

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN030620\
 Data File : VN060380.D
 Acq On : 6 Mar 2020 15:06
 Operator : JC/MD
 Sample : L1802-01
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 400304782.2-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_N\METHODS\82N022720W.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	1.976	55	63	74	rVB	185726	256792	6.22%	1.375%
2	3.793	603	628	645	rBV2	35399	91793	2.22%	0.491%
3	4.725	889	918	964	rBV	931413	3255312	78.85%	17.426%
4	6.777	1528	1556	1581	rBV	1347185	4128662	100.00%	22.102%
5	7.178	1659	1681	1723	rBV	625107	1733106	41.98%	9.278%
6	7.564	1783	1801	1813	rBV	126996	315164	7.63%	1.687%
7	7.641	1813	1825	1845	rVB	249326	587035	14.22%	3.143%
8	8.005	1920	1938	1958	rBV2	167392	425876	10.32%	2.280%
9	8.101	1959	1968	1984	rVB2	29144	65542	1.59%	0.351%
10	8.567	2095	2113	2130	rBV	374813	785989	19.04%	4.208%
11	9.368	2350	2362	2369	rBV	26978	51822	1.26%	0.277%
12	9.947	2529	2542	2557	rBV4	18282	52978	1.28%	0.284%
13	10.075	2569	2582	2596	rBV	600273	1117614	27.07%	5.983%
14	10.178	2607	2614	2627	rVB	53232	96506	2.34%	0.517%
15	10.709	2763	2779	2798	rVV	170549	307280	7.44%	1.645%
16	10.834	2808	2818	2838	rVB	15642	48286	1.17%	0.258%
17	11.400	2981	2994	3007	rBV	557564	972219	23.55%	5.205%
18	11.609	3046	3059	3070	rBV	82724	159405	3.86%	0.853%
19	11.940	3151	3162	3176	rVB	90622	156768	3.80%	0.839%
20	12.397	3292	3304	3323	rVB	460281	786966	19.06%	4.213%
21	13.034	3491	3502	3514	rBV2	35565	61733	1.50%	0.330%
22	13.159	3529	3541	3552	rBV4	80340	146845	3.56%	0.786%
23	13.339	3584	3597	3610	rBV	575590	1016900	24.63%	5.444%
24	13.403	3611	3617	3627	rVB	56048	88951	2.15%	0.476%
25	13.812	3734	3744	3755	rBV2	74423	138075	3.34%	0.739%
26	13.876	3756	3764	3776	rVB2	84635	140161	3.39%	0.750%
27	14.217	3857	3870	3886	rBV	633515	1097285	26.58%	5.874%
28	14.570	3973	3980	3995	rVB9	22369	46335	1.12%	0.248%
29	14.702	4015	4021	4034	rVB3	23048	42787	1.04%	0.229%
30	14.802	4040	4052	4065	rBV6	59493	147249	3.57%	0.788%
31	14.889	4069	4079	4094	rVV3	201790	358882	8.69%	1.921%

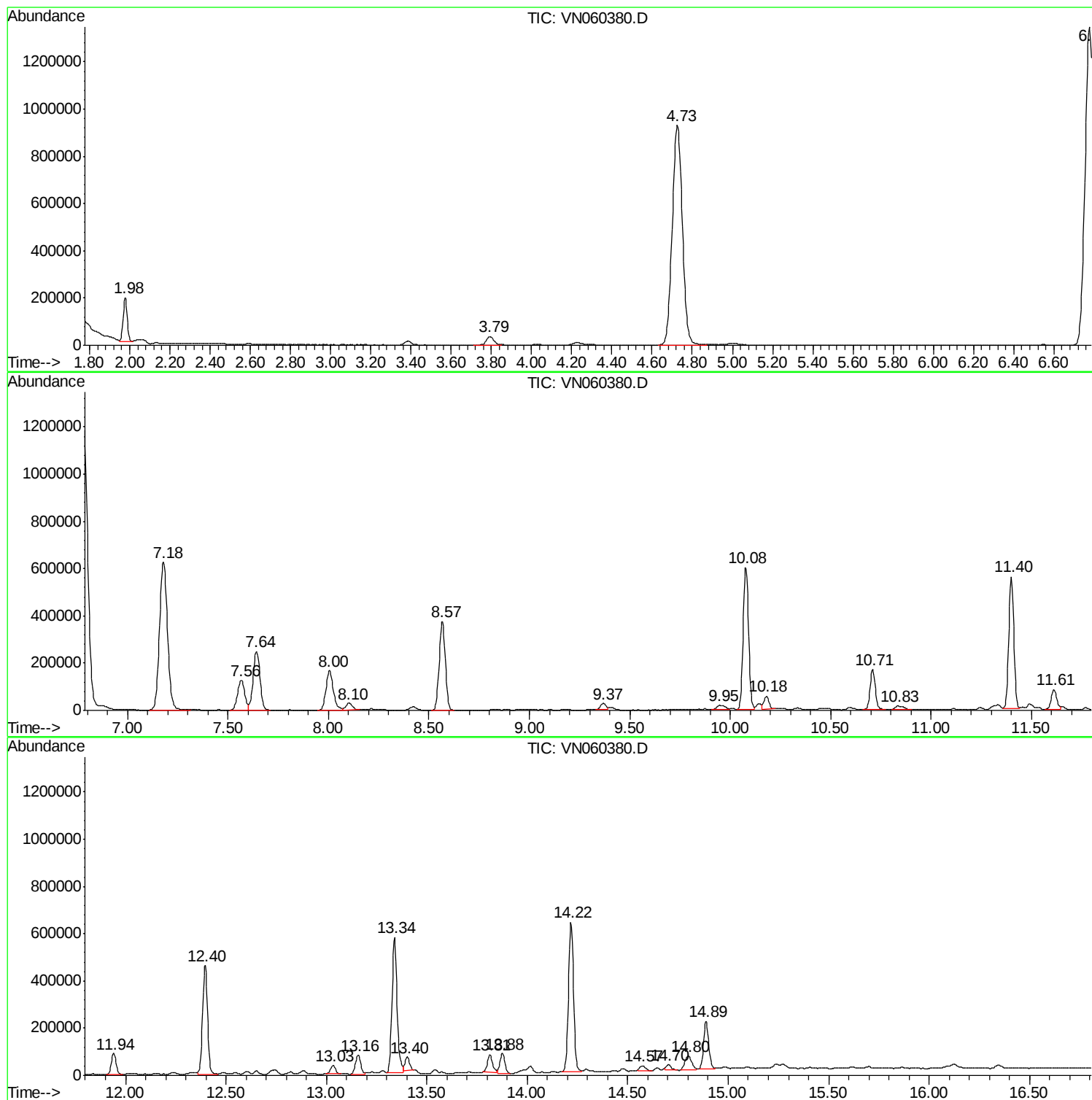
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ALS Vial : 12 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

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



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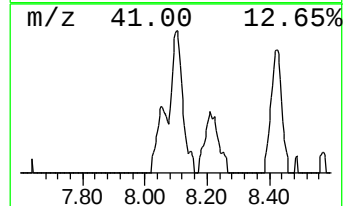
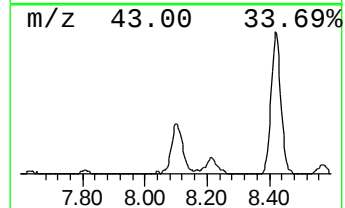
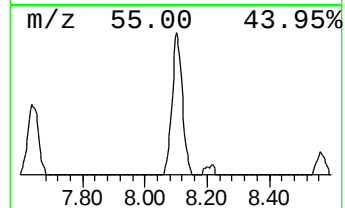
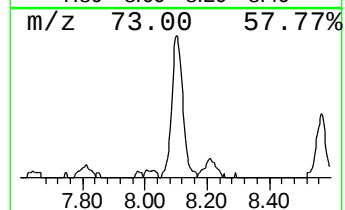
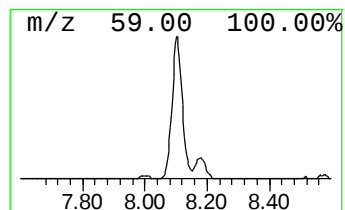
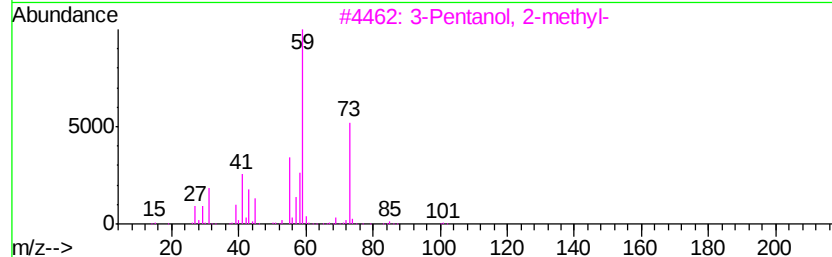
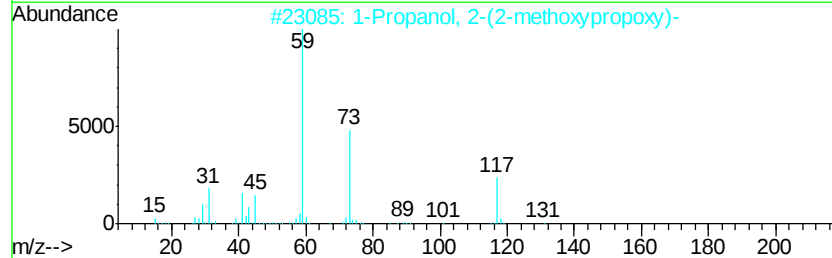
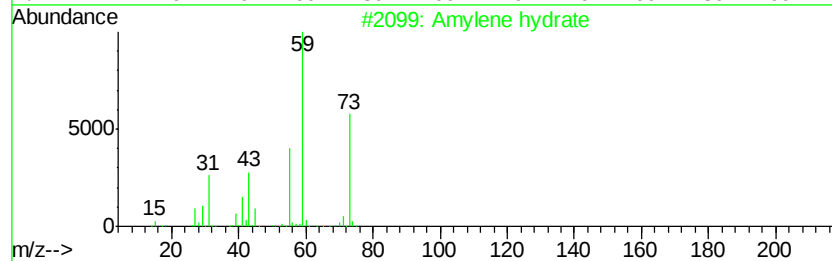
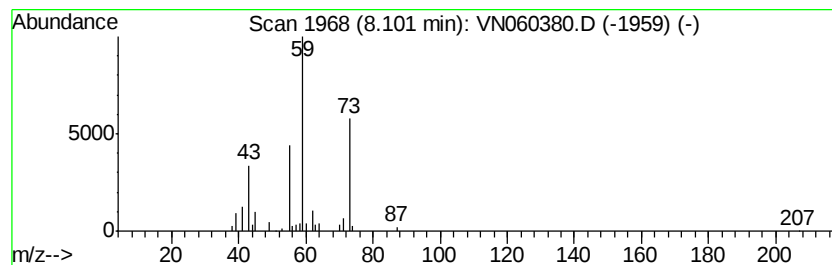
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Quant Title : SW846 8260

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

Peak Number 3 Amylene hydrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.10	5.58 ug/l	65542	Pentafluorobenzene	7.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Amylene hydrate	88	C5H12O	000075-85-4	53
2		1-Propanol, 2-(2-methoxypropoxy)-	148	C7H16O3	013588-28-8	38
3		3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	38
4		Butanamide	87	C4H9NO	000541-35-5	37
5		3-Hexanol	102	C6H14O	000623-37-0	28



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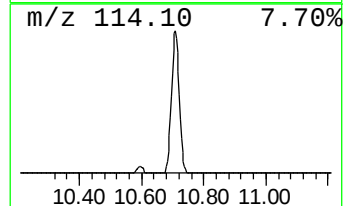
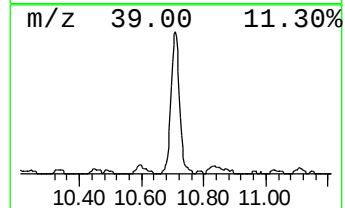
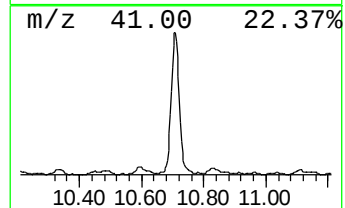
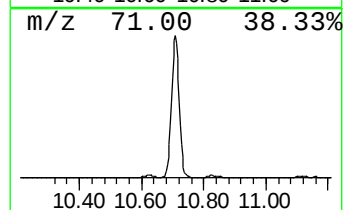
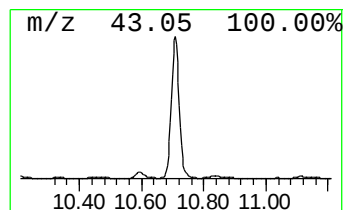
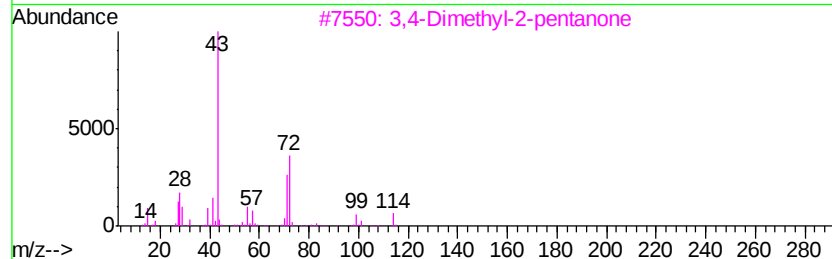
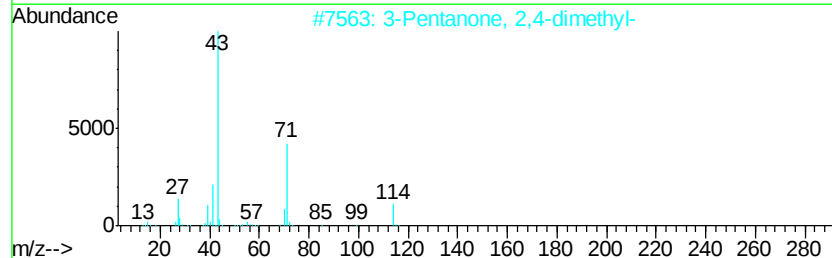
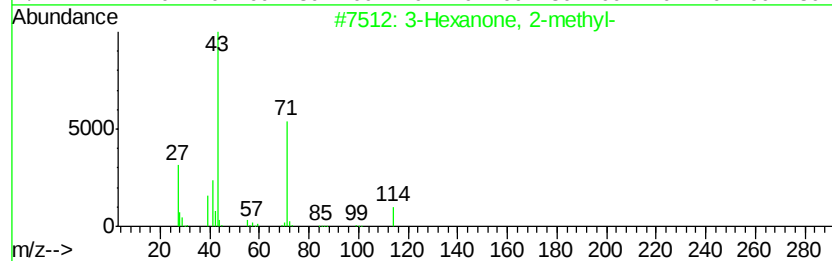
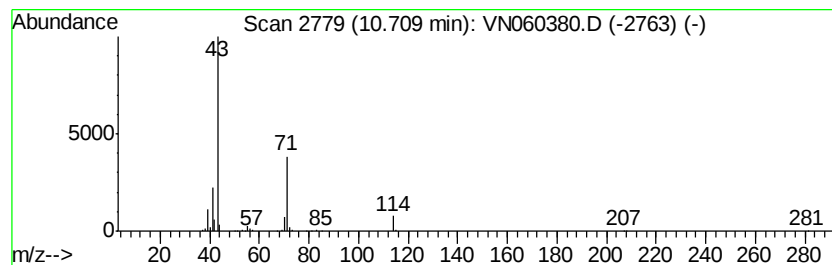
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Hexanone, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.71	15.80 ug/l	307280	Chlorobenzene-d5	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	86
2		3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	64
3		3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	50
4		Pyrrolidine	71	C4H9N	000123-75-1	45
5		4-Heptanone	114	C7H14O	000123-19-3	45



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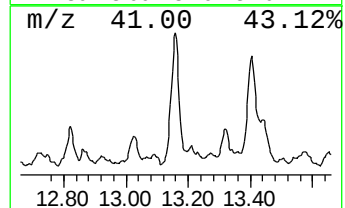
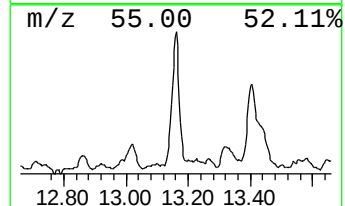
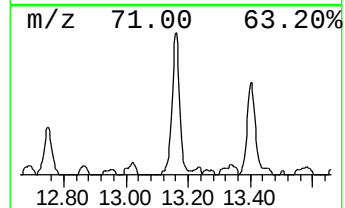
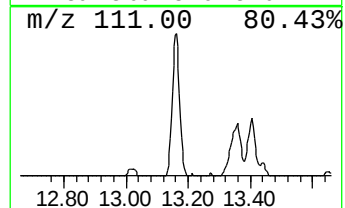
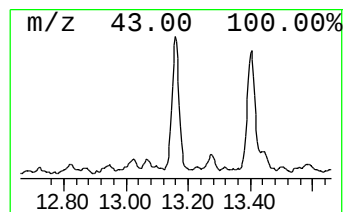
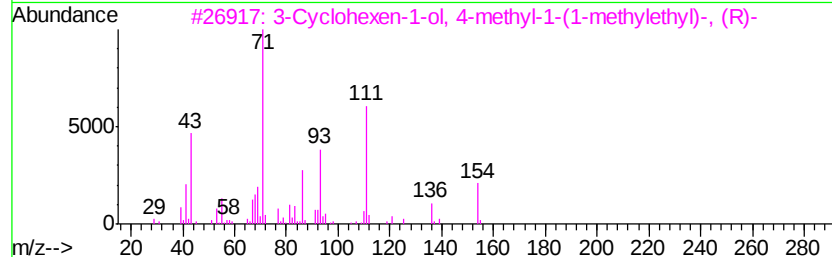
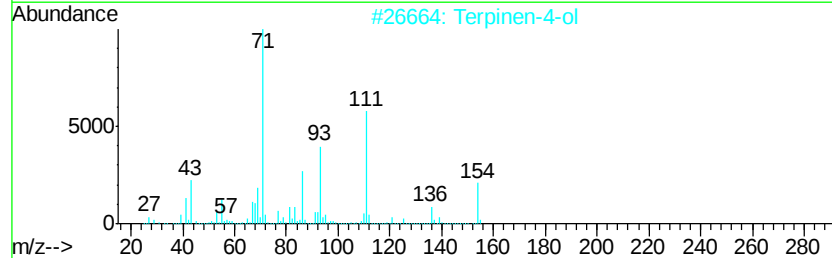
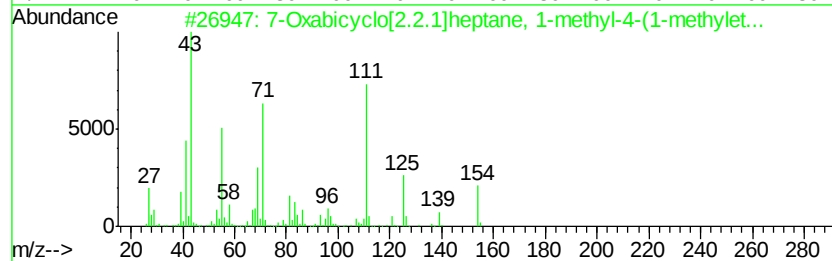
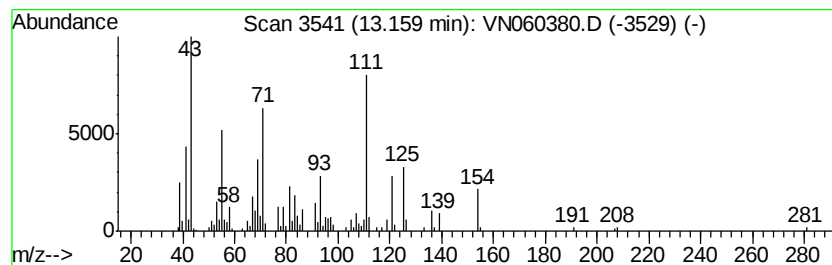
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.16	7.22 ug/l	146845	1,4-Dichlorobenzene-d4	13.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	90
2		Terpinen-4-ol	154	C10H18O	000562-74-3	60
3		3-Cyclohexen-1-ol, 4-methyl-1-(1...	154	C10H18O	020126-76-5	59
4		4a(2H)-Naphthalenol, octahydro-,...	154	C10H18O	001654-87-1	38
5		p-Menth-8-en-1-ol, stereoisomer	154	C10H18O	007299-40-3	38



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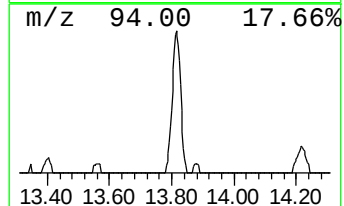
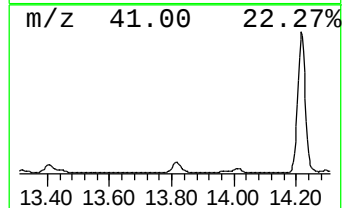
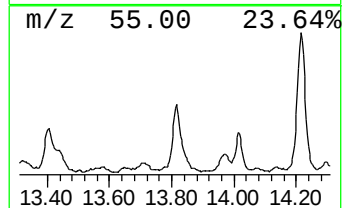
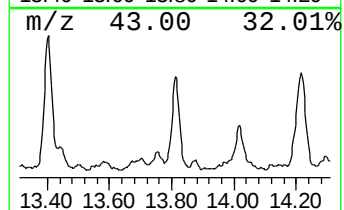
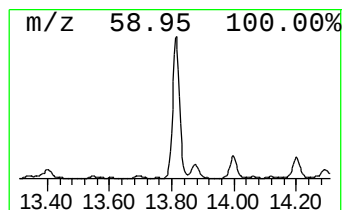
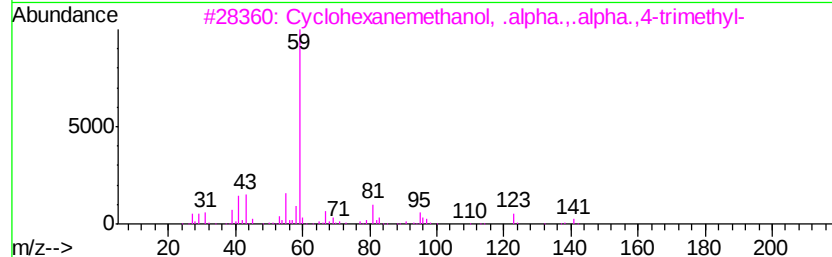
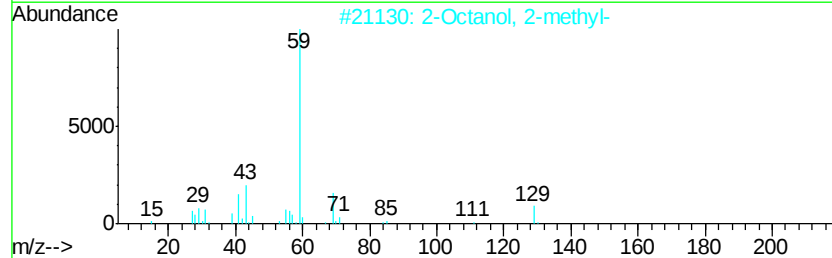
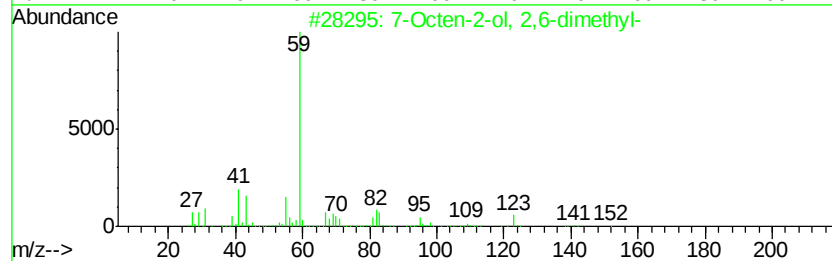
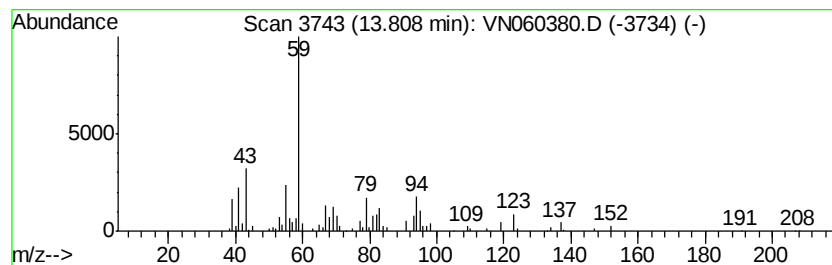
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	6.79 ug/l	138075	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	64
2		2-Octanol, 2-methyl-	144	C9H20O	000628-44-4	47
3		Cyclohexanemethanol, .alpha.,.alpha...	156	C10H20O	000498-81-7	47
4		2-(3,4-Dibromo-4-methylcyclohexy...	312	C10H18Br2O	110202-13-6	42
5		1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	42



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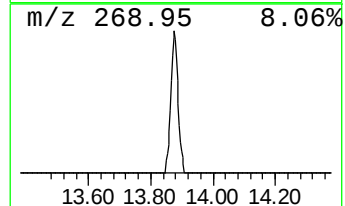
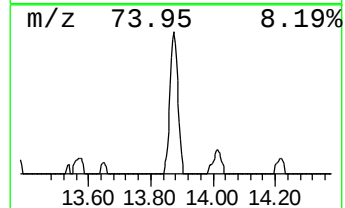
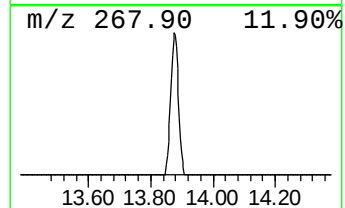
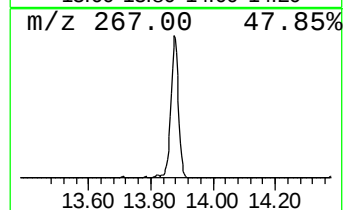
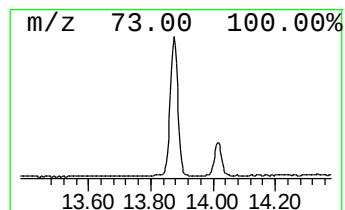
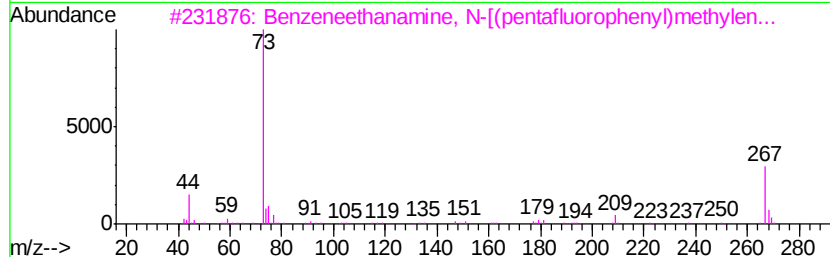
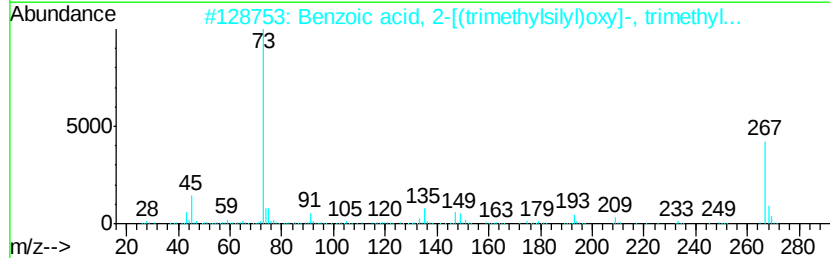
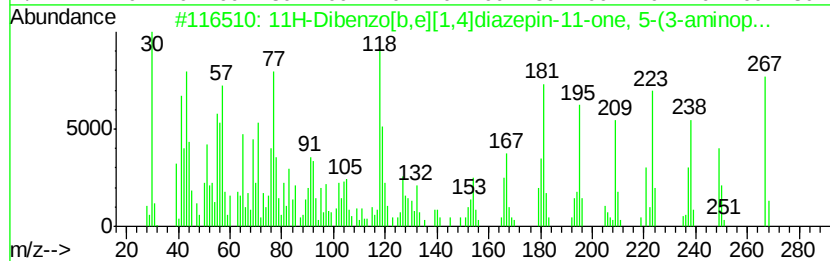
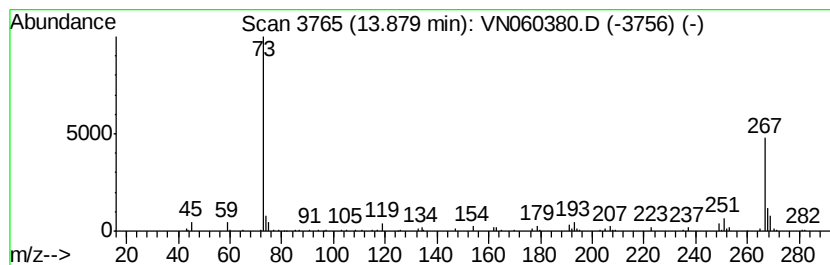
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Peak Number 7 unknown13.88 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	6.89 ug/l	140161	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	43
2		Benzoic acid, 2-[(trimethylsilyl)...	282	C13H22O3Si2	003789-85-3	39
3		Benzeneethanamine, N-[(pentafluo...	475	C21H26F5N02Si2	055429-85-1	32
4		3,5-Dimethoxyphenylacetic acid, ...	268	C13H20O4Si	1000071-82-4	10
5		Monobenzylidene-d-glucose	268	C13H16O6	1000127-04-3	9



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ALS Vial : 12 Sample Multiplier: 1

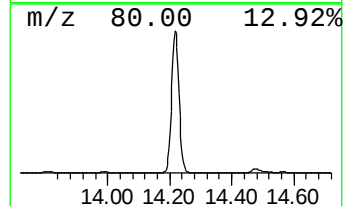
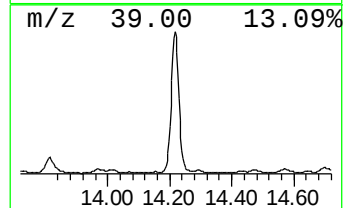
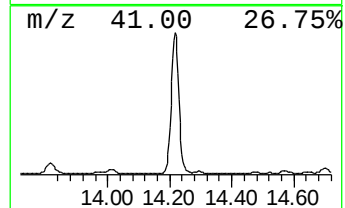
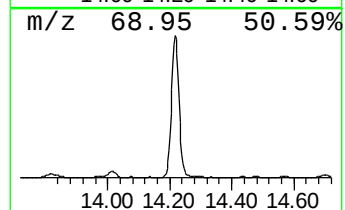
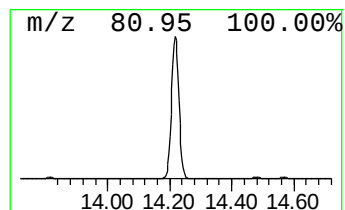
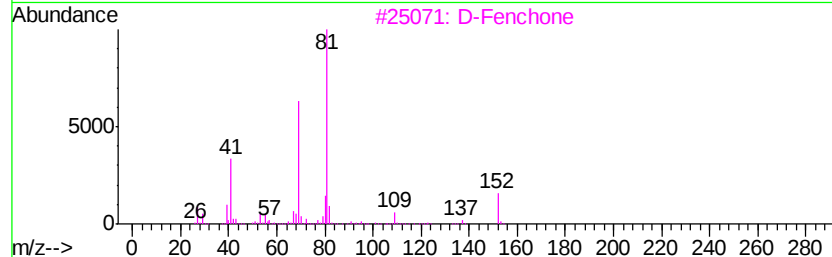
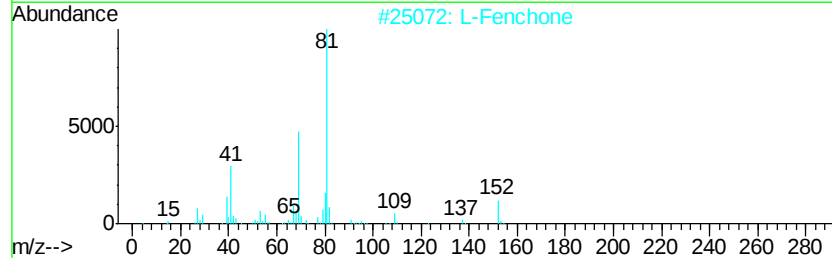
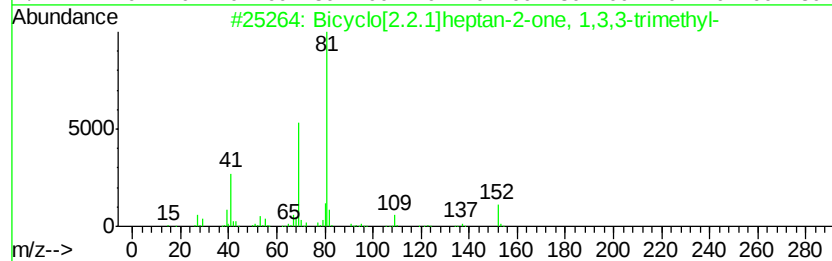
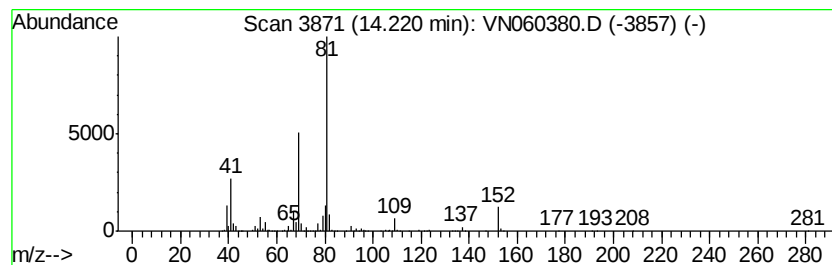
Instrument :
MSVOA_N
ClientSampleId :
400304782.2-VOA

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.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.	
14.22	53.95 ug/l	1097290	1,4-Dichlorobenzene-d4	13.34	
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	95
3	D-Fenchone	152	C10H16O	004695-62-9	94
4	Ethanone, 1-(2-methyl-2-cyclopen...	124	C8H12O	001767-84-6	45
5	2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN030620\
Data File : VN060380.D
Acq On : 6 Mar 2020 15:06
Operator : JC/MD
Sample : L1802-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
400304782.2-VOA

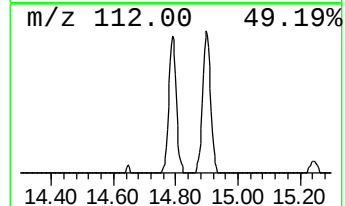
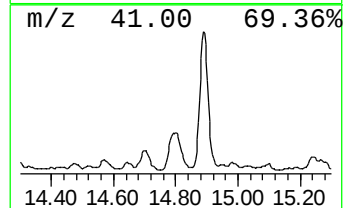
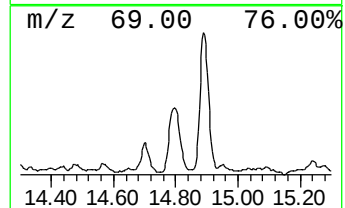
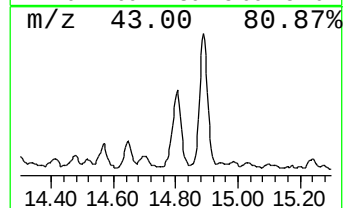
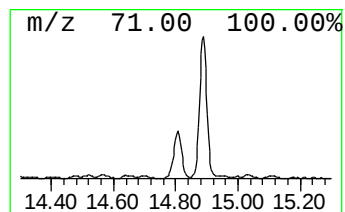
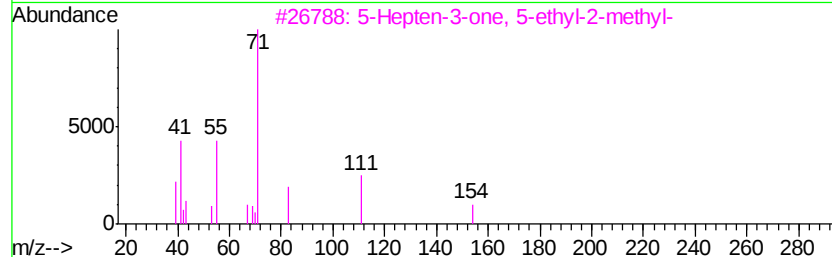
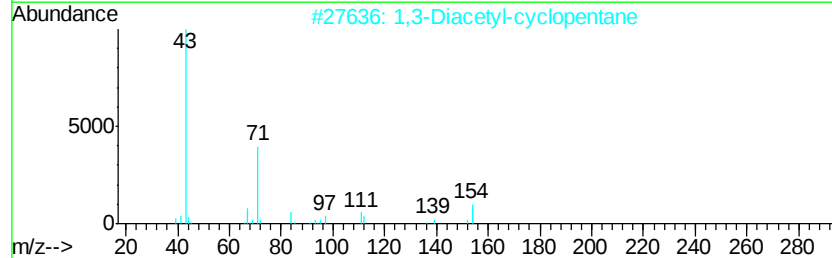
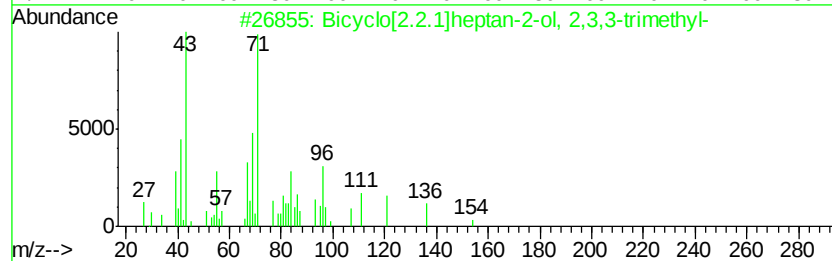
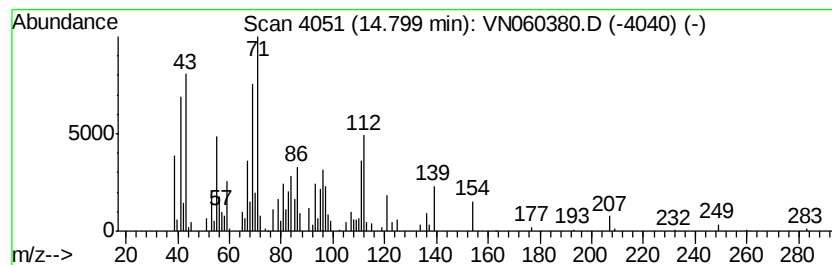
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

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

Peak Number 9 Bicyclo[2.2.1]heptan-2-ol, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	7.24 ug/l	147249	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-ol, 2,3,3...	154	C10H18O	000465-31-6	58
2		1,3-Diacetyl-cyclopentane	154	C9H14O2	1000143-37-1	50
3		5-Hepten-3-one, 5-ethyl-2-methyl-	154	C10H18O	049833-97-8	43
4		1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	38
5		2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN030620\
Data File : VN060380.D
Acq On : 6 Mar 2020 15:06
Operator : JC/MD
Sample : L1802-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
400304782.2-VOA

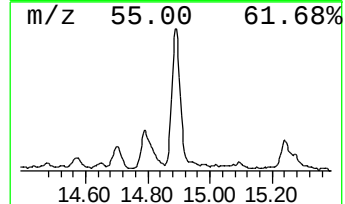
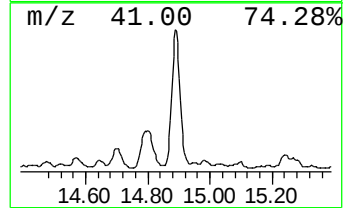
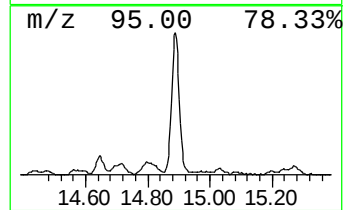
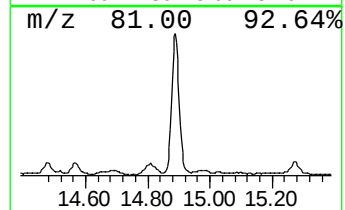
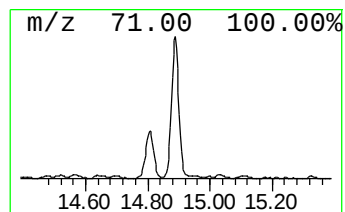
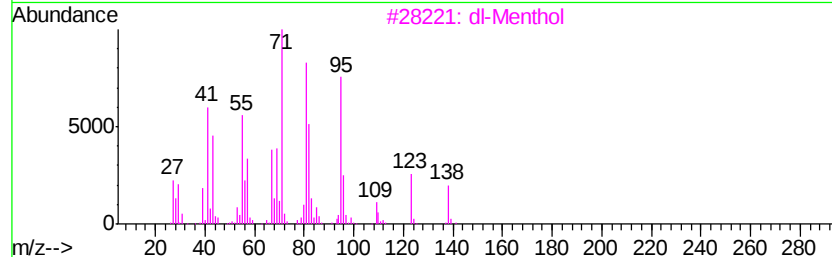
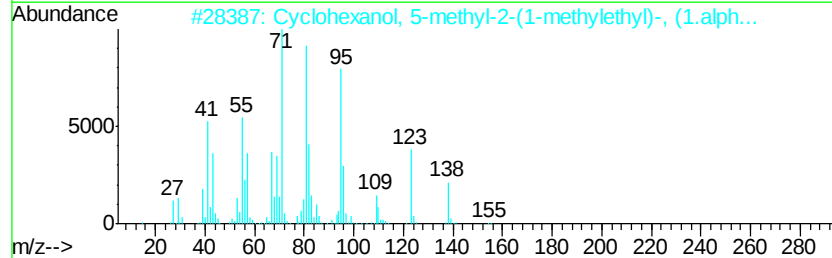
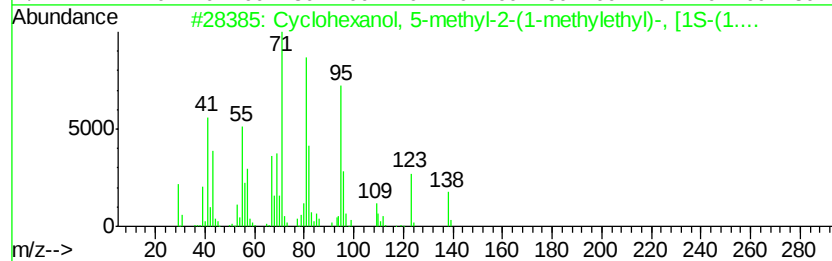
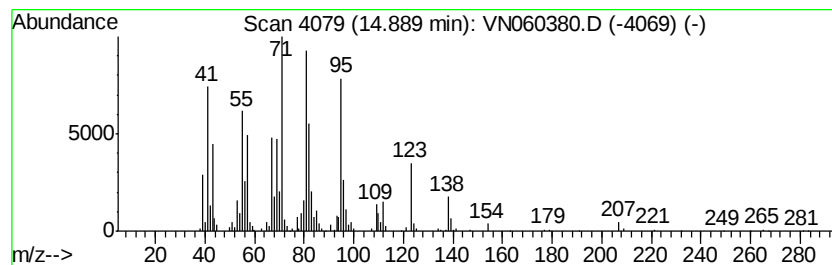
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

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

Peak Number 10 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	17.65 ug/l	358882	1,4-Dichlorobenzene-d4	13.34

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	91
3		dl-Menthol	156	C10H20O	000089-78-1	91
4		Levomenthol	156	C10H20O	002216-51-5	90
5		Cyclohexene,1-(2-methylpropyl)-	138	C10H18	003983-03-7	70



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN030620\
Data File : VN060380.D
Acq On : 6 Mar 2020 15:06
Operator : JC/MD
Sample : L1802-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
400304782.2-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.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
Amylene hydrate	8.10	5.6	ug/l	65542	1	7.64	587035	50.0
3-Hexanone, 2-met...	10.71	15.8	ug/l	307280	3	11.40	972219	50.0
7-Oxabicyclo[2.2...	13.16	7.2	ug/l	146845	4	13.34	1016900	50.0
7-Octen-2-ol, 2,6...	13.81	6.8	ug/l	138075	4	13.34	1016900	50.0
unknown13.88	13.88	6.9	ug/l	140161	4	13.34	1016900	50.0
Bicyclo[2.2.1]hep...	14.22	54.0	ug/l	1097290	4	13.34	1016900	50.0
Bicyclo[2.2.1]hep...	14.80	7.2	ug/l	147249	4	13.34	1016900	50.0
Cyclohexanol, 5-m...	14.89	17.6	ug/l	358882	4	13.34	1016900	50.0