

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091721\
 Data File : VY006083.D
 Acq On : 17 Sep 2021 20:15
 Operator : SY/MD
 Sample : M3797-03
 Misc : 5.00G/5ML/MSVOA_Y/SOIL
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20430

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\82Y091421S.M

Title : SW846 8260

Signal : TIC: VY006083.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.143	1032	1037	1038	rBV5	1058	1514	1.37%	0.960%
2	8.691	1122	1127	1133	rBV7	1813	4317	3.92%	2.737%
3	9.075	1187	1190	1192	rBV4	1574	2224	2.02%	1.410%
4	9.380	1239	1240	1243	rBV3	1485	1502	1.36%	0.952%
5	12.660	1770	1778	1779	rBV2	47431	110161	100.00%	69.830%
6	15.501	2239	2244	2254	rVB8	14109	38038	34.53%	24.112%

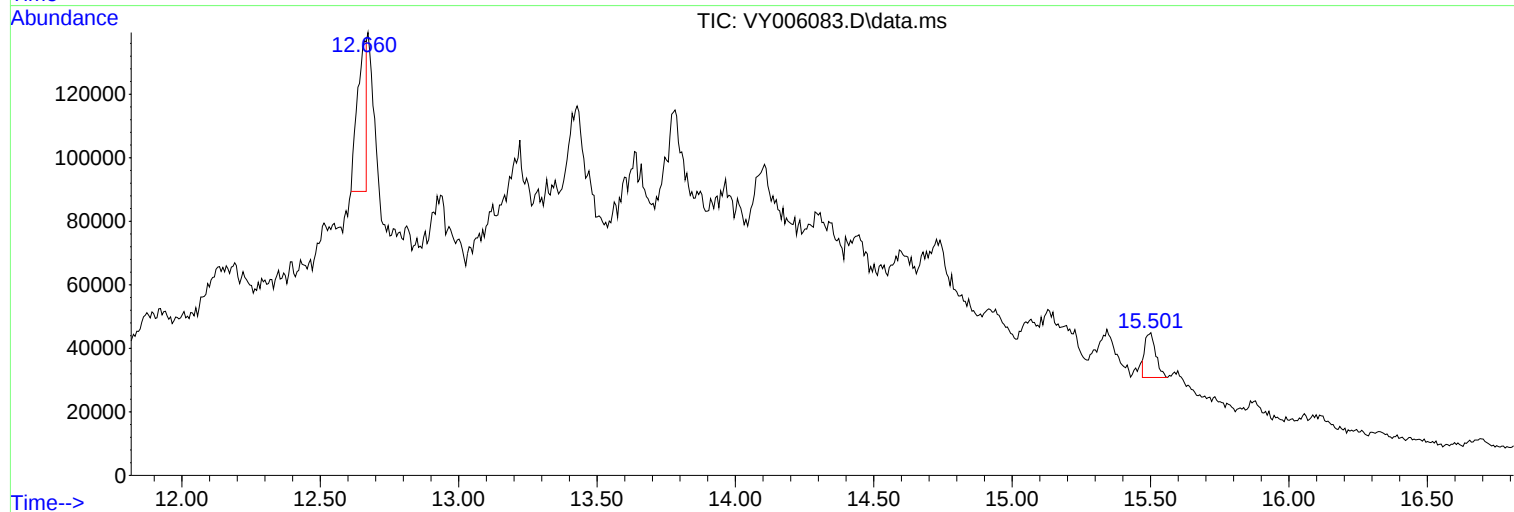
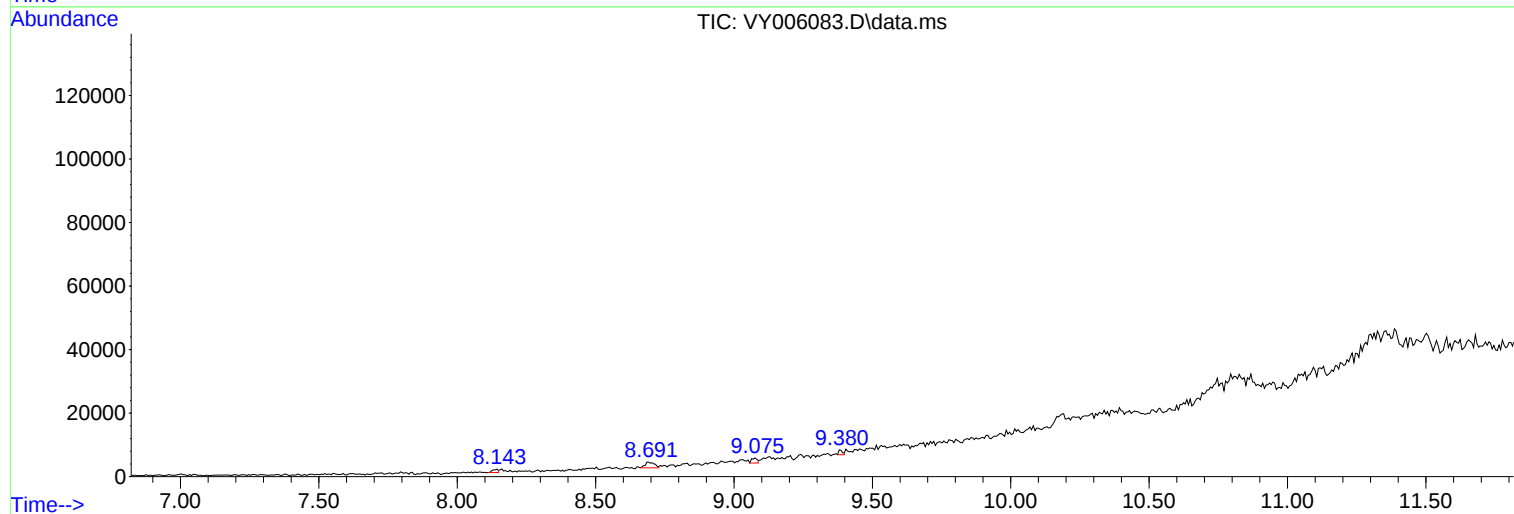
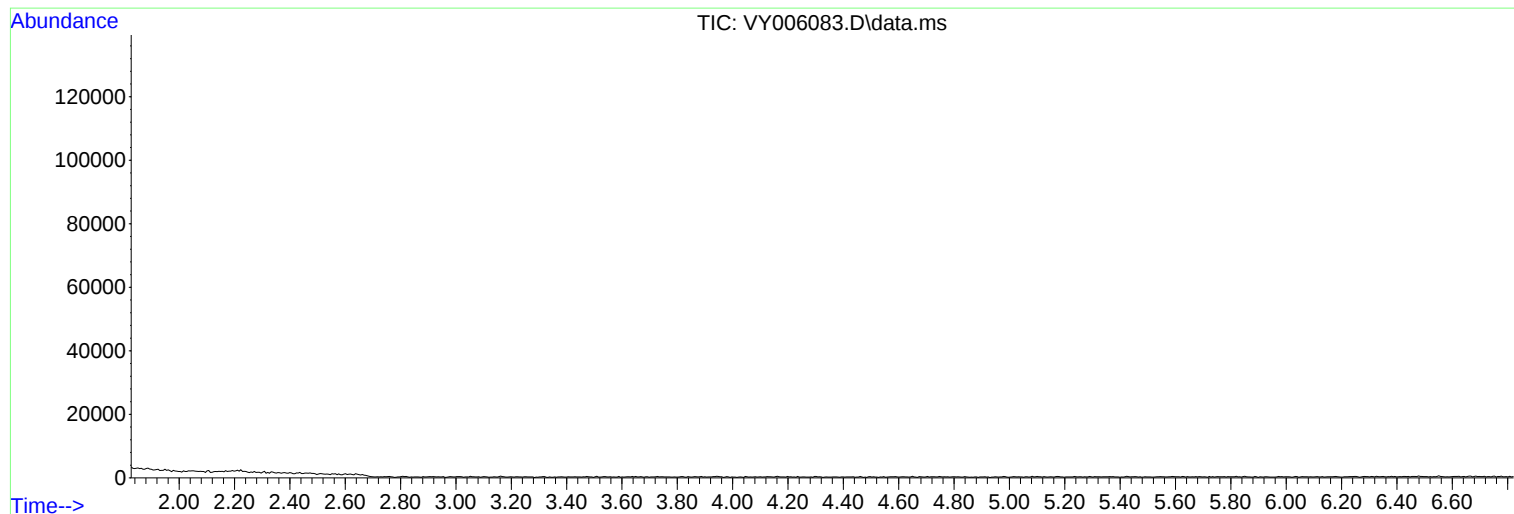
Sum of corrected areas: 157756

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



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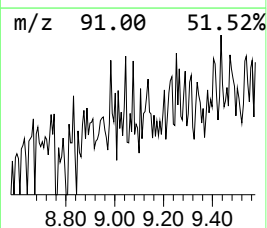
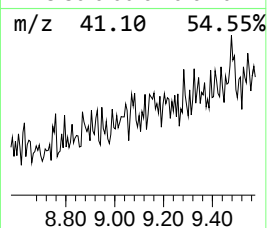
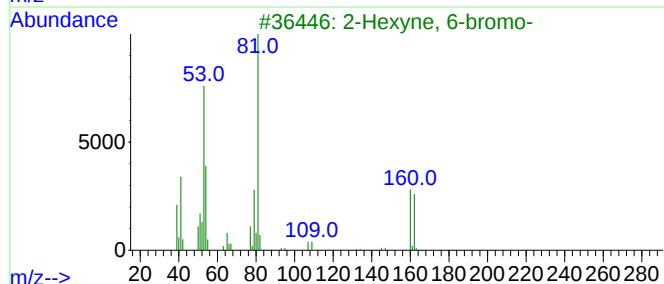
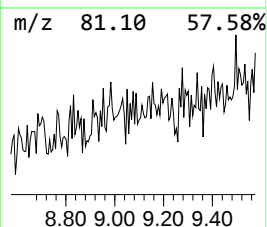
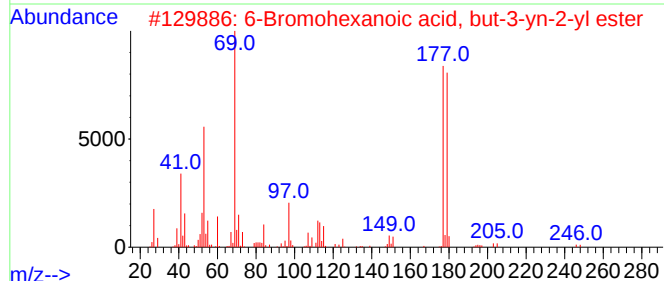
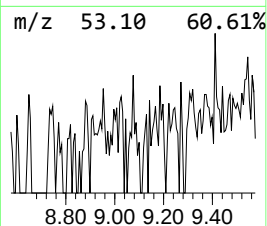
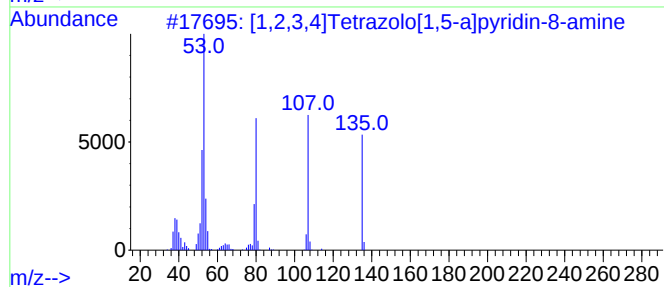
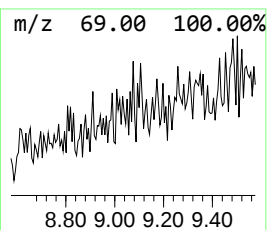
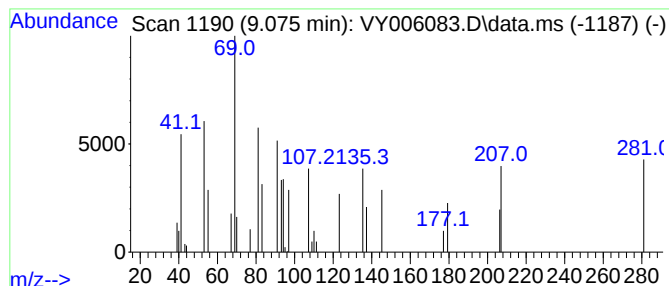
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown9.075 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.075	25.76 ug/l	2224	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	[1,2,3,4]Tetrazolo[1,5-a]pyridin...	135	C5H5N5	073721-28-5	32		
2	6-Bromohexanoic acid, but-3-yn-2...	246	C10H15BrO2	1000299-28-6	23		
3	2-Hexyne, 6-bromo-	160	C6H9Br	055402-12-5	9		
4	3,7-Dimethyl-1-phenylsulfonyl-2...	278	C16H22O2S	1000432-27-5	9		
5	2R-Acetoxymethyl-1,3,3-trimethyl...	282	C17H30O3	1000144-12-4	9		



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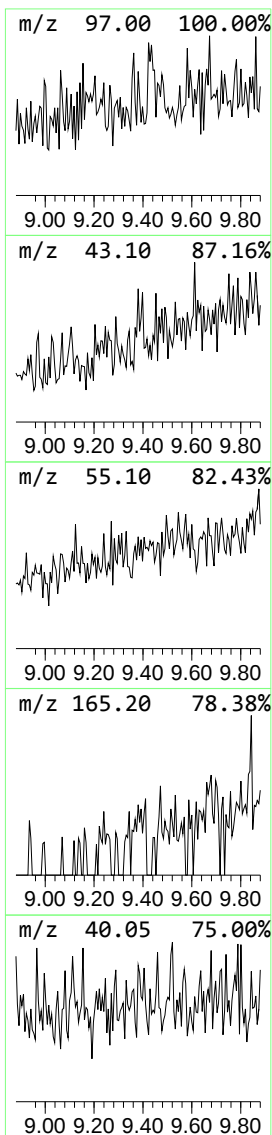
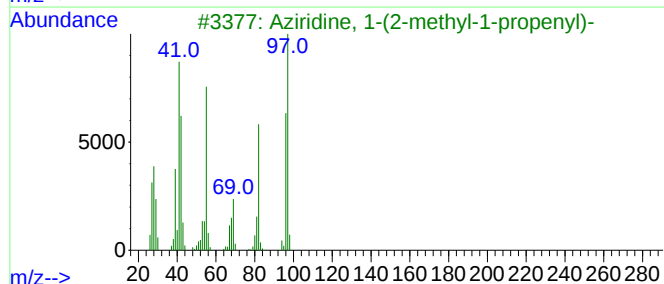
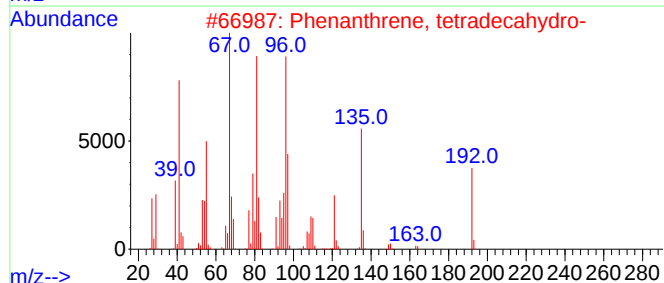
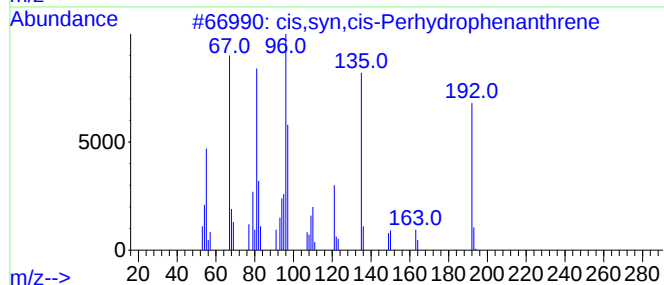
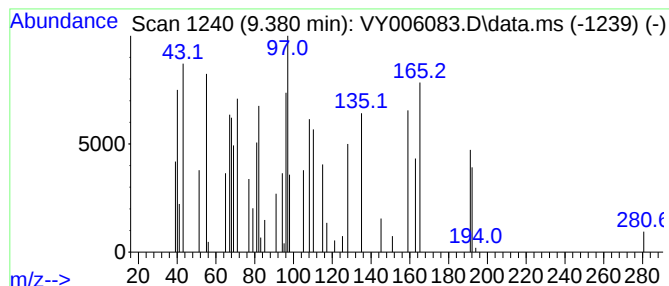
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Peak Number 2 unknown9.380 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.380	17.40 ug/l	1502	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis,syn,cis-Perhydrophenanthrene	192	C14H24	026634-41-3	30
2			Phenanthrene, tetradecahydro-	192	C14H24	005743-97-5	22
3			Aziridine, 1-(2-methyl-1-propenyl)-	97	C6H11N	080839-93-6	18
4			Perhydrophenanthrene, (4a.alpha....	192	C14H24	027389-76-0	16
5			trans-2-Methylcyclohexanol, 2-me...	184	C11H20O2	1000447-34-0	10



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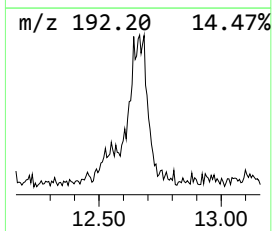
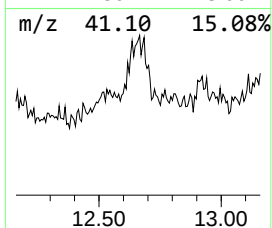
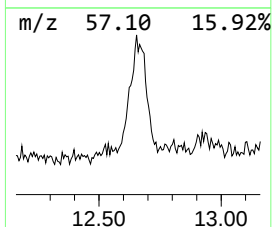
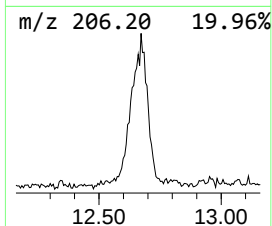
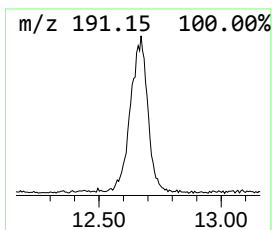
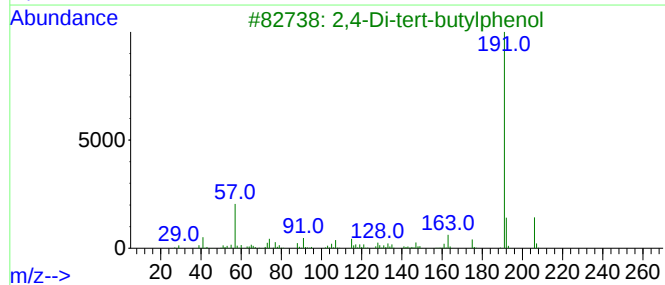
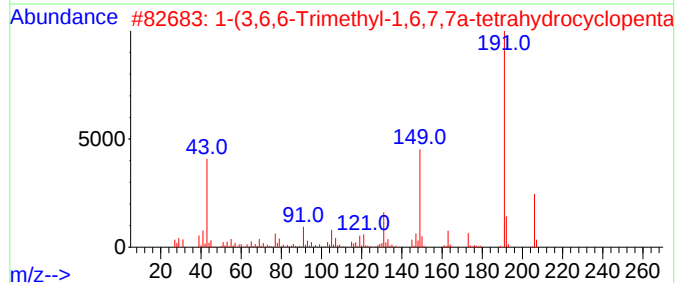
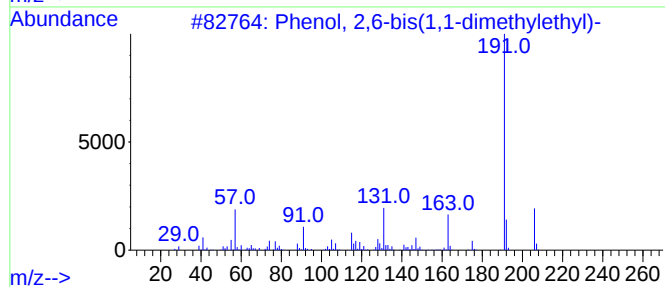
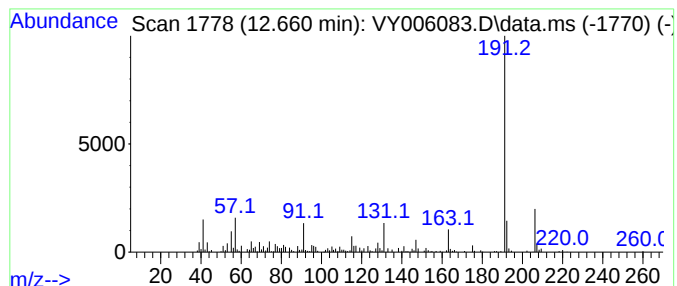
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Peak Number 3 Phenol, 2,6-bis(1,1-dimethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.660	50.00 ug/l	110161	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	95
2			1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	91
3			2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	87
4			3-(4-tert-Butylphenyl)propanoic ...	206	C13H18O2	001208-64-6	83
5			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	72



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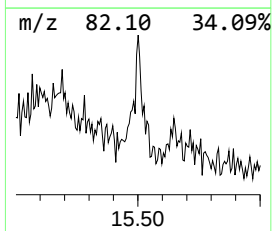
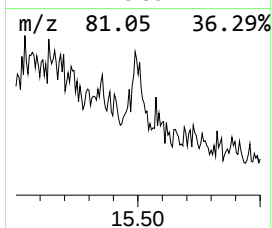
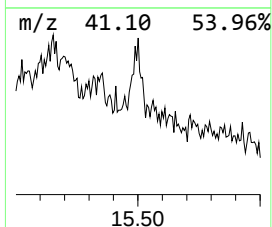
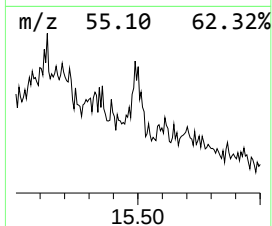
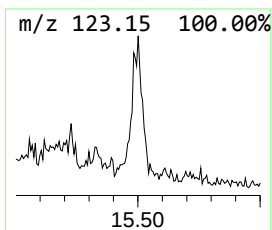
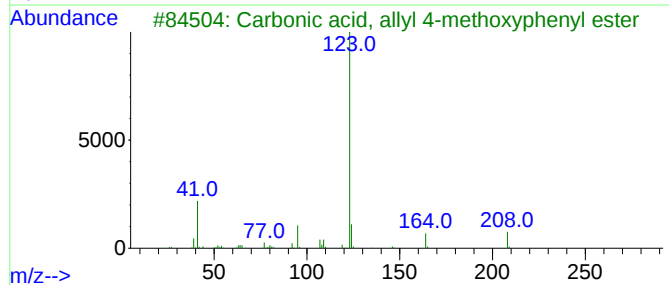
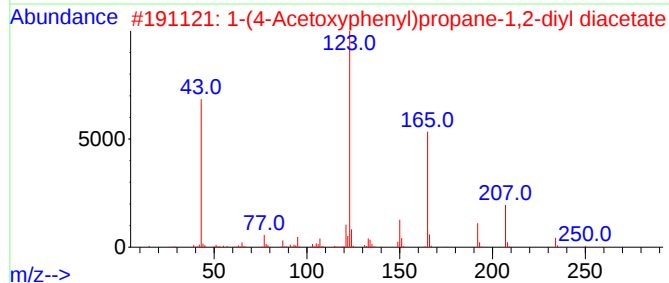
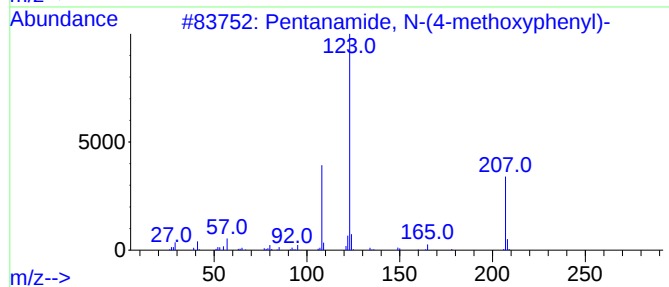
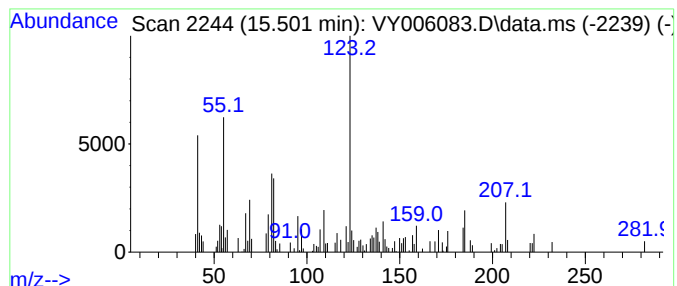
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Peak Number 4 unknown15.501 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.501	17.26 ug/l	38038	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	47
2			1-(4-Acetoxyphenyl)propane-1,2-d...	294	C15H18O6	1000495-87-2	43
3			Carbonic acid, allyl 4-methoxyph...	208	C11H12O4	1000357-81-0	38
4			4,6-Dimethyl-2(1H)pyridone, 3-(t...	232	C12H12N2OS	1000223-42-9	38
5			Ethanone, 1-[2-methyl-5-(1-methy...	166	C11H18O	074063-72-2	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown9.075	9.075	25.8	ug/l	2224	2	8.691	4317	50.0
unknown9.380	9.380	17.4	ug/l	1502	2	8.691	4317	50.0
Phenol, 2,6-bis...	12.660	50.0	ug/l	110161	4	13.422	110161	50.0
unknown15.501	15.501	17.3	ug/l	38038	4	13.422	110161	50.0