

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122324\
Data File : VX044470.D
Acq On : 23 Dec 2024 11:27
Operator : JC/MD
Sample : P5317-06 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-04-20241216

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\82X121124W.M
Title : SW846 8260

Signal : TIC: VX044470.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.593	69	83	84	rBV3	18527	56365	6.73%	1.278%
2	1.788	113	115	129	rVB6	3248	8935	1.07%	0.203%
3	5.379	693	704	720	rBV2	97731	293645	35.09%	6.657%
4	5.544	720	731	745	rBV2	157311	455625	54.44%	10.329%
5	5.952	788	798	811	rBV	108808	298696	35.69%	6.771%
6	6.757	921	930	945	rBV	251415	617737	73.81%	14.004%
7	8.647	1231	1240	1253	rBV	507239	836918	100.00%	18.973%
8	10.049	1465	1470	1484	rBV	511549	718055	85.80%	16.278%
9	11.079	1634	1639	1649	rBV	396947	513665	61.38%	11.645%
10	12.018	1788	1793	1806	rBV	481394	611436	73.06%	13.861%

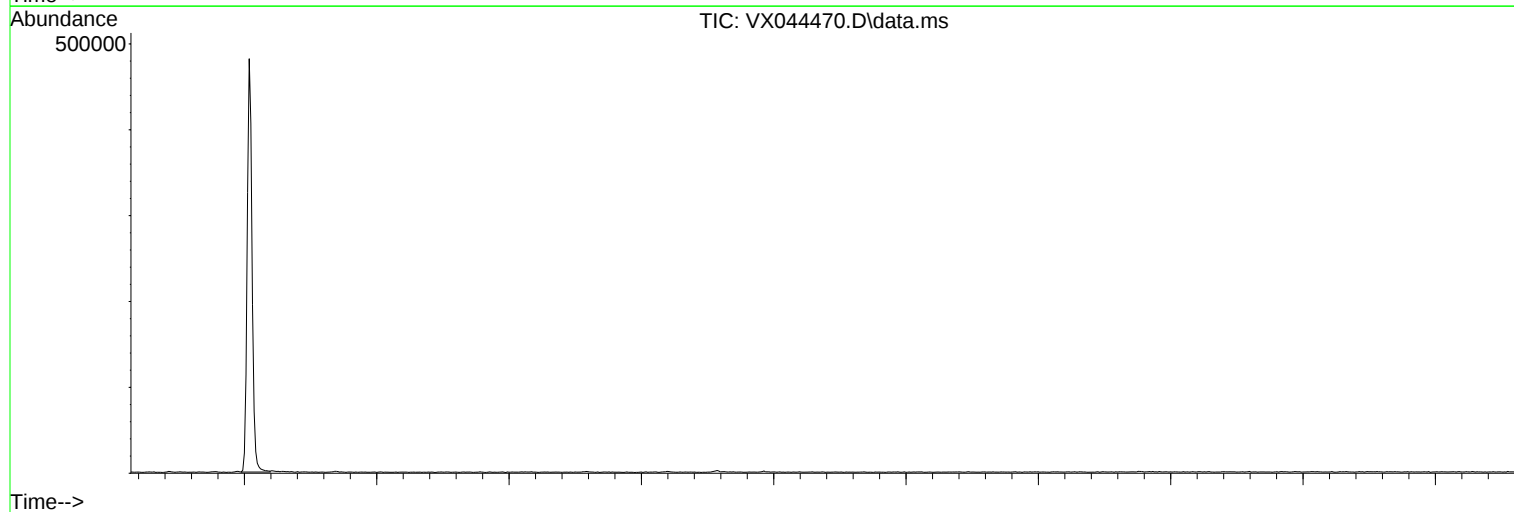
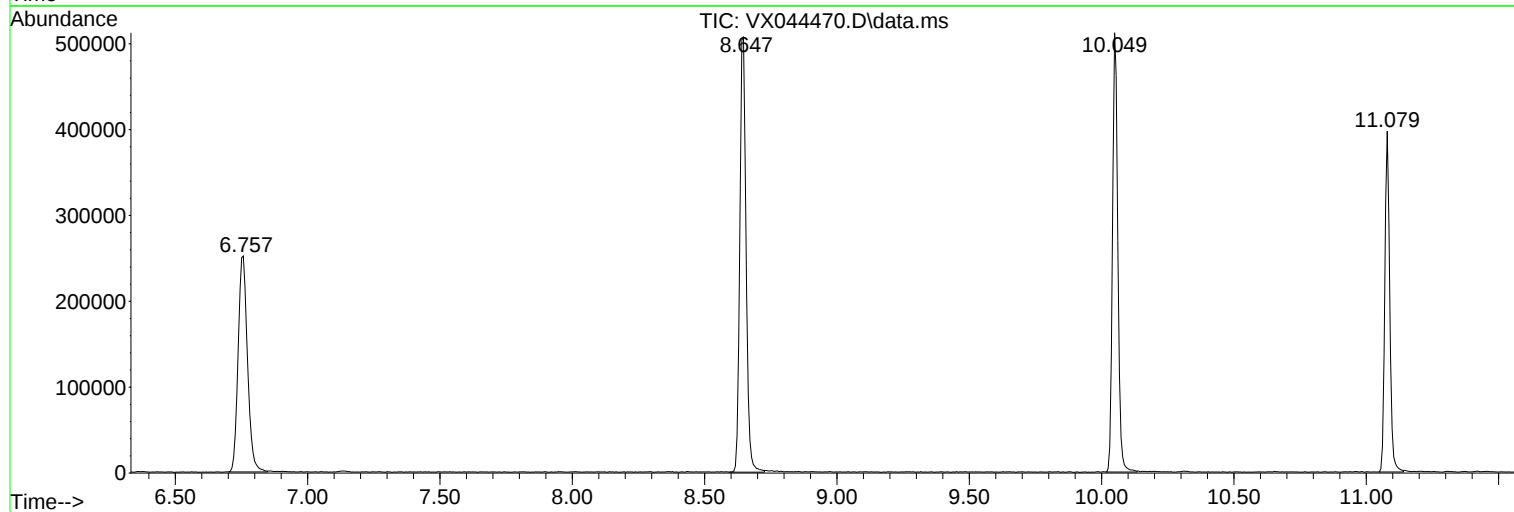
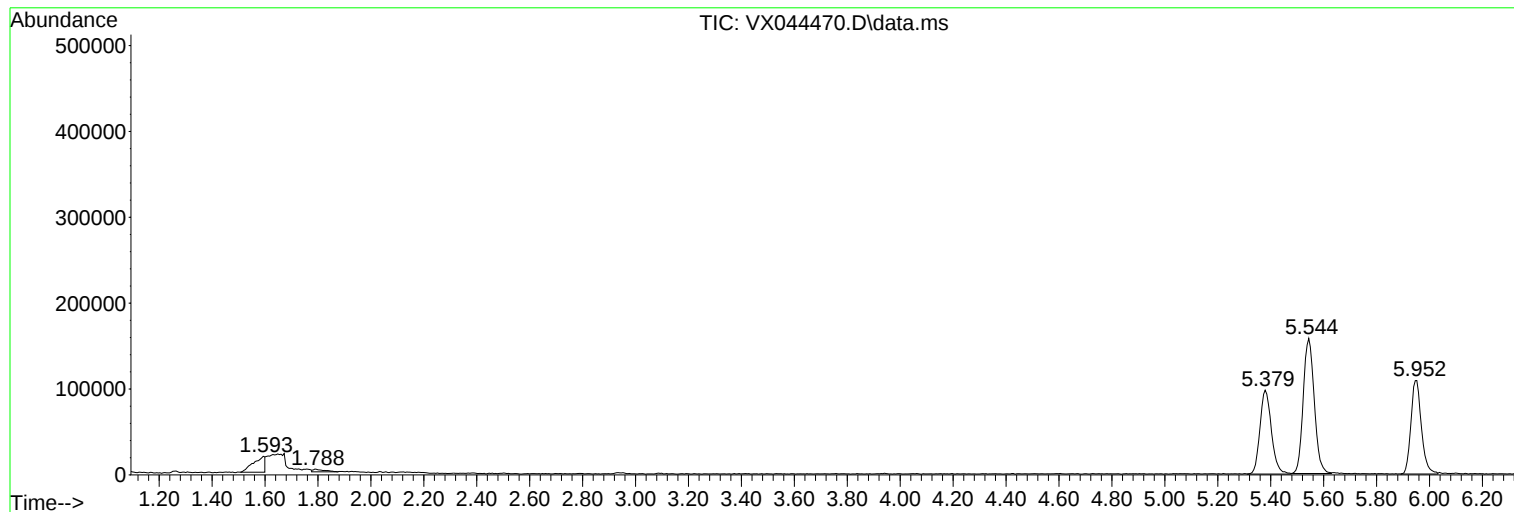
Sum of corrected areas: 4411077

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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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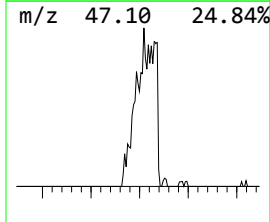
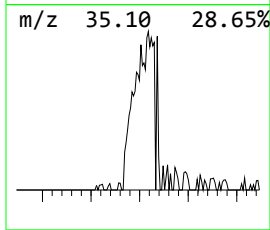
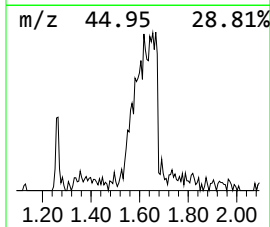
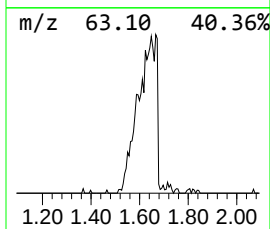
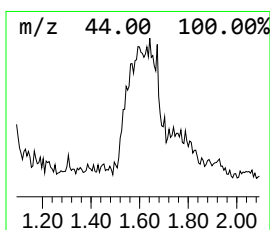
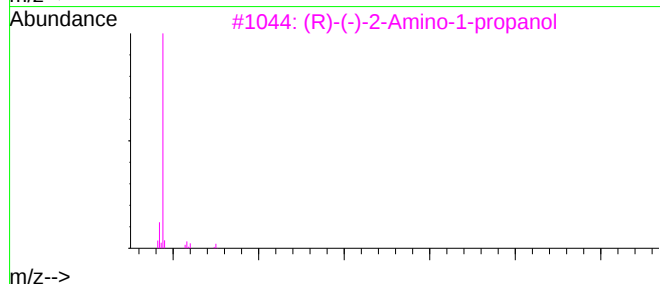
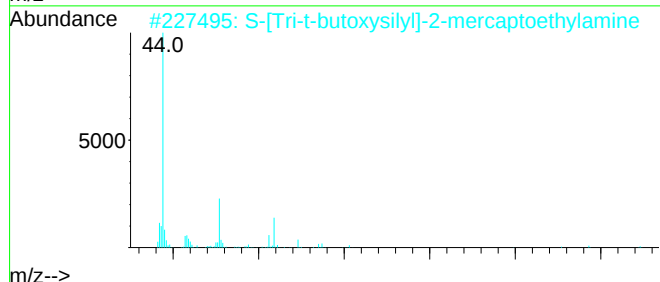
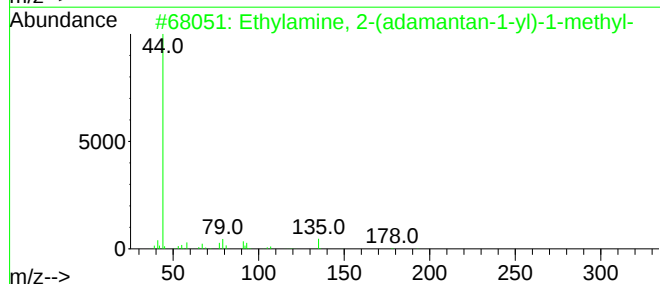
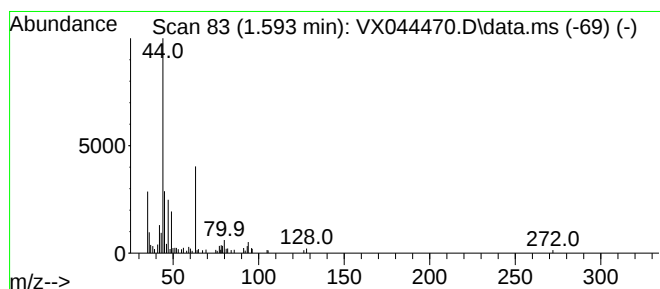
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Peak Number 1 unknown1.593 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.593	6.19 ug/l	56365	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylamine, 2-(adamantan-1-yl)-1...	193	C13H23N	1000310-59-0	10
2	S-[Tri-t-butoxysilyl]-2-mercapto...	323	C14H33NO3SSi	1000252-63-8	10
3	(R)-(-)-2-Amino-1-propanol	75	C3H9NO	035320-23-1	9
4	Propanoyl chloride	92	C3H5ClO	000079-03-8	9
5	Dimethyl-(6-methyl-2-thioxo-[1,3...	211	C6H14NOPS2	139575-19-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.593	1.593	6.2	ug/l	56365	1	5.544	455625	50.0