

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112524\
 Data File : VX043990.D
 Acq On : 25 Nov 2024 16:35
 Operator : JC/MD
 Sample : P4873-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FSND-MW-32-20241114

Integration Parameters: RTEINT.P
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
 Title : SW846 8260

Signal : TIC: VX043990.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	5	9	19	rVB	31786	34561	4.81%	0.765%
2	1.240	21	25	27	rBV	11523	12978	1.81%	0.287%
3	1.264	27	29	36	rVB3	6093	7230	1.01%	0.160%
4	1.368	41	46	53	rBV2	19610	35960	5.01%	0.796%
5	1.605	69	85	86	rVV5	15534	63057	8.78%	1.395%
6	1.636	86	90	96	rVB6	20017	44750	6.23%	0.990%
7	1.892	127	132	135	rBV4	6280	9607	1.34%	0.213%
8	2.569	235	243	249	rVB3	4167	8946	1.25%	0.198%
9	4.483	549	557	572	rBV2	46064	128809	17.94%	2.850%
10	5.379	693	704	721	rBV	84256	250140	34.83%	5.534%
11	5.544	721	731	744	rBV2	122728	363682	50.64%	8.046%
12	5.952	786	798	818	rBV	100992	273149	38.04%	6.043%
13	6.757	921	930	946	rBV	216016	525926	73.24%	11.635%
14	7.123	981	990	1003	rBV	214350	475276	66.18%	10.515%
15	8.647	1234	1240	1255	rBV	436909	718105	100.00%	15.887%
16	10.055	1465	1471	1484	rBV	420983	616735	85.88%	13.644%
17	11.079	1634	1639	1651	rBV	332116	440070	61.28%	9.736%
18	12.018	1788	1793	1802	rBV	391452	511134	71.18%	11.308%

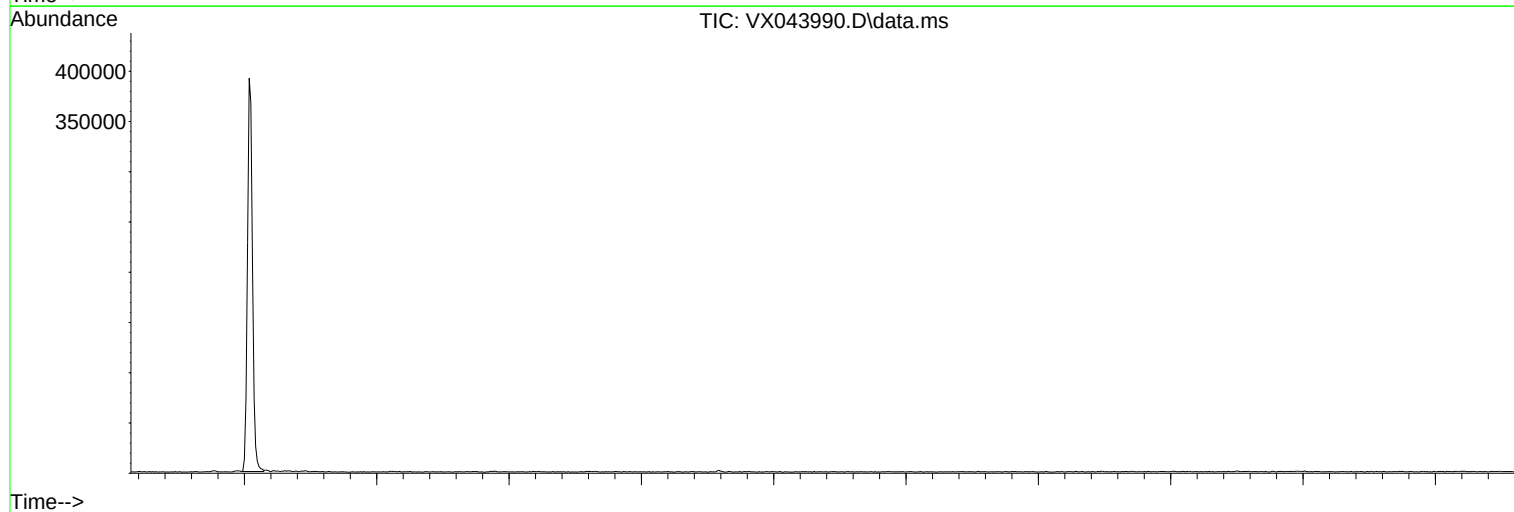
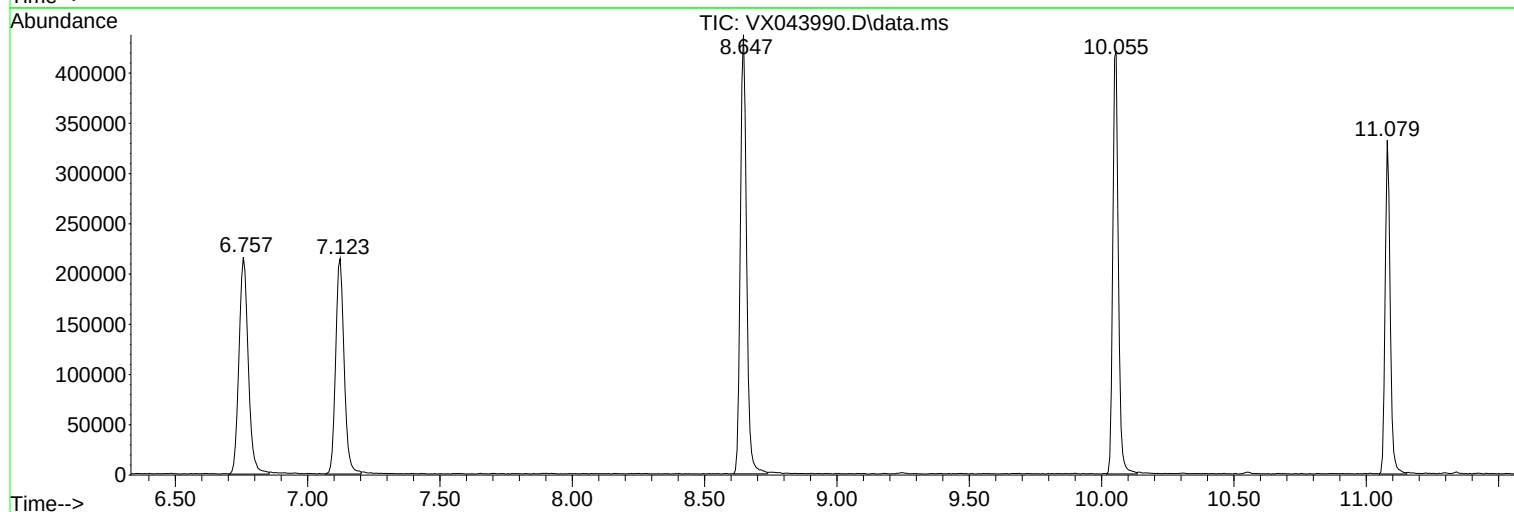
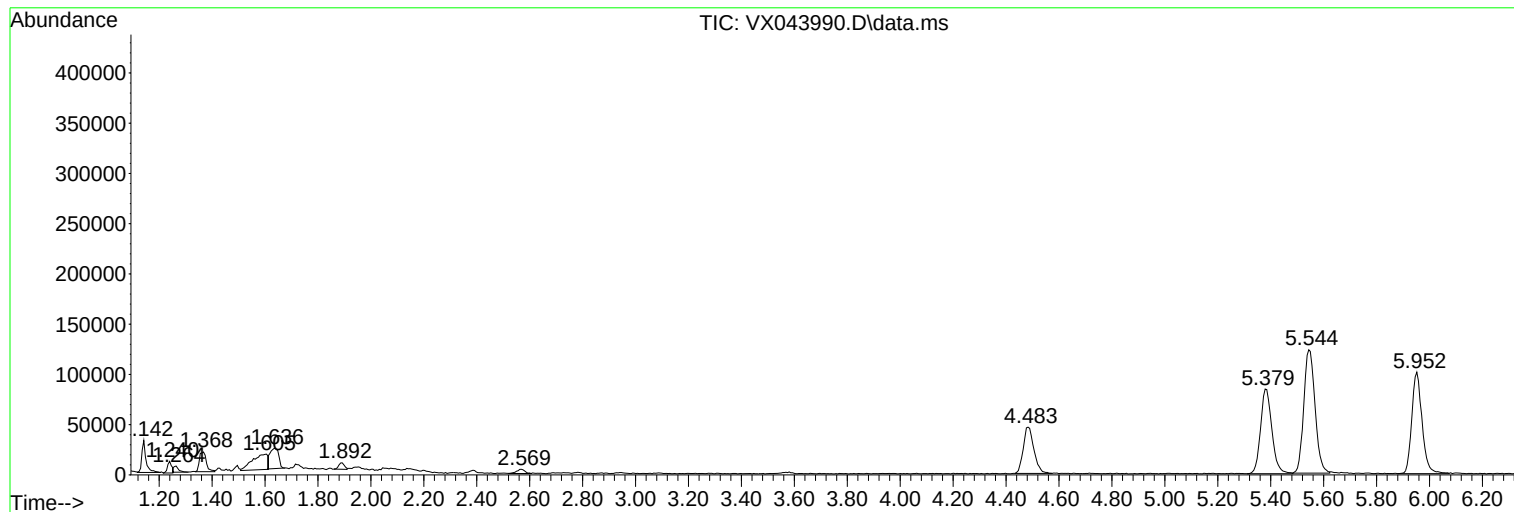
Sum of corrected areas: 4520115

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

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



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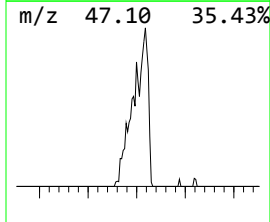
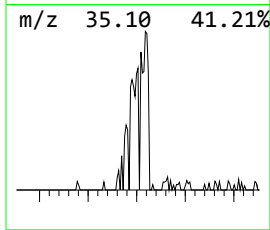
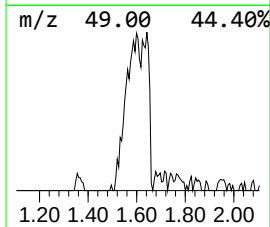
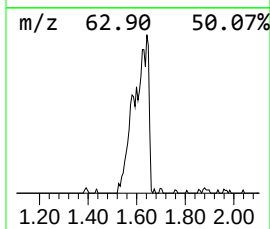
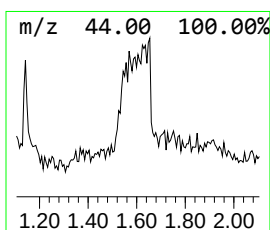
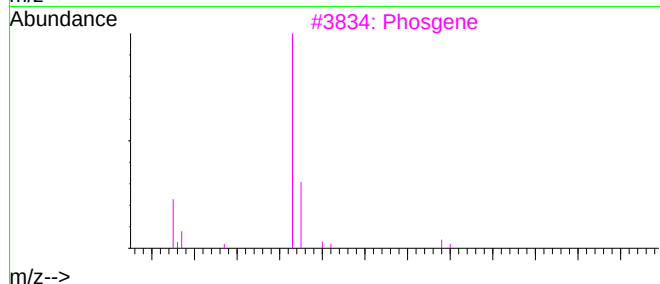
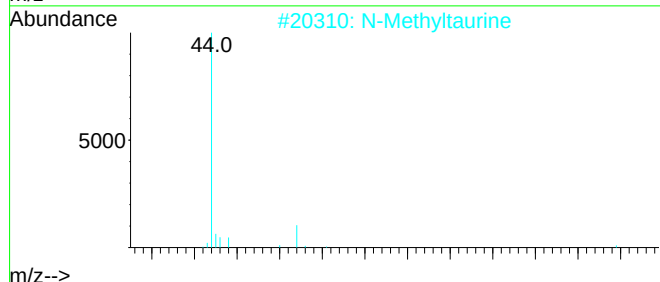
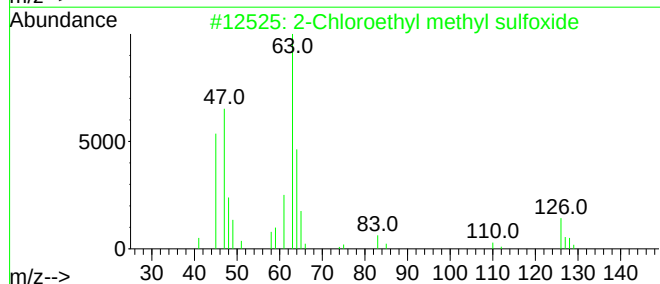
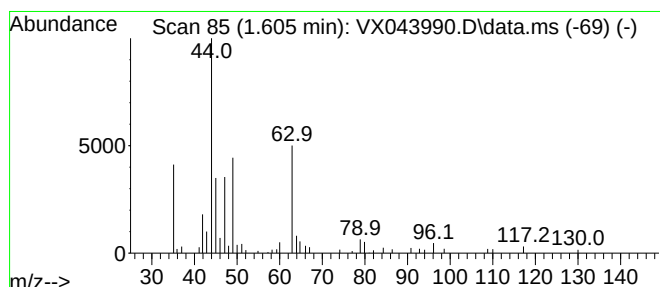
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.605 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.605	8.67 ug/l	63057	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl methyl sulfoxide	126	C3H7ClOS	005331-57-7	17
2	N-Methyltaurine	139	C3H9NO3S	000107-68-6	9
3	Phosgene	98	CCl2O	000075-44-5	7
4	Methan-d3-ol	35	CHD3O	001849-29-2	4
5	3-Azabicyclo[3.2.2]nonane	125	C8H15N	000283-24-9	4



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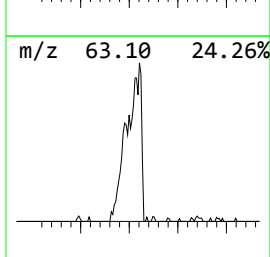
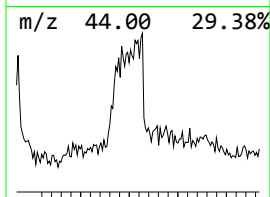
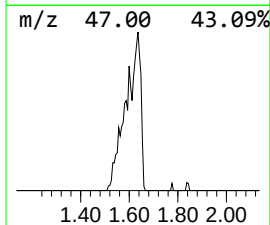
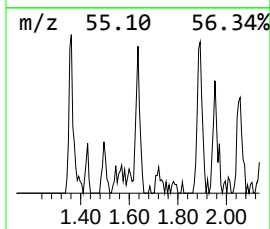
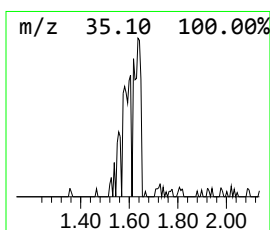
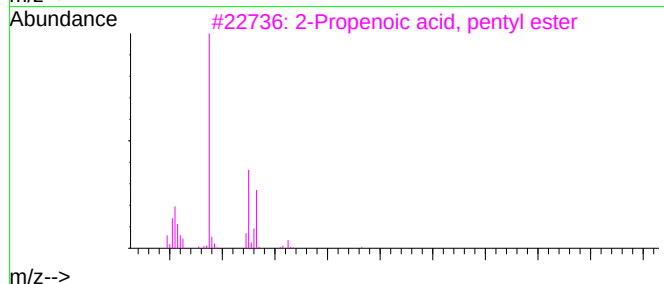
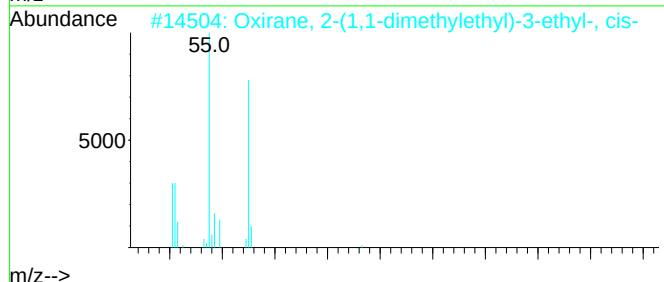
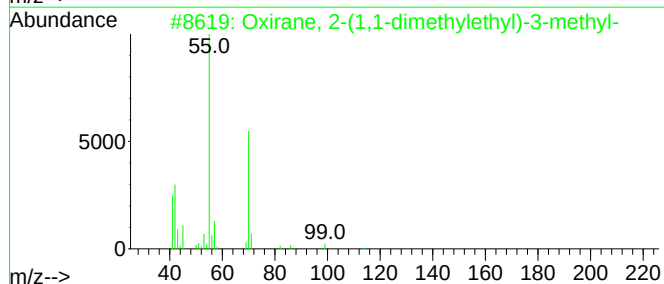
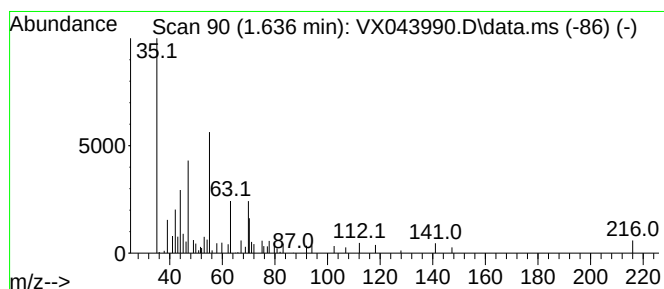
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown1.636 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.636	6.15 ug/l	44750	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, 2-(1,1-dimethylethyl)-3...	114	C7H14O	053897-30-6	22
2	Oxirane, 2-(1,1-dimethylethyl)-3...	128	C8H16O	036099-44-2	10
3	2-Propenoic acid, pentyl ester	142	C8H14O2	002998-23-4	4
4	Methan-d3-ol	35	CHD3O	001849-29-2	3
5	6-Tridecene, (Z)-	182	C13H26	006508-77-6	2



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.605	1.605	8.7	ug/l	63057	1	5.544	363682	50.0
unknown1.636	1.636	6.2	ug/l	44750	1	5.544	363682	50.0