

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042623\
 Data File : VY013471.D
 Acq On : 26 Apr 2023 14:19
 Operator : KP/MD
 Sample : 02401-04
 Misc : 3.59g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20230248-14-2

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_Y\methods\82Y042423S.M
 Title : SW846 8260

Signal : TIC: VY013471.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.863	3	7	18	rVB2	21495	40559	4.97%	0.673%
2	2.052	34	38	44	rBV2	4389	9242	1.13%	0.153%
3	2.217	60	65	68	rBV	16497	27485	3.37%	0.456%
4	3.253	229	235	240	rBV4	4574	9762	1.20%	0.162%
5	3.948	340	349	364	rBV2	8141	26490	3.25%	0.440%
6	4.192	382	389	402	rVB	25997	69219	8.48%	1.149%
7	4.710	463	474	487	rBV4	15813	55688	6.82%	0.924%
8	5.741	636	643	654	rVB5	3641	13364	1.64%	0.222%
9	6.984	842	847	859	rVB5	3445	10075	1.23%	0.167%
10	7.716	956	967	973	rBV	119865	290838	35.64%	4.827%
11	7.789	973	979	990	rVB	193690	440337	53.96%	7.309%
12	8.136	1027	1036	1051	rBV	133512	297745	36.49%	4.942%
13	8.685	1117	1126	1135	rBV	302656	604735	74.11%	10.038%
14	9.185	1204	1208	1215	rVB6	4443	8721	1.07%	0.145%
15	10.179	1363	1371	1378	rBV	474523	816051	100.00%	13.545%
16	10.240	1378	1381	1387	rVB2	8568	13720	1.68%	0.228%
17	10.368	1394	1402	1409	rVB9	3422	8184	1.00%	0.136%
18	11.142	1524	1529	1534	rBV3	5145	9022	1.11%	0.150%
19	11.288	1545	1553	1561	rVB10	3395	9311	1.14%	0.155%
20	11.490	1579	1586	1595	rBV	425455	715459	87.67%	11.875%
21	11.587	1597	1602	1612	rVB2	9945	19432	2.38%	0.323%
22	11.691	1612	1619	1626	rBV3	25844	59818	7.33%	0.993%
23	11.843	1638	1644	1647	rBV4	8987	17727	2.17%	0.294%
24	11.886	1647	1651	1656	rVB6	5182	12458	1.53%	0.207%
25	11.983	1662	1667	1672	rBV4	10942	22331	2.74%	0.371%
26	12.093	1680	1685	1693	rVB5	12117	28347	3.47%	0.471%
27	12.233	1696	1708	1714	rBV4	30396	92665	11.36%	1.538%
28	12.319	1714	1722	1727	rBV6	20387	53817	6.59%	0.893%
29	12.386	1727	1733	1736	rBV7	5144	9741	1.19%	0.162%
30	12.477	1742	1748	1755	rBV	327806	536412	65.73%	8.904%
31	12.569	1759	1763	1768	rBV7	11301	18756	2.30%	0.311%
32	12.727	1782	1789	1796	rBV5	41429	112268	13.76%	1.863%
33	12.806	1796	1802	1805	rBV6	27430	63198	7.74%	1.049%
34	12.947	1821	1825	1829	rBV5	22207	30532	3.74%	0.507%
35	13.062	1837	1844	1849	rBV4	28330	62305	7.63%	1.034%
36	13.123	1849	1854	1858	rBV5	27416	43576	5.34%	0.723%

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37	13.166	1858	1861	1863	rBV4	12209	16200	1.99%	0.269%
38	13.294	1878	1882	1887	rBV7	16831	36123	4.43%	0.600%
39	13.349	1888	1891	1896	rVV6	23663	41447	5.08%	0.688%
40	13.422	1897	1903	1911	rVB	404048	645253	79.07%	10.710%
41	13.562	1923	1926	1930	rVB6	18090	25976	3.18%	0.431%
42	13.611	1930	1934	1936	rBV4	10265	16705	2.05%	0.277%
43	13.745	1950	1956	1961	rBV8	42217	74578	9.14%	1.238%
44	13.965	1989	1992	2002	rVB6	36675	77198	9.46%	1.281%
45	14.074	2007	2010	2014	rVB3	14968	18616	2.28%	0.309%
46	14.148	2015	2022	2027	rVB10	18072	40305	4.94%	0.669%
47	14.202	2027	2031	2035	rBV4	17651	28613	3.51%	0.475%
48	14.251	2035	2039	2043	rBV5	22895	38542	4.72%	0.640%
49	14.422	2064	2067	2070	rVB3	18534	24512	3.00%	0.407%
50	14.544	2084	2087	2089	rBV4	10382	12417	1.52%	0.206%
51	14.611	2095	2098	2104	rVB5	13390	19289	2.36%	0.320%
52	14.678	2106	2109	2114	rVV7	17193	33291	4.08%	0.553%
53	14.733	2114	2118	2123	rVB6	20124	34978	4.29%	0.581%
54	14.843	2133	2136	2139	rVB5	12065	15726	1.93%	0.261%
55	14.934	2149	2151	2156	rVB6	13980	20448	2.51%	0.339%
56	15.001	2158	2162	2165	rBV6	12385	20691	2.54%	0.343%
57	15.117	2178	2181	2187	rVB6	14969	26015	3.19%	0.432%
58	15.446	2231	2235	2237	rBV5	7732	12494	1.53%	0.207%
59	15.605	2257	2261	2266	rVB5	23808	39632	4.86%	0.658%
60	16.159	2350	2352	2356	rVB5	7583	10468	1.28%	0.174%
61	16.476	2399	2404	2412	rVB5	10823	23813	2.92%	0.395%
62	16.598	2420	2424	2427	rBV5	6100	11960	1.47%	0.199%

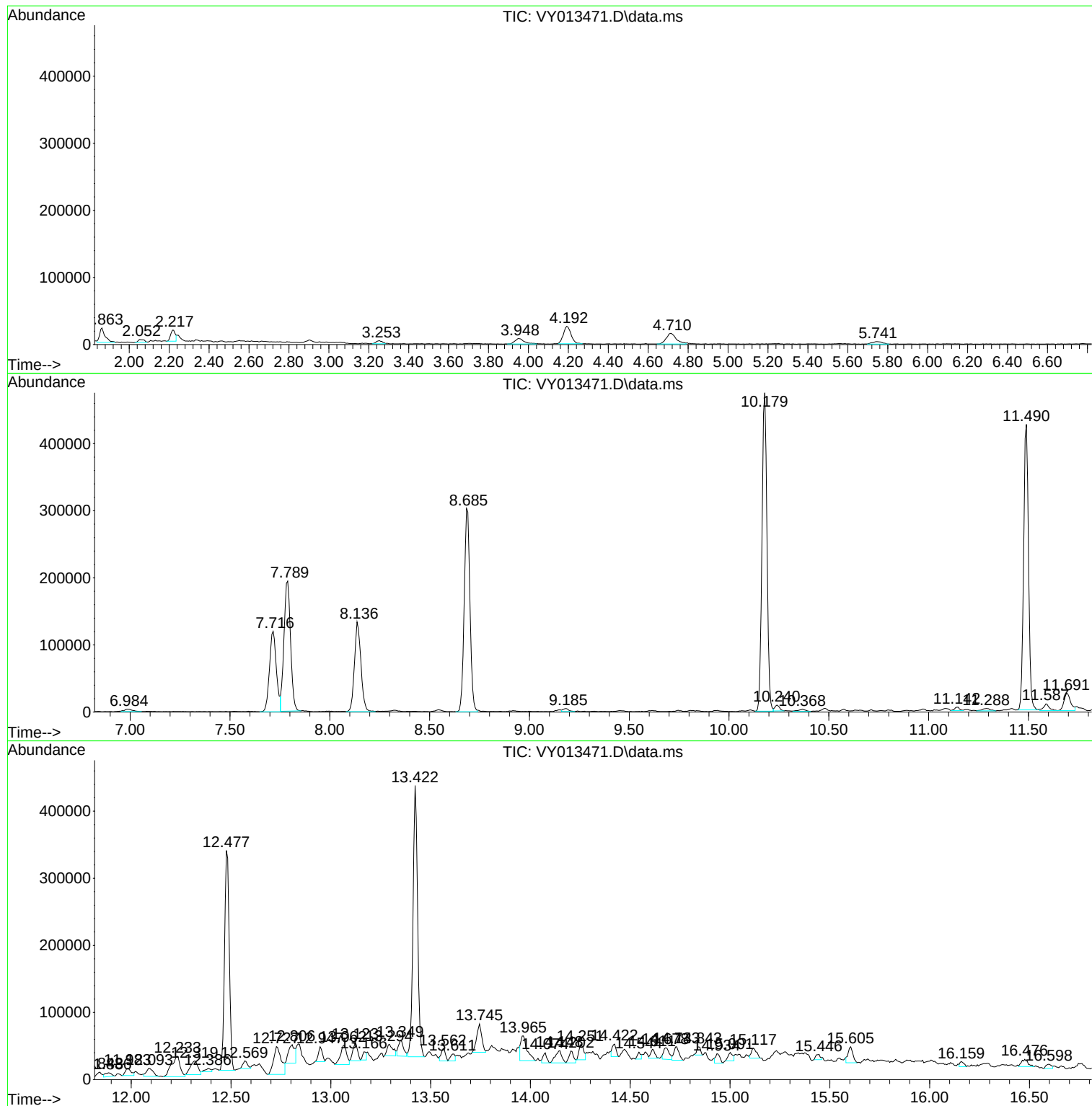
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Quant Title : SW846 8260

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



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Instrument :
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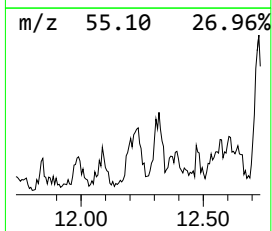
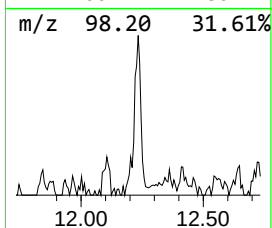
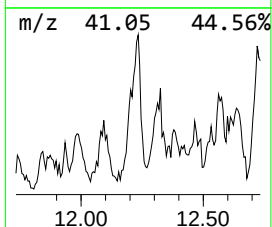
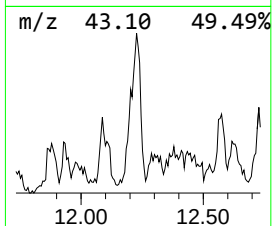
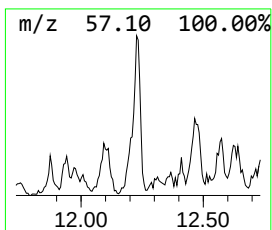
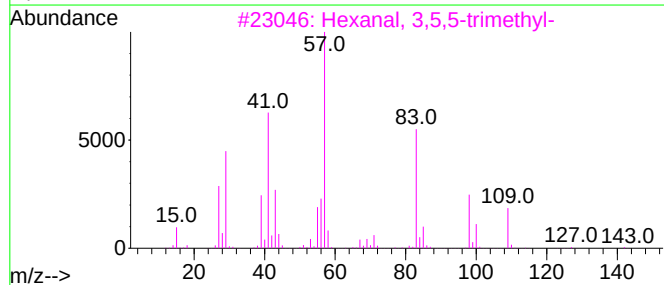
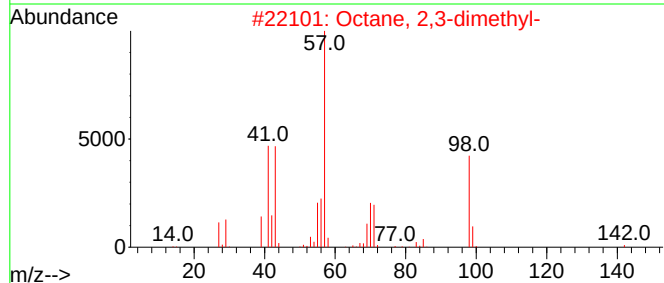
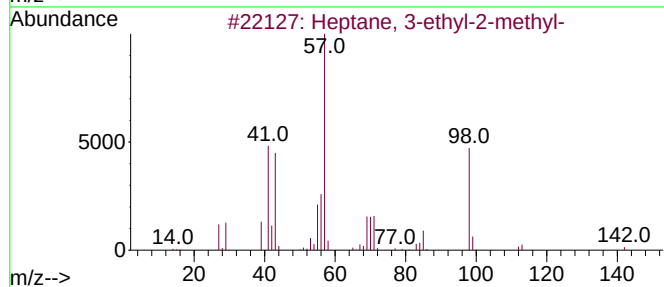
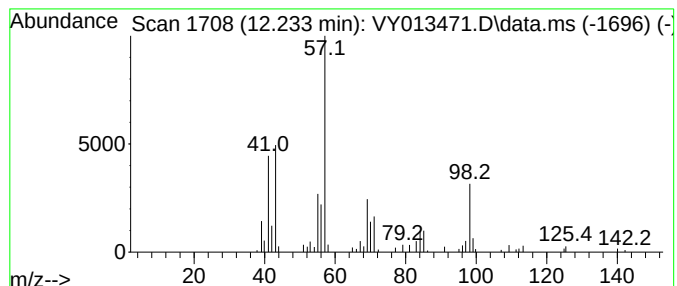
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane, 3-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.233	6.48 ug/l	92665	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	87
2			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	76
3			Hexanal, 3,5,5-trimethyl-	142	C9H18O	005435-64-3	58
4			Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	53
5			Hexane, 3-ethyl-2,5-dimethyl-	142	C10H22	052897-04-8	53



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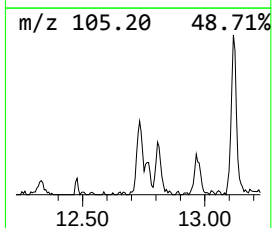
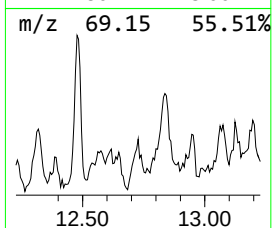
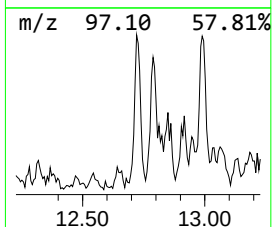
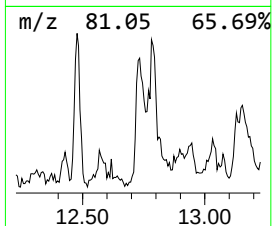
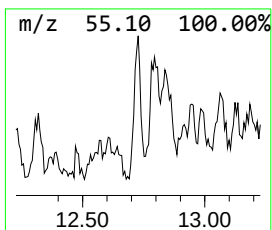
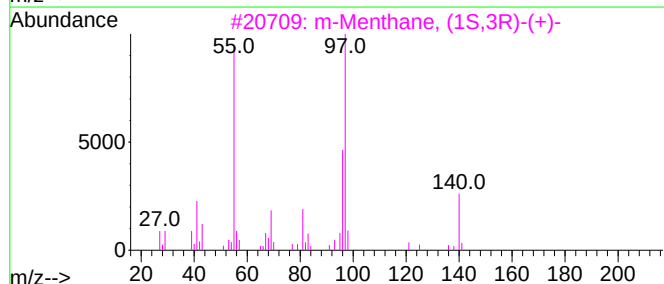
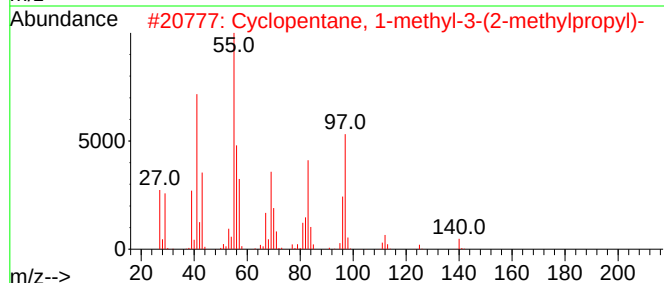
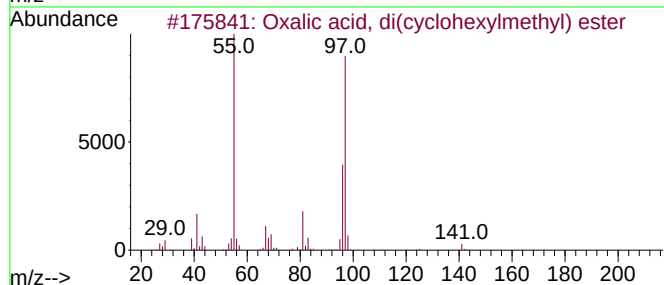
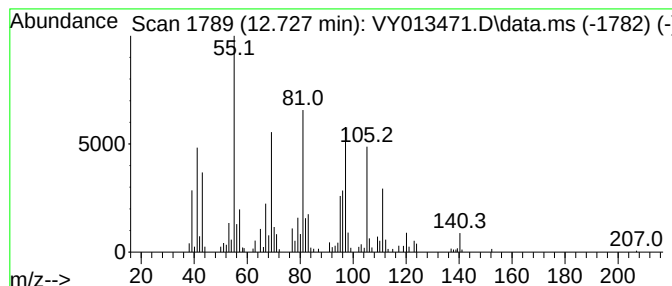
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Oxalic acid, di(cyclohexylm... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.727	8.70 ug/l	112268	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, di(cyclohexylmethyl... 282	C16H26O4	1000309-68-5	50	
2			Cyclopentane, 1-methyl-3-(2-meth... 140	C10H20	029053-04-1	49	
3			m-Menthane, (1S,3R)-(+)- 140	C10H20	013837-66-6	43	
4			m-Menthane, (1S,3S)-(+)- 140	C10H20	013837-67-7	43	
5			Cyclohexane, 1-methyl-4-(1-methy... 140	C10H20	006069-98-3	38	



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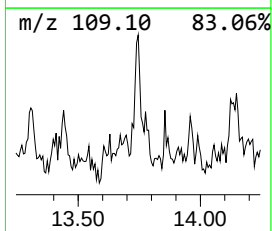
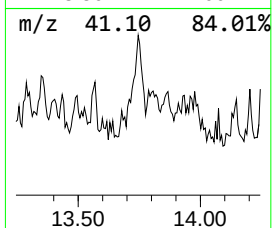
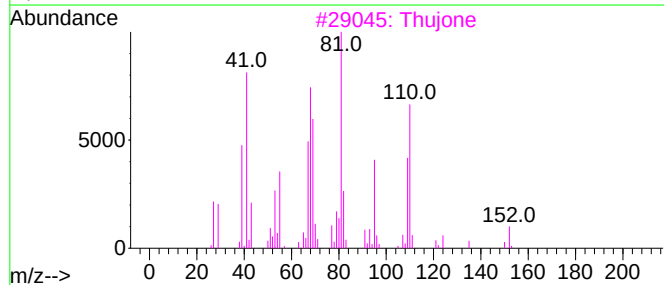
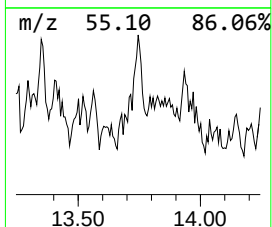
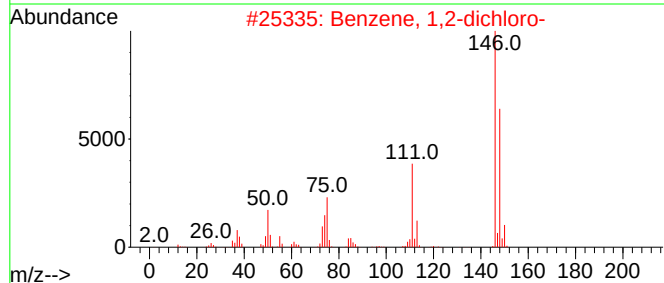
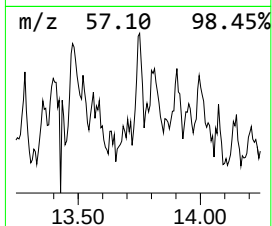
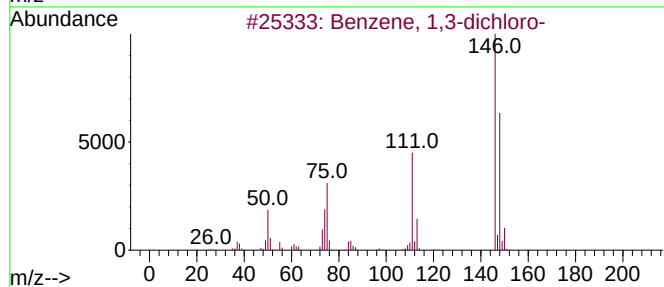
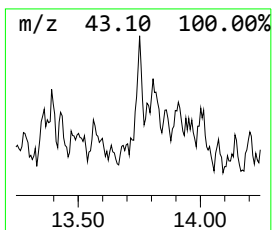
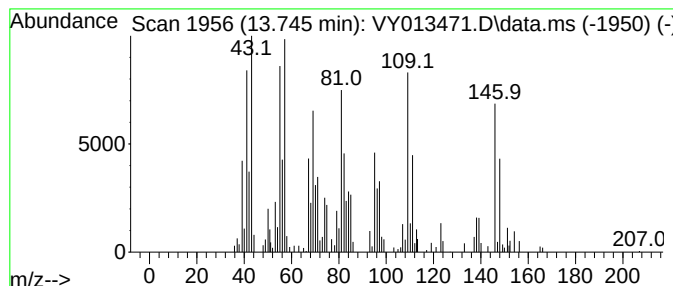
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown13.745 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	5.78 ug/l	74578	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dichloro-	146	C6H4Cl2	000541-73-1	35
2			Benzene, 1,2-dichloro-	146	C6H4Cl2	000095-50-1	25
3			Thujone	152	C10H16O	000546-80-5	20
4			Cyclohexene, 1-butyl-	138	C10H18	003282-53-9	18
5			Benzene, 1,4-dichloro-	146	C6H4Cl2	000106-46-7	18



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Heptane, 3-ethy...	12.233	6.5	ug/l	92665	3	11.490	715459	50.0
Oxalic acid, di...	12.727	8.7	ug/l	112268	4	13.422	645253	50.0
unknown13.745	13.745	5.8	ug/l	74578	4	13.422	645253	50.0
Benzamide, 4-me...	13.965	6.0	ug/l	77198	4	13.422	645253	50.0