

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD101221\
 Data File : VD070684.D
 Acq On : 12 Oct 2021 17:29
 Operator : VA/SY
 Sample : M4127-05
 Misc : 5.15G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 CHRT-20426

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_D\Method\82D100521S.M
 Title : SW846 8260

Signal : TIC: VD070684.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.315	62	67	73	rBV	26435	42111	1.65%	0.259%
2	7.914	1009	1019	1024	rBV	323783	797217	31.17%	4.910%
3	7.979	1024	1030	1041	rVB	526927	1169973	45.75%	7.205%
4	8.326	1080	1089	1103	rBV	293294	666837	26.07%	4.107%
5	8.861	1170	1180	1192	rBV	869523	1742610	68.14%	10.732%
6	10.338	1422	1431	1442	rBV	1382629	2557511	100.00%	15.750%
7	11.638	1645	1652	1660	rBV	1246225	2157124	84.34%	13.284%
8	12.479	1791	1795	1801	rBV	71760	110546	4.32%	0.681%
9	12.626	1813	1820	1826	rBV	914768	1612849	63.06%	9.932%
10	12.708	1826	1834	1851	rVB5	159472	732159	28.63%	4.509%
11	12.943	1868	1874	1875	rBV6	33098	64099	2.51%	0.395%
12	13.561	1973	1979	1997	rBV	1110494	2069844	80.93%	12.747%
13	13.779	2010	2016	2028	rVB5	195003	667318	26.09%	4.110%
14	13.885	2031	2034	2039	rVB7	37429	58596	2.29%	0.361%
15	14.390	2116	2120	2132	rVB4	115368	364745	14.26%	2.246%
16	14.555	2146	2148	2152	rVB3	68027	77323	3.02%	0.476%
17	15.137	2245	2247	2250	rBV4	42564	57636	2.25%	0.355%
18	15.426	2289	2296	2301	rBV4	144074	382681	14.96%	2.357%
19	16.667	2503	2507	2522	rVB5	332752	906955	35.46%	5.585%

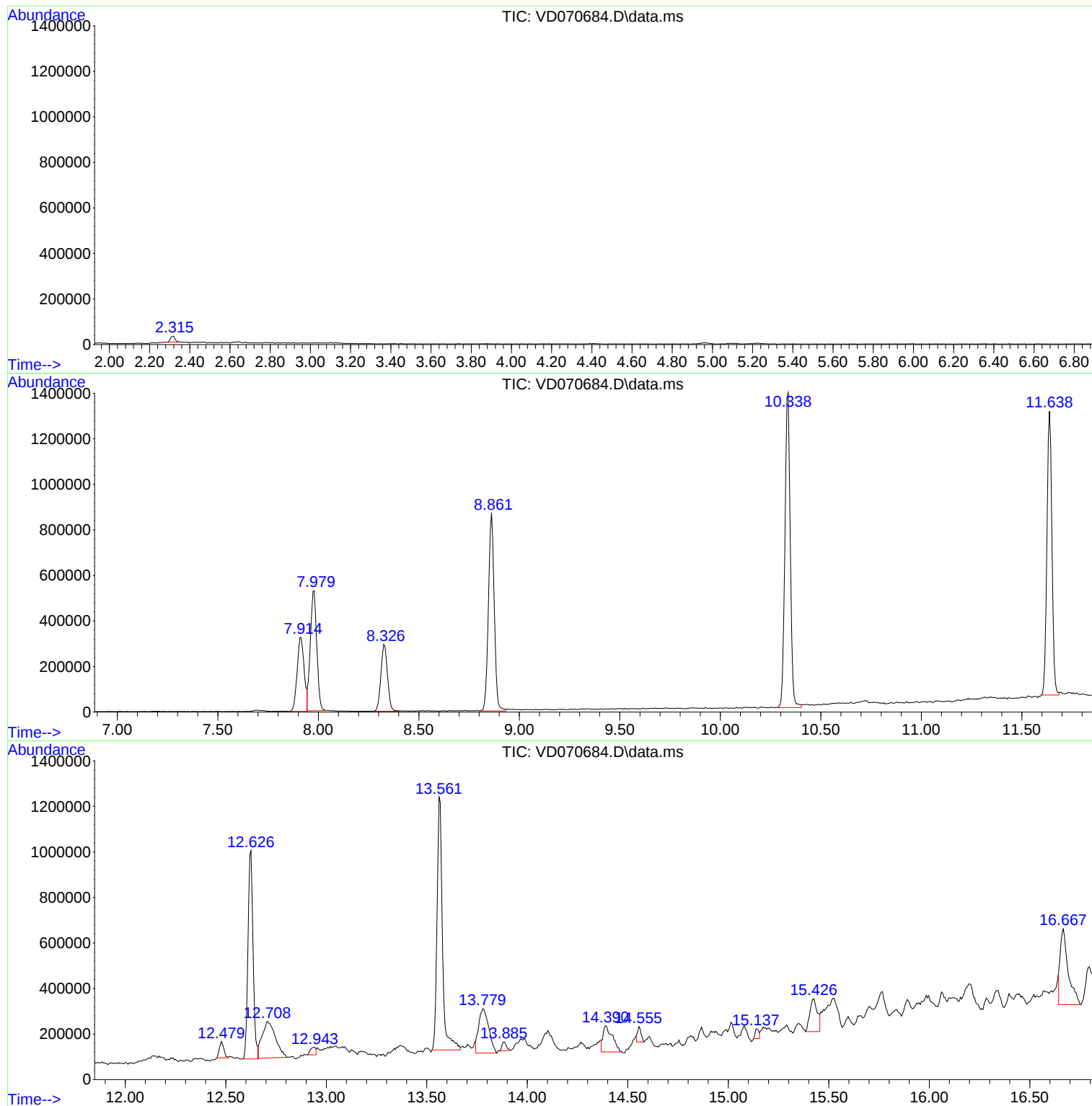
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D100521S.M
Quant Title : SW846 8260

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



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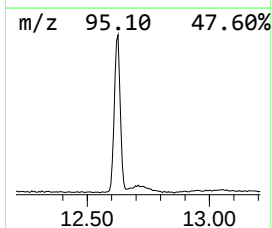
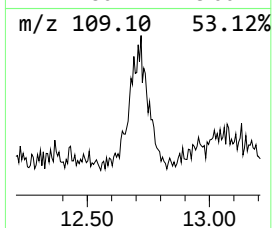
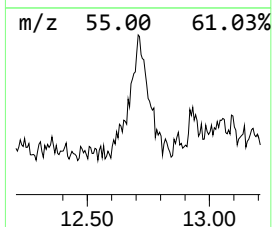
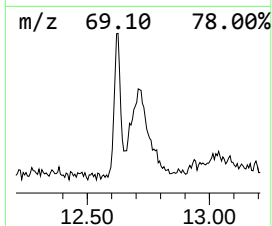
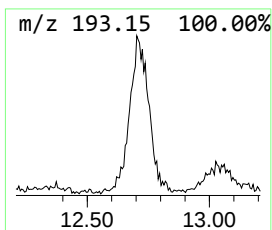
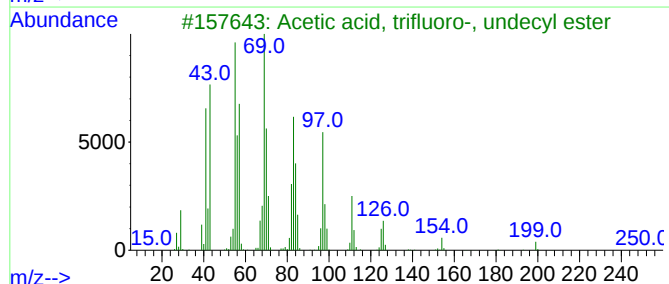
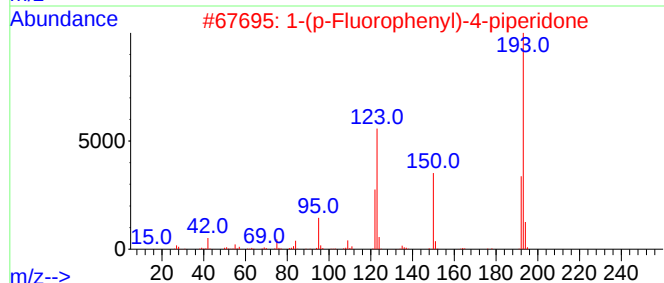
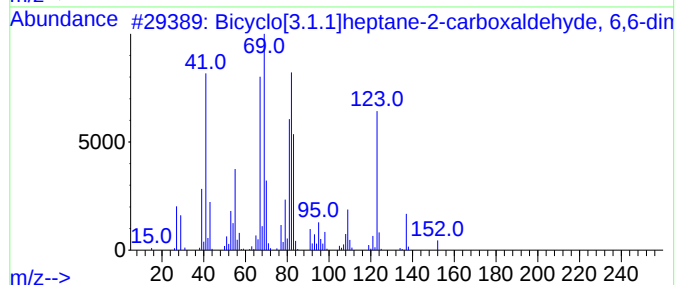
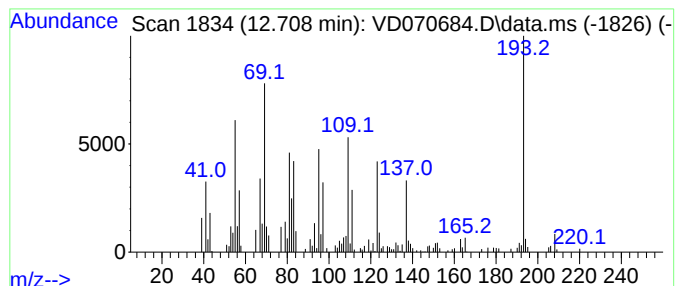
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D100521S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown12.708 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.708	17.69 ug/l	732159	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptane-2-carboxal...	152	C10H16O	004764-14-1	35
2			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	22
3			Acetic acid, trifluoro-, undecyl...	268	C13H23F3O2	053800-01-4	22
4			1,1'-Bicyclohexyl, 2-ethyl-, cis-	194	C14H26	050991-12-3	18
5			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	15



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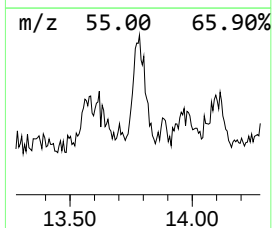
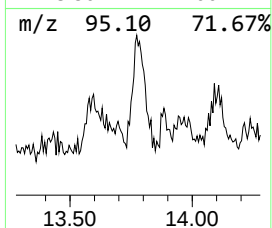
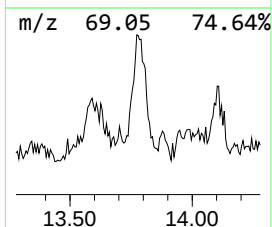
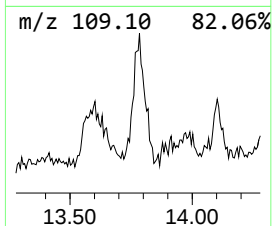
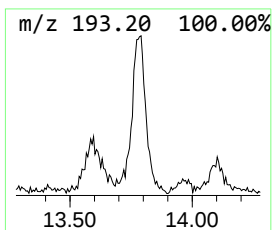
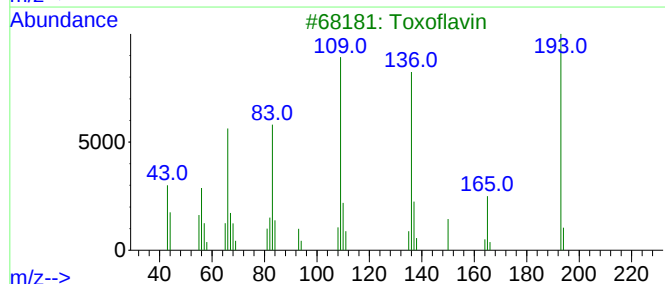
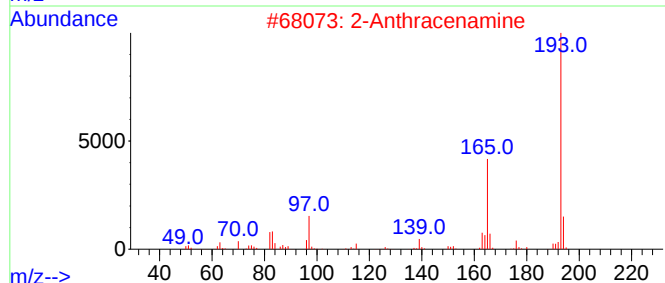
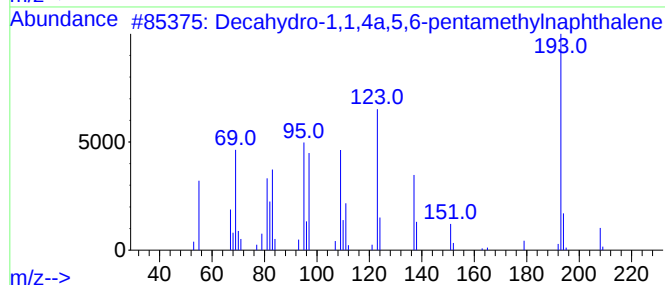
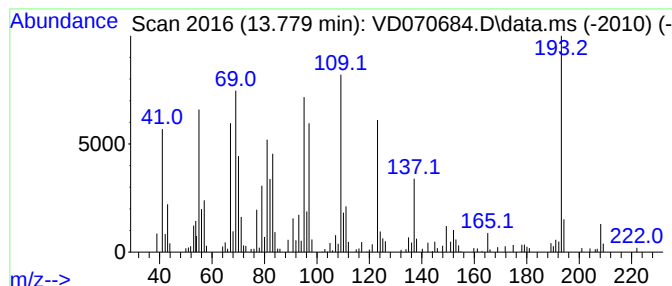
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D100521S.M
Quant Title : SW846 8260

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

Peak Number 2 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.779	16.12 ug/l	667318	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	86
2			2-Anthracenamine	193	C14H11N	000613-13-8	35
3			Toxoflavin	193	C7H7N5O2	000084-82-2	30
4			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	25
5			Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	25



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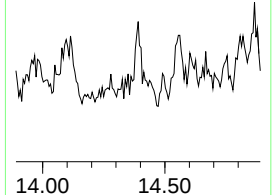
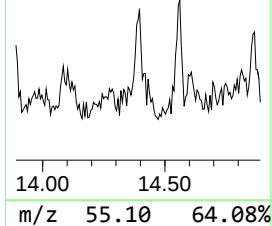
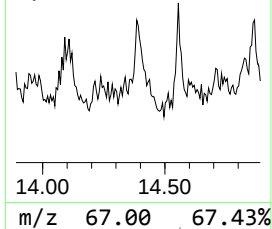
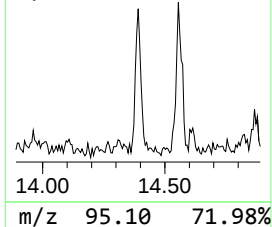
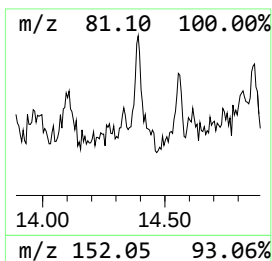
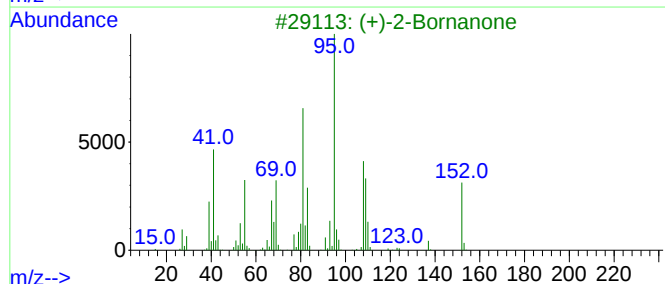
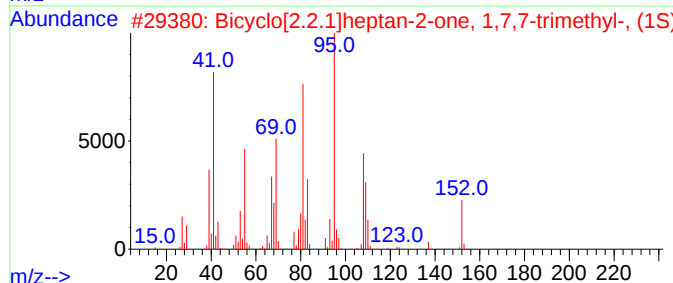
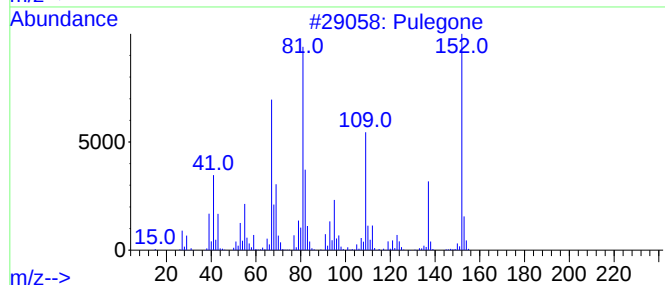
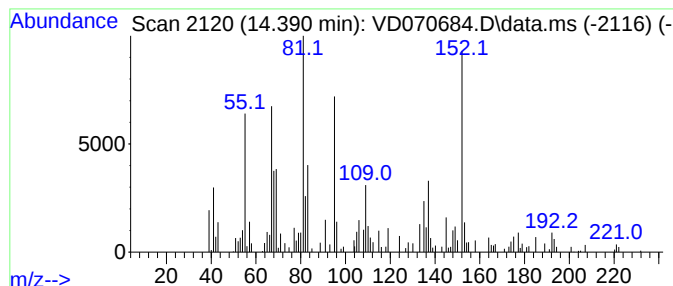
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Quant Title : SW846 8260

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

Peak Number 3 Pulegone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.390	8.81 ug/l	364745	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pulegone	152	C10H16O	000089-82-7	83
2			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	81
3			(+)-2-Bornanone	152	C10H16O	000464-49-3	74
4			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	72
5			Bicyclo[4.1.0]heptan-3-one, 4,7,...	152	C10H16O	004176-04-9	58



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ALS Vial : 15 Sample Multiplier: 1

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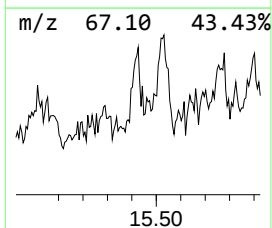
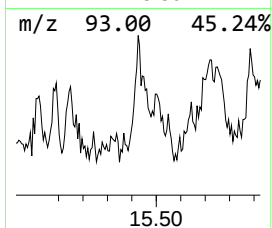
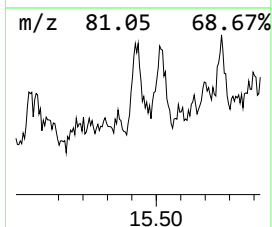
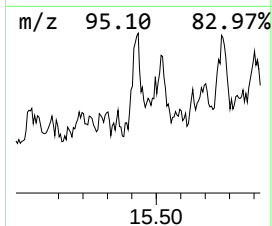
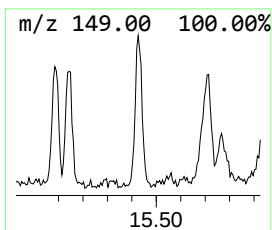
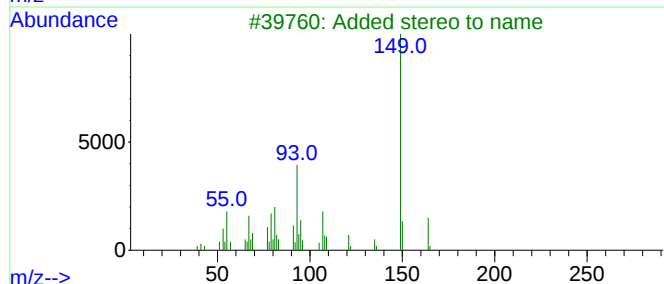
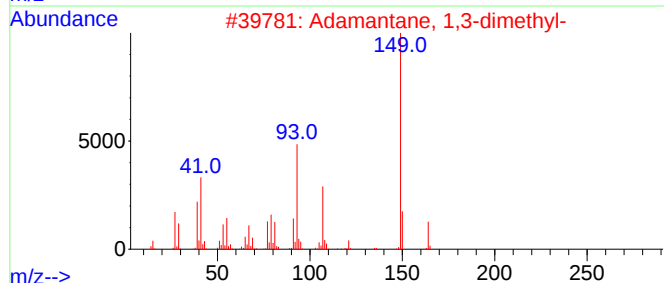
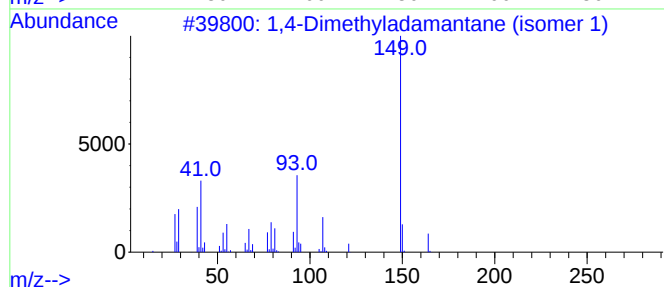
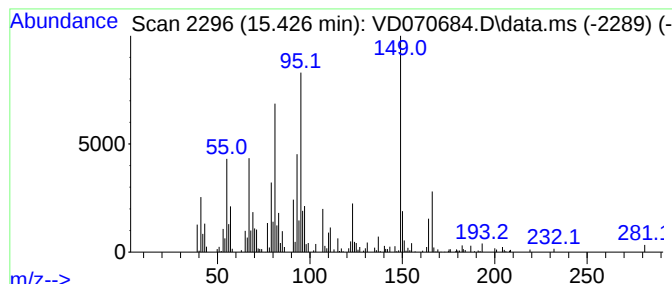
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown15.426 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.426	9.24 ug/l	382681	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	38
2			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	38
3			Added stereo to name	164	C12H20	024145-88-8	38
4			Added stereo to name	164	C12H20	024145-89-9	35
5			trans,cis-1,8-Dimethylspiro[4.5]...	166	C12H22	1000111-72-9	35



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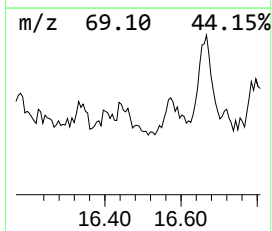
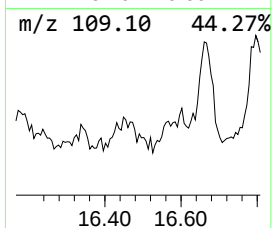
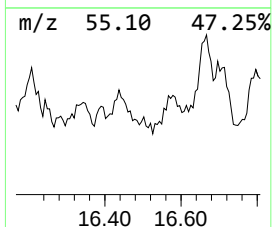
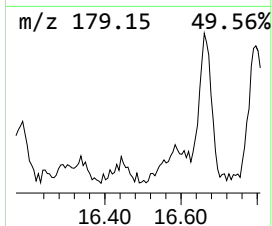
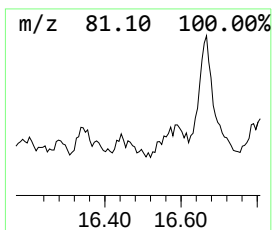
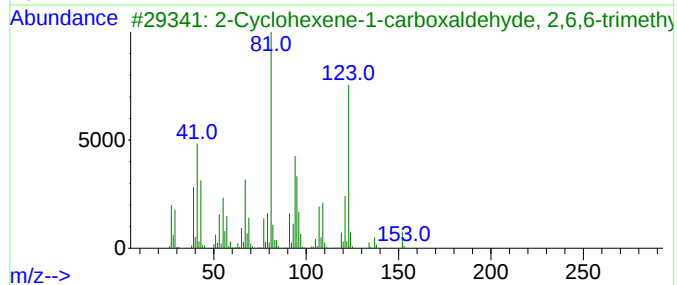
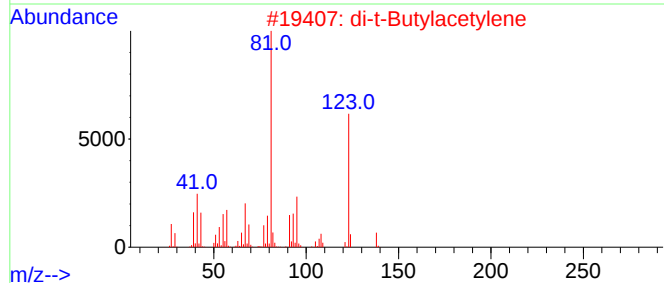
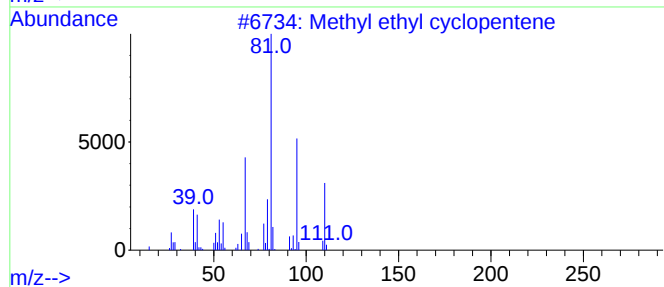
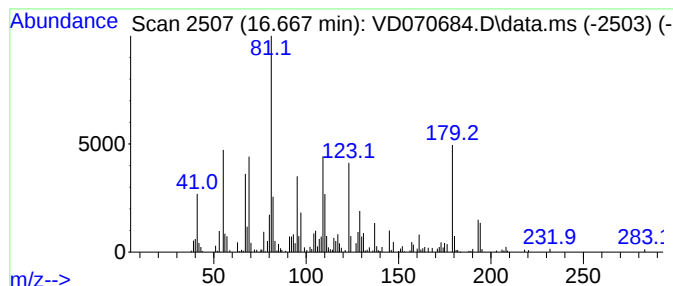
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown16.667 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.667	21.91 ug/l	906955	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl ethyl cyclopentene	110	C8H14	019780-56-4	42
2			di-t-Butylacetylene	138	C10H18	017530-24-4	38
3			2-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	000432-24-6	32
4			1-(2-Ethyl-1,3-dimethyl-cyclopent...	166	C11H18O	1010185-18-1	32
5			Cyclopentane, 1-isobutylidene-3-...	138	C10H18	1000150-62-1	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Decahydro-1,1,4...	13.779	16.1	ug/l	667318	4	13.561	2069840	50.0
Pulegone	14.390	8.8	ug/l	364745	4	13.561	2069840	50.0
unknown15.426	15.426	9.2	ug/l	382681	4	13.561	2069840	50.0
unknown16.667	16.667	21.9	ug/l	906955	4	13.561	2069840	50.0