

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
 Data File : VX042061.D
 Acq On : 26 Jun 2024 18:22
 Operator : JC/MD
 Sample : P3073-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW11-20240625

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\82X061824W.M
 Title : SW846 8260

Signal : TIC: VX042061.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	21	25	33	rBV	94414	110339	15.24%	1.978%
2	3.117	322	333	344	rBV	6133	15434	2.13%	0.277%
3	5.391	694	706	721	rBV2	84956	255023	35.23%	4.573%
4	5.550	722	732	752	rVB	145858	420395	58.07%	7.538%
5	5.958	787	799	817	rBV2	80766	218792	30.22%	3.923%
6	6.763	921	931	953	rBV	221059	531147	73.37%	9.524%
7	8.647	1234	1240	1257	rBV	450502	723949	100.00%	12.981%
8	9.275	1338	1343	1348	rBV2	6092	8653	1.20%	0.155%
9	10.055	1465	1471	1485	rBV	475251	655769	90.58%	11.758%
10	11.079	1634	1639	1650	rBV	423466	550241	76.01%	9.866%
11	11.305	1673	1676	1683	rVB	5131	7365	1.02%	0.132%
12	11.616	1721	1727	1734	rBV	8074	11293	1.56%	0.202%
13	11.756	1745	1750	1756	rBV	26786	35621	4.92%	0.639%
14	12.024	1788	1794	1801	rBV	514543	660428	91.23%	11.842%
15	12.085	1801	1804	1810	rVB	7398	10905	1.51%	0.196%
16	12.189	1816	1821	1823	rBV3	5078	9544	1.32%	0.171%
17	12.244	1826	1830	1838	rVV3	29447	47903	6.62%	0.859%
18	12.317	1838	1842	1848	rVB2	10514	15867	2.19%	0.284%
19	12.555	1872	1881	1885	rBV6	4387	12105	1.67%	0.217%
20	12.610	1885	1890	1895	rVB3	6628	11234	1.55%	0.201%
21	12.701	1900	1905	1909	rBV	12976	19296	2.67%	0.346%
22	12.969	1945	1949	1955	rVB4	5965	9350	1.29%	0.168%
23	13.103	1968	1971	1978	rVB8	3700	7489	1.03%	0.134%
24	13.170	1978	1982	1985	rBV	8598	10957	1.51%	0.196%
25	13.231	1985	1992	1994	rBV8	5019	10505	1.45%	0.188%
26	13.286	1998	2001	2006	rVB4	9791	14292	1.97%	0.256%
27	13.347	2007	2011	2014	rBV2	8146	12843	1.77%	0.230%
28	13.426	2020	2024	2030	rVB	25613	36314	5.02%	0.651%
29	13.506	2033	2037	2040	rVV5	5412	8604	1.19%	0.154%
30	13.542	2040	2043	2048	rVB4	5400	8247	1.14%	0.148%
31	13.774	2072	2081	2093	rBV	278311	376920	52.06%	6.758%
32	14.225	2149	2155	2159	rBV5	4304	8425	1.16%	0.151%
33	14.323	2167	2171	2177	rVB2	5510	9796	1.35%	0.176%
34	14.640	2211	2223	2233	rBV	114589	163276	22.55%	2.928%
35	14.780	2239	2246	2259	rBV	151020	201589	27.85%	3.615%
36	15.207	2308	2316	2322	rBV	18818	31764	4.39%	0.570%

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37	15.377	2339	2344	2347	rBV	13727	19803	2.74%	0.355%
38	15.481	2355	2361	2370	rBV	23963	43776	6.05%	0.785%
39	15.615	2377	2383	2387	rBV	36044	61418	8.48%	1.101%
40	15.652	2387	2389	2394	rVB	13890	17359	2.40%	0.311%
41	15.835	2410	2419	2425	rBV2	13858	36781	5.08%	0.659%
42	15.987	2439	2444	2451	rBV2	12055	23287	3.22%	0.418%
43	16.091	2455	2461	2469	rBV2	9471	17067	2.36%	0.306%
44	16.194	2473	2478	2485	rVB4	4992	8450	1.17%	0.152%
45	16.328	2492	2500	2506	rBV	52960	107542	14.85%	1.928%

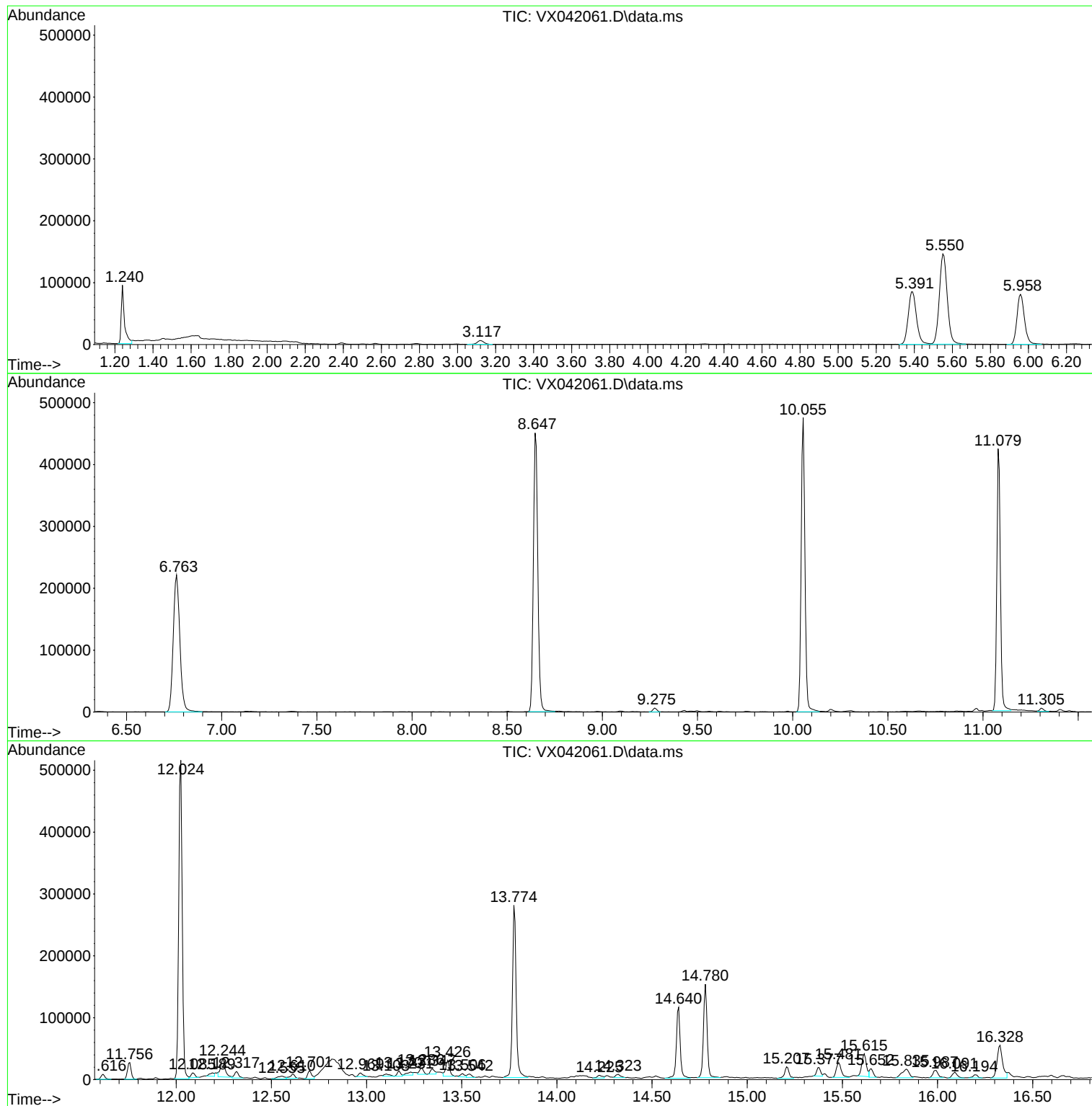
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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



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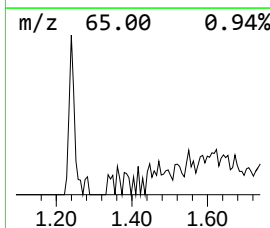
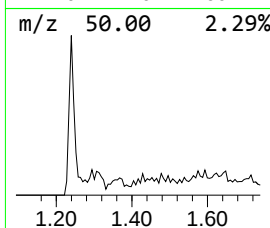
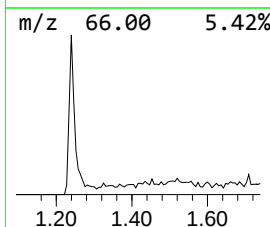
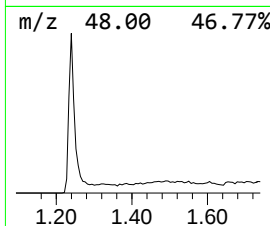
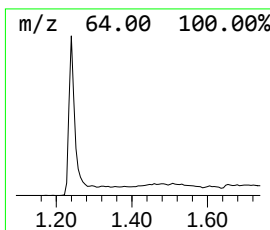
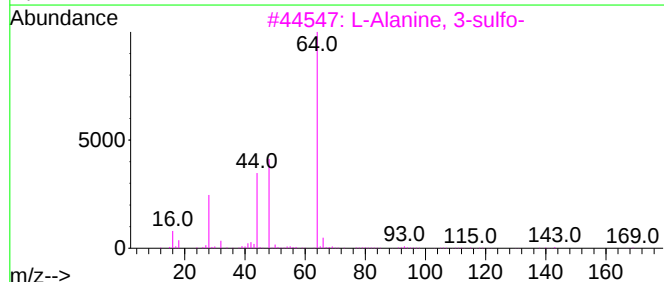
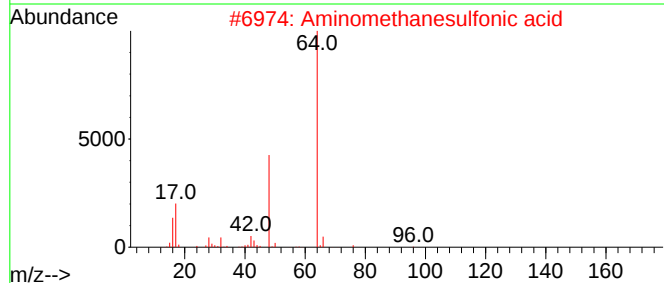
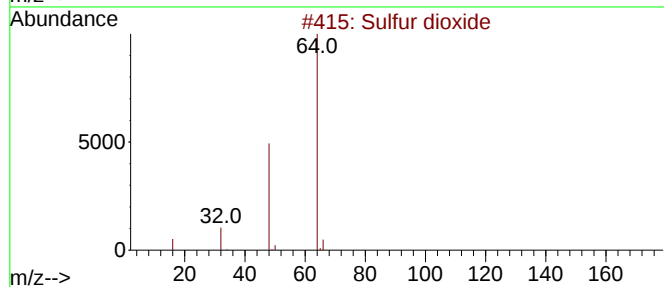
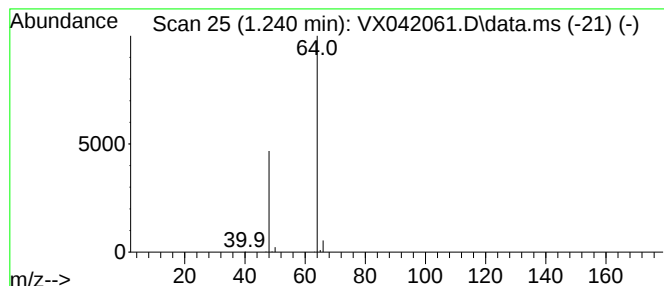
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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.
1.240	13.12 ug/l	110339	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	64
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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ClientSampleId :
MW11-20240625

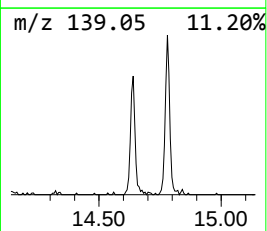
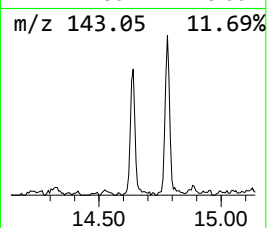
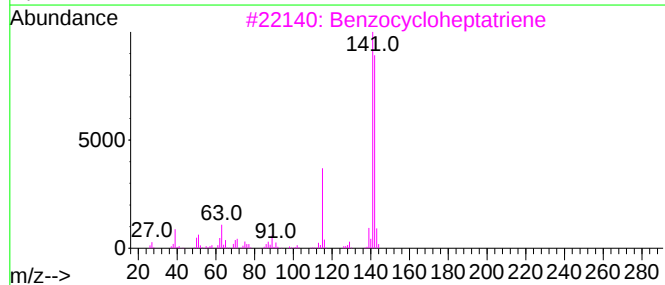
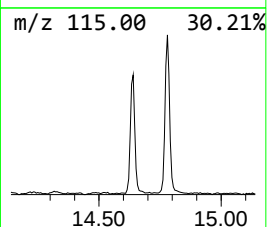
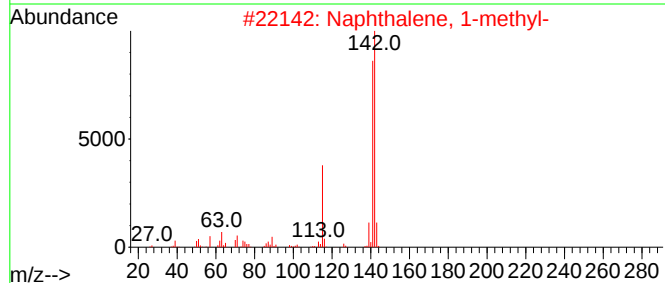
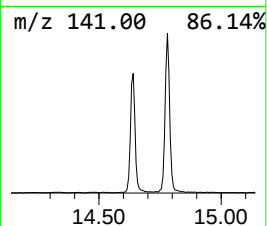
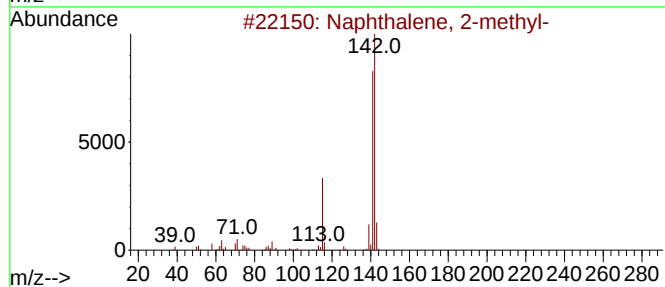
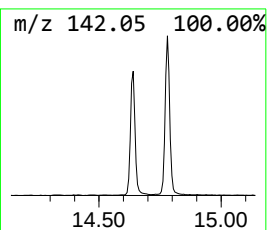
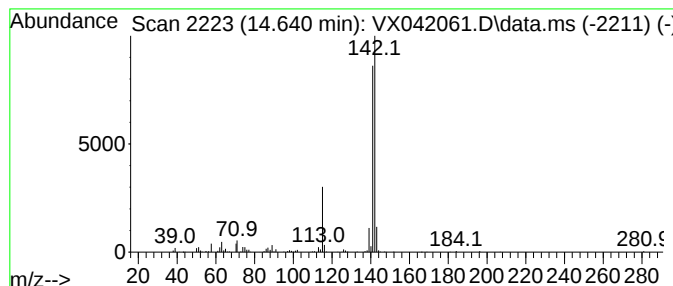
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	12.36 ug/l	163276	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			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1-Naphthaleneacetamide	185	C12H11NO	000086-86-2	59



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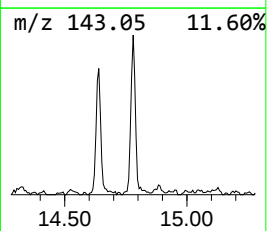
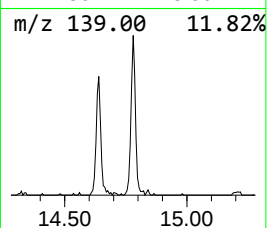
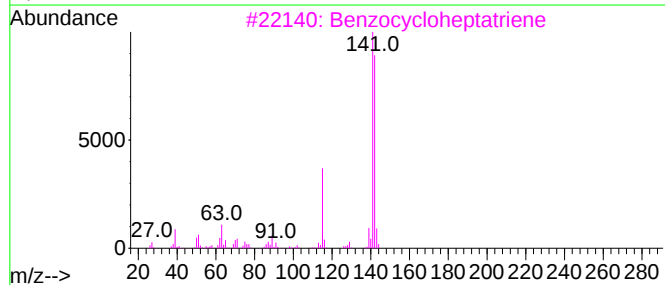
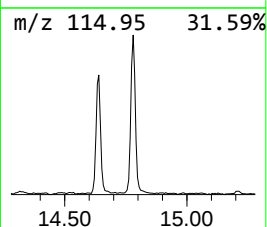
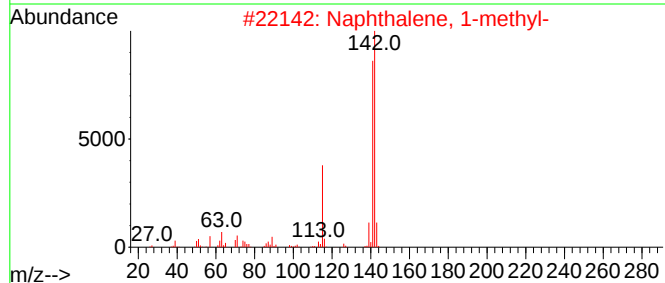
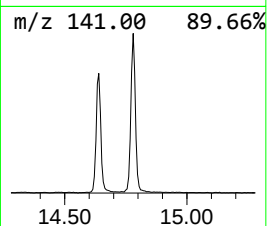
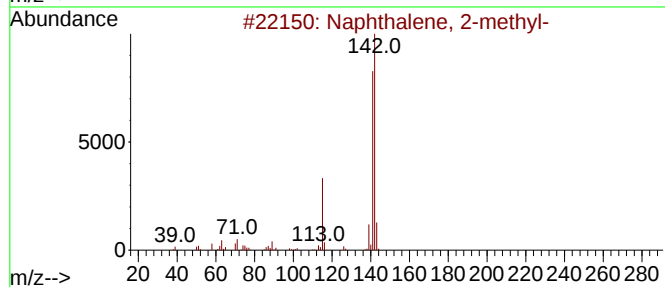
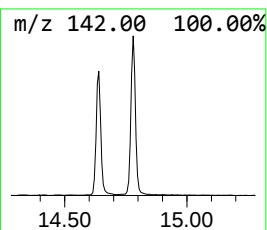
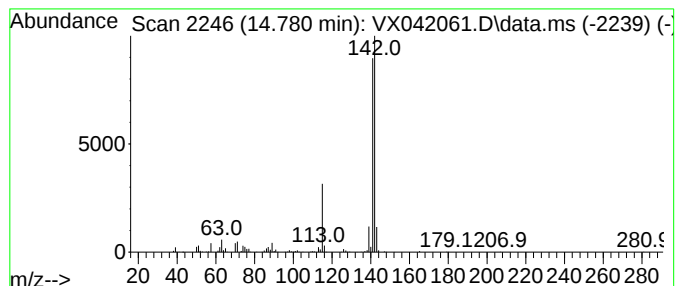
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	15.26 ug/l	201589	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			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91



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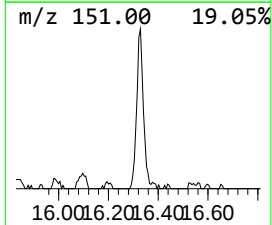
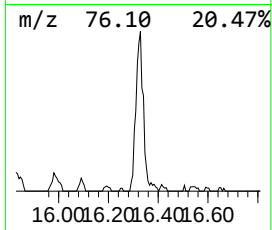
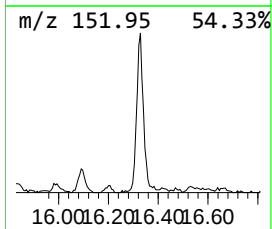
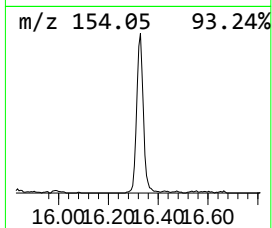
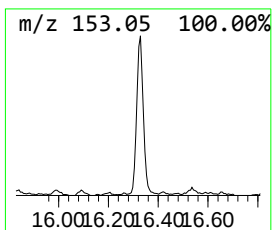
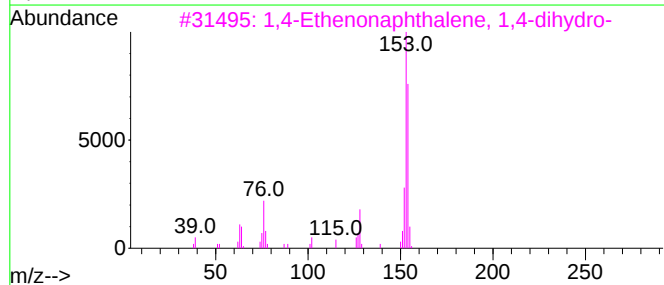
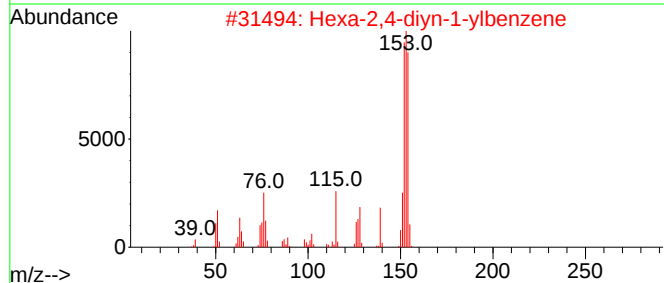
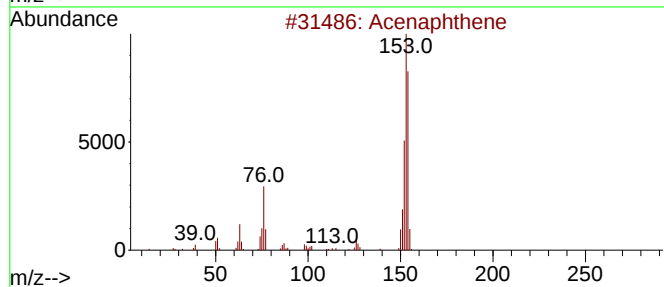
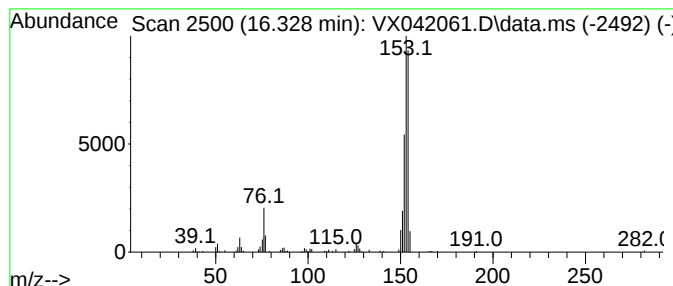
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Acenaphthene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	8.14 ug/l	107542	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	86
2			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
3			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	59
4			2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	50
5			3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	49



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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	1.240	13.1	ug/l	110339	1	5.556	420395	50.0
Naphthalene, 2-...	14.640	12.4	ug/l	163276	4	12.024	660428	50.0
Naphthalene, 1-...	14.780	15.3	ug/l	201589	4	12.024	660428	50.0
Acenaphthene	16.328	8.1	ug/l	107542	4	12.024	660428	50.0