

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
 Data File : VX033237.D
 Acq On : 05 Dec 2022 19:41
 Operator : JC/MD
 Sample : N5875-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-38

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\82X112222W.M
 Title : SW846 8260

Signal : TIC: VX033237.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	37	47	50	rBV4	19932	50185	9.86%	1.210%
2	1.752	105	109	119	rVB2	22706	34026	6.69%	0.821%
3	1.959	139	143	150	rVB2	8048	13232	2.60%	0.319%
4	2.069	158	161	166	rVB3	3532	5321	1.05%	0.128%
5	2.215	181	185	191	rVB2	4186	6675	1.31%	0.161%
6	2.782	271	278	282	rBV4	3212	7021	1.38%	0.169%
7	3.111	324	332	342	rVB3	13133	30270	5.95%	0.730%
8	4.306	519	528	542	rVB3	5533	15523	3.05%	0.374%
9	5.025	637	646	654	rBV4	7043	22953	4.51%	0.554%
10	5.385	694	705	716	rBV	61099	178555	35.09%	4.307%
11	5.550	723	732	754	rVB2	125100	365767	71.88%	8.822%
12	5.958	789	799	808	rBV	62119	162023	31.84%	3.908%
13	6.037	808	812	824	rVB3	5529	14508	2.85%	0.350%
14	6.251	841	847	858	rVB5	2092	6372	1.25%	0.154%
15	6.763	921	931	942	rBV	186335	447891	88.02%	10.803%
16	7.373	1025	1031	1038	rVB4	2317	6353	1.25%	0.153%
17	8.647	1234	1240	1247	rBV	273773	440739	86.61%	10.630%
18	8.720	1247	1252	1259	rVB	28678	44266	8.70%	1.068%
19	10.055	1465	1471	1480	rBV	369393	508863	100.00%	12.274%
20	10.195	1489	1494	1500	rVB	41413	54405	10.69%	1.312%
21	10.299	1506	1511	1520	rVB	84649	117023	23.00%	2.823%
22	10.640	1562	1567	1577	rBV	25007	35177	6.91%	0.848%
23	10.963	1616	1620	1624	rBV	9676	11865	2.33%	0.286%
24	11.079	1634	1639	1650	rBV	249104	321298	63.14%	7.750%
25	11.305	1672	1676	1683	rBV2	15126	20428	4.01%	0.493%
26	11.378	1683	1688	1696	rVV	24164	47780	9.39%	1.152%
27	11.451	1696	1700	1709	rVB	13550	16869	3.32%	0.407%
28	11.616	1722	1727	1731	rVB	14699	18761	3.69%	0.453%
29	11.750	1745	1749	1757	rVB	46476	59255	11.64%	1.429%
30	12.024	1788	1794	1800	rBV	394346	499842	98.23%	12.056%
31	12.085	1800	1804	1811	rVB	15212	19744	3.88%	0.476%
32	12.244	1825	1830	1838	rBV3	49414	68083	13.38%	1.642%
33	12.317	1838	1842	1850	rVB4	13113	23386	4.60%	0.564%
34	12.463	1862	1866	1870	rBV3	4136	5236	1.03%	0.126%
35	12.530	1873	1877	1879	rBV	5254	6559	1.29%	0.158%
36	12.616	1885	1891	1894	rBV	15290	18902	3.71%	0.456%

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Integrator: RTE

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37	12.701	1900	1905	1912	rBV3	21392	32365	6.36%	0.781%
38	12.847	1924	1929	1934	rVB2	4633	6611	1.30%	0.159%
39	12.920	1934	1941	1945	rBV	16349	21852	4.29%	0.527%
40	12.963	1945	1948	1954	rVB	9297	11012	2.16%	0.266%
41	13.024	1954	1958	1963	rBV5	2643	5758	1.13%	0.139%
42	13.170	1978	1982	1987	rVB	8891	10307	2.03%	0.249%
43	13.292	1998	2002	2007	rVB2	27371	35552	6.99%	0.858%
44	13.420	2019	2023	2029	rVB2	8677	12399	2.44%	0.299%
45	13.579	2046	2049	2055	rVV3	6146	9580	1.88%	0.231%
46	13.676	2061	2065	2070	rVB3	5800	11396	2.24%	0.275%
47	13.774	2073	2081	2090	rBV	47839	66910	13.15%	1.614%
48	13.853	2090	2094	2100	rVB4	3441	5296	1.04%	0.128%
49	13.926	2100	2106	2110	rBV3	6966	9220	1.81%	0.222%
50	14.127	2135	2139	2143	rVV2	3801	5516	1.08%	0.133%
51	14.213	2147	2153	2163	rBV3	5440	12501	2.46%	0.302%
52	14.323	2167	2171	2175	rBV3	4002	5420	1.07%	0.131%
53	14.377	2175	2180	2185	rVB3	5706	8803	1.73%	0.212%
54	14.481	2192	2197	2202	rBV4	4453	6040	1.19%	0.146%
55	14.633	2218	2222	2234	rVB	36666	53994	10.61%	1.302%
56	14.780	2240	2246	2255	rBV	58099	75019	14.74%	1.809%
57	15.481	2355	2361	2364	rBV2	3415	5218	1.03%	0.126%
58	15.615	2373	2383	2386	rBV	9349	14454	2.84%	0.349%
59	15.652	2386	2389	2394	rVB3	5480	7566	1.49%	0.182%
60	16.328	2493	2500	2508	rBV4	4338	8060	1.58%	0.194%

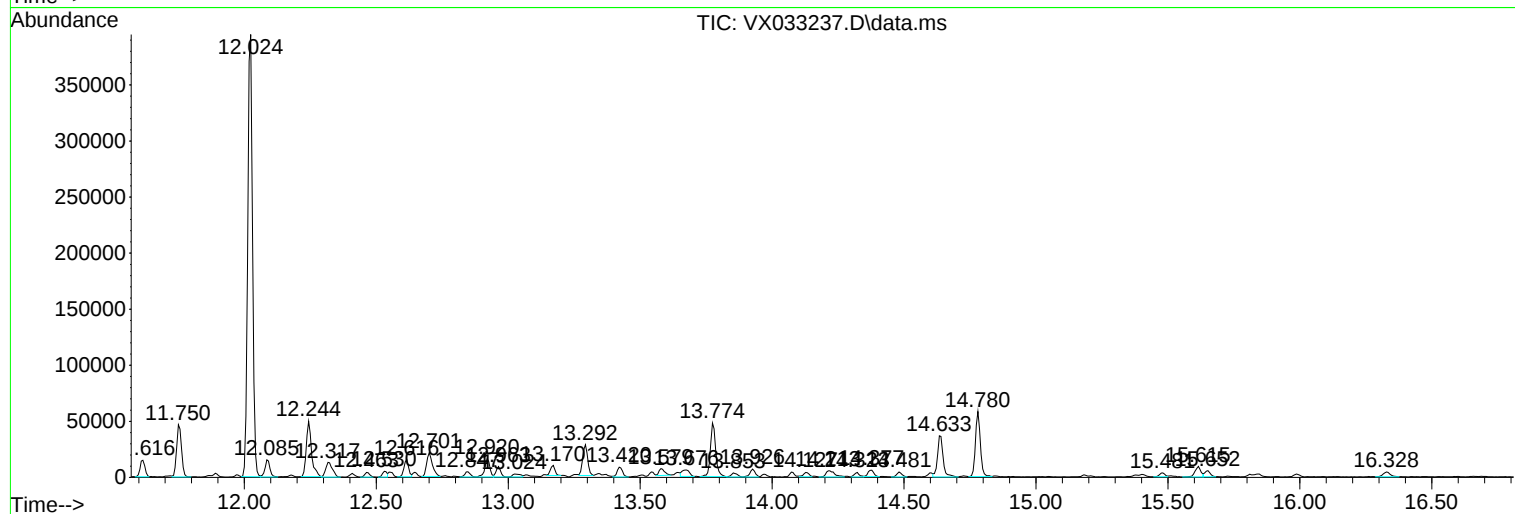
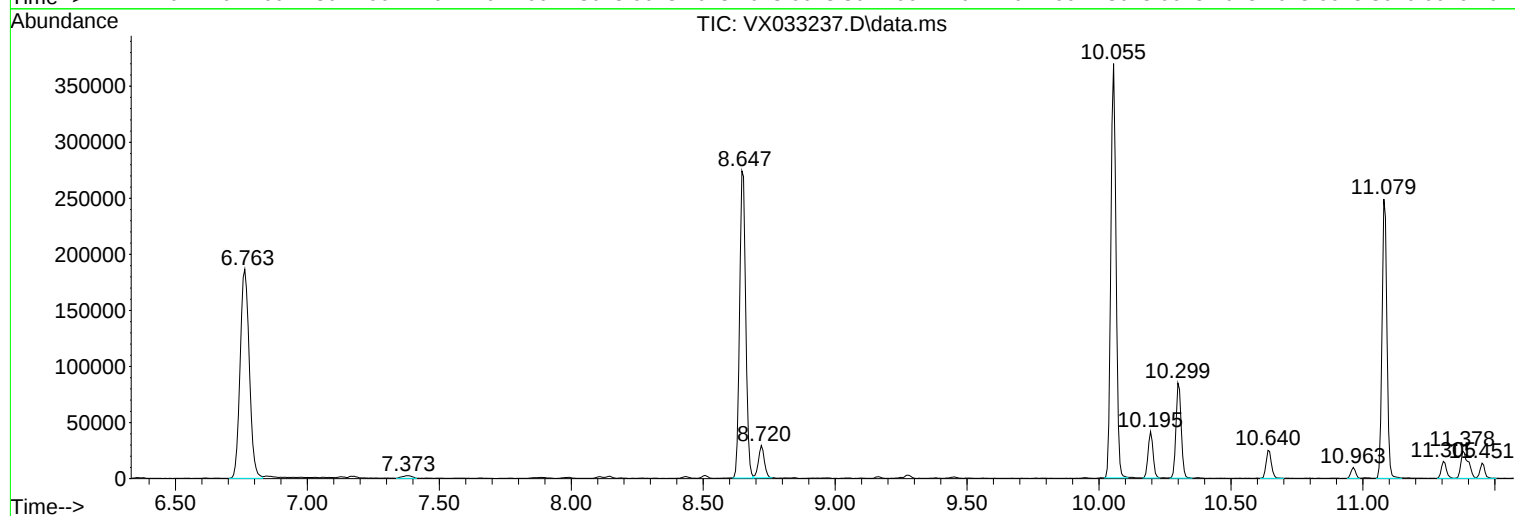
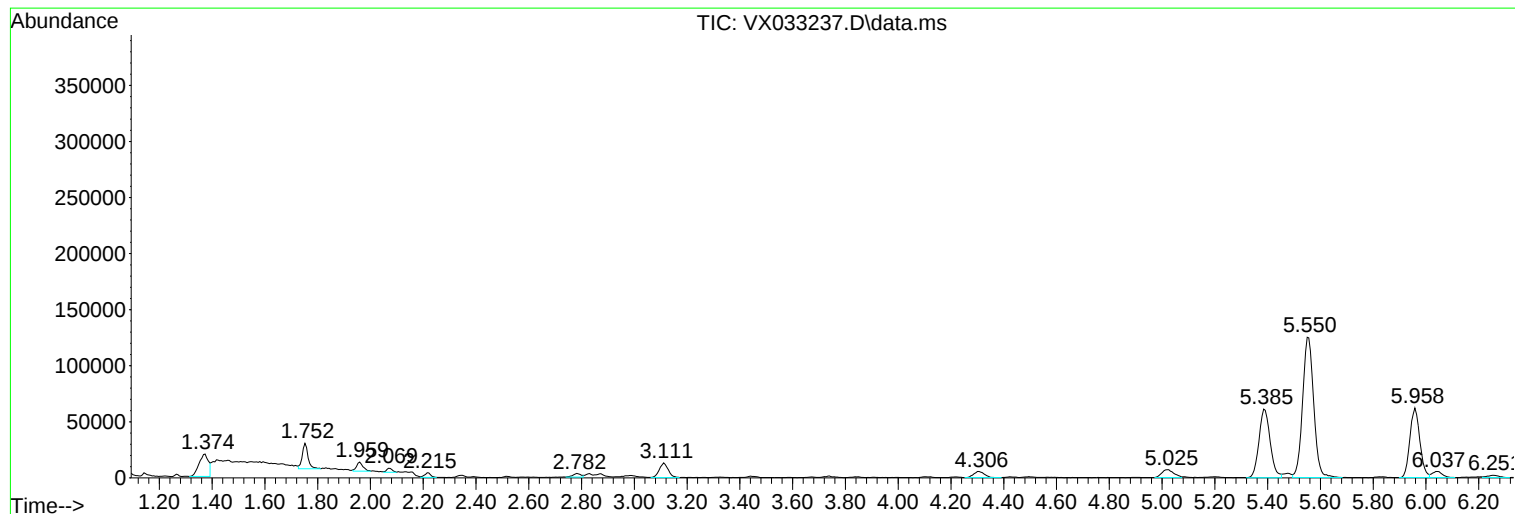
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Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
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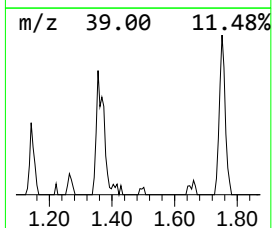
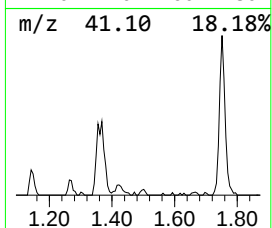
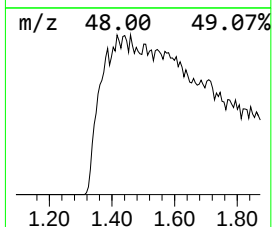
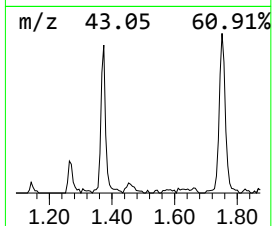
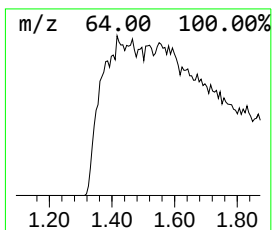
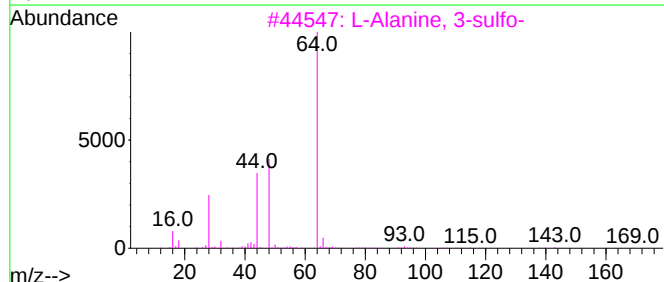
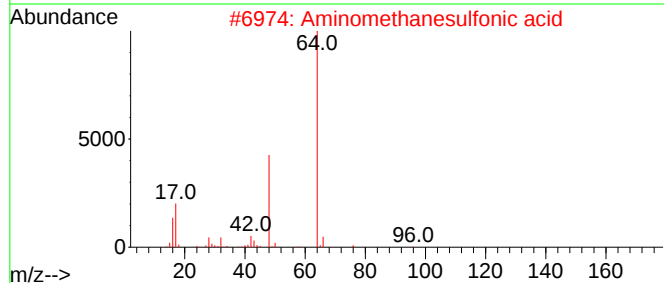
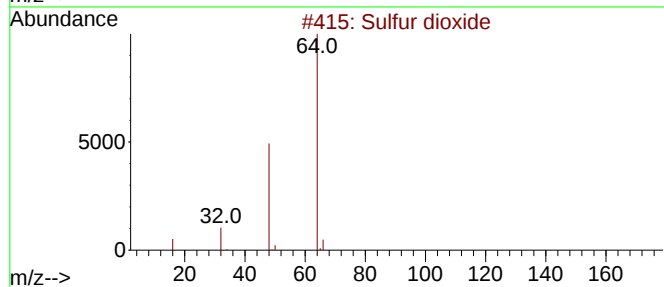
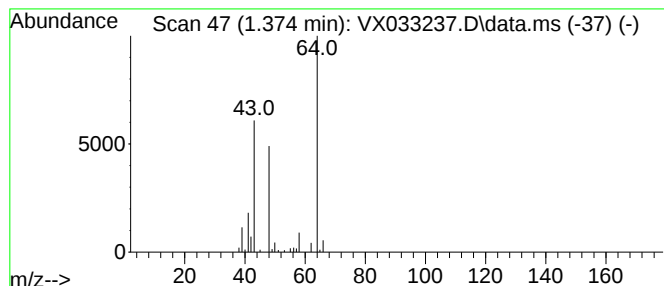
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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.
1.374	6.86 ug/l	50185	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	86
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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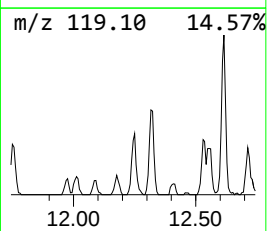
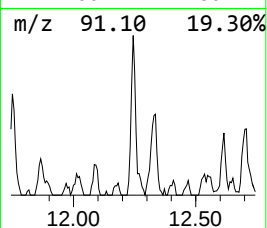
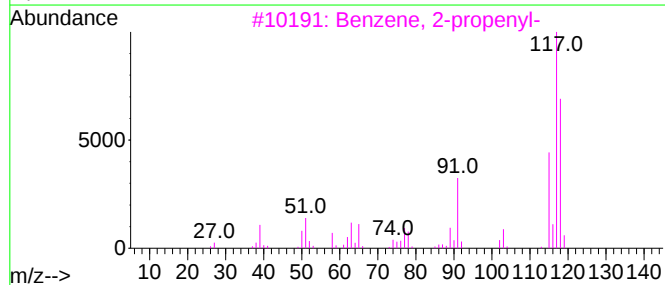
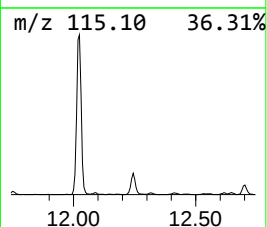
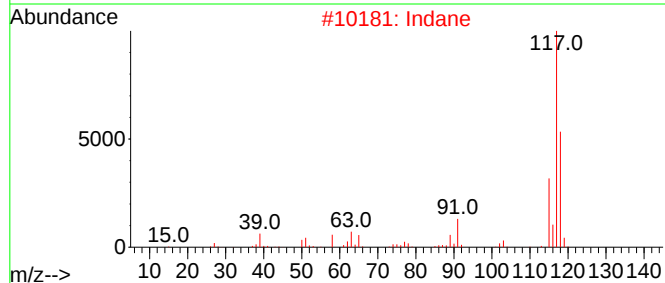
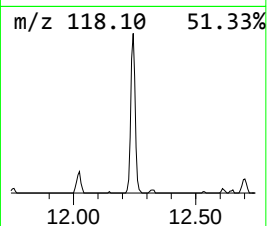
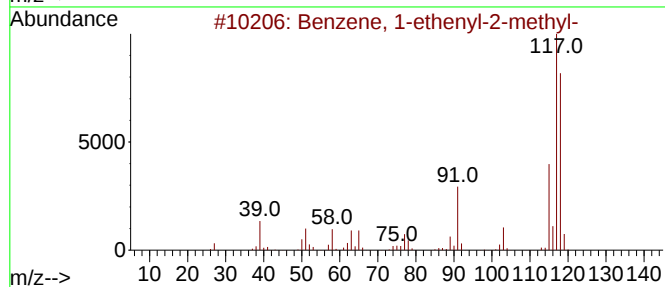
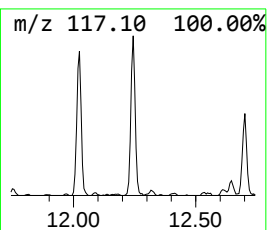
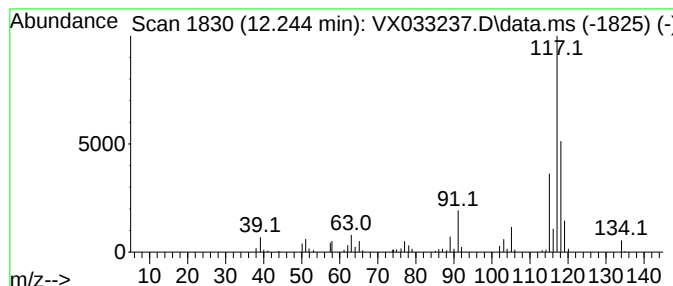
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1-ethenyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	6.81 ug/l	68083	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	87
2			Indane	118	C9H10	000496-11-7	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
5			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	70



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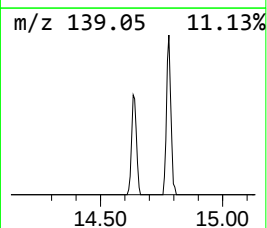
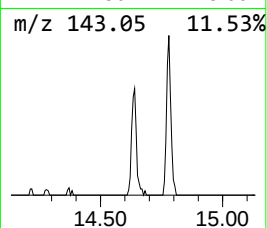
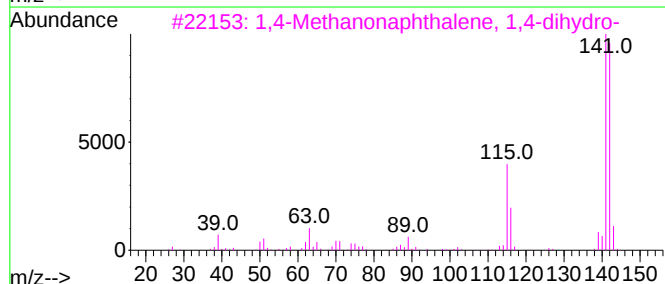
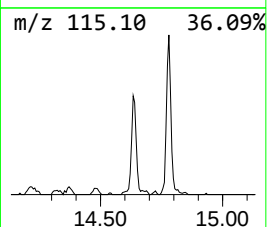
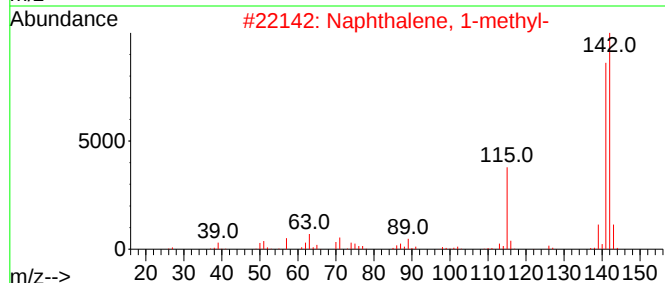
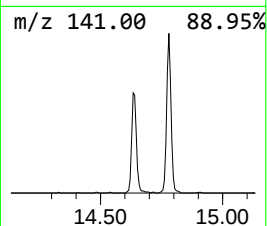
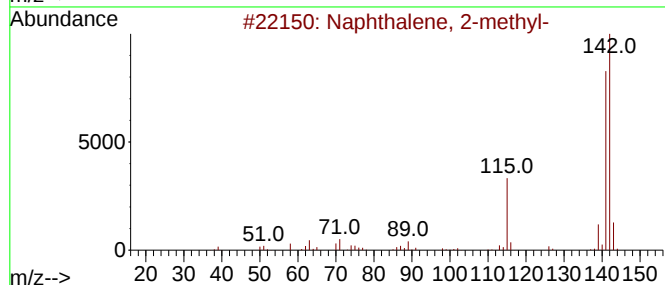
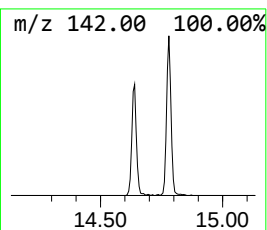
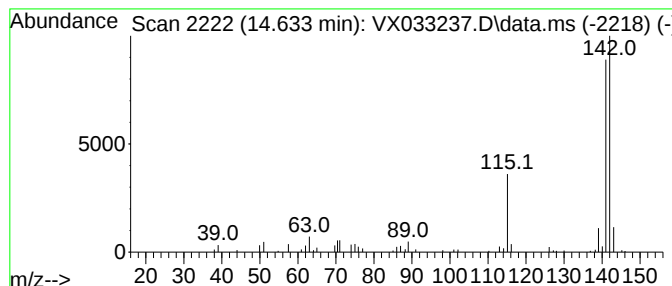
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	5.40 ug/l	53994	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4		Benzocycloheptatriene	142	C11H10	000264-09-5	91
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



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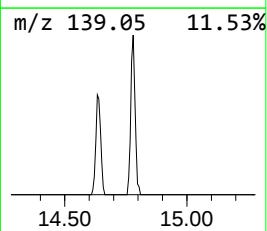
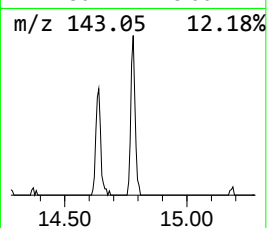
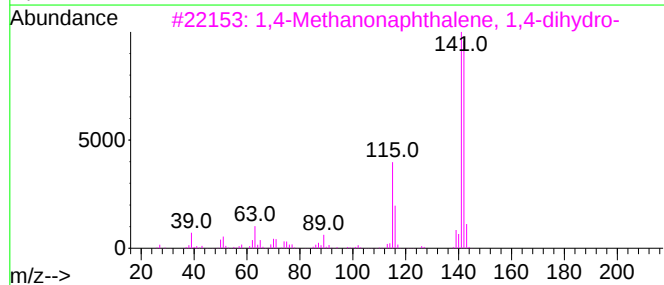
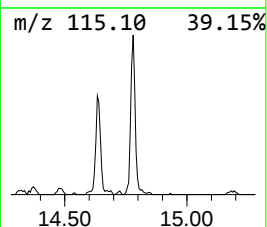
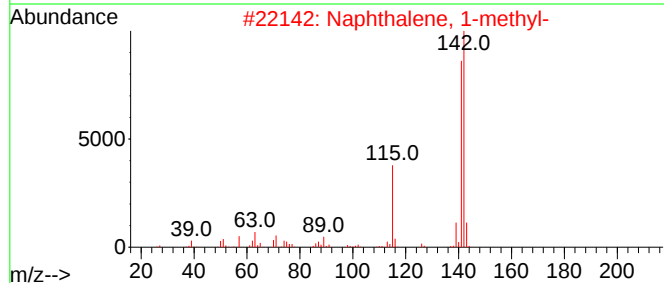
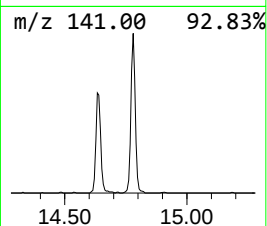
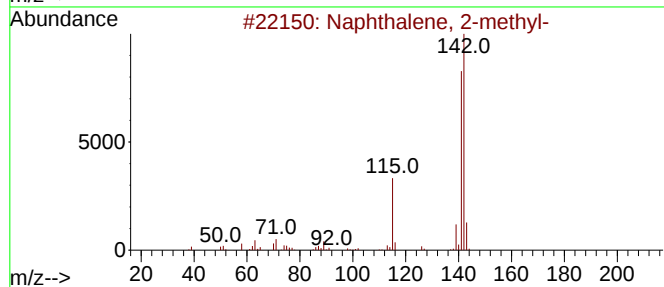
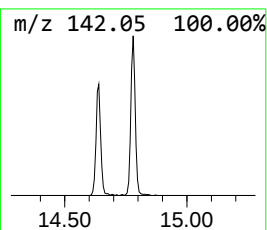
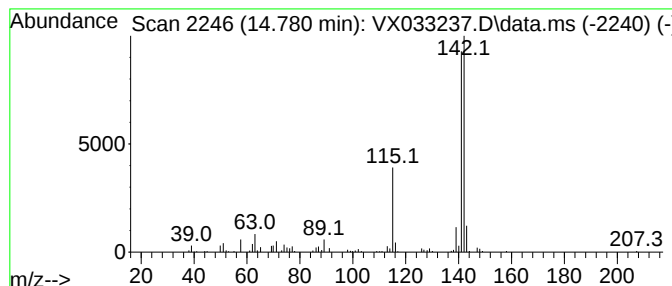
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	7.50 ug/l	75019	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	94
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.374	6.9	ug/l	50185	1	5.556	365767	50.0
Benzene, 1-ethe...	12.244	6.8	ug/l	68083	4	12.024	499842	50.0
Naphthalene, 2-...	14.634	5.4	ug/l	53994	4	12.024	499842	50.0
Naphthalene, 1-...	14.780	7.5	ug/l	75019	4	12.024	499842	50.0