

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101824\
 Data File : VX043431.D
 Acq On : 18 Oct 2024 14:00
 Operator : JC/MD
 Sample : P4427-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 241016059-01-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\82X100124W.M
 Title : SW846 8260

Signal : TIC: VX043431.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	25	28	36	rVB2	34152	48865	1.28%	0.292%
2	2.398	206	215	228	rBV2	41477	83409	2.18%	0.499%
3	2.941	296	304	308	rBV	54026	123518	3.23%	0.739%
4	3.038	308	320	370	rVB	875481	3819922	100.00%	22.850%
5	4.654	564	585	626	rBV	781563	3651011	95.58%	21.840%
6	5.013	633	644	669	rVB	423965	1387539	36.32%	8.300%
7	5.385	692	705	721	rBV	42799	129910	3.40%	0.777%
8	5.544	721	731	742	rBV	73905	203788	5.33%	1.219%
9	5.952	789	798	806	rBV	55740	146796	3.84%	0.878%
10	6.288	842	853	860	rBV3	18523	62985	1.65%	0.377%
11	6.757	921	930	948	rVB	116326	283196	7.41%	1.694%
12	8.647	1234	1240	1247	rVV	236008	372683	9.76%	2.229%
13	8.714	1247	1251	1261	rVV	55458	96796	2.53%	0.579%
14	8.805	1261	1266	1278	rVB	34387	65957	1.73%	0.395%
15	9.378	1353	1360	1368	rVB	99593	149768	3.92%	0.896%
16	10.055	1461	1471	1483	rBV	236943	410645	10.75%	2.456%
17	10.195	1489	1494	1506	rVV2	62140	107796	2.82%	0.645%
18	10.299	1506	1511	1520	rVV	80170	121108	3.17%	0.724%
19	10.640	1563	1567	1573	rBV	49430	69990	1.83%	0.419%
20	11.079	1634	1639	1645	rBV	192872	259699	6.80%	1.553%
21	11.506	1705	1709	1715	rVB	33796	45221	1.18%	0.271%
22	11.750	1745	1749	1754	rVB	30304	40414	1.06%	0.242%
23	11.884	1763	1771	1779	rVB4	38333	60076	1.57%	0.359%
24	12.018	1787	1793	1800	rVB2	266898	405244	10.61%	2.424%
25	12.104	1800	1807	1811	rBV2	123333	183152	4.79%	1.096%
26	12.579	1881	1885	1894	rVB	74963	102383	2.68%	0.612%
27	12.762	1905	1915	1920	rBV2	89507	137440	3.60%	0.822%
28	12.902	1927	1938	1944	rBV	570679	745862	19.53%	4.462%
29	12.963	1944	1948	1959	rVB3	49094	85088	2.23%	0.509%
30	13.213	1984	1989	1995	rVB2	32087	54087	1.42%	0.324%
31	13.335	2005	2009	2012	rBV	117491	146998	3.85%	0.879%
32	13.475	2027	2032	2034	rBV2	142973	219213	5.74%	1.311%
33	13.506	2034	2037	2045	rVB	1208189	1597814	41.83%	9.558%
34	13.585	2045	2050	2060	rBV2	410523	580556	15.20%	3.473%
35	13.731	2069	2074	2077	rBV	141557	172389	4.51%	1.031%
36	13.774	2077	2081	2086	rVB	156387	195185	5.11%	1.168%

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Instrument :
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ClientSampleId :
241016059-01-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\82X100124W.M
Title : SW846 8260

37	13.932	2100	2107	2112	rBV3	36051	83805	2.19%	0.501%
38	14.097	2128	2134	2145	rBV	181853	266936	6.99%	1.597%

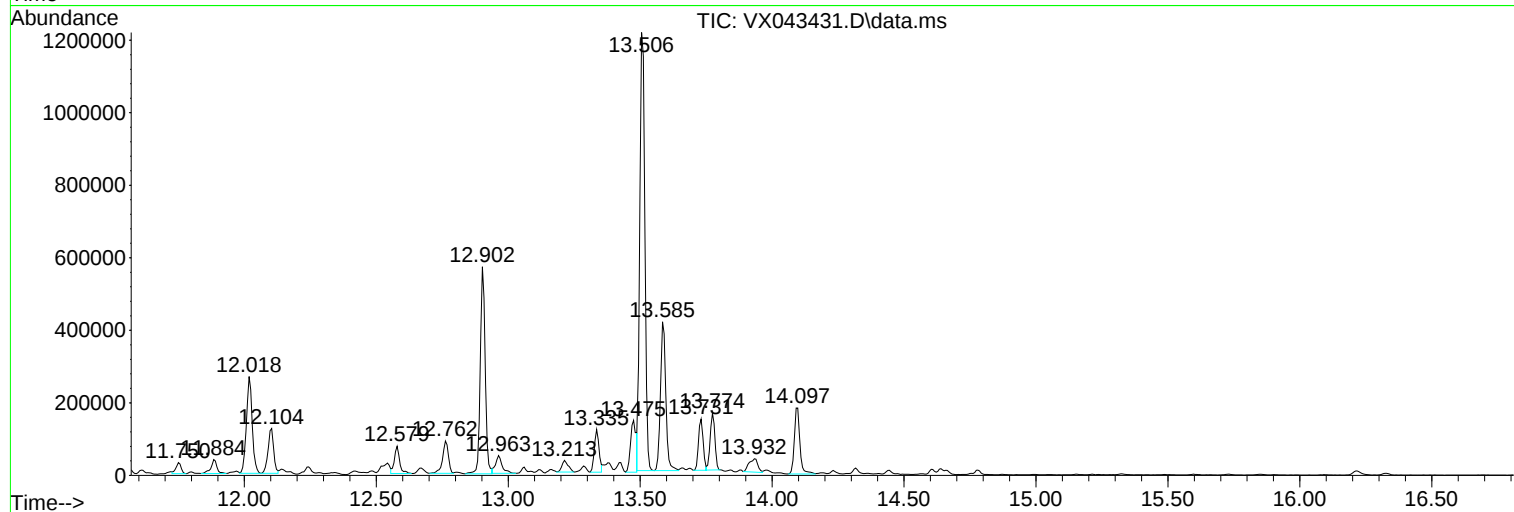
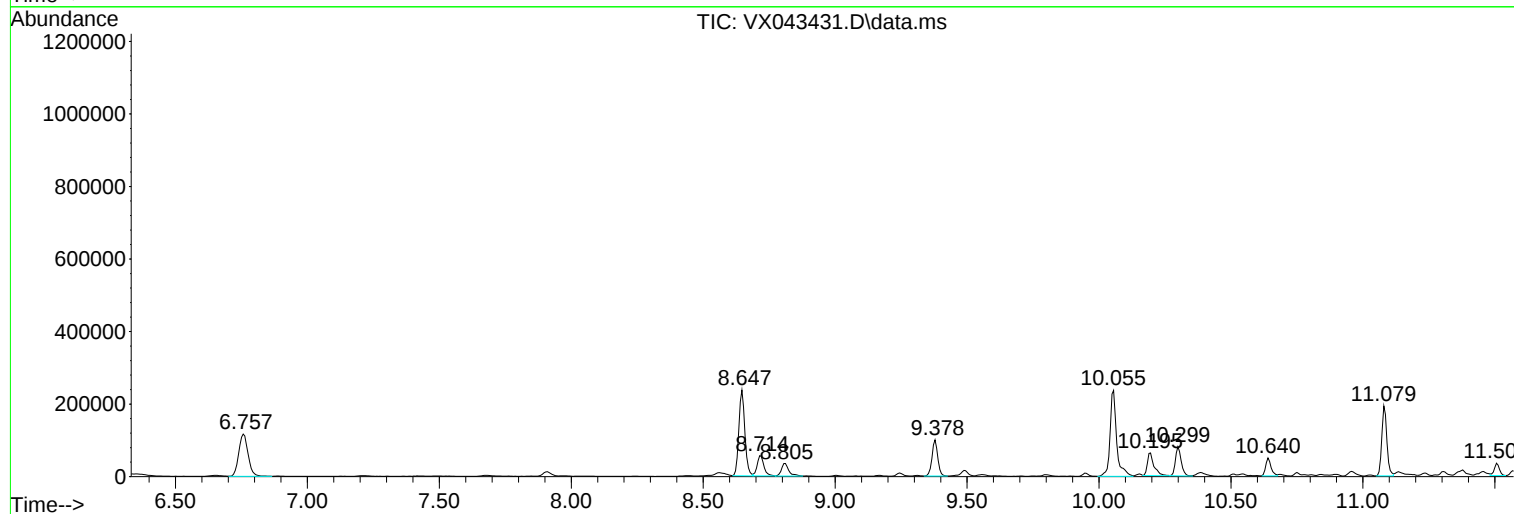
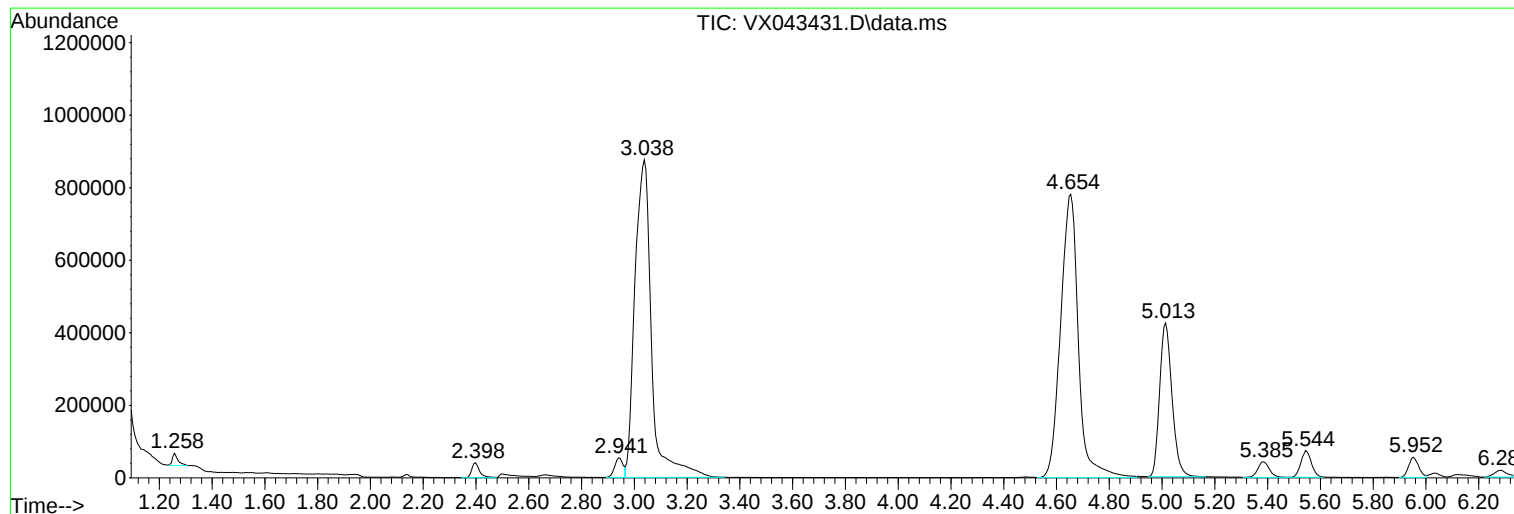
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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



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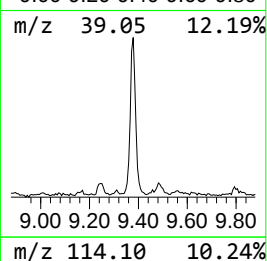
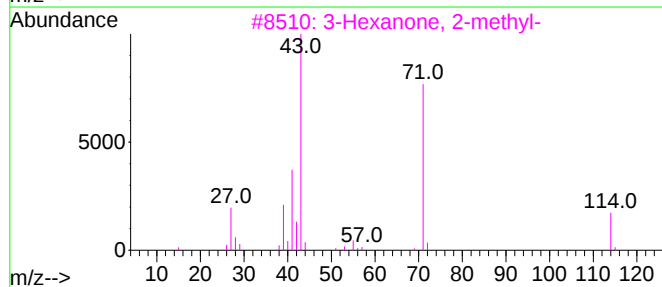
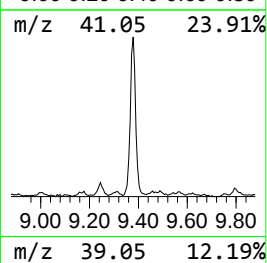
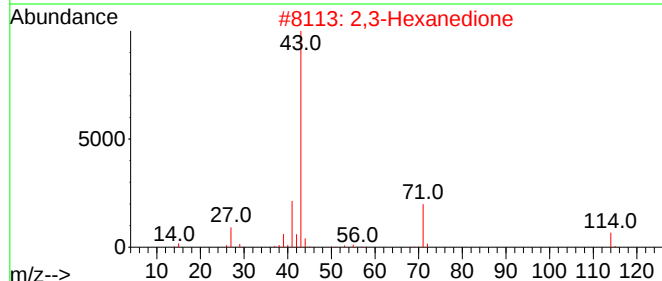
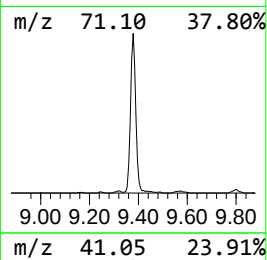
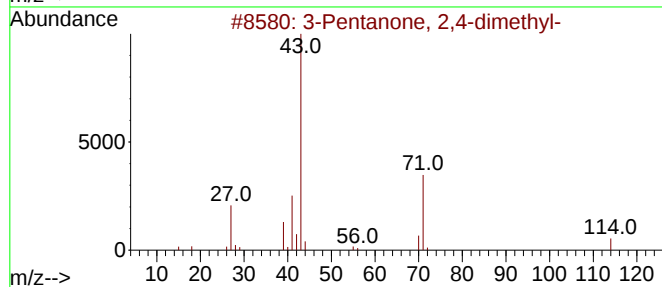
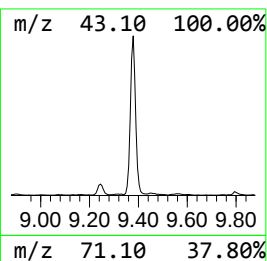
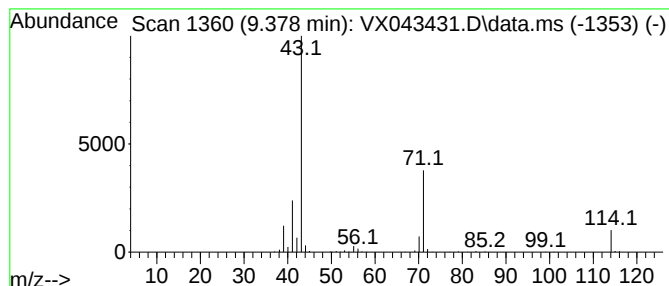
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 3 3-Pentanone, 2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	18.24 ug/l	149768	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2			2,3-Hexanedione	114	C6H10O2	003848-24-6	72
3			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	52
4			3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	50
5			2-Oxo-n-valeric acid	116	C5H8O3	001821-02-9	43



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Instrument :
MSVOA_X
ClientSampleId :
241016059-01-VOA

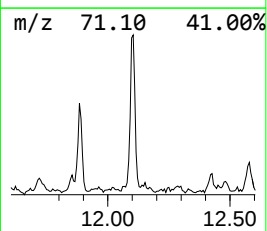
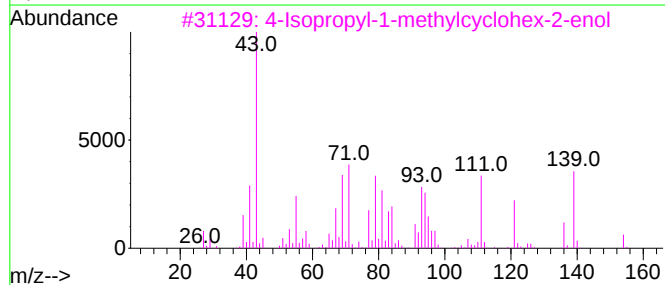
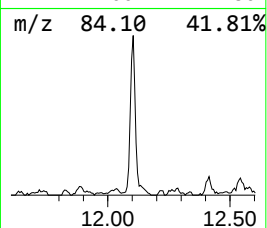
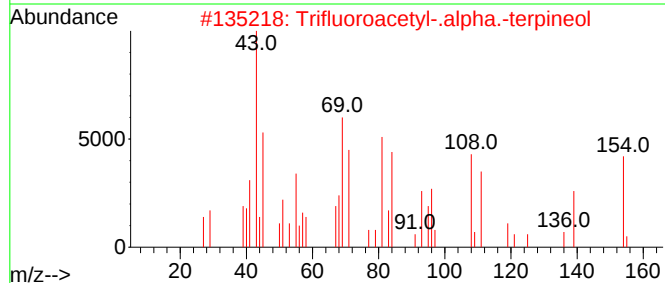
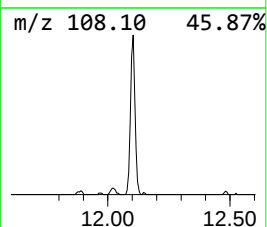
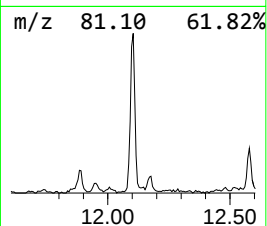
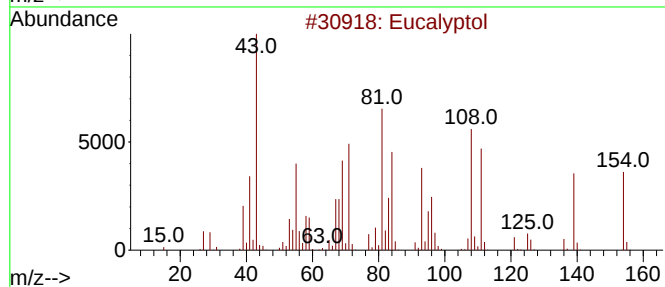
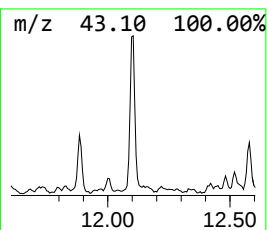
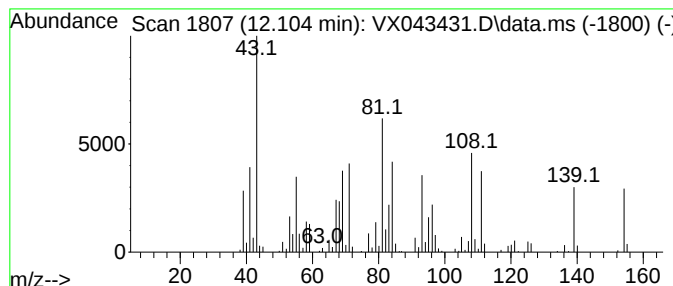
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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.
12.104	22.60 ug/l	183152	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	64
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	27
5			3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25



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ClientSampleId :
241016059-01-VOA

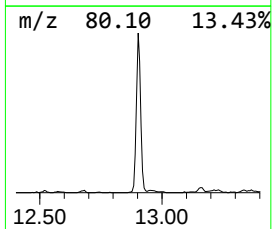
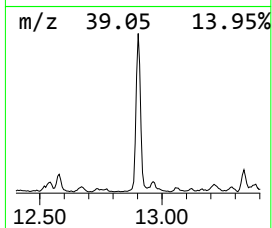
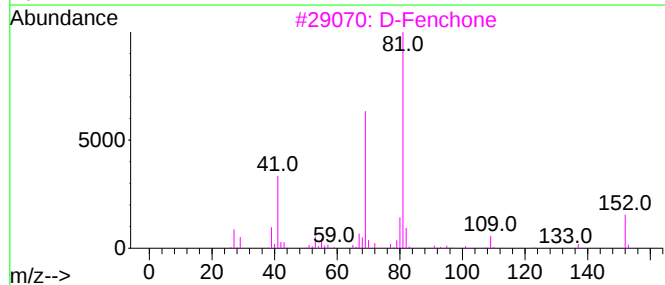
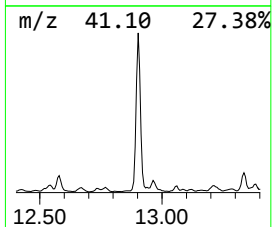
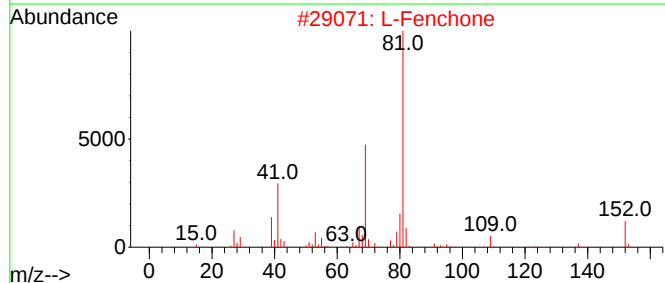
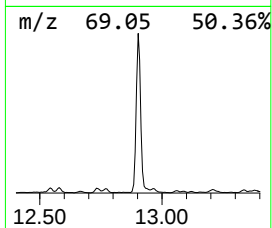
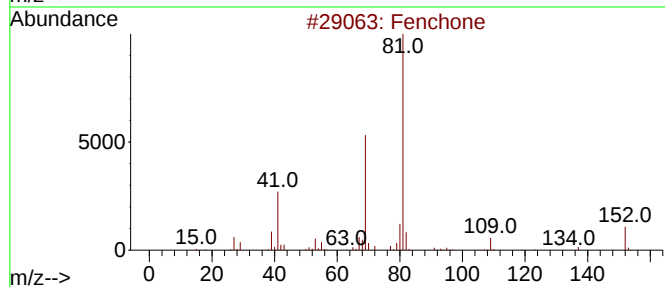
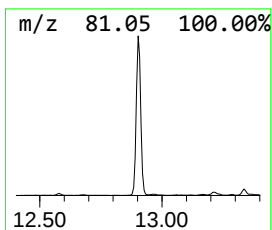
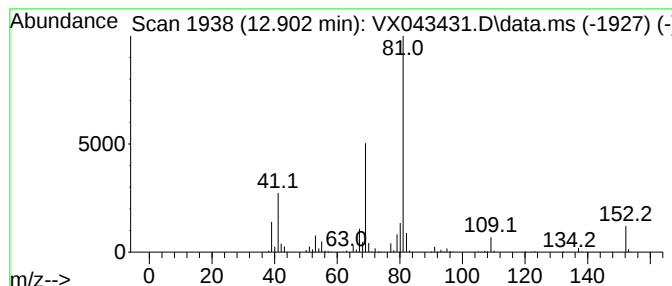
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 5 Fenchone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.902	92.03 ug/l	745862	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	95
3			D-Fenchone	152	C10H16O	004695-62-9	91
4			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	59
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45



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Sample : P4427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

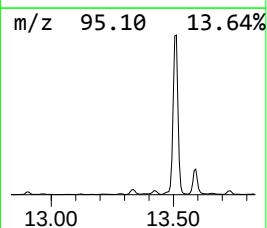
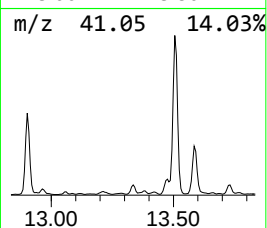
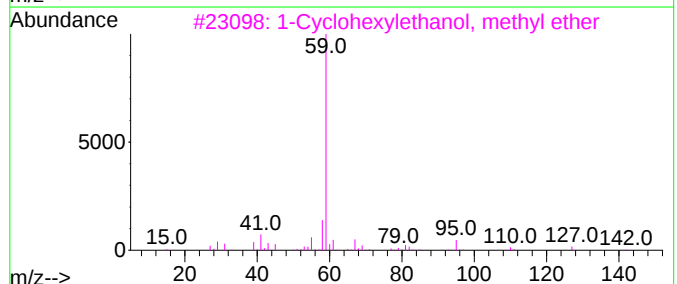
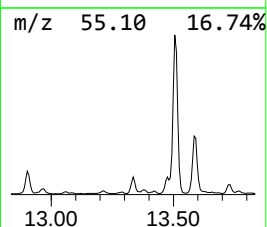
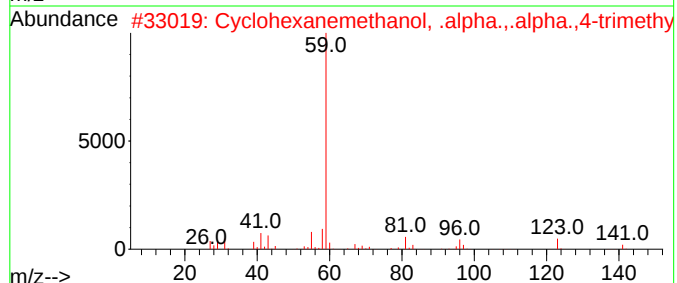
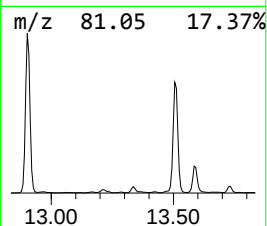
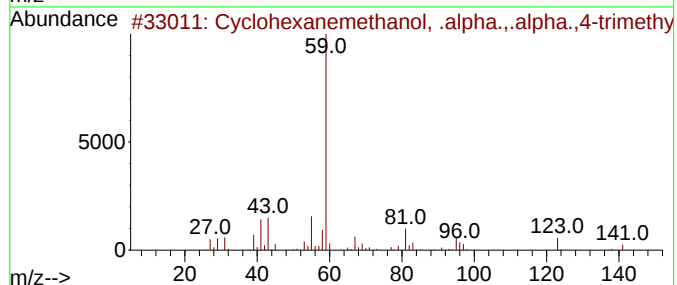
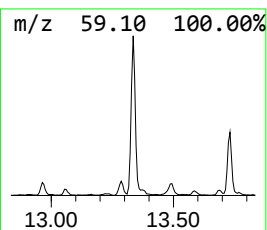
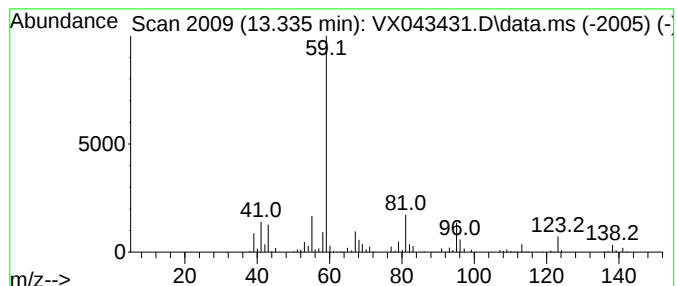
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexanemethanol, .alpha... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.335	18.14 ug/l	146998	1,4-Dichlorobenzene-d4		12.024	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, .alpha.,.al...		156	C10H20O	000498-81-7	64
2	Cyclohexanemethanol, .alpha.,.al...		156	C10H20O	007322-63-6	59
3	1-Cyclohexylethanol, methyl ether		142	C9H18O	1000365-12-8	50
4	2,4-Dimethyl-4-penten-2-ol		114	C7H14O	019781-53-4	50
5	Cyclohexanemethanol, .alpha.,.al...		156	C10H20O	005114-00-1	45



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Instrument :
MSVOA_X
ClientSampleId :
241016059-01-VOA

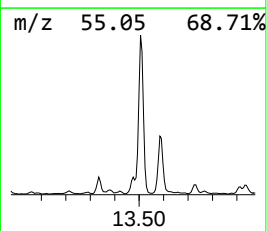
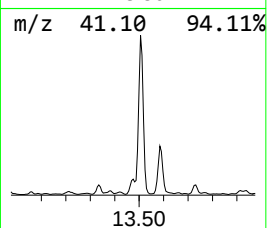
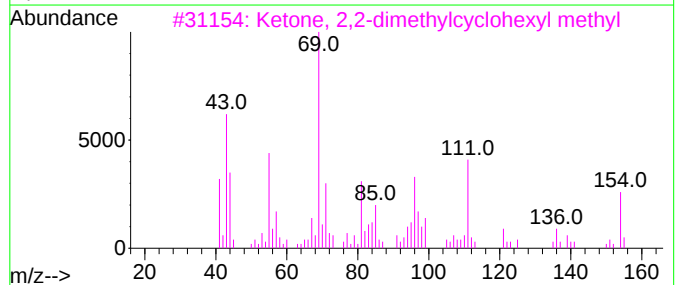
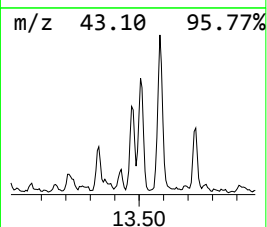
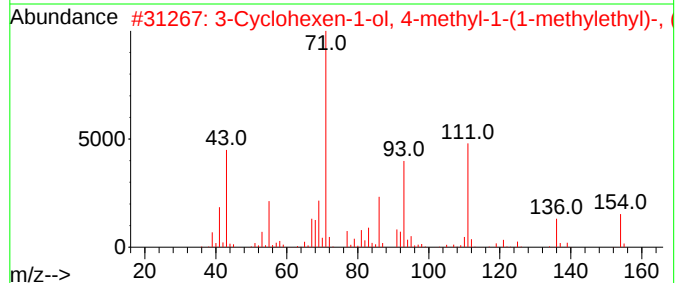
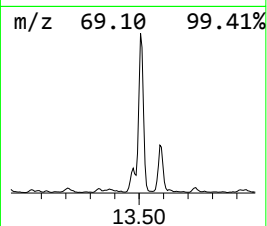
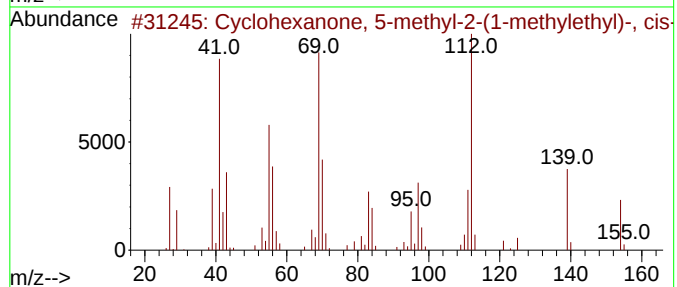
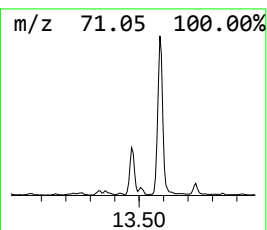
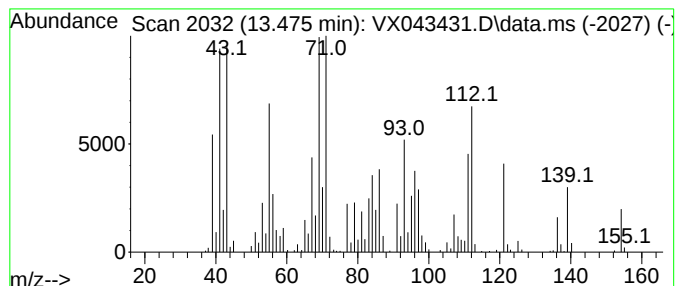
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 7 Cyclohexanone, 5-methyl-2-(... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.475	27.05 ug/l	219213	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000491-07-6	70
2			3-Cyclohexen-1-ol, 4-methyl-1-(1...	154	C10H18O	020126-76-5	46
3			Ketone, 2,2-dimethylcyclohexyl m...	154	C10H18O	017983-26-5	45
4			Terpinen-4-ol	154	C10H18O	000562-74-3	41
5			Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	010458-14-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101824\
Data File : VX043431.D
Acq On : 18 Oct 2024 14:00
Operator : JC/MD
Sample : P4427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
241016059-01-VOA

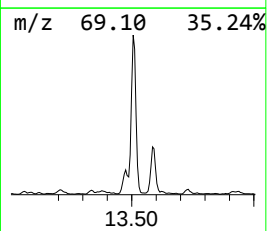
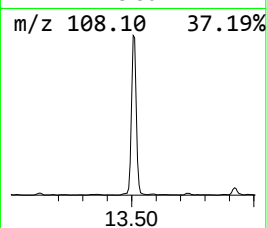
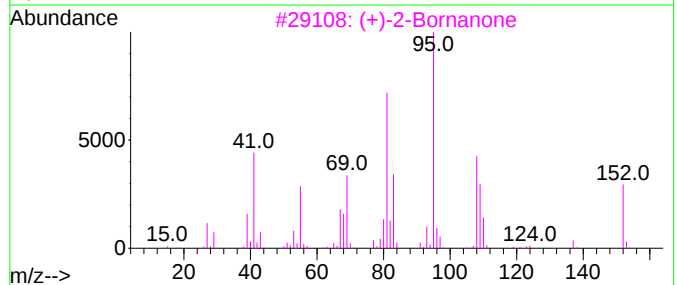
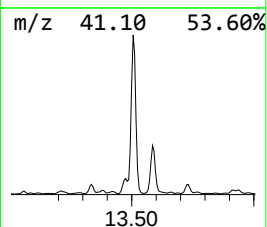
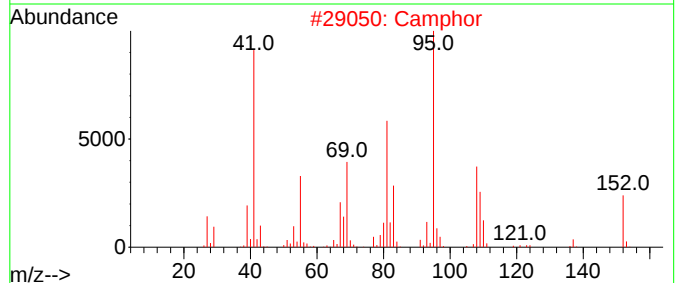
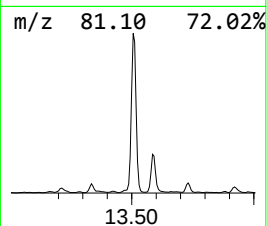
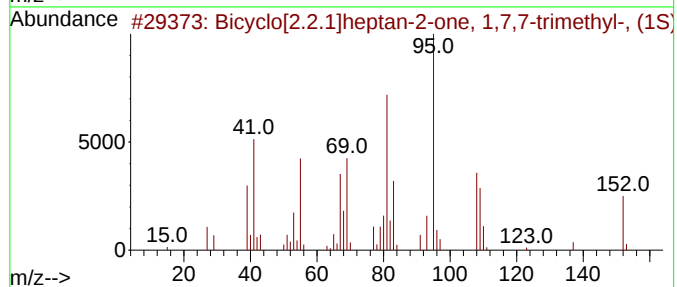
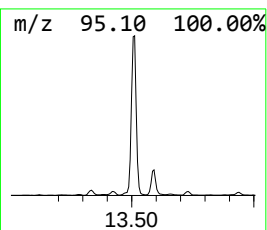
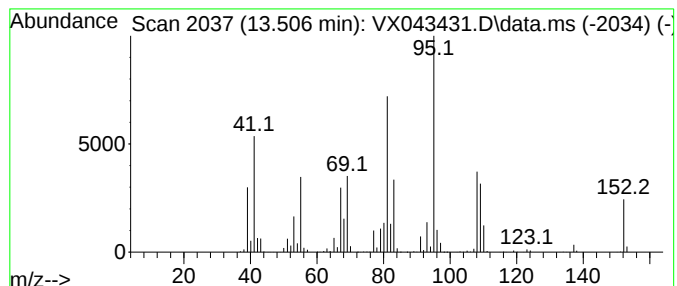
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Quant Title : SW846 8260

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

Peak Number 8 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.506	197.14 ug/l	1597810	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
2			Camphor	152	C10H16O	000076-22-2	97
3			(+)-2-Bornanone	152	C10H16O	000464-49-3	97
4			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	64
5			2-Furancarboxylic acid, 2-propen...	152	C8H8O3	004208-49-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101824\
Data File : VX043431.D
Acq On : 18 Oct 2024 14:00
Operator : JC/MD
Sample : P4427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
241016059-01-VOA

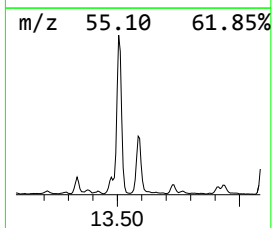
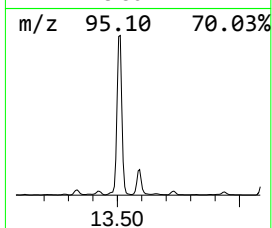
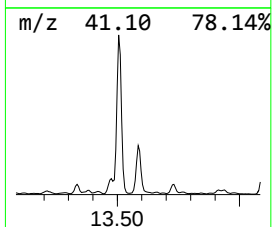
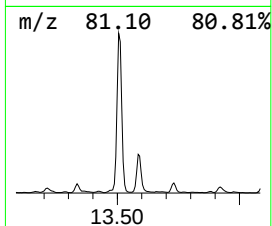
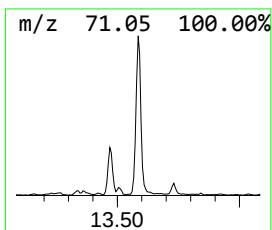
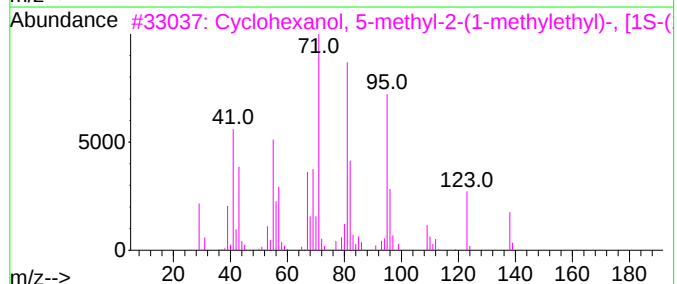
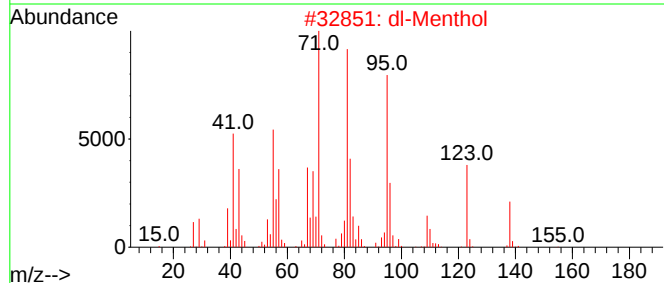
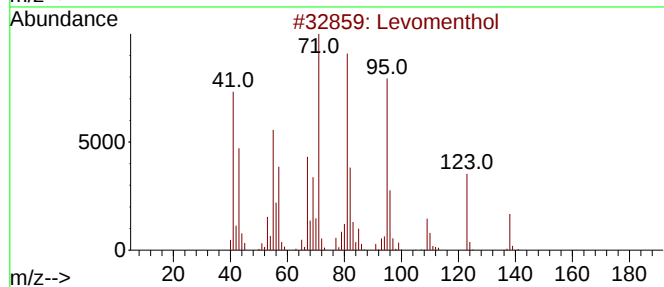
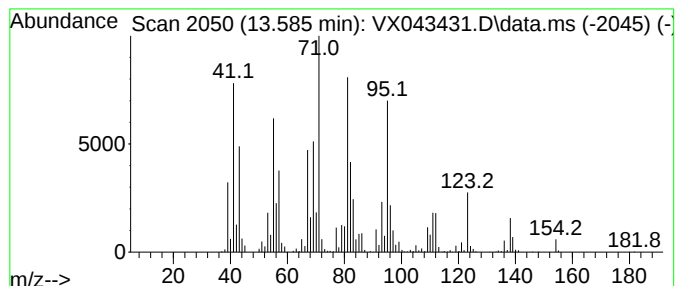
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Quant Title : SW846 8260

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

Peak Number 9 Levomenthol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.585	71.63 ug/l	580556	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Levomenthol	156	C10H20O	002216-51-5	91
2			dl-Menthol	156	C10H20O	000089-78-1	87
3			Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	87
4			Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	023283-97-8	72
5			Cyclohexanol, 1-methyl-4-(1-meth...	156	C10H20O	021129-27-1	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101824\
Data File : VX043431.D
Acq On : 18 Oct 2024 14:00
Operator : JC/MD
Sample : P4427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
241016059-01-VOA

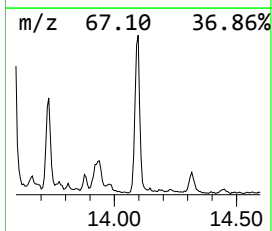
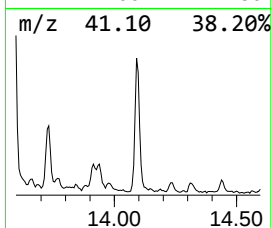
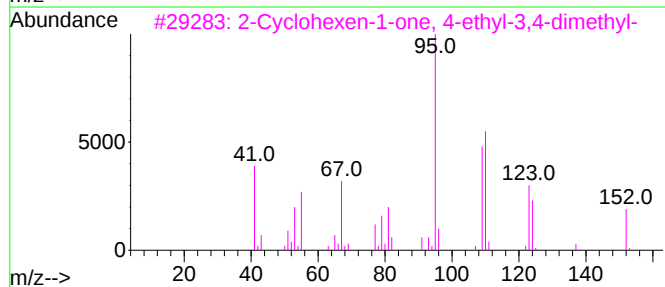
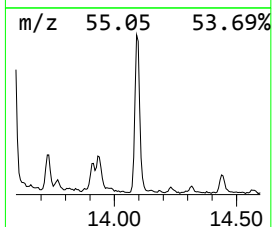
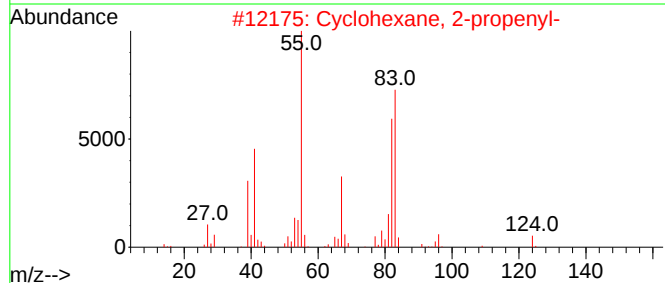
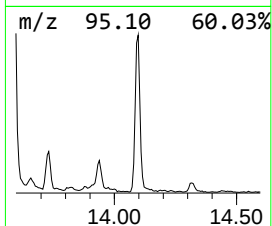
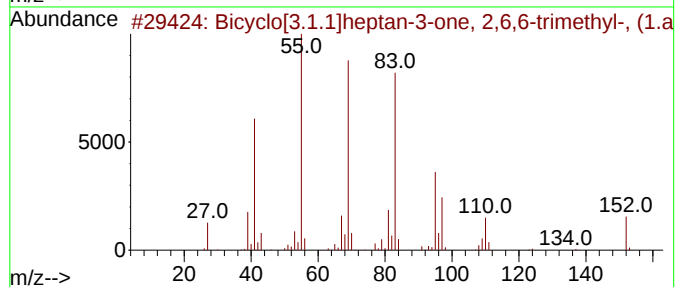
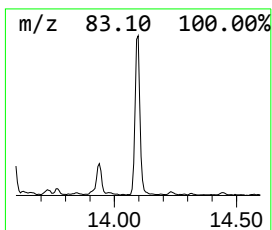
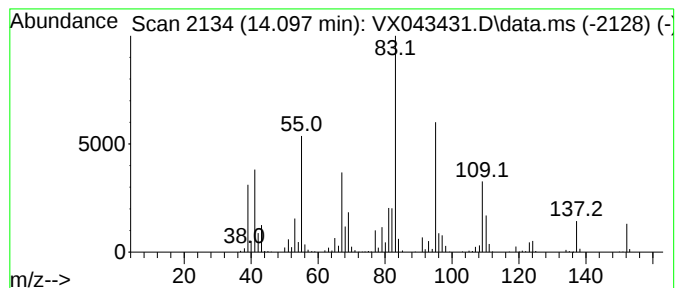
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 10 unknown14.097 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.097	32.94 ug/l	266936	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	015358-88-0	49
2		Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	38
3		2-Cyclohexen-1-one, 4-ethyl-3,4-...	152	C10H16O	017622-46-7	38
4		1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	35
5		2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101824\
Data File : VX043431.D
Acq On : 18 Oct 2024 14:00
Operator : JC/MD
Sample : P4427-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
241016059-01-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.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
3-Pentanone, 2,...	9.378	18.2	ug/l	149768	3	10.055	410645	50.0
Eucalyptol	12.104	22.6	ug/l	183152	4	12.024	405244	50.0
Fenchone	12.902	92.0	ug/l	745862	4	12.024	405244	50.0
Cyclohexanemeth...	13.335	18.1	ug/l	146998	4	12.024	405244	50.0
Cyclohexanone, ...	13.475	27.1	ug/l	219213	4	12.024	405244	50.0
Bicyclo[2.2.1]h...	13.506	197.1	ug/l	1597810	4	12.024	405244	50.0
Levomenthol	13.585	71.6	ug/l	580556	4	12.024	405244	50.0
unknown14.097	14.097	32.9	ug/l	266936	4	12.024	405244	50.0