

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030721\
 Data File : VX021046.D
 Acq On : 05 Mar 2021 19:29
 Operator : JC/MD
 Sample : M1553-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 30-31

Integration Parameters: RTEINT.P

Integrator: RTE

Smoother: 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\82X022421W.M

Title : SW846 8260

Signal : TIC: VX021046.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.629	761	772	786	rBV2	229150	627256	1.08%	0.676%
2	6.829	966	976	1001	rVB2	378084	920864	1.58%	0.992%
3	8.694	1286	1293	1299	rBV	841663	1292072	2.22%	1.392%
4	10.094	1520	1531	1541	rBV	835724	1161425	2.00%	1.251%
5	11.118	1700	1705	1717	rVB	682889	874687	1.50%	0.942%
6	12.059	1860	1865	1873	rVB	861419	1085589	1.87%	1.169%
7	12.141	1873	1879	1893	rVB	7238860	9142526	15.72%	9.849%
8	12.271	1894	1901	1928	rBV	36795762	58157056	100.00%	62.649%
9	13.012	2022	2027	2039	rBV	727129	1097587	1.89%	1.182%
10	13.106	2039	2043	2046	rVV	786688	1112116	1.91%	1.198%
11	13.136	2046	2048	2067	rVB	1420849	2130688	3.66%	2.295%
12	13.459	2098	2103	2114	rBV	2381607	3089274	5.31%	3.328%
13	13.553	2114	2119	2128	rVB	1677786	2285040	3.93%	2.462%
14	13.871	2168	2173	2180	rBV	7231850	8916592	15.33%	9.605%
15	13.930	2180	2183	2215	rVB3	380288	936958	1.61%	1.009%

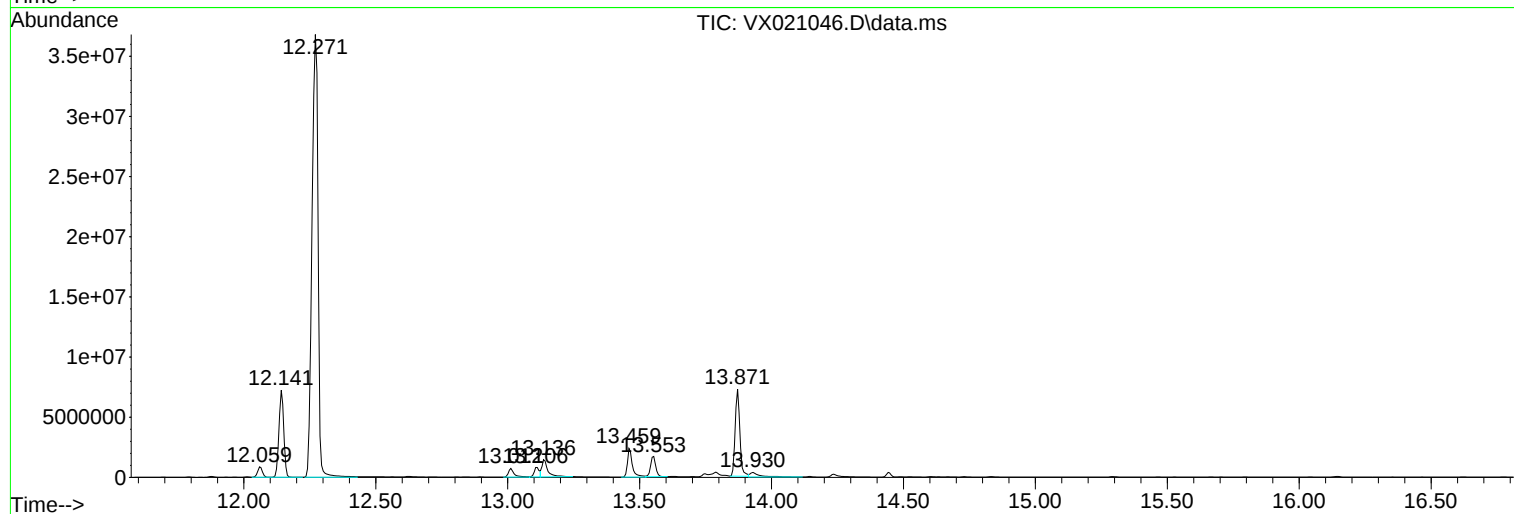
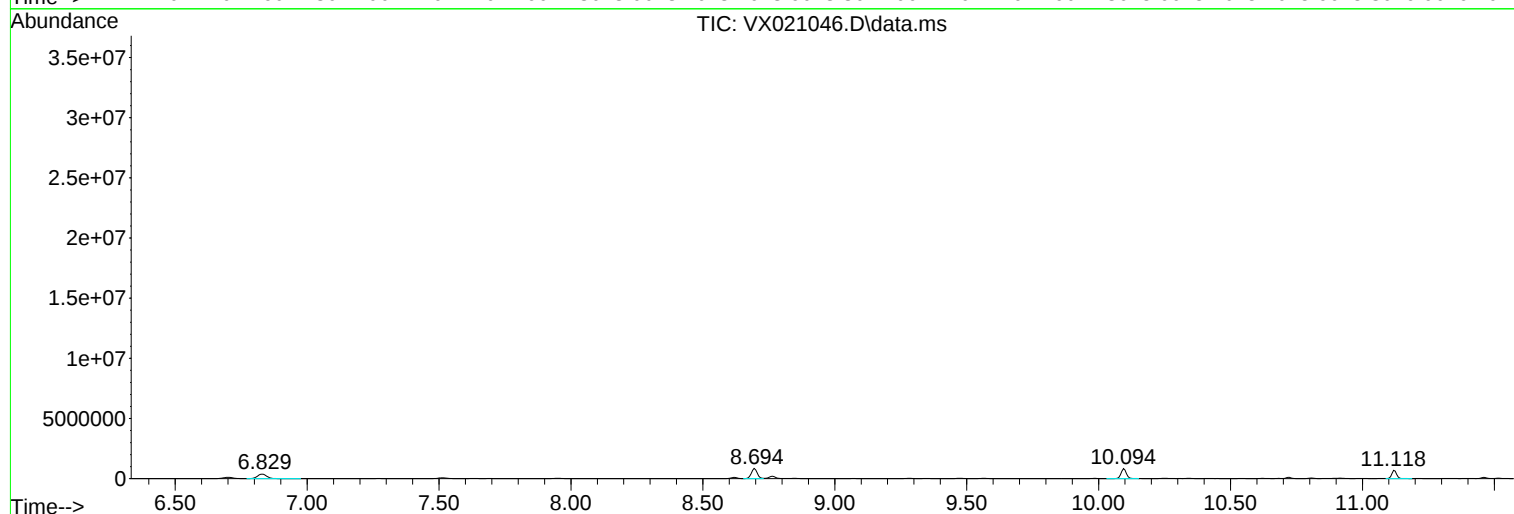
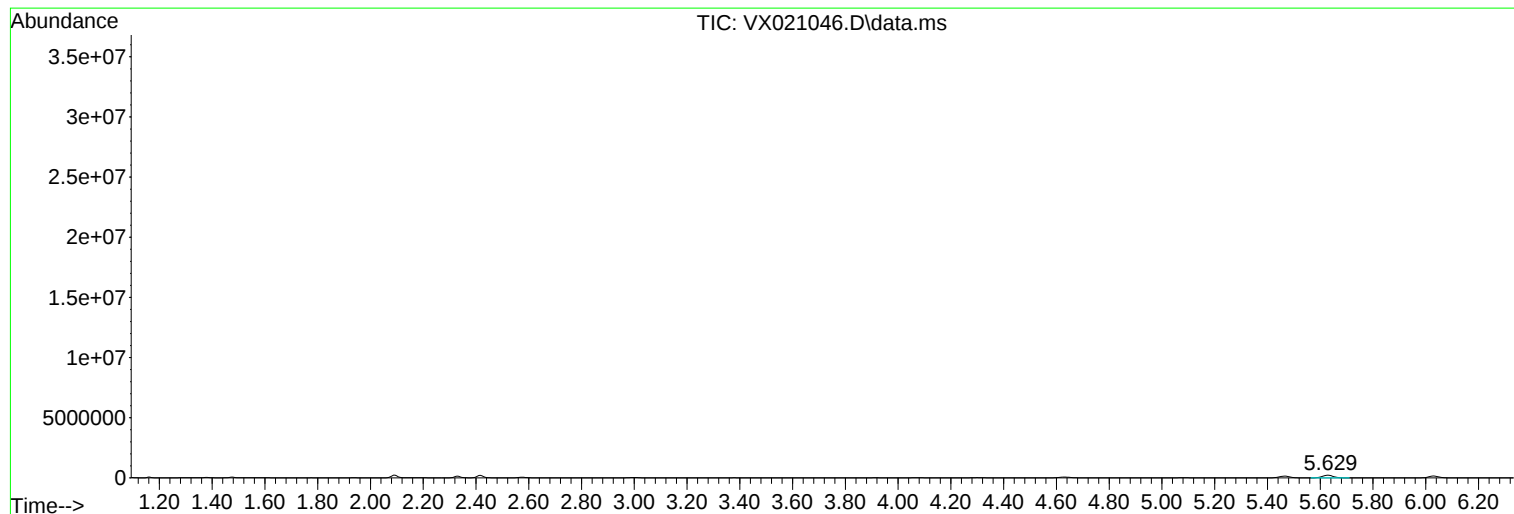
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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ClientSampleId :
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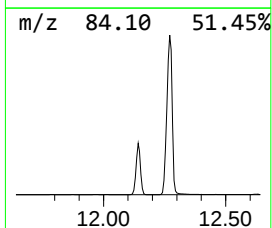
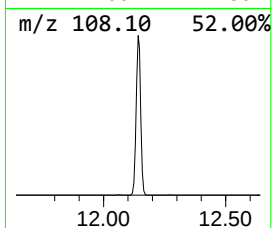
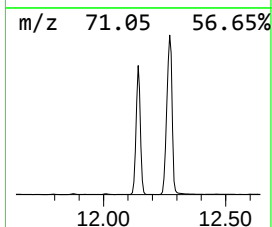
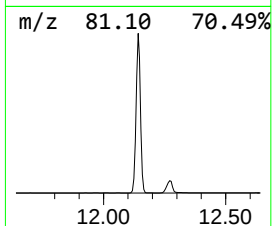
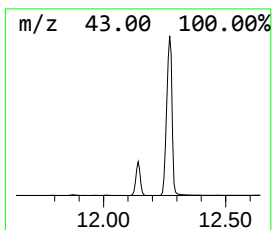
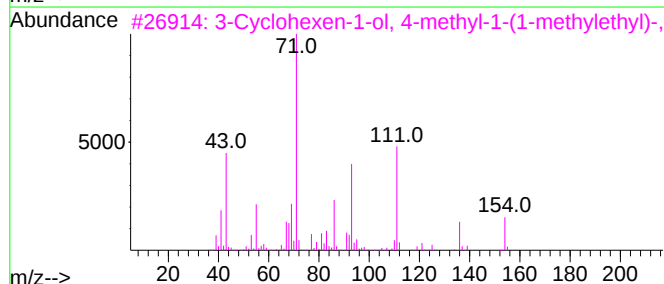
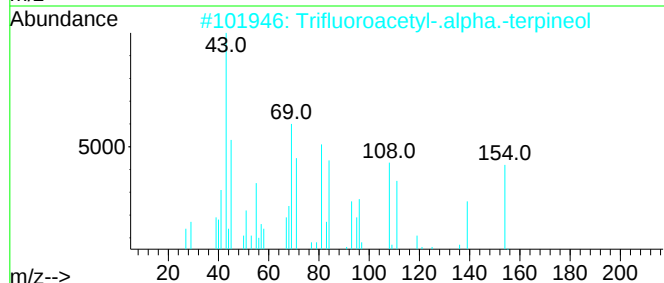
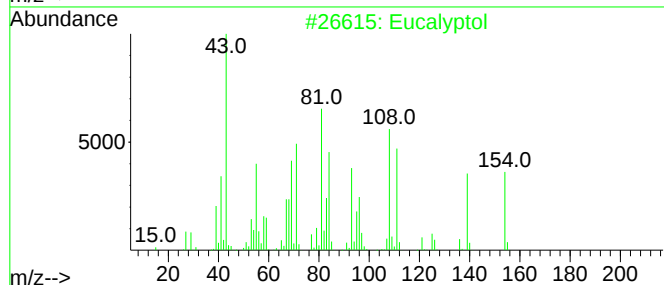
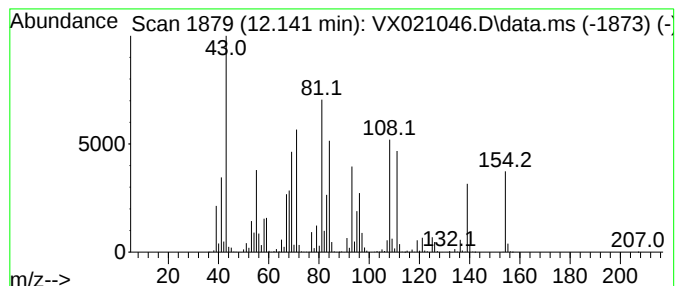
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Eucalyptol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.142	421.09 ug/l	9142530	1,4-Dichlorobenzene-d4	12.059

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	50
3			3-Cyclohexen-1-ol, 4-methyl-1-(1...	154	C10H18O	020126-76-5	35
4			Sulfurous acid, 2-pentyl propyl ...	194	C8H18O3S	1000309-15-1	22
5			2-Acetyl cyclohexanone	154	C9H14O2	006126-53-0	22



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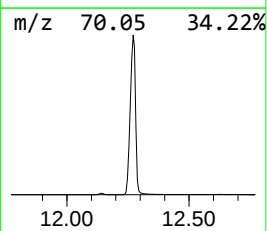
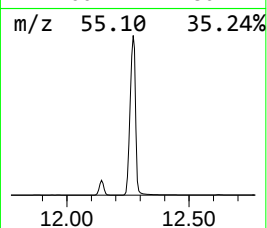
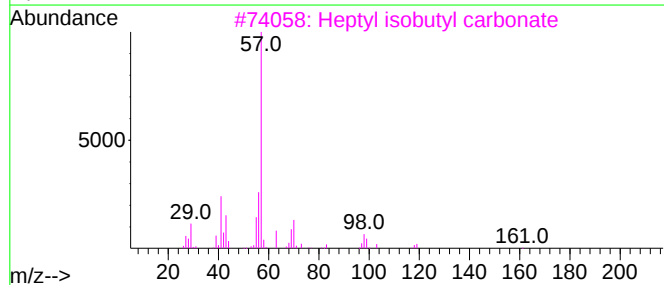
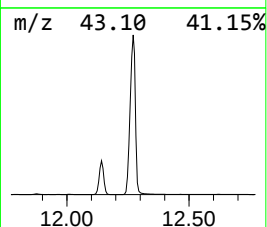
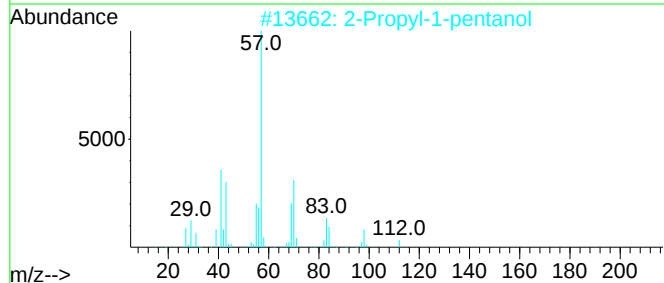
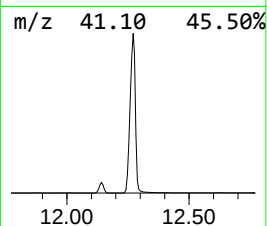
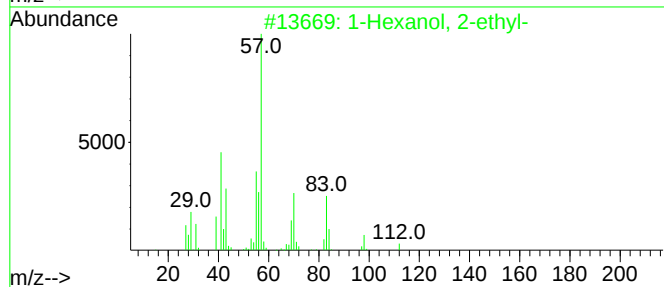
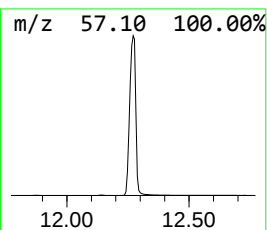
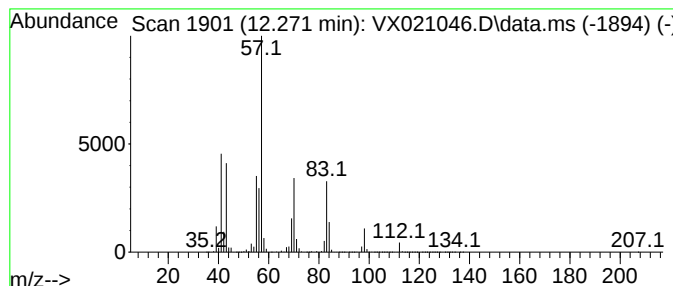
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.271	2678.59 ug/l	58157100	1,4-Dichlorobenzene-d4	12.059

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	72
3		Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	50
4		Bicyclo[3.1.0]hexan-2-ol	98	C6H10O	1000194-18-6	47
5		Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	46



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ClientSampleId :
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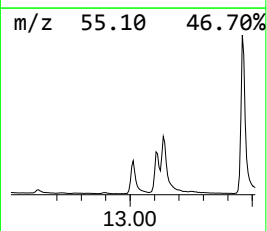
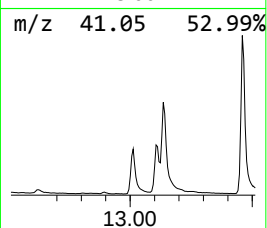
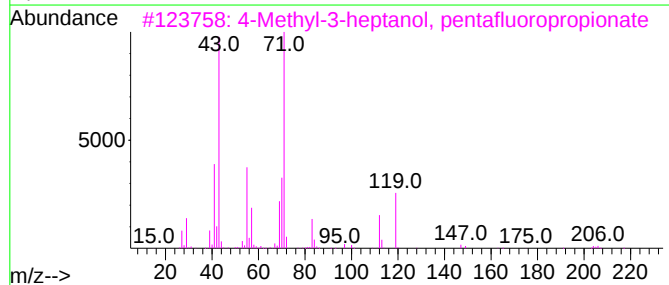
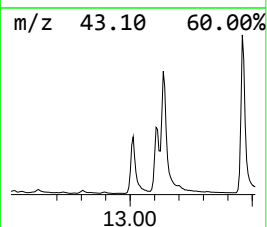
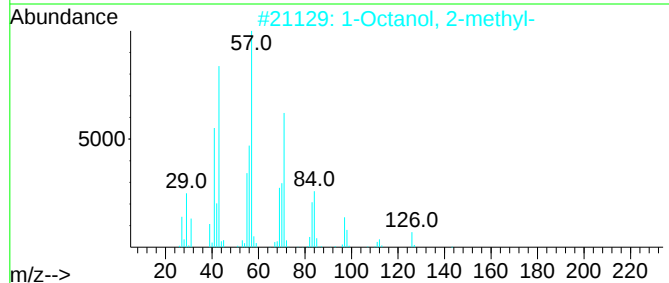
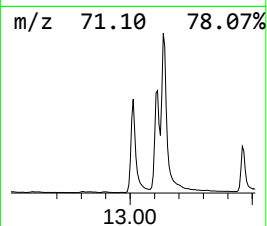
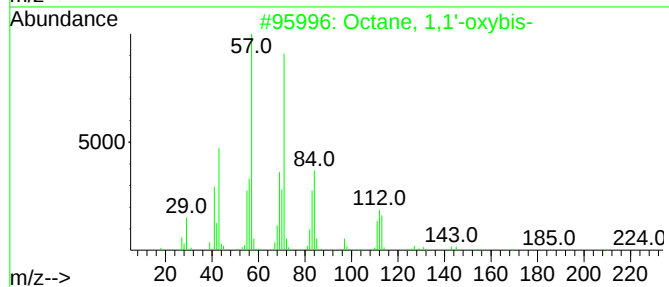
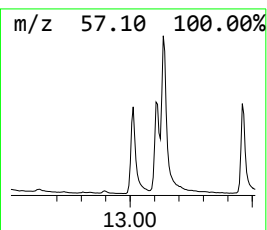
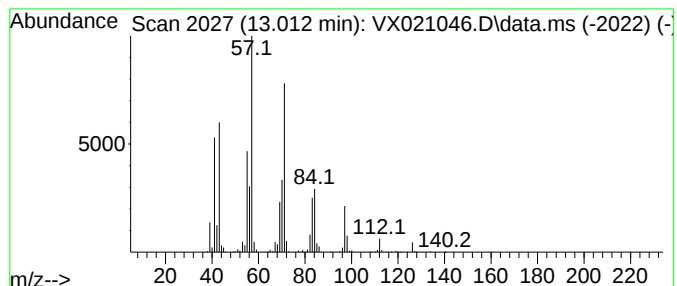
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octane, 1,1'-oxybis- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.012	50.55 ug/l	1097590	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	80
2			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	53
3			4-Methyl-3-heptanol, pentafluoro...	276	C11H17F5O2	1000365-51-7	47
4			1-Decene, 4-methyl-	154	C11H22	013151-29-6	47
5			Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	47



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Instrument :
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ClientSampleId :
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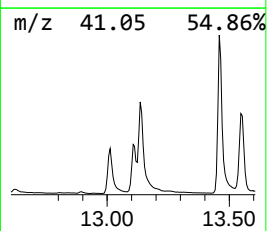
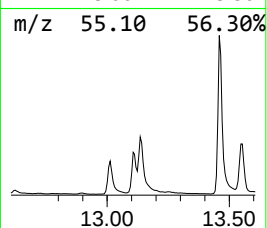
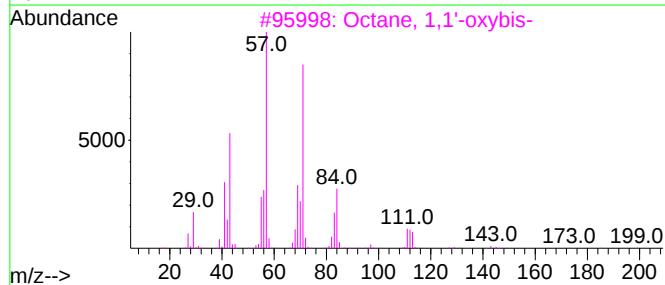
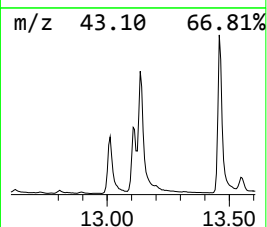
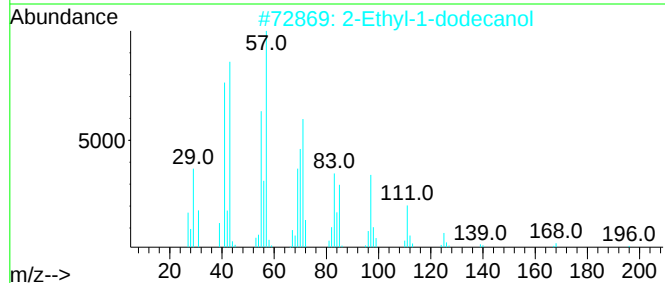
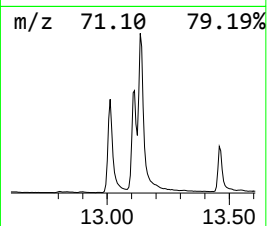
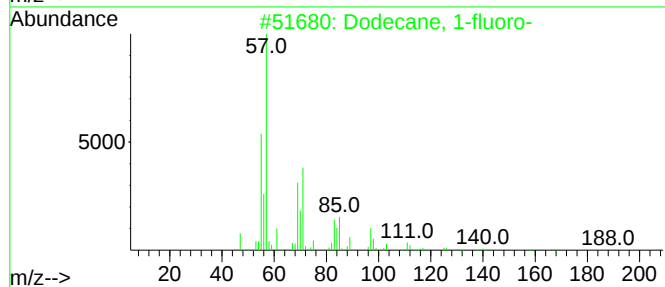
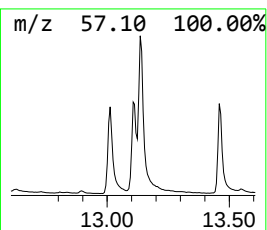
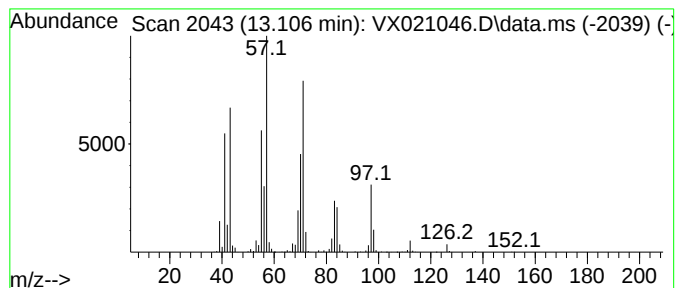
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecane, 1-fluoro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.106	51.22 ug/l	1112120	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	64
2			2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	59
3			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	50
4			n-Butyric acid 2-ethylhexyl ester	200	C12H24O2	025415-84-3	47
5			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	43



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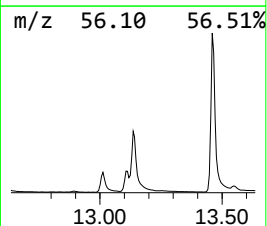
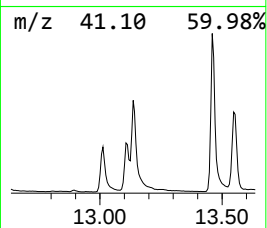
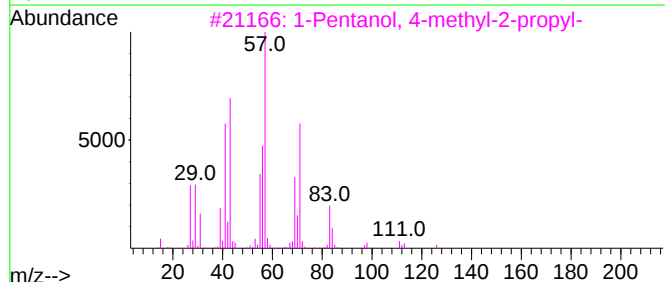
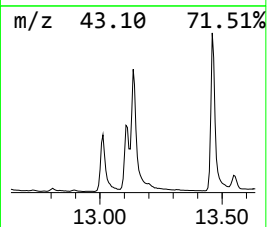
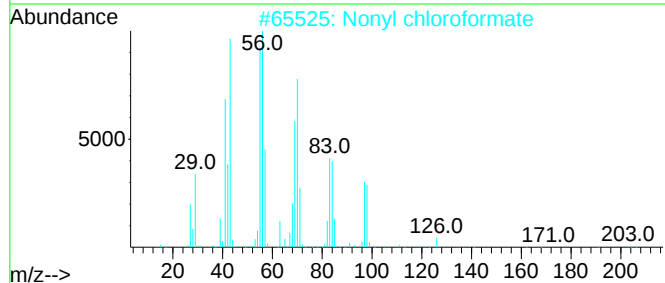
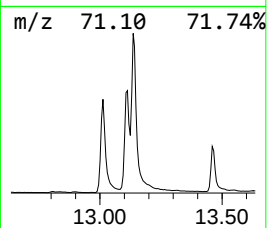
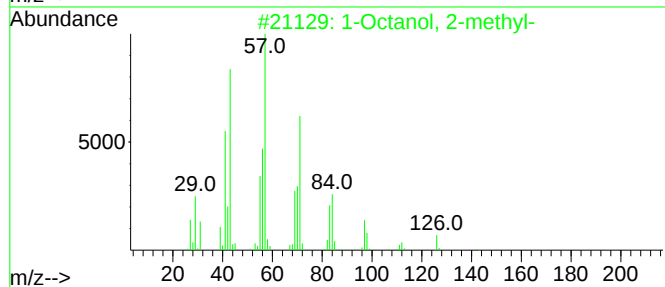
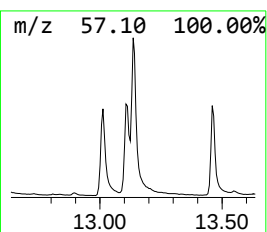
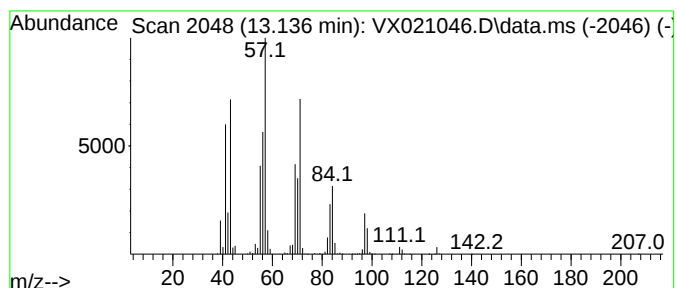
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Octanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.136	98.14 ug/l	2130690	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	72
2			Nonyl chloroformate	206	C10H19ClO2	057045-82-6	59
3			1-Pentanol, 4-methyl-2-propyl-	144	C9H20O	054004-41-0	59
4			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	59
5			Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	52



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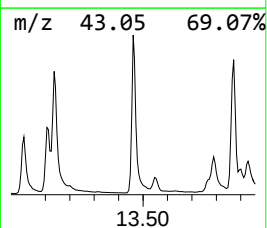
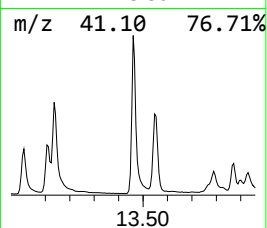
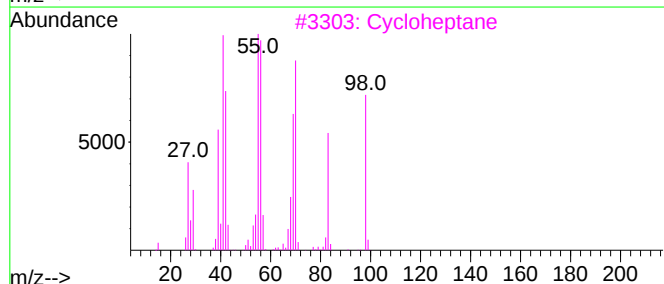
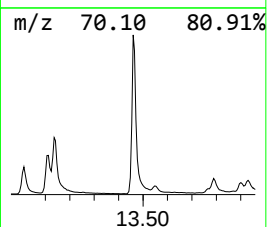
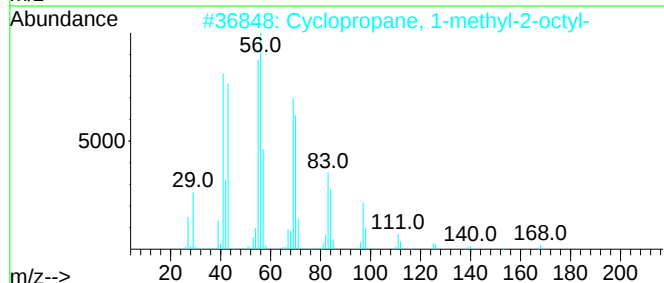
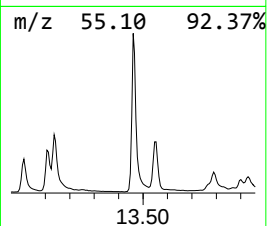
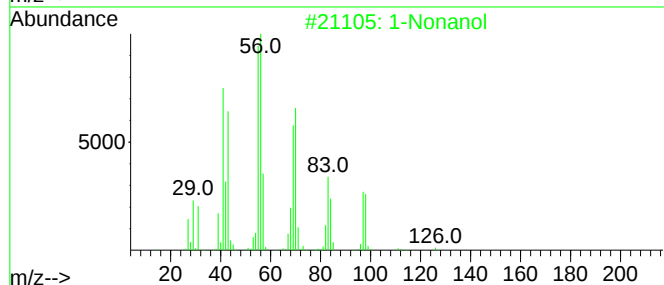
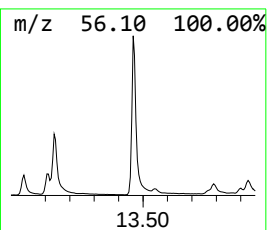
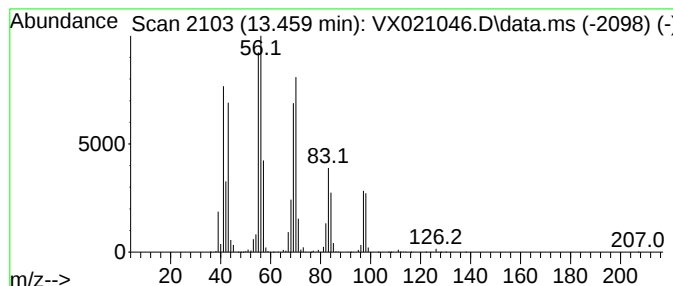
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Nonanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.459	142.29 ug/l	3089270	1,4-Dichlorobenzene-d4	12.059

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Nonanol	144	C9H20O	000143-08-8	91
2		Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	86
3		Cycloheptane	98	C7H14	000291-64-5	64
4		1-Octanol	130	C8H18O	000111-87-5	64
5		Formic acid, octyl ester	158	C9H18O2	000112-32-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030721\
Data File : VX021046.D
Acq On : 05 Mar 2021 19:29
Operator : JC/MD
Sample : M1553-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30-31

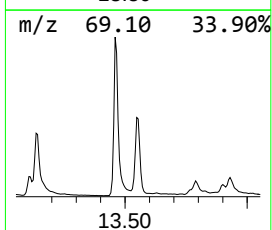
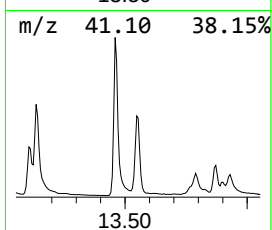
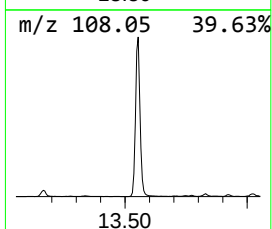
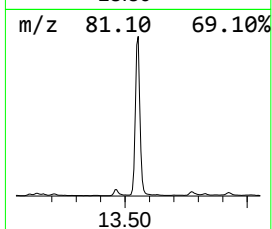
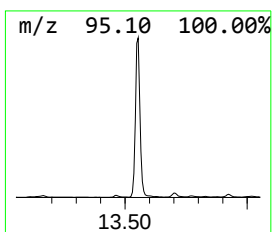
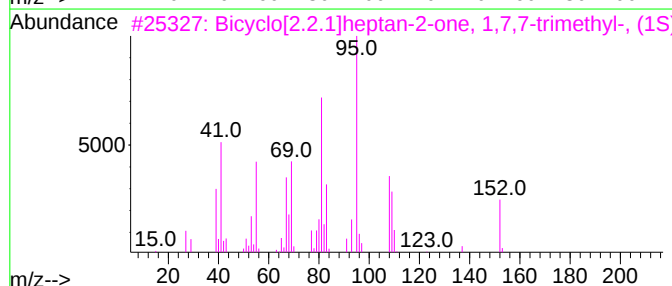
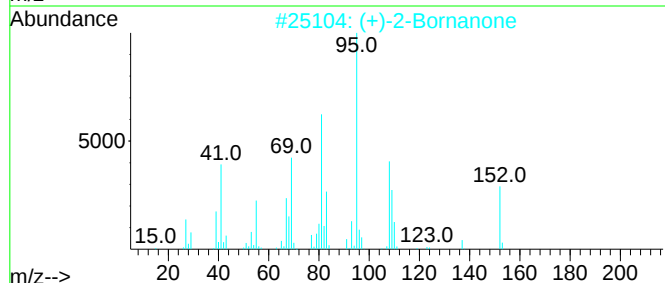
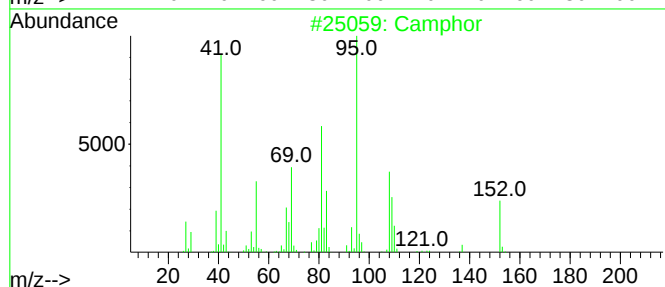
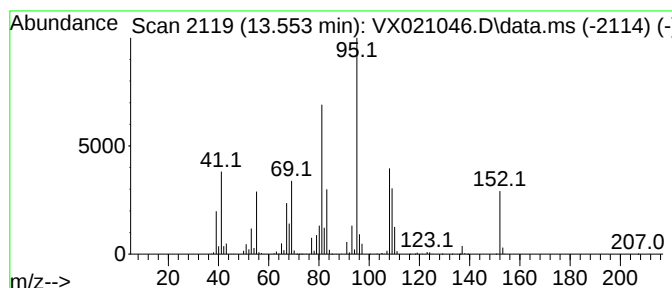
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Camphor Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.553	105.24 ug/l	2285040	1,4-Dichlorobenzene-d4	12.059

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	96
4			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46
5			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030721\
Data File : VX021046.D
Acq On : 05 Mar 2021 19:29
Operator : JC/MD
Sample : M1553-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30-31

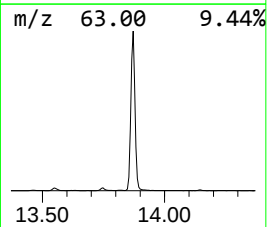
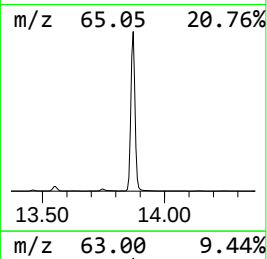
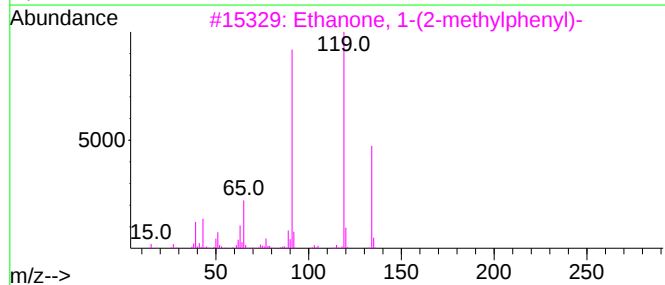
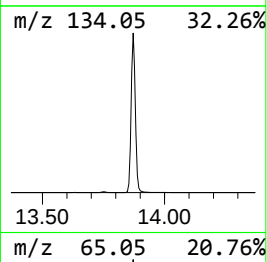
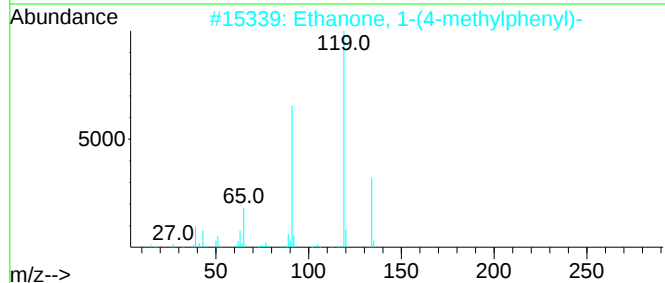
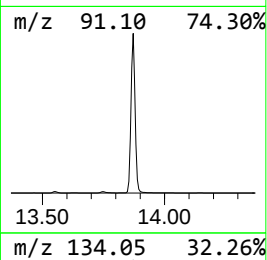
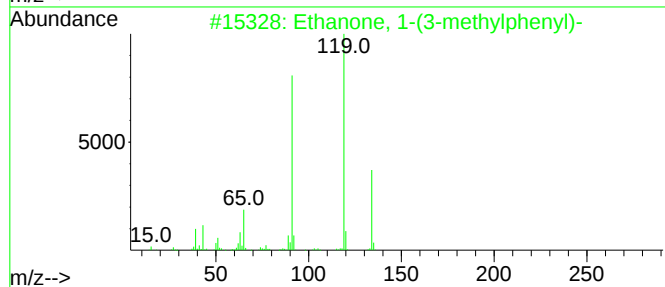
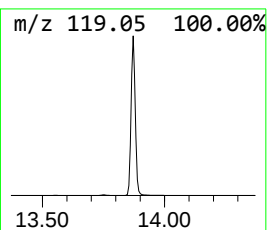
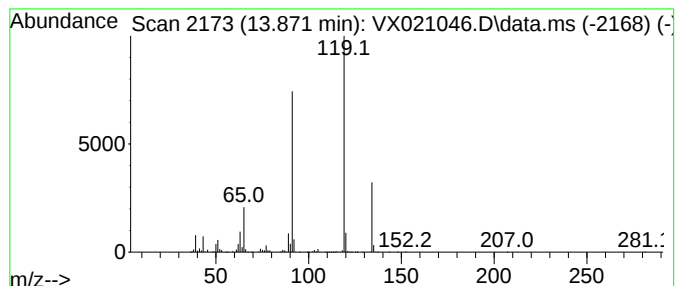
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Ethanone, 1-(3-methylphenyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	410.68 ug/l	8916590	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(3-methylphenyl)-	134	C9H10O	000585-74-0	97
2			Ethanone, 1-(4-methylphenyl)-	134	C9H10O	000122-00-9	95
3			Ethanone, 1-(2-methylphenyl)-	134	C9H10O	000577-16-2	94
4			4-Methylbenzoic acid, pentafluor...	302	C14H7F5O2	1000354-15-1	80
5			4-Methylbenzoic acid anhydride	254	C16H14O3	013222-85-0	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030721\
Data File : VX021046.D
Acq On : 05 Mar 2021 19:29
Operator : JC/MD
Sample : M1553-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30-31

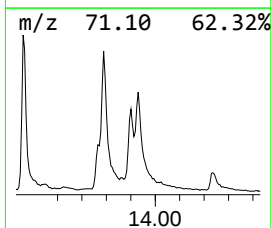
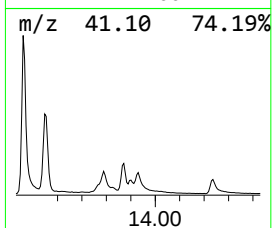
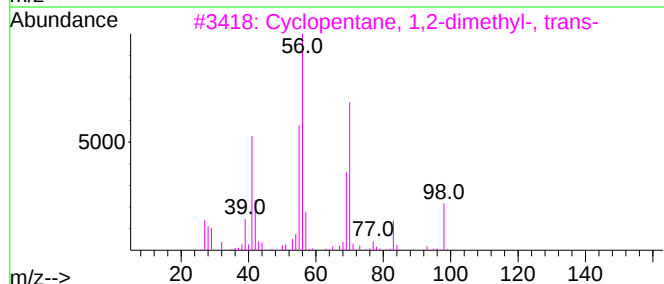
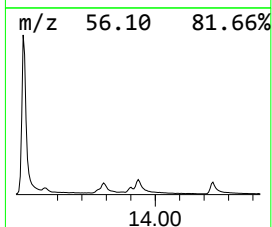
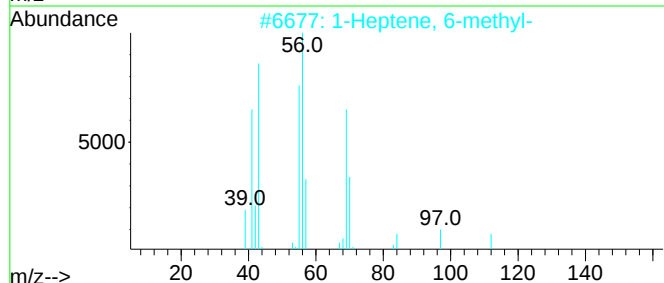
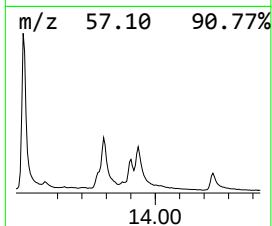
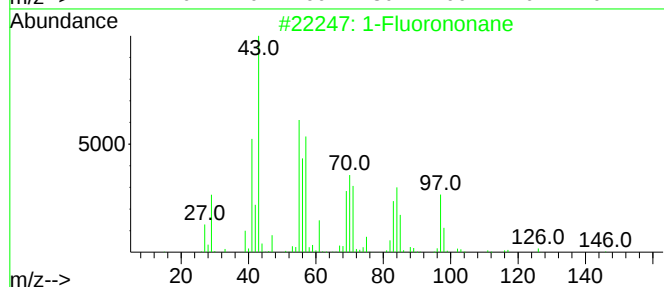
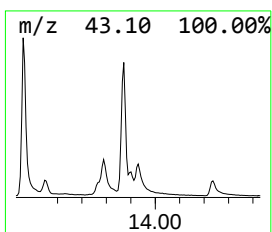
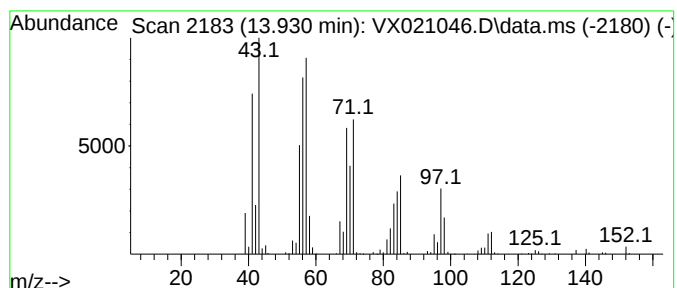
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown13.930 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.930	43.15 ug/l	936958	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Fluorononane	146	C9H19F	000463-18-3	49
2			1-Heptene, 6-methyl-	112	C8H16	005026-76-6	45
3			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	43
4			Cyclopentane, 1,1,2-trimethyl-	112	C8H16	004259-00-1	43
5			1-Heptene	98	C7H14	000592-76-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030721\
 Data File : VX021046.D
 Acq On : 05 Mar 2021 19:29
 Operator : JC/MD
 Sample : M1553-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 30-31

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
 Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Eucalyptol	12.142	421.1	ug/l	9142530	4	12.059	1085590	50.0
1-Hexanol, 2-et...	12.271	2678.6	ug/l	58157100	4	12.059	1085590	50.0
Octane, 1,1'-ox...	13.012	50.5	ug/l	1097590	4	12.059	1085590	50.0
Dodecane, 1-flu...	13.106	51.2	ug/l	1112120	4	12.059	1085590	50.0
1-Octanol, 2-me...	13.136	98.1	ug/l	2130690	4	12.059	1085590	50.0
1-Nonanol	13.459	142.3	ug/l	3089270	4	12.059	1085590	50.0
Camphor	13.553	105.2	ug/l	2285040	4	12.059	1085590	50.0
Ethanone, 1-(3-...	13.871	410.7	ug/l	8916590	4	12.059	1085590	50.0
unknown13.930	13.930	43.1	ug/l	936958	4	12.059	1085590	50.0