

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU021623\
 Data File : VU053116.D
 Acq On : 16 Feb 2023 11:09
 Operator : JC/MD
 Sample : VU0216WBL01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK015

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.1

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_U\Method\SFAMUSIM021523.M

Title : TRACE VOA SOM01.0

Signal : TIC: VU053116.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	95	100	110	rBV	9238	14873	26.73%	3.985%
2	2.564	231	237	250	rVB	3073	6110	10.98%	1.637%
3	3.045	295	297	301	rBV3	969	5651	10.16%	1.514%
4	5.040	399	403	413	rVB	669	2884	5.18%	0.773%
5	5.661	432	436	447	rBV2	5009	20279	36.44%	5.433%
6	6.207	460	465	476	rBV	13191	49387	88.75%	13.232%
7	6.508	477	481	484	rVV	424	1743	3.13%	0.467%
8	6.639	484	488	499	rVB	8467	31471	56.55%	8.432%
9	7.536	529	531	539	rVB2	338	1064	1.91%	0.285%
10	7.830	546	550	564	rBV	17011	54887	98.63%	14.706%
11	8.108	564	568	581	rVB	610	2138	3.84%	0.573%
12	9.346	644	648	664	rBV	16756	55370	99.50%	14.835%
13	10.679	721	725	736	rVB	5885	19115	34.35%	5.121%
14	11.742	782	787	805	rVB	16596	55647	100.00%	14.910%
15	12.119	805	809	824	rVB	15678	52612	94.55%	14.096%

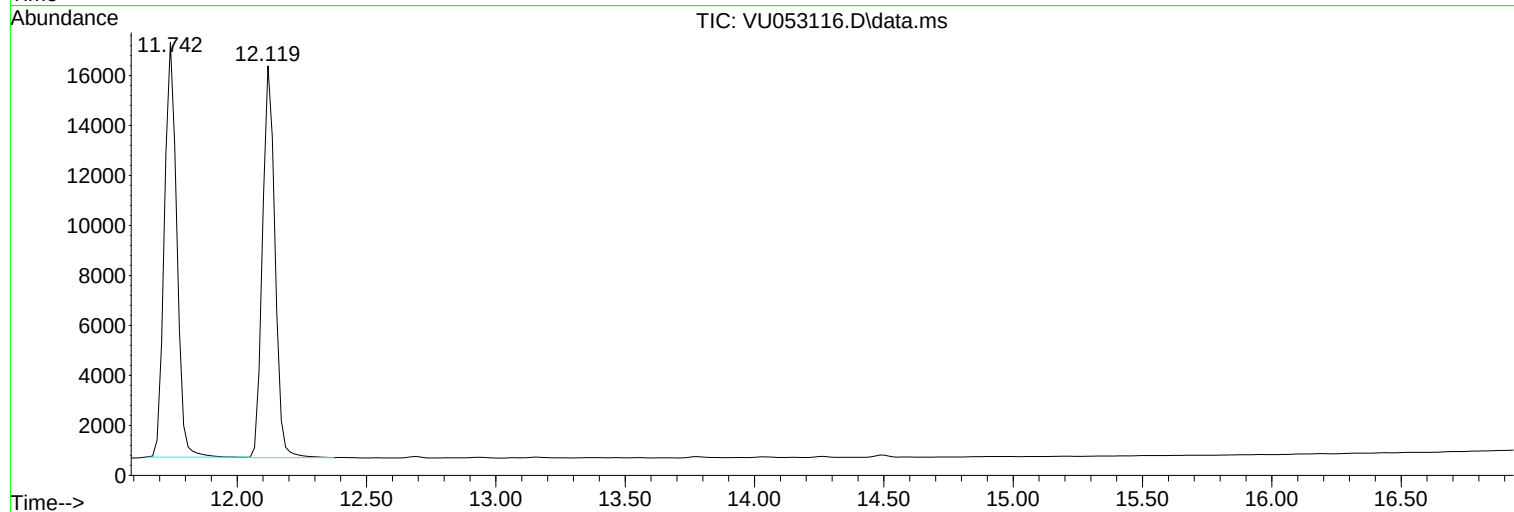
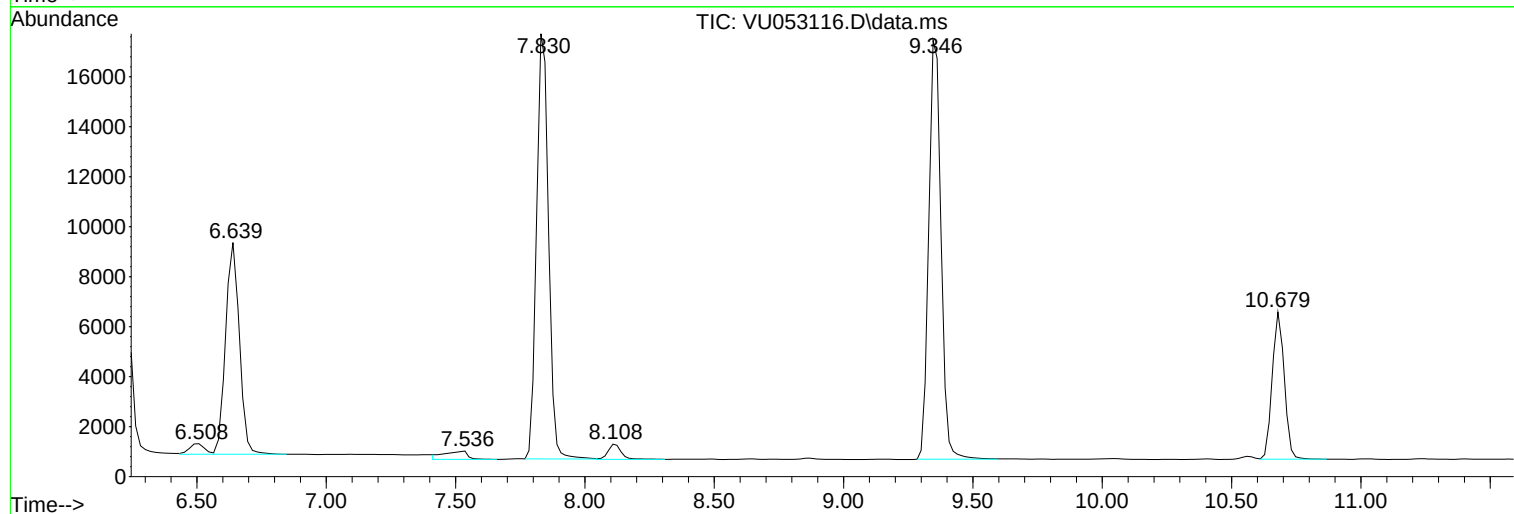
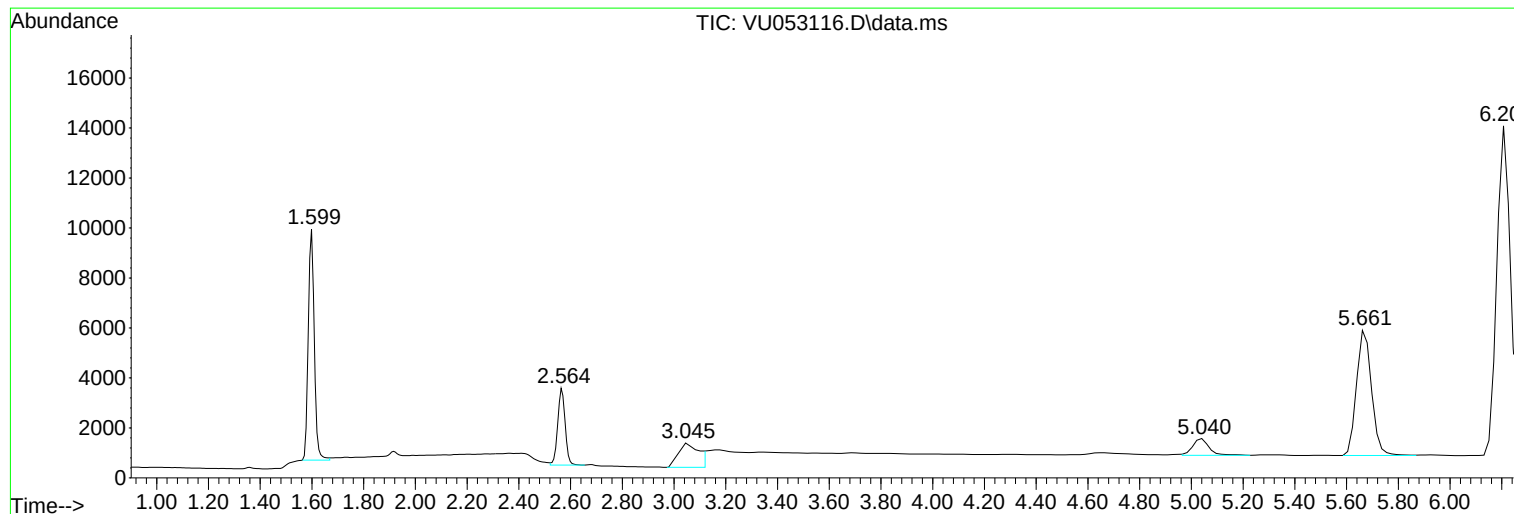
Sum of corrected areas: 373231

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUSIM021523.M
Quant Title : TRACE VOA SOM01.0

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



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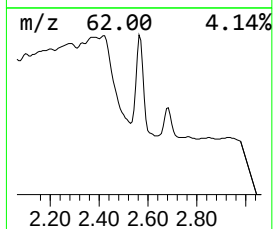
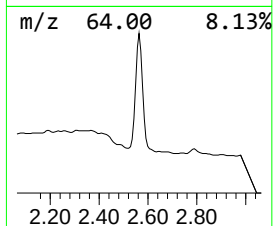
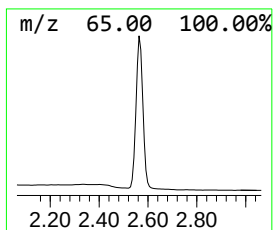
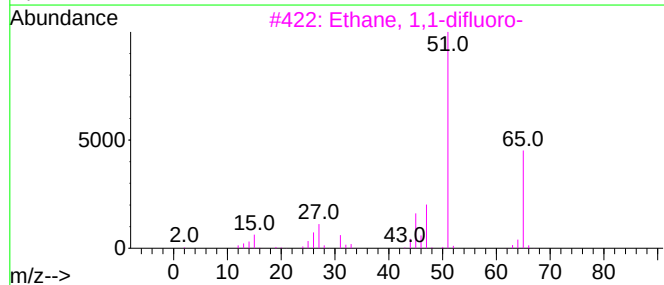
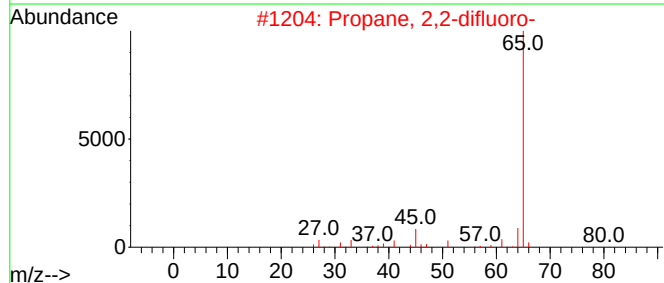
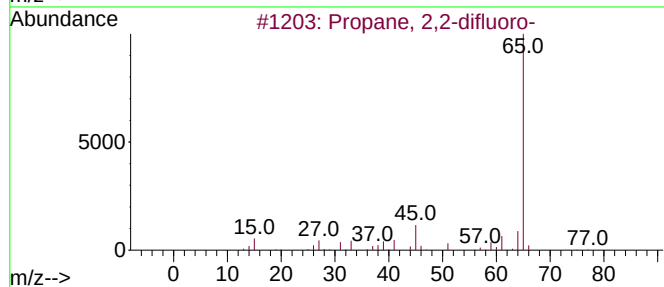
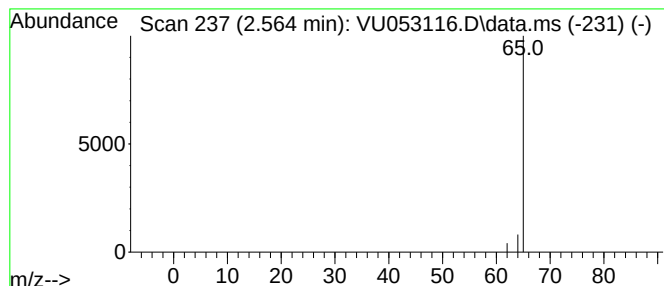
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.564	0.06 ug/L	6110	1,4-Difluorobenzene	6.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	1
2			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	1
3			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	1
4			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	1
5			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	1



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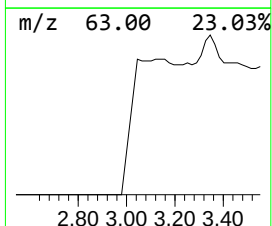
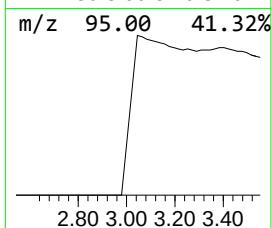
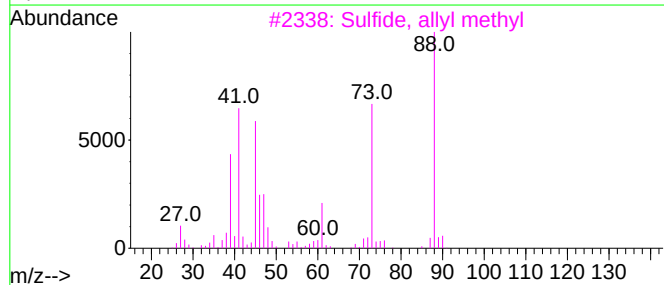
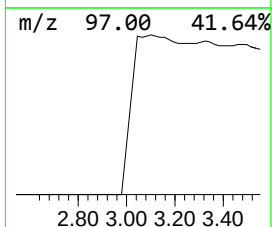
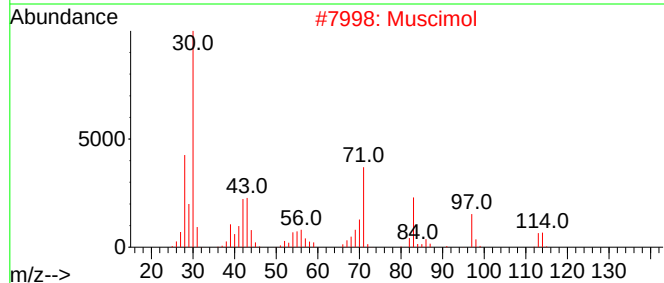
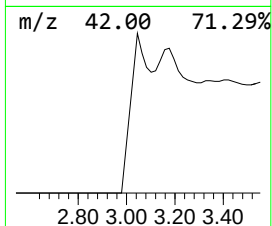
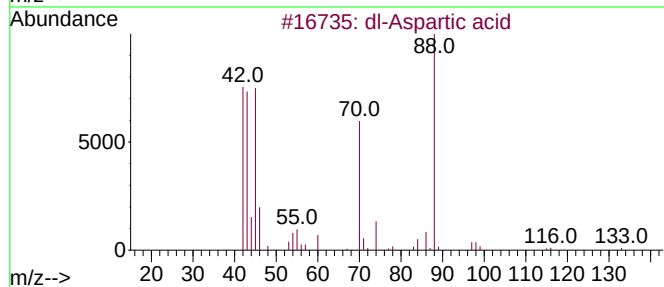
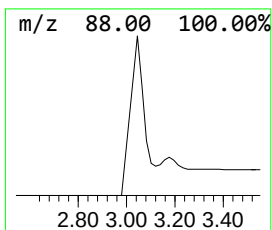
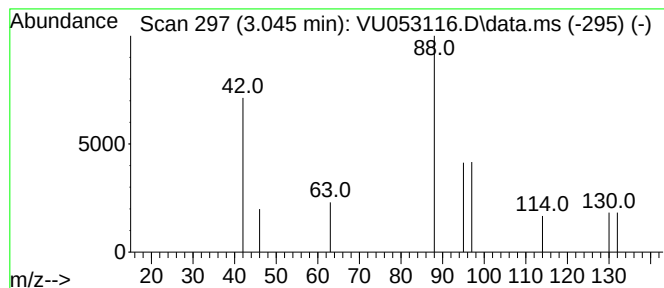
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Peak Number 2 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.045	0.06 ug/L	5651	1,4-Difluorobenzene	6.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			dl-Aspartic acid	133	C4H7NO4	000617-45-8	9
2			Muscimol	114	C4H6N2O2	002763-96-4	7
3			Sulfide, allyl methyl	88	C4H8S	010152-76-8	5
4			Sulfide, allyl methyl	88	C4H8S	010152-76-8	5
5			2,2-Dimethylthiirane	88	C4H8S	003772-13-2	5



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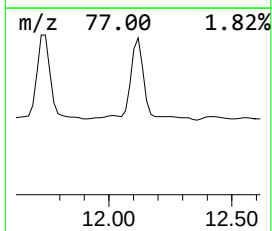
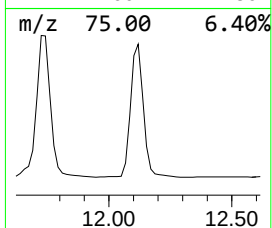
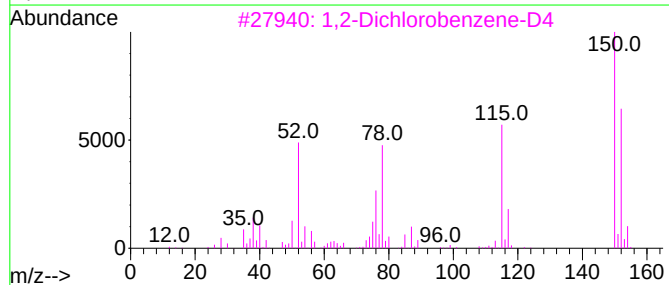
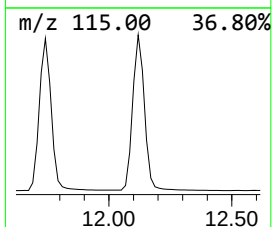
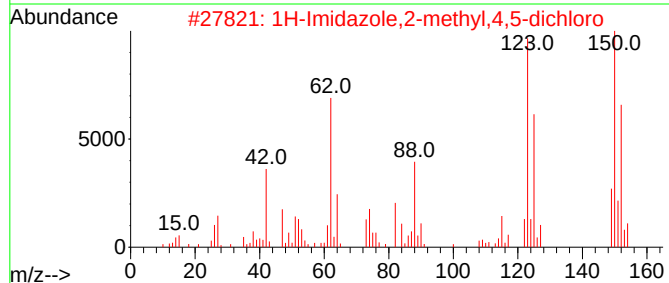
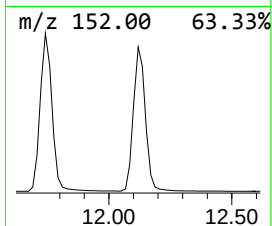
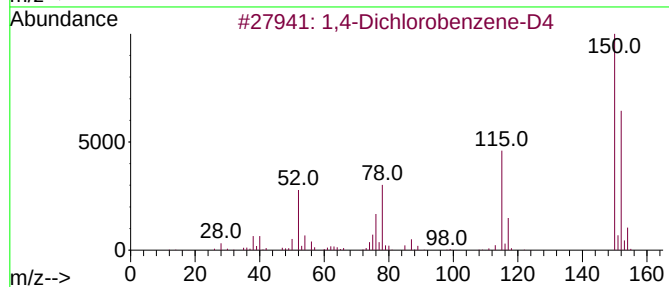
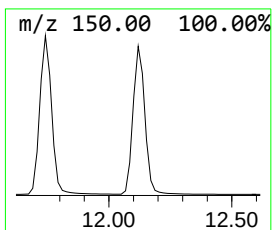
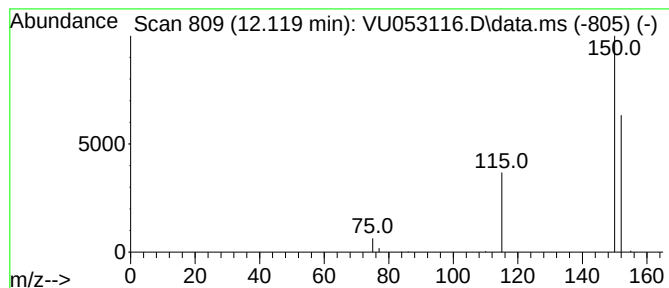
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Peak Number 3 unknown-03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.119	0.47 ug/L	52612	1,4-Dichlorobenzene-d4	11.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	9
2			1H-Imidazole,2-methyl,4,5-dichloro	150	C4H4Cl2N2	015965-33-0	5
3			1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	5
4			Acenaphthylene	152	C12H8	000208-96-8	5
5			3-Phospholene, 3-chloro-1-methyl...	150	C5H8ClOP	022356-34-9	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	2.564	0.1	ug/L	6110	1	6.207	49387	0.5
unknown-02	3.045	0.1	ug/L	5651	1	6.207	49387	0.5
unknown-03	12.119	0.5	ug/L	52612	3	11.742	55647	0.5