

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121824\
Data File : VX044392.D
Acq On : 18 Dec 2024 18:42
Operator : JC/MD
Sample : P5281-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RE115D1-20241213

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\82X121124W.M
Title : SW846 8260

Signal : TIC: VX044392.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.624	67	88	91	rBV4	21066	100129	2.27%	1.226%
2	2.313	194	201	213	rBV2	112672	225810	5.12%	2.766%
3	5.385	693	705	718	rBV2	77538	233414	5.29%	2.859%
4	5.550	721	732	742	rVV	124888	358089	8.11%	4.386%
5	5.952	787	798	809	rBV2	89919	245118	5.55%	3.002%
6	6.757	921	930	951	rBV	205045	497695	11.27%	6.095%
7	7.123	979	990	1017	rBV	2026796	4414164	100.00%	54.062%
8	8.647	1232	1240	1250	rBV	423098	664684	15.06%	8.141%
9	10.055	1465	1471	1484	rBV	402401	571361	12.94%	6.998%
10	11.079	1634	1639	1652	rBV	300203	400411	9.07%	4.904%
11	12.018	1788	1793	1803	rBV	347484	454144	10.29%	5.562%

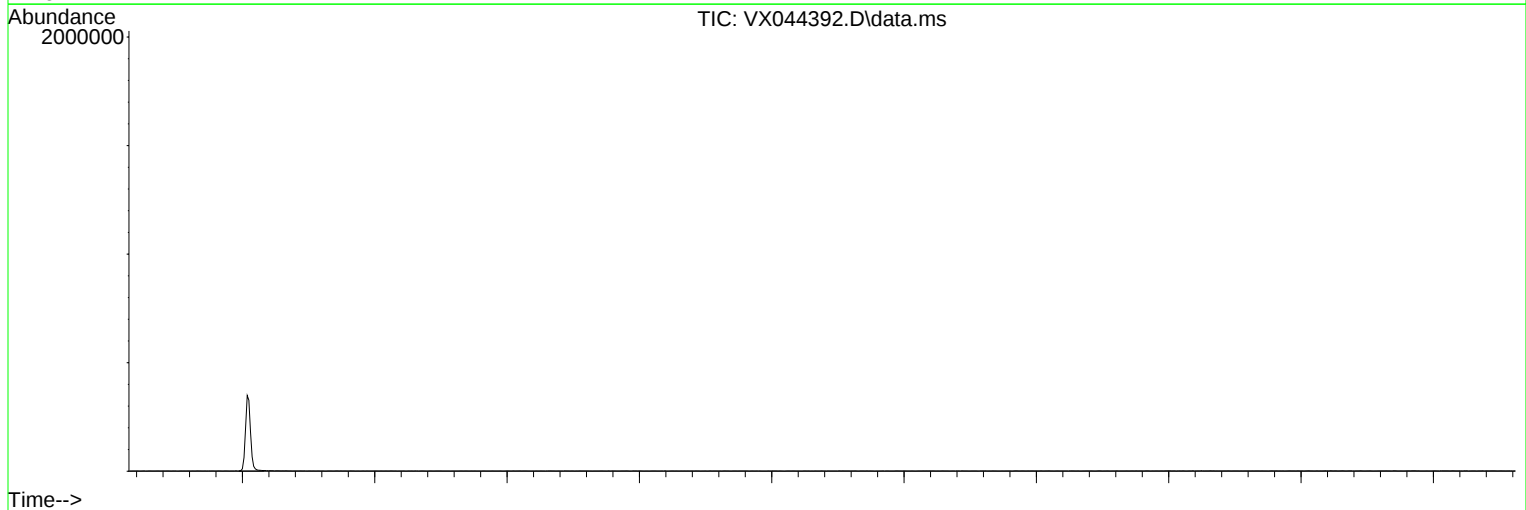
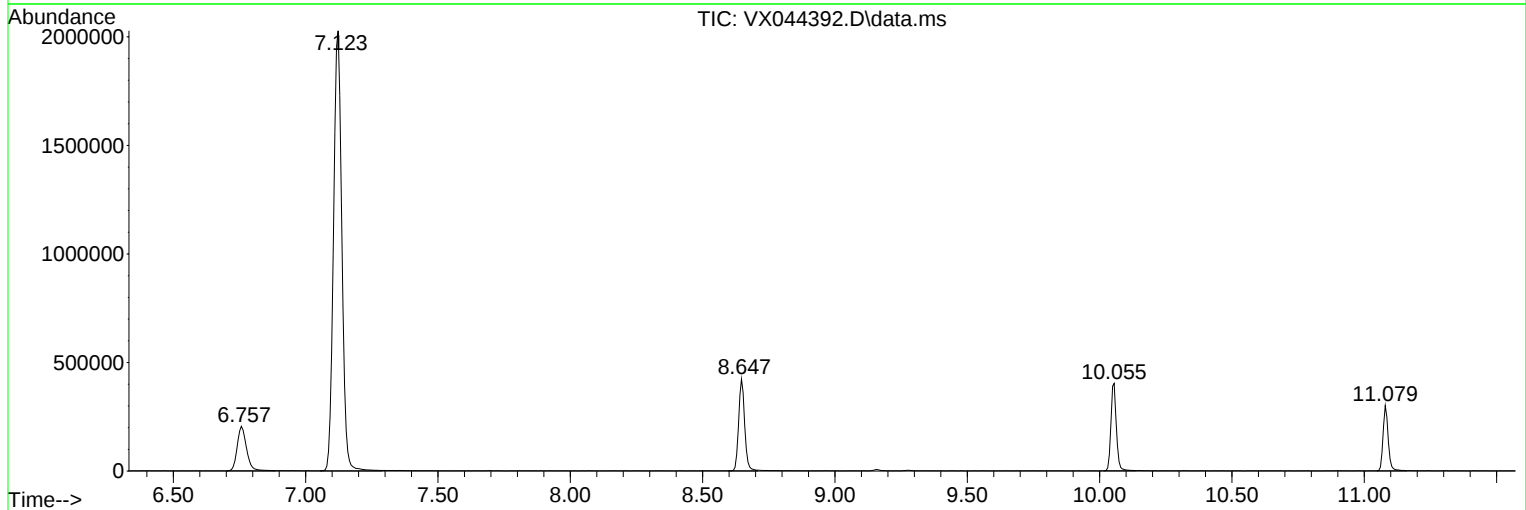
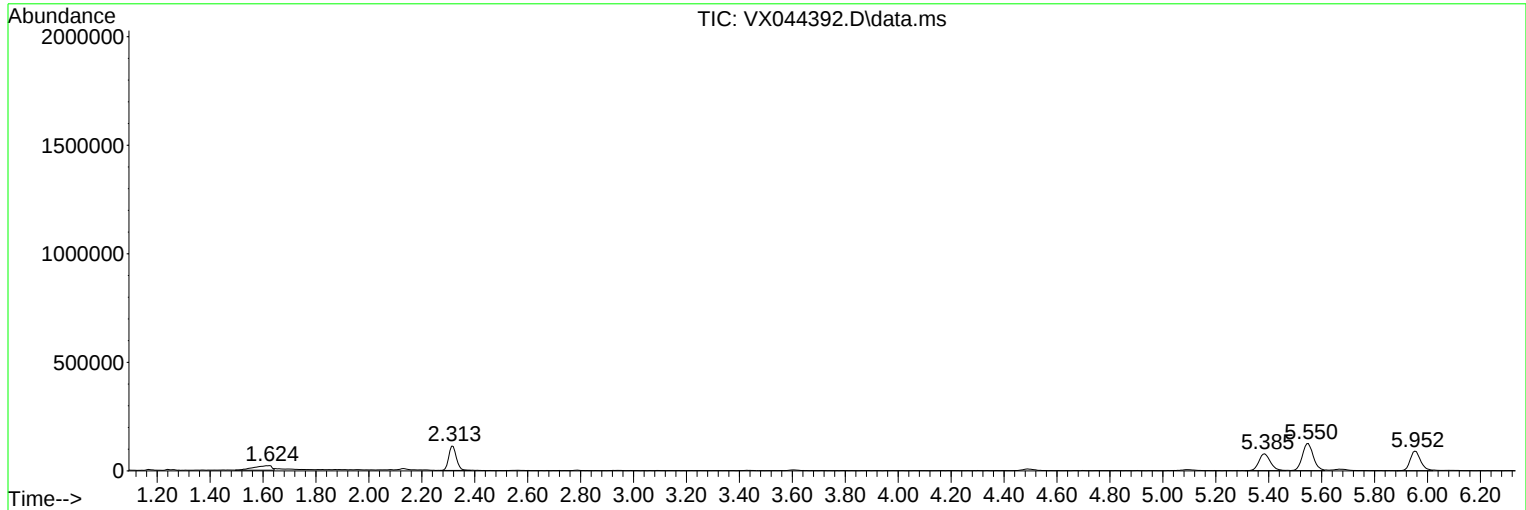
Sum of corrected areas: 8165019

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121124W.M
Quant Title : SW846 8260

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



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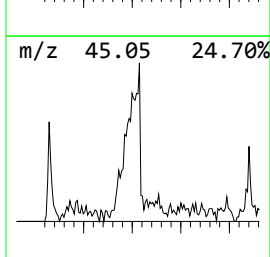
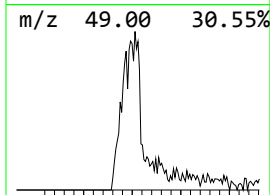
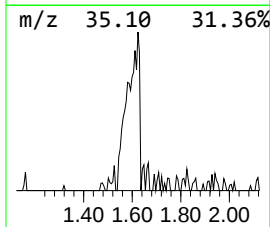
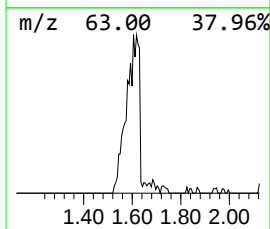
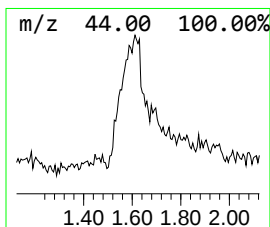
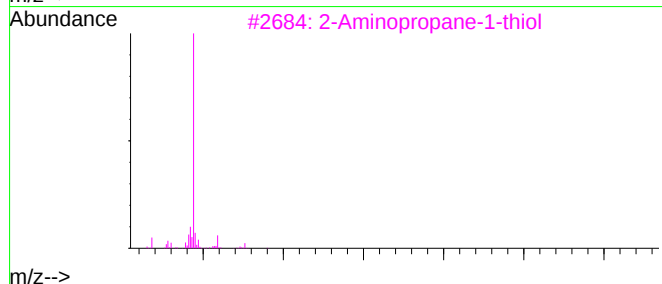
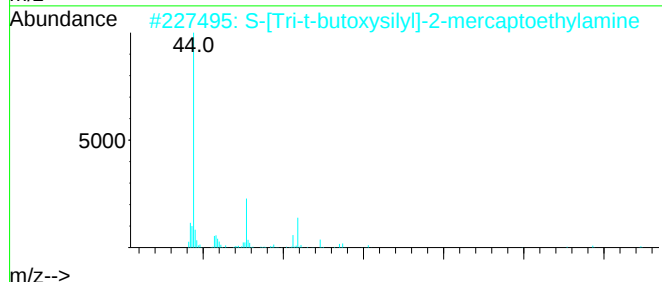
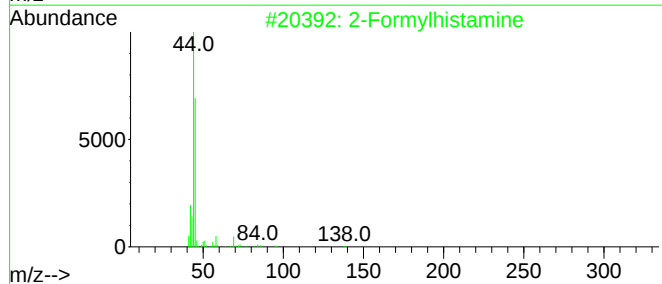
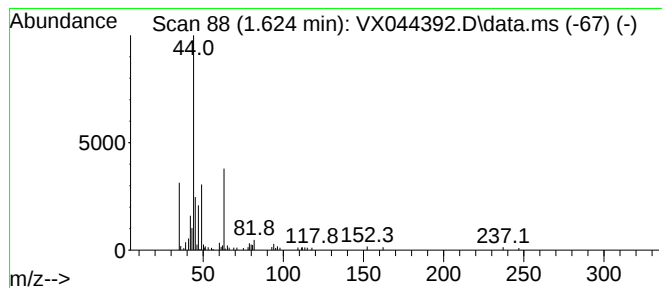
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121124W.M
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TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.624 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.624	13.98 ug/l	100129	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Formylhistamine	139	C6H9N3O	1000132-95-8	10
2			S-[Tri-t-butoxysilyl]-2-mercapto...	323	C14H33NO3SSi	1000252-63-8	10
3			2-Aminopropane-1-thiol	91	C3H9NS	010229-29-5	9
4			Dimethylamine	45	C2H7N	000124-40-3	9
5			D-Alanine	89	C3H7NO2	000338-69-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.624	1.624	14.0	ug/l	100129	1	5.550	358089	50.0