

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051520\
 Data File : VX016279.D
 Acq On : 15 May 2020 14:40
 Operator : JC/SP
 Sample : L2642-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 400513791-VOA

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.276	28	31	45	rVB	154613	188108	1.99%	0.469%
2	2.422	212	219	236	rVB2	98940	201010	2.12%	0.501%
3	3.007	305	315	332	rBV	3067209	6785645	71.70%	16.905%
4	4.666	562	587	599	rBV	2854985	9463289	100.00%	23.576%
5	5.086	645	656	680	rVB	1105234	3266615	34.52%	8.138%
6	5.464	708	718	730	rVV	141213	404987	4.28%	1.009%
7	5.629	734	745	759	rVB	246062	700568	7.40%	1.745%
8	6.031	801	811	819	rBV	156519	414284	4.38%	1.032%
9	6.117	819	825	838	rVV	66158	206608	2.18%	0.515%
10	6.239	838	845	850	rVV2	34247	106814	1.13%	0.266%
11	6.306	850	856	866	rVB	69255	187770	1.98%	0.468%
12	6.830	931	942	955	rBV	395243	930668	9.83%	2.319%
13	8.695	1241	1248	1254	rBV	853712	1328904	14.04%	3.311%
14	8.763	1254	1259	1268	rVB2	153769	263493	2.78%	0.656%
15	8.848	1268	1273	1278	rBV	102205	160118	1.69%	0.399%
16	9.421	1359	1367	1373	rBV	415472	600378	6.34%	1.496%
17	10.098	1467	1478	1490	rBV	942034	1427013	15.08%	3.555%
18	10.238	1496	1501	1511	rBV2	168918	293443	3.10%	0.731%
19	10.342	1511	1518	1524	rVV	341100	472034	4.99%	1.176%
20	10.427	1524	1532	1541	rVB2	130948	202783	2.14%	0.505%
21	10.683	1569	1574	1579	rBV	223784	297177	3.14%	0.740%
22	11.122	1640	1646	1651	rBV	783020	991630	10.48%	2.470%
23	11.421	1688	1695	1701	rVB3	50703	97931	1.03%	0.244%
24	11.543	1711	1715	1721	rVB	72648	94899	1.00%	0.236%
25	11.793	1744	1756	1760	rBV	126418	178444	1.89%	0.445%
26	11.927	1770	1778	1785	rVB2	152400	228546	2.42%	0.569%
27	12.061	1794	1800	1808	rVB3	1025637	1552756	16.41%	3.868%
28	12.140	1808	1813	1817	rBV2	194359	311694	3.29%	0.777%
29	12.286	1830	1837	1842	rBV	115173	167986	1.78%	0.419%
30	12.805	1914	1922	1926	rVB3	68273	111955	1.18%	0.279%
31	12.945	1938	1945	1950	rBV	1516362	1905763	20.14%	4.748%
32	13.000	1950	1954	1958	rVB2	85381	129324	1.37%	0.322%
33	13.256	1992	1996	2002	rVB	74077	119147	1.26%	0.297%
34	13.378	2012	2016	2019	rBV	158852	207036	2.19%	0.516%

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Sampling : 1 Min Area: 3 % of largest Peak
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35	13.469	2026	2031	2034	rVB	67400	95581	1.01%	0.238%
36	13.518	2034	2039	2041	rBV2	289474	418226	4.42%	1.042%
37	13.554	2041	2045	2052	rVB	2223186	2904422	30.69%	7.236%
38	13.634	2052	2058	2067	rBV2	473221	715327	7.56%	1.782%
39	13.774	2076	2081	2084	rBV	132495	168786	1.78%	0.420%
40	13.817	2084	2088	2095	rVB	838750	1006961	10.64%	2.509%
41	13.975	2107	2114	2120	rVB5	100182	234389	2.48%	0.584%
42	14.140	2134	2141	2146	rBV	376744	498687	5.27%	1.242%
43	14.682	2226	2230	2233	rBV	73220	98593	1.04%	0.246%

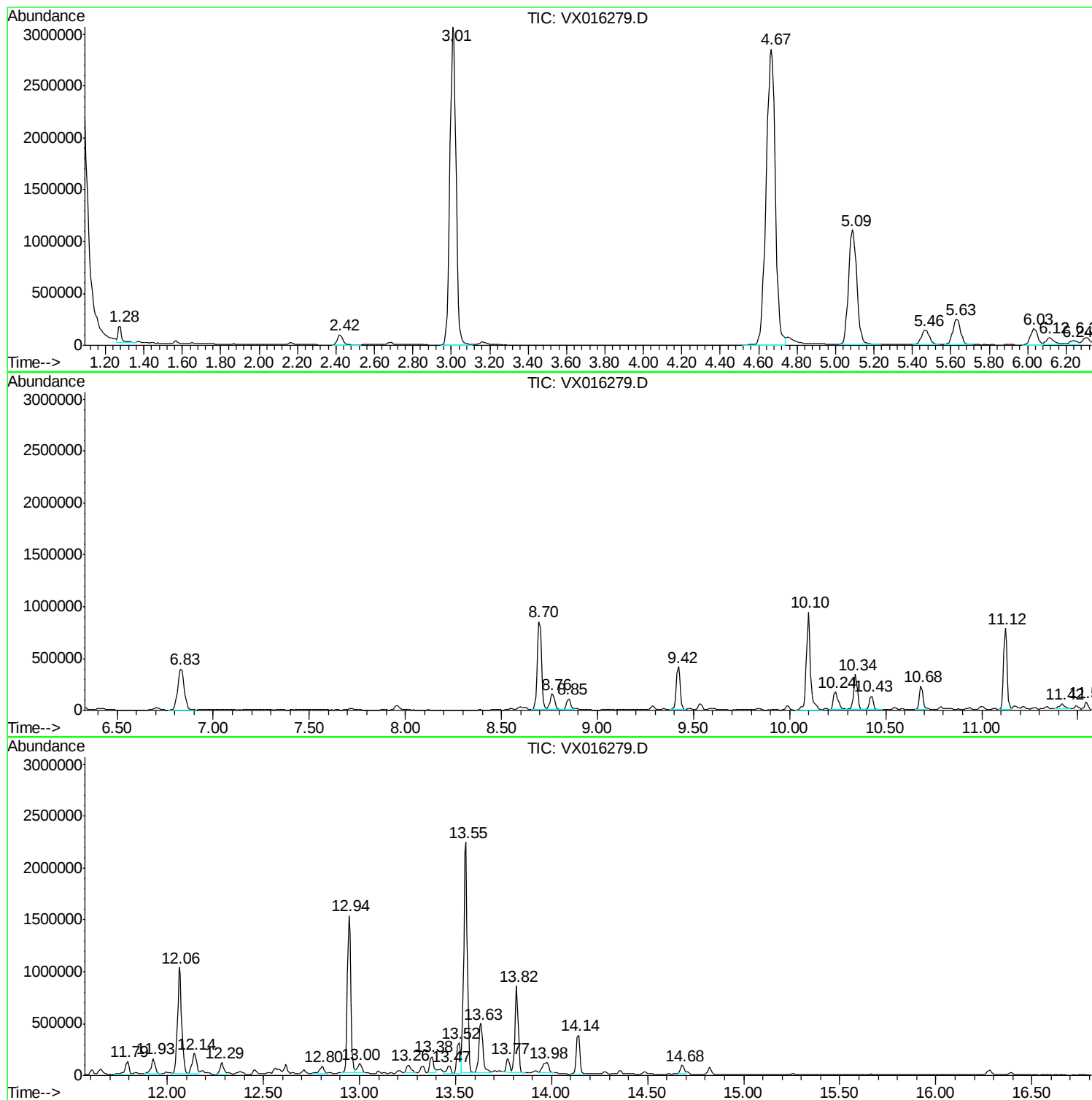
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Quant Title : SW846 8260

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



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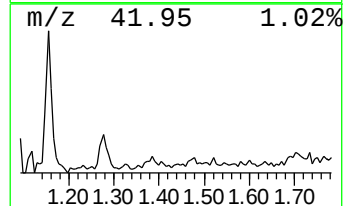
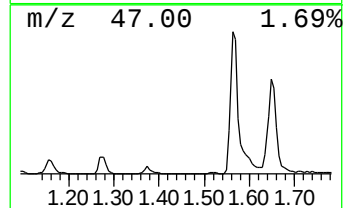
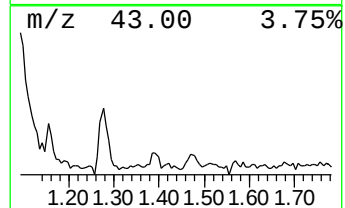
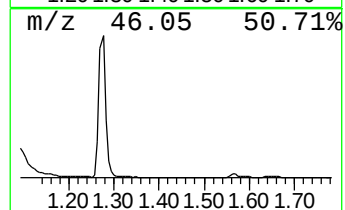
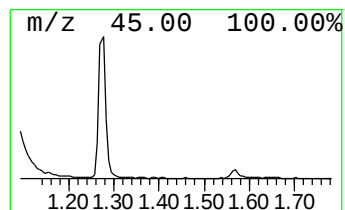
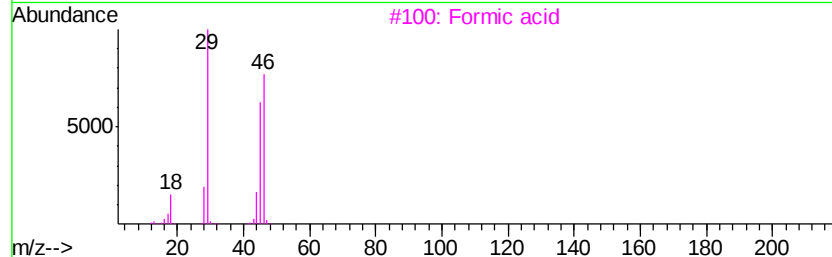
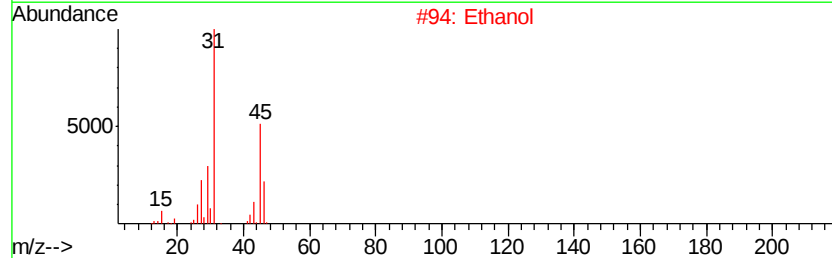
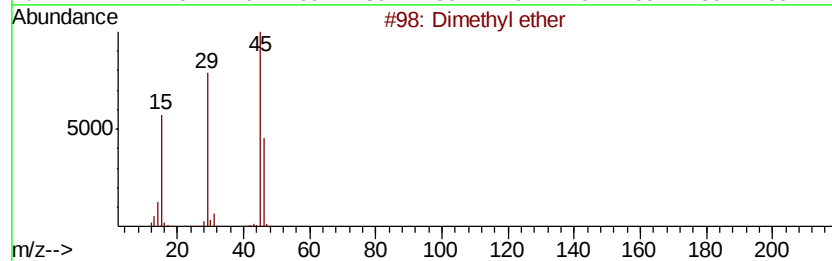
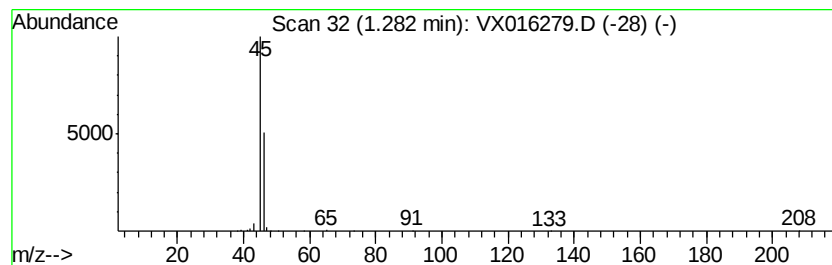
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

Peak Number 1 Dimethyl ether Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
1.28	13.43 ug/l	188108	Pentafluorobenzene	5.64		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dimethyl ether	46	C2H6O	000115-10-6	56
2		Ethanol	46	C2H6O	000064-17-5	7
3		Formic acid	46	CH2O2	000064-18-6	5
4		Hydrazine, methyl-	46	CH6N2	000060-34-4	4
5		Ethene, fluoro-	46	C2H3F	000075-02-5	4



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Instrument :
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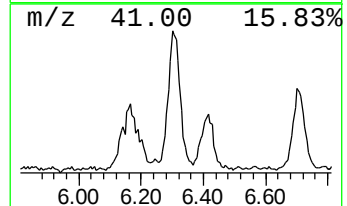
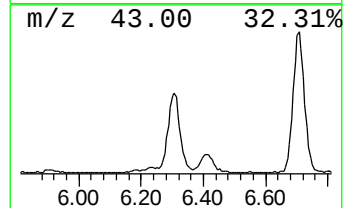
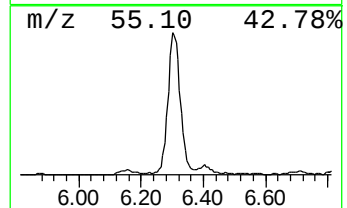
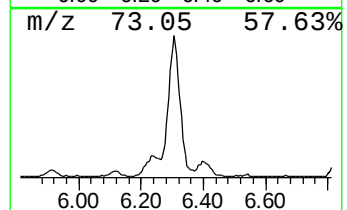
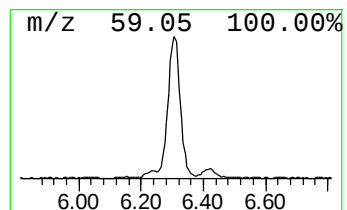
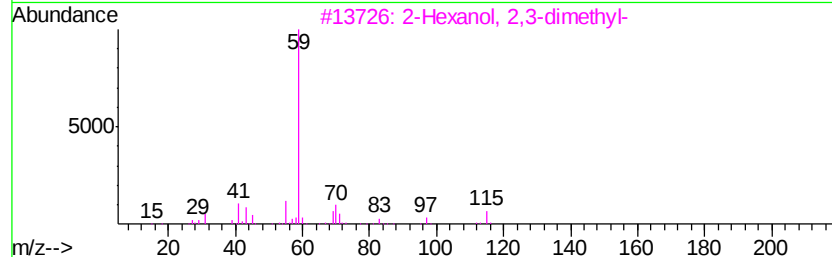
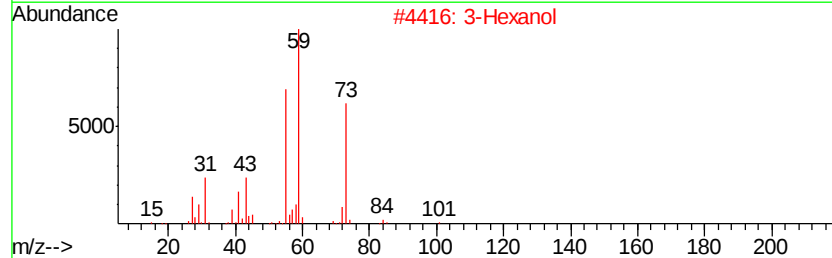
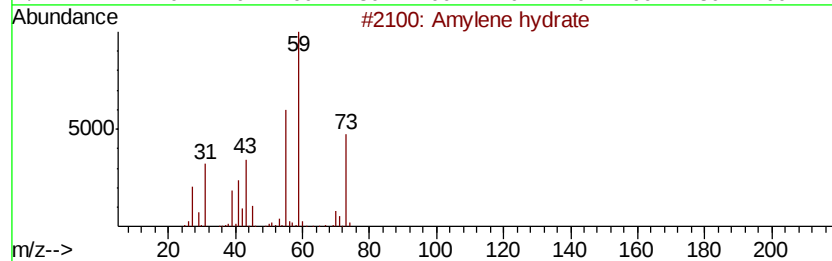
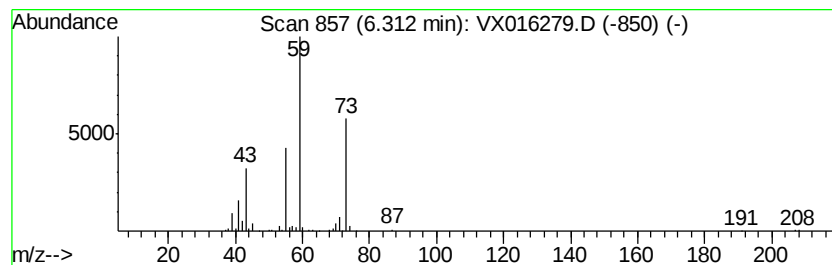
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
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Peak Number 3 Amylene hydrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.31	10.09 ug/l	187770	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Amylene hydrate	88	C5H12O	000075-85-4	78
2		3-Hexanol	102	C6H14O	000623-37-0	56
3		2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	38
4		Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	36
5		Guanidine	59	CH5N3	000113-00-8	36



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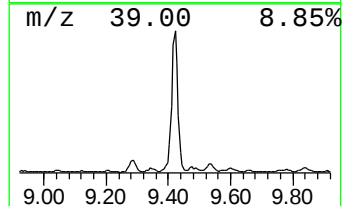
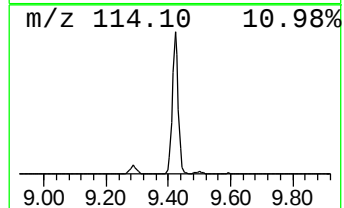
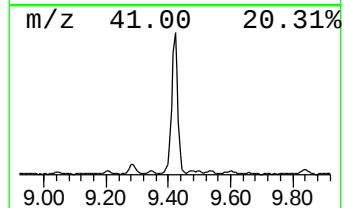
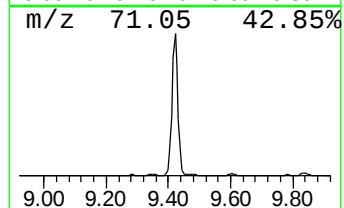
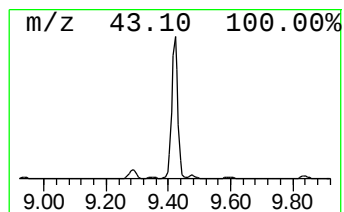
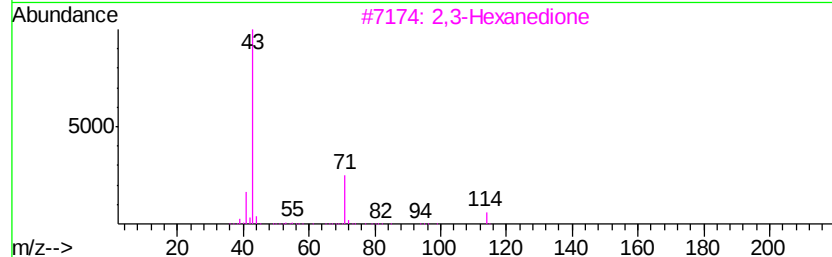
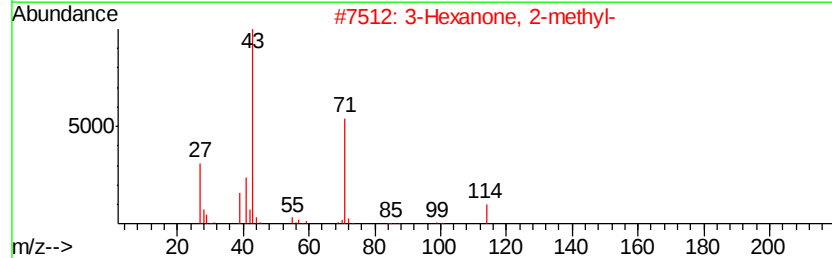
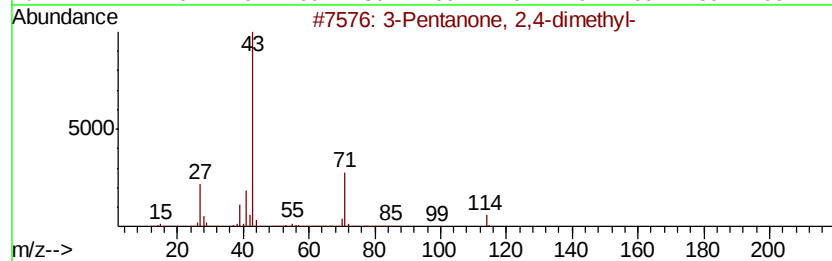
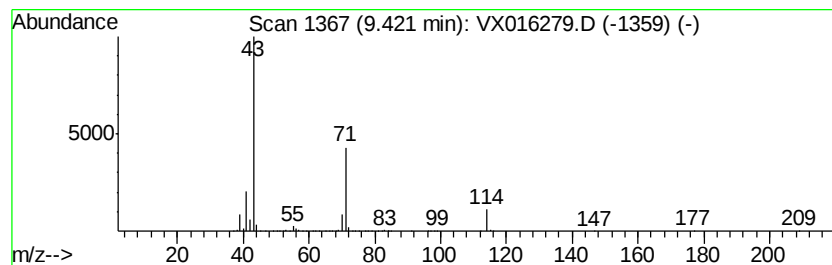
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Pentanone, 2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	21.04 ug/l	600378	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	90
2		3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	90
3		2,3-Hexanedione	114	C6H10O2	003848-24-6	80
4		4-Heptanone	114	C7H14O	000123-19-3	72
5		Heptane, 4-methyl-	114	C8H18	000589-53-7	64



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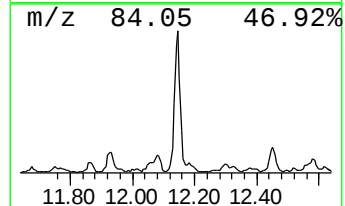
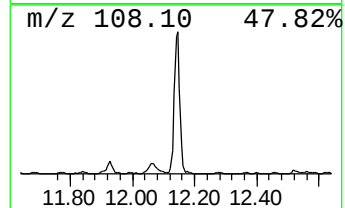
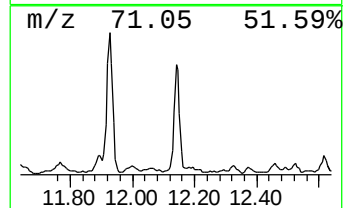
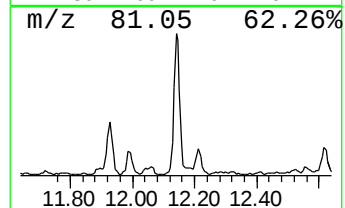
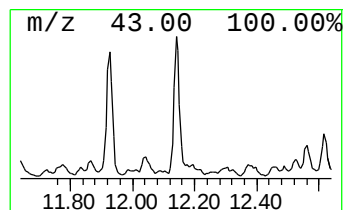
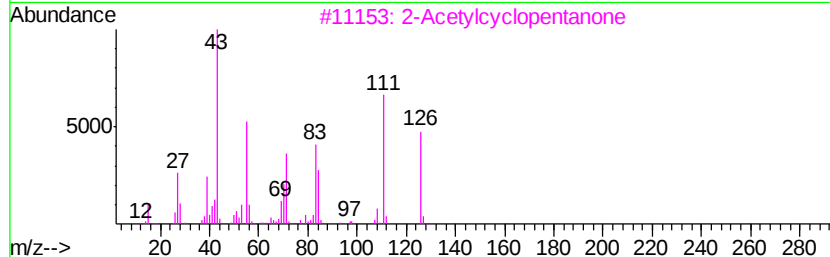
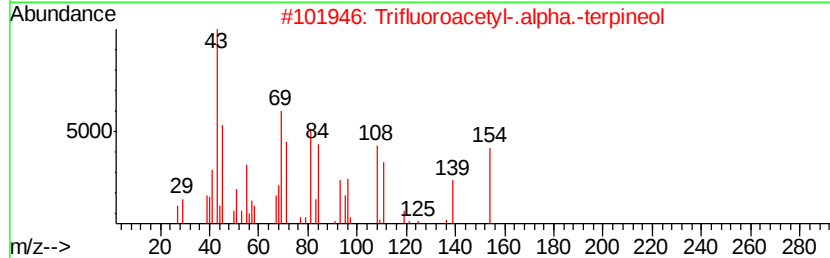
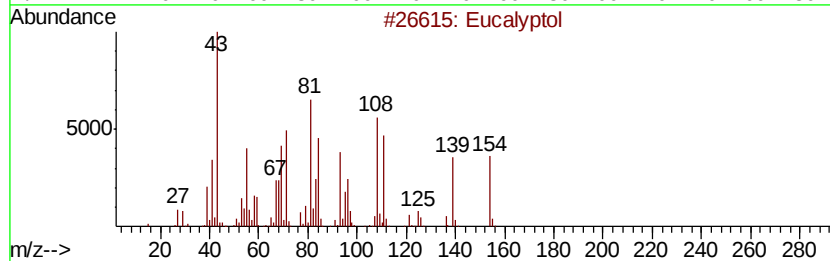
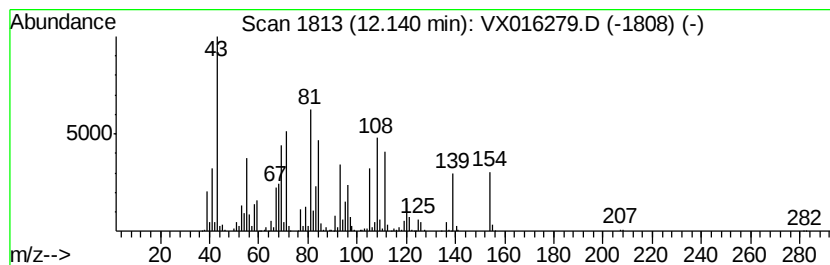
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Peak Number 5 Eucalyptol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.14	10.04 ug/l	311694	1,4-Dichlorobenzene-d4	12.06	
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	47
3	2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	35
4	3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25
5	2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	18



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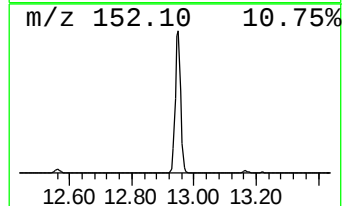
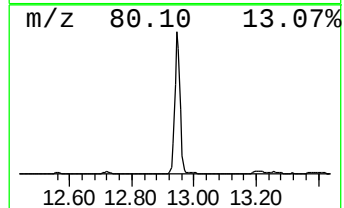
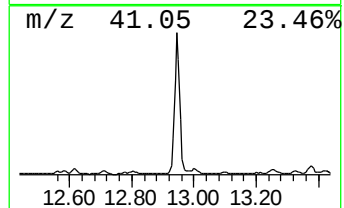
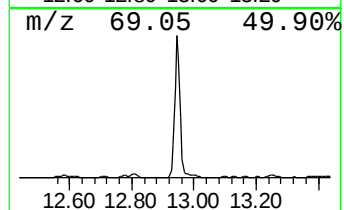
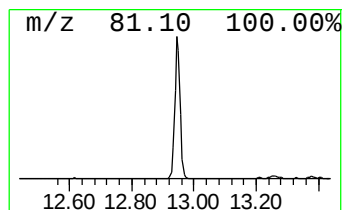
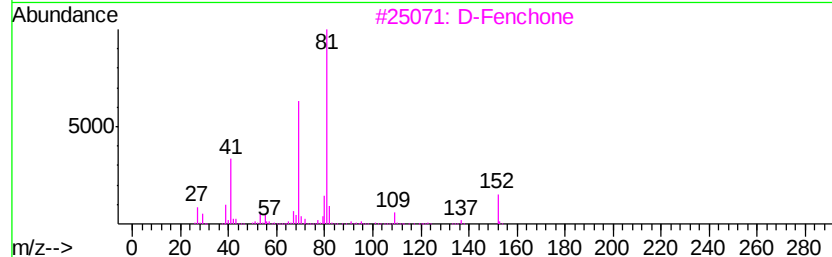
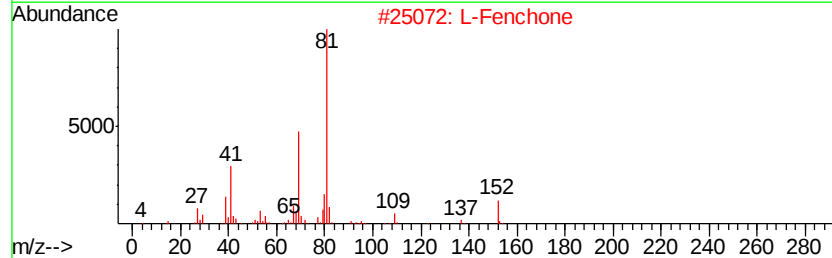
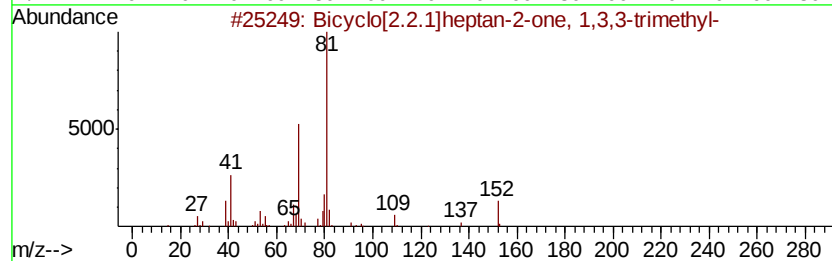
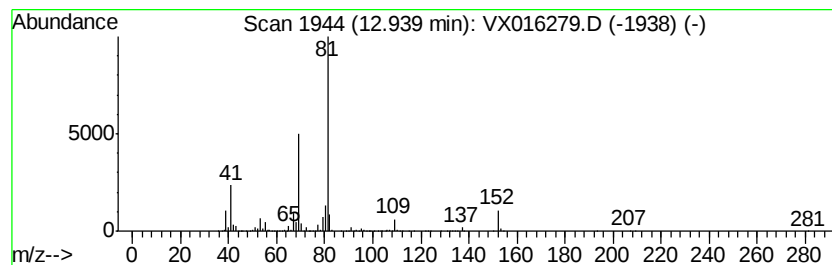
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.94	61.37 ug/l	1905760	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	95
2		L-Fenchone	152	C10H16O	007787-20-4	95
3		D-Fenchone	152	C10H16O	004695-62-9	94
4		2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	42
5		Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX051520\
Data File : VX016279.D
Acq On : 15 May 2020 14:40
Operator : JC/SP
Sample : L2642-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

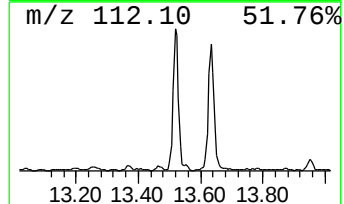
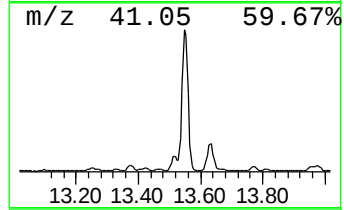
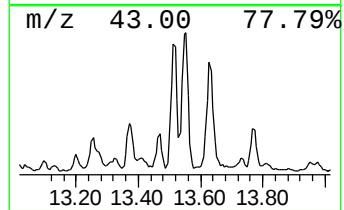
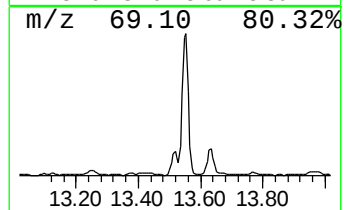
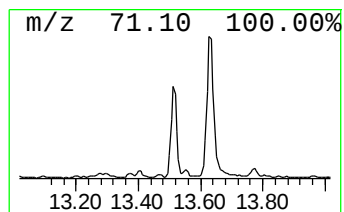
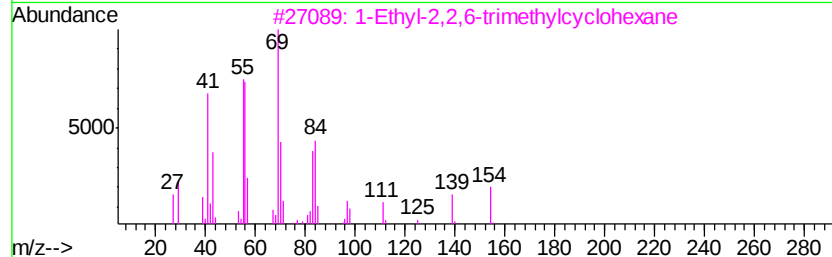
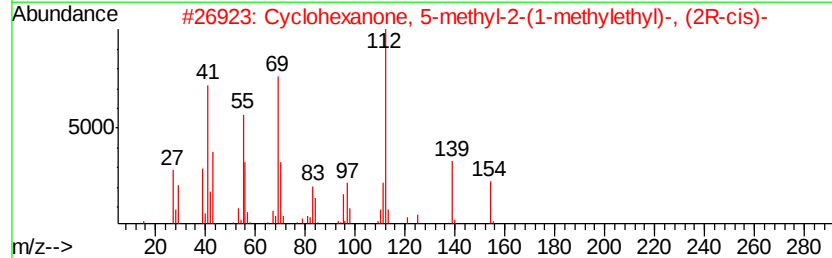
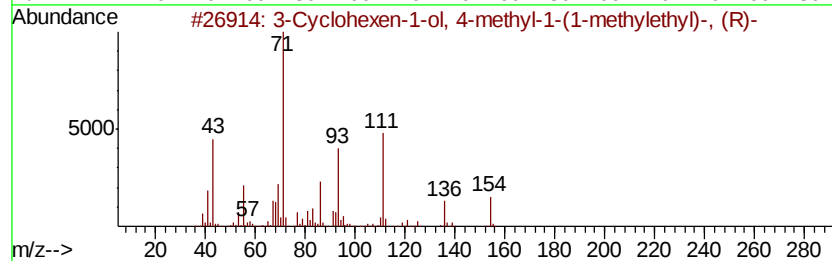
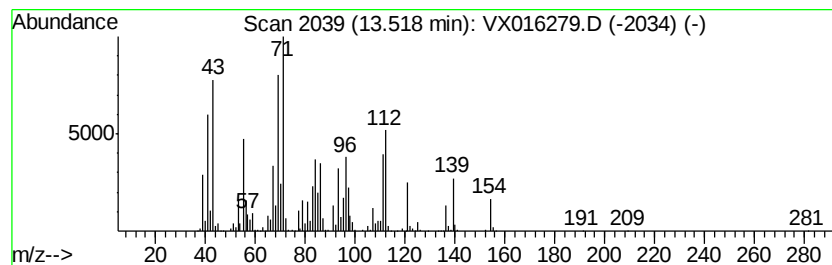
Instrument :
MSVOA_X
ClientSampleId :
400513791-VOA

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

Peak Number 7 unknown13.52 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	13.47 ug/l	418226	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	3-Cyclohexen-1-ol, 4-methyl-1-(1...	154 C10H18O	020126-76-5	38
2	Cyclohexanone, 5-methyl-2-(1-met...	154 C10H18O	001196-31-2	30
3	1-Ethyl-2,2,6-trimethylcyclohexane	154 C11H22	071186-27-1	30
4	1-Menthone	154 C10H18O	014073-97-3	25
5	Thieno[2,3-d]-1,3-thiaselenol-2-...	238 C5H2S3Se	081803-09-0	25



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX051520\
 Data File : VX016279.D
 Acq On : 15 May 2020 14:40
 Operator : JC/SP
 Sample : L2642-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 400513791-VOA

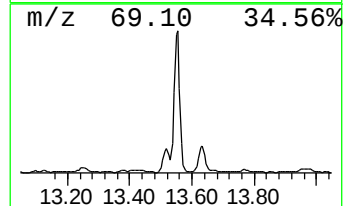
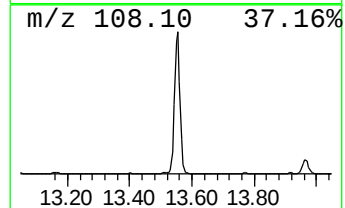
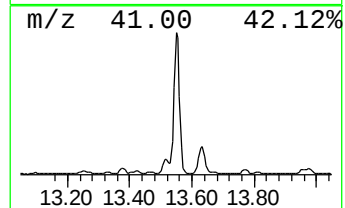
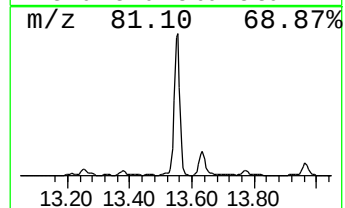
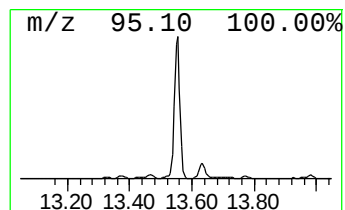
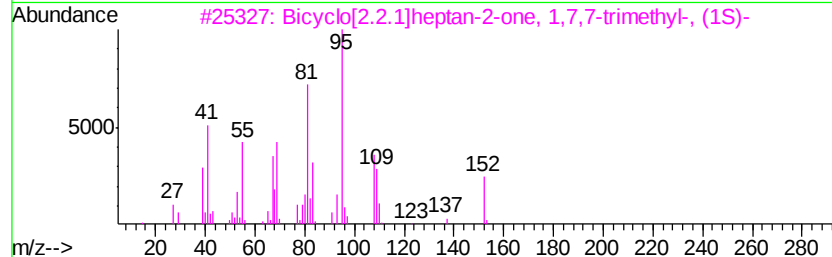
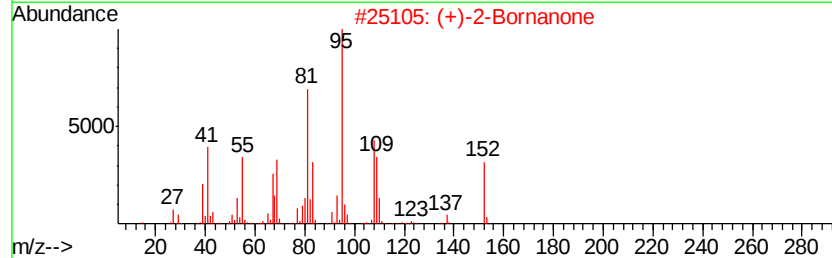
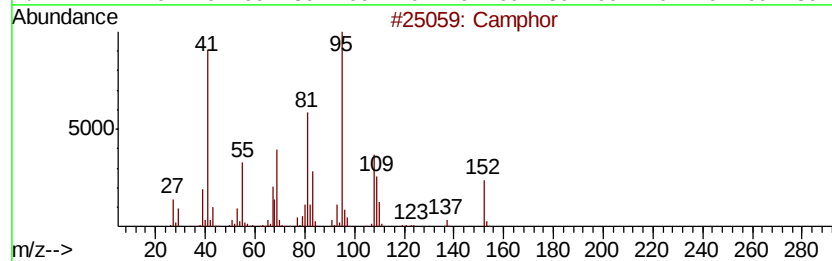
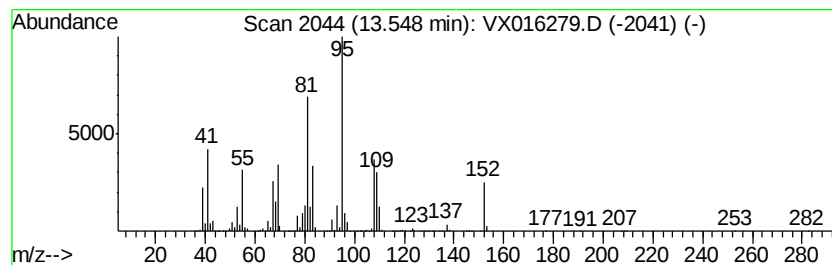
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 Quant Title : SW846 8260

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

 Peak Number 8 Camphor Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	93.52 ug/l	2904420	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Camphor	152	C10H16O	000076-22-2	98
2		(+)-2-Bornanone	152	C10H16O	000464-49-3	98
3		Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-	152	C10H16O	000464-48-2	96
4		2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49
5		1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	41



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX051520\
Data File : VX016279.D
Acq On : 15 May 2020 14:40
Operator : JC/SP
Sample : L2642-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

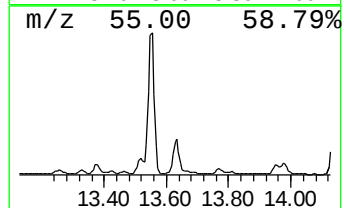
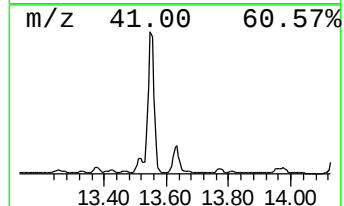
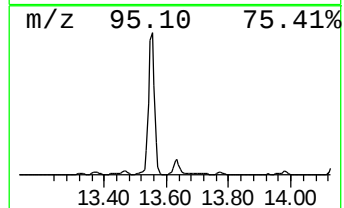
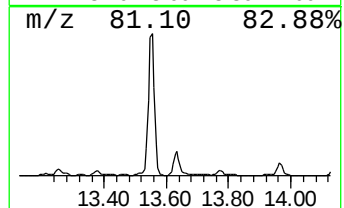
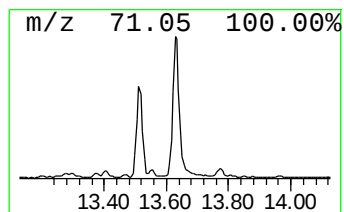
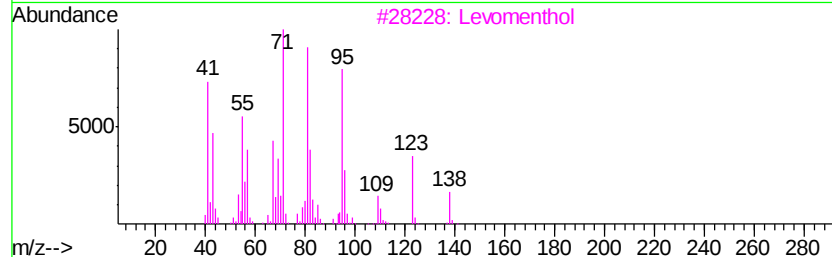
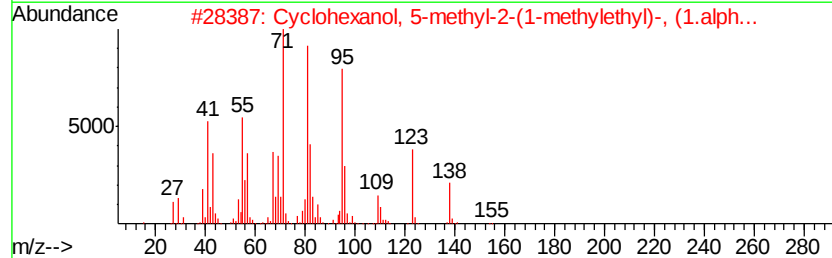
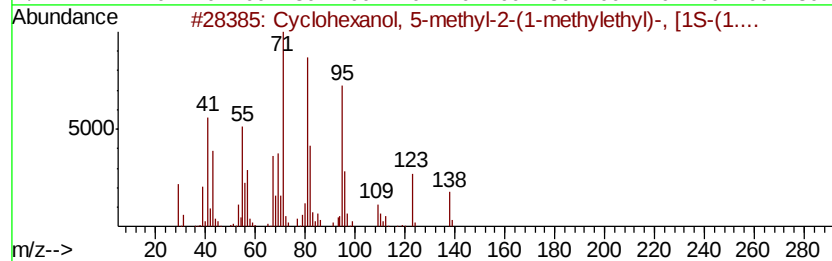
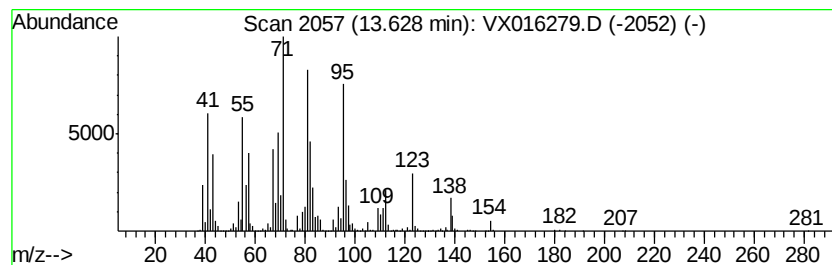
Instrument :
MSVOA_X
ClientSampleId :
400513791-VOA

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

Peak Number 9 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.63	23.03 ug/l	715327	1,4-Dichlorobenzene-d4	12.06		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	91
2		Cvclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	90
3		Levomenthol	156	C10H20O	002216-51-5	90
4		Cvclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	87
5		dl-Menthol	156	C10H20O	000089-78-1	87



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX051520\
Data File : VX016279.D
Acq On : 15 May 2020 14:40
Operator : JC/SP
Sample : L2642-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
400513791-VOA

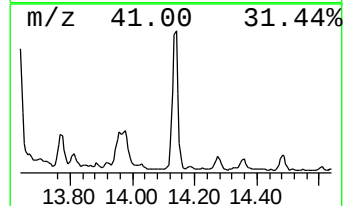
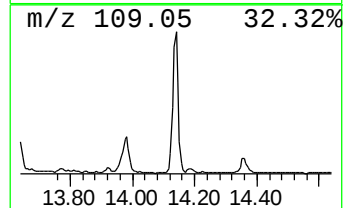
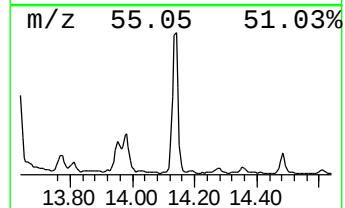
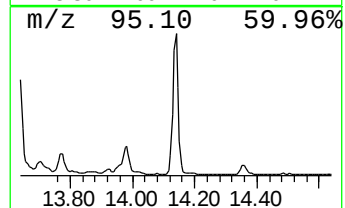
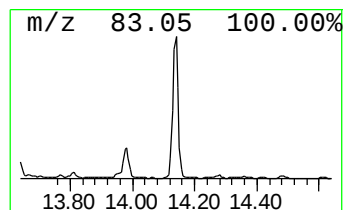
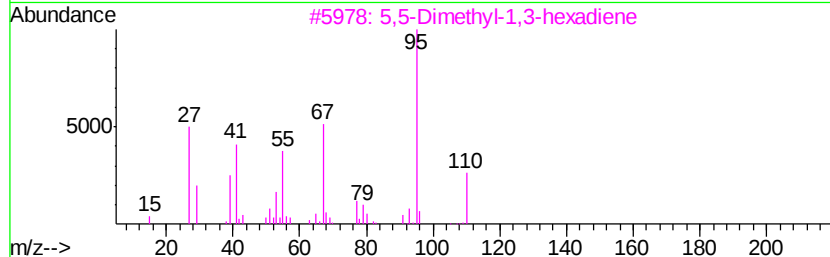
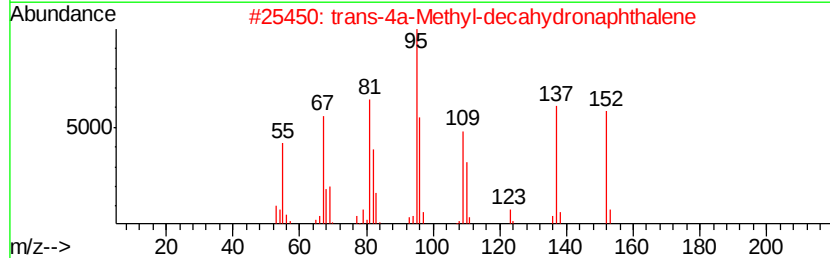
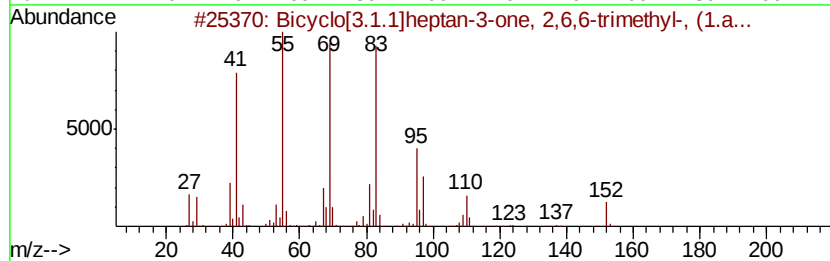
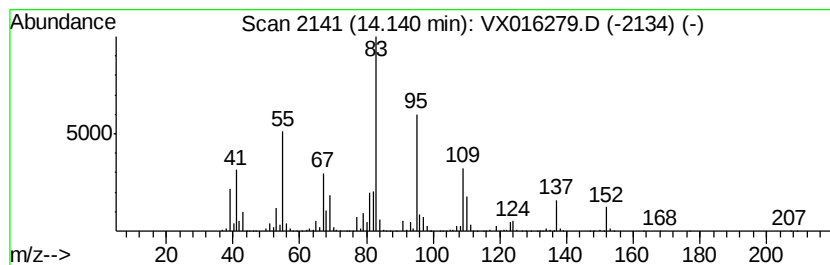
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

Peak Number 10 Bicyclo[3.1.1]heptan-3-one,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	16.06 ug/l	498687	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	64
2		trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	46
3		5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	35
4		2-Cyclohexen-1-one, 4-ethyl-3,4-...	152	C10H16O	017622-46-7	30
5		1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	25



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051520\
Data File : VX016279.D
Acq On : 15 May 2020 14:40
Operator : JC/SP
Sample : L2642-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
400513791-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.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
Dimethyl ether	1.28	13.4	ug/l	188108	1	5.64	700568	50.0
Amylene hydrate	6.31	10.1	ug/l	187770	2	6.83	930668	50.0
3-Pentanone, 2,4-...	9.42	21.0	ug/l	600378	3	10.10	1427010	50.0
Eucalyptol	12.14	10.0	ug/l	311694	4	12.06	1552760	50.0
Bicyclo[2.2.1]hep...	12.94	61.4	ug/l	1905760	4	12.06	1552760	50.0
unknown13.52	13.52	13.5	ug/l	418226	4	12.06	1552760	50.0
Camphor	13.55	93.5	ug/l	2904420	4	12.06	1552760	50.0
Cyclohexanol, 5-m...	13.63	23.0	ug/l	715327	4	12.06	1552760	50.0
Bicyclo[3.1.1]hep...	14.14	16.1	ug/l	498687	4	12.06	1552760	50.0