

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100720\
 Data File : VX018818.D
 Acq On : 07 Oct 2020 18:06
 Operator : JC/SP
 Sample : VIBLK69
 Misc : 25.0mL/MSVOA X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VIBLK69

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	45	49	52	rBV	60083	59647	9.82%	1.122%
2	1.459	52	61	62	rBV	19068	46684	7.69%	0.878%
3	1.697	96	100	104	rVB	56099	61590	10.14%	1.159%
4	2.191	179	181	193	rVB6	8289	25200	4.15%	0.474%
5	2.343	201	206	216	rVB	113184	177393	29.22%	3.338%
6	2.867	280	292	302	rVB4	38589	102701	16.92%	1.932%
7	2.989	306	312	315	rBV5	3590	7069	1.16%	0.133%
8	3.148	330	338	348	rBV	60799	141852	23.36%	2.669%
9	3.501	386	396	404	rBV	134994	303562	50.00%	5.712%
10	4.373	530	539	545	rBV5	4604	13674	2.25%	0.257%
11	4.562	559	570	583	rBV	56787	240564	39.62%	4.526%
12	5.135	653	664	677	rBV2	79623	242526	39.95%	4.563%
13	6.044	802	813	827	rBV3	184540	539798	88.91%	10.156%
14	6.830	930	942	950	rBV	141885	362974	59.79%	6.829%
15	7.366	1020	1030	1042	rVB	117762	264588	43.58%	4.978%
16	8.372	1188	1195	1204	rBV	73246	124512	20.51%	2.343%
17	8.695	1238	1248	1256	rBV	274260	426239	70.21%	8.020%
18	8.994	1289	1297	1304	rBV	56463	82162	13.53%	1.546%
19	9.427	1362	1368	1379	rBV	418134	607123	100.00%	11.423%
20	9.738	1413	1419	1429	rBV2	21443	34517	5.69%	0.649%
21	10.098	1472	1478	1490	rBV	278992	401333	66.10%	7.551%
22	11.232	1655	1664	1670	rBV	133004	170919	28.15%	3.216%
23	12.061	1794	1800	1806	rBV	301112	368321	60.67%	6.930%
24	12.359	1842	1849	1855	rBV	323243	401084	66.06%	7.547%
25	13.341	2003	2010	2011	rBV7	3934	8035	1.32%	0.151%
26	13.628	2046	2057	2063	rBV2	22987	42982	7.08%	0.809%
27	13.884	2095	2099	2107	rBV	28090	43626	7.19%	0.821%
28	13.999	2116	2118	2127	rVB10	4969	7398	1.22%	0.139%
29	15.664	2385	2391	2395	rBV9	3151	6732	1.11%	0.127%

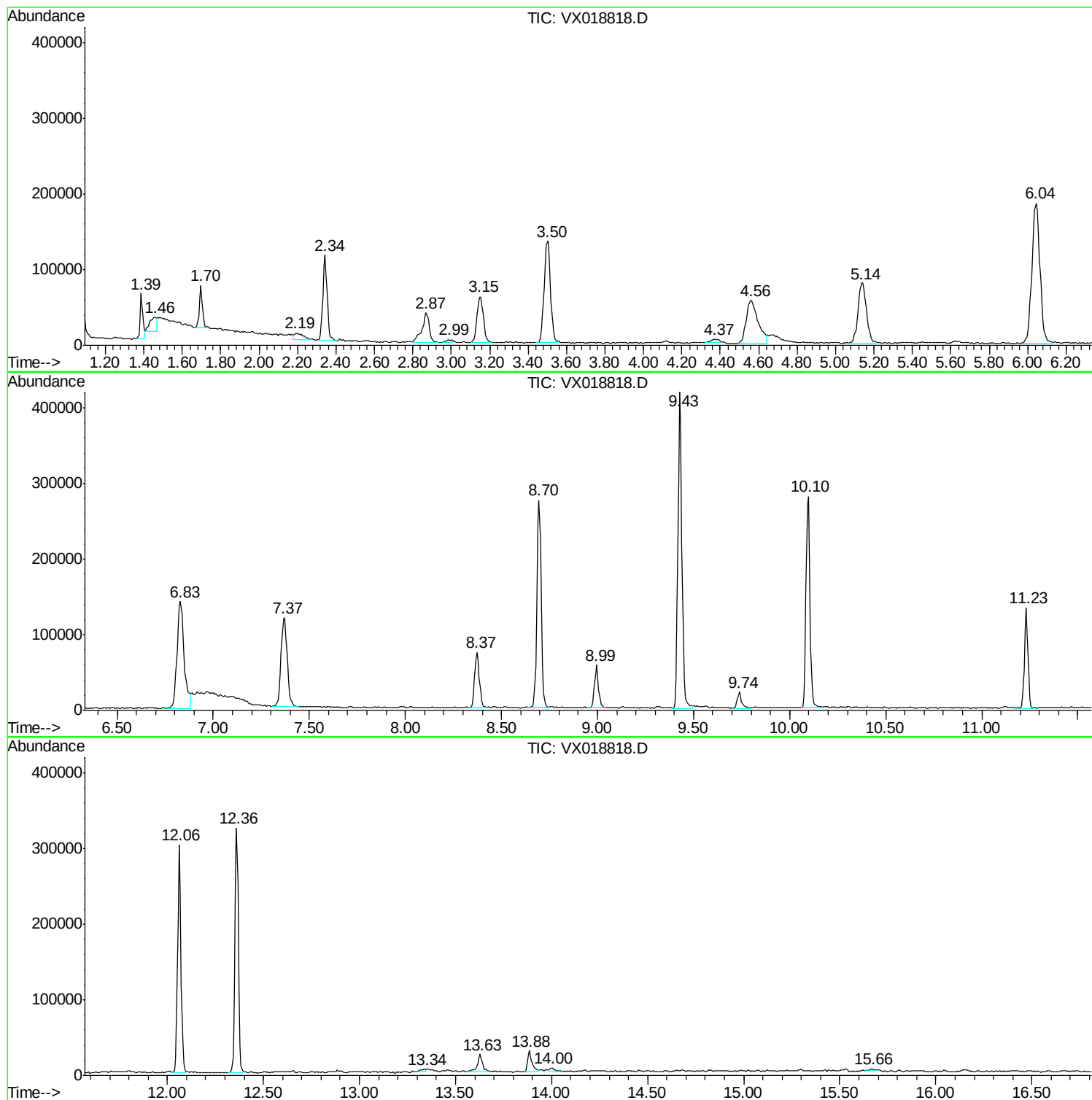
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VIBLK69

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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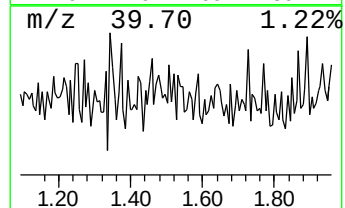
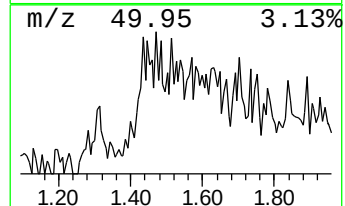
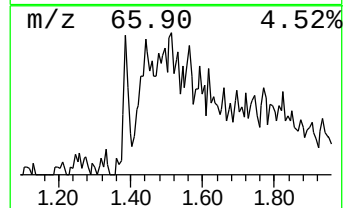
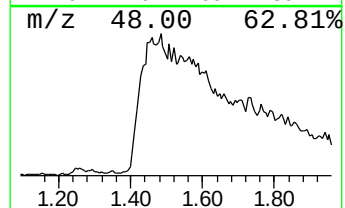
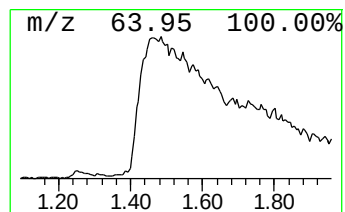
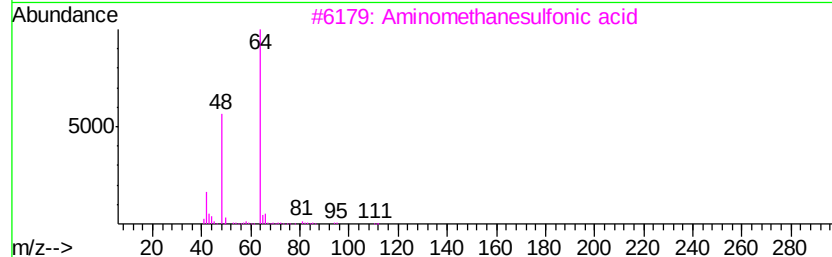
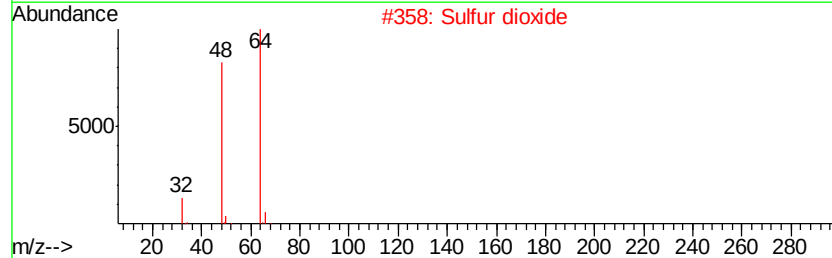
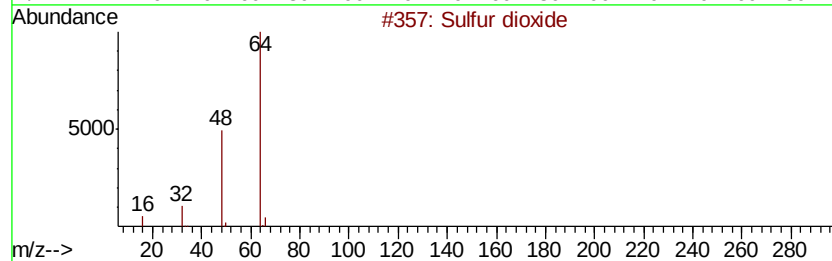
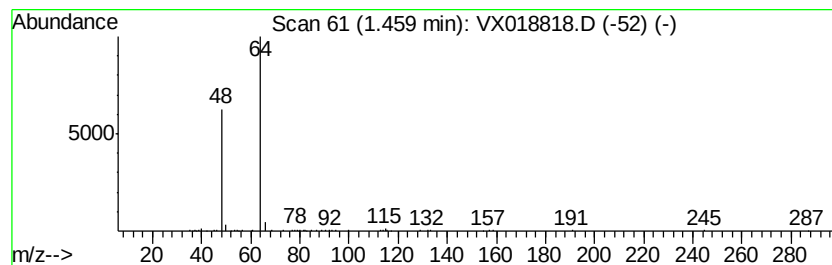
Instrument :
MSVOA_X
ClientSampleId :
VIBLK69

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 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.46	0.64 ug/L	46684	1,4-Difluorobenzene	6.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Sulfur dioxide	64 02S	007446-09-5	74
2	Sulfur dioxide	64 02S	007446-09-5	74
3	Aminomethanesulfonic acid	111 CH5N03S	013881-91-9	64
4	S-2-[4-Glutarimidobutylamino]eth...	324 C11H20N2O5S2	031701-78-7	9
5	Thiosulfuric acid (H2S2O3), S-(2...	320 C11H16N2O3S3	040284-00-2	9



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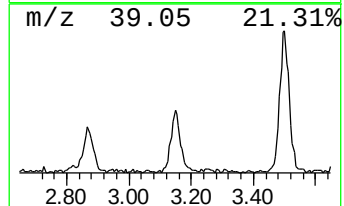
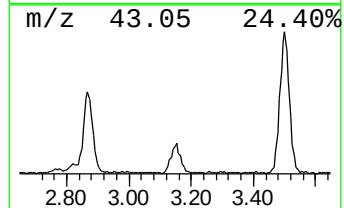
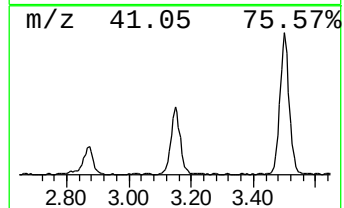
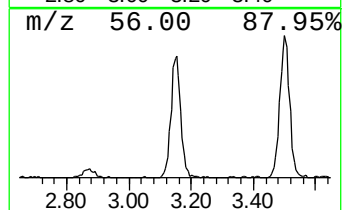
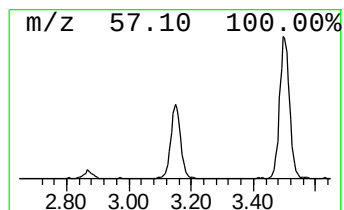
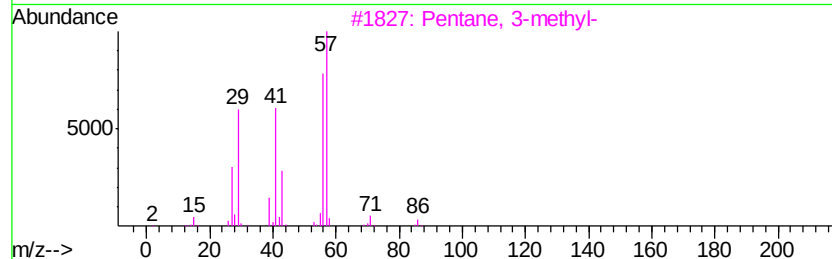
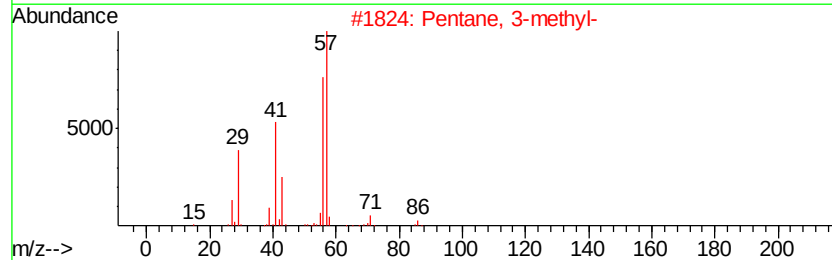
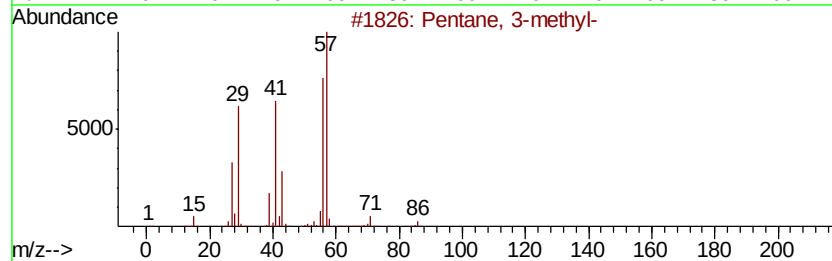
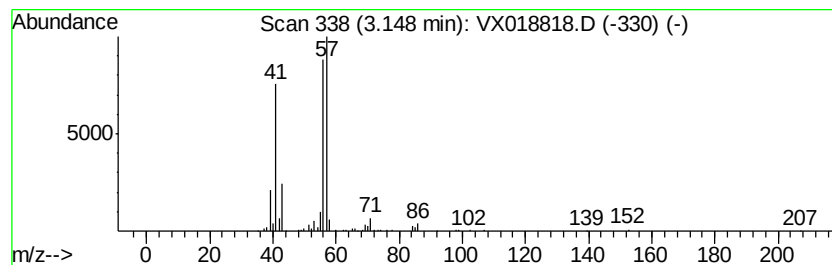
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	1.95 ug/L	141852	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	64
5		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	59



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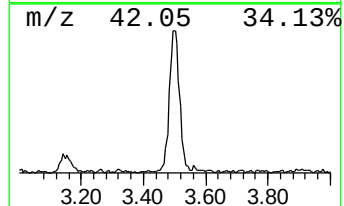
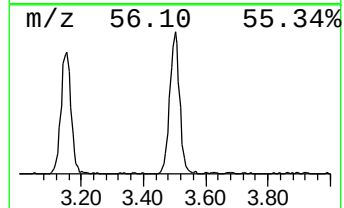
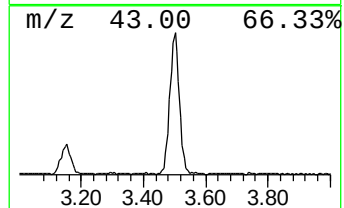
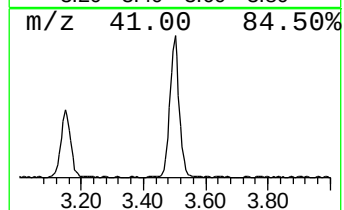
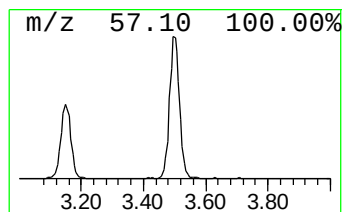
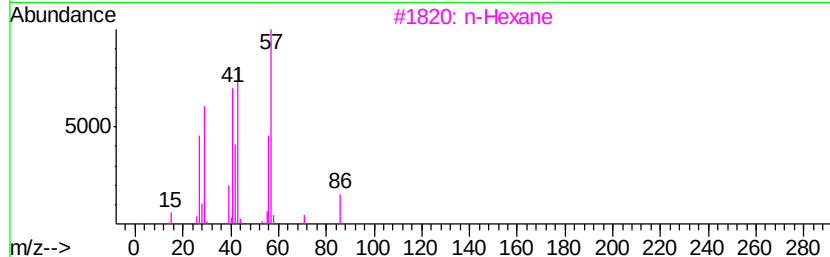
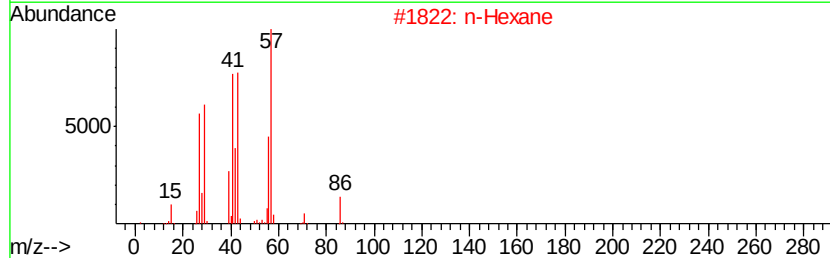
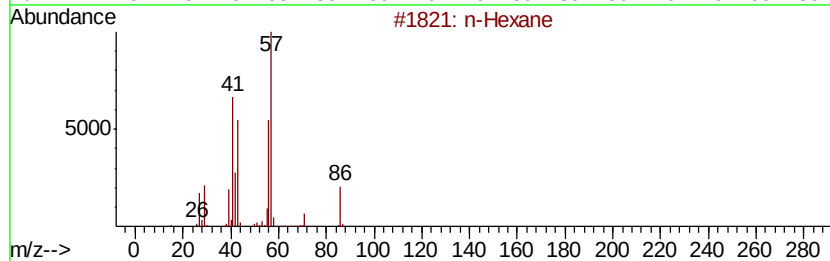
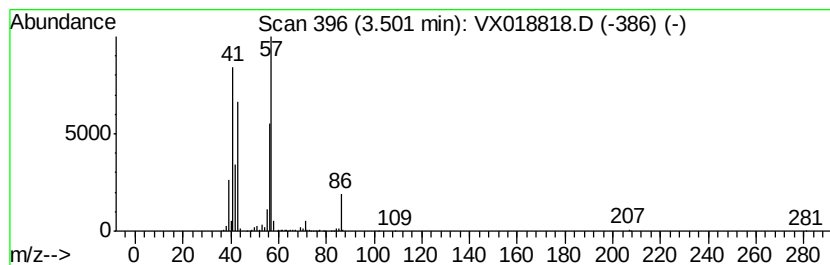
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	4.18 ug/L	303562	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	90
2		n-Hexane	86	C6H14	000110-54-3	64
3		n-Hexane	86	C6H14	000110-54-3	59
4		Oxirane, 2-methyl-3-(1-methyleth...	100	C6H12O	001192-31-0	43
5		Butanal, 2-methyl-	86	C5H10O	000096-17-3	43



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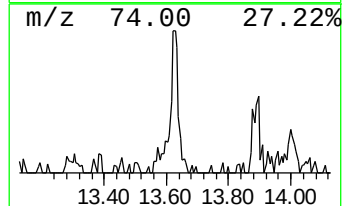
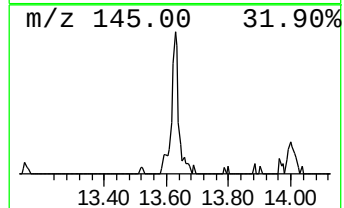
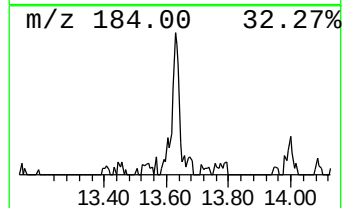
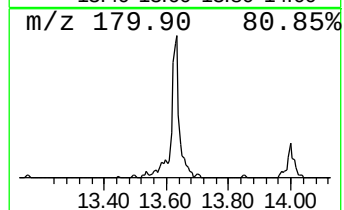
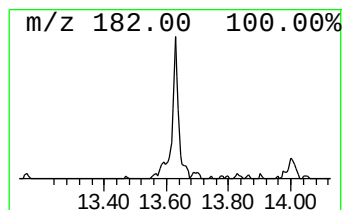
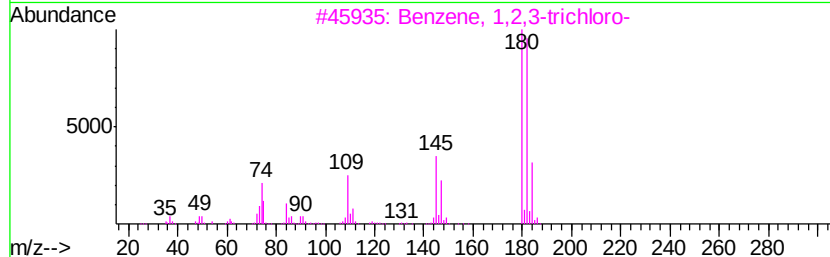
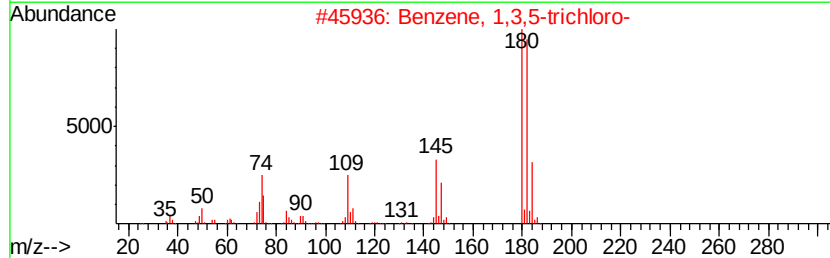
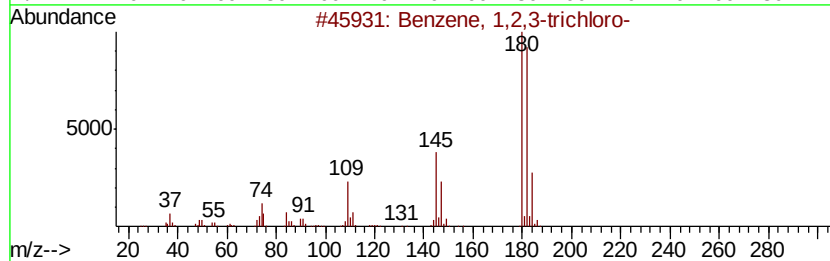
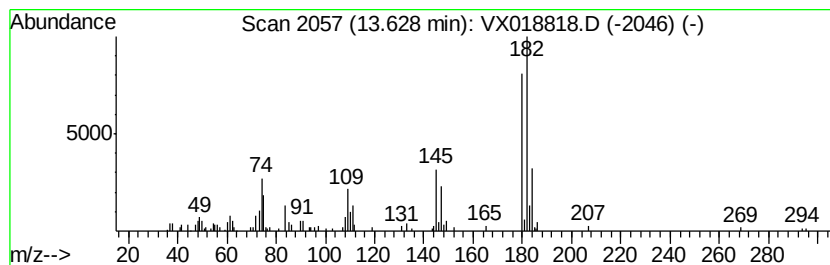
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzene, 1,2,3-trichloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	0.58 ug/L	42982	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	97
2		Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	96
3		Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	96
4		Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	96
5		Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	95



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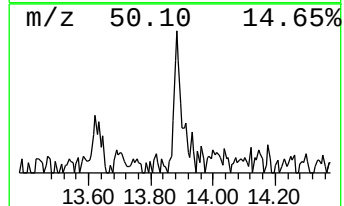
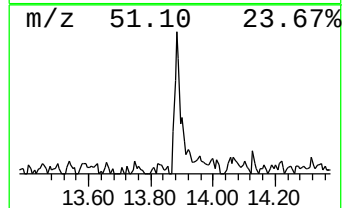
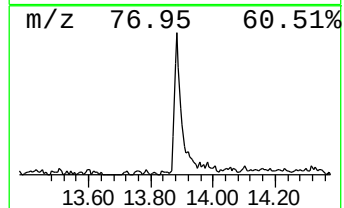
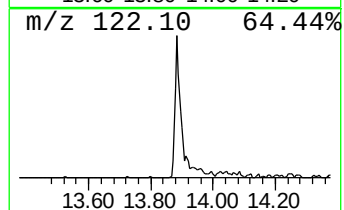
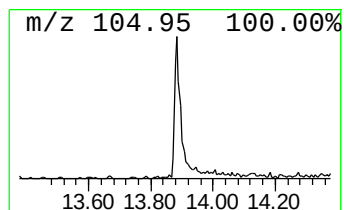
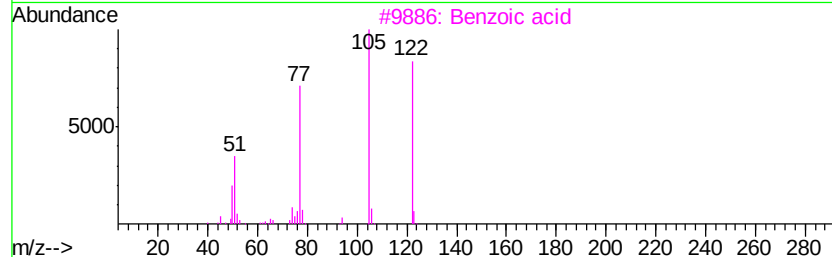
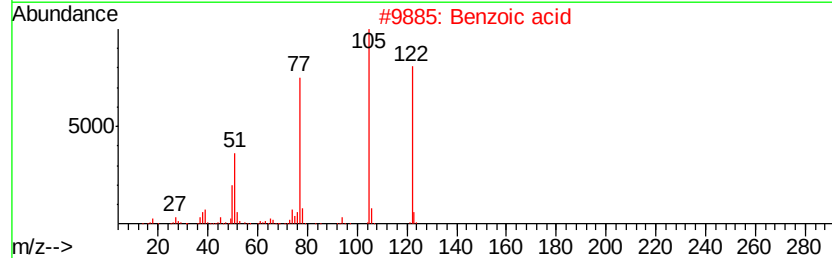
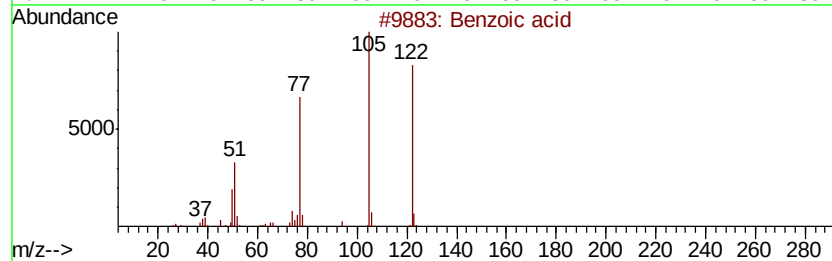
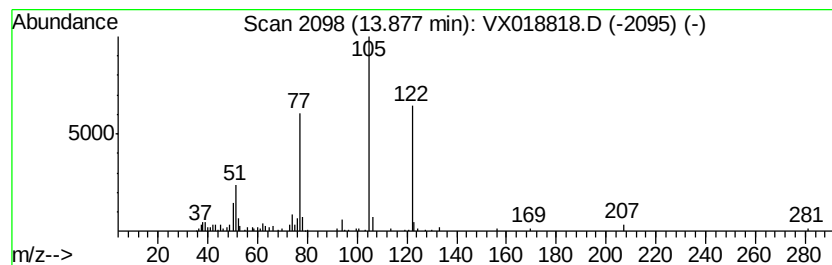
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Benzoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	0.59 ug/L	43626	1,4-Dichlorobenzene-d4	12.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid		122	C7H6O2	000065-85-0	95
2	Benzoic acid		122	C7H6O2	000065-85-0	95
3	Benzoic acid		122	C7H6O2	000065-85-0	95
4	Methanol, oxo-, benzoate		150	C8H6O3	1000305-65-2	90
5	2-Chloroethyl benzoate		184	C9H9ClO2	000939-55-9	83



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Sulfur dioxide	1.46	0.6	ug/L	46684	1	6.83	362974	5.0
(DEL) Alkane: Str...	3.15	2.0	ug/L	141852	1	6.83	362974	5.0
(DEL) Alkane: Str...	3.50	4.2	ug/L	303562	1	6.83	362974	5.0
Benzene, 1,2,3-tr...	13.63	0.6	ug/L	42982	3	12.06	368321	5.0
Benzoic acid	13.88	0.6	ug/L	43626	3	12.06	368321	5.0