

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX072220\
 Data File : VX017473.D
 Acq On : 22 Jul 2020 18:18
 Operator : JC/SP
 Sample : L3395-14
 Misc : 25.0mL/MSVOA X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GAY22

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\SOMXTR072120WMA.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	16	rVB	589924	508246	33.16%	2.882%
2	1.239	23	25	29	rVB4	15325	15599	1.02%	0.088%
3	1.282	29	32	36	rBV	104100	98948	6.46%	0.561%
4	1.386	44	49	54	rBV2	400730	525484	34.29%	2.980%
5	1.447	57	59	61	rVV3	16988	16338	1.07%	0.093%
6	1.471	61	63	67	rVB	28500	30326	1.98%	0.172%
7	1.514	67	70	75	rBV	34988	43689	2.85%	0.248%
8	1.575	77	80	81	rVV3	14885	18713	1.22%	0.106%
9	1.593	81	83	89	rVB7	21603	22898	1.49%	0.130%
10	1.691	95	99	106	rVB	163054	200069	13.05%	1.134%
11	1.776	108	113	117	rBV	97494	132432	8.64%	0.751%
12	1.934	135	139	143	rVB	37436	44966	2.93%	0.255%
13	1.983	143	147	156	rBV3	56013	111659	7.29%	0.633%
14	2.099	162	166	170	rVB2	21971	28866	1.88%	0.164%
15	2.197	178	182	186	rVB3	19620	26974	1.76%	0.153%
16	2.251	186	191	198	rVV3	21495	45678	2.98%	0.259%
17	2.343	200	206	214	rVB	374701	596367	38.91%	3.382%
18	2.416	214	218	222	rBV	28250	42037	2.74%	0.238%
19	2.550	233	240	242	rBV2	29211	50653	3.31%	0.287%
20	2.581	242	245	251	rVV	40959	66292	4.33%	0.376%
21	2.831	280	286	289	rBV5	19741	38558	2.52%	0.219%
22	2.867	290	292	295	rVV4	21913	30795	2.01%	0.175%
23	2.910	296	299	309	rVB3	21986	47877	3.12%	0.271%
24	3.148	332	338	346	rVB3	16683	43574	2.84%	0.247%
25	3.385	369	377	382	rBV8	14793	33981	2.22%	0.193%
26	3.501	386	396	403	rVB4	16800	40904	2.67%	0.232%
27	4.367	533	538	546	rVB4	12129	28630	1.87%	0.162%
28	4.532	554	565	576	rBV	191099	563456	36.77%	3.195%
29	4.653	576	585	599	rVV	88530	317173	20.70%	1.798%
30	4.794	599	608	623	rVB	237689	699447	45.64%	3.966%
31	5.141	653	665	676	rBV2	206686	624131	40.72%	3.539%
32	6.043	800	813	822	rBV3	523481	1532574	100.00%	8.690%
33	6.434	869	877	879	rBV8	10953	23845	1.56%	0.135%
34	6.830	932	942	952	rBV	475825	1139114	74.33%	6.459%

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 Title : TRACE VOA SOM01.0

35	7.171	993	998	1002	rBV7	8442	19931	1.30%	0.113%
36	7.372	1022	1031	1038	rBV	311426	688597	44.93%	3.905%
37	7.440	1040	1042	1047	rVB4	15096	22805	1.49%	0.129%
38	8.372	1188	1195	1203	rBV	210482	339905	22.18%	1.927%
39	8.695	1241	1248	1254	rBV	831295	1271757	82.98%	7.211%
40	8.762	1254	1259	1266	rVB	136449	216869	14.15%	1.230%
41	8.994	1288	1297	1306	rBV	142266	227578	14.85%	1.290%
42	9.311	1346	1349	1354	rVB7	10461	15591	1.02%	0.088%
43	9.427	1362	1368	1374	rBV	974152	1322093	86.27%	7.497%
44	9.738	1414	1419	1425	rBV2	55842	87498	5.71%	0.496%
45	10.098	1472	1478	1486	rBV	991963	1382808	90.23%	7.841%
46	10.238	1495	1501	1507	rBV	104289	146654	9.57%	0.832%
47	10.341	1511	1518	1524	rVV	257163	335400	21.88%	1.902%
48	10.683	1569	1574	1579	rVB	96043	121960	7.96%	0.692%
49	11.232	1658	1664	1671	rBV	309935	388332	25.34%	2.202%
50	11.341	1677	1682	1689	rVB	22444	33217	2.17%	0.188%
51	11.421	1689	1695	1703	rBV	45662	99980	6.52%	0.567%
52	11.488	1703	1706	1712	rVB2	23678	33769	2.20%	0.191%
53	11.652	1729	1733	1738	rVB	25140	36204	2.36%	0.205%
54	11.792	1752	1756	1762	rVB	102300	132323	8.63%	0.750%
55	12.061	1795	1800	1805	rBV	1061871	1312854	85.66%	7.444%
56	12.128	1807	1811	1814	rVB	26350	31014	2.02%	0.176%
57	12.256	1828	1832	1834	rBV2	22496	29980	1.96%	0.170%
58	12.286	1834	1837	1840	rVV	41648	58578	3.82%	0.332%
59	12.359	1844	1849	1857	rVB	925094	1141678	74.49%	6.474%
60	12.652	1891	1897	1900	rBV2	17597	24279	1.58%	0.138%
61	12.737	1908	1911	1918	rBV5	16926	27998	1.83%	0.159%
62	12.890	1932	1936	1939	rVV6	15009	19492	1.27%	0.111%
63	12.963	1942	1948	1951	rBV5	14302	27595	1.80%	0.156%
64	13.000	1951	1954	1960	rVB3	18787	25680	1.68%	0.146%
65	13.207	1981	1988	1991	rBV4	11444	19218	1.25%	0.109%
66	13.335	2004	2009	2014	rVB4	25734	42508	2.77%	0.241%
67	13.621	2052	2056	2060	rBV6	8923	16617	1.08%	0.094%
68	13.664	2060	2063	2066	rVV4	12292	16277	1.06%	0.092%
69	13.707	2068	2070	2078	rVB9	8647	16783	1.10%	0.095%
70	13.816	2081	2088	2092	rBV	33220	49828	3.25%	0.283%
71	14.676	2224	2229	2234	rBV	31647	45138	2.95%	0.256%

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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

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Title : TRACE VOA SOM01.0

72	14.822	2250	2253	2257	rBV5	13962	16750	1.09%	0.095%
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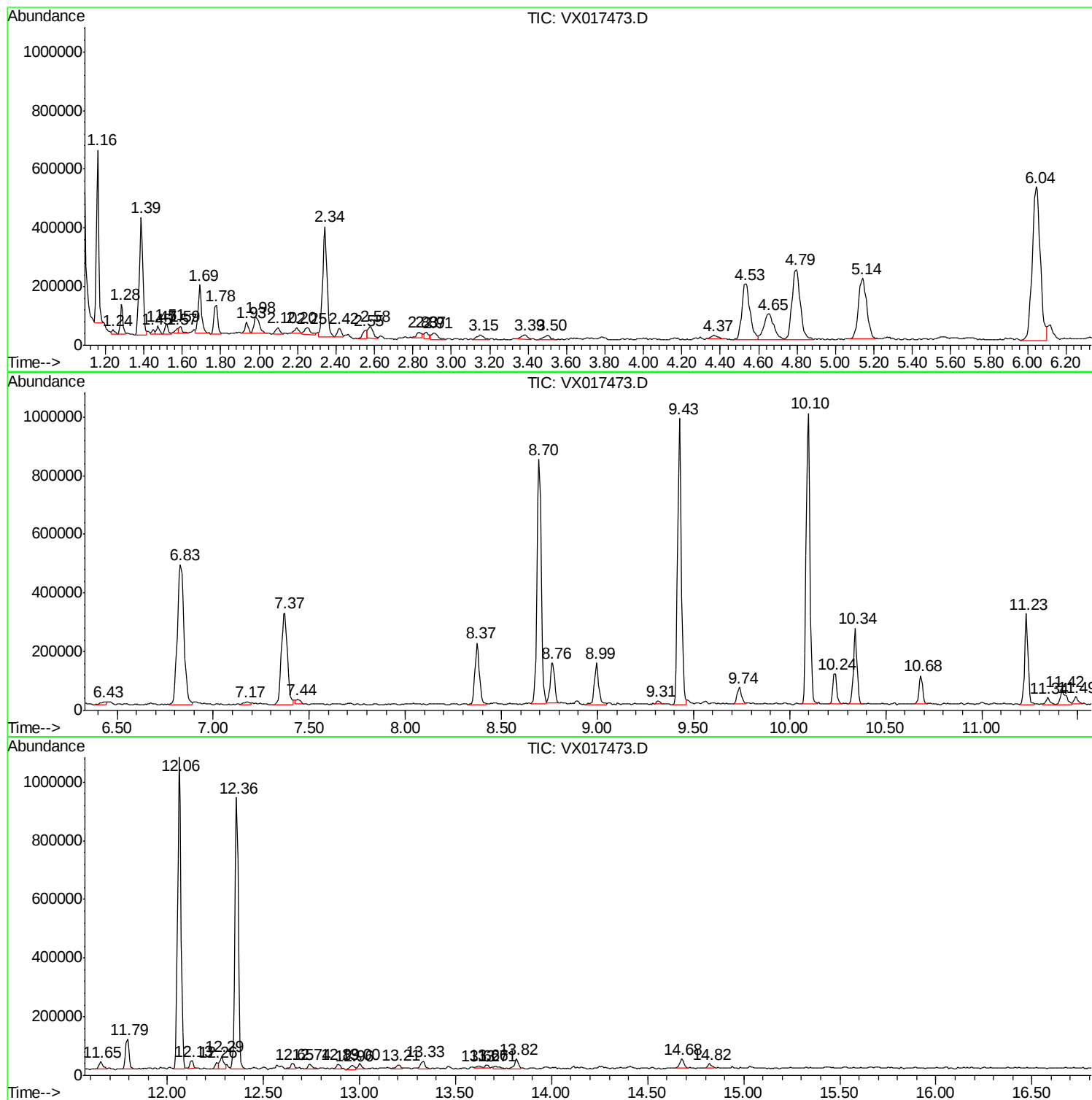
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

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



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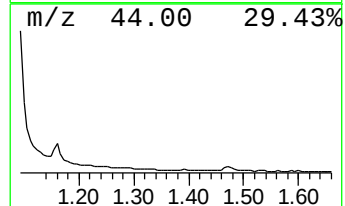
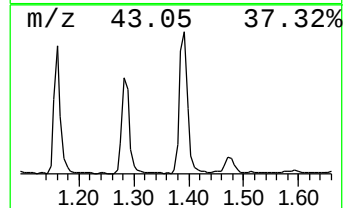
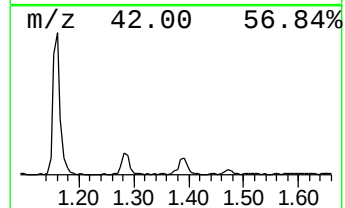
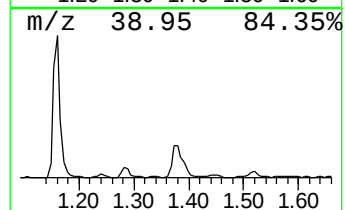
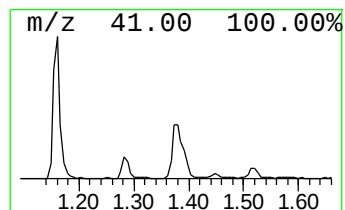
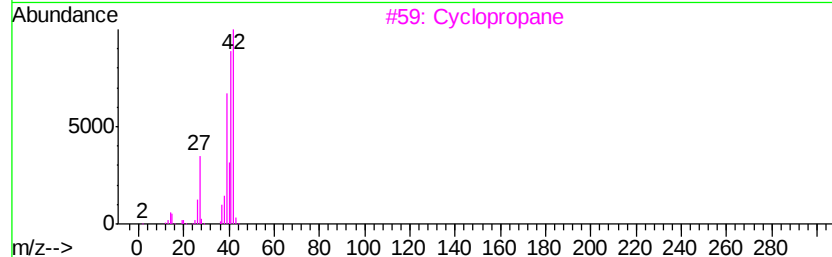
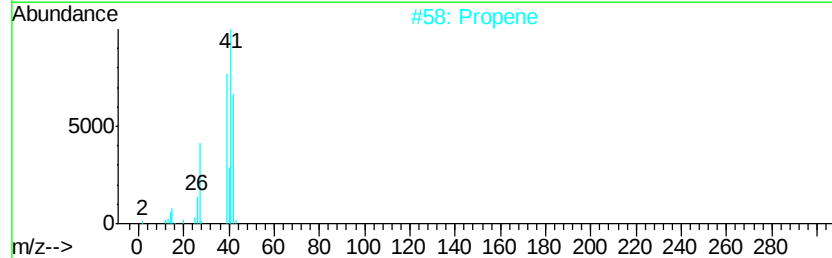
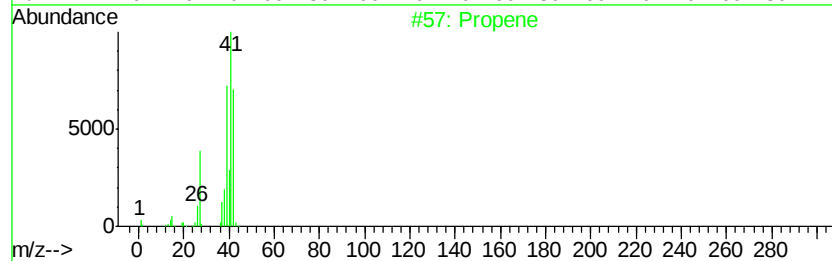
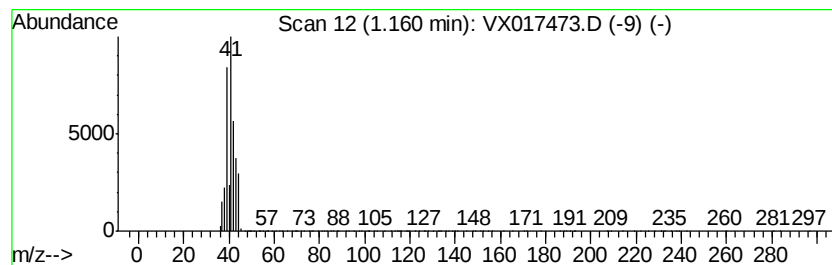
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.16	2.23 ug/L	508246	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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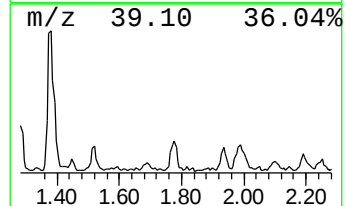
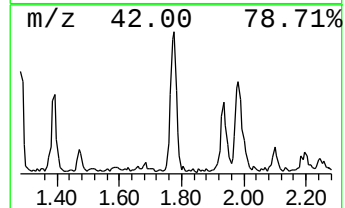
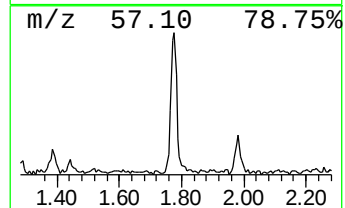
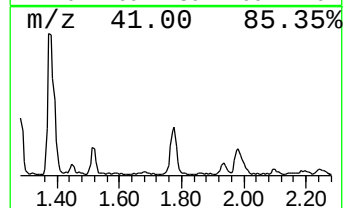
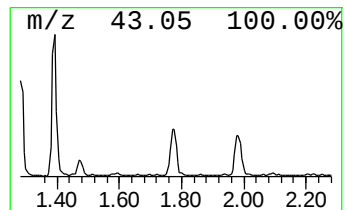
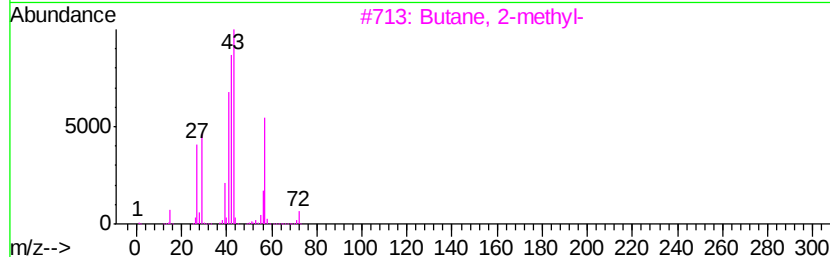
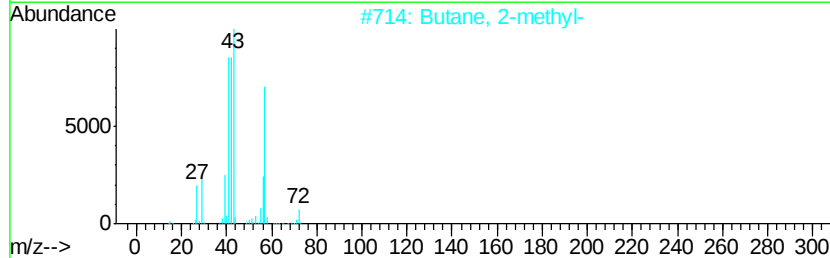
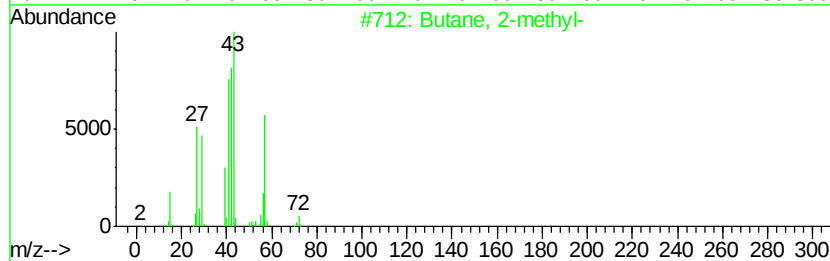
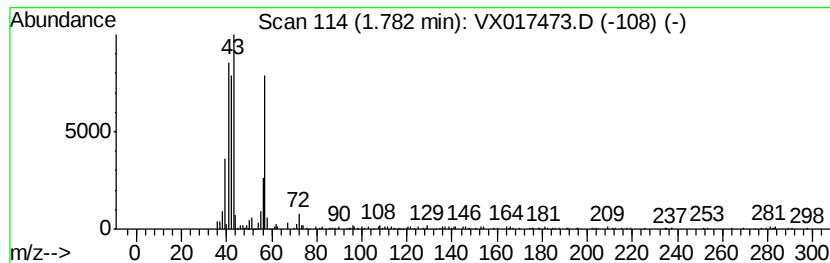
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	0.58 ug/L	132432	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2		Butane, 2-methyl-	72	C5H12	000078-78-4	86
3		Butane, 2-methyl-	72	C5H12	000078-78-4	80
4		Pentane	72	C5H12	000109-66-0	33
5		2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28



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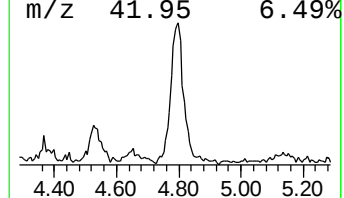
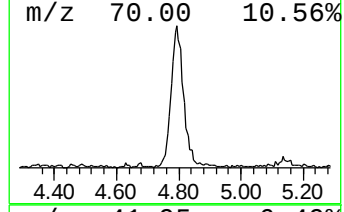
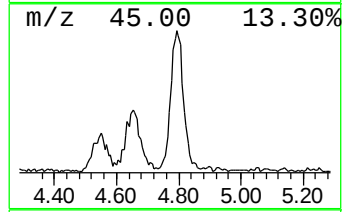
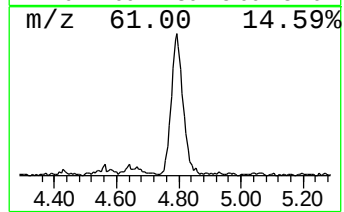
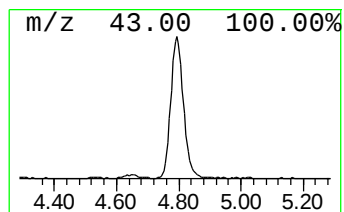
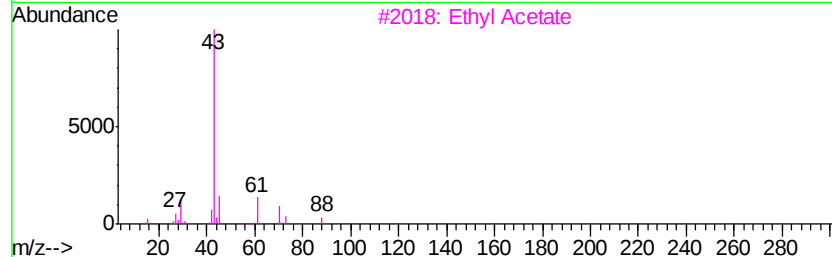
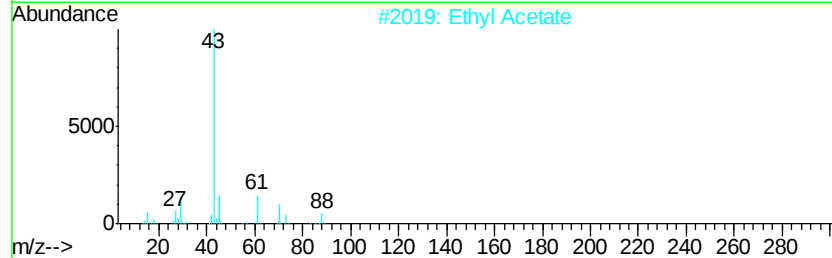
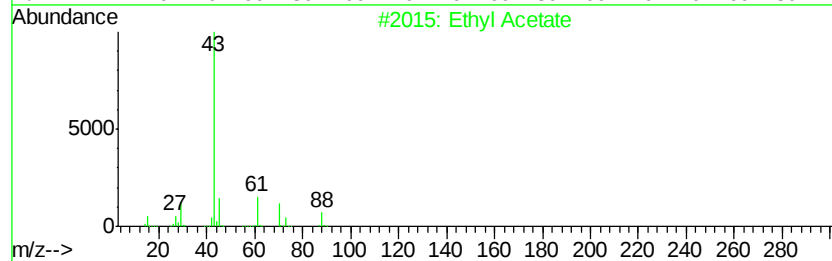
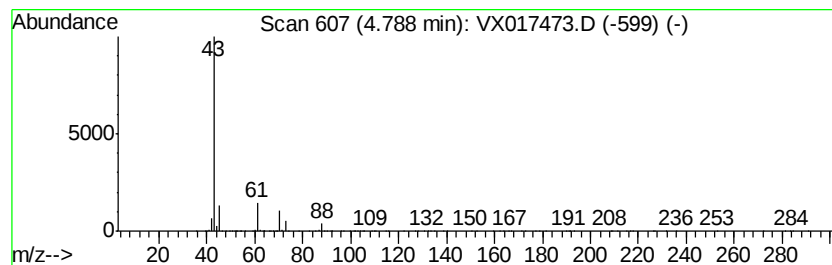
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	3.07 ug/L	699447	1,4-Difluorobenzene	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	90
2			Ethyl Acetate	88	C4H8O2	000141-78-6	90
3			Ethyl Acetate	88	C4H8O2	000141-78-6	86
4			Ethyl Acetate	88	C4H8O2	000141-78-6	72
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	33



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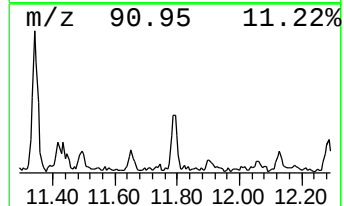
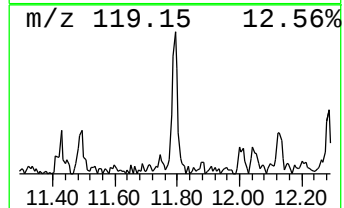
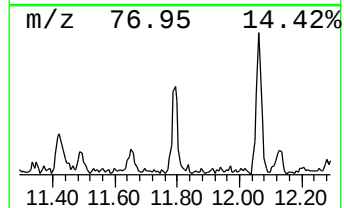
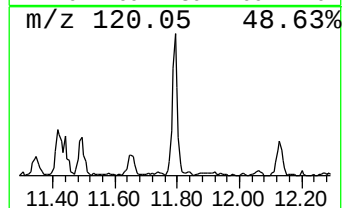
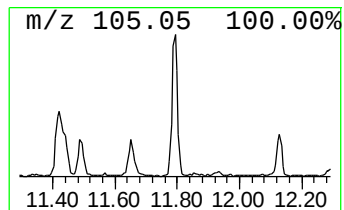
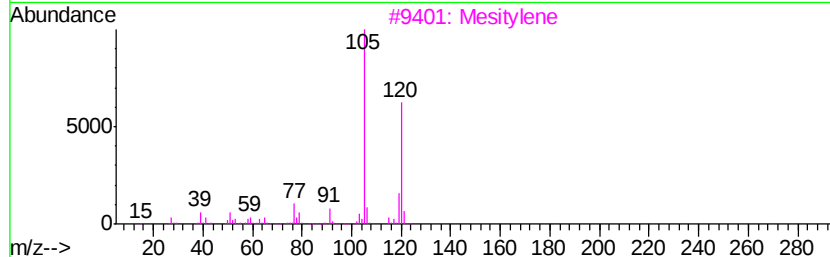
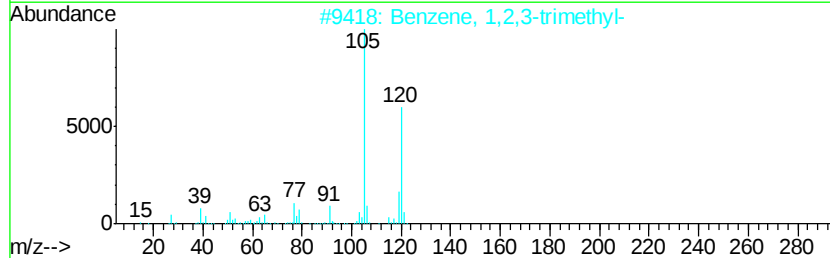
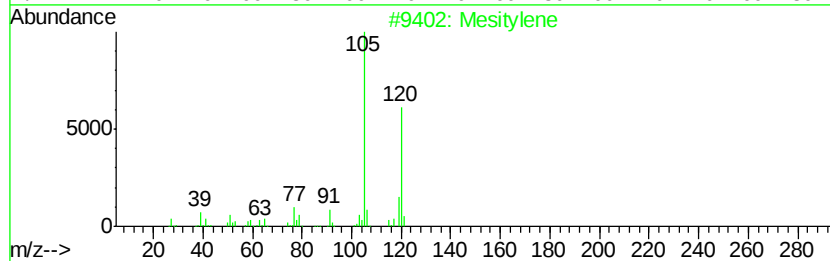
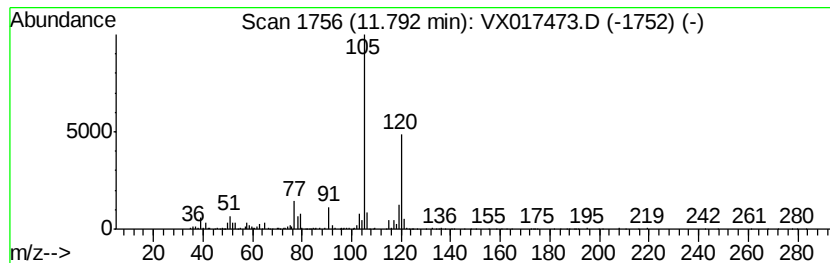
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Mesitylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	0.50 ug/L	132323	1,4-Dichlorobenzene-d4	12.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene		120	C9H12	000108-67-8	95
2	Benzene, 1,2,3-trimethyl-		120	C9H12	000526-73-8	94
3	Mesitylene		120	C9H12	000108-67-8	94
4	Benzene, 1,2,4-trimethyl-		120	C9H12	000095-63-6	91
5	Mesitylene		120	C9H12	000108-67-8	91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX072220\
Data File : VX017473.D
Acq On : 22 Jul 2020 18:18
Operator : JC/SP
Sample : L3395-14
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GAY22

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR072120WMA.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...	1.16	2.2	ug/L	508246	1	6.83	1139110	5.0
(DEL) Alkane: Str...	1.78	0.6	ug/L	132432	1	6.83	1139110	5.0
Ethyl Acetate	4.79	3.1	ug/L	699447	1	6.83	1139110	5.0
Mesitylene	11.79	0.5	ug/L	132323	3	12.06	1312850	5.0