

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
 Data File : VX020767.D
 Acq On : 26 Jan 2021 20:35
 Operator : JC/SP
 Sample : VSTDCCC050
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_X
 LabSampleId :
 VSTDCCC050

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M

Title : SW846 8260

Signal : TIC: VX020767.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.185	12	16	25	rBV	490448	468896	9.44%	0.337%
2	1.313	34	37	46	rVB	449059	426828	8.60%	0.307%
3	1.392	46	50	60	rBV	450952	438782	8.84%	0.316%
4	1.624	84	88	92	rVB	316261	299277	6.03%	0.215%
5	1.703	97	101	114	rVB	235448	306018	6.16%	0.220%
6	1.910	129	135	148	rBV	524867	772466	15.56%	0.556%
7	2.166	172	177	189	rBV	386425	547166	11.02%	0.394%
8	2.270	189	194	202	rVV	256428	402744	8.11%	0.290%
9	2.355	202	208	214	rVV2	869054	1626057	32.75%	1.170%
10	2.422	214	219	225	rVV	447919	770914	15.53%	0.555%
11	2.489	225	230	235	rVV	260178	446478	8.99%	0.321%
12	2.550	235	240	255	rVB	399378	694822	13.99%	0.500%
13	2.703	256	265	269	rBV	476972	886300	17.85%	0.638%
14	2.745	269	272	280	rVV	225629	405223	8.16%	0.292%
15	2.831	280	286	302	rVB	480849	920138	18.53%	0.662%
16	3.020	305	317	325	rBV	191041	431449	8.69%	0.310%
17	3.117	325	333	361	rVB3	832302	3883383	78.21%	2.794%
18	3.666	413	423	433	rBV	339726	820839	16.53%	0.591%
19	3.782	433	442	467	rVB2	1474249	4965078	100.00%	3.573%
20	4.556	554	569	576	rBV2	634142	1944152	39.16%	1.399%
21	4.635	576	582	590	rVV	455694	1289267	25.97%	0.928%
22	4.721	590	596	603	rVV	340181	986507	19.87%	0.710%
23	4.818	603	612	628	rVV2	222716	1005468	20.25%	0.723%
24	4.989	628	640	649	rVV3	372652	1351397	27.22%	0.972%
25	5.087	649	656	664	rVV	550746	1659794	33.43%	1.194%
26	5.172	664	670	687	rVB	331963	985684	19.85%	0.709%
27	5.464	705	718	725	rBV	576959	1766254	35.57%	1.271%
28	5.544	725	731	738	rVV	478930	1414066	28.48%	1.017%
29	5.629	738	745	749	rVV	397456	1089933	21.95%	0.784%
30	5.684	750	754	760	rVV	362704	987146	19.88%	0.710%
31	5.757	760	766	784	rVB2	674753	2006180	40.41%	1.444%
32	6.025	799	810	816	rBV2	248325	649411	13.08%	0.467%
33	6.111	816	824	830	rBV	687021	1812848	36.51%	1.304%
34	6.409	862	873	893	rVB	376809	944878	19.03%	0.680%
35	6.830	931	942	961	rBV	607729	1436557	28.93%	1.034%
36	7.184	991	1000	1013	rBV	598463	1284298	25.87%	0.924%

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37	7.440	1032	1042	1046	rBV	730407	1627968	32.79%	1.171%
38	7.489	1046	1050	1061	rVB	564540	1100598	22.17%	0.792%
39	7.635	1067	1074	1081	rBV	399504	760450	15.32%	0.547%
40	7.745	1081	1092	1102	rVB2	579573	1248378	25.14%	0.898%
41	7.854	1102	1110	1111	rBV	573850	887819	17.88%	0.639%
42	8.165	1152	1161	1174	rBV	118949	215629	4.34%	0.155%
43	8.287	1174	1181	1193	rVV	2114955	3328778	67.04%	2.395%
44	8.415	1195	1202	1210	rVV	720883	1126462	22.69%	0.811%
45	8.622	1228	1236	1242	rBV	2749794	4387337	88.36%	3.157%
46	8.696	1242	1248	1254	rVV	1273636	1962983	39.54%	1.412%
47	8.763	1254	1259	1270	rVB	1529741	2298372	46.29%	1.654%
48	9.019	1291	1301	1312	rBV	727166	1061379	21.38%	0.764%
49	9.159	1318	1324	1327	rBV	825373	1178334	23.73%	0.848%
50	9.196	1327	1330	1339	rVB	901892	1219093	24.55%	0.877%
51	9.317	1341	1350	1353	rBV	1141957	1765289	35.55%	1.270%
52	9.348	1353	1355	1361	rVB	768366	1010404	20.35%	0.727%
53	9.470	1369	1375	1384	rBV	2343406	3168547	63.82%	2.280%
54	9.561	1384	1390	1395	rVV	582660	848182	17.08%	0.610%
55	9.616	1395	1399	1402	rVV	831432	1095179	22.06%	0.788%
56	9.653	1402	1405	1413	rVB	465432	622274	12.53%	0.448%
57	10.098	1471	1478	1479	rBV	1240821	1707182	34.38%	1.228%
58	10.122	1479	1482	1489	rVV	1387476	1870143	37.67%	1.346%
59	10.201	1489	1495	1497	rVV	1055349	1377018	27.73%	0.991%
60	10.232	1497	1500	1506	rVB	1913858	2501949	50.39%	1.800%
61	10.342	1512	1518	1530	rVB	3621182	4776267	96.20%	3.437%
62	10.689	1568	1575	1584	rBV2	2607928	4537214	91.38%	3.265%
63	10.842	1594	1600	1603	rBV	498184	689762	13.89%	0.496%
64	10.878	1603	1606	1618	rVV	1142230	1310546	26.40%	0.943%
65	11.000	1621	1626	1631	rVV	2171253	2594892	52.26%	1.867%
66	11.055	1631	1635	1641	rVV	655631	825797	16.63%	0.594%
67	11.122	1641	1646	1653	rVB	1012328	1318253	26.55%	0.949%
68	11.238	1659	1665	1669	rBV2	1423427	2634261	53.06%	1.895%
69	11.281	1669	1672	1678	rVV2	912237	1810074	36.46%	1.302%
70	11.341	1678	1682	1687	rVV	2045337	2458218	49.51%	1.769%
71	11.402	1687	1692	1698	rVV	1643367	2045946	41.21%	1.472%
72	11.494	1701	1707	1715	rVB2	3482665	4554111	91.72%	3.277%
73	11.756	1744	1750	1753	rBV2	2572100	3646108	73.44%	2.624%
74	11.793	1753	1756	1761	rVB	2053250	2433363	49.01%	1.751%
75	11.927	1772	1778	1784	rBV	1917965	2344736	47.22%	1.687%
76	12.006	1786	1791	1794	rBV	1424063	1755017	35.35%	1.263%

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77	12.049	1794	1798	1802	rBV2	2324209	4069181	81.96%	2.928%
78	12.372	1846	1851	1859	rBV	3354125	3976194	80.08%	2.861%
79	12.579	1879	1885	1892	rBV	1031970	1323502	26.66%	0.952%
80	12.981	1943	1951	1960	rBV2	386848	556858	11.22%	0.401%
81	13.140	1973	1977	1983	rBV	54090	71006	1.43%	0.051%
82	13.323	2002	2007	2017	rBV	2085927	2451689	49.38%	1.764%
83	13.628	2051	2057	2064	rBV	1241403	1555826	31.34%	1.120%
84	13.762	2074	2079	2083	rBV	845928	1049189	21.13%	0.755%
85	13.817	2083	2088	2094	rVB	1757503	2107783	42.45%	1.517%
86	14.000	2113	2118	2126	rBV	1297495	1582608	31.87%	1.139%

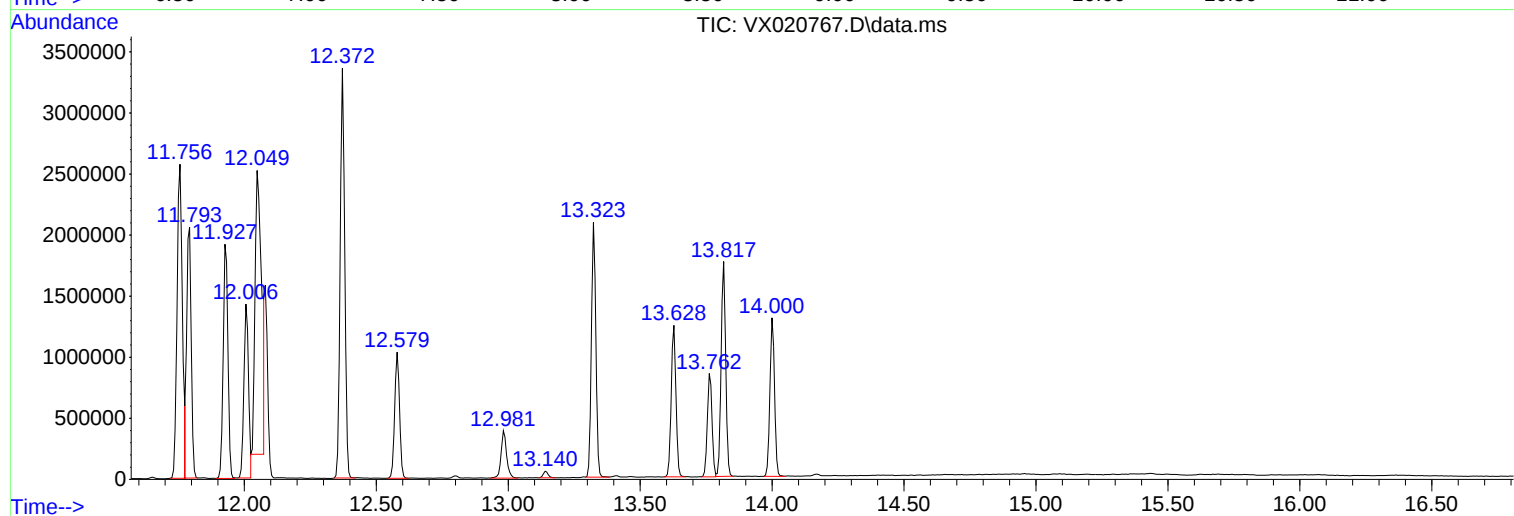
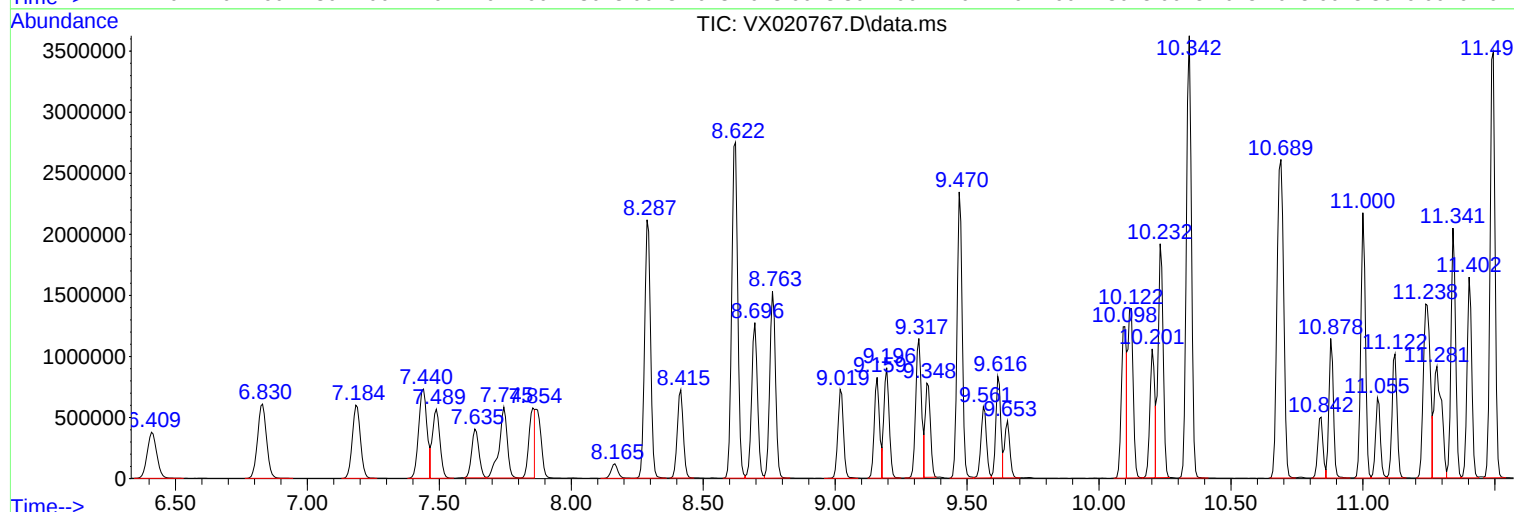
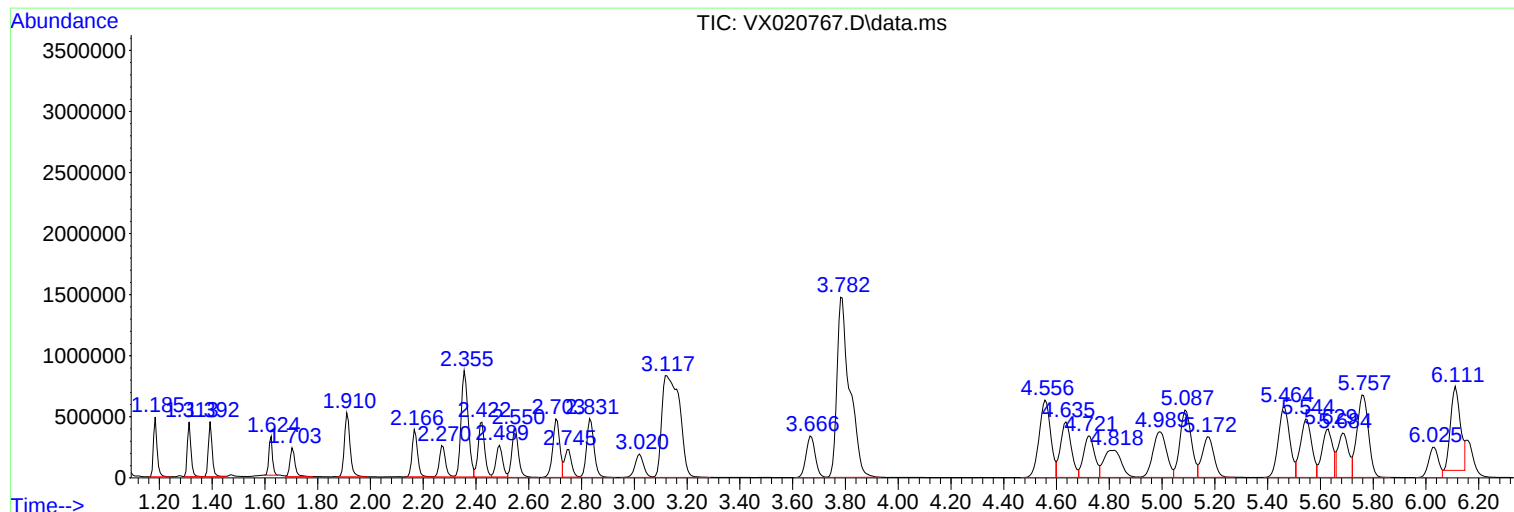
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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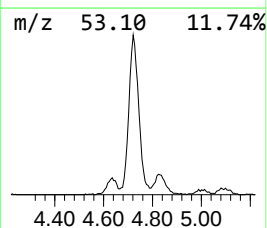
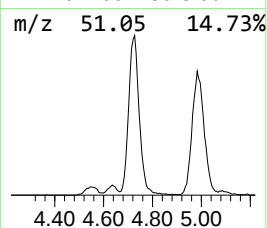
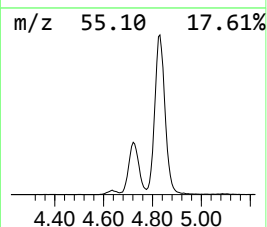
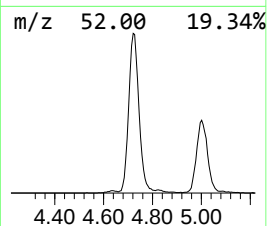
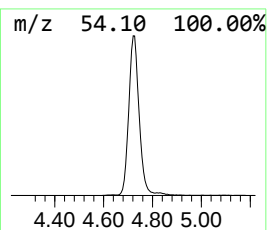
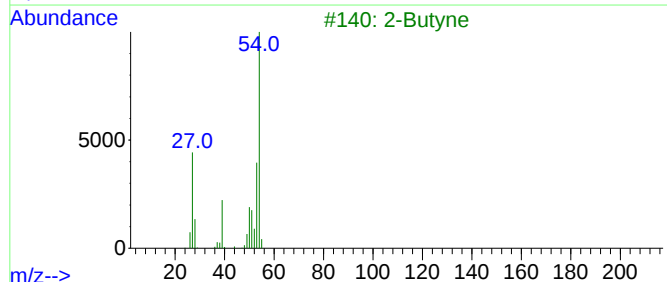
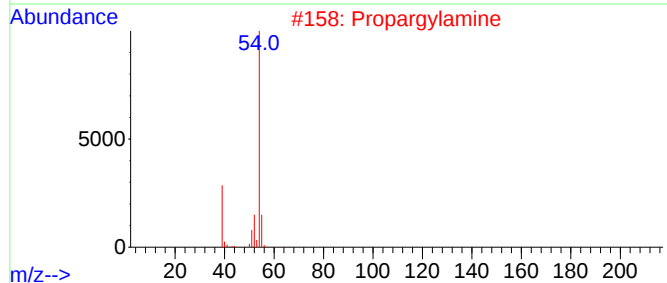
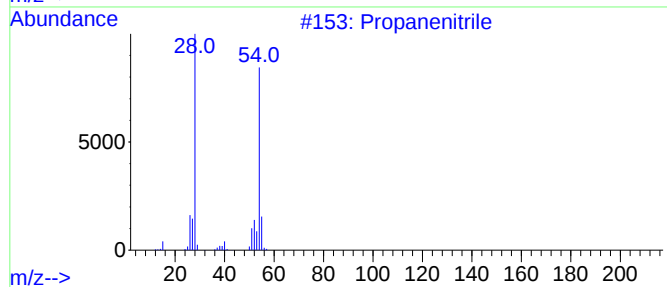
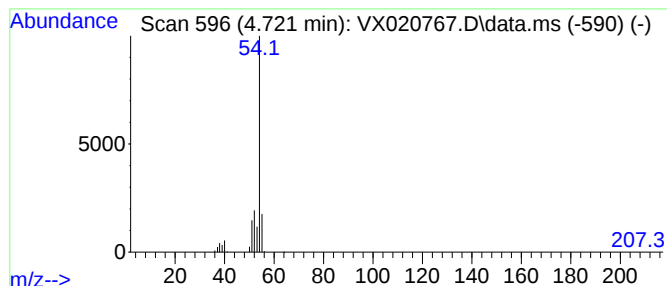
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanenitrile Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.721	45.26 ug/l	986507	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanenitrile	55	C3H5N	000107-12-0	59
2			Propargylamine	55	C3H5N	002450-71-7	7
3			2-Butyne	54	C4H6	000503-17-3	7
4			1-Butyne	54	C4H6	000107-00-6	4
5			1,2-Butadiene	54	C4H6	000590-19-2	3



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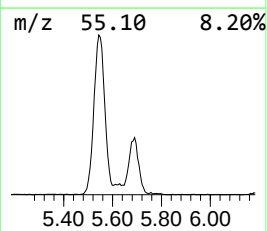
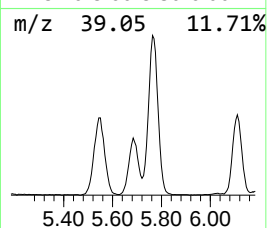
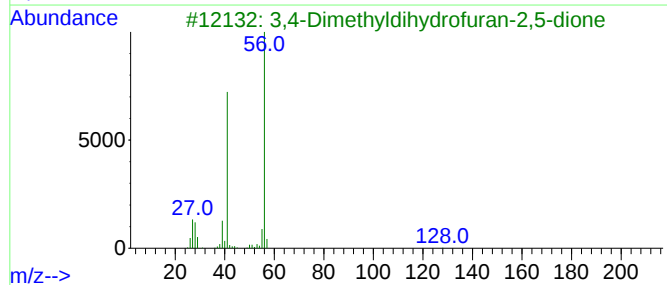
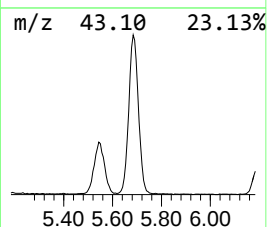
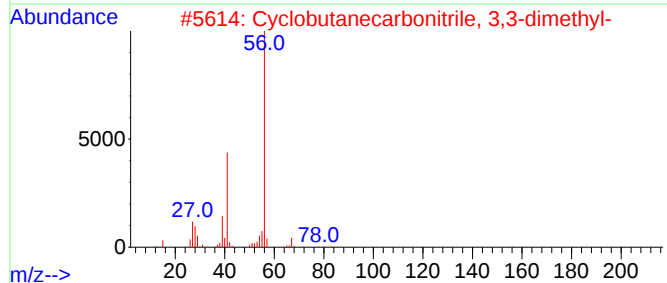
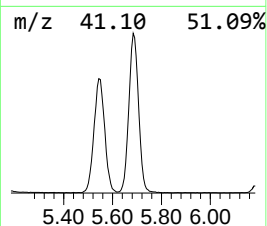
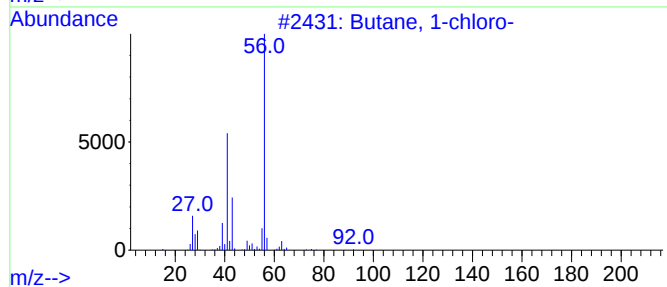
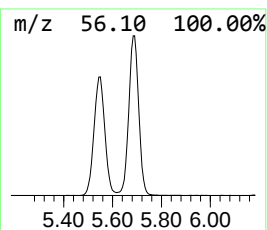
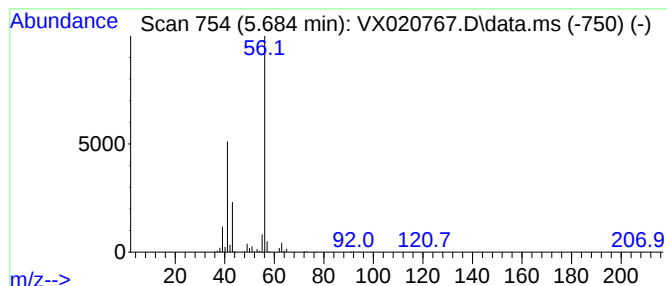
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 1-chloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.684	45.28 ug/l	987146	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	91
2			Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	50
3			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	50
4			Ethane, diazo-	56	C2H4N2	001117-96-0	9
5			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9



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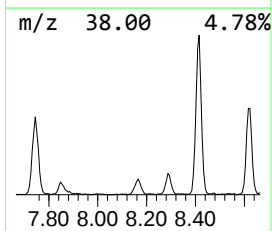
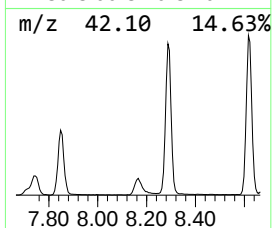
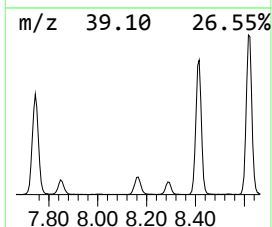
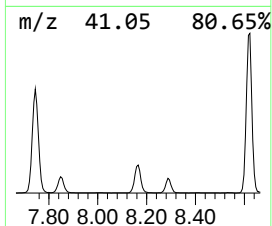
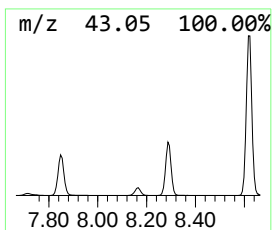
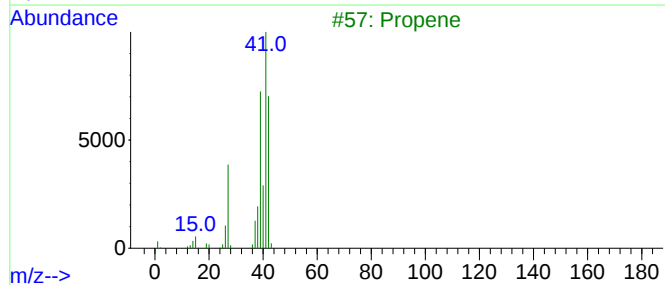
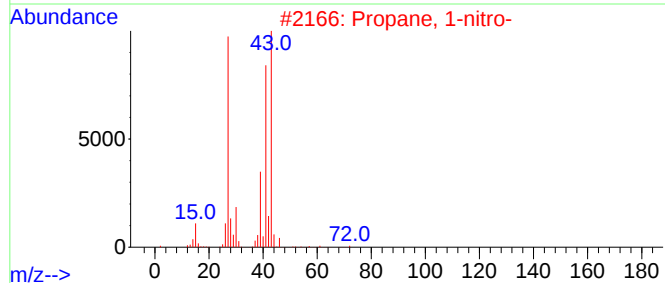
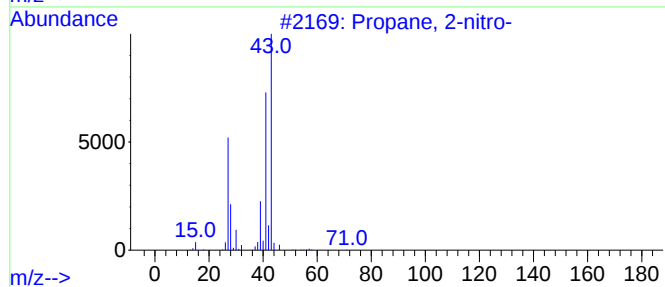
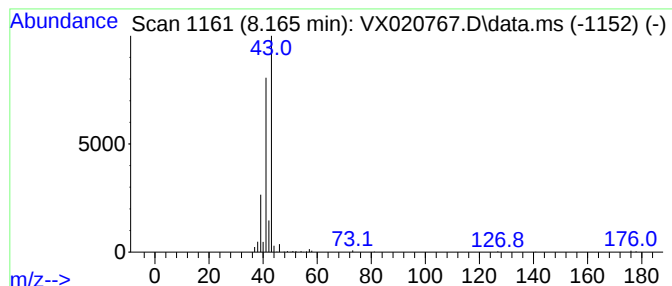
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 2-nitro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.165	7.51 ug/l	215629	1,4-Difluorobenzene	6.830

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	72
2			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	56
3			Propene	42	C3H6	000115-07-1	9
4			1H-Pyrazol-1-amine, 5-methyl-3-n...	142	C4H6N4O2	151588-03-3	9
5			Isobutyl nitrite	103	C4H9NO2	000542-56-3	9



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LabSampleId :
VSTDCCC050

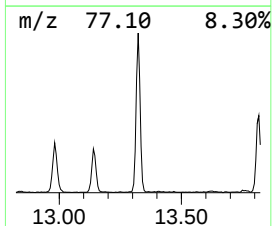
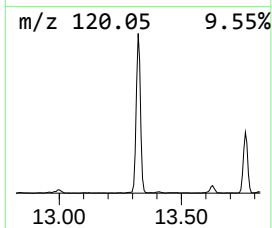
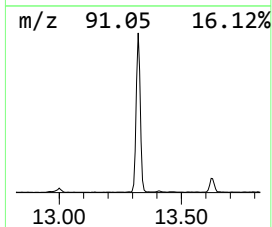
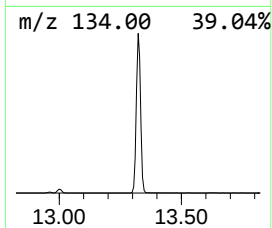
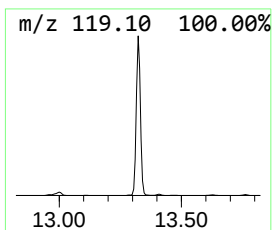
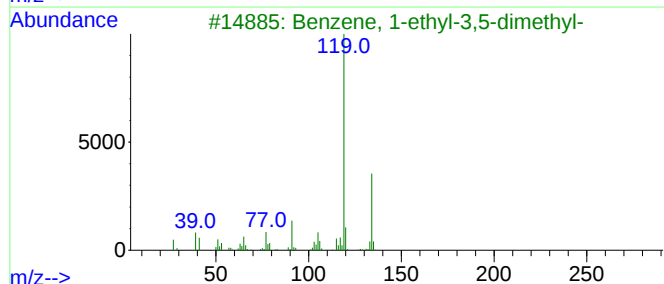
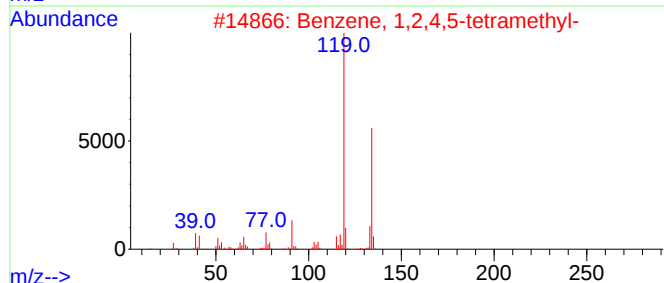
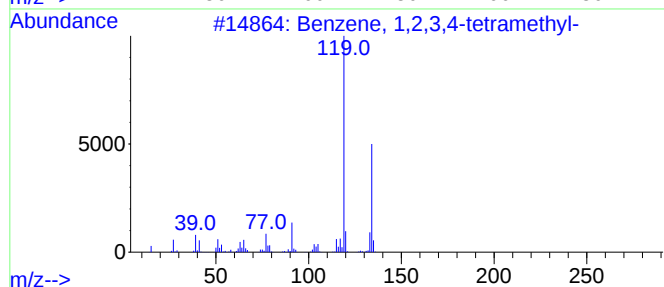
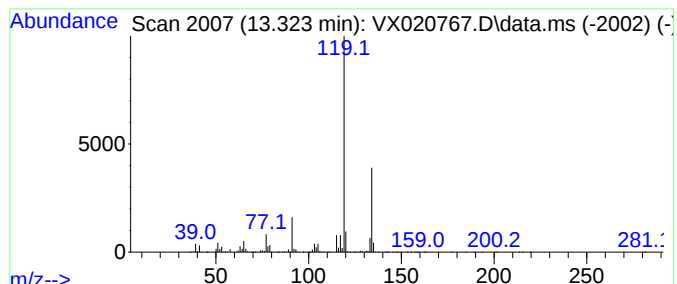
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.323	30.13 ug/l	2451690	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
3			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020767.D
Acq On : 26 Jan 2021 20:35
Operator : JC/SP
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
LabSampleId :
VSTDCCC050

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanenitrile	4.721	45.3	ug/l	986507	1	5.629	1089930	50.0
Butane, 1-chloro-	5.684	45.3	ug/l	987146	1	5.629	1089930	50.0
Propane, 2-nitro-	8.165	7.5	ug/l	215629	2	6.830	1436560	50.0
Benzene, 1,2,3,...	13.323	30.1	ug/l	2451690	4	12.061	4069180	50.0