

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
 Data File : VX025452.D
 Acq On : 03 Dec 2021 01:19
 Operator : JC/MD
 Sample : M4917-16
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-32

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\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025452.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	45	rBV	206301	353575	65.49%	7.506%
2	3.117	324	333	343	rVB3	5573	13936	2.58%	0.296%
3	3.764	431	439	448	rVB3	3064	8224	1.52%	0.175%
4	4.306	520	528	540	rVB4	3421	9257	1.71%	0.197%
5	5.391	695	706	716	rBV2	64096	185249	34.31%	3.932%
6	5.556	723	733	752	rVB	103038	300994	55.75%	6.390%
7	5.958	789	799	809	rBV	66553	176361	32.66%	3.744%
8	6.251	837	847	858	rVB	7920	24719	4.58%	0.525%
9	6.763	921	931	942	rBV	166878	393322	72.85%	8.349%
10	7.373	1020	1031	1042	rBV6	3519	9569	1.77%	0.203%
11	7.988	1125	1132	1138	rVB2	7755	15583	2.89%	0.331%
12	8.110	1145	1152	1161	rBV2	11197	26364	4.88%	0.560%
13	8.653	1222	1241	1248	rBV	334300	539932	100.00%	11.462%
14	8.958	1287	1291	1299	rVB	5889	10414	1.93%	0.221%
15	10.055	1465	1471	1488	rBV	349489	460475	85.28%	9.775%
16	10.195	1488	1494	1502	rVV	168864	214042	39.64%	4.544%
17	10.305	1504	1512	1519	rVB	16439	22170	4.11%	0.471%
18	10.647	1563	1568	1572	rBV	5529	7352	1.36%	0.156%
19	10.964	1616	1620	1626	rBV	14309	17661	3.27%	0.375%
20	11.079	1634	1639	1650	rBV	264402	348597	64.56%	7.400%
21	11.177	1650	1655	1661	rVB3	3921	5608	1.04%	0.119%
22	11.305	1671	1676	1683	rVB	39769	49354	9.14%	1.048%
23	11.402	1683	1692	1697	rVV	13666	23111	4.28%	0.491%
24	11.616	1722	1727	1734	rVB	31088	38898	7.20%	0.826%
25	11.756	1744	1750	1756	rBV	320499	396147	73.37%	8.409%
26	12.024	1789	1794	1801	rBV	353463	429440	79.54%	9.116%
27	12.091	1801	1805	1809	rVB	8904	11181	2.07%	0.237%
28	12.244	1824	1830	1838	rBV	124474	159357	29.51%	3.383%
29	12.317	1838	1842	1851	rVB3	12753	22352	4.14%	0.474%
30	12.415	1853	1858	1862	rVV2	7828	10579	1.96%	0.225%
31	12.463	1862	1866	1872	rVB	9791	12299	2.28%	0.261%
32	12.530	1872	1877	1879	rBV	16377	19764	3.66%	0.420%
33	12.555	1879	1881	1886	rVV	12746	14441	2.67%	0.307%
34	12.616	1886	1891	1894	rVV	27587	33419	6.19%	0.709%
35	12.646	1894	1896	1901	rVV3	6742	8776	1.63%	0.186%
36	12.701	1901	1905	1913	rVB2	21425	32778	6.07%	0.696%

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37	12.921	1934	1941	1945	rBV	18562	24057	4.46%	0.511%
38	12.963	1945	1948	1954	rVB	31832	36579	6.77%	0.777%
39	13.170	1978	1982	1986	rVB	17499	19955	3.70%	0.424%
40	13.292	1998	2002	2007	rVB2	42707	55296	10.24%	1.174%
41	13.427	2020	2024	2029	rVB2	12181	15885	2.94%	0.337%
42	13.548	2040	2044	2046	rBV	4738	5812	1.08%	0.123%
43	13.585	2046	2050	2056	rVB3	5390	9098	1.69%	0.193%
44	13.664	2061	2063	2069	rVB3	4931	7198	1.33%	0.153%
45	13.780	2076	2082	2089	rVB	64951	84579	15.66%	1.795%
46	14.219	2148	2154	2159	rBV2	4659	7626	1.41%	0.162%
47	14.780	2242	2246	2251	rBV	13785	17396	3.22%	0.369%
48	15.115	2296	2301	2308	rBV	15698	21959	4.07%	0.466%

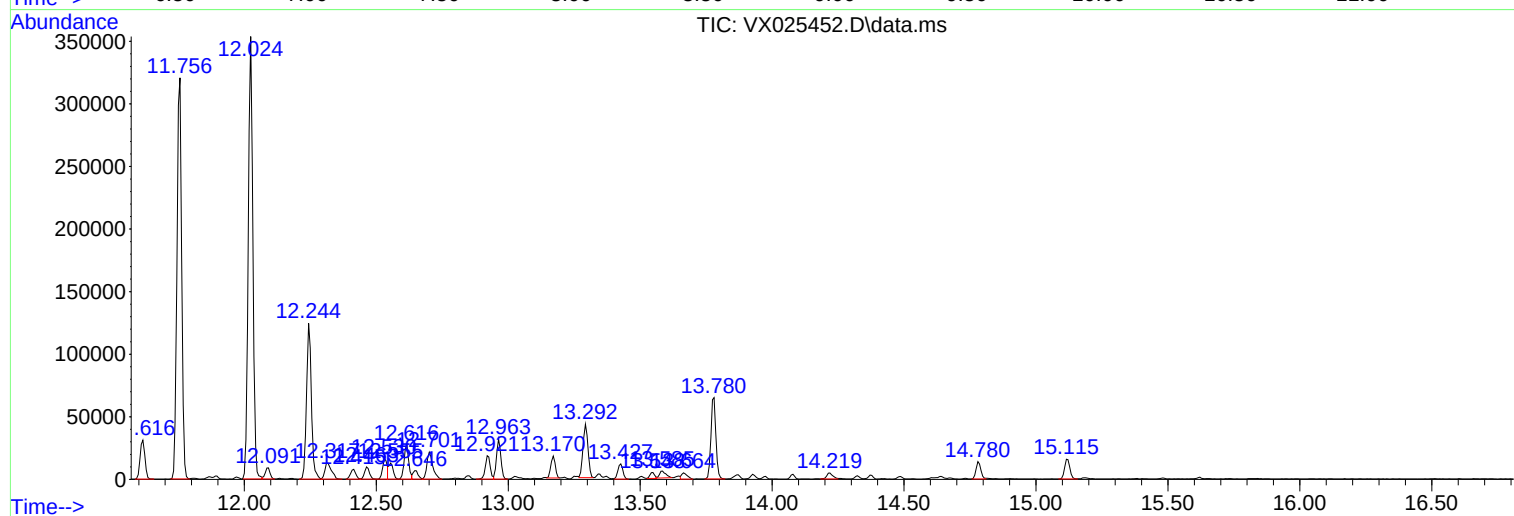
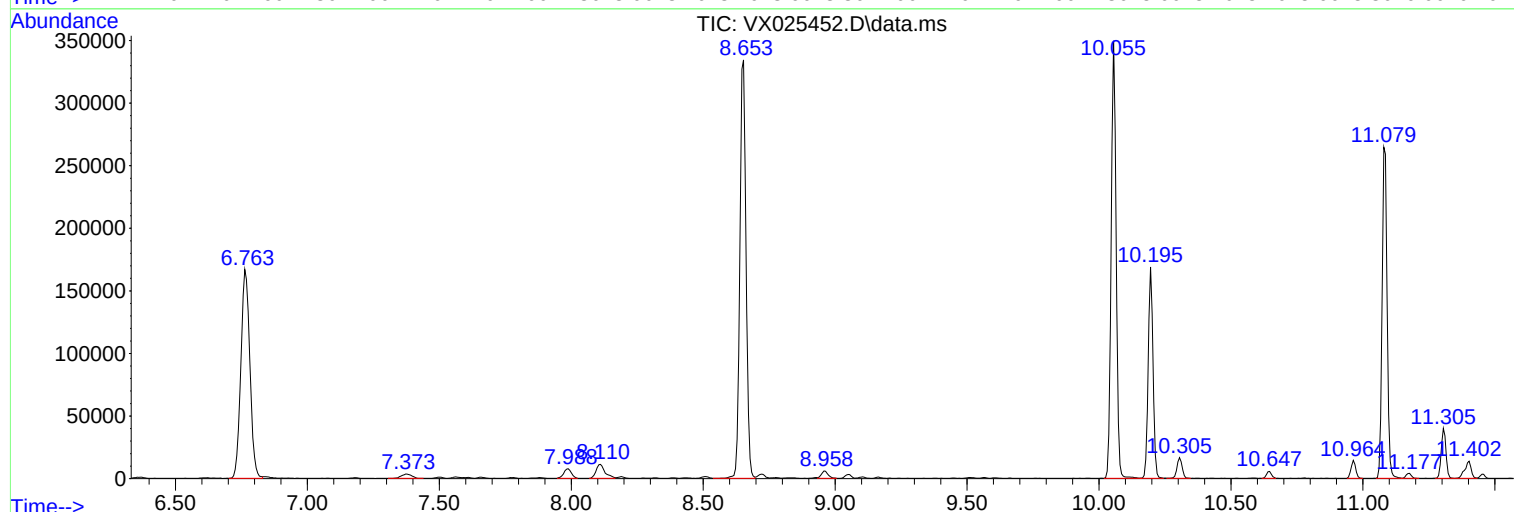
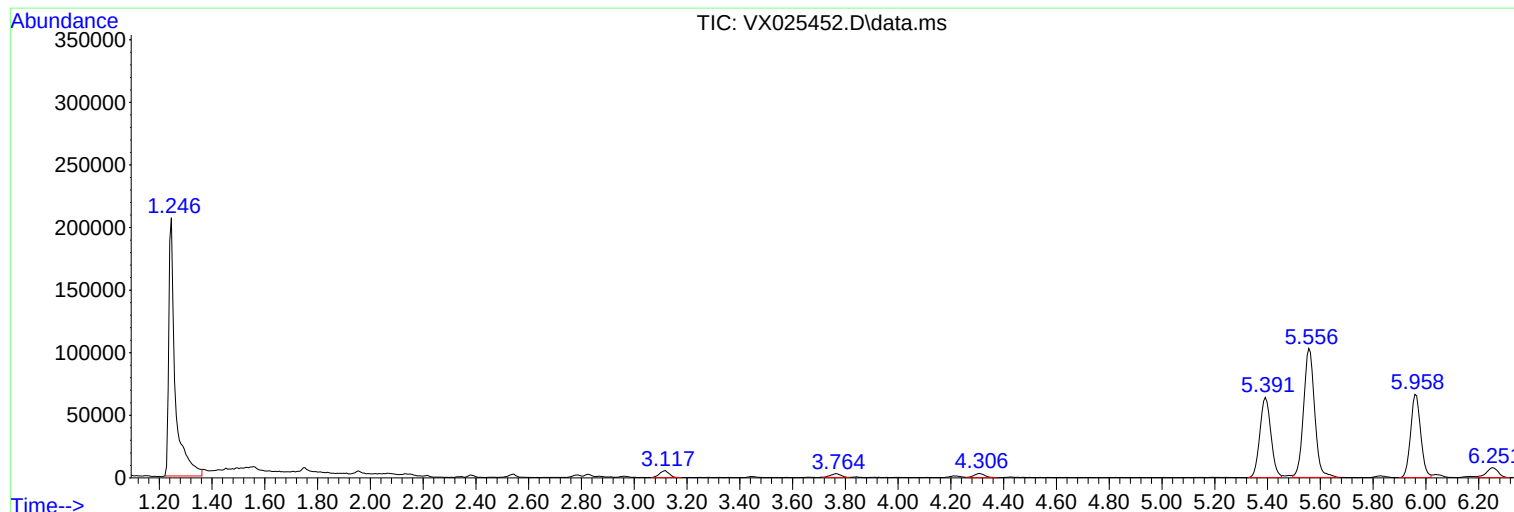
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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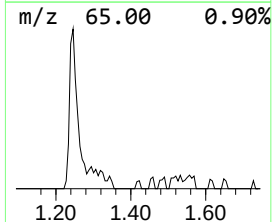
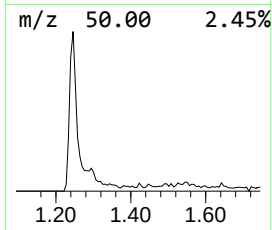
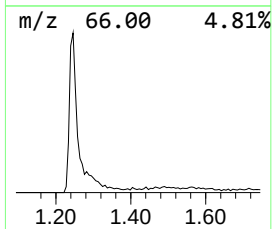
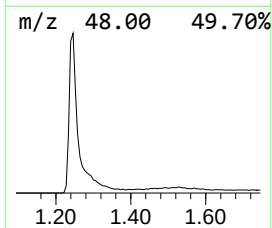
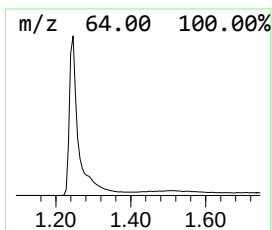
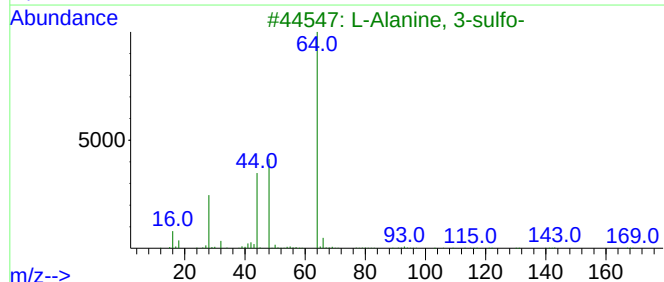
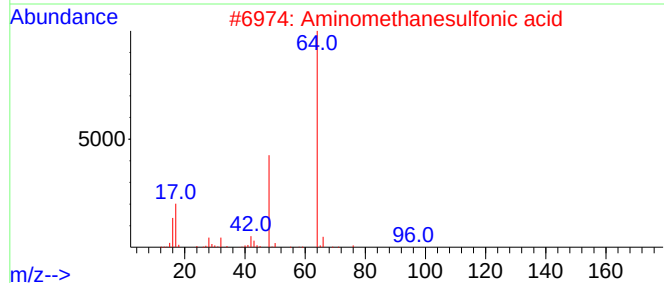
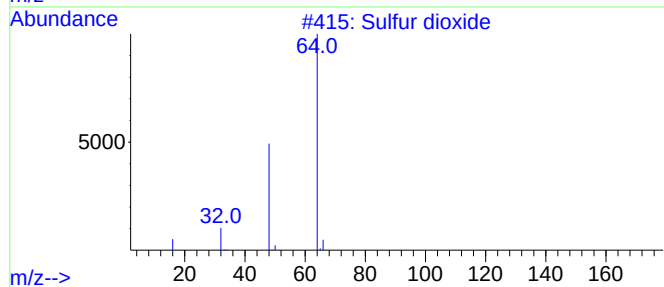
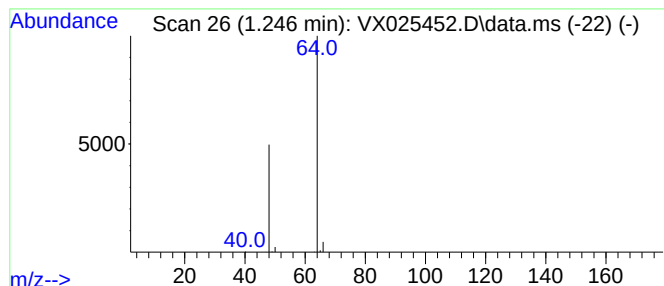
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	58.73 ug/l	353575	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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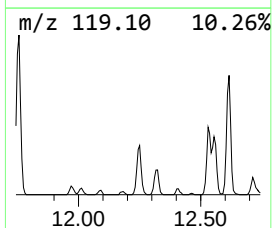
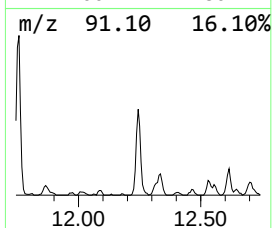
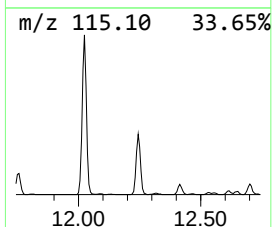
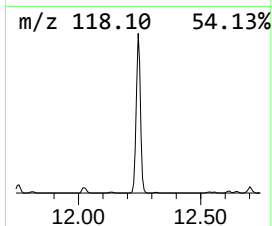
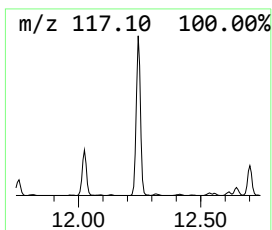
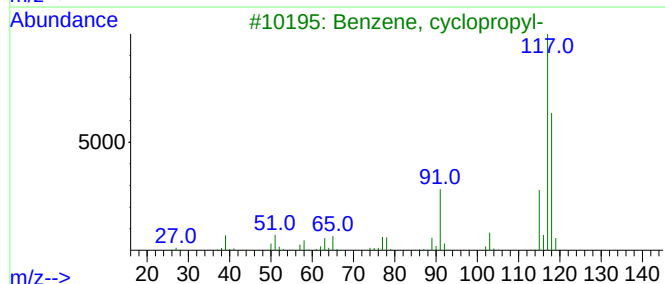
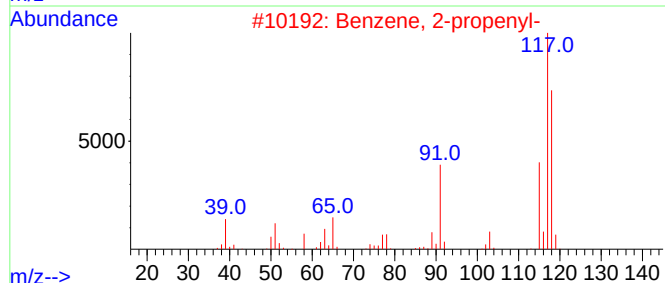
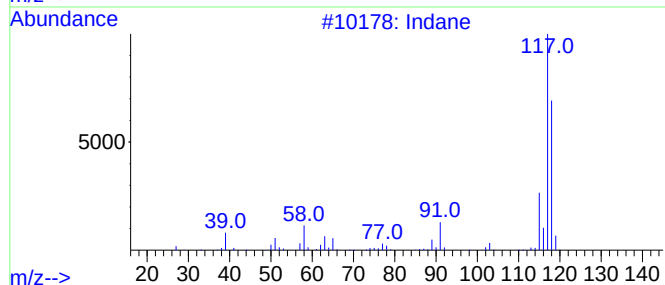
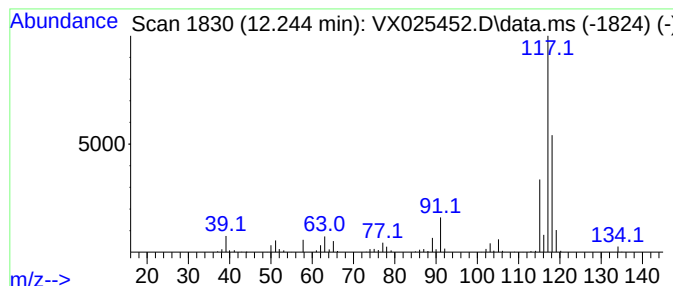
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Quant Title : SW846 8260

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

Peak Number 2 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	18.55 ug/l	159357	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	83
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
4			Deltacyclene	118	C9H10	007785-10-6	68
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64



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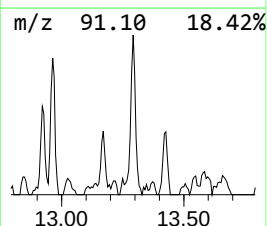
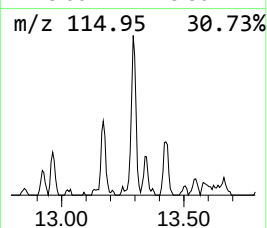
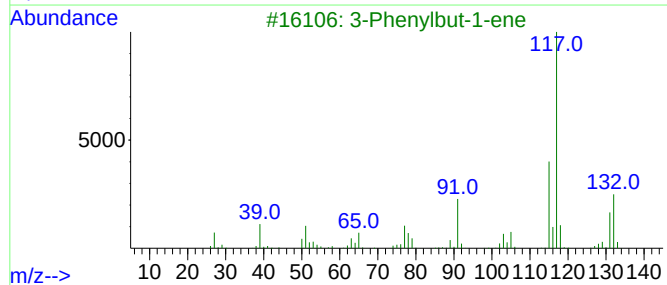
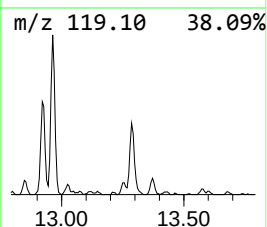
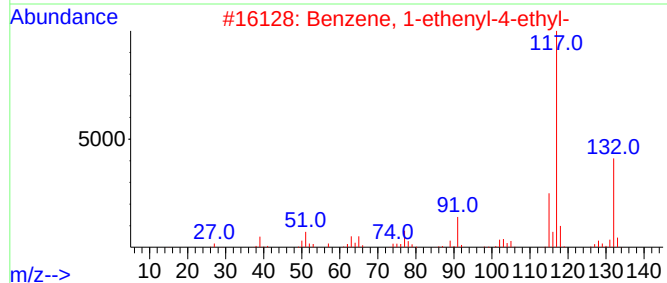
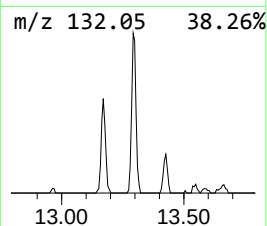
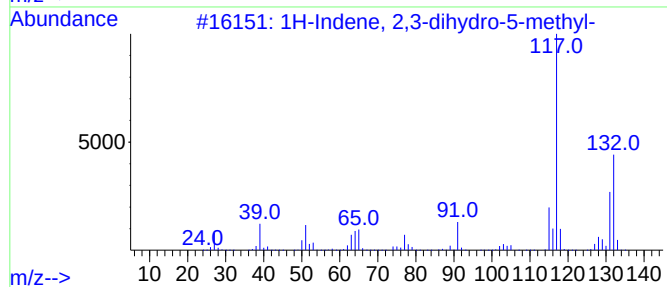
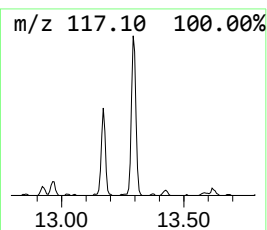
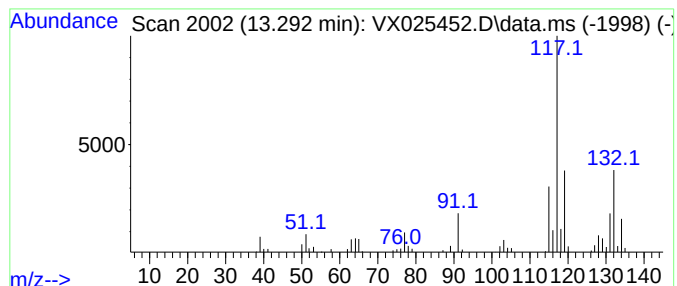
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	6.44 ug/l	55296	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	76
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	76
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70



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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
Sulfur dioxide	1.246	58.7	ug/l	353575	1	5.556	300994	50.0
Indane	12.244	18.6	ug/l	159357	4	12.024	429440	50.0
1H-Indene, 2,3-...	13.292	6.4	ug/l	55296	4	12.024	429440	50.0