

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX123124\
 Data File : VX044552.D
 Acq On : 30 Dec 2024 18:28
 Operator : JC/MD
 Sample : P5376-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TT149S1-20241218

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: VX044552.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.605	69	85	86	rBV2	17572	61267	8.89%	1.623%
2	3.117	324	333	342	rBV	38934	88097	12.78%	2.334%
3	5.385	691	705	720	rBV	86134	251086	36.42%	6.653%
4	5.543	722	731	744	rVV	125188	361357	52.41%	9.575%
5	5.952	788	798	811	rBV	94853	257562	37.35%	6.825%
6	6.757	920	930	944	rBV	203910	494063	71.65%	13.092%
7	7.129	984	991	1003	rVB3	15003	35045	5.08%	0.929%
8	8.647	1234	1240	1256	rBV	430784	689512	100.00%	18.271%
9	9.275	1338	1343	1350	rBV3	7044	11170	1.62%	0.296%
10	10.055	1465	1471	1482	rBV	400924	580601	84.20%	15.385%
11	11.079	1634	1639	1656	rBV	332423	437379	63.43%	11.590%
12	12.018	1788	1793	1807	rBV	390005	506738	73.49%	13.428%

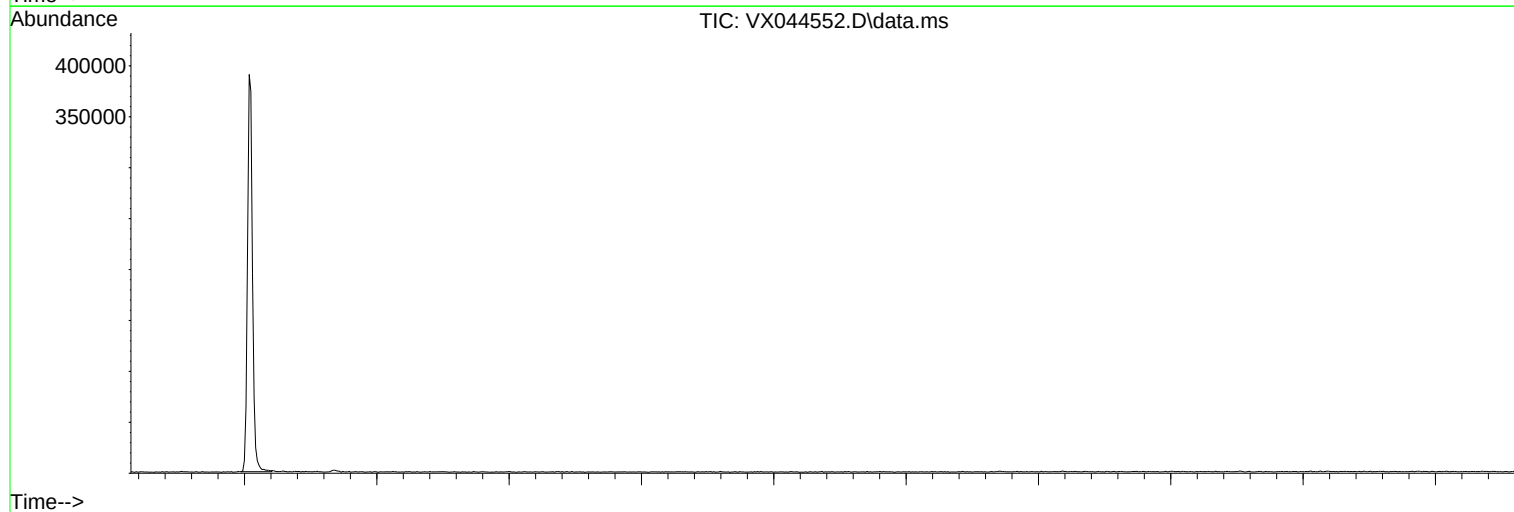
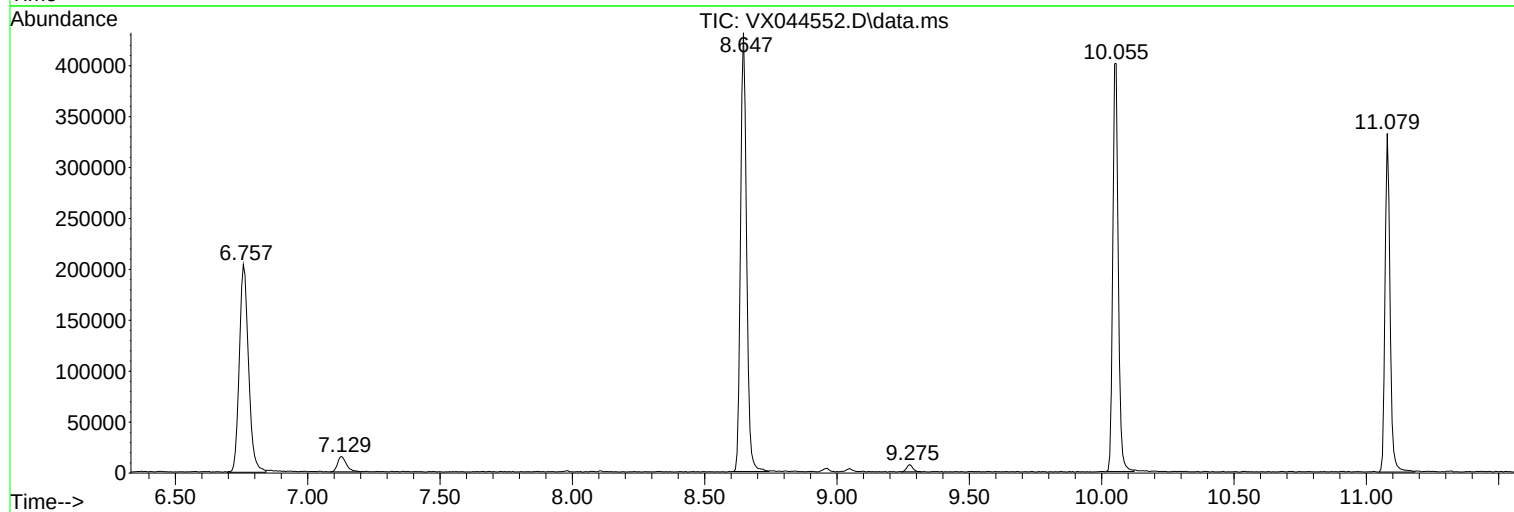
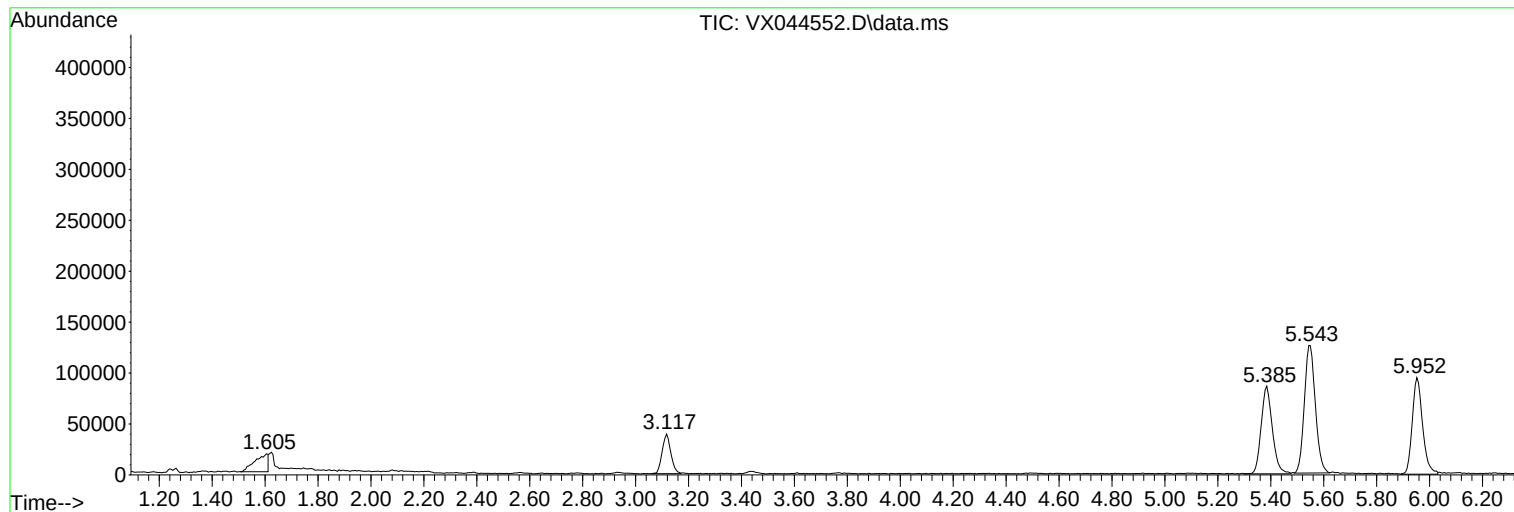
Sum of corrected areas: 3773877

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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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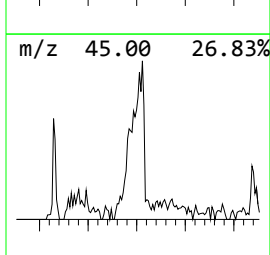
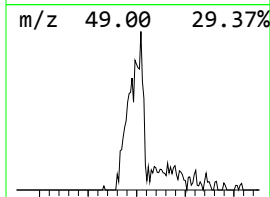
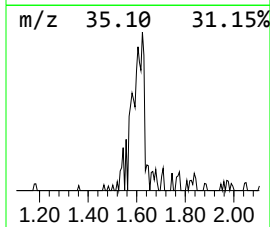
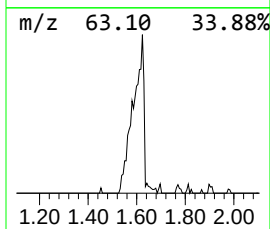
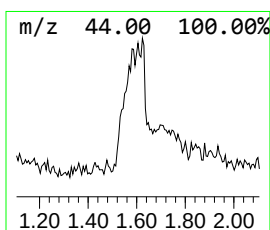
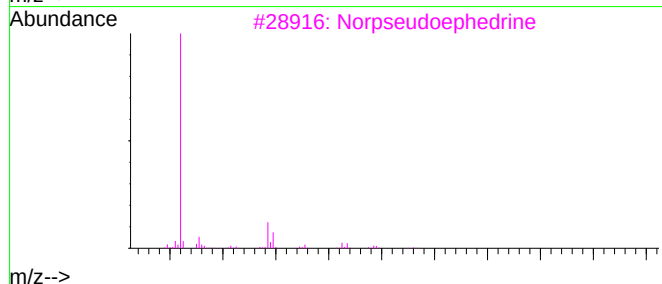
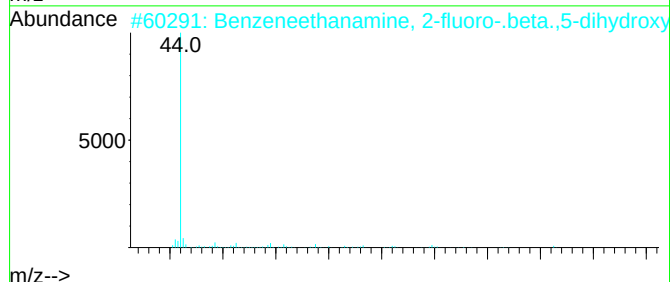
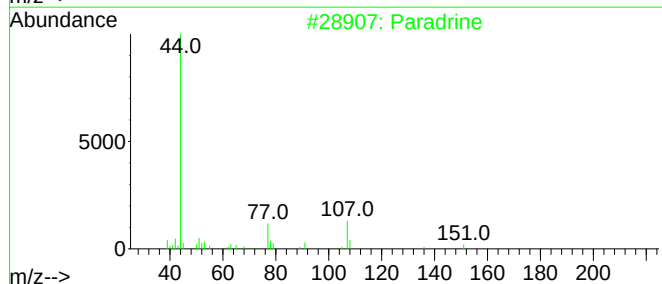
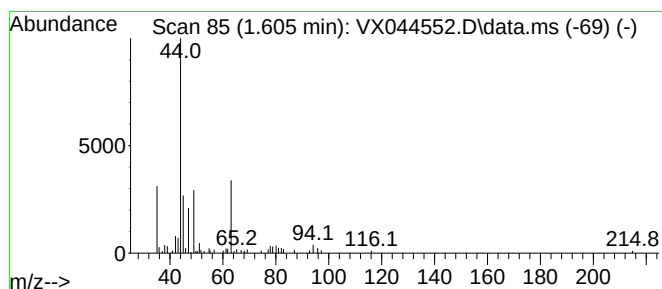
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Peak Number 1 unknown1.605 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.605	8.48 ug/l	61267	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Paradrine	151	C9H13NO	000103-86-6	10
2	Benzeneethanamine, 2-fluoro-.bet...	185	C9H12FNO2	103439-07-2	9
3	Norpseudoephedrine	151	C9H13NO	036393-56-3	9
4	2-Heptanamine, 5-methyl-	129	C8H19N	053907-81-6	9
5	Atomoxetine	255	C17H21NO	083015-26-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.605	1.605	8.5	ug/l	61267	1	5.550	361357	50.0