

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
 Data File : VX039411.D
 Acq On : 20 Dec 2023 18:53
 Operator : JC/MD
 Sample : 05808-10ME
 Misc : 4.90g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B04ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\SFAMXML120523WMA.M

Title : VOC Analysis

Signal : TIC: VX039411.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	66	rVB	92317	163485	12.37%	1.385%
2	1.648	89	92	99	rBV	33304	59055	4.47%	0.500%
3	2.282	190	196	211	rBV	248805	421020	31.86%	3.567%
4	2.709	265	266	269	rBV3	507	516	0.04%	0.004%
5	2.843	274	288	299	rVV	162067	324066	24.52%	2.745%
6	3.014	314	316	318	rBV2	254	264	0.02%	0.002%
7	3.062	322	324	326	rBV	287	274	0.02%	0.002%
8	3.123	329	334	335	rBV3	437	615	0.05%	0.005%
9	3.312	359	365	370	rVB2	533	1176	0.09%	0.010%
10	3.349	370	371	373	rBV	338	230	0.02%	0.002%
11	3.416	379	382	383	rBV2	285	263	0.02%	0.002%
12	3.587	409	410	413	rBV	209	223	0.02%	0.002%
13	3.648	418	420	423	rVB2	185	213	0.02%	0.002%
14	3.831	447	450	452	rBV	207	298	0.02%	0.003%
15	4.111	494	496	499	rVV	289	278	0.02%	0.002%
16	4.483	547	557	591	rBV2	70702	348666	26.38%	2.954%
17	4.873	619	621	624	rVB3	357	365	0.03%	0.003%
18	5.056	638	651	669	rBV	155899	518876	39.26%	4.395%
19	5.214	675	677	680	rBV3	300	364	0.03%	0.003%
20	5.355	697	700	702	rBV2	166	211	0.02%	0.002%
21	5.391	702	706	707	rBV2	305	363	0.03%	0.003%
22	5.531	726	729	731	rBV3	515	599	0.05%	0.005%
23	5.690	752	755	758	rBV2	226	287	0.02%	0.002%
24	5.964	788	800	818	rBV2	456896	1321624	100.00%	11.196%
25	6.287	852	853	855	rBV	327	215	0.02%	0.002%
26	6.470	882	883	887	rVB3	210	258	0.02%	0.002%
27	6.550	893	896	901	rBV2	286	428	0.03%	0.004%
28	6.757	921	930	948	rBV	286766	714845	54.09%	6.056%
29	7.110	983	988	995	rVV5	2067	5213	0.39%	0.044%
30	7.305	1011	1020	1037	rBV	261678	598669	45.30%	5.071%
31	7.488	1045	1050	1054	rVV5	770	1490	0.11%	0.013%
32	7.519	1054	1055	1058	rVB3	531	391	0.03%	0.003%
33	7.586	1064	1066	1070	rBV2	239	253	0.02%	0.002%
34	7.781	1094	1098	1100	rBV2	199	244	0.02%	0.002%
35	7.891	1113	1116	1117	rBV2	226	226	0.02%	0.002%
36	7.958	1122	1127	1130	rVV2	751	1117	0.08%	0.009%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
 Title : VOC Analysis

37	8.000	1132	1134	1137	rVV2	381	413	0.03%	0.003%
38	8.092	1145	1149	1151	rVB2	155	253	0.02%	0.002%
39	8.263	1174	1177	1181	rBV3	449	694	0.05%	0.006%
40	8.324	1181	1187	1201	rBV	161606	291844	22.08%	2.472%
41	8.500	1215	1216	1217	rBV	439	247	0.02%	0.002%
42	8.586	1226	1230	1232	rBV2	361	515	0.04%	0.004%
43	8.647	1233	1240	1250	rBV	605373	999065	75.59%	8.463%
44	8.811	1265	1267	1270	rVB	527	483	0.04%	0.004%
45	8.909	1281	1283	1284	rBV	350	327	0.02%	0.003%
46	8.952	1284	1290	1306	rVV	117465	190162	14.39%	1.611%
47	9.269	1339	1342	1348	rVB2	800	1268	0.10%	0.011%
48	9.354	1355	1356	1357	rBV	335	241	0.02%	0.002%
49	9.397	1357	1363	1376	rBV	408612	786728	59.53%	6.665%
50	9.714	1412	1415	1420	rBV2	784	1111	0.08%	0.009%
51	9.860	1437	1439	1441	rVB	263	227	0.02%	0.002%
52	9.896	1443	1445	1448	rVB2	292	219	0.02%	0.002%
53	10.055	1465	1471	1487	rVV	588405	842195	63.72%	7.134%
54	10.201	1492	1495	1500	rVB2	915	1030	0.08%	0.009%
55	10.311	1510	1513	1515	rBV3	441	493	0.04%	0.004%
56	10.610	1559	1562	1563	rBV	223	235	0.02%	0.002%
57	10.652	1566	1569	1573	rVV4	557	909	0.07%	0.008%
58	10.945	1615	1617	1618	rVV	434	353	0.03%	0.003%
59	10.957	1618	1619	1624	rVB3	651	859	0.06%	0.007%
60	11.085	1637	1640	1641	rBV2	287	342	0.03%	0.003%
61	11.195	1652	1658	1669	rVV	474195	625759	47.35%	5.301%
62	11.317	1673	1678	1682	rVB3	3164	4638	0.35%	0.039%
63	11.415	1693	1694	1697	rBV	247	279	0.02%	0.002%
64	11.457	1697	1701	1703	rVV2	688	1046	0.08%	0.009%
65	11.475	1703	1704	1709	rVB3	970	1384	0.10%	0.012%
66	11.530	1711	1713	1717	rBV2	227	254	0.02%	0.002%
67	11.756	1747	1750	1752	rBV3	658	850	0.06%	0.007%
68	11.829	1759	1762	1765	rVB2	189	270	0.02%	0.002%
69	11.884	1769	1771	1773	rVV	228	234	0.02%	0.002%
70	11.969	1780	1785	1789	rBV	100743	129996	9.84%	1.101%
71	12.024	1789	1794	1810	rVB2	709537	1004127	75.98%	8.506%
72	12.323	1837	1843	1857	rVV3	745575	1178013	89.13%	9.979%
73	12.500	1870	1872	1875	rVB2	229	225	0.02%	0.002%
74	12.573	1881	1884	1886	rBV	194	268	0.02%	0.002%
75	12.762	1910	1915	1920	rBV	7518	10076	0.76%	0.085%
76	12.798	1920	1921	1925	rVB2	200	218	0.02%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

77	13.067	1960	1965	1969	rVV4	1833	3371	0.26%	0.029%
78	13.115	1969	1973	1977	rVB3	904	1349	0.10%	0.011%
79	13.158	1977	1980	1981	rBV2	301	271	0.02%	0.002%
80	13.201	1983	1987	1992	rVV	2627	2891	0.22%	0.024%
81	13.268	1995	1998	2002	rBV4	524	649	0.05%	0.005%
82	13.585	2045	2050	2063	rVV	560760	696869	52.73%	5.903%
83	13.780	2079	2082	2087	rBV3	642	795	0.06%	0.007%
84	13.963	2106	2112	2122	rVB	174055	229421	17.36%	1.943%
85	14.127	2134	2139	2145	rVB	7973	10378	0.79%	0.088%
86	14.176	2145	2147	2150	rBV	172	212	0.02%	0.002%
87	14.262	2159	2161	2166	rVB3	162	218	0.02%	0.002%
88	14.426	2185	2188	2190	rVB2	235	253	0.02%	0.002%
89	14.542	2205	2207	2211	rVB2	337	329	0.02%	0.003%
90	14.585	2211	2214	2217	rVB3	256	267	0.02%	0.002%
91	14.621	2217	2220	2224	rBV4	568	690	0.05%	0.006%
92	14.780	2239	2246	2255	rVV2	23382	40835	3.09%	0.346%
93	14.920	2268	2269	2273	rVB	471	401	0.03%	0.003%
94	15.249	2317	2323	2329	rBV	167481	238855	18.07%	2.023%
95	15.383	2342	2345	2349	rBV3	904	1358	0.10%	0.012%
96	15.524	2366	2368	2371	rBV3	264	236	0.02%	0.002%
97	15.956	2436	2439	2441	rBV3	389	343	0.03%	0.003%
98	16.322	2496	2499	2500	rBV2	442	442	0.03%	0.004%
99	16.505	2523	2529	2536	rVB3	5334	9360	0.71%	0.079%
100	16.597	2541	2544	2546	rBV2	401	397	0.03%	0.003%

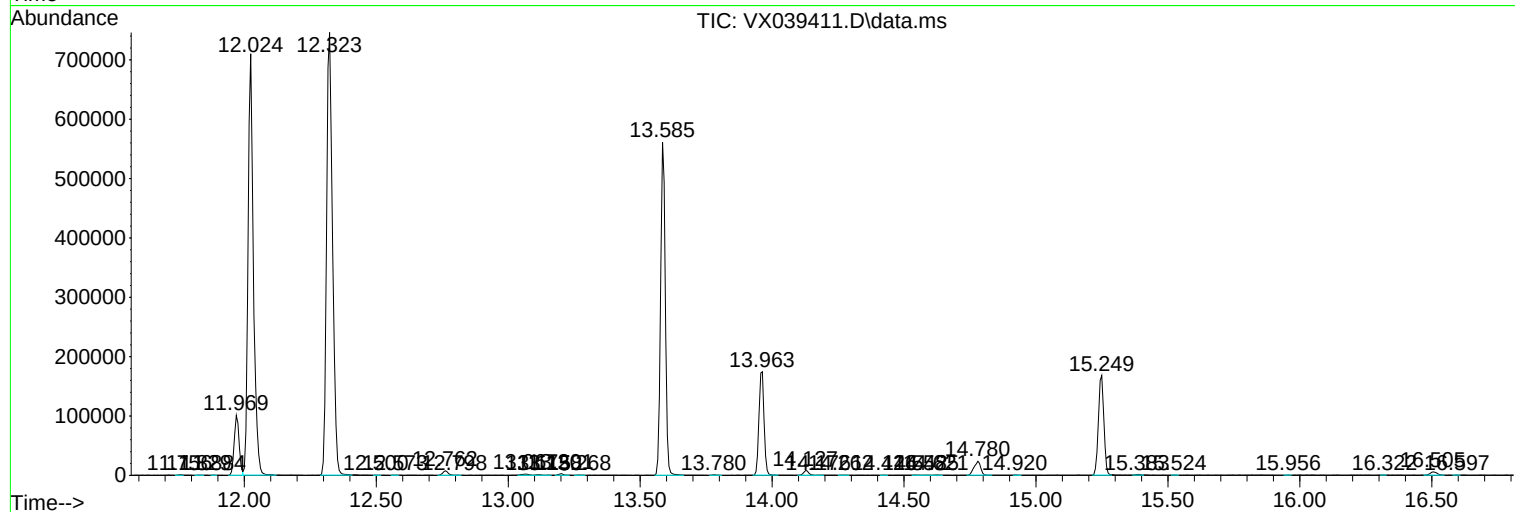
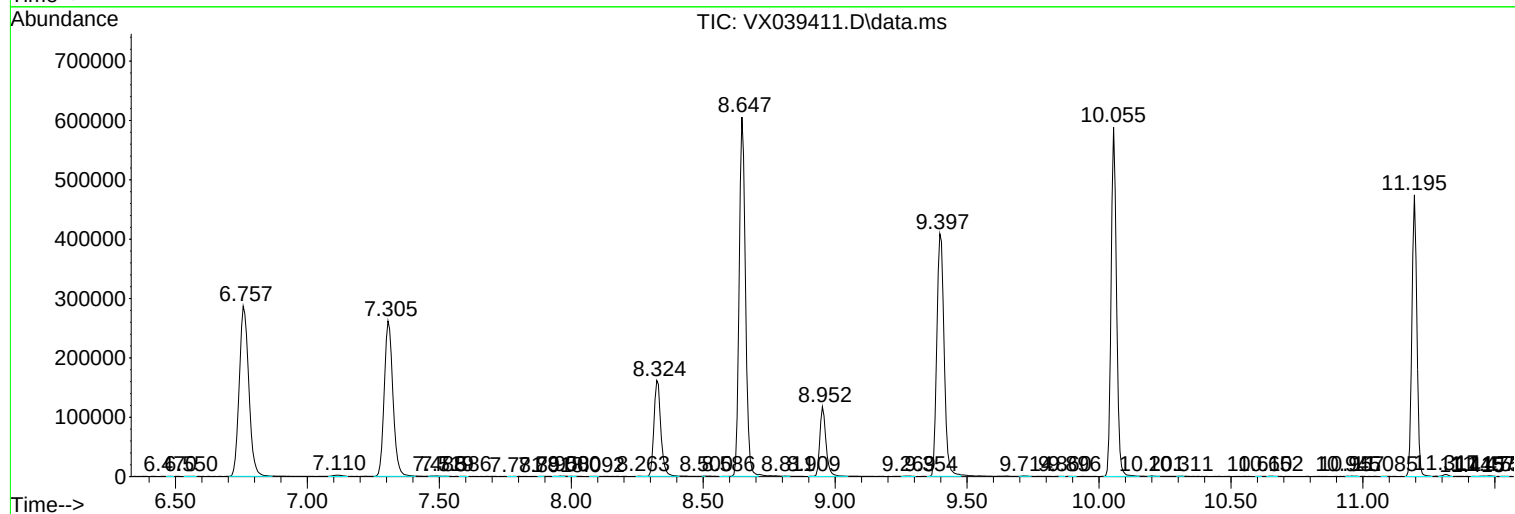
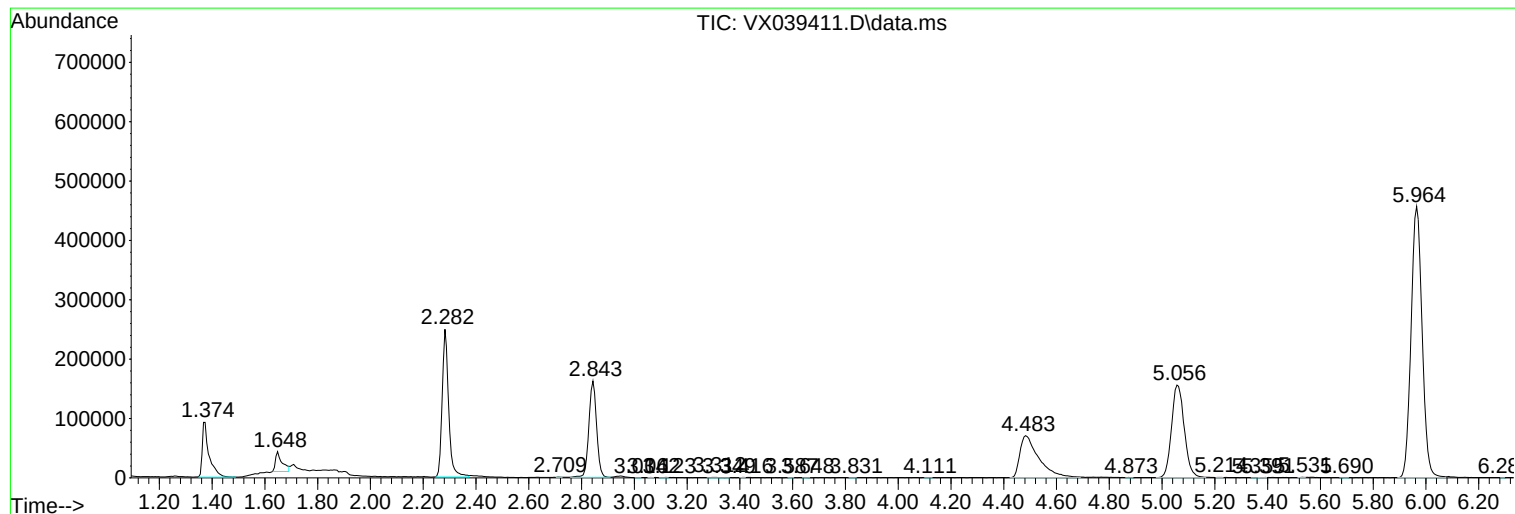
Sum of corrected areas: 11804720

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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B04ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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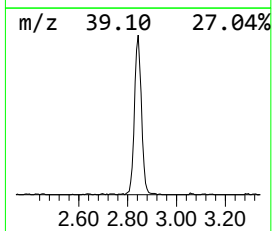
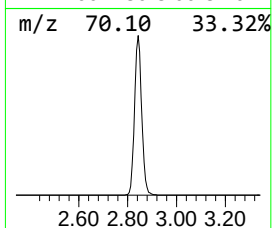
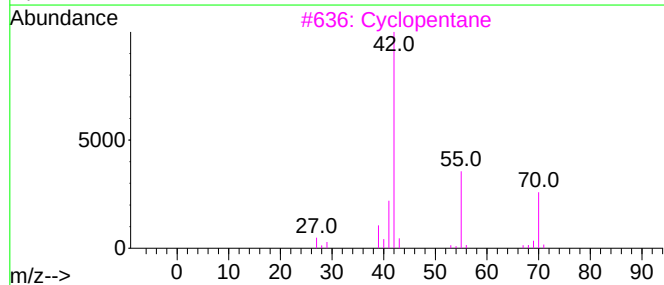
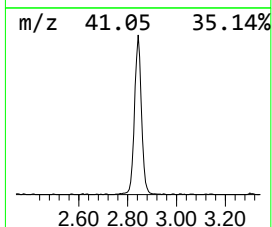
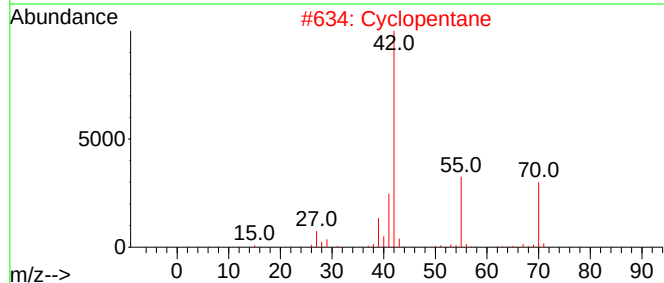
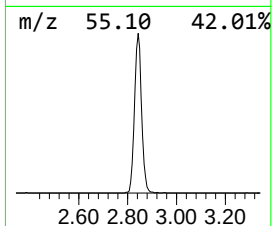
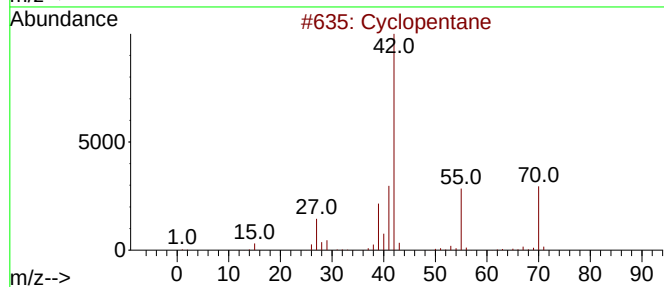
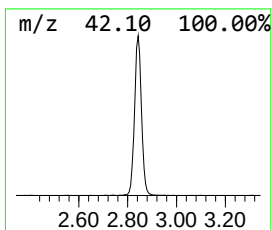
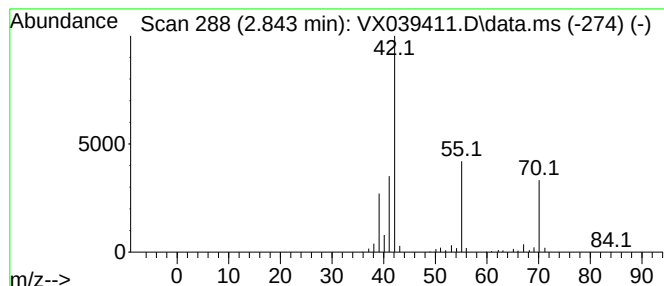
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic2.843 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.843	22.67 ug/L	324066	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	90
2			Cyclopentane	70	C5H10	000287-92-3	86
3			Cyclopentane	70	C5H10	000287-92-3	72
4			Cyclobutane, methyl-	70	C5H10	000598-61-8	72
5			Cyclobutane, methyl-	70	C5H10	000598-61-8	56



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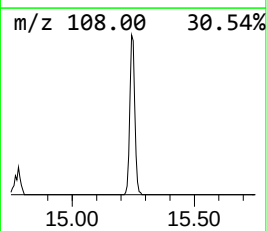
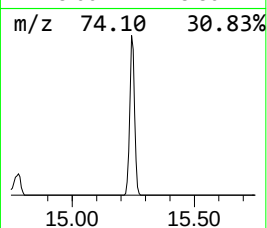
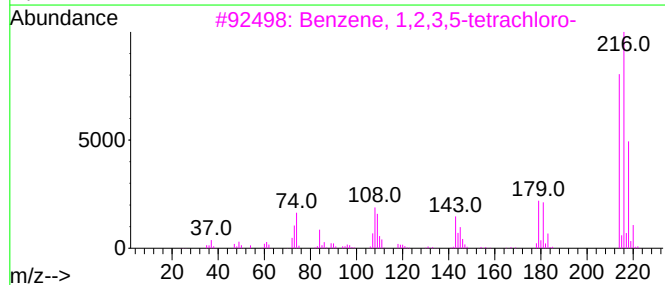
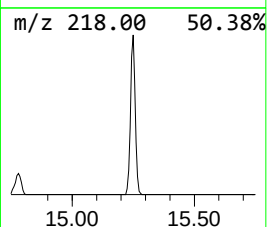
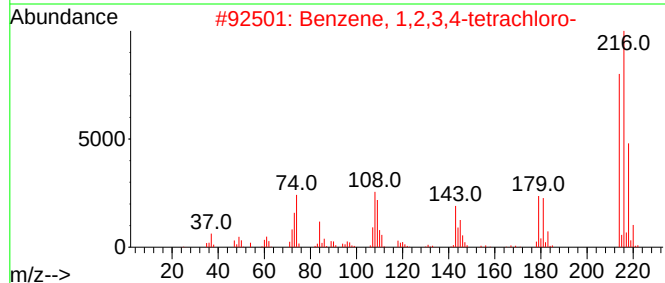
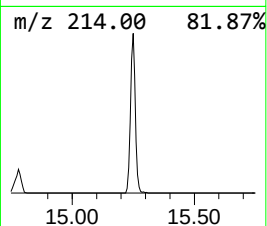
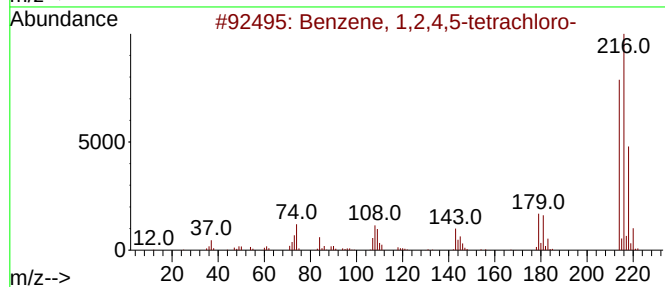
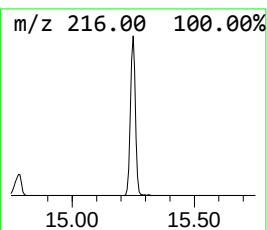
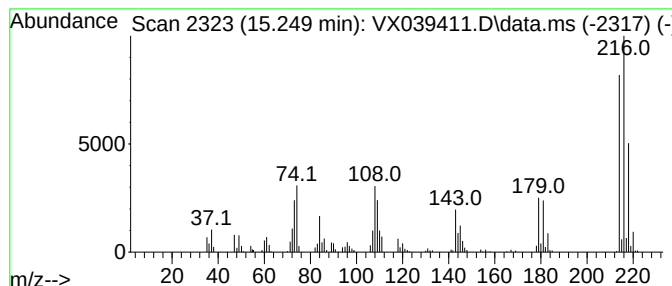
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,2,4,5-tetrachloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.249	11.89 ug/L	238855	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetrachloro-	214	C6H2Cl4	000095-94-3	99
2			Benzene, 1,2,3,4-tetrachloro-	214	C6H2Cl4	000634-66-2	99
3			Benzene, 1,2,3,5-tetrachloro-	214	C6H2Cl4	000634-90-2	99
4			Benzene, 1,2,4,5-tetrachloro-	214	C6H2Cl4	000095-94-3	99
5			Benzene, 1,2,3,4-tetrachloro-	214	C6H2Cl4	000634-66-2	98



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	2.843	22.7	ug/L	324066	1	6.757	714845	50.0
Benzene, 1,2,4,...	15.249	11.9	ug/L	238855	3	12.024	1004130	50.0