LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027973.D
Acq On : 04 Apr 2022 21:13
Operator : JC/MD
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 : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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\82X032922W.M
Title : SW846 8260

Signal : TIC: VX027973.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.166	9	13	21	rVB	39597	36542	4.33%	0.168%
2	1.288	31	33	42	rVB	35243	36969	4.38%	0.170%
3	1.374	43	47	54	rBV	36669	37197	4.41%	0.171%
4	1.599	79	84	88	rBV	25729	26067	3.09%	0.120%
5	1.678	93	97	104	rVB	23125	30081	3.57%	0.139%
6	1.886	125	131	140	rBV	55917	81786	9.70%	0.377%
7	2.136	166	172	181	rVB	49555	72743	8.63%	0.335%
8	2.233	183	188	196	rVV	44860	67408	7.99%	0.311%
9	2.325	196	203	208	rVV2	109346	212695	25.22%	0.980%
10	2.380	208	212	219	rVV	88696	146638	17.39%	0.676%
11	2.453	219	224	229	rVV	27737	46835	5.55%	0.216%
12	2.508	229	233	244	rVB	32203	52767	6.26%	0.243%
13	2.666	248	259	262	rBV2	71384	134941	16.00%	0.622%
14	2.703	262	265	273	rVV	44519	72795	8.63%	0.335%
15	2.788	273	279	290	rVB	72157	133144	15.79%	0.613%
16	2.965	299	308	317	rBV2	33305	85700	10.16%	0.395%
17	3.062	317	324	327	rBV	134056	266510	31.60%	1.228%
18	3.611	406	414	423	rBV	51012	120097	14.24%	0.553%
19	3.721	423	432	455	rVV2	258390	836350	99.17%	3.853%
20	4.483	541	557	563	rBV4	97112	288576	34.22%	1.330%
21	4.556	563	569	577	rVB2	72965	186940	22.17%	0.861%
22	4.647	577	584	590	rBV	48894	121172	14.37%	0.558%
23	4.721	590	596	598	rBV	18210	36534	4.33%	0.168%
24	4.910	615	627	635	rBV6	63901	209712	24.87%	0.966%
25	5.007	635	643	651	rVV	88852	277776	32.94%	1.280%
26	5.099	651	658	672	rVB2	50875	154155	18.28%	0.710%
27	5.385	693	705	713	rBV	92174	277155	32.86%	1.277%
28	5.470	713	719	726	rVV	47656	140788	16.69%	0.649%
29	5.556	726	733	738	rVV	64036	184357	21.86%	0.849%
30	5.617	738	743	747	rVV2	47797	124781	14.80%	0.575%
31	5.690	747	755	772	rVB3	90448	285595	33.86%	1.316%
32	5.958	789	799	805	rBV2	44569	115882	13.74%	0.534%
33	6.043	805	813	818	rBV	92068	245546	29.11%	1.131%
34	6.342	850	862	877	rBV2	66607	169352	20.08%	0.780%
35	6.763	917	931	944	rBV	109063	275997	32.73%	1.272%
36	7.129	982	991	1008	rVB2	79988	178049	21.11%	0.820%

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
LabSampleId :
VSTDCCC050

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Title : SW846 8260

37	7.379	1023	1032	1036	rBV	69083	148860	17.65%	0.686%
38	7.433	1036	1041	1055	rVB	85892	185769	22.03%	0.856%
39	7.586	1058	1066	1073	rBV	63711	125573	14.89%	0.579%
40	7.696	1073	1084	1094	rVV2	94176	210711	24.98%	0.971%
41	7.811	1094	1103	1116	rVB2	104801	302833	35.91%	1.395%
42	8.116	1145	1153	1165	rBV	26310	49218	5.84%	0.227%
43	8.244	1167	1174	1187	rVV	425679	655102	77.68%	3.018%
44	8.366	1187	1194	1202	rVB	112755	180563	21.41%	0.832%
45	8.574	1221	1228	1235	rBV	529275	843367	100.00%	3.886%
46	8.653	1235	1241	1247	rVV	191481	299885	35.56%	1.382%
47	8.720	1247	1252	1263	rVB	212591	321336	38.10%	1.481%
48	8.982	1287	1295	1305	rBV	117362	175938	20.86%	0.811%
49	9.116	1311	1317	1320	rBV	145907	205147	24.32%	0.945%
50	9.153	1320	1323	1334	rVB	149778	211211	25.04%	0.973%
51	9.275	1337	1343	1346	rBV	129411	193295	22.92%	0.891%
52	9.311	1346	1349	1355	rVB	131203	180038	21.35%	0.830%
53	9.433	1363	1369	1378	rBV	474641	623419	73.92%	2.872%
54	9.525	1378	1384	1389	rVV	98562	145434	17.24%	0.670%
55	9.579	1389	1393	1396	rVV	153346	201684	23.91%	0.929%
56	9.610	1396	1398	1406	rVB	76421	96420	11.43%	0.444%
57	10.055	1465	1471	1473	rBV	245103	330255	39.16%	1.522%
58	10.079	1473	1475	1484	rVV	221734	267922	31.77%	1.234%
59	10.165	1484	1489	1491	rVV	174284	237197	28.13%	1.093%
60	10.195	1491	1494	1506	rVB	270733	349914	41.49%	1.612%
61	10.305	1506	1512	1523	rBV	500983	691742	82.02%	3.187%
62	10.652	1562	1569	1579	rBV2	407994	718430	85.19%	3.310%
63	10.799	1587	1593	1597	rBV	92797	124953	14.82%	0.576%
64	10.848	1597	1601	1612	rVV	195210	239633	28.41%	1.104%
65	10.963	1615	1620	1625	rVV	306598	372603	44.18%	1.717%
66	11.018	1625	1629	1635	rVV	119771	149342	17.71%	0.688%
67	11.085	1635	1640	1650	rVB	182768	234830	27.84%	1.082%
68	11.201	1653	1659	1663	rBV2	239806	474935	56.31%	2.188%
69	11.244	1663	1666	1672	rVV2	174155	336343	39.88%	1.550%
70	11.305	1672	1676	1681	rVV	294324	355716	42.18%	1.639%
71	11.366	1681	1686	1692	rVV	272528	337332	40.00%	1.554%
72	11.457	1695	1701	1709	rVB2	545551	702682	83.32%	3.238%
73	11.719	1738	1744	1747	rBV2	435408	626380	74.27%	2.886%
74	11.756	1747	1750	1755	rVB	303252	369438	43.81%	1.702%
75	11.890	1764	1772	1778	rBV	282155	349053	41.39%	1.608%
76	11.969	1780	1785	1788	rBV	241429	297363	35.26%	1.370%

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LabSampleId :
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Title : SW846 8260

77	12.018	1788	1793	1796	rBV2	363148	676794	80.25%	3.118%
78	12.335	1840	1845	1854	rVB	515295	606047	71.86%	2.792%
79	12.542	1873	1879	1885	rBV	156153	204526	24.25%	0.942%
80	12.945	1939	1945	1953	rVB2	74232	100875	11.96%	0.465%
81	13.103	1966	1971	1976	rBV	10024	12095	1.43%	0.056%
82	13.286	1996	2001	2011	rVB	340885	389075	46.13%	1.793%
83	13.378	2011	2016	2023	rBV3	8126	12286	1.46%	0.057%
84	13.591	2045	2051	2058	rBV	191111	244126	28.95%	1.125%
85	13.725	2068	2073	2077	rBV	121998	144484	17.13%	0.666%
86	13.780	2077	2082	2091	rVB	278112	355848	42.19%	1.640%
87	13.963	2107	2112	2119	rBV	204100	250905	29.75%	1.156%
88	14.134	2135	2140	2147	rBV	11932	15439	1.83%	0.071%

Sum of corrected areas: 21703998

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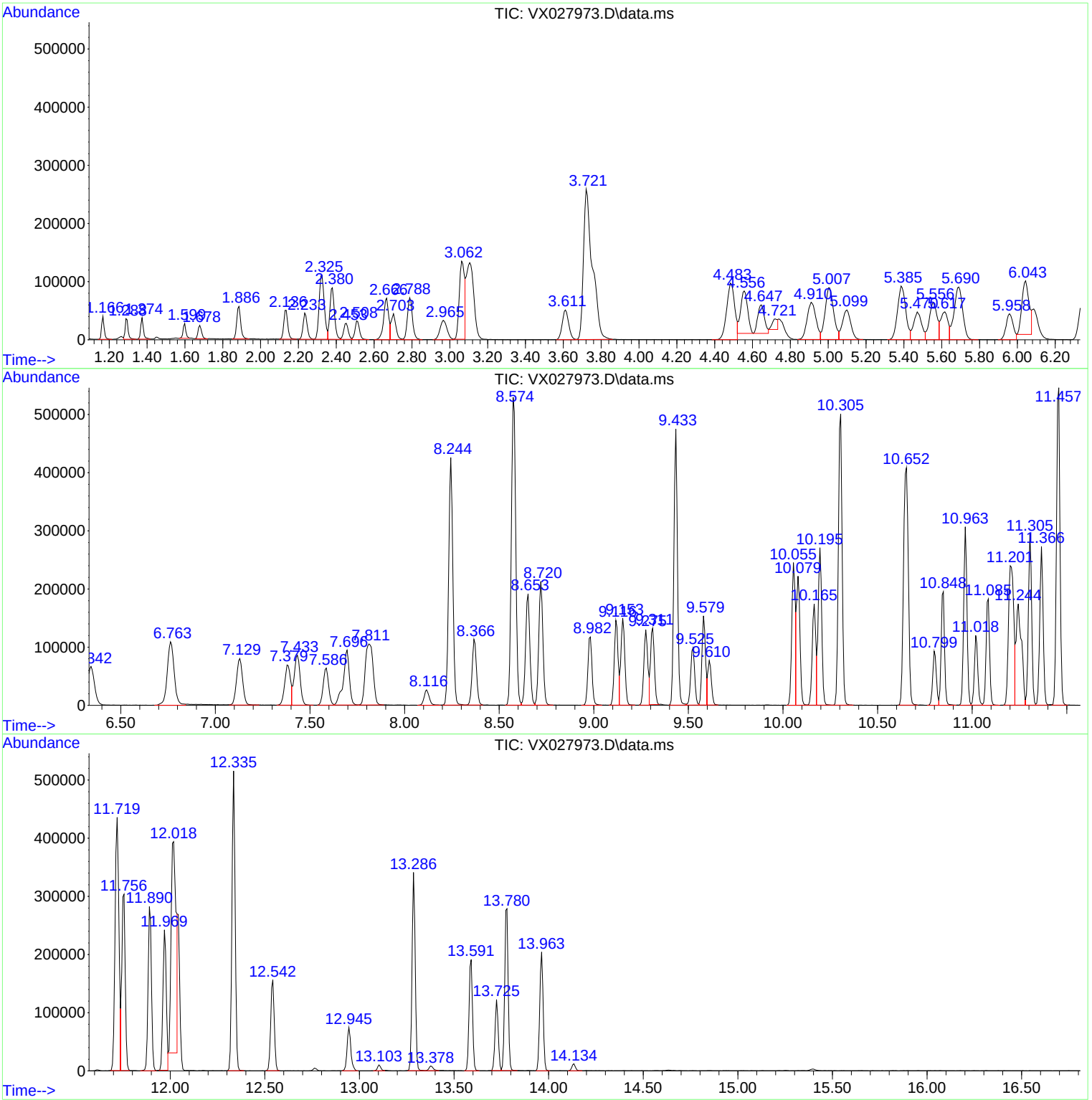
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
LabSampleId :
VSTDCCC050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

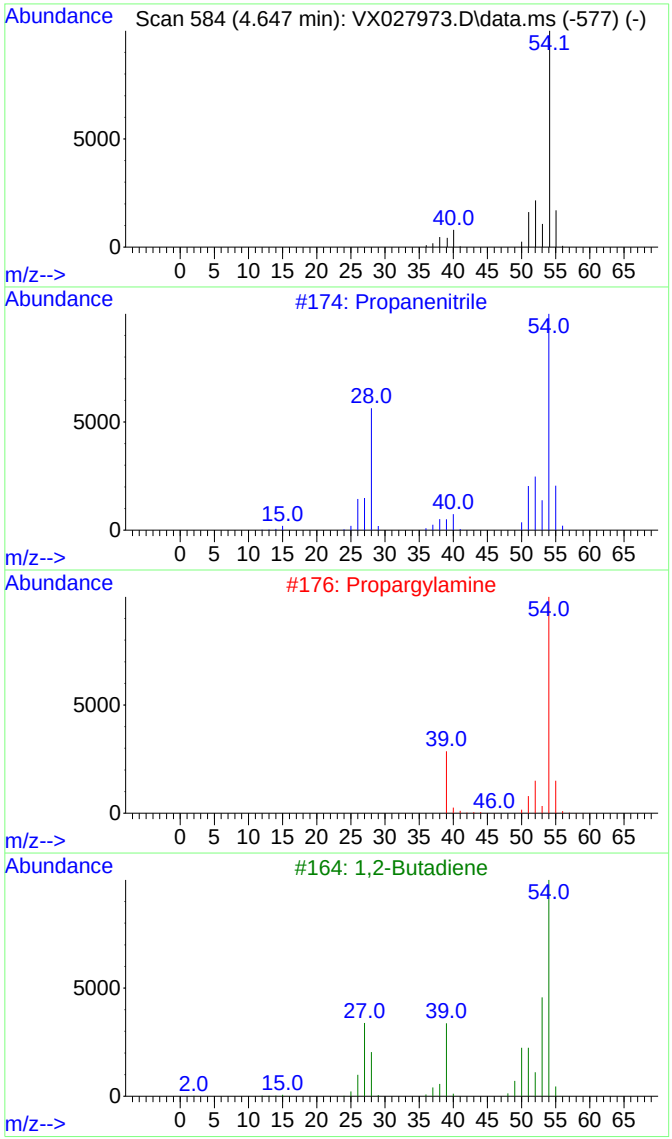
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

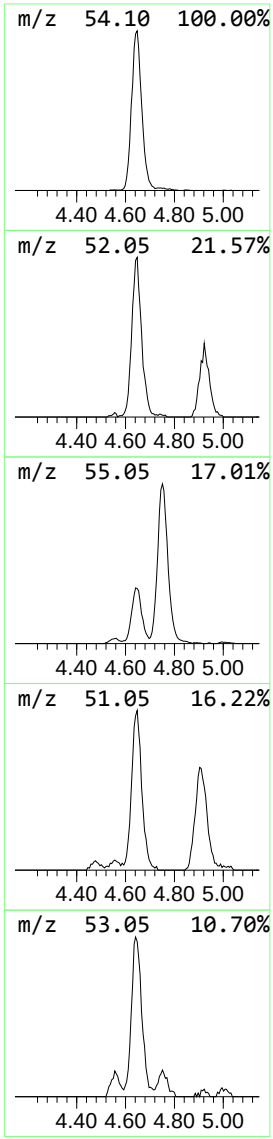
****

Peak Number 1 Propanenitrile Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.647	32.86 ug/l	121172	Pentafluorobenzene	5.556

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	4





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Data File : VX027973.D
Acq On : 04 Apr 2022 21:13
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
LabSampleId :
VSTDCCC050

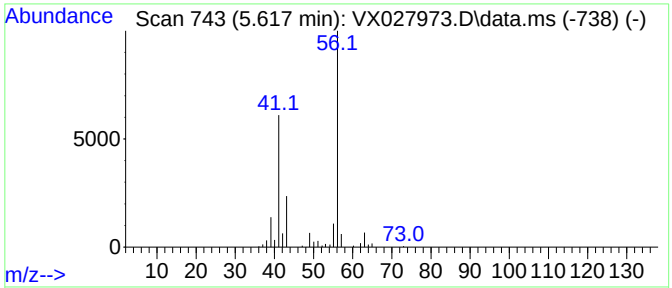
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

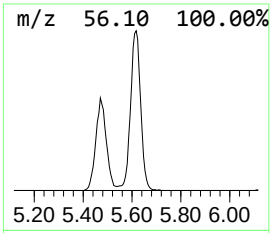
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

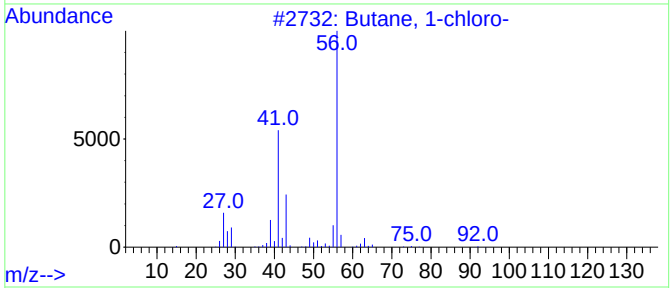
****
Peak Number 2 Butane, 1-chloro- Concentration Rank 1

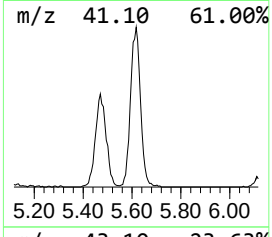
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.617	33.84 ug/l	124781	Pentafluorobenzene	5.556

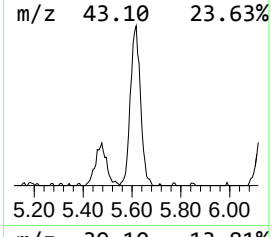
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	78
2	Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	72
3	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	64
4	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	50
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39

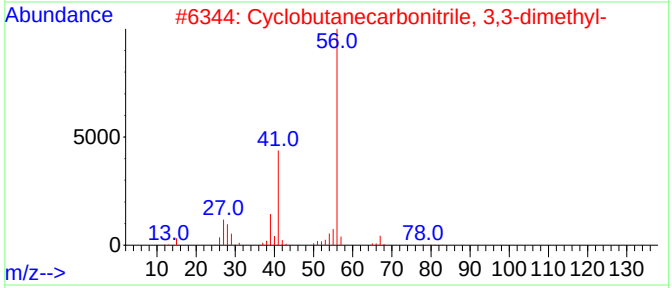


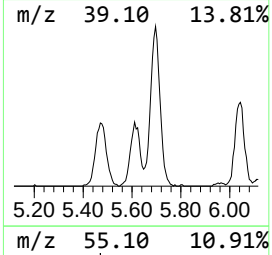


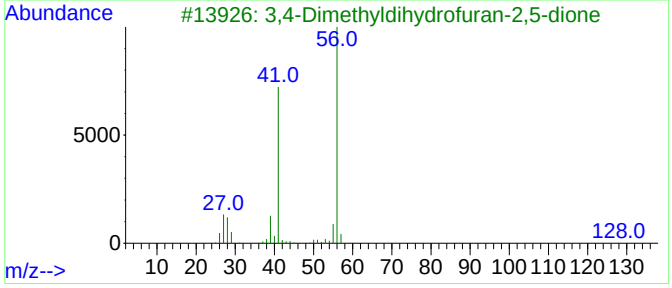


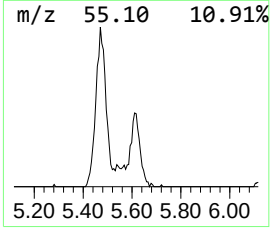












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LabSampleId :
VSTDCCC050

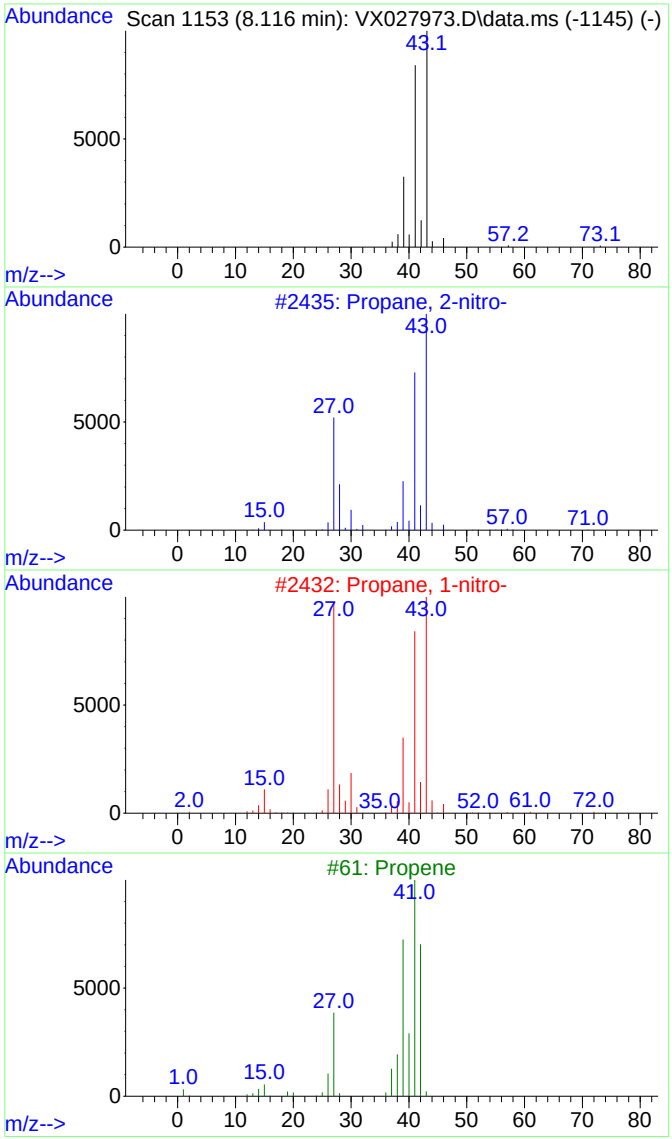
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

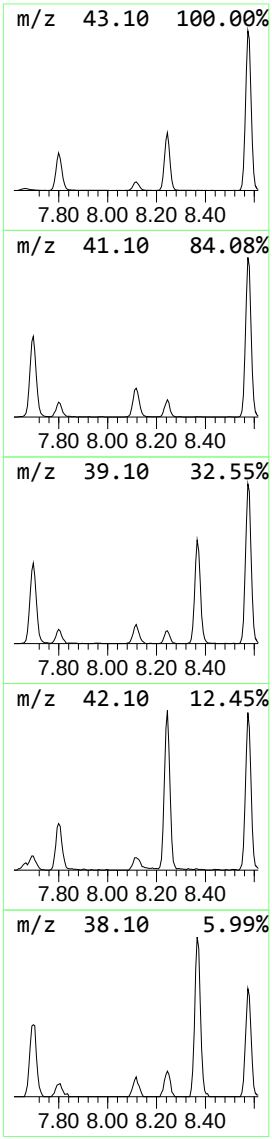
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.116	8.92 ug/l	49218	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	83
2	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	74
3	Propene	42	C3H6	000115-07-1	9
4	Oxirane, ethyl-	72	C4H8O	000106-88-7	9
5	Isobutyl nitrite	103	C4H9NO2	000542-56-3	9





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LabSampleId :
VSTDCCC050

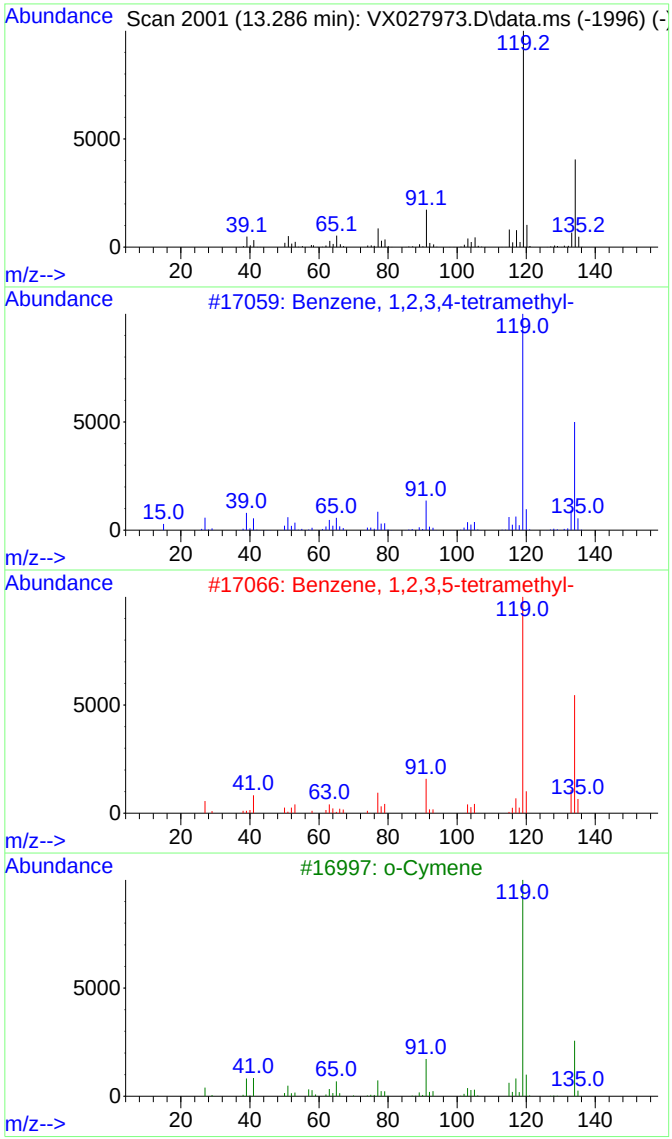
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

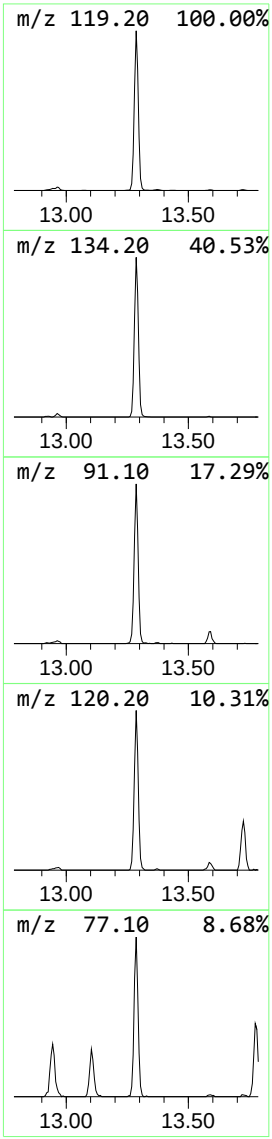
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	28.74 ug/l	389075	1,4-Dichlorobenzene-d4	12.024

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	p-Cymene	134	C10H14	000099-87-6	94





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propanenitrile	4.647	32.9	ug/l	121172	1	5.556	184357	50.0
Butane, 1-chloro-	5.617	33.8	ug/l	124781	1	5.556	184357	50.0
Propane, 2-nitro-	8.116	8.9	ug/l	49218	2	6.763	275997	50.0
Benzene, 1,2,3,...	13.286	28.7	ug/l	389075	4	12.024	676794	50.0