

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092922\
 Data File : VX031772.D
 Acq On : 29 Sep 2022 14:46
 Operator : JC/MD
 Sample : N4860-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-03

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\82X092622W.M
 Title : SW846 8260

Signal : TIC: VX031772.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	23	28	42	rBV	16547	44520	8.58%	1.329%
2	5.391	693	706	721	rBV2	66557	195372	37.66%	5.833%
3	5.550	721	732	749	rVB	74279	208955	40.28%	6.239%
4	5.958	788	799	812	rBV	69211	186895	36.03%	5.580%
5	6.763	920	931	951	rBV	104154	247108	47.63%	7.378%
6	8.647	1234	1240	1252	rBV	327915	518788	100.00%	15.489%
7	10.055	1465	1471	1478	rBV	261307	349648	67.40%	10.439%
8	11.079	1634	1639	1653	rBV	286512	365975	70.54%	10.927%
9	11.890	1768	1772	1776	rVB2	4831	6727	1.30%	0.201%
10	12.024	1788	1794	1803	rBV	376779	479619	92.45%	14.320%
11	12.177	1813	1819	1823	rBV	13751	18181	3.50%	0.543%
12	12.244	1823	1830	1835	rVV2	24535	34412	6.63%	1.027%
13	12.317	1838	1842	1848	rVB2	8246	13207	2.55%	0.394%
14	12.646	1886	1896	1901	rBV3	10953	22921	4.42%	0.684%
15	12.701	1901	1905	1910	rVV	13831	19235	3.71%	0.574%
16	12.762	1912	1915	1919	rVB3	5883	6985	1.35%	0.209%
17	12.841	1919	1928	1933	rBV	19848	30110	5.80%	0.899%
18	13.030	1955	1959	1965	rBV	14204	18353	3.54%	0.548%
19	13.146	1967	1978	1979	rBV4	14922	34393	6.63%	1.027%
20	13.195	1979	1986	1991	rVB5	21272	53691	10.35%	1.603%
21	13.292	1998	2002	2005	rBV5	5858	6952	1.34%	0.208%
22	13.347	2007	2011	2015	rBV3	7913	11136	2.15%	0.332%
23	13.622	2052	2056	2057	rBV	16856	20990	4.05%	0.627%
24	13.664	2057	2063	2073	rVB	84048	142579	27.48%	4.257%
25	13.750	2073	2077	2080	rBV	6717	9415	1.81%	0.281%
26	13.792	2080	2084	2090	rVB6	5310	11931	2.30%	0.356%
27	13.853	2090	2094	2098	rVB6	7090	10549	2.03%	0.315%
28	13.926	2098	2106	2111	rBV	26593	39767	7.67%	1.187%
29	13.975	2111	2114	2117	rBV2	4835	7013	1.35%	0.209%
30	14.097	2126	2134	2142	rBV2	7826	24484	4.72%	0.731%
31	14.207	2148	2152	2159	rVV7	6743	19212	3.70%	0.574%
32	14.286	2163	2165	2168	rVV3	6777	8097	1.56%	0.242%
33	14.323	2168	2171	2174	rVV5	4860	5514	1.06%	0.165%
34	14.378	2176	2180	2184	rVB2	10672	15217	2.93%	0.454%
35	14.487	2192	2198	2201	rBV2	10703	16627	3.20%	0.496%
36	14.524	2201	2204	2210	rVB8	2939	5289	1.02%	0.158%

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37	14.634	2216	2222	2225	rBV5	12832	23517	4.53%	0.702%
38	14.670	2227	2228	2234	rVB2	11020	12961	2.50%	0.387%
39	14.792	2241	2248	2251	rBV	12380	21720	4.19%	0.648%
40	14.914	2262	2268	2274	rVB8	9450	22001	4.24%	0.657%
41	15.182	2307	2312	2314	rBV5	6244	9227	1.78%	0.275%
42	15.262	2319	2325	2330	rVB5	6034	11197	2.16%	0.334%
43	15.396	2338	2347	2356	rVB8	8618	25553	4.93%	0.763%
44	15.597	2376	2380	2386	rVB8	3798	7670	1.48%	0.229%
45	15.658	2386	2390	2396	rVB7	2965	5651	1.09%	0.169%

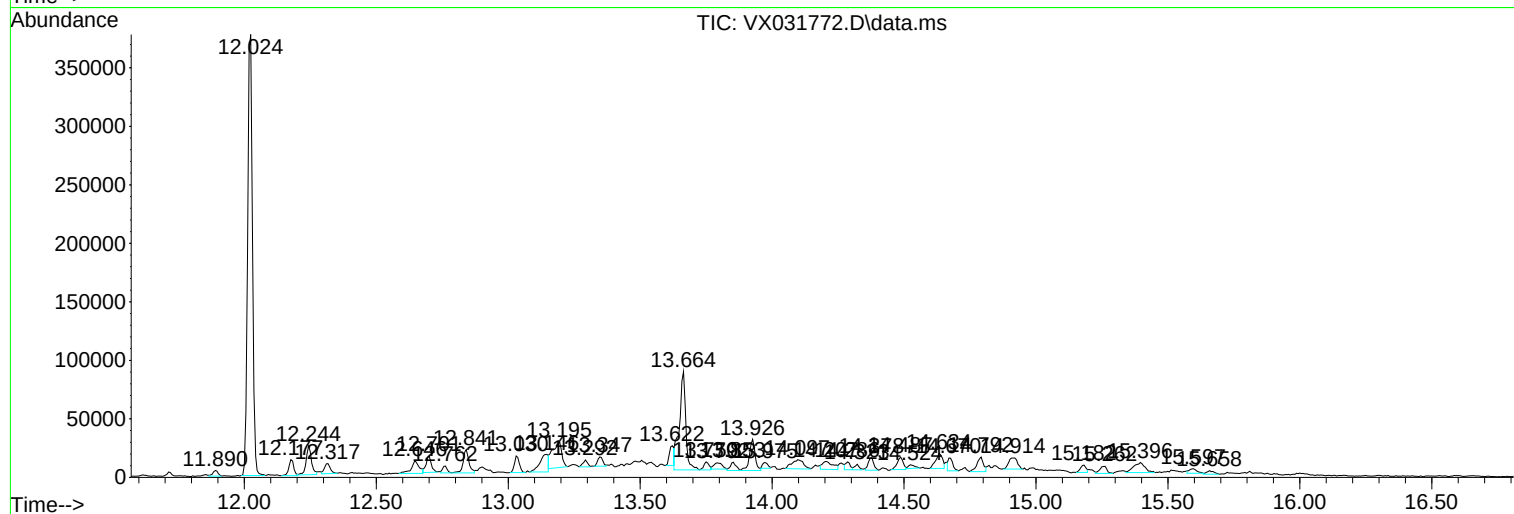
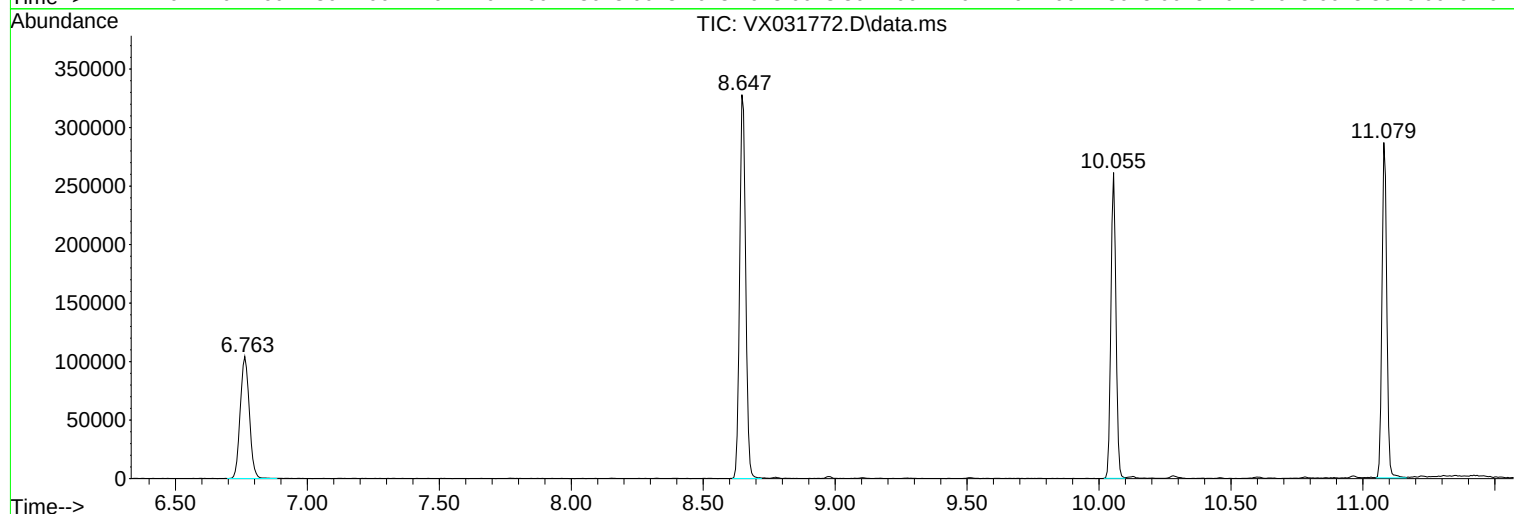
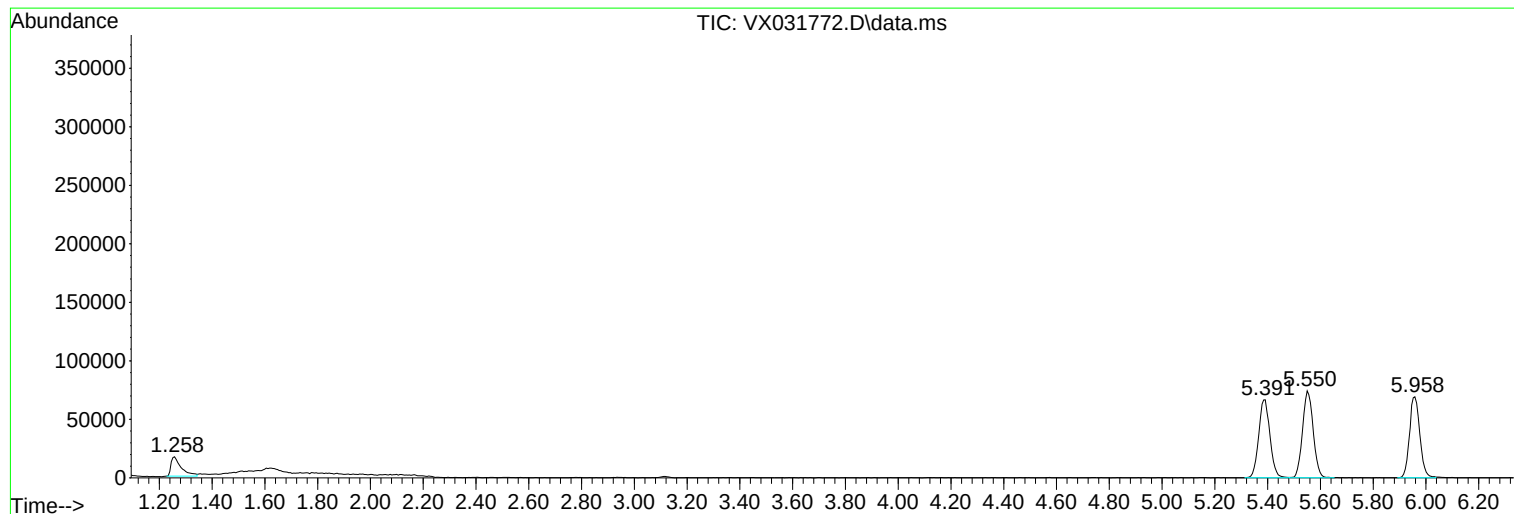
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092622W.M
Quant Title : SW846 8260

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



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Instrument :
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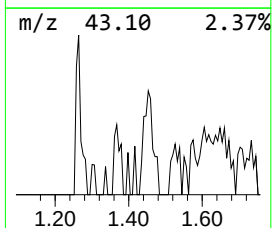
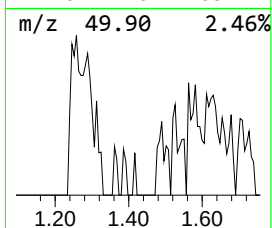
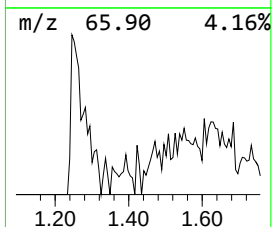
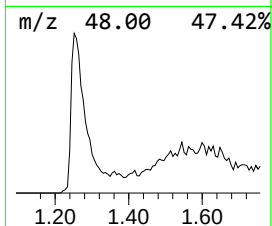
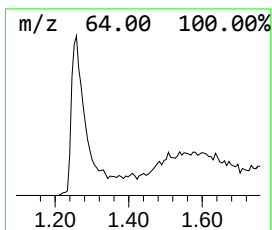
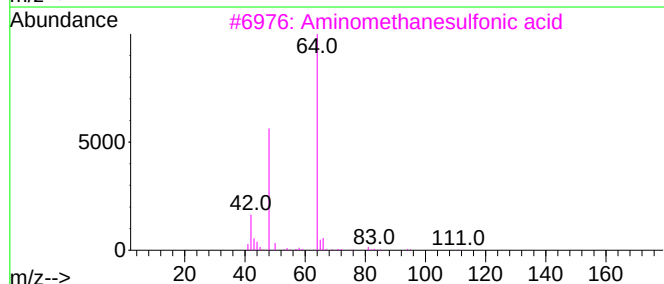
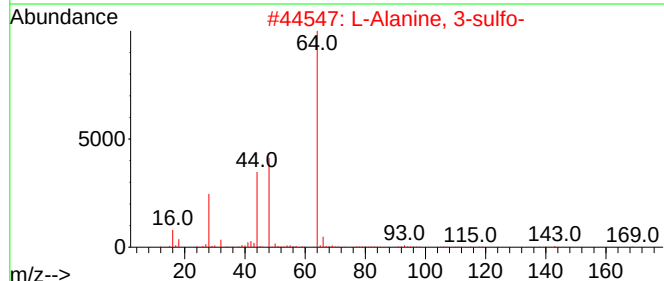
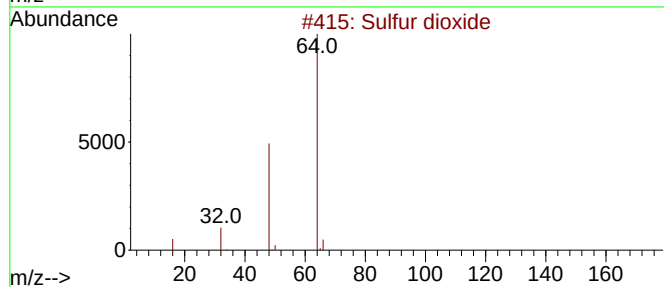
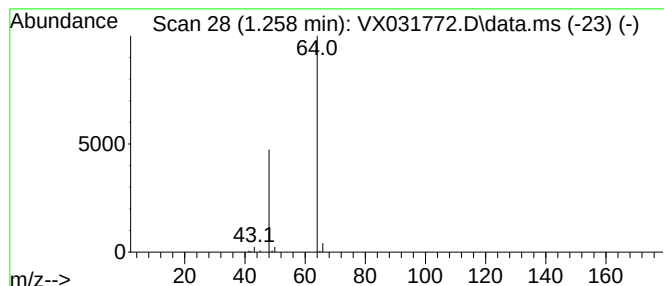
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092622W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	10.65 ug/l	44520	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	4



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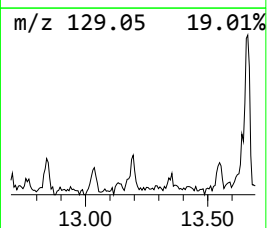
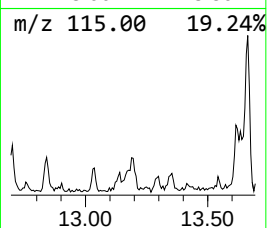
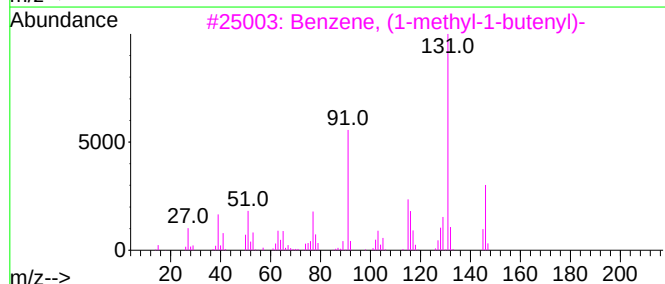
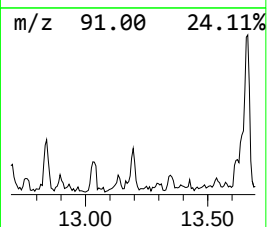
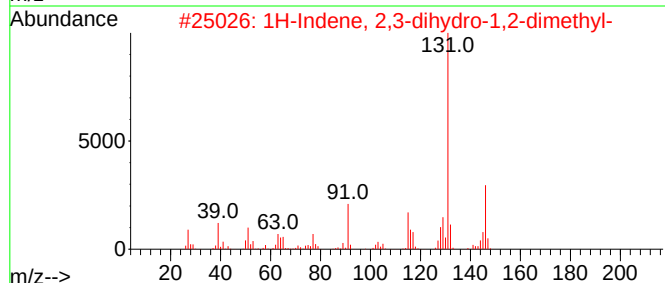
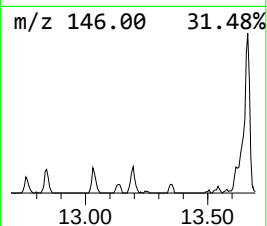
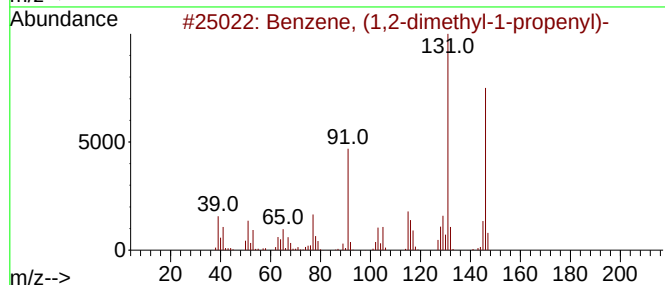
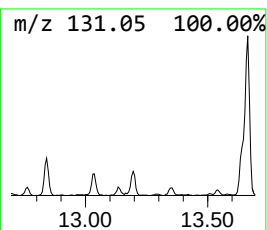
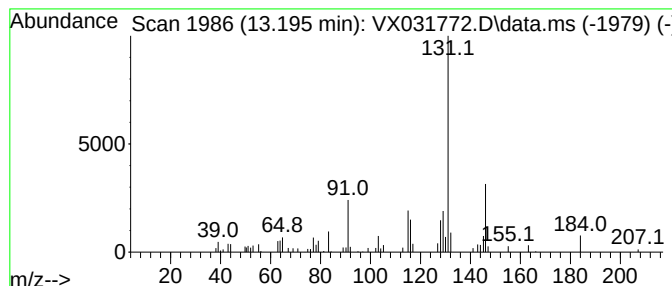
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Quant Title : SW846 8260

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

Peak Number 2 Benzene, (1,2-dimethyl-1-propenyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.195	5.60 ug/l	53691	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	94
2			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	91
3			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	91
4			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	90
5			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	87



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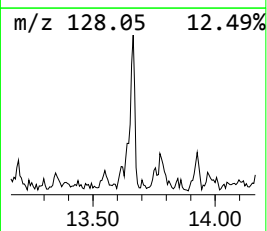
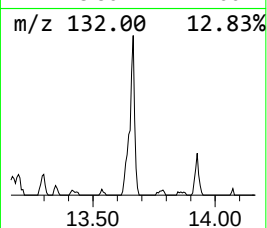
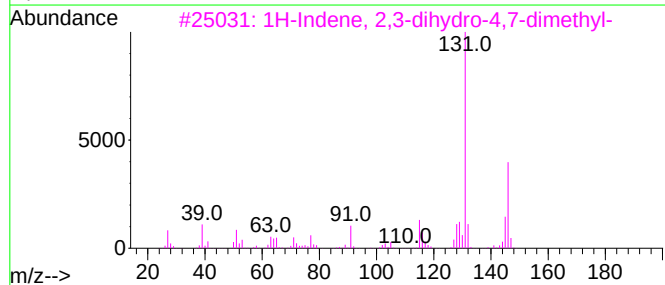
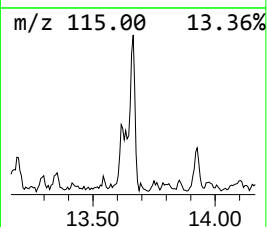
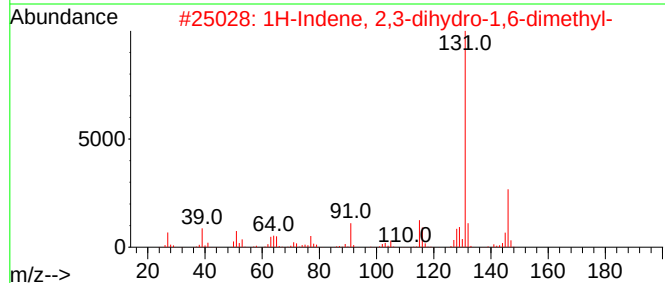
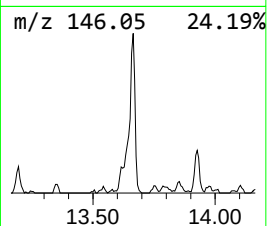
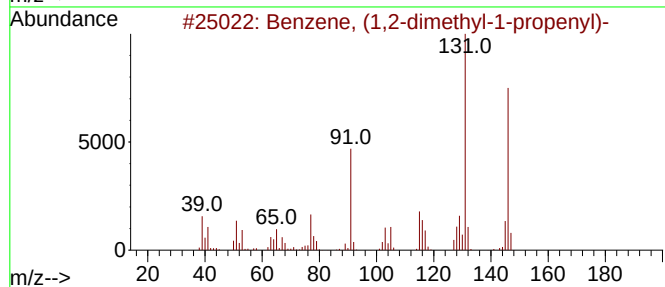
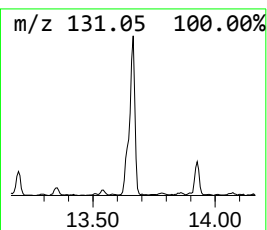
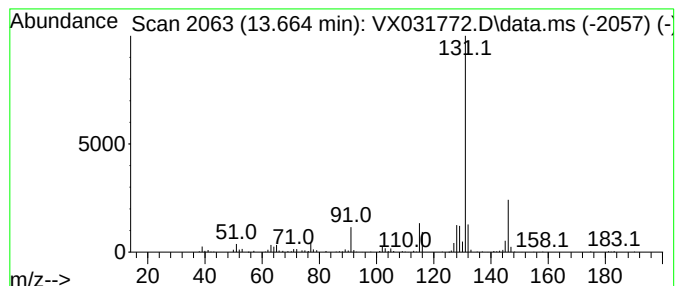
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092622W.M
Quant Title : SW846 8260

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Peak Number 3 1H-Indene, 2,3-dihydro-1,6-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.664	14.86 ug/l	142579	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	94
2			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	94
3			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	91
4			2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	91
5			1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.258	10.7	ug/l	44520	1	5.550	208955	50.0
Benzene, (1,2-d...	13.195	5.6	ug/l	53691	4	12.024	479619	50.0
1H-Indene, 2,3-...	13.664	14.9	ug/l	142579	4	12.024	479619	50.0