

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD101821\
 Data File : VD070742.D
 Acq On : 18 Oct 2021 21:00
 Operator : VA/SY
 Sample : M4248-03
 Misc : 5.03G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 72-12002

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\82D101521S.M
 Title : SW846 8260

Signal : TIC: VD070742.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.321	63	68	70	rBV3	12782	19076	1.11%	0.161%
2	4.962	507	517	529	rBV3	34983	118675	6.88%	1.001%
3	7.915	1007	1019	1024	rBV	269112	641951	37.22%	5.413%
4	7.979	1024	1030	1039	rVB	343273	785623	45.55%	6.624%
5	8.326	1078	1089	1102	rBV2	293396	657743	38.13%	5.546%
6	8.862	1170	1180	1194	rBV	607793	1223922	70.96%	10.320%
7	10.338	1422	1431	1439	rBV	932293	1724832	100.00%	14.544%
8	11.638	1644	1652	1666	rBV	857166	1484539	86.07%	12.518%
9	12.626	1811	1820	1829	rBV	569805	963913	55.88%	8.128%
10	12.950	1870	1875	1885	rVB9	14384	26664	1.55%	0.225%
11	13.261	1923	1928	1933	rBV3	18795	34048	1.97%	0.287%
12	13.561	1972	1979	1988	rBV	713282	1227071	71.14%	10.347%
13	13.691	1998	2001	2008	rBV9	10092	20903	1.21%	0.176%
14	13.879	2028	2033	2040	rBV7	50972	114290	6.63%	0.964%
15	14.097	2067	2070	2076	rVB8	24020	37112	2.15%	0.313%
16	14.208	2084	2089	2093	rBV7	25821	48427	2.81%	0.408%
17	14.267	2094	2099	2105	rBV8	38744	78505	4.55%	0.662%
18	14.338	2108	2111	2116	rVB6	18935	27345	1.59%	0.231%
19	14.397	2116	2121	2122	rBV3	72543	105750	6.13%	0.892%
20	14.426	2122	2126	2130	rVB2	76409	122448	7.10%	1.032%
21	14.555	2140	2148	2152	rBV3	78918	166856	9.67%	1.407%
22	14.744	2178	2180	2184	rBV5	23750	30524	1.77%	0.257%
23	14.802	2186	2190	2196	rVV5	83284	210119	12.18%	1.772%
24	14.867	2197	2201	2205	rVB4	88031	147710	8.56%	1.245%
25	15.014	2223	2226	2232	rVB3	92409	147470	8.55%	1.243%
26	15.085	2233	2238	2242	rVB6	106110	186364	10.80%	1.571%
27	15.144	2245	2248	2250	rBV3	69196	80407	4.66%	0.678%
28	15.426	2291	2296	2300	rBV5	133659	284205	16.48%	2.396%
29	16.667	2502	2507	2523	rVB6	379211	1143038	66.27%	9.638%

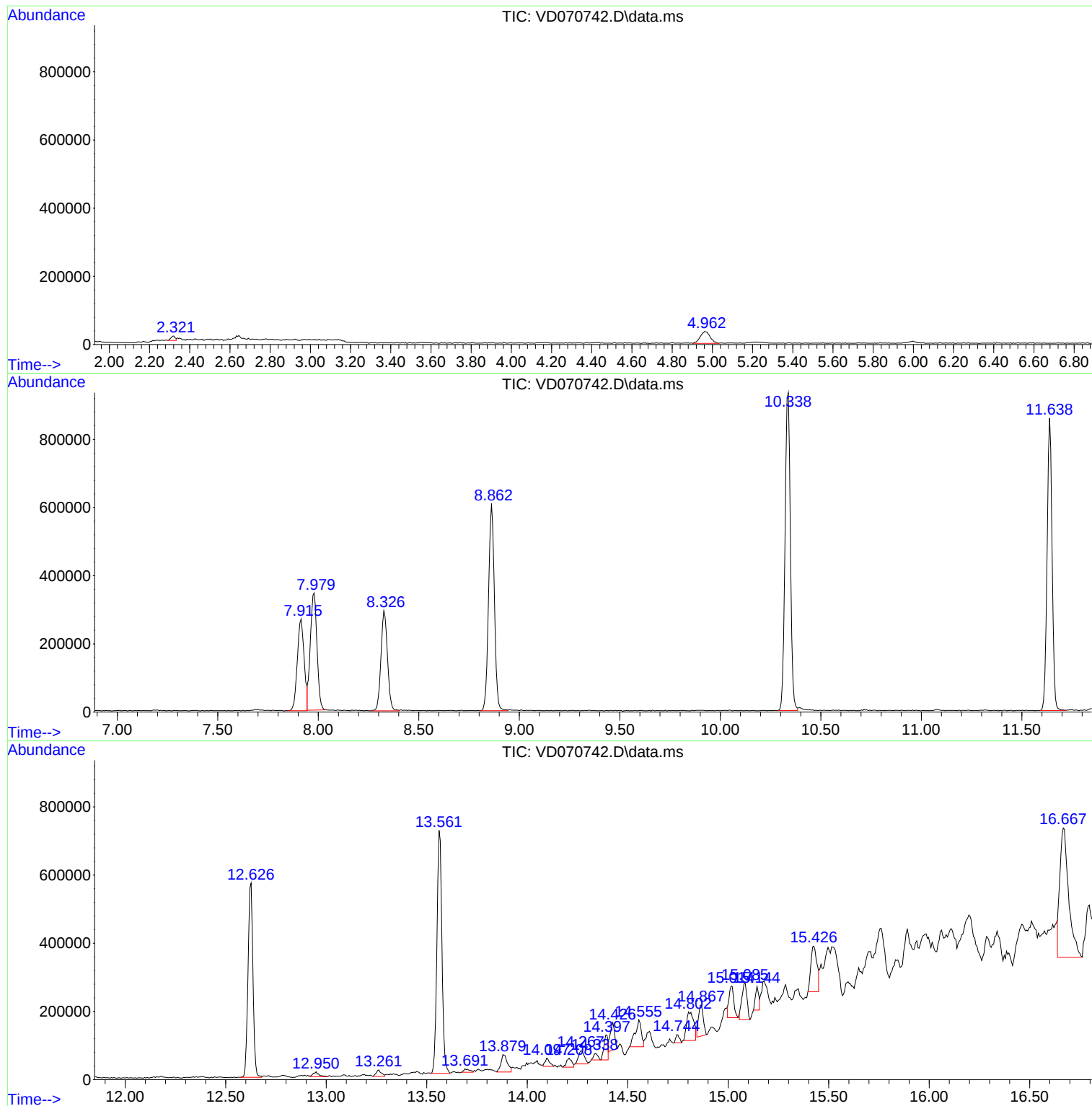
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD101821\
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Misc : 5.03G/5.00ml/MSVOA_D/SOIL
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
72-12002

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
Quant Title : SW846 8260

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



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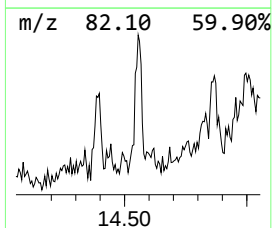
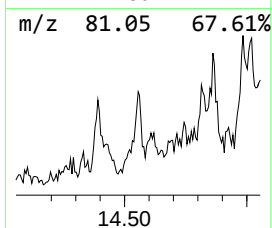
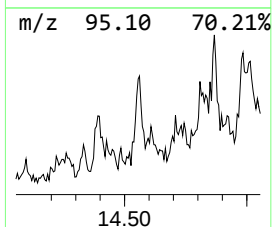
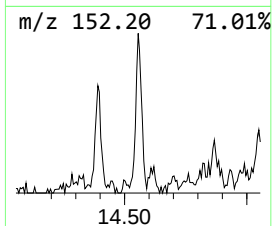
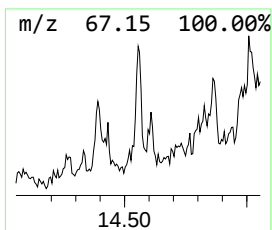
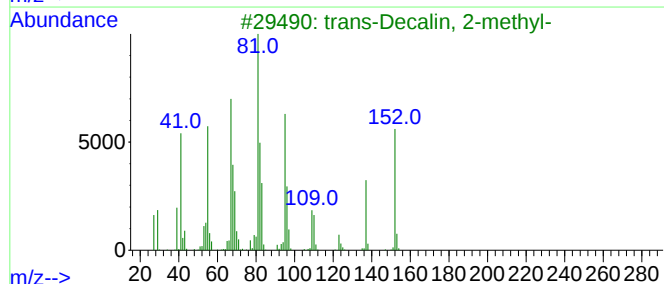
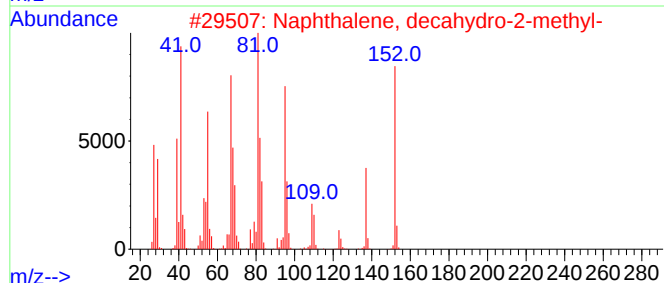
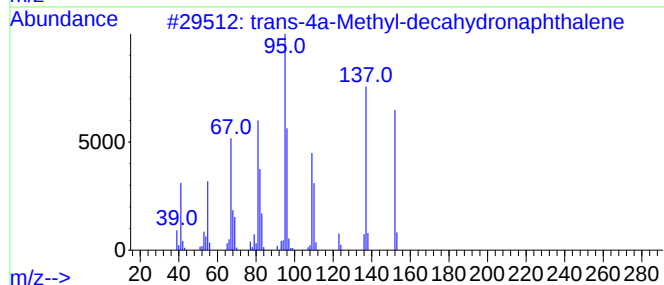
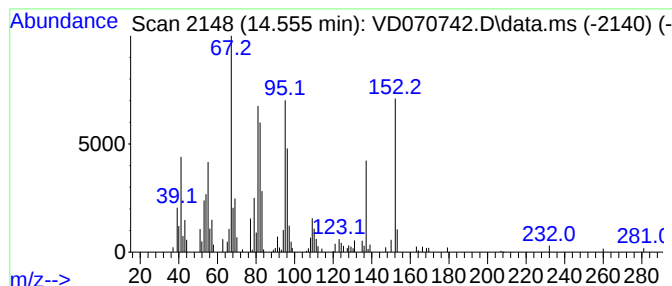
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
Quant Title : SW846 8260

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

Peak Number 2 trans-4a-Methyl-decahydrona... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.555	6.80 ug/l	166856	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	90
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	87
3			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	86
4			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	005948-04-9	74
5			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	007764-50-3	68



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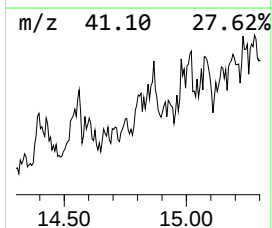
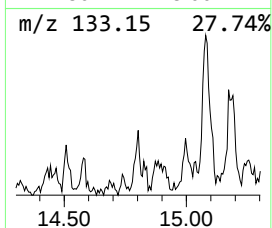
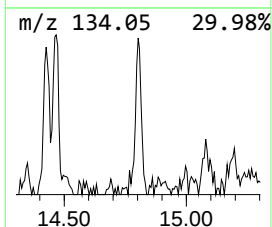
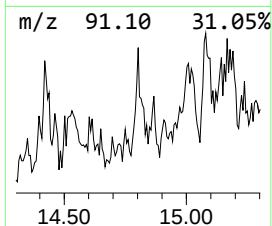
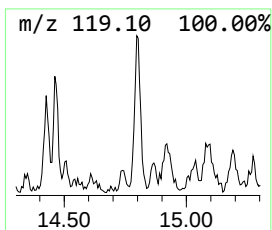
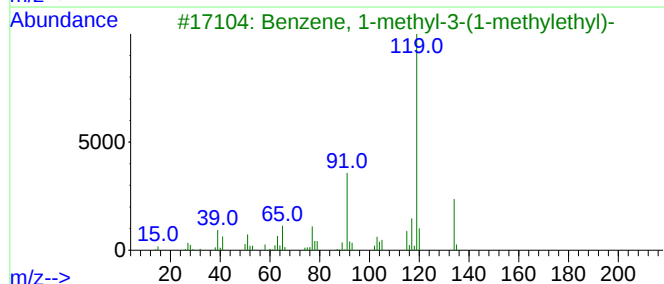
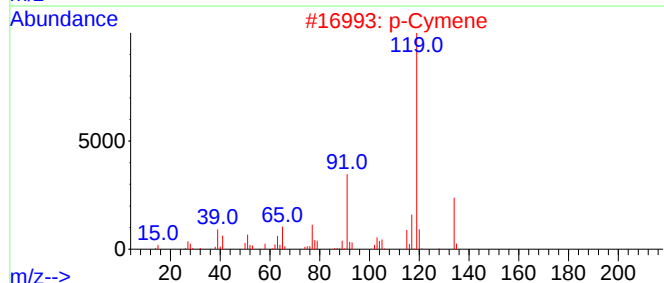
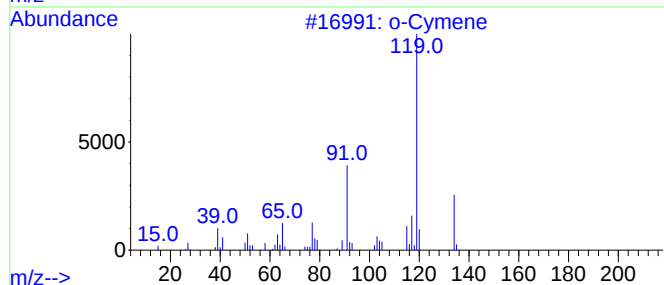
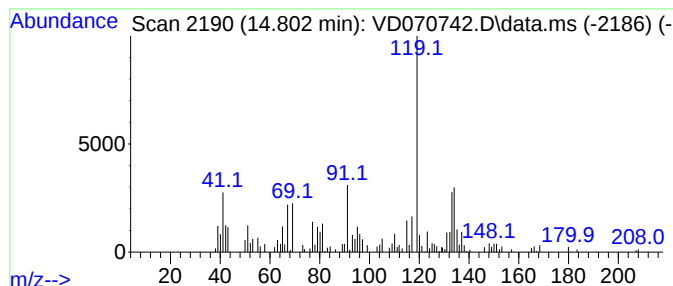
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
Quant Title : SW846 8260

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

Peak Number 3 o-Cymene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.802	8.56 ug/l	210119	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	60
2			p-Cymene	134	C10H14	000099-87-6	60
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	53
4			1,3,8-p-Menthatriene	134	C10H14	018368-95-1	49
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	49



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Misc : 5.03G/5.00ml/MSVOA_D/SOIL
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
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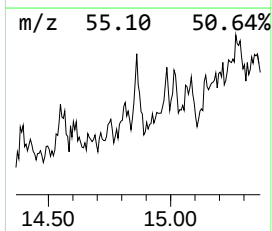
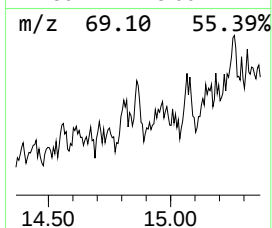
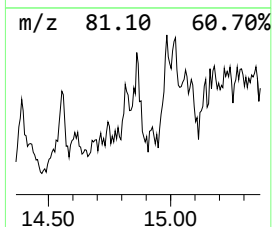
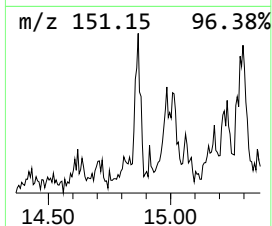
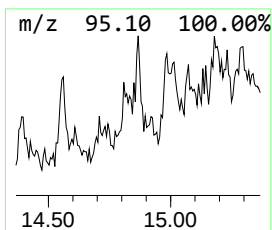
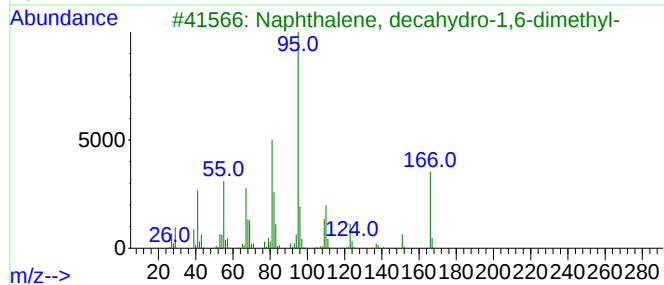
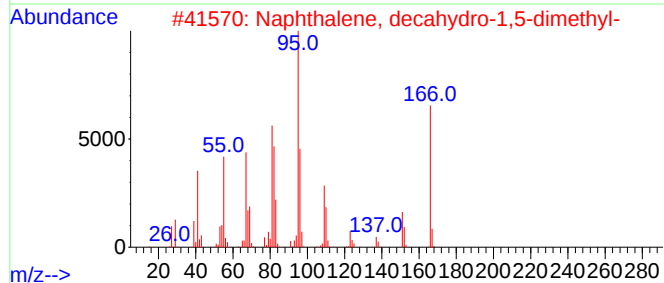
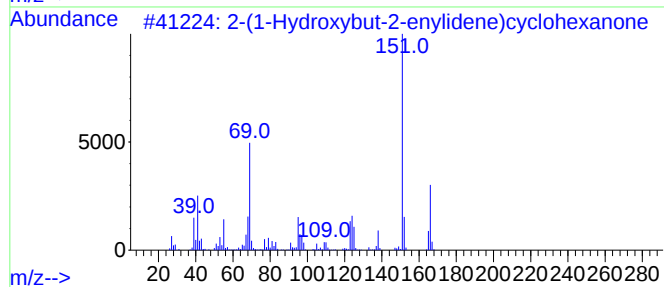
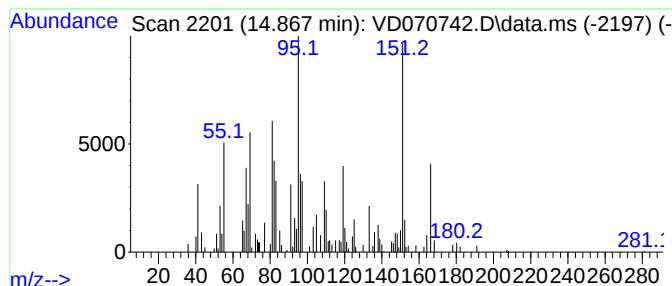
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
Quant Title : SW846 8260

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

Peak Number 4 2-(1-Hydroxybut-2-enylidene... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.867	6.02 ug/l	147710	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-(1-Hydroxybut-2-enylidene)cycl...	166	C10H14O2	1000186-18-9	64
2			Naphthalene, decahydro-1,5-dimet...	166	C12H22	066552-62-3	49
3			Naphthalene, decahydro-1,6-dimet...	166	C12H22	001750-51-2	43
4			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	38
5			(4aS,7S,7aR)-4,7-Dimethyl-5,6,7,...	166	C10H14O2	021651-62-7	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD101821\
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Misc : 5.03G/5.00ml/MSVOA_D/SOIL
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
72-12002

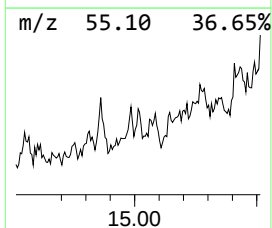
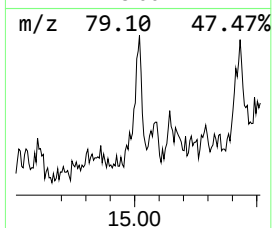
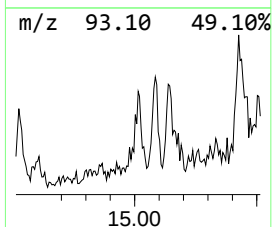
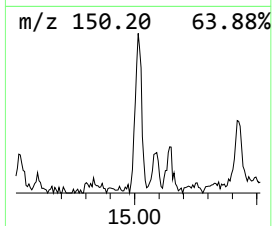
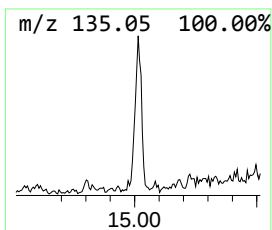
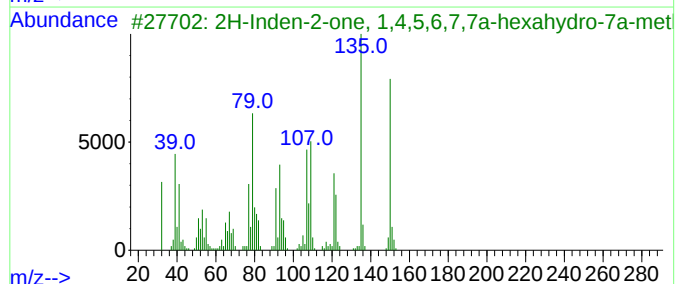
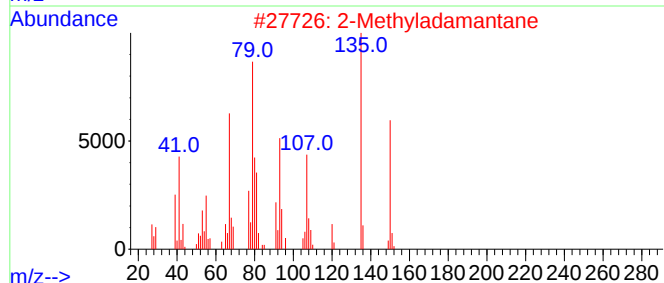
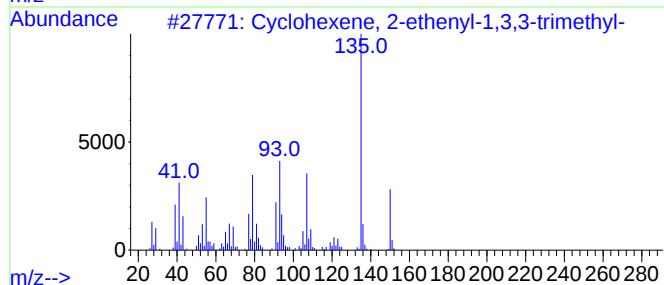
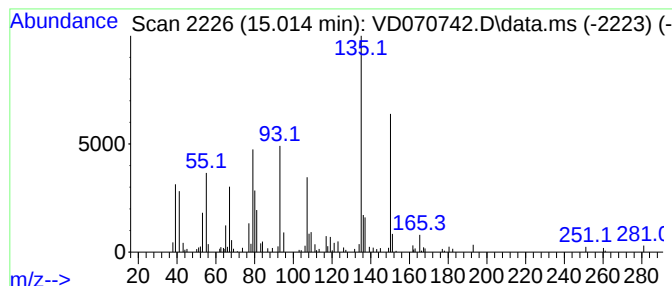
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclohexene, 2-ethenyl-1,3,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.014	6.01 ug/l	147470	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 2-ethenyl-1,3,3-tri...	150	C11H18	005293-90-3	90
2			2-Methyladamantane	150	C11H18	000700-56-1	83
3			2H-Inden-2-one, 1,4,5,6,7,7a-hex...	150	C10H14O	054725-16-5	74
4			Pyridinium, 1-(acetylamino)-2-me...	150	C8H10N2O	007584-27-2	47
5			Ethanone, 1-(2-hydroxy-5-methylp...	150	C9H10O2	001450-72-2	46



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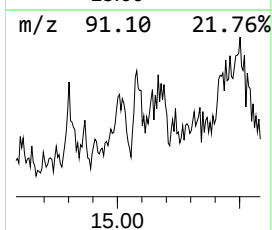
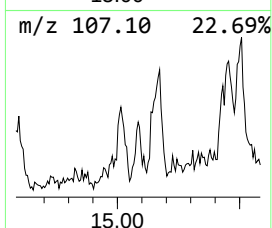
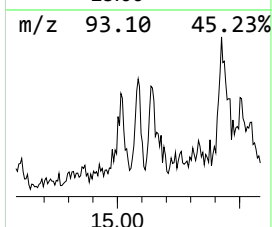
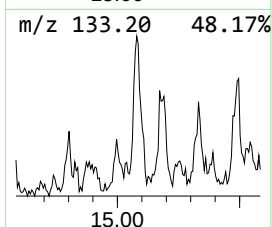
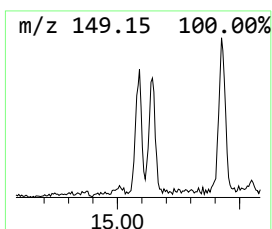
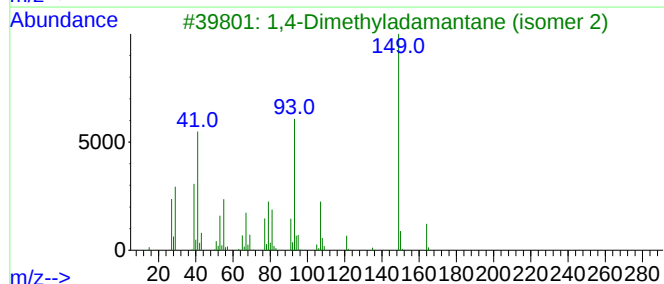
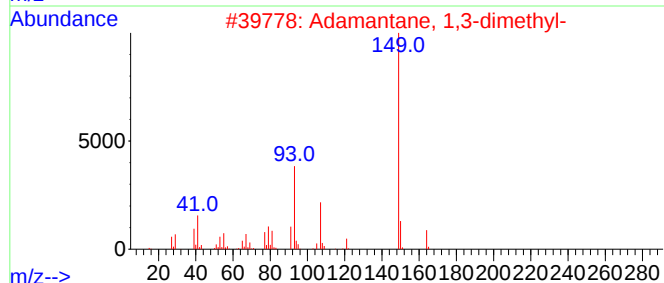
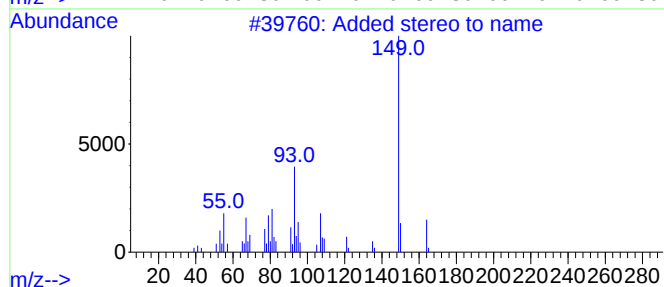
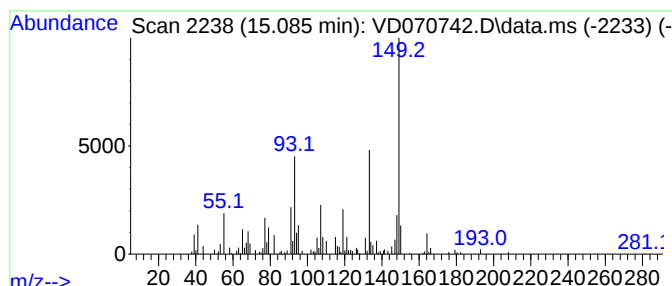
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
Quant Title : SW846 8260

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

Peak Number 6 Added stereo to name Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.085	7.59 ug/l	186364	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name			164	C12H20	024145-88-8	70
2	Adamantane, 1,3-dimethyl-			164	C12H20	000702-79-4	58
3	1,4-Dimethyladamantane (isomer 2)			164	C12H20	1000460-67-1	50
4	Methyl (1s,3s,5R,7S)-3-methylada...			208	C13H20O2	1010504-39-1	50
5	Added stereo to name			164	C12H20	024145-89-9	49



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ClientSampled :
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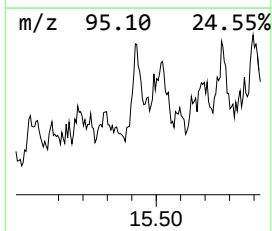
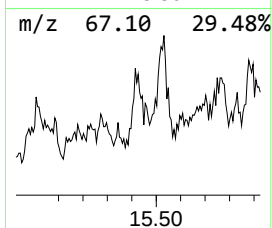
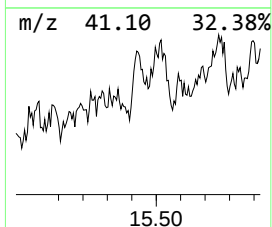
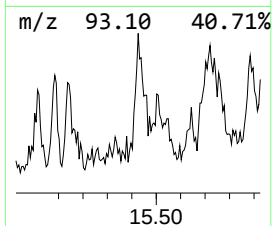
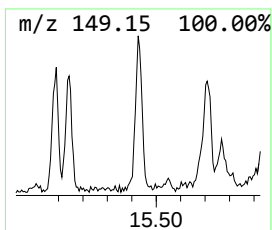
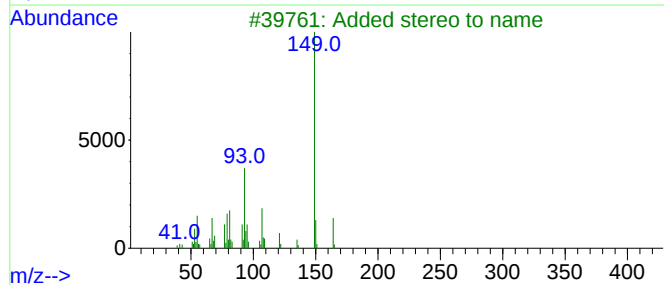
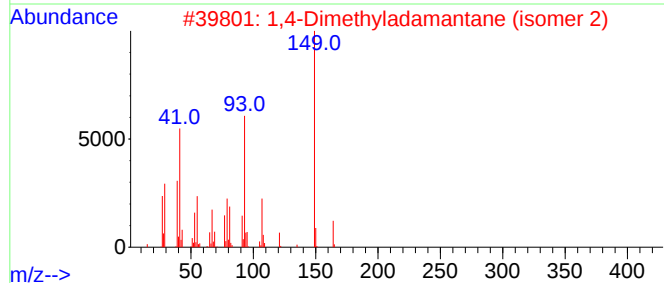
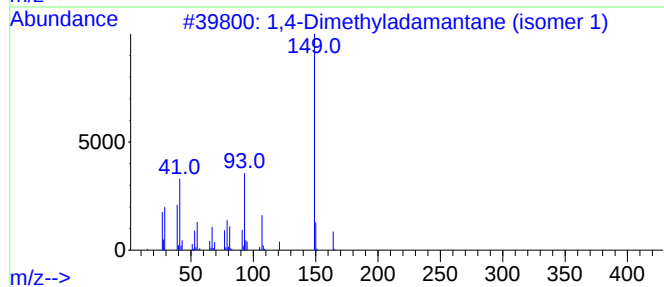
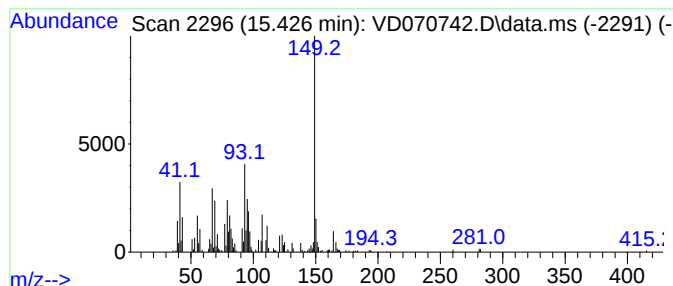
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Quant Title : SW846 8260

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

Peak Number 7 1,4-Dimethyladamantane (iso... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.426	11.58 ug/l	284205	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	68
2			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	62
3			Added stereo to name	164	C12H20	024145-89-9	62
4			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	58
5			Tricyclo[4.3.1.1(3,8)]undecane, ...	228	C11H17Br	021898-96-4	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD101821\
Data File : VD070742.D
Acq On : 18 Oct 2021 21:00
Operator : VA/SY
Sample : M4248-03
Misc : 5.03G/5.00ml/MSVOA_D/SOIL
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
72-12002

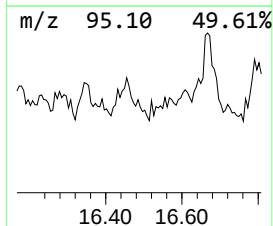
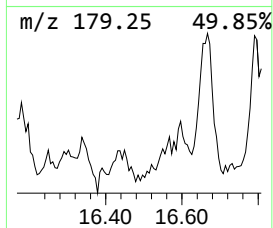
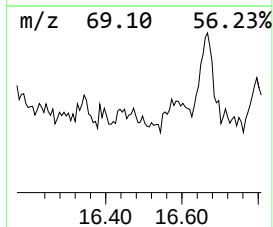
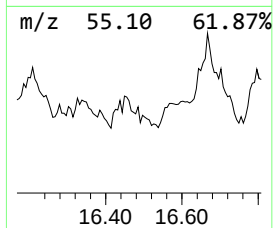
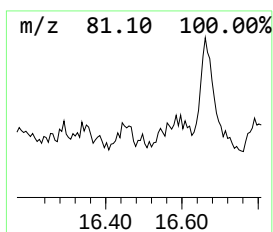
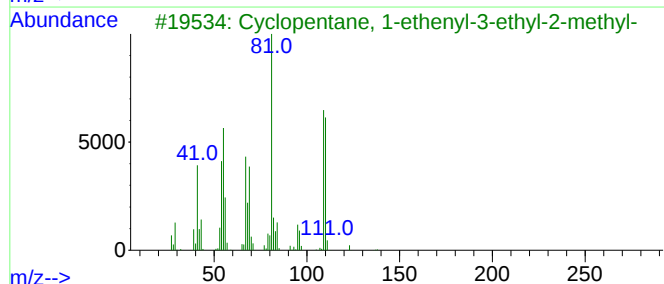
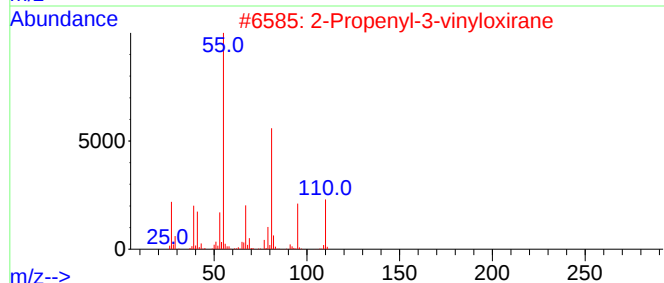
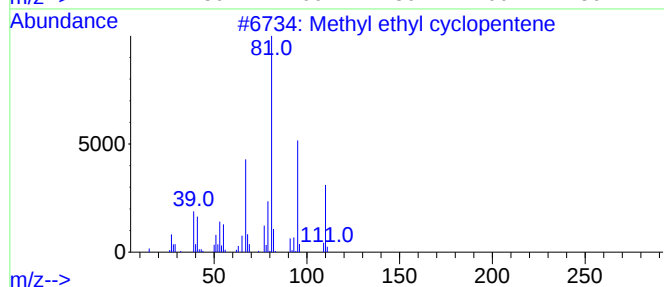
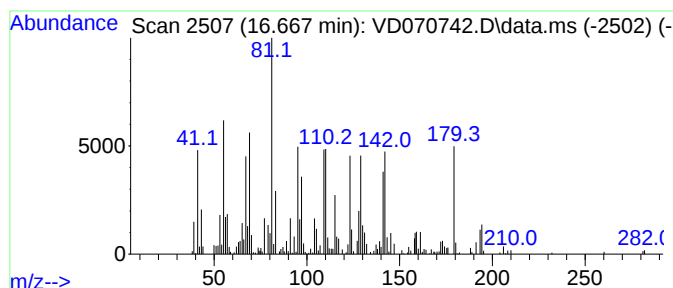
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
Quant Title : SW846 8260

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

Peak Number 8 unknown16.667 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.667	46.58 ug/l	1143040	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl ethyl cyclopentene	110	C8H14	019780-56-4	30
2			2-Propenyl-3-vinyloxirane	110	C7H10O	070597-49-8	27
3			Cyclopentane, 1-ethenyl-3-ethyl-...	138	C10H18	055170-98-4	27
4			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	22
5			Cyclopentane, 1-isobutylidene-3-...	138	C10H18	1000150-62-1	16



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD101821\
Data File : VD070742.D
Acq On : 18 Oct 2021 21:00
Operator : VA/SY
Sample : M4248-03
Misc : 5.03G/5.00ml/MSVOA_D/SOIL
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
72-12002

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.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
trans-4a-Methyl...	14.555	6.8	ug/l	166856	4	13.561	1227070	50.0
o-Cymene	14.802	8.6	ug/l	210119	4	13.561	1227070	50.0
2-(1-Hydroxybut...	14.867	6.0	ug/l	147710	4	13.561	1227070	50.0
Cyclohexene, 2-...	15.014	6.0	ug/l	147470	4	13.561	1227070	50.0
Added stereo to...	15.085	7.6	ug/l	186364	4	13.561	1227070	50.0
1,4-Dimethylada...	15.426	11.6	ug/l	284205	4	13.561	1227070	50.0
unknown16.667	16.667	46.6	ug/l	1143040	4	13.561	1227070	50.0