LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020741.D
Acq On : 26 Jan 2021 09:51
Operator : JC/SP
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 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: VX020741.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	464639	444254	10.37%	0.365%
2	1.313	33	37	46	rVB	373969	363749	8.49%	0.299%
3	1.392	46	50	59	rBV	388863	374795	8.75%	0.308%
4	1.624	84	88	96	rVB	287737	303920	7.10%	0.250%
5	1.703	96	101	113	rVB	208067	267798	6.25%	0.220%
6	1.910	129	135	145	rBV	484464	696008	16.25%	0.572%
7	2.166	171	177	185	rBV	335017	477195	11.14%	0.392%
8	2.270	189	194	201	rVV	220861	341839	7.98%	0.281%
9	2.355	201	208	214	rVV2	790210	1501373	35.05%	1.233%
10	2.416	214	218	225	rVV	423095	714827	16.69%	0.587%
11	2.489	225	230	235	rVV	215626	384488	8.98%	0.316%
12	2.544	235	239	254	rVB	364415	623532	14.56%	0.512%
13	2.703	254	265	269	rBV	412354	770479	17.99%	0.633%
14	2.745	269	272	279	rVV	199481	333896	7.80%	0.274%
15	2.831	279	286	299	rVB	415093	792085	18.49%	0.651%
16	3.014	304	316	325	rBV	156190	385658	9.00%	0.317%
17	3.117	325	333	357	rVB3	708904	3337016	77.91%	2.741%
18	3.666	410	423	433	rBV	296508	708773	16.55%	0.582%
19	3.782	433	442	473	rVB2	1313291	4283238	100.00%	3.519%
20	4.550	554	568	575	rBV2	564524	1746541	40.78%	1.435%
21	4.629	575	581	589	rVV	401541	1132539	26.44%	0.930%
22	4.721	589	596	602	rVV	286423	830678	19.39%	0.682%
23	4.812	602	611	626	rVV2	184721	845336	19.74%	0.694%
24	4.989	626	640	648	rVV3	314461	1132421	26.44%	0.930%
25	5.086	648	656	663	rVV	453244	1386556	32.37%	1.139%
26	5.172	663	670	685	rVB	288192	869426	20.30%	0.714%
27	5.458	703	717	724	rBV2	498884	1512096	35.30%	1.242%
28	5.544	724	731	738	rVV	420513	1288624	30.09%	1.059%
29	5.623	738	744	749	rVV2	353880	1002997	23.42%	0.824%
30	5.684	749	754	759	rVV	325953	890050	20.78%	0.731%
31	5.757	759	766	782	rVB2	599543	1790813	41.81%	1.471%
32	6.025	798	810	816	rBV	216441	564631	13.18%	0.464%
33	6.105	816	823	830	rBV	582923	1621119	37.85%	1.332%
34	6.403	862	872	884	rBV	310713	784226	18.31%	0.644%
35	6.824	930	941	953	rBV	516228	1200593	28.03%	0.986%
36	7.184	990	1000	1014	rBV	517956	1113107	25.99%	0.914%

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ALS Vial : 1 Sample Multiplier: 1

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LabSampleId : VSTDCCC050

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Title : SW846 8260

37	7.434	1030	1041	1046	rBV	688222	1548744	36.16%	1.272%
38	7.482	1046	1049	1060	rVB	480417	899278	21.00%	0.739%
39	7.635	1066	1074	1081	rBV	340950	656505	15.33%	0.539%
40	7.745	1081	1092	1102	rVV2	461833	1051482	24.55%	0.864%
41	7.866	1102	1112	1129	rVB2	500227	1487487	34.73%	1.222%
42	8.159	1153	1160	1174	rBV	105791	188244	4.39%	0.155%
43	8.287	1174	1181	1194	rBV	1789384	2765811	64.57%	2.272%
44	8.409	1194	1201	1209	rBV	621870	983356	22.96%	0.808%
45	8.616	1228	1235	1242	rBV	2370902	3662480	85.51%	3.009%
46	8.689	1242	1247	1253	rVV	1014824	1625409	37.95%	1.335%
47	8.763	1253	1259	1270	rVB	1323742	2006648	46.85%	1.648%
48	9.019	1293	1301	1317	rBV	653398	941698	21.99%	0.774%
49	9.159	1317	1324	1326	rBV	661837	932884	21.78%	0.766%
50	9.195	1326	1330	1339	rVB	756838	1113502	26.00%	0.915%
51	9.311	1341	1349	1353	rBV	987525	1598335	37.32%	1.313%
52	9.348	1353	1355	1361	rVB	693556	839581	19.60%	0.690%
53	9.470	1369	1375	1384	rBV	2010111	2640929	61.66%	2.169%
54	9.561	1384	1390	1395	rVV	544748	766002	17.88%	0.629%
55	9.616	1395	1399	1402	rVV	714137	923691	21.57%	0.759%
56	9.653	1402	1405	1412	rVB	401529	530984	12.40%	0.436%
57	10.092	1471	1477	1479	rBV	1103478	1522593	35.55%	1.251%
58	10.116	1479	1481	1488	rVV	1266258	1555743	36.32%	1.278%
59	10.201	1489	1495	1497	rVV	909195	1238670	28.92%	1.018%
60	10.232	1497	1500	1511	rVV	1722785	2159241	50.41%	1.774%
61	10.342	1511	1518	1529	rVB	3094738	4198719	98.03%	3.449%
62	10.683	1565	1574	1584	rBV2	2240137	3941770	92.03%	3.238%
63	10.835	1593	1599	1603	rBV	444067	614710	14.35%	0.505%
64	10.878	1603	1606	1619	rVV	943024	1071223	25.01%	0.880%
65	11.000	1620	1626	1631	rVV	1863712	2282399	53.29%	1.875%
66	11.055	1631	1635	1641	rVV	587693	729417	17.03%	0.599%
67	11.122	1641	1646	1654	rVB	828992	1111190	25.94%	0.913%
68	11.238	1659	1665	1669	rVV2	1260021	2307779	53.88%	1.896%
69	11.280	1669	1672	1678	rVV2	764028	1547064	36.12%	1.271%
70	11.341	1678	1682	1687	rVV	1844629	2200177	51.37%	1.807%
71	11.402	1687	1692	1698	rVV	1467732	1808278	42.22%	1.485%
72	11.488	1701	1706	1718	rVB2	3098644	4052424	94.61%	3.329%
73	11.756	1744	1750	1753	rBV2	2206248	3217873	75.13%	2.643%
74	11.786	1753	1755	1761	rVB	1770300	2128113	49.68%	1.748%
75	11.927	1770	1778	1784	rBV	1702291	2084665	48.67%	1.713%
76	12.006	1786	1791	1794	rBV	1255860	1576452	36.81%	1.295%

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77	12.049	1794	1798	1801	rBV2	2139966	3260966	76.13%	2.679%
78	12.372	1845	1851	1857	rBV	3032581	3612842	84.35%	2.968%
79	12.579	1877	1885	1891	rBV	918409	1189863	27.78%	0.977%
80	12.981	1941	1951	1959	rBV2	331981	464319	10.84%	0.381%
81	13.140	1970	1977	1982	rBV	49708	66911	1.56%	0.055%
82	13.323	2002	2007	2018	rBV	1851131	2098784	49.00%	1.724%
83	13.628	2050	2057	2067	rVB	1155648	1414685	33.03%	1.162%
84	13.762	2073	2079	2083	rBV	839814	1055499	24.64%	0.867%
85	13.817	2083	2088	2097	rVB	1522554	1811642	42.30%	1.488%
86	13.999	2111	2118	2125	rBV	1189741	1428152	33.34%	1.173%

Sum of corrected areas: 121731889

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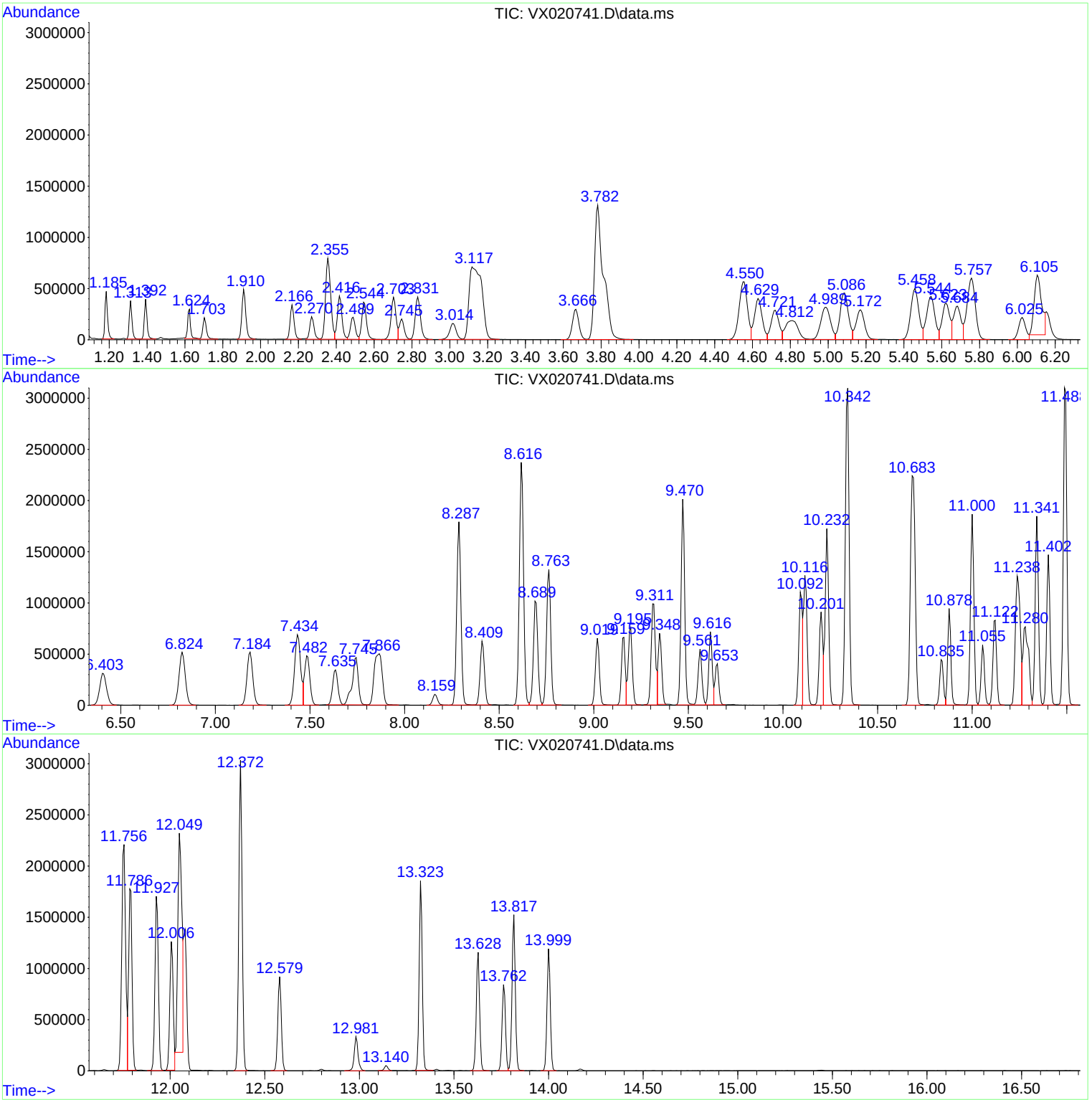
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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



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TIC Library : C:\DATABASE\NIST11.L
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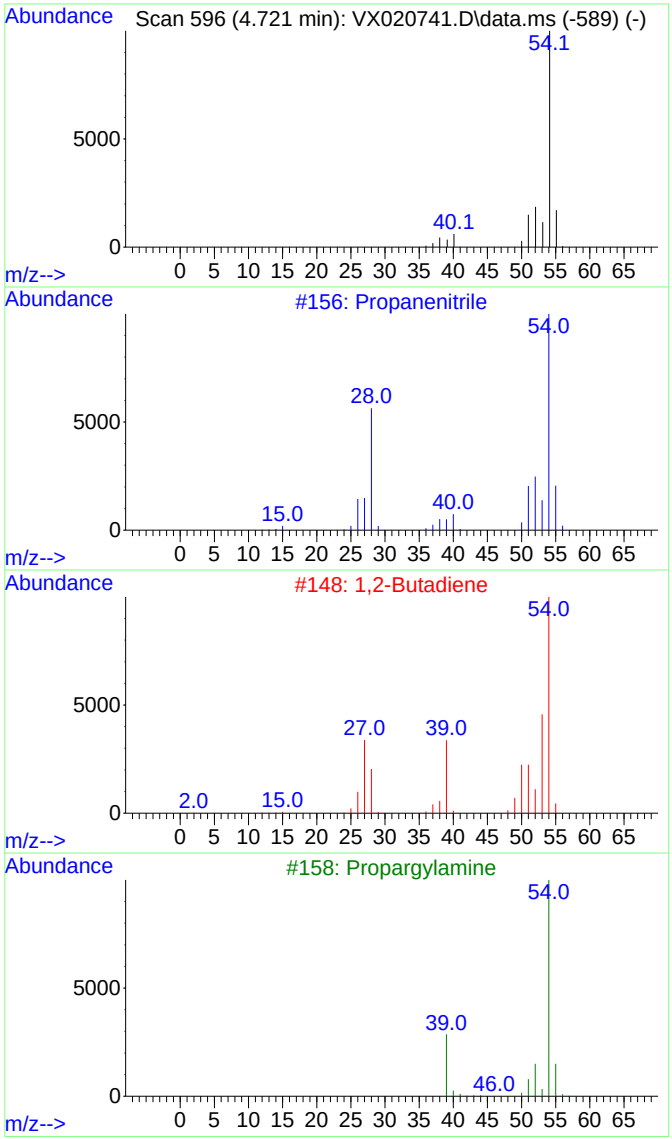
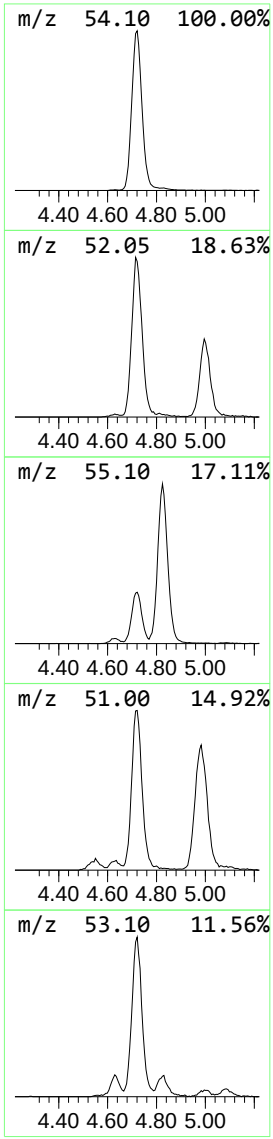
****

Peak Number 1 Propanenitrile Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.721	41.41 ug/l	830678	Pentafluorobenzene	5.617

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanenitrile	55	C3H5N	000107-12-0	86
2	1,2-Butadiene	54	C4H6	000590-19-2	9
3	Propargylamine	55	C3H5N	002450-71-7	5
4	2-Butyne	54	C4H6	000503-17-3	5
5	1-Butyne	54	C4H6	000107-00-6	3





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Instrument :
MSVOA_X
LabSampleId :
VSTDCCC050

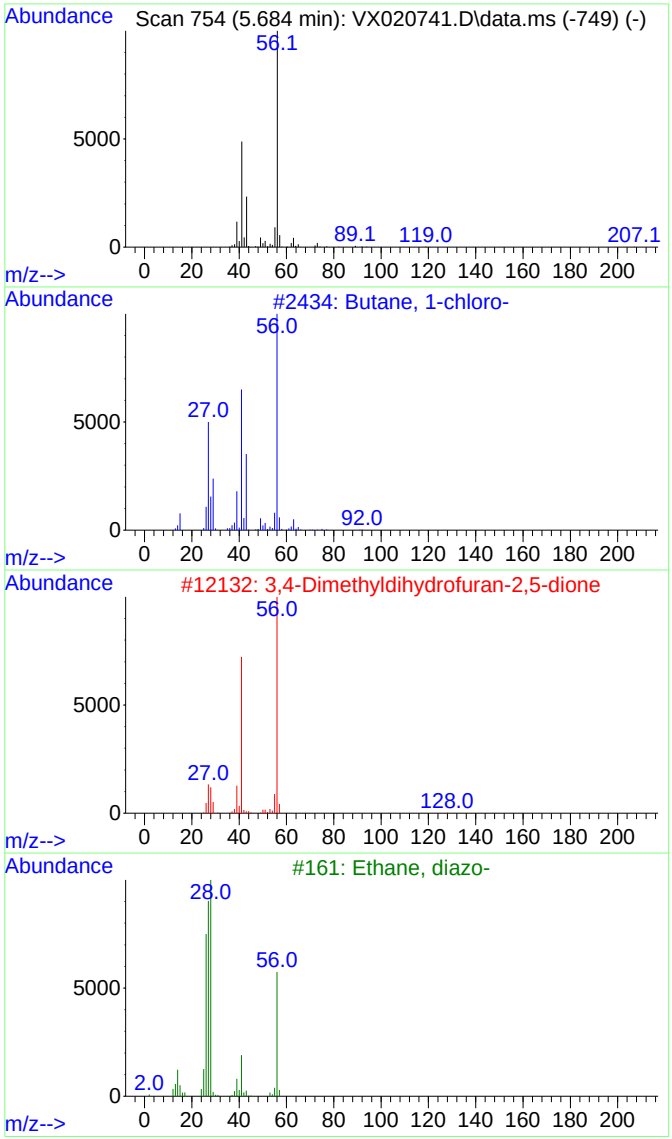
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

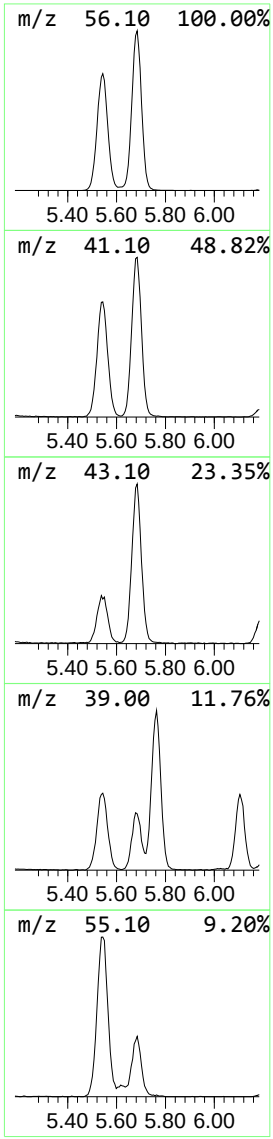
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.684	44.37 ug/l	890050	Pentafluorobenzene	5.617

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	90
2	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	64
3	Ethane, diazo-	56	C2H4N2	001117-96-0	9
4	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9
5	4-Propylcyclohexylamine	141	C9H19N	102653-37-2	9





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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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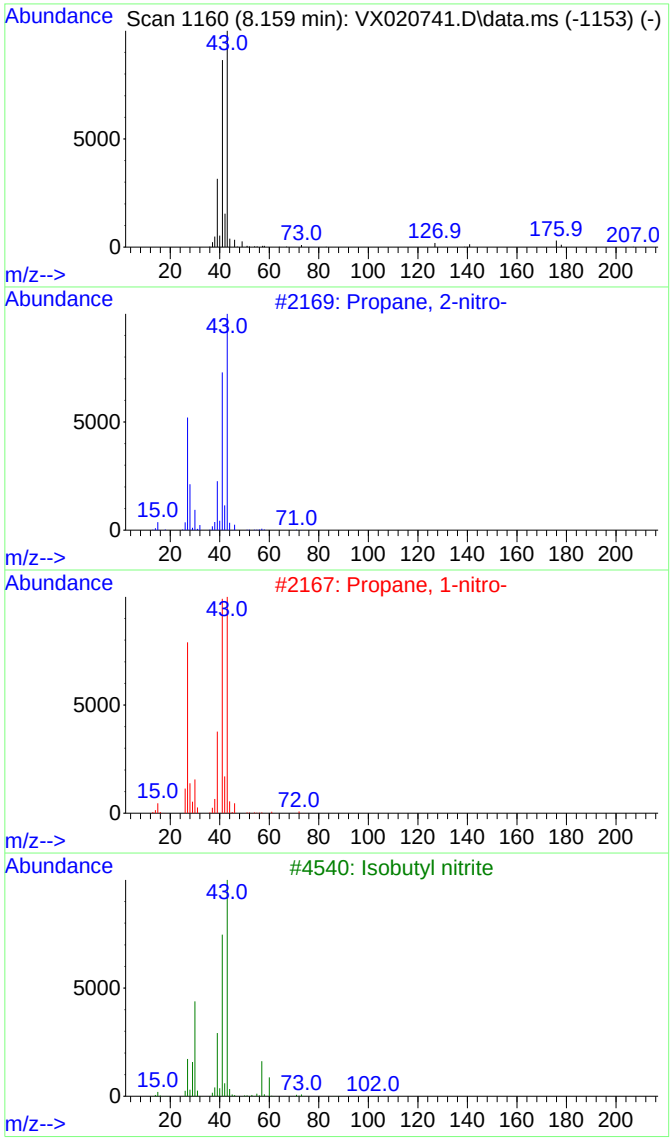
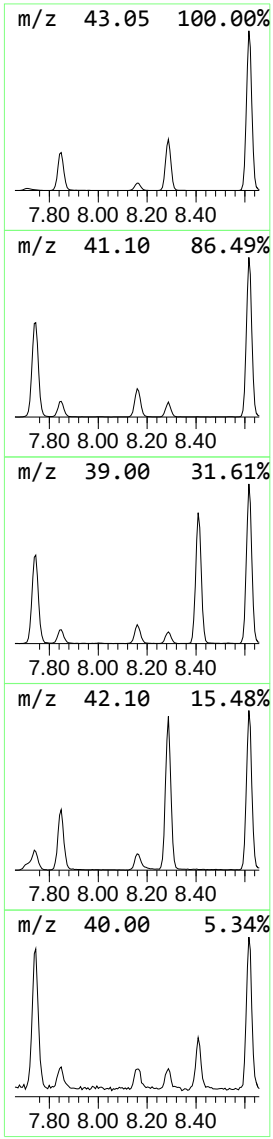
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.159	7.84 ug/l	188244	1,4-Difluorobenzene	6.824

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	64
2	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	64
3	Isobutyl nitrite	103	C4H9NO2	000542-56-3	9
4	1H-Pyrazol-1-amine, 5-methyl-3-n...	142	C4H6N4O2	151588-03-3	9
5	Propanamide, 2,2-dimethyl-	101	C5H11NO	000754-10-9	9





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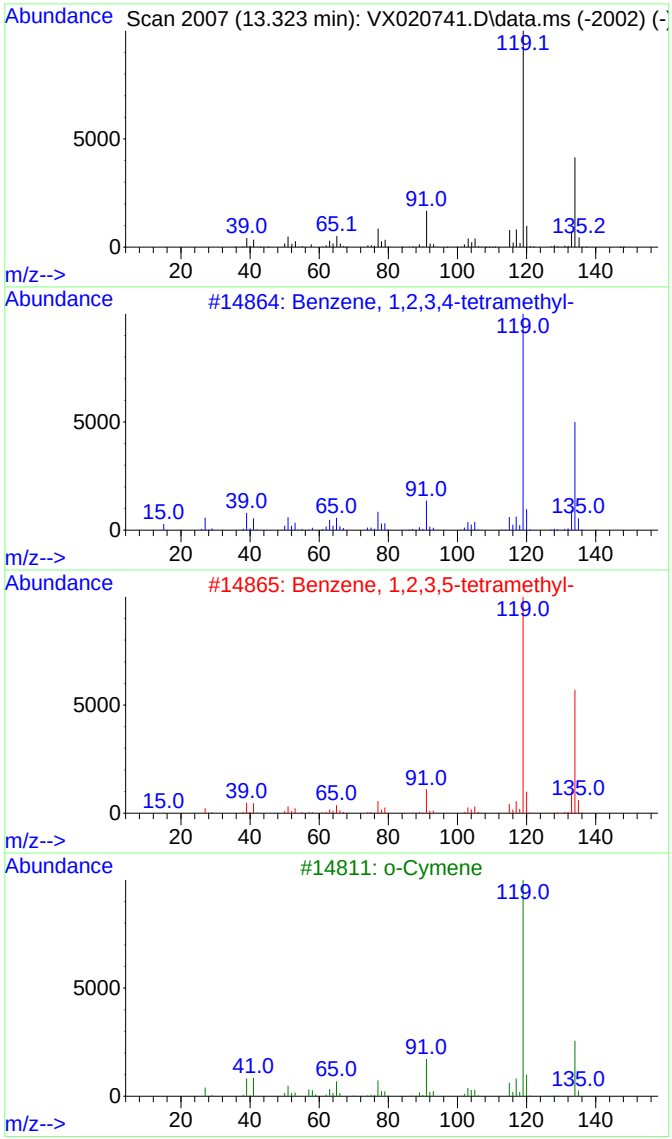
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

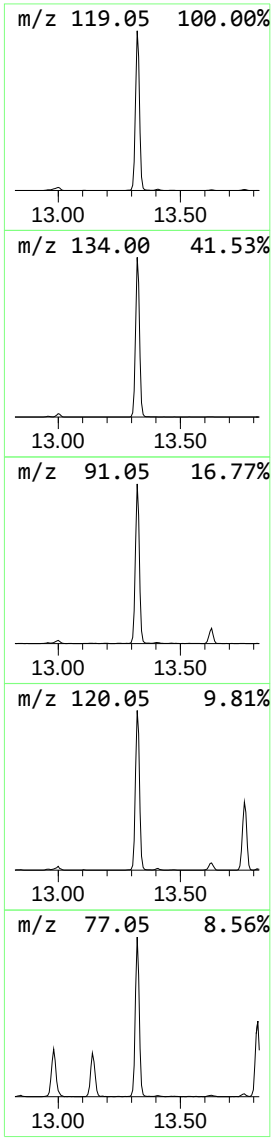
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.323	32.18 ug/l	2098780	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, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94





Tentatively Identified Compound (LSC) summary

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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propanenitrile	4.721	41.4	ug/l	830678	1	5.617	1003000	50.0
Butane, 1-chloro-	5.684	44.4	ug/l	890050	1	5.617	1003000	50.0
Propane, 2-nitro-	8.159	7.8	ug/l	188244	2	6.824	1200590	50.0
Benzene, 1,2,3,...	13.323	32.2	ug/l	2098780	4	12.061	3260970	50.0