

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100720\
 Data File : VX018820.D
 Acq On : 07 Oct 2020 18:57
 Operator : JC/SP
 Sample : L4240-15DL 40X
 Misc : 25.0mL/MSVOA X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BG3T7DL

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	57	rVB	56486	57283	9.80%	0.771%
2	1.508	61	69	71	rBV2	17545	40054	6.86%	0.539%
3	1.697	96	100	106	rVB	53979	63011	10.78%	0.848%
4	2.191	178	181	186	rVB3	4304	5876	1.01%	0.079%
5	2.343	199	206	215	rBV	106618	168569	28.85%	2.268%
6	2.825	277	285	287	rBV2	29780	55367	9.48%	0.745%
7	2.867	287	292	302	rVV	115357	241393	41.32%	3.248%
8	2.989	306	312	318	rBV4	3477	8666	1.48%	0.117%
9	3.148	329	338	347	rBV	212032	476276	81.52%	6.408%
10	3.501	386	396	409	rBV	244662	558421	95.58%	7.513%
11	4.117	488	497	503	rBV4	7426	23501	4.02%	0.316%
12	4.373	529	539	552	rVB3	103981	300054	51.36%	4.037%
13	4.556	558	569	583	rBV	52386	228540	39.12%	3.075%
14	5.135	653	664	678	rBV2	77238	243748	41.72%	3.279%
15	5.544	723	731	739	rBV6	7909	23360	4.00%	0.314%
16	6.043	801	813	829	rBV2	182255	533847	91.37%	7.182%
17	6.830	931	942	950	rBV2	134526	334454	57.24%	4.500%
18	6.940	950	960	961	rBV3	10034	27746	4.75%	0.373%
19	7.366	1021	1030	1044	rBV	112845	252192	43.16%	3.393%
20	8.372	1189	1195	1205	rBV	72237	119781	20.50%	1.611%
21	8.647	1233	1240	1242	rBV6	5595	9637	1.65%	0.130%
22	8.695	1242	1248	1256	rVB	261578	413575	70.79%	5.564%
23	8.817	1263	1268	1273	rBV7	4159	7212	1.23%	0.097%
24	8.994	1291	1297	1308	rVB2	50520	90176	15.43%	1.213%
25	9.147	1318	1322	1328	rVB6	4839	7824	1.34%	0.105%
26	9.427	1362	1368	1381	rBV	406324	584252	100.00%	7.860%
27	9.549	1384	1388	1394	rVV8	4160	9440	1.62%	0.127%
28	9.738	1413	1419	1424	rBV4	6593	9329	1.60%	0.126%
29	10.098	1471	1478	1479	rBV	300721	383739	65.68%	5.163%
30	10.122	1479	1482	1489	rVB	414285	549088	93.98%	7.387%
31	10.232	1497	1500	1504	rVB3	5560	7443	1.27%	0.100%
32	10.341	1512	1518	1525	rVB	9850	15646	2.68%	0.210%
33	11.232	1657	1664	1672	rBV	129058	167921	28.74%	2.259%
34	11.341	1676	1682	1688	rVB5	4273	7685	1.32%	0.103%

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35	11.414	1691	1694	1697	rBV5	8232	12514	2.14%	0.168%
36	11.494	1703	1707	1713	rVB4	6603	9942	1.70%	0.134%
37	11.792	1751	1756	1762	rVB2	18390	25301	4.33%	0.340%
38	12.006	1787	1791	1795	rBV	49913	66880	11.45%	0.900%
39	12.061	1795	1800	1808	rVV2	296847	472590	80.89%	6.358%
40	12.128	1808	1811	1815	rVB	8201	9803	1.68%	0.132%
41	12.286	1832	1837	1838	rBV5	7864	9680	1.66%	0.130%
42	12.311	1838	1841	1844	rVV2	9573	12753	2.18%	0.172%
43	12.359	1844	1849	1857	rVB	343604	423291	72.45%	5.695%
44	12.500	1868	1872	1876	rVB3	5935	8123	1.39%	0.109%
45	12.567	1879	1883	1885	rVV2	13394	16186	2.77%	0.218%
46	12.591	1885	1887	1892	rVB	14112	16618	2.84%	0.224%
47	12.652	1892	1897	1901	rBV	23453	28853	4.94%	0.388%
48	12.750	1907	1913	1921	rBV7	6476	15948	2.73%	0.215%
49	12.884	1931	1935	1940	rBV	8754	12578	2.15%	0.169%
50	12.963	1941	1948	1951	rVV	17768	24159	4.14%	0.325%
51	13.000	1951	1954	1960	rVB2	27394	36693	6.28%	0.494%
52	13.207	1981	1988	1994	rVB2	7557	12541	2.15%	0.169%
53	13.329	2004	2008	2015	rVB2	23318	33445	5.72%	0.450%
54	13.463	2027	2030	2035	rVB5	4284	5917	1.01%	0.080%
55	13.548	2038	2044	2047	rBV8	3049	6453	1.10%	0.087%
56	13.627	2052	2057	2065	rVV5	22038	40350	6.91%	0.543%
57	13.707	2065	2070	2075	rVB7	4342	9666	1.65%	0.130%
58	13.816	2081	2088	2095	rVB4	3285	6111	1.05%	0.082%
59	13.884	2095	2099	2107	rBV	25389	39827	6.82%	0.536%
60	13.963	2107	2112	2116	rVV8	4818	8541	1.46%	0.115%
61	14.005	2116	2119	2122	rVB5	5129	6133	1.05%	0.083%
62	14.262	2156	2161	2167	rBV6	5237	11152	1.91%	0.150%
63	14.524	2199	2204	2209	rBV8	4450	6356	1.09%	0.086%
64	14.676	2223	2229	2233	rBV5	6337	10458	1.79%	0.141%
65	14.828	2250	2254	2260	rBV7	4160	8960	1.53%	0.121%

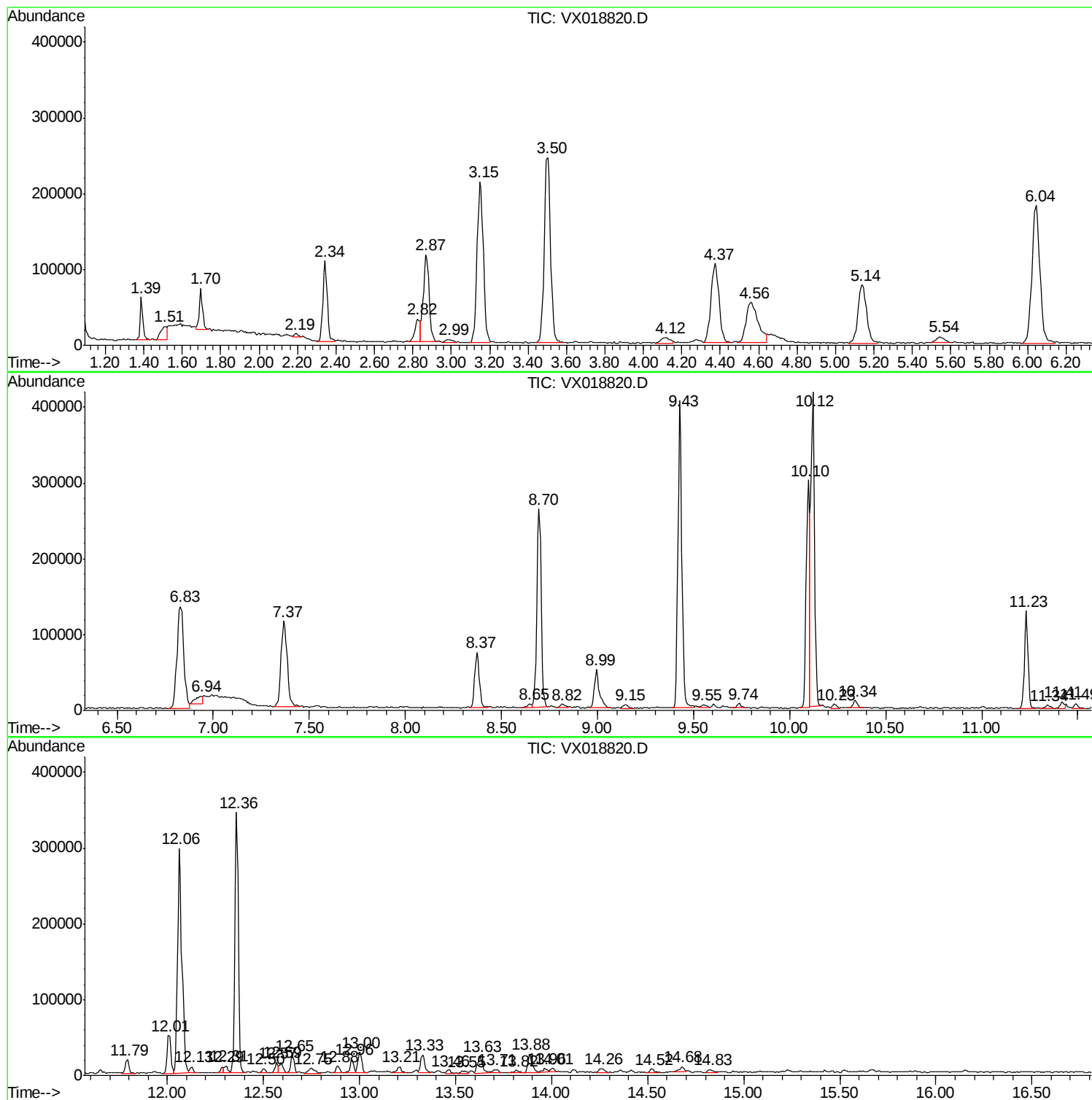
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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



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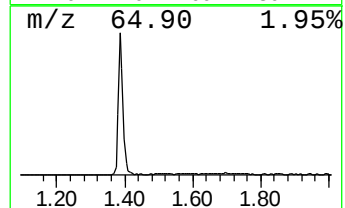
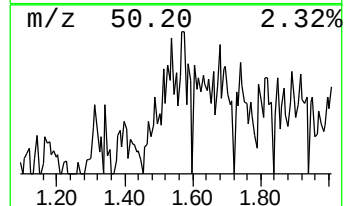
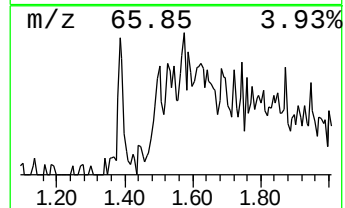
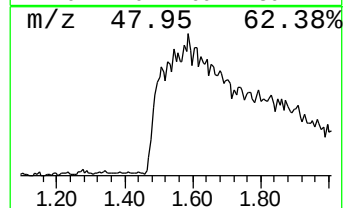
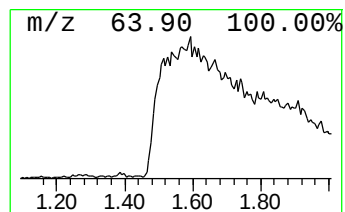
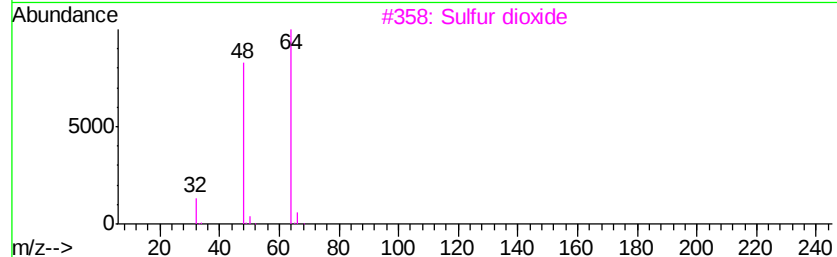
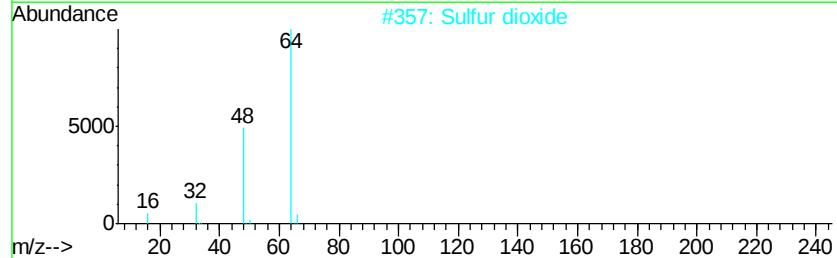
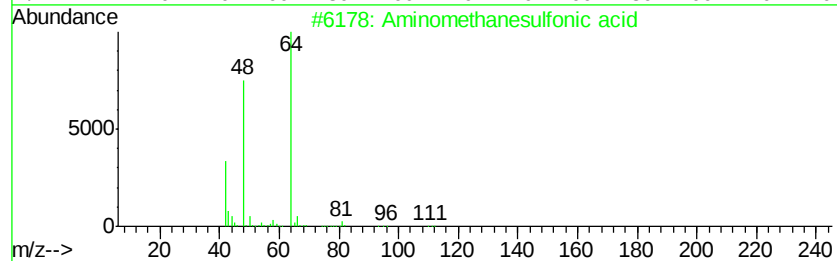
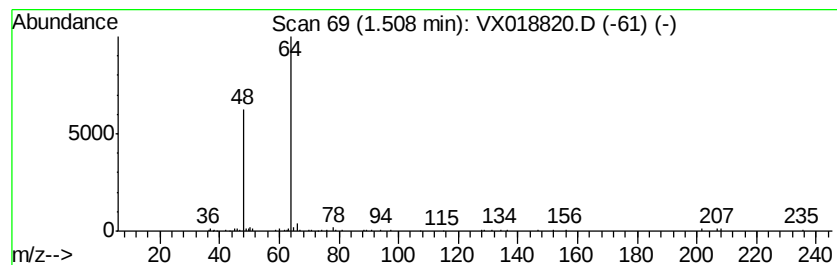
Instrument :
MSVOA_X
ClientSampleId :
BG3T7DL

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 Aminomethanesulfonic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.51	0.60 ug/L	40054	1,4-Difluorobenzene	6.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5N03S	013881-91-9	83
2	Sulfur dioxide	64	O2S	007446-09-5	74
3	Sulfur dioxide	64	O2S	007446-09-5	74
4	2-Aminoethyl hydrogen sulfate	141	C2H7N04S	000926-39-6	74
5	L-Alanine, 3-sulfo-	169	C3H7N05S	000498-40-8	74



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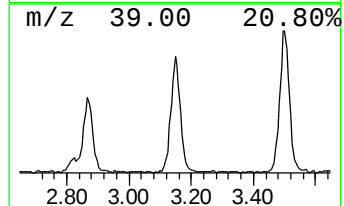
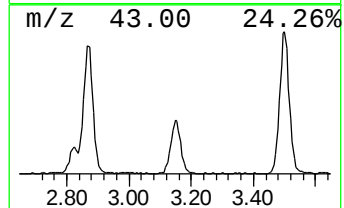
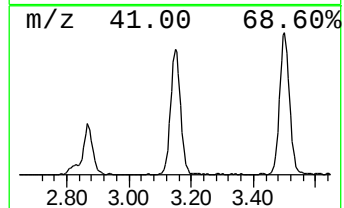
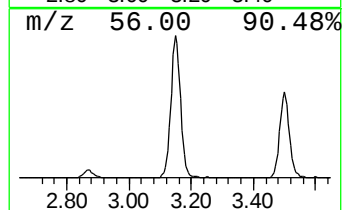
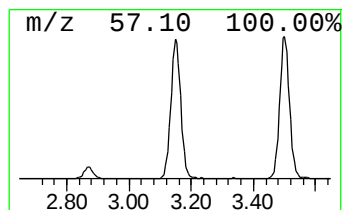
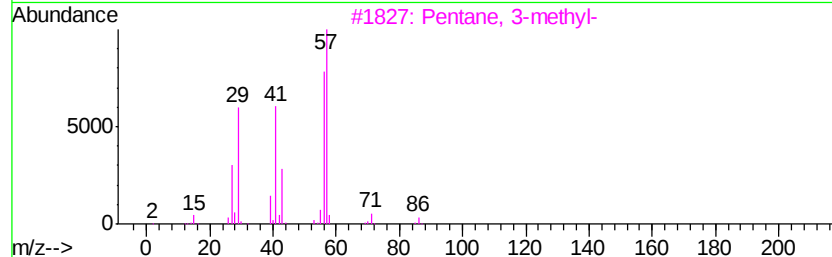
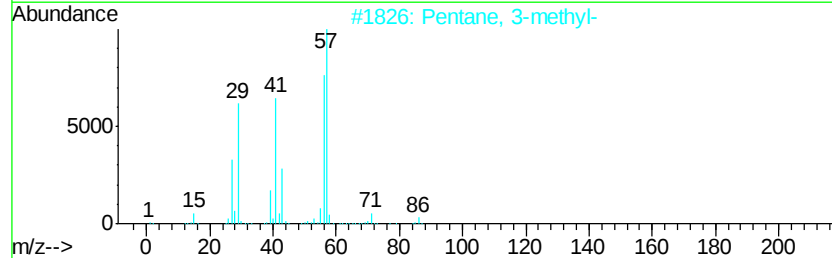
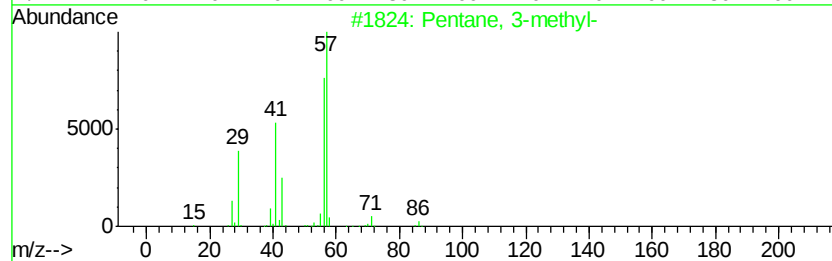
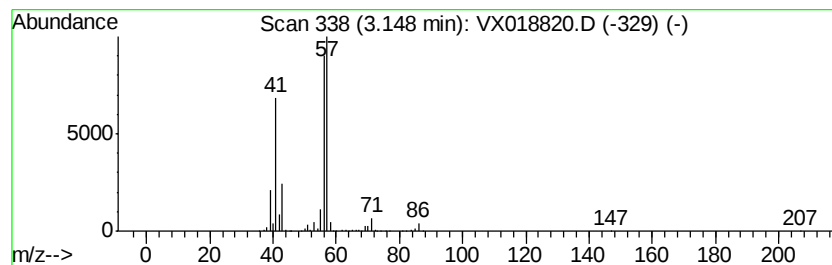
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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	7.12 ug/L	476276	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	78
5		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78



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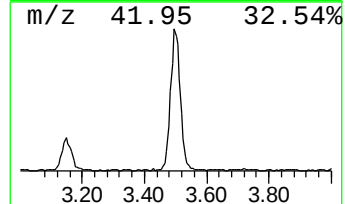
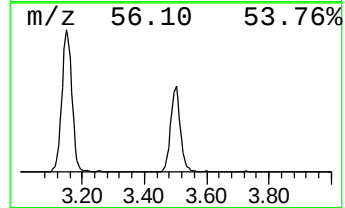
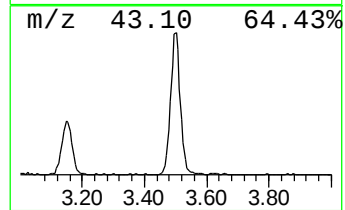
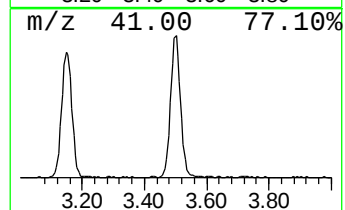
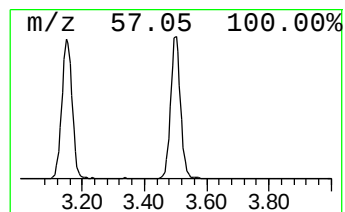
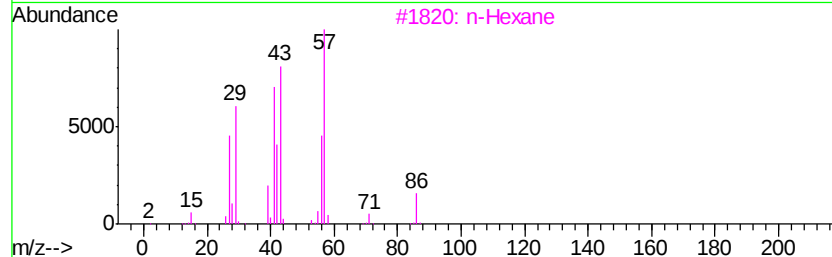
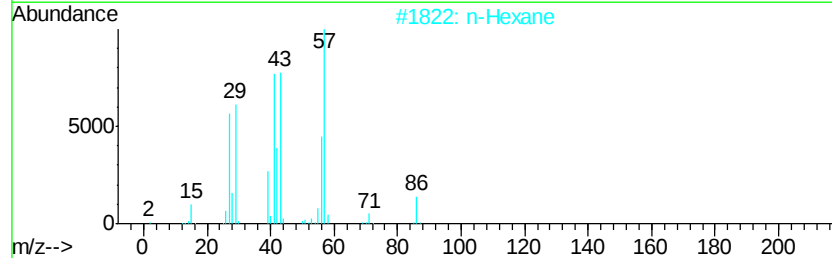
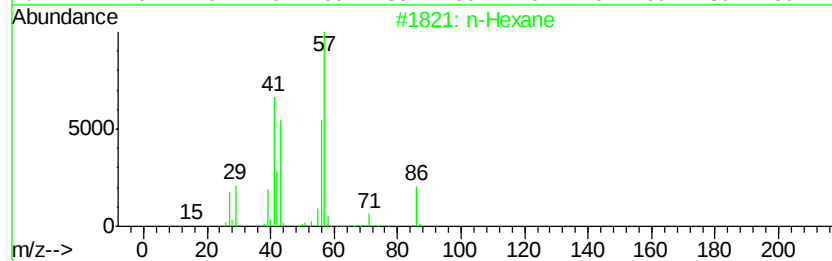
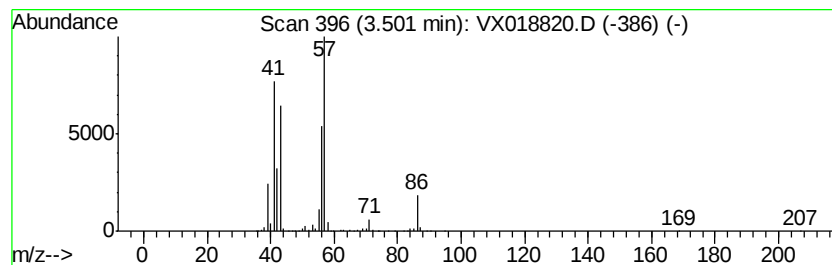
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	8.35 ug/L	558421	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		Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	47
5		Pentane, 3-methyl-	86	C6H14	000096-14-0	40



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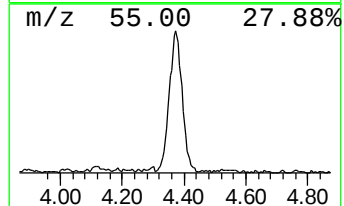
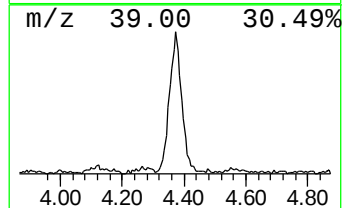
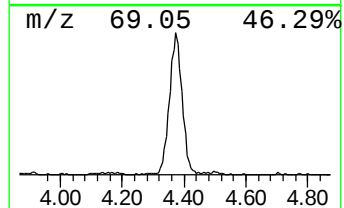
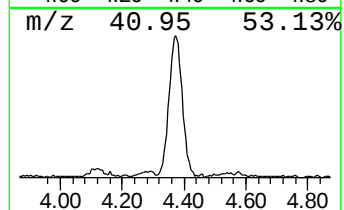
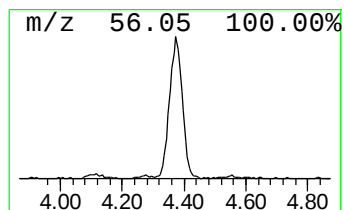
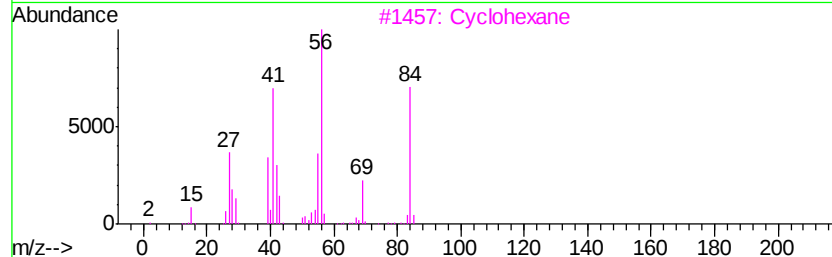
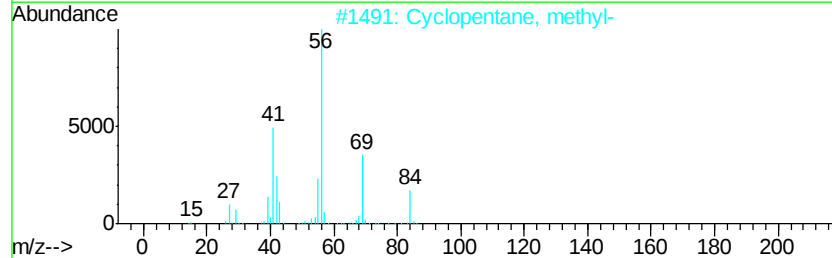
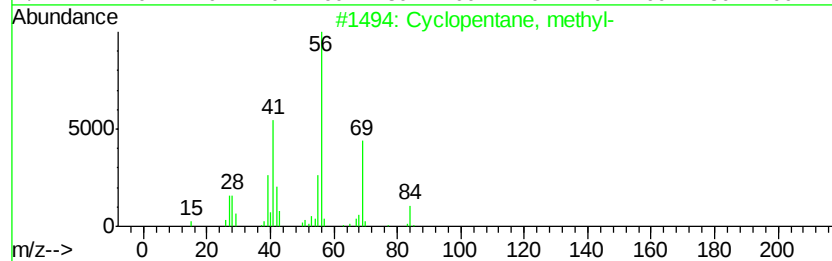
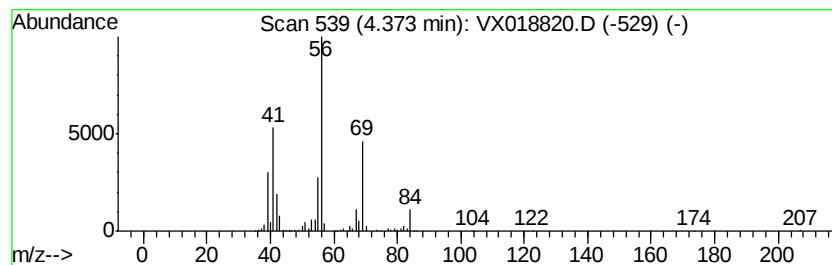
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 (DEL) Alkane: Cyclic4.37 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	4.49 ug/L	300054	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	80
3		Cyclohexane	84	C6H12	000110-82-7	80
4		Cyclopentane, methyl-	84	C6H12	000096-37-7	80
5		Cyclohexane	84	C6H12	000110-82-7	72



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BG3T7DL

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
Aminomethanesulfo...	1.51	0.6	ug/L	40054	1	6.83	334454	5.0
(DEL) Alkane: Str...	3.15	7.1	ug/L	476276	1	6.83	334454	5.0
(DEL) Alkane: Str...	3.50	8.3	ug/L	558421	1	6.83	334454	5.0
(DEL) Alkane: Cyc...	4.37	4.5	ug/L	300054	1	6.83	334454	5.0