

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101923\
 Data File : VX038385.D
 Acq On : 19 Oct 2023 15:01
 Operator : JC/MD
 Sample : 04966-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 231013059-VOA

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

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_X\Method\82X100523W.M
 Title : SW846 8260

Signal : TIC: VX038385.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	24	27	39	rVB	164310	209176	2.12%	0.664%
2	2.374	204	211	230	rBV	1887701	3138208	31.82%	9.961%
3	2.953	296	306	326	rBV	2455431	5292225	53.66%	16.798%
4	4.568	551	571	586	rBV2	2784494	9861986	100.00%	31.303%
5	4.995	631	641	669	rVB	684553	2097648	21.27%	6.658%
6	5.385	694	705	719	rBV	95359	277827	2.82%	0.882%
7	5.550	721	732	747	rVB	150931	427686	4.34%	1.358%
8	5.952	789	798	807	rBV	101582	273327	2.77%	0.868%
9	6.227	833	843	853	rVB2	42716	127691	1.29%	0.405%
10	6.757	922	930	946	rVV	236733	578048	5.86%	1.835%
11	7.452	1032	1044	1055	rBV	58559	158482	1.61%	0.503%
12	8.574	1220	1228	1234	rBV	317761	524593	5.32%	1.665%
13	8.647	1234	1240	1247	rVV	531592	836598	8.48%	2.655%
14	8.720	1247	1252	1259	rVB2	58147	102993	1.04%	0.327%
15	9.378	1352	1360	1365	rVB	83237	130996	1.33%	0.416%
16	10.055	1460	1471	1483	rBV	600075	905230	9.18%	2.873%
17	10.195	1489	1494	1504	rBV2	84441	140805	1.43%	0.447%
18	10.299	1507	1511	1518	rVV	102674	152898	1.55%	0.485%
19	10.768	1580	1588	1597	rBV	85095	135777	1.38%	0.431%
20	11.079	1634	1639	1645	rBV	518432	655695	6.65%	2.081%
21	12.024	1787	1794	1801	rVB	672875	966222	9.80%	3.067%
22	12.104	1801	1807	1811	rBV3	84837	139300	1.41%	0.442%
23	12.902	1927	1938	1943	rBV	576224	761843	7.73%	2.418%
24	12.963	1944	1948	1960	rVB6	59229	108994	1.11%	0.346%
25	13.335	2005	2009	2014	rBV	113568	149237	1.51%	0.474%
26	13.475	2027	2032	2034	rBV3	145825	224056	2.27%	0.711%
27	13.512	2034	2038	2045	rVV	1279527	1747689	17.72%	5.547%
28	13.591	2045	2051	2060	rVV3	186632	355089	3.60%	1.127%
29	13.731	2070	2074	2077	rVV	89343	123519	1.25%	0.392%
30	13.774	2077	2081	2087	rVB	450098	563225	5.71%	1.788%
31	13.933	2101	2107	2114	rBV5	48796	115481	1.17%	0.367%
32	14.097	2128	2134	2142	rBV	145531	221987	2.25%	0.705%

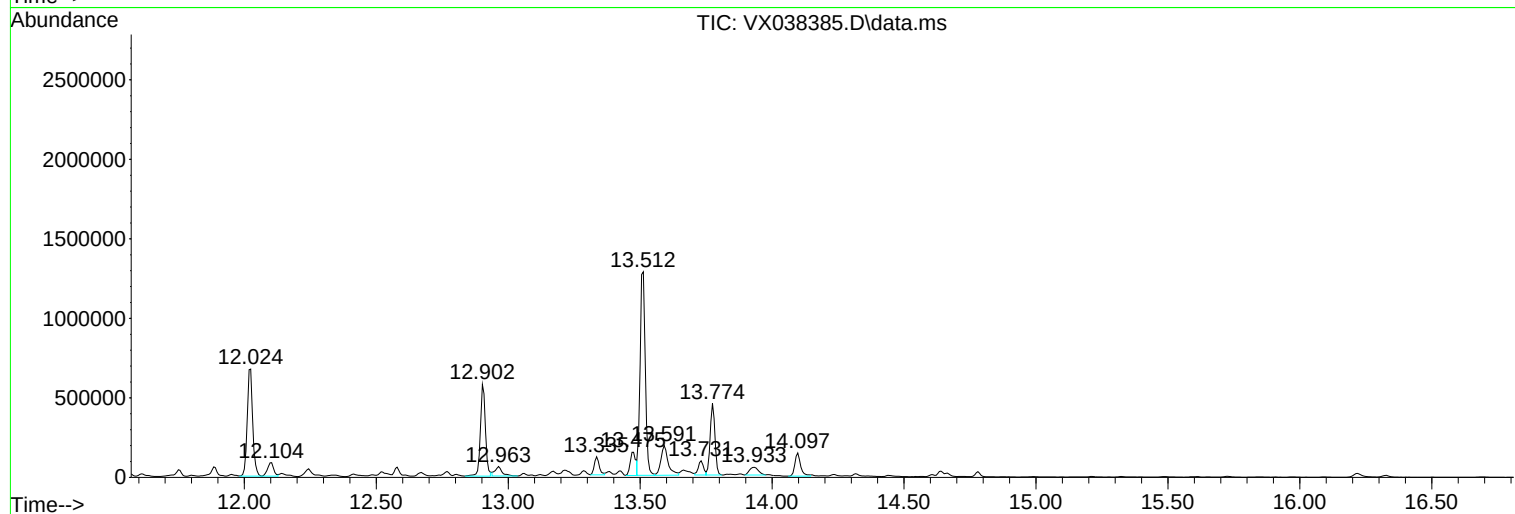
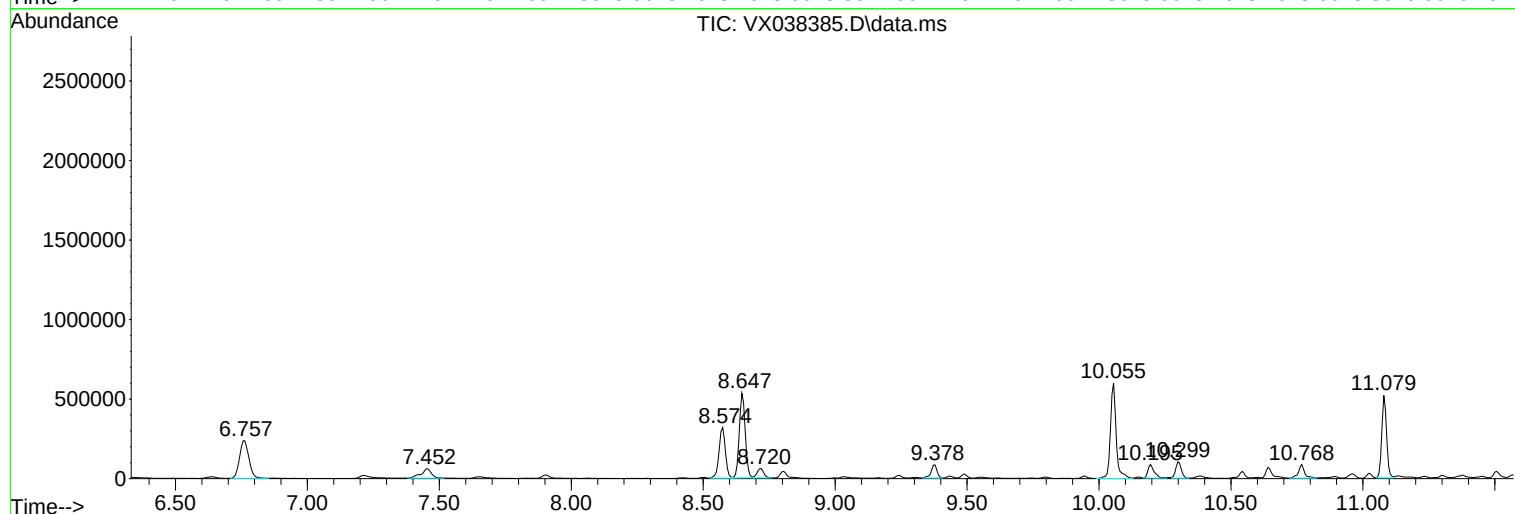
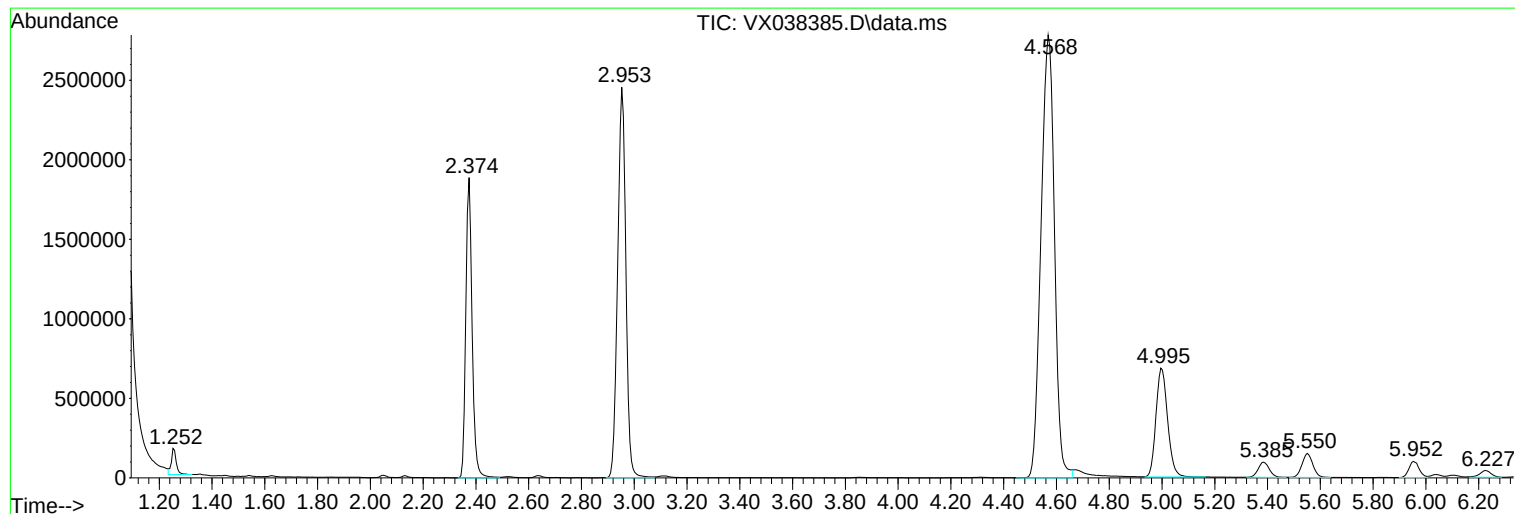
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ClientSampleId :
231013059-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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



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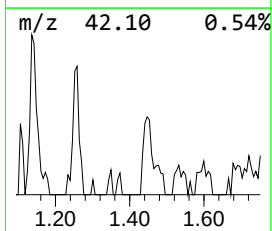
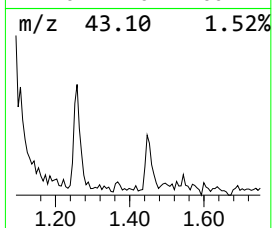
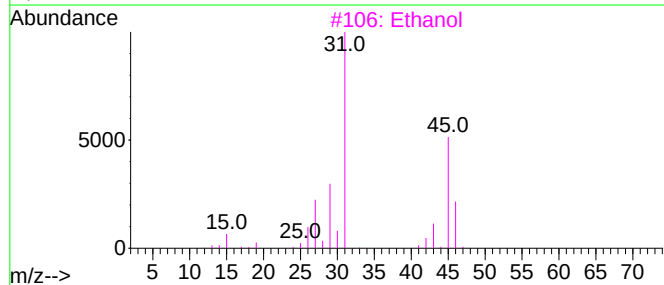
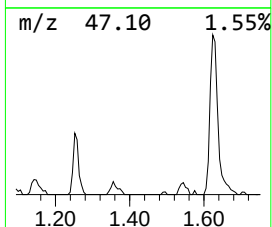
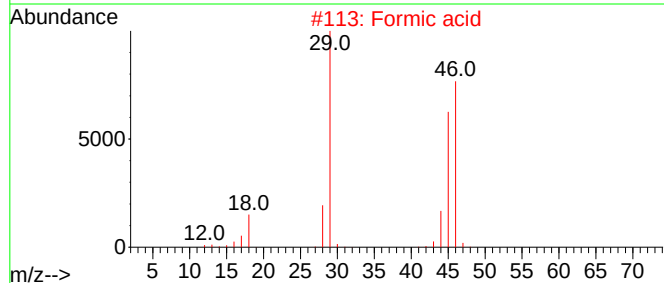
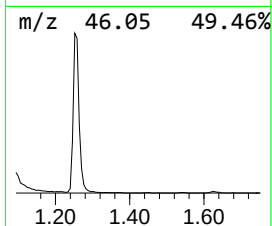
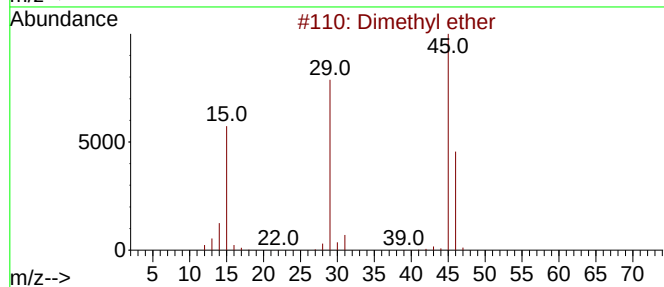
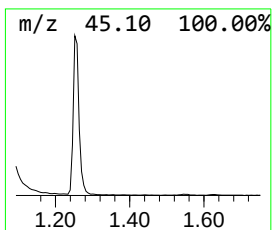
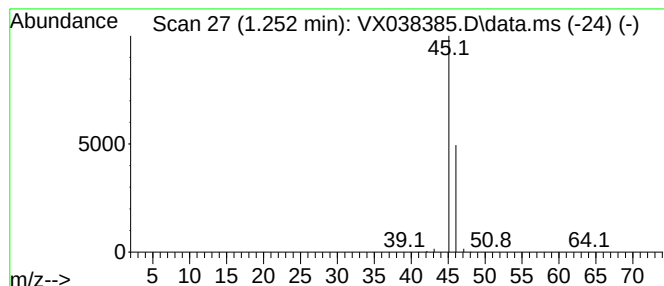
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 1 Dimethyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	24.45 ug/l	209176	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	64
2			Formic acid	46	CH2O2	000064-18-6	7
3			Ethanol	46	C2H6O	000064-17-5	7
4			Oxalic acid	90	C2H2O4	000144-62-7	4
5			Methane, nitroso-	45	CH3NO	000865-40-7	3



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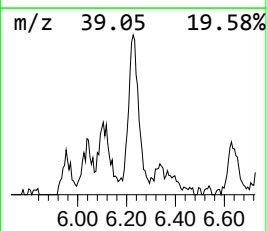
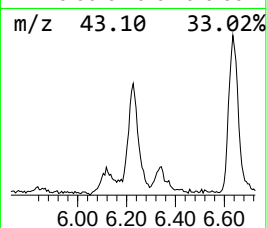
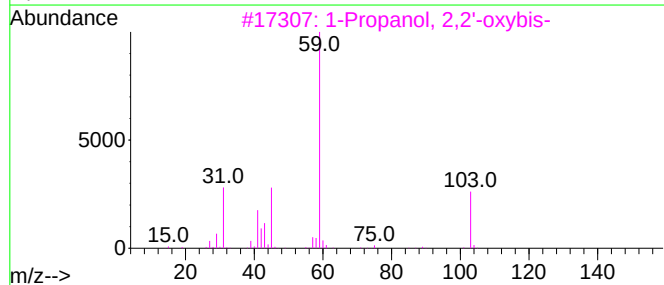
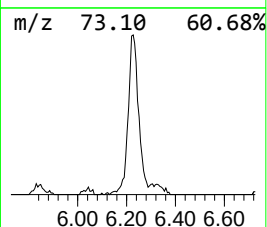
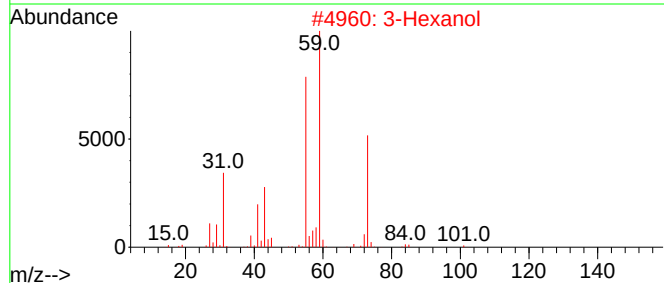
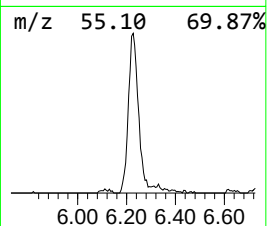
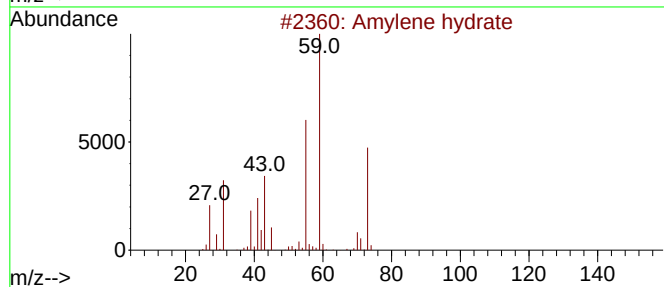
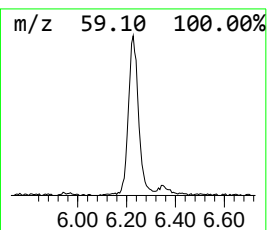
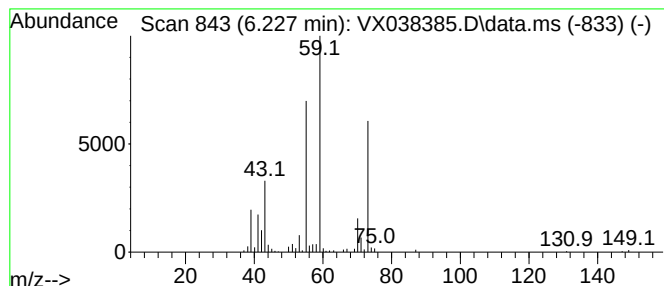
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 2 Amylene hydrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.227	11.05 ug/l	127691	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	64
2			3-Hexanol	102	C6H14O	000623-37-0	38
3			1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	33
4			Silane, trimethyl-	74	C3H10Si	000993-07-7	23
5			1-Butene, 3-methyl-	70	C5H10	000563-45-1	10



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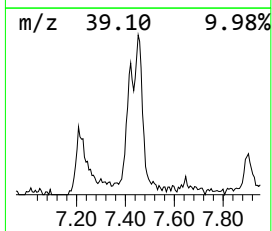
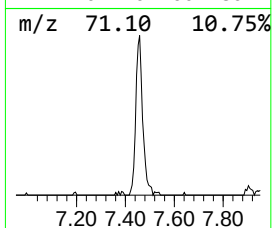
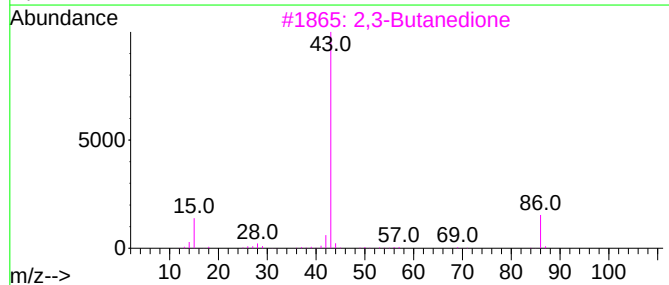
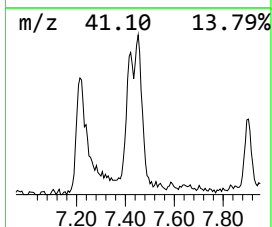
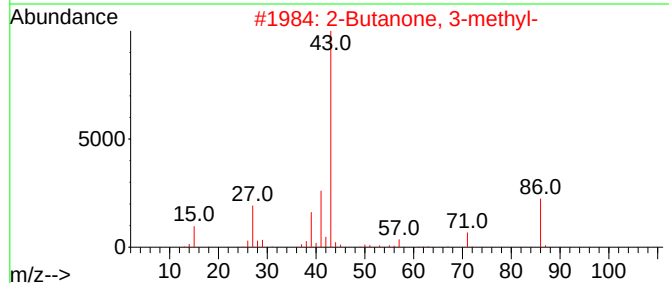
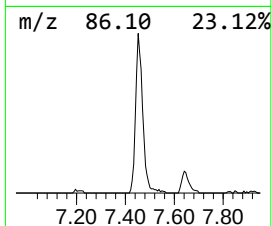
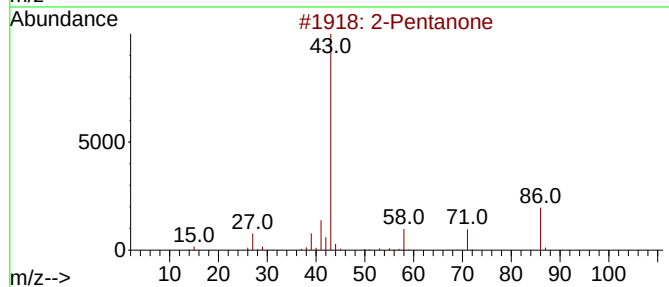
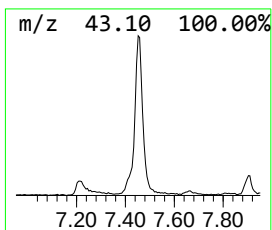
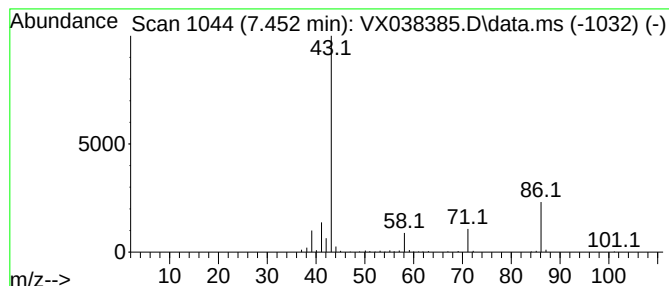
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 3 2-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.452	13.71 ug/l	158482	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone		86	C5H10O	000107-87-9	87
2	2-Butanone, 3-methyl-		86	C5H10O	000563-80-4	64
3	2,3-Butanedione		86	C4H6O2	000431-03-8	52
4	2-Propanone, methylhydrazone		86	C4H10N2	005771-02-8	9
5	2,3-Hexanedione		114	C6H10O2	003848-24-6	9



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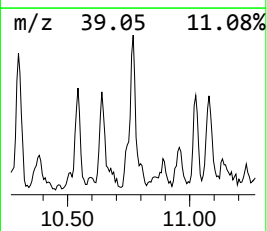
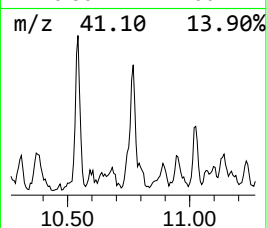
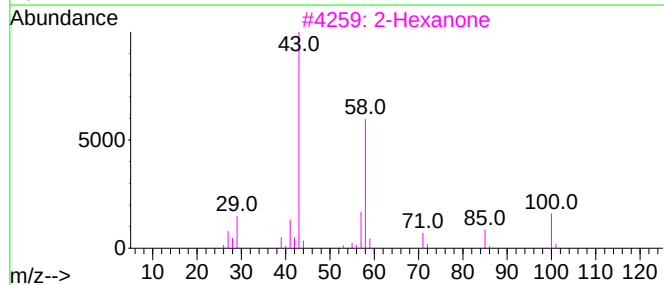
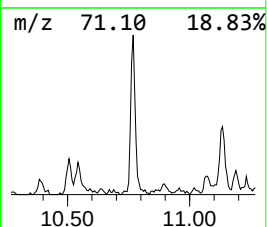
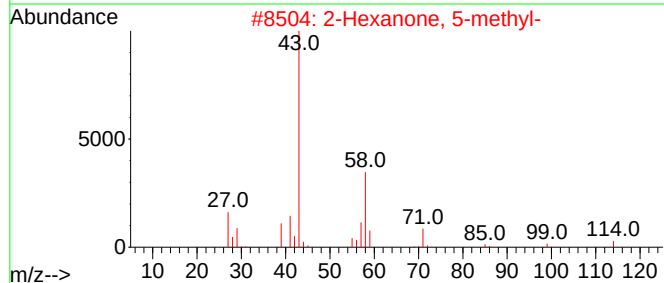
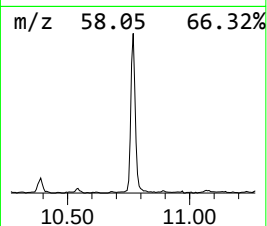
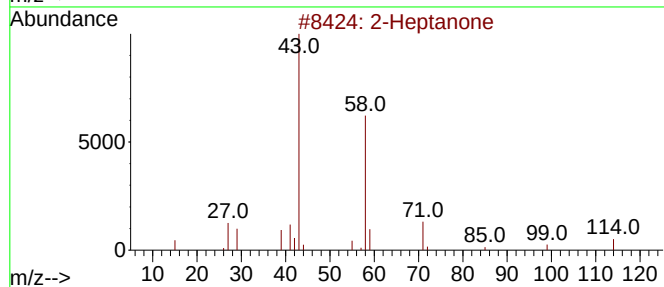
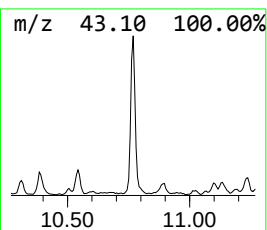
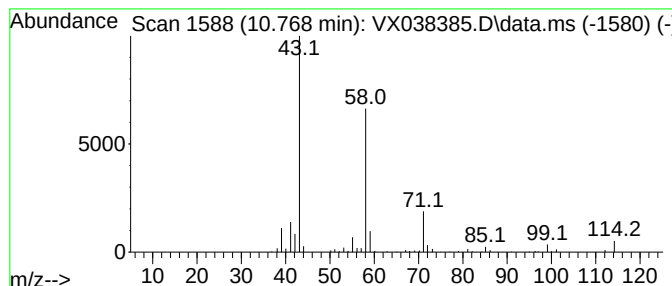
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Heptanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.769	7.50 ug/l	135777	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone	114	C7H14O	000110-43-0	91
2			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78
3			2-Hexanone	100	C6H12O	000591-78-6	59
4			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	59
5			2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	47



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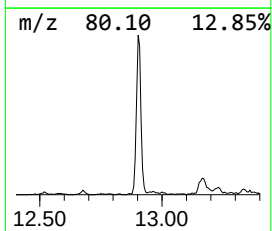
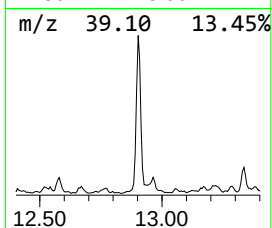
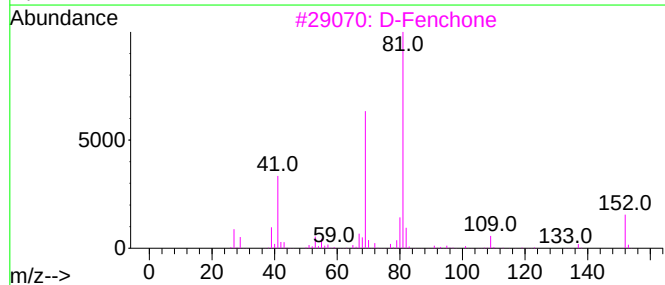
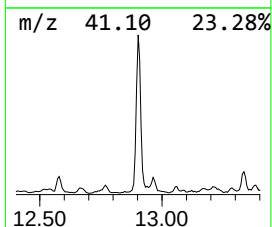
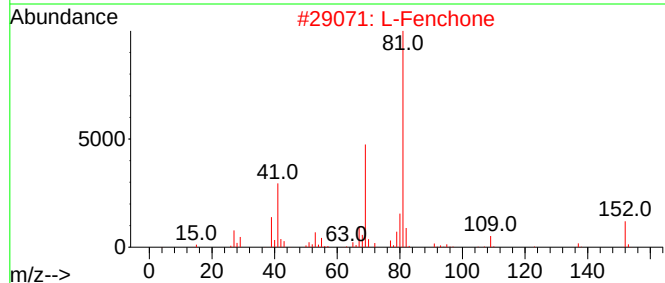
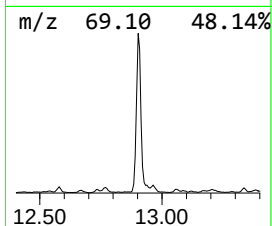
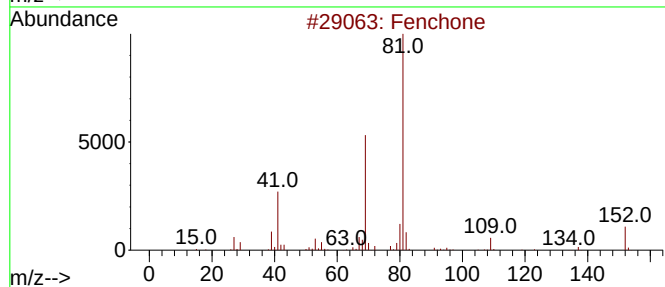
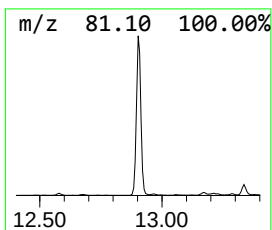
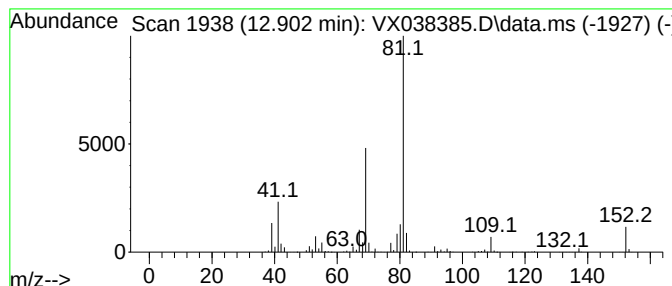
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 5 Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.902	39.42 ug/l	761843	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	95
2			L-Fenchone	152	C10H16O	007787-20-4	94
3			D-Fenchone	152	C10H16O	004695-62-9	91
4			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	45
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45



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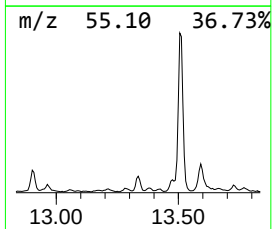
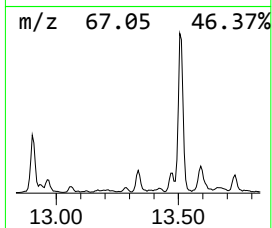
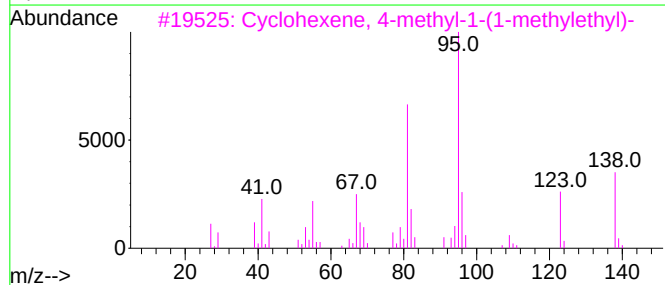
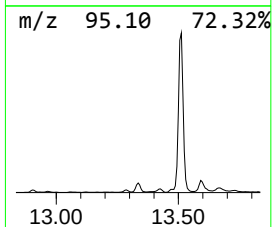
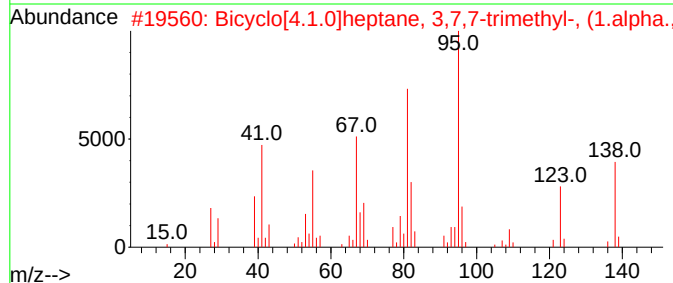
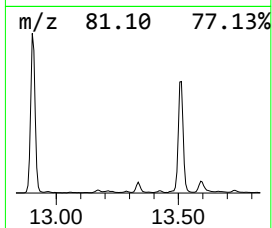
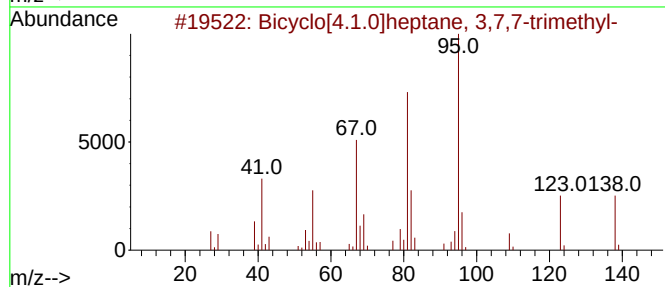
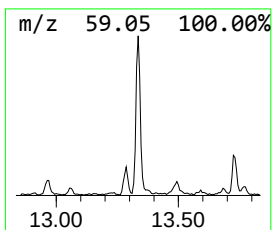
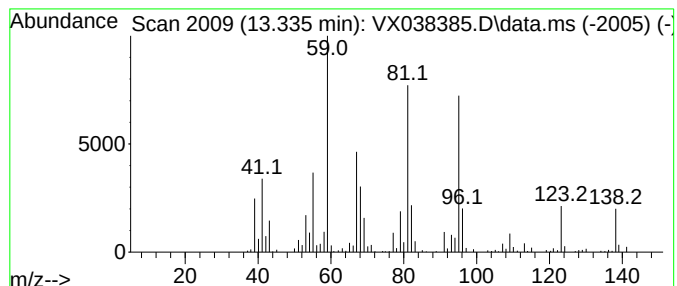
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Quant Title : SW846 8260

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

Peak Number 6 Bicyclo[4.1.0]heptane, 3,7,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	7.72 ug/l	149237	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	93
2			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	80
3			Cyclohexene, 4-methyl-1-(1-methy...	138	C10H18	000500-00-5	70
4			5H-Inden-5-one, octahydro-, trans-	138	C9H14O	004668-81-9	60
5			2H-Inden-2-one, octahydro-, cis-	138	C9H14O	005689-04-3	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101923\
Data File : VX038385.D
Acq On : 19 Oct 2023 15:01
Operator : JC/MD
Sample : 04966-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
231013059-VOA

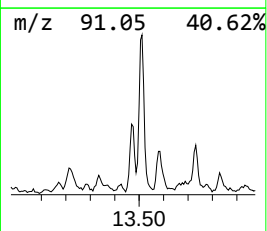
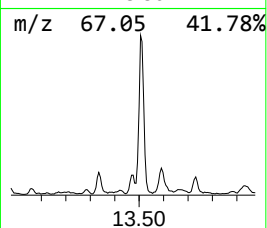
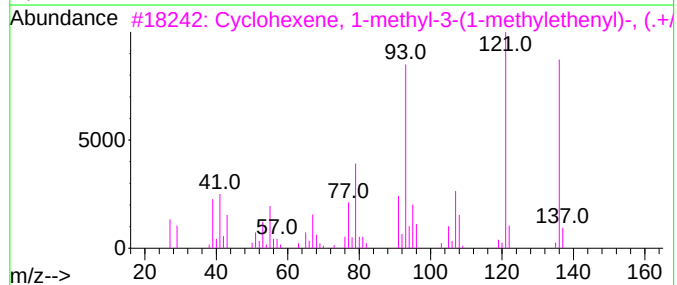
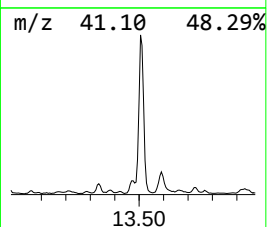
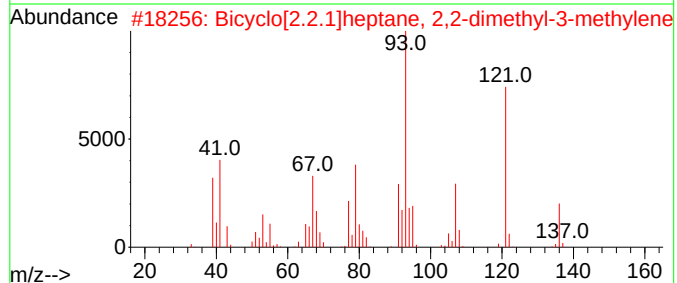
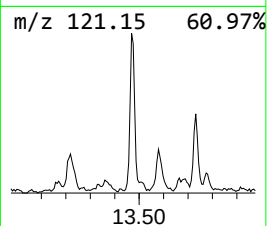
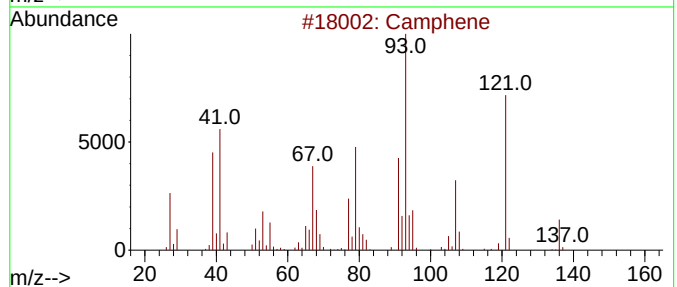
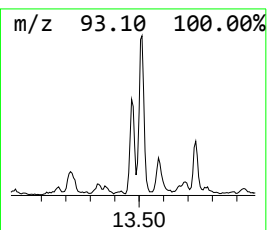
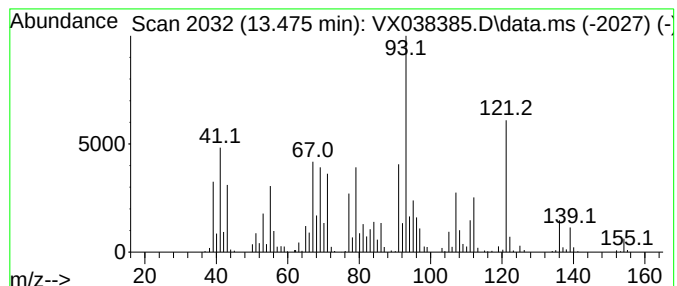
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Quant Title : SW846 8260

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

Peak Number 7 Camphene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.475	11.59 ug/l	224056	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphene	136	C10H16	000079-92-5	96
2			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	93
3			Cyclohexene, 1-methyl-3-(1-methy...	136	C10H16	000499-03-6	70
4			p-Menth-2-en-7-ol, trans-	154	C10H18O	019898-87-4	68
5			Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101923\
Data File : VX038385.D
Acq On : 19 Oct 2023 15:01
Operator : JC/MD
Sample : 04966-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
231013059-VOA

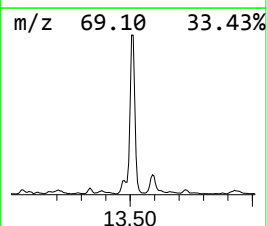
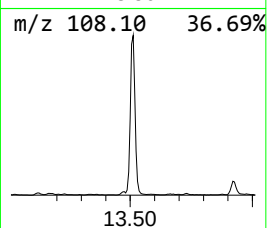
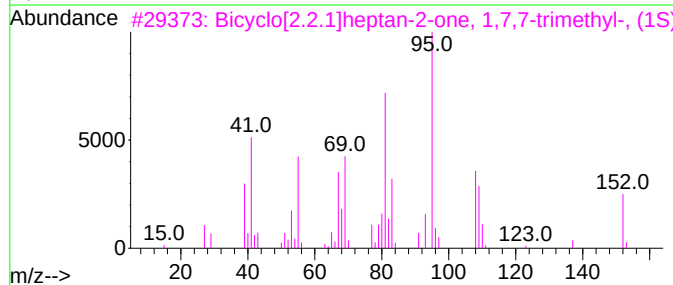
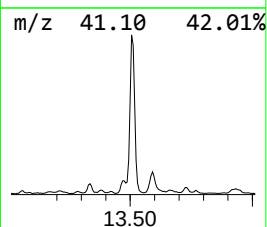
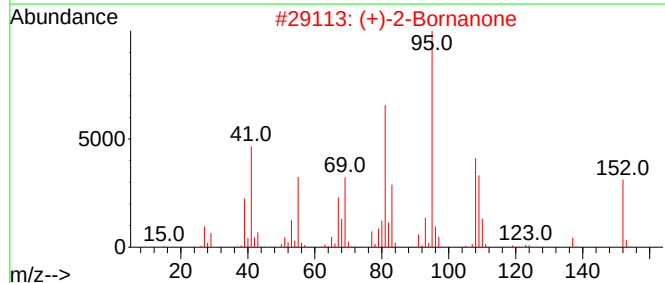
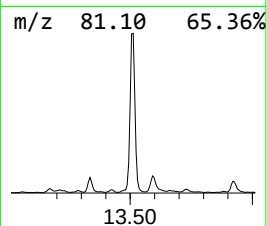
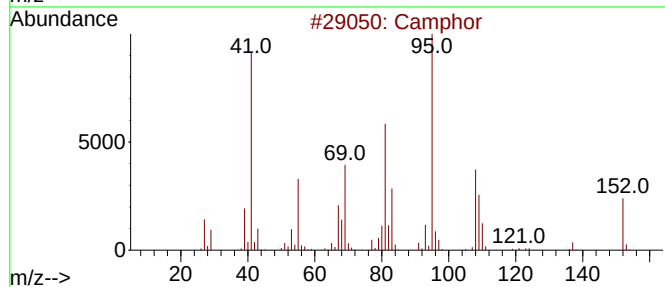
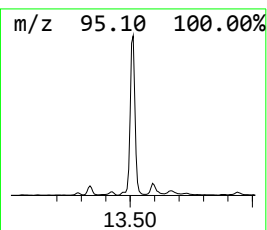
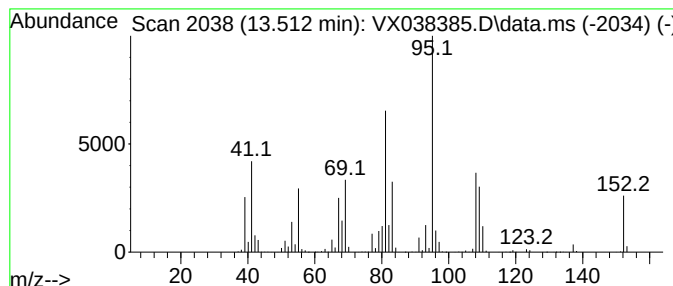
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Quant Title : SW846 8260

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

Peak Number 8 Camphor Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	90.44 ug/l	1747690	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphor	152	C10H16O	000076-22-2	98
2			(+)-2-Bornanone	152	C10H16O	000464-49-3	98
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
4			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49
5			2-Furancarboxylic acid, 2-propen...	152	C8H8O3	004208-49-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101923\
Data File : VX038385.D
Acq On : 19 Oct 2023 15:01
Operator : JC/MD
Sample : 04966-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
231013059-VOA

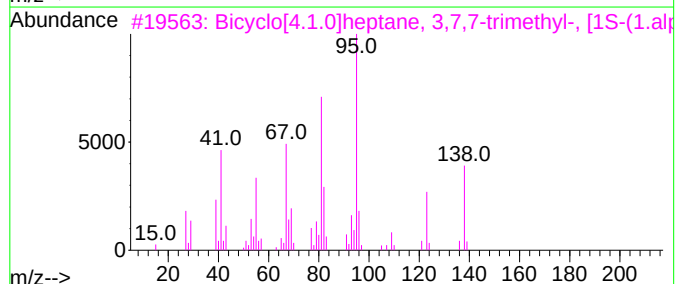
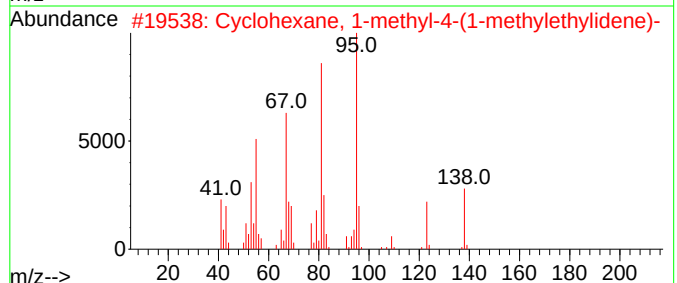
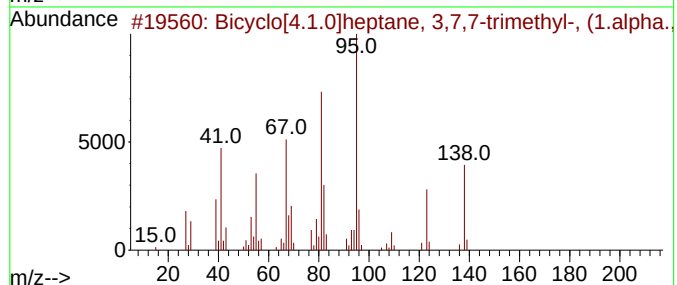
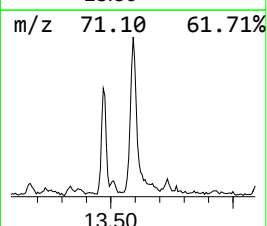
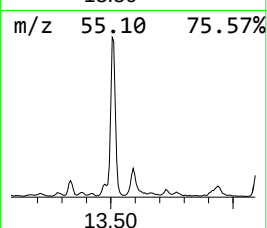
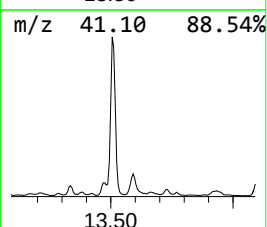
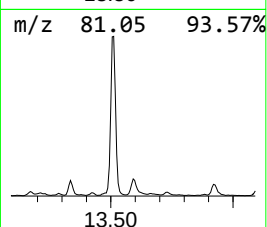
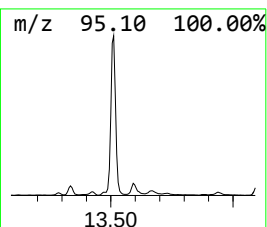
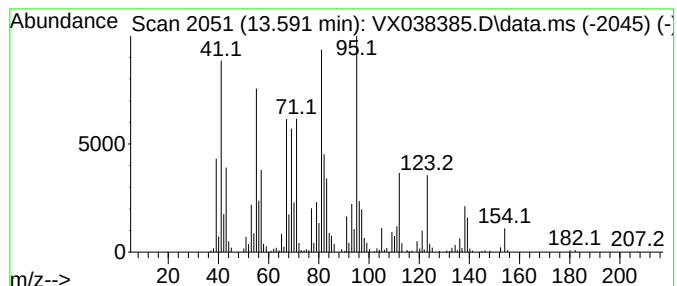
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 9 Cyclohexane, 1-methyl-4-(1-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.591	18.38 ug/l	355089	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	76
2			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-27-2	70
3			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	002778-68-9	70
4			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	70
5			Cyclohexanol, 5-methyl-2-(1-meth...	198	C12H22O2	016409-45-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101923\
Data File : VX038385.D
Acq On : 19 Oct 2023 15:01
Operator : JC/MD
Sample : 04966-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
231013059-VOA

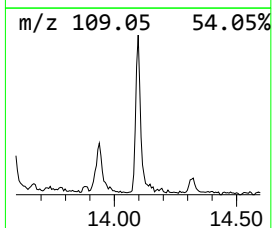
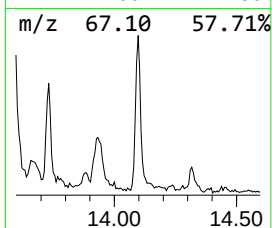
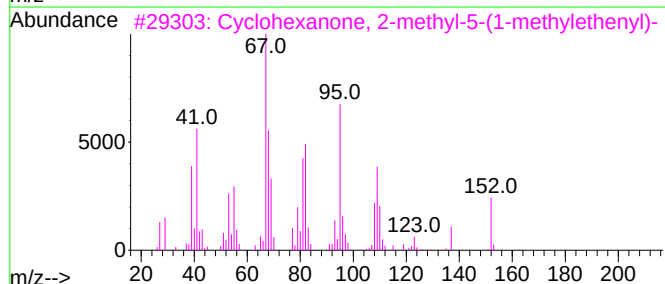
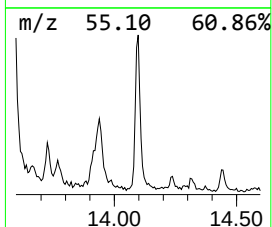
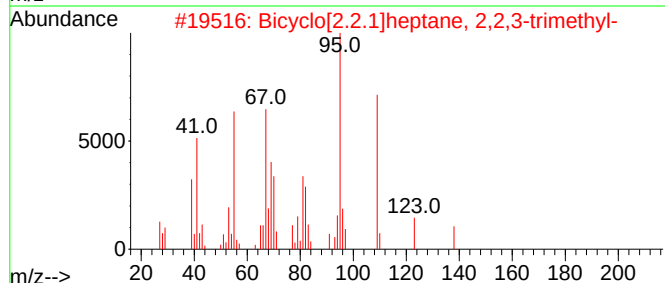
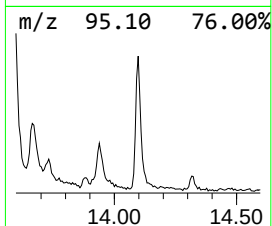
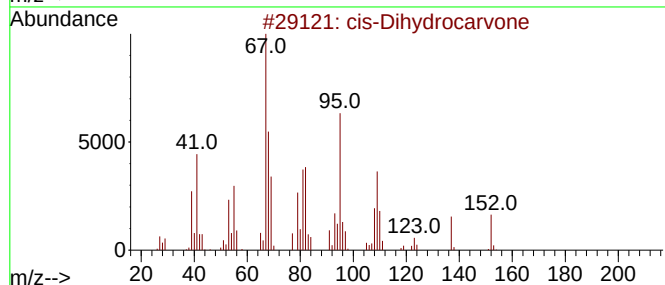
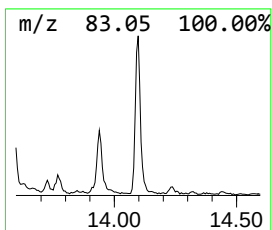
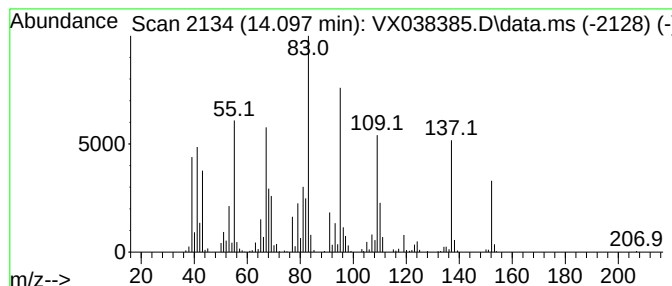
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 10 cis-Dihydrocarvone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.097	11.49 ug/l	221987	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Dihydrocarvone	152	C10H16O	003792-53-8	86
2			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	49
3			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	007764-50-3	43
4			Cyclopentane, (3-methylbutylidene)-	138	C10H18	053366-51-1	38
5			1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101923\
Data File : VX038385.D
Acq On : 19 Oct 2023 15:01
Operator : JC/MD
Sample : 04966-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
231013059-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl ether	1.252	24.4	ug/l	209176	1	5.550	427686	50.0
Amylene hydrate	6.227	11.1	ug/l	127691	2	6.763	578048	50.0
2-Pentanone	7.452	13.7	ug/l	158482	2	6.763	578048	50.0
2-Heptanone	10.769	7.5	ug/l	135777	3	10.055	905230	50.0
Fenchone	12.902	39.4	ug/l	761843	4	12.024	966222	50.0
Bicyclo[4.1.0]h...	13.335	7.7	ug/l	149237	4	12.024	966222	50.0
Camphene	13.475	11.6	ug/l	224056	4	12.024	966222	50.0
Camphor	13.512	90.4	ug/l	1747690	4	12.024	966222	50.0
Cyclohexane, 1-...	13.591	18.4	ug/l	355089	4	12.024	966222	50.0
cis-Dihydrocarvone	14.097	11.5	ug/l	221987	4	12.024	966222	50.0