LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012721\
Data File : VX020784.D
Acq On : 27 Jan 2021 20:38
Operator : JC/SP
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 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: VX020784.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	26	rVB	488351	472823	9.84%	0.350%
2	1.313	33	37	46	rBV	426437	415865	8.66%	0.308%
3	1.392	46	50	60	rVB	440054	422278	8.79%	0.312%
4	1.624	84	88	92	rBV	306747	298257	6.21%	0.221%
5	1.703	97	101	113	rVB	227845	293055	6.10%	0.217%
6	1.910	129	135	148	rVB	513052	759225	15.80%	0.562%
7	2.166	172	177	188	rBV	372868	520259	10.83%	0.385%
8	2.270	189	194	202	rVV	243875	383779	7.99%	0.284%
9	2.355	202	208	214	rVV2	852569	1627620	33.87%	1.204%
10	2.422	214	219	225	rVV	449155	769271	16.01%	0.569%
11	2.489	225	230	235	rVV	257188	439223	9.14%	0.325%
12	2.544	235	239	254	rVB	377728	663470	13.81%	0.491%
13	2.703	256	265	269	rBV	459250	848953	17.67%	0.628%
14	2.746	269	272	280	rVV	226207	402911	8.39%	0.298%
15	2.831	280	286	302	rVB	458023	881096	18.34%	0.652%
16	3.020	306	317	325	rBV	193988	450143	9.37%	0.333%
17	3.123	325	334	362	rVB3	832195	3818599	79.47%	2.825%
18	3.666	414	423	433	rBV	329199	790279	16.45%	0.585%
19	3.782	433	442	471	rVB2	1456256	4804873	100.00%	3.555%
20	4.556	554	569	576	rBV3	628001	1927230	40.11%	1.426%
21	4.635	576	582	590	rVV	462906	1300922	27.08%	0.963%
22	4.727	590	597	603	rVV	345086	1005767	20.93%	0.744%
23	4.812	603	611	627	rVV2	220292	994785	20.70%	0.736%
24	4.989	627	640	649	rVV3	367825	1329440	27.67%	0.984%
25	5.087	649	656	664	rVV	551333	1663981	34.63%	1.231%
26	5.172	664	670	685	rVB2	320126	960110	19.98%	0.710%
27	5.465	704	718	725	rBV	558181	1716167	35.72%	1.270%
28	5.544	725	731	738	rVV	459295	1360673	28.32%	1.007%
29	5.629	738	745	750	rVV	380669	1131364	23.55%	0.837%
30	5.684	750	754	759	rVV	358539	905013	18.84%	0.670%
31	5.763	759	767	784	rVB2	658349	2015536	41.95%	1.491%
32	6.032	800	811	816	rBV	240114	615649	12.81%	0.456%
33	6.111	816	824	830	rBV	659190	1751623	36.46%	1.296%
34	6.409	862	873	888	rBV	368091	921112	19.17%	0.682%
35	6.830	931	942	963	rVB	589255	1388160	28.89%	1.027%
36	7.184	990	1000	1011	rBV	585673	1261625	26.26%	0.933%

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ALS Vial : 18 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

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Peak separation: 5

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Title : SW846 8260

37	7.440	1030	1042	1046	rBV	664502	1486786	30.94%	1.100%
38	7.489	1046	1050	1061	rVB	538246	1052106	21.90%	0.778%
39	7.635	1067	1074	1081	rBV	396421	738055	15.36%	0.546%
40	7.745	1081	1092	1102	rVB2	562978	1213674	25.26%	0.898%
41	7.854	1102	1110	1111	rBV	553313	870960	18.13%	0.644%
42	8.165	1153	1161	1170	rBV	117100	209522	4.36%	0.155%
43	8.287	1174	1181	1195	rVV	2040857	3235194	67.33%	2.394%
44	8.415	1195	1202	1209	rVV	692869	1089585	22.68%	0.806%
45	8.623	1228	1236	1242	rBV	2718095	4363284	90.81%	3.228%
46	8.696	1242	1248	1254	rVV	1188199	1871107	38.94%	1.384%
47	8.763	1254	1259	1274	rVB	1519207	2247831	46.78%	1.663%
48	9.019	1292	1301	1315	rBV	719954	1031480	21.47%	0.763%
49	9.159	1318	1324	1327	rBV	811376	1142187	23.77%	0.845%
50	9.196	1327	1330	1340	rVB	858582	1177308	24.50%	0.871%
51	9.317	1340	1350	1353	rBV	1122652	1729441	35.99%	1.280%
52	9.348	1353	1355	1361	rVB	740267	968304	20.15%	0.716%
53	9.470	1369	1375	1384	rBV	2440046	3229658	67.22%	2.390%
54	9.561	1384	1390	1395	rVV	567468	824473	17.16%	0.610%
55	9.616	1395	1399	1402	rVV	836967	1083571	22.55%	0.802%
56	9.653	1402	1405	1413	rVB	450136	605065	12.59%	0.448%
57	10.098	1471	1478	1479	rBV	1234039	1667003	34.69%	1.233%
58	10.116	1479	1481	1489	rVV	1402259	1815099	37.78%	1.343%
59	10.201	1489	1495	1497	rVV	997872	1340182	27.89%	0.992%
60	10.232	1497	1500	1511	rVV	1874961	2449611	50.98%	1.812%
61	10.342	1512	1518	1535	rVB	3460939	4669287	97.18%	3.455%
62	10.689	1567	1575	1583	rBV2	2572393	4431631	92.23%	3.279%
63	10.842	1591	1600	1603	rBV	500208	692889	14.42%	0.513%
64	10.878	1603	1606	1619	rVV	1136333	1305896	27.18%	0.966%
65	11.000	1621	1626	1631	rVV	2077537	2523556	52.52%	1.867%
66	11.055	1631	1635	1641	rVV	689671	860374	17.91%	0.637%
67	11.122	1641	1646	1659	rVV	998659	1305672	27.17%	0.966%
68	11.238	1659	1665	1669	rVV2	1434261	2630474	54.75%	1.946%
69	11.281	1669	1672	1678	rVV2	925626	1845571	38.41%	1.366%
70	11.342	1678	1682	1687	rVV	1967948	2369081	49.31%	1.753%
71	11.402	1687	1692	1698	rVV	1610169	2017027	41.98%	1.492%
72	11.494	1701	1707	1719	rVB2	3358692	4421952	92.03%	3.272%
73	11.756	1740	1750	1753	rBV2	2387388	3472146	72.26%	2.569%
74	11.793	1753	1756	1761	rVB	1959516	2345400	48.81%	1.735%
75	11.927	1772	1778	1784	rBV	1733937	2132569	44.38%	1.578%
76	12.006	1786	1791	1794	rBV	1437096	1751460	36.45%	1.296%

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LabSampleId : VSTDCCC050

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
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Title : SW846 8260

77	12.049	1794	1798	1802	rBV2	2193167	3899060	81.15%	2.885%
78	12.372	1845	1851	1860	rBV	3098104	3731255	77.66%	2.761%
79	12.579	1877	1885	1891	rBV	945797	1230577	25.61%	0.911%
80	12.981	1939	1951	1961	rBV2	391341	557175	11.60%	0.412%
81	13.140	1973	1977	1984	rBV	55245	73161	1.52%	0.054%
82	13.323	2002	2007	2018	rBV	1903739	2254306	46.92%	1.668%
83	13.628	2050	2057	2066	rBV	1172143	1445023	30.07%	1.069%
84	13.762	2069	2079	2083	rBV	707185	880493	18.33%	0.651%
85	13.817	2083	2088	2096	rVB	1719068	2080623	43.30%	1.539%
86	14.000	2112	2118	2124	rBV	1186104	1472295	30.64%	1.089%

Sum of corrected areas: 135151575

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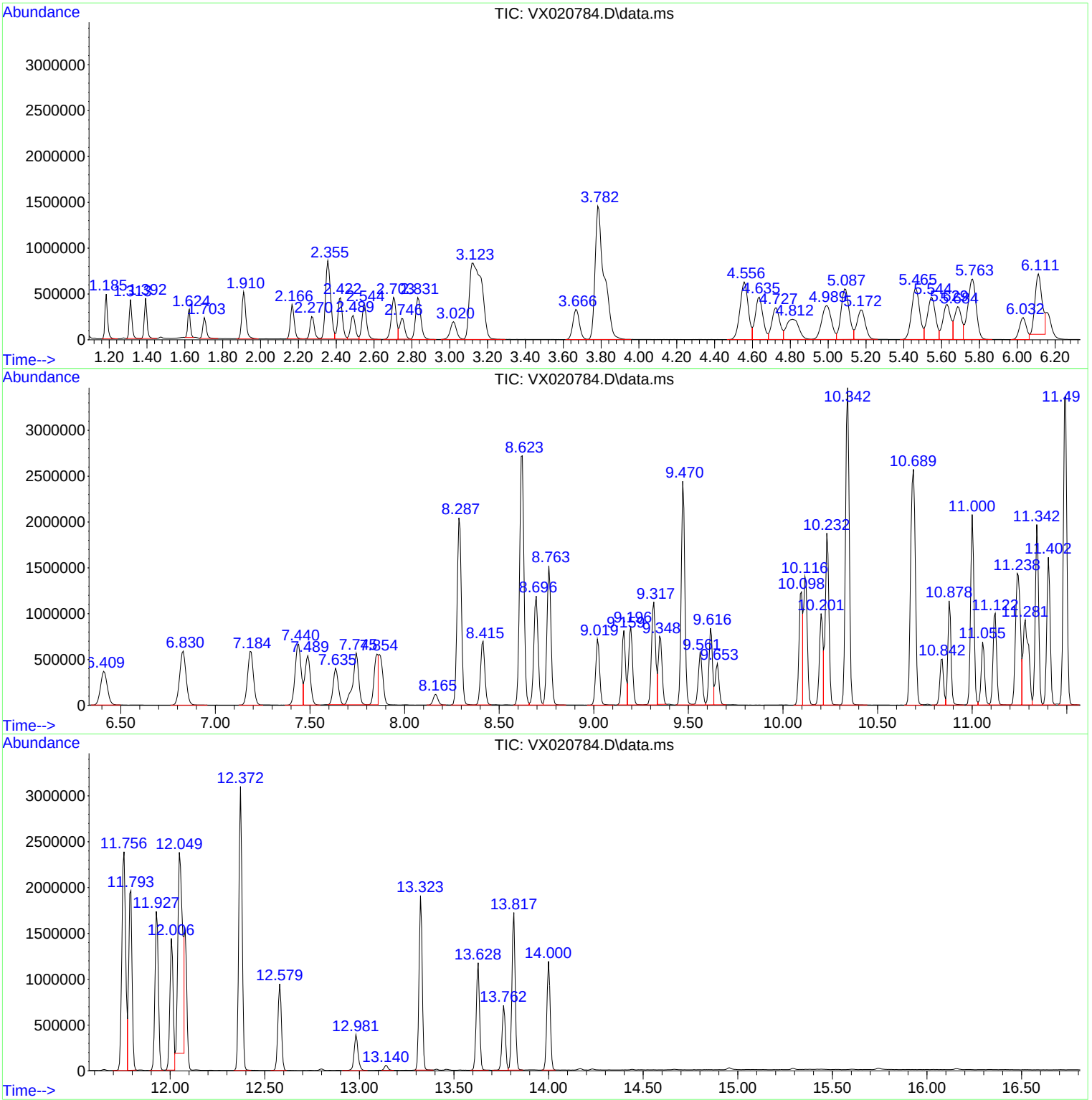
LabSampleId :
VSTDCCC050

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



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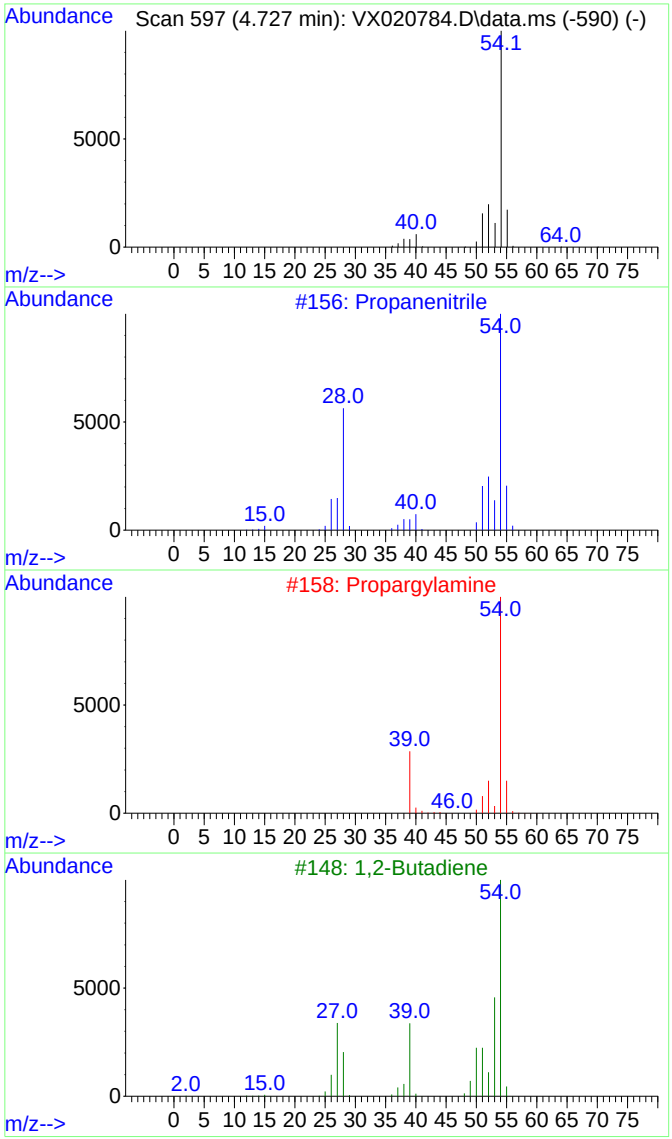
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

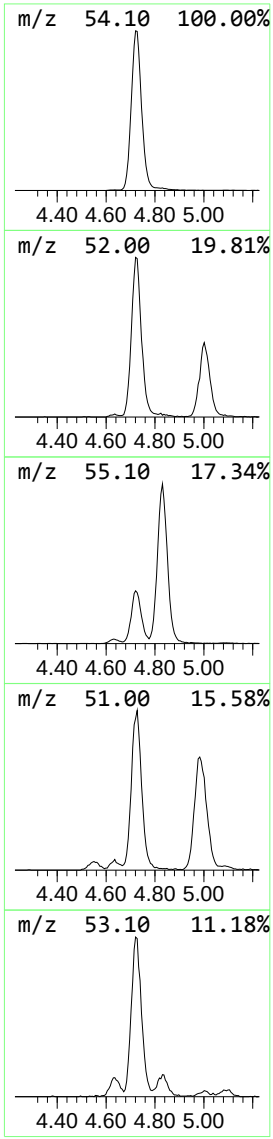
****

Peak Number 1 Propanenitrile Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.727	44.45 ug/l	1005770	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanenitrile	55	C3H5N	000107-12-0	64
2	Propargylamine	55	C3H5N	002450-71-7	5
3	1,2-Butadiene	54	C4H6	000590-19-2	5
4	2-Butyne	54	C4H6	000503-17-3	5
5	1-Butyne	54	C4H6	000107-00-6	3





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MSVOA_X
LabSampleId :
VSTDCCC050

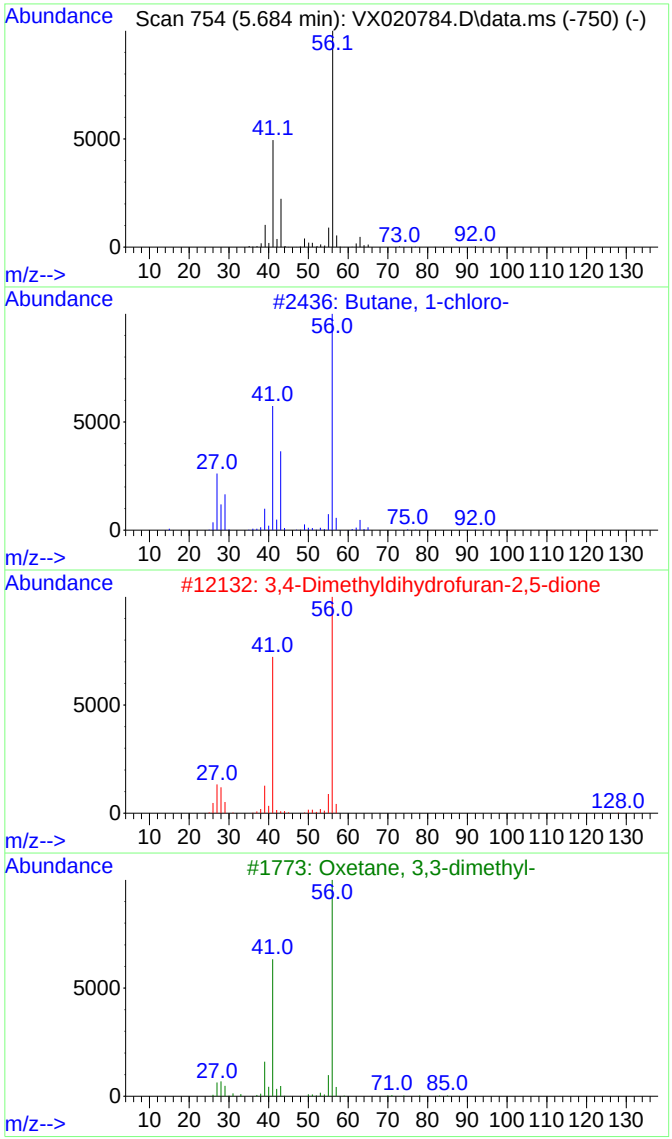
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

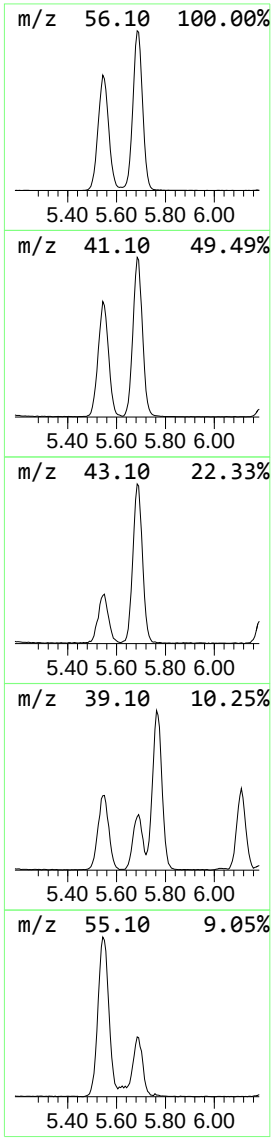
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.684	40.00 ug/l	905013	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	78
2	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	50
3	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	50
4	Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	50
5	Ethane, diazo-	56	C2H4N2	001117-96-0	9





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MSVOA_X
LabSampleId :
VSTDCCC050

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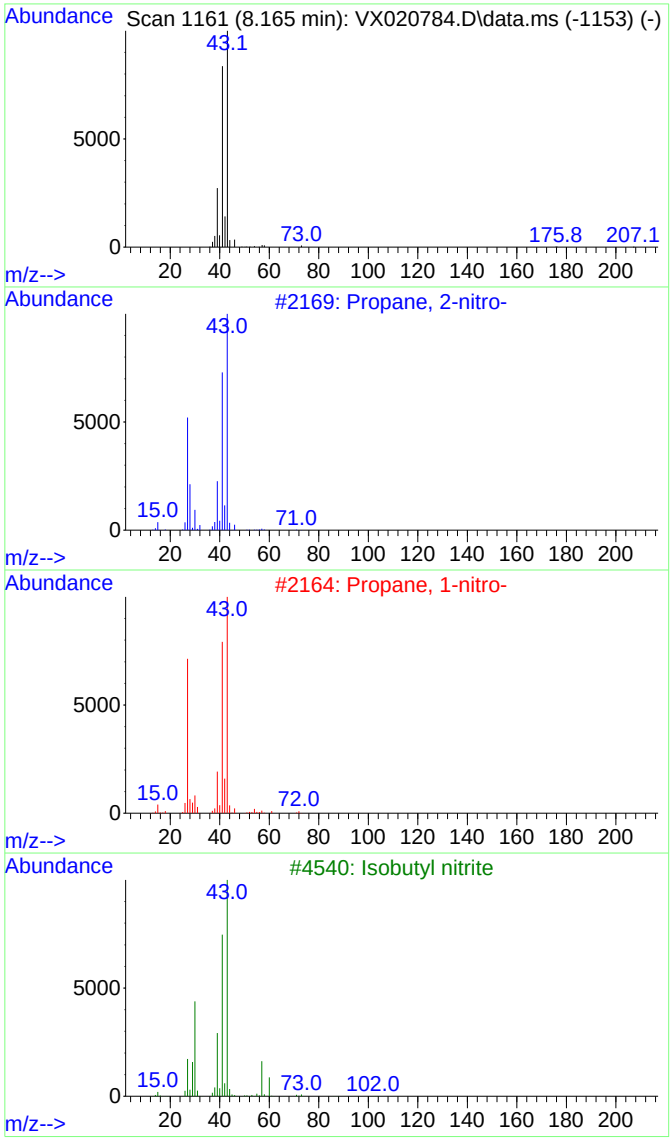
Quant Title : SW846 8260

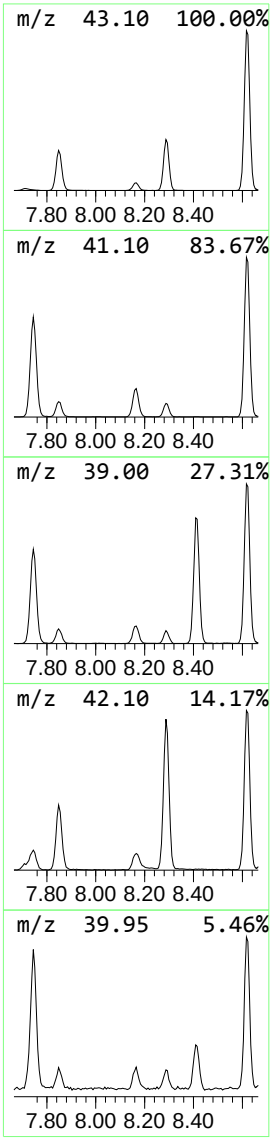
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.165	7.55 ug/l	209522	1,4-Difluorobenzene	6.830

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	78
2	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	50
3	Isobutyl nitrite	103	C4H9NO2	000542-56-3	9
4	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	9
5	1H-Pyrazol-1-amine, 5-methyl-3-n...	142	C4H6N4O2	151588-03-3	9





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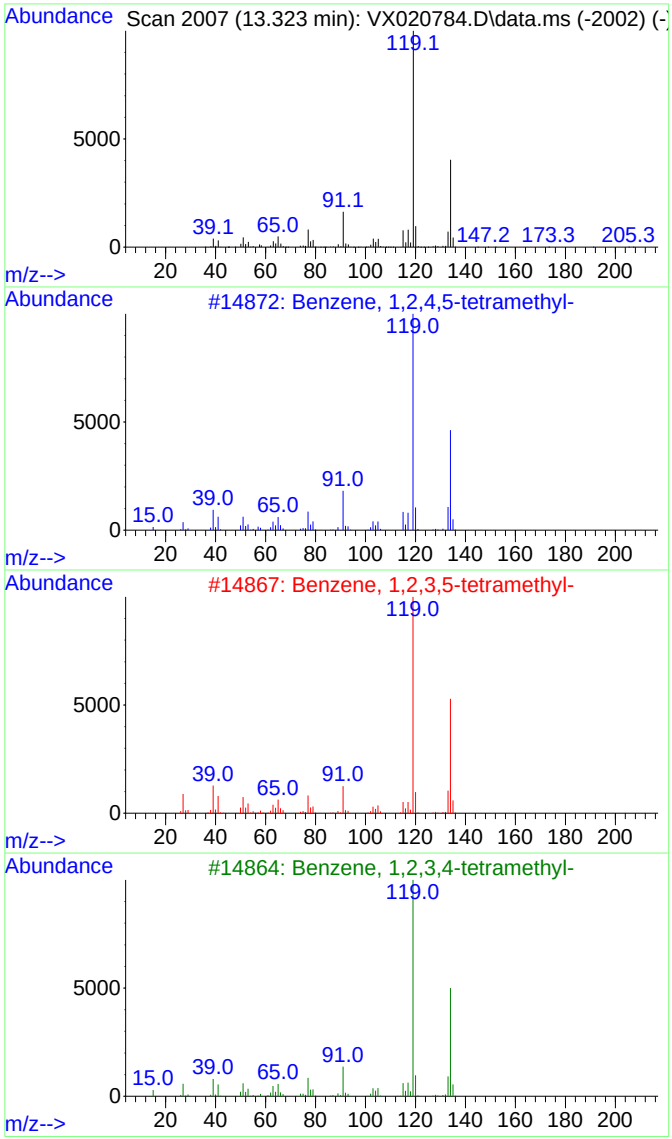
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

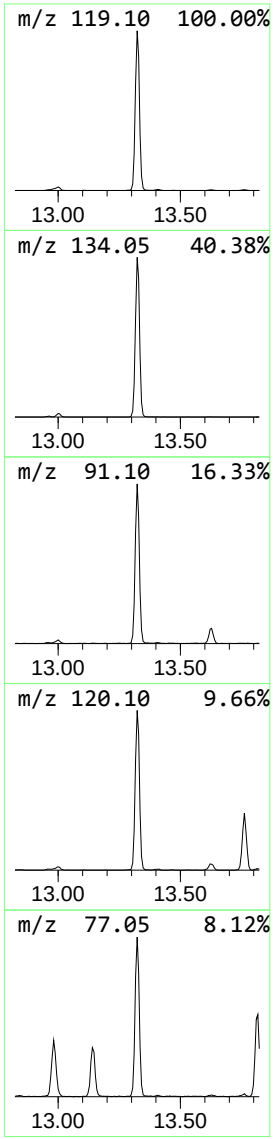
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.323	28.91 ug/l	2254310	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94





Tentatively Identified Compound (LSC) summary

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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propanenitrile	4.727	44.4	ug/l	1005770	1	5.629	1131360	50.0
Butane, 1-chloro-	5.684	40.0	ug/l	905013	1	5.629	1131360	50.0
Propane, 2-nitro-	8.165	7.5	ug/l	209522	2	6.830	1388160	50.0
Benzene, 1,2,4,...	13.323	28.9	ug/l	2254310	4	12.061	3899060	50.0