

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021623\
 Data File : VN076709.D
 Acq On : 16 Feb 2023 14:15
 Operator : JC\MD
 Sample : 01578-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 230215027-02-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\82N021323W.M
 Title : SW846 8260

Signal : TIC: VN076709.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.307	58	63	72	rVB	216214	342769	4.11%	0.816%
2	4.437	416	425	441	rBV	229025	737618	8.85%	1.756%
3	5.531	595	611	638	rBV2	1965153	6887559	82.63%	16.395%
4	7.442	924	936	954	rBV2	2646793	8335314	100.00%	19.842%
5	7.842	989	1004	1022	rBV	1413050	3671953	44.05%	8.741%
6	8.172	1050	1060	1065	rBV	258219	649534	7.79%	1.546%
7	8.231	1065	1070	1080	rVB	495426	1066800	12.80%	2.539%
8	8.584	1115	1130	1140	rBV3	332349	1064779	12.77%	2.535%
9	9.107	1210	1219	1230	rBV	705072	1443532	17.32%	3.436%
10	9.536	1285	1292	1301	rVB	116575	224922	2.70%	0.535%
11	10.572	1459	1468	1474	rBV	1088838	2034631	24.41%	4.843%
12	10.642	1474	1480	1492	rVB3	127814	379751	4.56%	0.904%
13	11.172	1560	1570	1580	rBV	180619	350927	4.21%	0.835%
14	11.866	1678	1688	1697	rBV	937876	1825621	21.90%	4.346%
15	11.966	1697	1705	1712	rVB2	264595	531951	6.38%	1.266%
16	12.072	1714	1723	1733	rVB	259029	559478	6.71%	1.332%
17	12.401	1770	1779	1785	rBV	178142	326585	3.92%	0.777%
18	12.854	1848	1856	1864	rVB	713390	1281387	15.37%	3.050%
19	13.483	1950	1963	1970	rBV2	110785	243438	2.92%	0.579%
20	13.607	1977	1984	1991	rBV4	98018	196664	2.36%	0.468%
21	13.795	2009	2016	2023	rBV	910361	1709690	20.51%	4.070%
22	13.860	2023	2027	2038	rVB3	235302	449838	5.40%	1.071%
23	13.995	2045	2050	2064	rVB	92438	210984	2.53%	0.502%
24	14.248	2086	2093	2098	rBV4	181125	346262	4.15%	0.824%
25	14.301	2098	2102	2113	rVB	171587	320115	3.84%	0.762%
26	14.448	2119	2127	2135	rVB7	74792	198322	2.38%	0.472%
27	14.677	2160	2166	2173	rVB	805319	1289444	15.47%	3.069%
28	15.030	2220	2226	2233	rBV8	68671	162536	1.95%	0.387%
29	15.101	2233	2238	2245	rVB2	185193	314710	3.78%	0.749%
30	15.283	2261	2269	2271	rBV6	135013	309387	3.71%	0.736%
31	15.330	2271	2277	2294	rVB2	1152307	3095927	37.14%	7.370%
32	15.642	2320	2330	2339	rVB	546978	1061404	12.73%	2.527%
33	15.801	2353	2357	2368	rVB4	60645	152645	1.83%	0.363%
34	16.012	2386	2393	2405	rBV3	98726	232530	2.79%	0.554%

Sum of corrected areas: 42009007

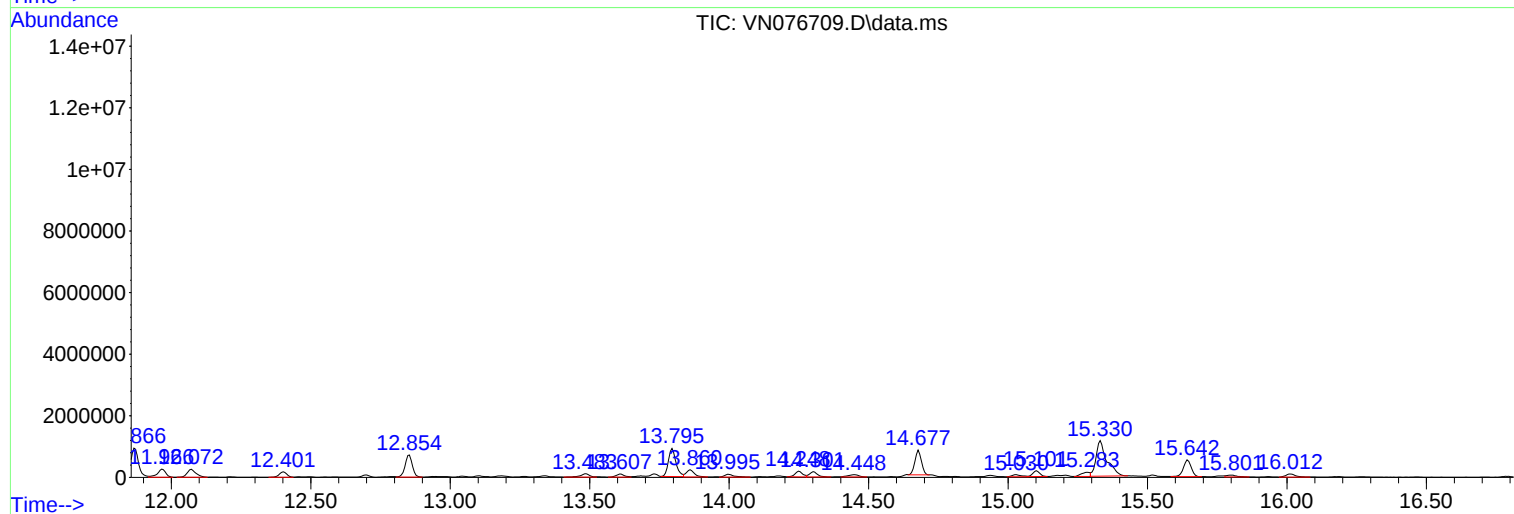
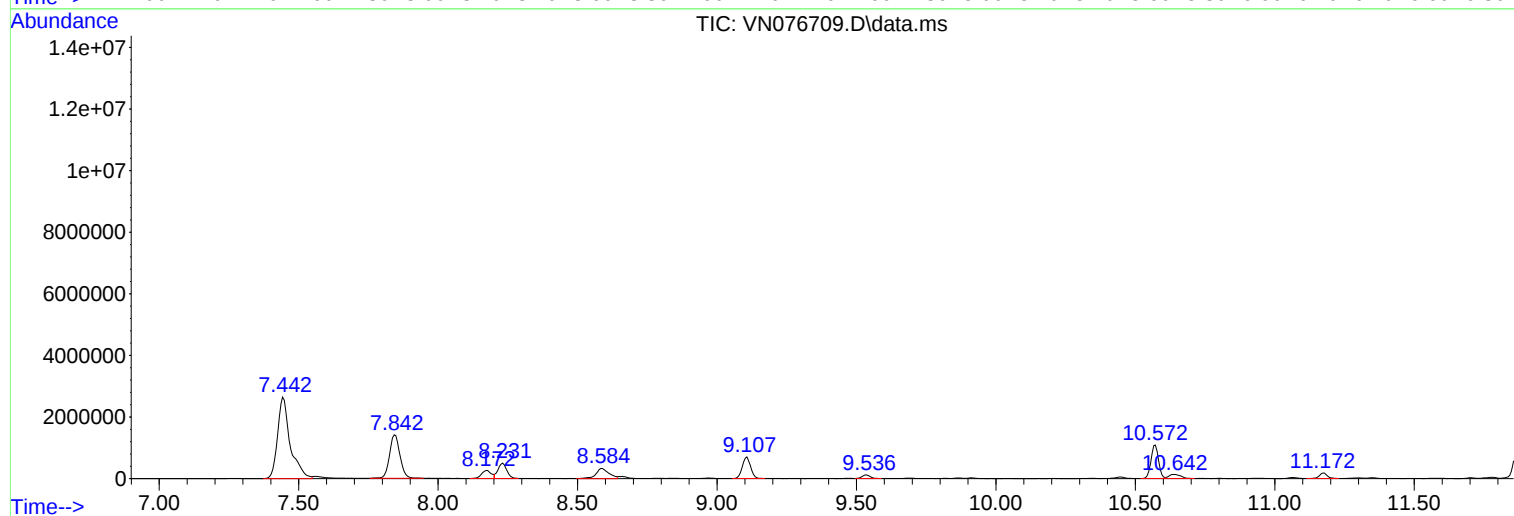
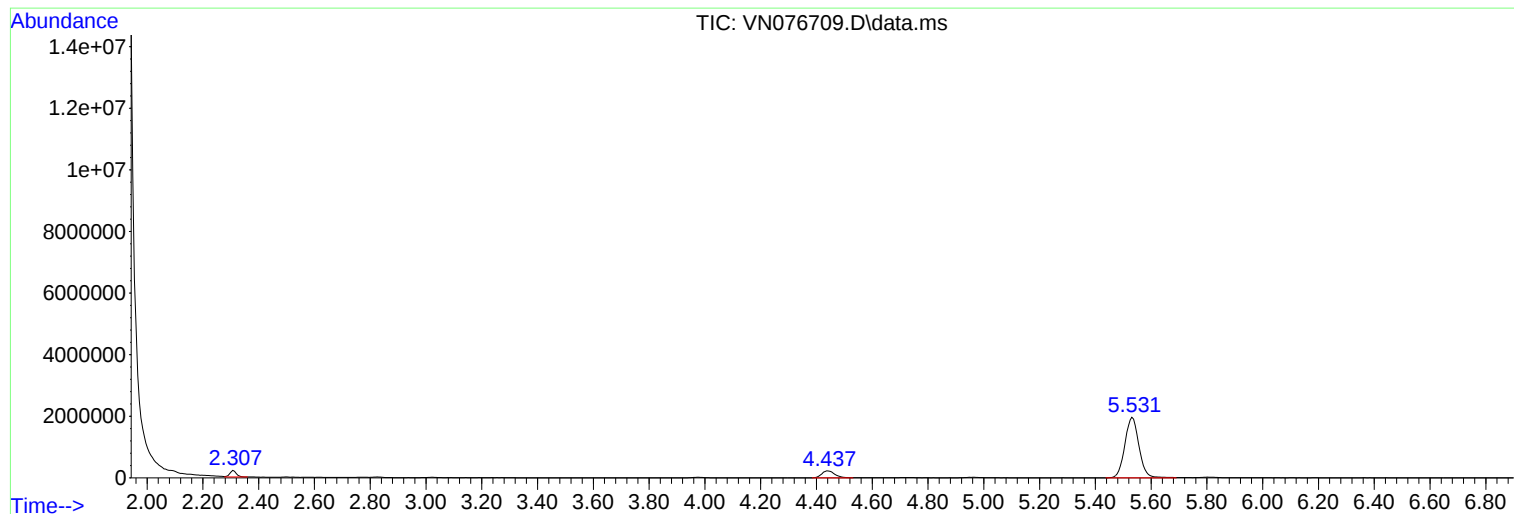
Instrument :
MSVOA_N
ClientSampleId :
230215027-02-VOA

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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



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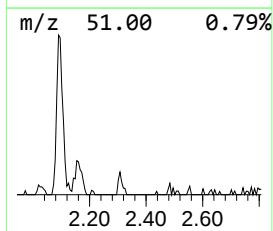
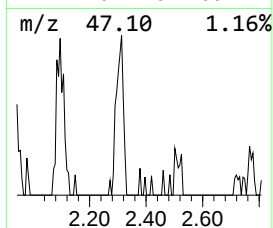
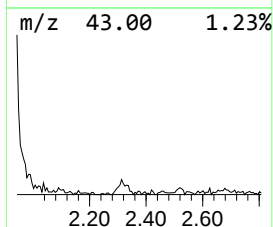
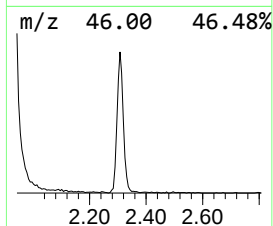
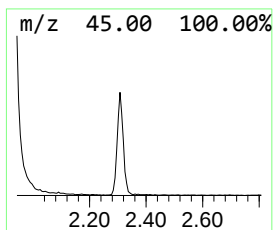
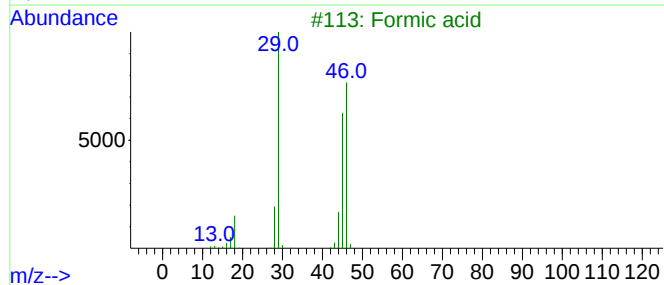
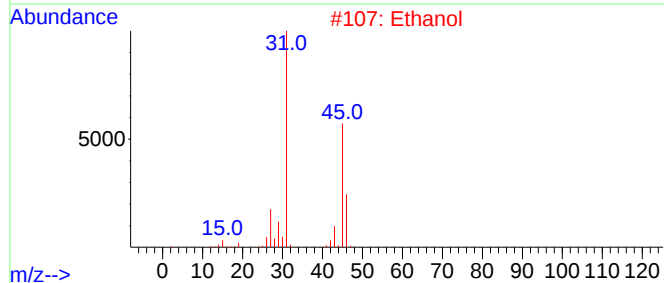
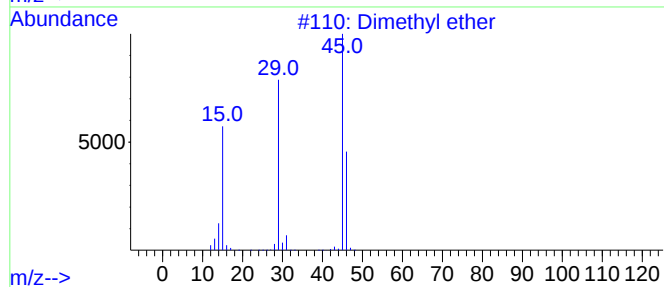
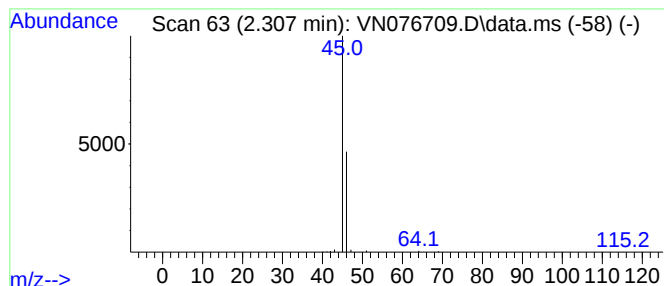
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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

Peak Number 1 Dimethyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.307	16.07 ug/l	342769	Pentafluorobenzene	8.231

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	64
2			Ethanol	46	C2H6O	000064-17-5	7
3			Formic acid	46	CH2O2	000064-18-6	4
4			Oxalic acid	90	C2H2O4	000144-62-7	4
5			Methane, nitroso-	45	CH3NO	000865-40-7	3



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230215027-02-VOA

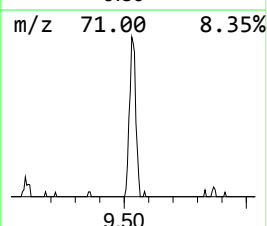
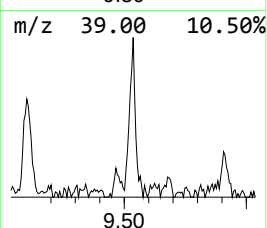
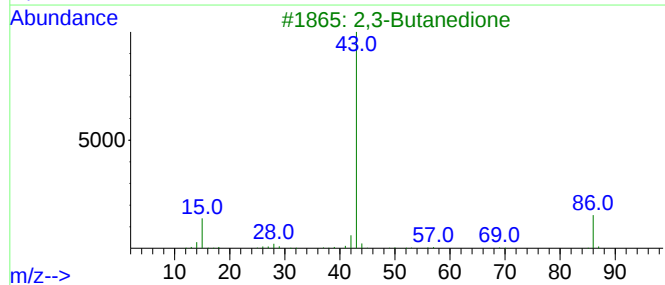
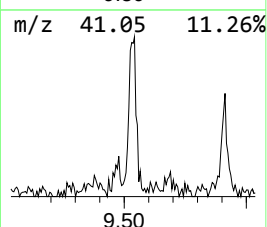
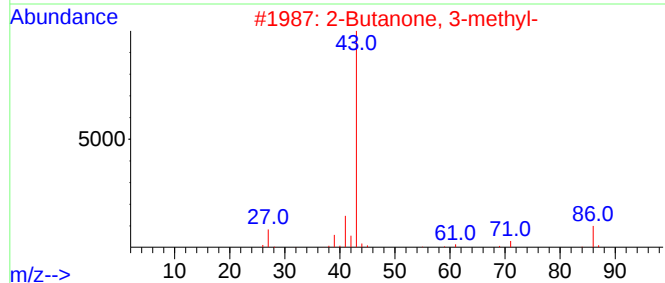
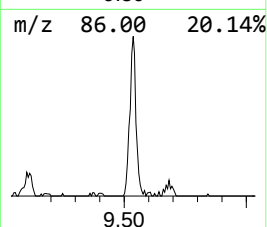
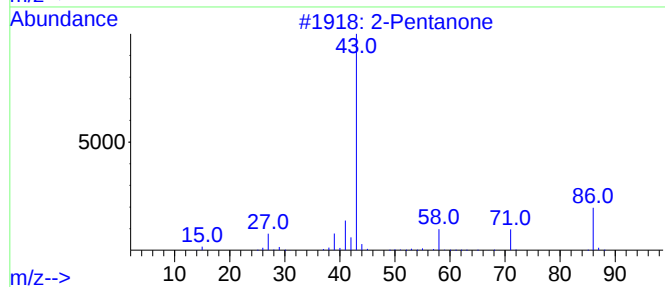
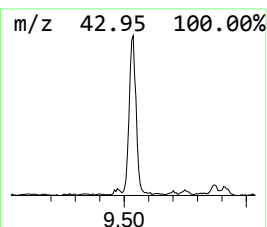
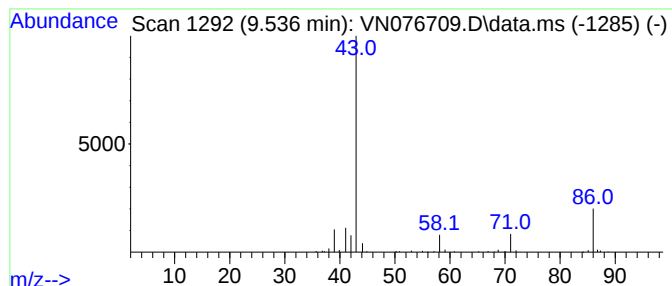
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Pentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.536	7.79 ug/l	224922	1,4-Difluorobenzene	9.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone	86	C5H10O	000107-87-9	86
2			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3			2,3-Butanedione	86	C4H6O2	000431-03-8	64
4			Propane, 2-(ethenyloxy)-	86	C5H10O	000926-65-8	53
5			3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	38



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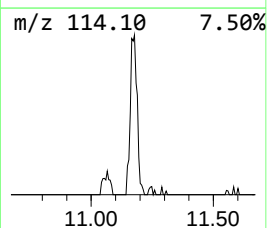
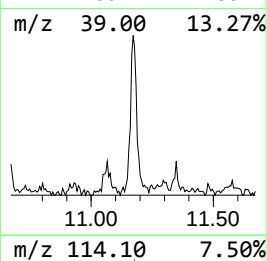
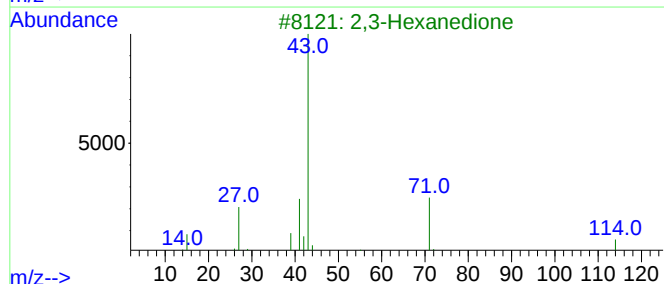
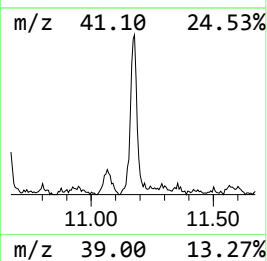
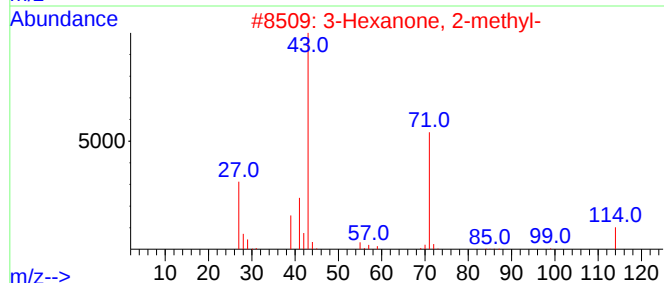
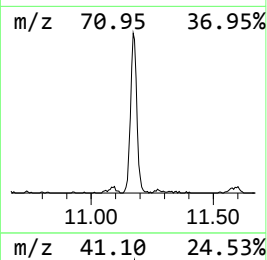
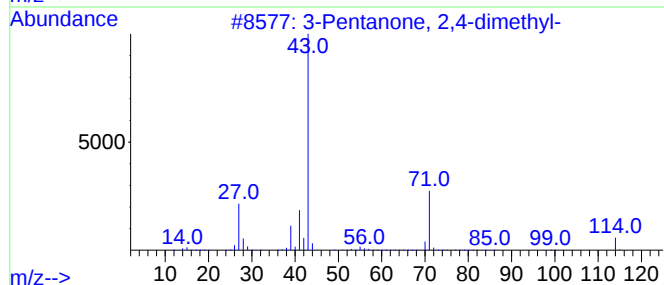
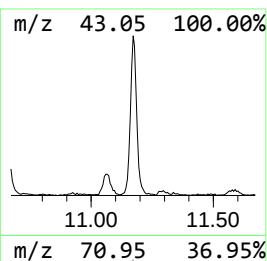
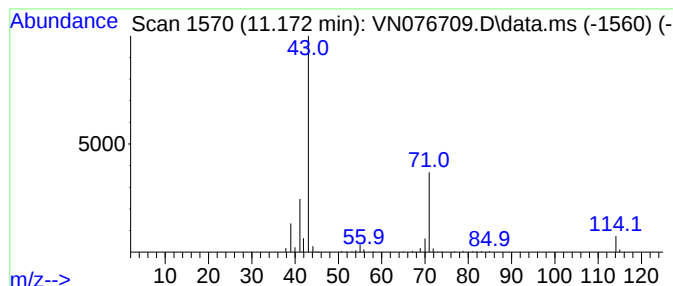
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.172	9.61 ug/l	350927	Chlorobenzene-d5			11.866

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	72	
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	59	
4	4-Heptanone	114	C7H14O	000123-19-3	53	
5	Pyrrolidine	71	C4H9N	000123-75-1	50	



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230215027-02-VOA

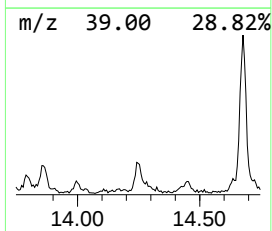
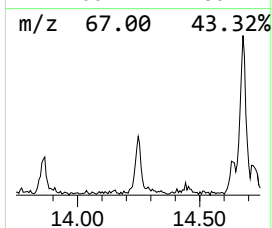
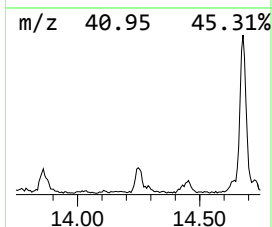
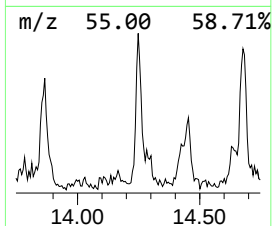
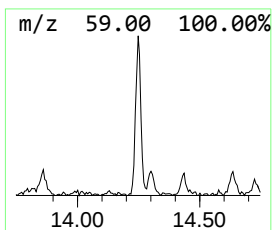
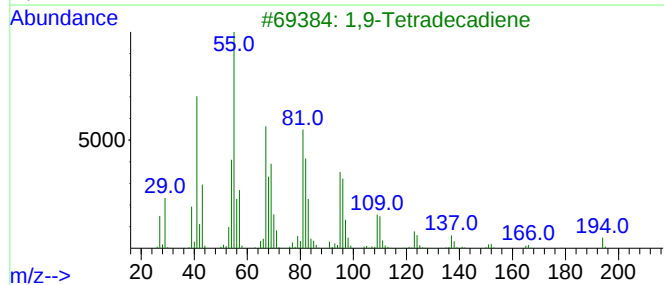
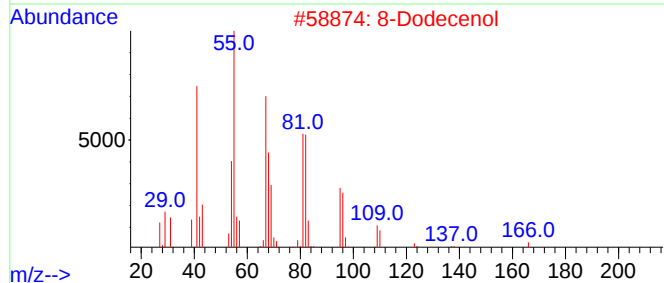
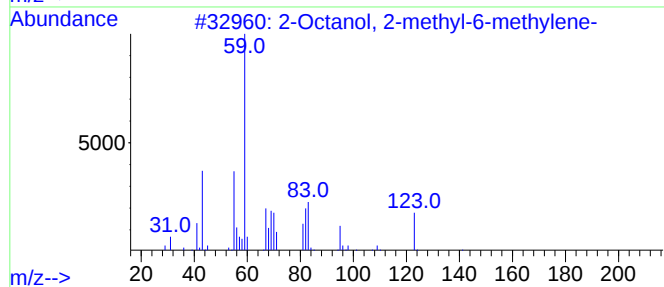
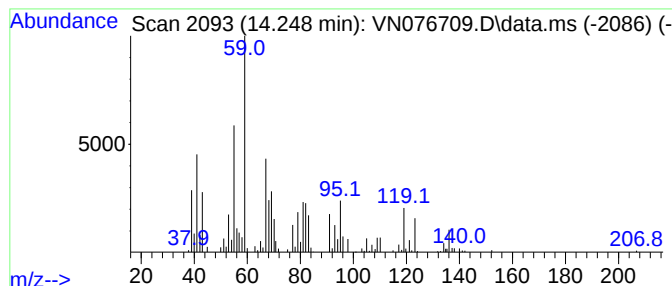
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown14.248 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.248	10.13 ug/l	346262	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	40
2			8-Dodecenol	184	C12H24O	042513-42-8	27
3			1,9-Tetradecadiene	194	C14H26	112929-06-3	25
4			3-Nonanol	144	C9H20O	000624-51-1	22
5			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	20



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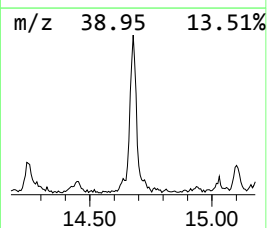
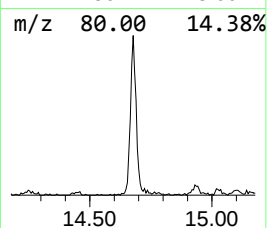
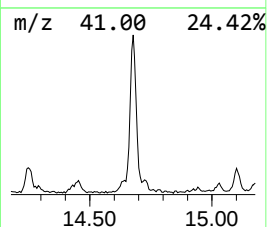
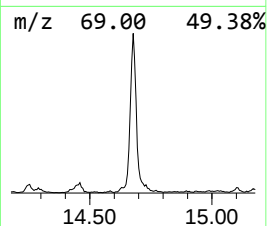
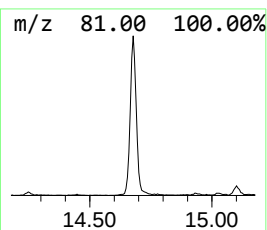
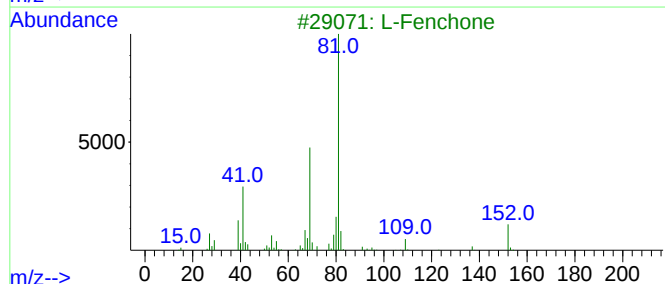
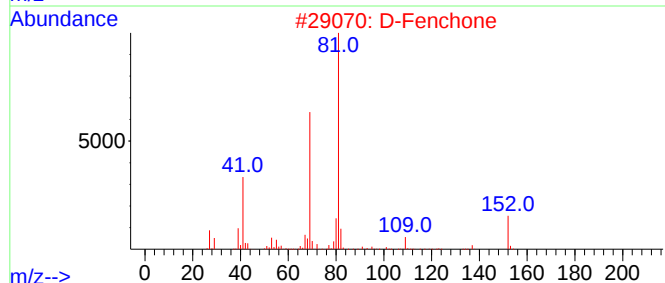
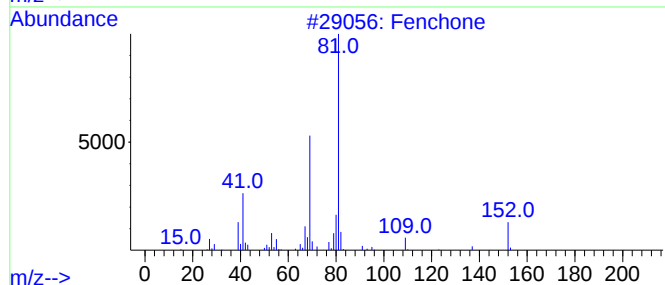
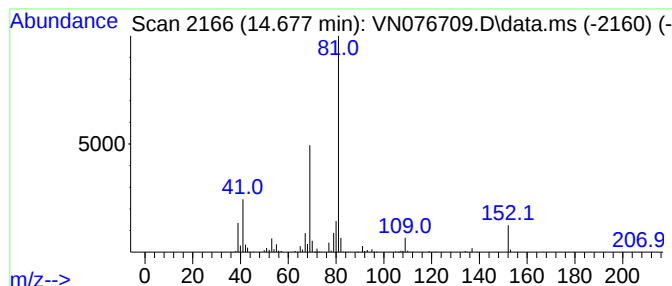
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Quant Title : SW846 8260

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

Peak Number 6 Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.677	37.71 ug/l	1289440	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	95
2			D-Fenchone	152	C10H16O	004695-62-9	94
3			L-Fenchone	152	C10H16O	007787-20-4	91
4			2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	53
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
230215027-02-VOA

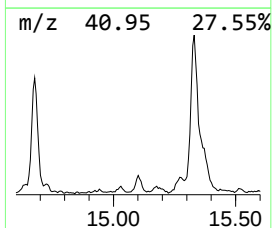
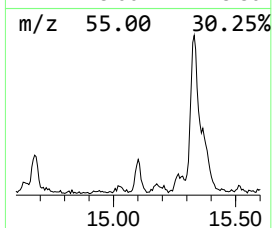
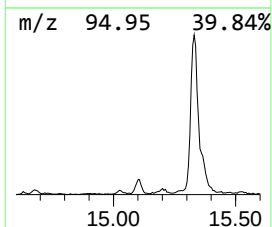
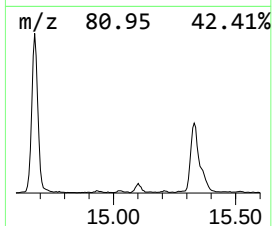
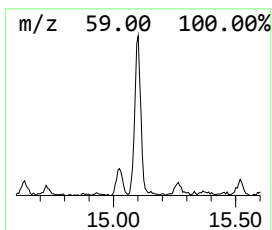
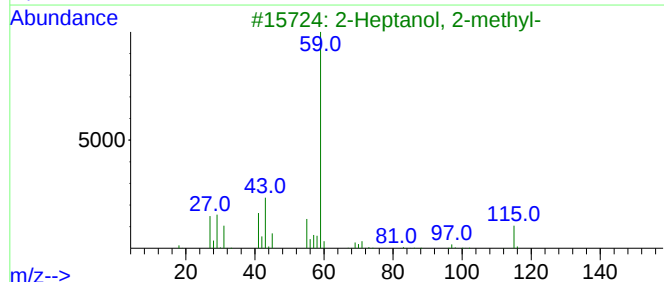
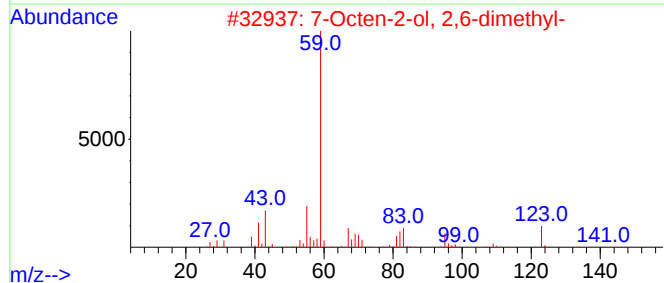
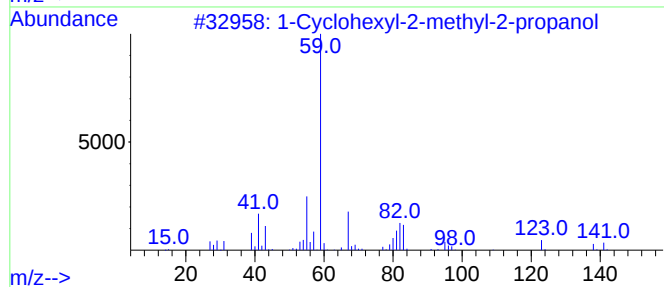
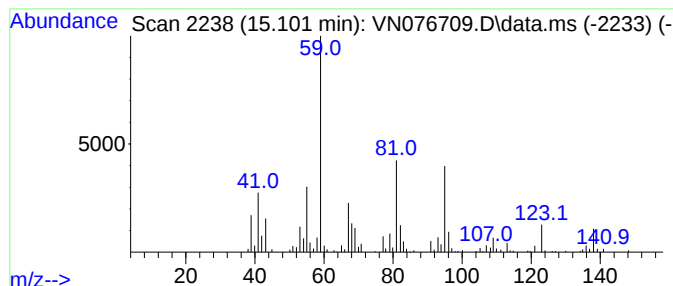
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Quant Title : SW846 8260

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

Peak Number 7 unknown15.101 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.101	9.20 ug/l	314710	1,4-Dichlorobenzene-d4	13.795

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Cyclohexyl-2-methyl-2-propanol	156	C10H20O	005531-30-6	33
2		7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	33
3		2-Heptanol, 2-methyl-	130	C8H18O	000625-25-2	27
4		6-Methylheptane-1,6-diol	146	C8H18O2	005392-57-4	25
5		Cyclohexanemethanol, .alpha.,.al...	154	C10H18O	007299-42-5	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021623\
Data File : VN076709.D
Acq On : 16 Feb 2023 14:15
Operator : JC\MD
Sample : 01578-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
230215027-02-VOA

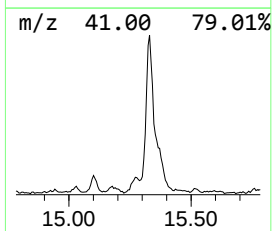
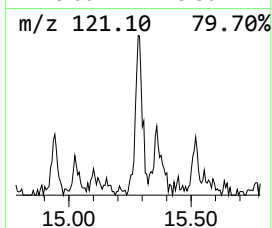
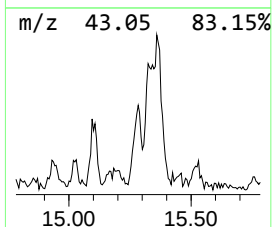
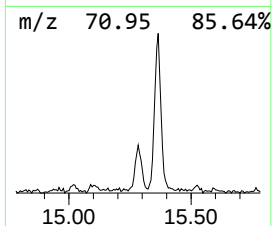
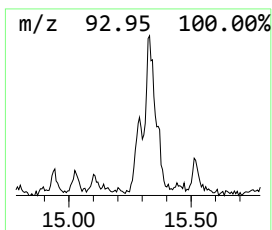
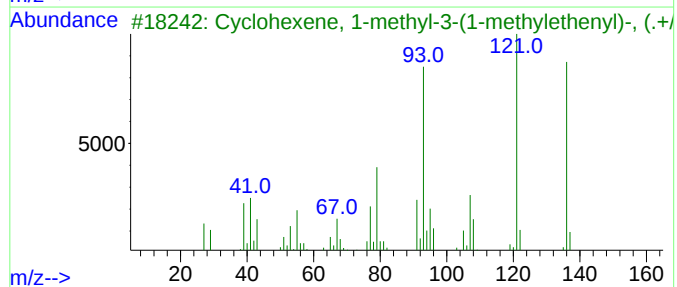
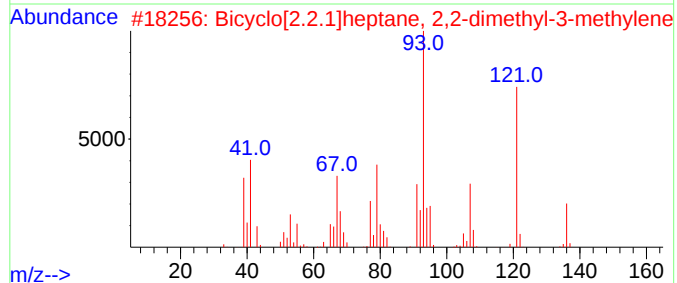
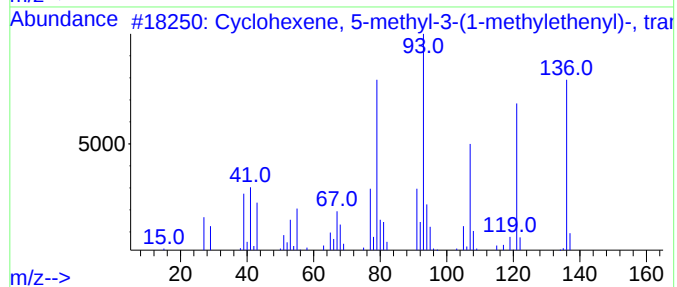
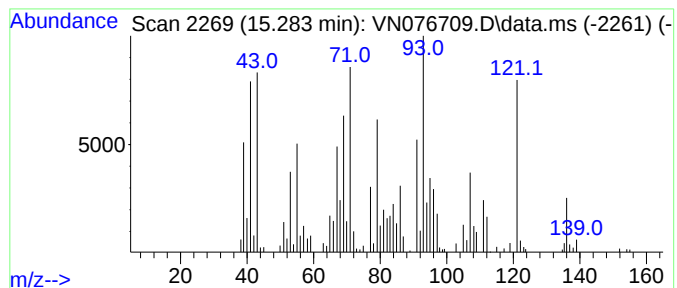
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.283	9.05 ug/l	309387	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 5-methyl-3-(1-methy...	136	C10H16	056816-08-1	80
2			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	78
3			Cyclohexene, 1-methyl-3-(1-methy...	136	C10H16	000499-03-6	60
4			Bicyclo[4.1.0]hept-2-ene, 3,7,7-...	136	C10H16	004497-92-1	50
5			Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021623\
Data File : VN076709.D
Acq On : 16 Feb 2023 14:15
Operator : JC\MD
Sample : 01578-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
230215027-02-VOA

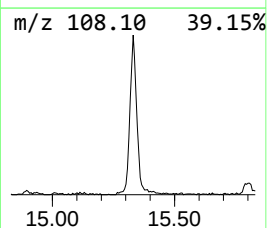
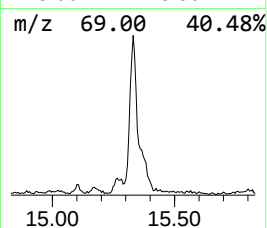
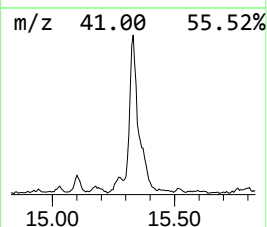
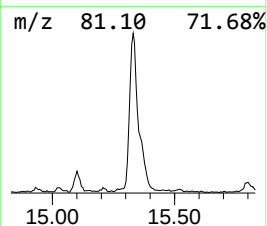
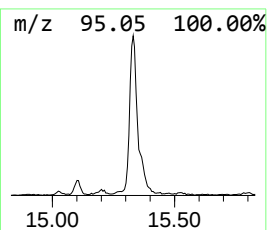
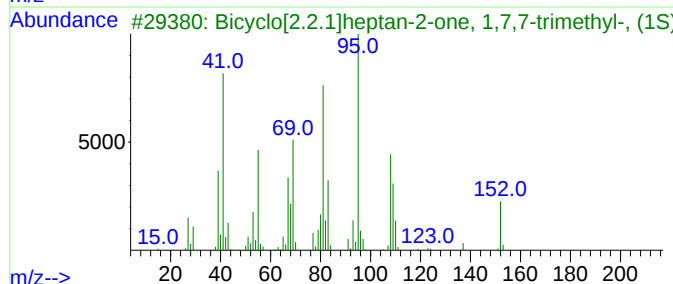
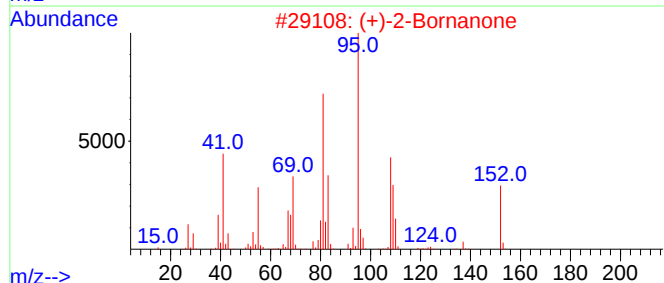
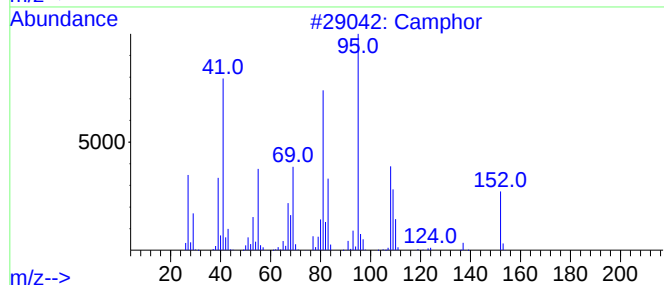
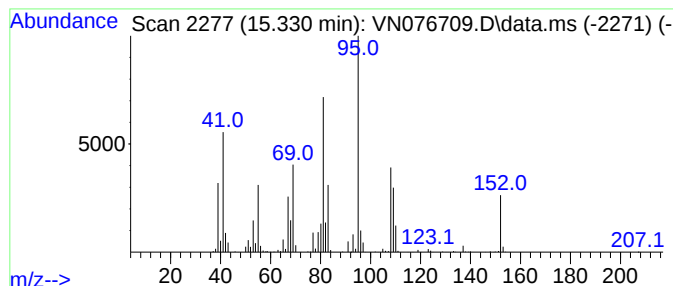
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Quant Title : SW846 8260

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

Peak Number 9 Camphor Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.330	90.54 ug/l	3095930	1,4-Dichlorobenzene-d4	13.795

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	97
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	94
4			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	43
5			Bicyclo[3.1.0]hexan-2-one, 4-met...	152	C10H16O	002506-61-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021623\
Data File : VN076709.D
Acq On : 16 Feb 2023 14:15
Operator : JC\MD
Sample : 01578-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
230215027-02-VOA

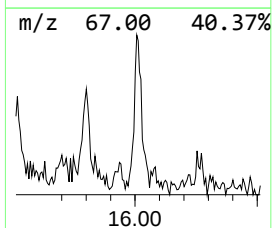
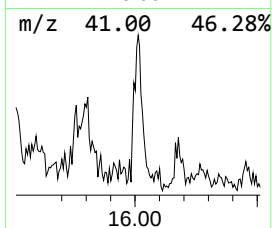
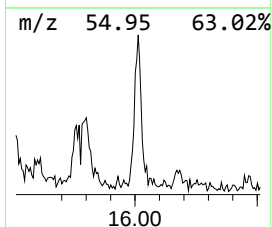
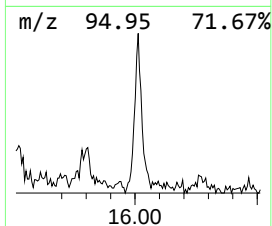
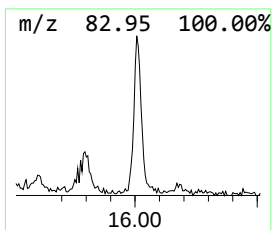
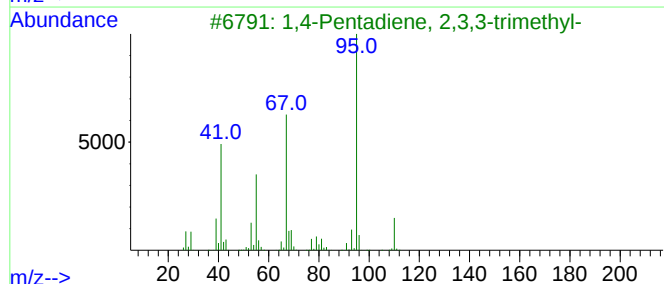
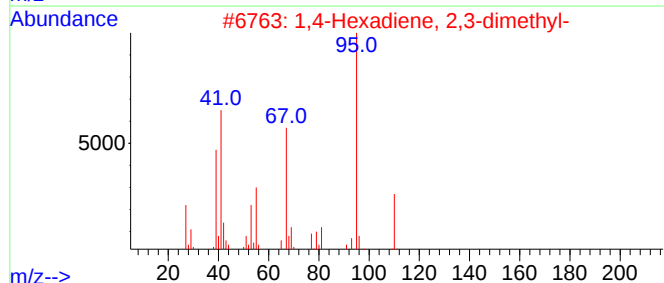
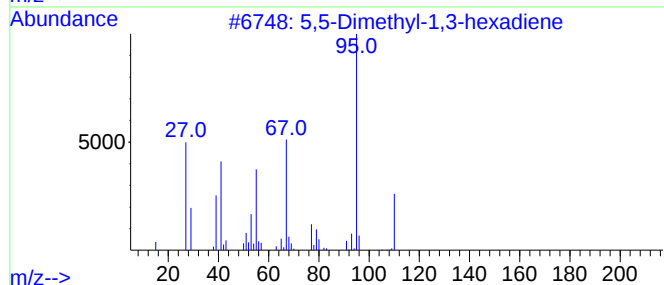
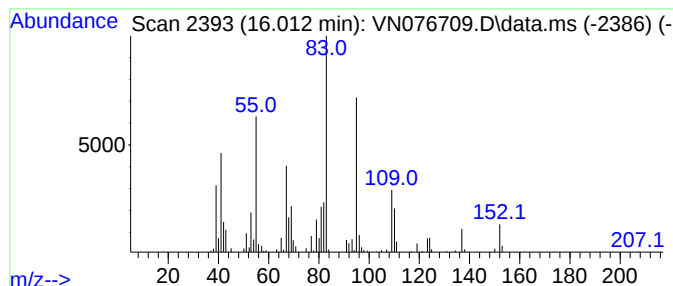
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Quant Title : SW846 8260

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

Peak Number 10 5,5-Dimethyl-1,3-hexadiene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.012	6.80 ug/l	232530	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	42
2			1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	38
3			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	38
4			Cyclobutene, 1,2,3,4-tetramethyl-	110	C8H14	090346-45-5	38
5			4-Methyl-1,3-heptadiene	110	C8H14	017603-57-5	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021623\
Data File : VN076709.D
Acq On : 16 Feb 2023 14:15
Operator : JC\MD
Sample : 01578-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
230215027-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl ether	2.307	16.1	ug/l	342769	1	8.231	1066800	50.0
2-Pentanone	9.536	7.8	ug/l	224922	2	9.107	1443530	50.0
3-Pentanone, 2,...	11.172	9.6	ug/l	350927	3	11.866	1825620	50.0
unknown14.248	14.248	10.1	ug/l	346262	4	13.795	1709690	50.0
Fenchone	14.677	37.7	ug/l	1289440	4	13.795	1709690	50.0
unknown15.101	15.101	9.2	ug/l	314710	4	13.795	1709690	50.0
Cyclohexene, 5-...	15.283	9.1	ug/l	309387	4	13.795	1709690	50.0
Camphor	15.330	90.5	ug/l	3095930	4	13.795	1709690	50.0
5,5-Dimethyl-1,...	16.012	6.8	ug/l	232530	4	13.795	1709690	50.0