

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100923\
 Data File : VV032322.D
 Acq On : 09 Oct 2023 12:34
 Operator : SY/MD
 Sample : 04708-12
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCJR2

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\SFAMVTR092923WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV032322.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	66	74	86	rBV	83592	91058	2.23%	0.988%
2	1.532	146	153	166	rVB	60196	70115	1.72%	0.761%
3	2.059	307	317	328	rBV	108890	158117	3.88%	1.716%
4	2.127	328	338	365	rVB	41837	98097	2.41%	1.064%
5	3.802	849	859	871	rBV	53494	140431	3.44%	1.524%
6	3.873	871	881	920	rVB	156121	450695	11.05%	4.891%
7	4.275	982	1006	1029	rBV3	248246	761140	18.66%	8.259%
8	4.963	1199	1220	1239	rBV2	156887	411060	10.08%	4.460%
9	5.538	1387	1399	1414	rBV	118477	246326	6.04%	2.673%
10	5.834	1476	1491	1503	rBV	2081969	4078062	100.00%	44.251%
11	5.992	1530	1540	1574	rVB2	88121	212536	5.21%	2.306%
12	6.436	1665	1678	1707	rBV2	60145	132414	3.25%	1.437%
13	6.918	1818	1828	1854	rBV2	40483	88475	2.17%	0.960%
14	7.246	1919	1930	1961	rBV	194478	371988	9.12%	4.036%
15	7.561	2019	2028	2045	rBV3	23883	48543	1.19%	0.527%
16	8.030	2164	2174	2185	rBV	221121	406485	9.97%	4.411%
17	8.185	2213	2222	2243	rVB4	21770	47465	1.16%	0.515%
18	8.789	2398	2410	2431	rBV	195728	343071	8.41%	3.723%
19	9.545	2635	2645	2663	rBV	32666	59292	1.45%	0.643%
20	9.654	2671	2679	2703	rBV	22141	42302	1.04%	0.459%
21	10.156	2825	2835	2852	rBV	68115	113133	2.77%	1.228%
22	10.882	3049	3061	3077	rBV3	38278	75793	1.86%	0.822%
23	10.988	3084	3094	3113	rBV	31449	58681	1.44%	0.637%
24	11.188	3146	3156	3181	rVB	217823	346461	8.50%	3.759%
25	11.564	3263	3273	3289	rVB	202624	313112	7.68%	3.398%
26	12.082	3426	3434	3449	rVB	31744	50808	1.25%	0.551%

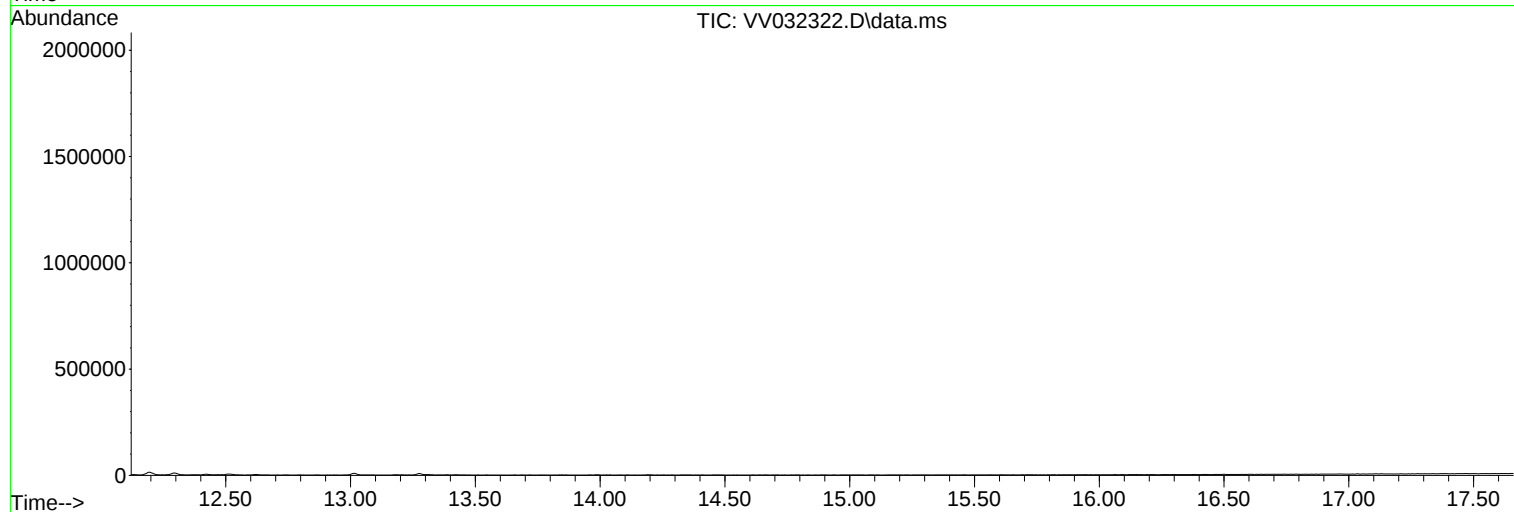
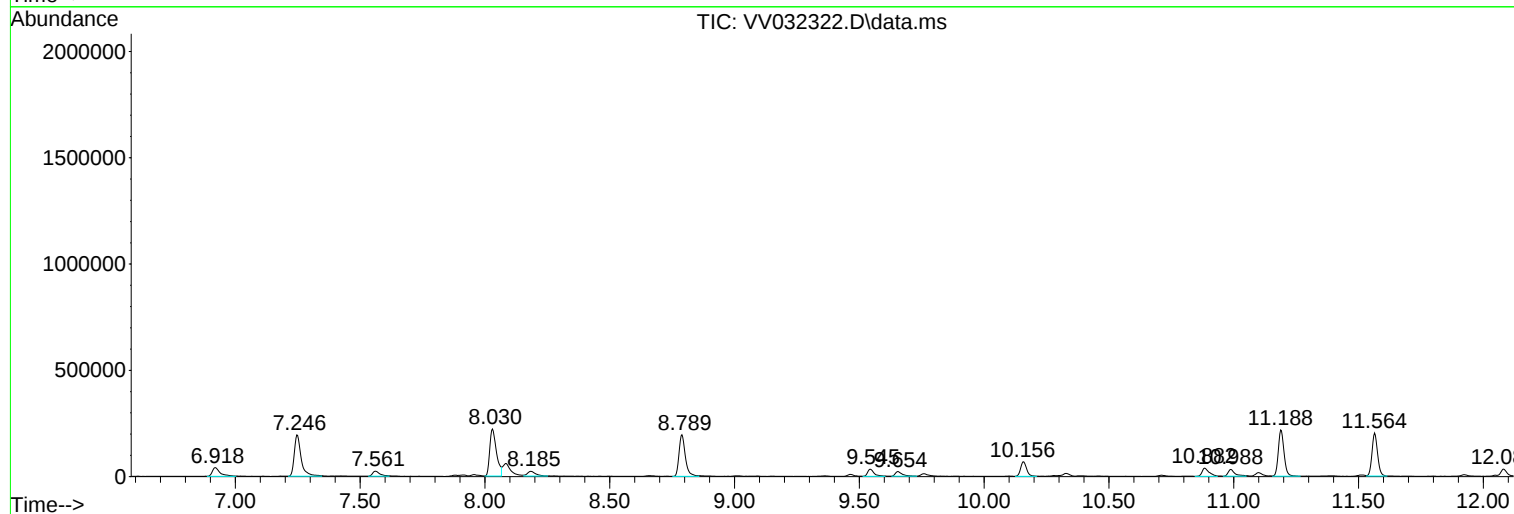
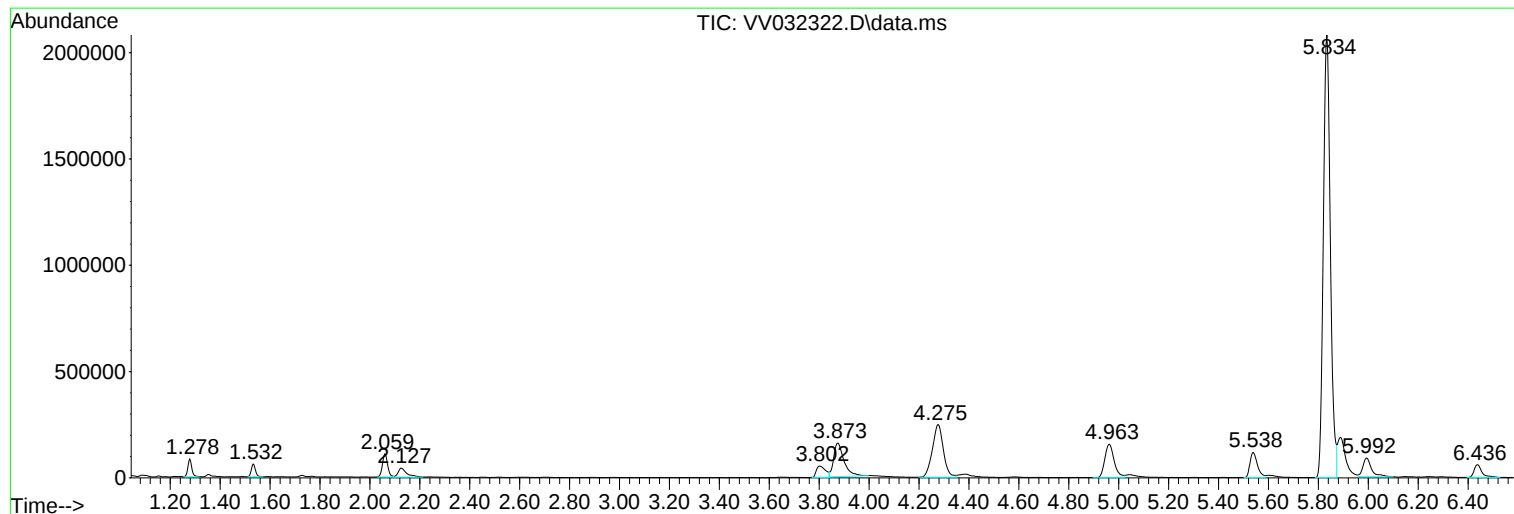
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Instrument :
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ClientSampleId :
DCJR2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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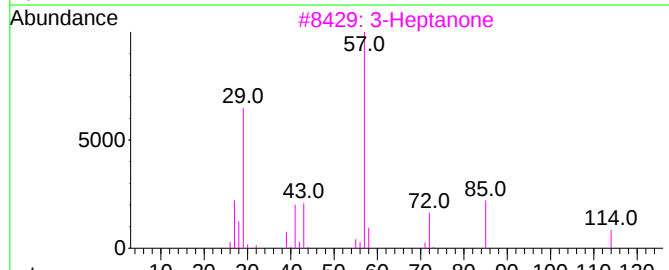
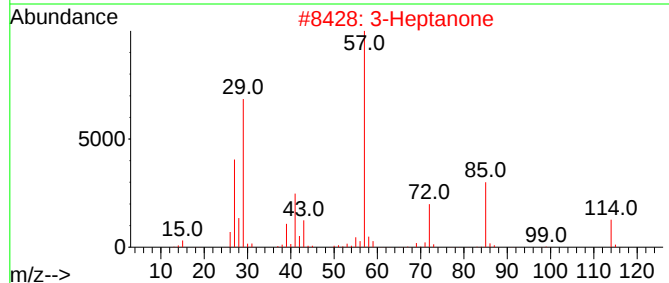
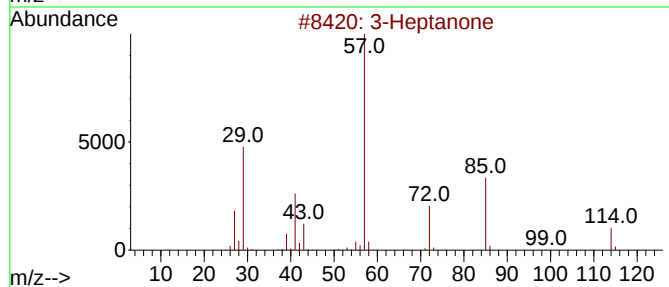
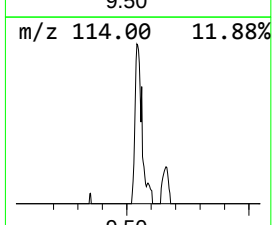
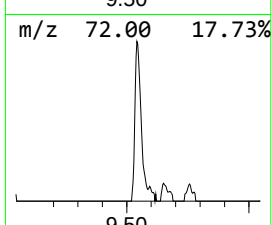
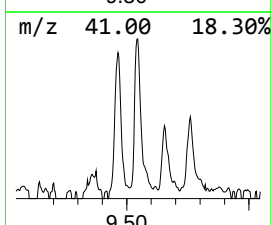
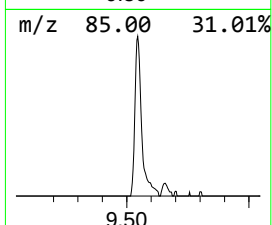
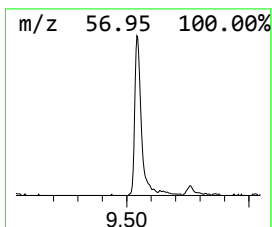
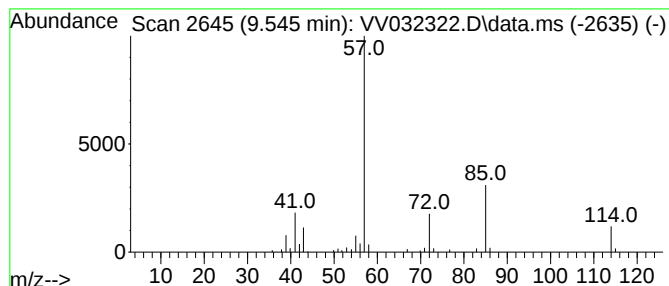
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 3-Heptanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.545	0.86 ug/L	59292	Chlorobenzene-d5	8.789

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Heptanone	114	C7H14O	000106-35-4	91
2		3-Heptanone	114	C7H14O	000106-35-4	86
3		3-Heptanone	114	C7H14O	000106-35-4	80
4		3-Heptanone	114	C7H14O	000106-35-4	80
5		3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	72



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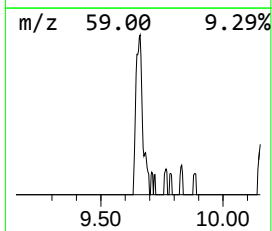
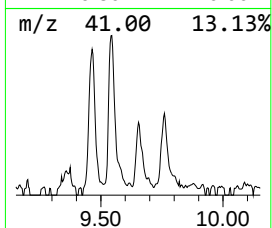
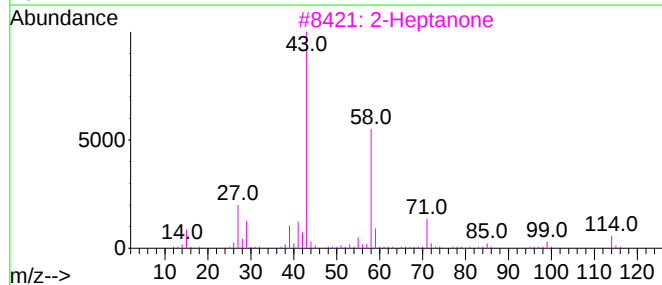
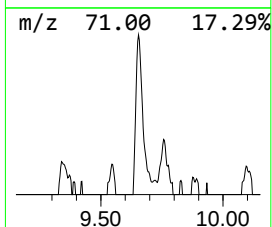
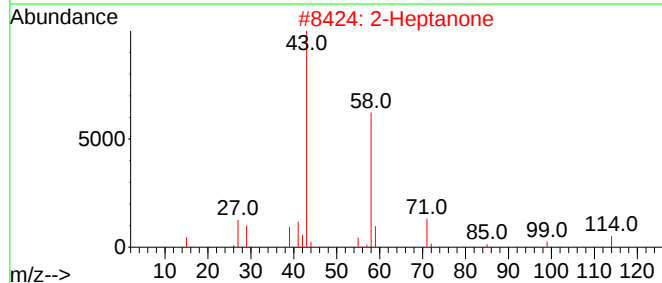
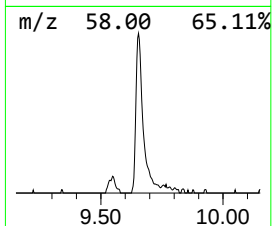
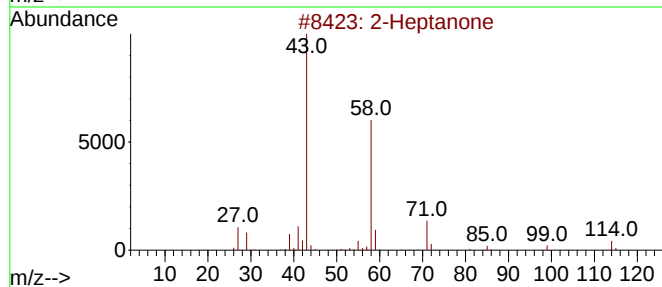
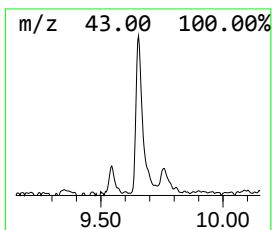
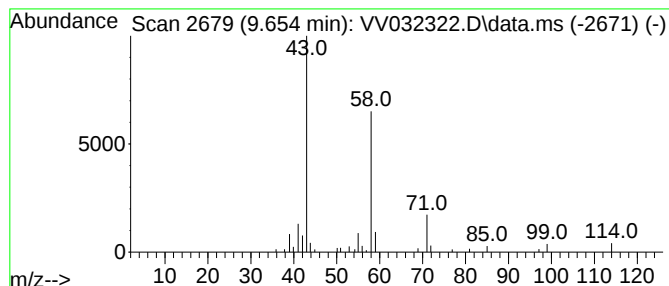
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 2-Heptanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.654	0.62 ug/L	42302	Chlorobenzene-d5	8.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone			114	C7H14O	000110-43-0	91
2	2-Heptanone			114	C7H14O	000110-43-0	90
3	2-Heptanone			114	C7H14O	000110-43-0	83
4	2-Heptanone			114	C7H14O	000110-43-0	83
5	2-Heptanone			114	C7H14O	000110-43-0	72



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Sample : 04708-12
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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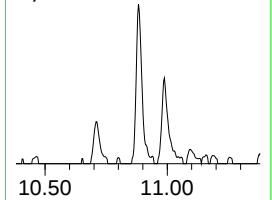
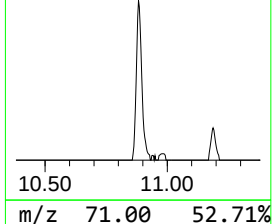
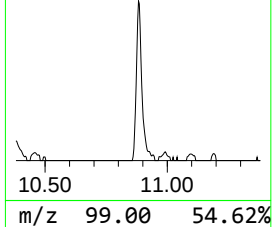
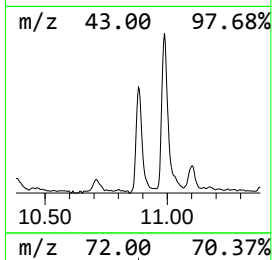
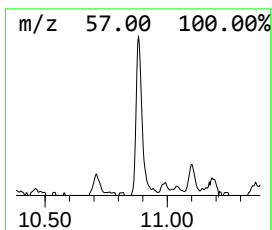
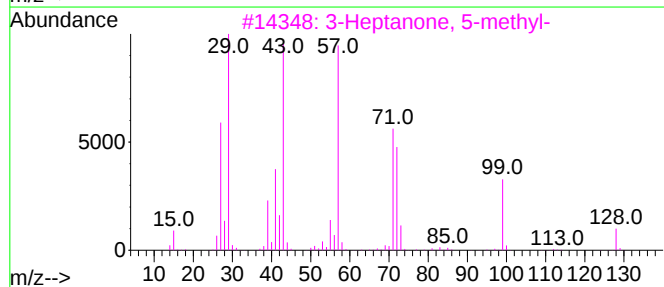
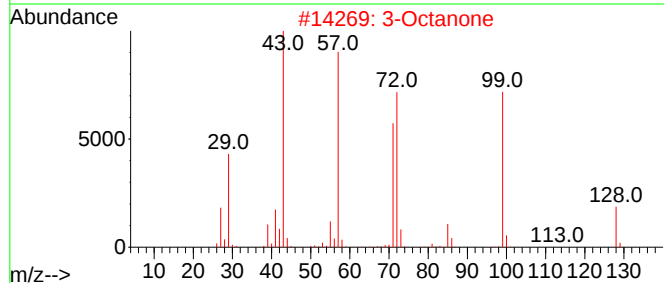
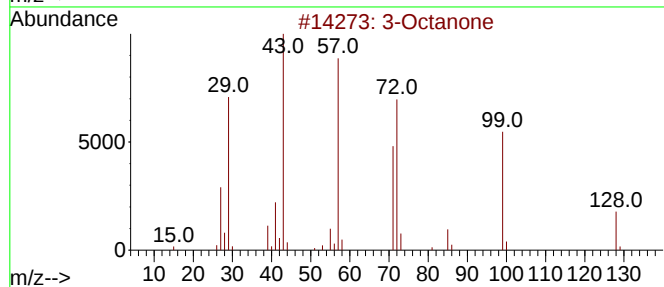
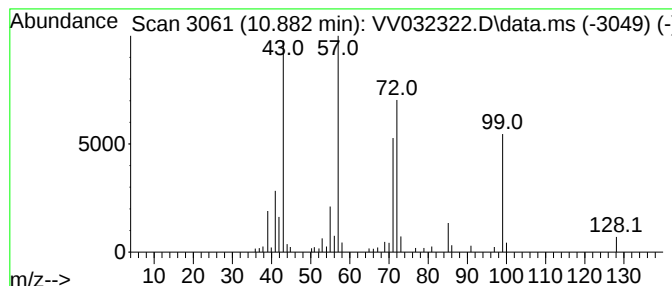
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 3-Octanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.882	1.09 ug/L	75793	1,4-Dichlorobenzene-d4	11.188

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octanone	128	C8H16O	000106-68-3	94
2			3-Octanone	128	C8H16O	000106-68-3	78
3			3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	59
4			3-Octanone	128	C8H16O	000106-68-3	59
5			Butanal, 2-ethyl-	100	C6H12O	000097-96-1	49



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Sample : 04708-12
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCJR2

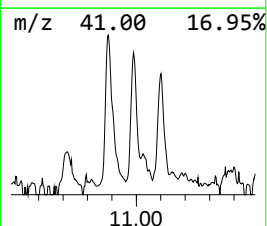
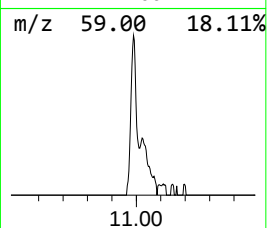
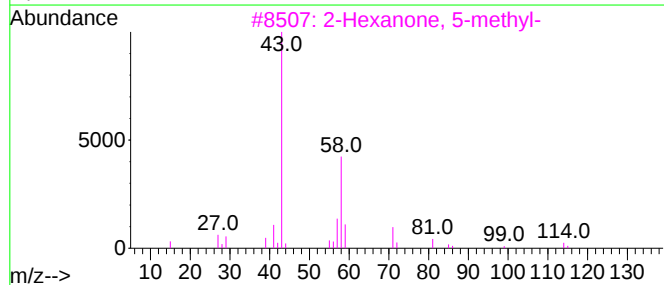
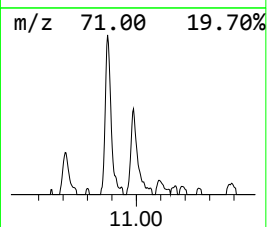
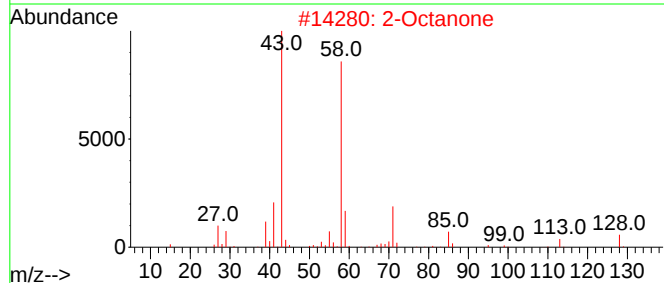
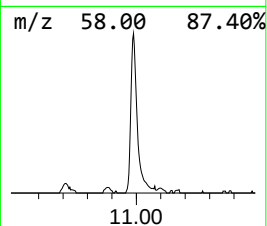
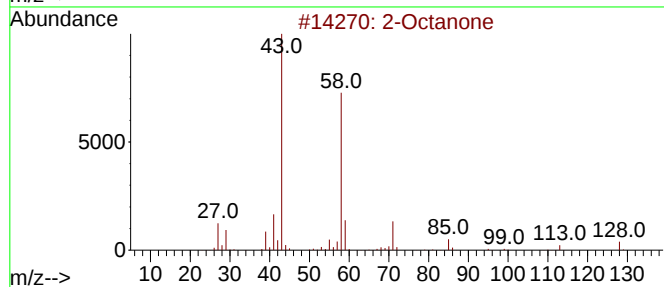
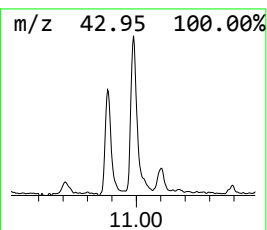
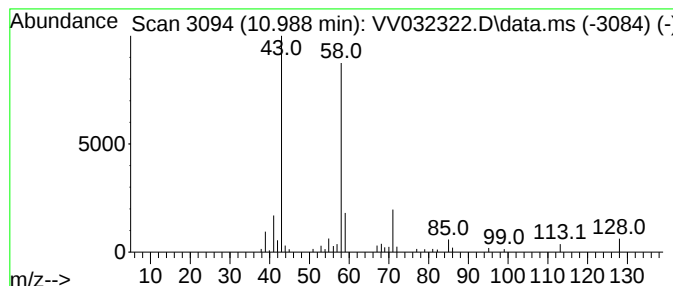
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 2-Octanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.988	0.85 ug/L	58681	1,4-Dichlorobenzene-d4	11.188

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octanone	128	C8H16O	000111-13-7	91
2			2-Octanone	128	C8H16O	000111-13-7	91
3			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78
4			2-Octanone	128	C8H16O	000111-13-7	74
5			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	72



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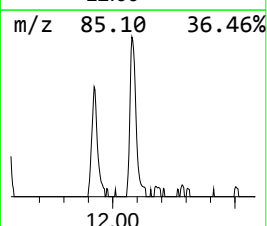
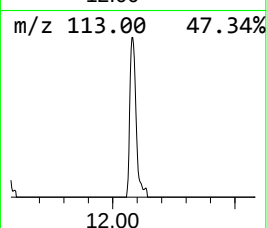
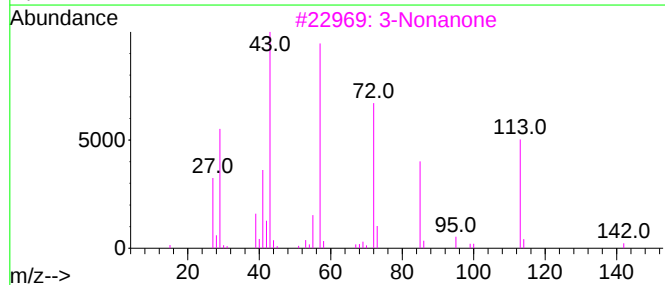
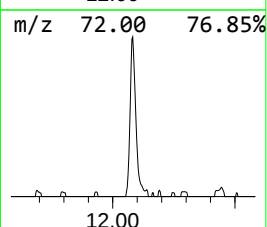
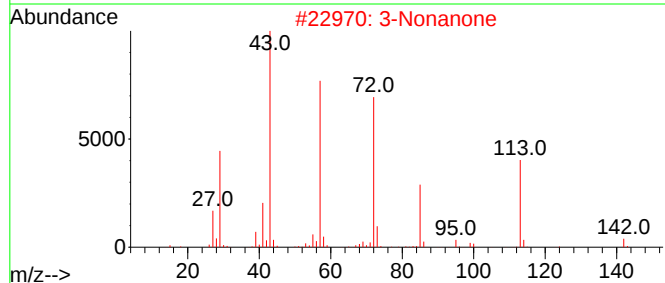
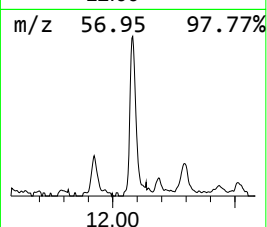
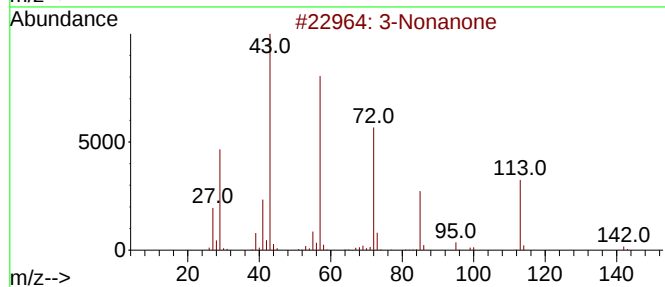
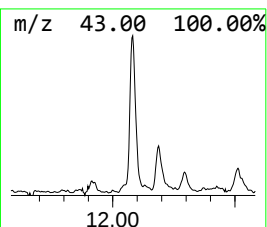
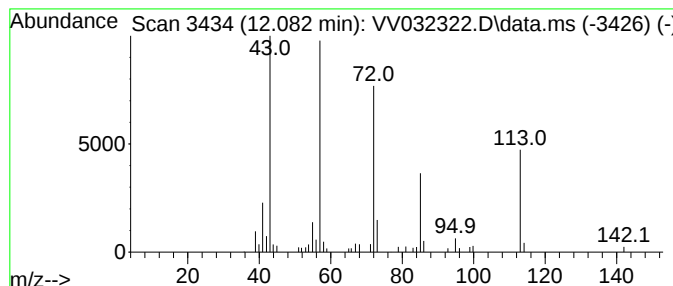
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 3-Nonanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.082	0.73 ug/L	50808	1,4-Dichlorobenzene-d4	11.188

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Nonanone		142	C9H18O	000925-78-0	95
2	3-Nonanone		142	C9H18O	000925-78-0	94
3	3-Nonanone		142	C9H18O	000925-78-0	91
4	3-Nonanone		142	C9H18O	000925-78-0	91
5	3-Nonanone		142	C9H18O	000925-78-0	83



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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
3-Heptanone	9.545	0.9	ug/L	59292	2	8.789	343071	5.0
2-Heptanone	9.654	0.6	ug/L	42302	2	8.789	343071	5.0
3-Octanone	10.882	1.1	ug/L	75793	3	11.188	346461	5.0
2-Octanone	10.988	0.8	ug/L	58681	3	11.188	346461	5.0
3-Nonanone	12.082	0.7	ug/L	50808	3	11.188	346461	5.0