

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
 Data File : VX041717.D
 Acq On : 03 Jun 2024 20:12
 Operator : JC/MD
 Sample : P2657-10 100X
 Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 3-AB-VOC

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\82X052924W.M

Title : SW846 8260

Signal : TIC: VX041717.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.245	22	26	27	rBV	7379	7495	1.16%	0.187%
2	1.258	27	28	34	rVB2	6245	6639	1.03%	0.166%
3	1.605	65	85	86	rBV7	9341	39234	6.09%	0.979%
4	5.385	695	705	721	rBV2	74804	220953	34.32%	5.511%
5	5.549	721	732	749	rVB	128724	371246	57.66%	9.260%
6	5.958	790	799	817	rBV	78563	210463	32.69%	5.249%
7	6.763	920	931	949	rBV	197726	471673	73.26%	11.765%
8	8.646	1234	1240	1250	rBV	398452	643810	100.00%	16.058%
9	10.055	1465	1471	1485	rBV	437844	600452	93.27%	14.977%
10	10.305	1507	1512	1521	rVB	5398	8090	1.26%	0.202%
11	11.079	1634	1639	1656	rBV	374737	488394	75.86%	12.182%
12	11.756	1746	1750	1755	rBV	5305	6493	1.01%	0.162%
13	12.024	1788	1794	1801	rBV	459666	585100	90.88%	14.594%
14	12.414	1853	1858	1869	rBV2	6058	8923	1.39%	0.223%
15	13.774	2076	2081	2093	rBV	244325	306234	47.57%	7.638%
16	14.639	2219	2223	2230	rBV	15195	19042	2.96%	0.475%
17	14.780	2239	2246	2253	rBV	10122	15026	2.33%	0.375%

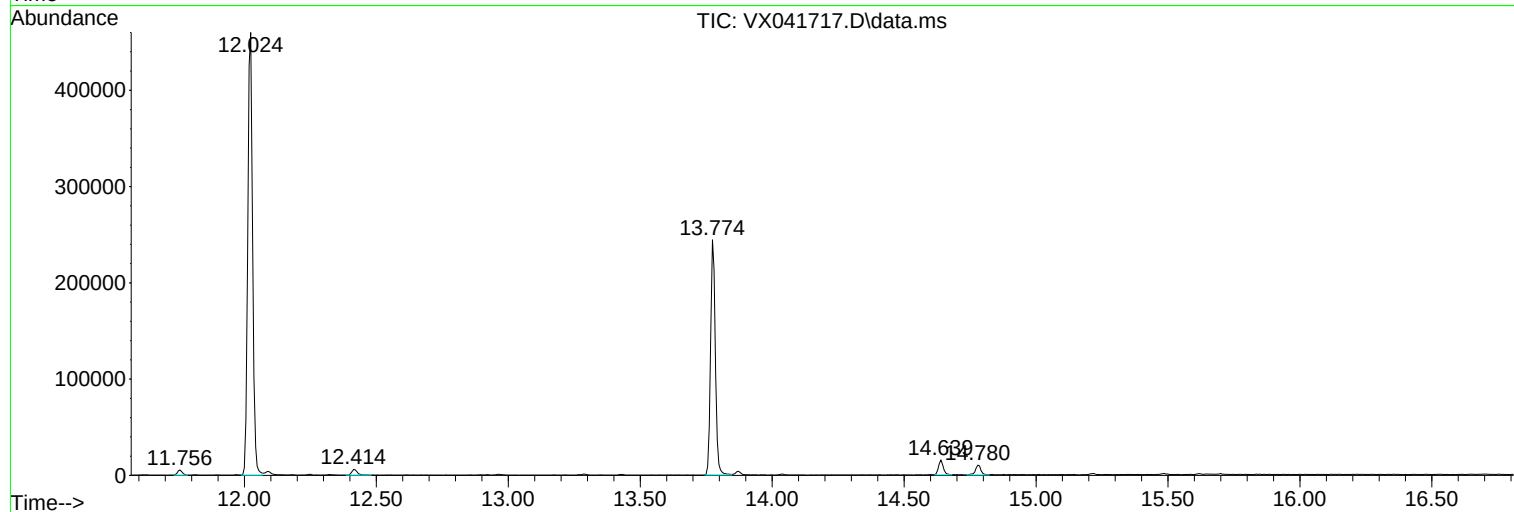
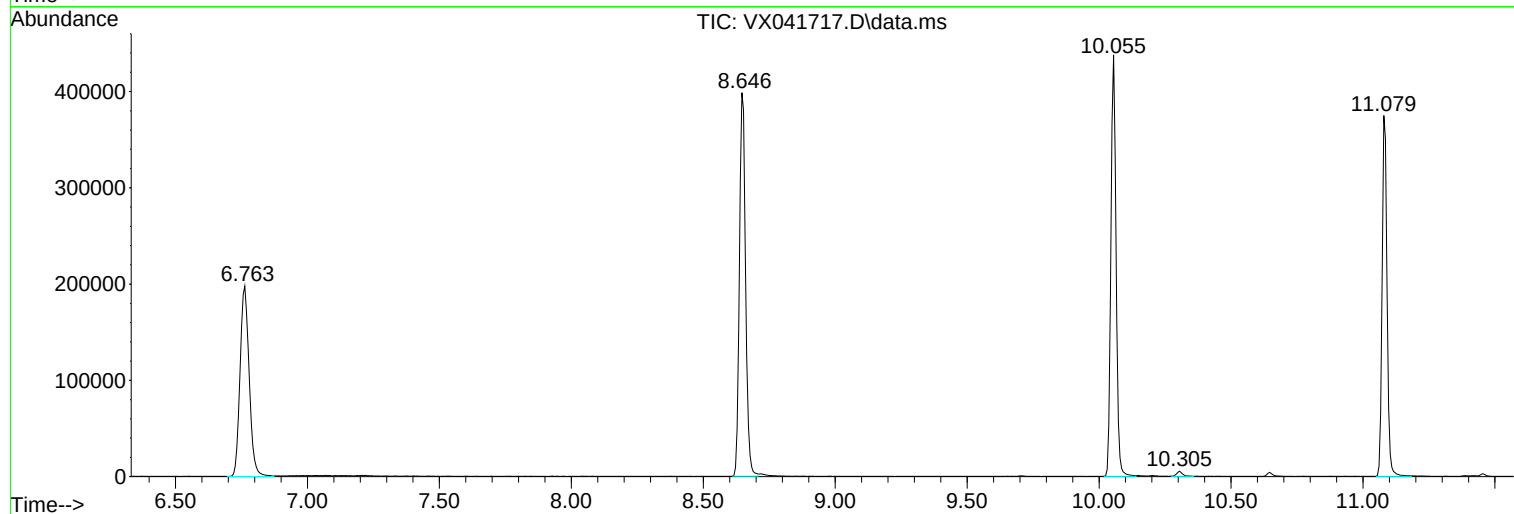
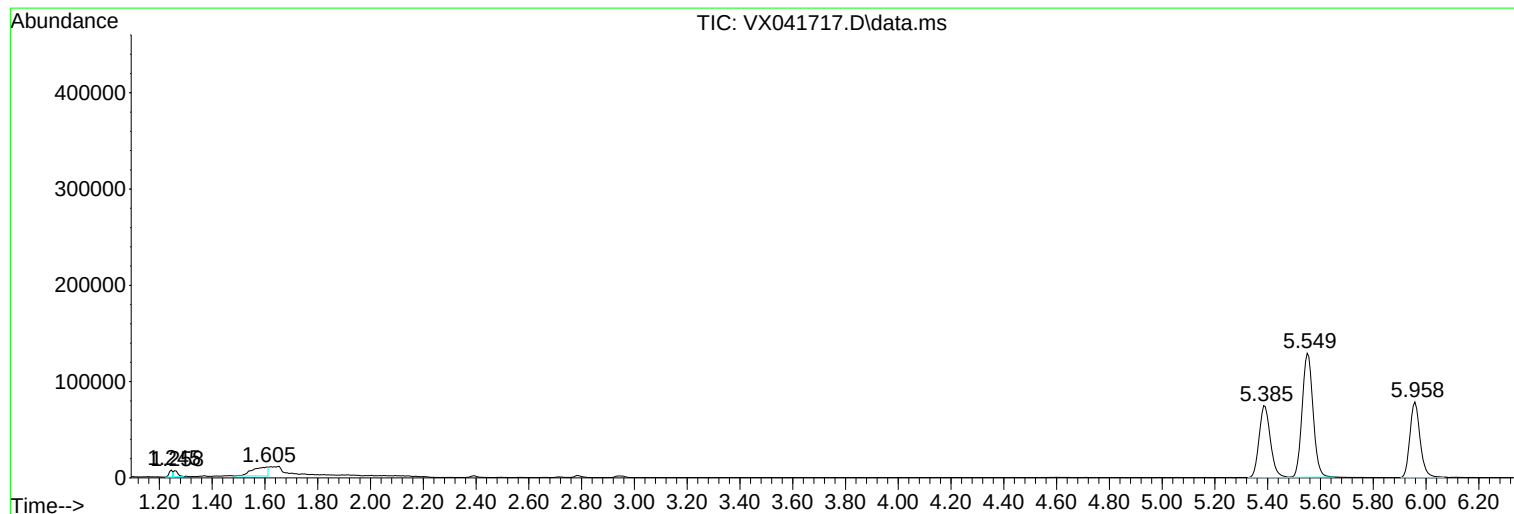
Sum of corrected areas: 4009267

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041717.D
Acq On : 03 Jun 2024 20:12
Operator : JC/MD
Sample : P2657-10 100X
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3-AB-VOC

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041717.D
Acq On : 03 Jun 2024 20:12
Operator : JC/MD
Sample : P2657-10 100X
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3-AB-VOC

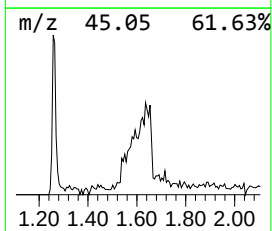
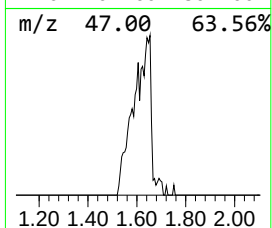
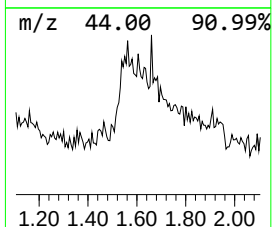
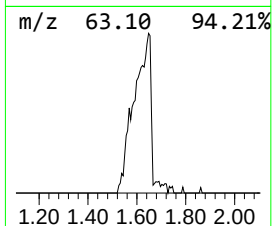
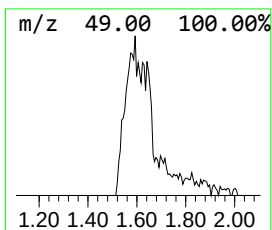
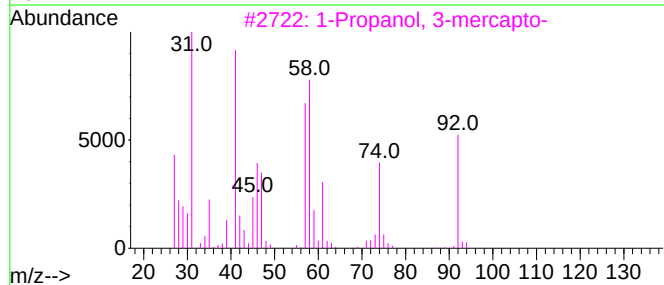
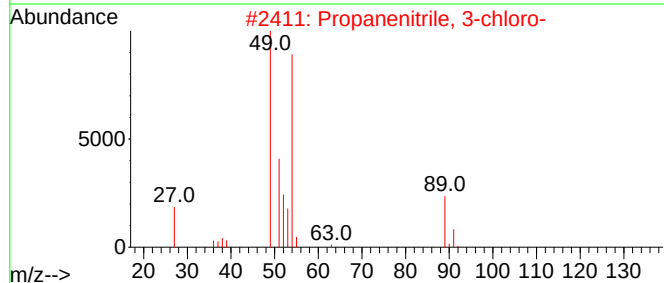
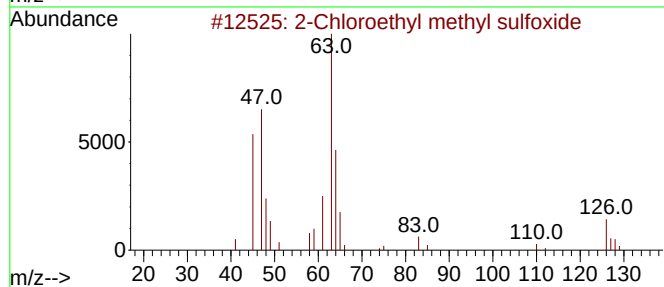
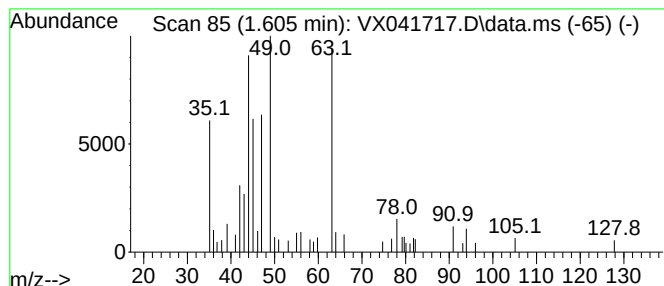
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.605 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.605	5.28 ug/l	39234	Pentafluorobenzene	5.549

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl methyl sulfoxide	126	C3H7ClOS	005331-57-7	17	
2	Propanenitrile, 3-chloro-	89	C3H4ClN	000542-76-7	9	
3	1-Propanol, 3-mercapto-	92	C3H8OS	019721-22-3	9	
4	bis(chloromethyl) carbonate	158	C3H4Cl2O3	1000404-37-0	9	
5	Propanoic acid, 2-chloro-, ethyl...	136	C5H9ClO2	000535-13-7	8	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041717.D
Acq On : 03 Jun 2024 20:12
Operator : JC/MD
Sample : P2657-10 100X
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3-AB-VOC

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
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
unknown1.605	1.605	5.3	ug/l	39234	1	5.549	371246	50.0