

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
 Data File : VN083842.D
 Acq On : 12 Sep 2024 19:30
 Operator : JC\MD
 Sample : P3966-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 VOA-240911078-02

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\82N091024W.M
 Title : SW846 8260

Signal : TIC: VN083842.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	68	rVB	81790	140498	2.96%	0.630%
2	2.942	164	168	175	rVB4	26127	52381	1.10%	0.235%
3	4.430	408	421	442	rBV2	105887	334540	7.04%	1.500%
4	5.542	588	610	630	rBV	999518	3880000	81.62%	17.392%
5	5.789	643	652	664	rVB2	17449	57267	1.20%	0.257%
6	7.447	920	934	949	rBV2	1462928	4753813	100.00%	21.309%
7	7.836	985	1000	1016	rBV	657355	1705108	35.87%	7.643%
8	8.165	1047	1056	1060	rBV	109633	260871	5.49%	1.169%
9	8.218	1060	1065	1075	rVB	179513	407530	8.57%	1.827%
10	8.577	1109	1126	1135	rBV2	129596	401061	8.44%	1.798%
11	8.665	1135	1141	1157	rVB3	80240	269271	5.66%	1.207%
12	9.100	1207	1215	1225	rVV	311512	637331	13.41%	2.857%
13	10.565	1457	1464	1470	rBV	456968	816875	17.18%	3.662%
14	10.629	1470	1475	1487	rVB3	66469	187355	3.94%	0.840%
15	11.171	1557	1567	1577	rVV	111966	220110	4.63%	0.987%
16	11.776	1662	1670	1675	rVV5	22526	62021	1.30%	0.278%
17	11.865	1675	1685	1694	rVV	545555	1044416	21.97%	4.682%
18	11.965	1694	1702	1708	rVV2	116782	231813	4.88%	1.039%
19	12.065	1712	1719	1731	rVV	93526	202236	4.25%	0.907%
20	12.394	1768	1775	1782	rBV2	65880	118573	2.49%	0.532%
21	12.847	1845	1852	1861	rVB	434606	765303	16.10%	3.431%
22	13.194	1902	1911	1918	rVB8	20948	66590	1.40%	0.298%
23	13.476	1948	1959	1967	rBV2	38229	90851	1.91%	0.407%
24	13.606	1975	1981	1986	rBV2	46094	75801	1.59%	0.340%
25	13.729	1995	2002	2006	rBV	82542	133008	2.80%	0.596%
26	13.794	2006	2013	2019	rVV	603474	1119081	23.54%	5.016%
27	13.859	2019	2024	2036	rVB3	141117	289849	6.10%	1.299%
28	13.994	2042	2047	2060	rVB3	30430	71697	1.51%	0.321%
29	14.247	2084	2090	2094	rVV2	113620	205000	4.31%	0.919%
30	14.294	2094	2098	2108	rVB	216411	375913	7.91%	1.685%
31	14.441	2114	2123	2132	rBV7	33380	88946	1.87%	0.399%
32	14.629	2149	2155	2157	rBV3	42829	65304	1.37%	0.293%
33	14.670	2157	2162	2169	rVV	455206	809114	17.02%	3.627%
34	14.929	2202	2206	2214	rVB8	25468	48818	1.03%	0.219%
35	15.023	2216	2222	2228	rBV4	28837	56477	1.19%	0.253%
36	15.094	2229	2234	2240	rVB	90363	151950	3.20%	0.681%

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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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Title : SW846 8260

37	15.264	2257	2263	2264	rBV2	74302	123269	2.59%	0.553%
38	15.323	2267	2273	2277	rBV	689303	1290857	27.15%	5.786%
39	15.511	2300	2305	2311	rVB3	49910	83878	1.76%	0.376%
40	15.641	2320	2327	2335	rVB	169633	344552	7.25%	1.544%
41	15.794	2350	2353	2370	rVB6	33959	85738	1.80%	0.384%
42	16.006	2382	2389	2398	rBV2	84943	183631	3.86%	0.823%

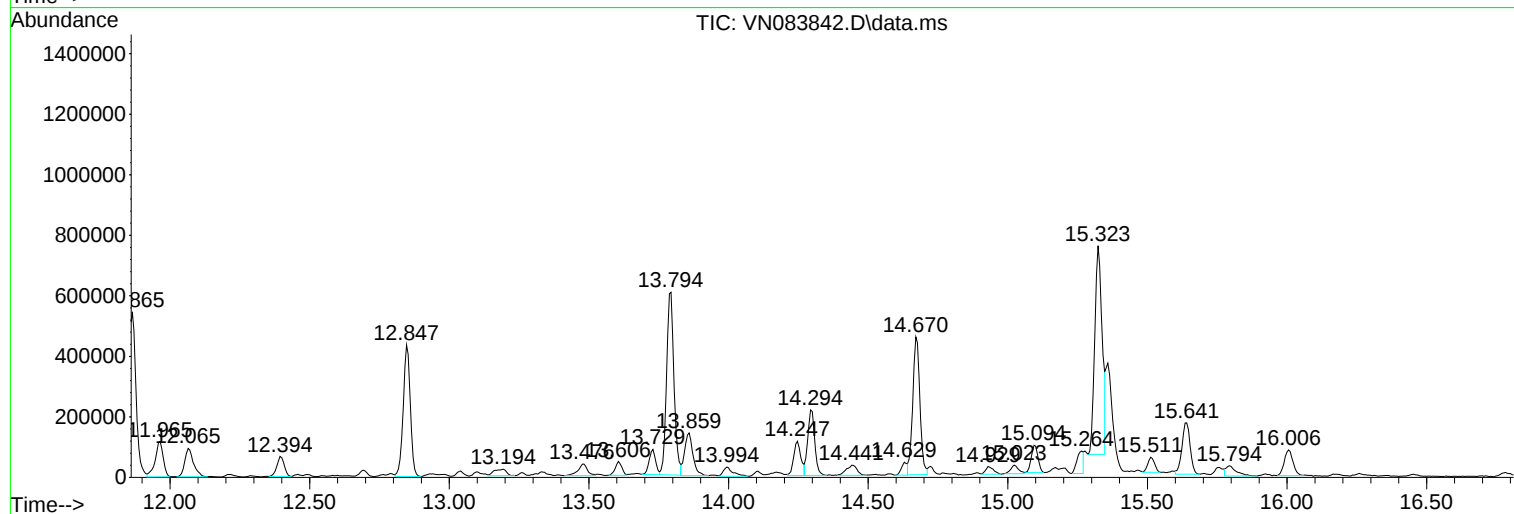
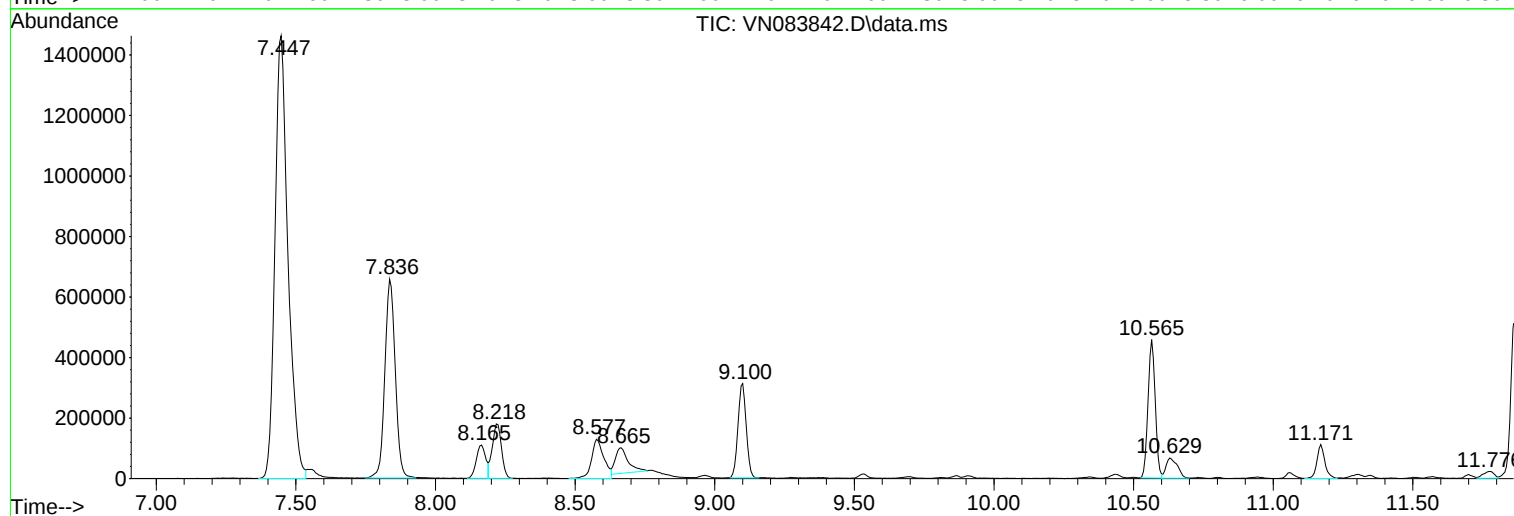
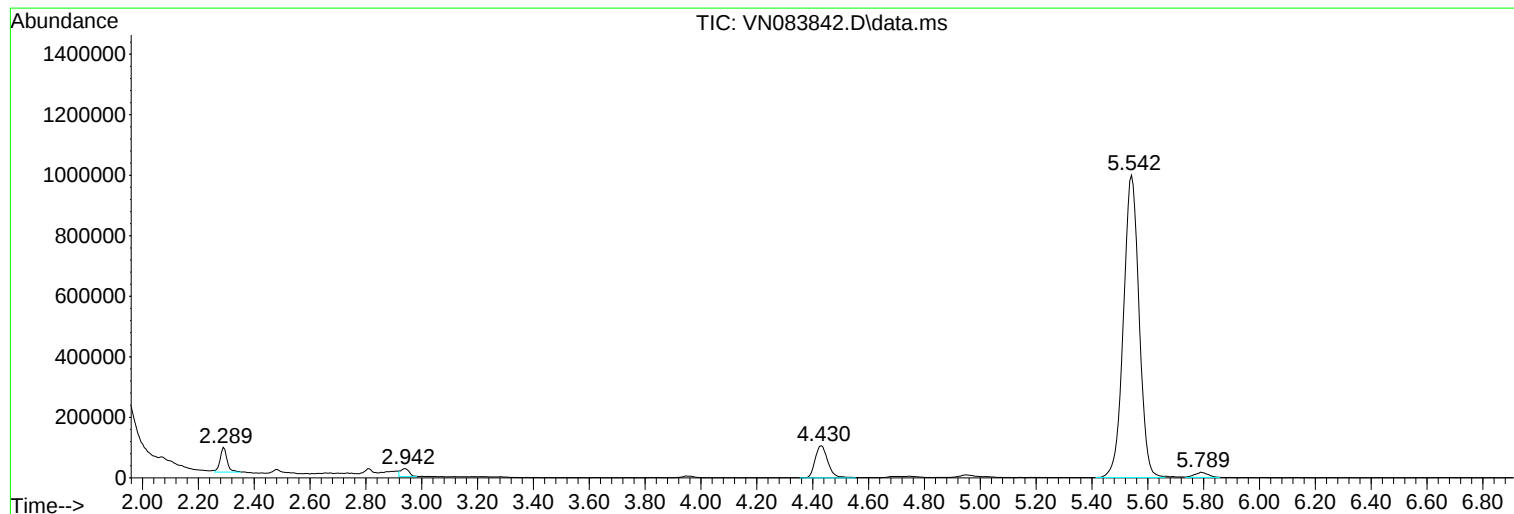
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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



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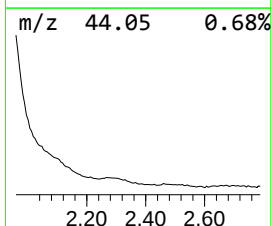
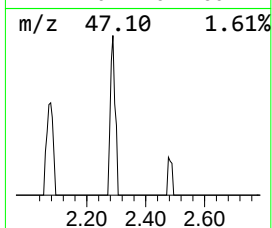
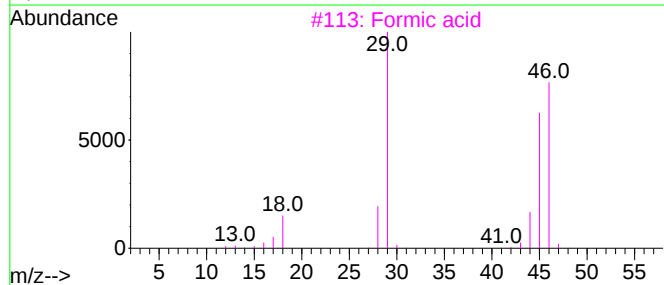
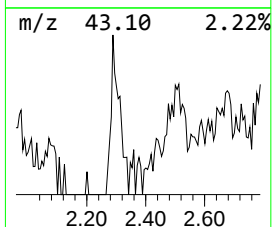
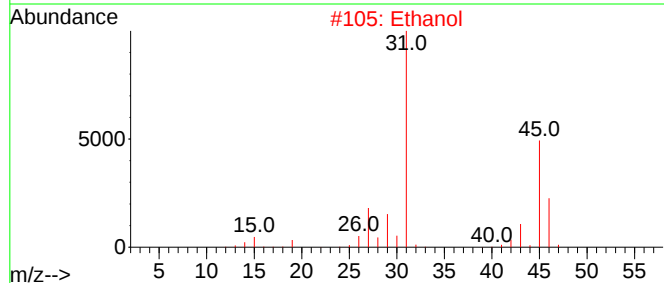
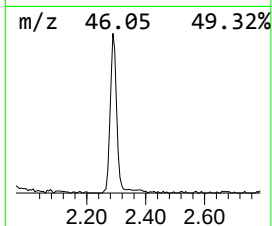
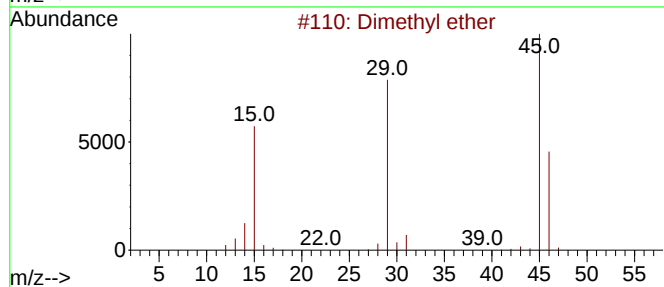
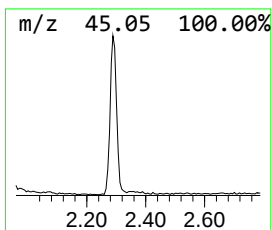
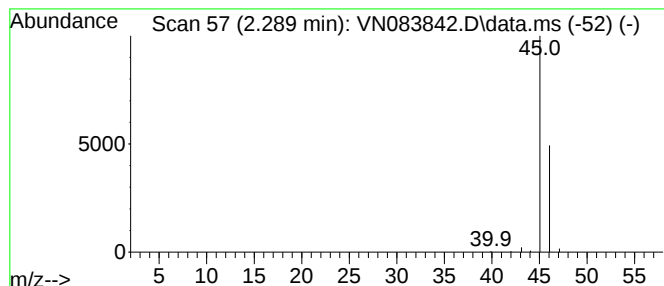
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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

Peak Number 1 Dimethyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.289	17.24 ug/l	140498	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	90
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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Instrument :
MSVOA_N
ClientSampleId :
VOA-240911078-02

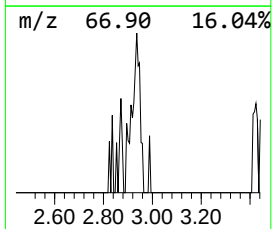
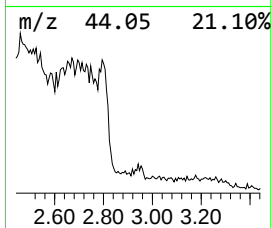
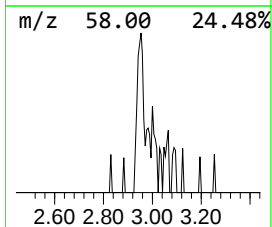
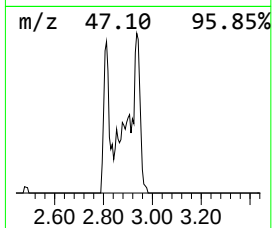
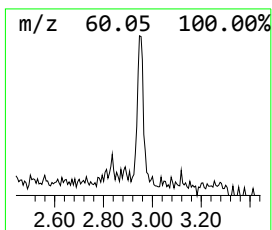
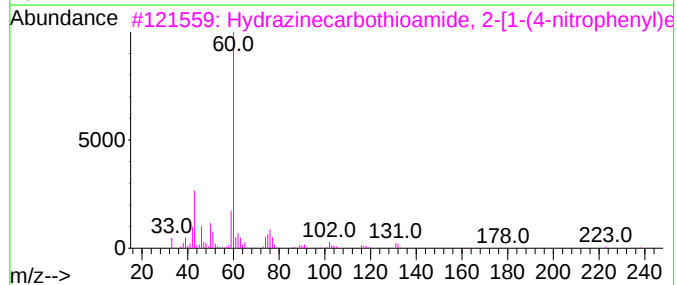
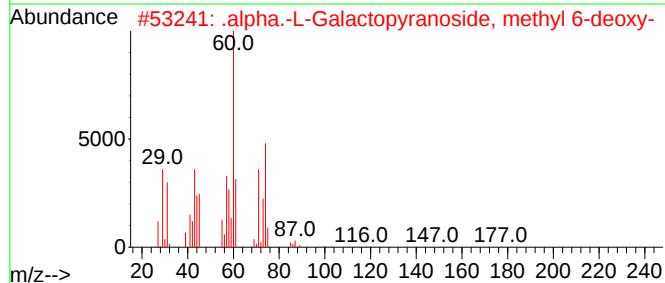
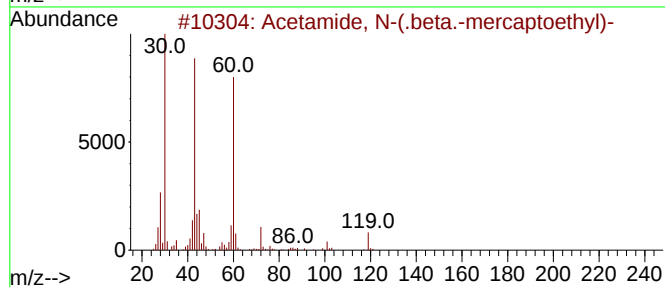
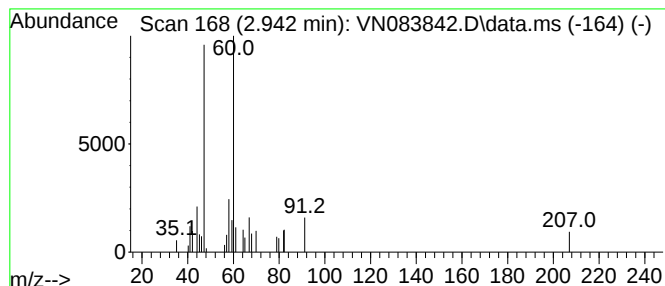
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown2.942 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.942	6.43 ug/l	52381	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetamide, N-(.beta.-mercaptoeth...	119	C4H9NOS	001190-73-4	25
2			.alpha.-L-Galactopyranoside, met...	178	C7H14O5	014687-15-1	17
3			Hydrazinecarbothioamide, 2-[1-(4...	238	C9H10N4O2S	005424-45-3	12
4			trans-Cyclohexene-4,5-diacetic acid	198	C10H14O4	025886-62-8	10
5			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	9



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ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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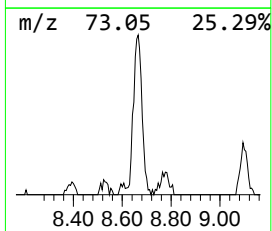
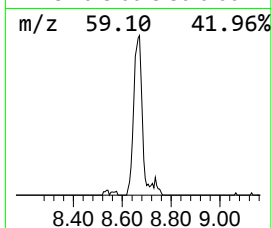
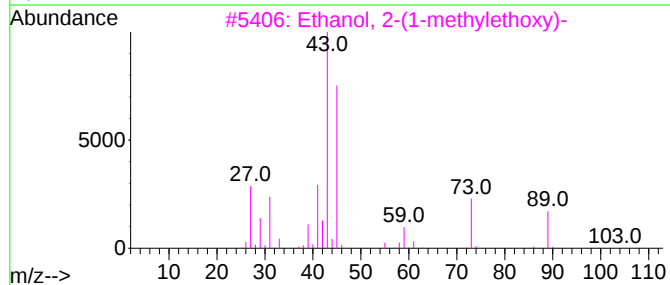
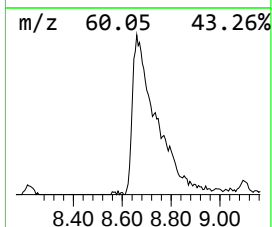
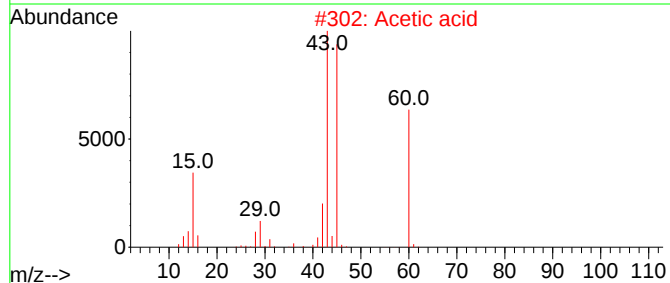
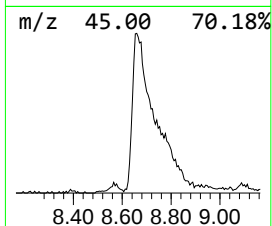
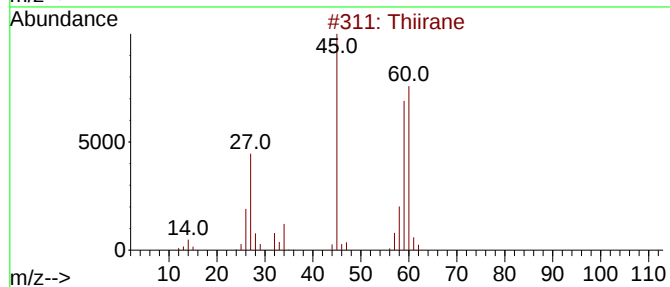
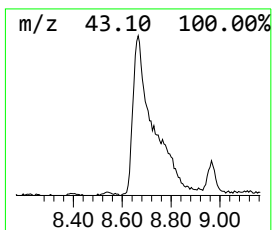
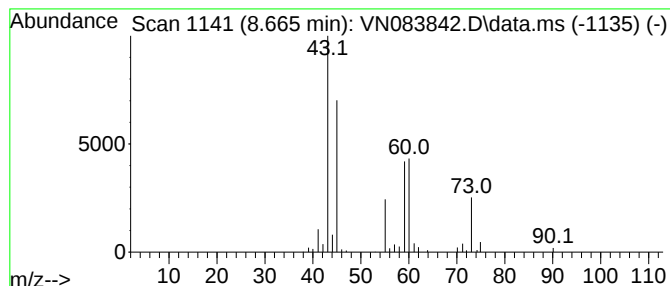
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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

Peak Number 3 Thiirane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.665	21.12 ug/l	269271	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiirane	60	C2H4S	000420-12-2	53
2			Acetic acid	60	C2H4O2	000064-19-7	43
3			Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	43
4			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	25
5			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	23



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ALS Vial : 26 Sample Multiplier: 1

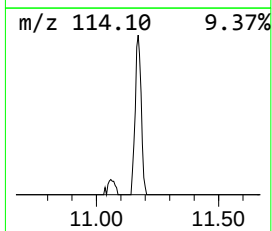
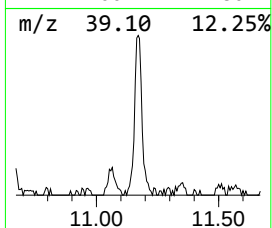
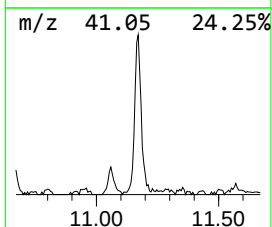
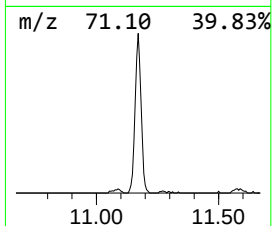
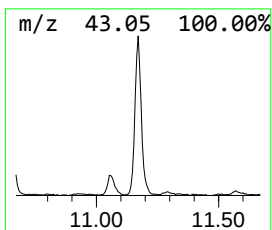
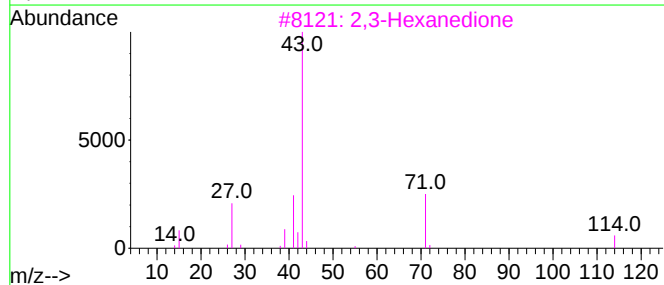
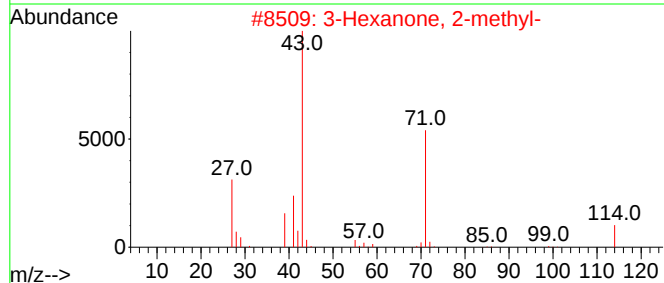
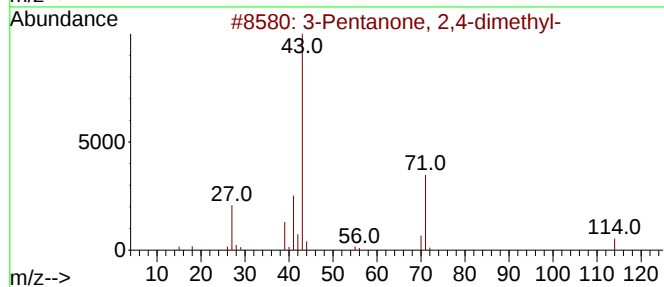
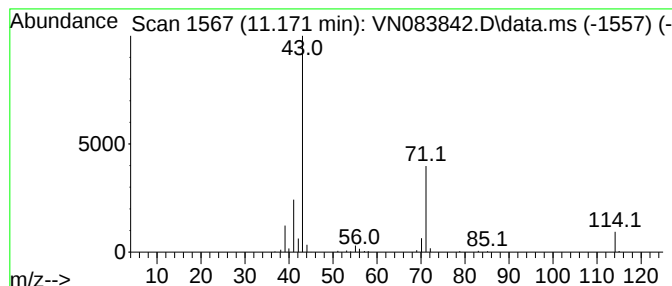
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Pentanone, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.171	10.54 ug/l	220110	Chlorobenzene-d5	11.865	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	90
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	86
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	72
4	Pyrrolidine	71	C4H9N	000123-75-1	42
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	38



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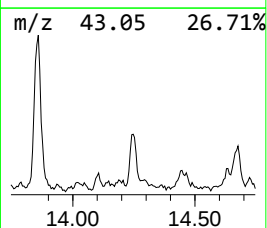
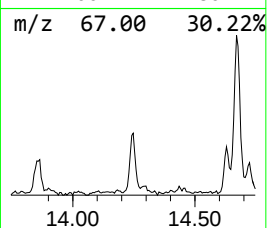
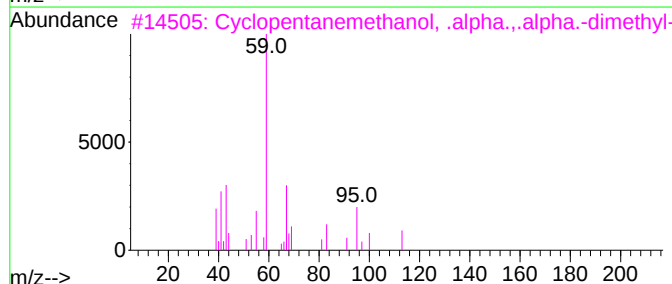
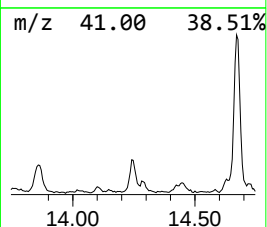
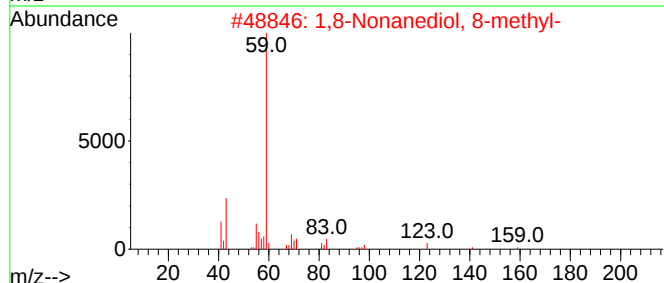
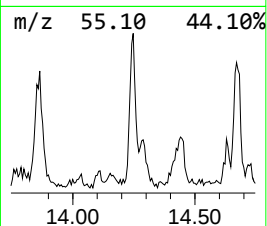
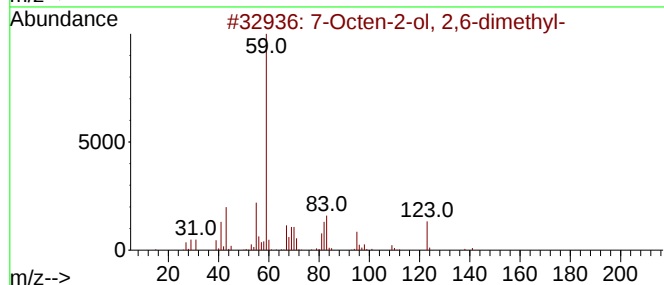
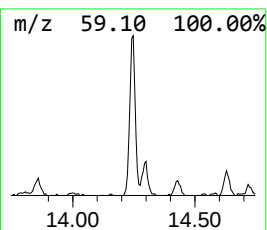
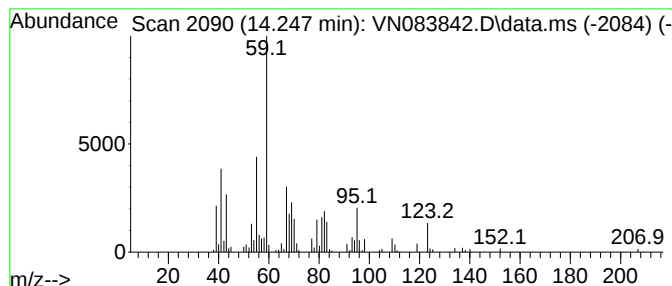
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Quant Title : SW846 8260

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

Peak Number 5 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.247	9.16 ug/l	205000	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	59
2			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	47
3			Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	45
4			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	42
5			d,l-trans-4-Methyl-5-methoxy-1-(...	184	C11H20O2	1000101-22-2	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083842.D
Acq On : 12 Sep 2024 19:30
Operator : JC\MD
Sample : P3966-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VOA-240911078-02

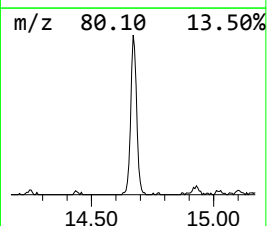
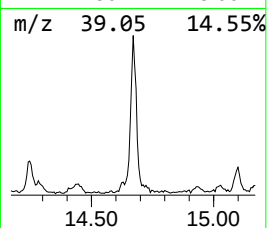
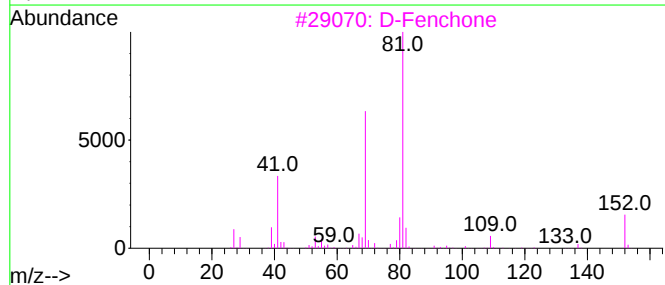
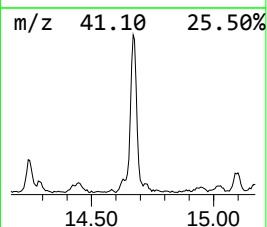
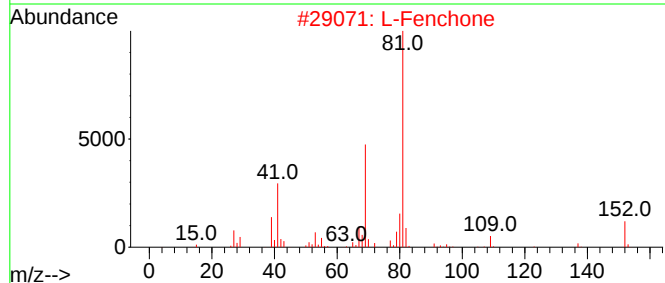
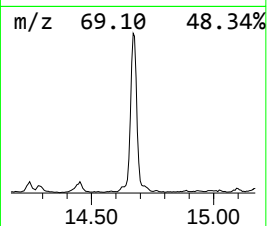
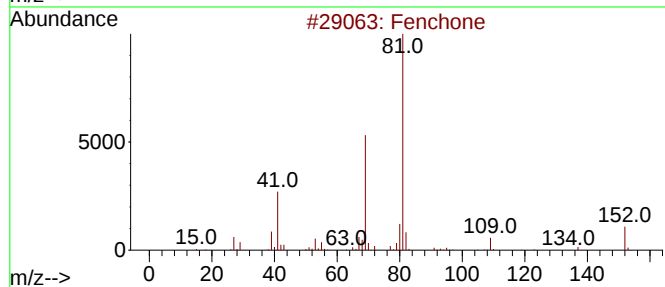
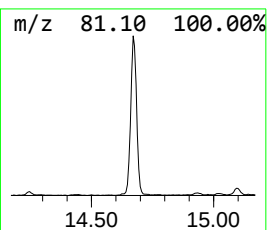
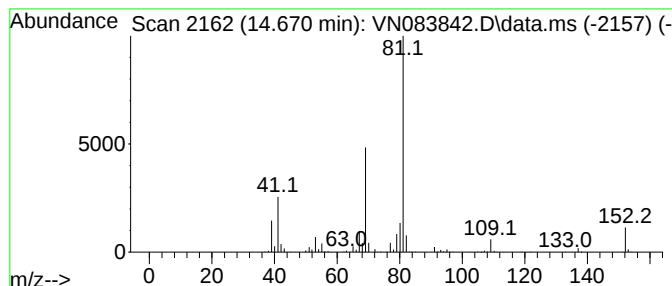
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Quant Title : SW846 8260

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

Peak Number 7 Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.670	36.15 ug/l	809114	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	91
4			2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	53
5			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083842.D
Acq On : 12 Sep 2024 19:30
Operator : JC\MD
Sample : P3966-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VOA-240911078-02

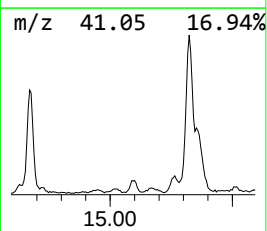
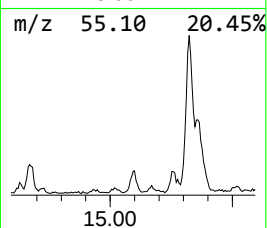
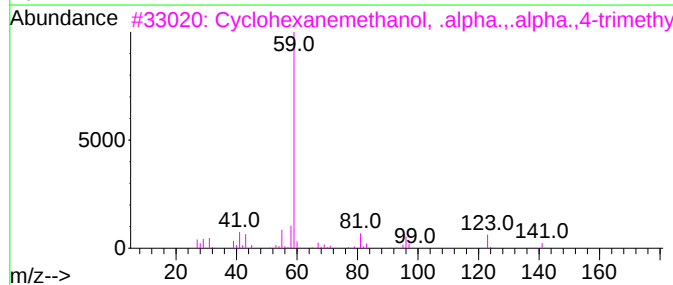
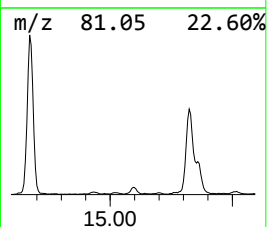
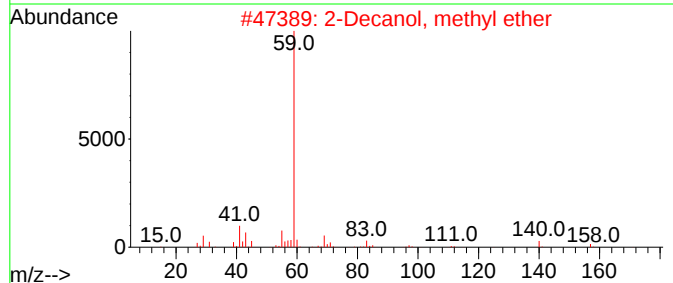
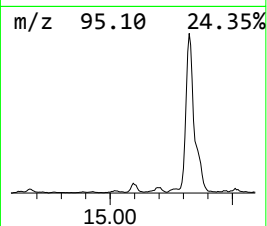
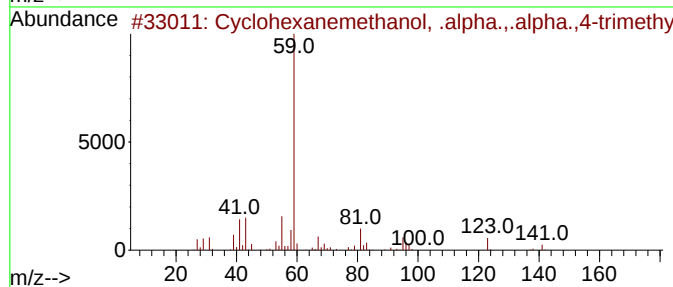
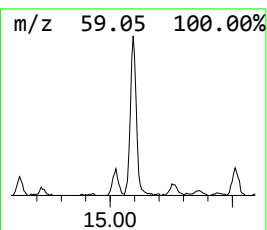
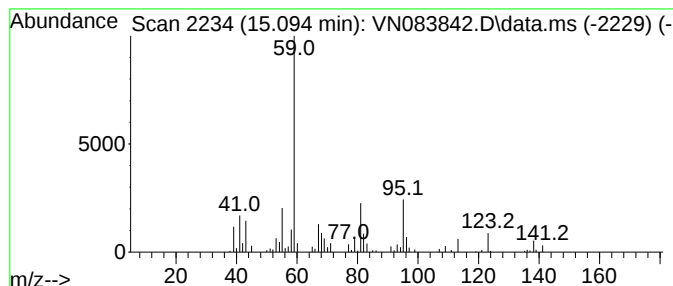
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Quant Title : SW846 8260

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

Peak Number 8 Cyclohexanemethanol, .alpha... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.094	6.79 ug/l	151950	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	59
2			2-Decanol, methyl ether	172	C11H24O	1000333-83-9	47
3			Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	005114-00-1	45
4			Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	007322-63-6	45
5			3-Pentanol	88	C5H12O	000584-02-1	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083842.D
Acq On : 12 Sep 2024 19:30
Operator : JC\MD
Sample : P3966-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VOA-240911078-02

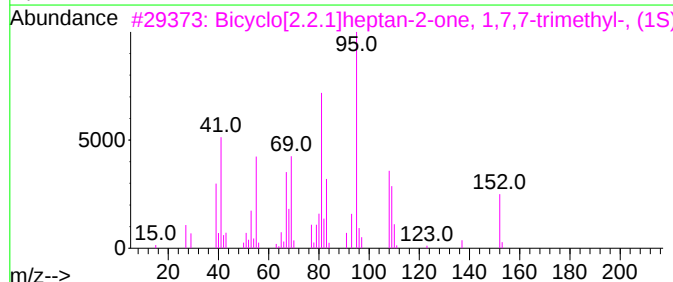
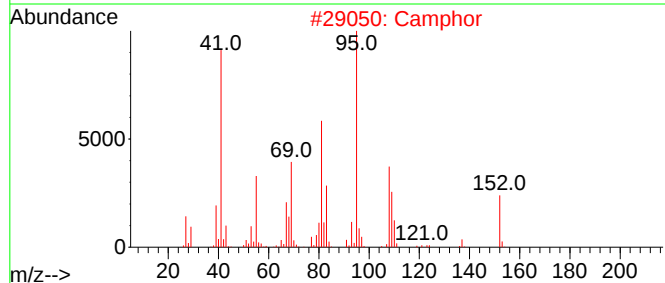
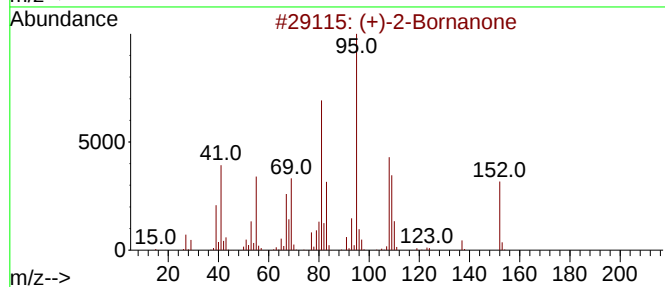
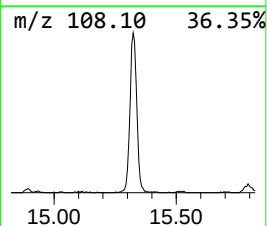
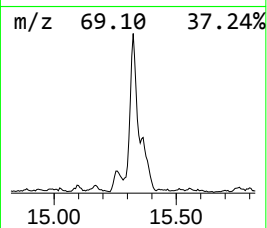
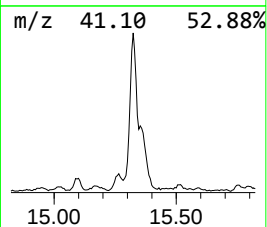
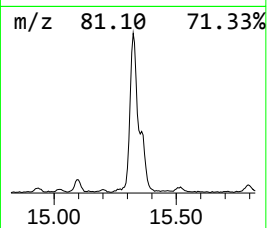
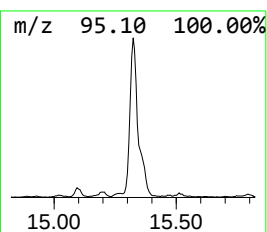
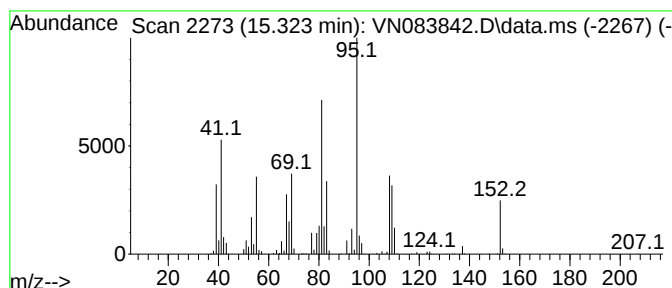
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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

Peak Number 9 (+)-2-Bornanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.323	57.67 ug/l	1290860	1,4-Dichlorobenzene-d4	13.794

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	97
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\VN091224\
Data File : VN083842.D
Acq On : 12 Sep 2024 19:30
Operator : JC\MD
Sample : P3966-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VOA-240911078-02

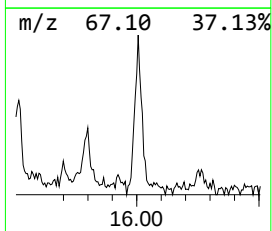
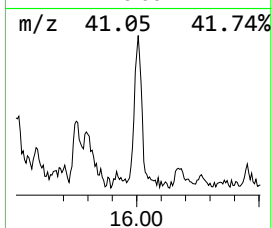
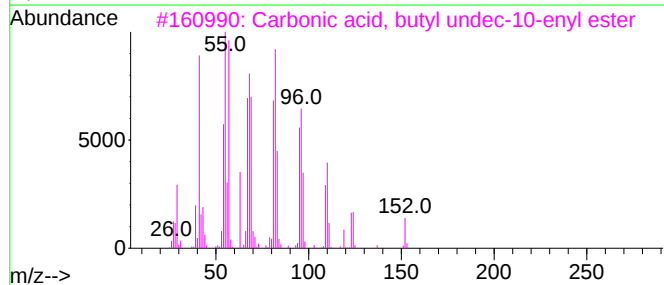
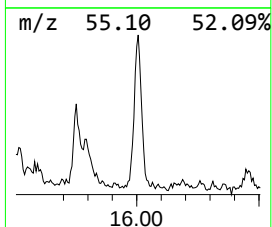
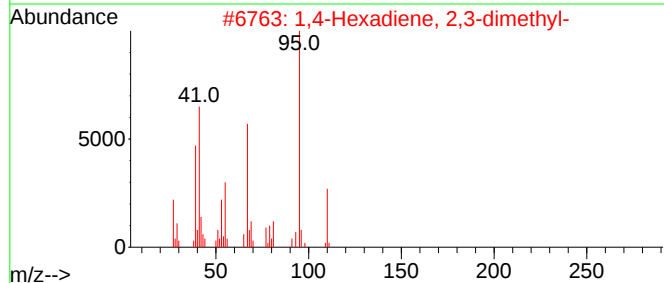
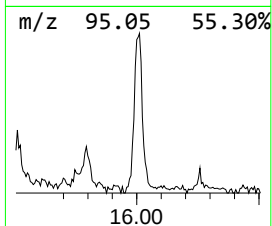
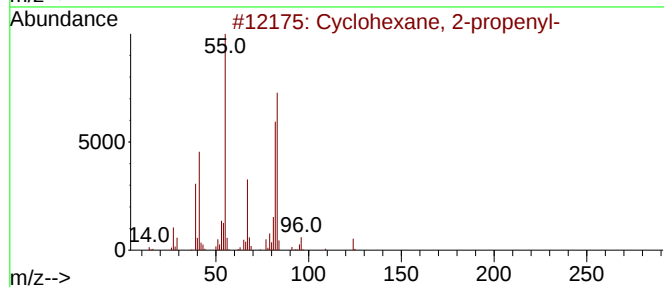
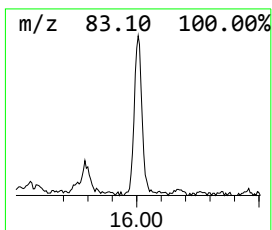
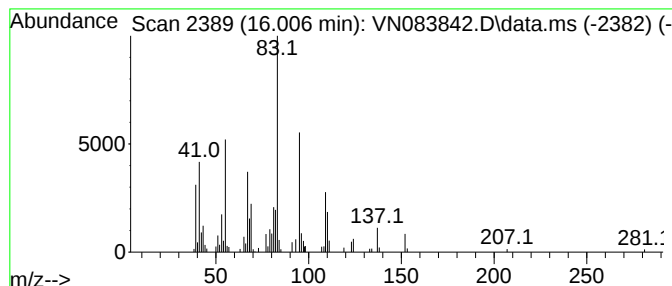
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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

Peak Number 10 unknown16.006 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.006	8.20 ug/l	183631	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	43
2			1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	38
3			Carbonic acid, butyl undec-10-en...	270	C16H30O3	1000314-63-8	35
4			1H-1,2,4-Triazole, 3-propyl-	111	C5H9N3	019932-60-6	27
5			4,4-Dimethyl-2-cyclopenten-1-one	110	C7H10O	022748-16-9	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083842.D
Acq On : 12 Sep 2024 19:30
Operator : JC\MD
Sample : P3966-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VOA-240911078-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.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
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unknown2.942	2.942	6.4	ug/l	52381	1	8.224	407530	50.0
Thiirane	8.665	21.1	ug/l	269271	2	9.100	637331	50.0
3-Pentanone, 2,...	11.171	10.5	ug/l	220110	3	11.865	1044420	50.0
7-Octen-2-ol, 2...	14.247	9.2	ug/l	205000	4	13.794	1119080	50.0
Fenchone	14.670	36.1	ug/l	809114	4	13.794	1119080	50.0
Cyclohexanemeth...	15.094	6.8	ug/l	151950	4	13.794	1119080	50.0
(+)-2-Bornanone	15.323	57.7	ug/l	1290860	4	13.794	1119080	50.0
unknown16.006	16.006	8.2	ug/l	183631	4	13.794	1119080	50.0