

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
 Data File : VX032740.D
 Acq On : 10 Nov 2022 19:47
 Operator : JC/MD
 Sample : N5565-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 221109054-02-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\82X102622W.M
 Title : SW846 8260

Signal : TIC: VX032740.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.105	157	167	181	rBV3	26844	101764	1.65%	0.571%
2	2.380	204	212	223	rBV	219306	380442	6.16%	2.134%
3	2.965	294	308	326	rBV	688310	1869547	30.27%	10.489%
4	4.586	553	574	589	rBV	1848526	6176154	100.00%	34.651%
5	5.007	632	643	661	rBV3	292861	938587	15.20%	5.266%
6	5.385	695	705	722	rVB	74887	222005	3.59%	1.246%
7	5.556	722	733	745	rBV	125035	354815	5.74%	1.991%
8	5.958	789	799	807	rBV	84217	223353	3.62%	1.253%
9	6.763	922	931	945	rVB	191201	453760	7.35%	2.546%
10	7.226	999	1007	1024	rBV	63681	169561	2.75%	0.951%
11	8.653	1234	1241	1247	rBV	399550	635746	10.29%	3.567%
12	8.720	1247	1252	1259	rVV	60166	96239	1.56%	0.540%
13	9.378	1356	1360	1366	rVB	119667	174383	2.82%	0.978%
14	10.055	1460	1471	1483	rBV	421566	633003	10.25%	3.551%
15	10.195	1489	1494	1501	rBV2	110692	165468	2.68%	0.928%
16	10.299	1504	1511	1518	rVB	98641	149809	2.43%	0.841%
17	10.640	1563	1567	1580	rVB	84263	136483	2.21%	0.766%
18	11.079	1634	1639	1645	rBV	382186	500998	8.11%	2.811%
19	11.890	1767	1772	1780	rVB	53470	76416	1.24%	0.429%
20	12.024	1788	1794	1801	rVB	449080	627098	10.15%	3.518%
21	12.103	1801	1807	1811	rBV2	91591	144660	2.34%	0.812%
22	12.908	1927	1939	1944	rBV	542933	734742	11.90%	4.122%
23	13.170	1977	1982	1986	rBV	92175	130267	2.11%	0.731%
24	13.335	2005	2009	2014	rBV2	50849	67442	1.09%	0.378%
25	13.475	2027	2032	2034	rBV2	73707	106929	1.73%	0.600%
26	13.512	2034	2038	2044	rVV	782098	1033068	16.73%	5.796%
27	13.591	2044	2051	2058	rVV3	177555	291988	4.73%	1.638%
28	13.658	2058	2062	2069	rVV	107973	171466	2.78%	0.962%
29	13.731	2069	2074	2077	rVV	212592	259858	4.21%	1.458%
30	13.774	2077	2081	2087	rVB	426248	526805	8.53%	2.956%
31	13.926	2101	2106	2121	rVB7	22439	70939	1.15%	0.398%
32	14.097	2125	2134	2146	rBV2	79552	130242	2.11%	0.731%
33	14.640	2218	2223	2232	rVB	40875	69737	1.13%	0.391%

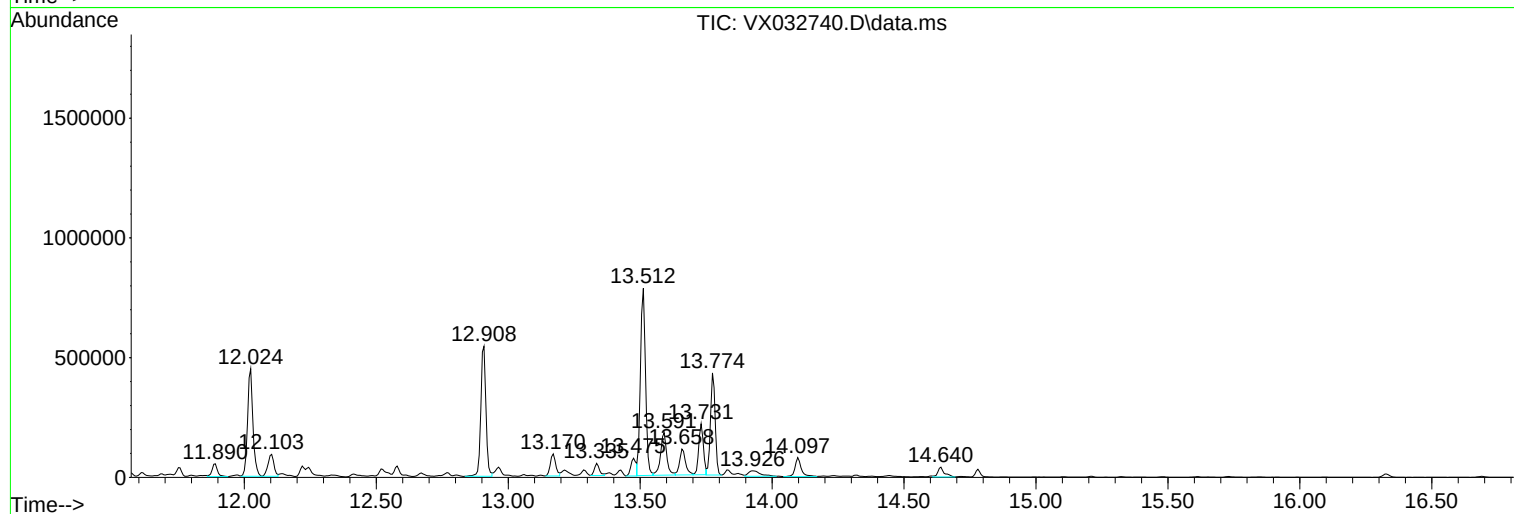
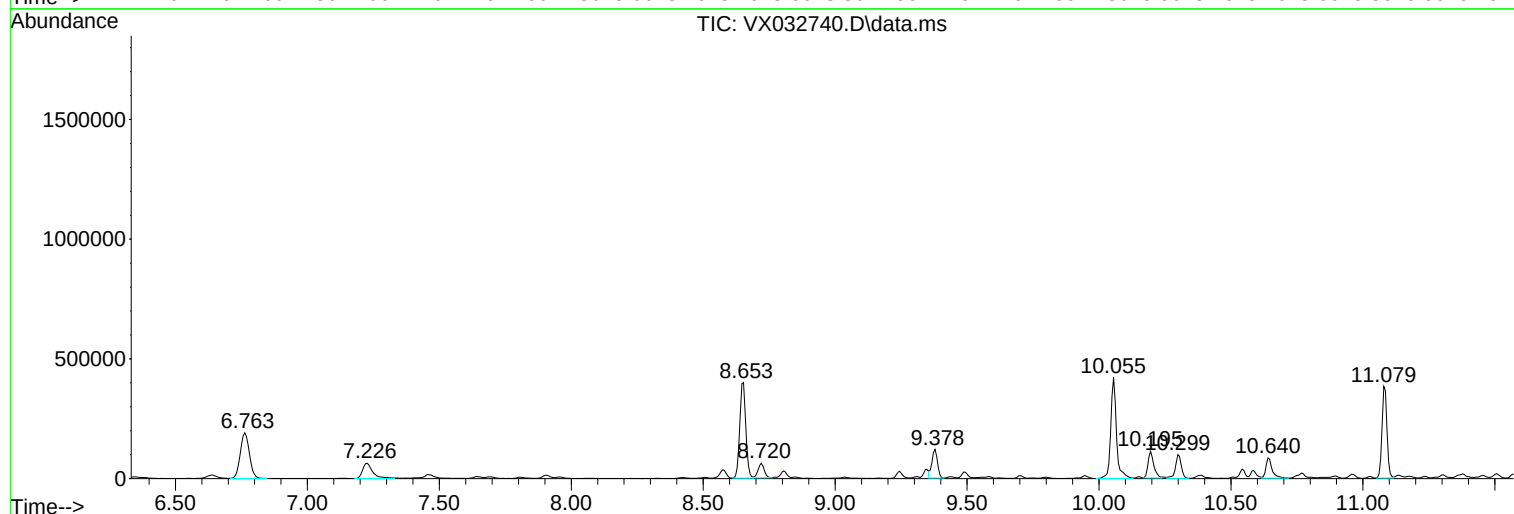
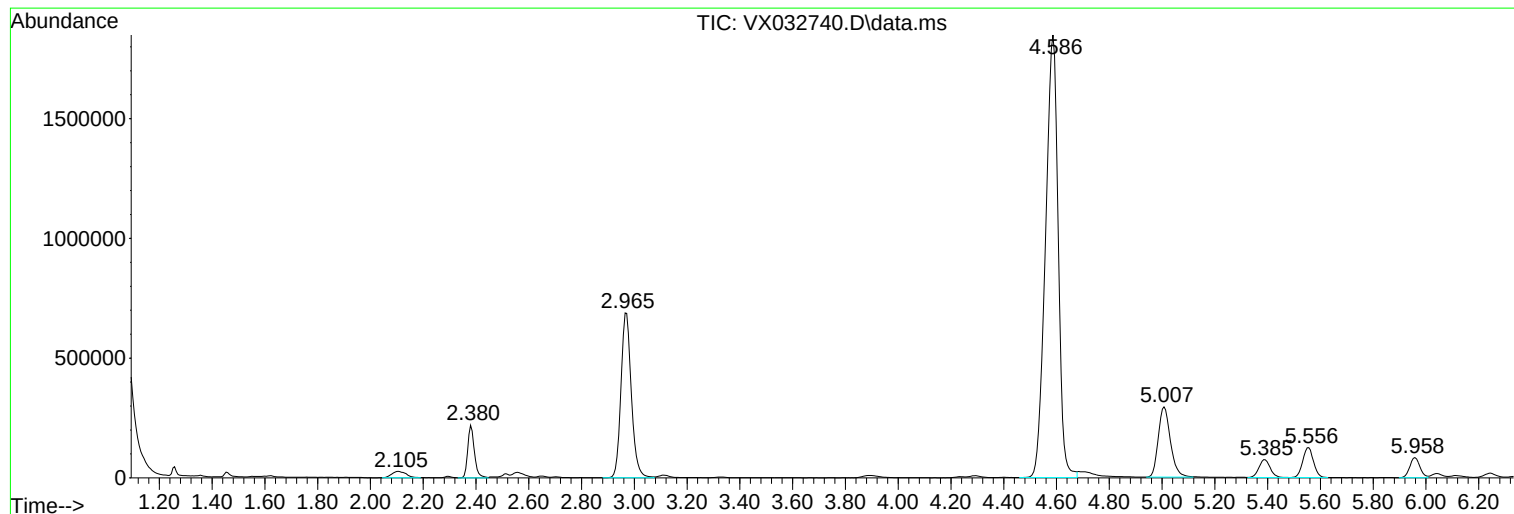
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ClientSampleId :
221109054-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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



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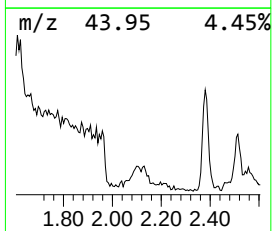
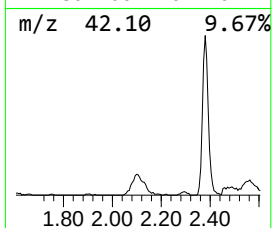
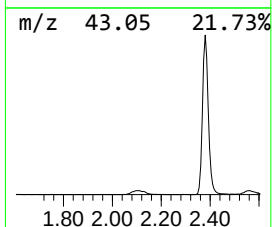
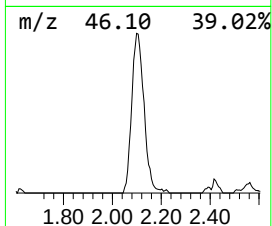
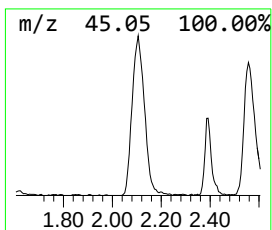
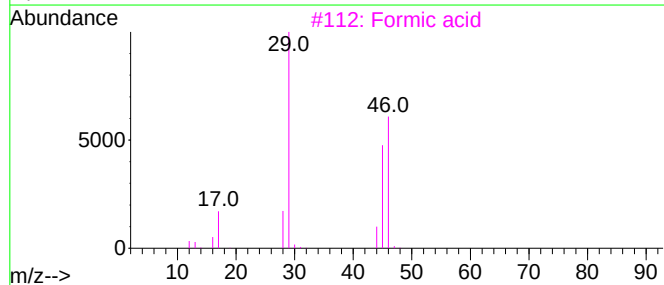
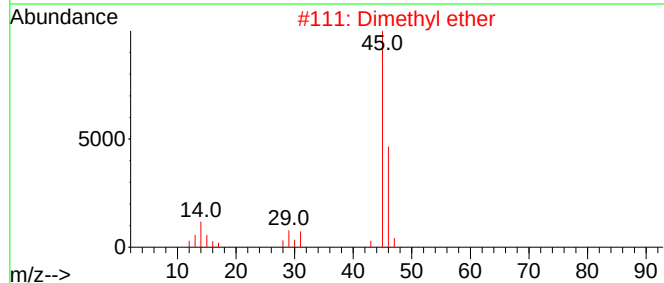
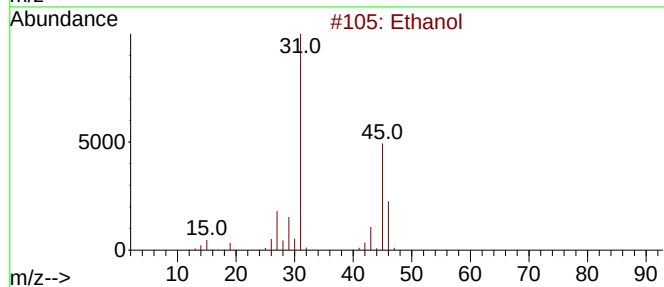
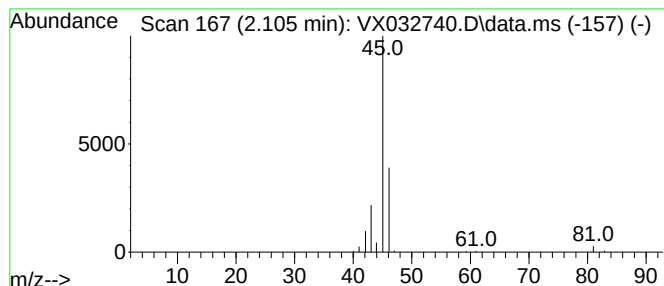
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.105 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.105	14.34 ug/l	101764	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	43
2	Dimethyl ether			46	C2H6O	000115-10-6	5
3	Formic acid			46	CH2O2	000064-18-6	4
4	Propanedioic acid, dihydroxy-			136	C3H4O6	000560-27-0	4
5	Methoxyacetic acid, pentyl ester			160	C8H16O3	168920-35-2	4



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221109054-02-VOA

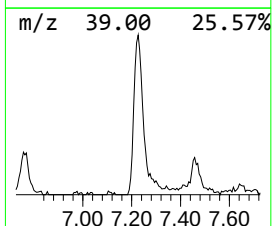
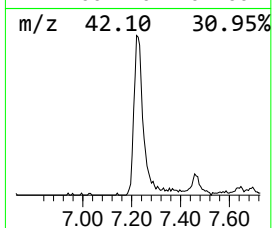
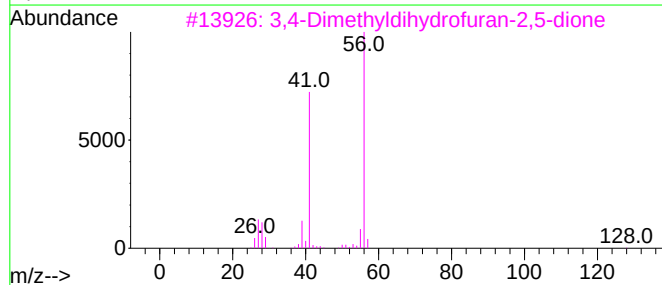
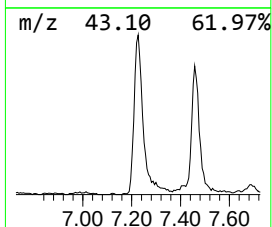
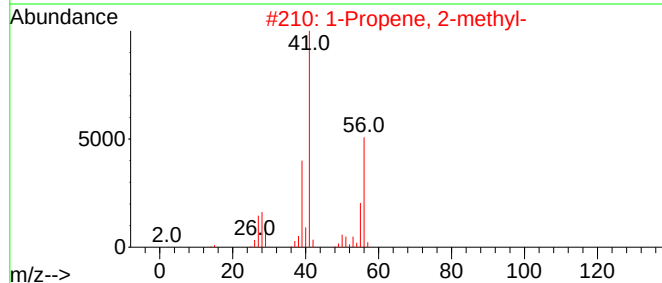
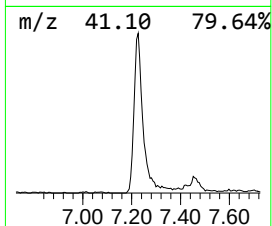
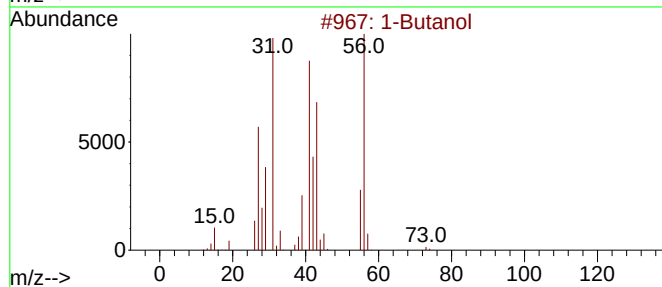
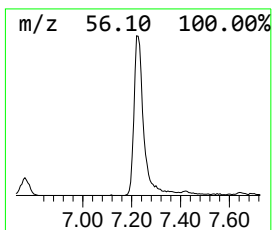
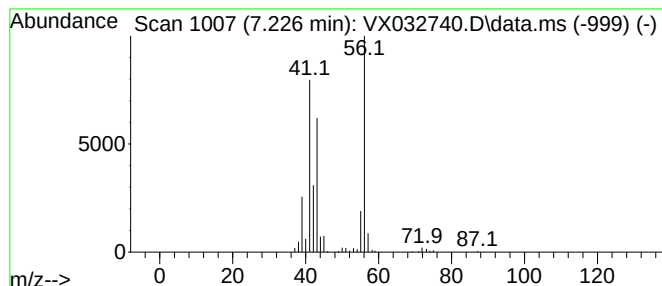
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.226	18.68 ug/l	169561	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			1-Propene, 2-methyl-	56	C4H8	000115-11-7	45
3			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	45
4			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
5			1-Hexanol	102	C6H14O	000111-27-3	38



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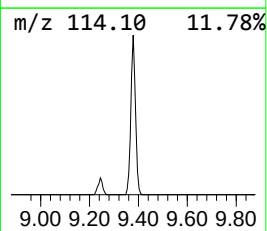
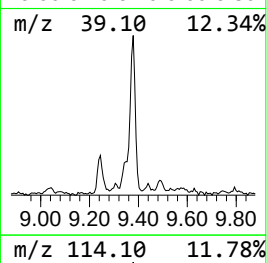
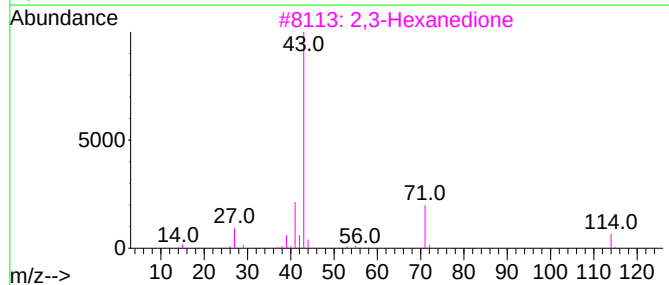
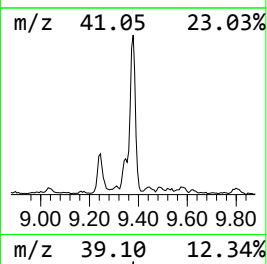
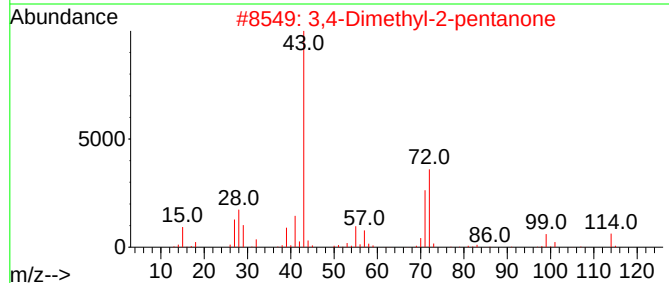
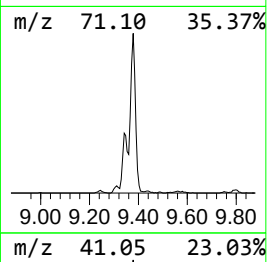
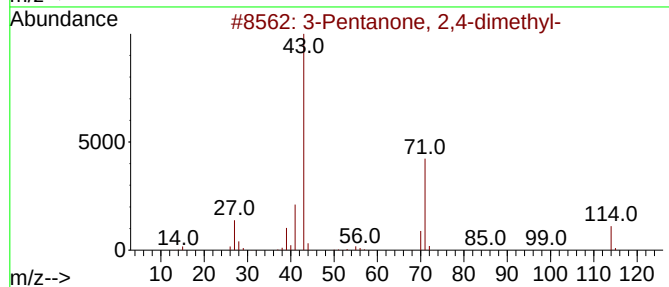
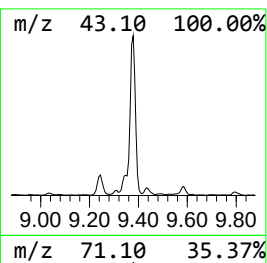
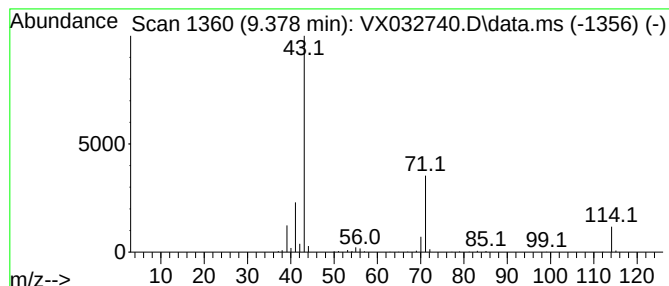
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Quant Title : SW846 8260

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

Peak Number 3 3-Pentanone, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	13.77 ug/l	174383	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	80
2			3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	50
3			2,3-Hexanedione	114	C6H10O2	003848-24-6	42
4			4-Heptanone	114	C7H14O	000123-19-3	40
5			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	38



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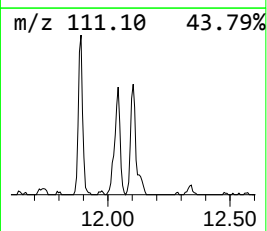
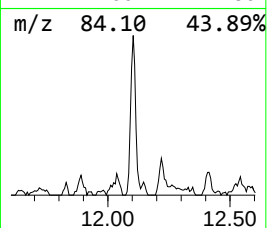
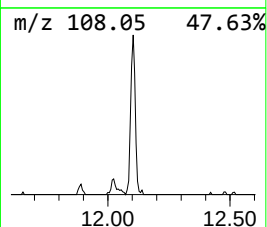
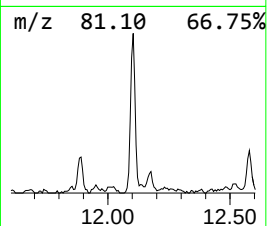
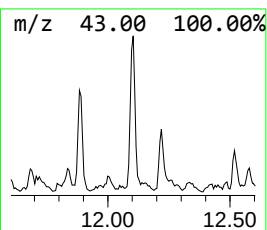
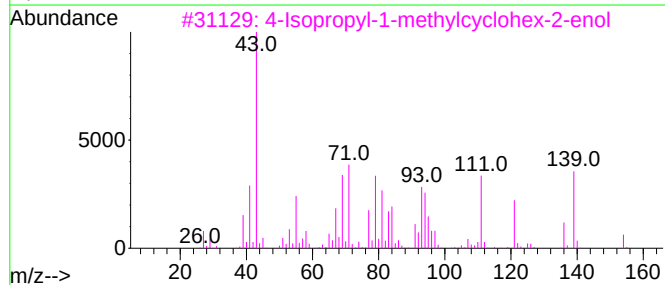
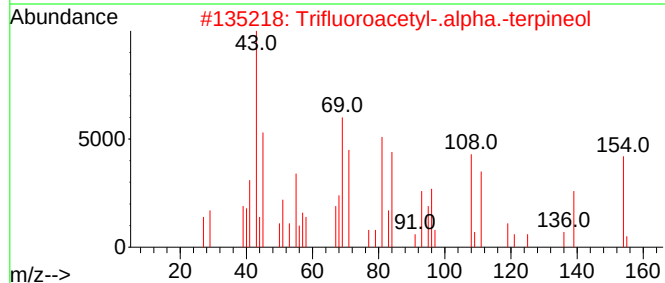
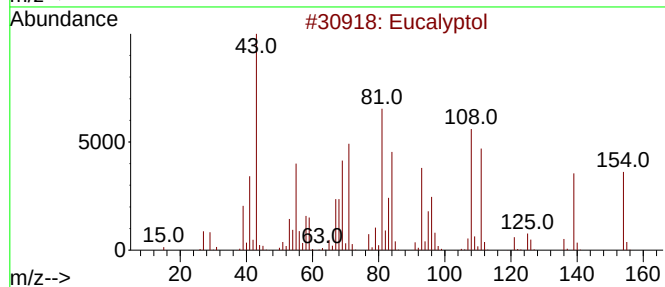
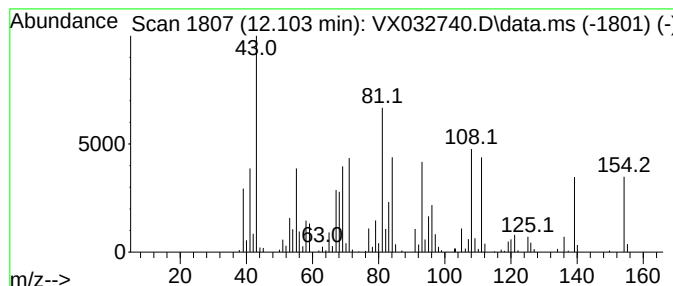
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eucalyptol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.103	11.53 ug/l	144660	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	99
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	74
3			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	32
4			2-Cyclohexen-1-ol, 1-methyl-4-(1...	154	C10H18O	029803-82-5	25
5			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	22



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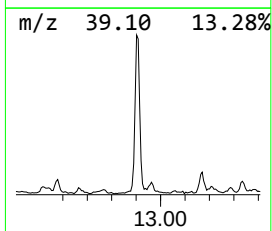
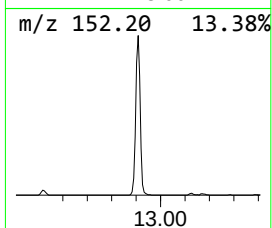
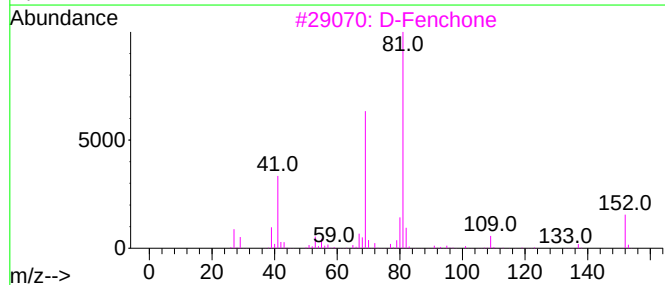
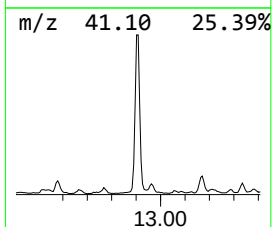
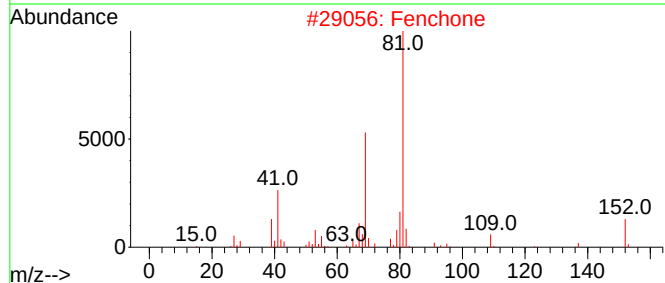
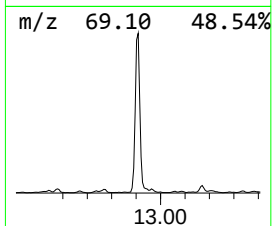
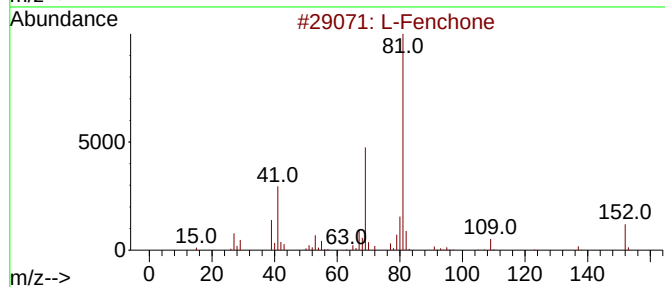
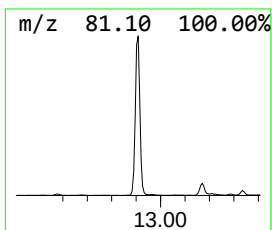
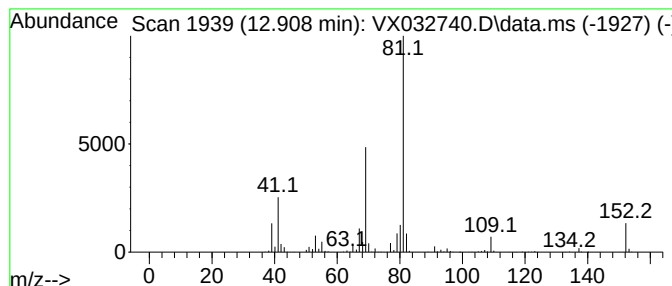
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Quant Title : SW846 8260

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

Peak Number 5 L-Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.908	58.58 ug/l	734742	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Fenchone	152	C10H16O	007787-20-4	95
2			Fenchone	152	C10H16O	001195-79-5	95
3			D-Fenchone	152	C10H16O	004695-62-9	91
4			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	45
5			Cyclohexane, 1,3-dichloro-, cis-	152	C6H10Cl2	024955-63-3	45



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221109054-02-VOA

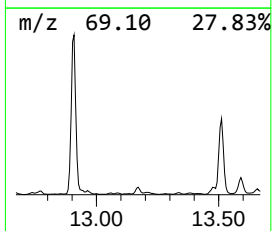
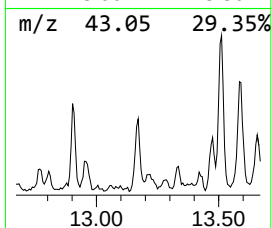
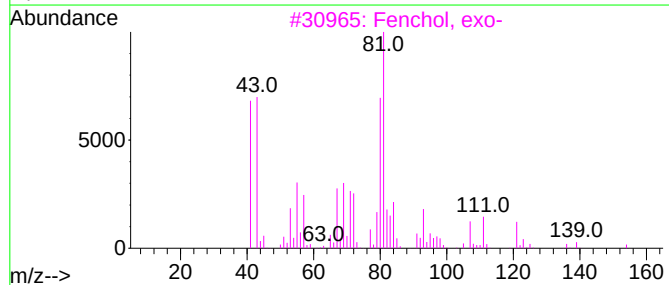
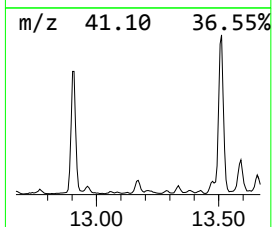
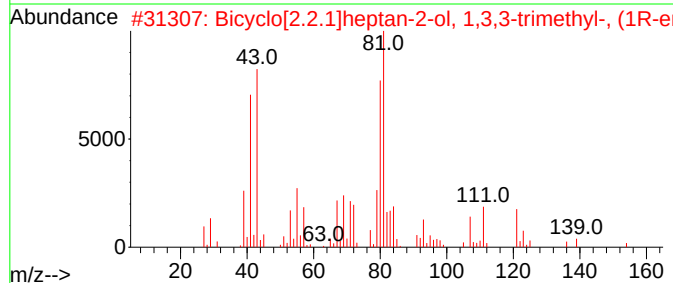
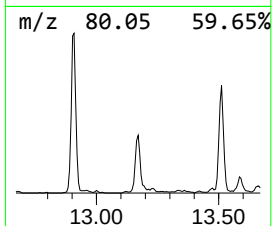
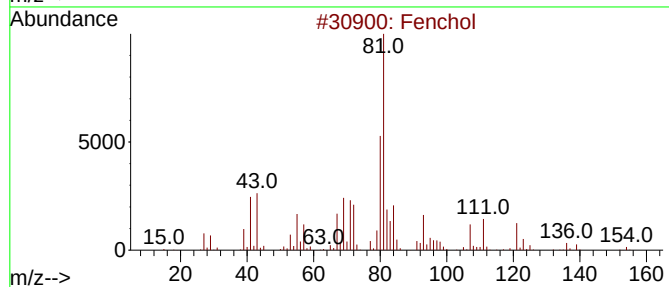
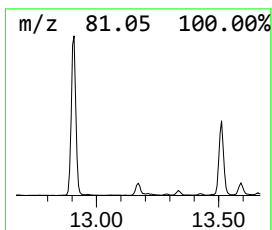
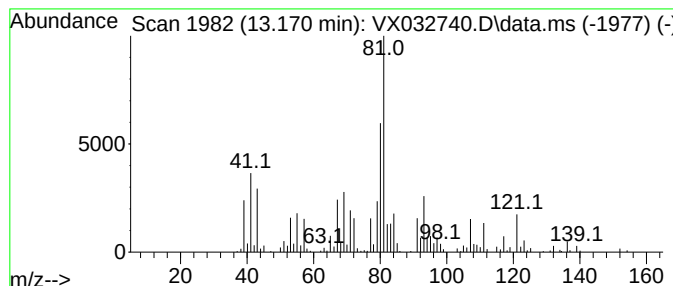
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Quant Title : SW846 8260

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

Peak Number 6 Fenchol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	10.39 ug/l	130267	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchol	154	C10H18O	001632-73-1	87
2			Bicyclo[2.2.1]heptan-2-ol, 1,3,3...	154	C10H18O	002217-02-9	86
3			Fenchol, exo-	154	C10H18O	022627-95-8	64
4			Fenchyl acetate	196	C12H20O2	013851-11-1	64
5			Bi-2-cyclohexen-1-yl	162	C12H18	001541-20-4	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
Data File : VX032740.D
Acq On : 10 Nov 2022 19:47
Operator : JC/MD
Sample : N5565-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

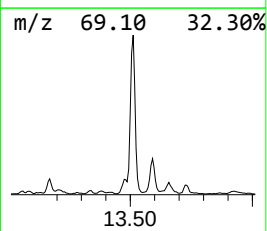
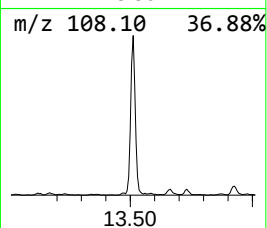
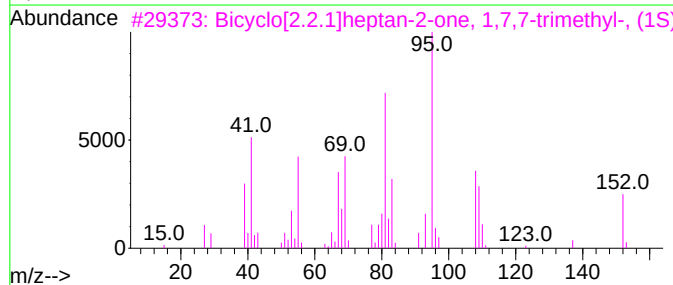
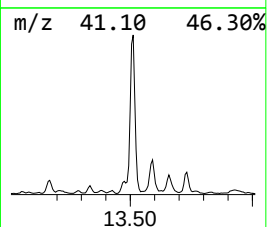
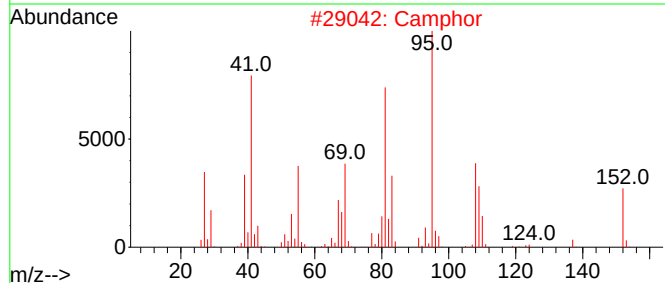
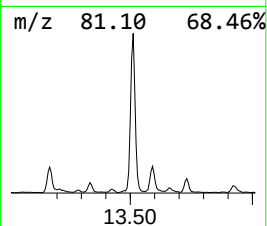
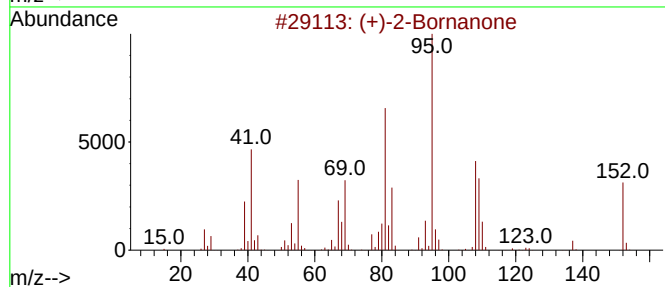
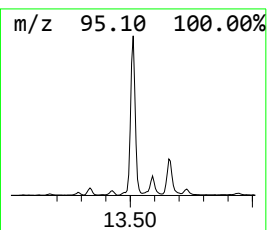
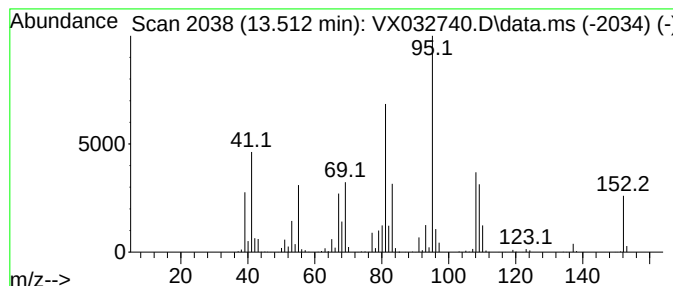
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ClientSampleId :
221109054-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 7 (+)-2-Bornanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.512	82.37 ug/l	1033070	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2	Camphor	152	C10H16O	000076-22-2	98
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
Data File : VX032740.D
Acq On : 10 Nov 2022 19:47
Operator : JC/MD
Sample : N5565-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
221109054-02-VOA

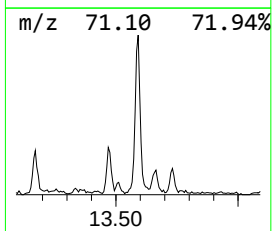
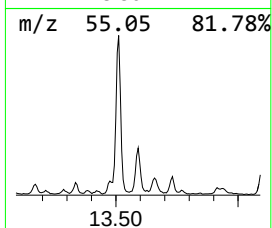
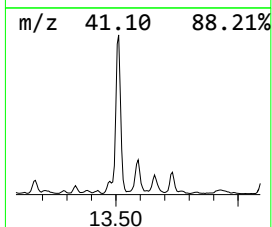
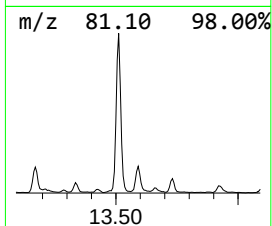
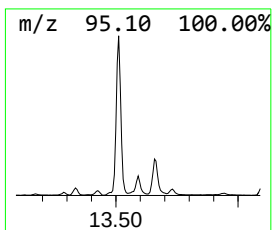
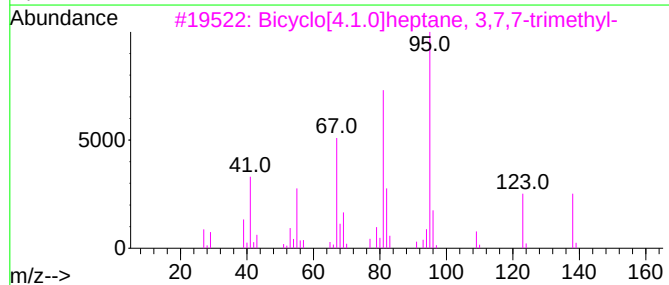
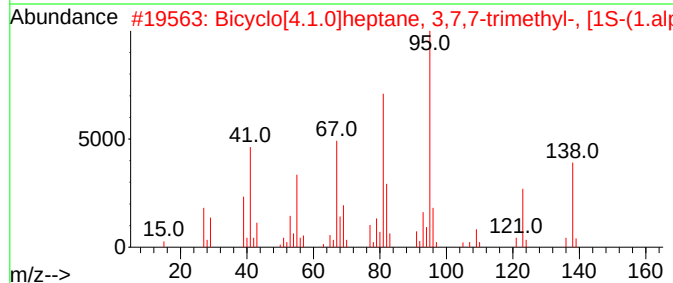
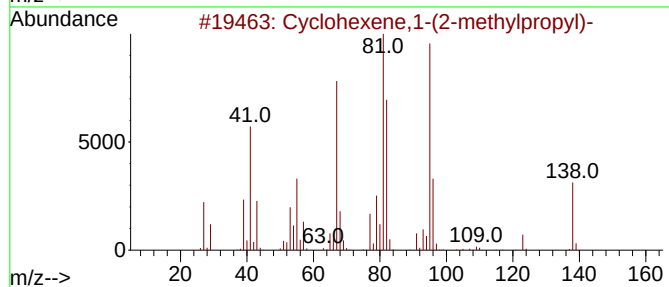
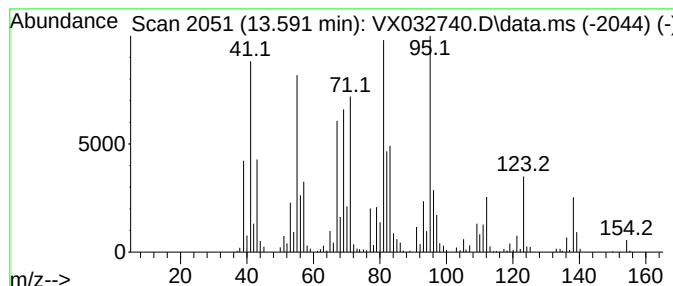
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Quant Title : SW846 8260

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

Peak Number 8 Cyclohexene,1-(2-methylprop... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.591	23.28 ug/l	291988	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexene,1-(2-methylpropyl)-	138	C10H18	003983-03-7	70
2		Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	002778-68-9	70
3		Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	64
4		Cyclohexene, 4-methyl-1-(1-methy...	138	C10H18	000500-00-5	62
5		(-)-Menthoxycetyl chloride	232	C12H21ClO2	015356-62-4	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
Data File : VX032740.D
Acq On : 10 Nov 2022 19:47
Operator : JC/MD
Sample : N5565-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
221109054-02-VOA

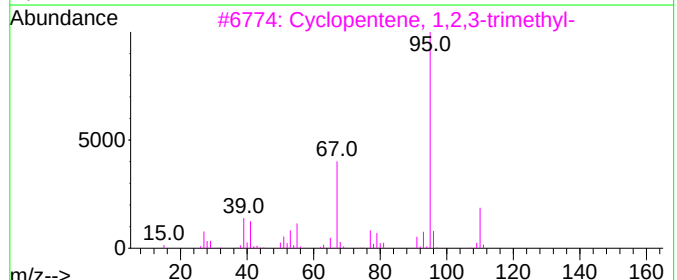
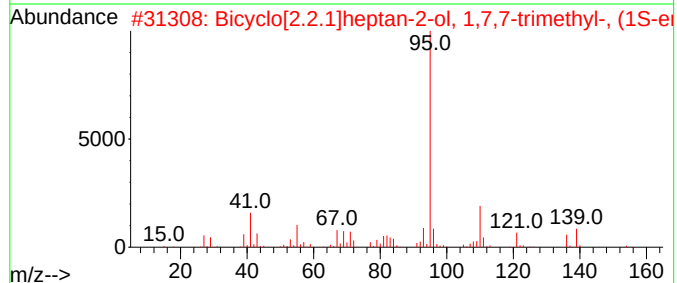
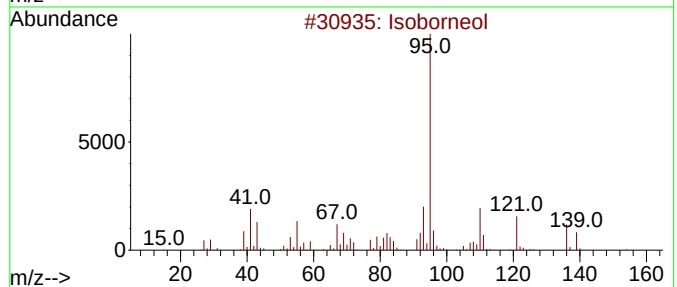
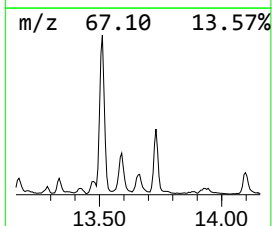
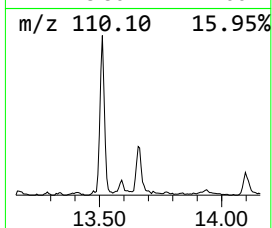
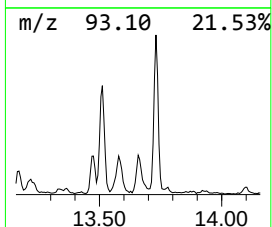
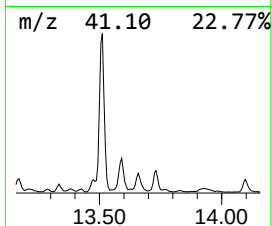
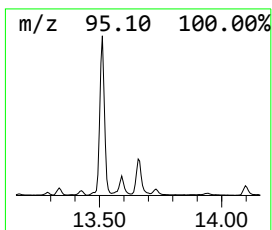
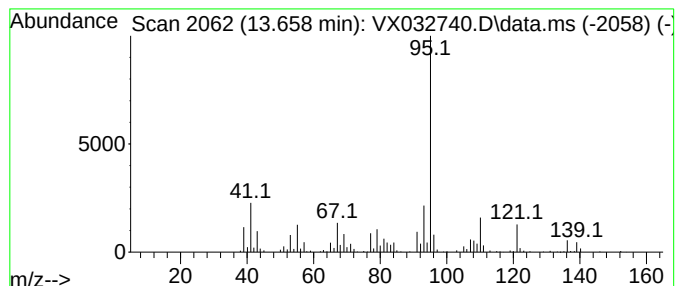
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Quant Title : SW846 8260

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

Peak Number 9 Isoborneol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.658	13.67 ug/l	171466	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isoborneol	154	C10H18O	000124-76-5	86
2			Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	154	C10H18O	000464-45-9	64
3			Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	62
4			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	58
5			Bicyclo[2.2.1]heptane-7-methanol...	170	C10H18O2	054831-21-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
Data File : VX032740.D
Acq On : 10 Nov 2022 19:47
Operator : JC/MD
Sample : N5565-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
221109054-02-VOA

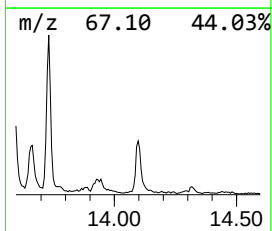
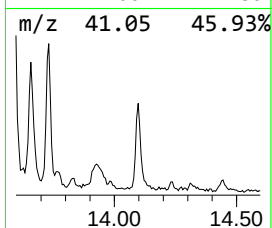
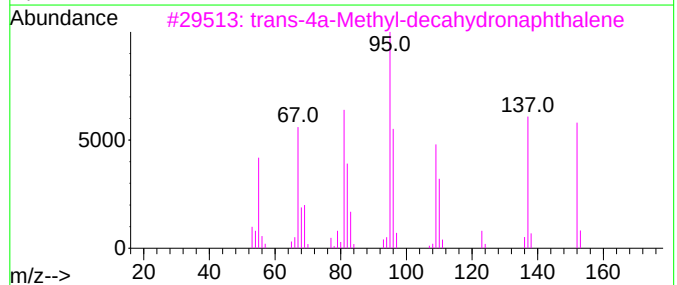
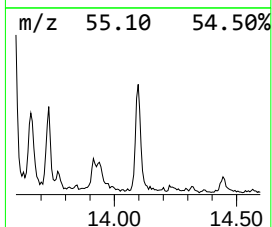
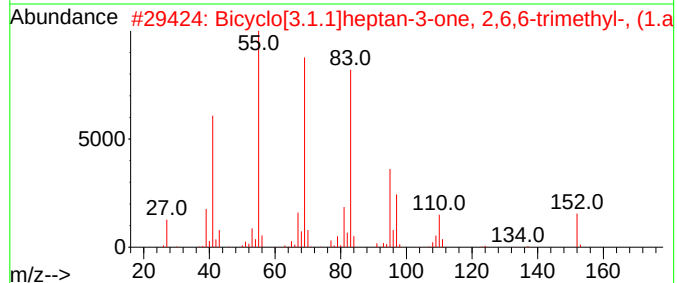
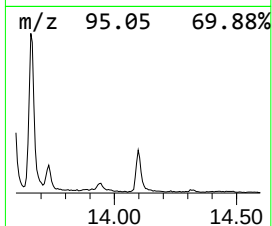
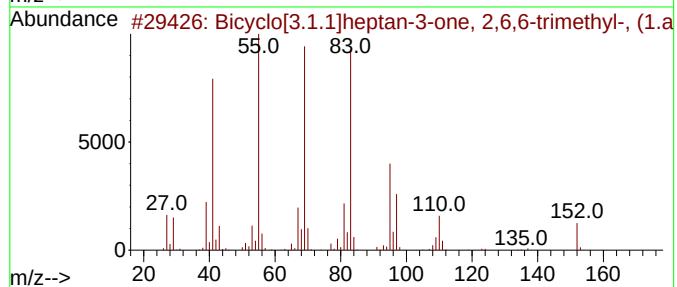
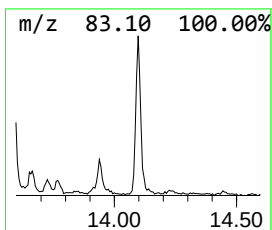
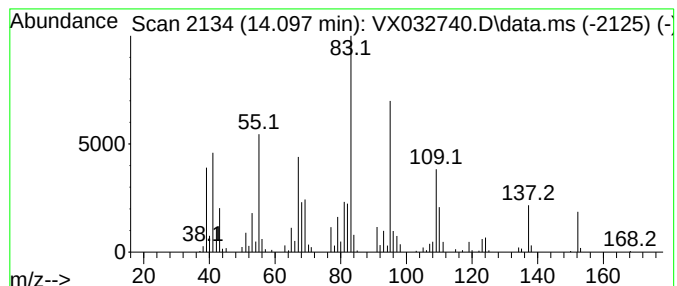
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Quant Title : SW846 8260

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

Peak Number 10 Bicyclo[3.1.1]heptan-3-one,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.097	10.38 ug/l	130242	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	52
2			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	49
3			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	43
4			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	38
5			Allyl 2,4-hexadienoate	152	C9H12O2	1000431-58-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
Data File : VX032740.D
Acq On : 10 Nov 2022 19:47
Operator : JC/MD
Sample : N5565-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
221109054-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.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
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1-Butanol	7.226	18.7	ug/l	169561	2	6.763	453760	50.0
3-Pentanone, 2,...	9.378	13.8	ug/l	174383	3	10.055	633003	50.0
Eucalyptol	12.103	11.5	ug/l	144660	4	12.024	627098	50.0
L-Fenchone	12.908	58.6	ug/l	734742	4	12.024	627098	50.0
Fenchol	13.170	10.4	ug/l	130267	4	12.024	627098	50.0
(+)-2-Bornanone	13.512	82.4	ug/l	1033070	4	12.024	627098	50.0
Cyclohexene,1-(...	13.591	23.3	ug/l	291988	4	12.024	627098	50.0
Isoborneol	13.658	13.7	ug/l	171466	4	12.024	627098	50.0
Bicyclo[3.1.1]h...	14.097	10.4	ug/l	130242	4	12.024	627098	50.0