

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100520\
 Data File : VX018766.D
 Acq On : 05 Oct 2020 15:21
 Operator : JC/SP
 Sample : L4239-02DL2 400X
 Misc : 25.0mL/MSVOA X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BG3N0DL2

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	1.386	46	49	58	rVB	70251	71940	6.55%	0.815%
2	1.697	96	100	105	rBV	56921	64599	5.88%	0.731%
3	2.343	198	206	215	rBV	126305	202595	18.44%	2.294%
4	2.830	279	286	287	rBV3	12315	20309	1.85%	0.230%
5	2.867	287	292	301	rVB	37254	80506	7.33%	0.911%
6	3.147	330	338	351	rVB	72157	162663	14.80%	1.842%
7	3.501	385	396	408	rBV	97485	221464	20.15%	2.507%
8	4.373	529	539	551	rBV	109416	314645	28.63%	3.562%
9	4.562	555	570	587	rBV2	78322	314804	28.65%	3.564%
10	5.141	652	665	676	rBV	80592	249967	22.75%	2.830%
11	5.464	704	718	727	rBV3	47642	157866	14.37%	1.787%
12	5.550	727	732	740	rVB5	10810	28243	2.57%	0.320%
13	6.043	800	813	826	rBV3	195497	574907	52.32%	6.509%
14	6.830	929	942	952	rBV	171053	407593	37.09%	4.615%
15	7.183	991	1000	1006	rBV	5276	13989	1.27%	0.158%
16	7.366	1021	1030	1041	rBV	121751	270256	24.59%	3.060%
17	8.372	1187	1195	1204	rBV	80615	132342	12.04%	1.498%
18	8.695	1238	1248	1254	rBV	303629	480310	43.71%	5.438%
19	8.762	1254	1259	1272	rVB	737653	1098844	100.00%	12.441%
20	8.994	1290	1297	1307	rBV	58007	86708	7.89%	0.982%
21	9.427	1362	1368	1383	rBV	399184	594196	54.07%	6.728%
22	9.738	1414	1419	1426	rVB2	12533	19898	1.81%	0.225%
23	10.097	1472	1478	1487	rBV	347586	477228	43.43%	5.403%
24	10.232	1496	1500	1505	rBV	34670	46652	4.25%	0.528%
25	10.341	1512	1518	1524	rVB	117906	157426	14.33%	1.782%
26	10.683	1567	1574	1582	rVB	63845	87283	7.94%	0.988%
27	11.000	1620	1626	1631	rBV2	14148	20610	1.88%	0.233%
28	11.231	1659	1664	1670	rBV	129886	167630	15.26%	1.898%
29	11.341	1677	1682	1689	rBV	36606	50055	4.56%	0.567%
30	11.420	1689	1695	1702	rVV	148984	266632	24.26%	3.019%
31	11.487	1702	1706	1715	rVB	73141	97500	8.87%	1.104%
32	11.609	1715	1726	1730	rBV	278217	336080	30.58%	3.805%
33	11.652	1730	1733	1741	rVB	80418	101731	9.26%	1.152%
34	11.792	1751	1756	1762	rBV	268721	327155	29.77%	3.704%

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ClientSampleId :
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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	11.865	1762	1768	1773	rVV2	8635	11862	1.08%	0.134%
36	12.061	1795	1800	1806	rBV	375717	477360	43.44%	5.405%
37	12.128	1806	1811	1819	rVB	69975	89813	8.17%	1.017%
38	12.280	1829	1836	1843	rBV2	29795	45253	4.12%	0.512%
39	12.359	1843	1849	1856	rVB	364022	458713	41.75%	5.194%
40	12.999	1951	1954	1962	rVB2	8374	11365	1.03%	0.129%
41	13.335	2003	2009	2015	rBV4	7406	11403	1.04%	0.129%
42	13.816	2084	2088	2093	rBV	16765	21916	1.99%	0.248%

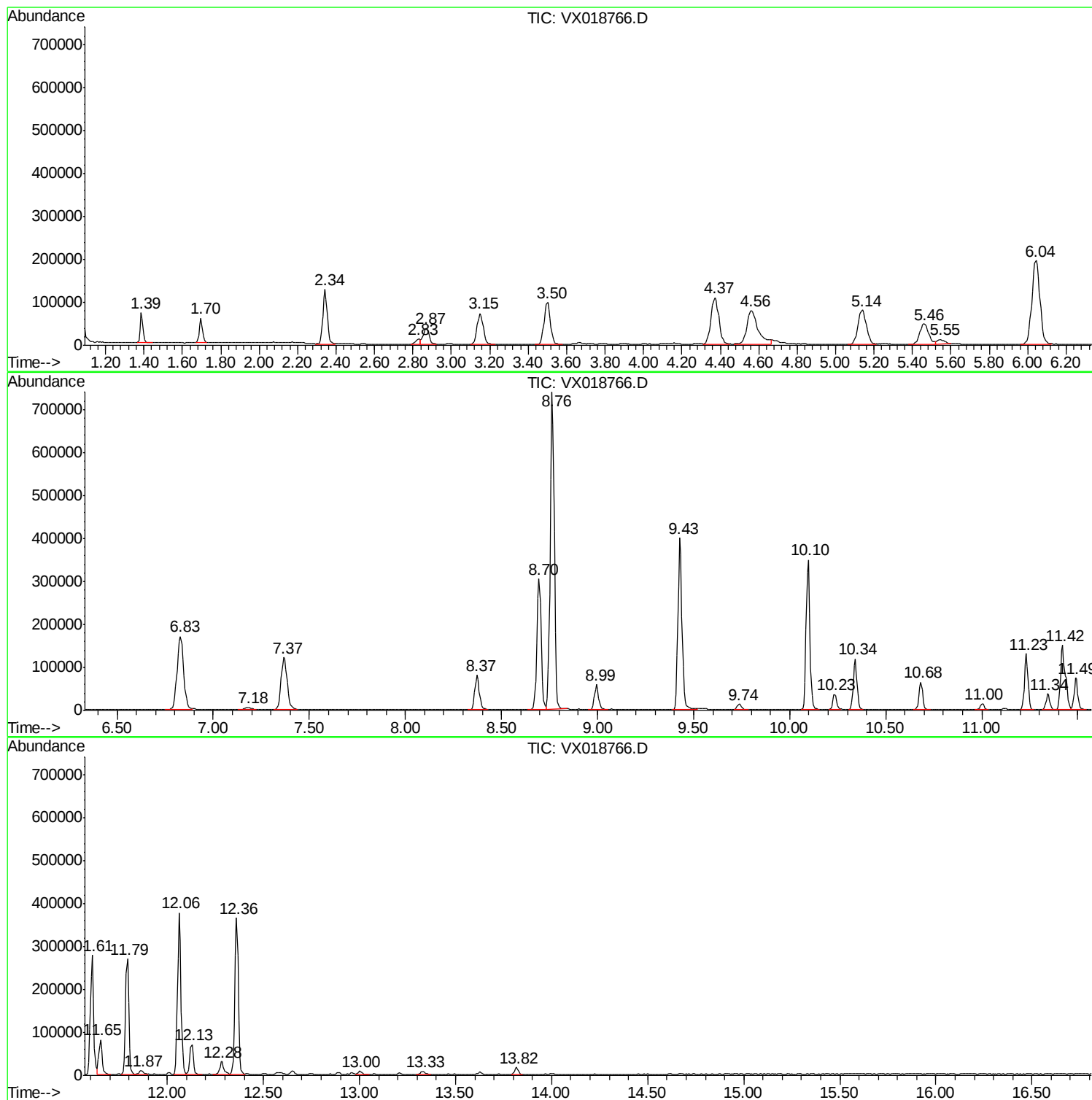
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Instrument :
MSVOA_X
ClientSampled :
BG3N0DL2

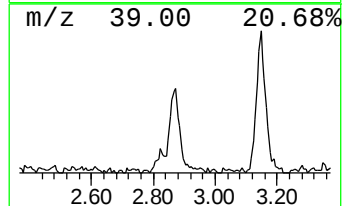
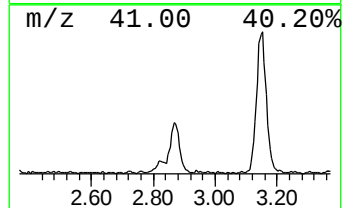
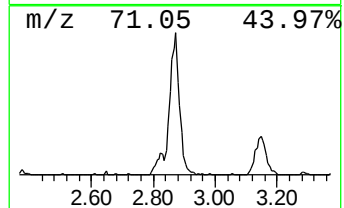
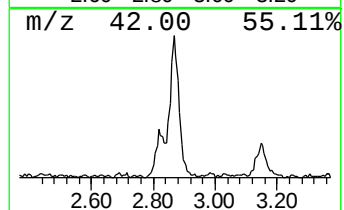
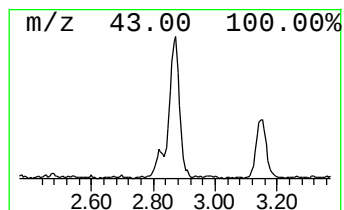
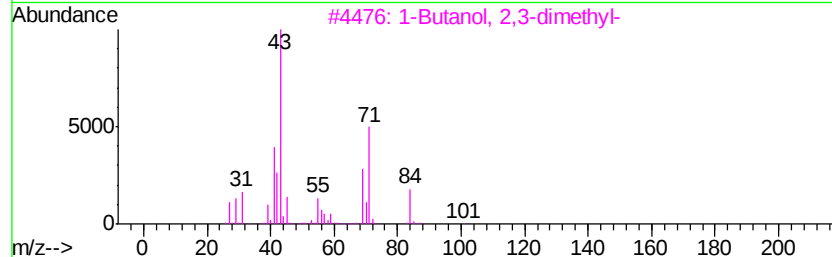
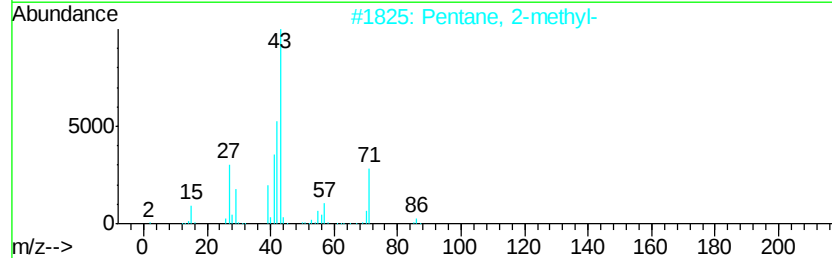
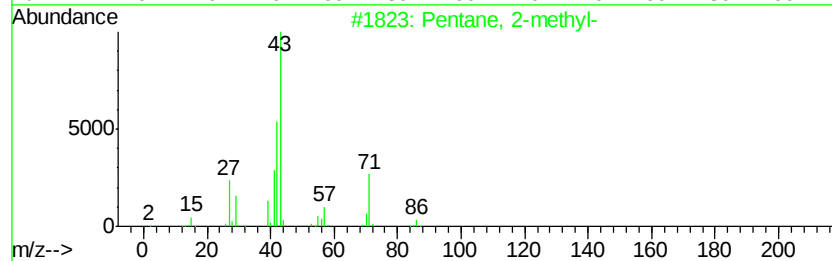
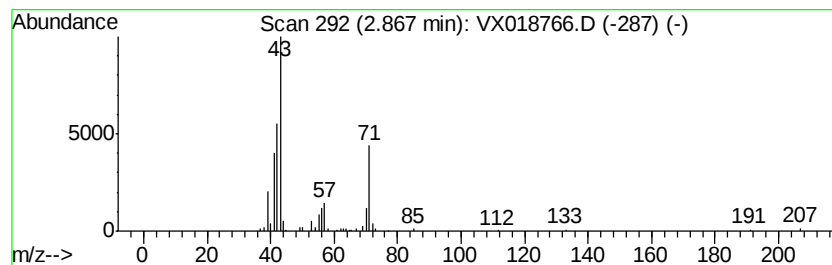
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.87	0.99 ug/L	80506	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2-methyl-	86	C6H14	000107-83-5	83
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	53
3		1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
4		Pentane	72	C5H12	000109-66-0	43
5		Pentane	72	C5H12	000109-66-0	43



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Instrument :
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ClientSampleId :
BG3N0DL2

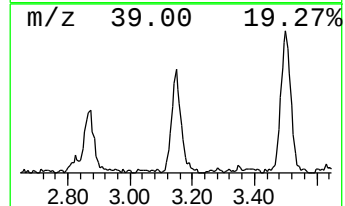
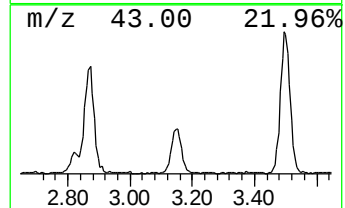
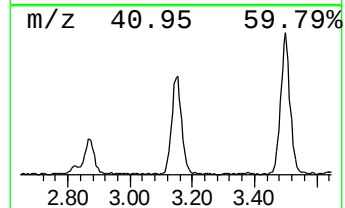
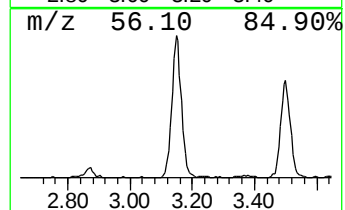
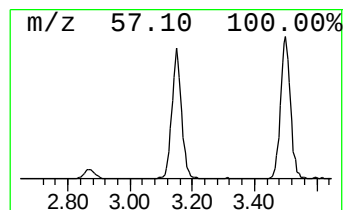
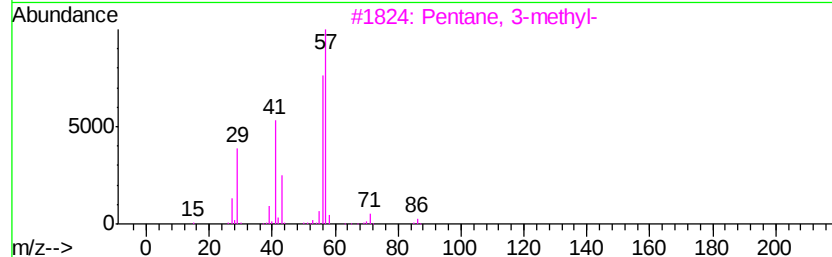
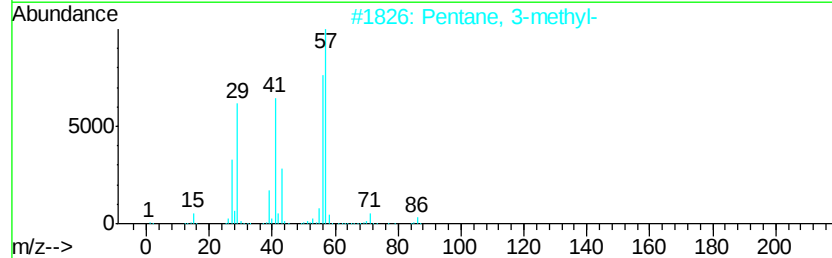
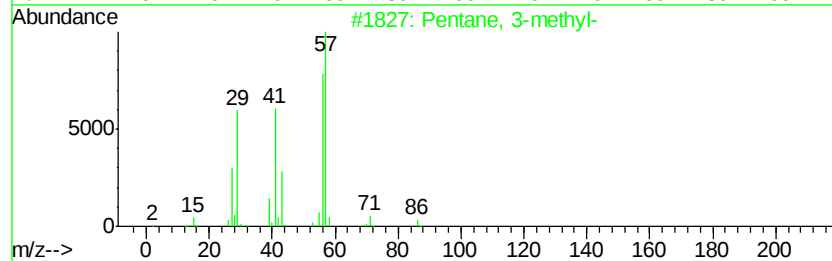
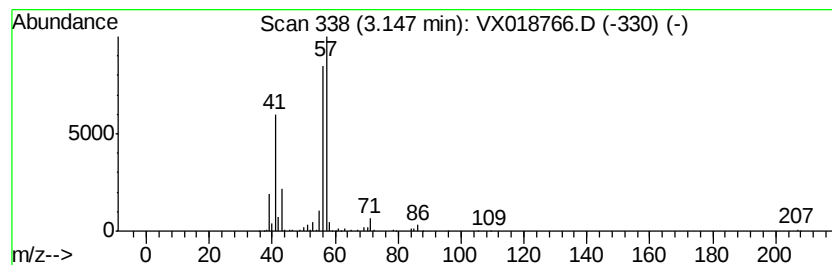
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	2.00 ug/L	162663	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	86
2		Pentane, 3-methyl-	86	C6H14	000096-14-0	86
3		Pentane, 3-methyl-	86	C6H14	000096-14-0	86
4		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	72
5		Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	72



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Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3N0DL2

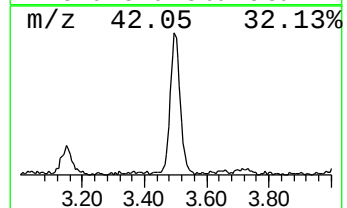
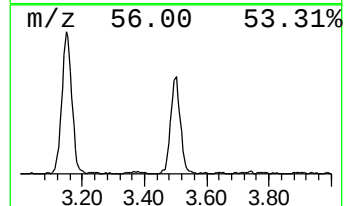
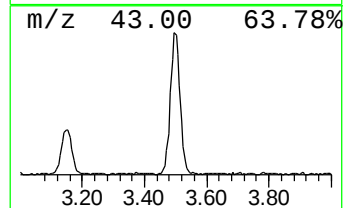
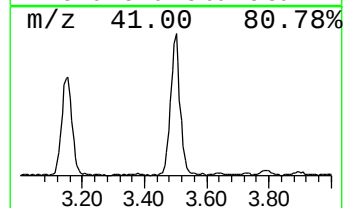
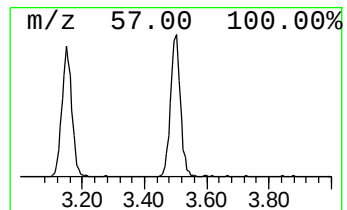
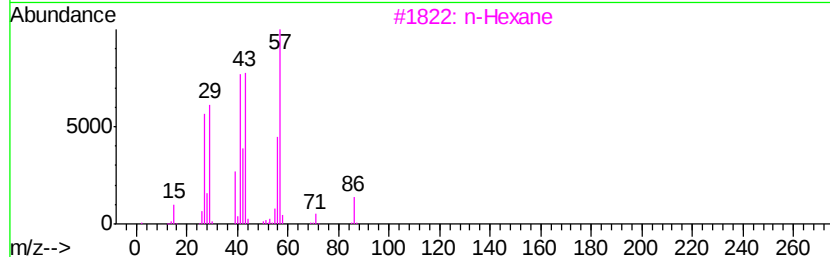
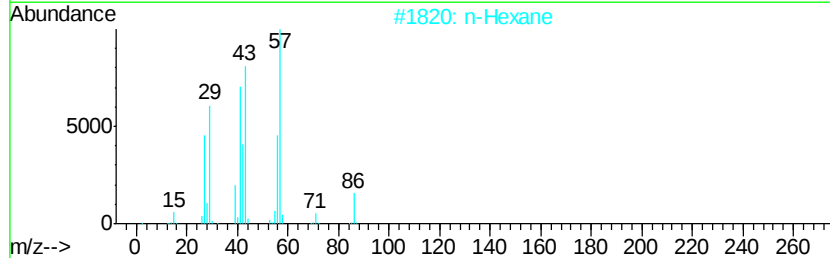
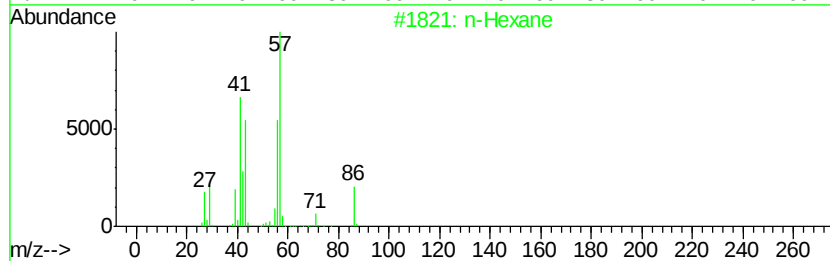
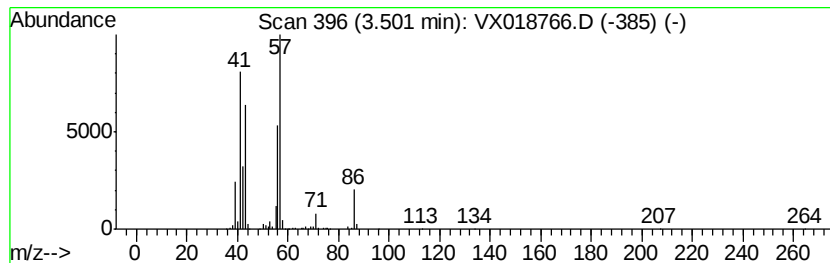
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	2.72 ug/L	221464	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	94
2		n-Hexane	86	C6H14	000110-54-3	72
3		n-Hexane	86	C6H14	000110-54-3	72
4		Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	50
5		Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	43



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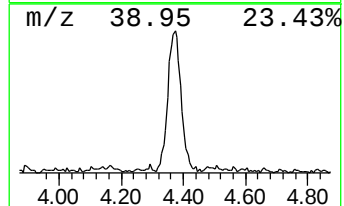
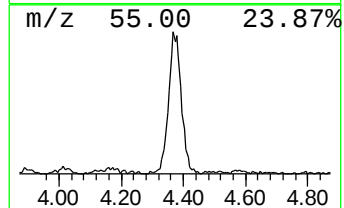
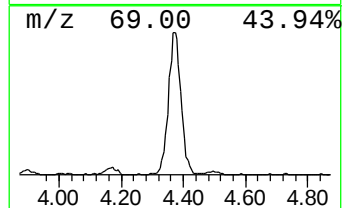
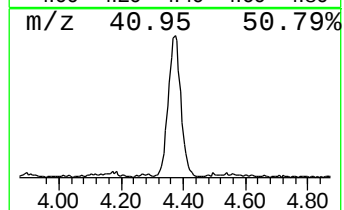
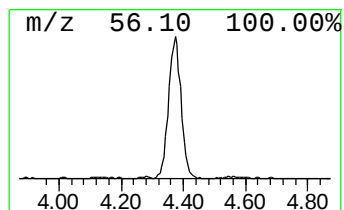
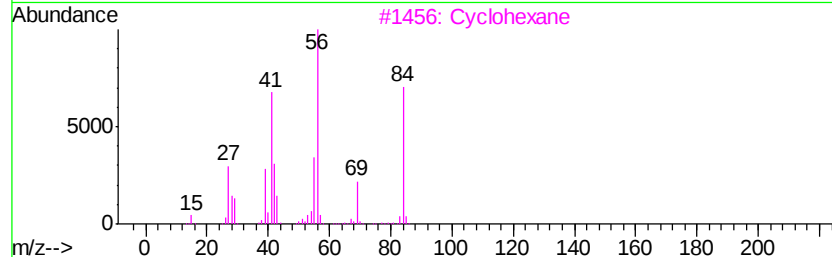
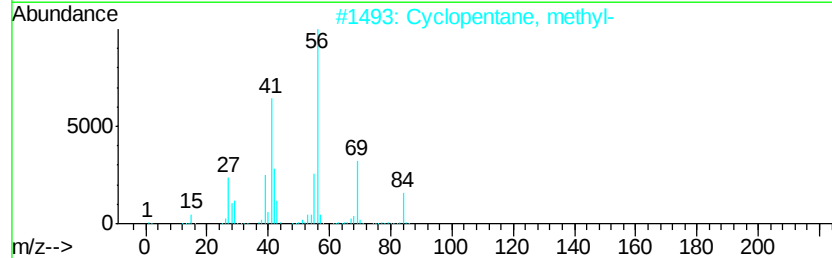
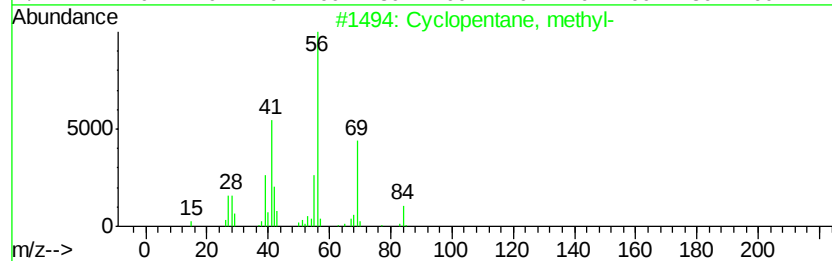
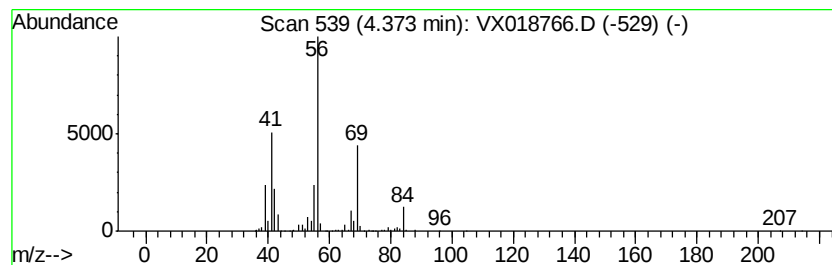
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Cyclic4.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	3.86 ug/L	314645	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	86
3		Cyclohexane	84	C6H12	000110-82-7	80
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64



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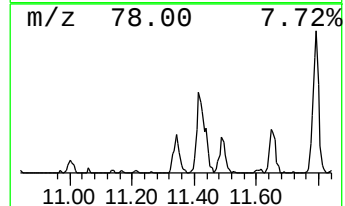
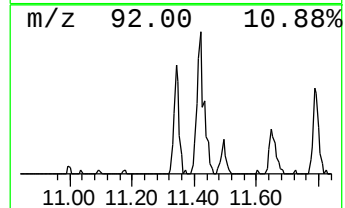
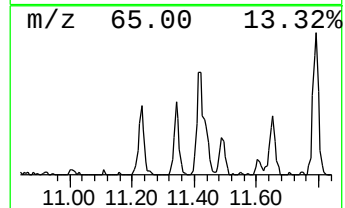
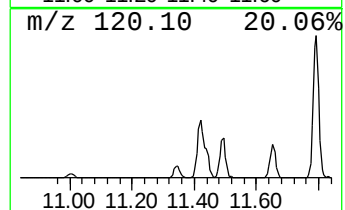
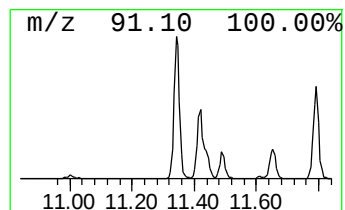
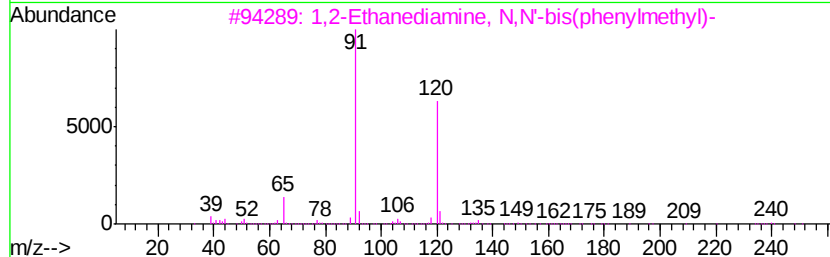
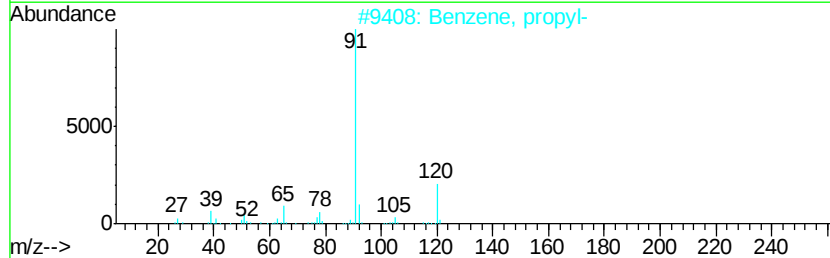
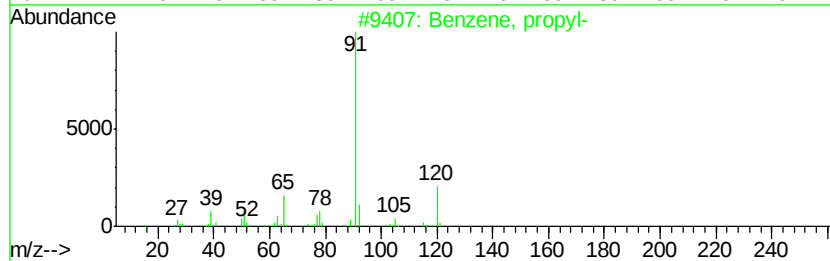
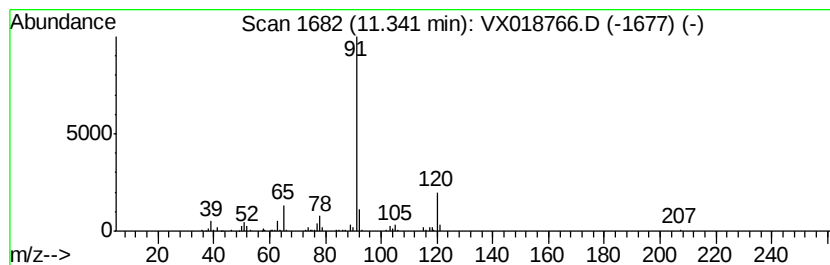
Instrument :
MSVOA_X
ClientSampled :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Benzene, propyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.34	0.52 ug/L	50055	1,4-Dichlorobenzene-d4	12.06	
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	1,2-Ethanediamine, N,N'-bis(phen...	240	C16H20N2	000140-28-3	83
4	Propanenitrile, 3-[(phenylmethyl)...	160	C10H12N2	000706-03-6	78
5	Ethanol, 2-[(phenylmethyl)amino]-	151	C9H13NO	000104-63-2	78



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018766.D
Acq On : 05 Oct 2020 15:21
Operator : JC/SP
Sample : L4239-02DL2 400X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
BG3N0DL2

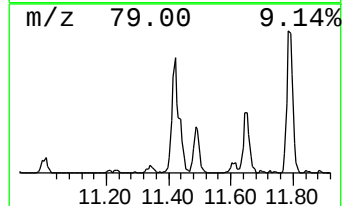
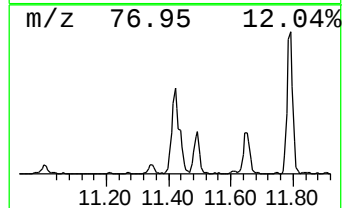
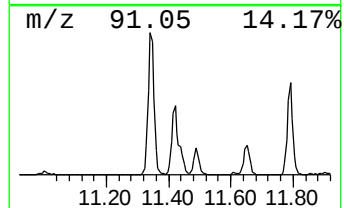
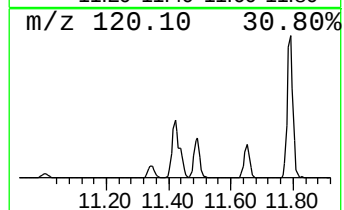
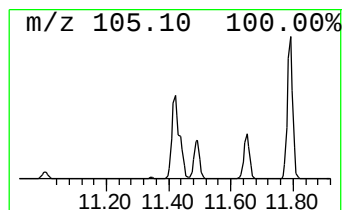
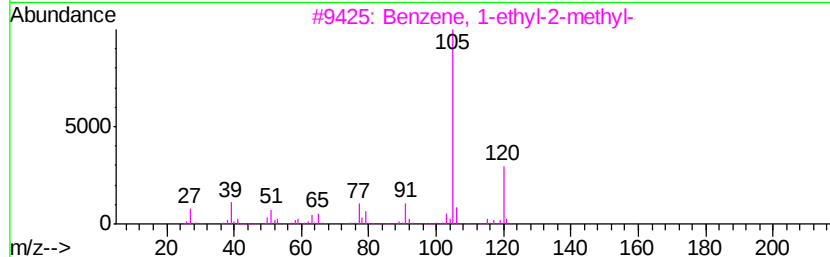
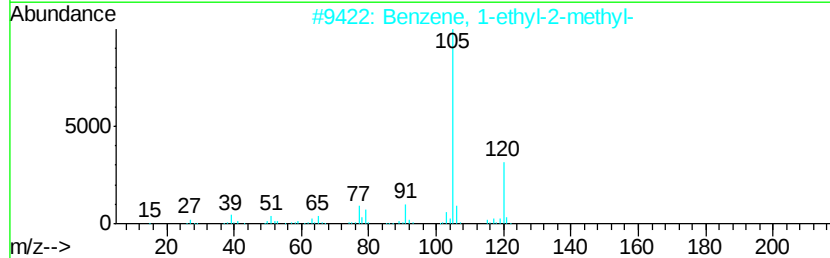
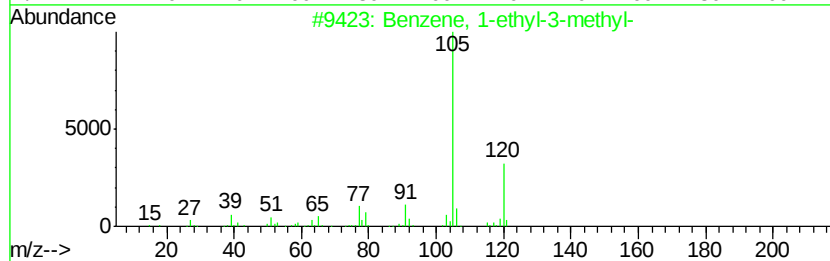
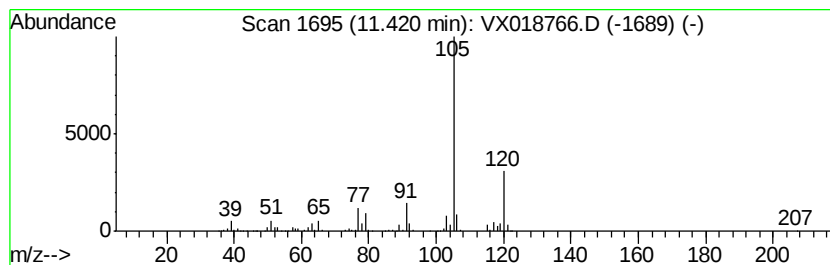
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 Benzene, 1-ethyl-3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	2.79 ug/L	266632	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
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:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018766.D
Acq On : 05 Oct 2020 15:21
Operator : JC/SP
Sample : L4239-02DL2 400X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3N0DL2

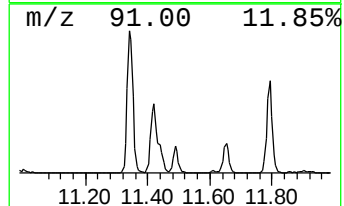
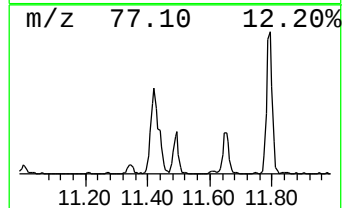
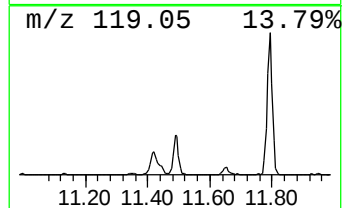
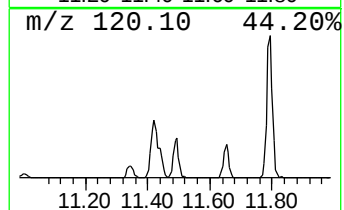
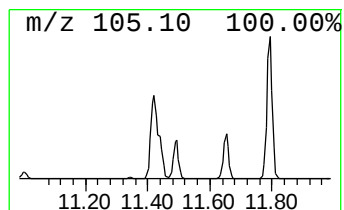
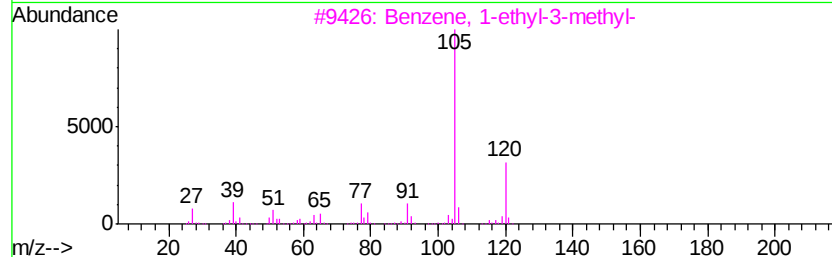
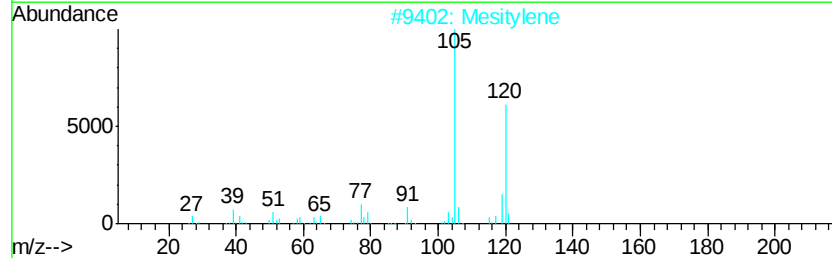
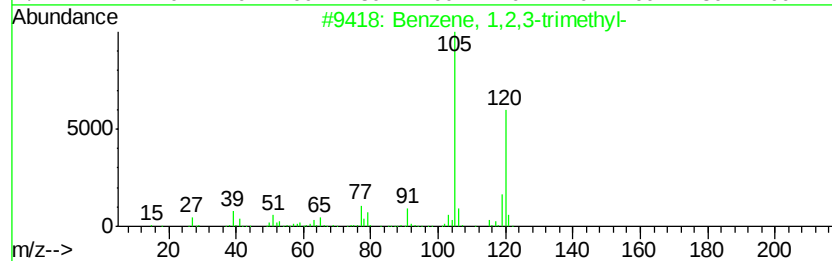
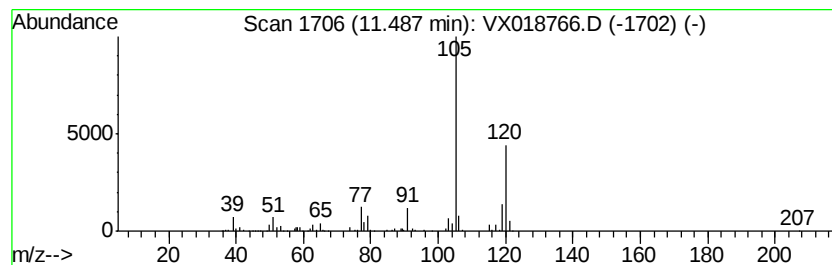
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.49	1.02 ug/L	97500	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		Mesitylene	120	C9H12	000108-67-8	91
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5		Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018766.D
Acq On : 05 Oct 2020 15:21
Operator : JC/SP
Sample : L4239-02DL2 400X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 7 Sample Multiplier: 1

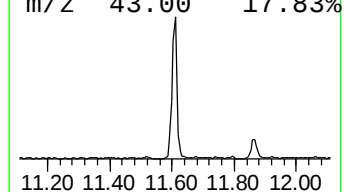
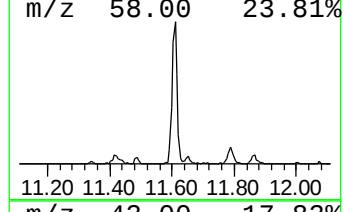
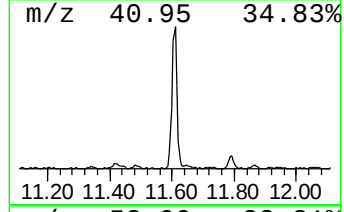
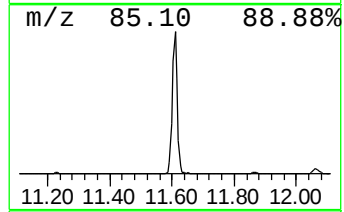
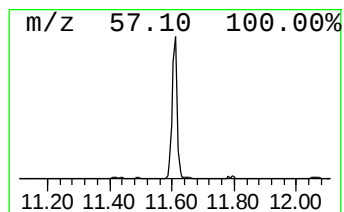
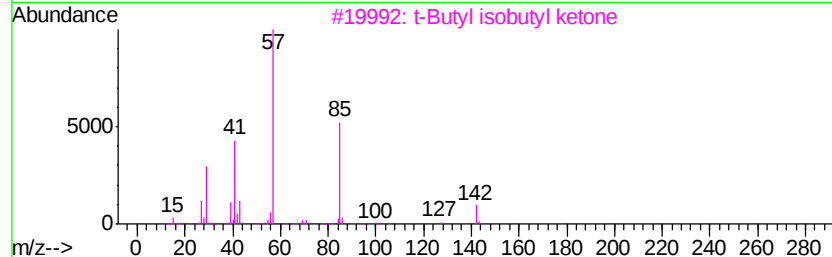
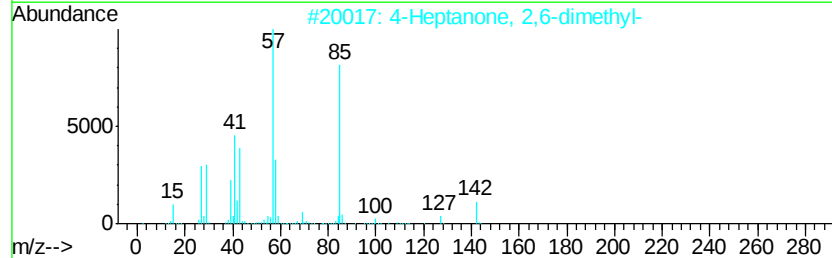
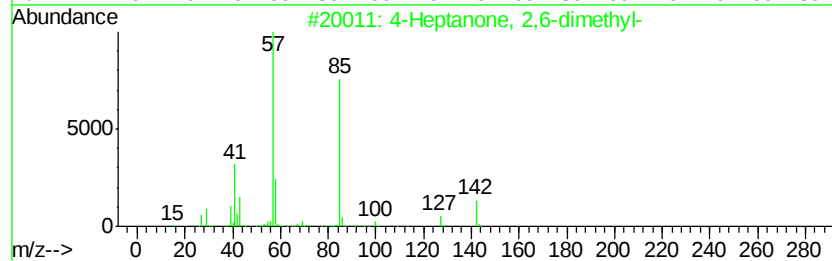
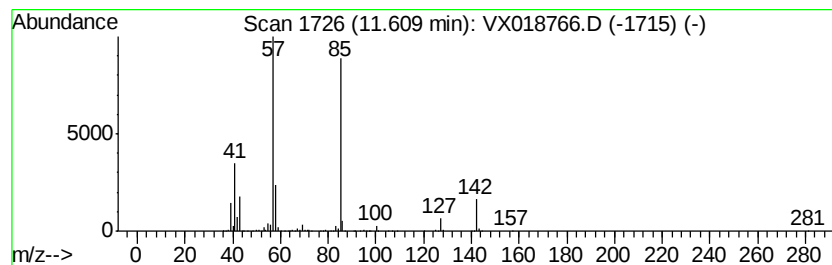
Instrument :
MSVOA_X
ClientSampleId :
BG3N0DL2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 4-Heptanone, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.61	3.52 ug/L	336080	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	t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	64
4	5-Nonanone	142	C9H18O	000502-56-7	59
5	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018766.D
Acq On : 05 Oct 2020 15:21
Operator : JC/SP
Sample : L4239-02DL2 400X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3N0DL2

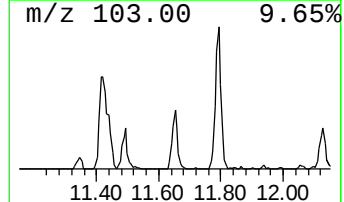
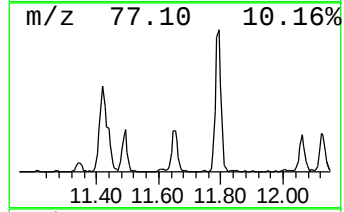
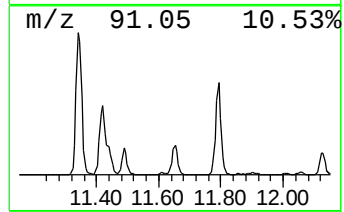
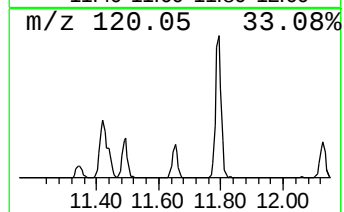
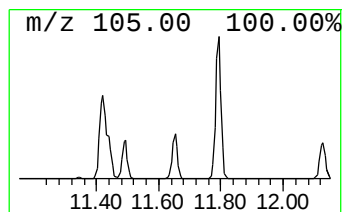
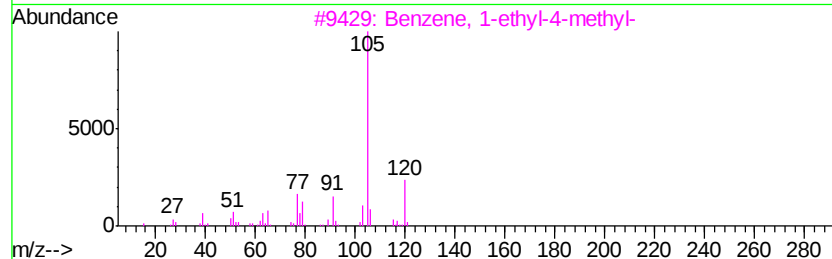
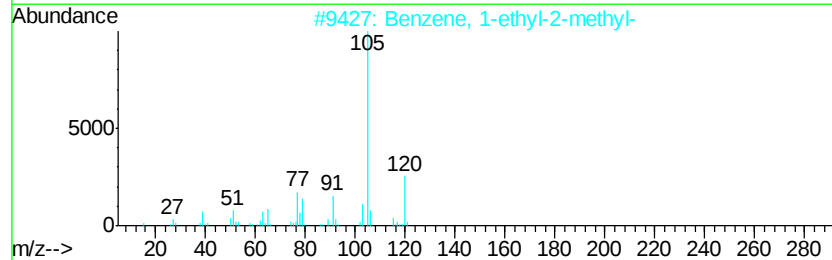
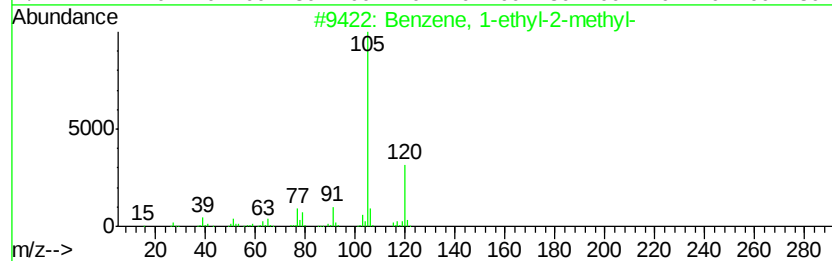
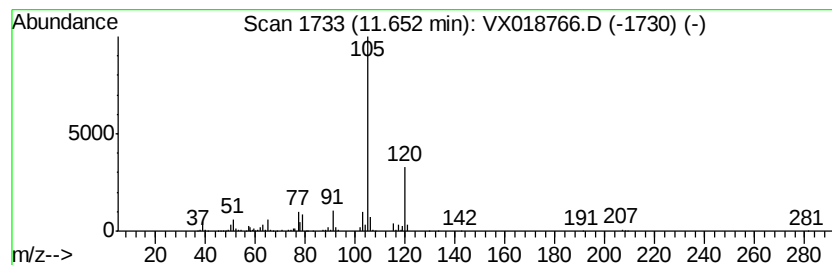
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	1.07 ug/L	101731	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-4-methyl-	120	C9H12	000622-96-8	94
4		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
5		Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018766.D
Acq On : 05 Oct 2020 15:21
Operator : JC/SP
Sample : L4239-02DL2 400X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
BG3N0DL2

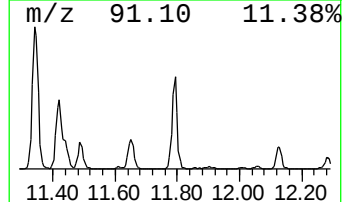
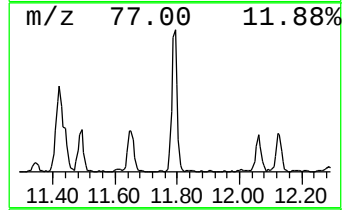
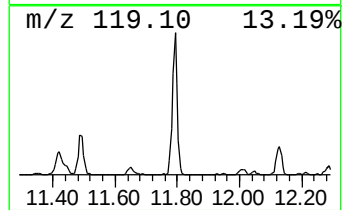
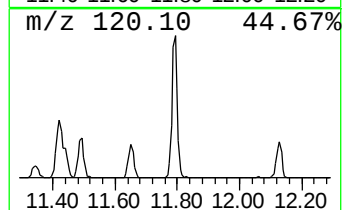
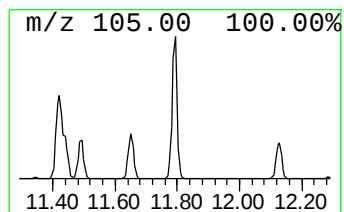
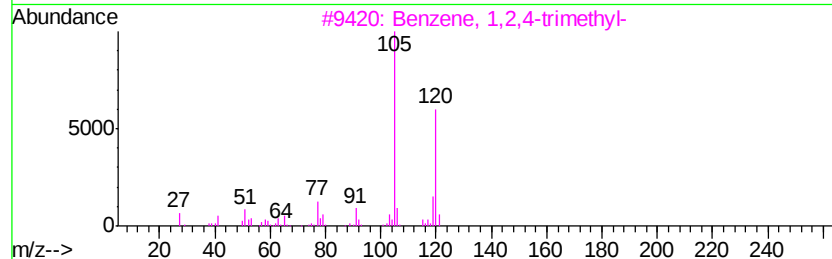
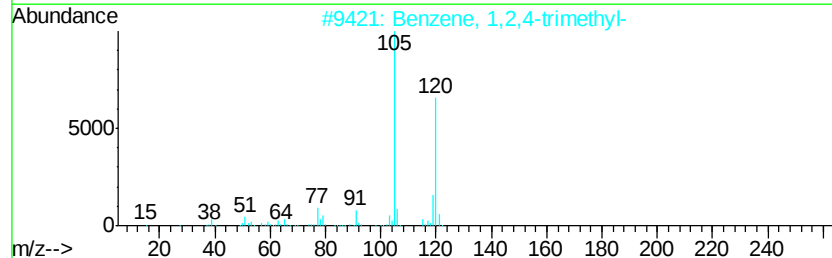
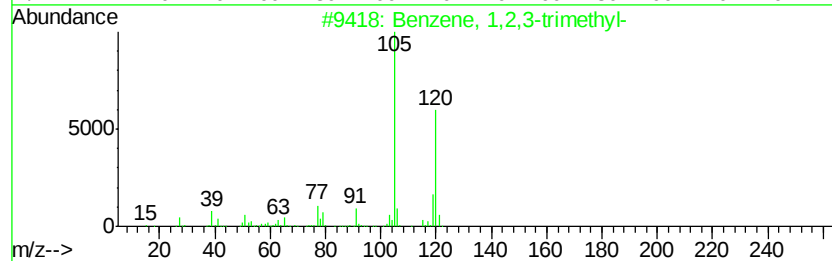
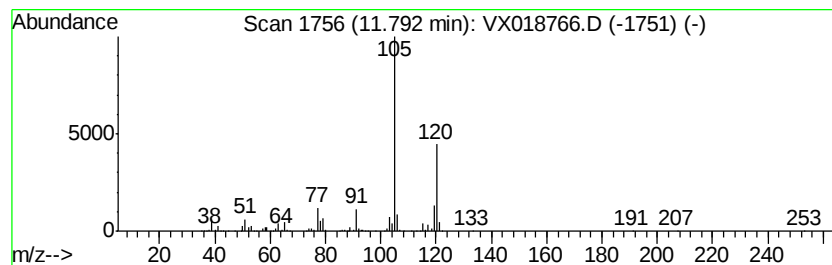
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 11 Benzene, 1,2,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	3.43 ug/L	327155	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, 1,2,4-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	93



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100520\
 Data File : VX018766.D
 Acq On : 05 Oct 2020 15:21
 Operator : JC/SP
 Sample : L4239-02DL2 400X
 Misc : 25.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BG3N0DL2

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...	2.87	1.0	ug/L	80506	1	6.83	407593	5.0
(DEL) Alkane: Str...	3.15	2.0	ug/L	162663	1	6.83	407593	5.0
(DEL) Alkane: Str...	3.50	2.7	ug/L	221464	1	6.83	407593	5.0
(DEL) Alkane: Cyc...	4.37	3.9	ug/L	314645	1	6.83	407593	5.0
Benzene, propyl-	11.34	0.5	ug/L	50055	3	12.06	477360	5.0
Benzene, 1-ethyl-...	11.42	2.8	ug/L	266632	3	12.06	477360	5.0
Benzene, 1,2,3-tr...	11.49	1.0	ug/L	97500	3	12.06	477360	5.0
4-Heptanone, 2,6-...	11.61	3.5	ug/L	336080	3	12.06	477360	5.0
Benzene, 1-ethyl-...	11.65	1.1	ug/L	101731	3	12.06	477360	5.0
Benzene, 1,2,4-tr...	11.79	3.4	ug/L	327155	3	12.06	477360	5.0