

Data Path : Z:\VOASRV\HPCHEM1\MSVOA D\DATA\VD080819\
 Data File : VD063442.D
 Acq On : 8 Aug 2019 16:58
 Operator : JC/SY
 Sample : K4223-08
 Misc : 4.24g/5ml/MSVOA D/SOIL
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 SP-4

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\82D072919S.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.480	3	5	27	rVB	2781831	7379317	100.00%	31.909%
2	3.262	177	186	203	rBV2	1116535	3085141	41.81%	13.341%
3	3.823	238	243	253	rVV	86336	236740	3.21%	1.024%
4	6.077	468	472	481	rBV2	31951	96169	1.30%	0.416%
5	6.934	552	559	566	rBV	481485	1345860	18.24%	5.820%
6	7.052	566	571	585	rVB	632624	1804205	24.45%	7.802%
7	7.465	607	613	625	rBV	423088	1082664	14.67%	4.682%
8	8.233	685	691	703	rBV	832968	2084561	28.25%	9.014%
9	10.094	872	880	889	rBV2	129999	302455	4.10%	1.308%
10	10.418	908	913	920	rBV	853332	1849585	25.06%	7.998%
11	12.377	1108	1112	1119	rBV	821554	1432413	19.41%	6.194%
12	13.401	1212	1216	1220	rVB	43520	75215	1.02%	0.325%
13	13.559	1229	1232	1237	rBV	664078	937171	12.70%	4.052%
14	13.953	1269	1272	1281	rVB2	76559	130161	1.76%	0.563%
15	14.524	1325	1330	1334	rVB2	673076	875404	11.86%	3.785%
16	15.350	1411	1414	1417	rBV	96234	124827	1.69%	0.540%
17	15.892	1466	1469	1472	rVB	100015	133538	1.81%	0.577%
18	16.591	1537	1540	1543	rBV2	112056	150419	2.04%	0.650%

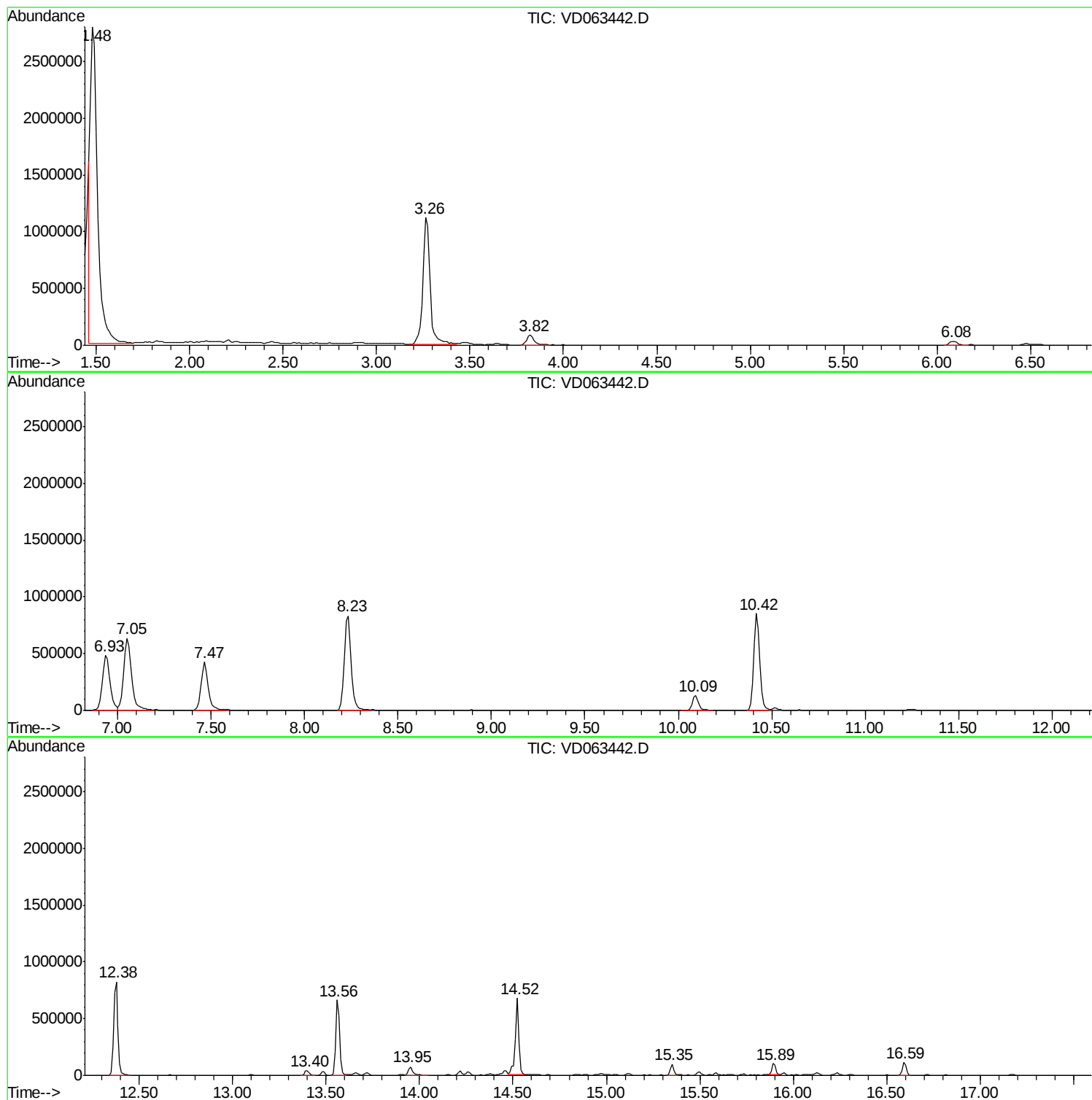
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_D\METHOD\82D072919S.M
Quant Title : SW846 8260

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



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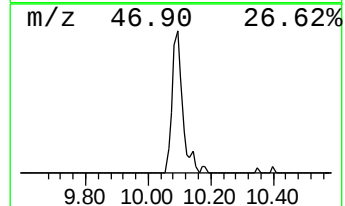
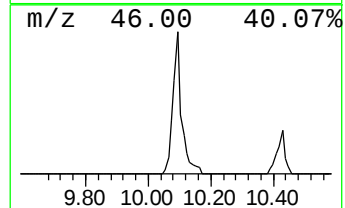
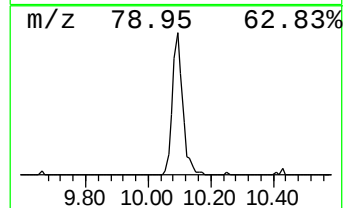
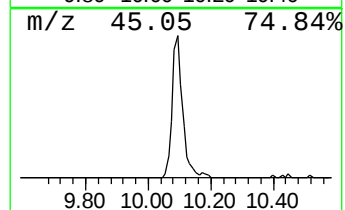
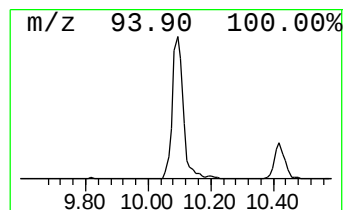
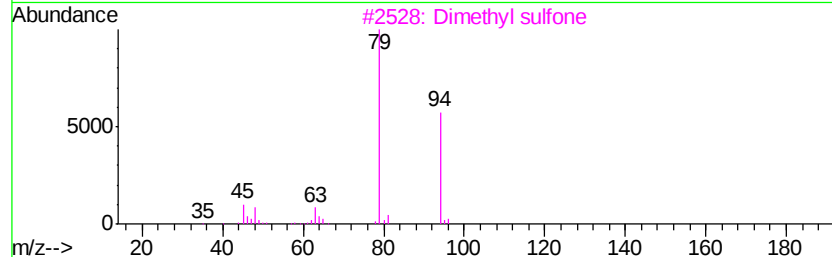
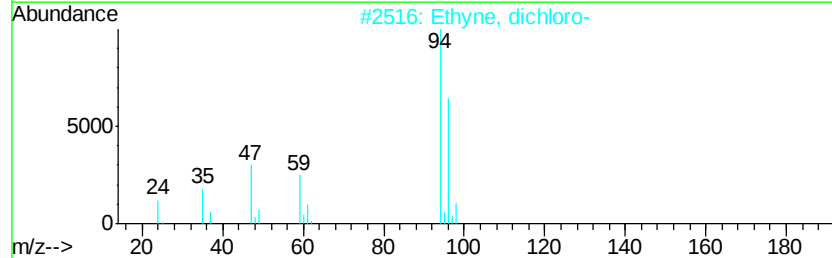
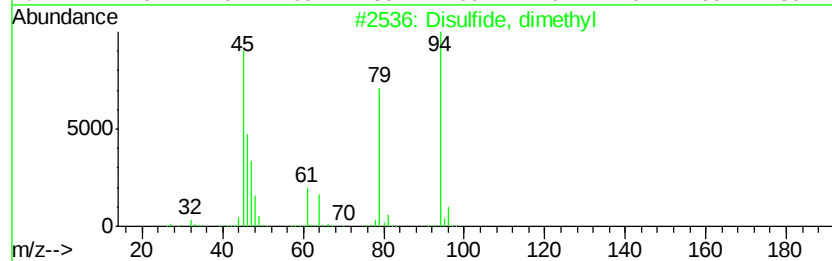
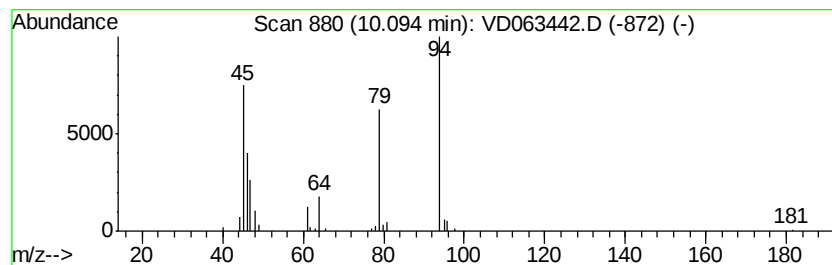
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Quant Title : SW846 8260

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

Peak Number 2 Disulfide, dimethyl Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.09	7.25 ug/l	302455	1,4-Difluorobenzene	8.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Disulfide, dimethyl	94	C2H6S2	000624-92-0	87
2		Ethyne, dichloro-	94	C2Cl2	007572-29-4	27
3		Dimethyl sulfone	94	C2H6O2S	000067-71-0	27
4		Ethyl 3-methyl-8-[p-sulfamylbenz...	416	C18H20N6O4S	021271-88-5	17
5		Sulfonium, dimethyl-, cyanonitro...	146	C4H6N2O2S	058992-18-0	17



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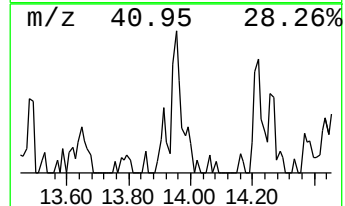
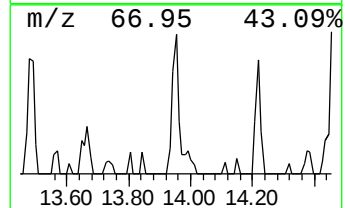
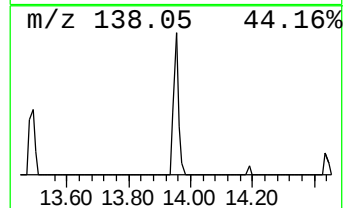
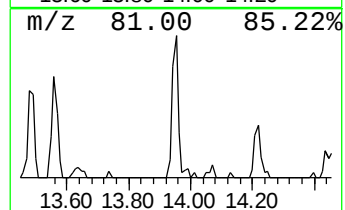
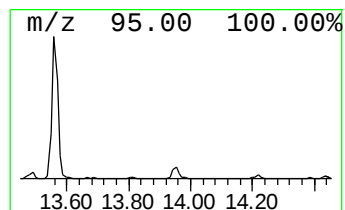
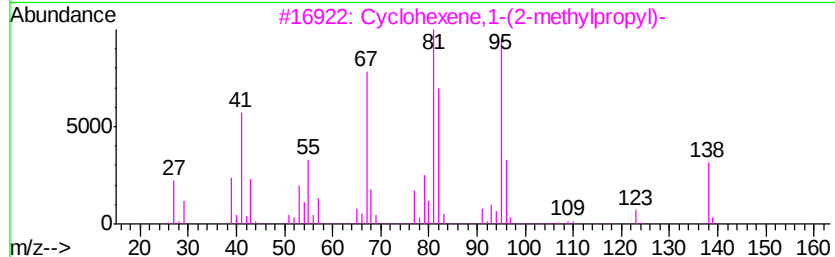
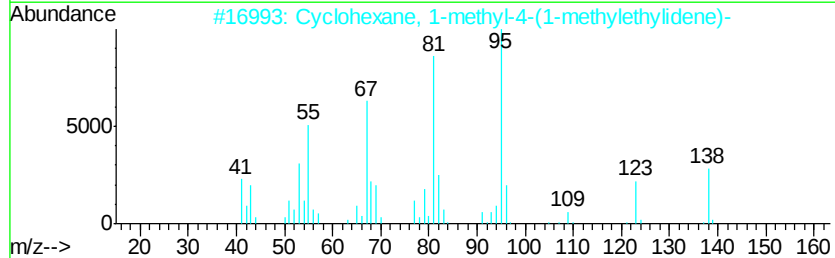
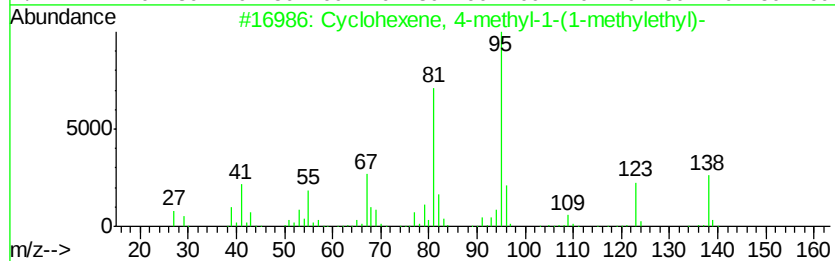
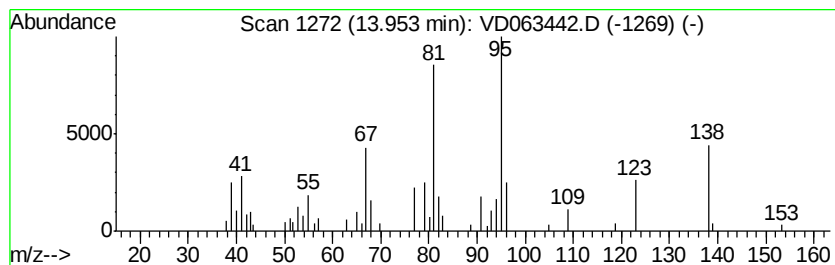
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Quant Title : SW846 8260

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

Peak Number 3 Cyclohexene, 4-methyl-1-(1-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	7.43 ug/l	130161	1,4-Dichlorobenzene-d4	14.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexene, 4-methyl-1-(1-methyl-...	138	C10H18	000500-00-5	93
2		Cyclohexane, 1-methyl-4-(1-methyl-...	138	C10H18	001124-27-2	90
3		Cyclohexene, 1-(2-methylpropyl)-	138	C10H18	003983-03-7	80
4		Cyclohexene, 4-methyl-1-(1-methyl-...	138	C10H18	000619-52-3	76
5		Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	72



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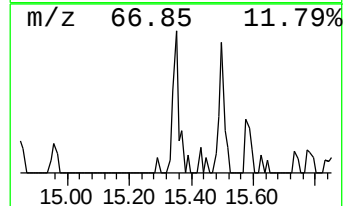
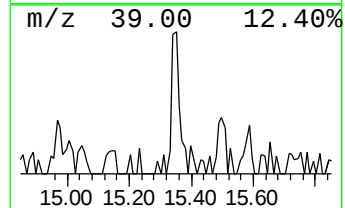
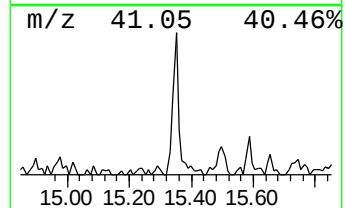
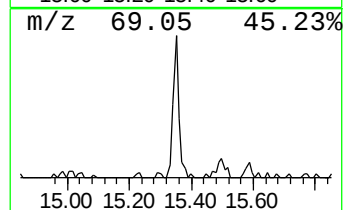
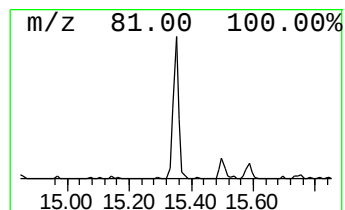
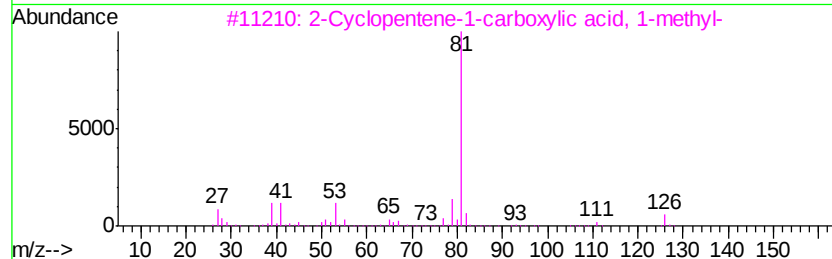
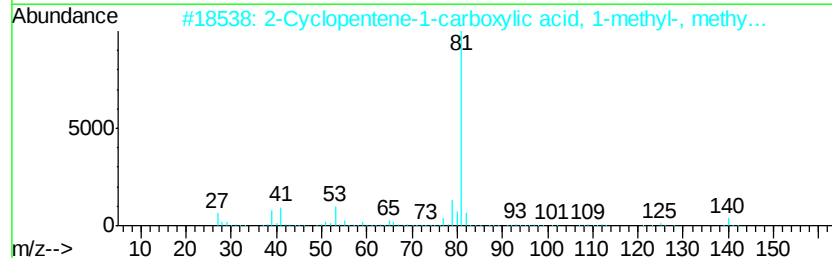
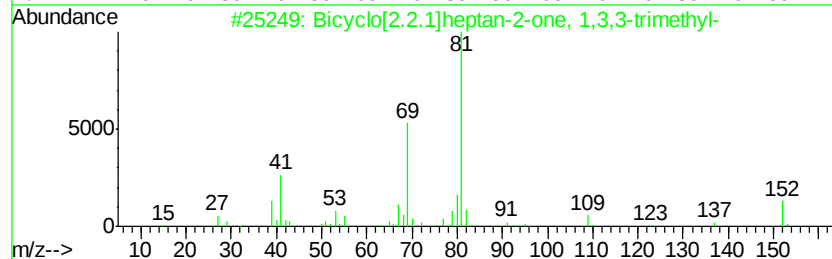
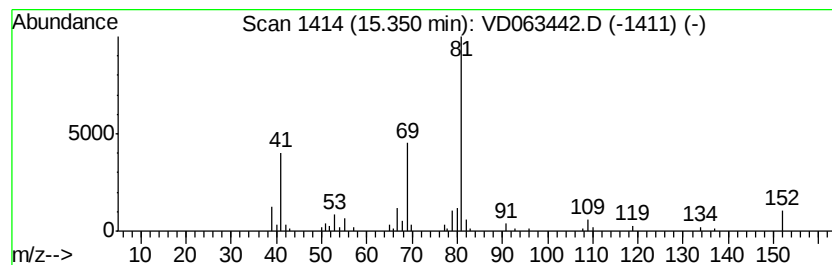
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Peak Number 4 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.35	7.13 ug/l	124827	1,4-Dichlorobenzene-d4	14.52	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicvclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	91
2	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	53
3	2-Cyclopentene-1-carboxylic acid...	126	C7H10O2	068317-77-1	50
4	Cyclohexane, 1,3-dichloro-, cis-	152	C6H10Cl2	024955-63-3	45
5	Cyclohexene,3-(2-propenyl)-	122	C9H14	015232-95-8	40



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampled :
SP-4

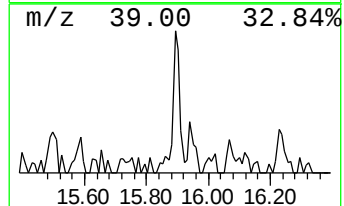
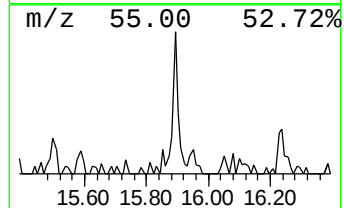
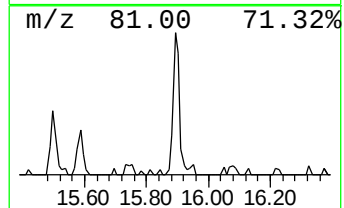
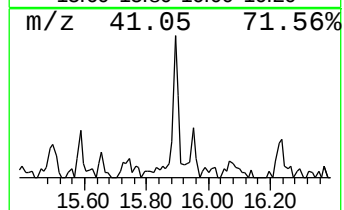
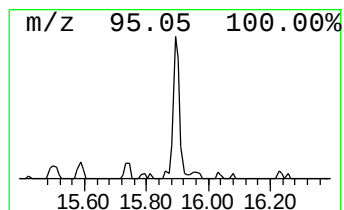
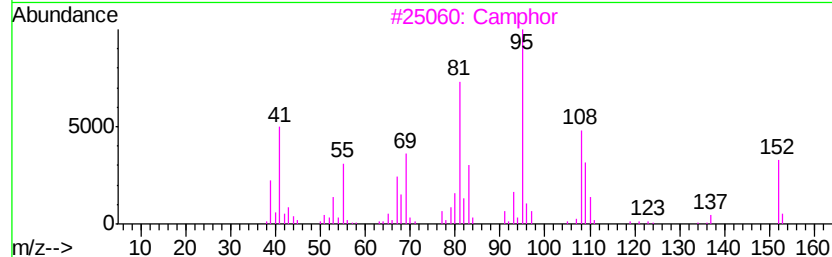
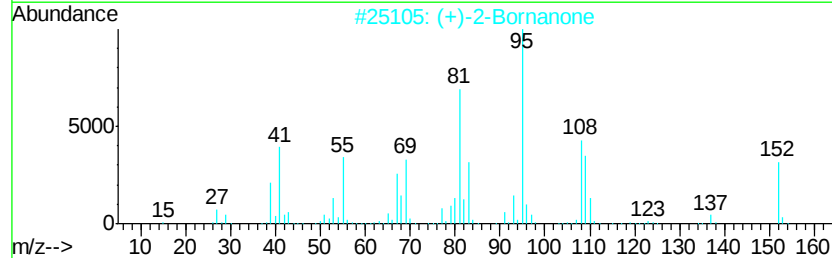
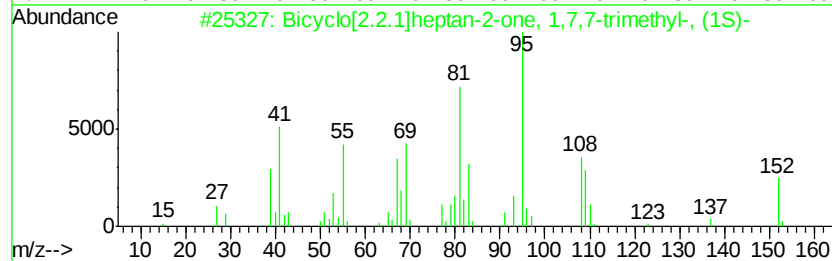
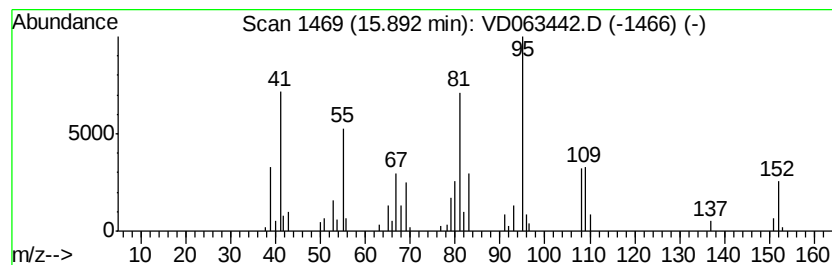
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Peak Number 5 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	7.63 ug/l	133538	1,4-Dichlorobenzene-d4	14.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	95
2		(+)-2-Bornanone	152	C10H16O	000464-49-3	94
3		Camphor	152	C10H16O	000076-22-2	83
4		1-Adamantanol	152	C10H16O	000768-95-6	47
5		Diisopropylaminoacrylonitril	152	C9H16N2	038691-28-0	47



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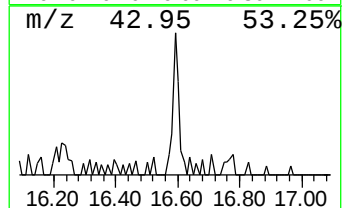
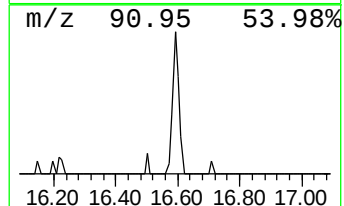
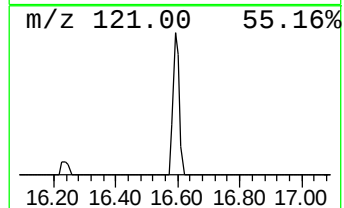
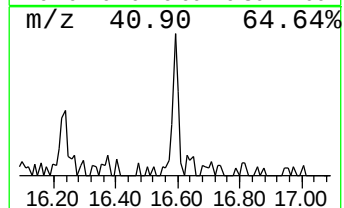
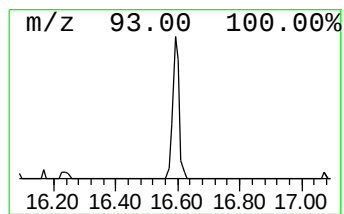
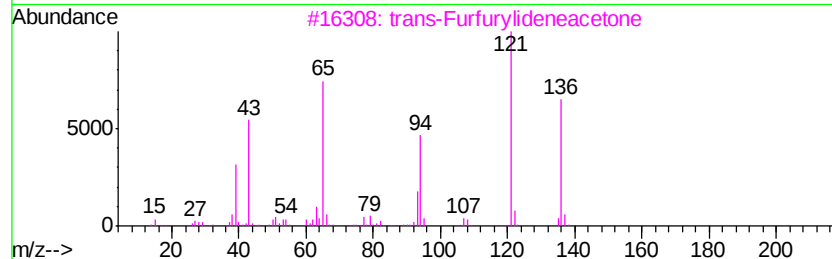
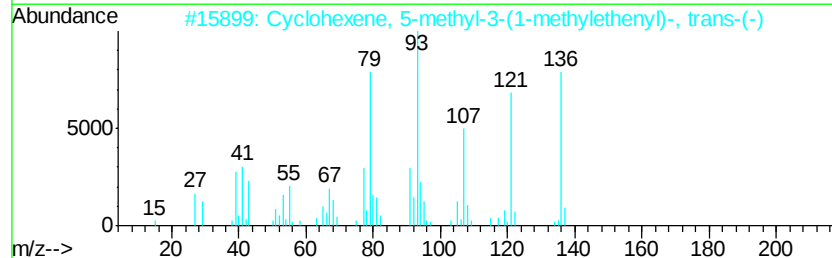
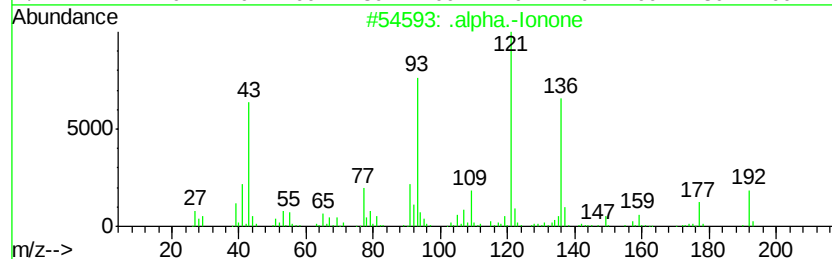
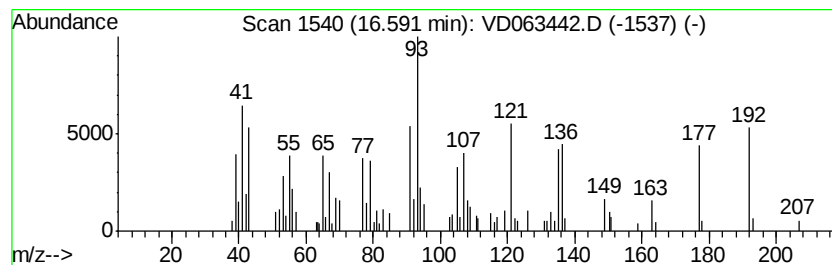
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown16.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	8.59 ug/l	150419	1,4-Dichlorobenzene-d4	14.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.alpha.-Ionone	192	C13H20O	000127-41-3	42
2		Cyclohexene, 5-methyl-3-(1-methy...	136	C10H16	056816-08-1	38
3		trans-Furfurylideneacetone	136	C8H8O2	041438-24-8	38
4		3-Buten-2-one, 4-(2-furanvl)-	136	C8H8O2	000623-15-4	38
5		Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	38



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Disulfide, dimethyl	10.09	7.3	ug/l	302455	2	8.23	2084560	50.0
Cyclohexene, 4-me...	13.95	7.4	ug/l	130161	4	14.52	875404	50.0
Bicyclo[2.2.1]hep...	15.35	7.1	ug/l	124827	4	14.52	875404	50.0
Bicyclo[2.2.1]hep...	15.89	7.6	ug/l	133538	4	14.52	875404	50.0
unknown16.59	16.59	8.6	ug/l	150419	4	14.52	875404	50.0