

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121523\
 Data File : VU056880.D
 Acq On : 15 Dec 2023 15:34
 Operator : MD/SY
 Sample : 05684-08 100X
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E06J4

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\SFAMUTR121123WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU056880.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	86	95	107	rVB	126973	142206	15.58%	1.909%
2	1.907	184	192	211	rVB	94248	130066	14.25%	1.746%
3	2.563	383	396	412	rBV	195046	321082	35.17%	4.311%
4	3.039	530	544	557	rBV4	15118	29265	3.21%	0.393%
5	3.181	574	588	599	rBV	6074	13597	1.49%	0.183%
6	4.624	1026	1037	1087	rBV2	116813	337125	36.93%	4.526%
7	5.055	1154	1171	1192	rBV	185325	414681	45.42%	5.567%
8	5.718	1358	1377	1408	rBV3	349057	912951	100.00%	12.257%
9	6.245	1526	1541	1564	rBV	276591	539169	59.06%	7.239%
10	6.685	1664	1678	1697	rBV	219256	433689	47.50%	5.822%
11	7.563	1937	1951	1971	rBV2	100409	187854	20.58%	2.522%
12	7.894	2039	2054	2085	rBV	386049	703715	77.08%	9.448%
13	8.177	2129	2142	2158	rBV2	58644	108049	11.84%	1.451%
14	8.467	2218	2232	2247	rBV3	10751	19545	2.14%	0.262%
15	8.631	2272	2283	2319	rBV	430578	875739	95.92%	11.757%
16	9.412	2513	2526	2551	rBV	386564	683777	74.90%	9.180%
17	10.753	2930	2943	2961	rBV2	155057	257365	28.19%	3.455%
18	10.888	2974	2985	2996	rBV	13277	20775	2.28%	0.279%
19	11.807	3260	3271	3296	rBV	352534	586400	64.23%	7.873%
20	12.187	3377	3389	3407	rBV	346060	598005	65.50%	8.029%
21	14.312	4040	4050	4057	rBV5	7181	10119	1.11%	0.136%
22	16.762	4802	4812	4825	rBV3	75084	123353	13.51%	1.656%

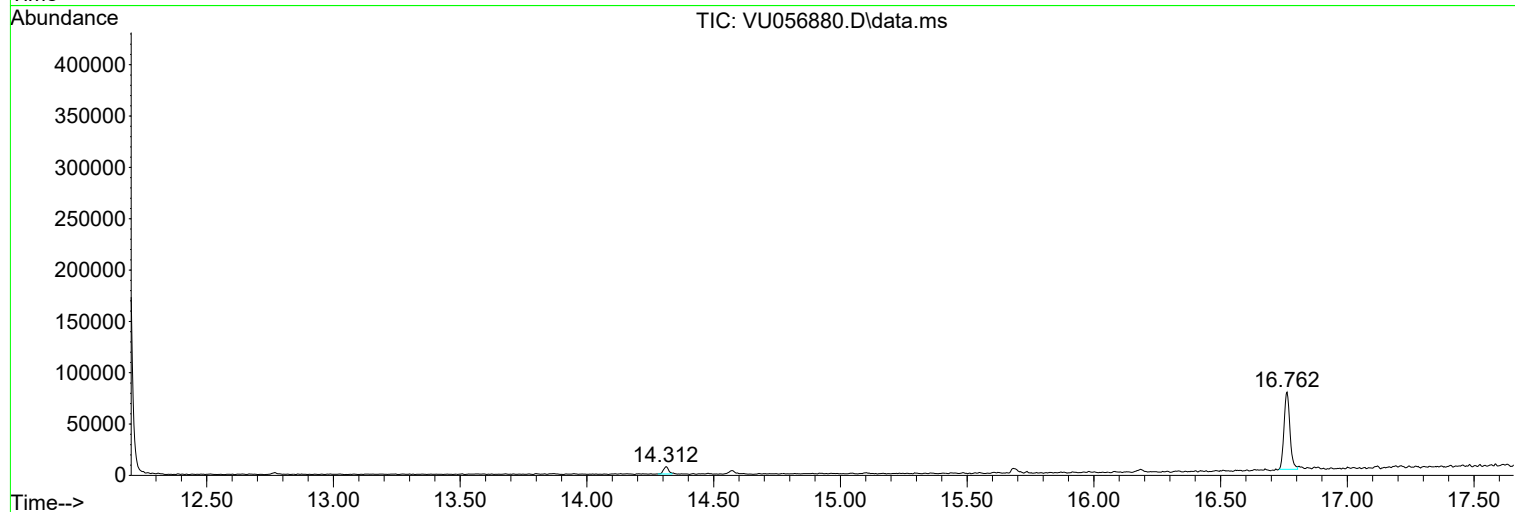
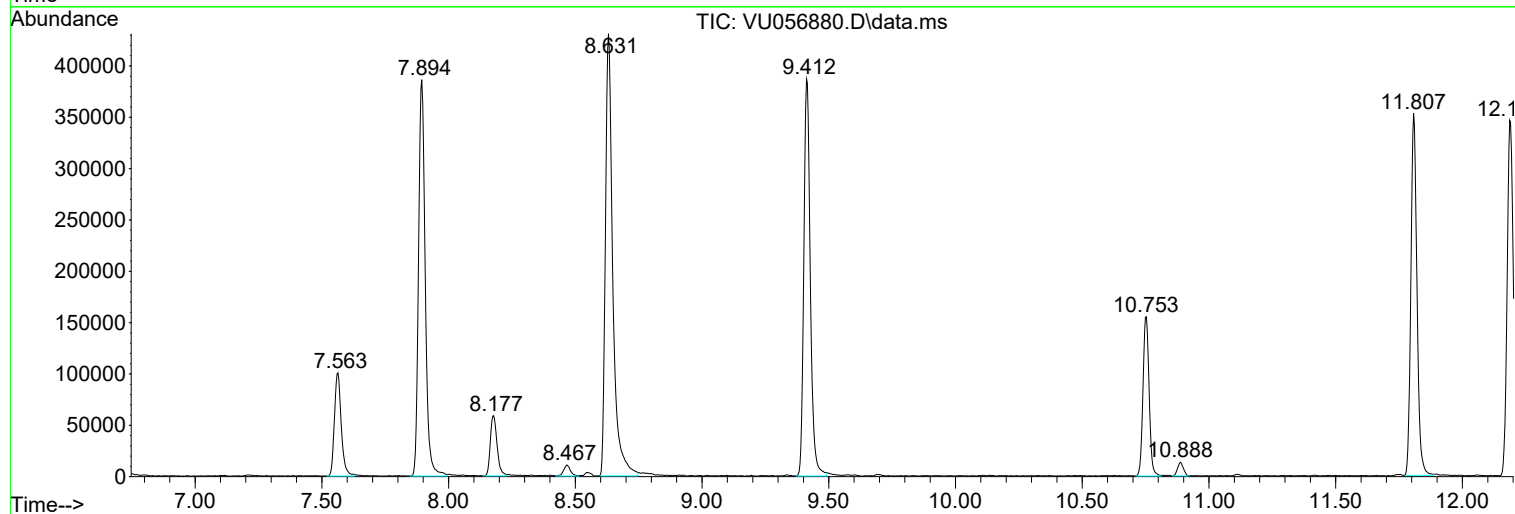
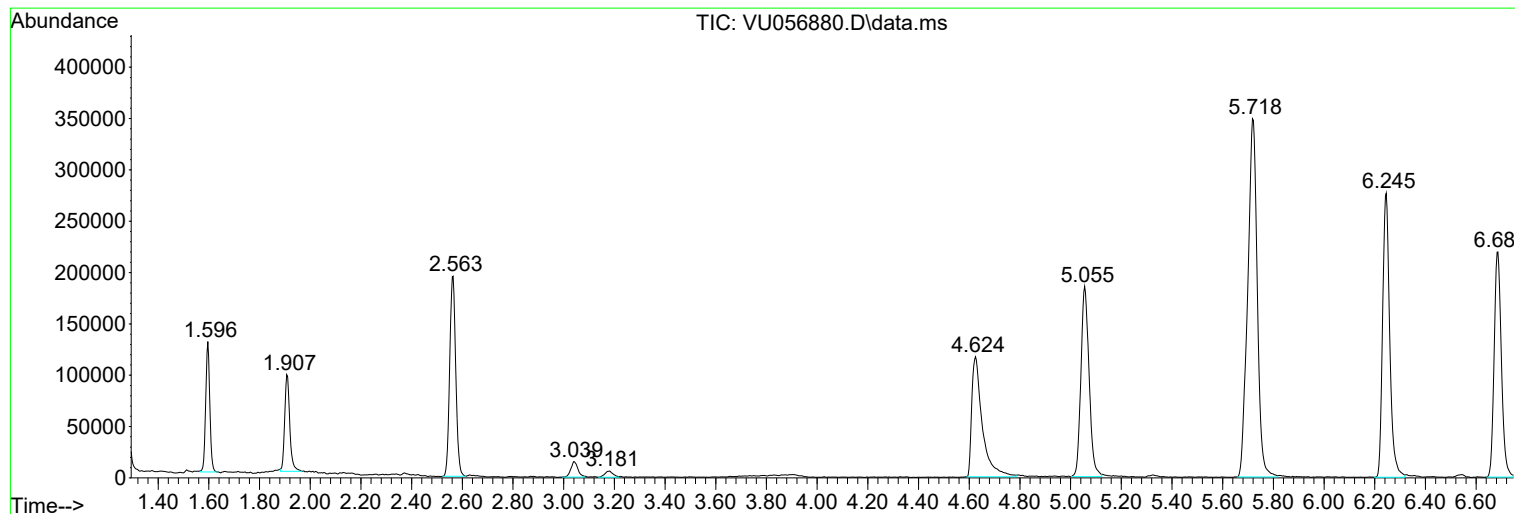
Sum of corrected areas: 7448527

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.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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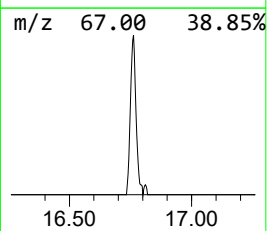
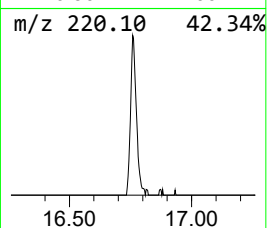
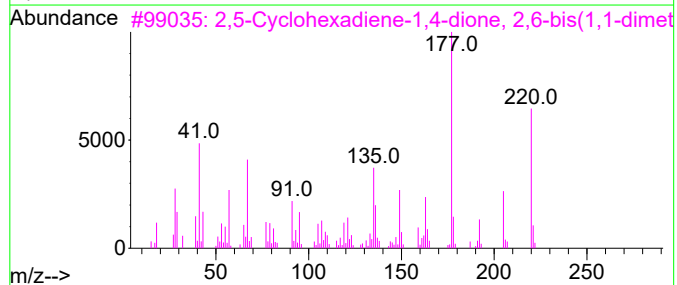
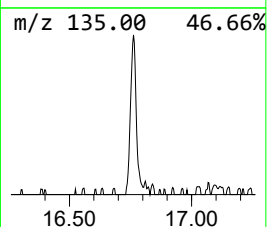
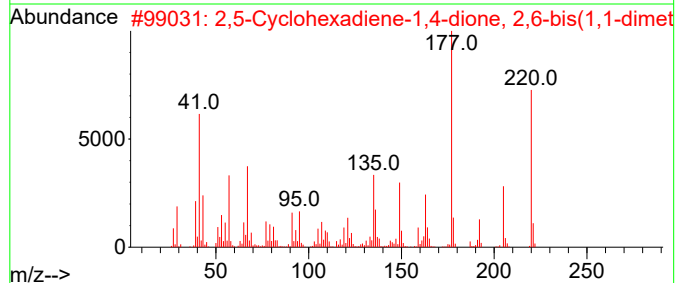
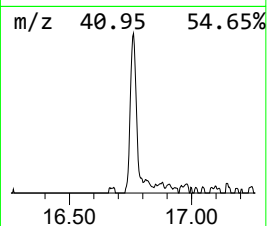
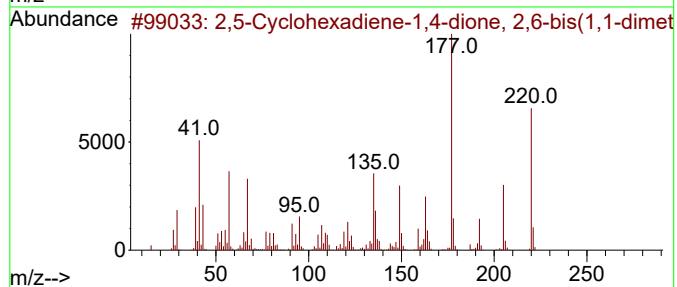
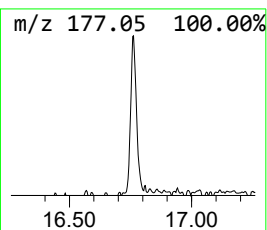
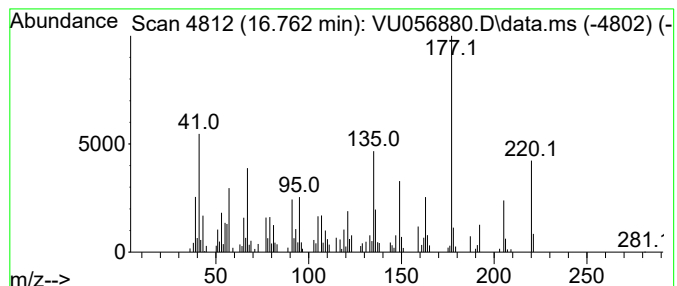
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.762	1.05 ug/L	123353	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	97		
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	96		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	96		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	89		
5	2-Acetyl-3,4,5,6-tetrafluorobenz...	220	C9H4F402	1000461-12-2	46		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,5-Cyclohexadi...	16.762	1.1	ug/L	123353	3	11.807	586400	5.0