

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121824\
Data File : VX044401.D
Acq On : 19 Dec 2024 00:13
Operator : JC/MD
Sample : P5317-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RE114D2-20241216

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: VX044401.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.179	10	15	22	rVB2	6956	9516	1.10%	0.216%
2	1.593	69	83	84	rBV2	17808	55106	6.37%	1.249%
3	2.130	166	171	175	rBV3	6683	9409	1.09%	0.213%
4	2.319	195	202	210	rBV2	48247	92466	10.69%	2.096%
5	4.489	551	558	567	rBV4	4653	13363	1.55%	0.303%
6	5.379	691	704	721	rBV	75178	227862	26.35%	5.165%
7	5.544	721	731	748	rVV2	117119	342263	39.58%	7.758%
8	5.952	789	798	811	rBV2	85714	236346	27.33%	5.357%
9	6.757	921	930	944	rBV2	195748	470366	54.39%	10.661%
10	7.117	978	989	1003	rBV	392741	864797	100.00%	19.601%
11	8.647	1234	1240	1250	rBV	409983	650757	75.25%	14.750%
12	10.055	1465	1471	1479	rBV	392355	558551	64.59%	12.660%
13	11.079	1634	1639	1650	rBV	311473	403304	46.64%	9.141%
14	12.018	1788	1793	1803	rBV	356663	477867	55.26%	10.831%

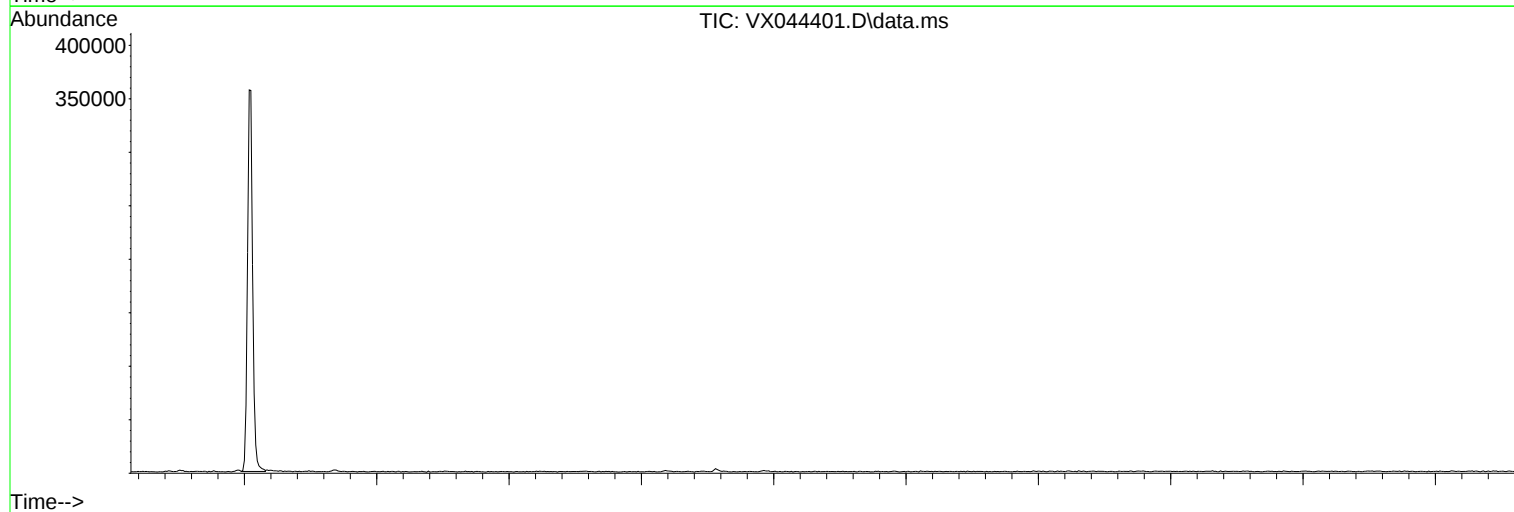
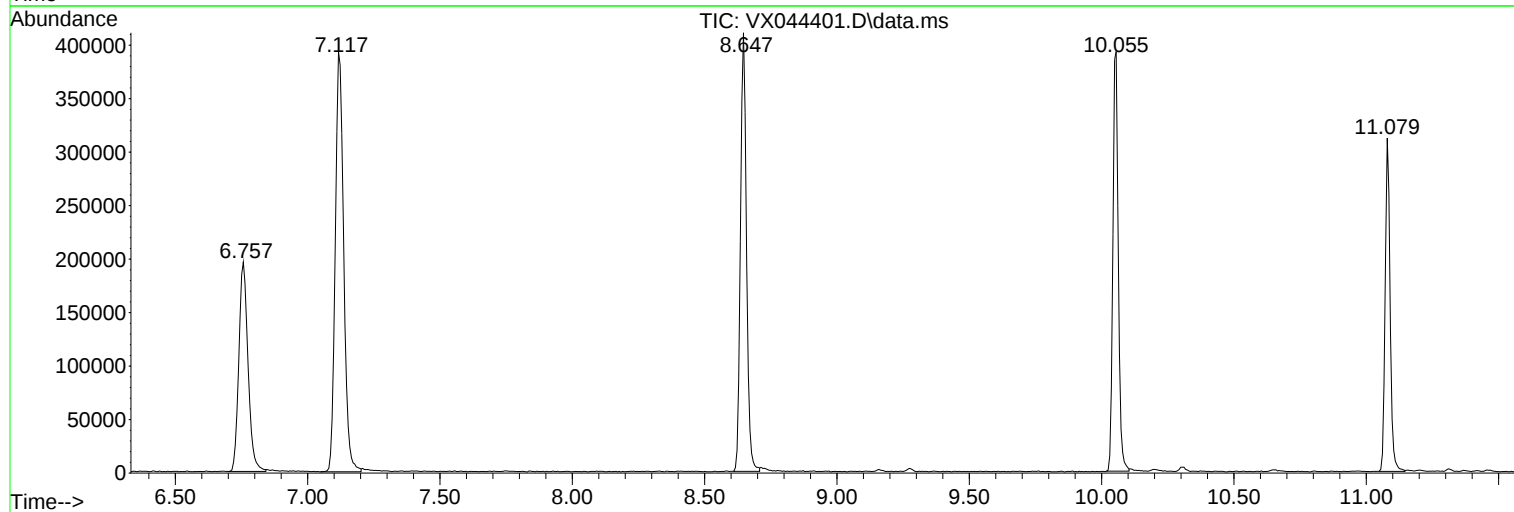
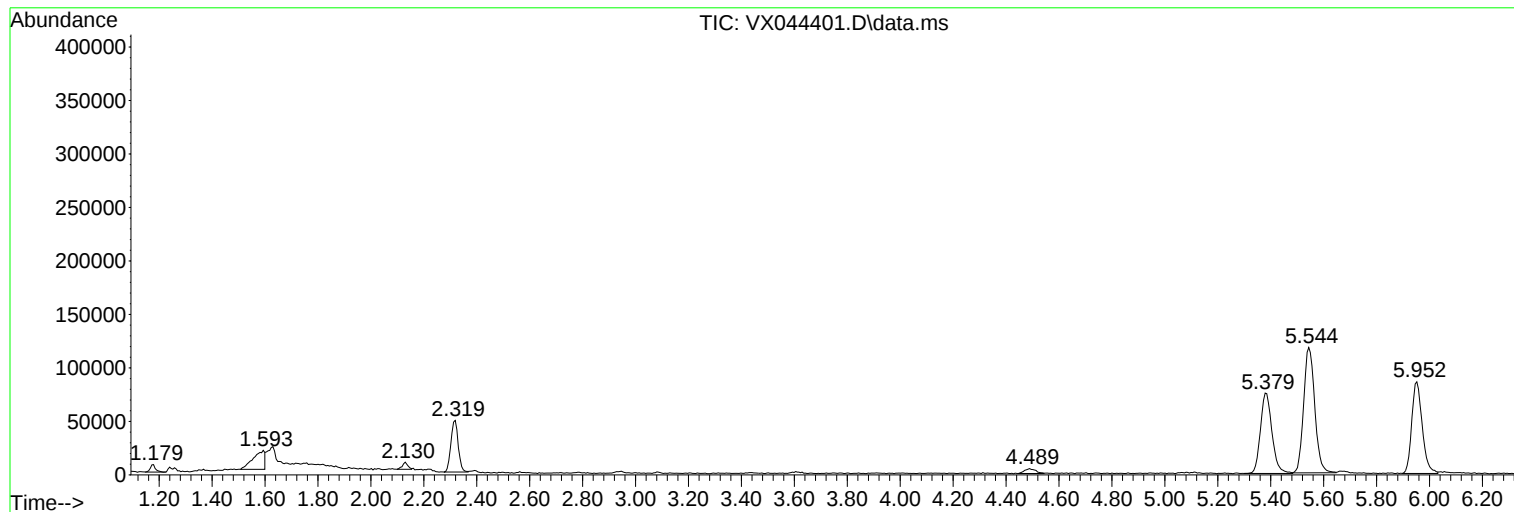
Sum of corrected areas: 4411973

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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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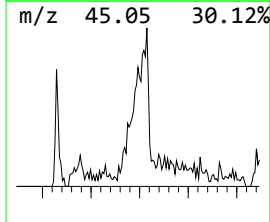
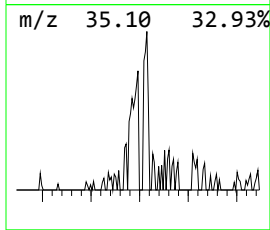
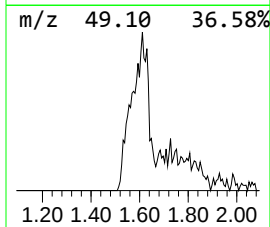
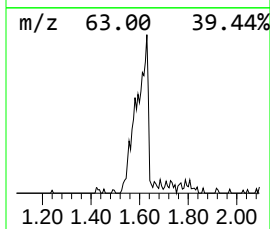
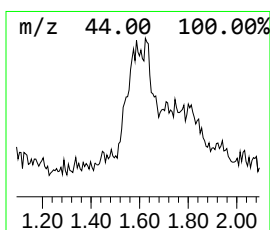
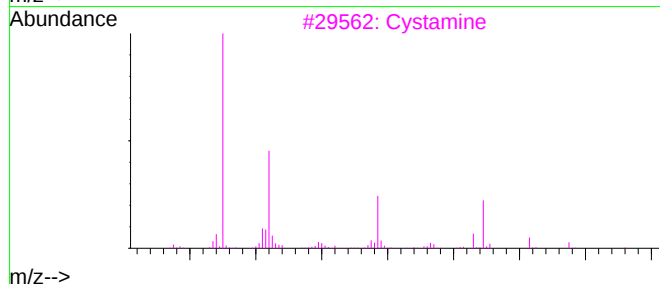
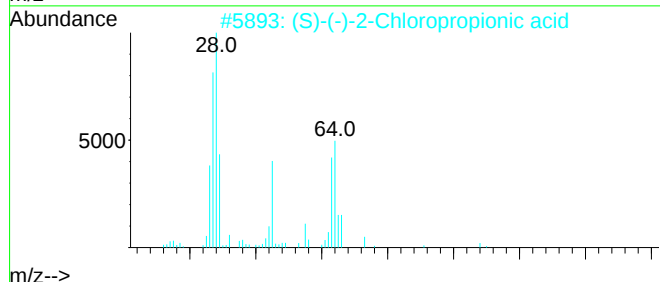
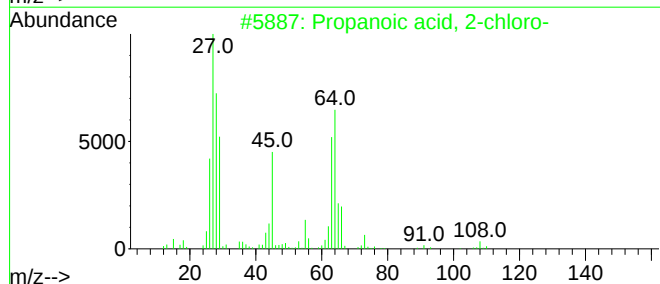
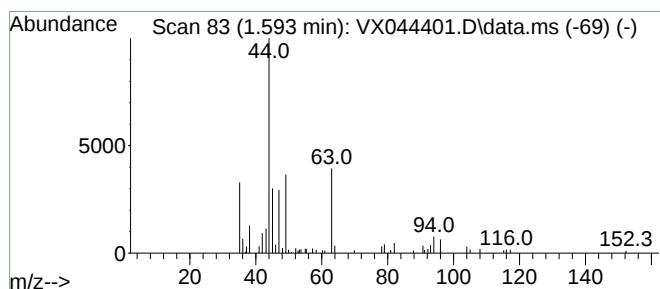
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.593 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.593	8.05 ug/l	55106	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	12
2	(S)-(-)-2-Chloropropionic acid	108	C3H5ClO2	029617-66-1	12
3	Cystamine	152	C4H12N2S2	000051-85-4	9
4	Norpseudoephedrine	151	C9H13NO	036393-56-3	9
5	Topotecan	421	C23H23N3O5	1000131-70-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.593	1.593	8.1	ug/l	55106	1	5.550	342263	50.0