

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111424\
 Data File : VN084848.D
 Acq On : 14 Nov 2024 13:48
 Operator : JC\MD
 Sample : P4844-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 241113075-01-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\82N103024W.M
 Title : SW846 8260

Signal : TIC: VN084848.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	52	57	67	rVB	83751	127469	2.37%	0.477%
2	2.947	164	169	179	rVB6	27006	78717	1.46%	0.294%
3	4.430	411	421	434	rBV2	48779	144732	2.69%	0.541%
4	5.547	587	611	635	rBV	1072907	5386926	100.00%	20.151%
5	7.453	918	935	946	rBV	1602895	5038039	93.52%	18.846%
6	7.829	988	999	1016	rBV	949688	2446358	45.41%	9.151%
7	8.159	1045	1055	1059	rBV	131999	305539	5.67%	1.143%
8	8.218	1059	1065	1075	rVB	245583	562277	10.44%	2.103%
9	8.571	1116	1125	1136	rBV4	152709	463553	8.61%	1.734%
10	8.665	1136	1141	1149	rVB	35136	84012	1.56%	0.314%
11	9.094	1205	1214	1226	rVV	349111	708236	13.15%	2.649%
12	10.559	1456	1463	1470	rBV	511847	957406	17.77%	3.581%
13	10.623	1470	1474	1488	rVB3	125487	325498	6.04%	1.218%
14	11.164	1558	1566	1576	rVV	167134	312570	5.80%	1.169%
15	11.776	1662	1670	1675	rVV5	29806	83508	1.55%	0.312%
16	11.864	1675	1685	1694	rVV	450195	887988	16.48%	3.322%
17	11.959	1694	1701	1710	rVB	136808	265658	4.93%	0.994%
18	12.064	1710	1719	1729	rBV	130418	277076	5.14%	1.036%
19	12.394	1768	1775	1782	rBV2	91323	167452	3.11%	0.626%
20	12.847	1844	1852	1860	rVB	394356	686828	12.75%	2.569%
21	13.188	1902	1910	1918	rVV6	30322	95241	1.77%	0.356%
22	13.476	1948	1959	1966	rBV2	49227	110227	2.05%	0.412%
23	13.605	1973	1981	1988	rBV2	58375	119902	2.23%	0.449%
24	13.723	1996	2001	2006	rBV	115288	187435	3.48%	0.701%
25	13.788	2006	2012	2019	rVV	469563	862805	16.02%	3.227%
26	13.853	2019	2023	2035	rVB3	221881	405667	7.53%	1.517%
27	14.241	2083	2089	2093	rBV	150323	255352	4.74%	0.955%
28	14.294	2093	2098	2108	rVB	320500	553898	10.28%	2.072%
29	14.447	2112	2124	2133	rBV5	45455	117722	2.19%	0.440%
30	14.629	2150	2155	2156	rBV2	52790	69579	1.29%	0.260%
31	14.670	2156	2162	2168	rVV	665988	1154914	21.44%	4.320%
32	14.929	2201	2206	2213	rBV7	29964	62652	1.16%	0.234%
33	15.023	2216	2222	2228	rBV7	30756	63586	1.18%	0.238%
34	15.094	2228	2234	2241	rBV	135845	243324	4.52%	0.910%
35	15.258	2256	2262	2267	rBV5	112248	288896	5.36%	1.081%
36	15.323	2267	2273	2277	rBV	1079495	2069457	38.42%	7.741%

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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

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37	15.511	2300	2305	2310	rVB3	58751	98650	1.83%	0.369%
38	15.635	2320	2326	2334	rVB	157873	312848	5.81%	1.170%
39	15.752	2340	2346	2349	rBV5	34172	65256	1.21%	0.244%
40	16.005	2380	2389	2399	rBV2	126347	285919	5.31%	1.070%

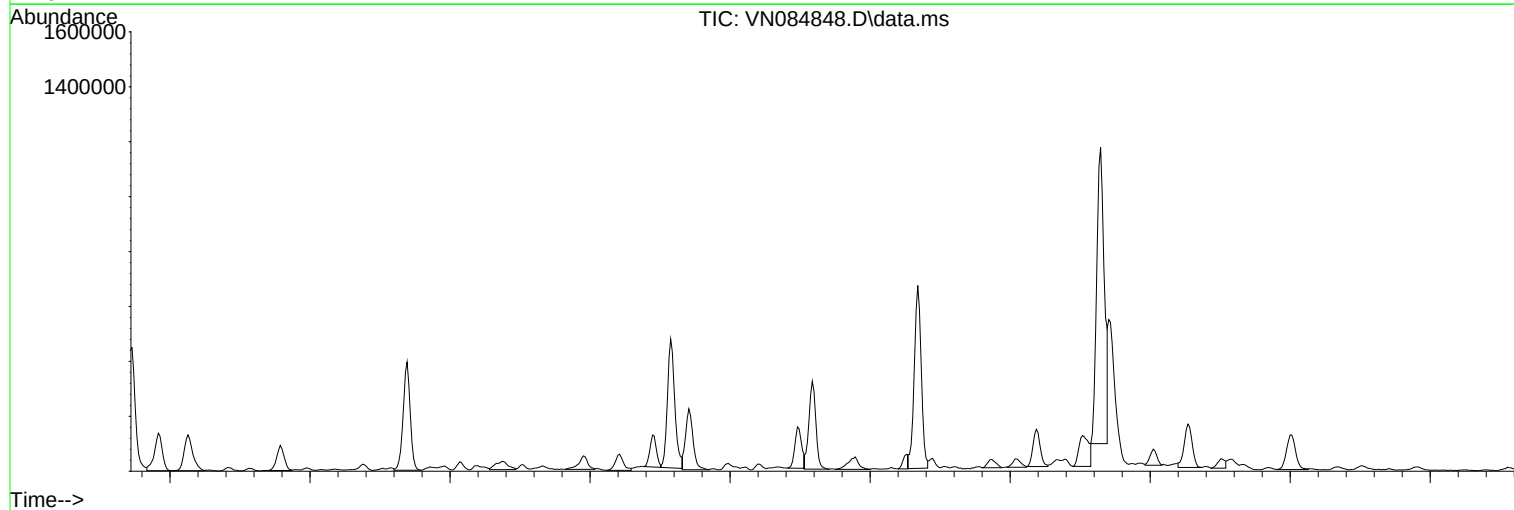
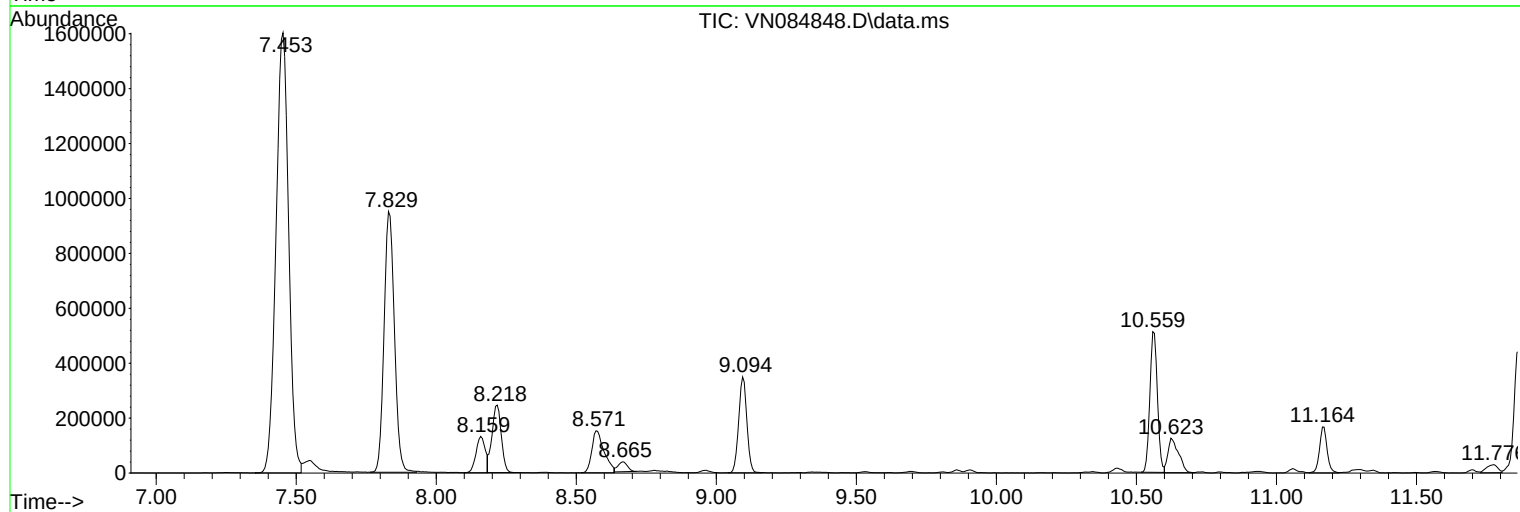
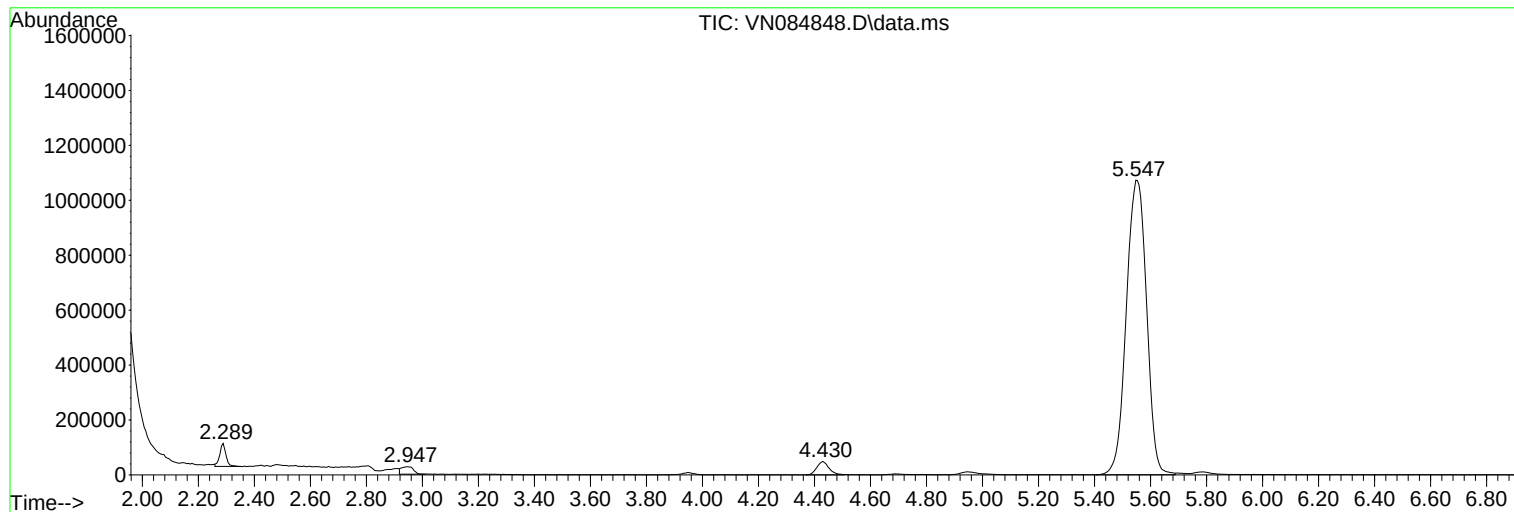
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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



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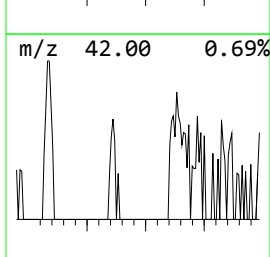
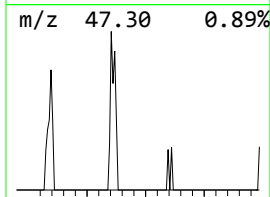
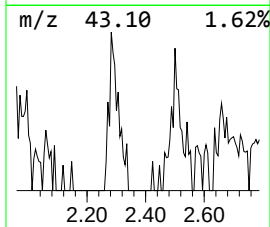
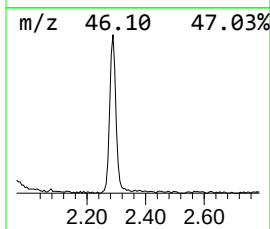
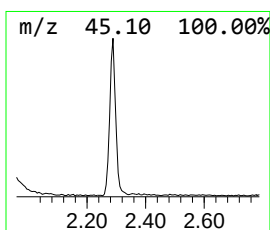
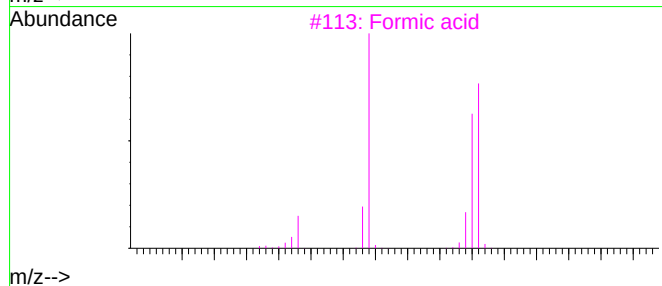
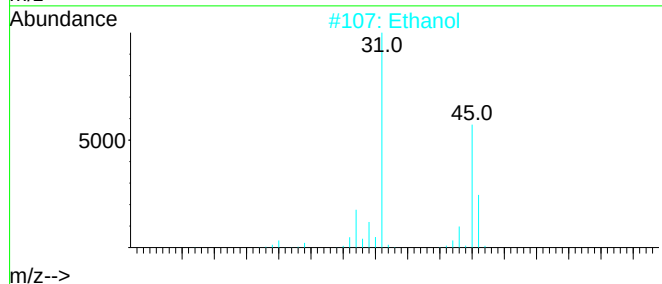
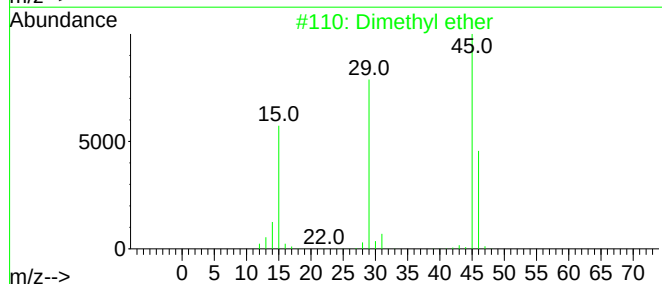
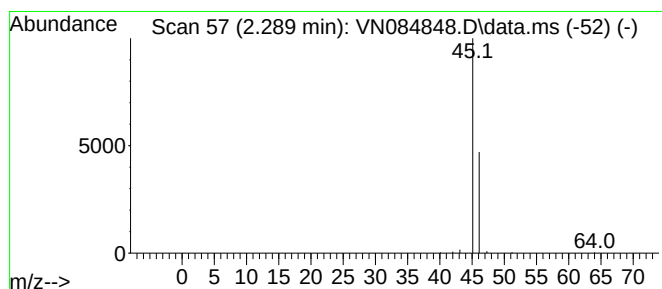
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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

Peak Number 1 Dimethyl ether Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.289	11.34 ug/l	127469	Pentafluorobenzene	8.212

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	74
2	Ethanol	46	C2H6O	000064-17-5	4
3	Formic acid	46	CH2O2	000064-18-6	4
4	Oxalic acid	90	C2H2O4	000144-62-7	4
5	Formamide	45	CH3NO	000075-12-7	2



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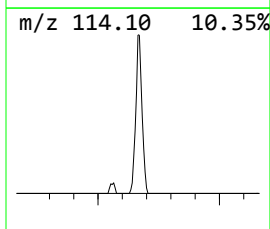
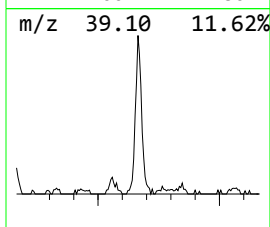
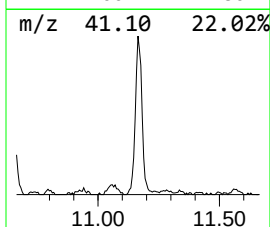
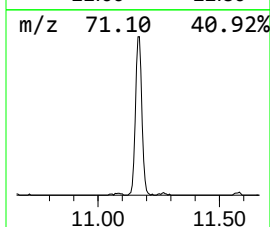
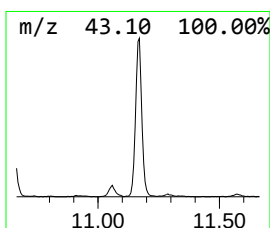
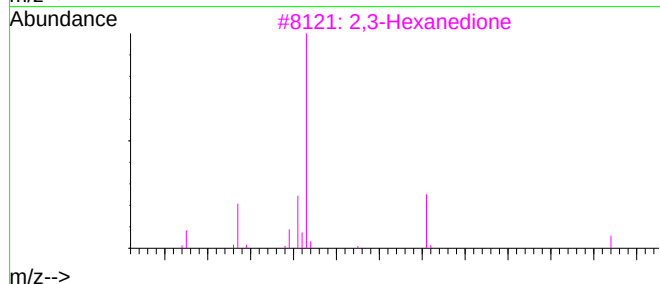
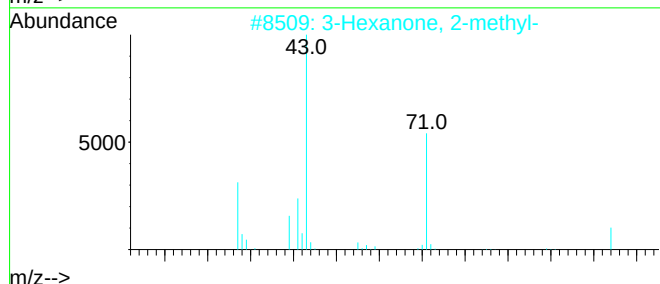
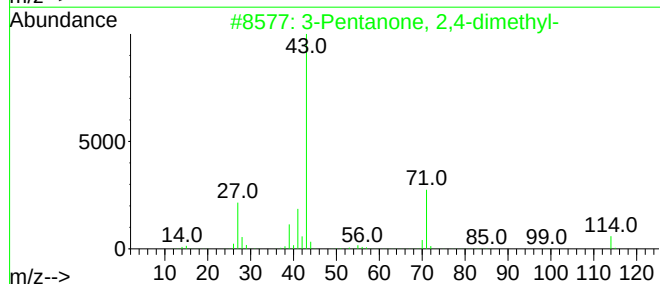
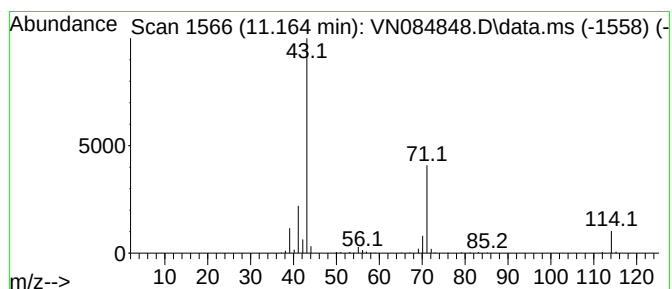
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.165	17.60 ug/l	312570	Chlorobenzene-d5	11.864

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	53
5	Pentane, 2-methyl-	86	C6H14	000107-83-5	36



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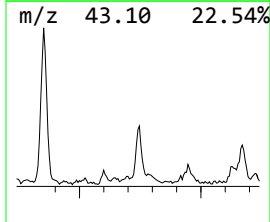
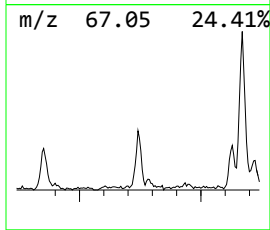
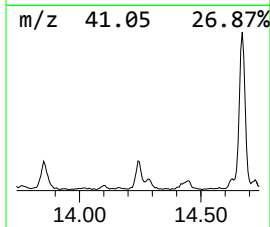
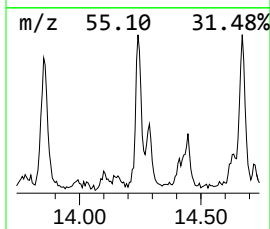
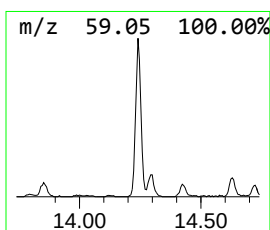
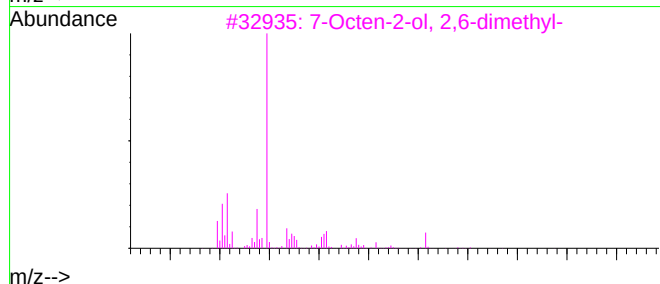
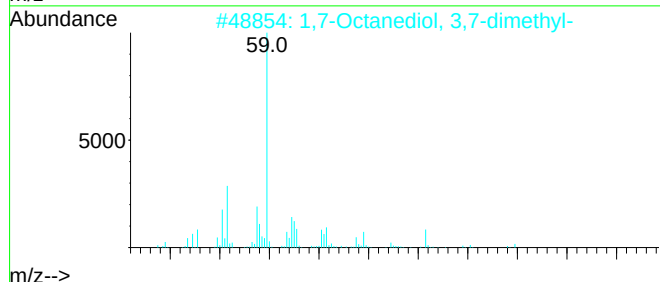
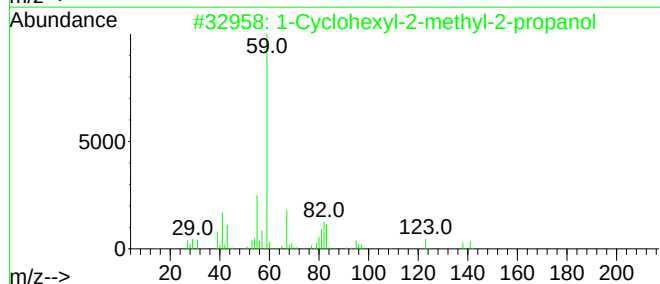
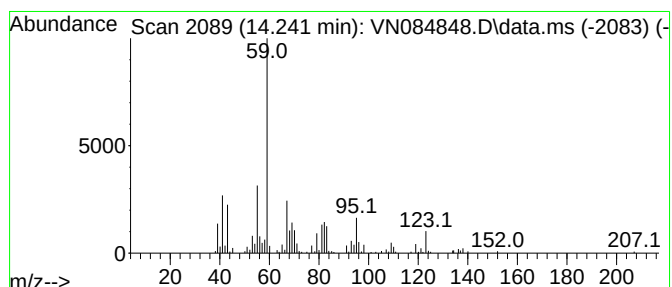
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Cyclohexyl-2-methyl-2-pro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.241	14.80 ug/l	255352	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cyclohexyl-2-methyl-2-propanol	156	C10H20O	005531-30-6	64
2	1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	53
3	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	50
4	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	50
5	3-(2-Hydroxy-2-methyl-propyl)-5,...	196	C12H20O2	077822-60-7	45



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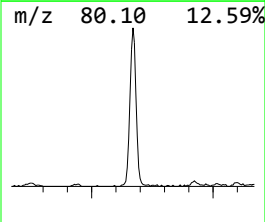
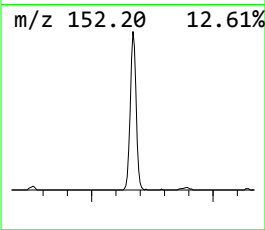
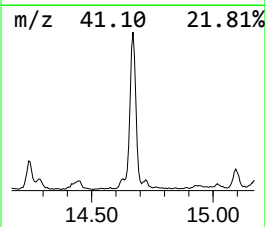
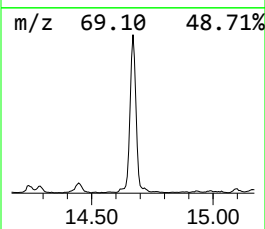
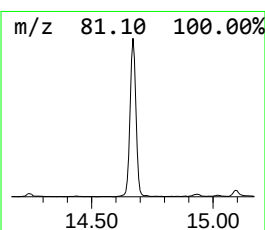
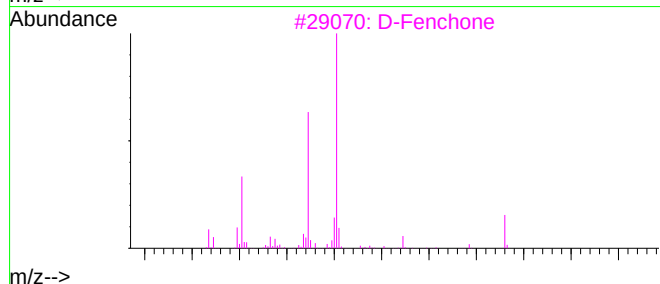
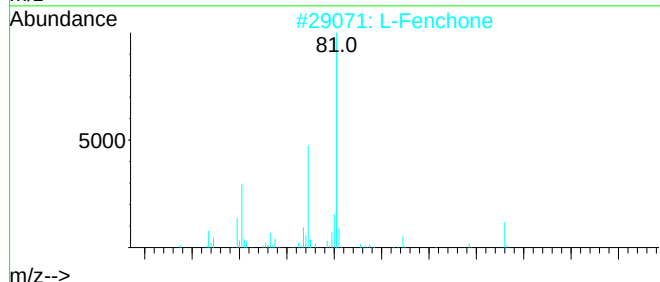
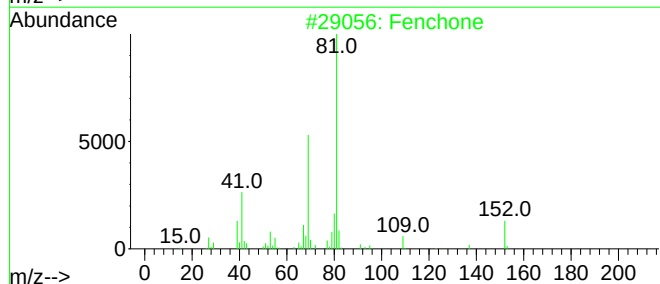
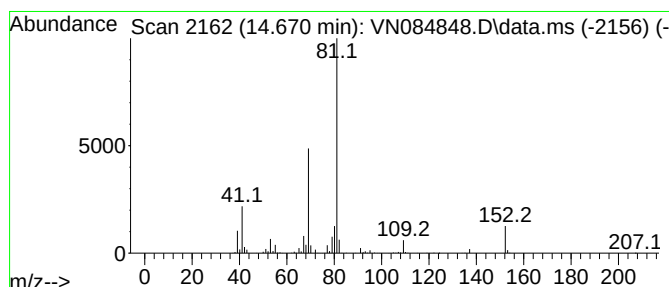
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Fenchone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.670	66.93 ug/l	1154910	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fenchone	152	C10H16O	001195-79-5	95
2	L-Fenchone	152	C10H16O	007787-20-4	94
3	D-Fenchone	152	C10H16O	004695-62-9	46
4	1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3N02	1000301-43-3	42
5	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	42



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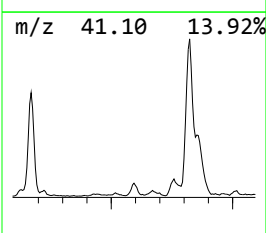
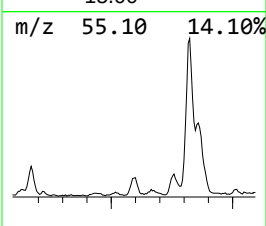
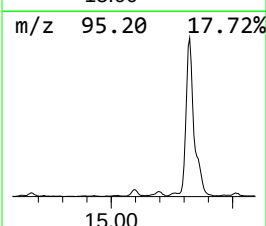
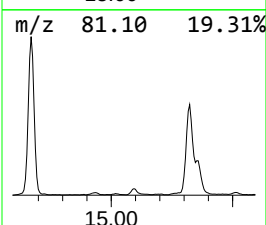
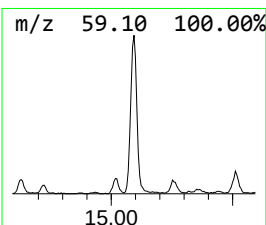
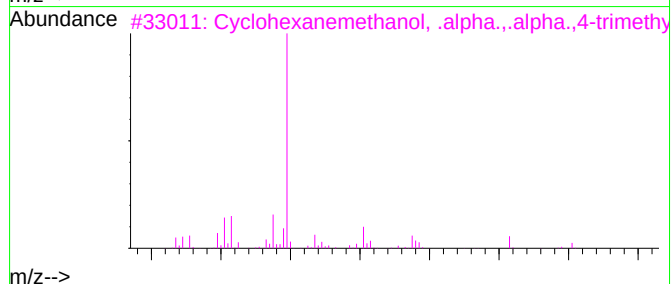
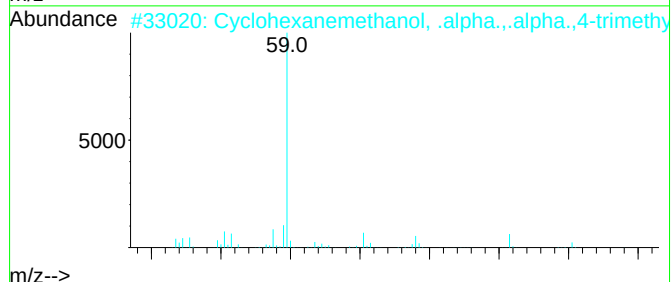
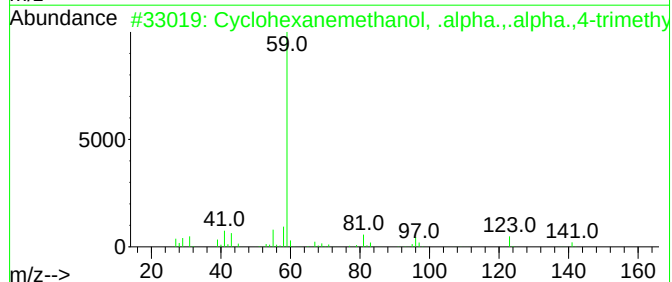
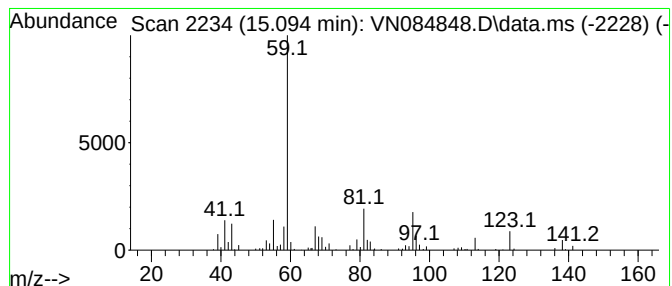
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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

Peak Number 7 Cyclohexanemethanol, .alpha... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.094	14.10 ug/l	243324	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	007322-63-6	64
2	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	005114-00-1	64
3	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	64
4	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	59
5	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111424\
Data File : VN084848.D
Acq On : 14 Nov 2024 13:48
Operator : JC\MD
Sample : P4844-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
241113075-01-VOA

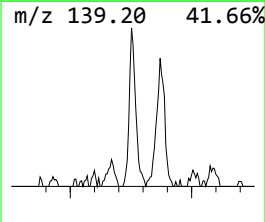
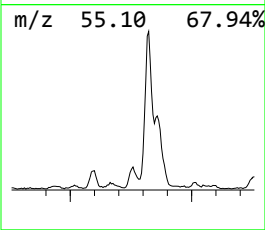
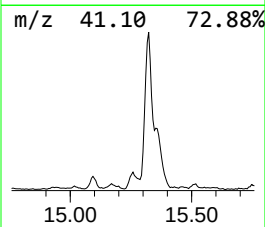
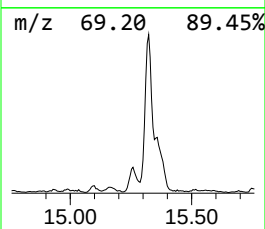
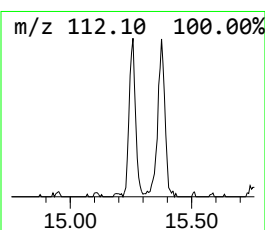
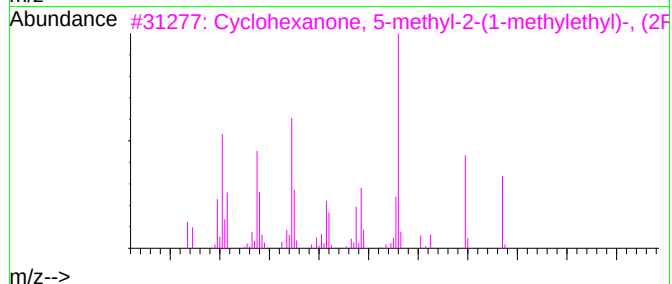
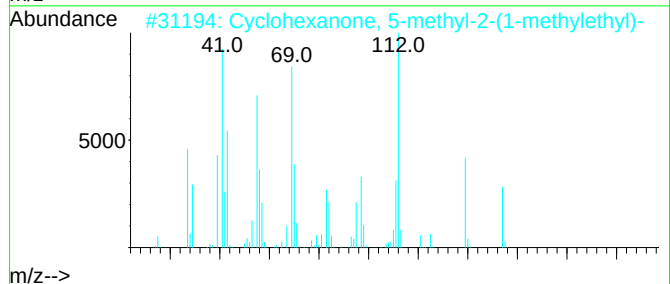
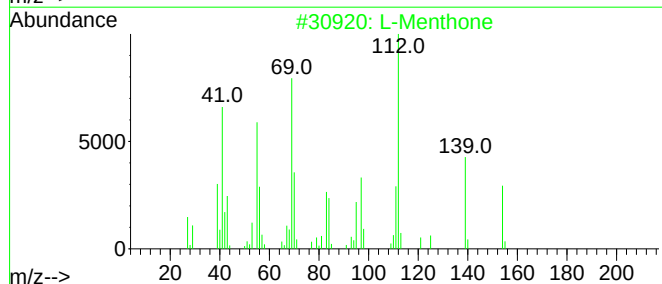
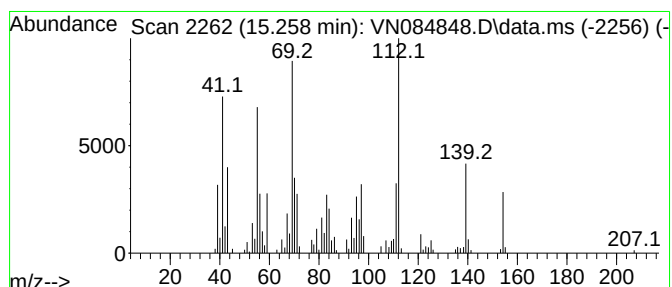
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Quant Title : SW846 8260

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

Peak Number 8 L-Menthone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.258	16.74 ug/l	288896	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Menthone	154	C10H18O	014073-97-3	98
2	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	010458-14-7	93
3	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	001196-31-2	91
4	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000491-07-6	91
5	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000089-80-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111424\
Data File : VN084848.D
Acq On : 14 Nov 2024 13:48
Operator : JC\MD
Sample : P4844-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

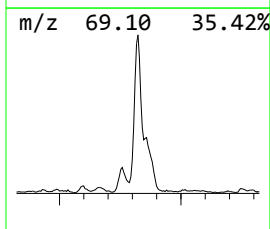
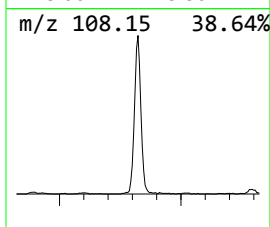
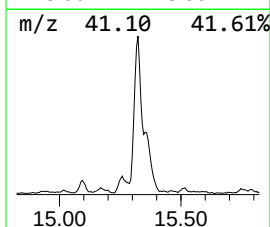
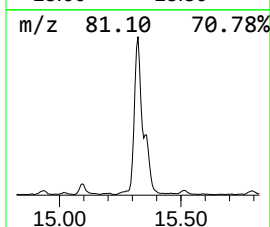
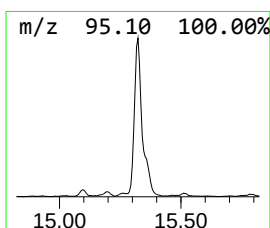
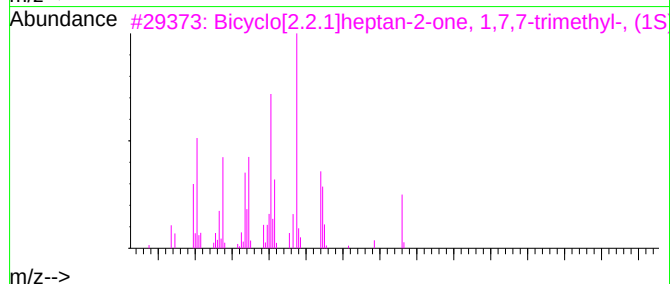
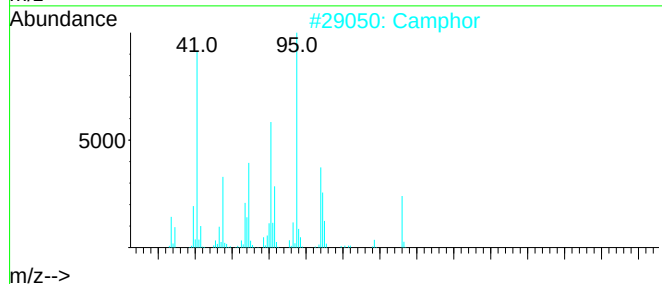
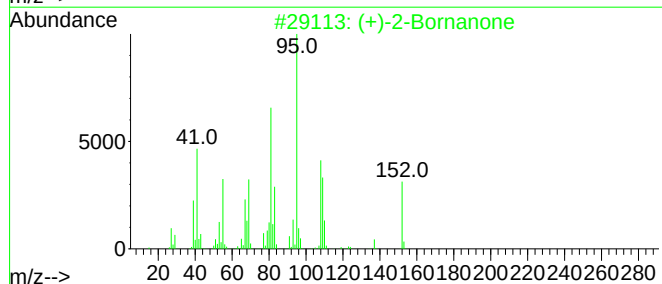
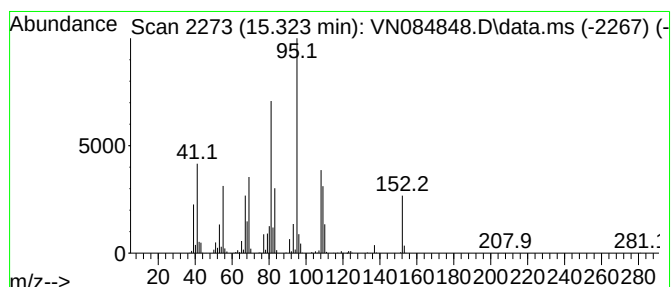
Instrument :
MSVOA_N
ClientSampleId :
241113075-01-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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

Peak Number 9 (+)-2-Bornanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.323	119.93 ug/l	2069460	1,4-Dichlorobenzene-d4	13.788	
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	49
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111424\
Data File : VN084848.D
Acq On : 14 Nov 2024 13:48
Operator : JC\MD
Sample : P4844-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
241113075-01-VOA

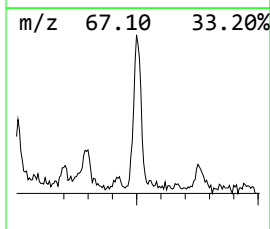
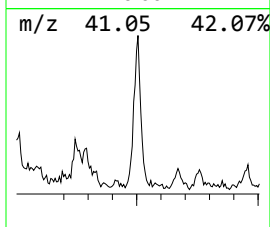
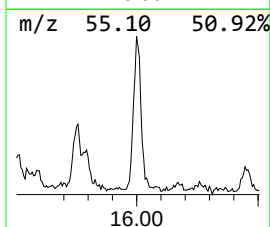
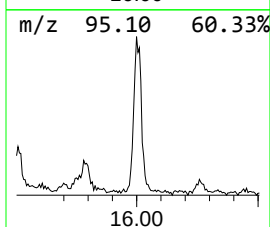
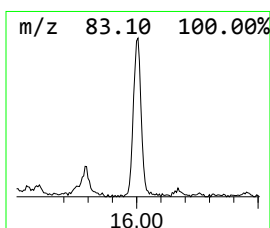
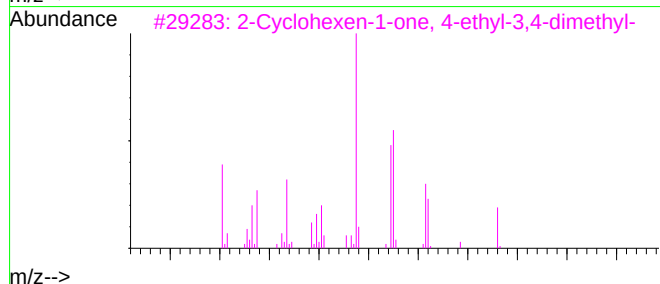
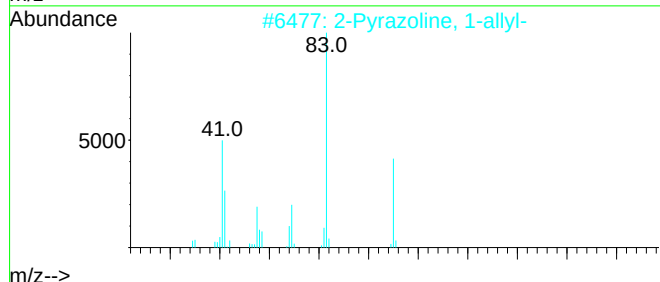
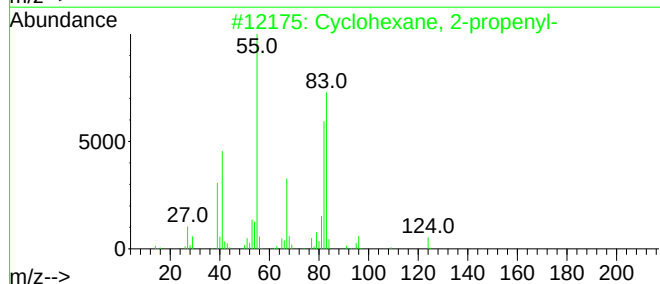
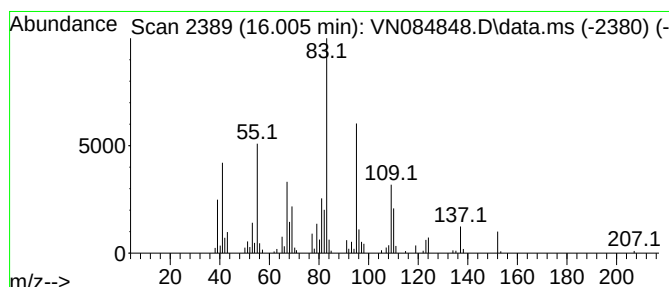
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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

Peak Number 10 unknown16.005 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.005	16.57 ug/l	285919	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	43
2	2-Pyrazoline, 1-allyl-	110	C6H10N2	019804-38-7	35
3	2-Cyclohexen-1-one, 4-ethyl-3,4-...	152	C10H16O	017622-46-7	30
4	3-Methyl-2-butenic acid, oct-3-...	210	C13H22O2	1000299-31-2	27
5	Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	1000150-99-3	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111424\
Data File : VN084848.D
Acq On : 14 Nov 2024 13:48
Operator : JC\MD
Sample : P4844-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
241113075-01-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.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
Dimethyl ether	2.289	11.3	ug/l	127469	1	8.212	562277	50.0
3-Pentanone, 2,...	11.165	17.6	ug/l	312570	3	11.864	887988	50.0
1-Cyclohexyl-2-...	14.241	14.8	ug/l	255352	4	13.788	862805	50.0
Fenchone	14.670	66.9	ug/l	1154910	4	13.788	862805	50.0
Cyclohexanemeth...	15.094	14.1	ug/l	243324	4	13.788	862805	50.0
L-Menthone	15.258	16.7	ug/l	288896	4	13.788	862805	50.0
(+)-2-Bornanone	15.323	119.9	ug/l	2069460	4	13.788	862805	50.0
unknown16.005	16.005	16.6	ug/l	285919	4	13.788	862805	50.0