

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112524\
Data File : VX043978.D
Acq On : 25 Nov 2024 11:55
Operator : JC/MD
Sample : VX1125MBL01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VX1125MBL01

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\82X112124W.M
Title : SW846 8260

Signal : TIC: VX043978.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	31	rBV4	5130	7918	1.09%	0.204%
2	1.612	68	86	87	rBV7	17681	75412	10.34%	1.941%
3	2.941	297	304	310	rBV5	4272	10533	1.44%	0.271%
4	5.379	693	704	716	rBV	87828	256696	35.20%	6.608%
5	5.538	719	730	747	rBV2	128786	378361	51.88%	9.740%
6	5.946	788	797	813	rBV	101086	276451	37.90%	7.117%
7	6.751	918	929	944	rBV	219337	535091	73.37%	13.775%
8	8.647	1233	1240	1254	rBV	443273	729348	100.00%	18.775%
9	10.049	1465	1470	1489	rBV	439884	628568	86.18%	16.181%
10	11.079	1634	1639	1654	rBV	339907	450356	61.75%	11.593%
11	12.018	1788	1793	1807	rBV	412206	535898	73.48%	13.795%

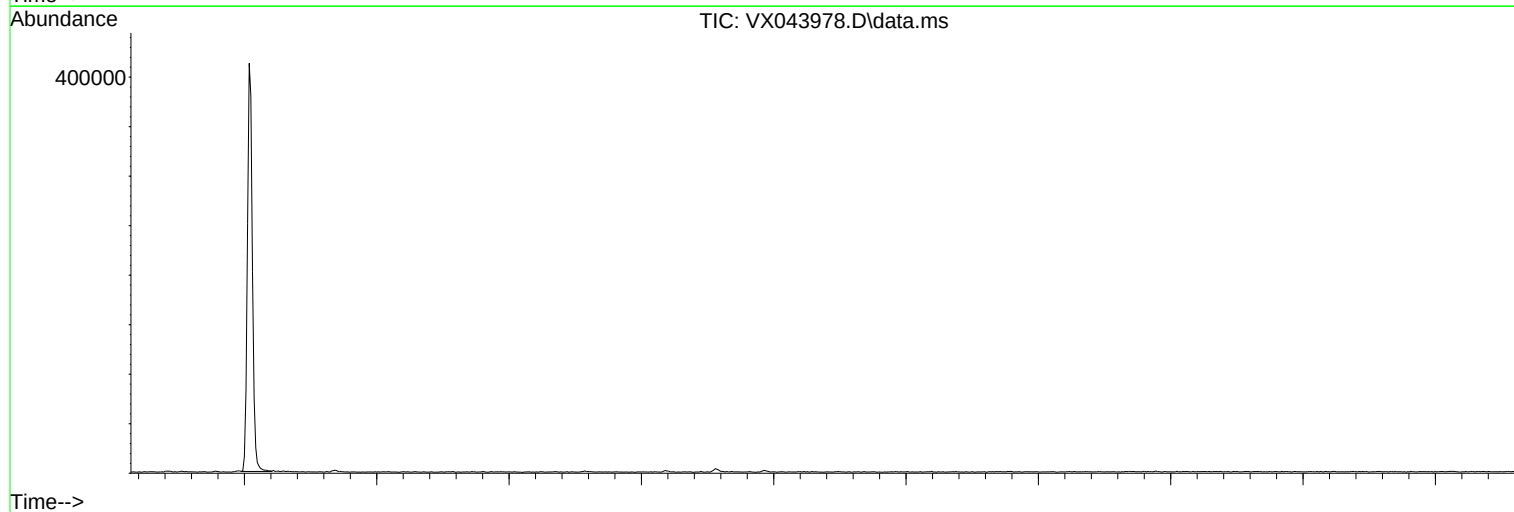
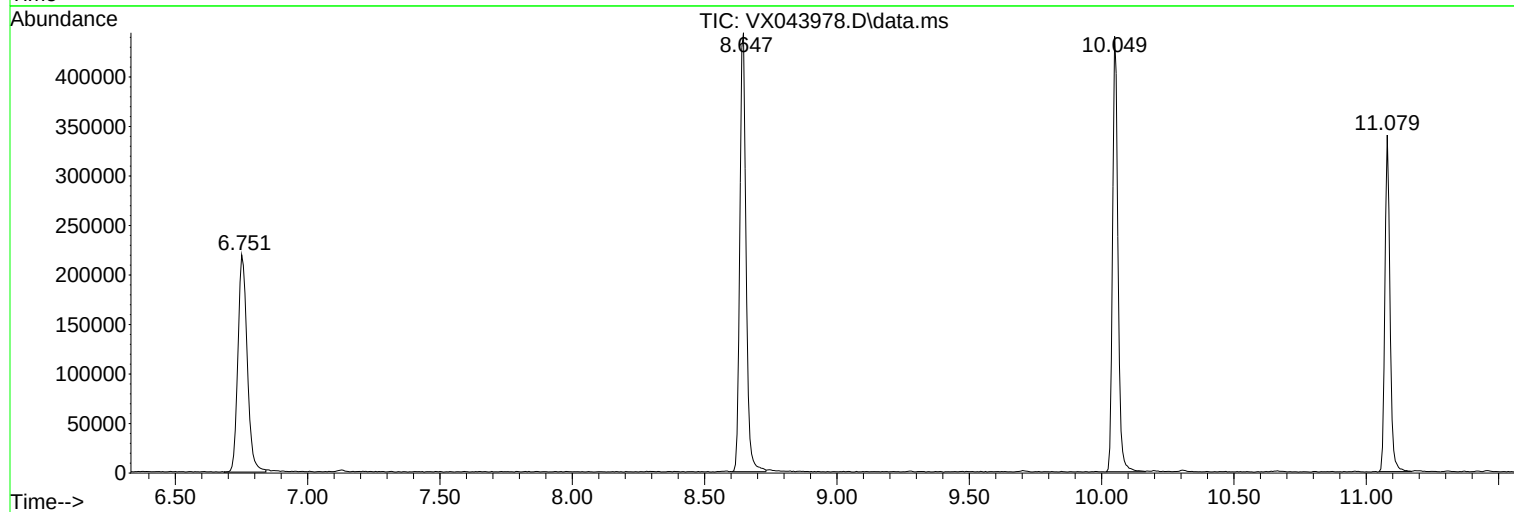
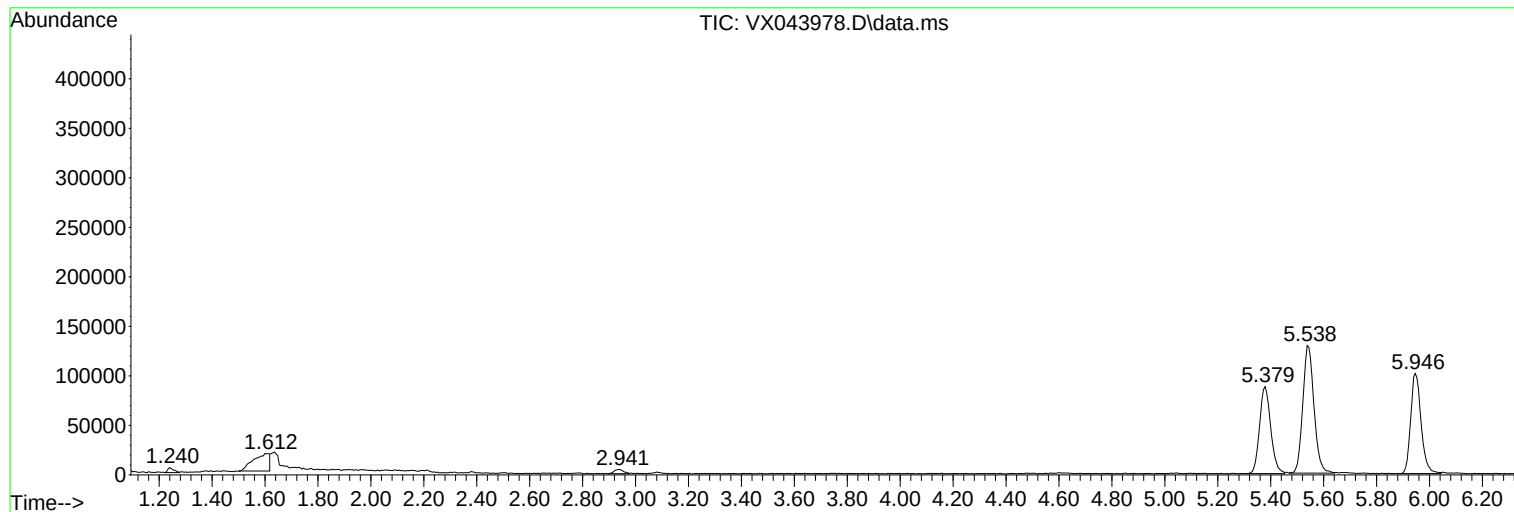
Sum of corrected areas: 3884632

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112524\
Data File : VX043978.D
Acq On : 25 Nov 2024 11:55
Operator : JC/MD
Sample : VX1125MBL01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VX1125MBL01

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112524\
Data File : VX043978.D
Acq On : 25 Nov 2024 11:55
Operator : JC/MD
Sample : VX1125MBL01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VX1125MBL01

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

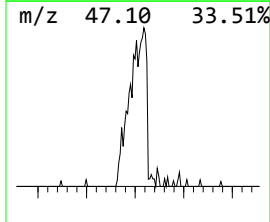
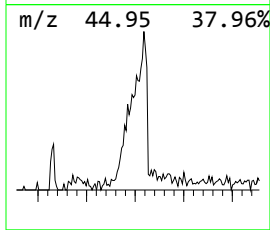
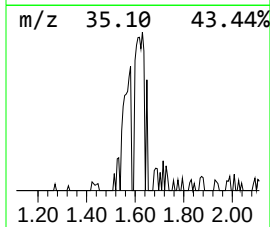
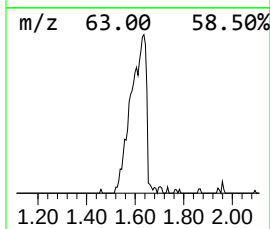
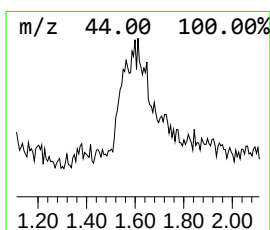
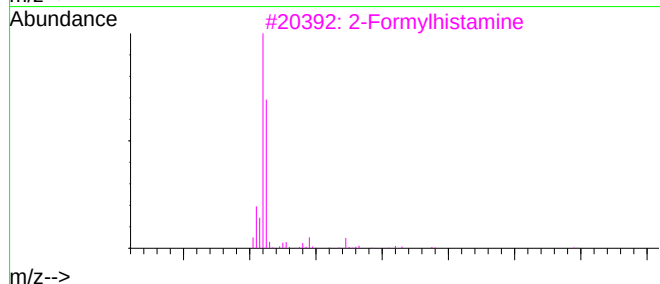
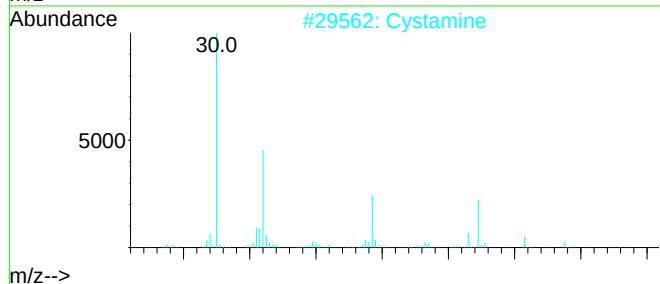
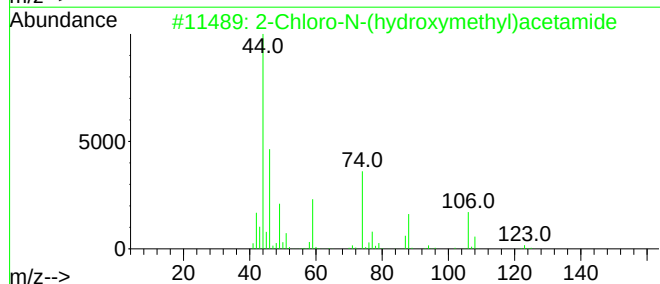
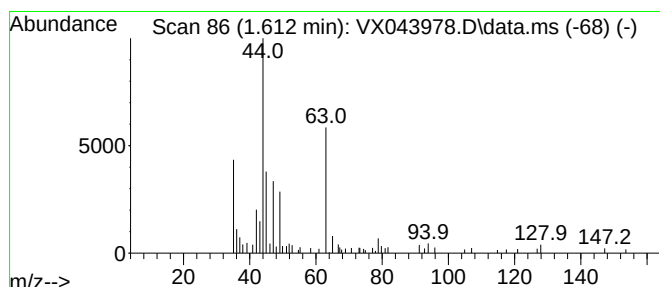
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.612 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.612	9.97 ug/l	75412	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloro-N-(hydroxymethyl)acetamide	123	C3H6ClNO2	002832-19-1	17
2			Cystamine	152	C4H12N2S2	000051-85-4	9
3			2-Formylhistamine	139	C6H9N3O	1000132-95-8	9
4			Phenylephrine	167	C9H13NO2	000059-42-7	9
5			Amidephrine	244	C10H16N2O3S	003354-67-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112524\
Data File : VX043978.D
Acq On : 25 Nov 2024 11:55
Operator : JC/MD
Sample : VX1125MBL01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VX1125MBL01

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.612	1.612	10.0	ug/l	75412	1	5.544	378361	50.0