

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041924\
 Data File : VN081813.D
 Acq On : 19 Apr 2024 16:52
 Operator : JC\MD
 Sample : P2211-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 240418097-02

Integration Parameters: RTEINT3.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\624N041024W.M

Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

Signal : TIC: VN081813.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.665	114	121	125	rBV2	4289	7839	2.29%	0.392%
2	2.818	136	147	155	rBV3	29316	67370	19.72%	3.372%
3	3.789	305	312	322	rBV3	7055	19491	5.71%	0.976%
4	4.430	411	421	429	rBV	19695	57932	16.96%	2.900%
5	4.524	431	437	448	rVB2	17887	49556	14.51%	2.481%
6	4.700	460	467	469	rBV3	10065	16868	4.94%	0.844%
7	7.812	983	996	1007	rBV3	41700	104344	30.55%	5.223%
8	7.965	1012	1022	1031	rBV	21251	51942	15.21%	2.600%
9	8.582	1118	1127	1139	rVB2	61855	143253	41.94%	7.171%
10	9.106	1208	1216	1224	rBV	92930	195221	57.15%	9.772%
11	10.376	1425	1432	1441	rBV3	32569	68351	20.01%	3.421%
12	10.571	1456	1465	1471	rBV	186282	341591	100.00%	17.099%
13	10.629	1471	1475	1484	rVB2	23837	43712	12.80%	2.188%
14	11.865	1678	1685	1699	rVB	189378	336755	98.58%	16.857%
15	12.847	1845	1852	1861	rBV	163127	289176	84.66%	14.475%
16	13.453	1948	1955	1959	rBV6	7603	13907	4.07%	0.696%
17	13.706	1994	1998	2006	rVB6	6842	11153	3.27%	0.558%
18	13.864	2018	2025	2033	rBV6	21431	46164	13.51%	2.311%
19	14.247	2082	2090	2095	rBV3	37984	61701	18.06%	3.089%
20	14.300	2095	2099	2105	rVB	14849	21369	6.26%	1.070%
21	14.447	2122	2124	2128	rVB3	4493	4259	1.25%	0.213%
22	14.494	2128	2132	2140	rVB4	27658	45773	13.40%	2.291%

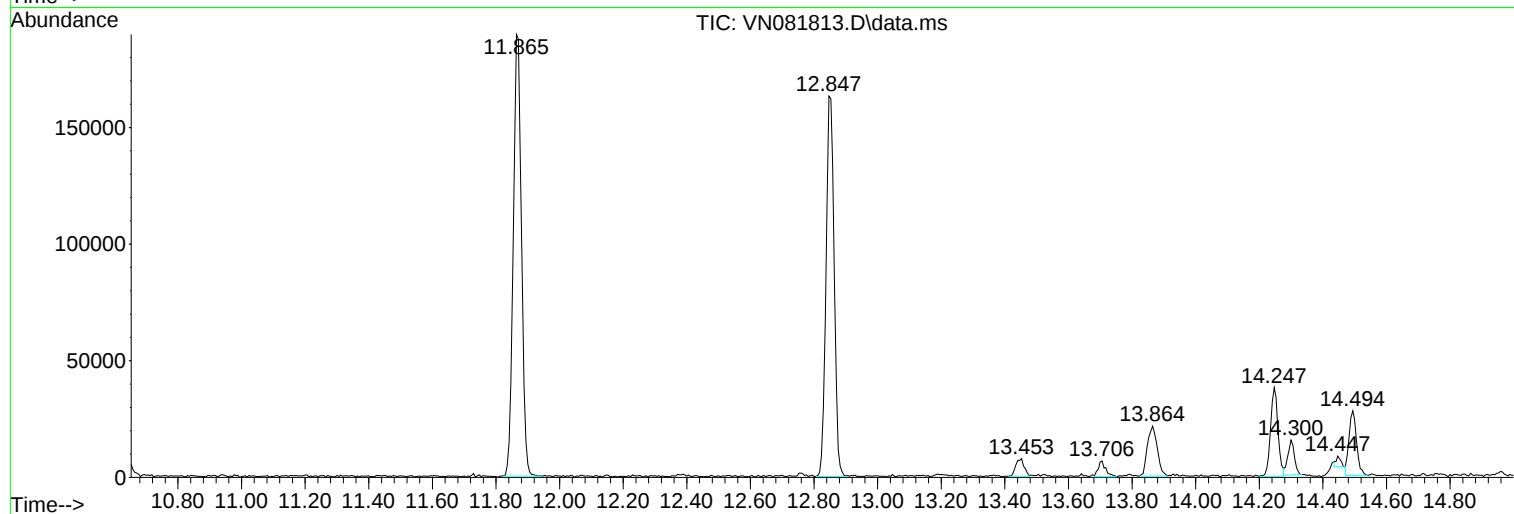
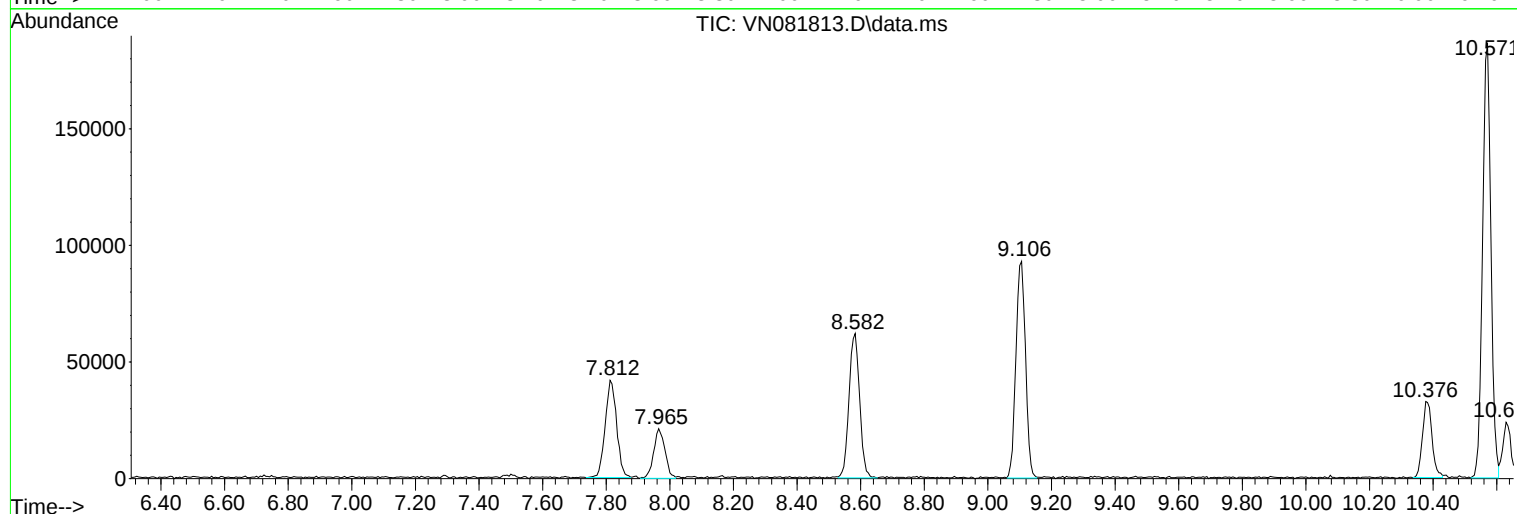
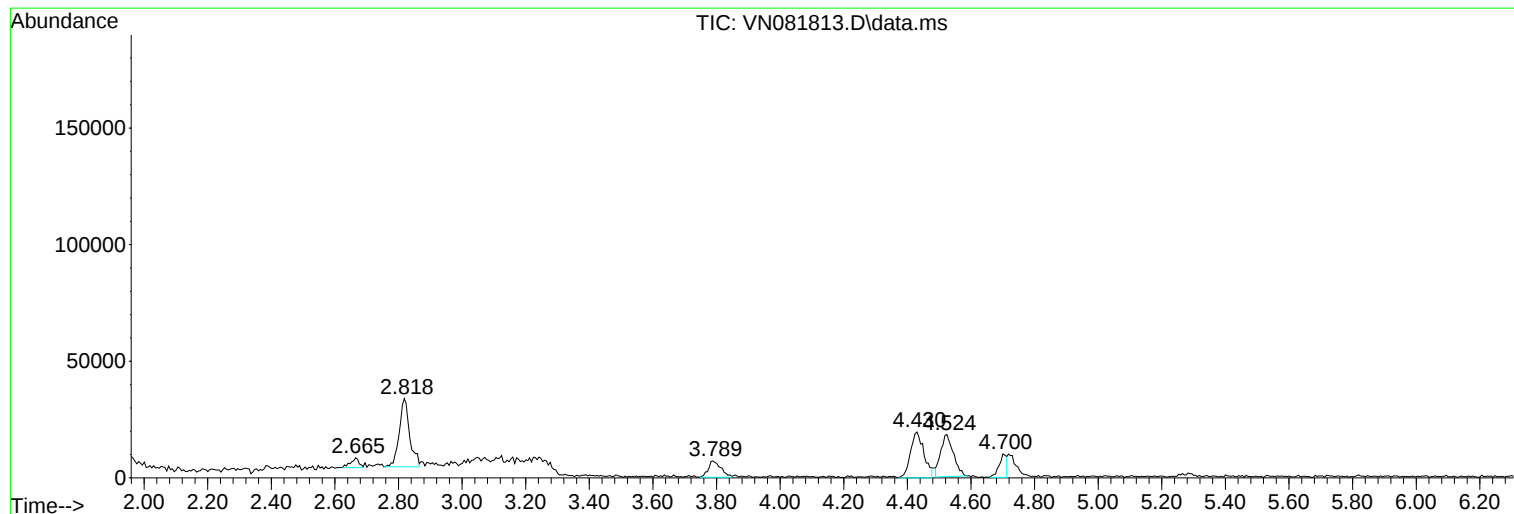
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240418097-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\624N041024W.M
Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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



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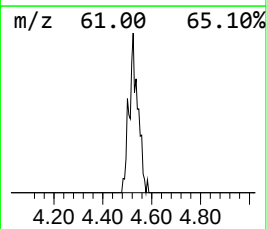
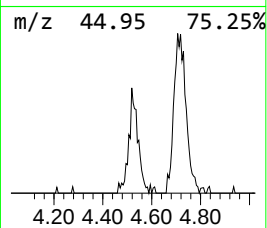
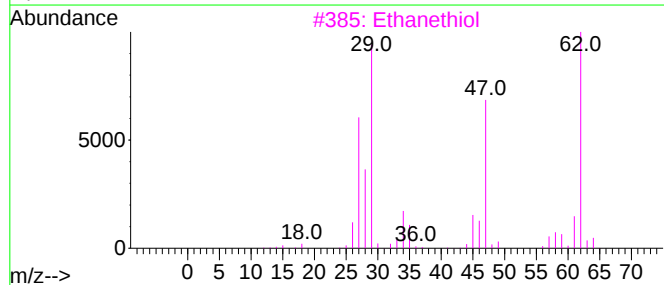
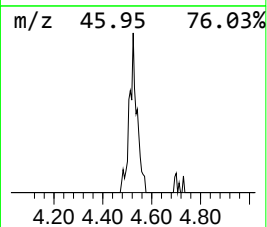
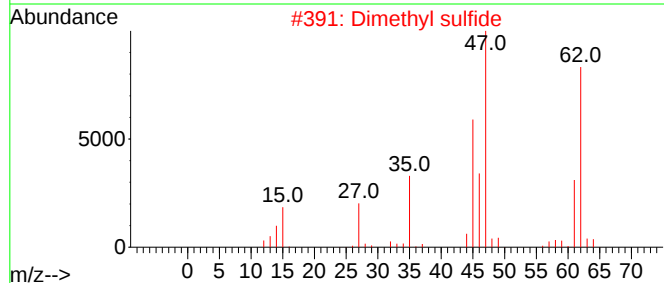
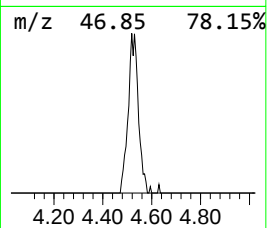
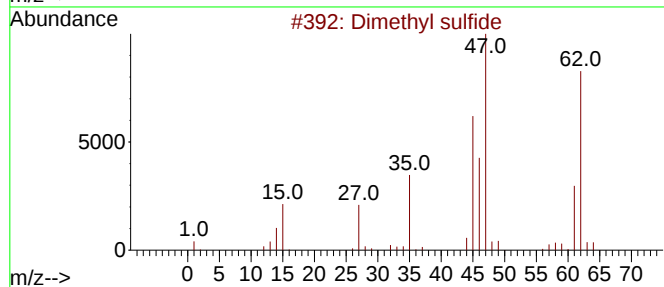
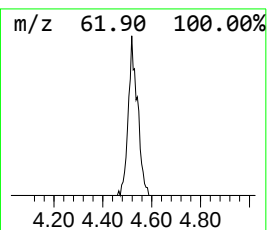
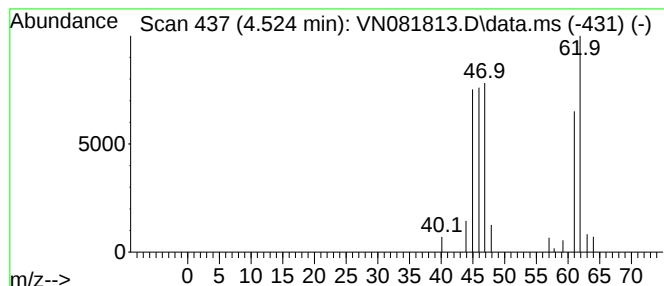
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Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 3 Dimethyl sulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.524	14.25 ug/l	49556	Bromochloromethane	7.818

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	64
2			Dimethyl sulfide	62	C2H6S	000075-18-3	64
3			Ethanethiol	62	C2H6S	000075-08-1	53
4			Ethanethiol	62	C2H6S	000075-08-1	53
5			Ethanethiol	62	C2H6S	000075-08-1	42



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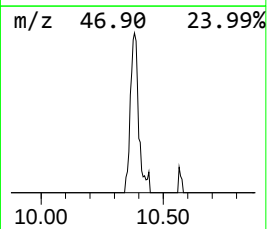
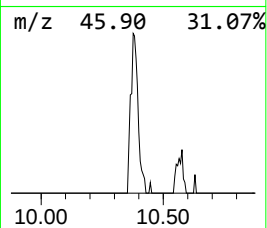
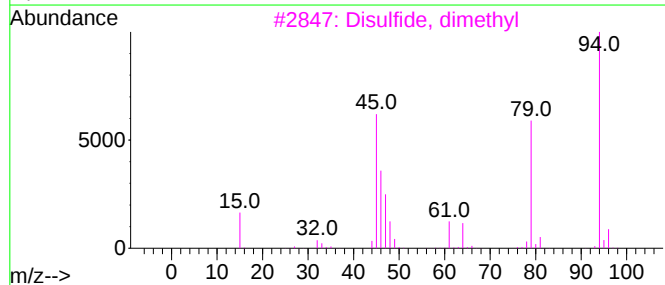
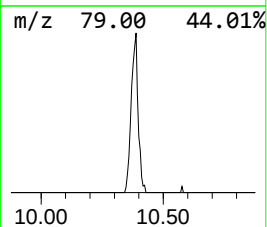
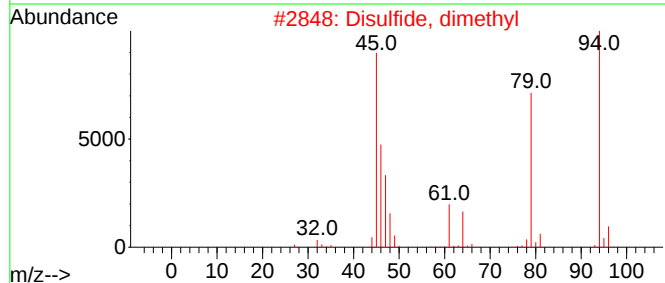
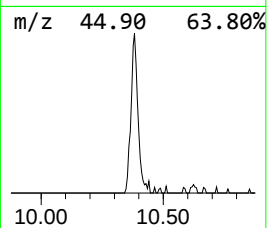
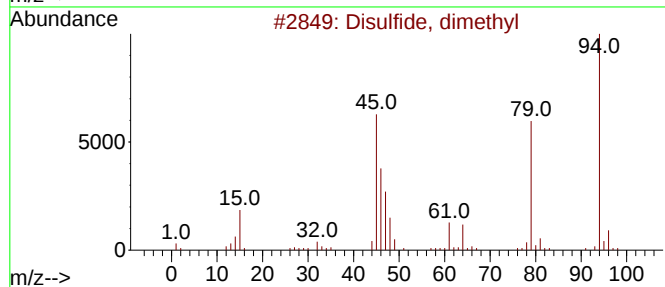
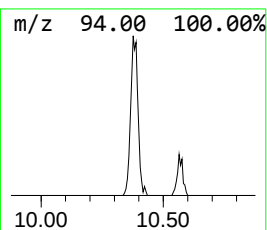
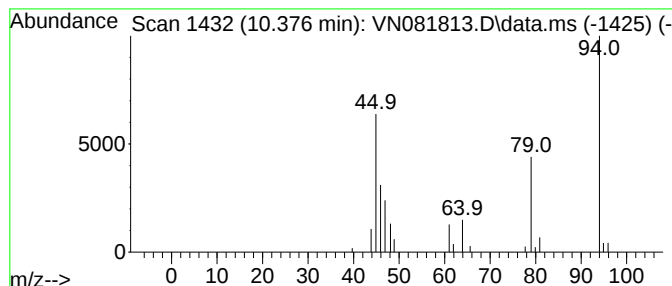
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\624N041024W.M
Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 5 Disulfide, dimethyl Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.377	10.50 ug/l	68351	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
2			Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
3			Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
4			Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
5			Disulfide, dimethyl	94	C2H6S2	000624-92-0	81



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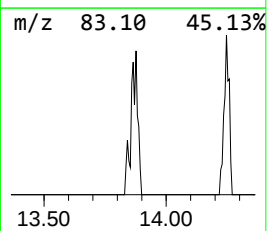
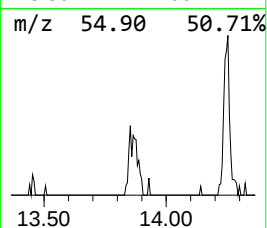
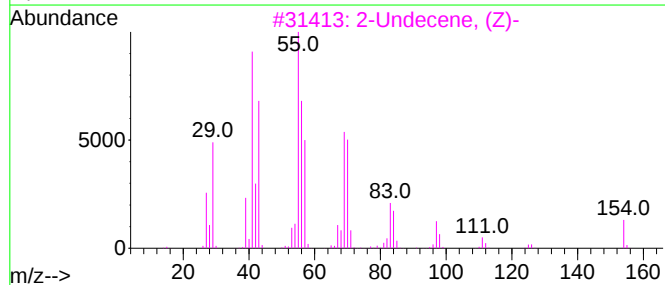
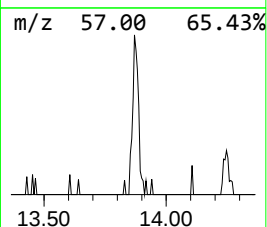
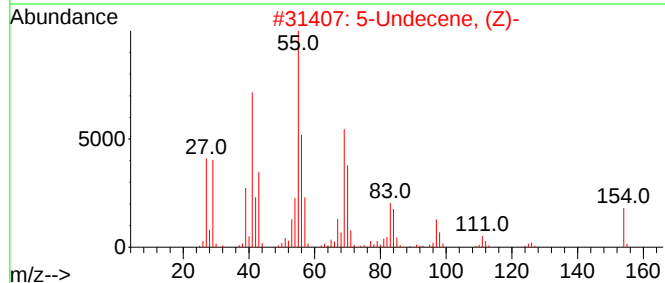
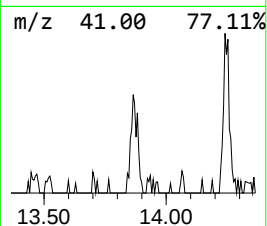
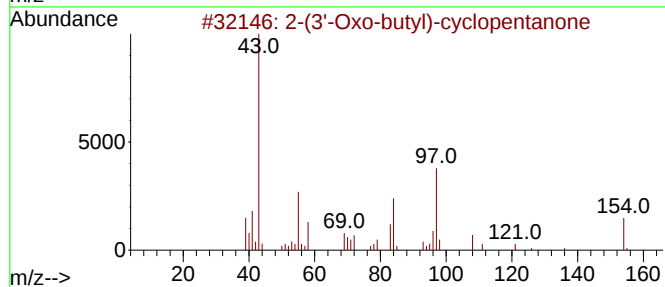
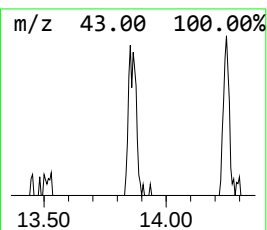
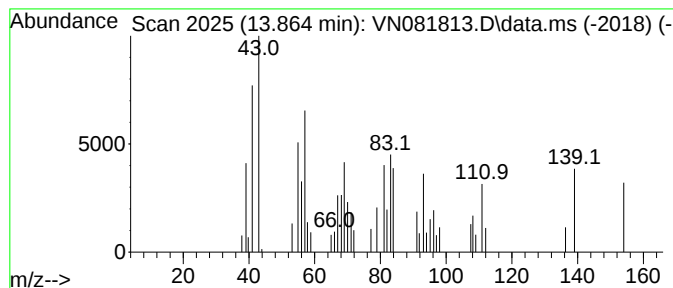
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\624N041024W.M
Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 6 unknown13.865 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.865	4.11 ug/l	46164	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(3'-Oxo-butyl)-cyclopentanone		154	C9H14O2		1010143-37-2	38
2	5-Undecene, (Z)-		154	C11H22		000764-96-5	35
3	2-Undecene, (Z)-		154	C11H22		000821-96-5	35
4	4-Heptenal, (E)-		112	C7H12O		000929-22-6	27
5	4-Nonenal, (E)-		140	C9H16O		002277-16-9	22



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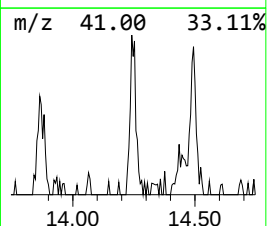
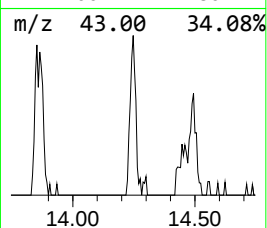
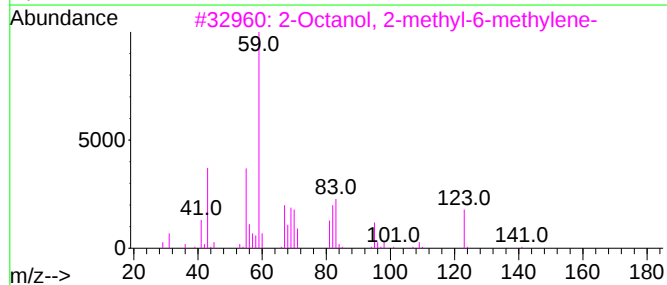
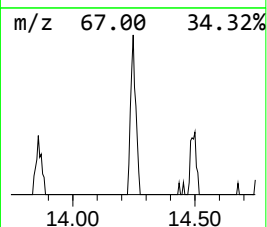
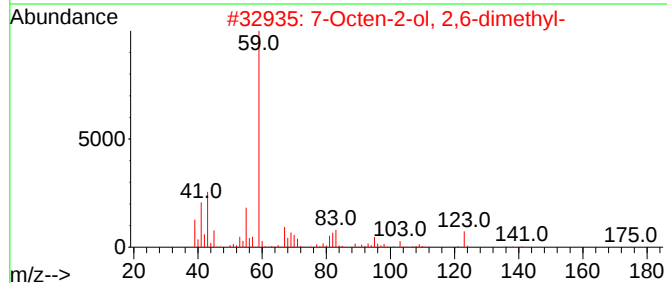
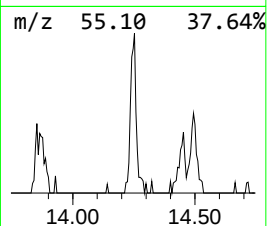
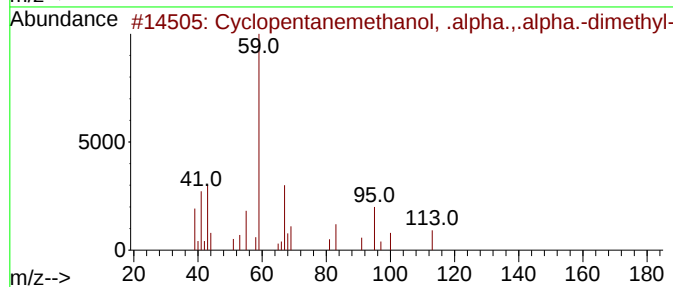
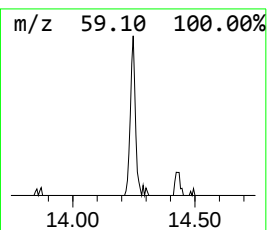
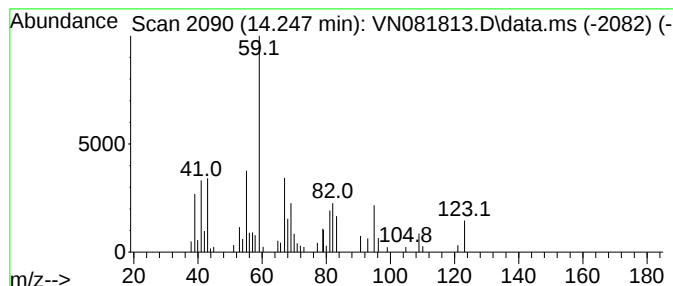
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Cyclopentanemethanol, .alph... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.247	5.50 ug/l	61701	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	53
2			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	45
3			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	36
4			1,2,4-Thiadiazole, 5-chloro-	120	C2HClN2S	038362-15-1	28
5			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	27



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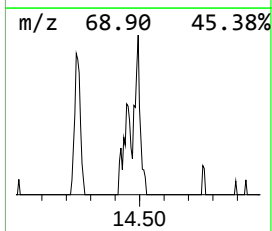
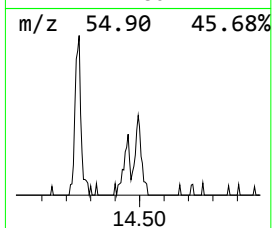
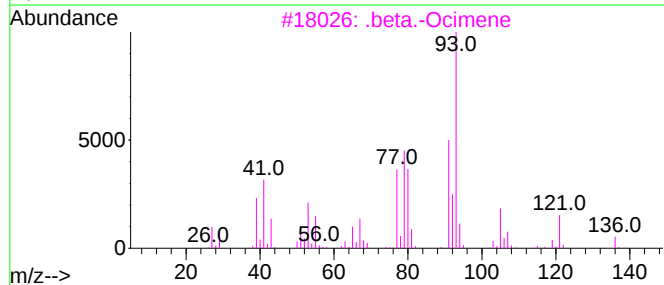
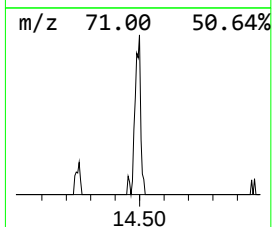
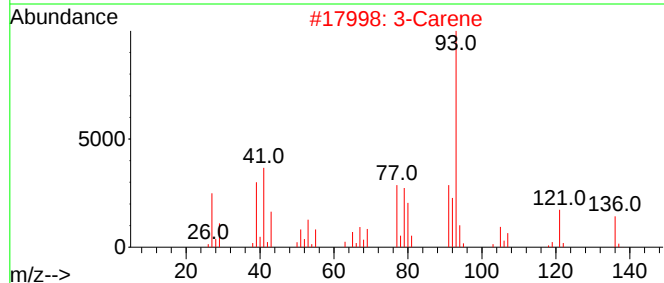
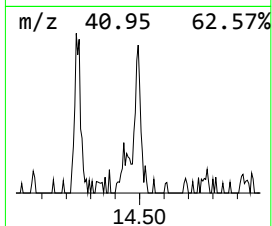
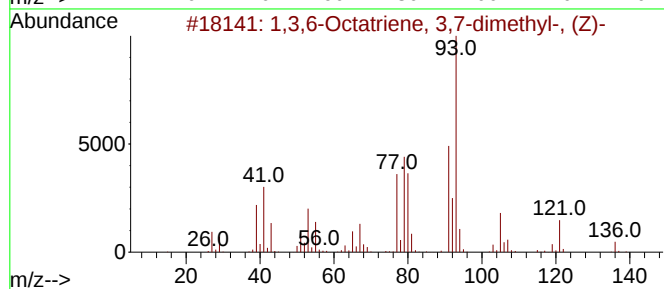
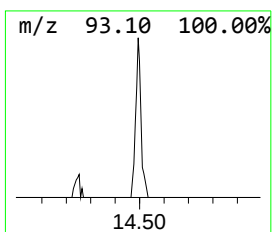
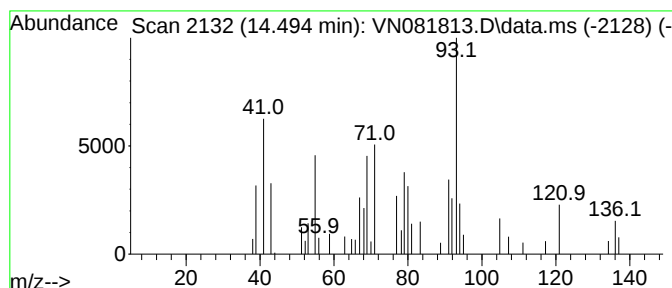
Instrument :
MSVOA_N
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1,3,6-Octatriene, 3,7-dimet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.494	4.08 ug/l	45773	Chlorobenzene-d5	11.865	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	83
2	3-Carene	136	C10H16	013466-78-9	64
3	.beta.-Ocimene	136	C10H16	013877-91-3	64
4	3-Carene	136	C10H16	013466-78-9	58
5	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	53



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl sulfide	4.524	14.3	ug/l	49556	1	7.818	104344	30.0
Disulfide, dime...	10.377	10.5	ug/l	68351	2	9.106	195221	30.0
unknown13.865	13.865	4.1	ug/l	46164	3	11.865	336755	30.0
Cyclopentanemet...	14.247	5.5	ug/l	61701	3	11.865	336755	30.0
1,3,6-Octatrien...	14.494	4.1	ug/l	45773	3	11.865	336755	30.0