

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
 Data File : VX027950.D
 Acq On : 04 Apr 2022 11:35
 Operator : JC/MD
 Sample : VX0404WBS01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VX0404WBS01

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: VX027950.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	10	13	18	rVB	14939	12801	2.50%	0.147%
2	1.288	30	33	39	rVB	12780	14207	2.78%	0.164%
3	1.374	44	47	50	rBV	13292	12274	2.40%	0.141%
4	1.605	81	85	94	rVB	12812	13788	2.70%	0.159%
5	1.685	94	98	104	rBV	9104	10324	2.02%	0.119%
6	1.886	127	131	139	rBV	20726	30148	5.89%	0.347%
7	2.130	166	171	179	rVB	17915	26853	5.25%	0.309%
8	2.233	179	188	195	rVV	14333	21944	4.29%	0.253%
9	2.325	197	203	208	rVV2	42448	80387	15.72%	0.926%
10	2.373	208	211	219	rVV	30074	50055	9.79%	0.577%
11	2.453	219	224	229	rVV	9469	15734	3.08%	0.181%
12	2.514	229	234	240	rVB	12475	19291	3.77%	0.222%
13	2.666	250	259	262	rBV2	23749	44649	8.73%	0.514%
14	2.703	262	265	273	rVV	14140	22864	4.47%	0.263%
15	2.788	273	279	288	rVB	25798	45805	8.96%	0.528%
16	2.965	300	308	317	rBV2	8621	25181	4.92%	0.290%
17	3.062	317	324	327	rVV	44296	89144	17.43%	1.027%
18	3.105	327	331	345	rVB3	47395	121190	23.70%	1.396%
19	3.611	405	414	424	rBV	17620	41279	8.07%	0.476%
20	3.721	424	432	455	rVV2	80297	264944	51.80%	3.053%
21	4.483	543	557	563	rBV3	36812	109611	21.43%	1.263%
22	4.556	563	569	577	rVB	25917	63400	12.40%	0.730%
23	4.641	577	583	590	rBV	16480	41208	8.06%	0.475%
24	4.721	590	596	598	rBV2	6738	14155	2.77%	0.163%
25	4.910	615	627	635	rBV5	24867	81009	15.84%	0.933%
26	5.007	635	643	651	rVV	33546	105783	20.68%	1.219%
27	5.093	651	657	673	rVB2	20413	61621	12.05%	0.710%
28	5.385	694	705	713	rBV2	56987	165428	32.34%	1.906%
29	5.471	713	719	725	rVB3	11708	24874	4.86%	0.287%
30	5.556	725	733	739	rBV2	51666	135028	26.40%	1.556%
31	5.690	747	755	766	rVB4	33601	103215	20.18%	1.189%
32	5.958	789	799	806	rBV	39942	105653	20.66%	1.217%
33	6.037	806	812	818	rBV	30830	81355	15.91%	0.937%
34	6.342	852	862	874	rVB	21245	53868	10.53%	0.621%
35	6.763	920	931	945	rBV	92164	215534	42.14%	2.483%
36	7.129	979	991	1003	rVB2	30243	66108	12.93%	0.762%

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37	7.379	1022	1032	1037	rBV	27331	62993	12.32%	0.726%
38	7.434	1037	1041	1049	rVB2	29245	57424	11.23%	0.662%
39	7.586	1059	1066	1073	rBV	23281	45146	8.83%	0.520%
40	7.696	1073	1084	1094	rVB2	31263	70468	13.78%	0.812%
41	7.818	1094	1104	1115	rBV2	35553	101732	19.89%	1.172%
42	8.116	1146	1153	1162	rBV2	8687	15901	3.11%	0.183%
43	8.244	1167	1174	1184	rVV	134380	212773	41.60%	2.451%
44	8.366	1187	1194	1205	rVB	40947	65861	12.88%	0.759%
45	8.574	1221	1228	1235	rBV	169522	266634	52.13%	3.072%
46	8.647	1235	1240	1247	rVV	170507	272937	53.37%	3.145%
47	8.720	1247	1252	1262	rVB	76462	116296	22.74%	1.340%
48	8.982	1287	1295	1305	rBV	40491	61331	11.99%	0.707%
49	9.116	1312	1317	1320	rBV	44943	63390	12.39%	0.730%
50	9.153	1320	1323	1333	rVB	53517	75793	14.82%	0.873%
51	9.275	1336	1343	1346	rBV	61214	90695	17.73%	1.045%
52	9.311	1346	1349	1355	rVB	47078	64448	12.60%	0.743%
53	9.433	1363	1369	1377	rBV	150293	206489	40.37%	2.379%
54	9.525	1378	1384	1389	rVV	37493	54601	10.68%	0.629%
55	9.580	1389	1393	1396	rVV	47825	64902	12.69%	0.748%
56	9.610	1396	1398	1406	rVB	27706	34773	6.80%	0.401%
57	10.055	1465	1471	1484	rBV2	202929	371187	72.58%	4.277%
58	10.165	1484	1489	1491	rVV	61143	83539	16.33%	0.962%
59	10.195	1491	1494	1502	rVB	97329	122853	24.02%	1.415%
60	10.305	1506	1512	1521	rVB	179805	248253	48.54%	2.860%
61	10.653	1562	1569	1578	rBV2	138991	247111	48.32%	2.847%
62	10.799	1588	1593	1597	rBV	33774	45193	8.84%	0.521%
63	10.842	1597	1600	1609	rVB	53435	65801	12.87%	0.758%
64	10.963	1615	1620	1625	rBV	107897	132255	25.86%	1.524%
65	11.018	1625	1629	1635	rVV	38073	46530	9.10%	0.536%
66	11.079	1635	1639	1651	rVB	155642	206008	40.28%	2.374%
67	11.201	1653	1659	1663	rBV2	83699	161856	31.65%	1.865%
68	11.244	1663	1666	1672	rVV2	56882	109346	21.38%	1.260%
69	11.305	1672	1676	1681	rVV	104343	128240	25.07%	1.478%
70	11.366	1681	1686	1692	rVV	97801	120417	23.54%	1.387%
71	11.457	1695	1701	1712	rVB	195992	253780	49.62%	2.924%
72	11.719	1738	1744	1747	rBV2	147670	212085	41.47%	2.444%
73	11.756	1747	1750	1756	rVB	111388	133436	26.09%	1.537%
74	11.890	1767	1772	1778	rVB	104298	128461	25.12%	1.480%
75	11.969	1780	1785	1788	rBV	87422	109027	21.32%	1.256%
76	12.018	1788	1793	1804	rVB4	251399	511452	100.00%	5.893%

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77	12.335	1840	1845	1857	rVB	188024	225427	44.08%	2.597%
78	12.542	1874	1879	1884	rBV	56842	74344	14.54%	0.857%
79	12.945	1939	1945	1952	rBV2	28331	37045	7.24%	0.427%
80	13.103	1967	1971	1979	rVB	4481	5941	1.16%	0.068%
81	13.286	1996	2001	2012	rVB	117254	136415	26.67%	1.572%
82	13.591	2046	2051	2057	rVB	74003	91404	17.87%	1.053%
83	13.725	2068	2073	2077	rBV	48991	56654	11.08%	0.653%
84	13.780	2077	2082	2091	rVB	95764	125896	24.62%	1.451%
85	13.963	2107	2112	2120	rVB	78903	94185	18.42%	1.085%

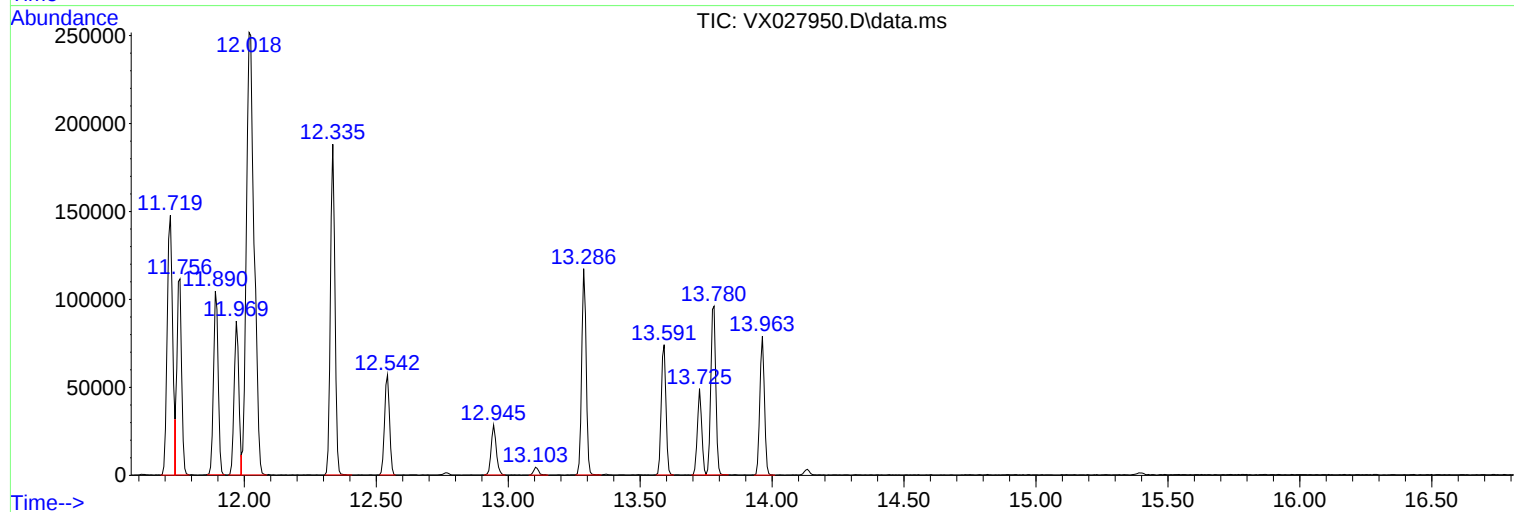
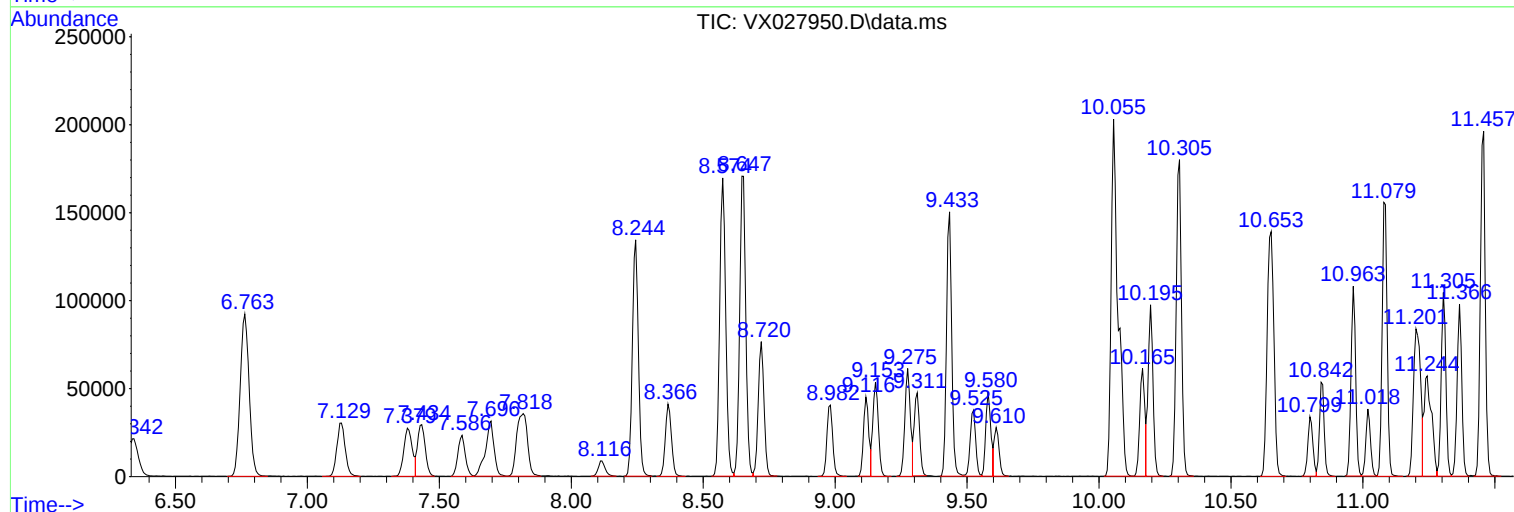
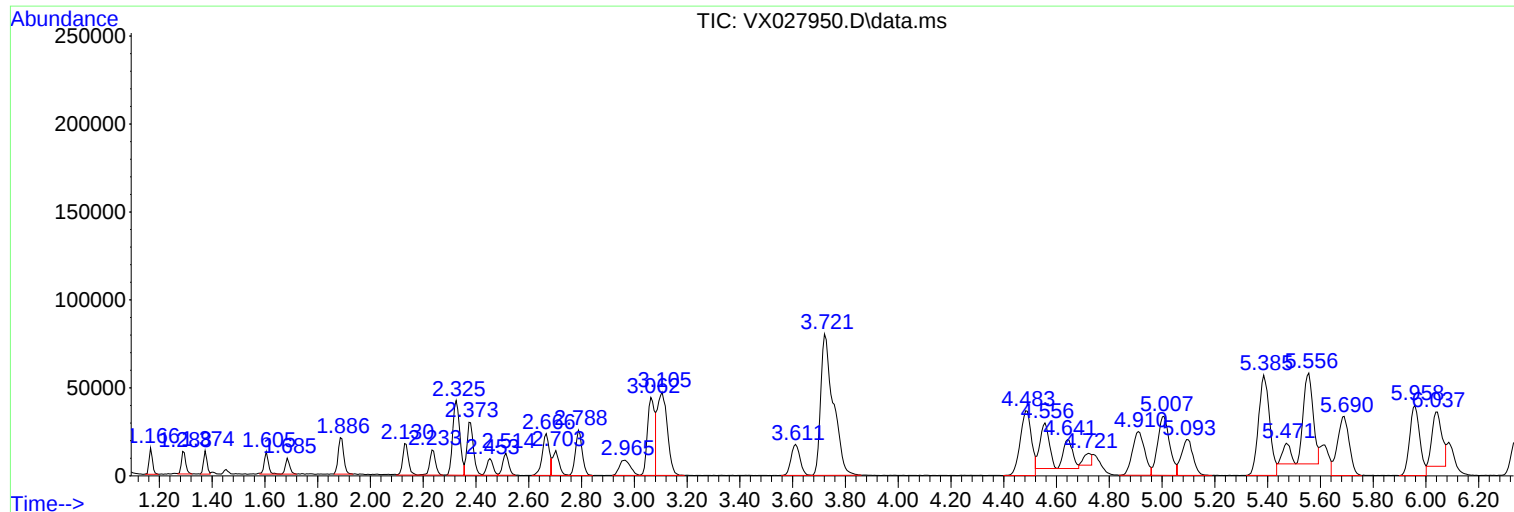
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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



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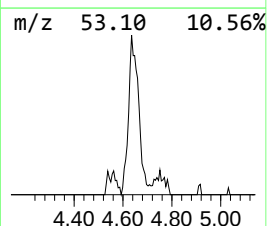
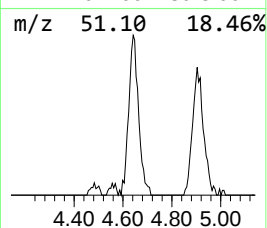
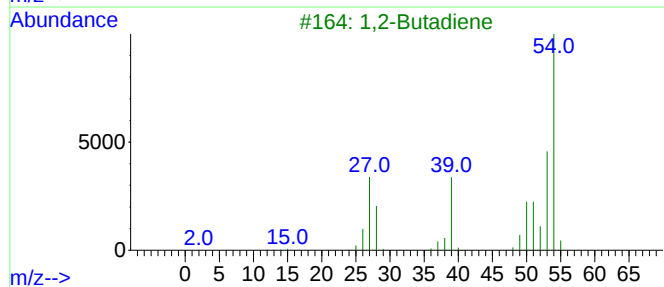
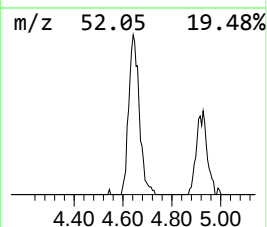
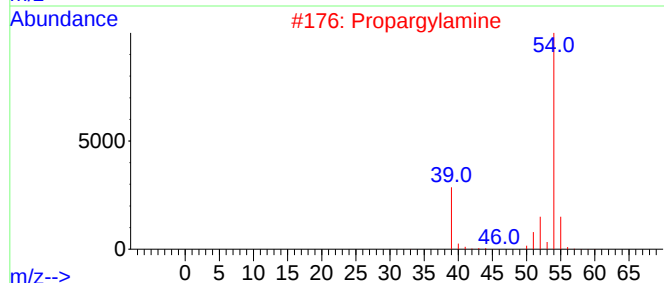
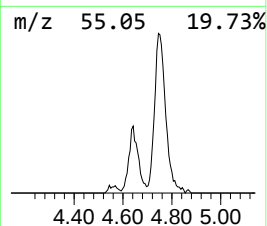
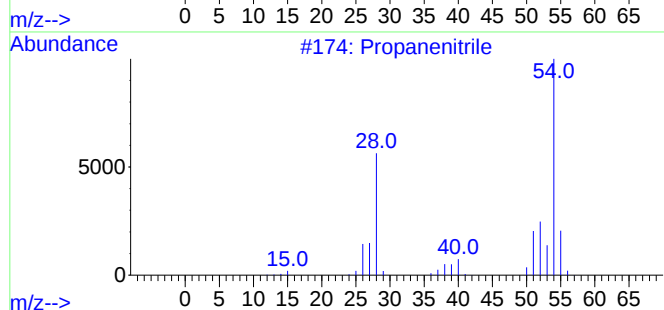
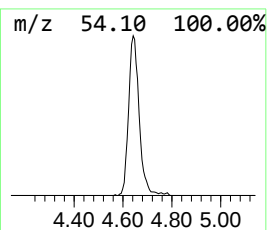
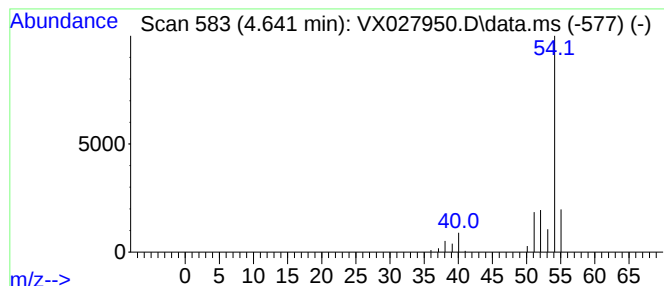
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanenitrile Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.641	15.26 ug/l	41208	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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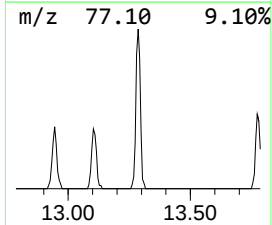
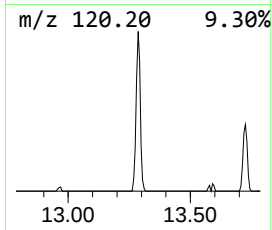
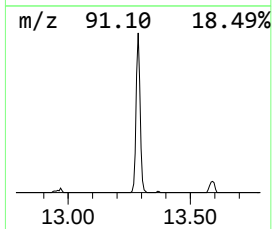
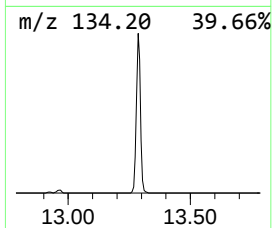
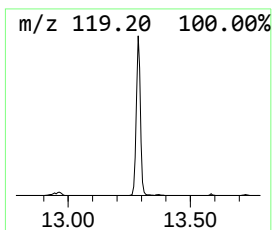
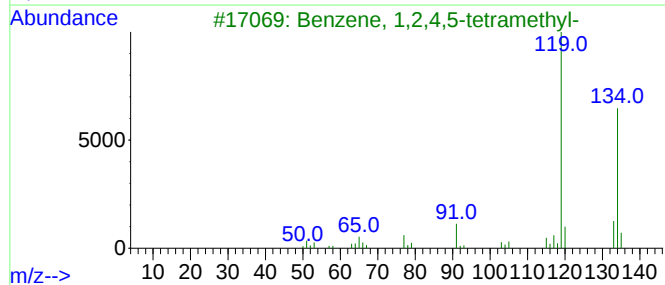
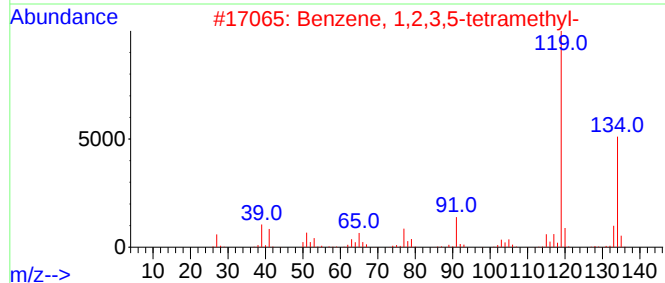
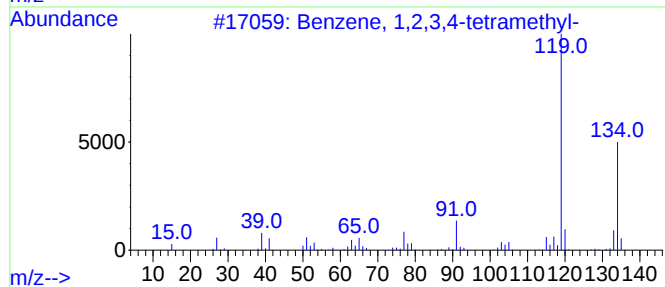
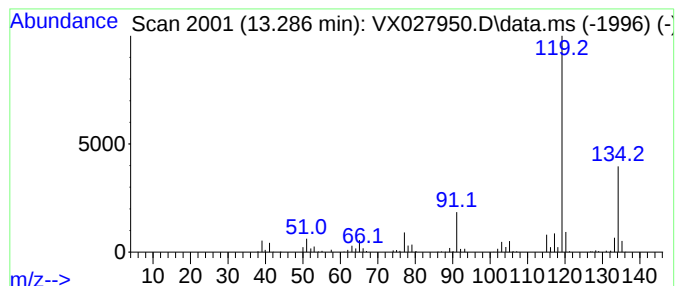
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	13.34 ug/l	136415	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	94
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
4			o-Cymene	134	C10H14	000527-84-4	94
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93



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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanenitrile	4.641	15.3	ug/l	41208	1	5.556	135028	50.0
Benzene, 1,2,3,...	13.286	13.3	ug/l	136415	4	12.024	511452	50.0