

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031424\
Data File : VN081407.D
Acq On : 14 Mar 2024 14:05
Operator : JC\MD
Sample : P1727-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240313044-02-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\82N030524W.M
Title : SW846 8260

Signal : TIC: VN081407.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	52	58	67	rVB	261941	420190	4.10%	0.915%
2	4.442	411	423	434	rBV3	45635	147956	1.44%	0.322%
3	5.512	590	605	629	rBV	2739117	9608773	93.78%	20.915%
4	5.794	643	653	665	rVB2	39654	130184	1.27%	0.283%
5	7.435	919	932	947	rBV	3908781	10246083	100.00%	22.302%
6	7.835	989	1000	1024	rVB	1702287	4336991	42.33%	9.440%
7	8.171	1047	1057	1061	rBV	256457	610365	5.96%	1.329%
8	8.224	1061	1066	1079	rVB	488767	1093379	10.67%	2.380%
9	8.577	1110	1126	1136	rBV3	335214	1085426	10.59%	2.363%
10	8.653	1137	1139	1145	rVB2	66993	112691	1.10%	0.245%
11	9.100	1206	1215	1226	rBV	687880	1420198	13.86%	3.091%
12	10.571	1457	1465	1472	rBV	1053472	1960399	19.13%	4.267%
13	10.653	1472	1479	1488	rVB4	111123	298249	2.91%	0.649%
14	11.171	1557	1567	1577	rBV	243118	459775	4.49%	1.001%
15	11.776	1662	1670	1675	rVV6	54072	150647	1.47%	0.328%
16	11.870	1675	1686	1695	rVV	924666	1890704	18.45%	4.115%
17	11.965	1695	1702	1711	rVB3	126268	308978	3.02%	0.673%
18	12.070	1713	1720	1730	rVV	208680	441764	4.31%	0.962%
19	12.400	1768	1776	1782	rBV	151544	277541	2.71%	0.604%
20	12.853	1845	1853	1861	rVB	679186	1232721	12.03%	2.683%
21	13.194	1903	1911	1916	rVB5	44688	111981	1.09%	0.244%
22	13.482	1947	1960	1967	rBV3	90856	210919	2.06%	0.459%
23	13.612	1973	1982	1987	rBV2	112147	221239	2.16%	0.482%
24	13.794	2005	2013	2020	rBV	823485	1571851	15.34%	3.421%
25	13.859	2020	2024	2036	rVB2	239783	455390	4.44%	0.991%
26	13.994	2042	2047	2062	rVB2	81357	191547	1.87%	0.417%
27	14.241	2082	2089	2095	rBV3	378318	757456	7.39%	1.649%
28	14.300	2095	2099	2108	rVB3	124528	245727	2.40%	0.535%
29	14.447	2112	2124	2131	rBV8	85238	252850	2.47%	0.550%
30	14.635	2150	2156	2157	rBV2	103170	141217	1.38%	0.307%
31	14.676	2157	2163	2169	rVB	1176165	1956772	19.10%	4.259%
32	14.941	2202	2208	2215	rVB6	60014	105624	1.03%	0.230%
33	15.029	2216	2223	2230	rBV3	73962	150249	1.47%	0.327%
34	15.170	2244	2247	2257	rVB5	42525	109791	1.07%	0.239%
35	15.282	2257	2266	2268	rBV6	198497	477381	4.66%	1.039%
36	15.329	2268	2274	2278	rBV	1011647	1936107	18.90%	4.214%

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ClientSampleId :
240313044-02-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\82N030524W.M
Title : SW846 8260

37	15.800	2349	2354	2366	rVB4	104578	269065	2.63%	0.586%
38	16.011	2382	2390	2403	rBV2	252521	543870	5.31%	1.184%

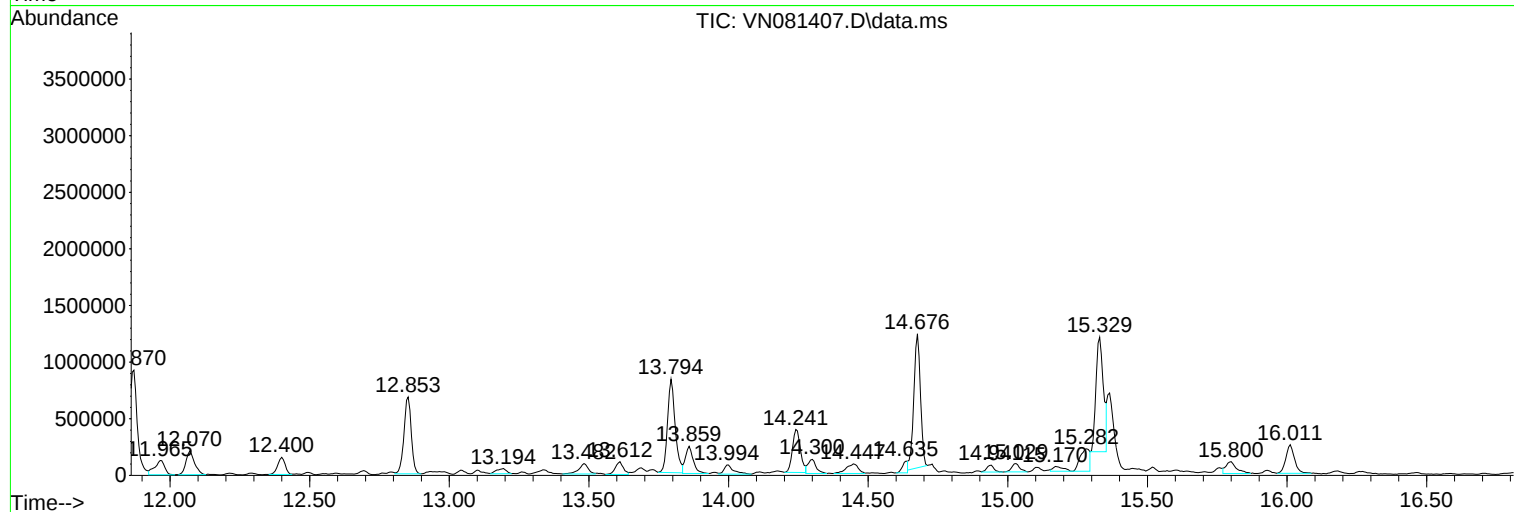
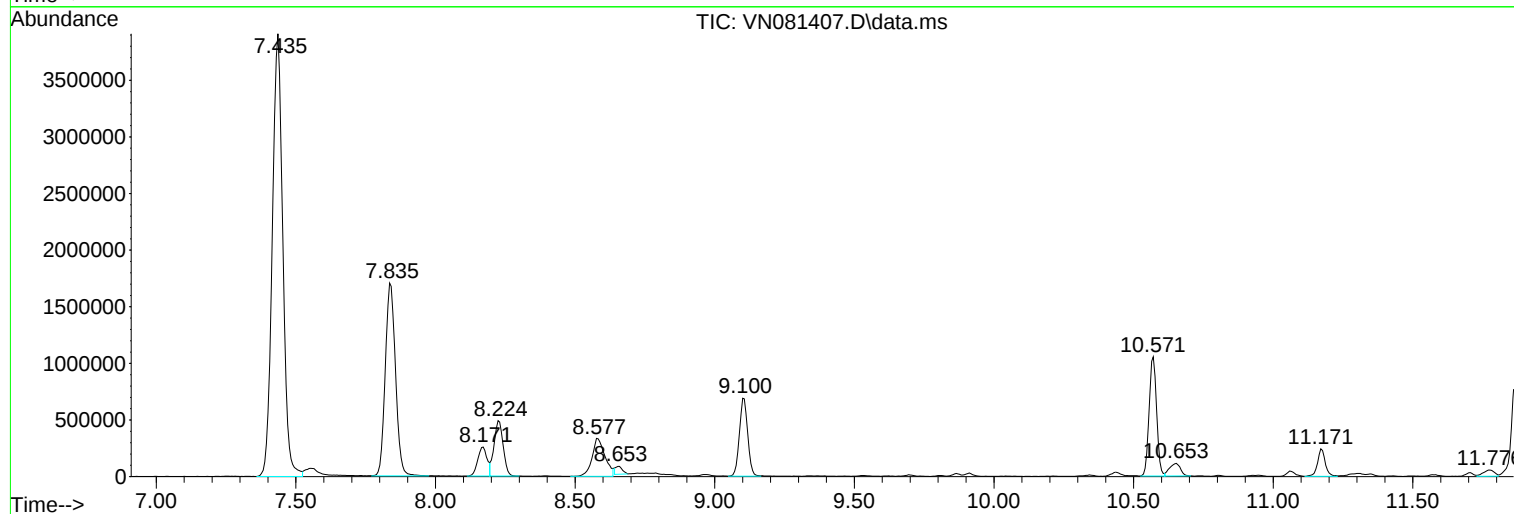
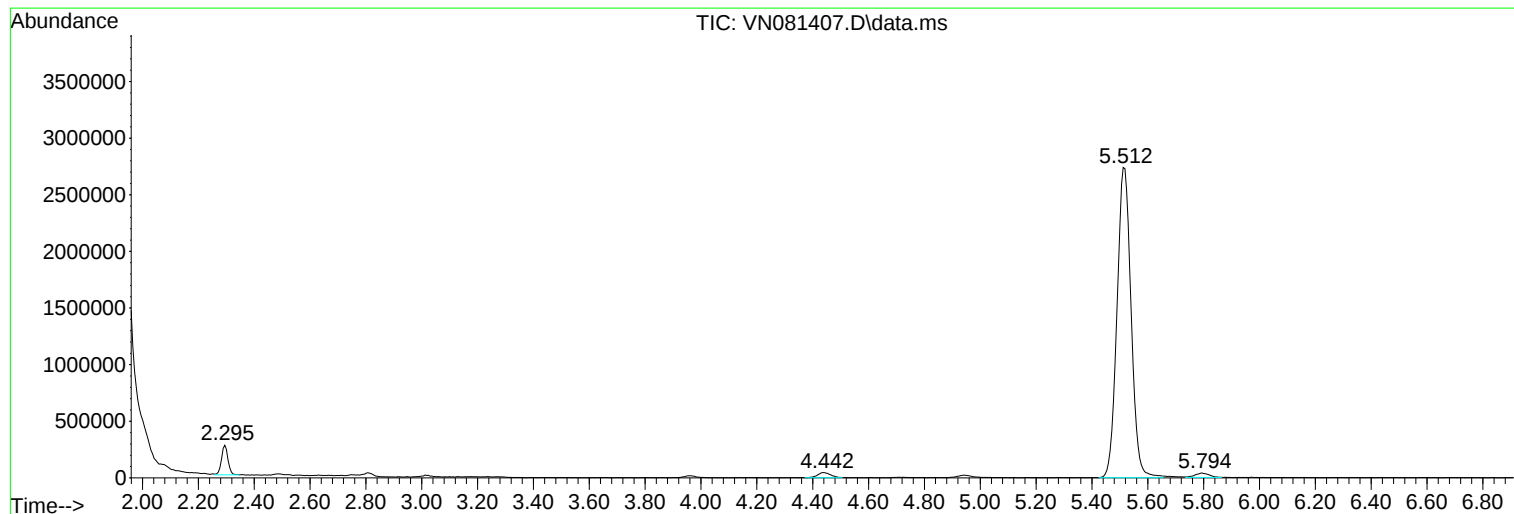
Sum of corrected areas: 45942050

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240313044-02-VOA

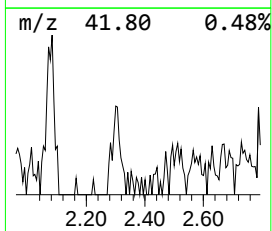
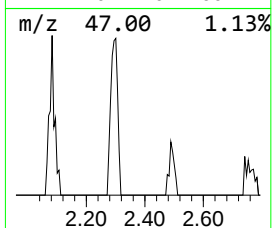
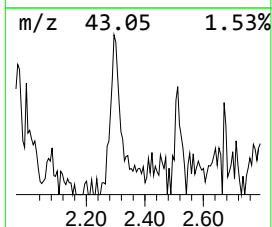
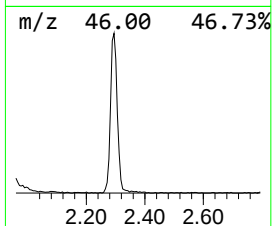
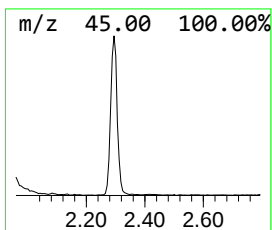
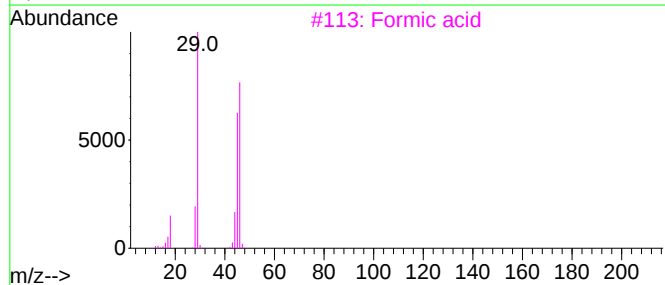
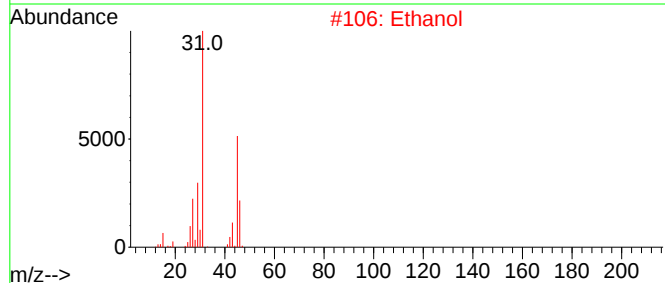
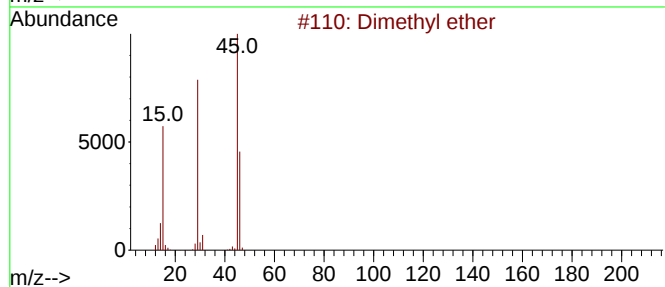
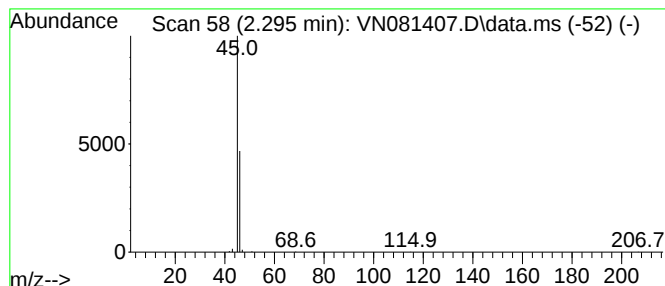
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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

Peak Number 1 Dimethyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.295	19.22 ug/l	420190	Pentafluorobenzene	8.230

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	7
3			Formic acid	46	CH2O2	000064-18-6	7
4			Oxalic acid	90	C2H2O4	000144-62-7	4
5			Methane, nitroso-	45	CH3NO	000865-40-7	3



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Sample : P1727-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

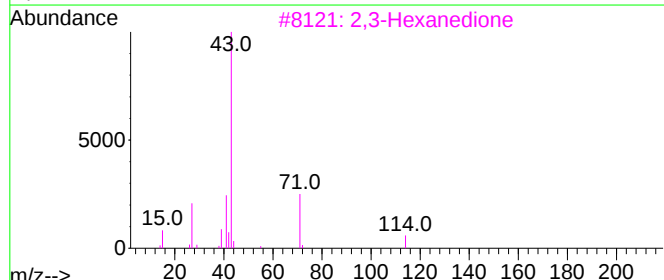
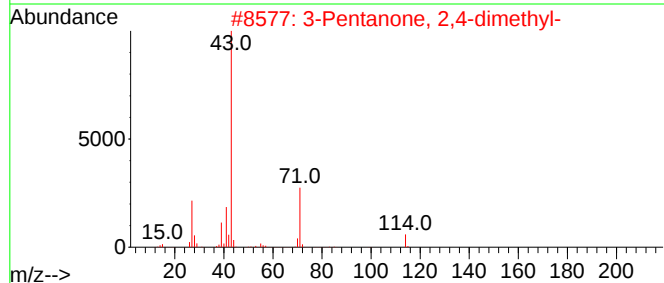
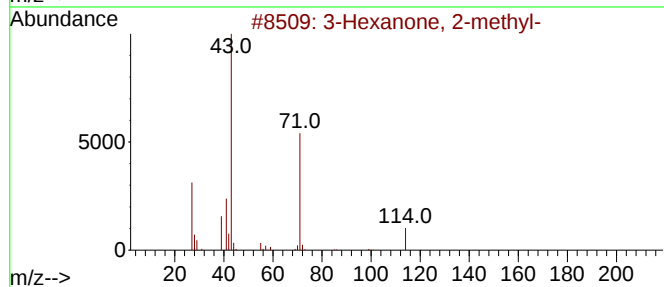
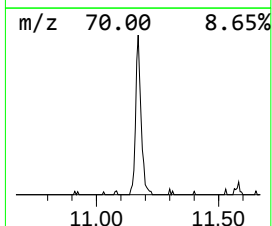
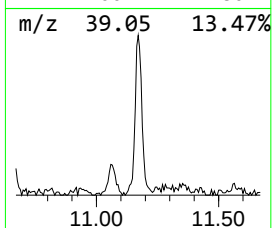
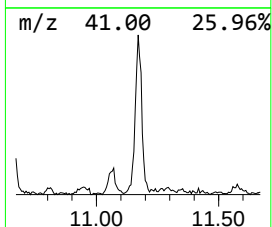
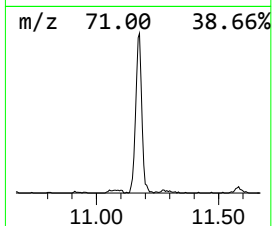
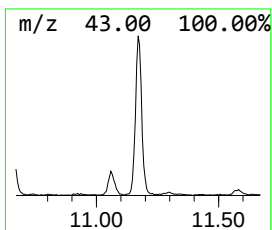
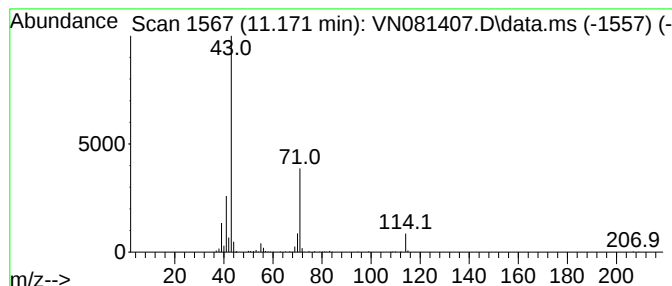
Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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

Peak Number 3 3-Hexanone, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.171	12.16 ug/l	459775	Chlorobenzene-d5		11.871	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-Hexanone, 2-methyl-		114	C7H14O	007379-12-6	86
2	3-Pentanone, 2,4-dimethyl-		114	C7H14O	000565-80-0	86
3	2,3-Hexanedione		114	C6H10O2	003848-24-6	64
4	Pyrrolidine		71	C4H9N	000123-75-1	53
5	4-Heptanone		114	C7H14O	000123-19-3	42



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240313044-02-VOA

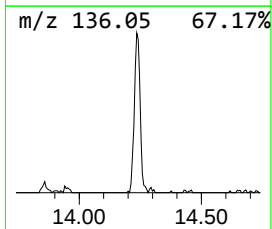
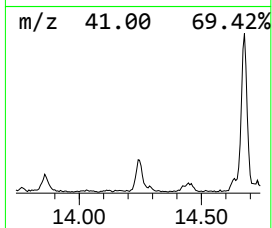
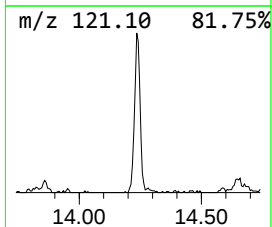
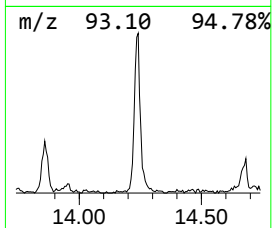
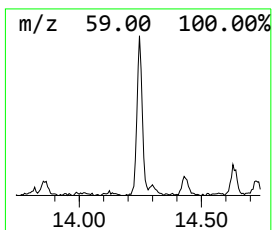
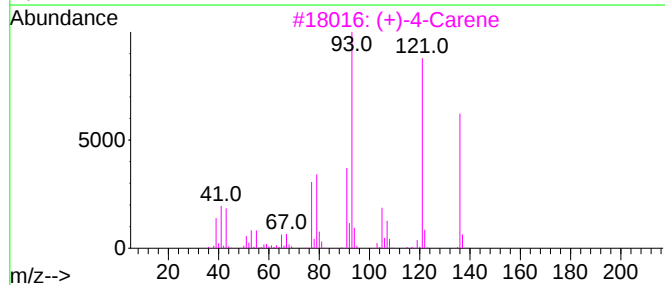
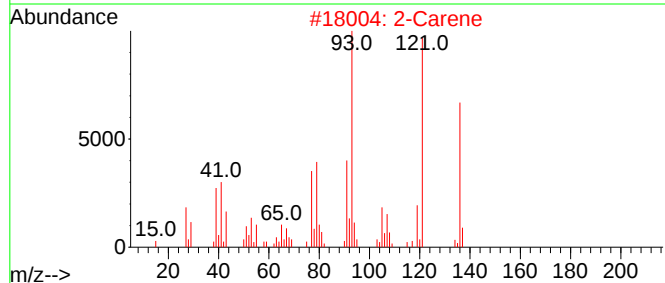
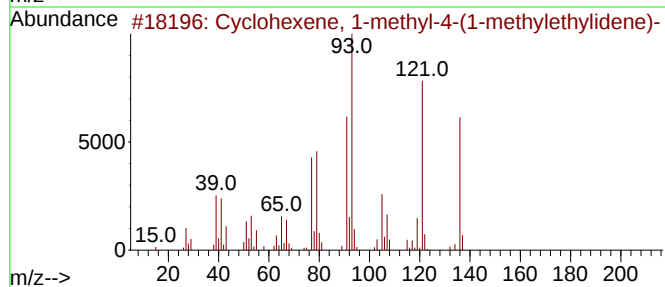
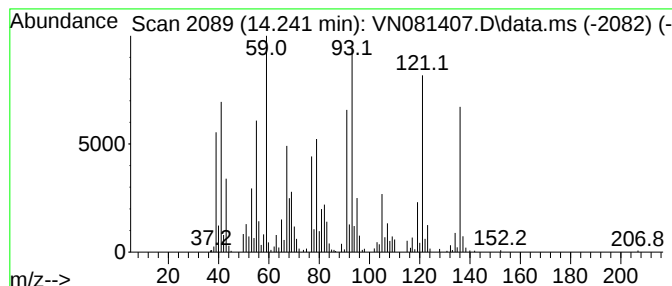
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.241	24.09 ug/l	757456	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	97
2			2-Carene	136	C10H16	000554-61-0	92
3			(+)-4-Carene	136	C10H16	029050-33-7	91
4			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	83
5			Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	000586-63-0	64



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Instrument :
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ClientSampleId :
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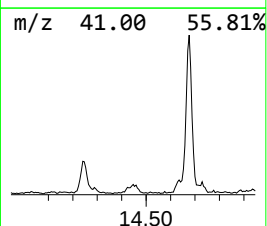
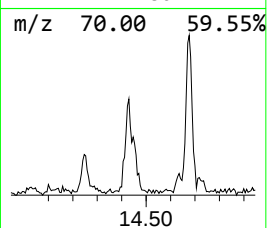
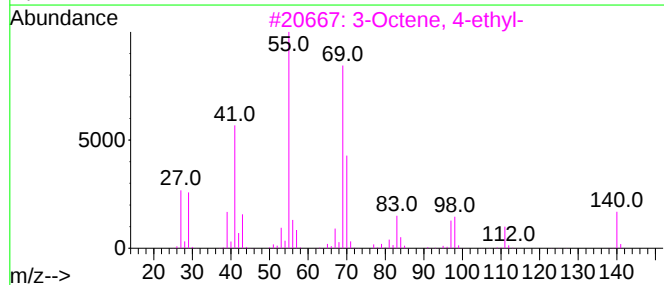
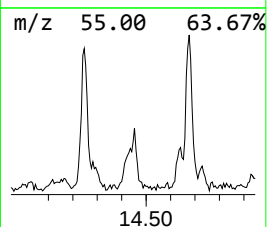
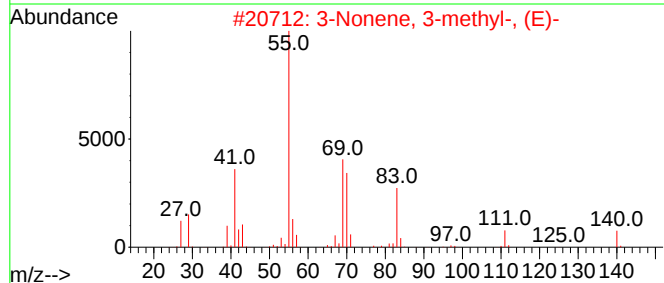
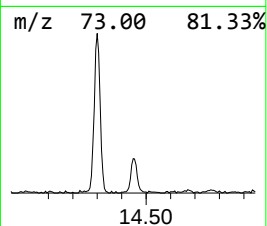
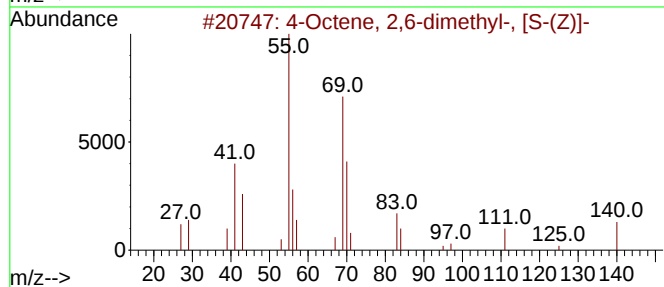
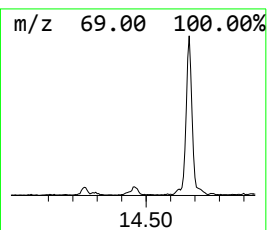
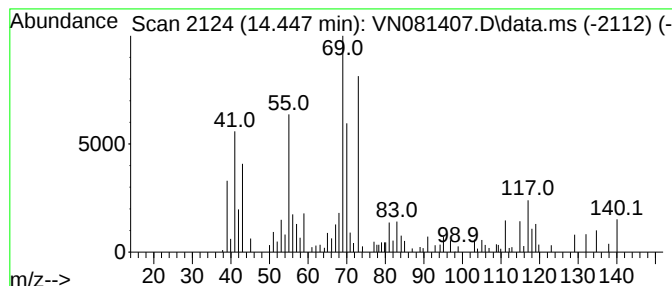
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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

Peak Number 5 4-Octene, 2,6-dimethyl-, [S... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	8.04 ug/l	252850	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Octene, 2,6-dimethyl-, [S-(Z)]-	140	C10H20	062960-77-4	53
2			3-Nonene, 3-methyl-, (E)-	140	C10H20	069405-42-1	53
3			3-Octene, 4-ethyl-	140	C10H20	053966-51-1	53
4			2-Octene, 4-ethyl-, (E)-	140	C10H20	074630-09-4	47
5			Cyclopentane, pentyl-	140	C10H20	003741-00-2	47



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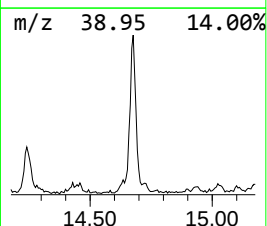
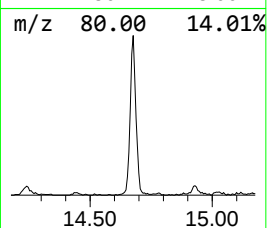
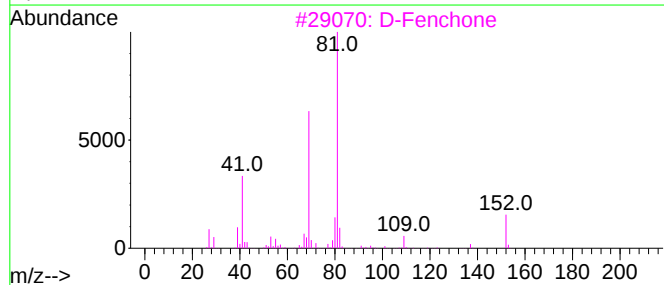
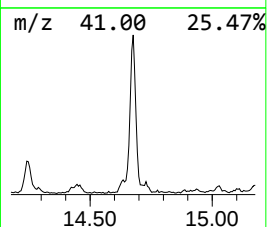
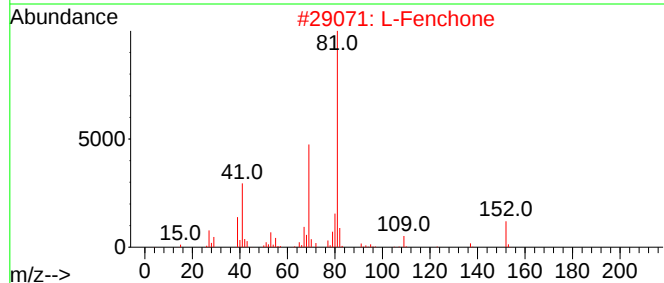
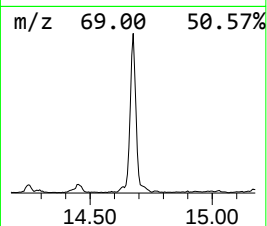
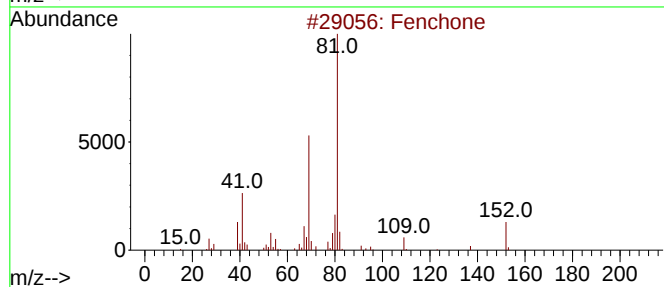
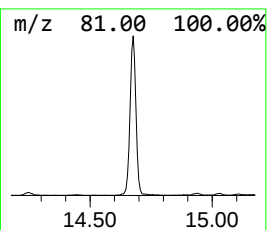
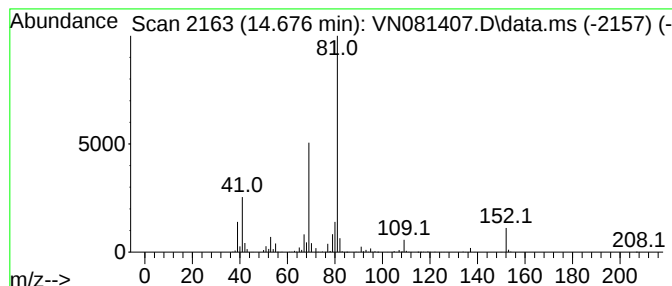
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Quant Title : SW846 8260

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.
14.676	62.24 ug/l	1956770	1,4-Dichlorobenzene-d4	13.794

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	95
3			D-Fenchone	152	C10H16O	004695-62-9	94
4			1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3NO2	1000301-43-3	36
5			2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	36



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031424\
Data File : VN081407.D
Acq On : 14 Mar 2024 14:05
Operator : JC\MD
Sample : P1727-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240313044-02-VOA

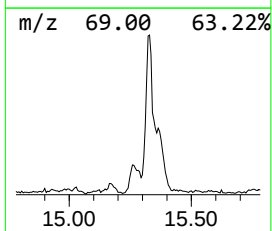
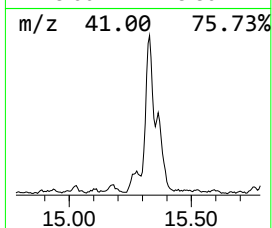
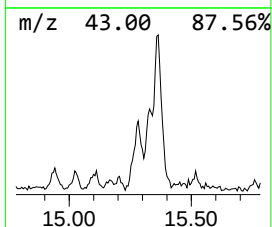
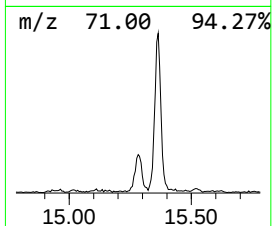
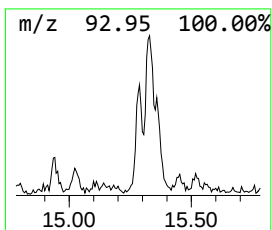
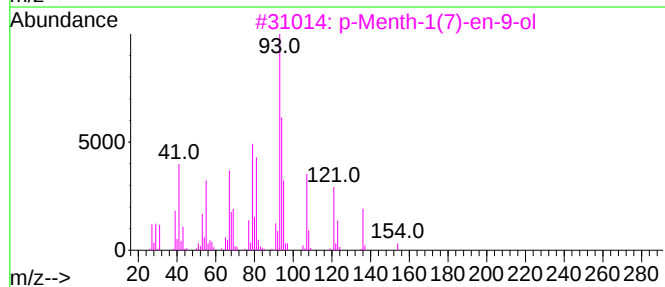
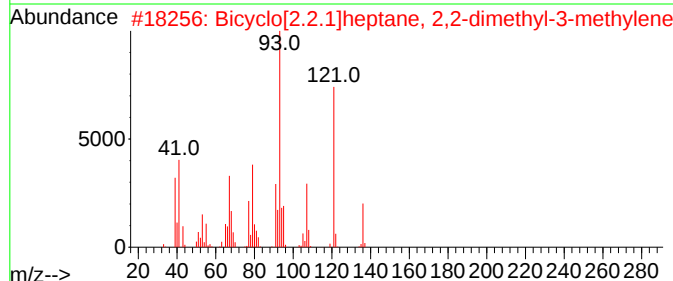
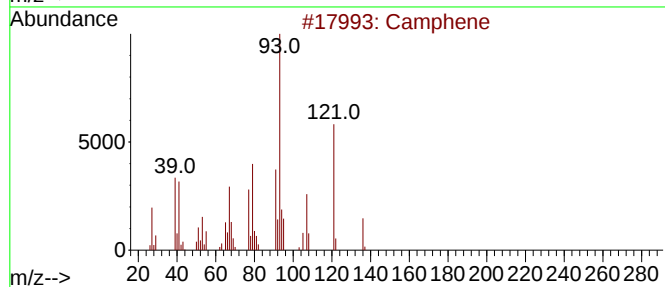
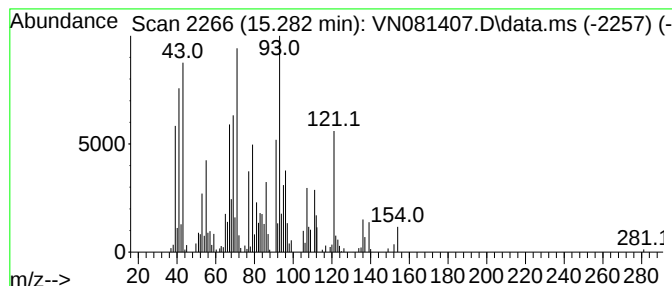
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Quant Title : SW846 8260

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

Peak Number 7 Camphene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.282	15.19 ug/l	477381	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphene	136	C10H16	000079-92-5	86
2			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	80
3			p-Menth-1(7)-en-9-ol	154	C10H18O	029548-16-1	49
4			Cyclohexene, 1-methyl-3-(1-methy...	136	C10H16	000499-03-6	46
5			p-Menth-2-en-7-ol, trans-	154	C10H18O	019898-87-4	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031424\
Data File : VN081407.D
Acq On : 14 Mar 2024 14:05
Operator : JC\MD
Sample : P1727-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240313044-02-VOA

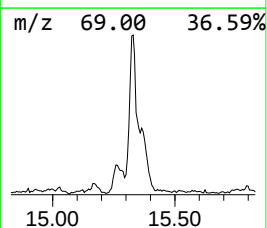
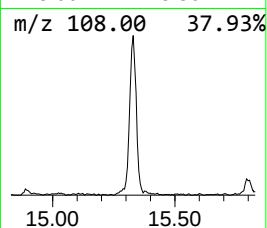
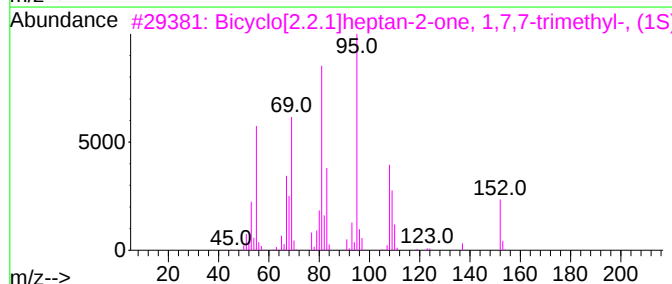
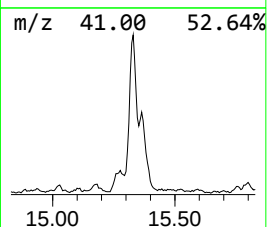
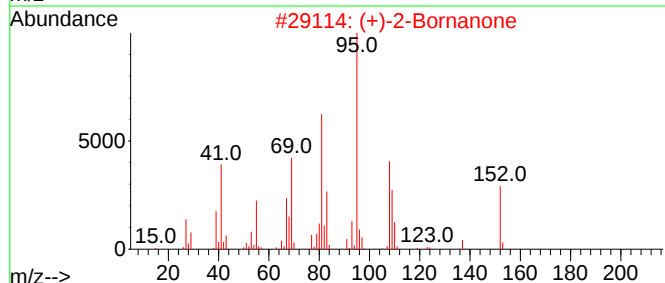
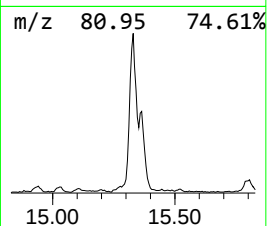
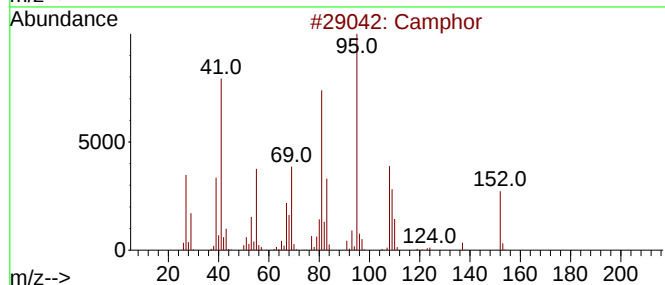
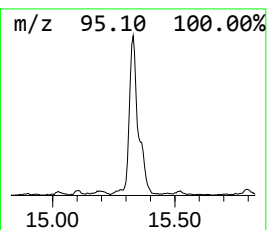
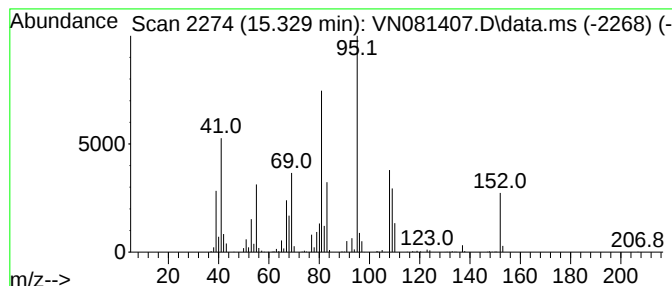
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Quant Title : SW846 8260

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

Peak Number 8 Camphor Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.329	61.59 ug/l	1936110	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphor	152	C10H16O	000076-22-2	96
2			(+)-2-Bornanone	152	C10H16O	000464-49-3	94
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	94
4			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	45
5			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031424\
Data File : VN081407.D
Acq On : 14 Mar 2024 14:05
Operator : JC\MD
Sample : P1727-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240313044-02-VOA

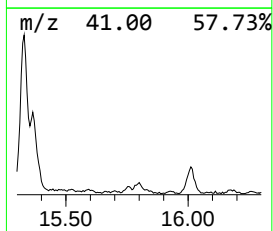
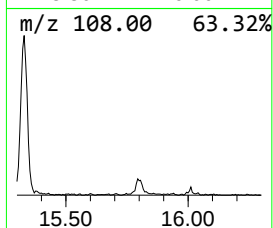
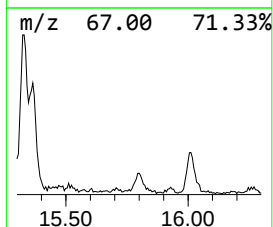
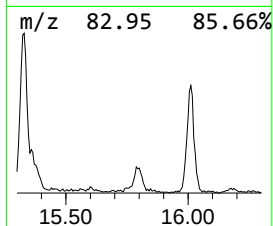
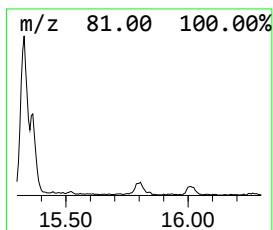
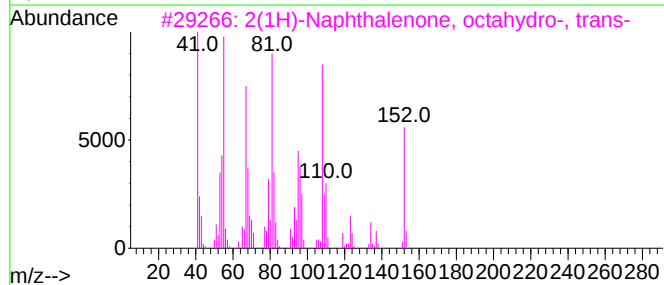
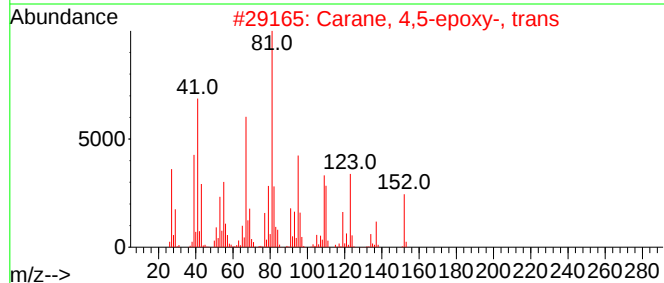
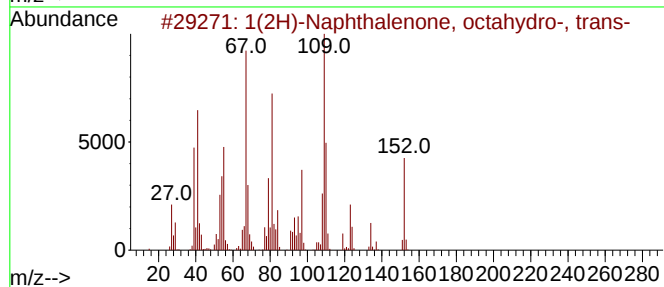
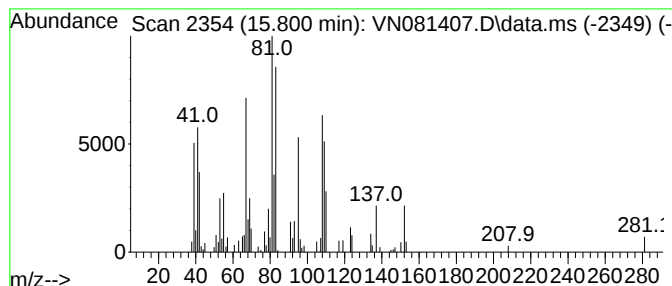
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Quant Title : SW846 8260

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

Peak Number 9 1(2H)-Naphthalenone, octahy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.800	8.56 ug/l	269065	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1(2H)-Naphthalenone, octahydro-,...	152	C10H16O	021370-71-8	70
2			Carane, 4,5-epoxy-, trans	152	C10H16O	006909-20-2	60
3			2(1H)-Naphthalenone, octahydro-,...	152	C10H16O	016021-08-2	58
4			Pulegone	152	C10H16O	000089-82-7	46
5			Bicyclo[3.1.0]hexan-3-one, 4-met...	152	C10H16O	001125-12-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031424\
Data File : VN081407.D
Acq On : 14 Mar 2024 14:05
Operator : JC\MD
Sample : P1727-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240313044-02-VOA

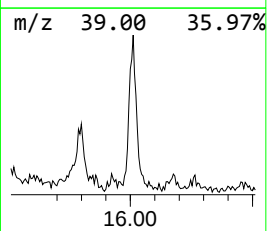
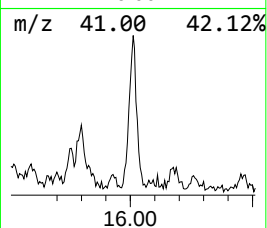
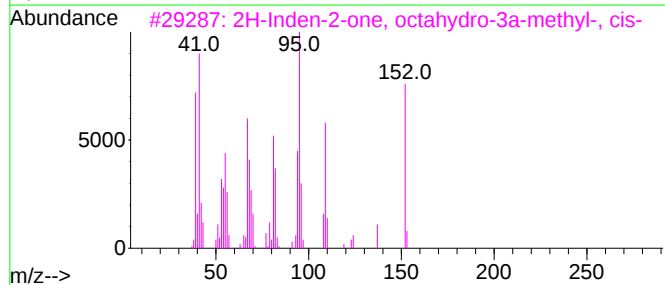
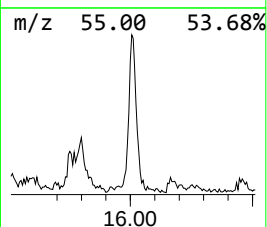
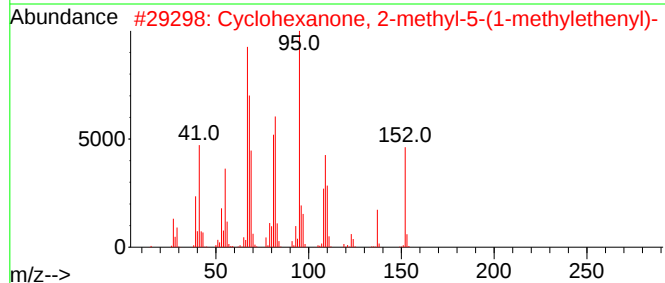
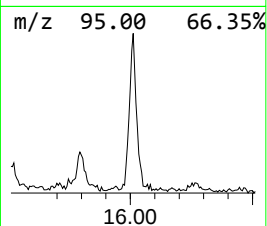
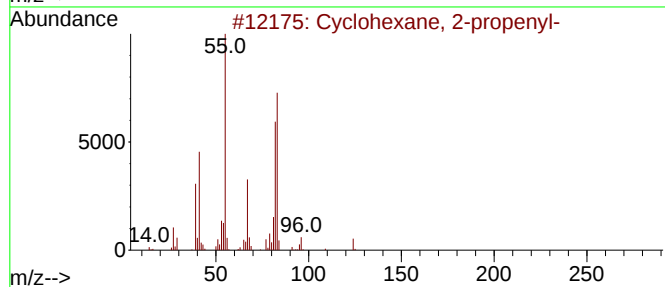
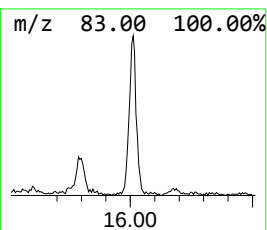
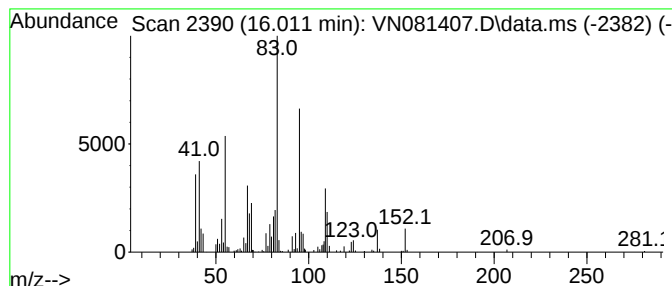
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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

Peak Number 10 Cyclohexane, 2-propenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.011	17.30 ug/l	543870	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	50
2			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	007764-50-3	46
3			2H-Inden-2-one, octahydro-3a-met...	152	C10H16O	013351-29-6	43
4			Bicyclo[2.2.1]heptane, 2-butyl-	152	C11H20	061177-16-0	38
5			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031424\
Data File : VN081407.D
Acq On : 14 Mar 2024 14:05
Operator : JC\MD
Sample : P1727-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240313044-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.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	2.295	19.2	ug/l	420190	1	8.230	1093380	50.0
3-Hexanone, 2-m...	11.171	12.2	ug/l	459775	3	11.871	1890700	50.0
Cyclohexene, 1-...	14.241	24.1	ug/l	757456	4	13.794	1571850	50.0
4-Octene, 2,6-d...	14.447	8.0	ug/l	252850	4	13.794	1571850	50.0
Fenchone	14.676	62.2	ug/l	1956770	4	13.794	1571850	50.0
Camphene	15.282	15.2	ug/l	477381	4	13.794	1571850	50.0
Camphor	15.329	61.6	ug/l	1936110	4	13.794	1571850	50.0
1(2H)-Naphthale...	15.800	8.6	ug/l	269065	4	13.794	1571850	50.0
Cyclohexane, 2-...	16.011	17.3	ug/l	543870	4	13.794	1571850	50.0