

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112322\
 Data File : VU052104.D
 Acq On : 23 Nov 2022 22:23
 Operator : JC/MD
 Sample : N5739-02
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBNK2

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\SFAMUTR111822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU052104.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	69	80	97	rVB2	121219	210463	22.71%	2.972%
2	1.687	102	108	120	rVB	10278	13524	1.46%	0.191%
3	1.912	170	178	206	rVB	91386	132638	14.31%	1.873%
4	2.568	369	382	395	rBV	160403	269704	29.10%	3.809%
5	2.633	395	402	415	rVB2	6459	12215	1.32%	0.173%
6	3.192	562	576	597	rBV2	26799	76468	8.25%	1.080%
7	3.588	678	699	716	rBV	3860	13118	1.42%	0.185%
8	3.880	761	790	805	rBV	13019	52699	5.69%	0.744%
9	4.440	948	964	979	rBV4	8950	23503	2.54%	0.332%
10	4.623	1005	1021	1054	rBV	144141	383090	41.34%	5.410%
11	5.060	1139	1157	1183	rBV	167225	374739	40.43%	5.292%
12	5.723	1342	1363	1388	rBV2	310425	826871	89.22%	11.678%
13	6.247	1512	1526	1548	rBV	261813	503698	54.35%	7.114%
14	6.687	1650	1663	1683	rBV2	203322	402692	43.45%	5.687%
15	7.163	1791	1811	1823	rBV	28106	57671	6.22%	0.814%
16	7.565	1923	1936	1954	rBV	86945	158135	17.06%	2.233%
17	7.896	2026	2039	2054	rBV	340650	591246	63.80%	8.350%
18	7.970	2057	2062	2073	rVB	8155	13301	1.44%	0.188%
19	8.179	2114	2127	2147	rBV	53913	93786	10.12%	1.325%
20	8.632	2253	2268	2311	rBV2	485157	926779	100.00%	13.089%
21	9.414	2495	2511	2530	rBV	394658	660802	71.30%	9.332%
22	10.755	2916	2928	2949	rBV	170148	277514	29.94%	3.919%
23	11.809	3244	3256	3274	rBV	311288	497513	53.68%	7.026%
24	12.192	3361	3375	3393	rBV	308761	508511	54.87%	7.182%

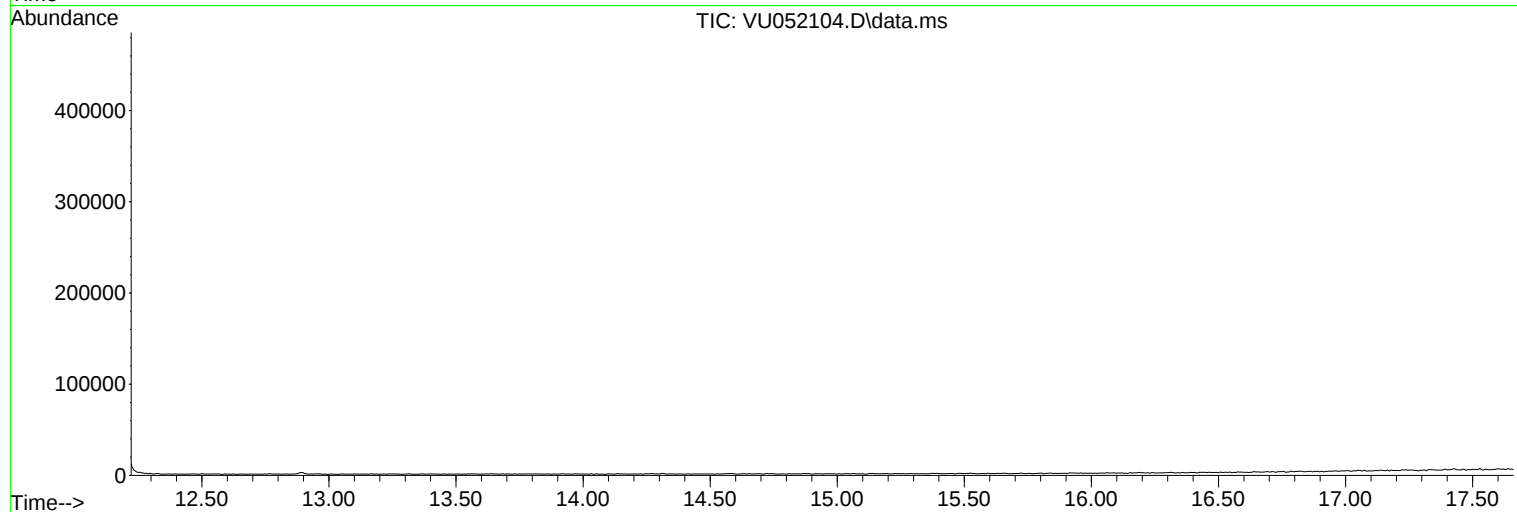
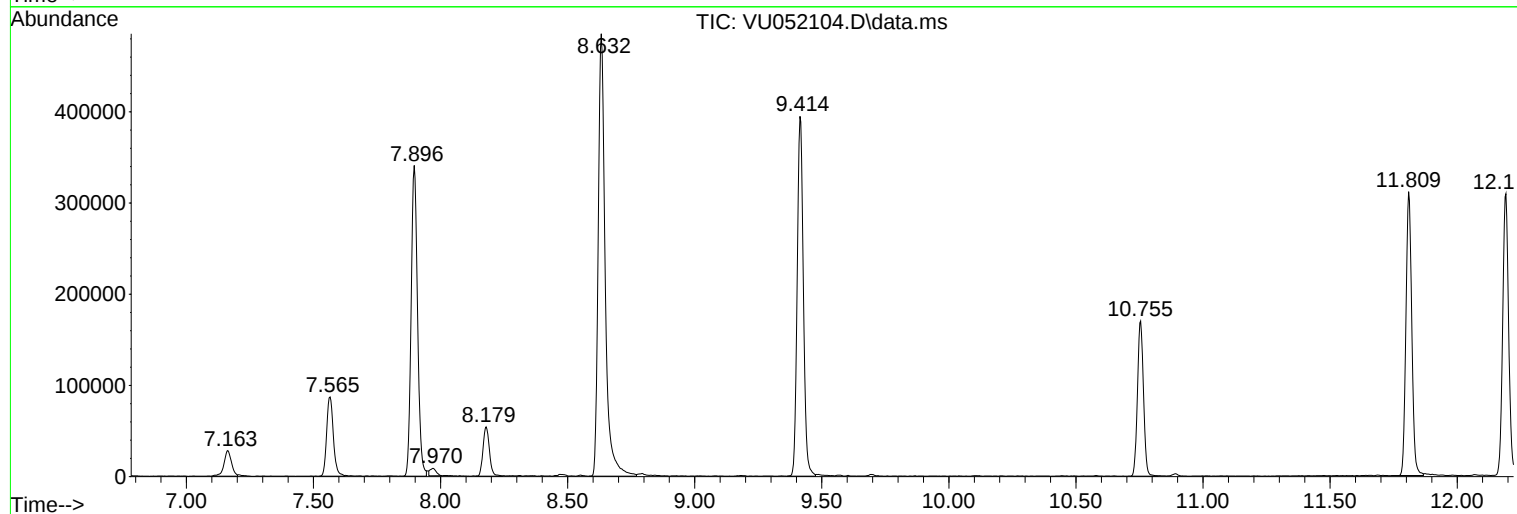
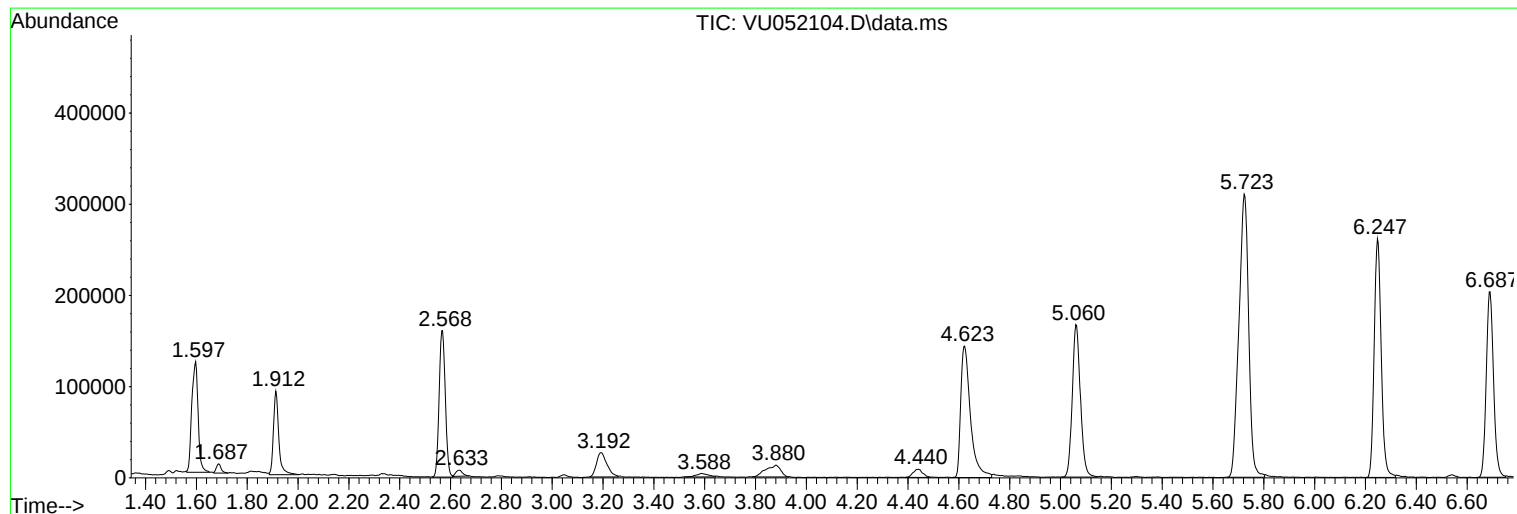
Sum of corrected areas: 7080680

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112322\
Data File : VU052104.D
Acq On : 23 Nov 2022 22:23
Operator : JC/MD
Sample : N5739-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBNK2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112322\
Data File : VU052104.D
Acq On : 23 Nov 2022 22:23
Operator : JC/MD
Sample : N5739-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBNK2

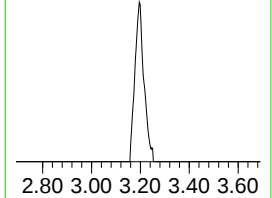
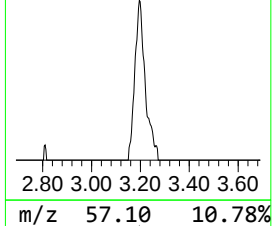
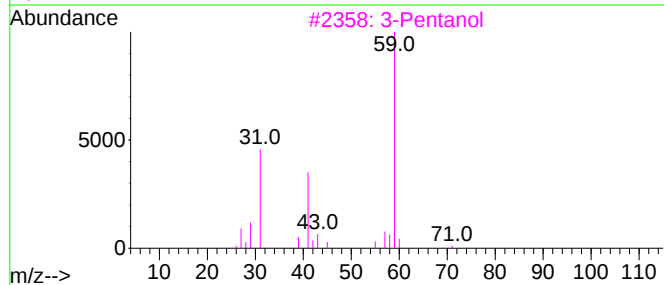
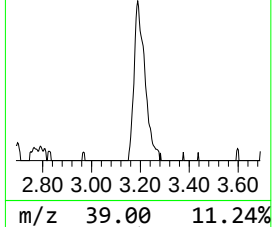
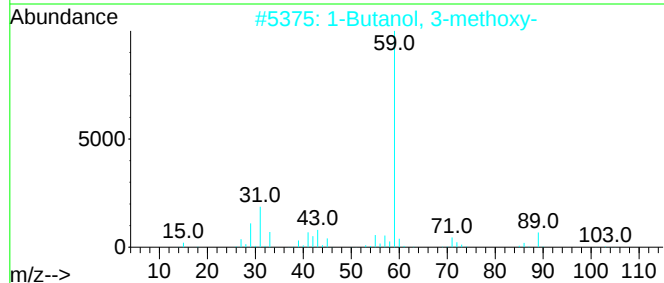
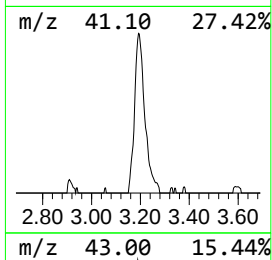
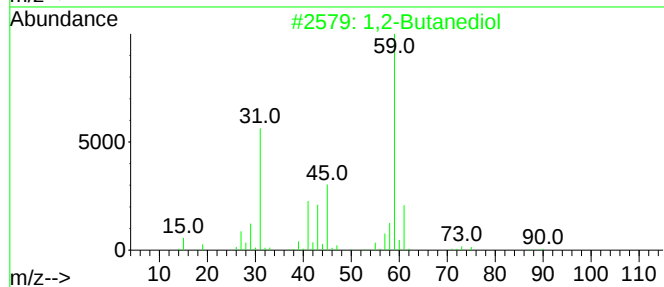
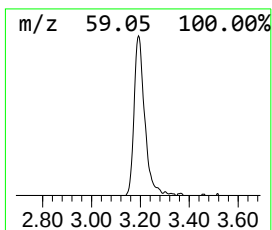
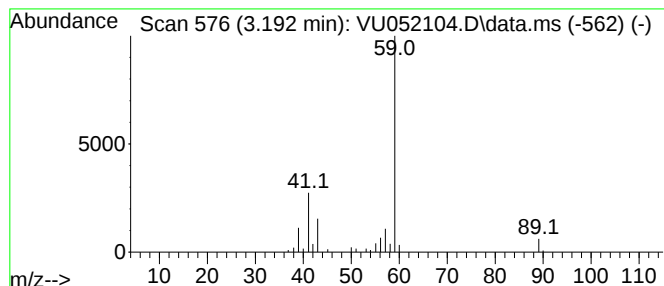
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 1,2-Butanediol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.192	0.76 ug/L	76468	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Butanediol			90	C4H10O2	000584-03-2	72
2	1-Butanol, 3-methoxy-			104	C5H12O2	002517-43-3	56
3	3-Pentanol			88	C5H12O	000584-02-1	50
4	Pentanamide			101	C5H11NO	000626-97-1	40
5	1-Butanol, 3-methoxy-			104	C5H12O2	002517-43-3	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112322\
Data File : VU052104.D
Acq On : 23 Nov 2022 22:23
Operator : JC/MD
Sample : N5739-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBNK2

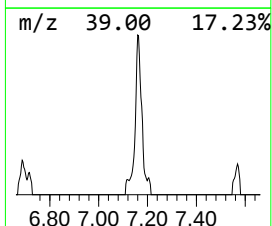
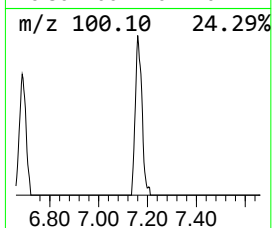
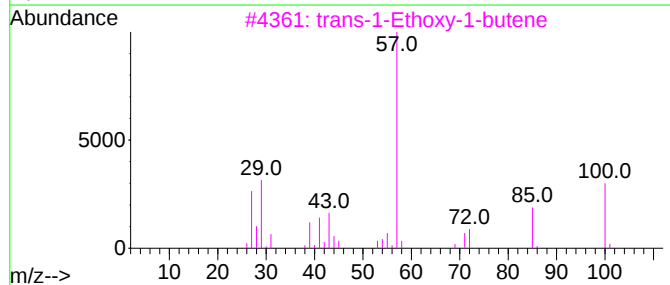
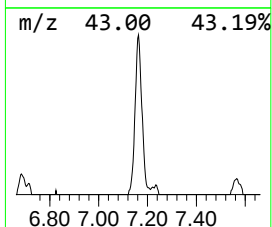
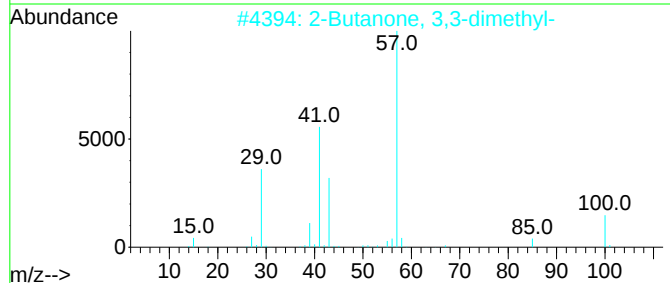
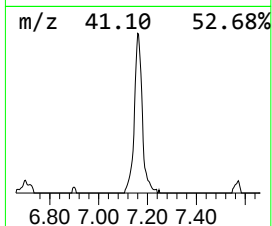
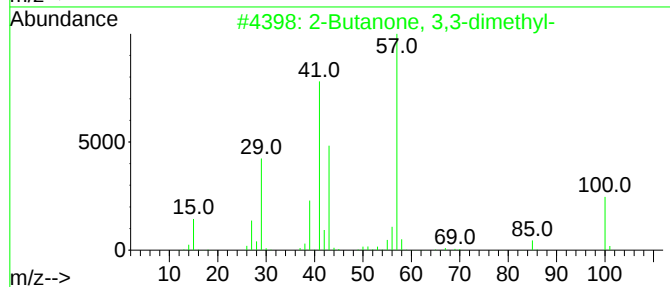
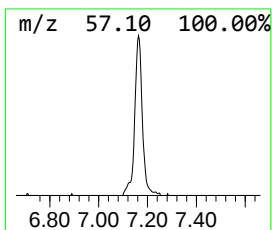
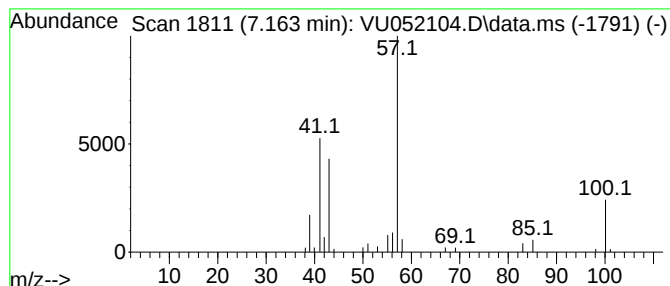
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.163	0.57 ug/L	57671	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	72
2	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	72
3	trans-1-Ethoxy-1-butene			100	C6H12O	1000139-43-9	58
4	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	58
5	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112322\
Data File : VU052104.D
Acq On : 23 Nov 2022 22:23
Operator : JC/MD
Sample : N5739-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBNK2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.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
1,2-Butanediol	3.192	0.8	ug/L	76468	1	6.247	503698	5.0
2-Butanone, 3,3...	7.163	0.6	ug/L	57671	1	6.247	503698	5.0