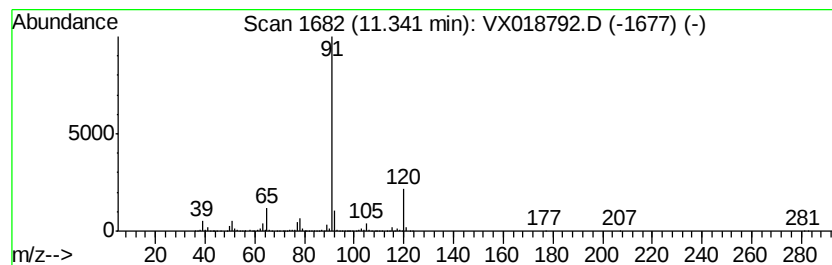
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Benzene, propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.34	7.72 ug/L	2249340	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, propyl-	120	C9H12	000103-65-1	90
2		Benzene, propyl-	120	C9H12	000103-65-1	90
3		Benzene, propyl-	120	C9H12	000103-65-1	86
4		N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	83
5		N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX100620\
Data File : VX018792.D
Acq On : 06 Oct 2020 12:08
Operator : JC/SP
Sample : L4240-02
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3Q9

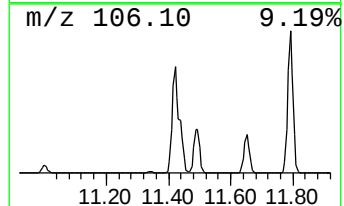
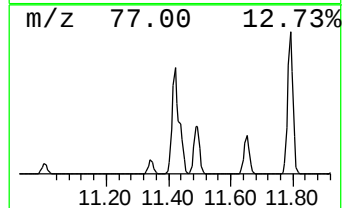
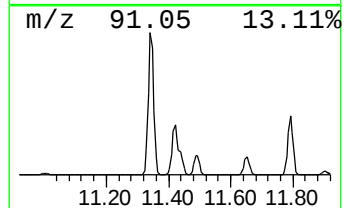
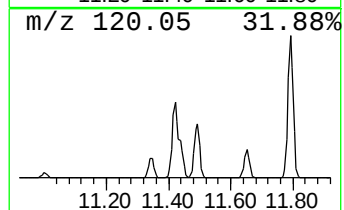
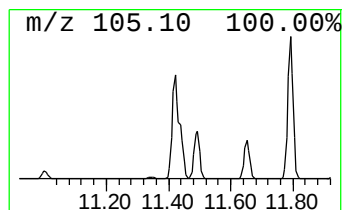
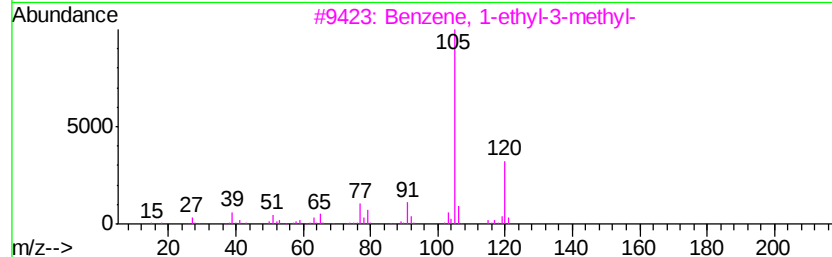
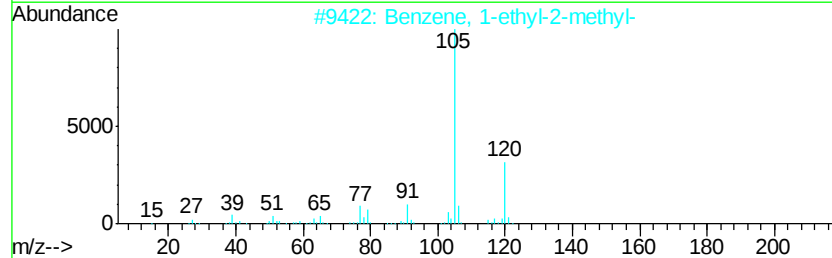
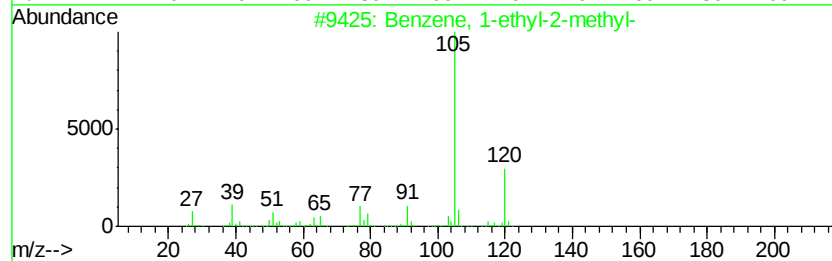
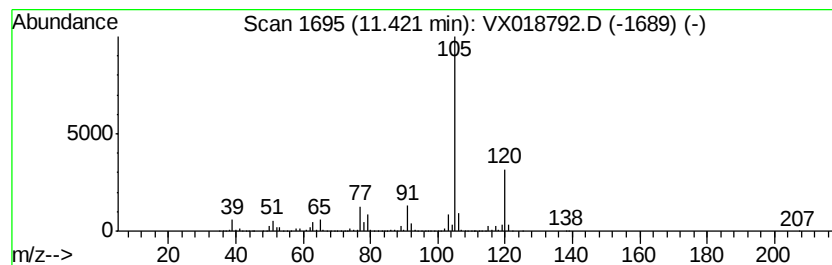
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	36.82 ug/L	10725700	1,4-Dichlorobenzene-d4	12.06

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100620\
Data File : VX018792.D
Acq On : 06 Oct 2020 12:08
Operator : JC/SP
Sample : L4240-02
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 6 Sample Multiplier: 1

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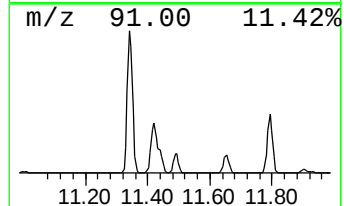
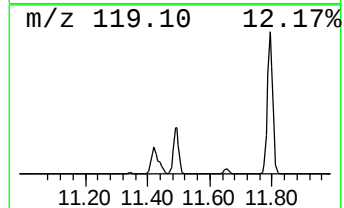
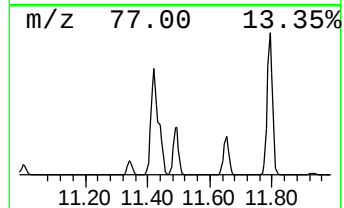
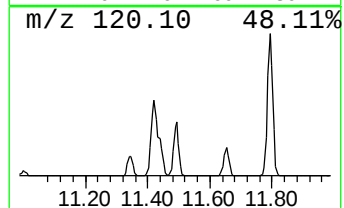
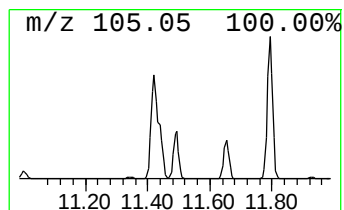
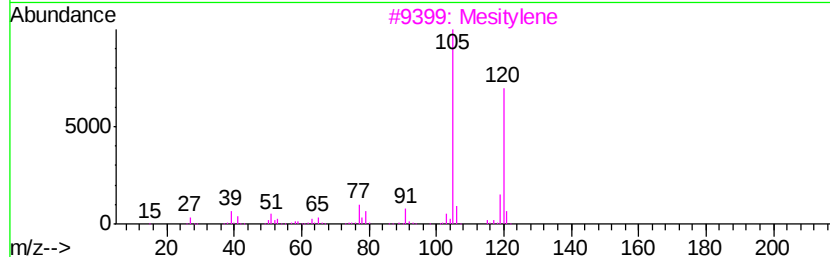
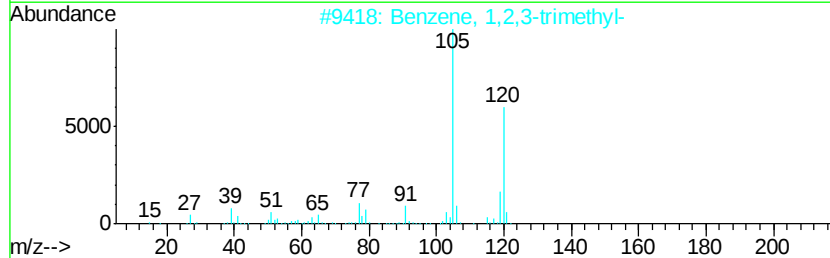
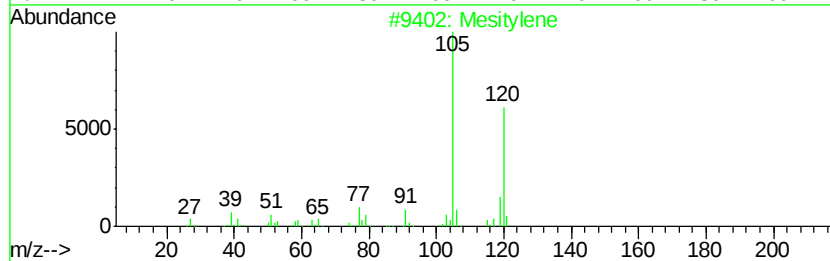
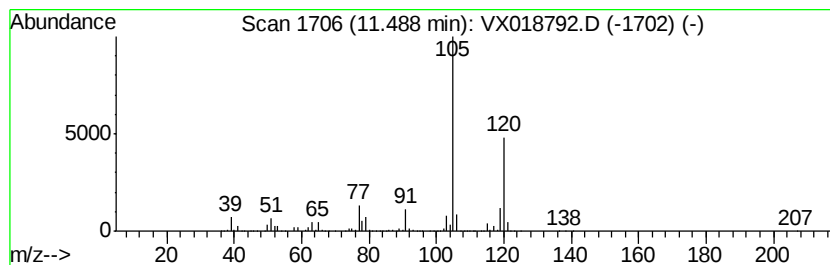
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 Mesitylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.49	13.45 ug/L	3918290	1,4-Dichlorobenzene-d4	12.06

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100620\
Data File : VX018792.D
Acq On : 06 Oct 2020 12:08
Operator : JC/SP
Sample : L4240-02
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3Q9

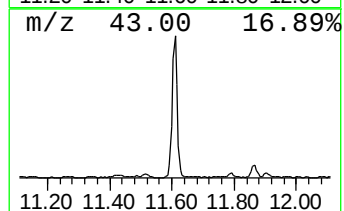
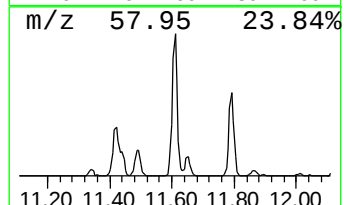
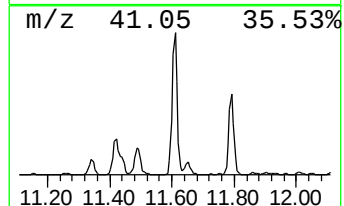
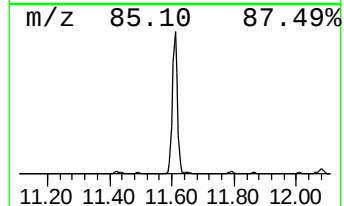
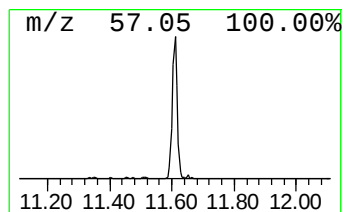
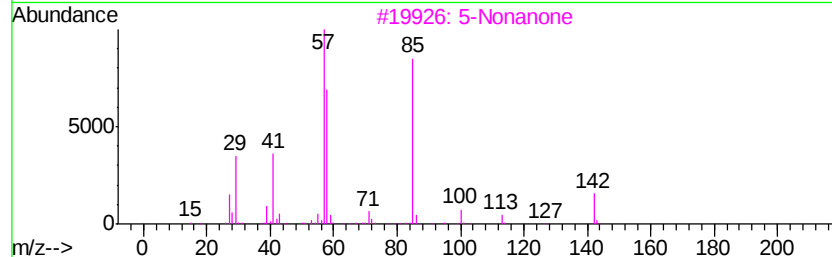
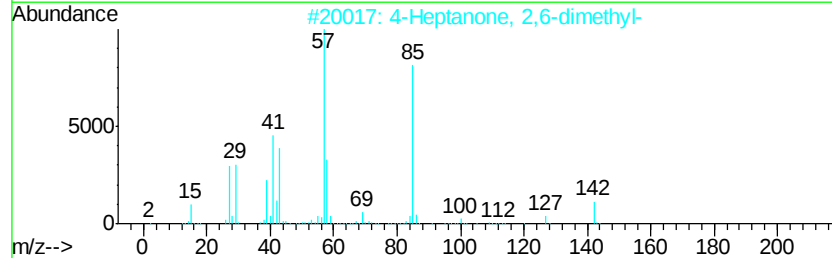
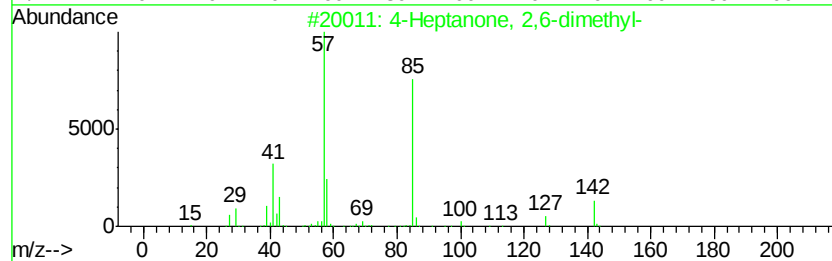
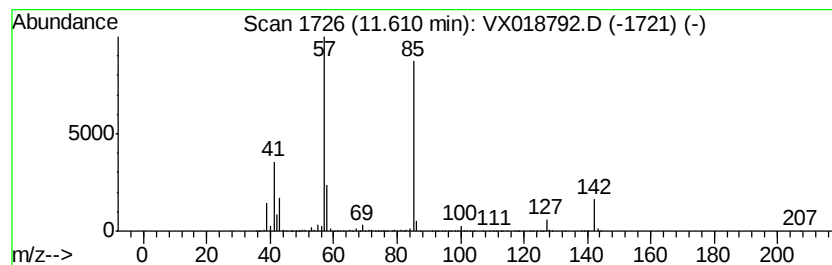
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 11 4-Heptanone, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.61	6.03 ug/L	1755620	1,4-Dichlorobenzene-d4	12.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	64
3			5-Nonanone	142	C9H18O	000502-56-7	59
4			3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	50
5			2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX100620\
Data File : VX018792.D
Acq On : 06 Oct 2020 12:08
Operator : JC/SP
Sample : L4240-02
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 6 Sample Multiplier: 1

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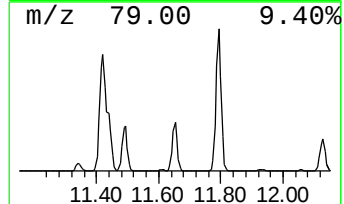
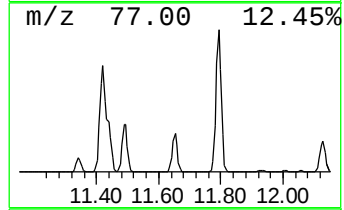
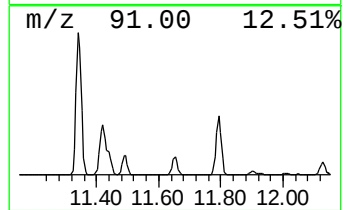
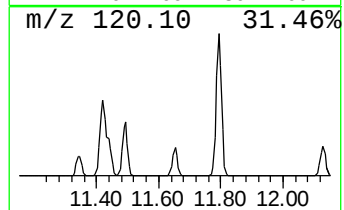
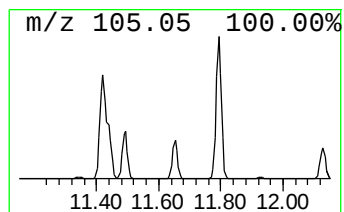
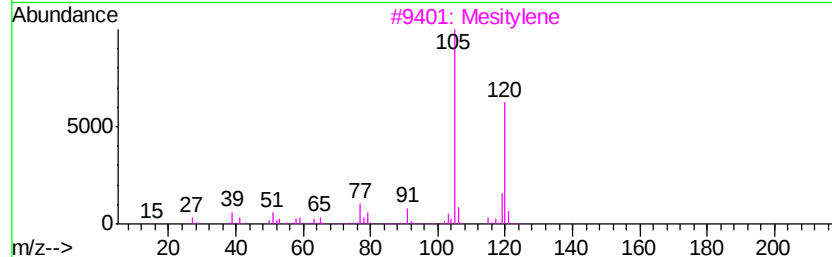
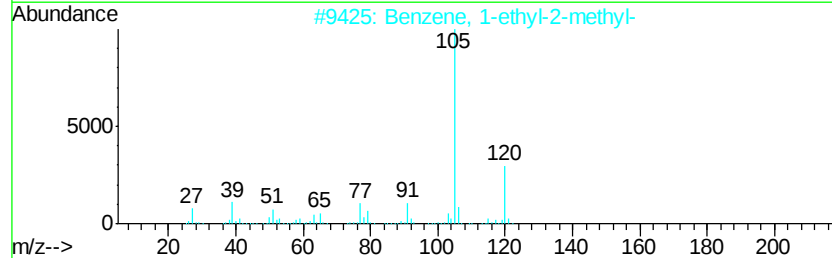
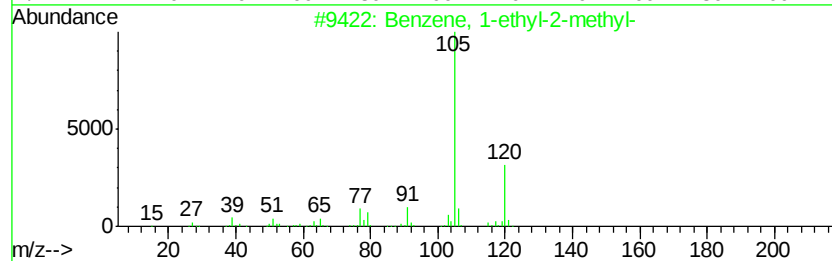
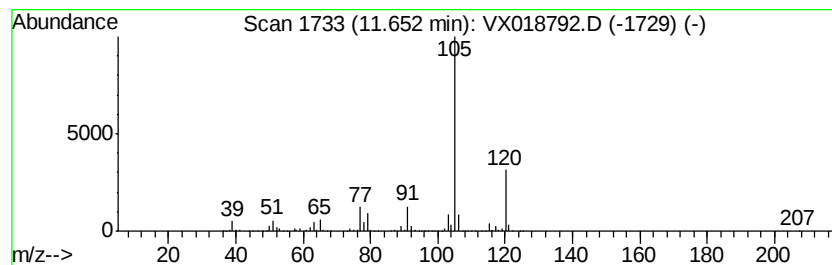
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 12 Benzene, 1-ethyl-4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	9.62 ug/L	2803030	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3		Mesitylene	120	C9H12	000108-67-8	91
4		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100620\
Data File : VX018792.D
Acq On : 06 Oct 2020 12:08
Operator : JC/SP
Sample : L4240-02
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3Q9

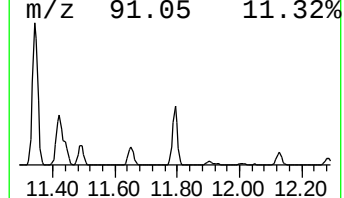
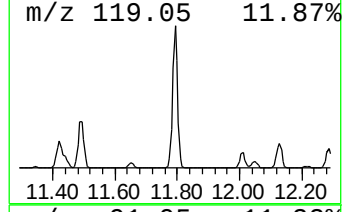
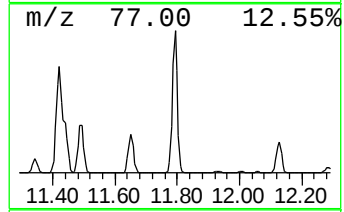
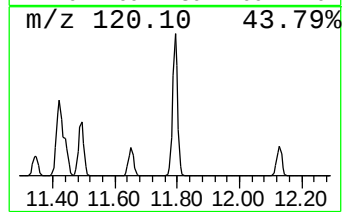
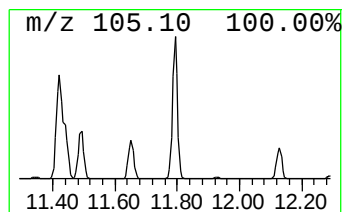
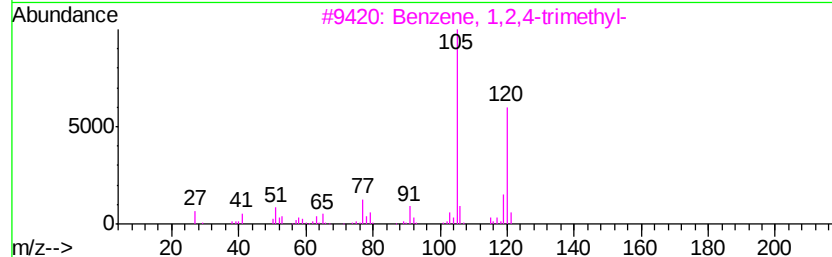
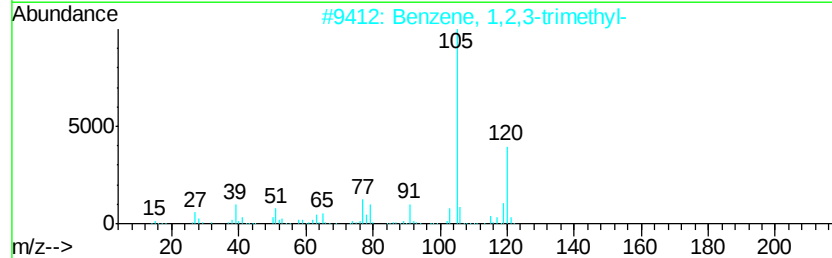
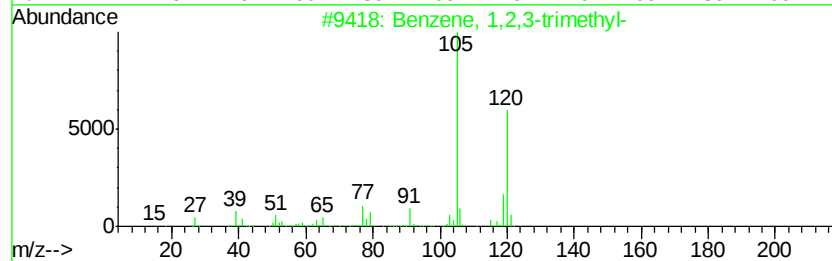
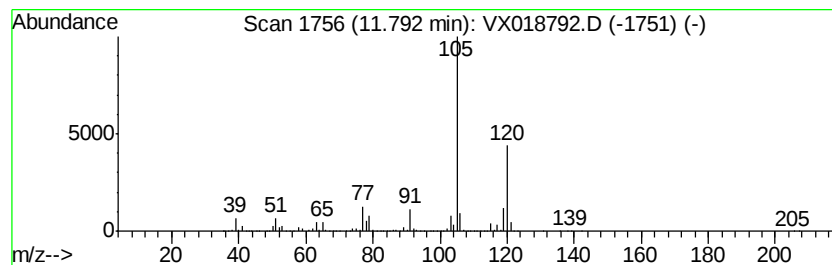
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 13 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	37.25 ug/L	10852900	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	93
5		Mesitylene	120	C9H12	000108-67-8	93



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\WX100620\
 Data File : VX018792.D
 Acq On : 06 Oct 2020 12:08
 Operator : JC/SP
 Sample : L4240-02
 Misc : 25.0mL/MSVOA_X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BG3Q9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.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...	2.83	3.2	ug/L	5315750	1	6.83	8399420	5.0
(DEL) Alkane: Str...	2.87	26.8	ug/L	45056400	1	6.83	8399420	5.0
(DEL) Alkane: Str...	3.16	43.4	ug/L	72817300	1	6.83	8399420	5.0
(DEL) Alkane: Str...	3.54	84.3	ug/L	141584000	1	6.83	8399420	5.0
(DEL) Alkane: Str...	4.12	2.7	ug/L	4475770	1	6.83	8399420	5.0
(DEL) Alkane: Str...	4.29	1.7	ug/L	2780260	1	6.83	8399420	5.0
(DEL) Alkane: Cyc...	4.40	50.5	ug/L	84770000	1	6.83	8399420	5.0
Benzene, propyl-	11.34	7.7	ug/L	2249340	3	12.06	1456610	5.0
Benzene, 1-ethyl-...	11.42	36.8	ug/L	10725700	3	12.06	1456610	5.0
Mesitylene	11.49	13.4	ug/L	3918290	3	12.06	1456610	5.0
4-Heptanone, 2,6-...	11.61	6.0	ug/L	1755620	3	12.06	1456610	5.0
Benzene, 1-ethyl-...	11.65	9.6	ug/L	2803030	3	12.06	1456610	5.0
Benzene, 1,2,3-tr...	11.79	37.3	ug/L	10852900	3	12.06	1456610	5.0