

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
 Data File : VX035448.D
 Acq On : 01 May 2023 18:14
 Operator : JC/MD
 Sample : 02515-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 22-MW-01S

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\82X042523W.M
 Title : SW846 8260

Signal : TIC: VX035448.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	22	25	40	rBV	852783	1017846	86.63%	11.502%
2	1.374	44	47	51	rVV	15097	17871	1.52%	0.202%
3	4.495	549	559	575	rBV	20288	58681	4.99%	0.663%
4	5.385	693	705	721	rBV	128449	376494	32.04%	4.255%
5	5.550	721	732	749	rVB	233292	660300	56.20%	7.462%
6	5.952	788	798	815	rBV2	136927	372559	31.71%	4.210%
7	6.763	921	931	943	rBV	358962	855749	72.83%	9.670%
8	8.647	1233	1240	1253	rBV	747388	1174916	100.00%	13.277%
9	10.055	1465	1471	1488	rBV	752545	1032772	87.90%	11.671%
10	10.195	1488	1494	1500	rVB	9391	13719	1.17%	0.155%
11	11.079	1634	1639	1648	rBV	636368	823797	70.12%	9.309%
12	11.750	1745	1749	1755	rVB	18815	26474	2.25%	0.299%
13	12.024	1788	1794	1801	rBV	779334	1008808	85.86%	11.400%
14	12.244	1824	1830	1838	rBV	21601	34313	2.92%	0.388%
15	12.701	1900	1905	1912	rVB	10470	15096	1.28%	0.171%
16	12.853	1912	1930	1946	rBV3	32580	184001	15.66%	2.079%
17	13.170	1977	1982	1988	rVB2	14119	20193	1.72%	0.228%
18	13.286	1992	2001	2007	rBV4	20315	46360	3.95%	0.524%
19	13.426	2020	2024	2032	rVB5	14249	26620	2.27%	0.301%
20	13.774	2071	2081	2092	rBV	167039	240143	20.44%	2.714%
21	14.639	2215	2223	2232	rBV	101864	147758	12.58%	1.670%
22	14.780	2239	2246	2254	rVB	180611	235250	20.02%	2.658%
23	15.206	2306	2316	2321	rBV	42755	63853	5.43%	0.722%
24	15.377	2339	2344	2347	rBV2	15400	23295	1.98%	0.263%
25	15.408	2347	2349	2354	rVB3	9219	12141	1.03%	0.137%
26	15.481	2354	2361	2371	rBV	30587	54888	4.67%	0.620%
27	15.615	2373	2383	2387	rVV	52518	93689	7.97%	1.059%
28	15.652	2387	2389	2396	rVB3	17215	24000	2.04%	0.271%
29	15.840	2410	2420	2430	rBV4	17681	51719	4.40%	0.584%
30	15.987	2438	2444	2454	rVB3	15385	27756	2.36%	0.314%
31	16.328	2493	2500	2510	rBV	46822	94830	8.07%	1.072%
32	16.670	2550	2556	2566	rVB8	4721	13333	1.13%	0.151%

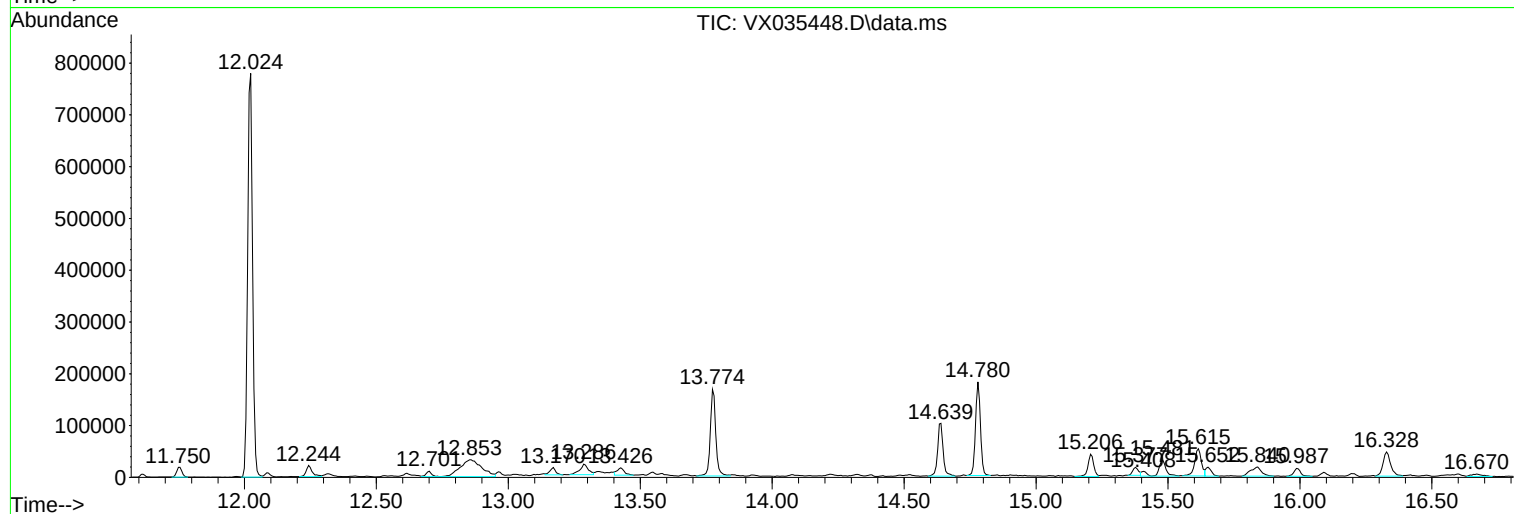
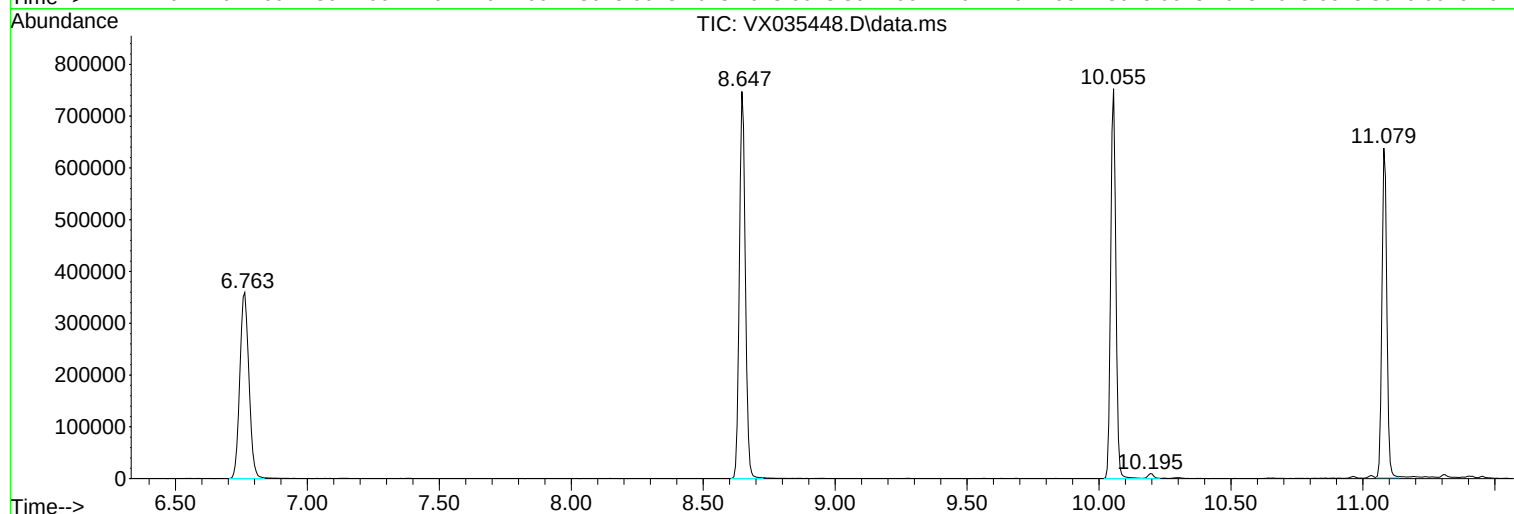
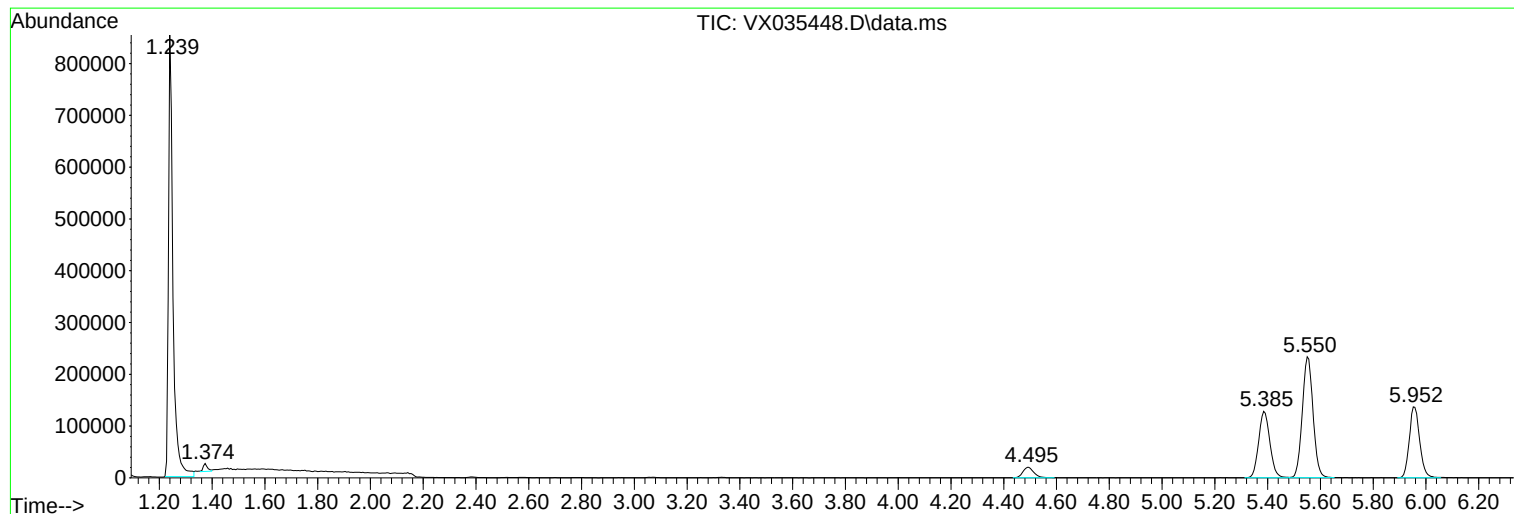
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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



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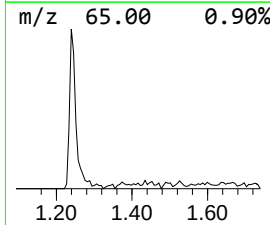
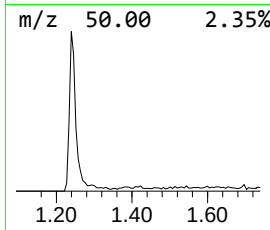
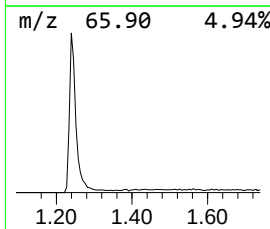
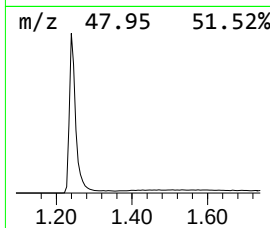
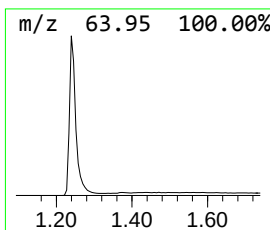
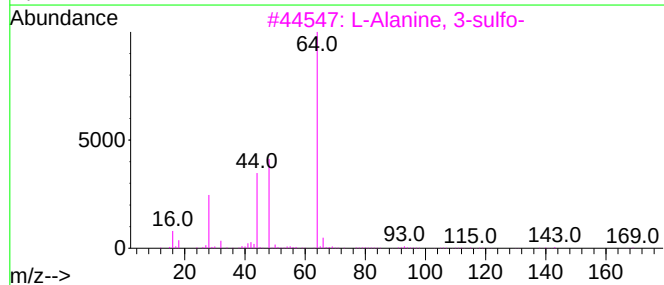
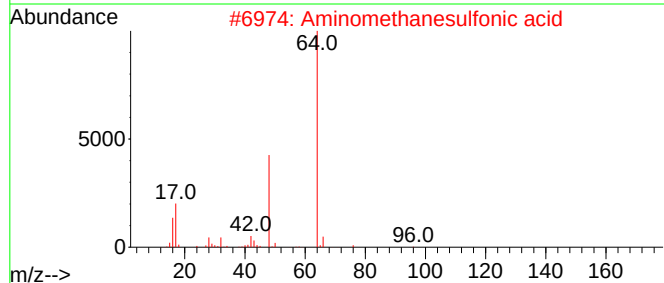
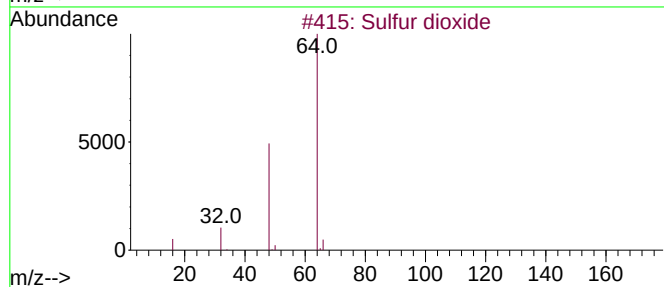
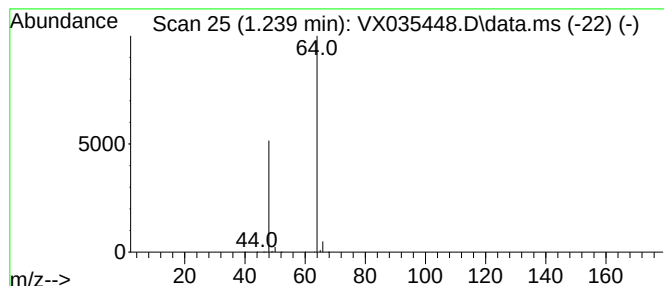
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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.
1.239	77.07 ug/l	1017850	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
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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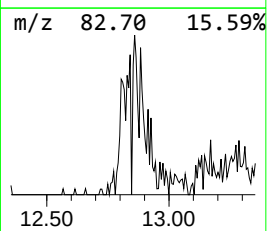
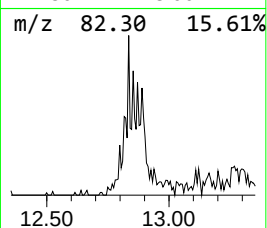
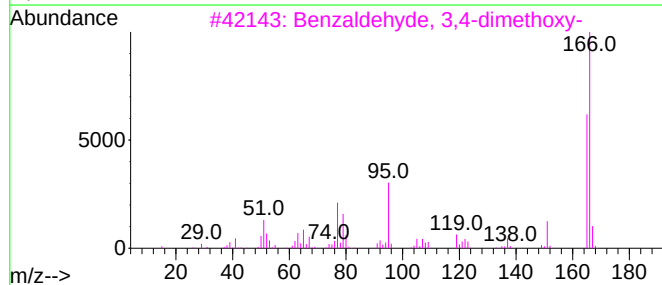
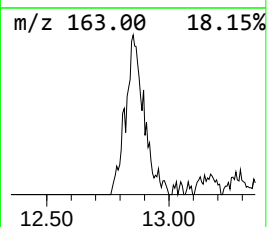
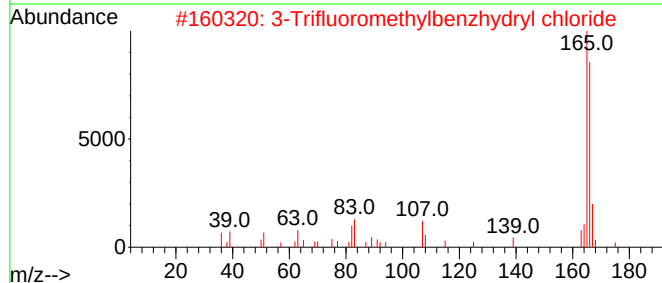
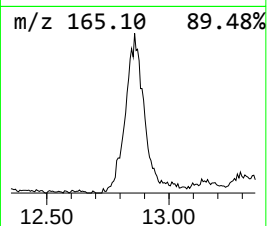
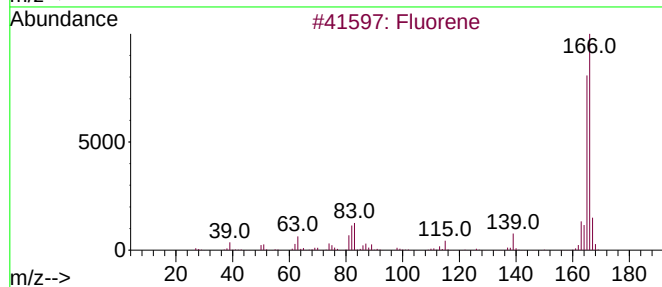
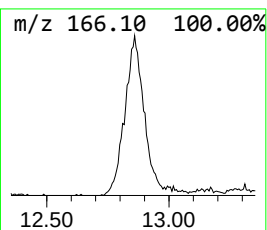
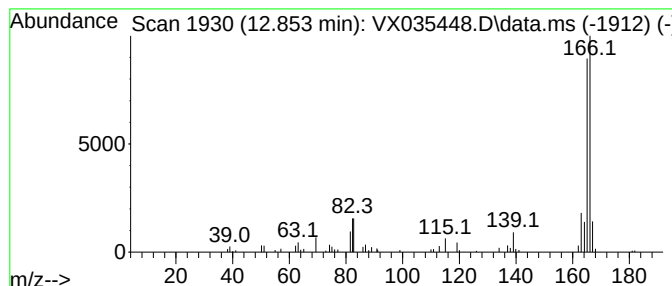
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 2 Fluorene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.853	9.12 ug/l	184001	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluorene	166	C13H10	000086-73-7	95
2			3-Trifluoromethylbenzhydryl chlo...	270	C14H10ClF3	067240-79-3	64
3			Benzaldehyde, 3,4-dimethoxy-	166	C9H10O3	000120-14-9	59
4			1H-Phenylene	166	C13H10	000203-80-5	53
5			1,3-Benzodioxole-5-carboxylic acid	166	C8H6O4	000094-53-1	42



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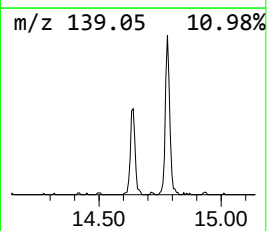
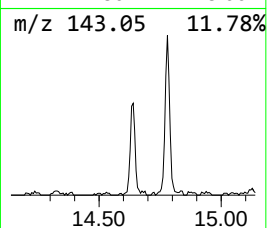
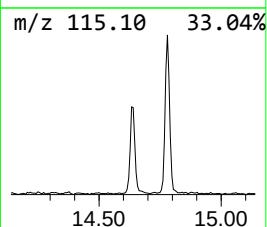
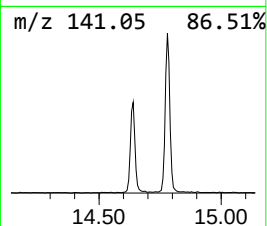
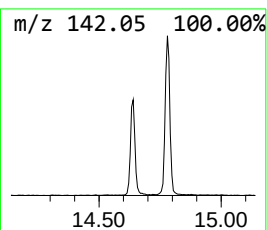
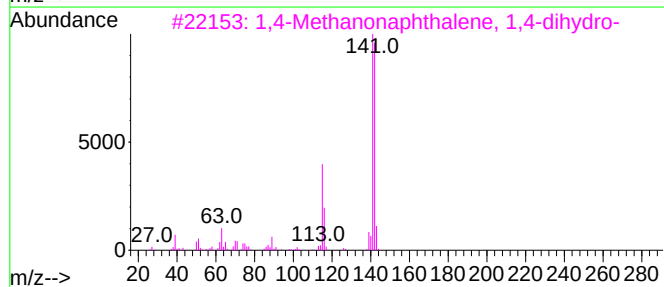
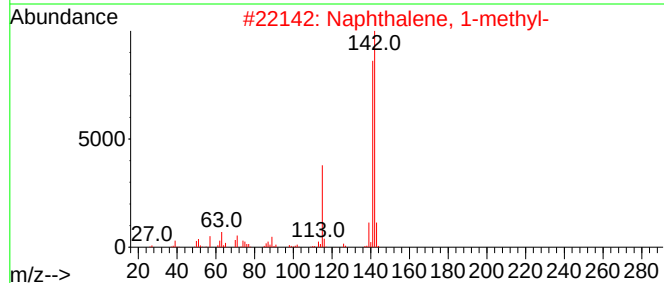
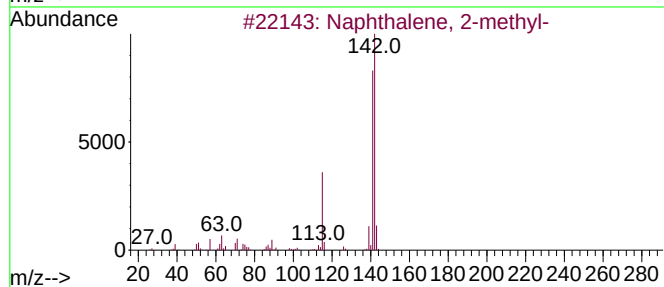
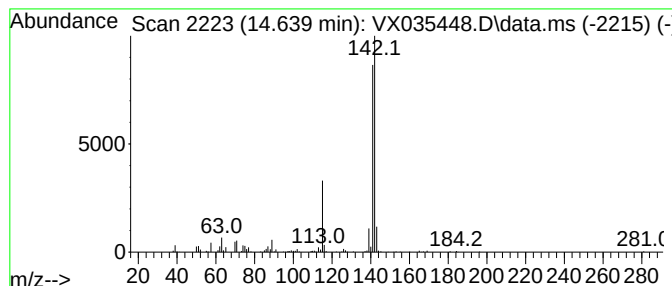
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 3 1,4-Methanonaphthalene, 1,4... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	7.32 ug/l	147758	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	91
4		Benzocycloheptatriene	142	C11H10	000264-09-5	90
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59



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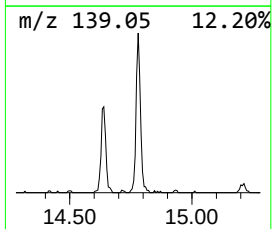
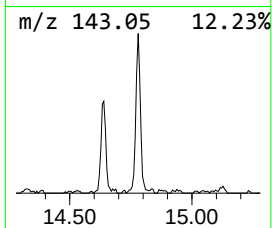
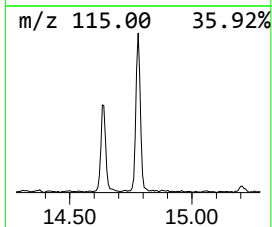
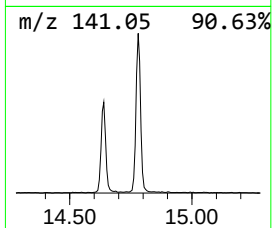
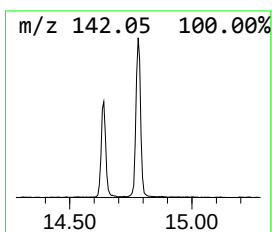
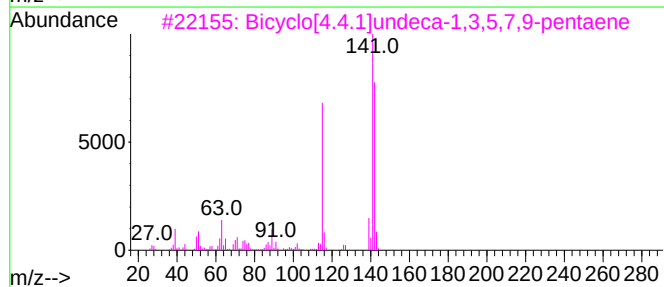
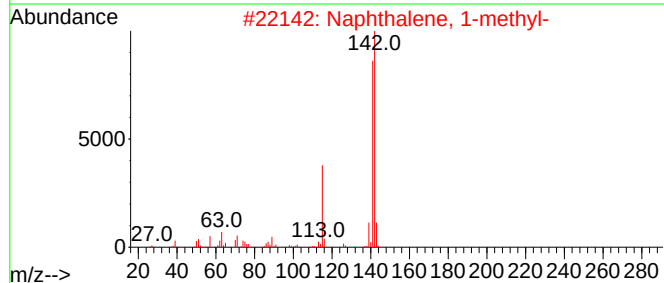
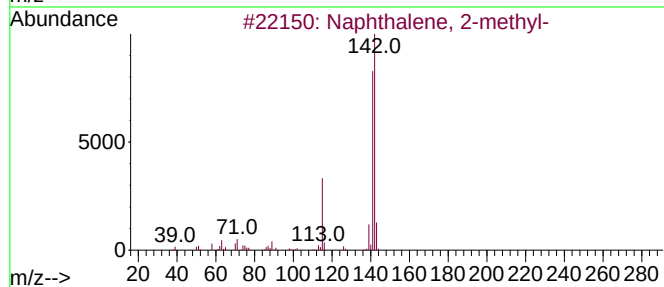
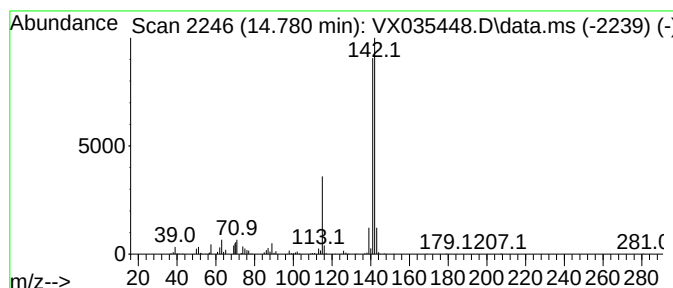
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Bicyclo[4.4.1]undeca-1,3,5,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	11.66 ug/l	235250	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			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.239	77.1	ug/l	1017850	1	5.556	660300	50.0
Fluorene	12.853	9.1	ug/l	184001	4	12.024	1008810	50.0
1,4-Methanonaph...	14.640	7.3	ug/l	147758	4	12.024	1008810	50.0
Bicyclo[4.4.1]u...	14.780	11.7	ug/l	235250	4	12.024	1008810	50.0