

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041224\
 Data File : VU058675.D
 Acq On : 13 Apr 2024 00:05
 Operator : MD/SY
 Sample : P2055-12
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0BN1

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\SFAMUTR040424WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU058675.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.593	86	94	105	rVB	25218	29104	13.14%	1.473%
2	1.725	130	135	149	rVB	4428	5824	2.63%	0.295%
3	1.905	183	191	201	rVB	24384	31025	14.01%	1.571%
4	2.448	352	360	369	rVB2	5075	7813	3.53%	0.396%
5	2.560	383	395	409	rBV	40275	66000	29.80%	3.341%
6	2.789	453	466	493	rBV3	7983	21656	9.78%	1.096%
7	3.191	576	591	615	rVB4	7948	25322	11.43%	1.282%
8	4.618	1018	1035	1060	rBV	32393	94298	42.57%	4.774%
9	5.052	1156	1170	1190	rBV	44801	100201	45.24%	5.073%
10	5.718	1359	1377	1398	rBV2	85085	221506	100.00%	11.214%
11	6.242	1527	1540	1566	rBV	83983	163850	73.97%	8.295%
12	6.683	1663	1677	1696	rBV2	56421	110259	49.78%	5.582%
13	7.560	1940	1950	1973	rBV2	21883	39714	17.93%	2.011%
14	7.891	2041	2053	2074	rBV	93071	163772	73.94%	8.291%
15	8.178	2132	2142	2159	rBV2	11994	21410	9.67%	1.084%
16	8.547	2245	2257	2273	rBV	42979	75250	33.97%	3.810%
17	8.631	2273	2283	2316	rBV2	97911	206508	93.23%	10.454%
18	9.412	2513	2526	2555	rBV	124261	212539	95.95%	10.760%
19	10.750	2932	2942	2957	rBV	35882	58432	26.38%	2.958%
20	10.888	2976	2985	2994	rBV5	1607	2532	1.14%	0.128%
21	11.808	3257	3271	3295	rBV	106497	179209	80.90%	9.072%
22	12.187	3378	3389	3410	rBV	81475	136530	61.64%	6.912%
23	12.766	3561	3569	3577	rBV2	1624	2554	1.15%	0.129%

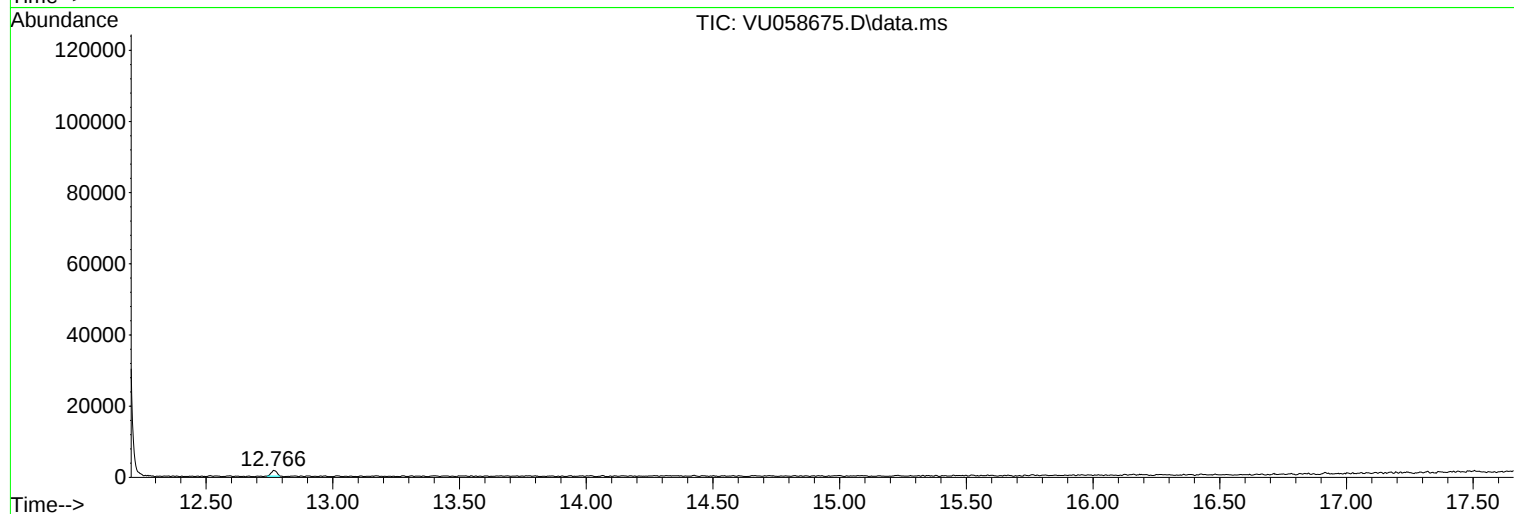
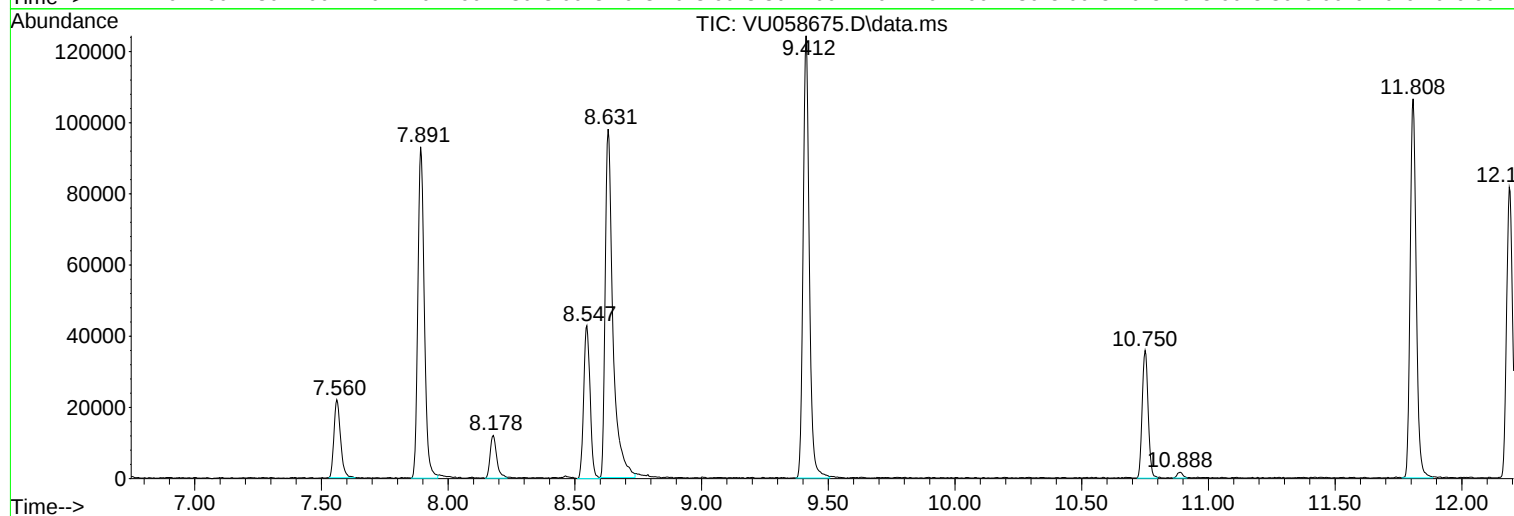
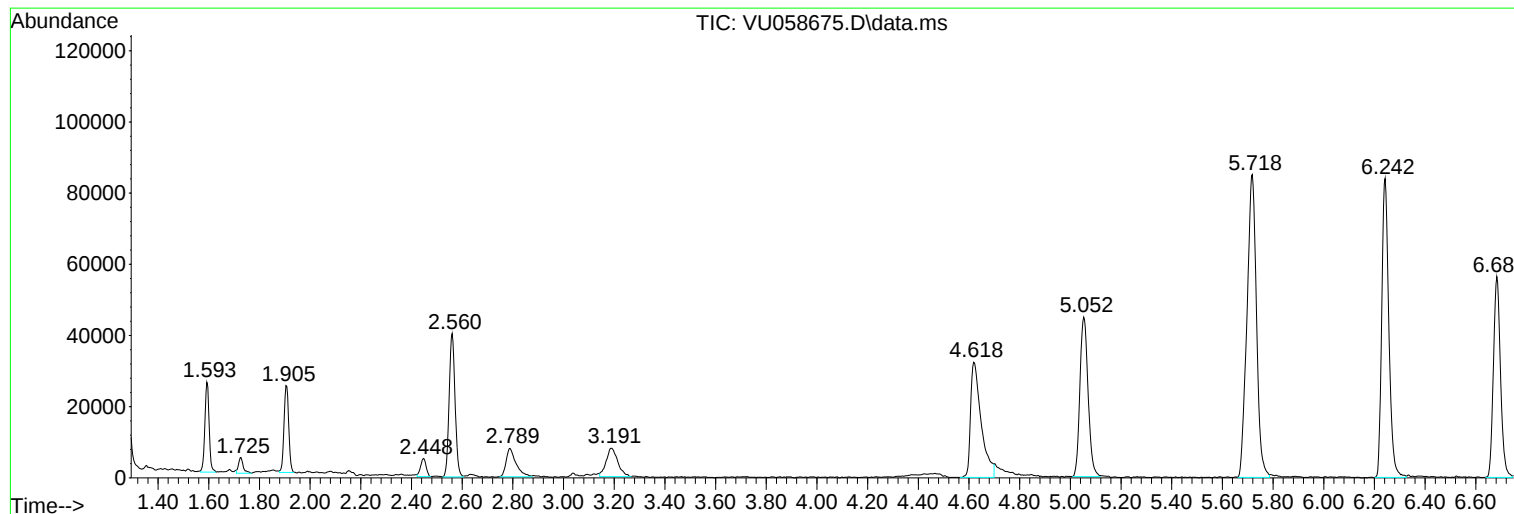
Sum of corrected areas: 1975308

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Instrument :
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ClientSampleId :
COBN1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR040424WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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ClientSampleId :
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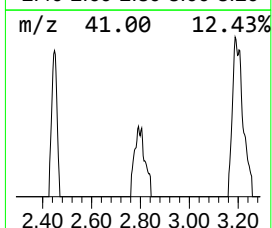
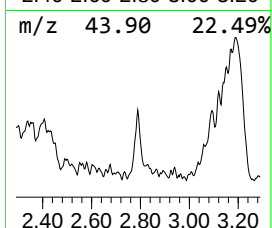
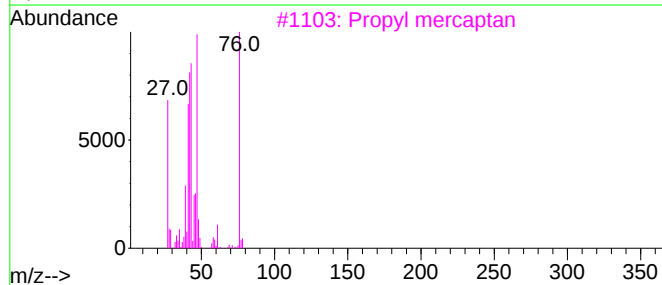
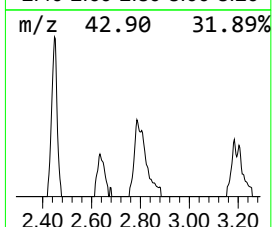
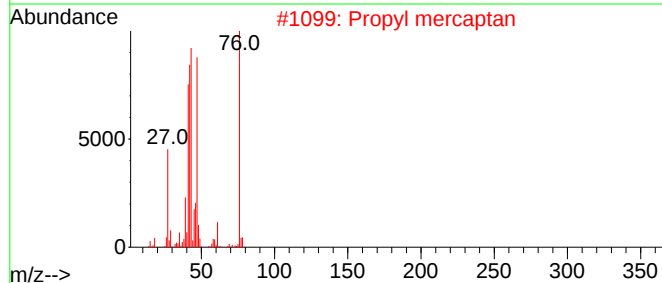
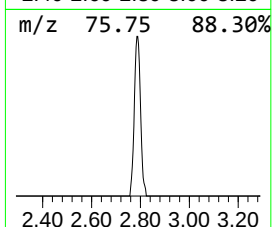
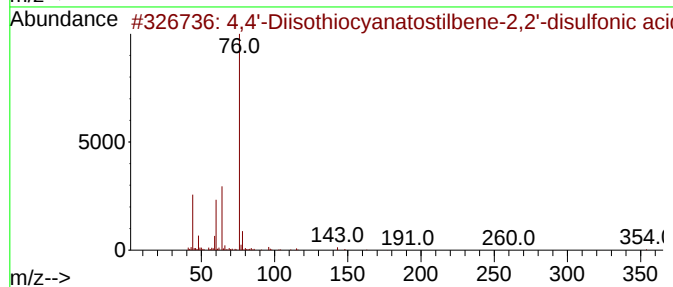
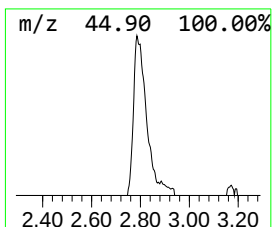
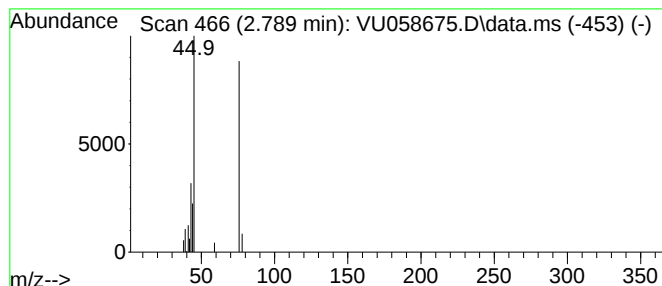
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR040424WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.789	0.66 ug/L	21656	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,4'-Diisothiocyanatostilbene-2,...	454	C16H10N2O6S4	053005-05-3	9
2			Propyl mercaptan	76	C3H8S	000107-03-9	7
3			Propyl mercaptan	76	C3H8S	000107-03-9	7
4			Carbon disulfide	76	CS2	000075-15-0	7
5			Thiourea	76	CH4N2S	000062-56-6	7



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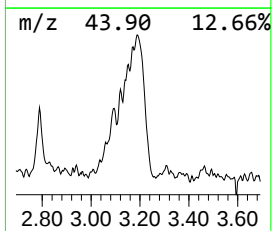
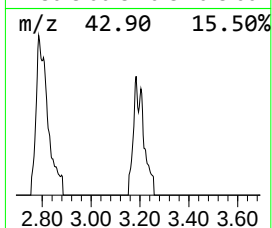
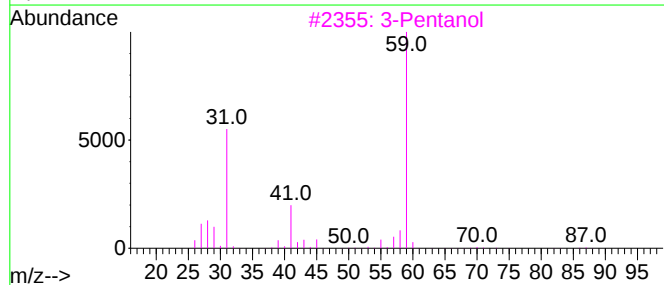
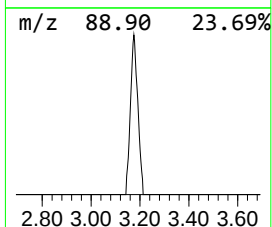
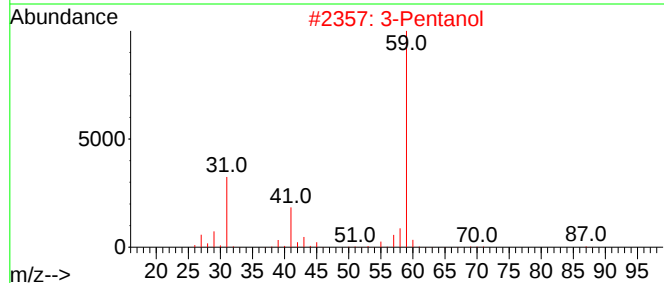
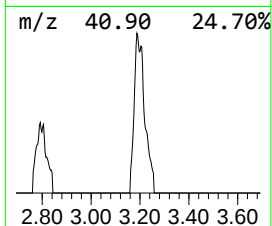
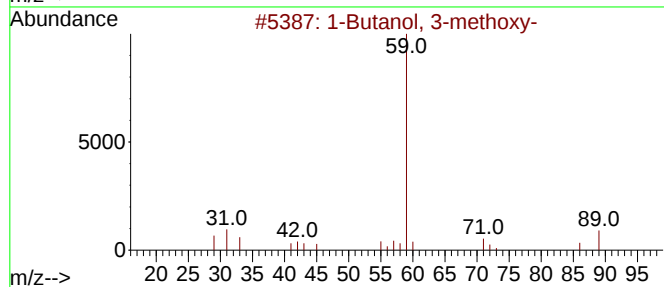
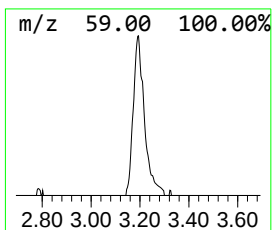
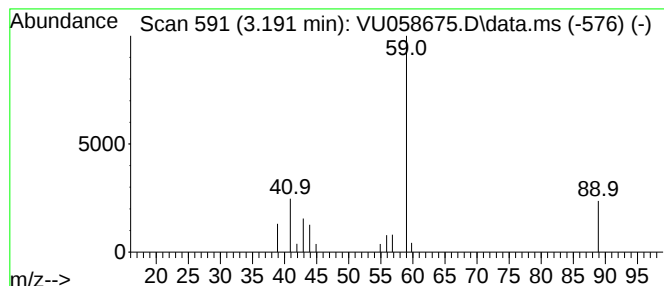
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR040424WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.191	0.77 ug/L	25322	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	39
2			3-Pentanol	88	C5H12O	000584-02-1	38
3			3-Pentanol	88	C5H12O	000584-02-1	38
4			3-Pentanol	88	C5H12O	000584-02-1	38
5			3-Pentanol	88	C5H12O	000584-02-1	38



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ClientSampleId :
C0BN1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR040424WMA.M
Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	2.789	0.7	ug/L	21656	1	6.242	163850	5.0
unknown-02	3.191	0.8	ug/L	25322	1	6.242	163850	5.0