

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052621\
 Data File : VY004882.D
 Acq On : 26 May 2021 13:31
 Operator : SY/MD
 Sample : M2519-01
 Misc : 4.33G/5ML/MSVOA_Y/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 26878

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\82Y051021S.M

Title : SW846 8260

Signal : TIC: VY004882.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.229	386	395	405	rBV2	4615	18073	1.05%	0.253%
2	4.729	466	477	493	rBV3	13753	47963	2.79%	0.671%
3	7.728	958	969	974	rBV	128336	305056	17.73%	4.268%
4	7.795	974	980	999	rVB	209852	468198	27.21%	6.550%
5	8.149	1028	1038	1050	rBV	148761	317912	18.48%	4.448%
6	8.697	1119	1128	1141	rBV	341133	671262	39.01%	9.391%
7	10.179	1364	1371	1379	rBV	542470	932067	54.17%	13.040%
8	11.490	1579	1586	1596	rBV	477598	771828	44.86%	10.798%
9	12.489	1742	1750	1759	rBV2	1006244	1720567	100.00%	24.071%
10	13.428	1890	1904	1910	rVV	315574	507289	29.48%	7.097%
11	13.751	1951	1957	1960	rBV6	12424	21503	1.25%	0.301%
12	13.965	1986	1992	2001	rVB	62071	108999	6.34%	1.525%
13	14.129	2015	2019	2026	rVB10	8442	17283	1.00%	0.242%
14	14.257	2035	2040	2042	rBV3	18248	31048	1.80%	0.434%
15	14.282	2042	2044	2055	rVB	22106	42368	2.46%	0.593%
16	14.398	2055	2063	2064	rBV	22750	42337	2.46%	0.592%
17	14.422	2064	2067	2070	rVV2	24263	36558	2.12%	0.511%
18	14.465	2071	2074	2082	rVB6	15403	35307	2.05%	0.494%
19	14.733	2114	2118	2123	rVB5	25021	41857	2.43%	0.586%
20	14.879	2139	2142	2146	rVB2	33715	47399	2.75%	0.663%
21	14.946	2149	2153	2157	rVB2	37365	58091	3.38%	0.813%
22	15.007	2158	2163	2164	rBV2	29795	47202	2.74%	0.660%
23	15.093	2173	2177	2180	rBV4	16943	26625	1.55%	0.372%
24	15.275	2202	2207	2210	rBV4	54390	112241	6.52%	1.570%
25	16.476	2399	2404	2412	rVB4	127917	271191	15.76%	3.794%
26	16.598	2420	2424	2439	rVB4	73463	265319	15.42%	3.712%
27	16.763	2447	2451	2455	rVB3	104545	182242	10.59%	2.550%

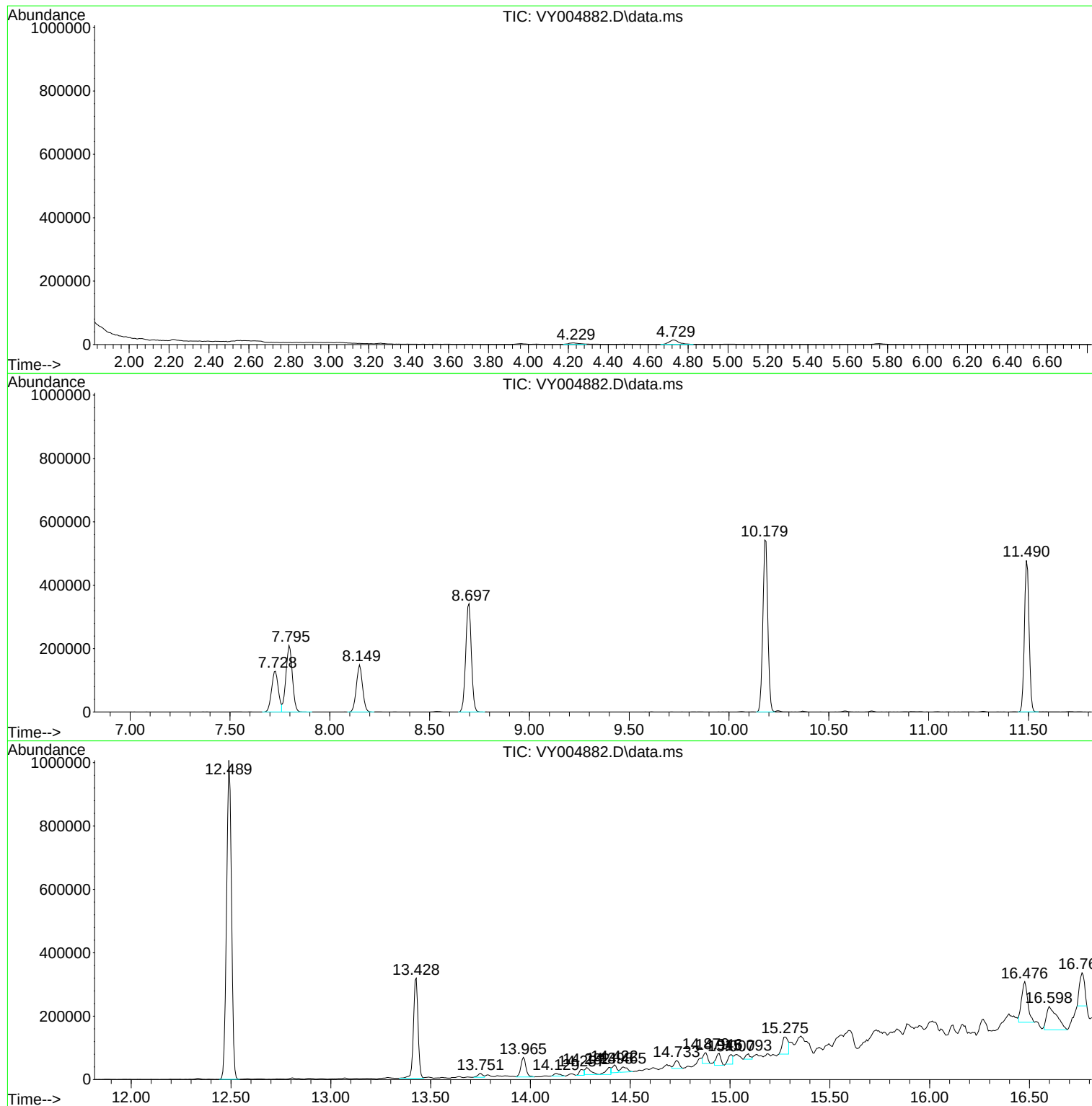
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
26878

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051021S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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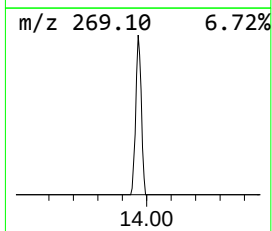
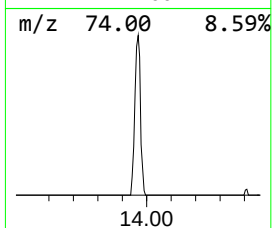
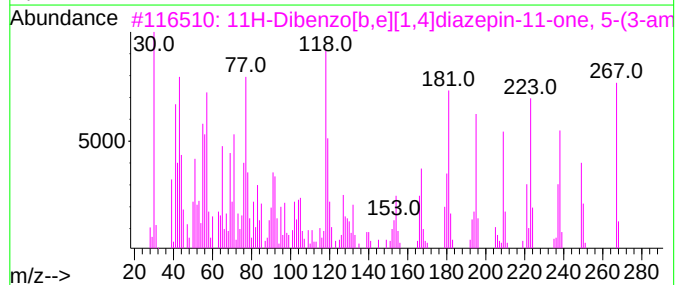
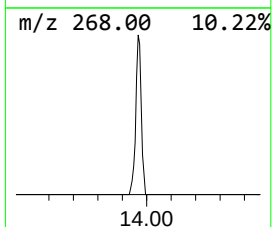
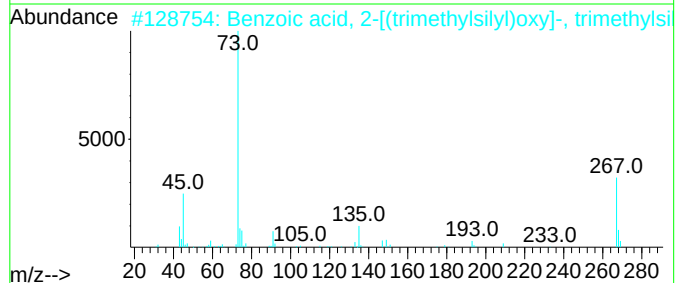
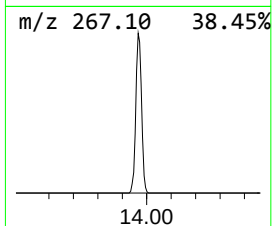
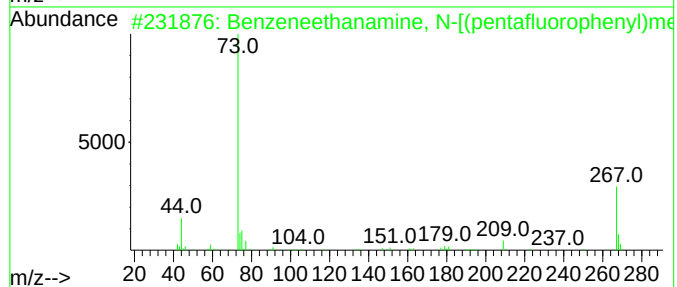
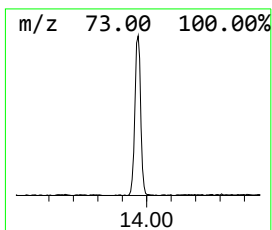
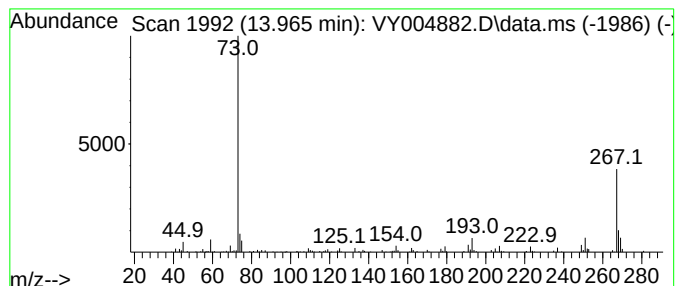
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051021S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzeneethanamine, N-[(pent... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	10.74 ug/l	108999	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneethanamine, N-[(pentafluoro...]	475	C21H26F5NO2Si2	055429-85-1	64
2			Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	282	C13H22O3Si2	003789-85-3	45
3			11H-Dibenzo[b,e][1,4]diazepin-11-one, 5-(3-aminophenyl)-	267	C16H17N3O	013450-73-2	43
4			3,5-Dimethoxyphenylacetic acid, methyl ester	268	C13H20O4Si	1000071-82-4	12
5			4-Methylcatechol, bis(trimethylsilyl) ether	268	C13H24O2Si2	1000332-79-9	9



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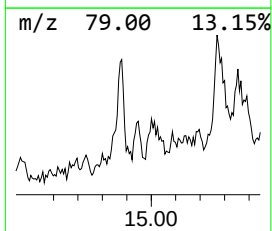
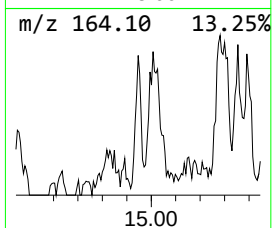
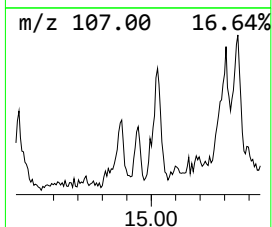
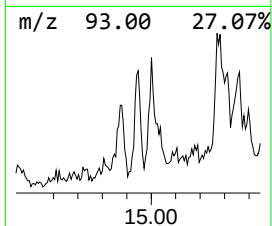
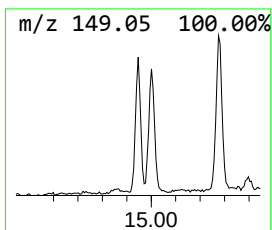
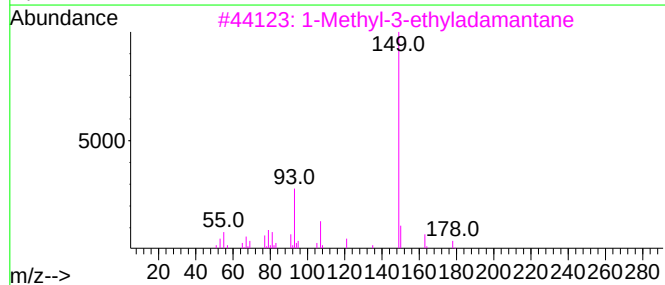
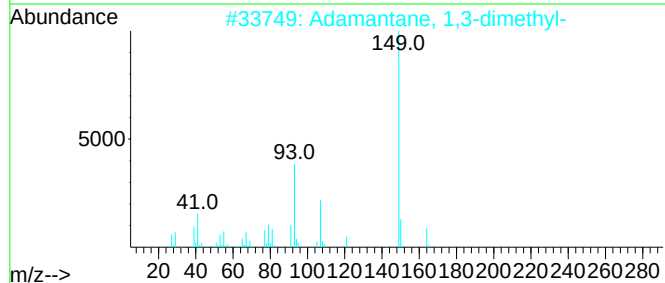
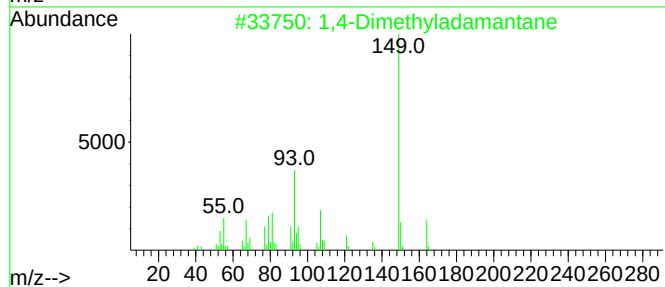
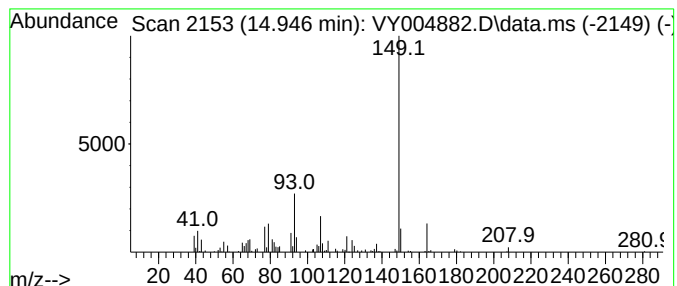
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051021S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,4-Dimethyladamantane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.946	5.73 ug/l	58091	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyladamantane	164	C12H20	024145-89-9	87
2			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	72
3			1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	64
4			1,3-Cyclohexadiene, 1,3,5,5,6,6-...	164	C12H20	1000150-39-4	64
5			2-(3-Methylbuta-1,3-dienyl)cyclo...	164	C11H16O	1000191-75-5	59



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Instrument :
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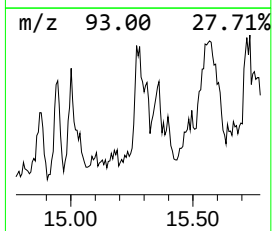
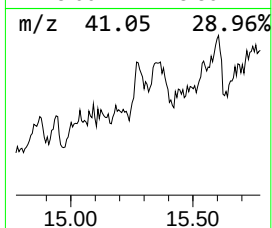
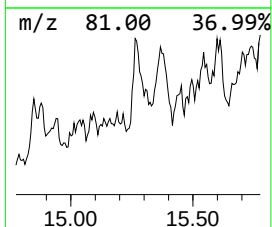
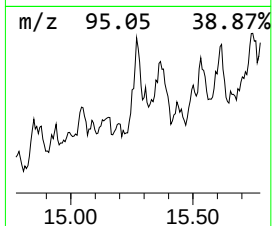
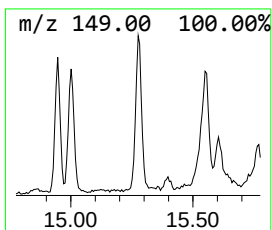
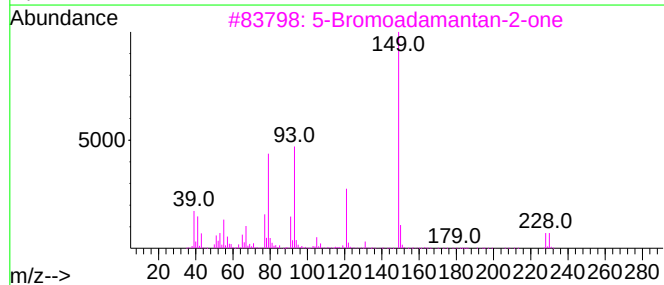
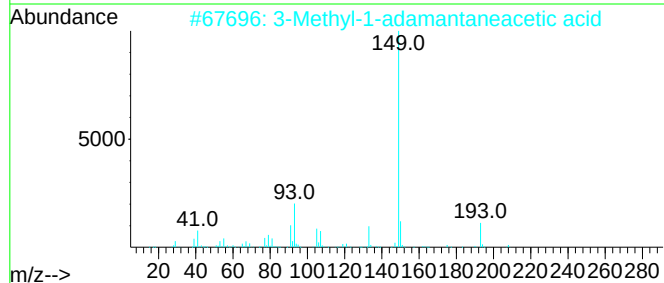
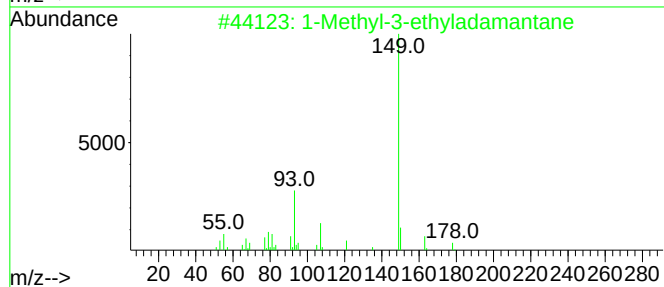
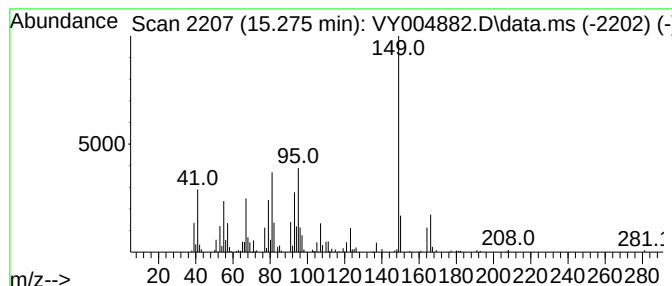
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051021S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown15.275 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.275	11.06 ug/l	112241	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	47
2			3-Methyl-1-adamantaneacetic acid	208	C13H20O2	014202-13-2	46
3			5-Bromoadamantan-2-one	228	C10H13BrO	020098-20-8	43
4			1,4-Dimethyladamantane	164	C12H20	024145-89-9	41
5			Pyridinium, 1-(acetyl-amino)-2,6-...	164	C9H12N2O	031020-35-6	38



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Misc : 4.33G/5ML/MSVOA_Y/SOIL
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Instrument :
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ClientSampleId :
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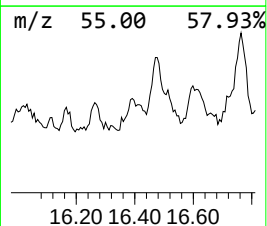
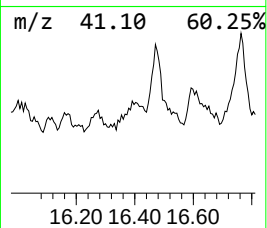
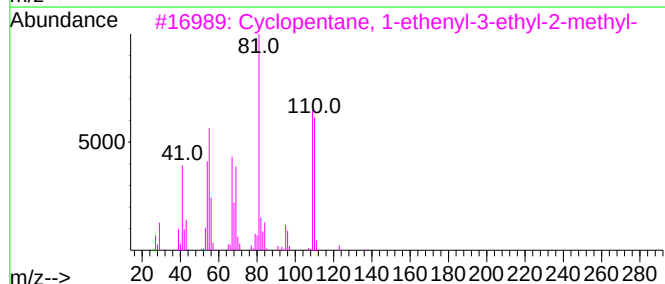
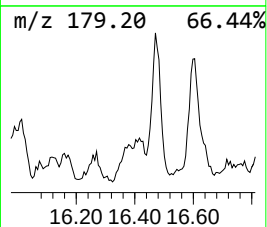
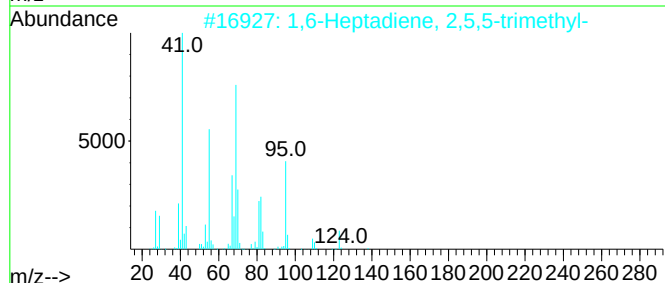
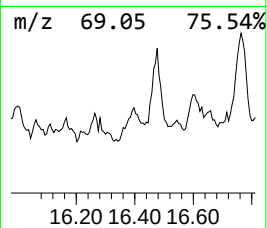
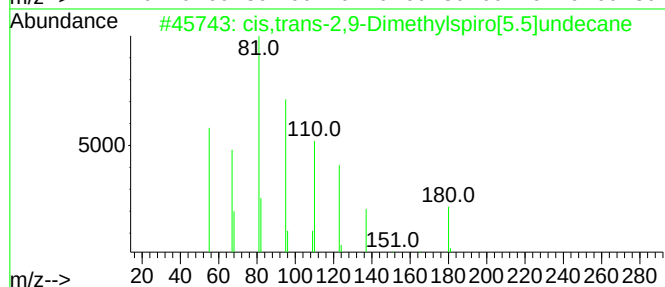
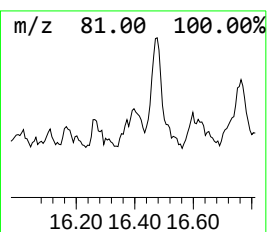
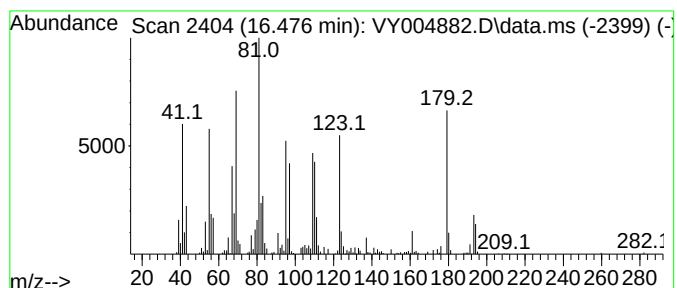
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 cis,trans-2,9-Dimethylspiro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.477	26.73 ug/l	271191	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis,trans-2,9-Dimethylspiro[5.5]...	180	C13H24	095530-74-8	50
2			1,6-Heptadiene, 2,5,5-trimethyl-	138	C10H18	062238-28-2	38
3			Cyclopentane, 1-ethenyl-3-ethyl-...	138	C10H18	055170-98-4	35
4			Methyl ethyl cyclopentene	110	C8H14	019780-56-4	35
5			2-(2-Hydroxycyclooctyl)-furan	194	C12H18O2	115754-90-0	30



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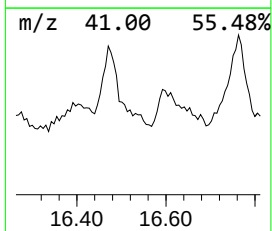
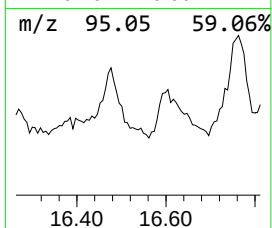
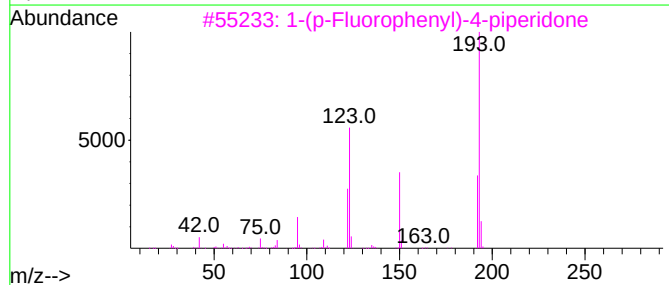
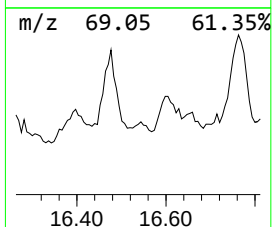
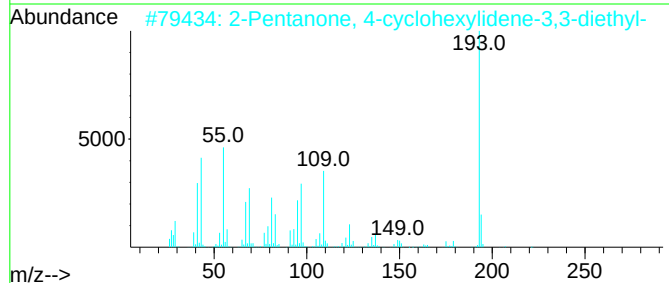
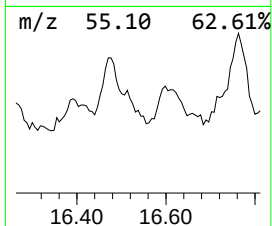
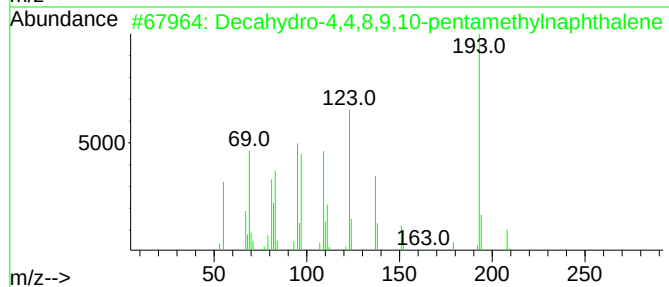
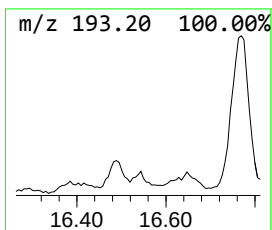
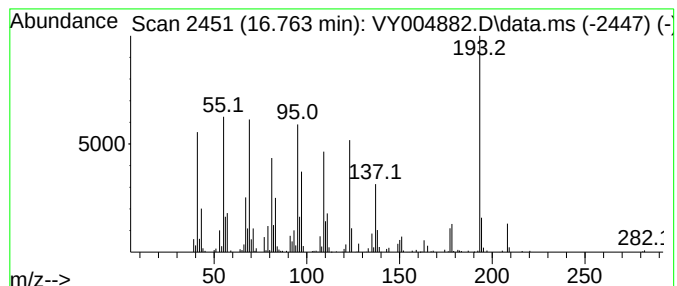
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Decahydro-4,4,8,9,10-pentam... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.763	17.96 ug/l	182242	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	59
2			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	50
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
4			1-(2-Hydroxyethyl)-1,2,5,5-tetra...	238	C16H30O	1000298-97-4	38
5			Pyrazolo[5,1-c]-as-triazine-3-ca...	193	C6H7N7O	016111-78-7	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzeneethanami...	13.965	10.7	ug/l	108999	4	13.428	507289	50.0
1,4-Dimethylada...	14.946	5.7	ug/l	58091	4	13.428	507289	50.0
unknown15.275	15.275	11.1	ug/l	112241	4	13.428	507289	50.0
cis,trans-2,9-D...	16.477	26.7	ug/l	271191	4	13.428	507289	50.0
Decahydro-4,4,8...	16.763	18.0	ug/l	182242	4	13.428	507289	50.0