

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051523\
 Data File : VV031036.D
 Acq On : 15 May 2023 19:22
 Operator : SY/MD
 Sample : 02768-05
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 CONN3

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: VV031036.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.085	11	14	28	rVB2	14316	21854	4.38%	0.523%
2	1.217	49	55	63	rBV	12360	14291	2.86%	0.342%
3	1.269	65	71	82	rVB	23781	25690	5.15%	0.614%
4	1.368	95	102	112	rVB4	6071	10277	2.06%	0.246%
5	1.539	148	155	166	rVB	69114	84305	16.89%	2.017%
6	2.449	425	438	446	rBV2	10829	21485	4.30%	0.514%
7	3.815	852	863	902	rBV	49379	187828	37.63%	4.493%
8	4.259	984	1001	1023	rBV	100081	275094	55.11%	6.580%
9	4.966	1202	1221	1244	rBV3	185966	499204	100.00%	11.941%
10	5.542	1387	1400	1421	rBV	136398	289906	58.07%	6.934%
11	5.844	1483	1494	1505	rVB	7286	16223	3.25%	0.388%
12	5.995	1523	1541	1560	rBV	126931	273898	54.87%	6.551%
13	6.236	1608	1616	1627	rBV8	5482	10044	2.01%	0.240%
14	6.445	1670	1681	1689	rBV6	7331	15308	3.07%	0.366%
15	7.175	1900	1908	1918	rVB6	3964	7709	1.54%	0.184%
16	7.883	2126	2128	2136	rVB7	4437	5160	1.03%	0.123%
17	8.034	2164	2175	2205	rBV	224188	465480	93.24%	11.134%
18	8.188	2214	2223	2232	rBV10	15523	25073	5.02%	0.600%
19	8.793	2398	2411	2431	rBV	232057	400134	80.15%	9.571%
20	8.879	2431	2438	2446	rVB5	9919	16816	3.37%	0.402%
21	9.754	2700	2710	2724	rBV2	47708	78371	15.70%	1.875%
22	10.159	2823	2836	2850	rBV	97252	160904	32.23%	3.849%
23	10.313	2869	2884	2903	rBV2	134457	240261	48.13%	5.747%
24	10.432	2911	2921	2940	rBV2	50873	91847	18.40%	2.197%
25	11.098	3121	3128	3136	rBV10	8484	14006	2.81%	0.335%
26	11.191	3146	3157	3175	rBV	241717	391287	78.38%	9.359%
27	11.493	3242	3251	3262	rBV6	17165	32366	6.48%	0.774%
28	11.567	3262	3274	3294	rVV	248629	419785	84.09%	10.041%
29	12.294	3493	3500	3508	rBV	11295	16982	3.40%	0.406%
30	12.474	3546	3556	3557	rBV7	15094	16773	3.36%	0.401%
31	12.757	3632	3644	3653	rBV7	6725	13578	2.72%	0.325%
32	13.387	3834	3840	3847	rVB7	5380	8004	1.60%	0.191%
33	13.818	3967	3974	3984	rVB7	8154	12543	2.51%	0.300%
34	14.615	4211	4222	4227	rBV10	4036	7003	1.40%	0.168%
35	15.728	4557	4568	4573	rBV10	6945	11243	2.25%	0.269%

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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

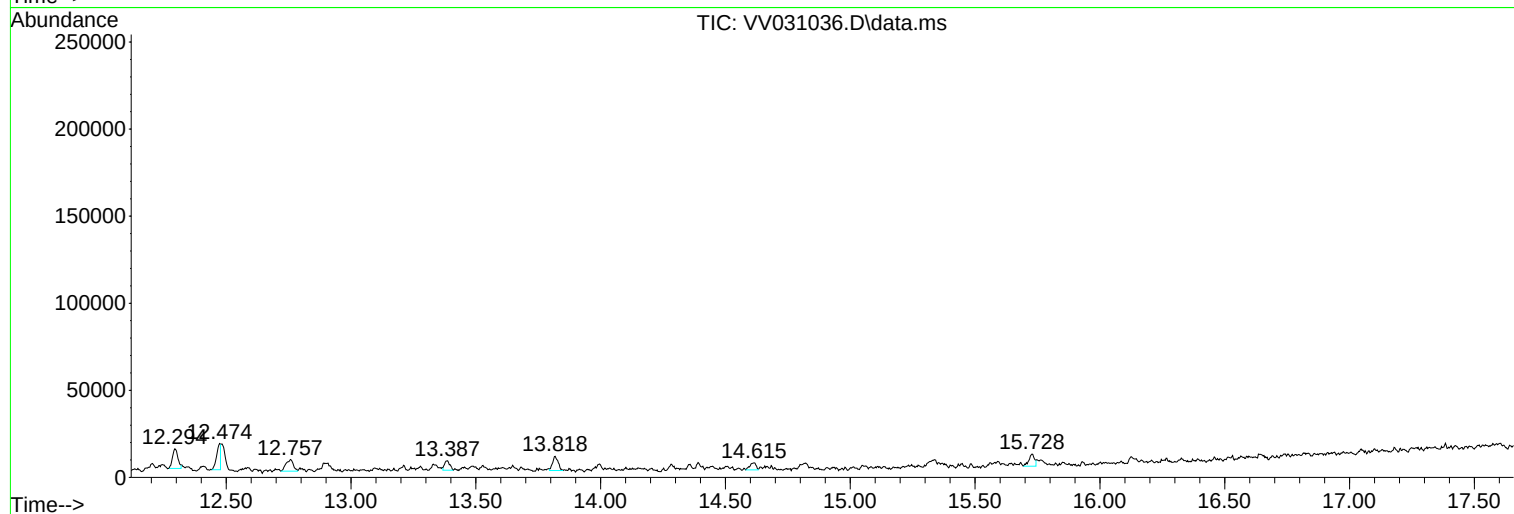
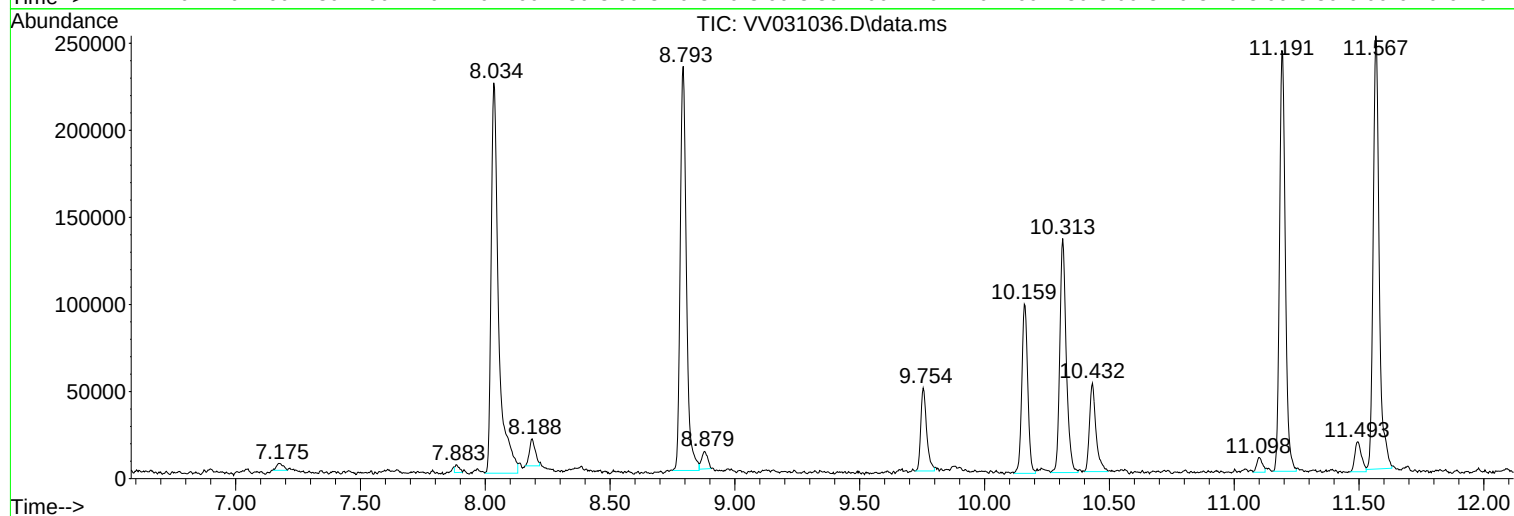
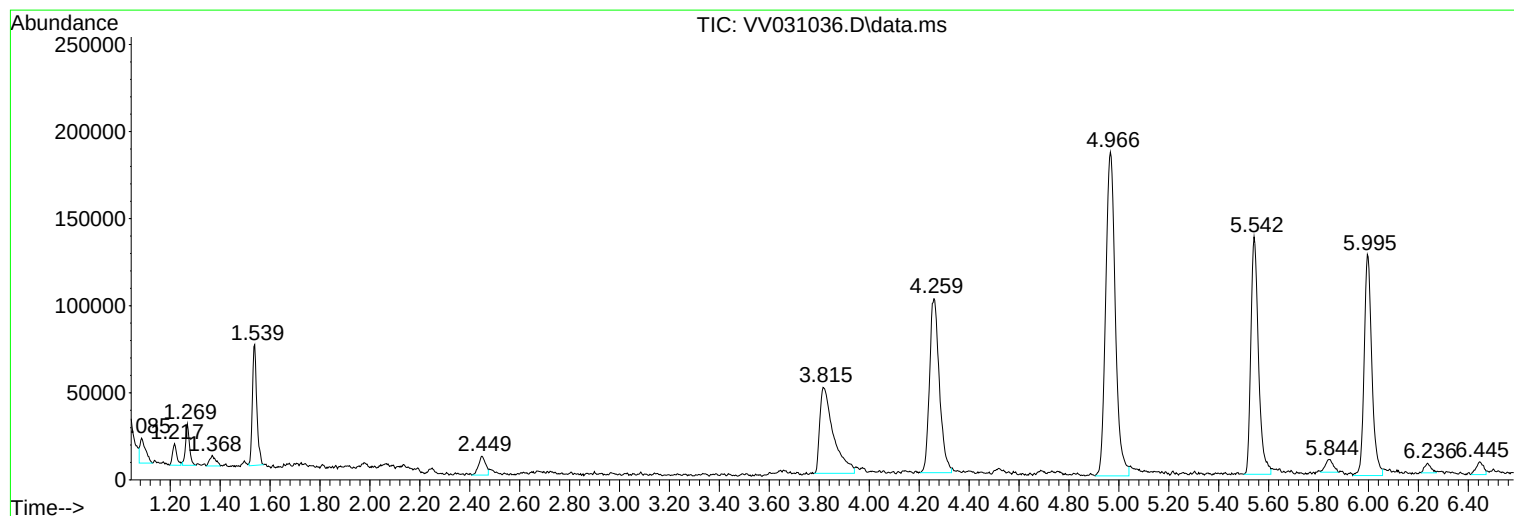
Sum of corrected areas: 4180732

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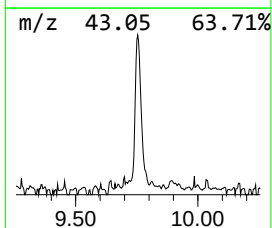
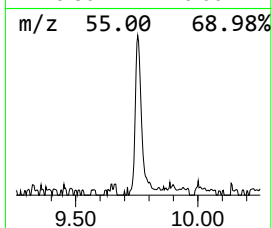
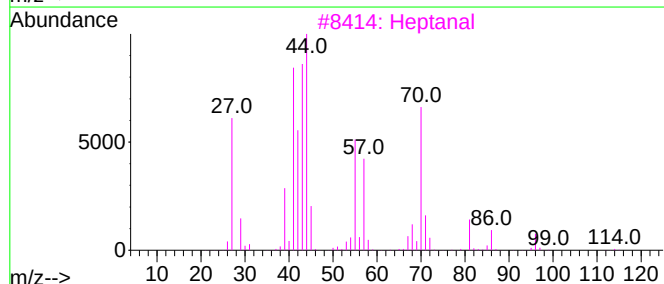
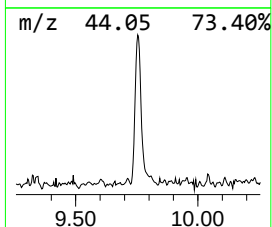
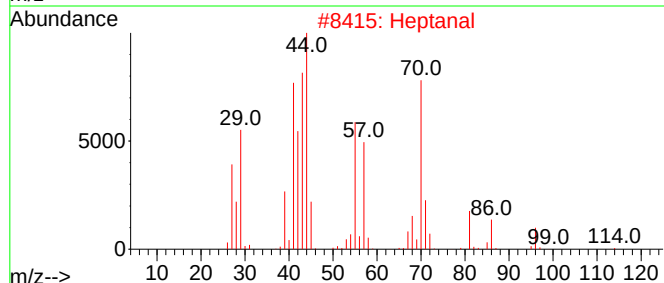
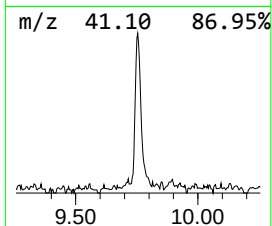
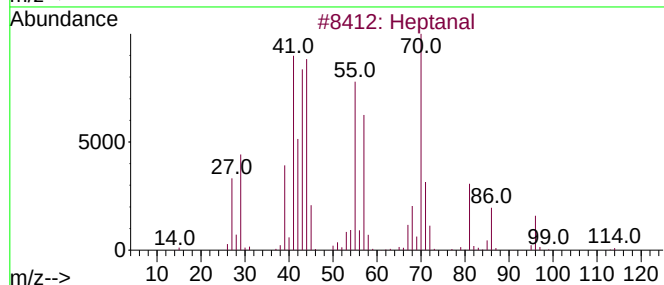
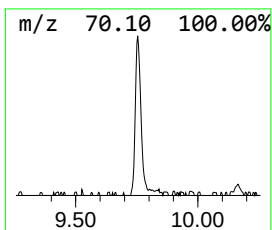
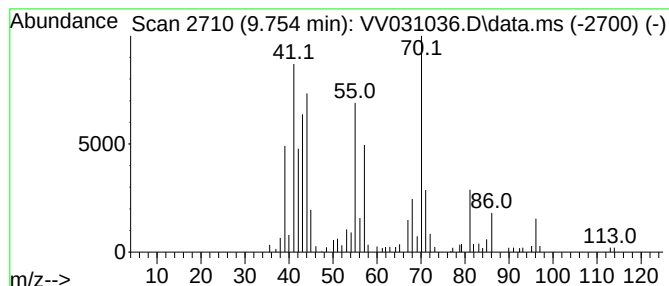
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR042823WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Heptanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.754	0.98 ug/L	78371	Chlorobenzene-d5	8.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal			114	C7H14O	000111-71-7	80
2	Heptanal			114	C7H14O	000111-71-7	72
3	Heptanal			114	C7H14O	000111-71-7	72
4	Heptanal			114	C7H14O	000111-71-7	70
5	Heptanal			114	C7H14O	000111-71-7	50



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Instrument :
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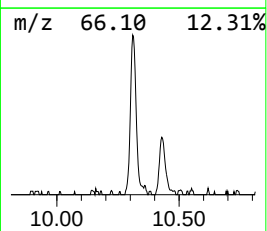
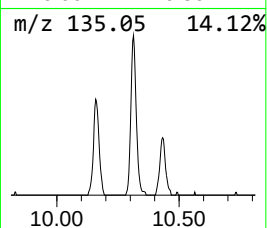
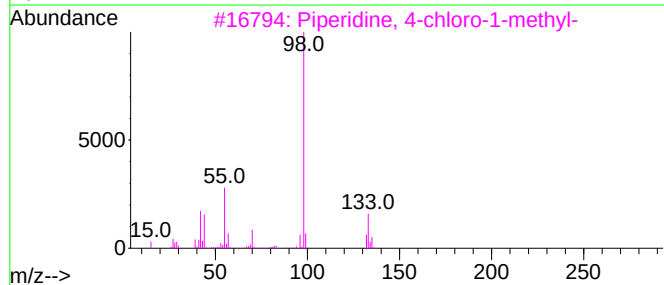
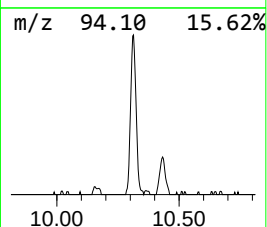
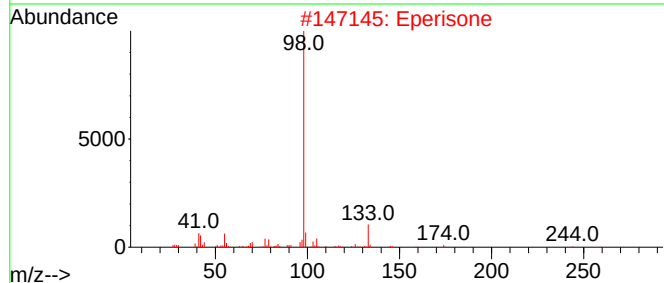
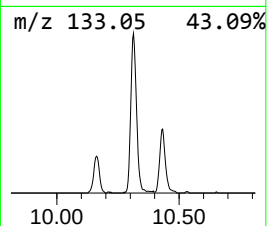
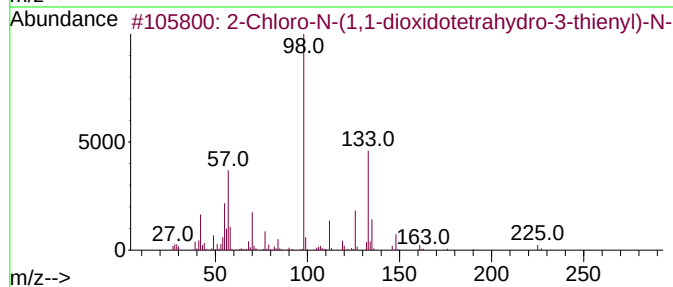
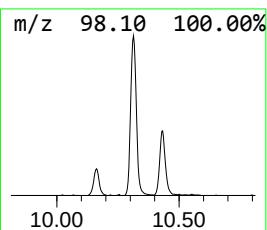
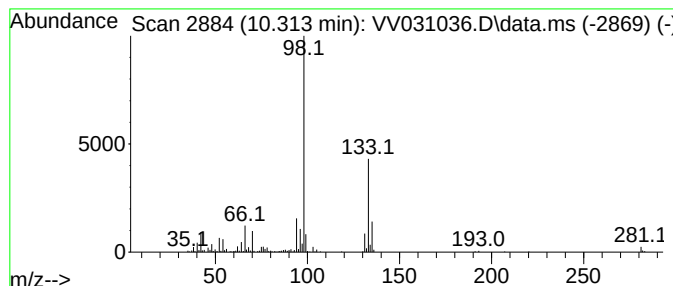
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR042823WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.313	3.07 ug/L	240261	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloro-N-(1,1-dioxidotetrahydr...	225	C7H12ClNO3S	007365-23-3	59
2			Eperisone	259	C17H25NO	064840-90-0	53
3			Piperidine, 4-chloro-1-methyl-	133	C6H12ClN	005570-77-4	45
4			1-Pyrrolidinecarbonyl chloride	133	C5H8ClNO	001192-63-8	42
5			Eperisone	259	C17H25NO	064840-90-0	36



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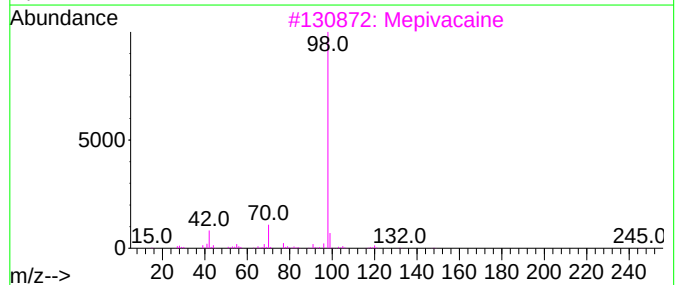
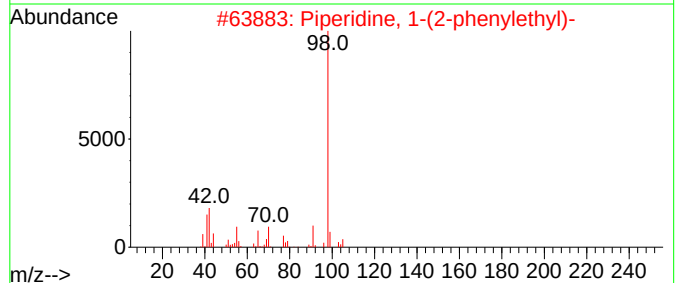
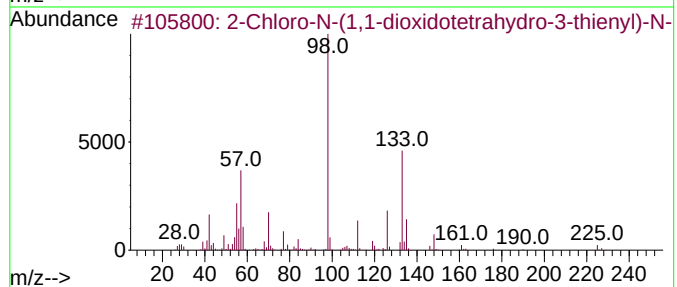
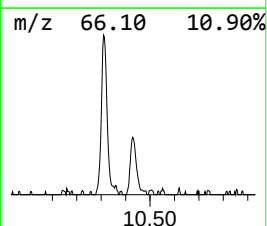
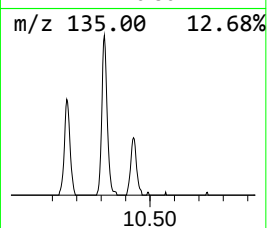
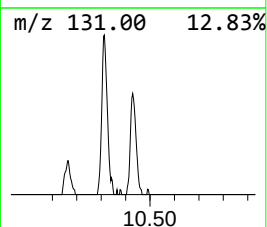
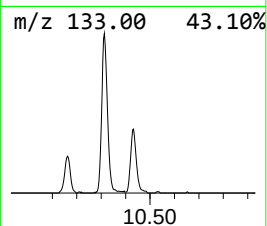
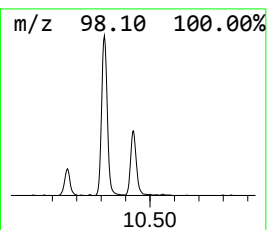
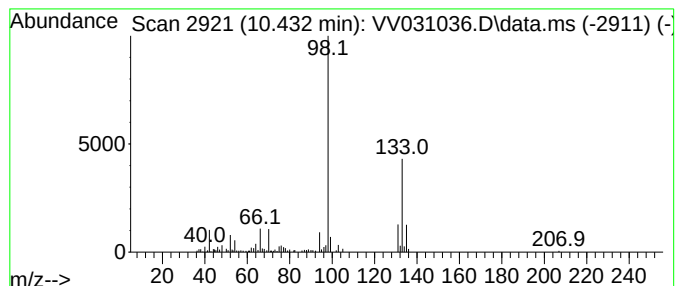
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Quant Title : TRACE VOA SFAM1.0

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	1.17 ug/L	91847	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloro-N-(1,1-dioxidotetrahydr...	225	C7H12ClNO3S	007365-23-3	50
2			Piperidine, 1-(2-phenylethyl)-	189	C13H19N	000332-14-9	38
3			Mepivacaine	246	C15H22N2O	000096-88-8	38
4			2-Benzyl-1-methylpiperidine	189	C13H19N	031414-56-9	38
5			4H-1,2,4-Triazole-3(2H)-thione, ...	278	C13H18N4OS	1000272-44-7	37



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Heptanal	9.754	1.0	ug/L	78371	2	8.793	400134	5.0
2-Chloro-N-(1,1...	10.313	3.1	ug/L	240261	3	11.191	391287	5.0
unknown-01	10.432	1.2	ug/L	91847	3	11.191	391287	5.0