

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
 Data File : VN069097.D
 Acq On : 21 Oct 2021 18:59
 Operator : JC/MD
 Sample : M4301-03
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 211020075-02-VOA

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
 Title : SW846 8260

Signal : TIC: VN069097.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.285	834	856	880	rBV	140184	410893	7.38%	1.663%
2	4.575	946	964	991	rVB	26978	84684	1.52%	0.343%
3	5.363	1218	1258	1322	rBV	948532	3476602	62.43%	14.069%
4	7.316	1956	1986	2056	rBV2	1783421	5568833	100.00%	22.536%
5	7.686	2094	2124	2166	rVB2	415253	1204691	21.63%	4.875%
6	8.024	2228	2250	2261	rBV	232786	557242	10.01%	2.255%
7	8.088	2262	2274	2305	rVB	444700	1025801	18.42%	4.151%
8	8.440	2382	2405	2426	rBV	267482	648201	11.64%	2.623%
9	8.533	2427	2440	2458	rVB2	47404	110399	1.98%	0.447%
10	8.971	2583	2603	2636	rBV	653314	1366882	24.55%	5.531%
11	10.443	3135	3152	3170	rBV	1024680	1922450	34.52%	7.780%
12	10.542	3182	3189	3210	rVB2	33680	62606	1.12%	0.253%
13	11.060	3359	3382	3403	rBV	61809	130103	2.34%	0.526%
14	11.746	3620	3638	3660	rBV	946712	1724111	30.96%	6.977%
15	11.846	3660	3675	3693	rVB3	39820	101052	1.81%	0.409%
16	11.953	3695	3715	3723	rBV2	26643	55897	1.00%	0.226%
17	12.733	3991	4006	4027	rVV	755203	1308343	23.49%	5.295%
18	12.838	4029	4045	4069	rVB	25133	67370	1.21%	0.273%
19	13.079	4117	4135	4147	rBV7	32422	81341	1.46%	0.329%
20	13.495	4272	4290	4302	rBV4	47774	91793	1.65%	0.371%
21	13.677	4342	4358	4373	rBV	861606	1518893	27.27%	6.147%
22	13.742	4373	4382	4411	rVB6	69039	172410	3.10%	0.698%
23	14.144	4520	4532	4541	rBV2	37825	65125	1.17%	0.264%
24	14.562	4664	4688	4720	rBV	549505	1012875	18.19%	4.099%
25	14.986	4834	4846	4860	rBV6	51096	98778	1.77%	0.400%
26	15.158	4893	4910	4913	rBV8	67684	123615	2.22%	0.500%
27	15.203	4914	4927	4940	rVV	737450	1285805	23.09%	5.203%
28	15.509	5028	5041	5057	rVB	106304	206098	3.70%	0.834%
29	15.665	5089	5099	5117	rVB3	35562	72499	1.30%	0.293%
30	15.871	5158	5176	5193	rBV4	67474	155748	2.80%	0.630%

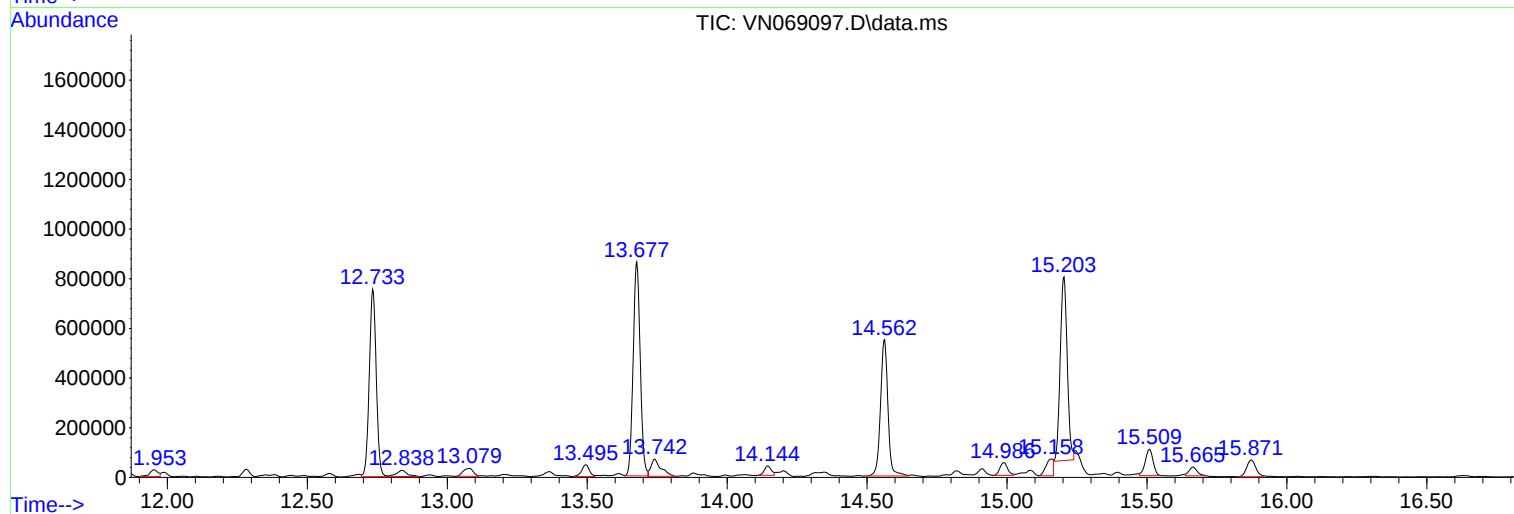
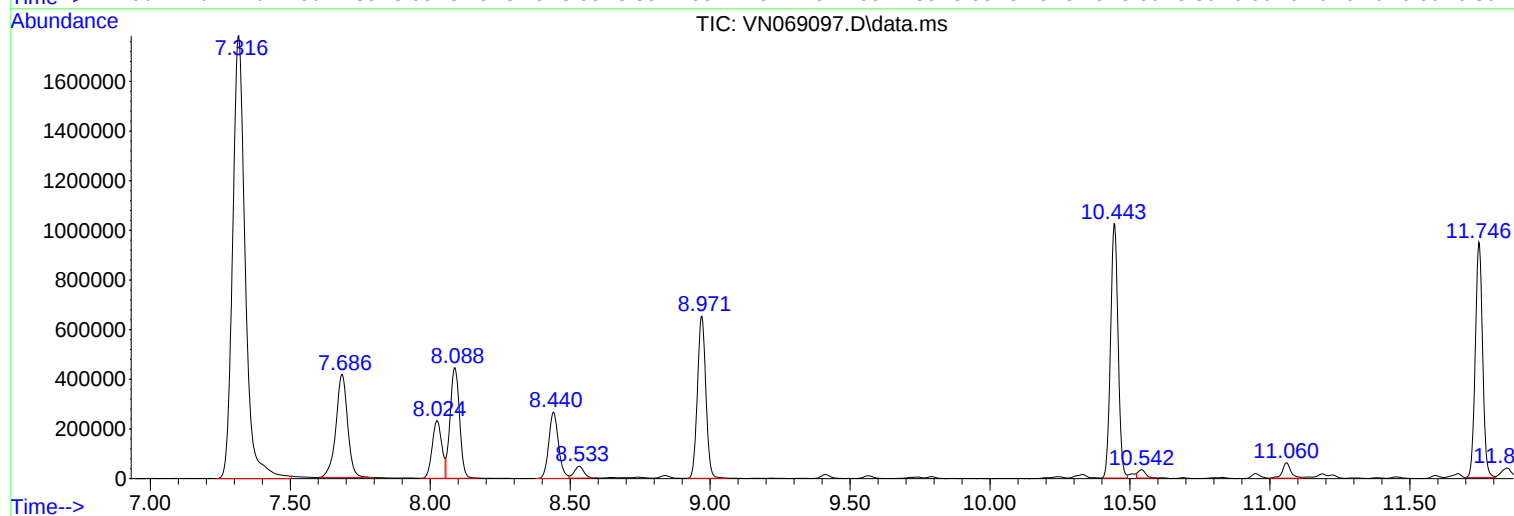
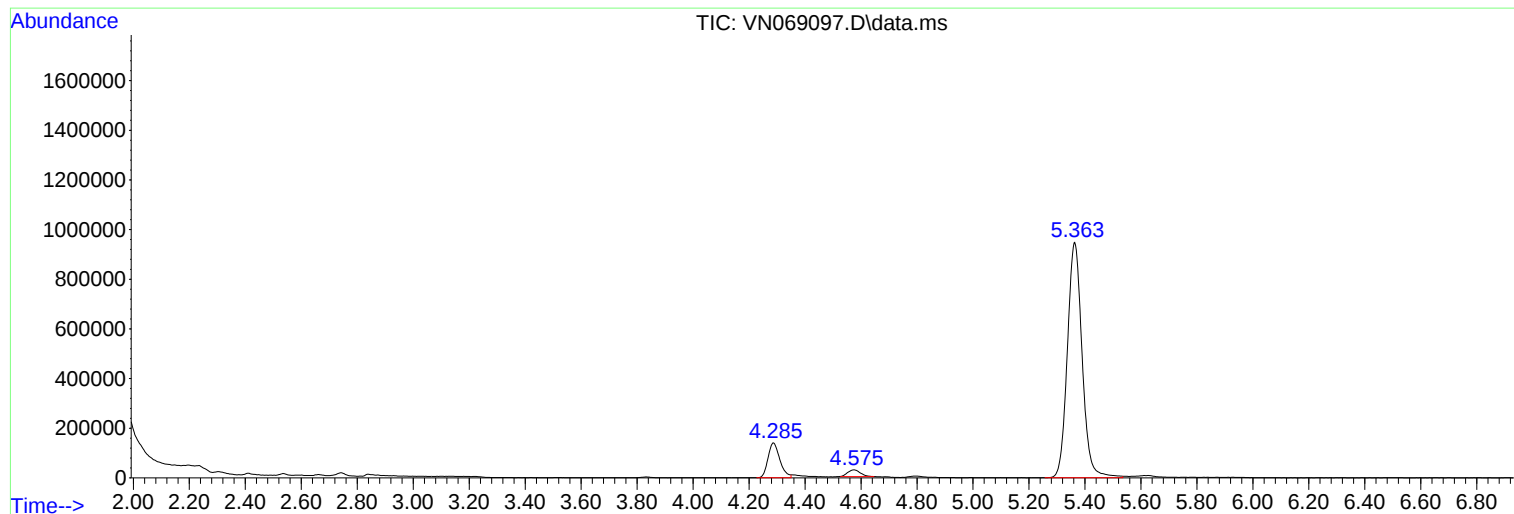
Sum of corrected areas: 24711140

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
Data File : VN069097.D
Acq On : 21 Oct 2021 18:59
Operator : JC/MD
Sample : M4301-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
211020075-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
Data File : VN069097.D
Acq On : 21 Oct 2021 18:59
Operator : JC/MD
Sample : M4301-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
211020075-02-VOA

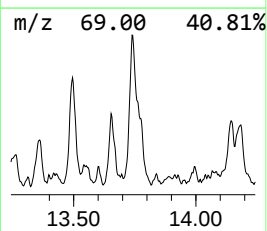
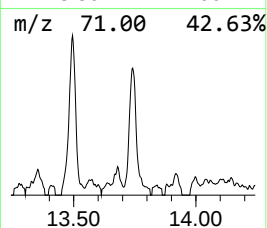
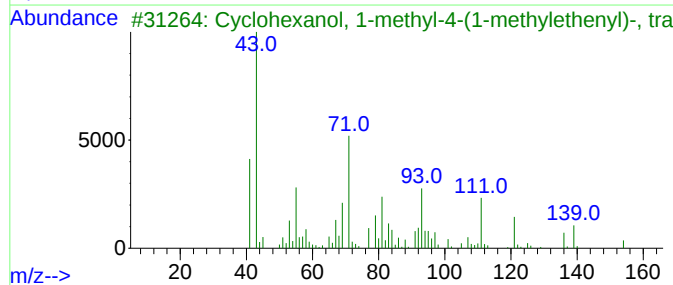
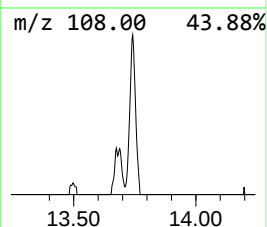
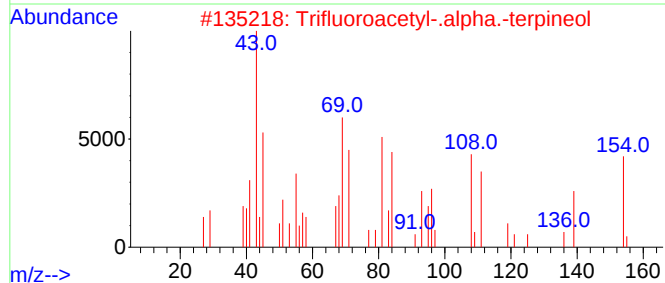
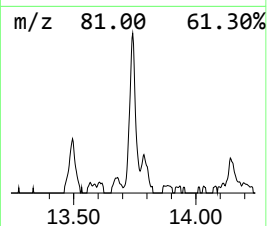
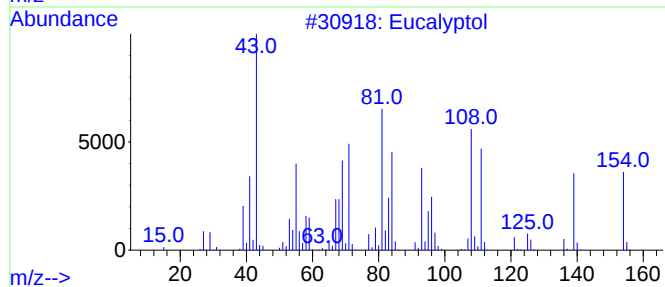
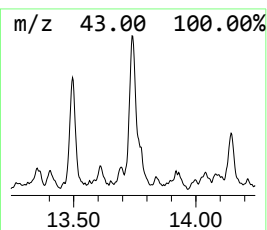
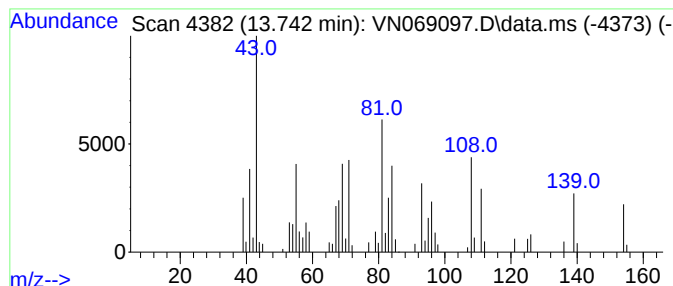
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 1 Eucalyptol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.742	5.68 ug/l	172410	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	95
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	90
3			Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-40-3	43
4			2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	27
5			5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
Data File : VN069097.D
Acq On : 21 Oct 2021 18:59
Operator : JC/MD
Sample : M4301-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
211020075-02-VOA

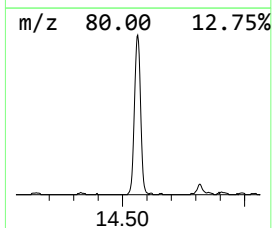
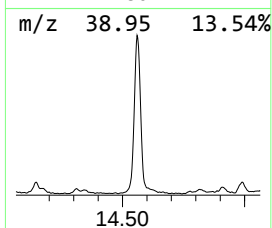
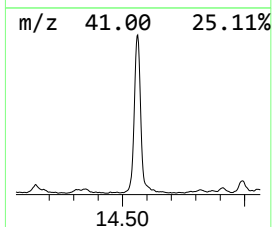
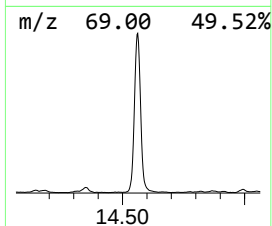
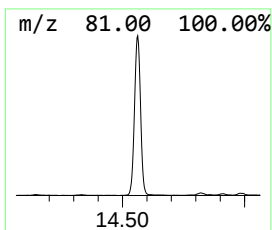
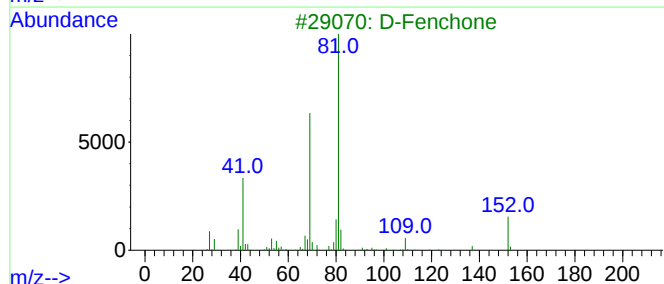
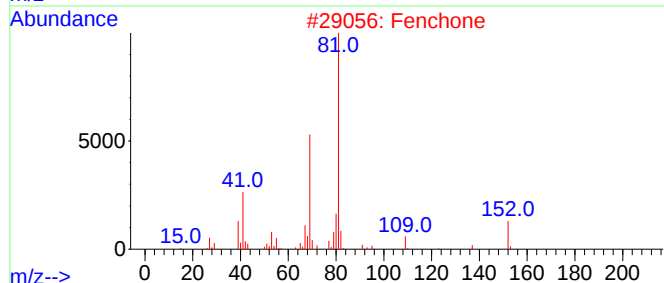
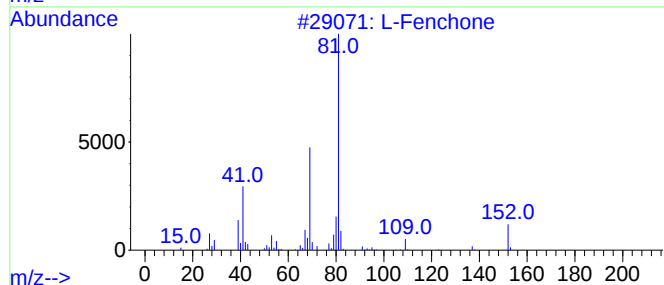
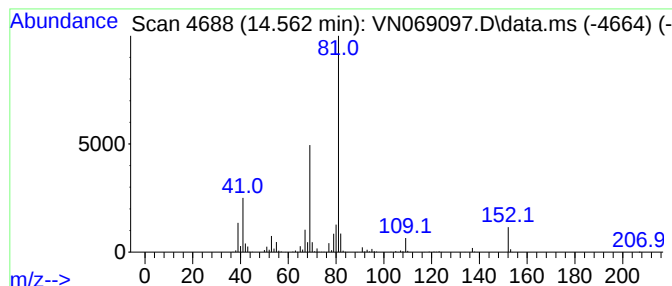
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 2 L-Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.563	33.34 ug/l	1012880	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Fenchone	152	C10H16O	007787-20-4	95
2			Fenchone	152	C10H16O	001195-79-5	95
3			D-Fenchone	152	C10H16O	004695-62-9	94
4			Ethanone, 1-(2-methyl-2-cyclopenten-1-yl)-	124	C8H12O	001767-84-6	45
5			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
Data File : VN069097.D
Acq On : 21 Oct 2021 18:59
Operator : JC/MD
Sample : M4301-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
211020075-02-VOA

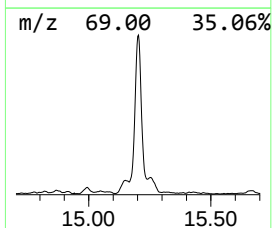
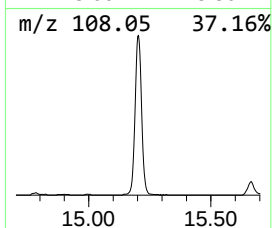
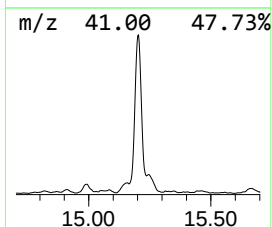
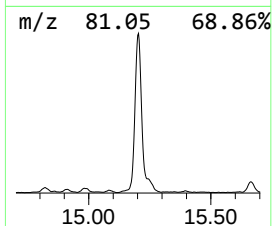
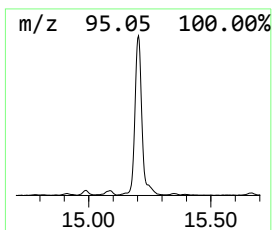
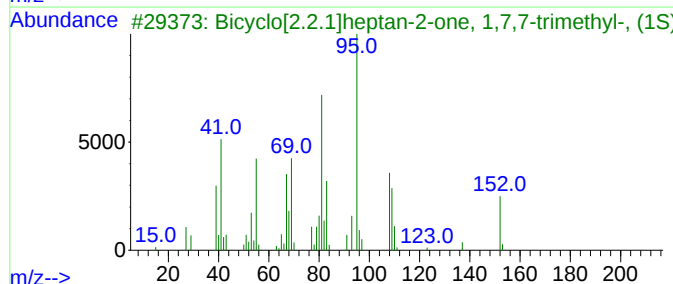
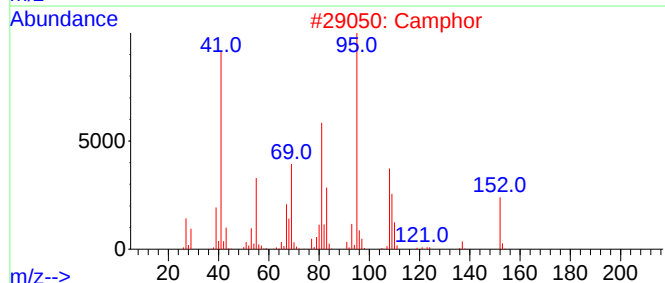
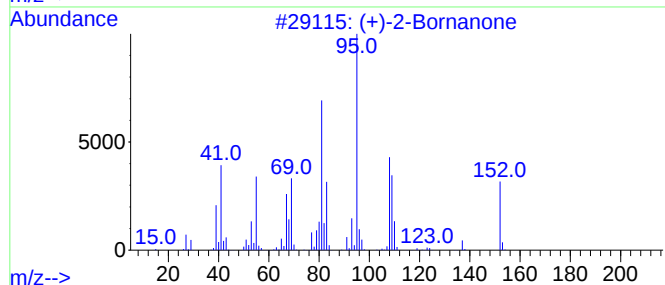
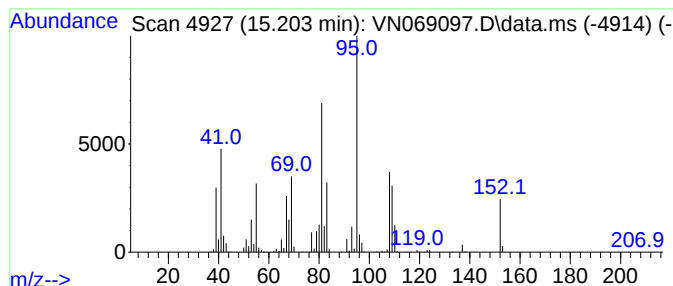
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 3 (+)-2-Bornanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.203	42.33 ug/l	1285810	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-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	98
4			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
Data File : VN069097.D
Acq On : 21 Oct 2021 18:59
Operator : JC/MD
Sample : M4301-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
211020075-02-VOA

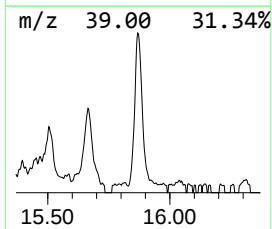
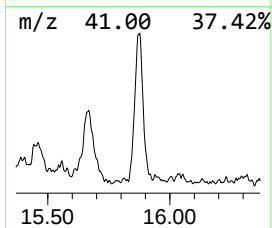
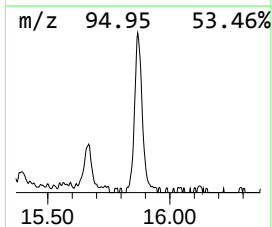
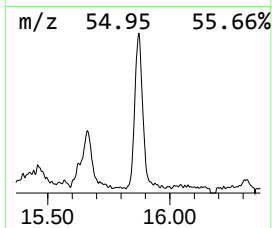
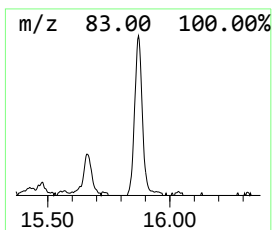
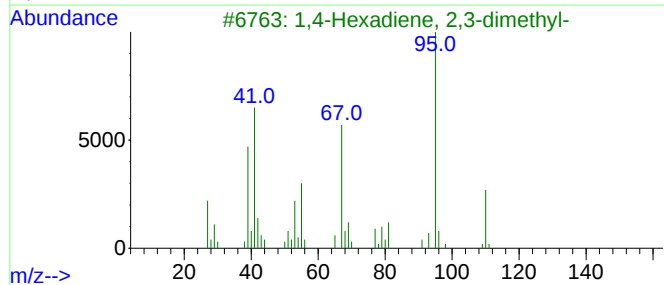
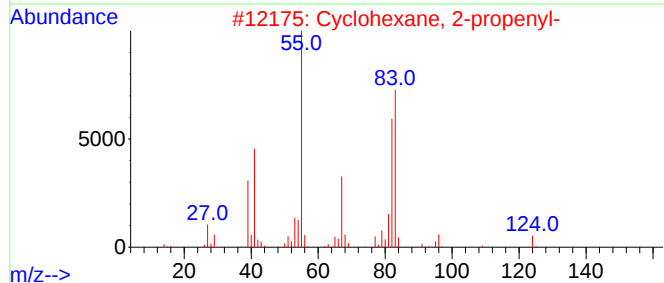
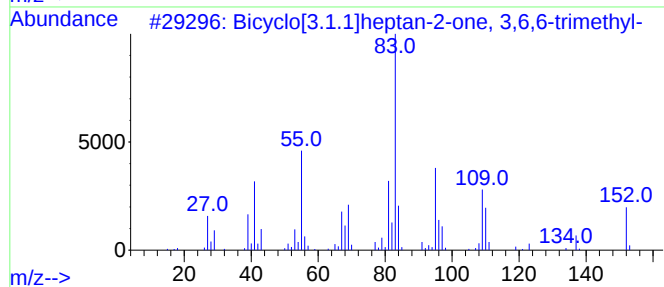
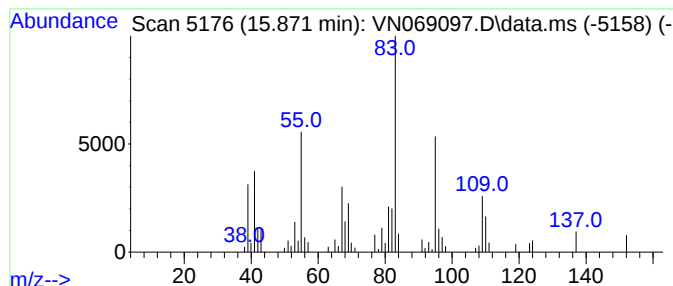
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 4 Bicyclo[3.1.1]heptan-2-one,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.871	5.13 ug/l	155748	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptan-2-one, 3,6,...	152	C10H16O	016022-08-5	53
2			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	43
3			1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	38
4			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	30
5			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
Data File : VN069097.D
Acq On : 21 Oct 2021 18:59
Operator : JC/MD
Sample : M4301-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
211020075-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Eucalyptol	13.742	5.7	ug/l	172410	4	13.677	1518890	50.0
L-Fenchone	14.563	33.3	ug/l	1012880	4	13.677	1518890	50.0
(+)-2-Bornanone	15.203	42.3	ug/l	1285810	4	13.677	1518890	50.0
Bicyclo[3.1.1]h...	15.871	5.1	ug/l	155748	4	13.677	1518890	50.0