

Data Path : Z:\VOASRV\HPCHEM1\MSVOA D\DATA\VD080819\
 Data File : VD063460.D
 Acq On : 9 Aug 2019 2:58
 Operator : JC/SY
 Sample : K4223-28
 Misc : 3.55g/5ml/MSVOA D/SOIL
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 SP-14

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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	3.266	178	187	202	rBV	941742	2504254	100.00%	26.383%
2	3.463	202	207	215	rVB3	21061	71383	2.85%	0.752%
3	3.817	238	243	249	rBV2	22222	58260	2.33%	0.614%
4	6.081	469	473	478	rBV	13203	35234	1.41%	0.371%
5	6.928	553	559	566	rBV	206591	586358	23.41%	6.177%
6	7.046	566	571	589	rVB	308964	911416	36.39%	9.602%
7	7.459	607	613	624	rBV2	205993	592596	23.66%	6.243%
8	8.227	685	691	701	rBV	443534	1099896	43.92%	11.588%
9	10.088	875	880	892	rBV	171838	405386	16.19%	4.271%
10	10.413	908	913	921	rBV	365055	799455	31.92%	8.422%
11	12.372	1108	1112	1120	rBV	590432	923272	36.87%	9.727%
12	13.563	1230	1233	1237	rBV	387320	528286	21.10%	5.566%
13	13.947	1269	1272	1275	rBV	25529	32939	1.32%	0.347%
14	14.518	1326	1330	1334	rBV	451003	612814	24.47%	6.456%
15	15.345	1411	1414	1418	rBV	69923	92128	3.68%	0.971%
16	15.502	1426	1430	1433	rBV2	22033	33893	1.35%	0.357%
17	15.896	1467	1470	1473	rBV	82941	118064	4.71%	1.244%
18	16.595	1537	1541	1544	rBV	65498	86292	3.45%	0.909%

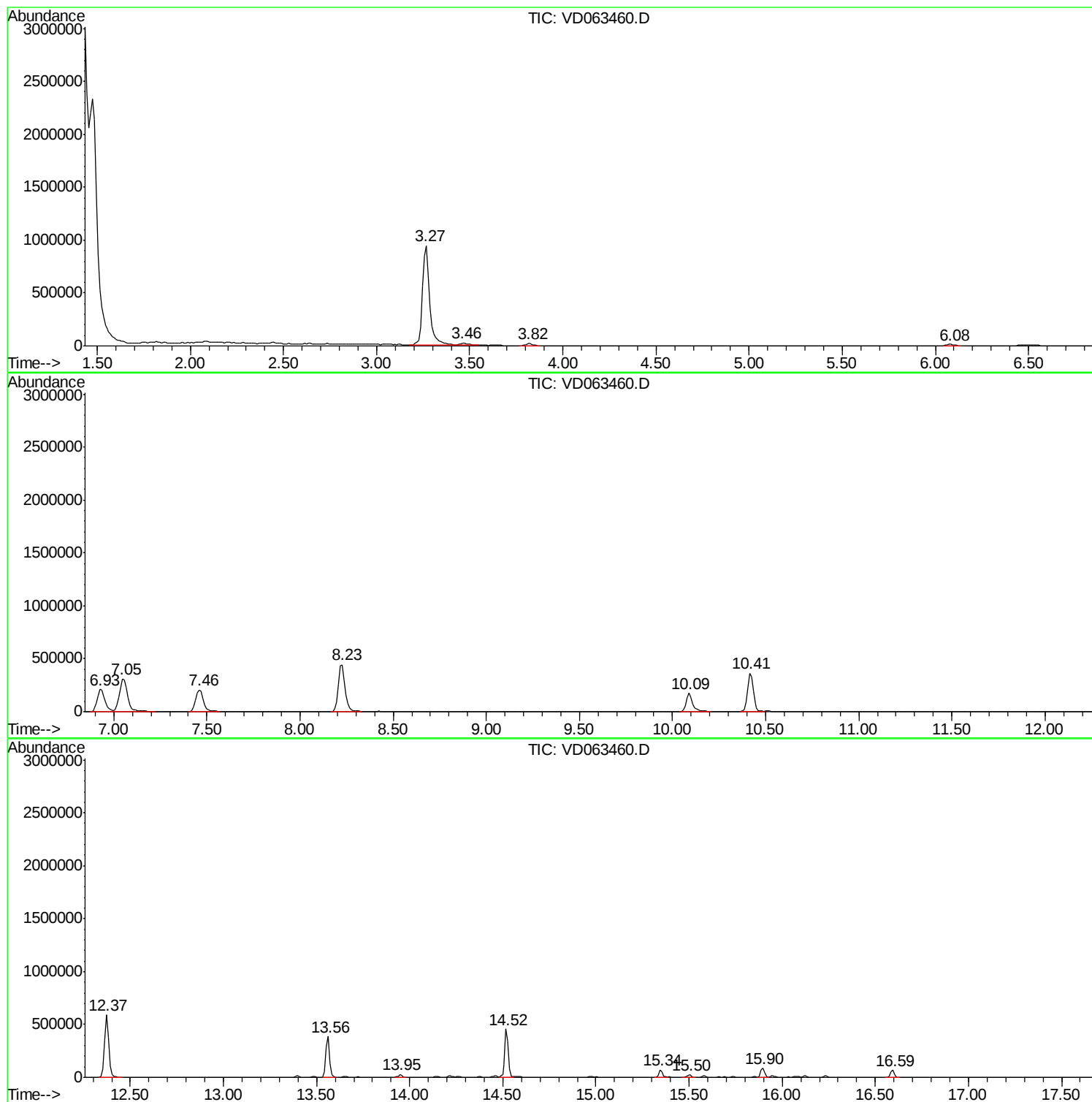
Sum of corrected areas: 9491926

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Quant Title : SW846 8260

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



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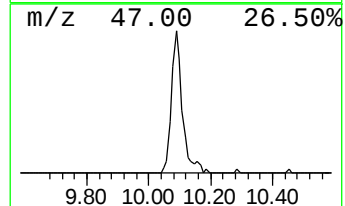
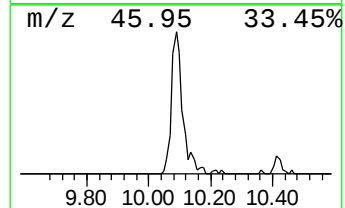
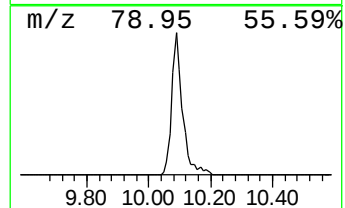
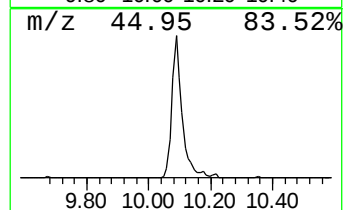
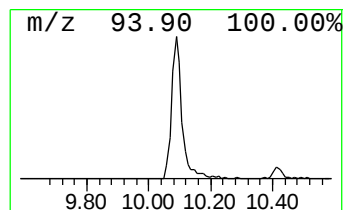
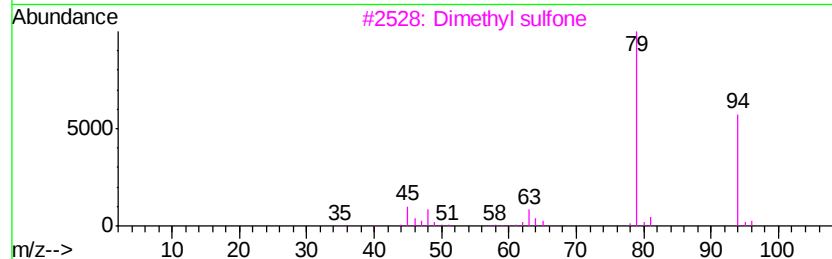
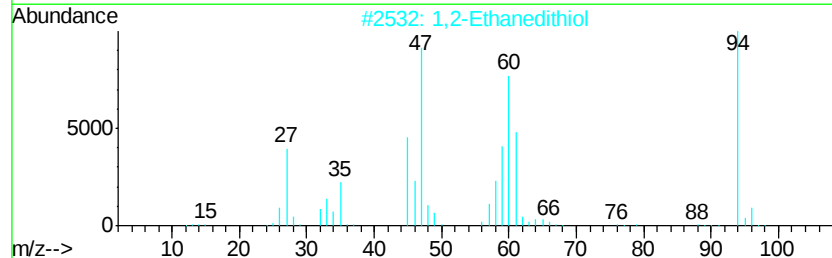
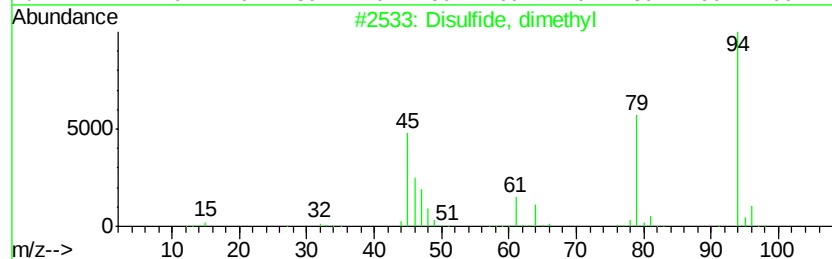
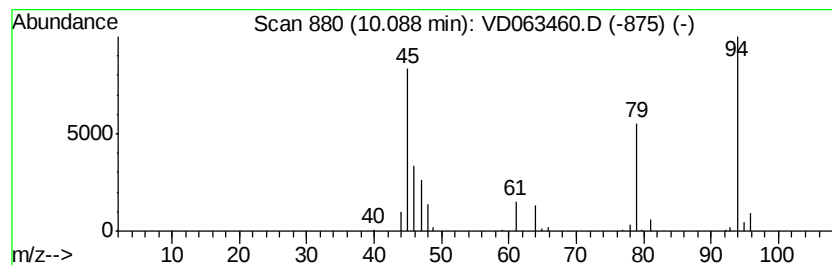
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_D\METHOD\82D072919S.M
Quant Title : SW846 8260

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

Peak Number 1 Disulfide, dimethyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.09	18.43 ug/l	405386	1,4-Difluorobenzene	8.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
2	1,2-Ethanedithiol	94	C2H6S2	000540-63-6	38
3	Dimethyl sulfone	94	C2H6O2S	000067-71-0	35
4	Fluoroacetic acid	78	C2H3FO2	000144-49-0	9
5	Pyrazine, methyl-	94	C5H6N2	000109-08-0	9



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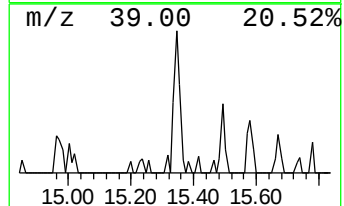
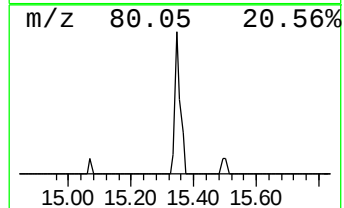
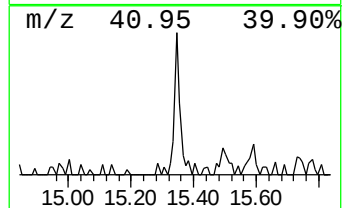
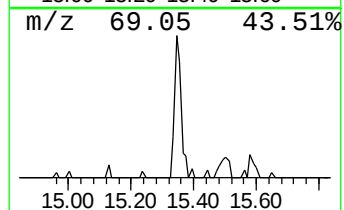
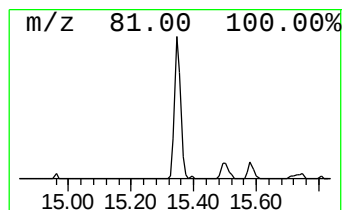
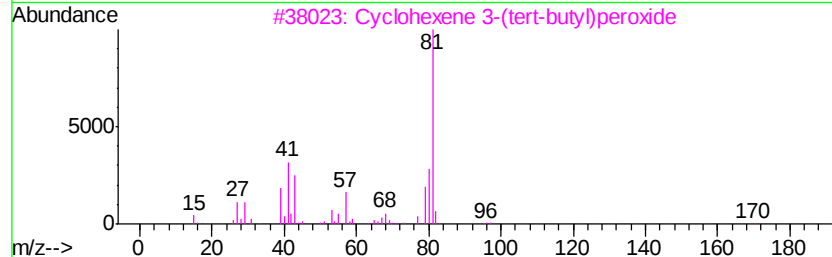
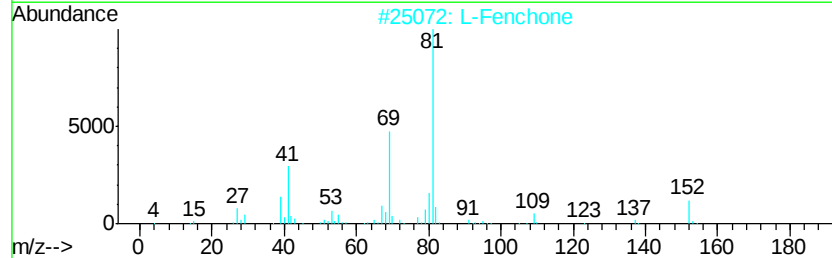
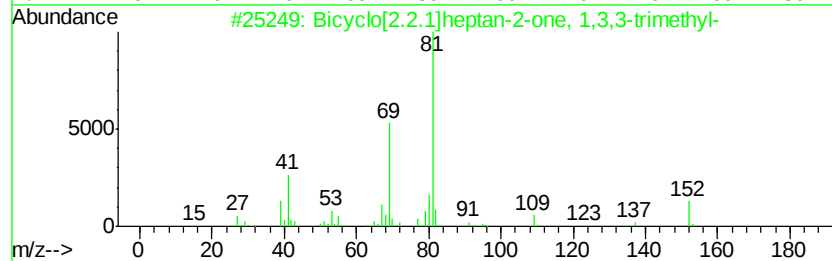
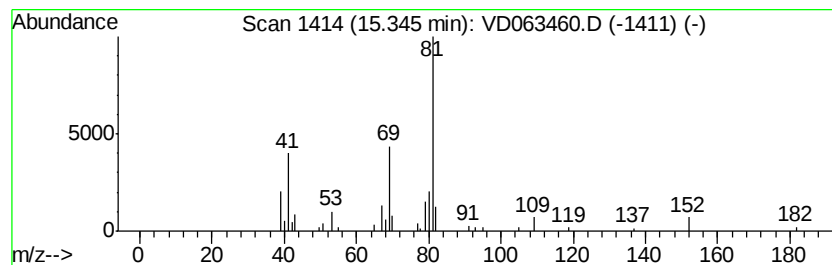
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.34	7.52 ug/l	92128	1,4-Dichlorobenzene-d4	14.53	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	87
2	L-Fenchone	152	C10H16O	007787-20-4	78
3	Cyclohexene 3-(tert-butyl)peroxide	170	C10H18O2	051437-25-3	59
4	D-Fenchone	152	C10H16O	004695-62-9	59
5	1,E-4,Z-8-Dodecatriene	164	C12H20	083489-22-9	53



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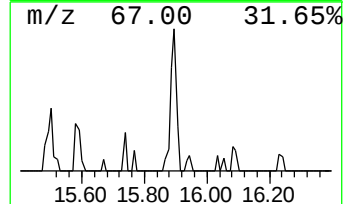
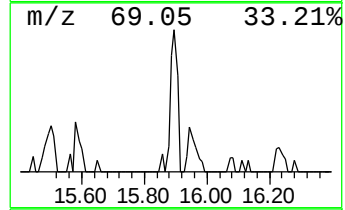
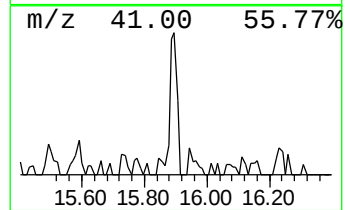
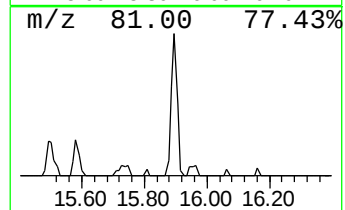
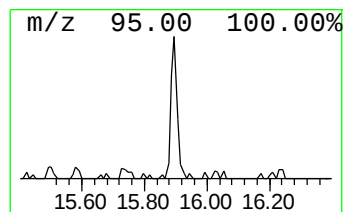
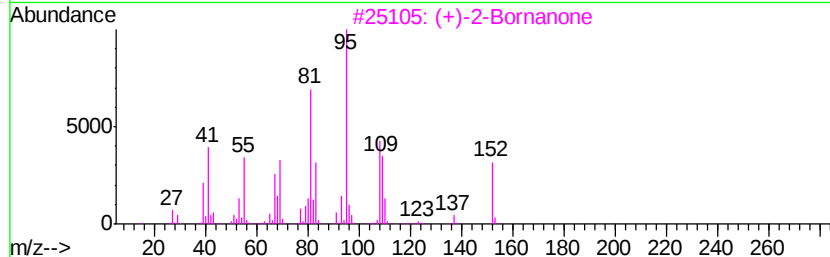
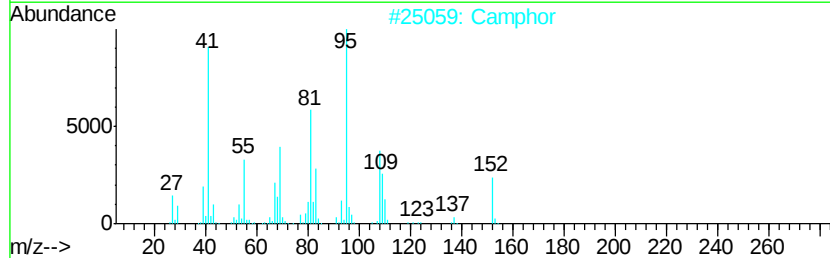
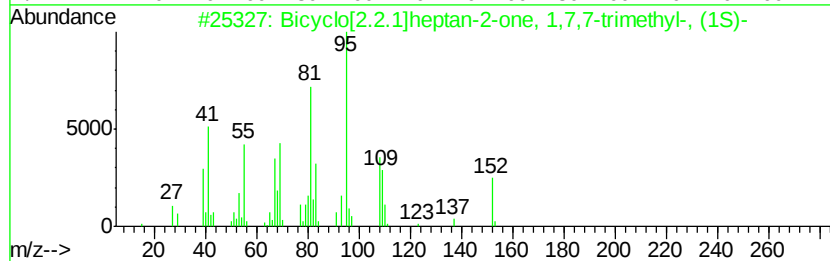
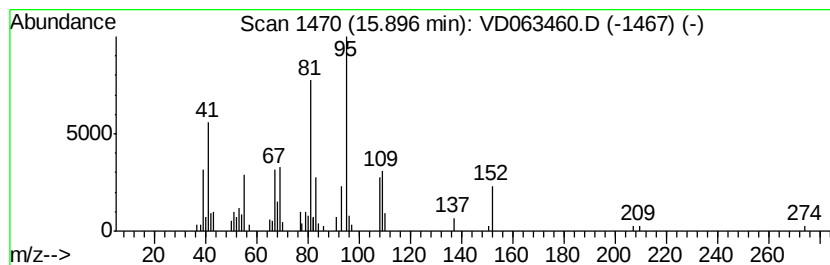
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Peak Number 3 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	9.63 ug/l	118064	1,4-Dichlorobenzene-d4	14.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	94
2		Camphor	152	C10H16O	000076-22-2	60
3		(+)-2-Bornanone	152	C10H16O	000464-49-3	50
4		5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	43
5		Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	38



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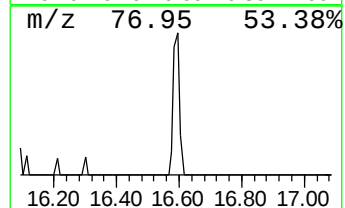
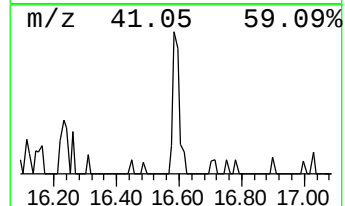
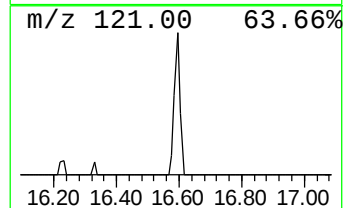
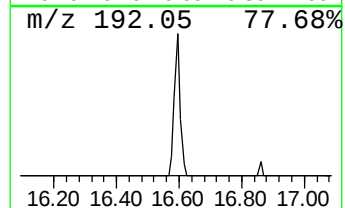
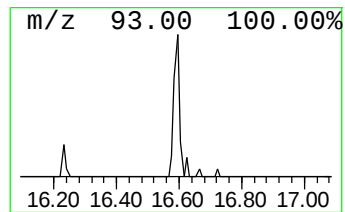
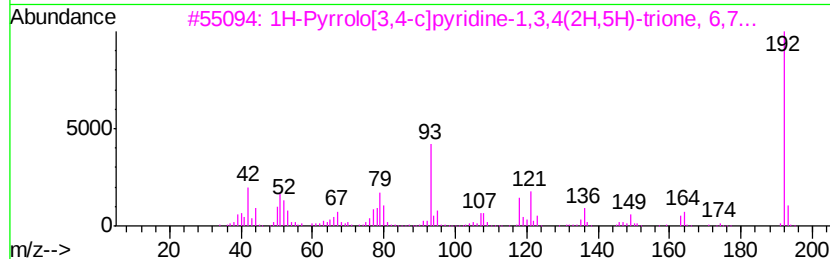
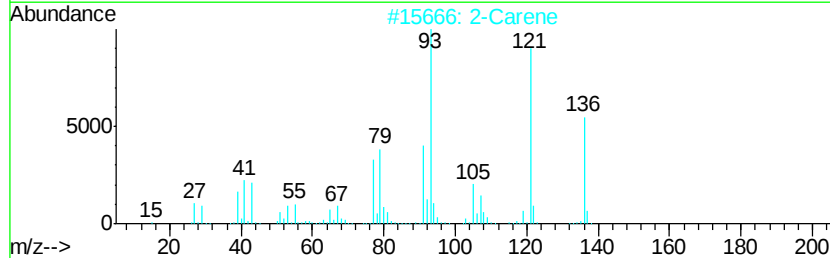
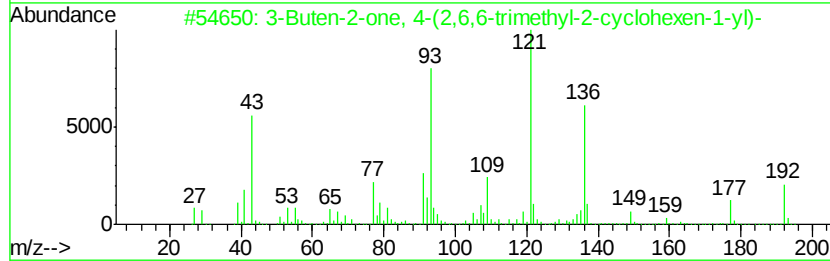
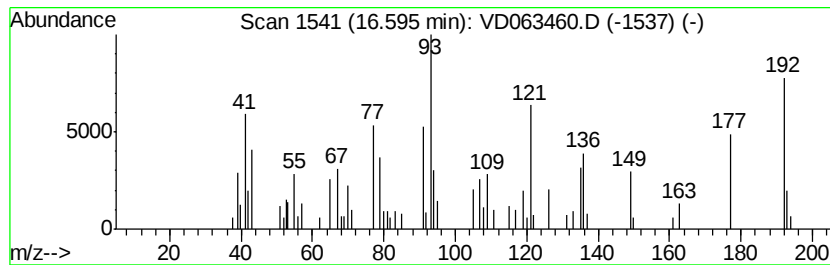
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Peak Number 4 3-Buten-2-one, 4-(2,6,6-tri... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.59	7.04 ug/l	86292	1,4-Dichlorobenzene-d4	14.53		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	006901-97-9	58	
2	2-Carene	136	C10H16	000554-61-0	38	
3	1H-Pyrrolo[3,4-c]pyridine-1,3,4(...	192	C9H8N2O3	298688-33-2	38	
4	Methyl m-tolyl carbinol	136	C9H12O	1000342-29-9	30	
5	Scopoletin	192	C10H8O4	000092-61-5	27	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Disulfide, dimethyl	10.09	18.4	ug/l	405386	2	8.23	1099900	50.0
Bicyclo[2.2.1]hep...	15.34	7.5	ug/l	92128	4	14.53	612814	50.0
Bicyclo[2.2.1]hep...	15.90	9.6	ug/l	118064	4	14.53	612814	50.0
3-Buten-2-one, 4-...	16.59	7.0	ug/l	86292	4	14.53	612814	50.0