

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012721\
 Data File : VX020772.D
 Acq On : 27 Jan 2021 16:04
 Operator : JC/SP
 Sample : VX0127WBSD01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VX0127WBSD01

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: VX020772.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	13	16	24	rVB	161877	154777	5.55%	0.325%
2	1.313	34	37	44	rVB	140626	131928	4.73%	0.277%
3	1.392	46	50	57	rBV	136279	131975	4.73%	0.277%
4	1.624	76	88	93	rBV	116804	147834	5.30%	0.310%
5	1.709	97	102	111	rVB	70613	95224	3.41%	0.200%
6	1.916	129	136	146	rBV	165842	253909	9.10%	0.533%
7	2.166	171	177	184	rBV	118129	168076	6.02%	0.353%
8	2.270	189	194	201	rVB	62227	93659	3.36%	0.197%
9	2.355	201	208	214	rBV2	274528	532116	19.07%	1.117%
10	2.416	214	218	225	rVB	137842	225873	8.10%	0.474%
11	2.489	225	230	235	rBV	77235	125926	4.51%	0.264%
12	2.544	235	239	253	rVB	127813	219373	7.86%	0.461%
13	2.703	257	265	269	rBV	141765	264787	9.49%	0.556%
14	2.745	269	272	280	rVB	69671	116166	4.16%	0.244%
15	2.831	280	286	302	rVB	154450	293711	10.53%	0.617%
16	3.014	305	316	325	rBV	60608	148848	5.34%	0.313%
17	3.117	325	333	335	rBV	241895	493391	17.68%	1.036%
18	3.666	413	423	433	rBV	109022	254888	9.14%	0.535%
19	3.782	433	442	468	rVB2	437729	1496596	53.64%	3.143%
20	4.556	554	569	576	rBV3	203384	640314	22.95%	1.345%
21	4.629	576	581	589	rVB	118571	289422	10.37%	0.608%
22	4.715	589	595	602	rBV	84623	209419	7.51%	0.440%
23	4.800	602	609	610	rBV2	36028	65806	2.36%	0.138%
24	4.989	628	640	648	rBV4	115279	404646	14.50%	0.850%
25	5.086	648	656	664	rVV	165342	507522	18.19%	1.066%
26	5.172	664	670	685	rVB	106842	313137	11.22%	0.658%
27	5.458	703	717	725	rBV	305114	912966	32.72%	1.917%
28	5.544	725	731	737	rVV	103291	236718	8.48%	0.497%
29	5.623	737	744	751	rBV	287512	745754	26.73%	1.566%
30	5.757	759	766	782	rVB2	212647	647402	23.20%	1.359%
31	6.025	799	810	817	rBV2	211509	562359	20.16%	1.181%
32	6.105	817	823	829	rBV	193259	488227	17.50%	1.025%
33	6.409	862	873	885	rBV	109492	273830	9.81%	0.575%
34	6.824	931	941	956	rBV	488467	1164740	41.75%	2.446%
35	7.184	990	1000	1010	rBV	186427	405159	14.52%	0.851%
36	7.434	1030	1041	1046	rBV	239179	546794	19.60%	1.148%

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 ClientSampleId :
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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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37	7.482	1046	1049	1060	rVV	172052	331032	11.86%	0.695%
38	7.635	1063	1074	1081	rVV	129949	245167	8.79%	0.515%
39	7.744	1081	1092	1102	rVV2	160111	374124	13.41%	0.786%
40	7.866	1102	1112	1122	rVB2	178759	521731	18.70%	1.096%
41	8.159	1154	1160	1168	rBV	33323	59637	2.14%	0.125%
42	8.287	1174	1181	1194	rBV	644440	995455	35.68%	2.090%
43	8.409	1195	1201	1211	rVB	214734	347120	12.44%	0.729%
44	8.616	1228	1235	1242	rBV	837895	1303511	46.72%	2.737%
45	8.695	1242	1248	1254	rVV	1017143	1617420	57.97%	3.396%
46	8.763	1254	1259	1269	rVB	469718	725130	25.99%	1.523%
47	9.019	1293	1301	1317	rBV	223023	323304	11.59%	0.679%
48	9.159	1317	1324	1326	rBV	222408	314206	11.26%	0.660%
49	9.195	1326	1330	1340	rVB	274980	412900	14.80%	0.867%
50	9.317	1343	1350	1353	rBV	383653	595380	21.34%	1.250%
51	9.348	1353	1355	1361	rVB	246500	304803	10.92%	0.640%
52	9.470	1369	1375	1384	rBV	709593	940943	33.73%	1.976%
53	9.561	1384	1390	1395	rVV	188496	274665	9.84%	0.577%
54	9.616	1395	1399	1402	rVV	247455	320944	11.50%	0.674%
55	9.653	1402	1405	1412	rVB	143791	192805	6.91%	0.405%
56	10.092	1469	1477	1489	rBV2	1063180	1997559	71.60%	4.195%
57	10.201	1489	1495	1497	rVV	327068	449131	16.10%	0.943%
58	10.232	1497	1500	1509	rVB	610634	764330	27.40%	1.605%
59	10.342	1511	1518	1524	rBV	1090169	1472041	52.76%	3.091%
60	10.683	1568	1574	1585	rBV2	776973	1378979	49.43%	2.896%
61	10.835	1593	1599	1603	rBV	155091	217902	7.81%	0.458%
62	10.878	1603	1606	1617	rVV	322888	376036	13.48%	0.790%
63	11.000	1620	1626	1631	rVV	670995	811947	29.10%	1.705%
64	11.055	1631	1635	1640	rVV	207971	256202	9.18%	0.538%
65	11.116	1640	1645	1655	rVV	860416	1121876	40.21%	2.356%
66	11.238	1659	1665	1669	rVV2	471001	855251	30.65%	1.796%
67	11.274	1669	1671	1678	rVV2	286292	572594	20.52%	1.202%
68	11.341	1678	1682	1687	rVV	671718	776441	27.83%	1.630%
69	11.402	1687	1692	1697	rVV	546487	654457	23.46%	1.374%
70	11.488	1701	1706	1718	rVB2	1098277	1449324	51.95%	3.043%
71	11.756	1738	1750	1753	rBV2	799472	1160694	41.60%	2.437%
72	11.786	1753	1755	1763	rVB	643869	759717	27.23%	1.595%
73	11.927	1772	1778	1784	rBV	611867	738052	26.45%	1.550%
74	12.006	1786	1791	1794	rVV	477252	581900	20.86%	1.222%
75	12.061	1794	1800	1810	rVB4	1333805	2789995	100.00%	5.859%
76	12.372	1845	1851	1859	rBV	1065578	1277079	45.77%	2.682%

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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VX0127WBSD01

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

77	12.579	1878	1885	1891	rBV	328566	425893	15.27%	0.894%
78	12.981	1944	1951	1958	rBV2	114162	158545	5.68%	0.333%
79	13.323	2002	2007	2018	rVB	573187	684841	24.55%	1.438%
80	13.628	2051	2057	2065	rBV	387890	480652	17.23%	1.009%
81	13.762	2074	2079	2083	rBV2	305986	369757	13.25%	0.776%
82	13.817	2083	2088	2096	rVB	493040	588189	21.08%	1.235%
83	13.999	2112	2118	2124	rBV	397486	487724	17.48%	1.024%

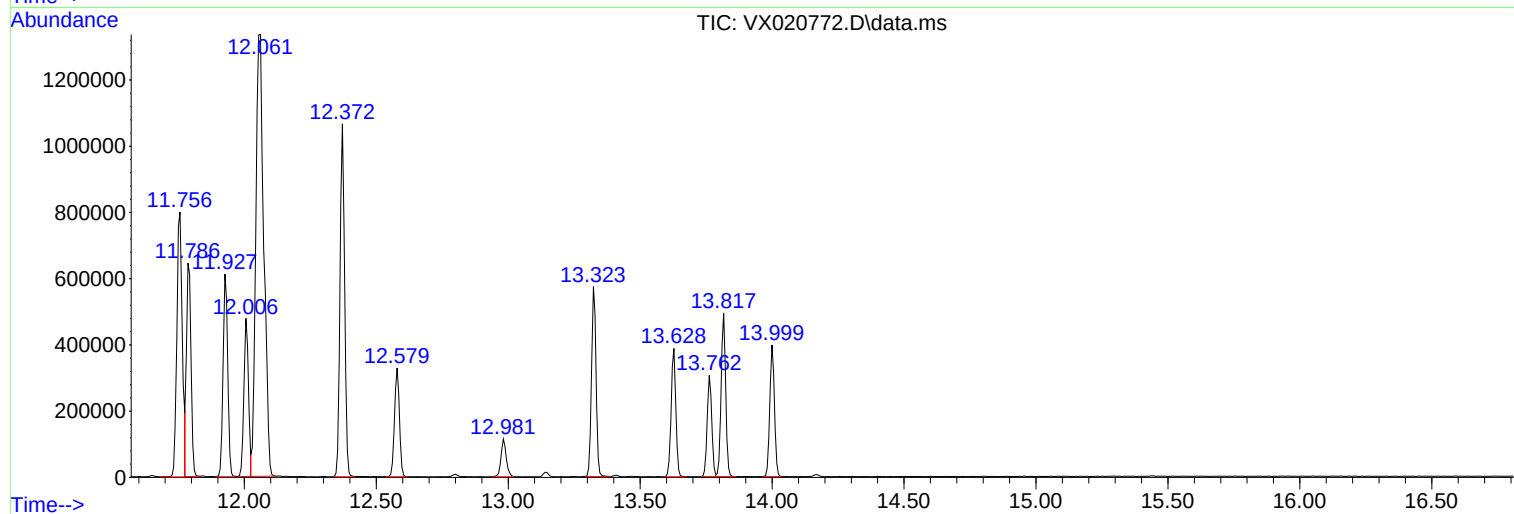
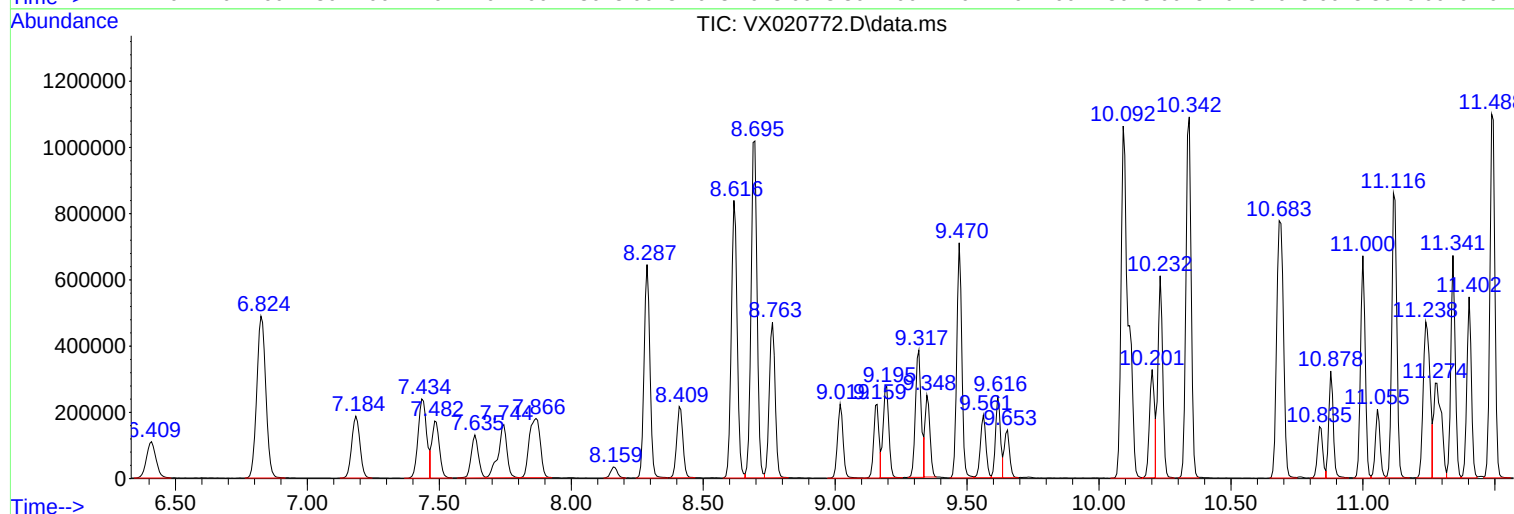
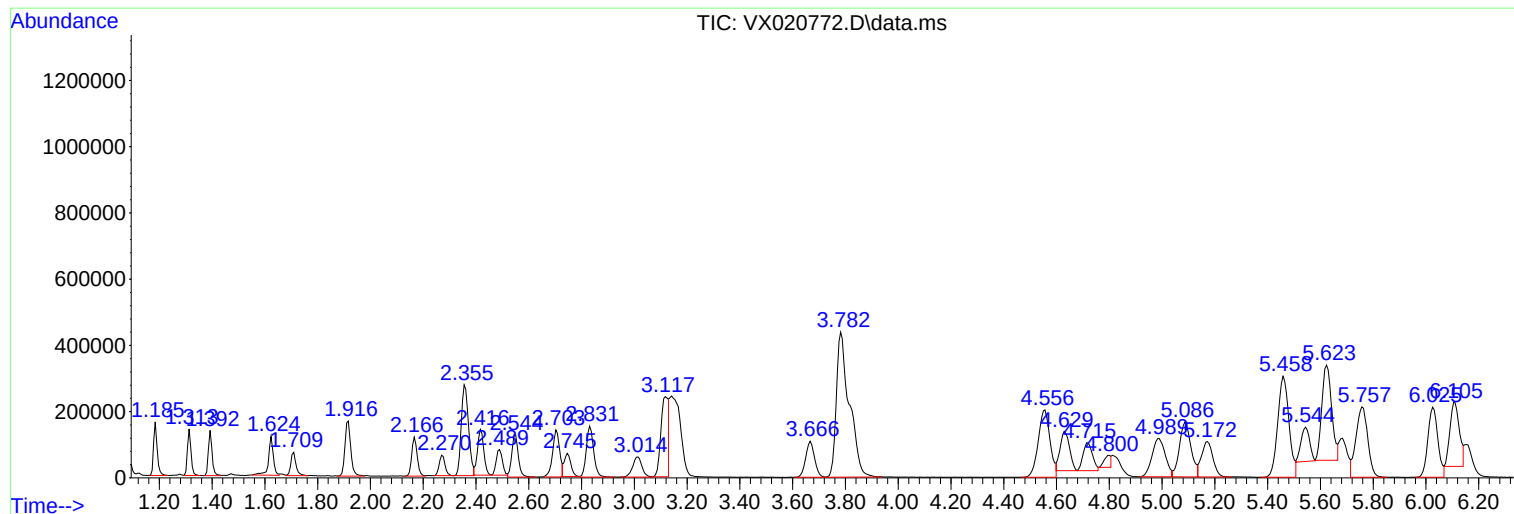
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VX0127WBSD01

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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Sample : VX0127WBSD01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VX0127WBSD01

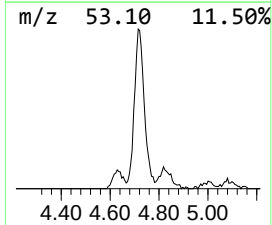
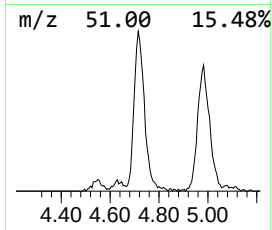
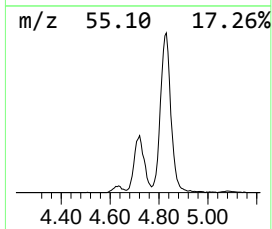
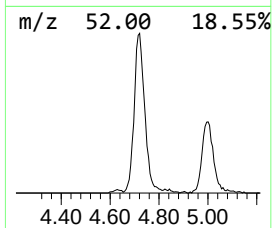
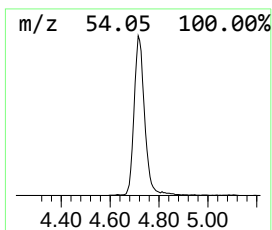
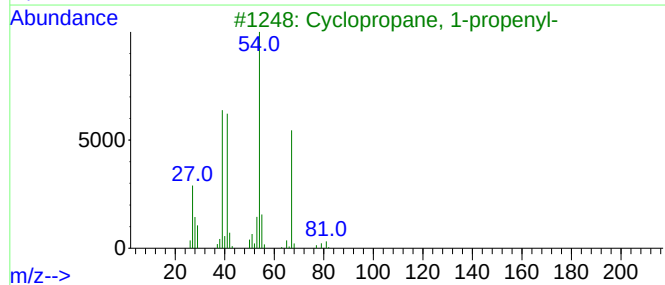
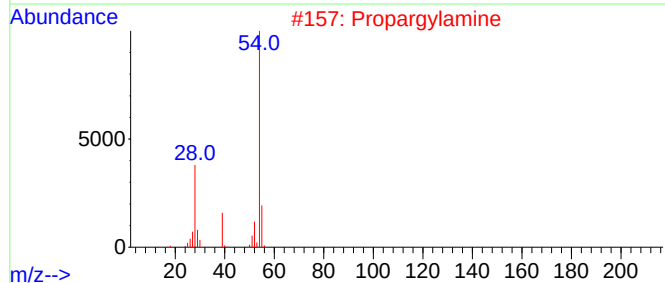
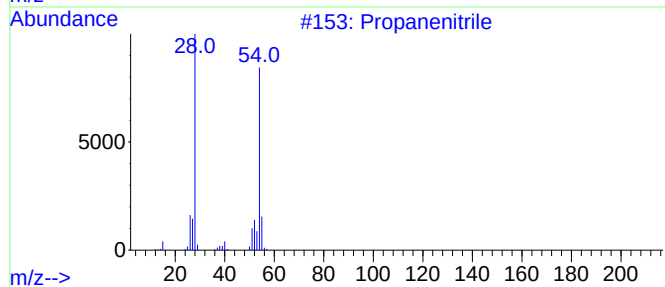
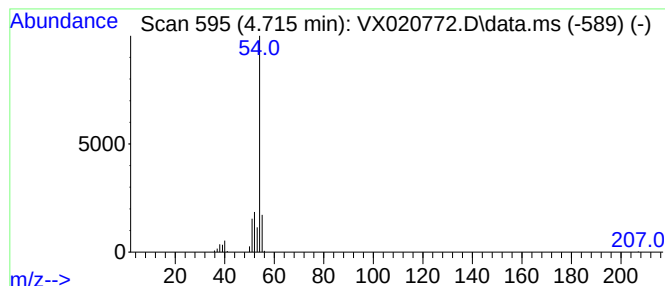
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanenitrile Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.715	14.04 ug/l	209419	Pentafluorobenzene	5.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanenitrile	55	C3H5N	000107-12-0	78
2			Propargylamine	55	C3H5N	002450-71-7	9
3			Cyclopropane, 1-propenyl-	82	C6H10	004663-21-2	9
4			3-Oxabicyclo[3.2.0]heptane-2,4-d...	126	C6H6O3	118554-23-7	9
5			1,2-Butadiene	54	C4H6	000590-19-2	5



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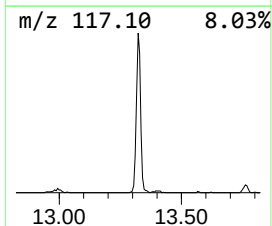
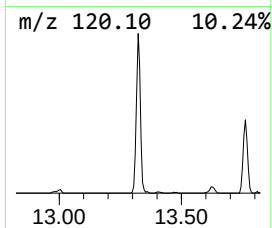
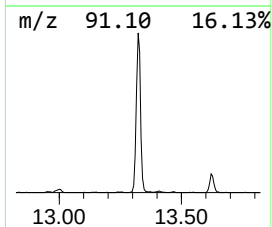
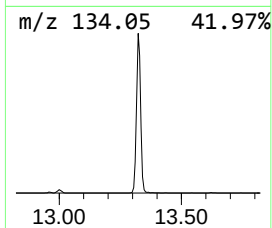
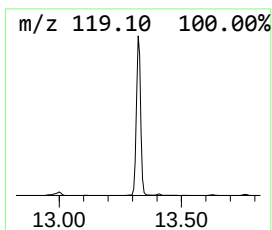
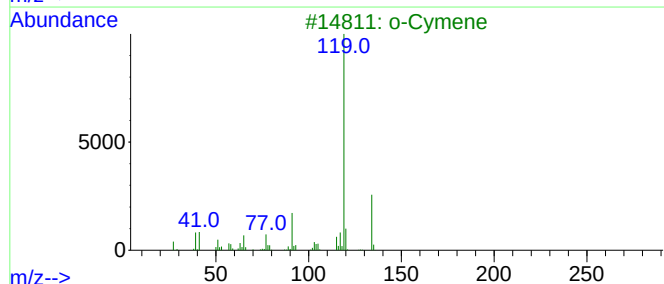
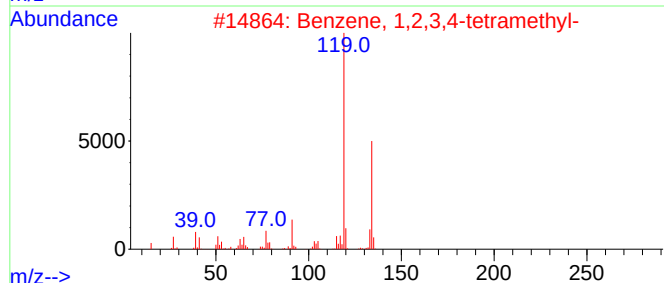
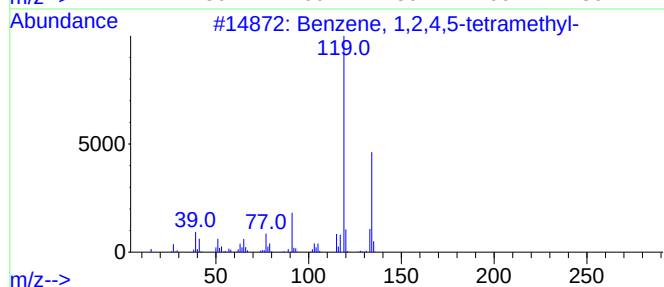
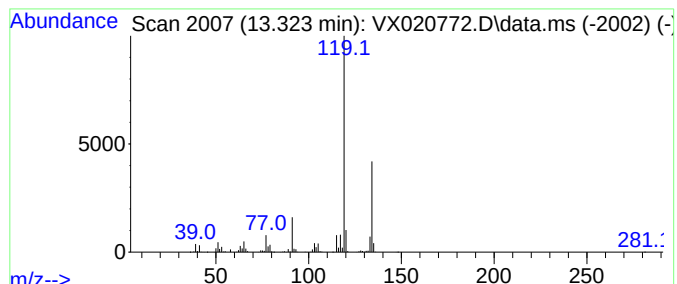
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
13.323	12.27 ug/l	684841	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, 1,2,3,4-tetramethyl-		134	C10H14	000488-23-3	95
3	o-Cymene		134	C10H14	000527-84-4	95
4	Benzene, 1,2,3,5-tetramethyl-		134	C10H14	000527-53-7	94
5	Benzene, 1-ethyl-3,5-dimethyl-		134	C10H14	000934-74-7	94



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanenitrile	4.715	14.0	ug/l	209419	1	5.623	745754	50.0
Benzene, 1,2,4,...	13.323	12.3	ug/l	684841	4	12.061	2790000	50.0