

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX072219\
 Data File : VX011041.D
 Acq On : 22 Jul 2019 19:20
 Operator : JC/SP
 Sample : K3934-13
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TP-1

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.276	13	20	27	rBV	25562	38844	3.63%	0.487%
2	2.440	206	211	218	rBV	8067	14962	1.40%	0.188%
3	5.208	657	665	674	rBV2	6719	19855	1.86%	0.249%
4	5.500	700	713	725	rBV	126877	366384	34.25%	4.595%
5	5.659	727	739	761	rVB	212682	612764	57.28%	7.685%
6	6.061	795	805	814	rBV	125279	328929	30.75%	4.125%
7	6.147	814	819	829	rVB2	9408	23655	2.21%	0.297%
8	6.860	925	936	951	rBV	323174	764414	71.46%	9.587%
9	7.457	1024	1034	1044	rVB8	6487	18453	1.72%	0.231%
10	7.848	1090	1098	1105	rBV4	11791	24846	2.32%	0.312%
11	8.031	1121	1128	1139	rVB7	8158	21824	2.04%	0.274%
12	8.293	1167	1171	1177	rVB4	6027	11102	1.04%	0.139%
13	8.451	1192	1197	1206	rBV6	4296	11051	1.03%	0.139%
14	8.573	1211	1217	1224	rVB6	5587	13402	1.25%	0.168%
15	8.665	1224	1232	1234	rBV3	14872	25064	2.34%	0.314%
16	8.713	1234	1240	1248	rVV	697358	1069755	100.00%	13.417%
17	8.780	1248	1251	1256	rVV	7419	13921	1.30%	0.175%
18	8.841	1256	1261	1265	rVV3	10268	19452	1.82%	0.244%
19	8.908	1269	1272	1280	rVB3	10533	16286	1.52%	0.204%
20	9.043	1288	1294	1305	rVB2	41719	71792	6.71%	0.900%
21	9.164	1307	1314	1319	rVB3	8830	14782	1.38%	0.185%
22	9.329	1337	1341	1349	rVB4	6401	13320	1.25%	0.167%
23	9.567	1374	1380	1385	rBV5	16064	35214	3.29%	0.442%
24	9.622	1385	1389	1393	rVB5	6718	10956	1.02%	0.137%
25	9.677	1393	1398	1402	rBV	78477	124242	11.61%	1.558%
26	9.713	1402	1404	1408	rVB2	11259	15910	1.49%	0.200%
27	9.817	1414	1421	1427	rBV2	16261	28189	2.64%	0.354%
28	9.890	1427	1433	1447	rVB3	38280	69702	6.52%	0.874%
29	10.109	1464	1469	1475	rVV	681570	935073	87.41%	11.727%
30	10.164	1475	1478	1485	rVB6	8331	17079	1.60%	0.214%
31	10.237	1485	1490	1496	rBV3	19458	34403	3.22%	0.431%
32	10.359	1502	1510	1515	rBV6	33782	91357	8.54%	1.146%
33	10.408	1515	1518	1530	rVB2	20626	43756	4.09%	0.549%
34	10.512	1530	1535	1541	rBV2	19017	32443	3.03%	0.407%

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Integrator: RTE
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35	10.640	1548	1556	1563	rBV5	49795	112022	10.47%	1.405%
36	10.713	1563	1568	1579	rVB5	14510	32746	3.06%	0.411%
37	10.810	1579	1584	1585	rBV	27732	34882	3.26%	0.437%
38	10.835	1585	1588	1592	rVV2	53505	67781	6.34%	0.850%
39	10.914	1596	1601	1612	rVV6	31616	75373	7.05%	0.945%
40	11.060	1620	1625	1631	rBV5	15787	27563	2.58%	0.346%
41	11.134	1632	1637	1642	rBV	592585	752599	70.35%	9.439%
42	11.182	1642	1645	1648	rVB2	17172	19593	1.83%	0.246%
43	11.274	1653	1660	1669	rVB4	51674	87809	8.21%	1.101%
44	11.365	1669	1675	1676	rBV3	7184	12576	1.18%	0.158%
45	11.390	1676	1679	1684	rBV2	11149	15282	1.43%	0.192%
46	11.445	1684	1688	1692	rBV3	21512	34046	3.18%	0.427%
47	11.536	1700	1703	1706	rVB2	12280	15627	1.46%	0.196%
48	11.579	1706	1710	1715	rVB4	19846	28794	2.69%	0.361%
49	11.670	1719	1725	1732	rBV6	19199	41499	3.88%	0.520%
50	11.737	1732	1736	1738	rBV5	8185	11425	1.07%	0.143%
51	11.762	1738	1740	1743	rVV3	11347	11945	1.12%	0.150%
52	11.804	1743	1747	1757	rVB8	19891	55930	5.23%	0.701%
53	11.908	1757	1764	1767	rBV8	13303	30970	2.90%	0.388%
54	11.944	1767	1770	1774	rVB5	13965	18385	1.72%	0.231%
55	11.999	1775	1779	1781	rBV4	9120	10885	1.02%	0.137%
56	12.079	1786	1792	1797	rVV	689126	896631	83.82%	11.245%
57	12.121	1797	1799	1803	rVV5	10739	13047	1.22%	0.164%
58	12.182	1804	1809	1811	rVV6	7114	14184	1.33%	0.178%
59	12.298	1824	1828	1832	rBV4	11000	15330	1.43%	0.192%
60	12.365	1835	1839	1846	rVB2	38560	66929	6.26%	0.839%
61	12.518	1862	1864	1869	rVB6	7890	12986	1.21%	0.163%
62	12.566	1869	1872	1877	rBV6	6066	12123	1.13%	0.152%
63	12.871	1918	1922	1928	rVB2	37538	56007	5.24%	0.702%
64	12.950	1928	1935	1937	rBV6	19252	32773	3.06%	0.411%
65	13.042	1945	1950	1953	rBV2	12435	19605	1.83%	0.246%
66	13.078	1953	1956	1961	rVB4	12376	21529	2.01%	0.270%
67	13.347	1996	2000	2006	rVB5	21324	33874	3.17%	0.425%
68	13.456	2011	2018	2028	rBV8	20941	62724	5.86%	0.787%
69	13.578	2033	2038	2043	rBV6	7737	19173	1.79%	0.240%
70	13.633	2043	2047	2051	rBV3	12432	20195	1.89%	0.253%
71	13.676	2051	2054	2059	rVV5	7505	11472	1.07%	0.144%

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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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72	13.719	2059	2061	2065	rVB3	12532	16745	1.57%	0.210%
73	13.804	2072	2075	2078	rBV2	13799	17704	1.65%	0.222%
74	13.901	2087	2091	2096	rVB5	12088	19037	1.78%	0.239%
75	13.962	2096	2101	2102	rBV5	8747	12085	1.13%	0.152%
76	14.029	2108	2112	2116	rBV2	9715	15732	1.47%	0.197%
77	14.121	2124	2127	2131	rBV5	9934	13404	1.25%	0.168%
78	14.267	2147	2151	2159	rVB	19256	29335	2.74%	0.368%
79	14.426	2173	2177	2181	rBV2	13912	18238	1.70%	0.229%
80	14.474	2181	2185	2190	rVB4	11363	17673	1.65%	0.222%
81	14.548	2191	2197	2204	rBV9	8742	22030	2.06%	0.276%
82	14.670	2214	2217	2223	rVB6	10261	15723	1.47%	0.197%
83	14.724	2223	2226	2231	rVB3	12679	16157	1.51%	0.203%

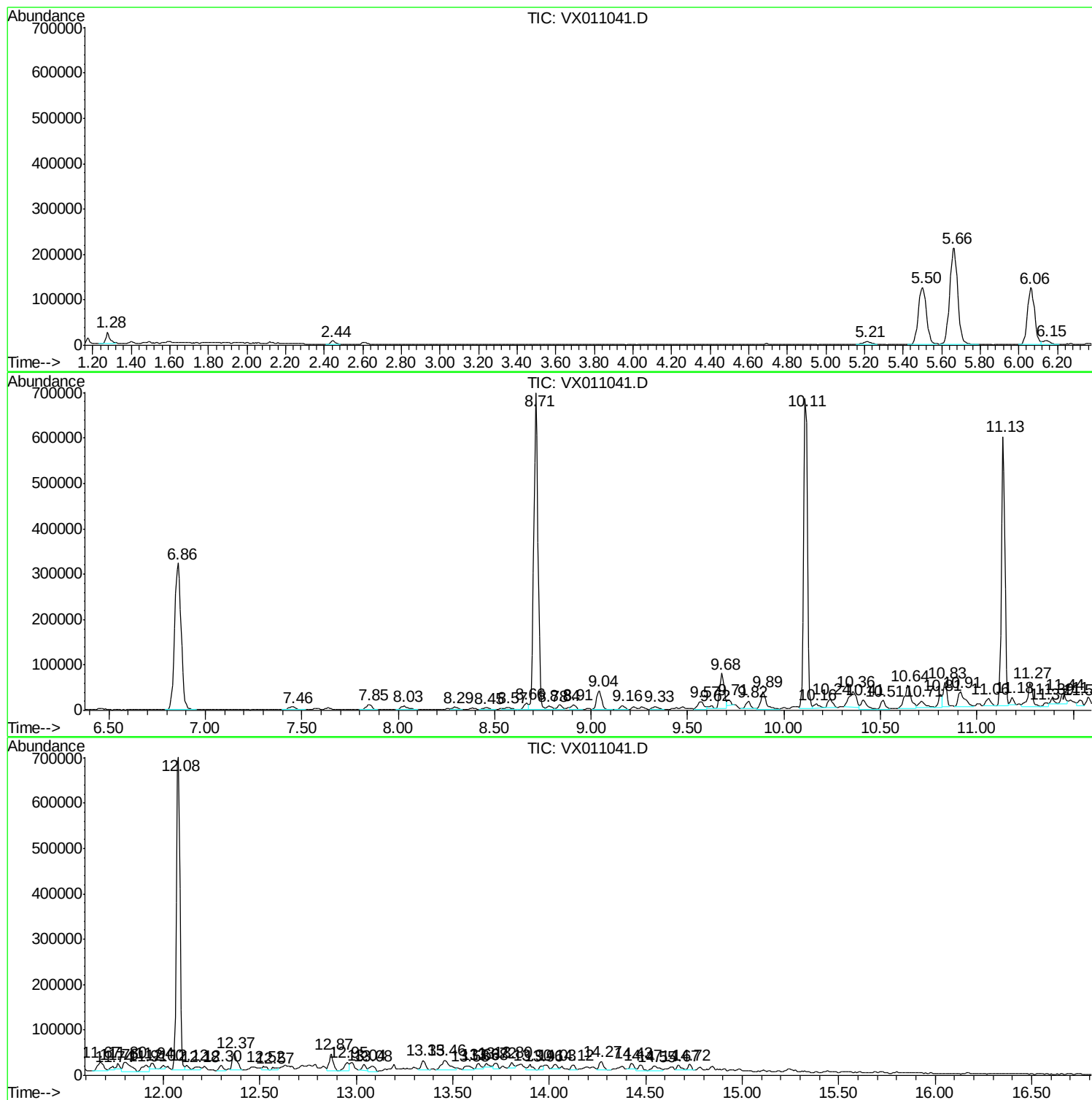
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

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



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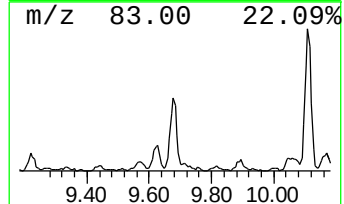
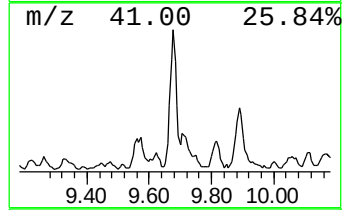
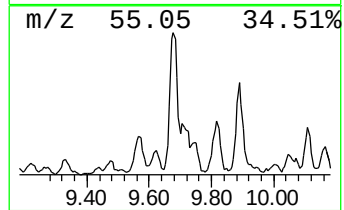
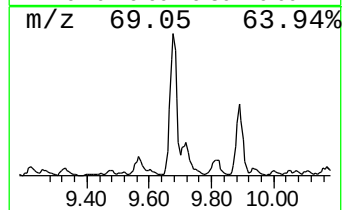
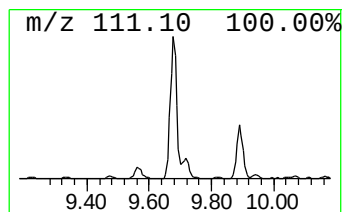
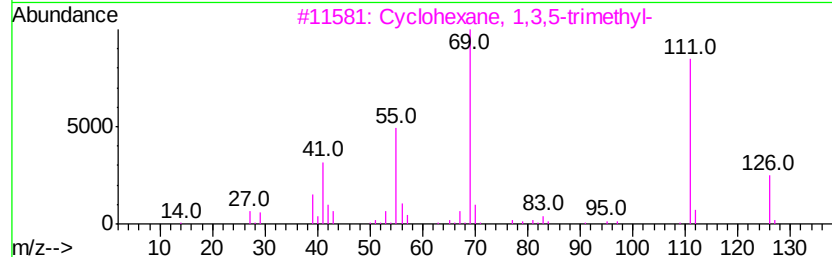
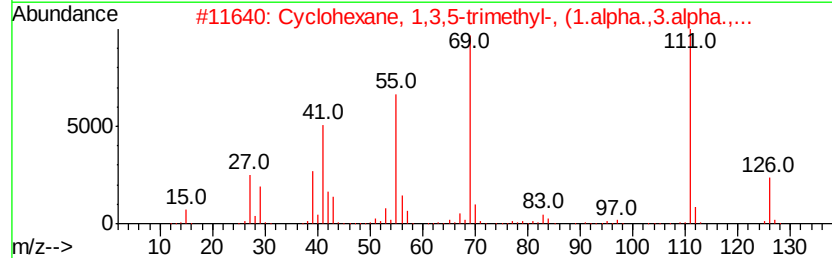
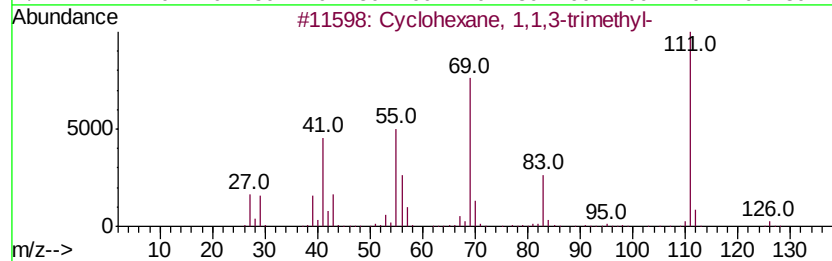
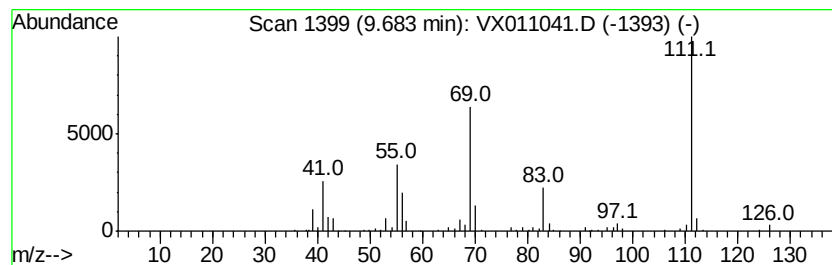
Instrument :
MSVOA_X
ClientSampled :
TP-1

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
9.68	6.64 ug/l	124242	Chlorobenzene-d5	10.11		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	91
2		Cvclohexane, 1,3,5-trimethyl-, (...)	126	C9H18	001795-27-3	64
3		Cvclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	59
4		2(1H)-Pvridinone, 5-hydroxy-	111	C5H5N02	005154-01-8	53
5		2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	50



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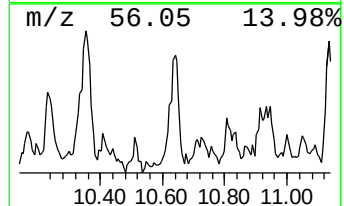
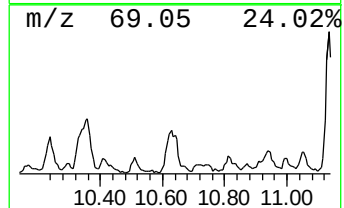
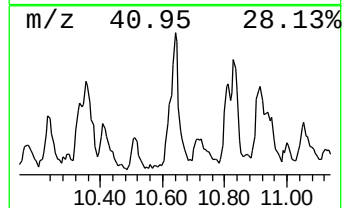
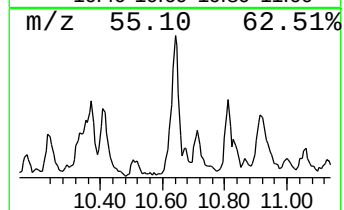
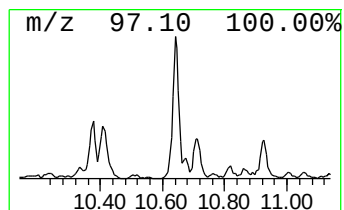
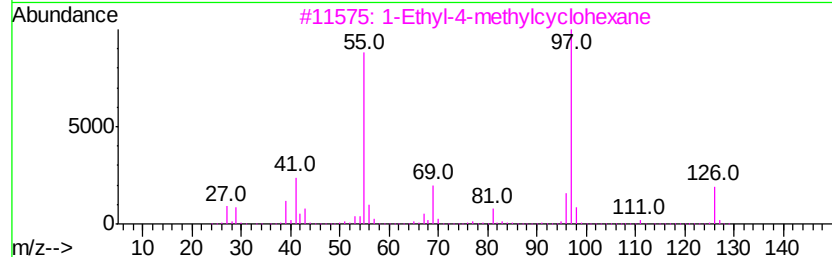
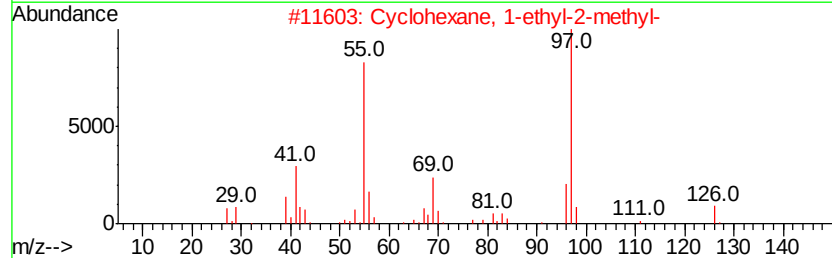
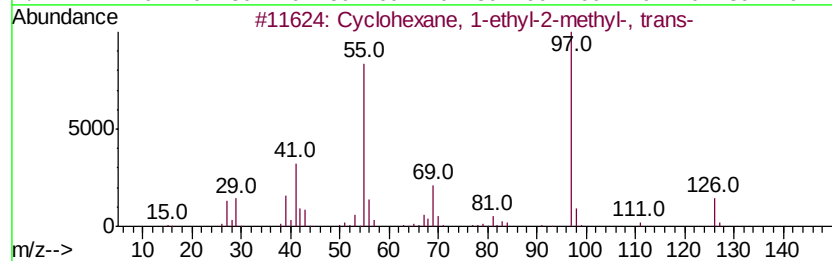
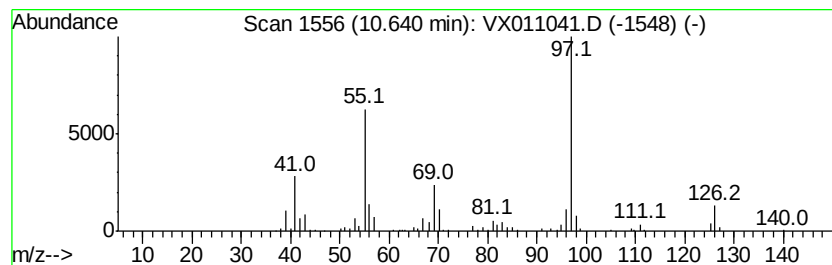
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	5.99 ug/l	112022	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	87
2		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	87
3		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	87
4		4-Octen-3-one	126	C8H14O	014129-48-7	64
5		3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexane, 1,1,...	9.68	6.6	ug/l	124242	3	10.11	935073	50.0
Cyclohexane, 1-et...	10.64	6.0	ug/l	112022	3	10.11	935073	50.0