

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX093020\
 Data File : VX018723.D
 Acq On : 01 Oct 2020 01:40
 Operator : JC/SP
 Sample : L4202-04
 Misc : 25.0mL/MSVOA X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BFSB7

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\SOMXTR092820WMA.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	1.160	9	12	20	rVB	709336	598717	81.17%	7.010%
2	1.239	22	25	29	rBV	8361	7922	1.07%	0.093%
3	1.282	29	32	34	rBV	51976	40739	5.52%	0.477%
4	1.313	34	37	41	rVB	26888	28100	3.81%	0.329%
5	1.386	44	49	54	rBV2	248521	390334	52.92%	4.570%
6	1.477	62	64	68	rVB2	6178	8584	1.16%	0.101%
7	1.520	68	71	74	rBV2	21540	23512	3.19%	0.275%
8	1.697	95	100	105	rBV2	75900	99678	13.51%	1.167%
9	1.776	108	113	118	rVB2	42072	52863	7.17%	0.619%
10	1.934	134	139	144	rBV	67159	88619	12.01%	1.038%
11	1.983	144	147	154	rVB2	49510	69612	9.44%	0.815%
12	2.099	162	166	173	rVV4	8495	15479	2.10%	0.181%
13	2.197	176	182	184	rVV4	16624	29034	3.94%	0.340%
14	2.233	184	188	195	rVB	29640	51745	7.02%	0.606%
15	2.343	201	206	214	rBV	139077	220090	29.84%	2.577%
16	2.440	218	222	230	rVB2	10195	19948	2.70%	0.234%
17	2.648	248	256	258	rBV8	7125	15254	2.07%	0.179%
18	2.873	288	293	299	rVB3	18131	35575	4.82%	0.417%
19	3.154	332	339	346	rVB2	25845	59084	8.01%	0.692%
20	3.391	369	378	386	rVB4	16116	41581	5.64%	0.487%
21	3.501	388	396	404	rVB3	40333	95004	12.88%	1.112%
22	3.715	426	431	441	rBV3	3670	9585	1.30%	0.112%
23	4.544	557	567	580	rBV	90308	297770	40.37%	3.486%
24	5.135	652	664	675	rBV2	106387	326311	44.24%	3.821%
25	5.629	740	745	750	rBV9	3598	8154	1.11%	0.095%
26	5.897	782	789	794	rBV9	4521	10795	1.46%	0.126%
27	6.043	802	813	827	rBV4	224631	677193	91.81%	7.929%
28	6.513	884	890	900	rBV4	6499	15668	2.12%	0.183%
29	6.684	913	918	924	rBV9	4798	11018	1.49%	0.129%
30	6.830	932	942	960	rBV2	260068	626331	84.92%	7.333%
31	7.183	995	1000	1006	rBV9	4803	10162	1.38%	0.119%
32	7.366	1021	1030	1042	rBV	152792	334370	45.33%	3.915%
33	8.232	1167	1172	1177	rBV9	4531	9066	1.23%	0.106%
34	8.372	1190	1195	1203	rVB	86440	149308	20.24%	1.748%

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 Sampling : 1
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 Stop Thrs : 0
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 Max Peaks: 100
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 Peak separation: 5

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 Title : TRACE VOA SOM01.0

35	8.537	1216	1222	1228	rVB	19706	36471	4.94%	0.427%
36	8.695	1242	1248	1255	rBV	337325	543227	73.65%	6.360%
37	8.762	1255	1259	1263	rVB5	7218	11551	1.57%	0.135%
38	8.994	1293	1297	1304	rVB	61929	87977	11.93%	1.030%
39	9.317	1343	1350	1357	rBV	219680	328096	44.48%	3.841%
40	9.427	1362	1368	1376	rBV	524061	728550	98.78%	8.530%
41	9.561	1387	1390	1395	rVB7	8430	10665	1.45%	0.125%
42	10.098	1470	1478	1488	rBV	536081	737581	100.00%	8.636%
43	10.890	1604	1608	1614	rBV8	4708	7609	1.03%	0.089%
44	11.232	1658	1664	1669	rBV	165386	209844	28.45%	2.457%
45	11.347	1678	1683	1688	rVB4	17111	26688	3.62%	0.312%
46	11.421	1688	1695	1696	rBV7	6758	10741	1.46%	0.126%
47	12.061	1794	1800	1808	rVV	549551	681434	92.39%	7.978%
48	12.256	1827	1832	1839	rBV2	30812	54984	7.45%	0.644%
49	12.359	1844	1849	1855	rVV	410690	514536	69.76%	6.024%
50	12.658	1893	1898	1900	rVB4	7607	10883	1.48%	0.127%
51	12.890	1931	1936	1940	rBV5	14396	19801	2.68%	0.232%
52	12.999	1951	1954	1960	rBV8	6990	10225	1.39%	0.120%
53	13.627	2052	2057	2062	rBV6	8321	14975	2.03%	0.175%
54	13.725	2068	2073	2075	rBV5	8386	9616	1.30%	0.113%
55	13.902	2098	2102	2105	rBV6	4857	8353	1.13%	0.098%

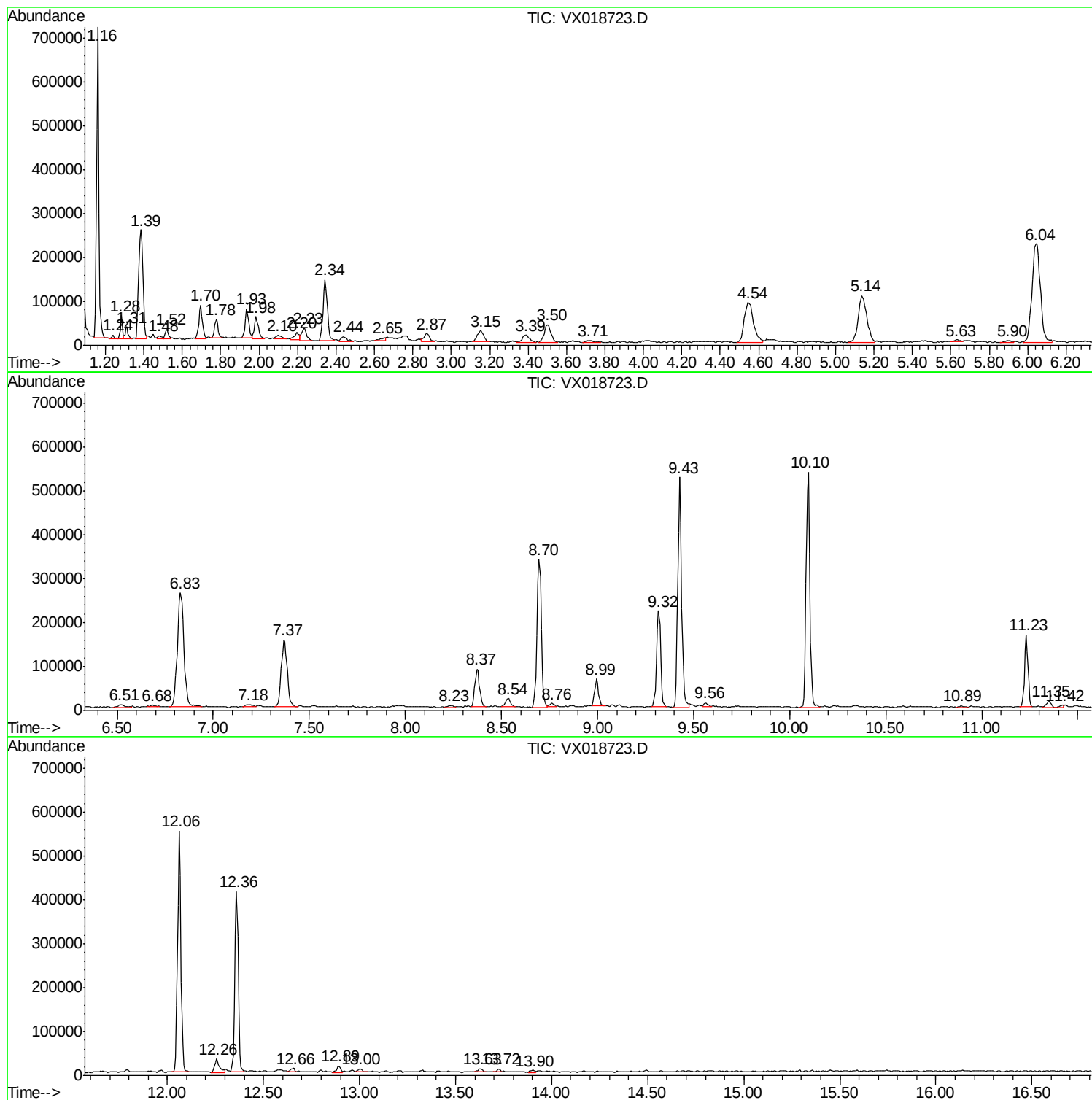
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR092820WMA.M
Quant Title : TRACE VOA SOM01.0

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



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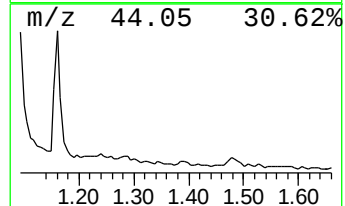
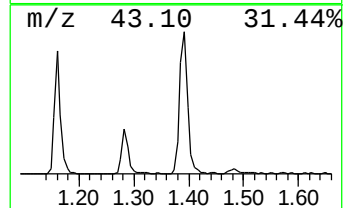
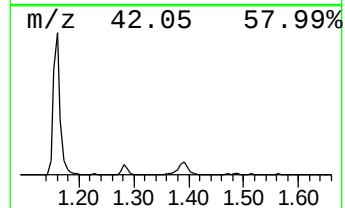
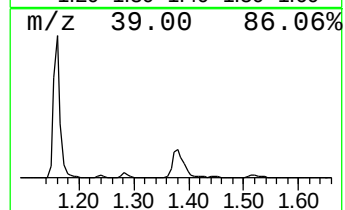
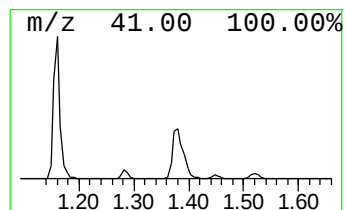
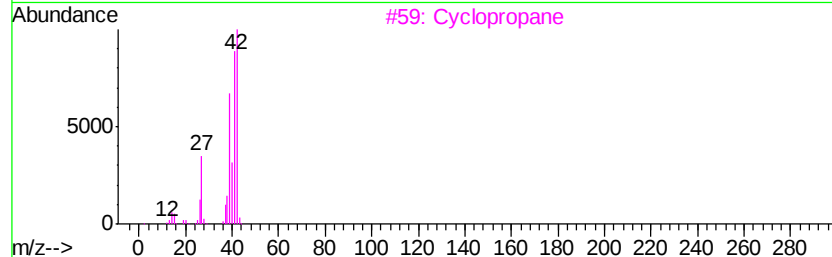
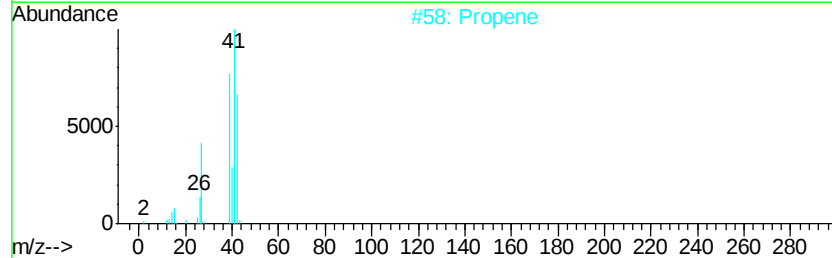
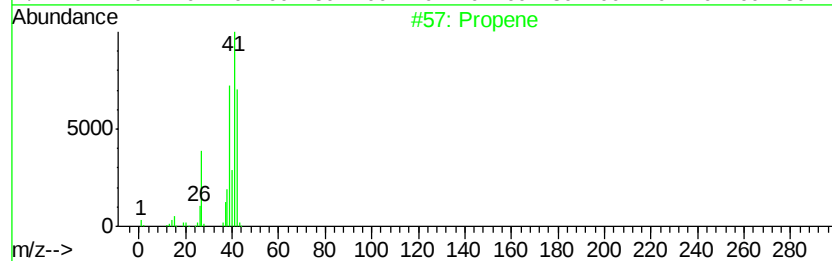
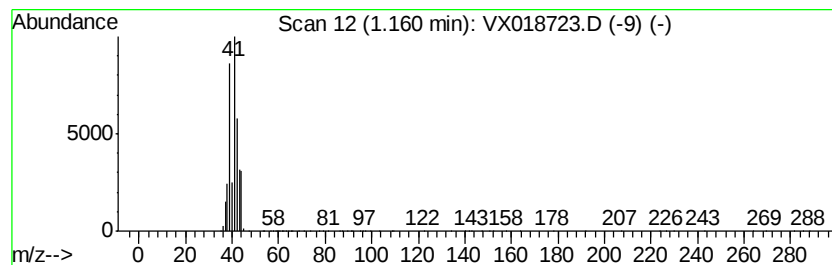
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.16	4.78 ug/L	598717	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propene	42	C3H6	000115-07-1	90
2		Propene	42	C3H6	000115-07-1	42
3		Cyclopropane	42	C3H6	000075-19-4	10
4		Cyclopropane	42	C3H6	000075-19-4	7
5		Cyclopropene	40	C3H4	002781-85-3	5



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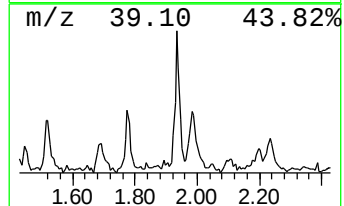
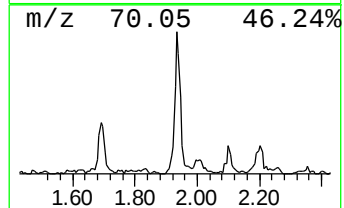
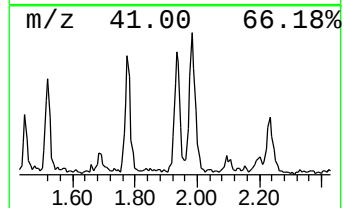
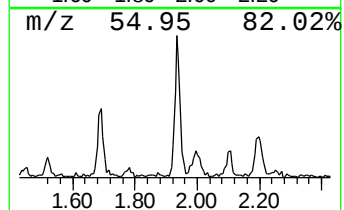
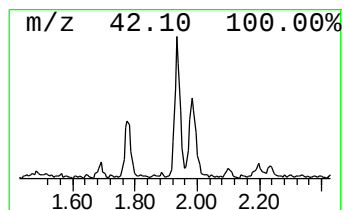
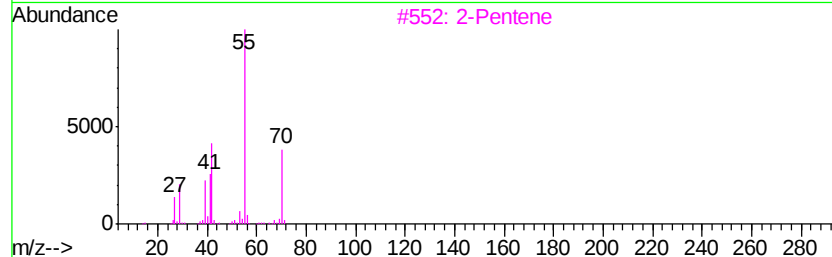
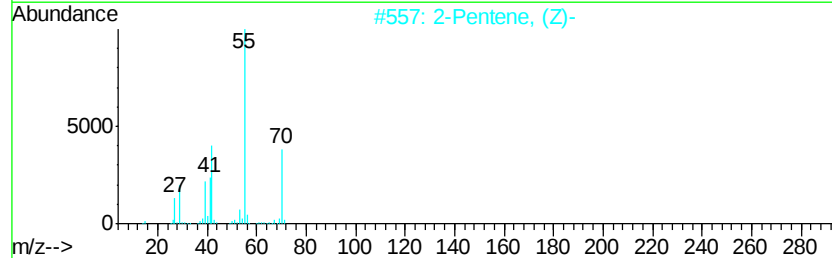
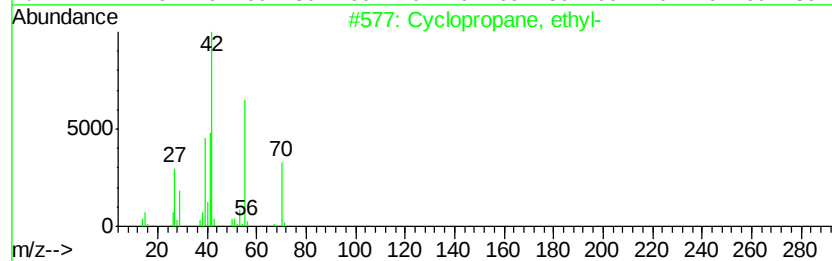
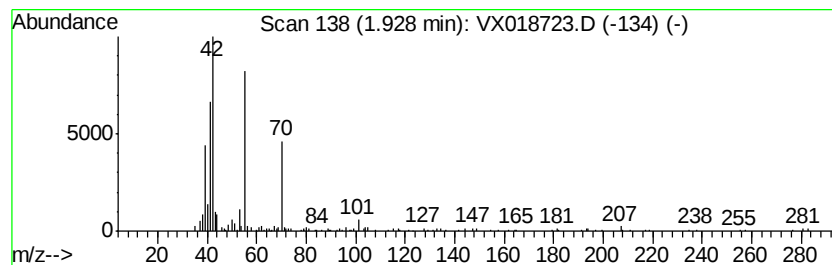
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR092820WMA.M
 Quant Title : TRACE VOA SOM01.0

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

 Peak Number 2 (DEL) Alkane: Cyclic1.93 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.93	0.71 ug/L	88619	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	91
2		2-Pentene, (Z)-	70	C5H10	000627-20-3	83
3		2-Pentene	70	C5H10	000109-68-2	83
4		2(3H)-Furanone, dihydro-3,5-dime...	114	C6H10O2	005145-01-7	78
5		1-Pentene	70	C5H10	000109-67-1	64



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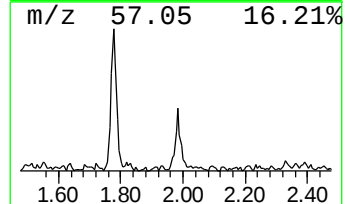
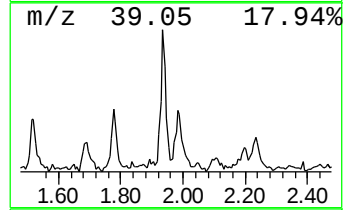
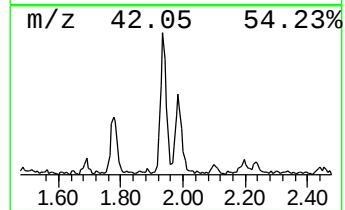
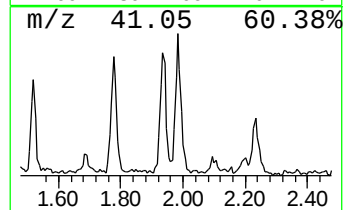
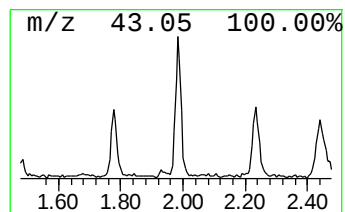
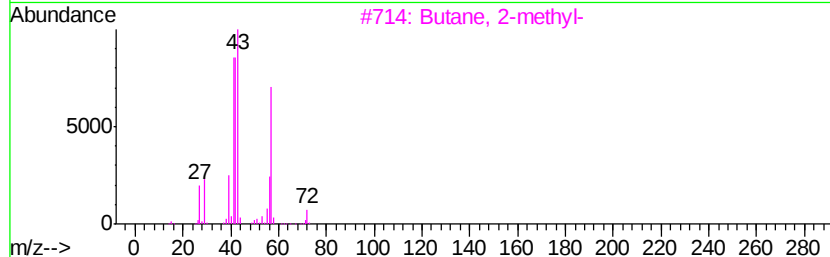
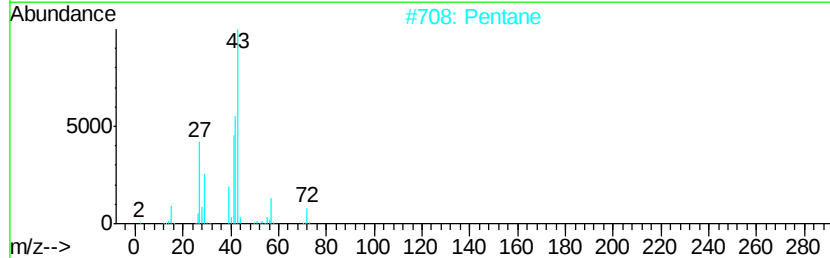
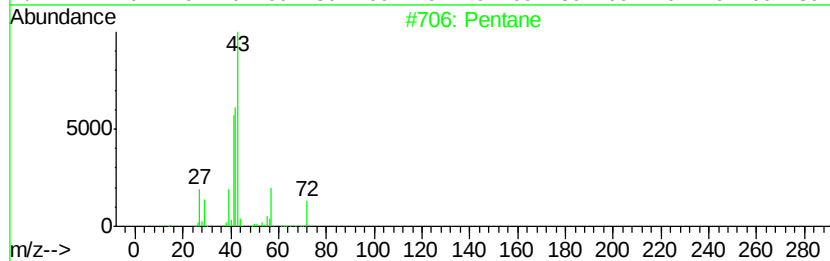
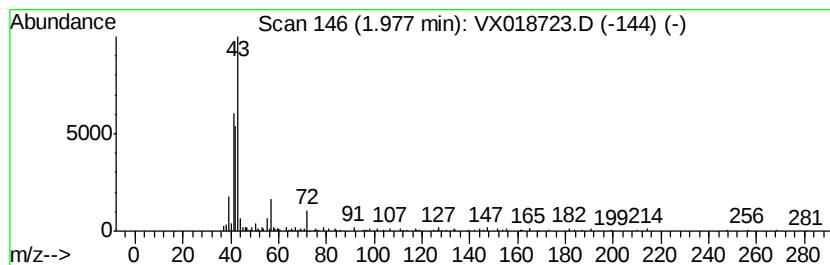
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.98	0.56 ug/L	69612	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	80
2		Pentane	72	C5H12	000109-66-0	72
3		Butane, 2-methyl-	72	C5H12	000078-78-4	25
4		Isobutylene epoxide	72	C4H8O	000558-30-5	17
5		Pentane	72	C5H12	000109-66-0	9



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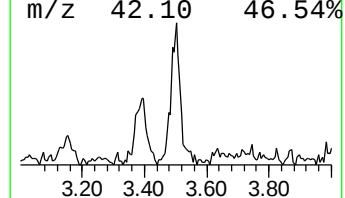
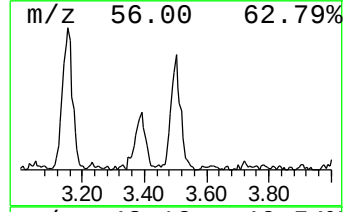
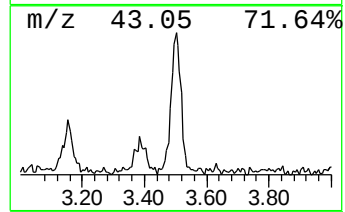
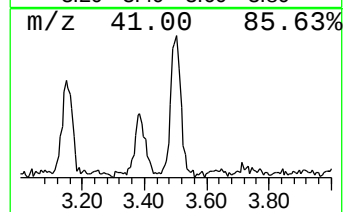
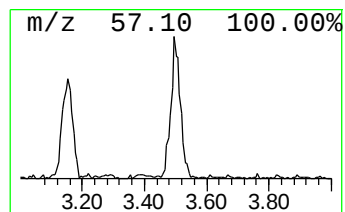
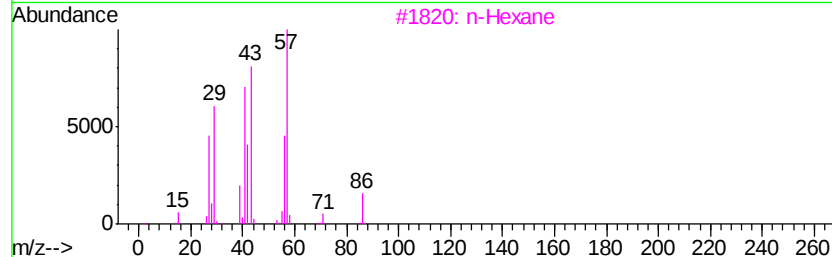
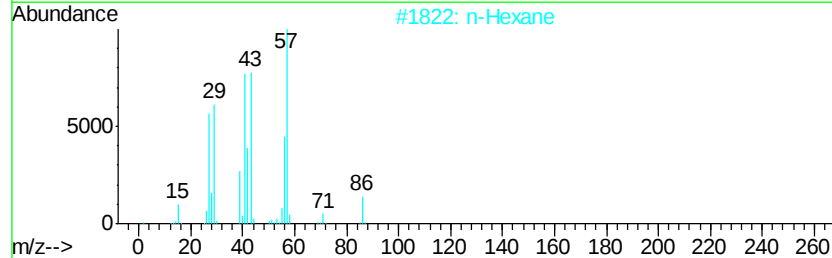
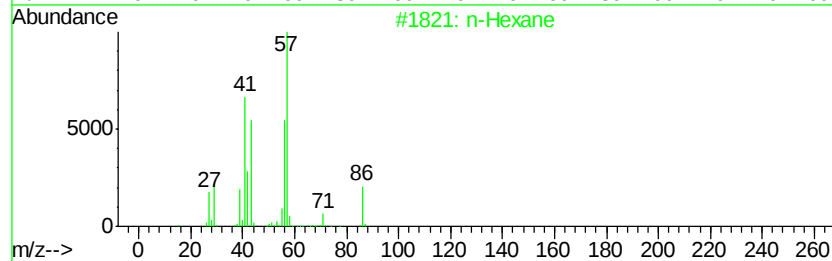
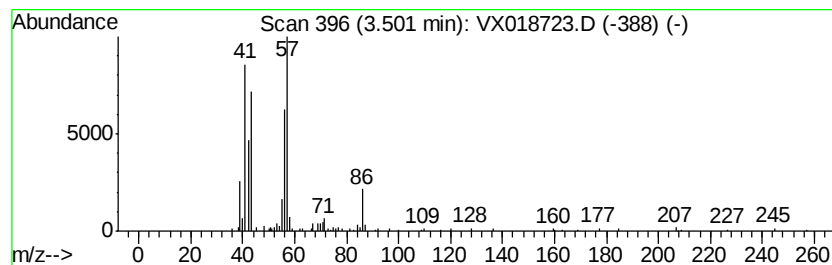
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	0.76 ug/L	95004	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	72
2		n-Hexane	86	C6H14	000110-54-3	72
3		n-Hexane	86	C6H14	000110-54-3	64
4		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	50
5		Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Str...	1.16	4.8	ug/L	598717	1	6.83	626331	5.0
(DEL) Alkane: Cyc...	1.93	0.7	ug/L	88619	1	6.83	626331	5.0
(DEL) Alkane: Str...	1.98	0.6	ug/L	69612	1	6.83	626331	5.0
(DEL) Alkane: Str...	3.50	0.8	ug/L	95004	1	6.83	626331	5.0