

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012721\
 Data File : VX020769.D
 Acq On : 27 Jan 2021 14:04
 Operator : JC/SP
 Sample : VSTDCCC050
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 2 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: VX020769.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	23	rBV	446667	438067	10.64%	0.375%
2	1.313	33	37	46	rVB	364254	356585	8.66%	0.306%
3	1.392	46	50	57	rBV	379959	367256	8.92%	0.315%
4	1.624	84	88	92	rBV	262662	267385	6.50%	0.229%
5	1.703	97	101	111	rVB	197550	251695	6.11%	0.216%
6	1.910	129	135	152	rVB	478018	697948	16.96%	0.598%
7	2.166	171	177	184	rBV	314064	444856	10.81%	0.381%
8	2.270	190	194	201	rVB	181154	269070	6.54%	0.231%
9	2.355	201	208	214	rVV2	768411	1455361	35.36%	1.247%
10	2.416	214	218	225	rVV	486129	801282	19.47%	0.687%
11	2.489	225	230	235	rVV	212563	373955	9.08%	0.320%
12	2.544	235	239	254	rVB	366718	615039	14.94%	0.527%
13	2.703	254	265	269	rBV	396635	737255	17.91%	0.632%
14	2.746	269	272	280	rVV	186968	313398	7.61%	0.269%
15	2.831	280	286	299	rVB	407375	771189	18.74%	0.661%
16	3.014	305	316	325	rBV	143126	334287	8.12%	0.286%
17	3.117	325	333	334	rBV	662160	1104417	26.83%	0.947%
18	3.666	413	423	433	rBV	289317	688476	16.73%	0.590%
19	3.782	433	442	474	rVB2	1222777	4040824	98.17%	3.463%
20	4.550	555	568	575	rBV3	560406	1720553	41.80%	1.475%
21	4.629	575	581	589	rVV	402394	1141038	27.72%	0.978%
22	4.715	589	595	602	rVV	262956	766318	18.62%	0.657%
23	4.812	602	611	626	rVV3	174514	783882	19.04%	0.672%
24	4.989	626	640	648	rVV3	309221	1099124	26.70%	0.942%
25	5.087	648	656	663	rVV	425147	1277381	31.03%	1.095%
26	5.172	663	670	683	rVB	280709	846507	20.56%	0.725%
27	5.458	703	717	724	rBV2	493172	1499205	36.42%	1.285%
28	5.544	724	731	738	rVV	411429	1262656	30.67%	1.082%
29	5.623	738	744	749	rVV	344126	984103	23.91%	0.843%
30	5.684	749	754	759	rVV	351751	946154	22.99%	0.811%
31	5.757	759	766	783	rVB2	591058	1771112	43.03%	1.518%
32	6.025	798	810	816	rBV	207772	548403	13.32%	0.470%
33	6.105	816	823	829	rBV	563128	1476828	35.88%	1.266%
34	6.409	862	873	886	rBV	287245	726504	17.65%	0.623%
35	6.824	930	941	954	rBV	488746	1153971	28.03%	0.989%
36	7.184	989	1000	1011	rBV	524010	1113037	27.04%	0.954%

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37	7.434	1028	1041	1046	rBV	677104	1516824	36.85%	1.300%
38	7.482	1046	1049	1060	rVB	458309	879696	21.37%	0.754%
39	7.635	1066	1074	1081	rBV	328300	641881	15.59%	0.550%
40	7.745	1081	1092	1102	rVV2	428797	962200	23.38%	0.825%
41	7.867	1102	1112	1126	rVB2	487726	1401998	34.06%	1.202%
42	8.159	1153	1160	1173	rBV	91951	166634	4.05%	0.143%
43	8.287	1173	1181	1193	rBV	1817724	2749310	66.79%	2.356%
44	8.409	1195	1201	1209	rBV	592086	937617	22.78%	0.804%
45	8.616	1228	1235	1242	rBV	2227549	3432878	83.40%	2.942%
46	8.696	1242	1248	1253	rVV	1008666	1619443	39.34%	1.388%
47	8.763	1253	1259	1269	rVB	1306947	1953280	47.45%	1.674%
48	9.019	1291	1301	1314	rBV	636901	889274	21.60%	0.762%
49	9.159	1317	1324	1326	rBV	627171	866417	21.05%	0.743%
50	9.196	1326	1330	1340	rVB	728282	1086840	26.40%	0.931%
51	9.318	1340	1350	1353	rBV	1018855	1628694	39.57%	1.396%
52	9.348	1353	1355	1361	rVB	658881	805862	19.58%	0.691%
53	9.470	1369	1375	1384	rBV	2029780	2656368	64.53%	2.277%
54	9.561	1384	1390	1395	rVV	511570	734260	17.84%	0.629%
55	9.616	1395	1399	1402	rVV	657020	858972	20.87%	0.736%
56	9.653	1402	1405	1411	rVB	380973	508488	12.35%	0.436%
57	10.092	1470	1477	1479	rBV	1064048	1457034	35.40%	1.249%
58	10.116	1479	1481	1489	rVV	1228206	1537132	37.34%	1.317%
59	10.201	1489	1495	1497	rVV	877485	1183000	28.74%	1.014%
60	10.232	1497	1500	1512	rVV	1699487	2142190	52.04%	1.836%
61	10.342	1512	1518	1533	rVB	3069079	4116274	100.00%	3.528%
62	10.689	1568	1575	1584	rBV2	2241091	3871063	94.04%	3.318%
63	10.836	1593	1599	1603	rBV	427916	593764	14.42%	0.509%
64	10.878	1603	1606	1617	rVV	899872	1038174	25.22%	0.890%
65	11.000	1620	1626	1631	rVV	1848675	2258593	54.87%	1.936%
66	11.055	1631	1635	1641	rVV	583010	702155	17.06%	0.602%
67	11.122	1641	1646	1656	rVB	861571	1140436	27.71%	0.977%
68	11.238	1659	1665	1669	rBV2	1258438	2283799	55.48%	1.957%
69	11.281	1669	1672	1674	rVV	741460	1141259	27.73%	0.978%
70	11.342	1678	1682	1687	rVV	1834820	2181393	52.99%	1.870%
71	11.402	1687	1692	1698	rVV	1464873	1799504	43.72%	1.542%
72	11.488	1701	1706	1719	rVB2	3112288	4055112	98.51%	3.475%
73	11.756	1744	1750	1753	rBV2	2215965	3195686	77.64%	2.739%
74	11.787	1753	1755	1761	rVB	1798928	2131257	51.78%	1.827%
75	11.927	1773	1778	1784	rBV	1739450	2084648	50.64%	1.787%
76	12.006	1786	1791	1794	rBV	1339610	1610250	39.12%	1.380%

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77	12.049	1794	1798	1801	rBV2	2236626	3351288	81.42%	2.872%
78	12.372	1845	1851	1869	rVB	3086110	3664433	89.02%	3.141%
79	12.579	1877	1885	1892	rBV	925760	1183820	28.76%	1.015%
80	12.981	1941	1951	1963	rVB2	307047	435271	10.57%	0.373%
81	13.140	1973	1977	1983	rVB	41595	54072	1.31%	0.046%
82	13.323	2002	2007	2018	rBV	1881145	2094927	50.89%	1.795%
83	13.628	2050	2057	2063	rBV	1143350	1404101	34.11%	1.203%
84	13.762	2074	2079	2083	rBV	861065	1062715	25.82%	0.911%
85	13.817	2083	2088	2099	rVB	1501721	1752358	42.57%	1.502%
86	14.000	2112	2118	2128	rVB	1181004	1415195	34.38%	1.213%

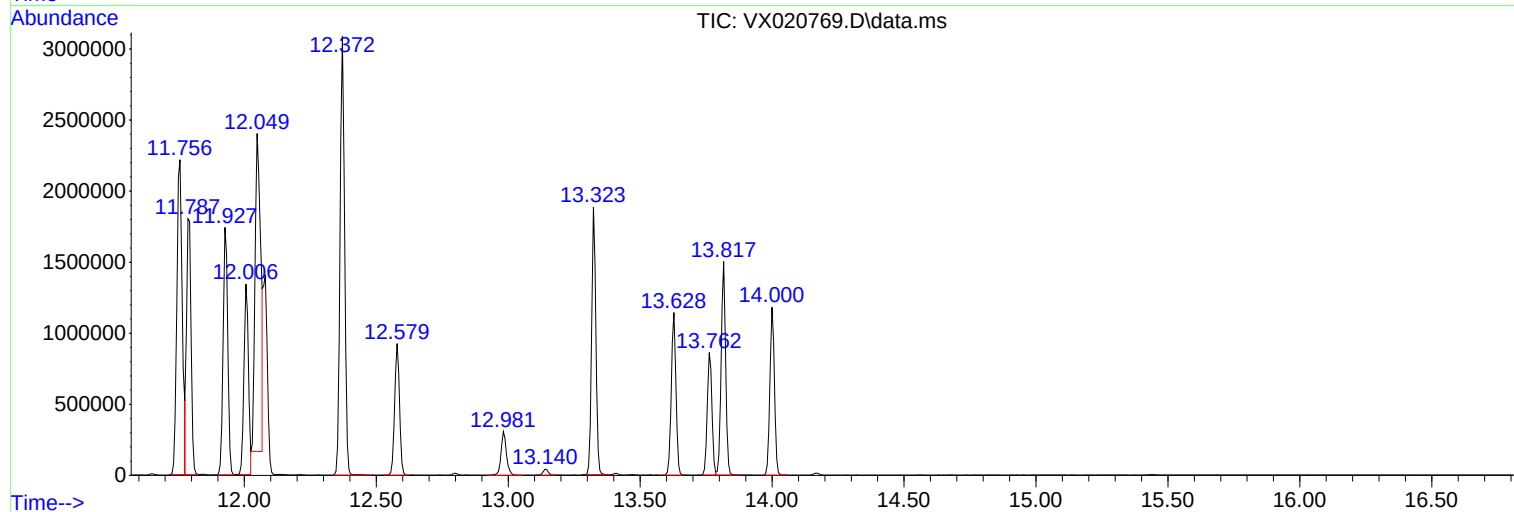
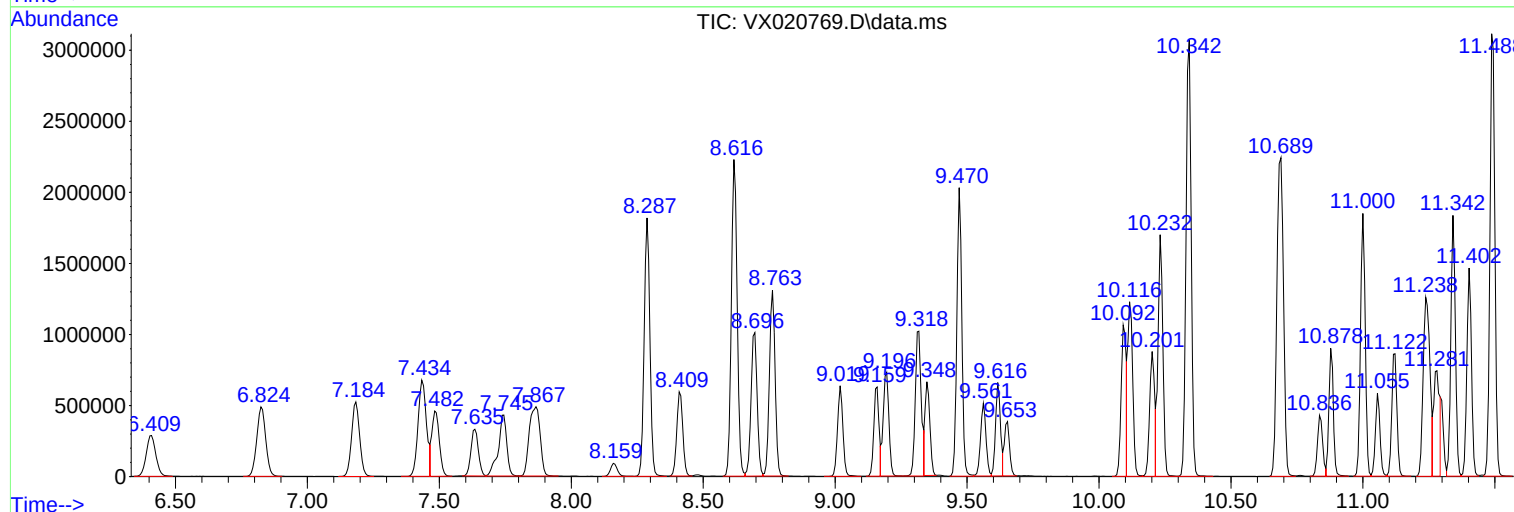
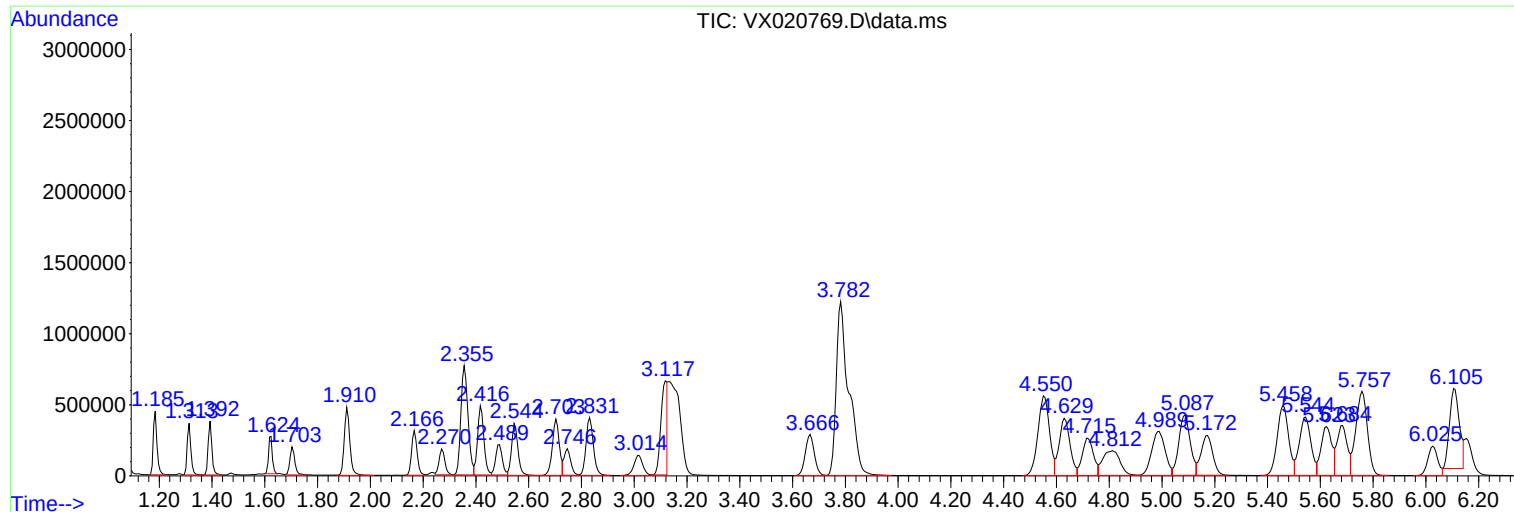
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Instrument :
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LabSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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



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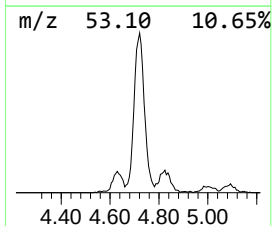
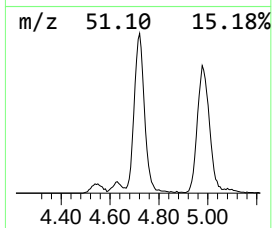
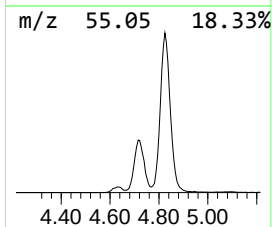
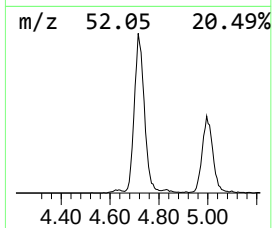
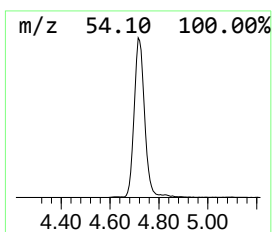
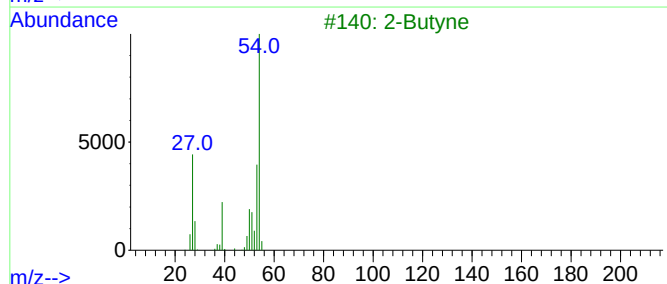
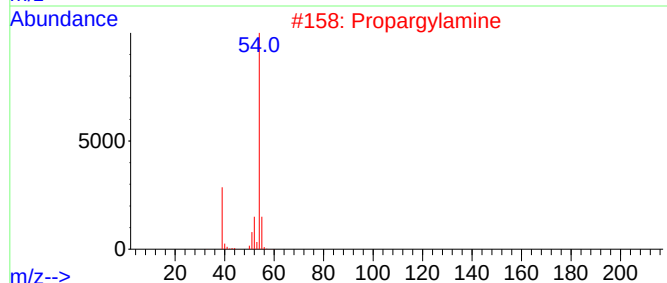
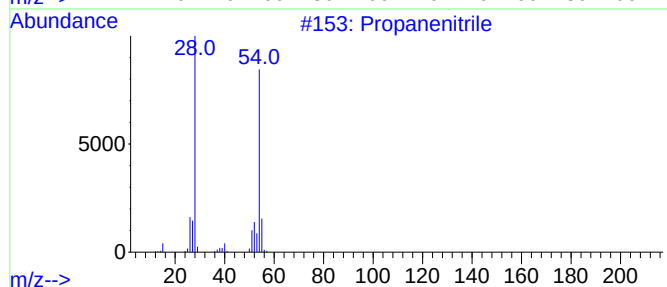
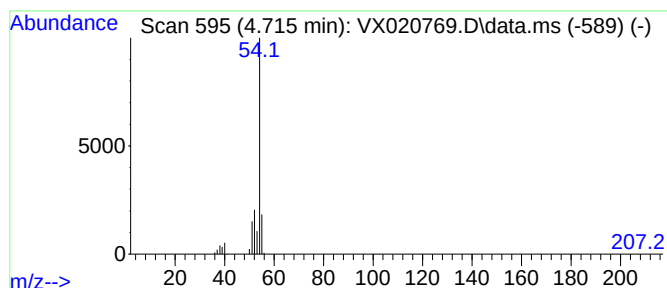
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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.
4.715	38.93 ug/l	766318	Pentafluorobenzene	5.623

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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LabSampleId :
VSTDCCC050

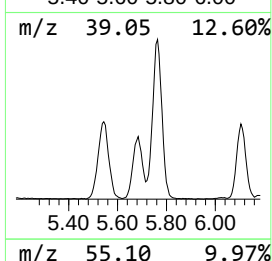
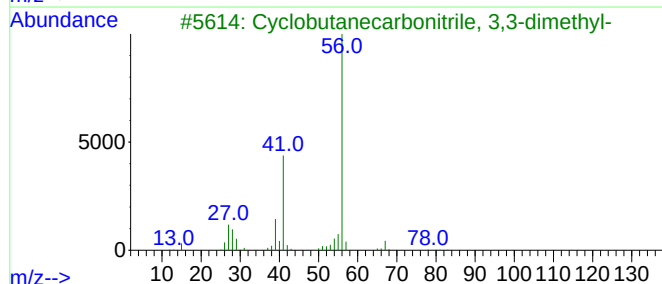
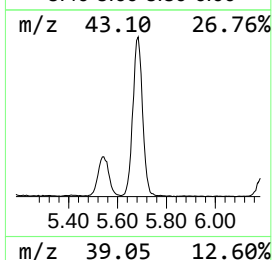
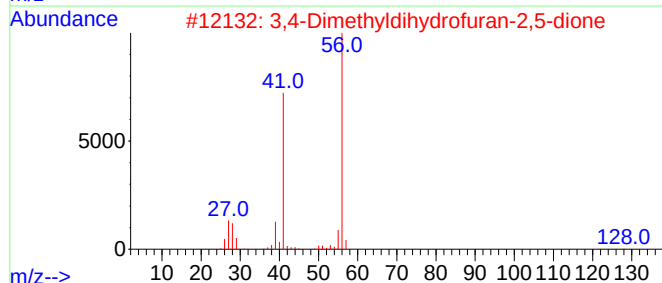
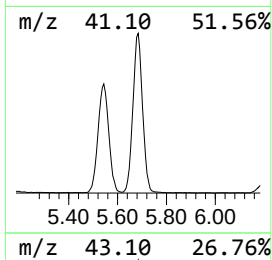
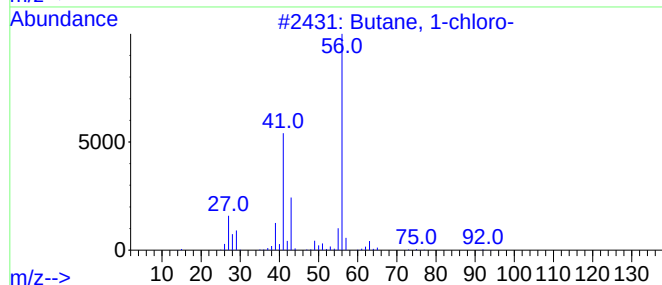
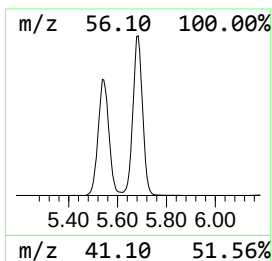
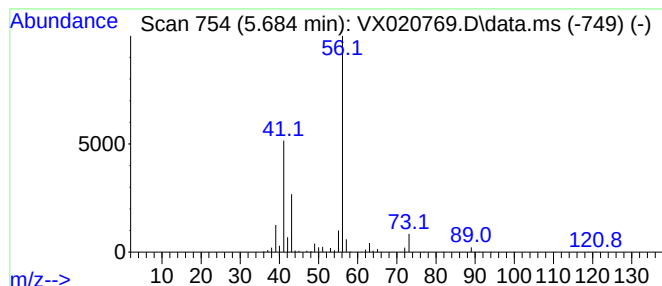
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.684	48.07 ug/l	946154	Pentafluorobenzene	5.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	72
2			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	59
3			Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	45
4			Formic acid, butyl ester	102	C5H10O2	000592-84-7	45
5			Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	38



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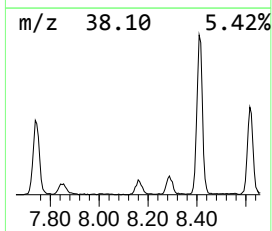
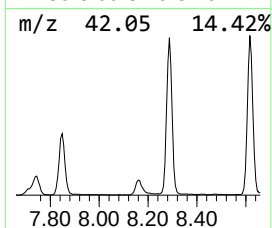
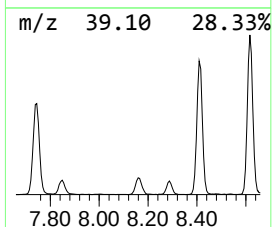
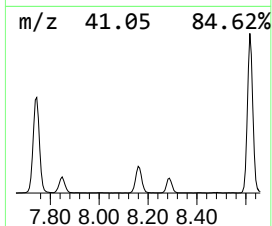
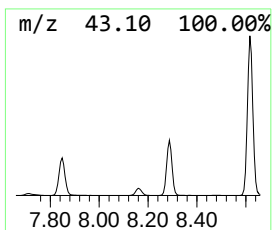
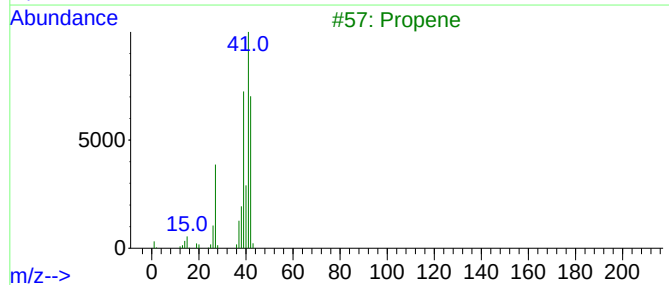
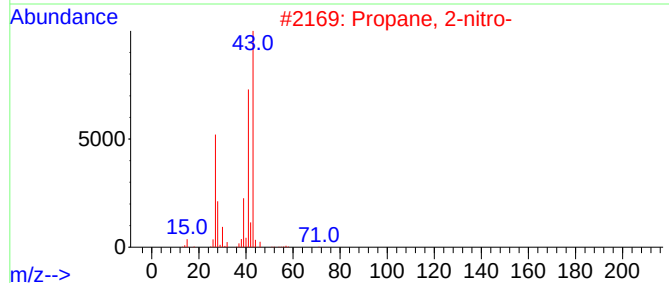
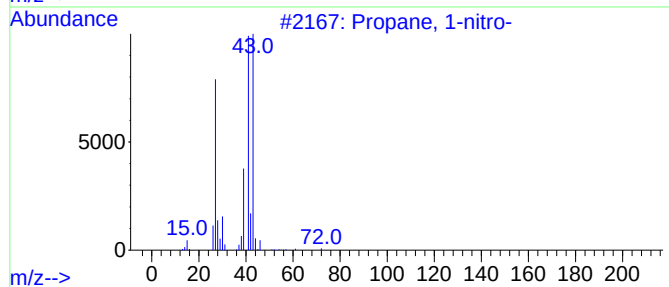
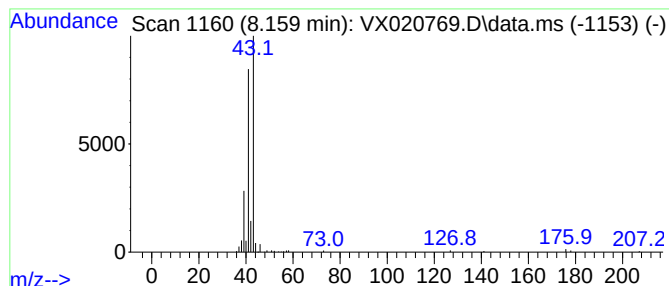
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Quant Title : SW846 8260

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

Peak Number 3 Propane, 1-nitro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.159	7.22 ug/l	166634	1,4-Difluorobenzene	6.824

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	78
2			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	78
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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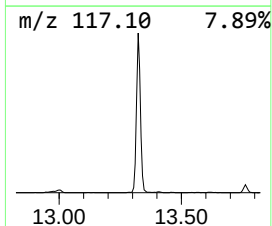
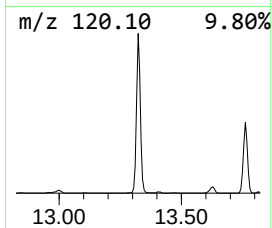
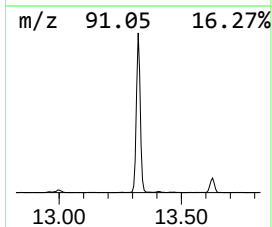
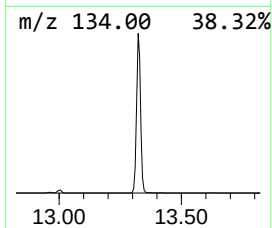
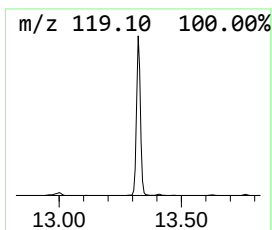
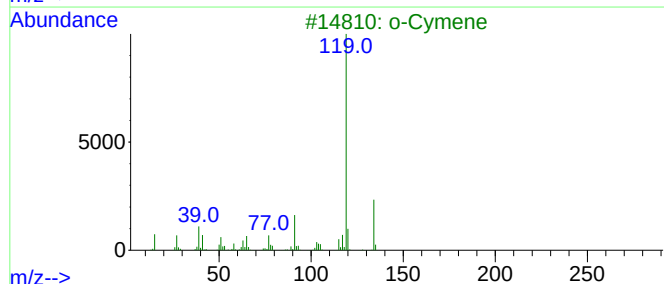
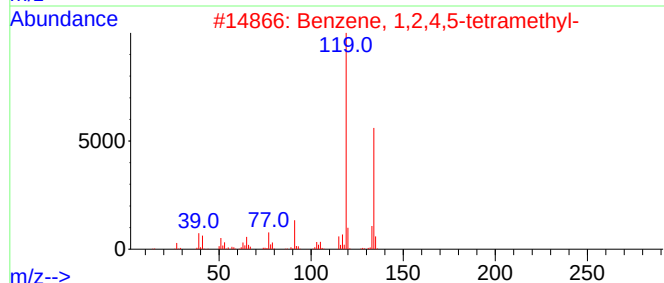
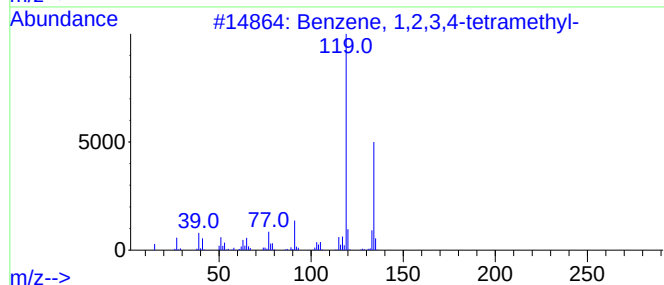
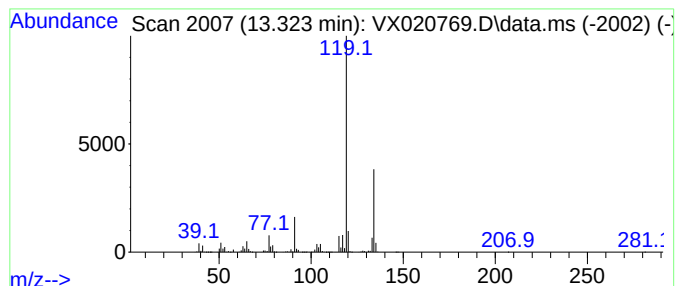
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Quant Title : SW846 8260

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	31.26 ug/l	2094930	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			o-Cymene	134	C10H14	000527-84-4	95
4			p-Cymene	134	C10H14	000099-87-6	95
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012721\
Data File : VX020769.D
Acq On : 27 Jan 2021 14:04
Operator : JC/SP
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 2 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	4.715	38.9	ug/l	766318	1	5.623	984103	50.0
Butane, 1-chloro-	5.684	48.1	ug/l	946154	1	5.623	984103	50.0
Propane, 1-nitro-	8.159	7.2	ug/l	166634	2	6.824	1153970	50.0
Benzene, 1,2,3,...	13.323	31.3	ug/l	2094930	4	12.061	3351290	50.0