

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081924\
 Data File : VY019128.D
 Acq On : 19 Aug 2024 19:51
 Operator : SY/MD
 Sample : P3641-04
 Misc : 6.90g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 S-908-K1-0.5-1.0-081524

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_Y\methods\82Y081524S.M
 Title : SW846 8260

Signal : TIC: VY019128.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.604	462	473	484	rVB2	13532	41278	4.79%	1.005%
2	5.635	632	642	653	rVB6	2986	9809	1.14%	0.239%
3	7.622	959	968	974	rBV	81440	196899	22.83%	4.796%
4	7.695	974	980	992	rVB	133184	305246	35.39%	7.435%
5	8.049	1030	1038	1051	rBV2	68363	153087	17.75%	3.729%
6	8.604	1120	1129	1140	rBV	211441	415810	48.21%	10.129%
7	10.103	1367	1375	1383	rBV	310004	520158	60.31%	12.670%
8	11.414	1582	1590	1600	rBV	281986	451708	52.38%	11.003%
9	11.969	1674	1681	1689	rVB	26435	41961	4.87%	1.022%
10	12.261	1721	1729	1738	rBV	540945	862415	100.00%	21.007%
11	12.408	1746	1753	1761	rBV2	228907	408971	47.42%	9.962%
12	12.505	1763	1769	1775	rVB2	35268	59577	6.91%	1.451%
13	12.816	1814	1820	1827	rBV2	8340	15272	1.77%	0.372%
14	12.999	1834	1850	1851	rBV3	17339	40069	4.65%	0.976%
15	13.347	1901	1907	1914	rVB	225935	350593	40.65%	8.540%
16	13.603	1935	1949	1955	rBV	14096	64366	7.46%	1.568%
17	13.889	1989	1996	2001	rBV2	39937	64213	7.45%	1.564%
18	14.060	2012	2024	2031	rBV9	17601	62915	7.30%	1.533%
19	14.413	2073	2082	2087	rBV5	6259	20667	2.40%	0.503%
20	14.487	2090	2094	2100	rVB6	4575	11143	1.29%	0.271%
21	14.932	2160	2167	2174	rBV4	4371	9149	1.06%	0.223%

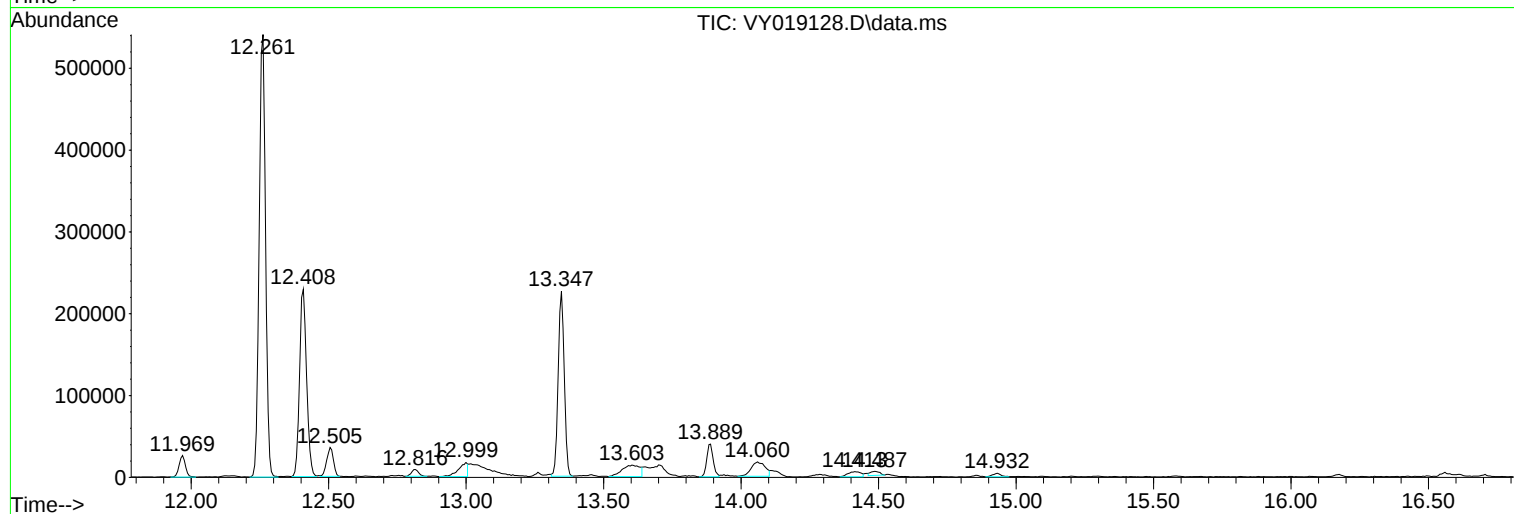
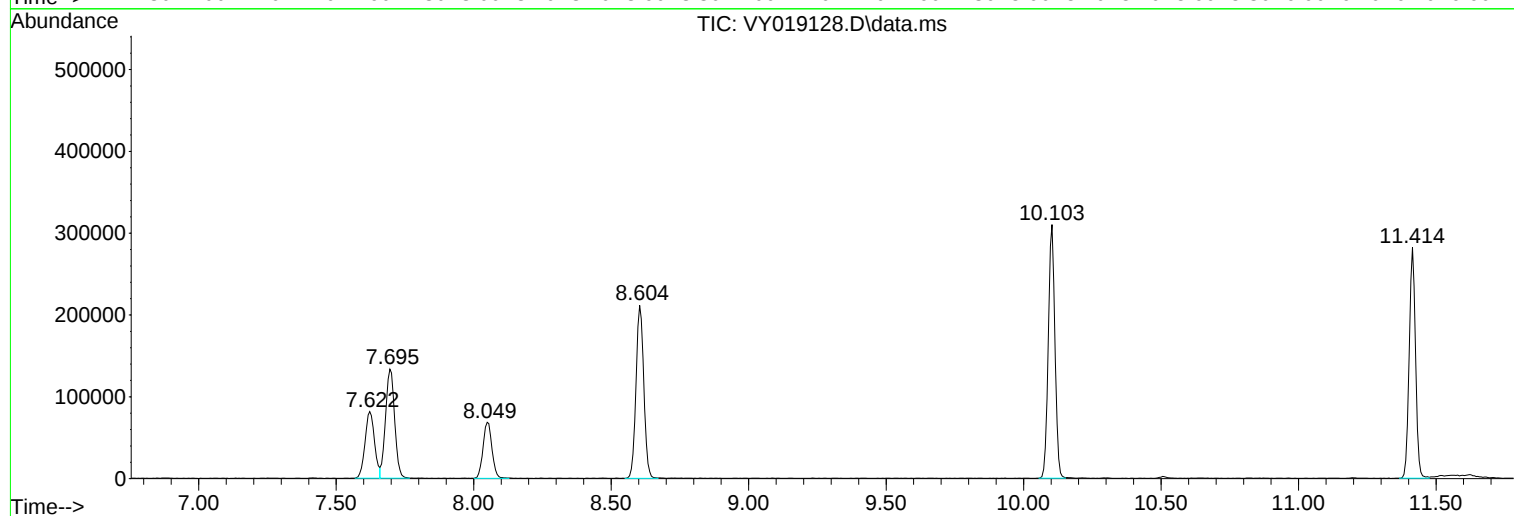
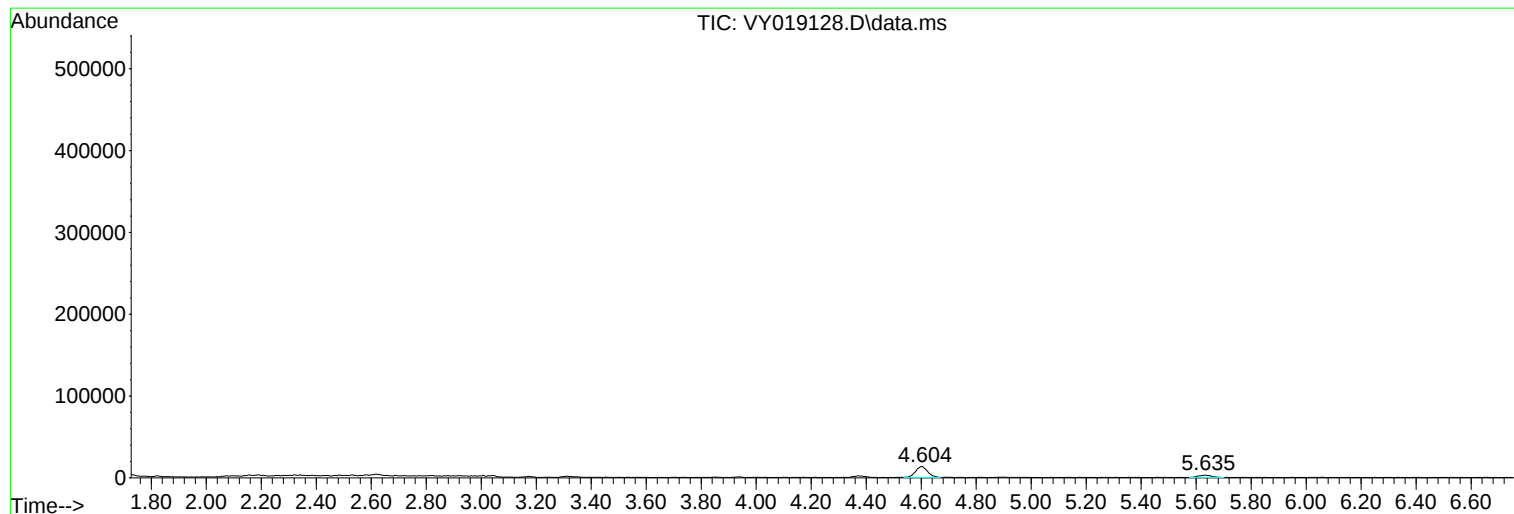
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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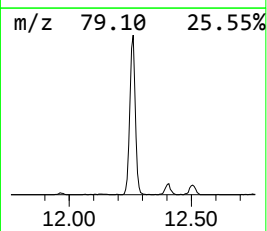
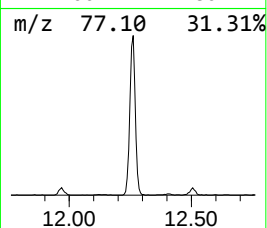
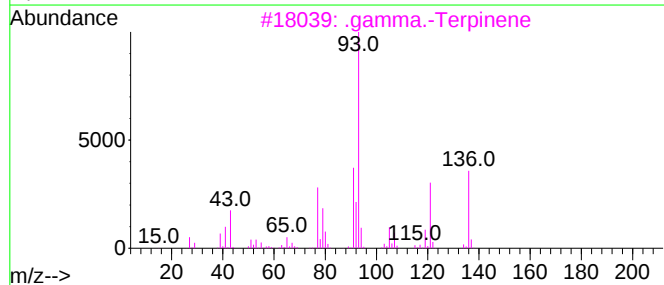
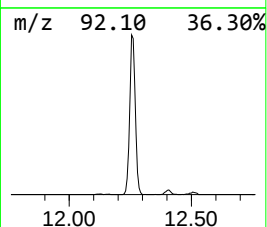
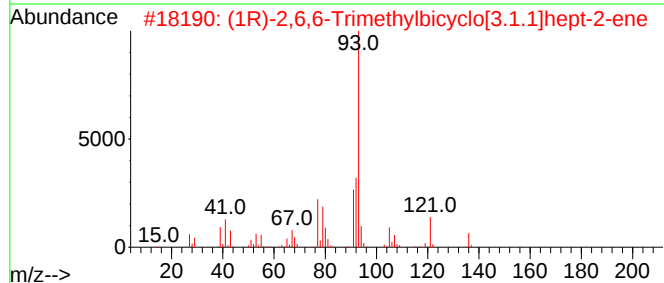
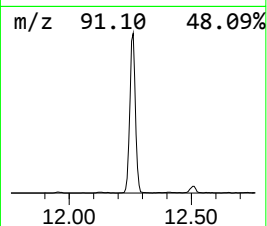
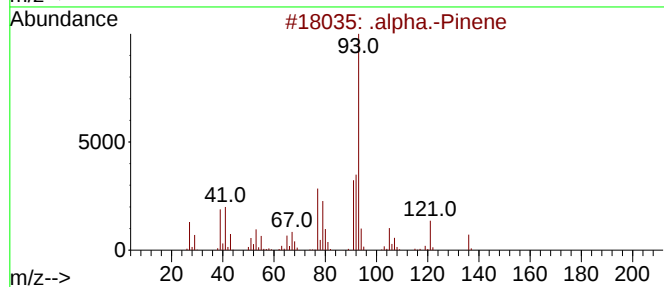
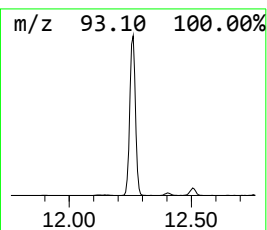
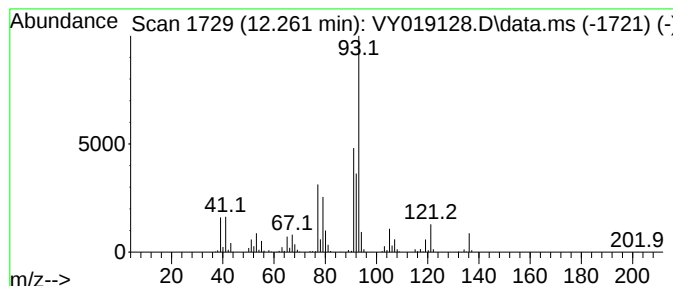
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
Quant Title : SW846 8260

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

Peak Number 2 .alpha.-Pinene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.261	95.46 ug/l	862415	Chlorobenzene-d5	11.414

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Pinene	136	C10H16	000080-56-8	97
2			(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	94
3			.gamma.-Terpinene	136	C10H16	000099-85-4	91
4			(+)-3-Carene	136	C10H16	000498-15-7	91
5			Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	91



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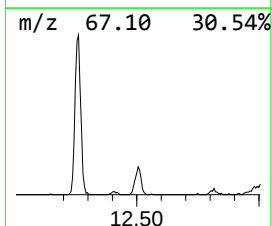
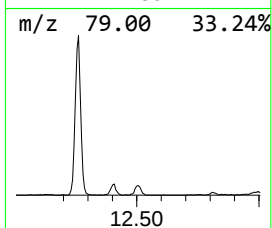
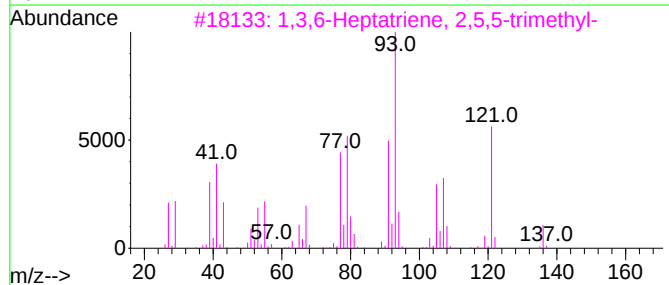
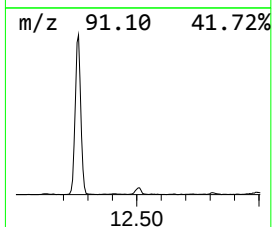
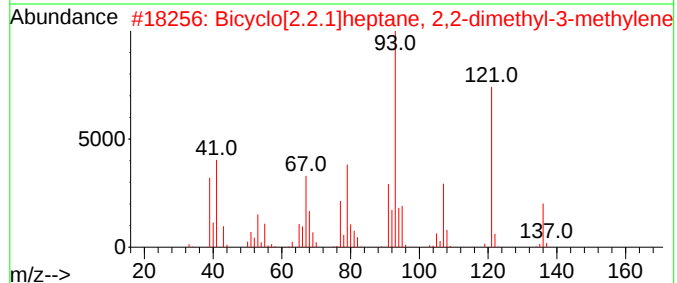
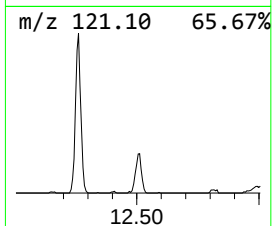
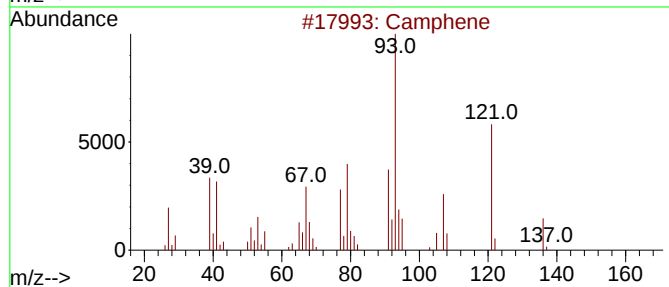
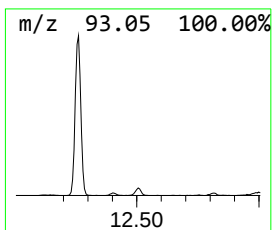
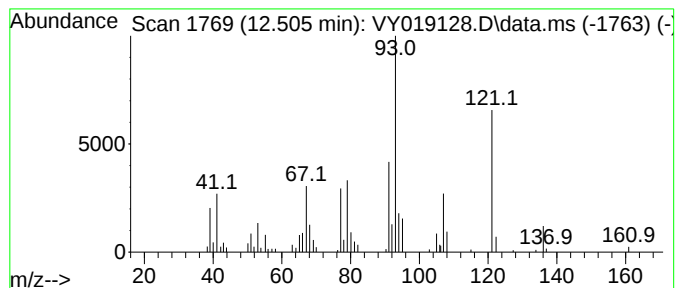
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
Quant Title : SW846 8260

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Peak Number 3 Camphene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.505	8.50 ug/l	59577	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphene	136	C10H16	000079-92-5	97
2			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	94
3			1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	029548-02-5	91
4			2-Carene	136	C10H16	000554-61-0	87
5			(+)-4-Carene	136	C10H16	029050-33-7	87



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Instrument :
MSVOA_Y
ClientSampleId :
S-908-K1-0.5-1.0-081524

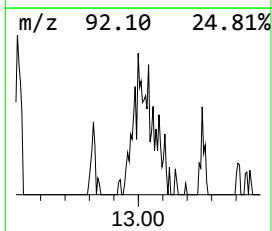
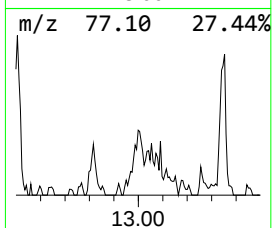
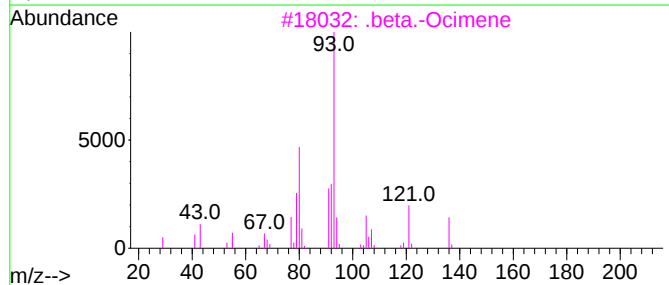
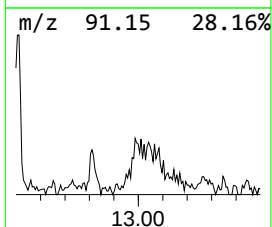
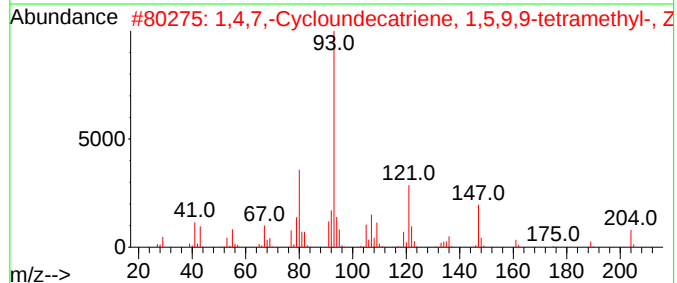
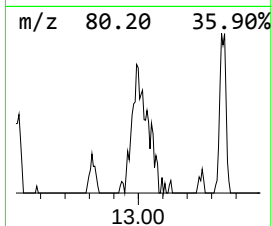
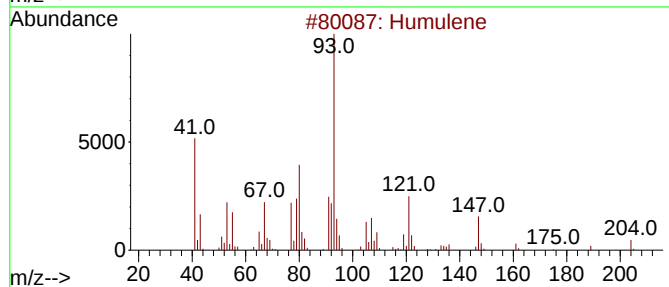
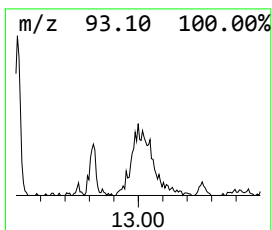
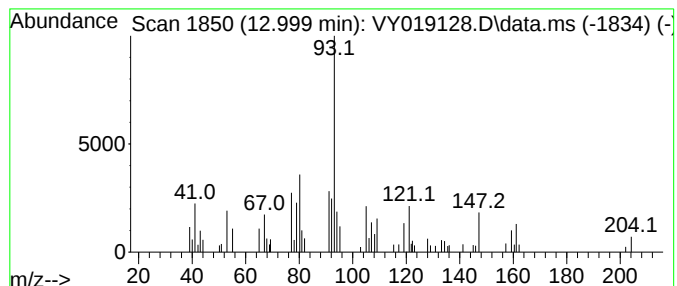
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
Quant Title : SW846 8260

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

Peak Number 4 Humulene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.999	5.71 ug/l	40069	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Humulene	204	C15H24	006753-98-6	93
2			1,4,7,-Cycloundecatriene, 1,5,9,...	204	C15H24	1000062-61-9	83
3			.beta.-Ocimene	136	C10H16	013877-91-3	53
4			1,2-Dihydropyridine, 1-(1-oxobut...	151	C9H13NO	1000132-46-2	50
5			Bicyclo[3.1.1]hept-2-ene, 2,6-di...	204	C15H24	017699-05-7	49



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MSVOA_Y
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S-908-K1-0.5-1.0-081524

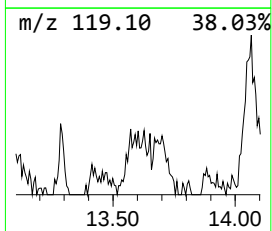
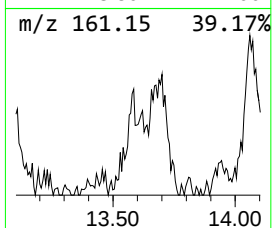
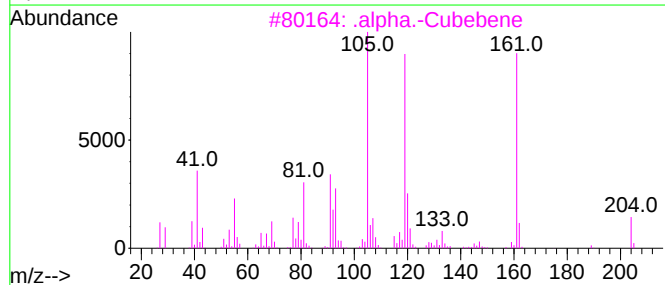
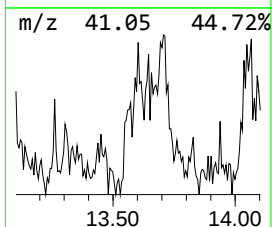
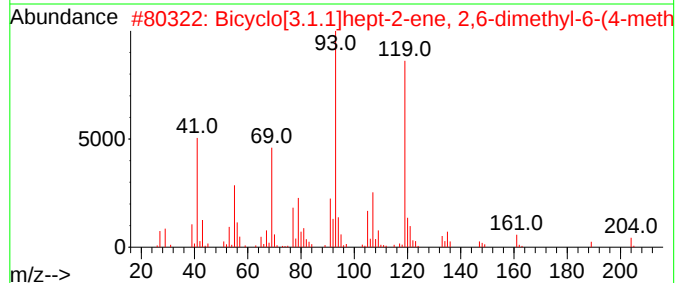
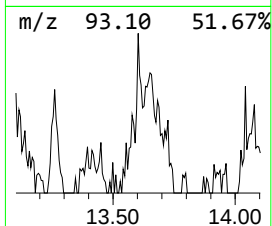
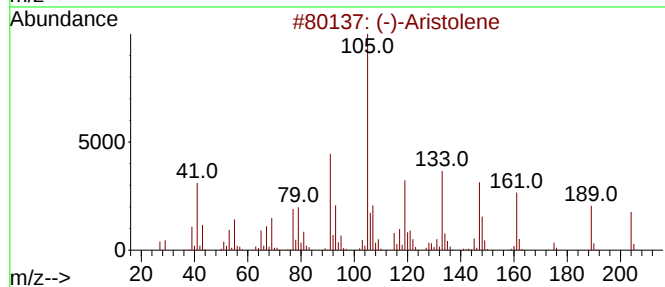
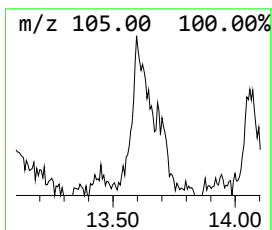
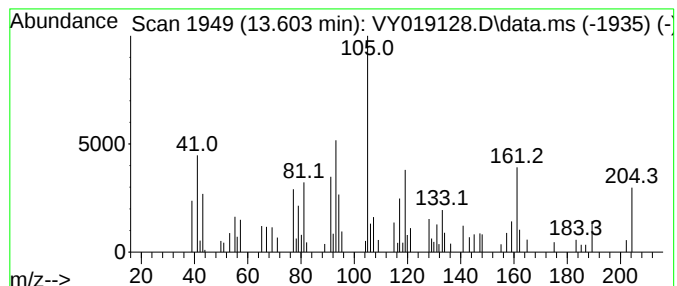
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.603 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.603	9.18 ug/l	64366	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(-)-Aristolene			204	C15H24	006831-16-9	46
2	Bicyclo[3.1.1]hept-2-ene, 2,6-di...			204	C15H24	017699-05-7	38
3	.alpha.-Cubebene			204	C15H24	017699-14-8	27
4	Bicyclo[5.2.0]nonane, 2-methylen...			204	C15H24	242794-76-9	18
5	Dimethyl(1-methylvinyl)chlorosilane			134	C5H11ClSi	104583-59-7	14



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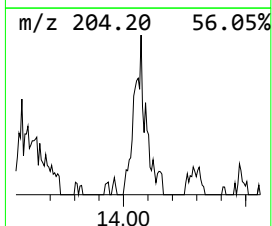
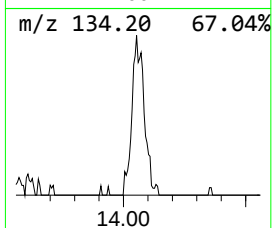
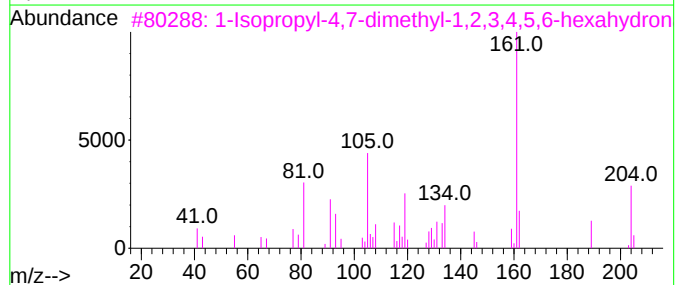
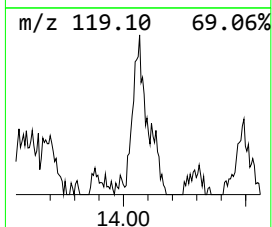
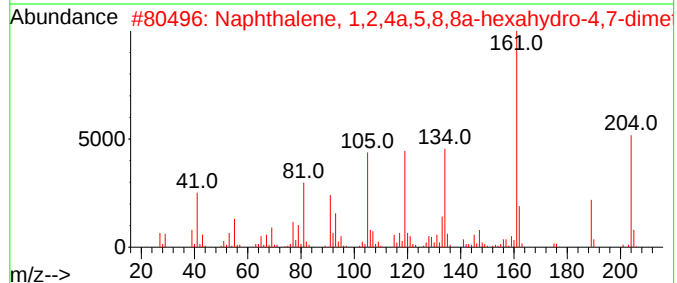
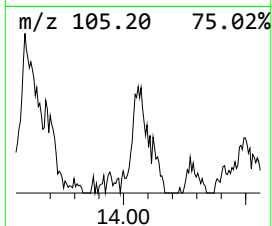
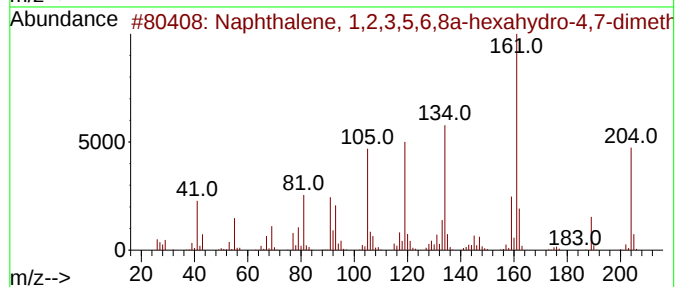
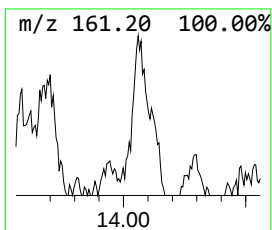
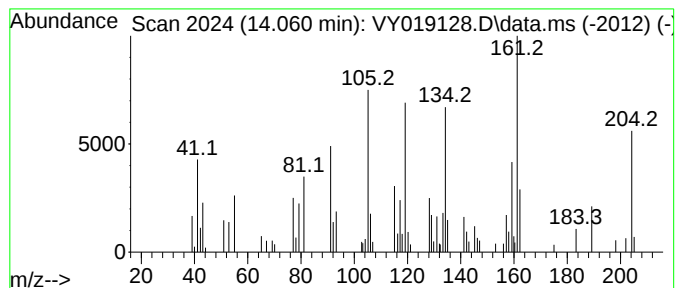
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,5,6,8a-h... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.060	8.97 ug/l	62915	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	90
2			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	70
3			1-Isopropyl-4,7-dimethyl-1,2,3,4...	204	C15H24	016729-00-3	55
4			cis-murola-3,5-diene	204	C15H24	1000365-95-4	55
5			isolekene	204	C15H24	095910-36-4	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
.alpha.-Pinene	12.261	95.5	ug/l	862415	3	11.414	451708	50.0
Camphene	12.505	8.5	ug/l	59577	4	13.347	350593	50.0
Humulene	12.999	5.7	ug/l	40069	4	13.347	350593	50.0
unknown13.603	13.603	9.2	ug/l	64366	4	13.347	350593	50.0
Naphthalene, 1,...	14.060	9.0	ug/l	62915	4	13.347	350593	50.0