

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
 Data File : VX027951.D
 Acq On : 04 Apr 2022 12:13
 Operator : JC/MD
 Sample : VX0404WBSD01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VX0404WBSD01

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: VX027951.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.167	10	13	19	rVB	20878	18117	3.53%	0.196%
2	1.252	21	27	31	rBV3	3367	7611	1.48%	0.082%
3	1.288	31	33	43	rVB	14678	16602	3.24%	0.180%
4	1.374	43	47	50	rBV	16219	15178	2.96%	0.164%
5	1.605	81	85	94	rVB	13888	18240	3.56%	0.198%
6	1.685	94	98	106	rBV	9694	13034	2.54%	0.141%
7	1.886	126	131	140	rVB	26908	38755	7.56%	0.420%
8	2.130	166	171	181	rVB	20525	29685	5.79%	0.322%
9	2.233	183	188	196	rBV	14898	22981	4.48%	0.249%
10	2.325	196	203	208	rVV2	52370	101260	19.74%	1.097%
11	2.374	208	211	219	rVV	35156	54999	10.72%	0.596%
12	2.453	219	224	229	rVV	11197	18664	3.64%	0.202%
13	2.508	229	233	243	rVB	14863	25293	4.93%	0.274%
14	2.660	249	258	262	rBV2	28712	56464	11.01%	0.612%
15	2.703	262	265	272	rVV	15718	25465	4.97%	0.276%
16	2.788	272	279	290	rVB	27944	51912	10.12%	0.562%
17	2.953	299	306	317	rBV2	13442	31660	6.17%	0.343%
18	3.063	317	324	326	rVV	49791	91883	17.92%	0.995%
19	3.105	327	331	346	rVB2	55383	137167	26.75%	1.486%
20	3.611	403	414	423	rBV	20701	48422	9.44%	0.525%
21	3.721	423	432	454	rVV2	93841	312707	60.97%	3.387%
22	4.477	544	556	563	rBV2	42207	129804	25.31%	1.406%
23	4.550	563	568	576	rVB2	27858	69710	13.59%	0.755%
24	4.635	576	582	589	rBV	18946	47417	9.25%	0.514%
25	4.715	589	595	597	rBV	7025	13140	2.56%	0.142%
26	4.910	616	627	635	rBV5	27641	91333	17.81%	0.989%
27	5.001	635	642	650	rVV	36813	113695	22.17%	1.232%
28	5.093	650	657	671	rVB2	22074	69786	13.61%	0.756%
29	5.385	694	705	713	rBV2	62293	185330	36.14%	2.008%
30	5.471	713	719	725	rVB2	14432	32584	6.35%	0.353%
31	5.550	725	732	739	rBV	59396	154621	30.15%	1.675%
32	5.684	747	754	767	rVB4	41666	123838	24.15%	1.341%
33	5.952	788	798	805	rBV	43443	114773	22.38%	1.243%
34	6.038	805	812	817	rBV2	35809	84623	16.50%	0.917%
35	6.336	852	861	875	rBV2	23064	60470	11.79%	0.655%
36	6.763	921	931	945	rBV	100526	238897	46.58%	2.588%

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37	7.123	983	990	1002	rBV	33954	75002	14.62%	0.812%
38	7.379	1025	1032	1037	rBV2	35302	80980	15.79%	0.877%
39	7.428	1037	1040	1050	rVB	31726	61822	12.05%	0.670%
40	7.580	1058	1065	1073	rBV2	24983	48024	9.36%	0.520%
41	7.690	1073	1083	1095	rVV2	32027	73863	14.40%	0.800%
42	7.818	1095	1104	1120	rVB2	40470	112341	21.90%	1.217%
43	8.116	1146	1153	1159	rBV	9572	17052	3.32%	0.185%
44	8.238	1167	1173	1185	rBV	139139	225381	43.95%	2.441%
45	8.366	1188	1194	1204	rVB	44869	70416	13.73%	0.763%
46	8.574	1220	1228	1234	rBV	191726	301008	58.69%	3.261%
47	8.647	1234	1240	1247	rVV	190024	302875	59.06%	3.281%
48	8.720	1247	1252	1264	rVB	85377	130291	25.40%	1.411%
49	8.976	1289	1294	1302	rBV	45022	67082	13.08%	0.727%
50	9.116	1311	1317	1320	rBV	50939	70793	13.80%	0.767%
51	9.153	1320	1323	1330	rVB	54638	76081	14.83%	0.824%
52	9.275	1337	1343	1346	rBV	67486	100819	19.66%	1.092%
53	9.305	1346	1348	1355	rVB	46223	63121	12.31%	0.684%
54	9.427	1363	1368	1377	rBV	145562	200035	39.00%	2.167%
55	9.519	1378	1383	1388	rVV	37615	54765	10.68%	0.593%
56	9.580	1388	1393	1396	rVV	45696	63893	12.46%	0.692%
57	9.610	1396	1398	1406	rVB	27925	34367	6.70%	0.372%
58	10.055	1465	1471	1483	rBV2	198163	365241	71.22%	3.956%
59	10.165	1483	1489	1491	rVV	60074	86984	16.96%	0.942%
60	10.195	1491	1494	1506	rVV	102927	129057	25.16%	1.398%
61	10.299	1506	1511	1522	rVB	183157	251308	49.00%	2.722%
62	10.647	1562	1568	1578	rBV2	127966	233562	45.54%	2.530%
63	10.799	1588	1593	1597	rBV	32680	43899	8.56%	0.476%
64	10.842	1597	1600	1607	rVB	48128	56085	10.94%	0.608%
65	10.964	1615	1620	1625	rBV	111020	135242	26.37%	1.465%
66	11.018	1625	1629	1634	rVV	33475	41906	8.17%	0.454%
67	11.079	1634	1639	1649	rVB	151159	198197	38.65%	2.147%
68	11.201	1653	1659	1663	rVV2	76580	149787	29.21%	1.623%
69	11.238	1663	1665	1672	rVV2	51759	98160	19.14%	1.063%
70	11.305	1672	1676	1681	rVV	108195	129306	25.21%	1.401%
71	11.366	1681	1686	1692	rVV	91729	114411	22.31%	1.239%
72	11.451	1695	1700	1711	rVB2	191407	247318	48.22%	2.679%
73	11.720	1738	1744	1747	rBV2	146861	214082	41.74%	2.319%
74	11.750	1747	1749	1758	rVB	110279	131197	25.58%	1.421%
75	11.890	1767	1772	1780	rVB	112723	137157	26.74%	1.486%
76	11.969	1780	1785	1788	rVV	89246	108268	21.11%	1.173%

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77	12.018	1788	1793	1804	rVB4	254287	512861	100.00%	5.556%
78	12.335	1840	1845	1852	rVB	196248	231866	45.21%	2.512%
79	12.543	1874	1879	1884	rBV	63420	81855	15.96%	0.887%
80	12.945	1936	1945	1951	rBV2	27224	37152	7.24%	0.402%
81	13.103	1967	1971	1976	rVB	4424	5728	1.12%	0.062%
82	13.286	1996	2001	2009	rVB	138321	159610	31.12%	1.729%
83	13.591	2046	2051	2058	rBV	84802	106518	20.77%	1.154%
84	13.725	2068	2073	2077	rBV	68768	80618	15.72%	0.873%
85	13.780	2077	2082	2090	rVB	109411	138292	26.96%	1.498%
86	13.963	2107	2112	2118	rBV	88064	109680	21.39%	1.188%

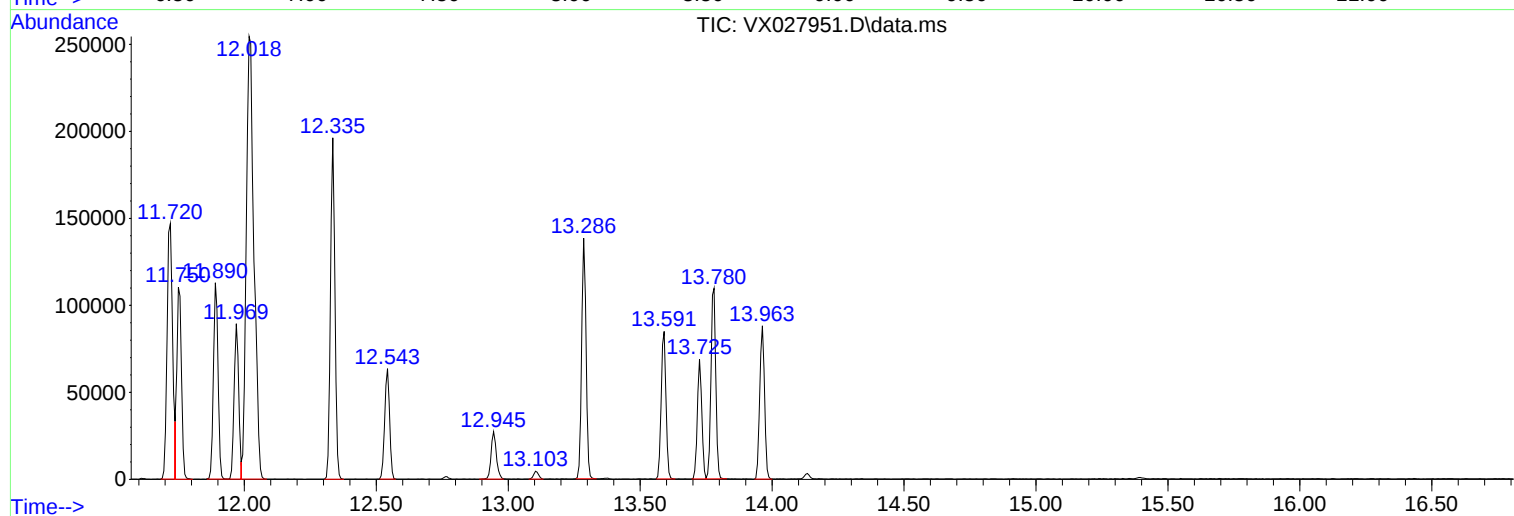
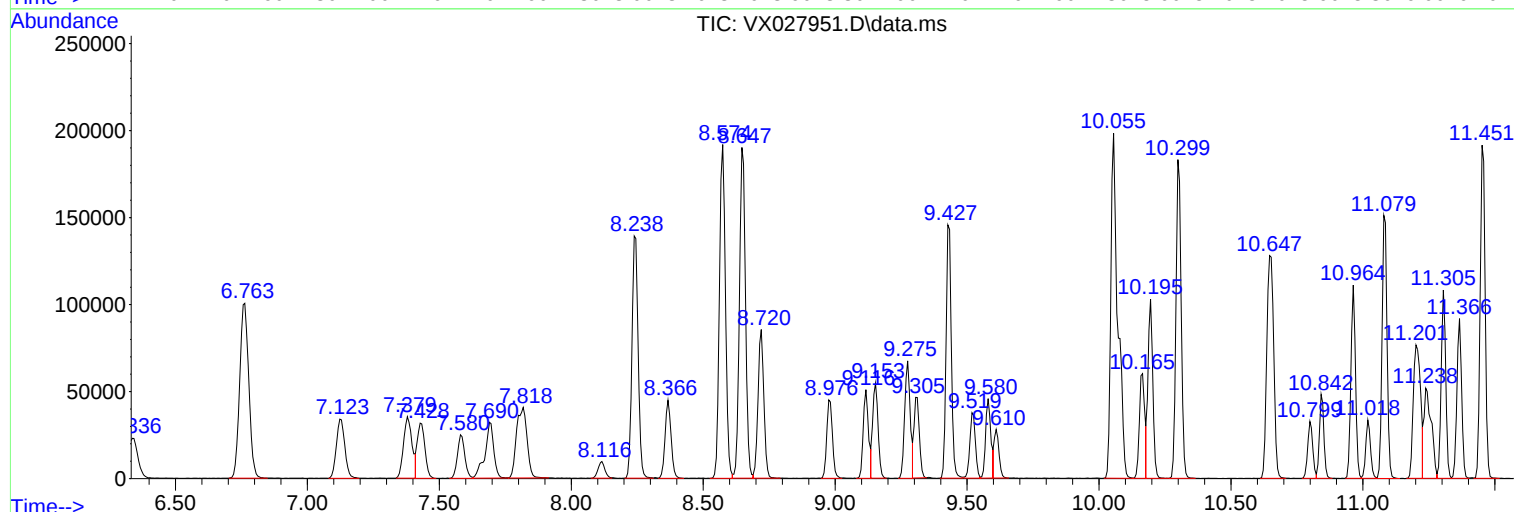
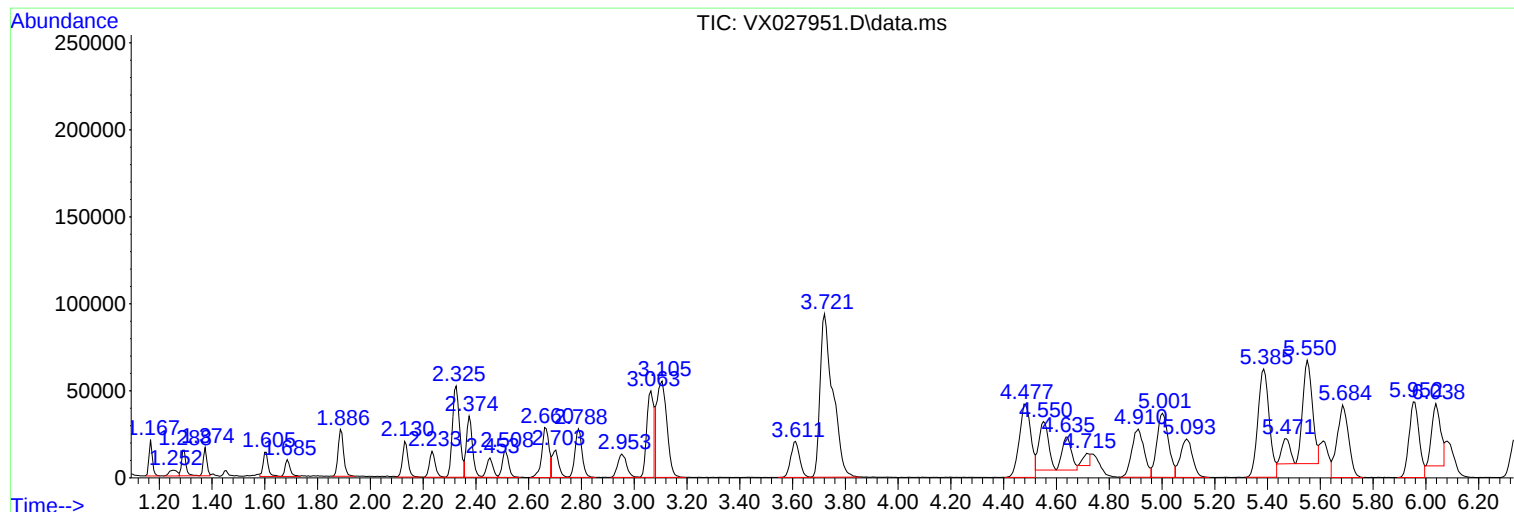
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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



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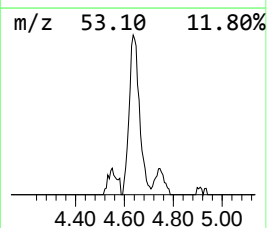
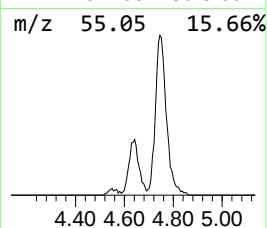
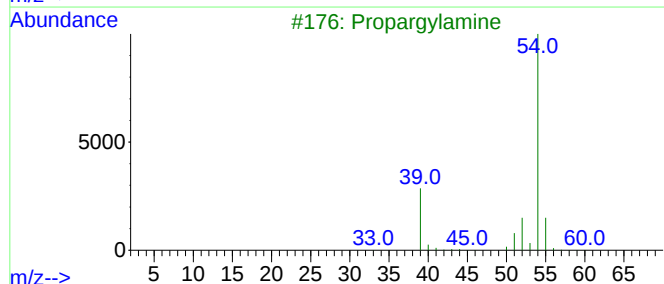
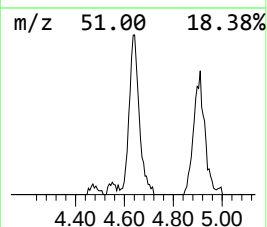
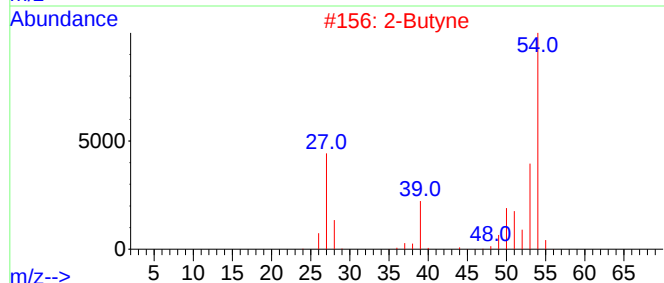
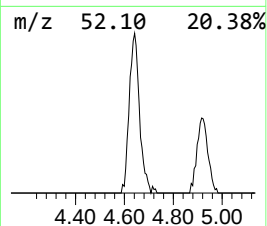
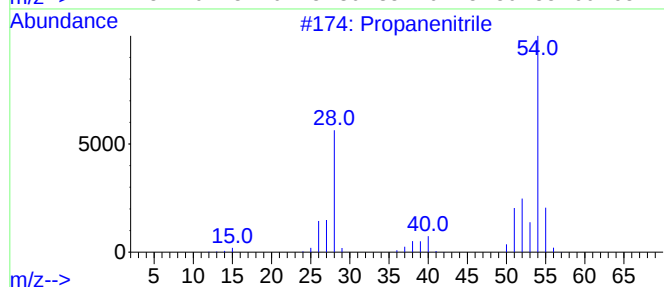
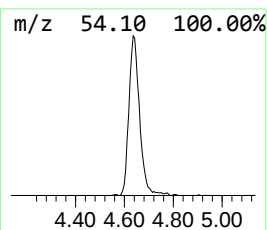
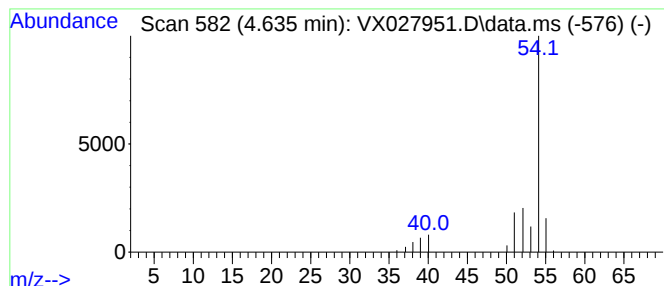
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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.
4.635	15.33 ug/l	47417	Pentafluorobenzene	5.550

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



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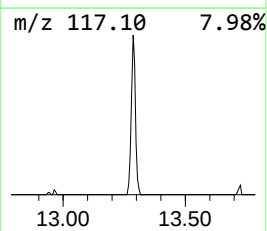
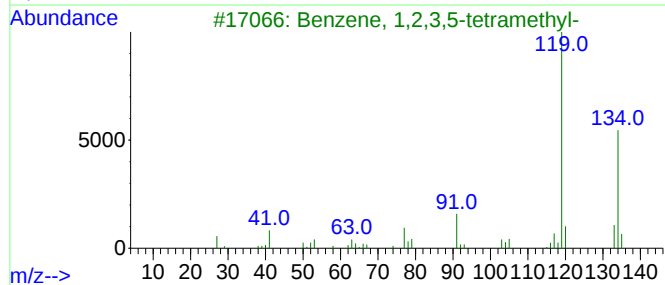
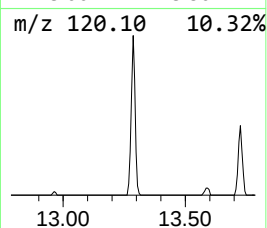
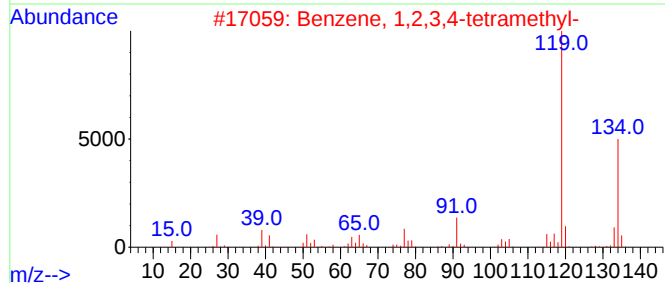
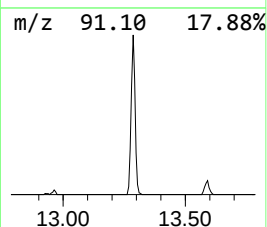
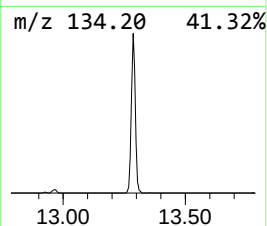
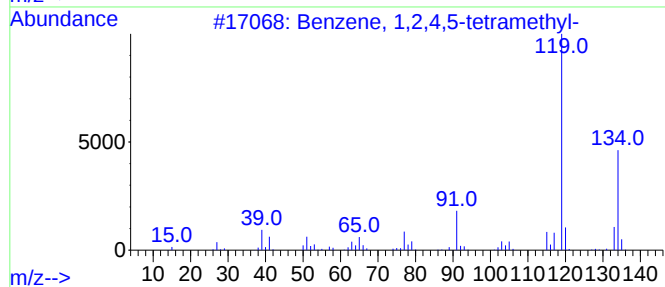
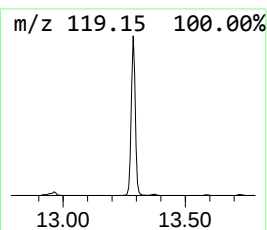
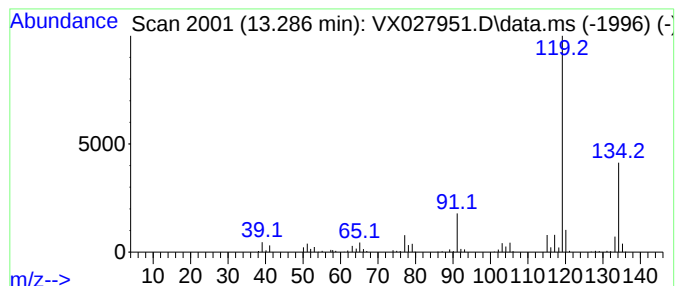
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	15.56 ug/l	159610	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanenitrile	4.635	15.3	ug/l	47417	1	5.550	154621	50.0
Benzene, 1,2,4,...	13.286	15.6	ug/l	159610	4	12.024	512861	50.0