

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX102220\
 Data File : VX019065.D
 Acq On : 23 Oct 2020 06:33
 Operator : JC/SP
 Sample : L4490-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 56 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 201021073-02-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\82X102120W.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	1.270	28	30	42	rVB	92058	119543	2.34%	0.441%
2	2.416	212	218	230	rBV2	99543	191047	3.74%	0.705%
3	3.008	303	315	331	rBV	1766991	3918647	76.79%	14.452%
4	4.647	561	584	597	rBV	1583360	5103126	100.00%	18.820%
5	5.086	643	656	678	rBV	526765	1591218	31.18%	5.868%
6	5.464	706	718	731	rBV	175213	500600	9.81%	1.846%
7	5.629	733	745	762	rVB	285787	799706	15.67%	2.949%
8	6.031	800	811	819	rBV	177683	469787	9.21%	1.733%
9	6.111	819	824	843	rVV	34234	121805	2.39%	0.449%
10	6.300	847	855	865	rVB2	33559	92163	1.81%	0.340%
11	6.830	932	942	955	rBV	446288	1057967	20.73%	3.902%
12	8.696	1241	1248	1254	rBV	968628	1495341	29.30%	5.515%
13	8.763	1254	1259	1268	rVB2	78123	136623	2.68%	0.504%
14	8.848	1268	1273	1278	rBV	52327	82936	1.63%	0.306%
15	9.421	1358	1367	1373	rBV	169427	259192	5.08%	0.956%
16	10.098	1466	1478	1489	rBV	980073	1457279	28.56%	5.374%
17	10.238	1496	1501	1507	rBV2	143468	223831	4.39%	0.825%
18	10.342	1510	1518	1524	rVB	237649	333639	6.54%	1.230%
19	10.683	1569	1574	1586	rVB	144217	201509	3.95%	0.743%
20	11.122	1640	1646	1651	rBV	822500	1069535	20.96%	3.944%
21	11.415	1688	1694	1701	rBV3	43190	79501	1.56%	0.293%
22	11.543	1711	1715	1721	rVB2	58480	81930	1.61%	0.302%
23	11.652	1728	1733	1741	rVB	39062	62417	1.22%	0.230%
24	11.793	1743	1756	1760	rBV	90710	135705	2.66%	0.500%
25	11.927	1770	1778	1785	rVB2	85344	128532	2.52%	0.474%
26	12.061	1794	1800	1807	rVB	1210783	1617838	31.70%	5.967%
27	12.140	1807	1813	1817	rBV2	98188	171663	3.36%	0.633%
28	12.280	1829	1836	1845	rBV	87232	145118	2.84%	0.535%
29	12.451	1859	1864	1869	rBV2	34486	57684	1.13%	0.213%
30	12.561	1878	1882	1888	rBV4	36085	77535	1.52%	0.286%
31	12.616	1888	1891	1895	rVB	57116	61913	1.21%	0.228%
32	12.798	1914	1921	1926	rVB	120944	170878	3.35%	0.630%
33	12.945	1938	1945	1950	rBV	1017551	1288138	25.24%	4.751%
34	13.000	1950	1954	1959	rVB3	57256	86312	1.69%	0.318%

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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\82X102120W.M
Title : SW846 8260

35	13.250	1991	1995	2001	rVB2	31232	54826	1.07%	0.202%
36	13.329	2001	2008	2011	rBV2	39784	56481	1.11%	0.208%
37	13.371	2011	2015	2019	rBV2	93479	124779	2.45%	0.460%
38	13.463	2026	2030	2034	rVB	49020	63252	1.24%	0.233%
39	13.512	2034	2038	2040	rBV2	151906	205392	4.02%	0.757%
40	13.548	2040	2044	2051	rVB	1358988	1728153	33.86%	6.373%
41	13.628	2051	2057	2066	rBV2	346992	480208	9.41%	1.771%
42	13.768	2076	2080	2084	rBV	76167	100029	1.96%	0.369%
43	13.817	2084	2088	2093	rVB	307781	391411	7.67%	1.444%
44	13.975	2107	2114	2120	rVB4	46830	106458	2.09%	0.393%
45	14.134	2134	2140	2146	rBV	192063	254145	4.98%	0.937%
46	14.676	2225	2229	2233	rBV	62849	79799	1.56%	0.294%
47	14.822	2246	2253	2258	rVB	57172	79617	1.56%	0.294%

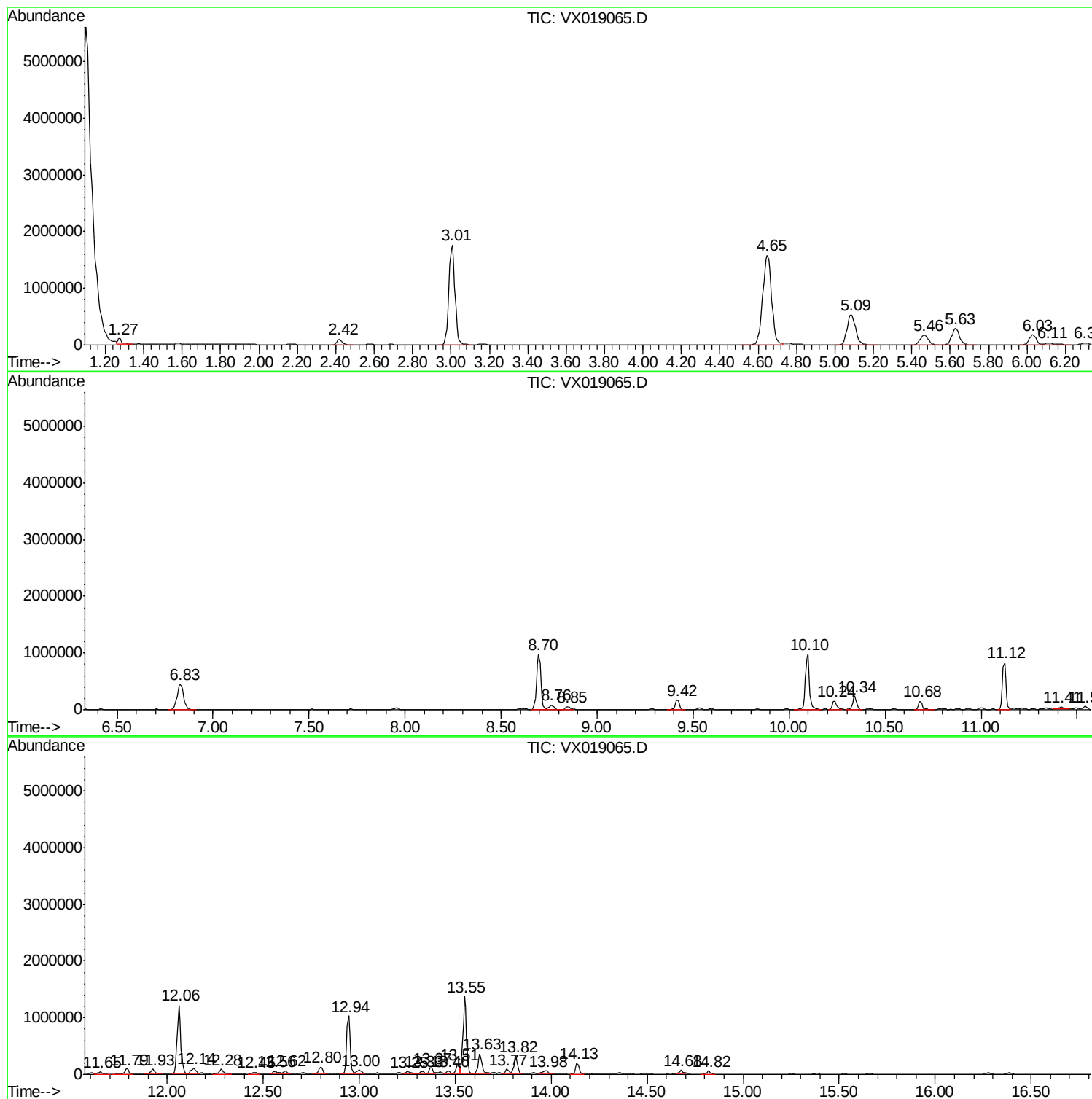
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.M
Quant Title : SW846 8260

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



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Instrument :
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201021073-02-VOA

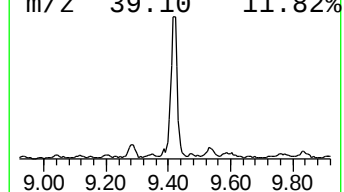
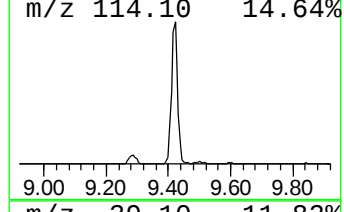
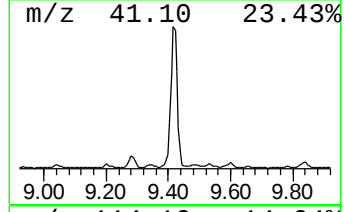
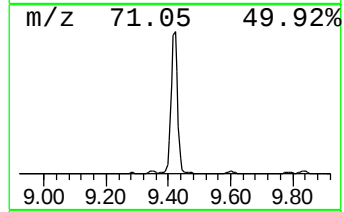
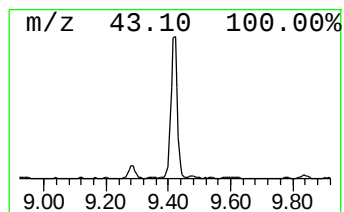
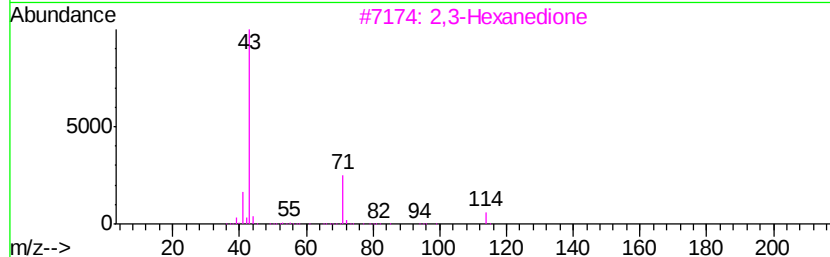
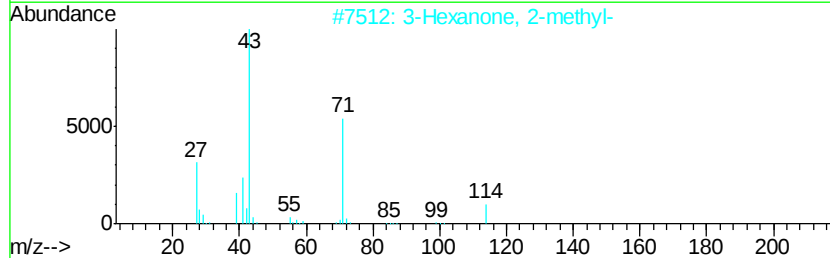
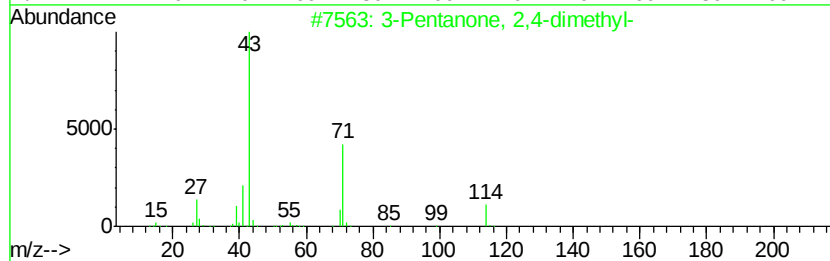
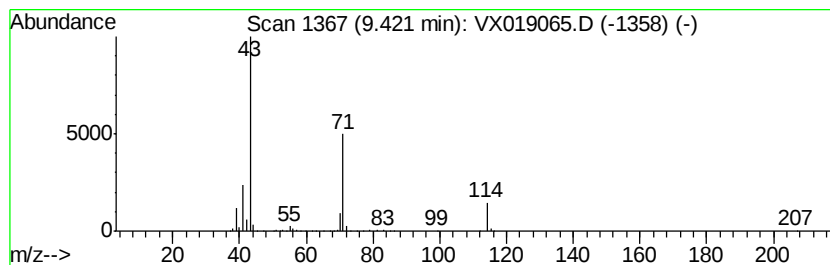
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	8.89 ug/l	259192	Chlorobenzene-d5	10.10

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	80
3			2,3-Hexanedione	114	C6H10O2	003848-24-6	64
4			4-Heptanone	114	C7H14O	000123-19-3	59
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	42



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ALS Vial : 56 Sample Multiplier: 1

Instrument :
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ClientSampleId :
201021073-02-VOA

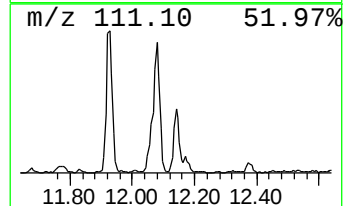
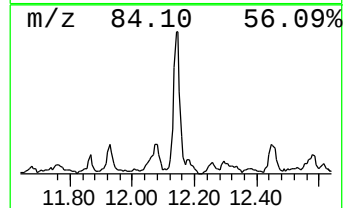
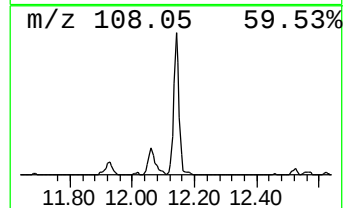
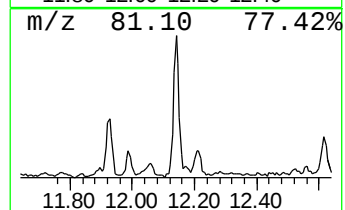
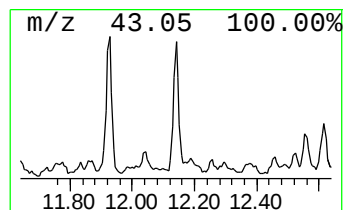
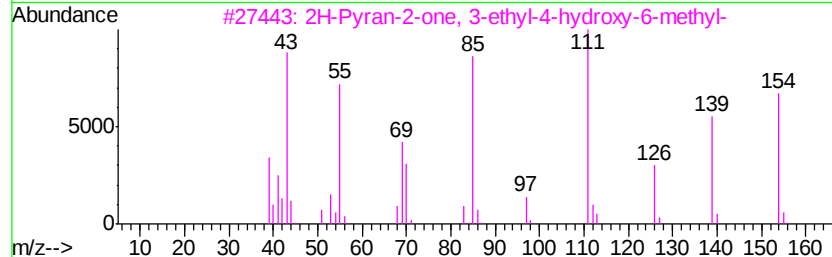
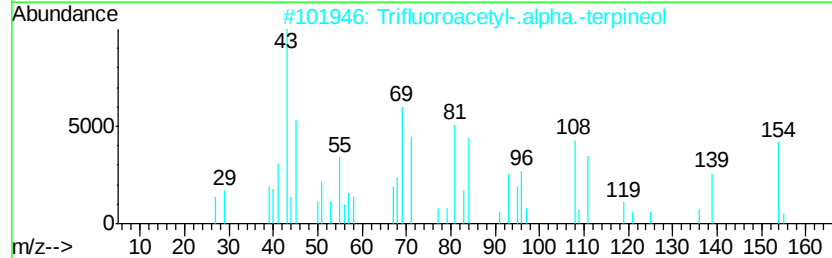
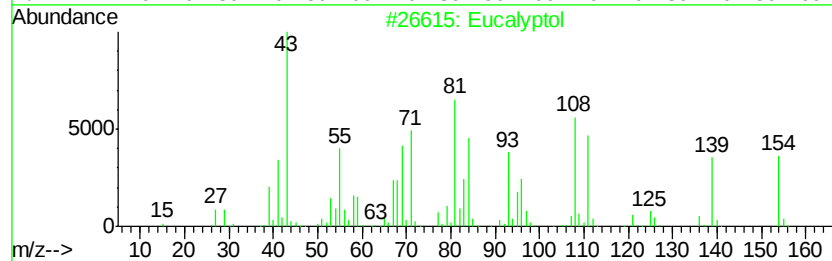
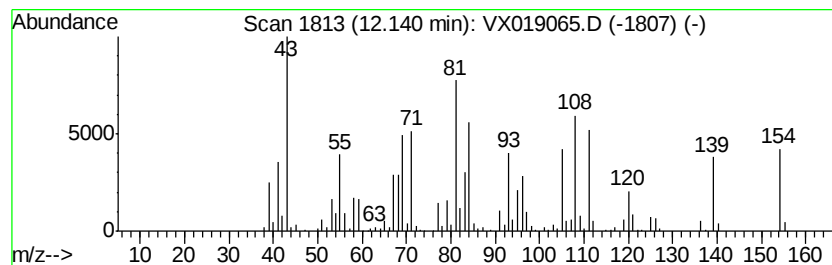
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.M
Quant Title : SW846 8260

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

Peak Number 3 Eucalyptol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	5.31 ug/l	171663	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	49
3	2H-Pyran-2-one, 3-ethyl-4-hydrox...		154	C8H10O3	050607-35-7	35
4	3-Hepten-2-one, 3-propyl-		154	C10H18O	032064-69-0	25
5	Terpinen-4-ol		154	C10H18O	000562-74-3	22



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ALS Vial : 56 Sample Multiplier: 1

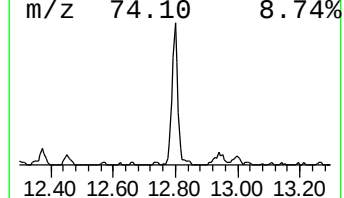
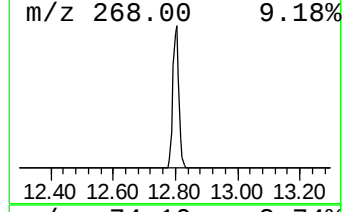
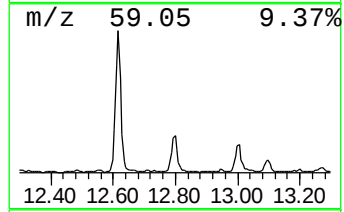
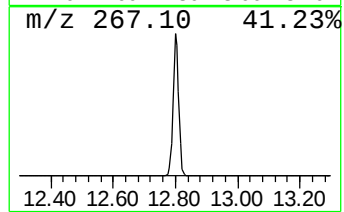
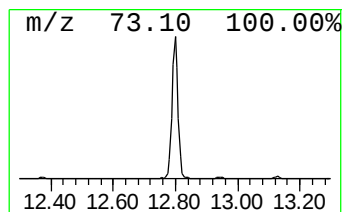
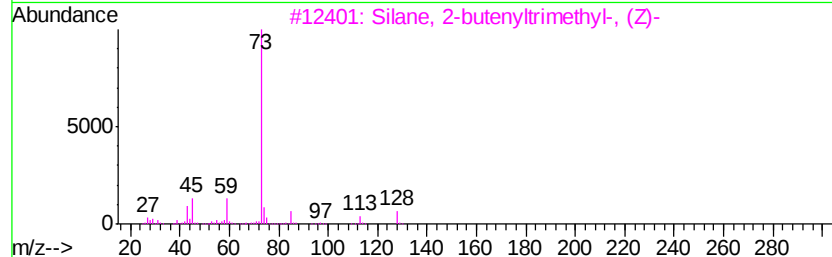
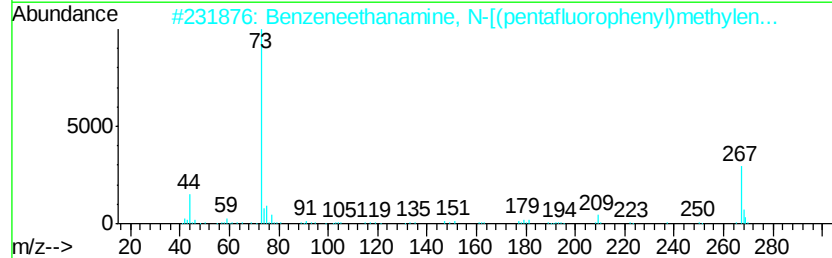
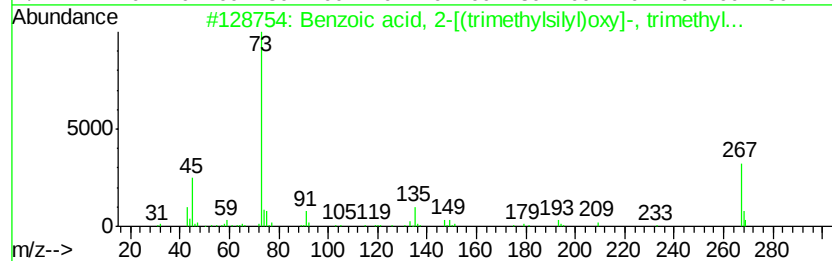
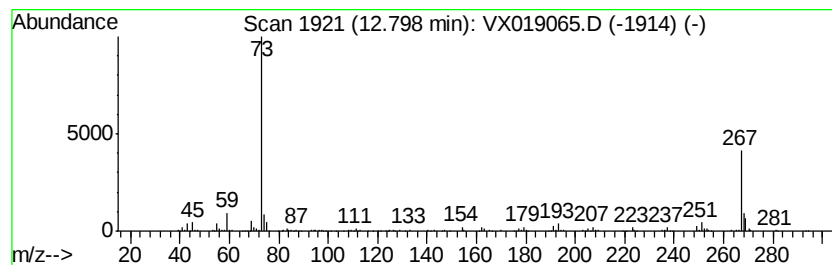
Instrument :
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ClientSampleId :
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Quant Title : SW846 8260

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

Peak Number 4 unknown12.80 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	5.28 ug/l	170878	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethyl...	282	C13H22O3Si2	003789-85-3 45
2	Benzenethanamine, N-[(pentafluorophenyl)methyl]-, (Z)-	475	C21H26F5N2Si2	055429-85-1 42
3	Silane, 2-butenyltrimethyl-, (Z)-	128	C7H16Si	017486-13-4 14
4	Tetrasiloxane, 1,1,3,3,5,5,7,7-octa-	282	C8H26O3Si4	001000-05-1 12
5	1-(3-Chlorophenyl)piperazine, 4-(3-chlorophenyl)-	268	C13H21ClN2Si	1000373-99-3 12



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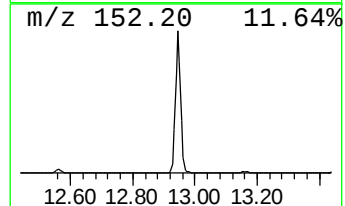
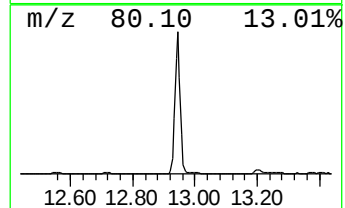
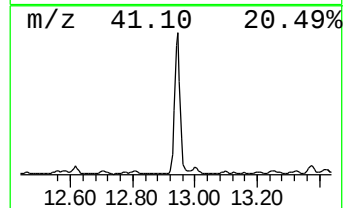
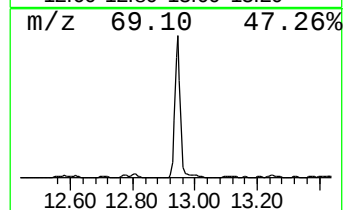
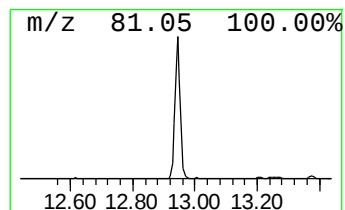
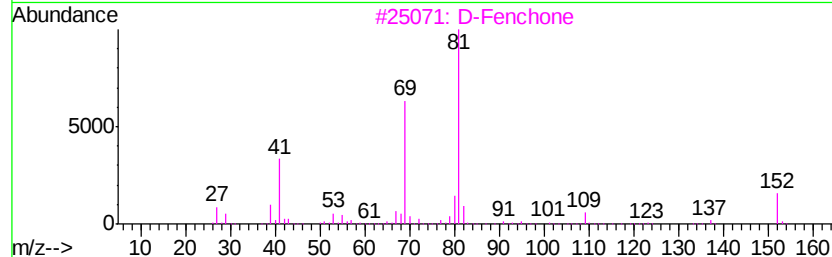
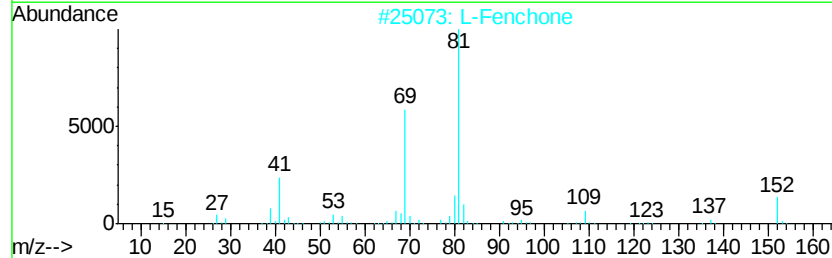
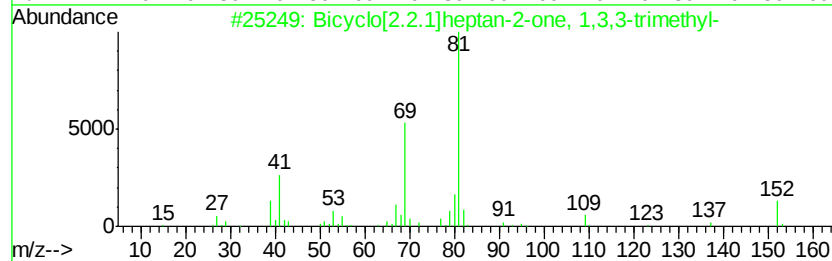
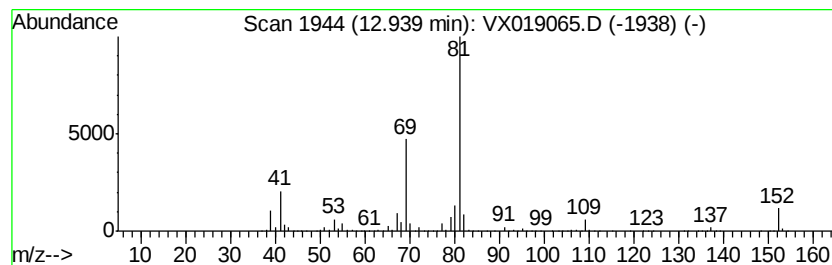
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.94	39.81 ug/l	1288140	1,4-Dichlorobenzene-d4	12.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicvclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	95
2	L-Fenchone	152	C10H16O	007787-20-4	94
3	D-Fenchone	152	C10H16O	004695-62-9	94
4	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45
5	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	42



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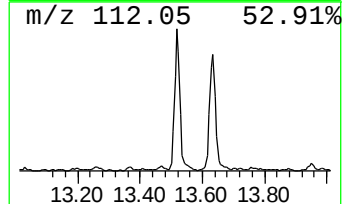
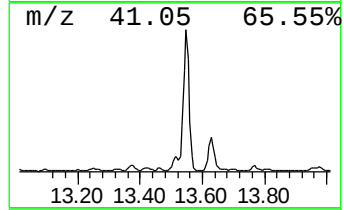
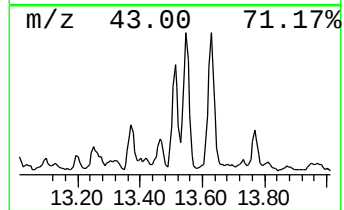
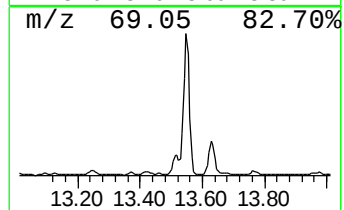
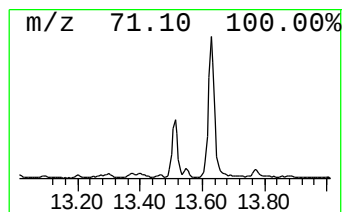
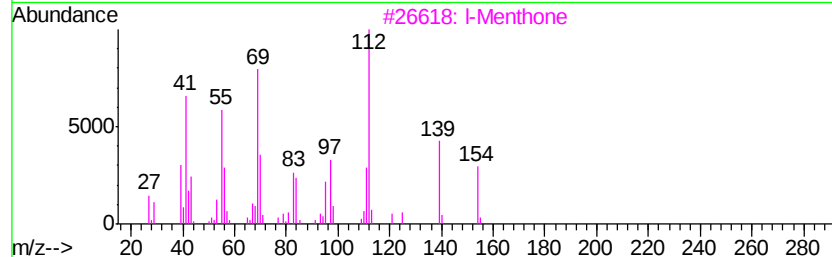
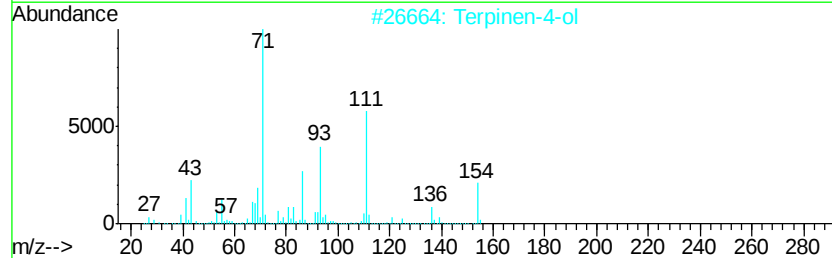
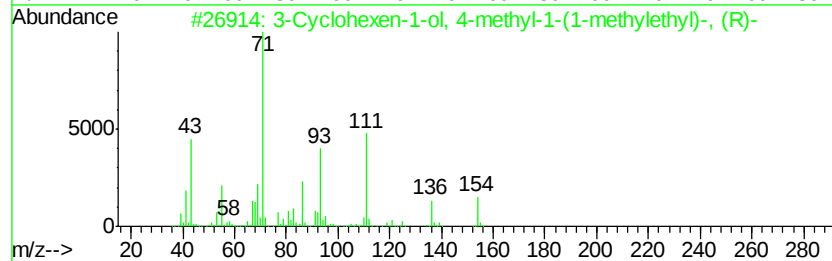
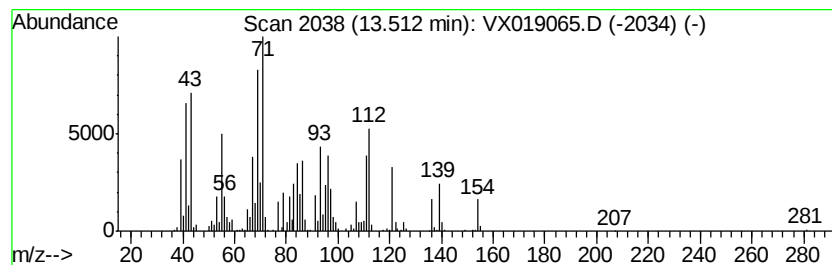
Instrument :
MSVOA_X
ClientSampleId :
201021073-02-VOA

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.M
Quant Title : SW846 8260

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

Peak Number 6 unknown13.51 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.51	6.35 ug/l	205392	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	30
2	Terpinen-4-ol	154	C10H18O	000562-74-3	30
3	l-Menthone	154	C10H18O	014073-97-3	25
4	Eucalyptol	154	C10H18O	000470-82-6	25
5	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	010458-14-7	25



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX102220\
Data File : VX019065.D
Acq On : 23 Oct 2020 06:33
Operator : JC/SP
Sample : L4490-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 56 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
201021073-02-VOA

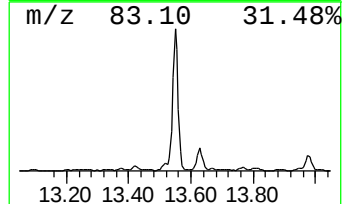
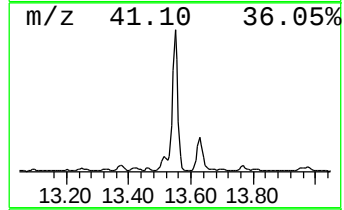
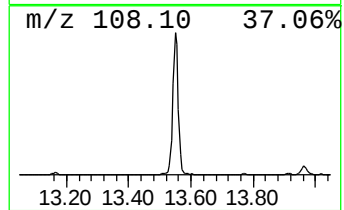
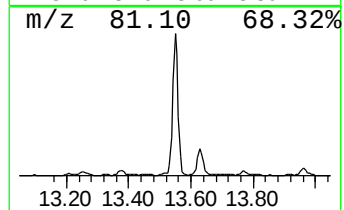
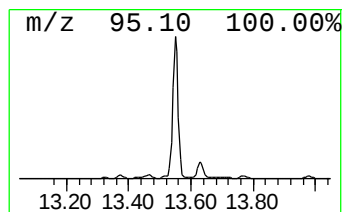
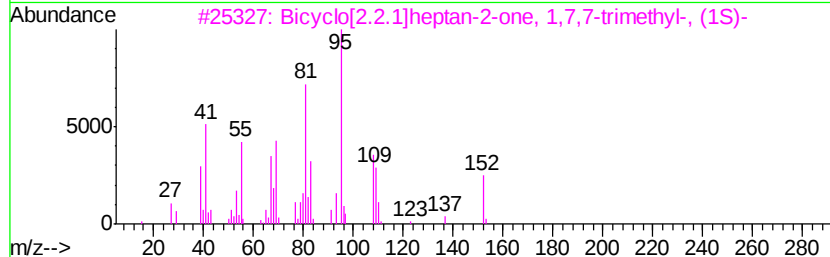
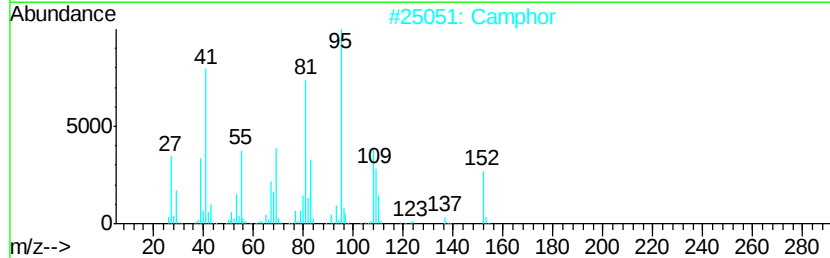
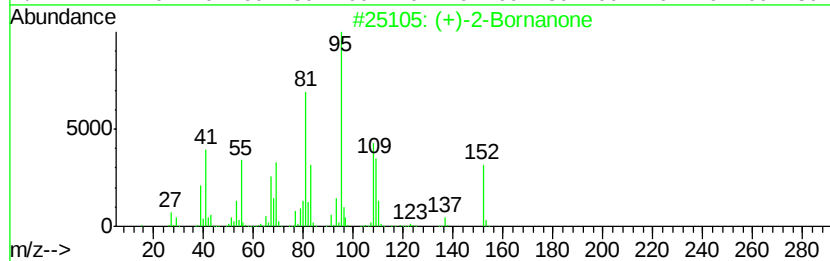
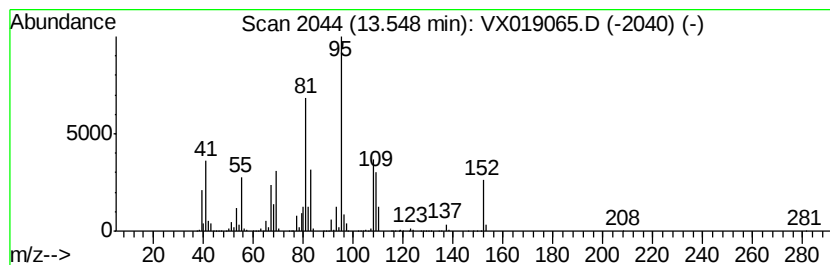
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	53.41 ug/l	1728150	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(+)-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	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\VX102220\
Data File : VX019065.D
Acq On : 23 Oct 2020 06:33
Operator : JC/SP
Sample : L4490-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 56 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
201021073-02-VOA

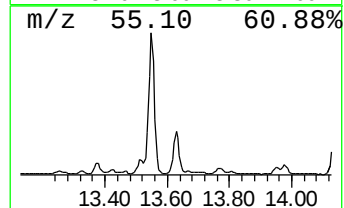
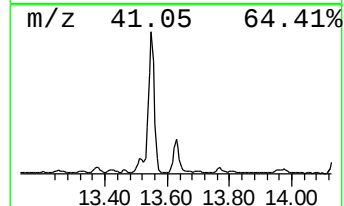
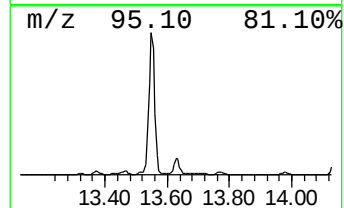
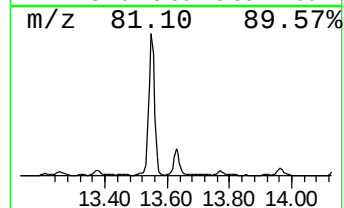
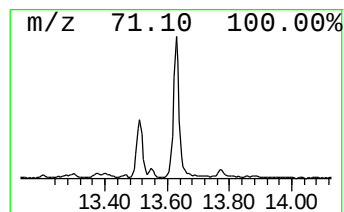
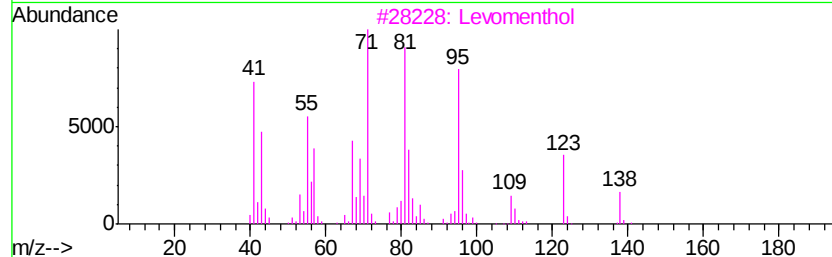
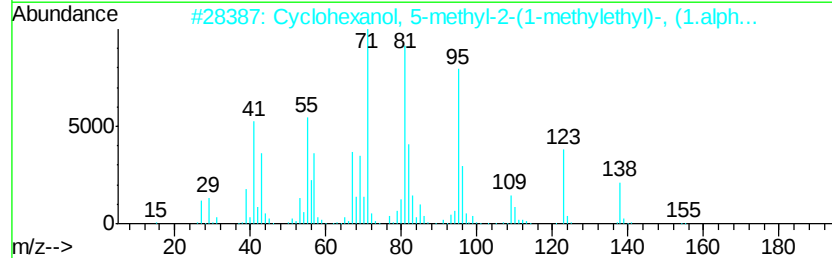
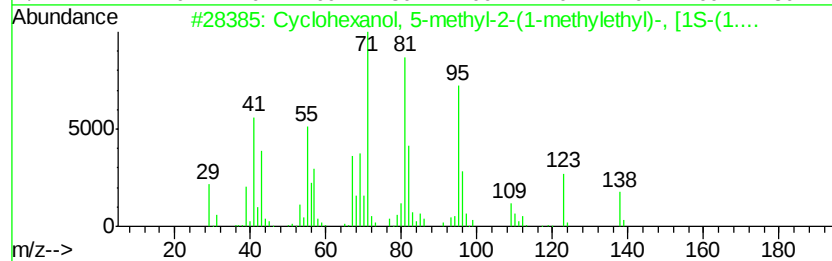
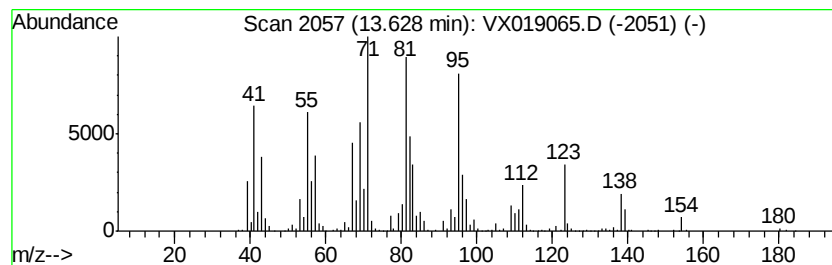
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.M
Quant Title : SW846 8260

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

Peak Number 8 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	14.84 ug/l	480208	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	91
2		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	90
3		Levomenthol	156	C10H20O	002216-51-5	90
4		dl-Menthol	156	C10H20O	000089-78-1	87
5		d-Menthol	156	C10H20O	015356-60-2	80



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX102220\
Data File : VX019065.D
Acq On : 23 Oct 2020 06:33
Operator : JC/SP
Sample : L4490-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 56 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
201021073-02-VOA

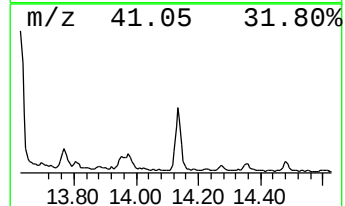
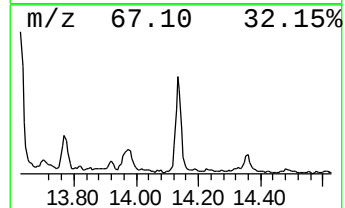
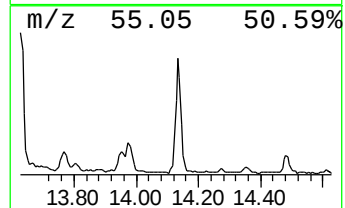
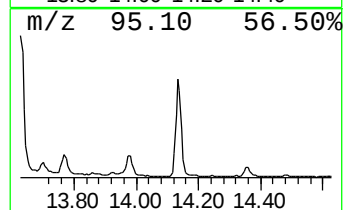
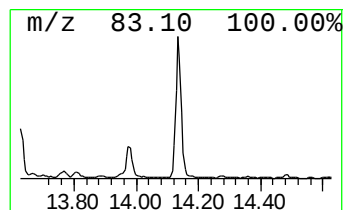
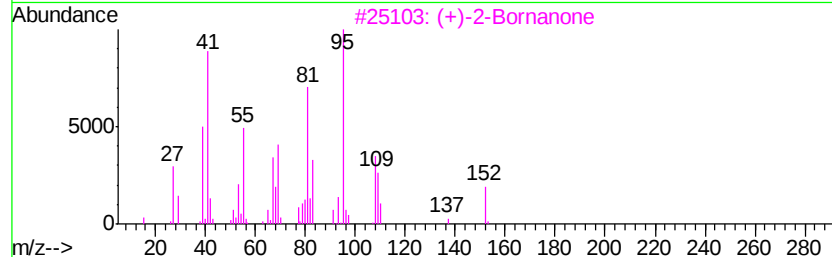
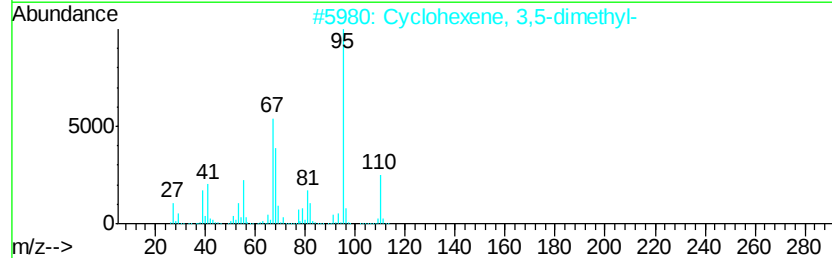
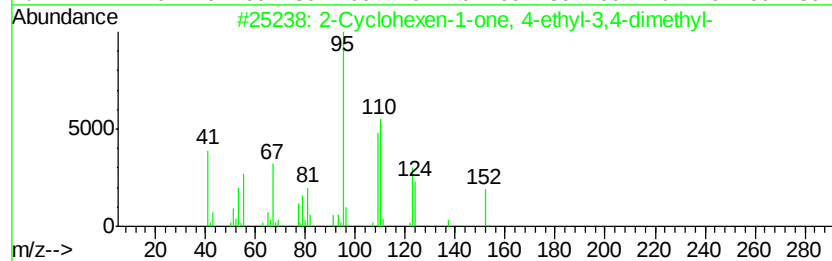
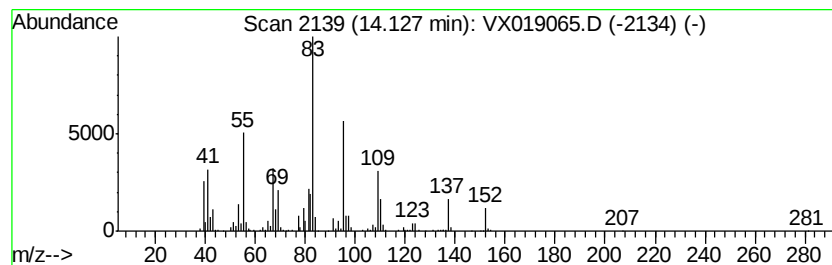
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.M
Quant Title : SW846 8260

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

Peak Number 9 unknown14.13 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	7.85 ug/l	254145	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Cyclohexen-1-one, 4-ethyl-3,4-...	152	C10H16O	017622-46-7	30
2		Cyclohexene, 3,5-dimethyl-	110	C8H14	000823-17-6	25
3		(+)-2-Bornanone	152	C10H16O	000464-49-3	25
4		Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	25
5		Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	1000150-99-3	25



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX102220\
Data File : VX019065.D
Acq On : 23 Oct 2020 06:33
Operator : JC/SP
Sample : L4490-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 56 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
201021073-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.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
3-Pentanone, 2,4-...	9.42	8.9	ug/l	259192	3	10.10	1457280	50.0
Eucalyptol	12.14	5.3	ug/l	171663	4	12.06	1617840	50.0
unknown12.80	12.80	5.3	ug/l	170878	4	12.06	1617840	50.0
Bicyclo[2.2.1]hep...	12.94	39.8	ug/l	1288140	4	12.06	1617840	50.0
unknown13.51	13.51	6.3	ug/l	205392	4	12.06	1617840	50.0
(+)-2-Bornanone	13.55	53.4	ug/l	1728150	4	12.06	1617840	50.0
Cyclohexanol, 5-m...	13.63	14.8	ug/l	480208	4	12.06	1617840	50.0
unknown14.13	14.13	7.8	ug/l	254145	4	12.06	1617840	50.0