

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100520\
 Data File : VX018782.D
 Acq On : 05 Oct 2020 22:35
 Operator : JC/SP
 Sample : L4240-03 40X
 Misc : 25.0mL/MSVOA X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BG3R0

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	56	rVB	66838	64782	2.79%	0.522%
2	1.477	56	64	66	rBV2	25243	71225	3.07%	0.574%
3	1.697	96	100	107	rVB	54157	66697	2.87%	0.537%
4	2.343	200	206	218	rVB	126461	197507	8.51%	1.591%
5	2.825	278	285	287	rBV2	59918	120081	5.18%	0.967%
6	2.867	287	292	304	rVV	366129	751538	32.39%	6.054%
7	3.148	329	338	353	rBV	639004	1429178	61.59%	11.514%
8	3.501	383	396	413	rBV	1031193	2320339	100.00%	18.693%
9	4.117	486	497	511	rBV2	51630	161618	6.97%	1.302%
10	4.276	513	523	530	rVV2	35273	106361	4.58%	0.857%
11	4.373	530	539	551	rVB	286398	817177	35.22%	6.583%
12	4.556	557	569	581	rBV	49449	201035	8.66%	1.620%
13	5.141	652	665	680	rBV	78257	251841	10.85%	2.029%
14	5.550	723	732	740	rBV2	20929	64370	2.77%	0.519%
15	6.043	800	813	827	rBV2	185509	545762	23.52%	4.397%
16	6.830	932	942	950	rBV	132050	358396	15.45%	2.887%
17	7.366	1021	1030	1038	rBV	117306	257723	11.11%	2.076%
18	8.372	1190	1195	1202	rVB	83630	137640	5.93%	1.109%
19	8.647	1233	1240	1243	rBV2	27191	50990	2.20%	0.411%
20	8.695	1243	1248	1256	rVB	298716	472641	20.37%	3.808%
21	8.817	1263	1268	1273	rBV	23704	38708	1.67%	0.312%
22	8.994	1293	1297	1299	rVV	54456	85193	3.67%	0.686%
23	9.019	1299	1301	1310	rVB	59420	87211	3.76%	0.703%
24	9.147	1316	1322	1327	rVB2	21010	34449	1.48%	0.278%
25	9.427	1362	1368	1379	rBV	381042	561492	24.20%	4.523%
26	9.555	1384	1389	1393	rVV4	14393	23770	1.02%	0.191%
27	10.098	1472	1478	1479	rBV	294820	382248	16.47%	3.079%
28	10.122	1479	1482	1488	rVB	478130	644461	27.77%	5.192%
29	10.342	1509	1518	1525	rBV	16068	26473	1.14%	0.213%
30	11.232	1659	1664	1670	rBV	125900	161235	6.95%	1.299%
31	11.421	1689	1695	1702	rBV	18657	38109	1.64%	0.307%
32	11.792	1751	1756	1761	rVB	39686	48801	2.10%	0.393%
33	12.006	1785	1791	1796	rBV	86169	119233	5.14%	0.961%
34	12.061	1796	1800	1808	rVV2	313148	562316	24.23%	4.530%

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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	12.305	1832	1840	1844	rBV3	23914	47771	2.06%	0.385%
36	12.359	1844	1849	1856	rVB	384875	500117	21.55%	4.029%
37	12.573	1878	1884	1885	rBV	27333	35310	1.52%	0.284%
38	12.591	1885	1887	1892	rVB	29528	33011	1.42%	0.266%
39	12.652	1892	1897	1900	rBV	56503	66234	2.85%	0.534%
40	12.756	1908	1914	1919	rBV6	15923	35180	1.52%	0.283%
41	12.884	1931	1935	1940	rVB2	18844	26660	1.15%	0.215%
42	12.963	1940	1948	1951	rBV	41002	55995	2.41%	0.451%
43	13.000	1951	1954	1960	rVB	63733	80253	3.46%	0.647%
44	13.207	1981	1988	1992	rVB3	17856	27958	1.20%	0.225%
45	13.329	2004	2008	2014	rVV2	47844	78340	3.38%	0.631%
46	13.628	2052	2057	2064	rVV3	39063	71070	3.06%	0.573%
47	13.890	2096	2100	2106	rBV2	16287	25053	1.08%	0.202%
48	14.255	2154	2160	2168	rBV5	14000	30883	1.33%	0.249%
49	14.676	2222	2229	2233	rBV3	20264	38594	1.66%	0.311%

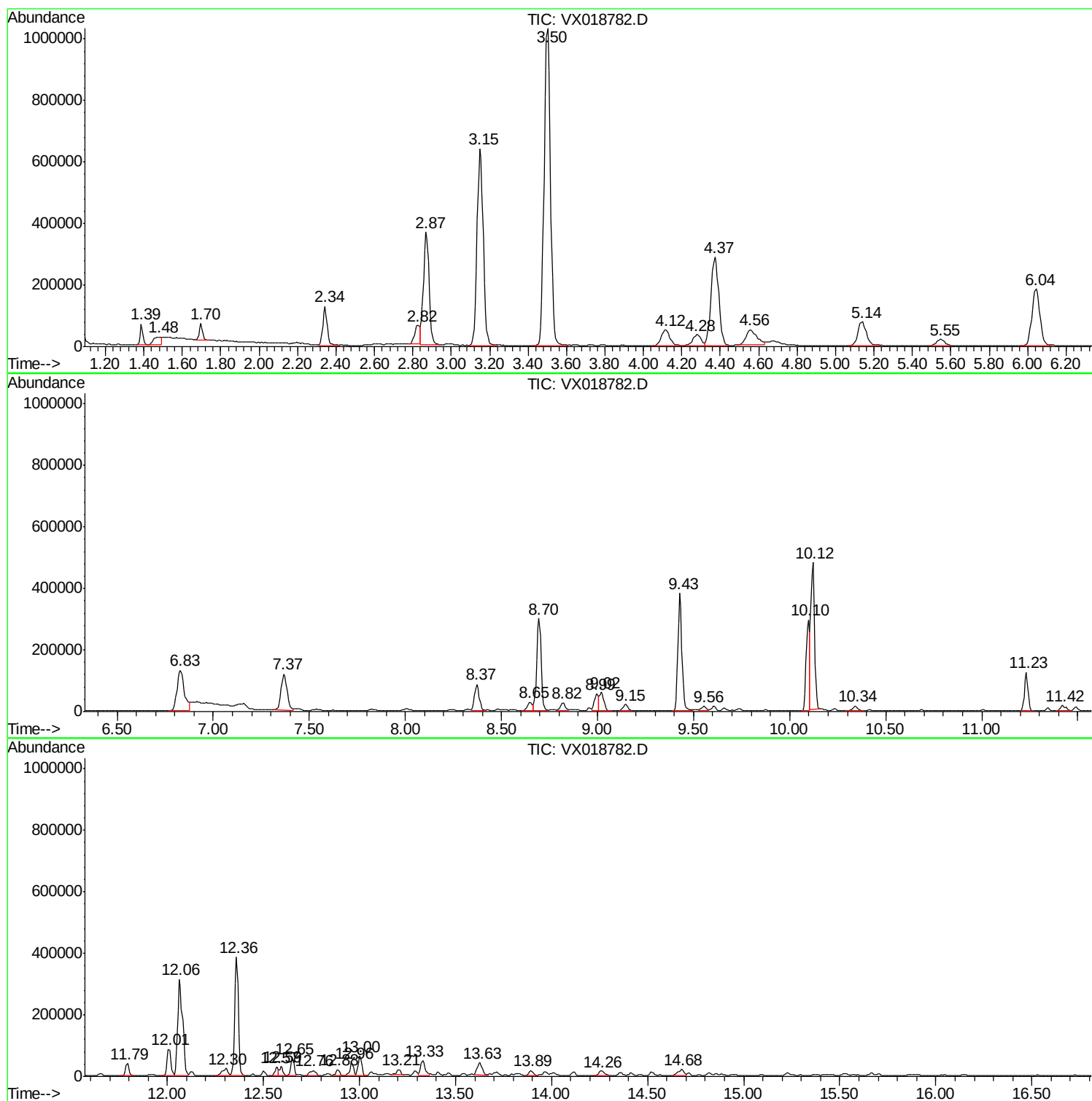
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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



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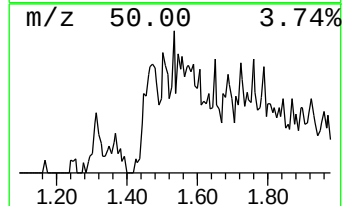
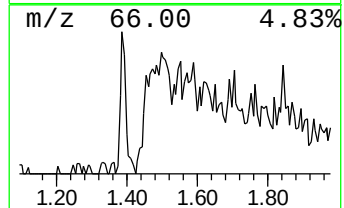
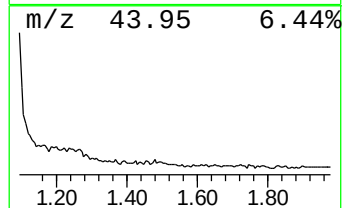
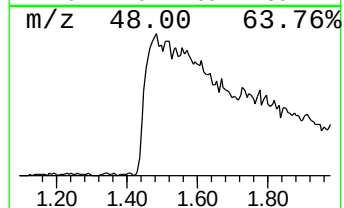
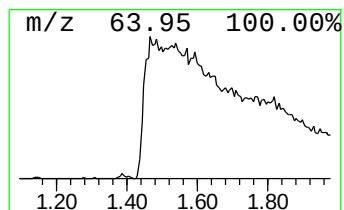
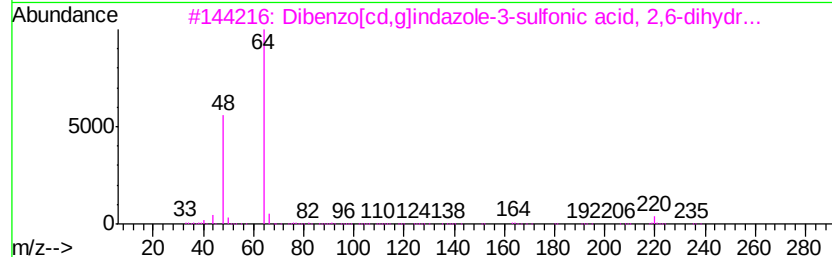
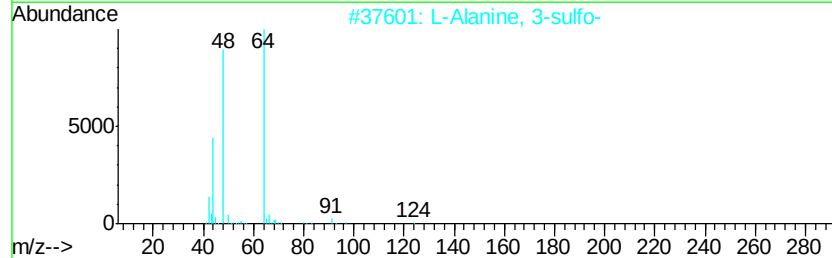
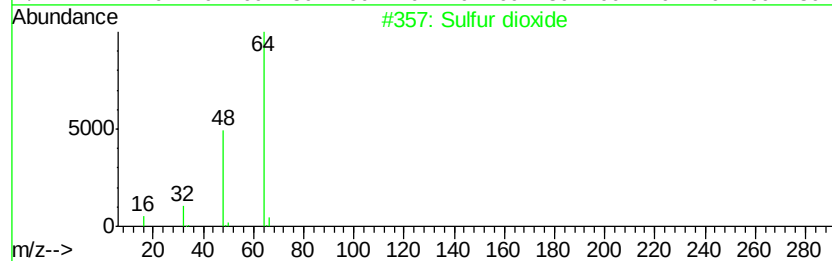
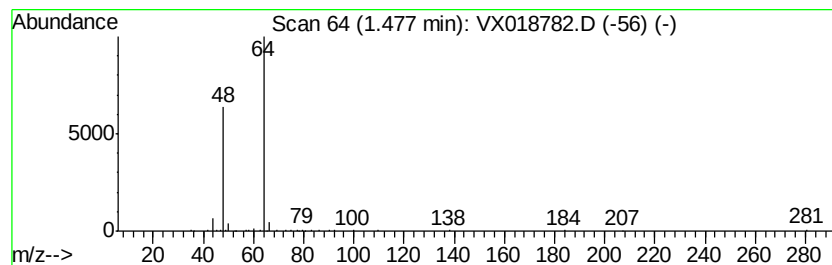
Instrument :
MSVOA_X
ClientSampleId :
BG3R0

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

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	0.99 ug/L	71225	1,4-Difluorobenzene	6.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Sulfur dioxide	64 O2S	007446-09-5 90
2		L-Alanine, 3-sulfo-	169 C3H7NO5S	000498-40-8 64
3		Dibenzo[cd,g]indazole-3-sulfonic...	300 C14H8N2O4S	293765-87-4 64
4		Aminomethanesulfonic acid	111 CH5NO3S	013881-91-9 64
5		Methanethiol, (N-cycloheptylmeth...	280 C10H20N2O3S2	040283-61-2 9



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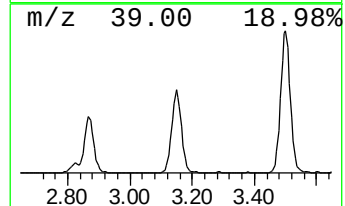
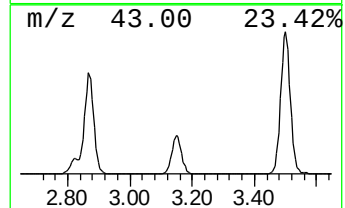
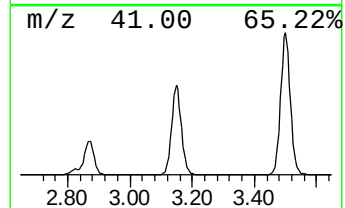
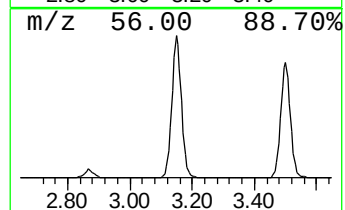
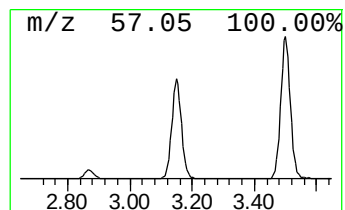
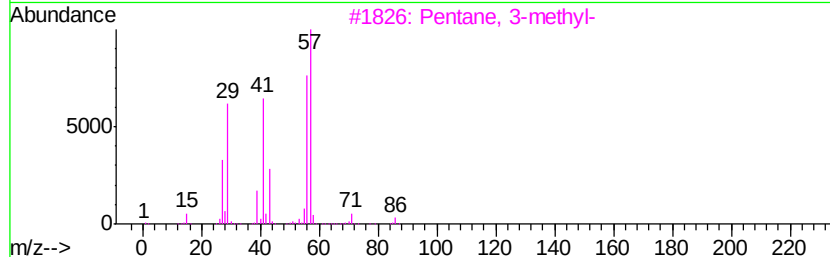
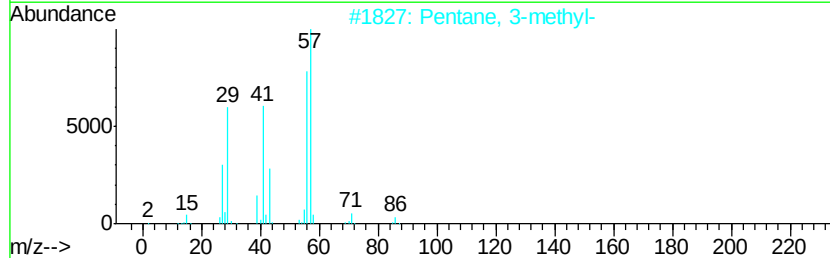
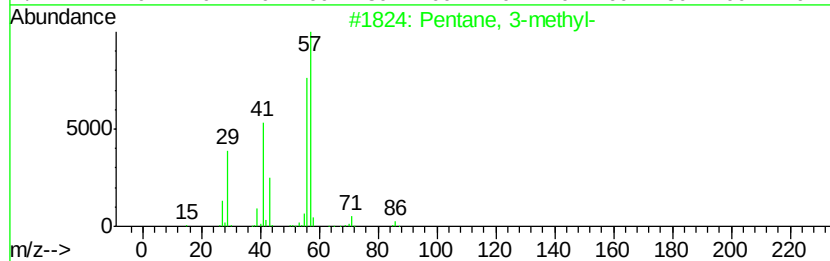
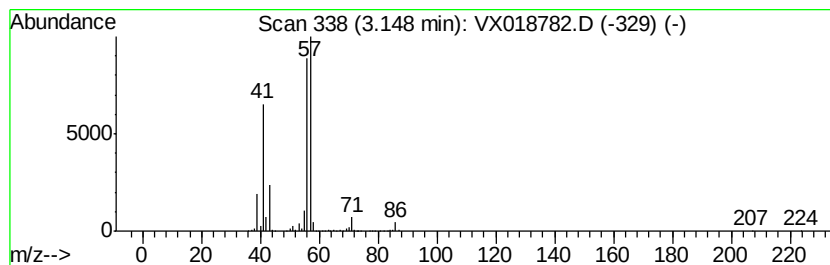
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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	19.94 ug/L	1429180	1,4-Difluorobenzene	6.83

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	90
3		Pentane, 3-methyl-	86	C6H14	000096-14-0	90
4		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
5		3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	53



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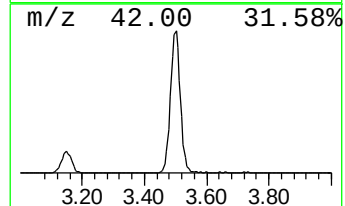
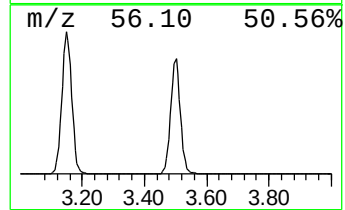
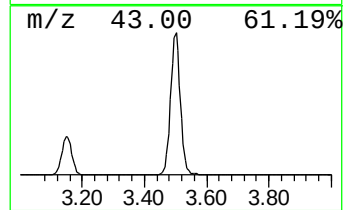
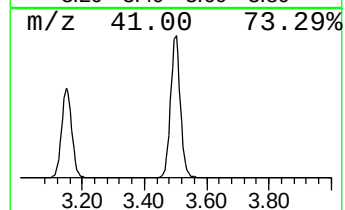
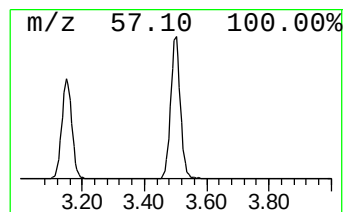
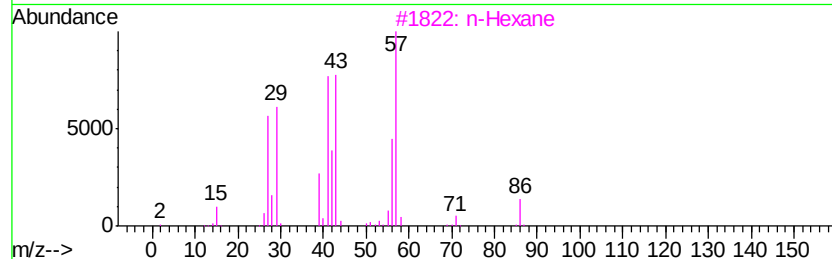
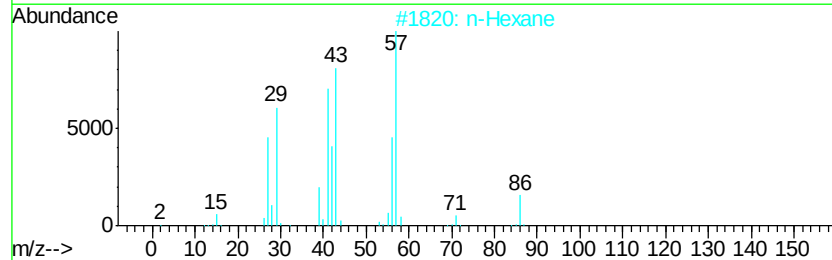
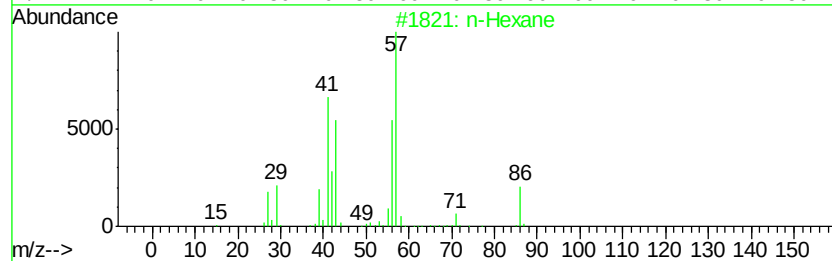
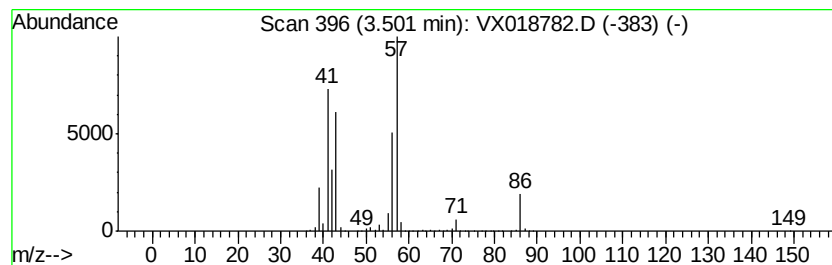
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Quant Title : TRACE VOA SOM01.0

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.
3.50	32.37 ug/L	2320340	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	64
4		Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	53
5		Butanal, 2-methyl-	86	C5H10O	000096-17-3	43



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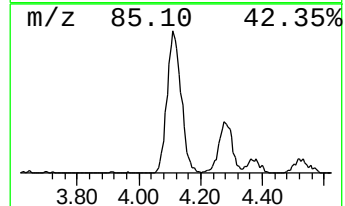
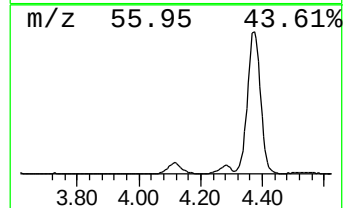
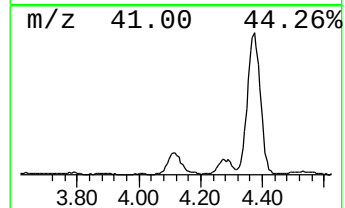
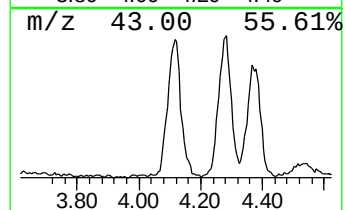
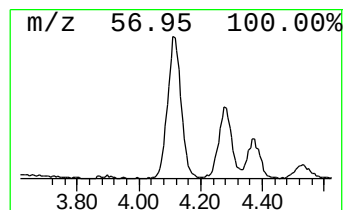
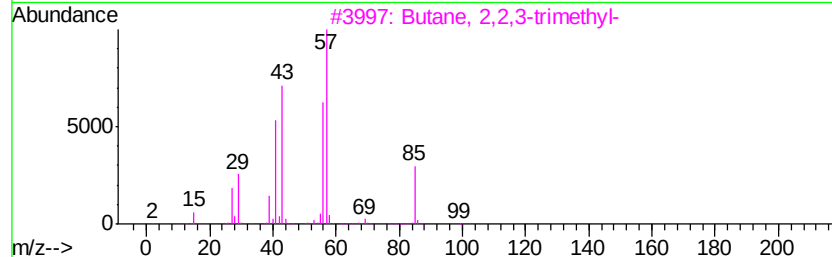
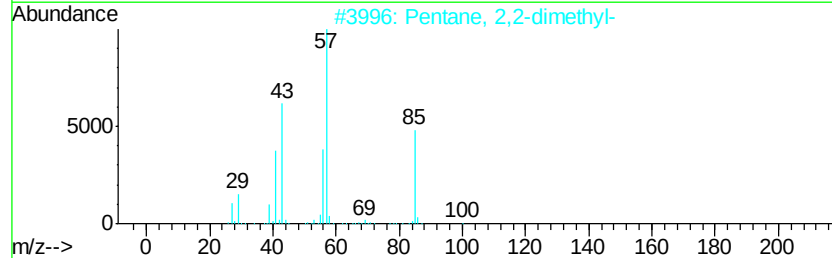
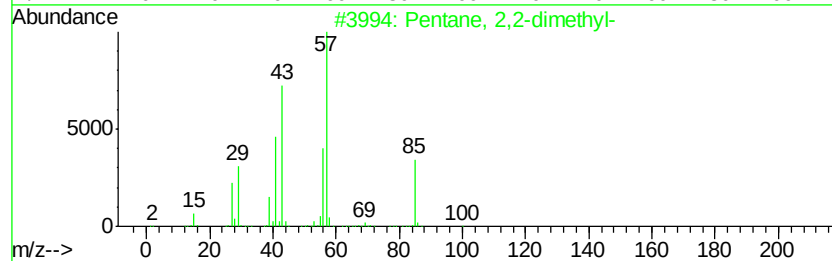
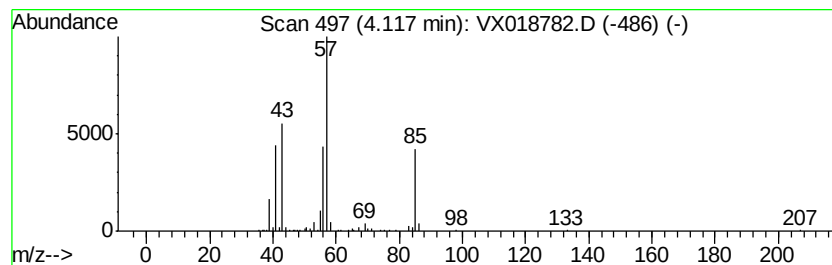
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.12	2.25 ug/L	161618	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	78
2		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	78
3		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
4		Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	74
5		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	64



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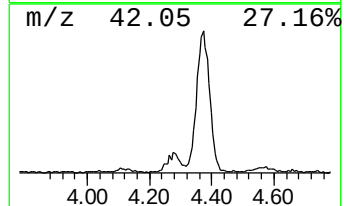
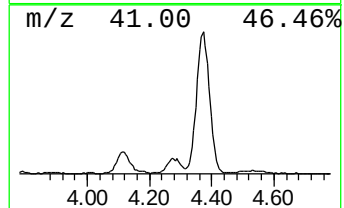
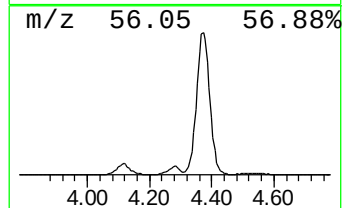
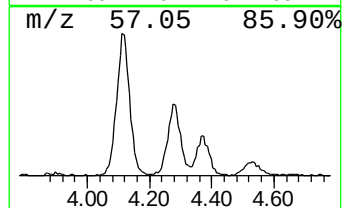
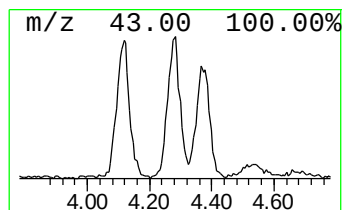
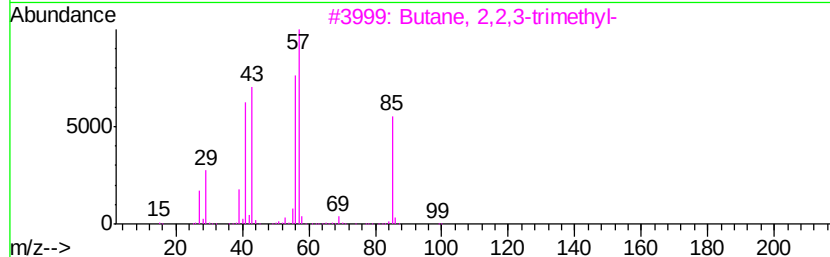
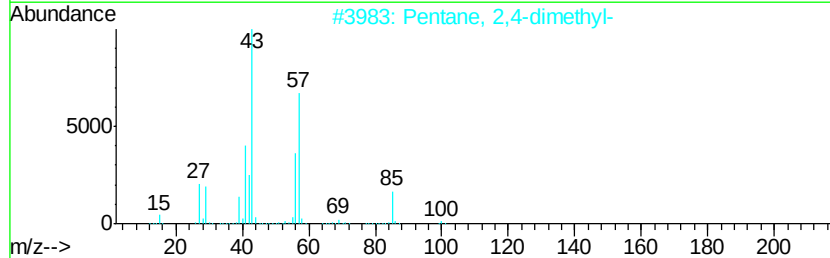
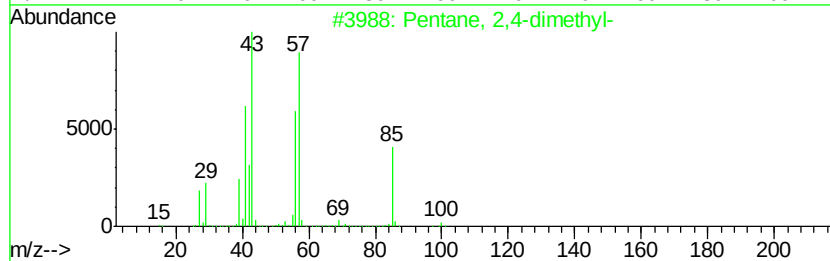
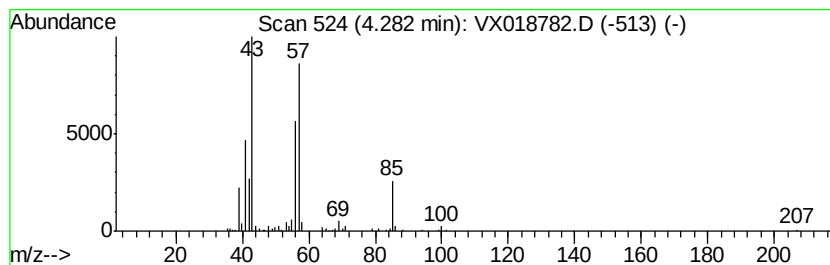
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.28	1.48 ug/L	106361	1,4-Difluorobenzene	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	93
2			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	76
3			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53
4			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	50
5			Hexane, 2-methyl-	100	C7H16	000591-76-4	47



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018782.D
Acq On : 05 Oct 2020 22:35
Operator : JC/SP
Sample : L4240-03 40X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3R0

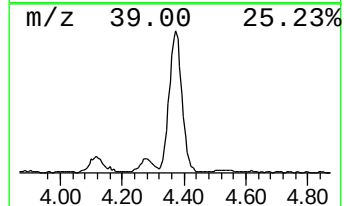
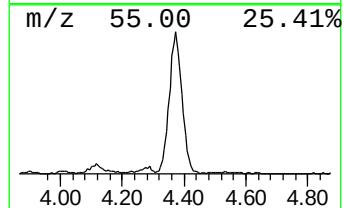
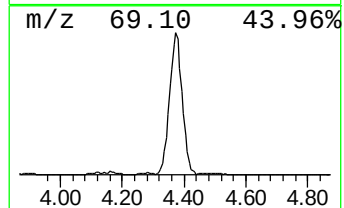
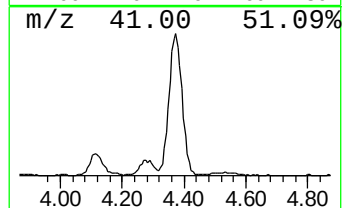
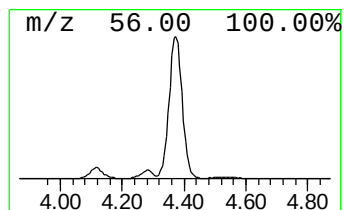
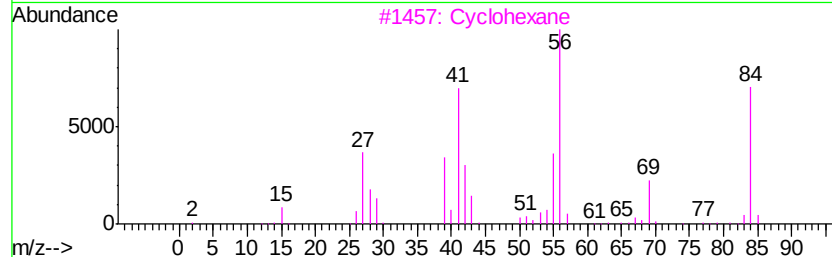
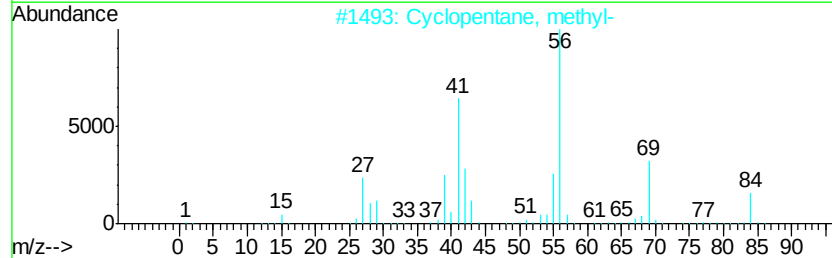
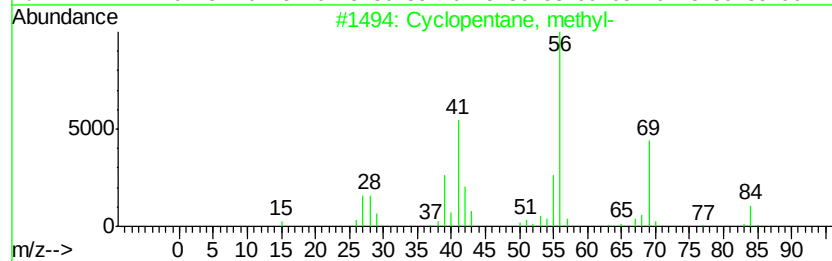
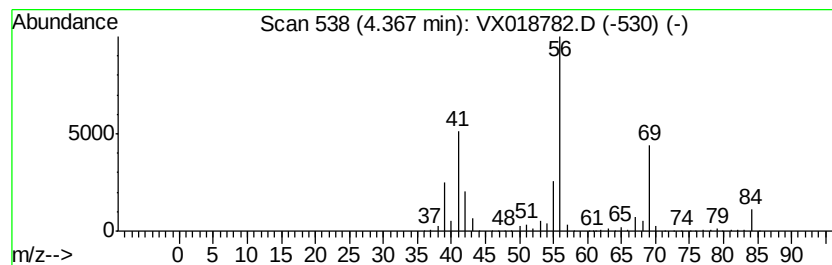
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 (DEL) Alkane: Cyclic4.37 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	11.40 ug/L	817177	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	90
3		Cyclohexane	84	C6H12	000110-82-7	86
4		Cyclohexane	84	C6H12	000110-82-7	86
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	80



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018782.D
Acq On : 05 Oct 2020 22:35
Operator : JC/SP
Sample : L4240-03 40X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 24 Sample Multiplier: 1

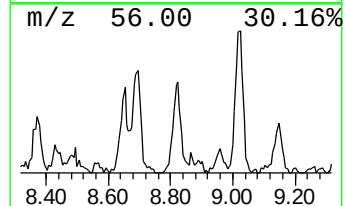
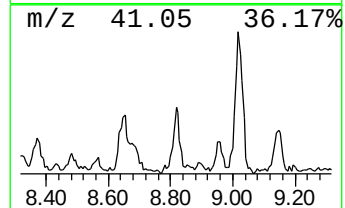
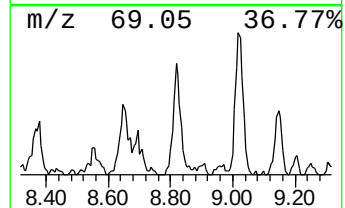
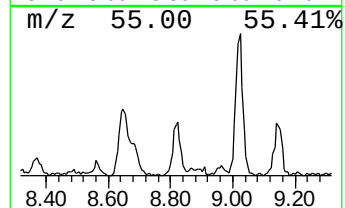
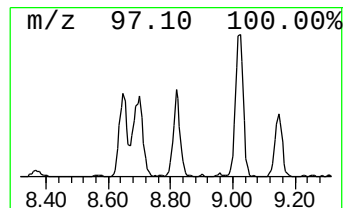
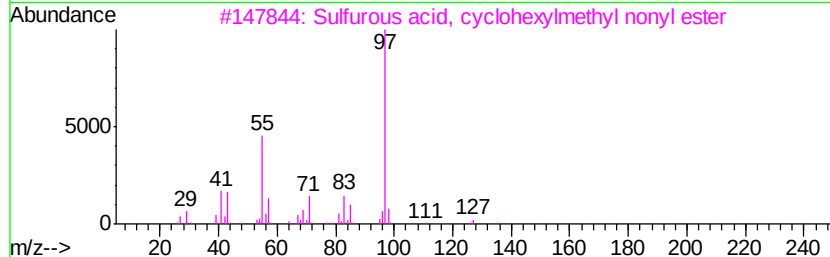
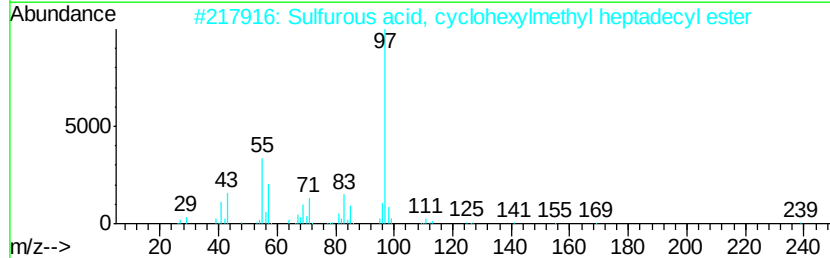
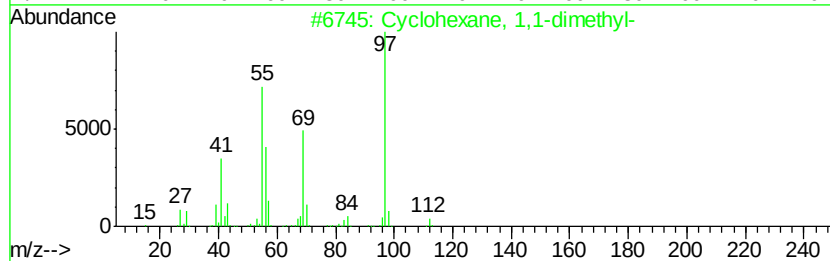
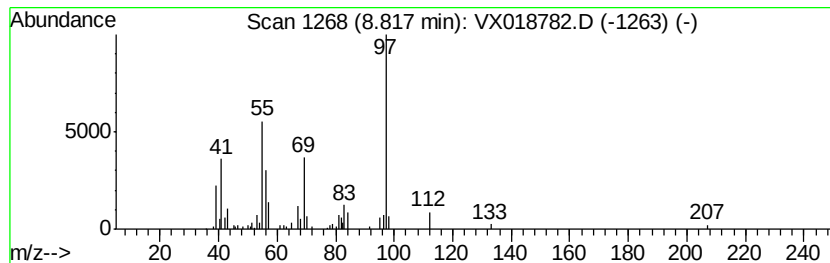
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ClientSampled :
BG3R0

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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 (DEL) Alkane: Cyclic8.82 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.82	0.51 ug/L	38708	Chlorobenzene-d5	10.10	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	68
2	Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	59
3	Sulfurous acid, cyclohexylmethyl...	304	C16H32O3S	1000309-21-8	59
4	Cyclohexanepropanoic acid	156	C9H16O2	000701-97-3	53
5	Cyclohexane, 1-bromo-2-methyl-	176	C7H13Br	006294-39-9	53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018782.D
Acq On : 05 Oct 2020 22:35
Operator : JC/SP
Sample : L4240-03 40X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 24 Sample Multiplier: 1

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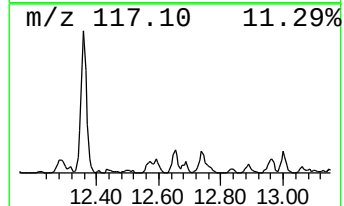
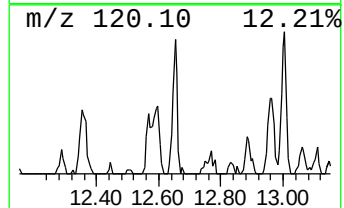
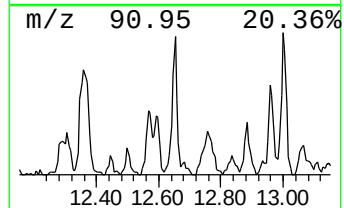
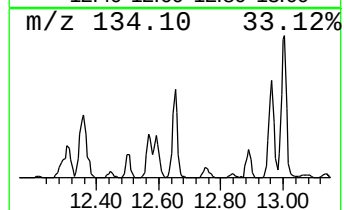
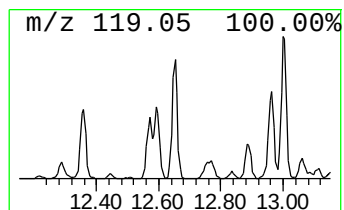
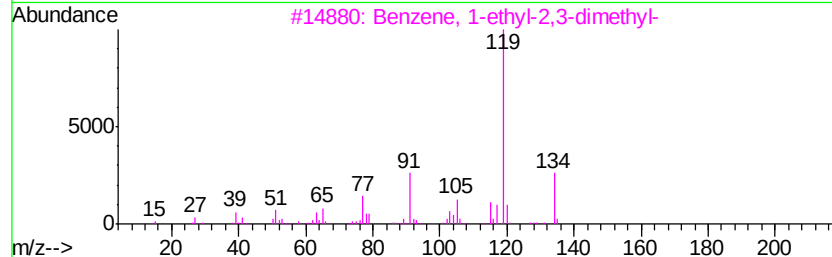
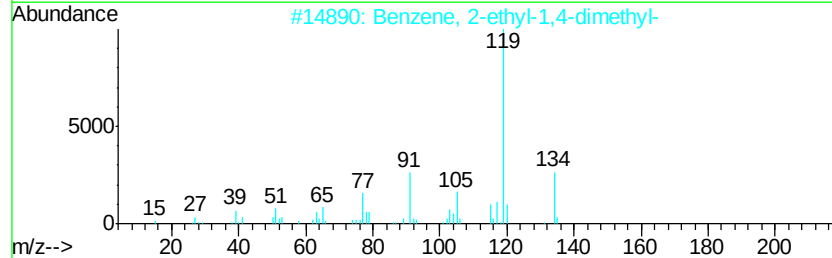
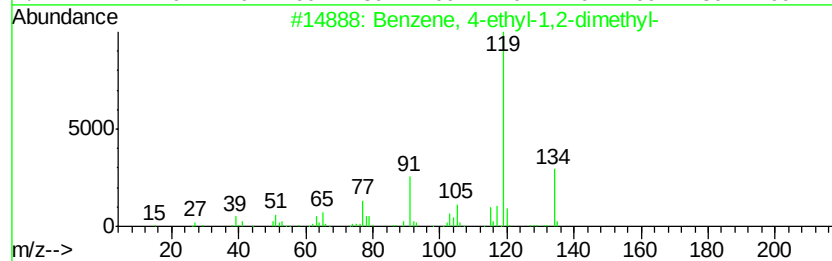
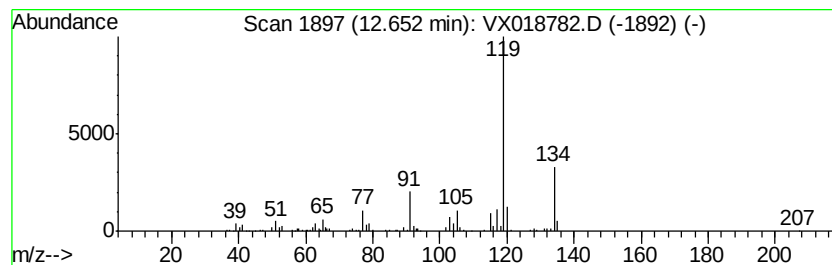
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	0.59 ug/L	66234	1,4-Dichlorobenzene-d4	12.06

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	97
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
4	o-Cymene	134	C10H14	000527-84-4	95
5	o-Cymene	134	C10H14	000527-84-4	95



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018782.D
Acq On : 05 Oct 2020 22:35
Operator : JC/SP
Sample : L4240-03 40X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
BG3R0

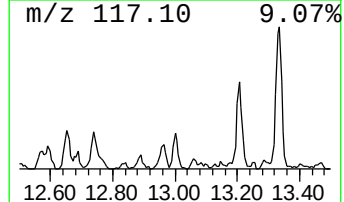
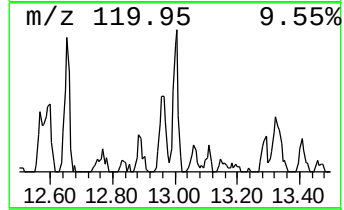
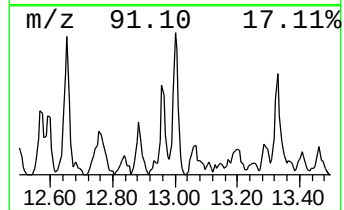
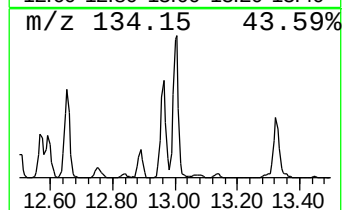
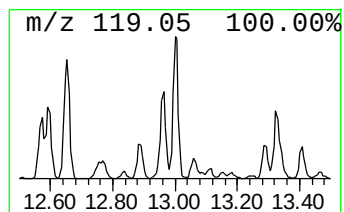
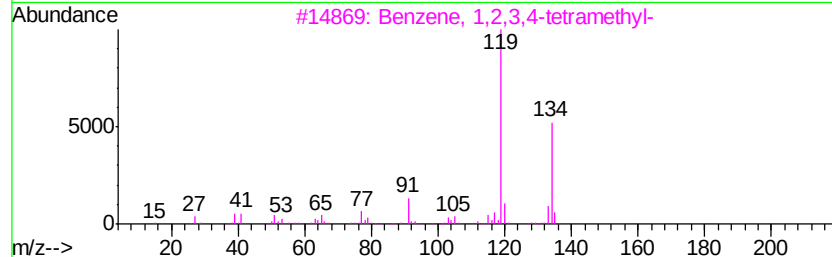
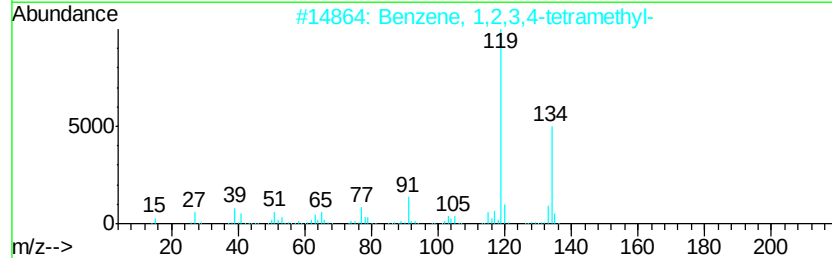
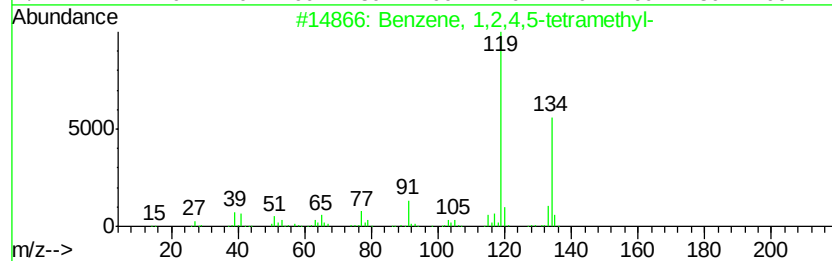
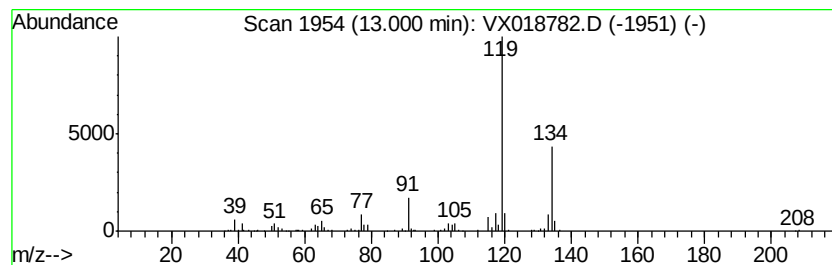
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.00	0.71 ug/L	80253	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
4		p-Cymene	134	C10H14	000099-87-6	91
5		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX100520\
Data File : VX018782.D
Acq On : 05 Oct 2020 22:35
Operator : JC/SP
Sample : L4240-03 40X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3R0

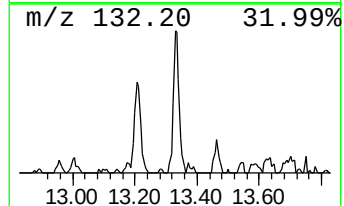
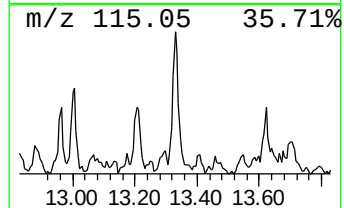
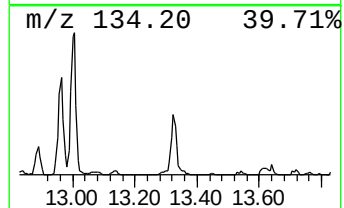
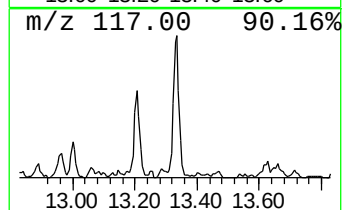
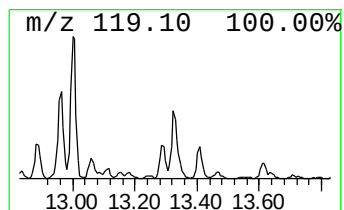
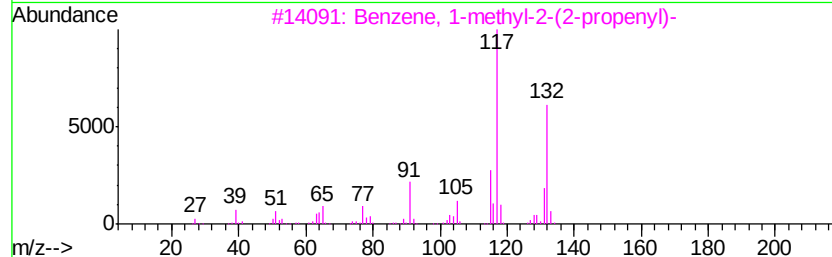
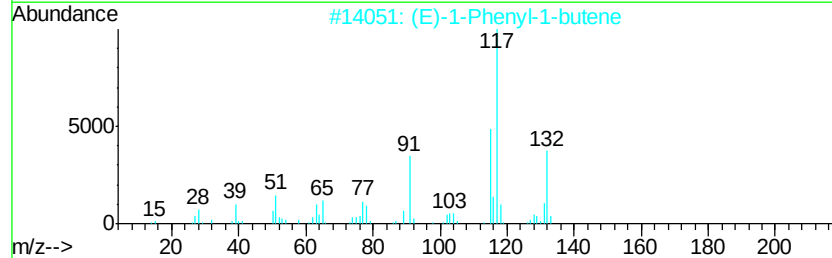
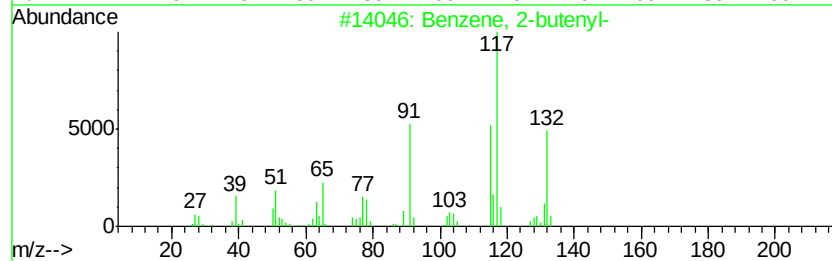
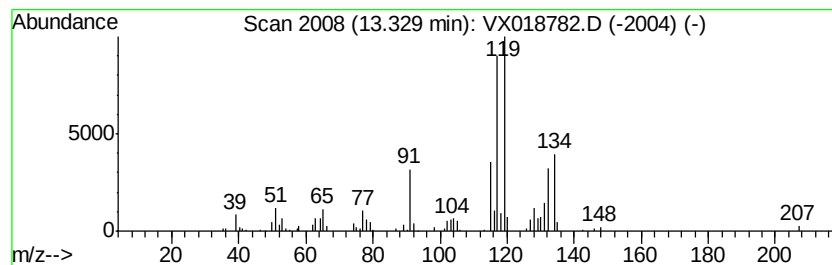
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 11 Benzene, 2-butenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	0.70 ug/L	78340	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	64
2		(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	64
3		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	50
4		3-Phenylbut-1-ene	132	C10H12	000934-10-1	50
5		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100520\
Data File : VX018782.D
Acq On : 05 Oct 2020 22:35
Operator : JC/SP
Sample : L4240-03 40X
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3R0

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
Sulfur dioxide	1.48	1.0	ug/L	71225	1	6.83	358396	5.0
(DEL) Alkane: Str...	3.15	19.9	ug/L	1429180	1	6.83	358396	5.0
(DEL) Alkane: Str...	3.50	32.4	ug/L	2320340	1	6.83	358396	5.0
(DEL) Alkane: Str...	4.12	2.3	ug/L	161618	1	6.83	358396	5.0
(DEL) Alkane: Str...	4.28	1.5	ug/L	106361	1	6.83	358396	5.0
(DEL) Alkane: Cyc...	4.37	11.4	ug/L	817177	1	6.83	358396	5.0
(DEL) Alkane: Cyc...	8.82	0.5	ug/L	38708	2	10.10	382248	5.0
Benzene, 4-ethyl-...	12.65	0.6	ug/L	66234	3	12.06	562316	5.0
Benzene, 1,2,4,5-...	13.00	0.7	ug/L	80253	3	12.06	562316	5.0
Benzene, 2-butenyl-	13.33	0.7	ug/L	78340	3	12.06	562316	5.0