

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
 Data File : VX035449.D
 Acq On : 01 May 2023 18:37
 Operator : JC/MD
 Sample : 02515-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 LEA-12I

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: VX035449.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	22	25	49	rBV	730023	935314	73.11%	11.023%
2	5.385	693	705	721	rBV	141916	413678	32.33%	4.875%
3	5.550	721	732	748	rVV	257154	726417	56.78%	8.561%
4	5.958	788	799	815	rBV	150536	406356	31.76%	4.789%
5	6.757	921	930	948	rBV	390758	938633	73.37%	11.062%
6	7.129	984	991	1002	rBV3	10977	24973	1.95%	0.294%
7	8.647	1233	1240	1251	rBV	819637	1279353	100.00%	15.077%
8	10.055	1465	1471	1485	rBV	814305	1121428	87.66%	13.216%
9	11.079	1634	1639	1652	rBV	701297	878636	68.68%	10.355%
10	11.750	1745	1749	1759	rVB	25299	32870	2.57%	0.387%
11	12.018	1788	1793	1801	rBV	817471	1070541	83.68%	12.616%
12	12.244	1825	1830	1838	rBV2	21159	29300	2.29%	0.345%
13	12.701	1901	1905	1914	rVB	16017	21460	1.68%	0.253%
14	12.963	1944	1948	1954	rVB	11184	13504	1.06%	0.159%
15	13.170	1977	1982	1987	rVB	16563	21629	1.69%	0.255%
16	13.286	1991	2001	2007	rBV2	22818	36406	2.85%	0.429%
17	13.427	2019	2024	2033	rVB4	11415	17587	1.37%	0.207%
18	13.774	2076	2081	2091	rBV	106108	141782	11.08%	1.671%
19	14.640	2213	2223	2233	rBV	59178	87720	6.86%	1.034%
20	14.780	2241	2246	2255	rVB	102163	127272	9.95%	1.500%
21	15.207	2309	2316	2322	rBV	16577	26420	2.07%	0.311%
22	15.377	2338	2344	2348	rBV6	8393	14471	1.13%	0.171%
23	15.481	2354	2361	2367	rBV2	13531	23754	1.86%	0.280%
24	15.615	2370	2383	2386	rVV3	21023	41327	3.23%	0.487%
25	15.841	2410	2420	2424	rBV6	6988	20463	1.60%	0.241%
26	16.335	2492	2501	2509	rBV3	15251	34064	2.66%	0.401%

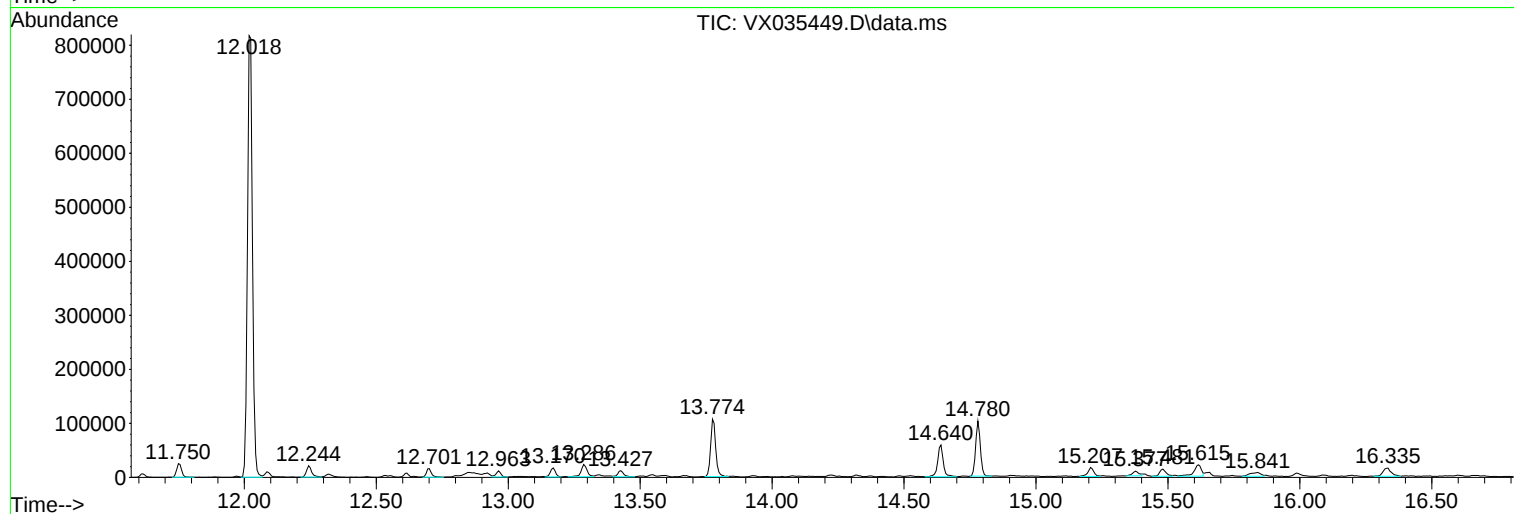
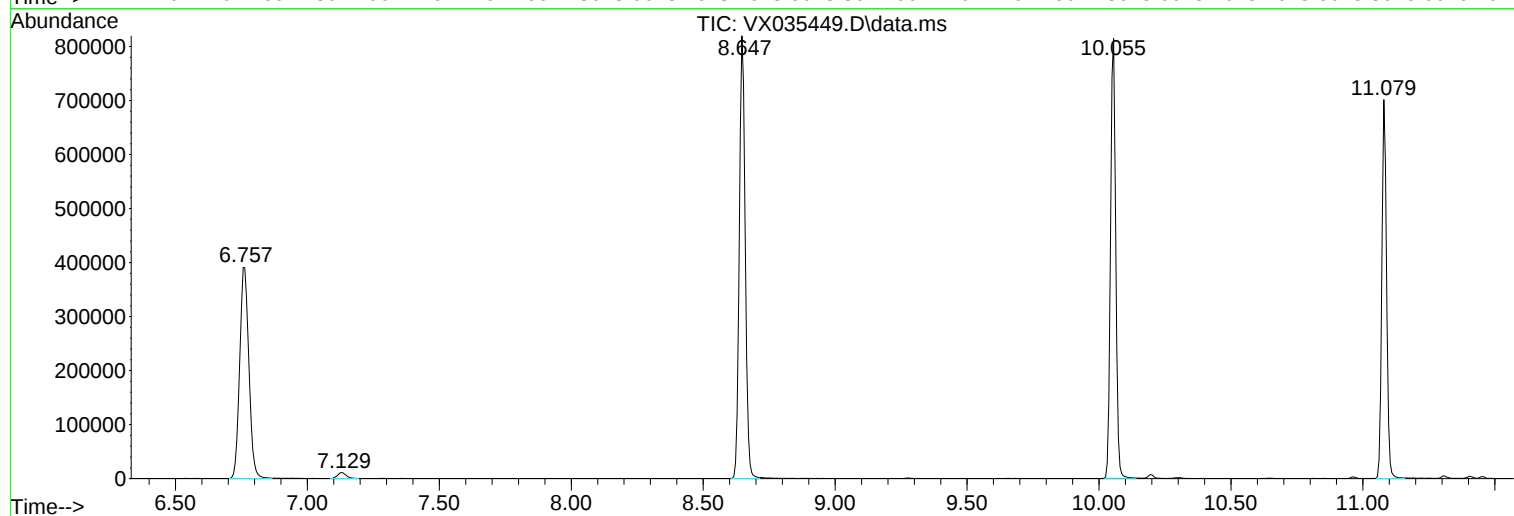
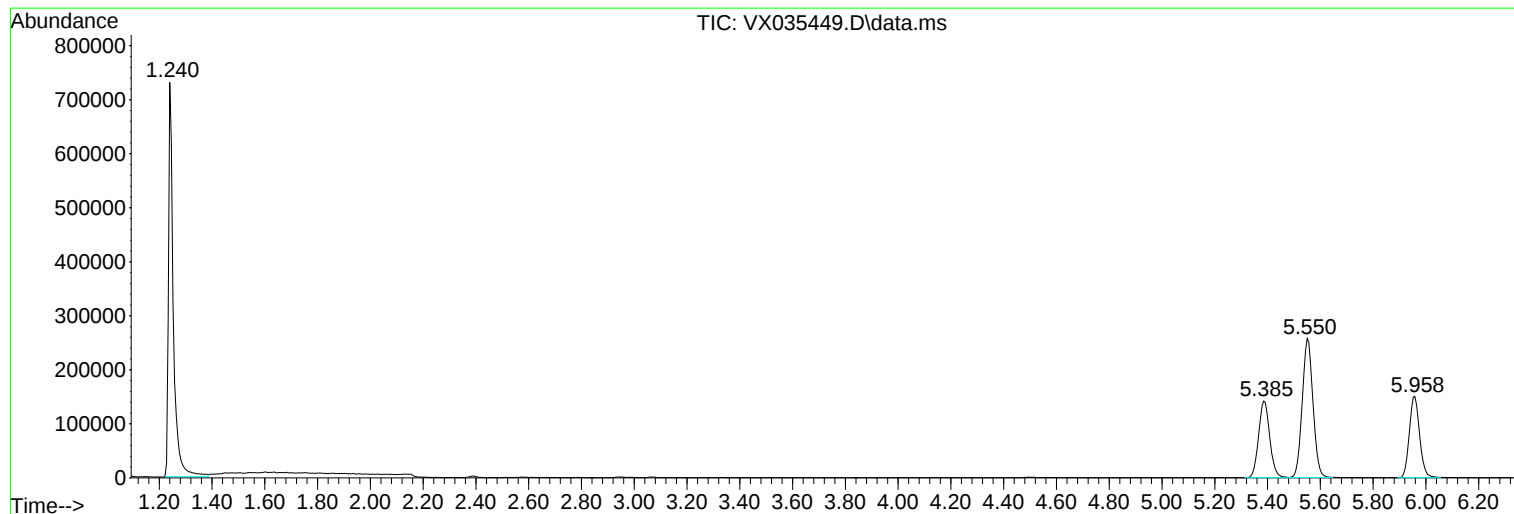
Sum of corrected areas: 8485358

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
Data File : VX035449.D
Acq On : 01 May 2023 18:37
Operator : JC/MD
Sample : 02515-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
LEA-12I

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
Data File : VX035449.D
Acq On : 01 May 2023 18:37
Operator : JC/MD
Sample : 02515-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
LEA-12I

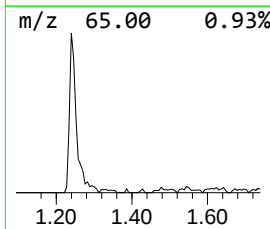
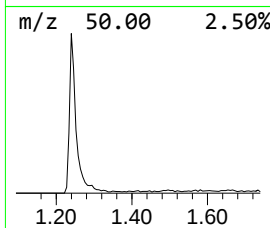
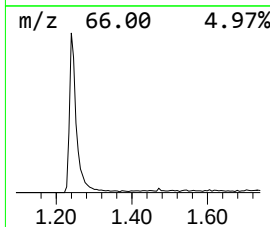
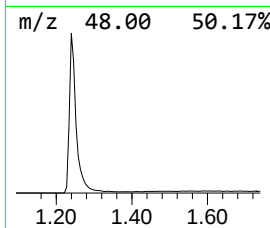
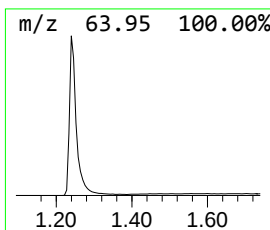
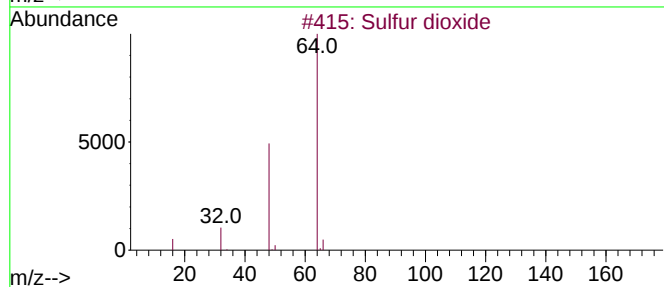
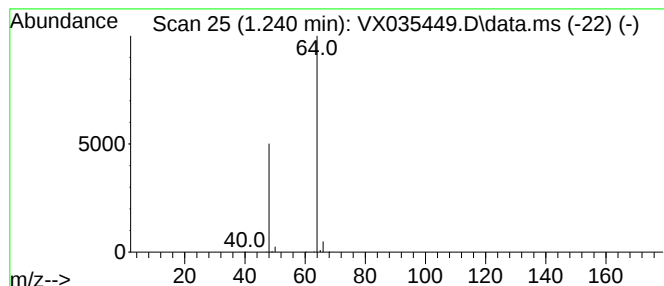
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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.
1.240	64.38 ug/l	935314	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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
Data File : VX035449.D
Acq On : 01 May 2023 18:37
Operator : JC/MD
Sample : 02515-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
LEA-12I

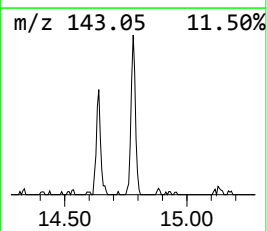
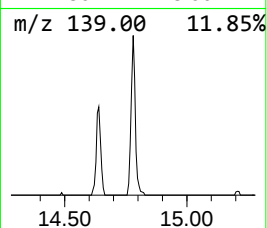
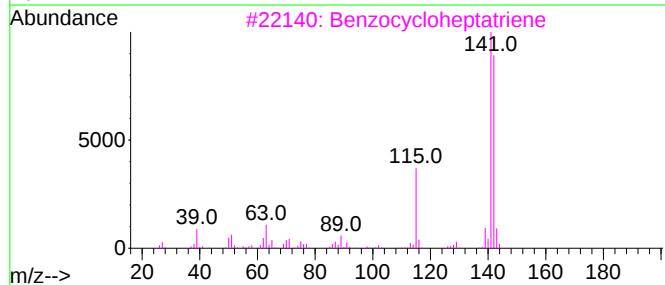
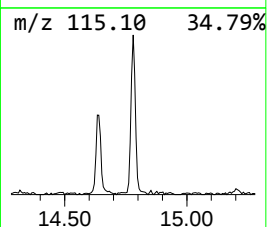
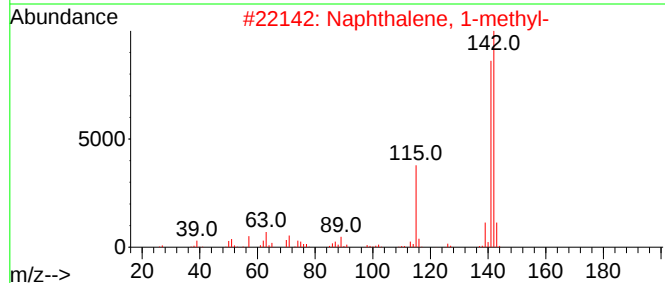
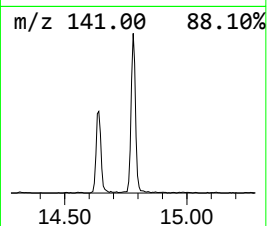
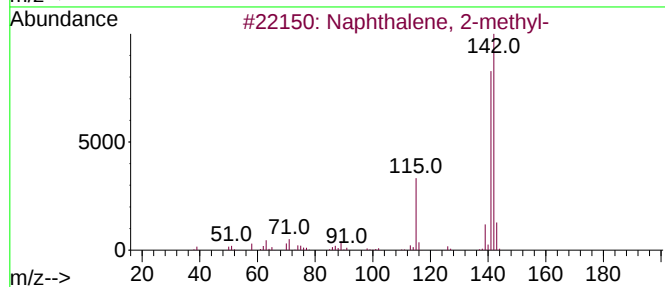
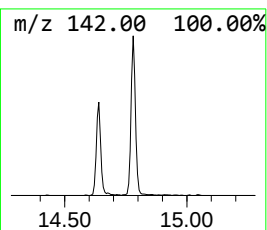
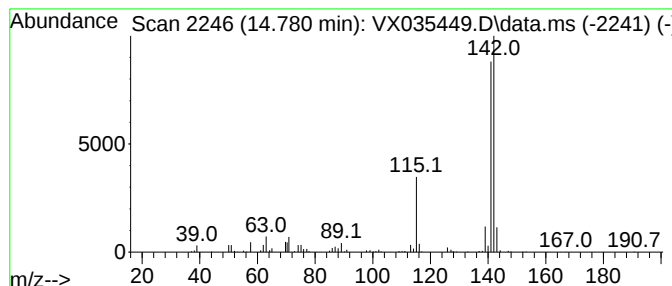
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	5.94 ug/l	127272	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			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
Data File : VX035449.D
Acq On : 01 May 2023 18:37
Operator : JC/MD
Sample : 02515-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
LEA-12I

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	64.4	ug/l	935314	1	5.556	726417	50.0
Benzocyclohepta...	14.780	5.9	ug/l	127272	4	12.024	1070540	50.0