

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051623\
 Data File : VV031055.D
 Acq On : 16 May 2023 16:03
 Operator : SY/MD
 Sample : 02768-05RE
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 CONN3RE

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_V\Method\SFAMVTR042823WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV031055.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.217	50	55	66	rBV	32728	35711	7.72%	0.873%
2	1.539	148	155	168	rVB	57412	71138	15.38%	1.739%
3	2.066	309	319	331	rBV	65338	97777	21.15%	2.390%
4	2.449	431	438	447	rBV3	11289	19432	4.20%	0.475%
5	3.818	848	864	892	rBV2	45747	159185	34.43%	3.890%
6	4.262	988	1002	1025	rBV3	83467	234172	50.64%	5.723%
7	4.741	1144	1151	1170	rVB9	6517	18152	3.93%	0.444%
8	4.970	1207	1222	1244	rBV3	161261	425290	91.98%	10.393%
9	5.545	1389	1401	1427	rBV	166690	344065	74.41%	8.408%
10	5.838	1484	1492	1494	rBV7	4726	5606	1.21%	0.137%
11	5.998	1528	1542	1560	rBV	101573	215567	46.62%	5.268%
12	6.236	1605	1616	1618	rBV10	4250	6602	1.43%	0.161%
13	6.445	1673	1681	1693	rBV6	7958	16565	3.58%	0.405%
14	6.896	1809	1821	1822	rBV10	7490	9438	2.04%	0.231%
15	6.924	1823	1830	1843	rVB3	24544	44720	9.67%	1.093%
16	7.043	1858	1867	1874	rVB3	4187	7486	1.62%	0.183%
17	7.175	1898	1908	1909	rBV6	4319	5972	1.29%	0.146%
18	7.256	1920	1933	1954	rVB	41964	82909	17.93%	2.026%
19	7.564	2018	2029	2038	rBV3	16476	29443	6.37%	0.720%
20	7.879	2119	2127	2136	rBV3	8130	14903	3.22%	0.364%
21	8.034	2165	2175	2199	rBV	193400	371394	80.32%	9.076%
22	8.194	2213	2225	2235	rBV10	12606	23824	5.15%	0.582%
23	8.371	2274	2280	2289	rVB10	5783	9470	2.05%	0.231%
24	8.793	2401	2411	2431	rBV	254213	421388	91.13%	10.298%
25	9.757	2703	2711	2721	rBV5	16312	28066	6.07%	0.686%
26	10.162	2820	2837	2849	rBV	81094	136407	29.50%	3.334%
27	10.313	2872	2884	2902	rBV2	107131	207146	44.80%	5.062%
28	10.432	2912	2921	2937	rBV2	38159	70415	15.23%	1.721%
29	10.648	2976	2988	2997	rBV2	4365	9855	2.13%	0.241%
30	10.889	3053	3063	3065	rBV9	4780	7445	1.61%	0.182%
31	11.104	3118	3130	3137	rBV10	8963	17594	3.80%	0.430%
32	11.194	3145	3158	3175	rBV	290129	462394	100.00%	11.300%
33	11.493	3241	3251	3263	rBV5	19539	40201	8.69%	0.982%
34	11.567	3263	3274	3293	rVV	208078	353039	76.35%	8.628%
35	12.201	3462	3471	3481	rBV3	13610	22361	4.84%	0.546%
36	12.297	3493	3501	3507	rBV7	9945	16052	3.47%	0.392%

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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_V\Method\SFAMVTR042823WMA.M
Title : TRACE VOA SFAM1.0

37	12.763	3636	3646	3652	rVB7	7519	13571	2.93%	0.332%
38	13.384	3831	3839	3848	rBV10	7197	10770	2.33%	0.263%
39	13.821	3966	3975	3983	rBV10	7504	10746	2.32%	0.263%
40	13.992	4020	4028	4029	rBV	7899	8049	1.74%	0.197%
41	15.725	4562	4567	4573	rBV8	6298	7577	1.64%	0.185%

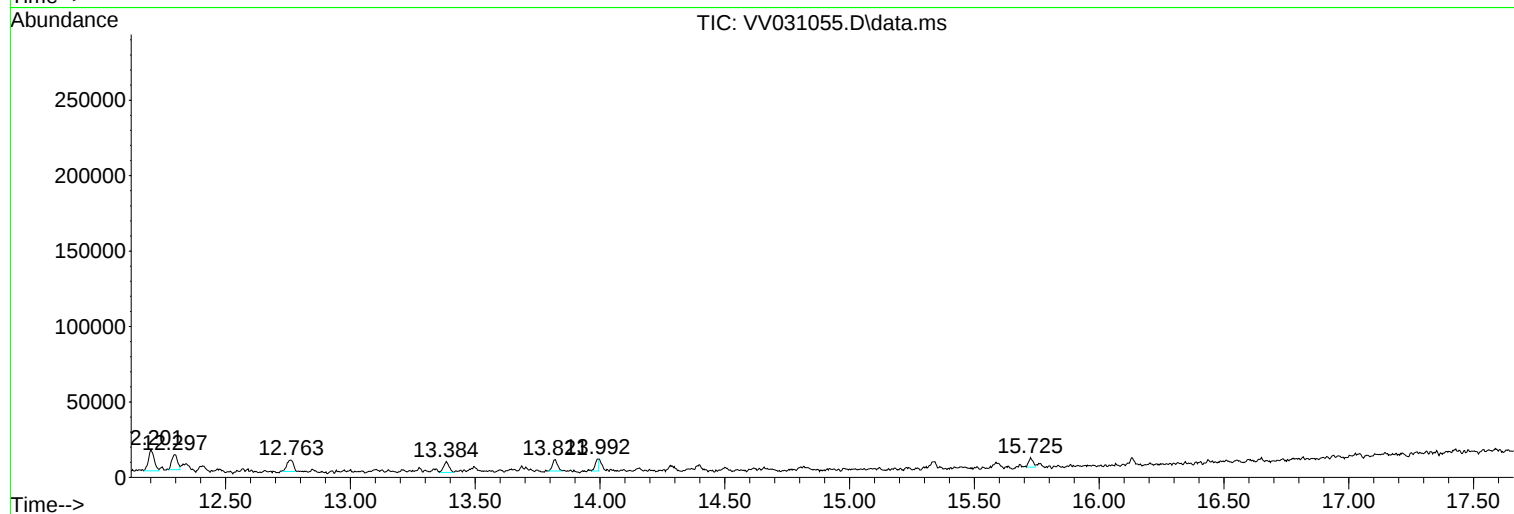
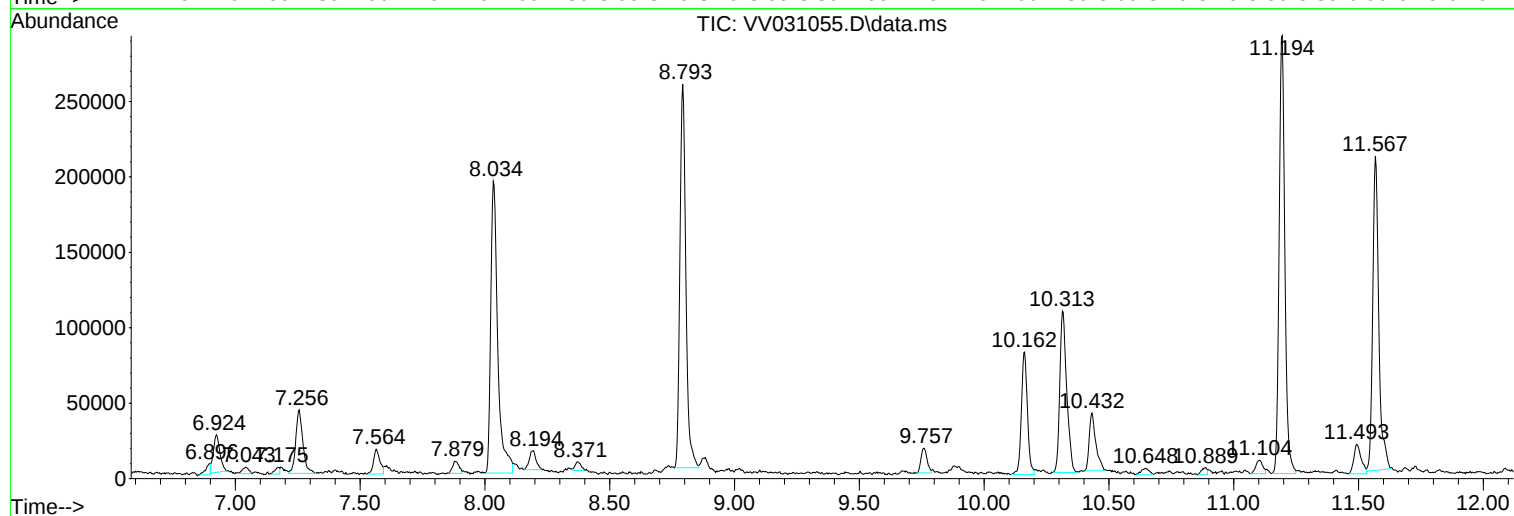
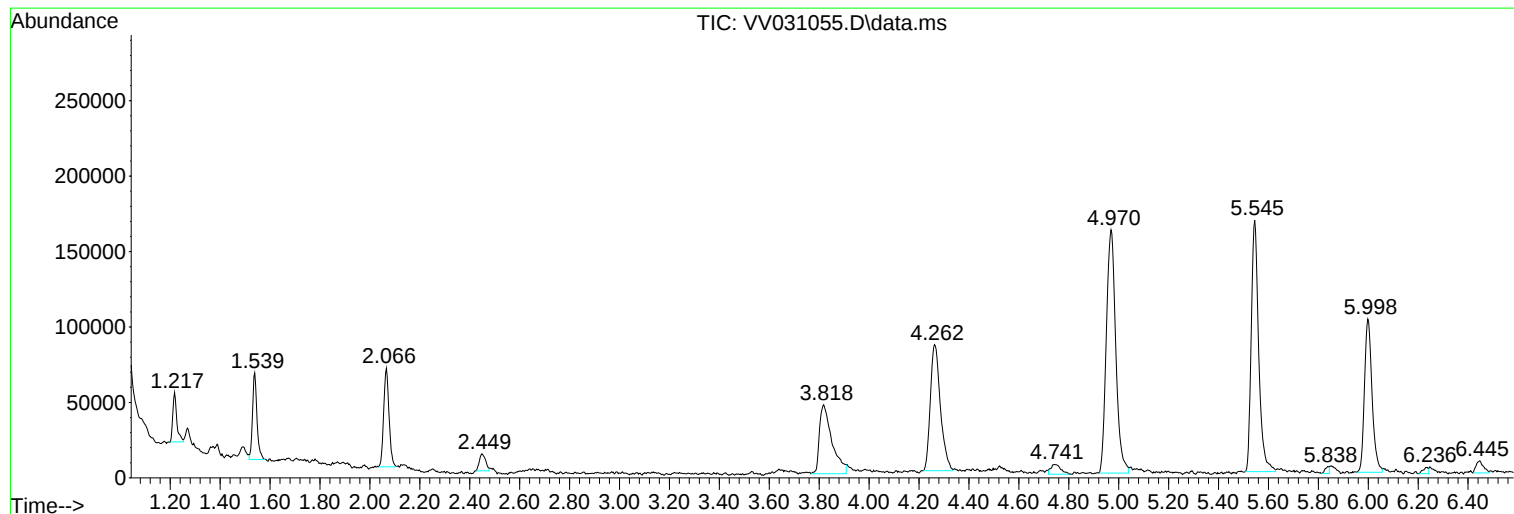
Sum of corrected areas: 4091897

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR042823WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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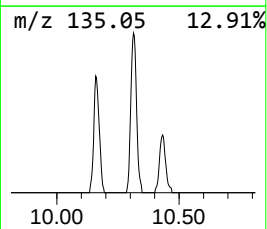
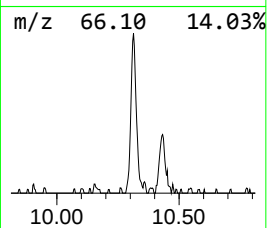
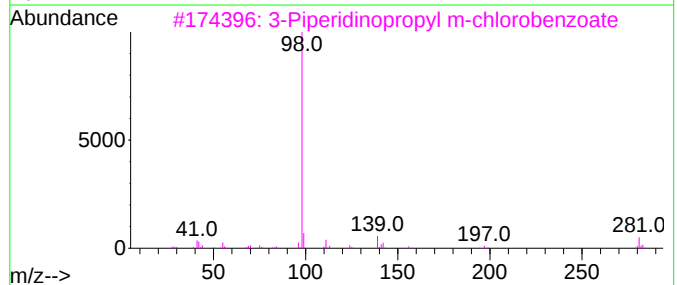
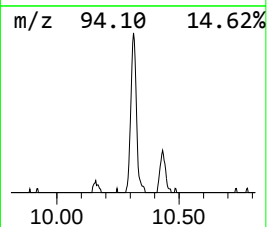
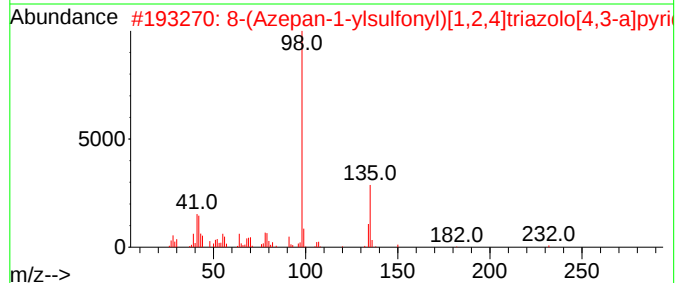
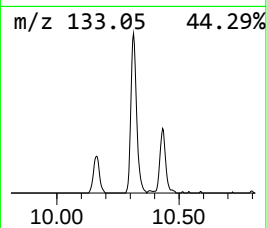
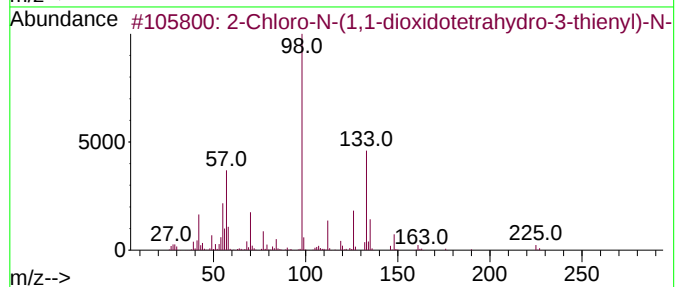
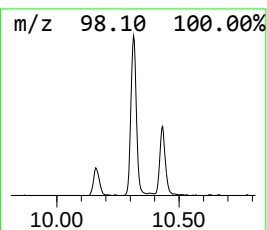
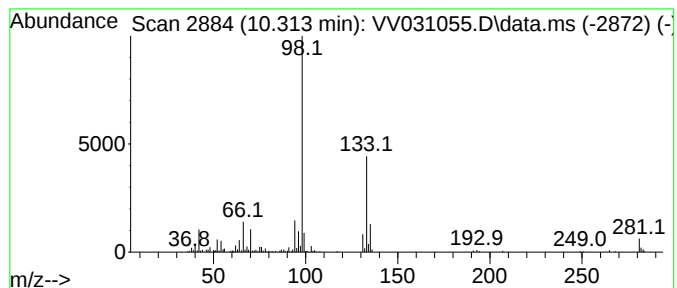
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR042823WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 2-Chloro-N-(1,1-dioxidotetr... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.313	2.24 ug/L	207146	1,4-Dichlorobenzene-d4	11.194

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloro-N-(1,1-dioxidotetrahydr...	225	C7H12ClNO3S	007365-23-3	59
2			8-(Azepan-1-ylsulfonyl)[1,2,4]tr...	296	C12H16N4O3S	1291486-98-0	43
3			3-Piperidinopropyl m-chlorobenzoate	281	C15H20ClNO2	1000240-41-2	38
4			3-Piperidinopropyl p-chlorobenzoate	281	C15H20ClNO2	1000240-42-7	38
5			N-[(3-Ethylisoxazol-5-yl)methyl]...	373	C20H27N3O4	1000482-49-0	37



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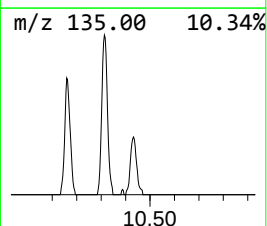
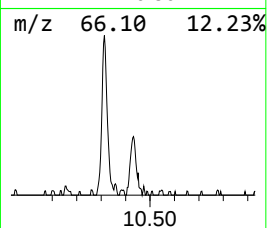
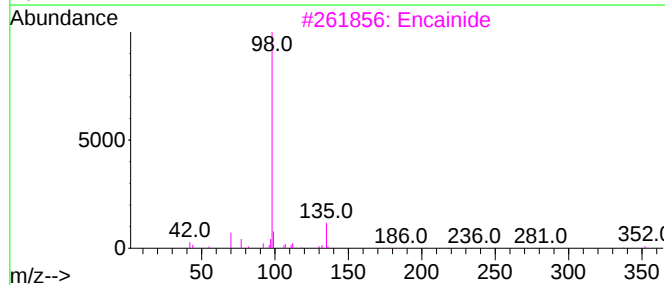
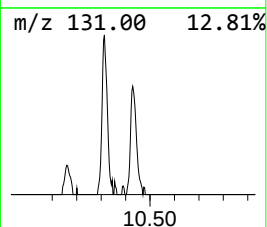
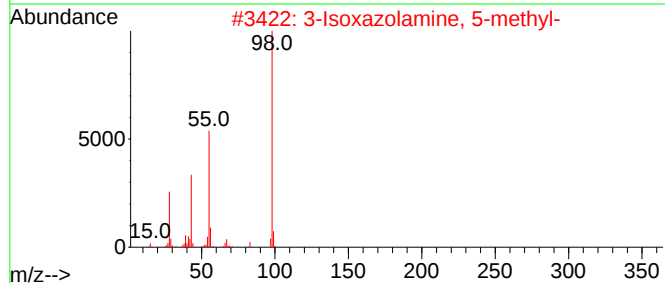
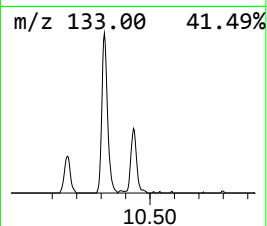
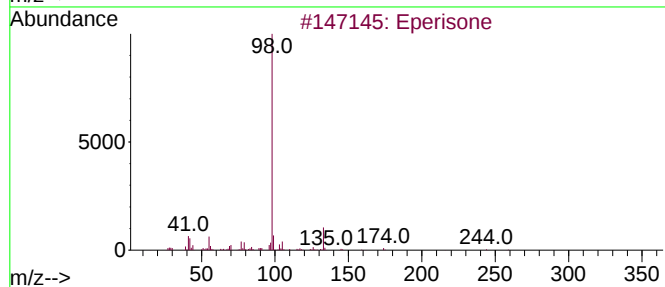
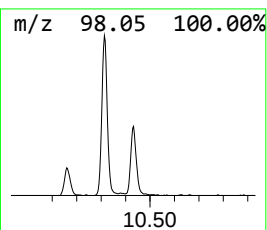
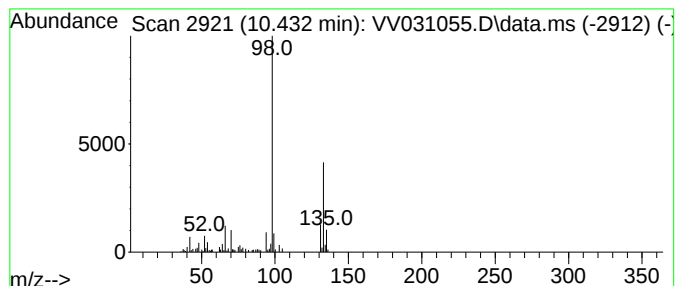
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.432	0.76 ug/L	70415	1,4-Dichlorobenzene-d4	11.194

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eperisone	259	C17H25NO	064840-90-0	45
2			3-Isoxazamine, 5-methyl-	98	C4H6N2O	001072-67-9	38
3			Encainide	352	C22H28N2O2	037612-13-8	37
4			4-[4-[(1-Methyl-2-piperidyl)met...	471	C20H24Cl3N5O2	1000253-80-5	25
5			2-Azabutan-3-one, 1-(1-methylaza...	328	C16H22Cl2N2O	184637-52-3	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Chloro-N-(1,1...	10.313	2.2	ug/L	207146	3	11.194	462394	5.0
unknown-01	10.432	0.8	ug/L	70415	3	11.194	462394	5.0