

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX090623\  
 Data File : VX037550.D  
 Acq On : 06 Sep 2023 13:21  
 Operator : JC/MD  
 Sample : 04220-03 20X  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 MW7

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\82X081723W.M  
 Title : SW846 8260

Signal : TIC: VX037550.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.971	296	309	323	rBV2	105384	267003	15.18%	3.787%
2	3.117	323	333	349	rVB	764421	1758503	100.00%	24.941%
3	4.587	561	574	590	rBV	120208	401803	22.85%	5.699%
4	5.019	635	645	660	rBV2	23727	73628	4.19%	1.044%
5	5.385	694	705	723	rBV	72391	212629	12.09%	3.016%
6	5.550	723	732	749	rVB	135043	382462	21.75%	5.425%
7	5.958	789	799	806	rBV	75839	201143	11.44%	2.853%
8	6.038	806	812	825	rVB	26591	71578	4.07%	1.015%
9	6.330	853	860	873	rVB2	12916	38241	2.17%	0.542%
10	6.763	918	931	948	rBV	197551	479458	27.27%	6.800%
11	8.647	1234	1240	1249	rBV	405554	636962	36.22%	9.034%
12	9.378	1354	1360	1368	rBV	20421	30721	1.75%	0.436%
13	9.494	1368	1379	1394	rVV	68933	112255	6.38%	1.592%
14	10.055	1465	1471	1486	rBV	406529	629979	35.82%	8.935%
15	10.195	1490	1494	1501	rVV	30534	41294	2.35%	0.586%
16	10.305	1505	1512	1519	rVB2	18512	30586	1.74%	0.434%
17	10.963	1615	1620	1625	rBV	34912	42397	2.41%	0.601%
18	11.079	1634	1639	1654	rBV	320860	420609	23.92%	5.966%
19	11.305	1670	1676	1684	rBV	39967	54204	3.08%	0.769%
20	11.616	1723	1727	1734	rVB	15100	19061	1.08%	0.270%
21	11.890	1765	1772	1778	rVB3	13707	22140	1.26%	0.314%
22	12.024	1789	1794	1801	rBV	413617	523055	29.74%	7.419%
23	12.091	1801	1805	1812	rVV2	11168	20794	1.18%	0.295%
24	12.189	1815	1821	1825	rBV	15950	20389	1.16%	0.289%
25	12.244	1825	1830	1838	rVV	99101	125785	7.15%	1.784%
26	12.542	1872	1879	1887	rBV3	14678	32358	1.84%	0.459%
27	12.616	1887	1891	1894	rBV	35169	42612	2.42%	0.604%
28	12.701	1900	1905	1913	rVB2	21315	31666	1.80%	0.449%
29	12.920	1934	1941	1946	rBV2	34425	49193	2.80%	0.698%
30	13.170	1978	1982	1991	rVB	25353	31576	1.80%	0.448%
31	13.292	1997	2002	2006	rBV2	69959	91766	5.22%	1.302%
32	13.512	2032	2038	2041	rBV2	12616	18327	1.04%	0.260%
33	13.774	2076	2081	2089	rBV	74679	92800	5.28%	1.316%
34	14.640	2218	2223	2231	rVB	19247	25271	1.44%	0.358%
35	14.780	2240	2246	2254	rVB	14696	18303	1.04%	0.260%

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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

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

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X081723W.M  
Title : SW846 8260

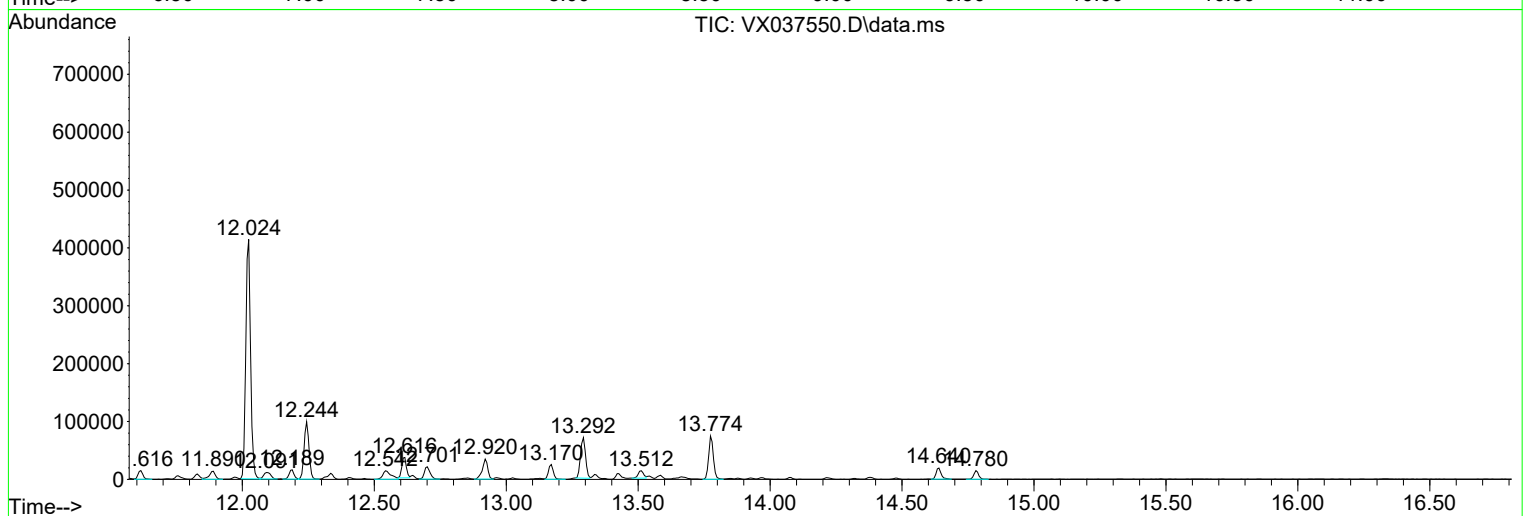
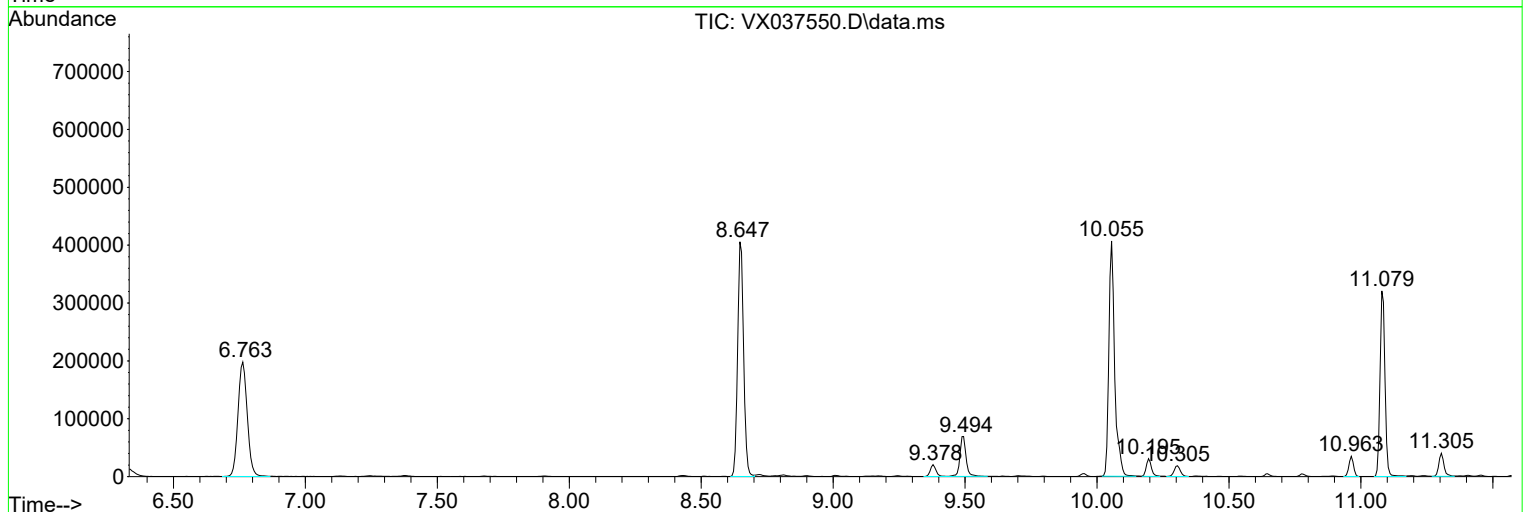
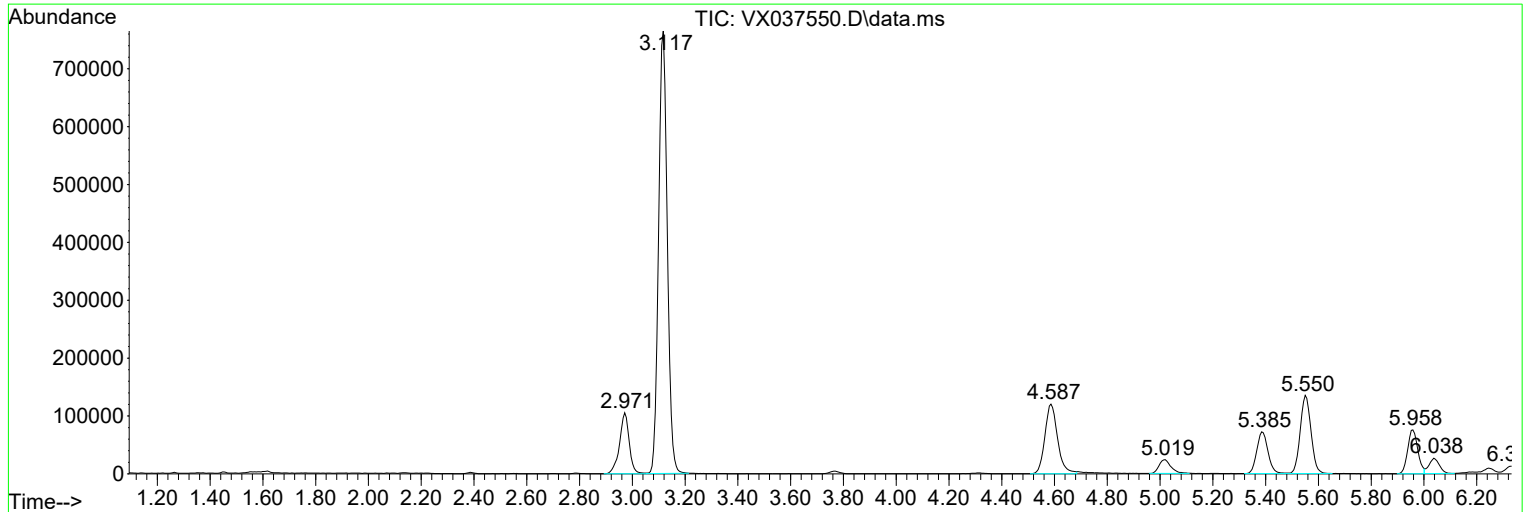
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 MSVOA\_X  
**ClientSampleId :**  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X081723W.M  
 Quant Title : SW846 8260

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



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Instrument :  
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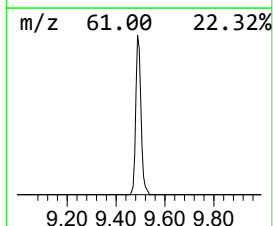
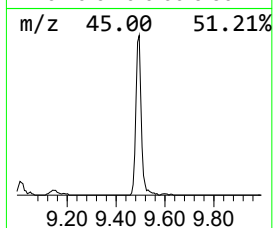
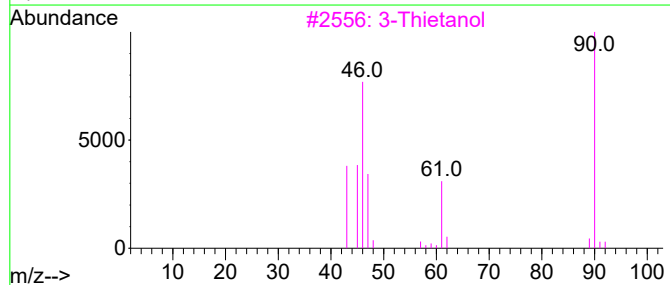
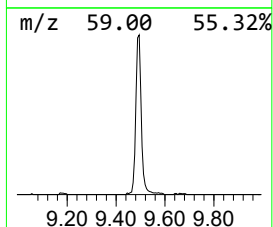
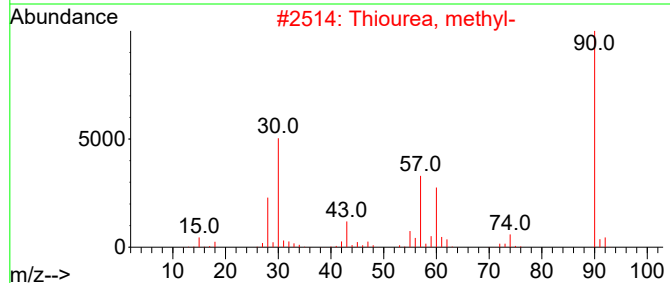
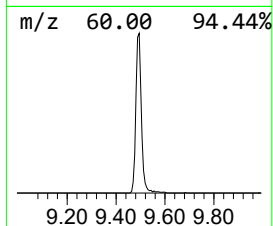
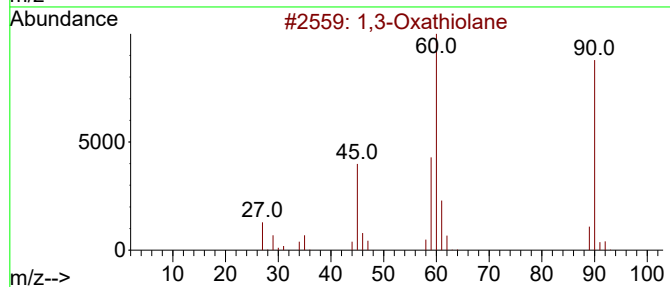
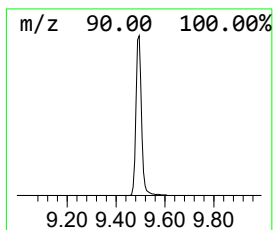
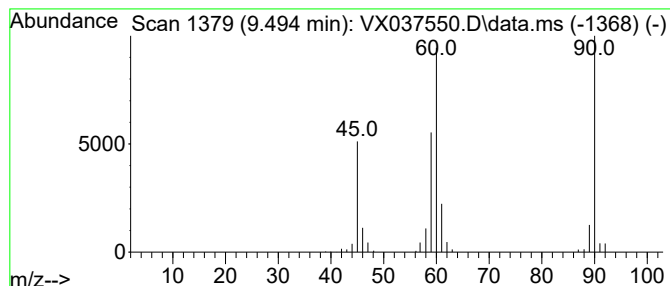
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X081723W.M  
 Quant Title : SW846 8260

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

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 Peak Number 2 1,3-Oxathiolane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.494	8.91 ug/l	112255	Chlorobenzene-d5	10.055

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Oxathiolane	90	C3H6OS	002094-97-5	94
2		Thiourea, methyl-	90	C2H6N2S	000598-52-7	50
3		3-Thietanol	90	C3H6OS	010304-16-2	40
4		Hydrazinecarboxylic acid, methyl...	90	C2H6N2O2	006294-89-9	38
5		Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	36



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Instrument :  
 MSVOA\_X  
 ClientSampleId :  
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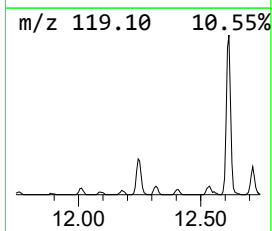
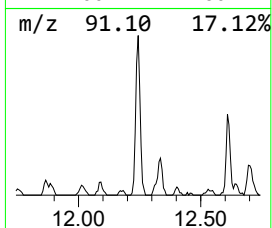
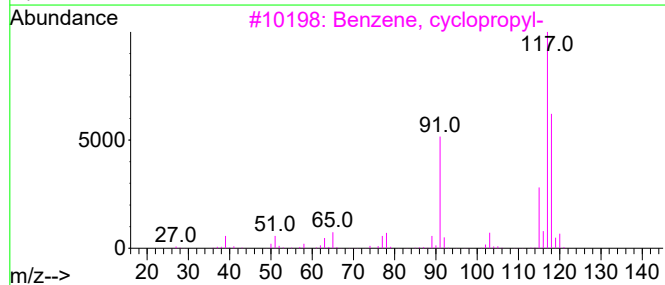
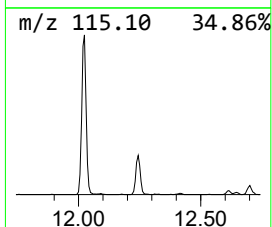
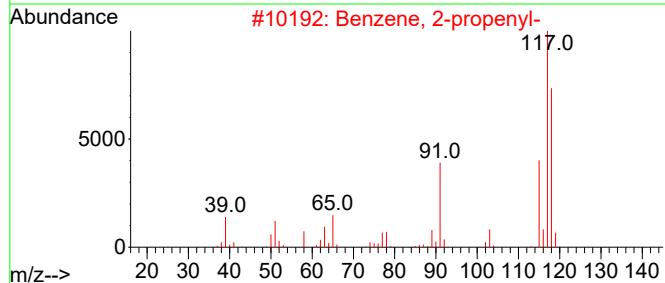
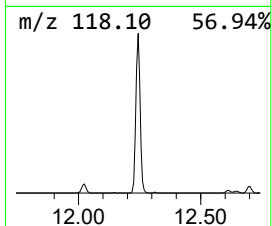
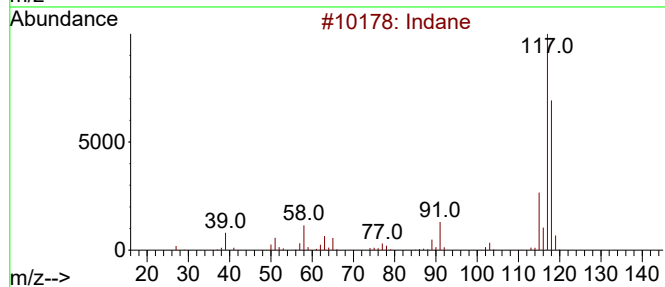
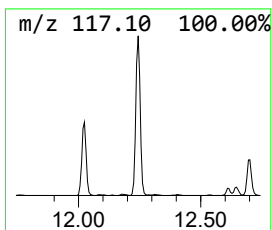
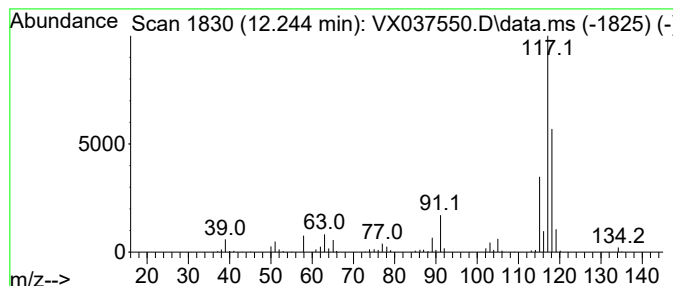
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 Peak Number 3 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	12.02 ug/l	125785	1,4-Dichlorobenzene-d4	12.024

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indane	118	C9H10	000496-11-7	87
2		Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3		Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
4		Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64
5		Deltacyclene	118	C9H10	007785-10-6	53



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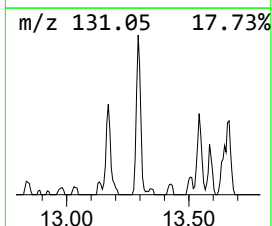
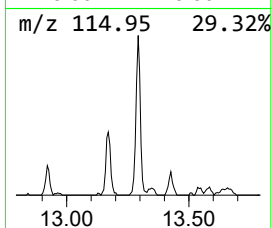
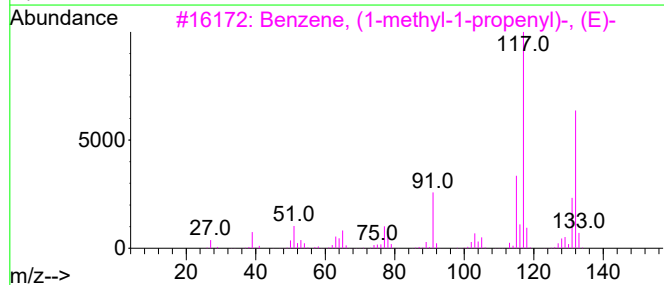
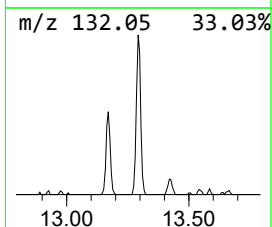
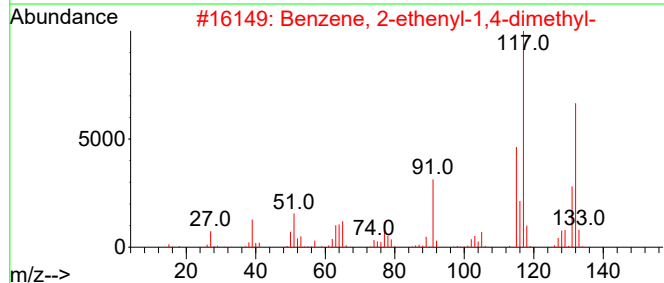
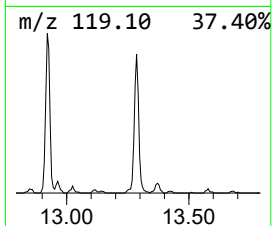
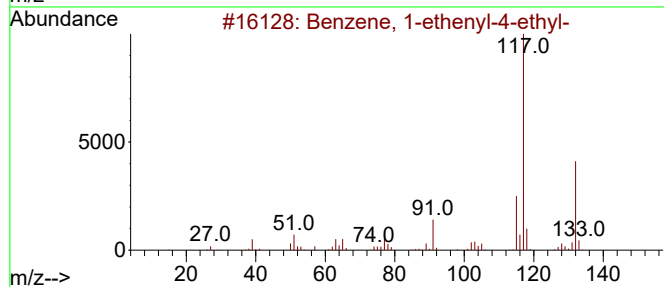
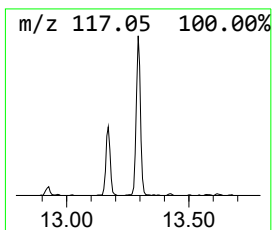
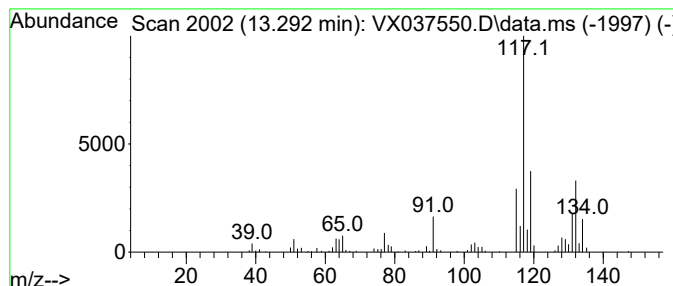
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X081723W.M  
 Quant Title : SW846 8260

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

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 Peak Number 4 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	8.77 ug/l	91766	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	81
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	76



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Oxathiolane	9.494	8.9	ug/l	112255	3	10.055	629979	50.0
Indane	12.244	12.0	ug/l	125785	4	12.024	523055	50.0
Benzene, 1-ethe...	13.292	8.8	ug/l	91766	4	12.024	523055	50.0