

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111025\
 Data File : VX048544.D
 Acq On : 10 Nov 2025 16:49
 Operator : JC/MD
 Sample : Q3569-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-12

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\82X110725W.M
 Title : SW846 8260

Signal : TIC: VX048544.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.136	166	172	199	rVB	734007	1235023	20.34%	5.947%
2	2.934	295	303	316	rBV	48269	125746	2.07%	0.606%
3	3.751	422	437	469	rBV	872951	2590861	42.66%	12.477%
4	4.538	554	566	587	rBV2	57039	224265	3.69%	1.080%
5	4.983	628	639	672	rBV	506788	1827585	30.09%	8.801%
6	5.373	694	703	720	rBV2	109974	362674	5.97%	1.746%
7	5.544	720	731	749	rVB	156465	492858	8.12%	2.373%
8	5.946	786	797	802	rBV	118141	318948	5.25%	1.536%
9	6.025	802	810	831	rVV	620638	1806091	29.74%	8.697%
10	6.202	831	839	853	rVV	83353	268356	4.42%	1.292%
11	6.324	853	859	881	rVB2	44779	139890	2.30%	0.674%
12	6.745	919	928	952	rBV	286773	771026	12.70%	3.713%
13	8.635	1231	1238	1247	rBV	608528	999120	16.45%	4.811%
14	8.787	1257	1263	1275	rVB	45503	81553	1.34%	0.393%
15	9.159	1318	1324	1330	rBV	44066	76117	1.25%	0.367%
16	10.061	1463	1472	1478	rBV2	3685027	6073302	100.00%	29.247%
17	10.110	1478	1480	1489	rVB	121789	183447	3.02%	0.883%
18	10.945	1611	1617	1623	rBV	340560	443625	7.30%	2.136%
19	11.061	1631	1636	1648	rBV	581261	838720	13.81%	4.039%
20	11.829	1753	1762	1765	rBV	75352	126535	2.08%	0.609%
21	11.866	1765	1768	1773	rVB2	97044	133072	2.19%	0.641%
22	12.000	1785	1790	1798	rBV	837672	1206760	19.87%	5.811%
23	12.225	1820	1827	1834	rBV2	68142	107534	1.77%	0.518%
24	12.402	1850	1856	1868	rBV6	37575	83575	1.38%	0.402%
25	12.817	1917	1924	1929	rBV2	47648	80648	1.33%	0.388%
26	13.103	1967	1971	1974	rBV	54147	70329	1.16%	0.339%
27	13.140	1974	1977	1982	rVB3	73919	98243	1.62%	0.473%

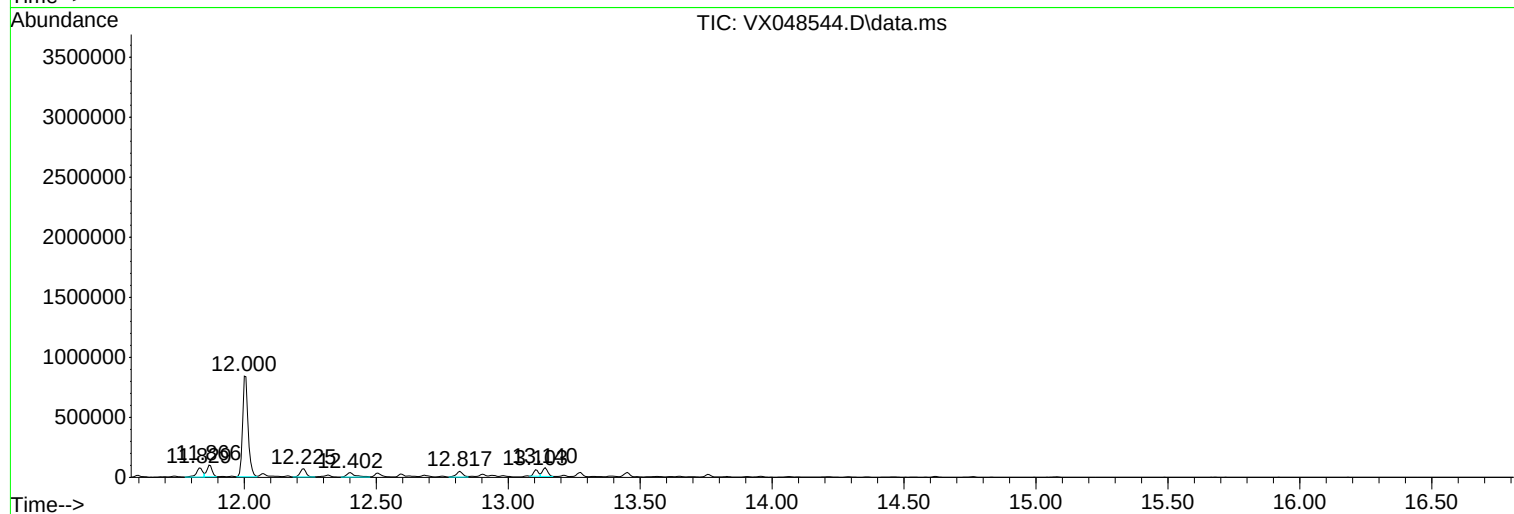
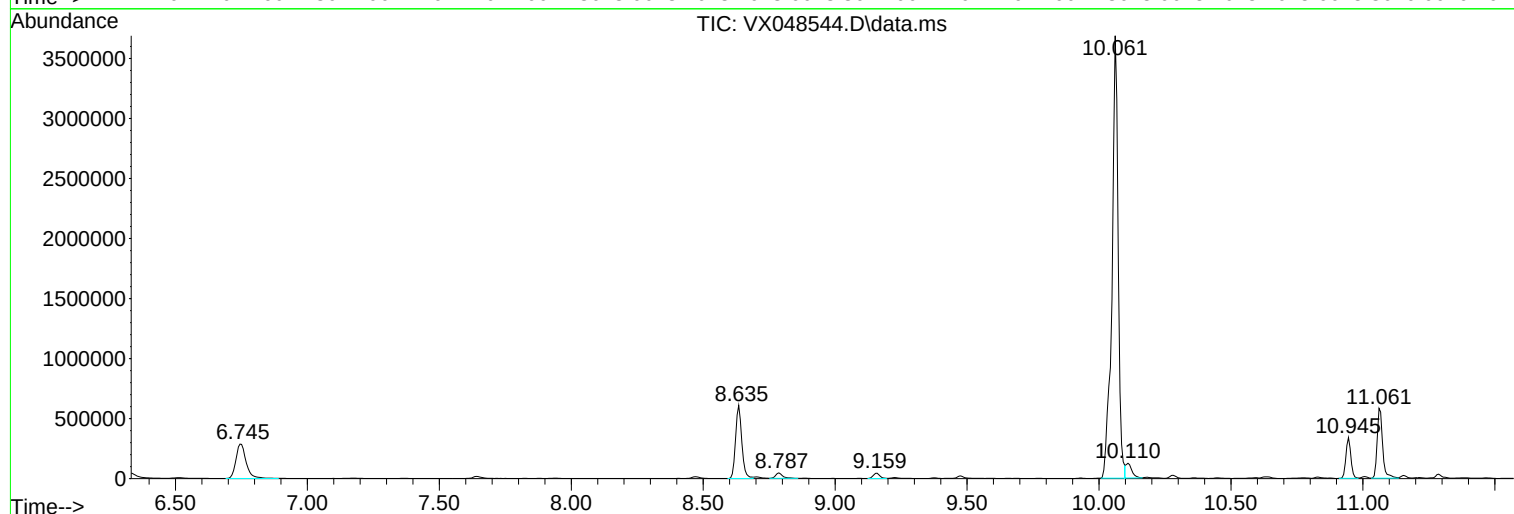
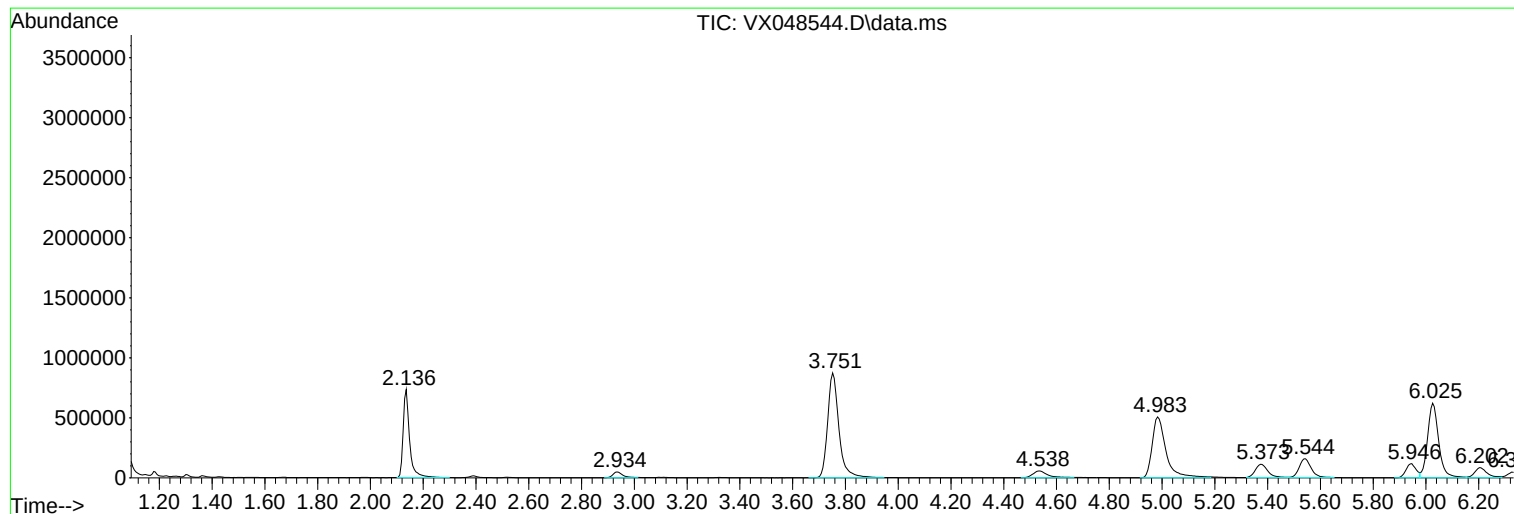
Sum of corrected areas: 20765903

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Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110725W.M
Quant Title : SW846 8260

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



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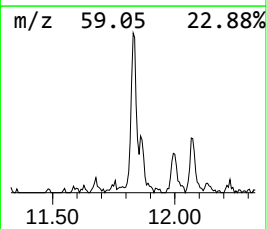
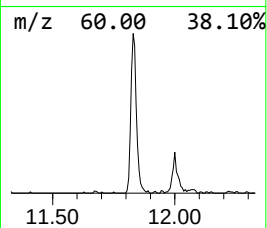
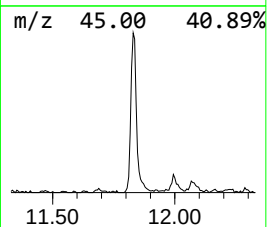
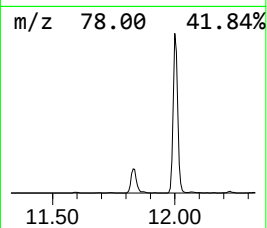
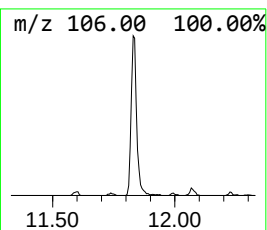
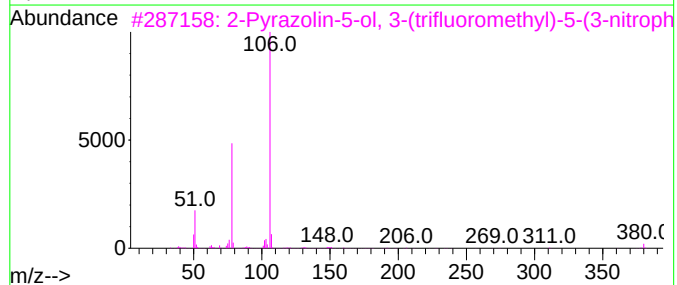
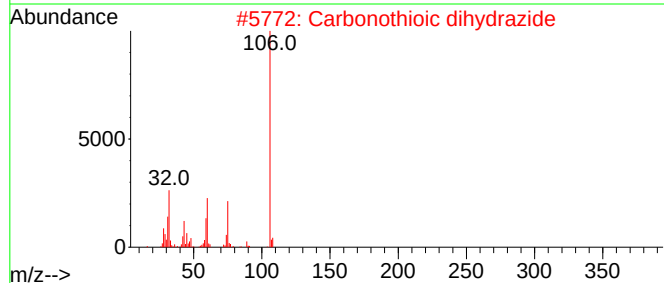
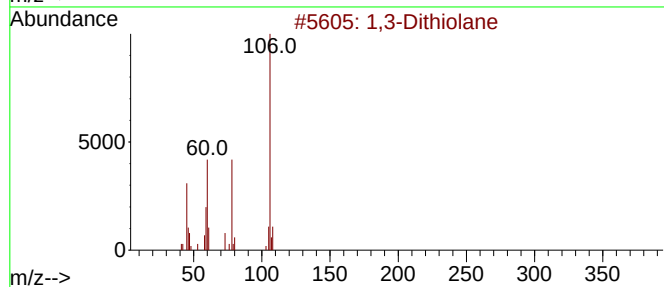
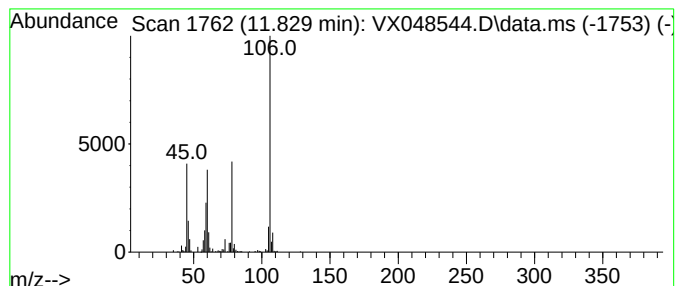
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110725W.M
Quant Title : SW846 8260

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

Peak Number 4 1,3-Dithiolane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.829	5.24 ug/l	126535	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dithiolane	106	C3H6S2	004829-04-3	91
2			Carbonothioic dihydrazide	106	CH6N4S	002231-57-4	23
3			2-Pyrazolin-5-ol, 3-(trifluorome...	380	C16H11F3N4O4	331865-32-8	17
4			2,4-Pentanedione, ion(1-), lithium	106	C5H7LiO2	018115-70-3	10
5			3-Pyridinecarboxylic acid, 2-pro...	163	C9H9NO2	025635-12-5	9



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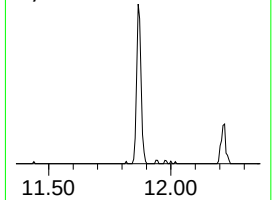
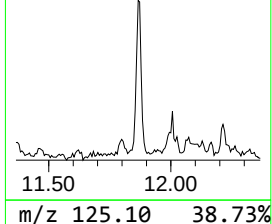
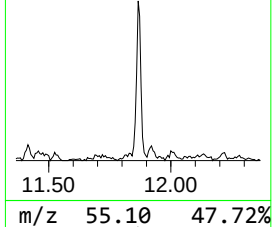
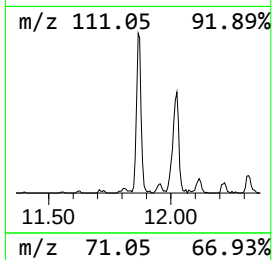
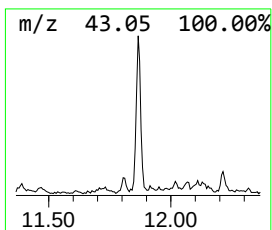
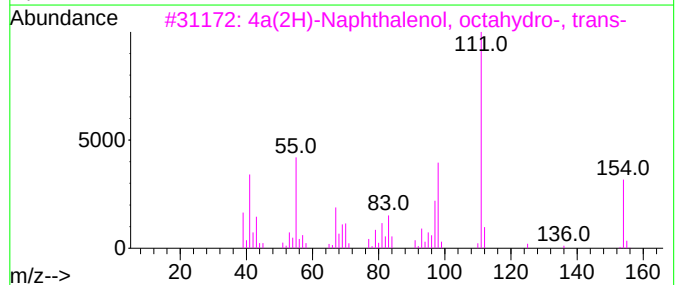
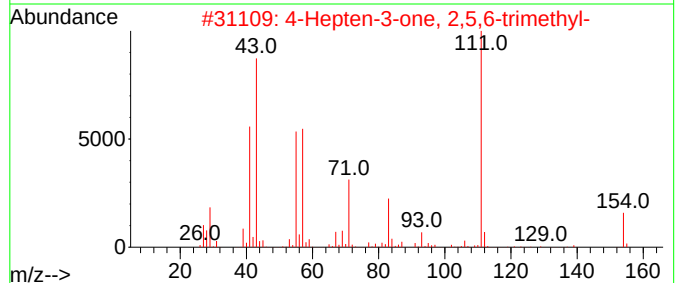
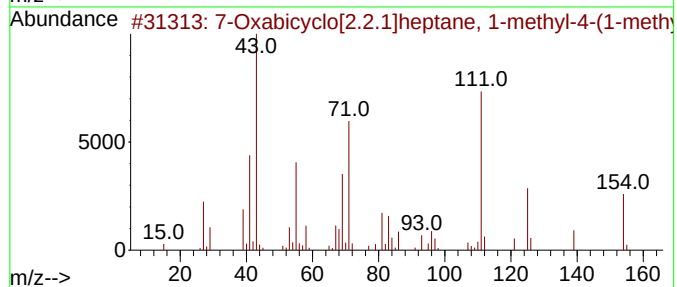
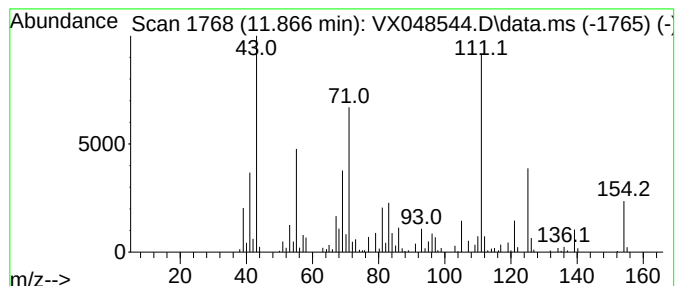
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TIC Integration Parameters: LSCINT.P

Peak Number 5 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.866	5.51 ug/l	133072	1,4-Dichlorobenzene-d4			12.006
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	7-Oxabicyclo[2.2.1]heptane, 1-me...		154	C10H18O	000470-67-7	95
2	4-Hepten-3-one, 2,5,6-trimethyl-		154	C10H18O	016466-21-0	43
3	4a(2H)-Naphthalenol, octahydro-,...		154	C10H18O	001654-87-1	38
4	Benzenamine, 3-fluoro-		111	C6H6FN	000372-19-0	30
5	4-Butyl-5-methylpyrazalone		154	C8H14N2O	1010289-28-0	30



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Dithiolane	11.829	5.2	ug/l	126535	4	12.006	1206760	50.0
7-Oxabicyclo[2....	11.866	5.5	ug/l	133072	4	12.006	1206760	50.0