

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD081423\
 Data File : VD077006.D
 Acq On : 14 Aug 2023 17:35
 Operator : JC/SY
 Sample : 03973-01
 Misc : 5.05G/5.0ml/MSVOA_D/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 SB-01-14.5-15.0

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\82D080823S.M
 Title : SW846 8260

Signal : TIC: VD077006.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.734	18	25	41	rVB	169995	317990	66.07%	27.495%
2	2.152	91	96	97	rBV2	4155	5167	1.07%	0.447%
3	2.352	127	130	138	rVB4	4196	8919	1.85%	0.771%
4	7.799	1049	1056	1057	rBV4	6458	9656	2.01%	0.835%
5	7.875	1062	1069	1076	rVB4	8403	18969	3.94%	1.640%
6	8.222	1121	1128	1133	rBV3	6350	15291	3.18%	1.322%
7	8.775	1215	1222	1228	rBV3	14673	29769	6.18%	2.574%
8	9.746	1383	1387	1388	rVV4	4952	5098	1.06%	0.441%
9	10.269	1468	1476	1484	rBV	30102	63351	13.16%	5.478%
10	10.628	1534	1537	1538	rBV3	6964	8506	1.77%	0.735%
11	10.657	1540	1542	1547	rVV6	8090	14162	2.94%	1.225%
12	11.581	1696	1699	1704	rVB	26856	37283	7.75%	3.224%
13	13.645	2043	2050	2065	rVB5	135496	481322	100.00%	41.618%
14	15.651	2386	2391	2402	rVB9	47431	141046	29.30%	12.196%

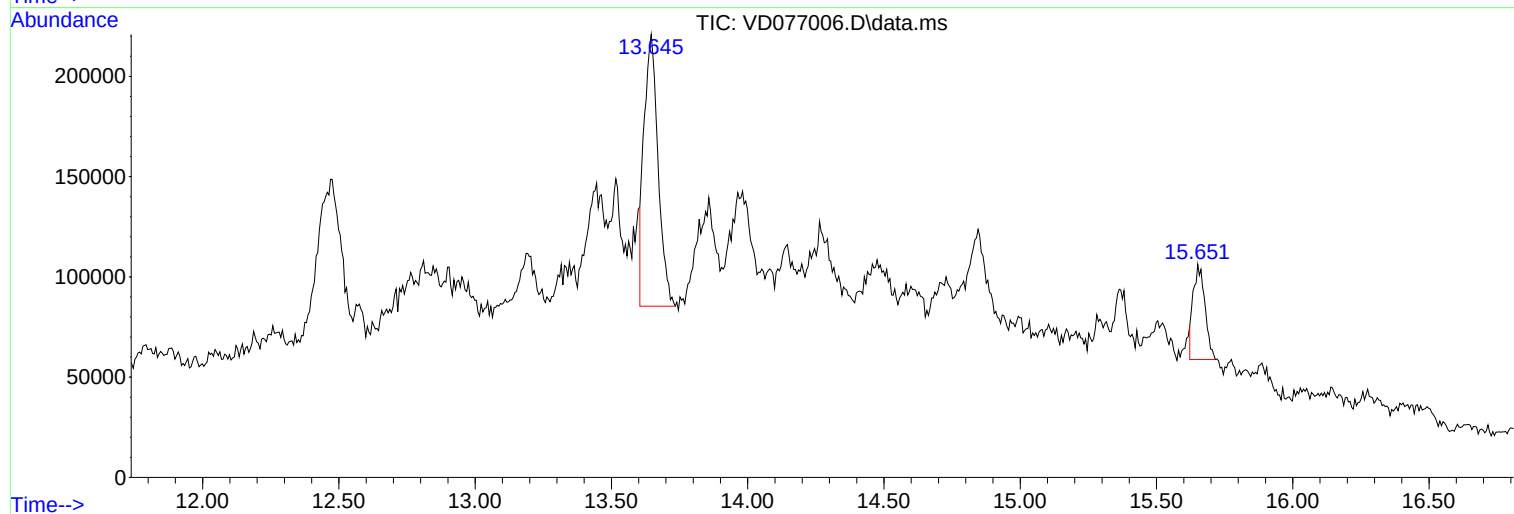
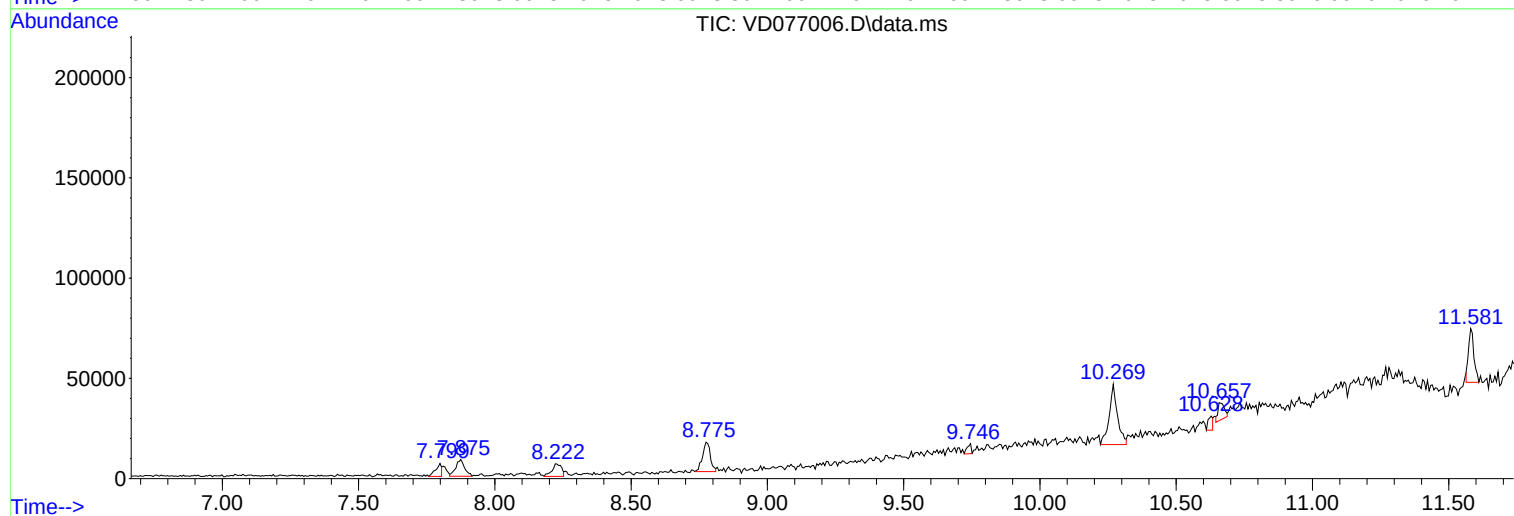
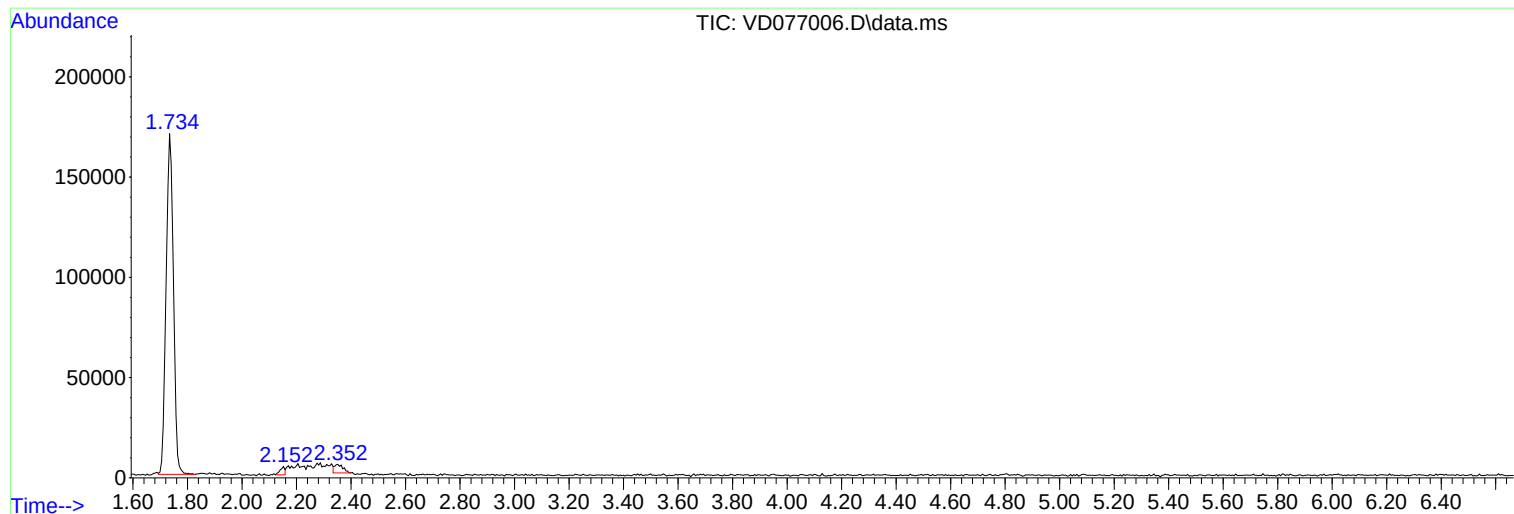
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D080823S.M
Quant Title : SW846 8260

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



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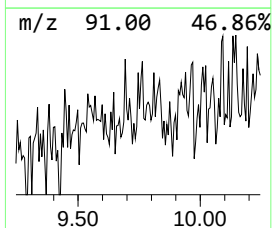
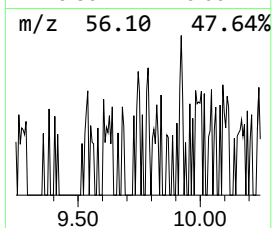
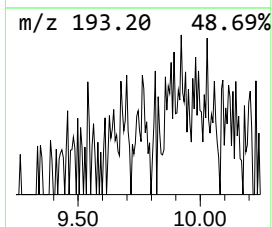
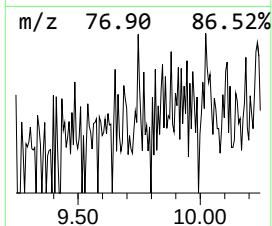
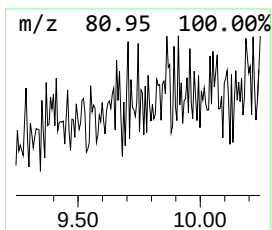
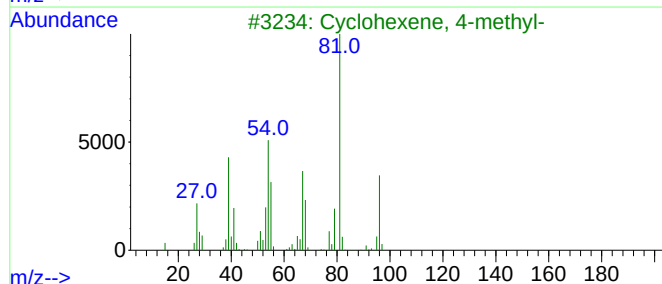
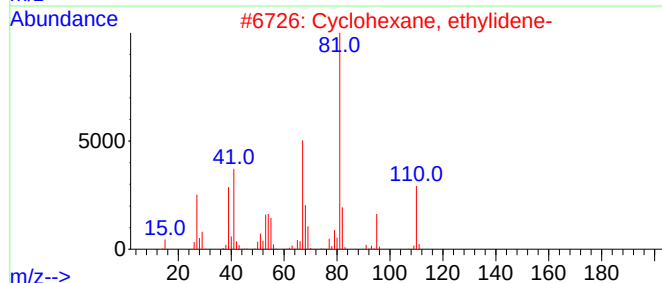
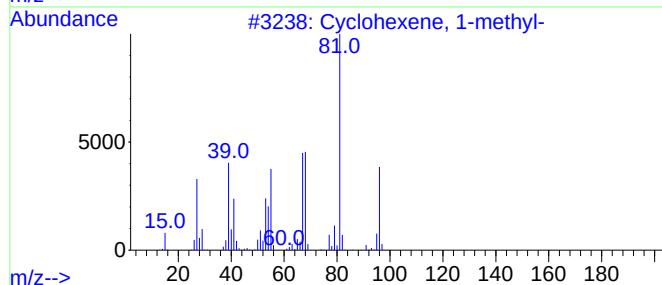
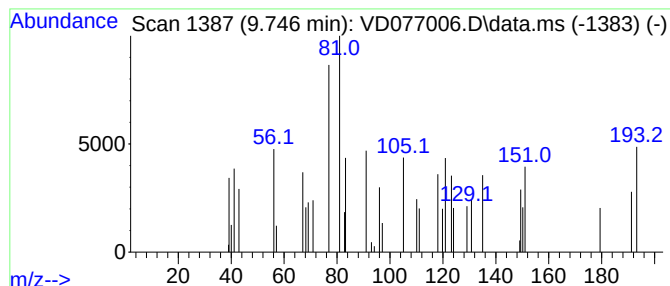
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D080823S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown9.746 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.746	8.56 ug/l	5098	1,4-Difluorobenzene	8.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	10
2			Cyclohexane, ethylidene-	110	C8H14	001003-64-1	10
3			Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	10
4			Cyclohexene,1-propyl-	124	C9H16	002539-75-5	9
5			Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	9



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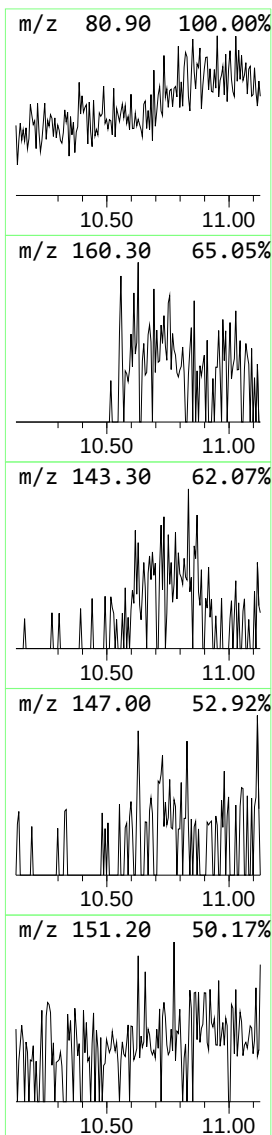
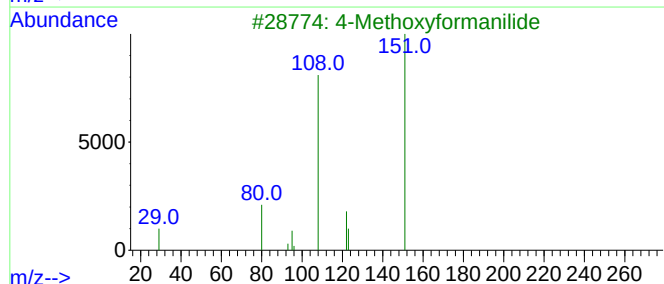
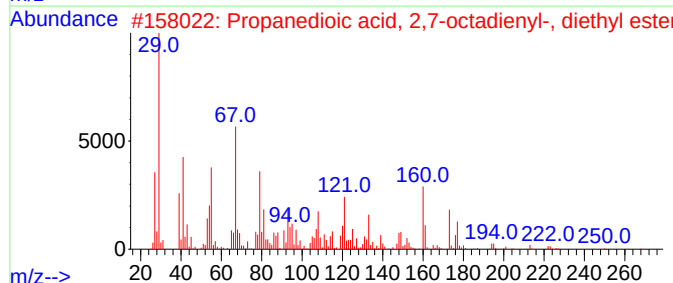
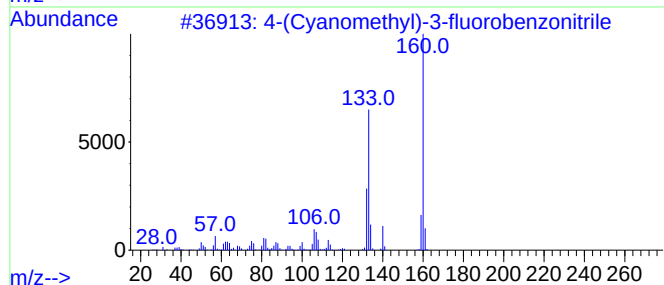
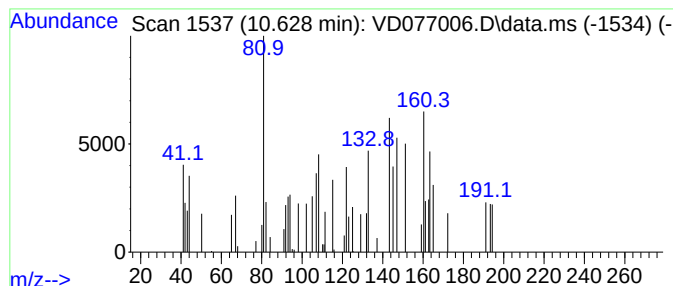
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown10.628 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.628	11.41 ug/l	8506	Chlorobenzene-d5	11.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(Cyanomethyl)-3-fluorobenzonitrile	160	C9H5FN2	1000516-58-4	11
2			Propanedioic acid, 2,7-octadieny...	268	C15H24O4	029330-87-8	10
3			4-Methoxyformanilide	151	C8H9NO2	005470-34-8	10
4			Benzonitrile, 2-fluoro-6-methoxy-	151	C8H6FNO	094088-46-7	10
5			Benzaldehyde, 2-amino-5-methoxy-	151	C8H9NO2	026831-52-7	9



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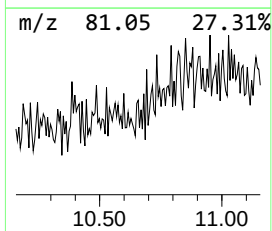
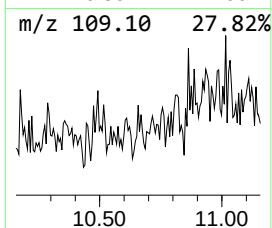
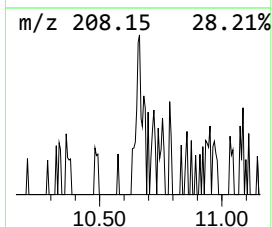
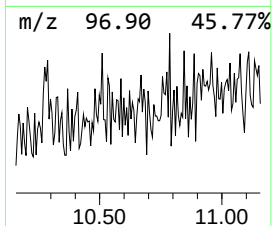
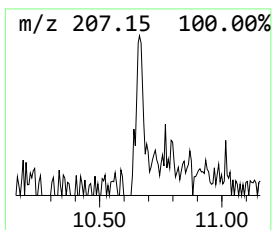
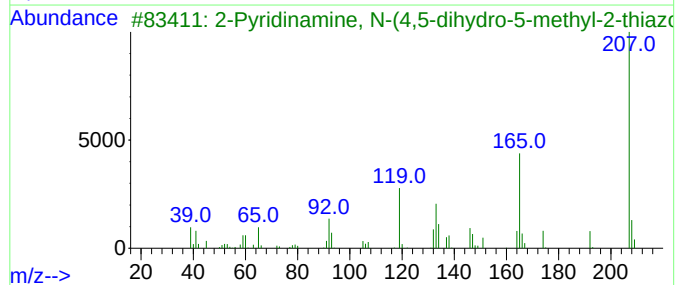
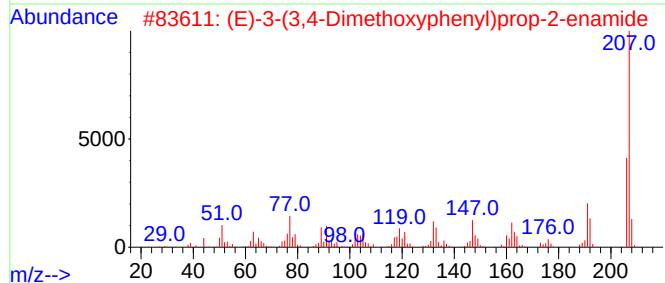
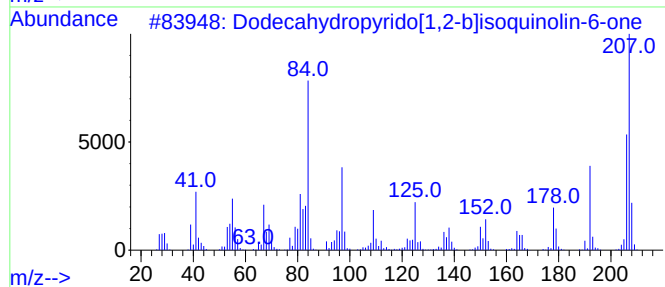
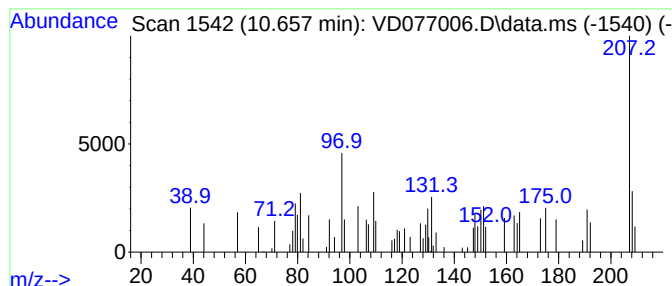
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 unknown10.657 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.657	18.99 ug/l	14162	Chlorobenzene-d5	11.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecahydropyrido[1,2-b]isoquino...	207	C13H21NO	108873-36-5	32
2			(E)-3-(3,4-Dimethoxyphenyl)prop-...	207	C11H13NO3	130973-10-3	25
3			2-Pyridinamine, N-(4,5-dihydro-5...	207	C10H13N3S	1000362-45-9	22
4			Corydaldine	207	C11H13NO3	000493-49-2	22
5			5,7-Dimethyl-2-thioxo-2,3-dihydr...	207	C9H9N3OS	049600-56-8	22



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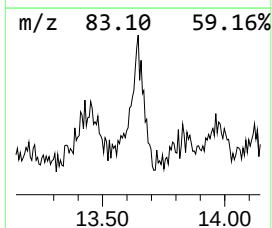
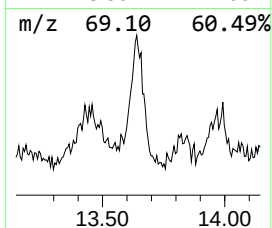
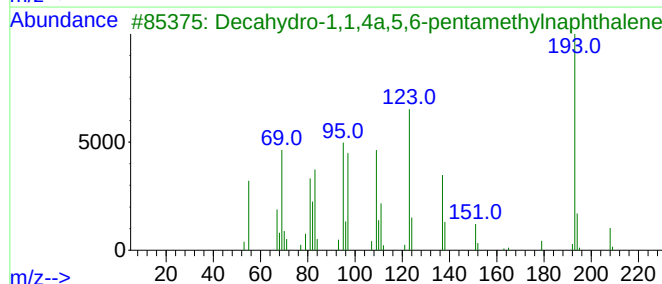
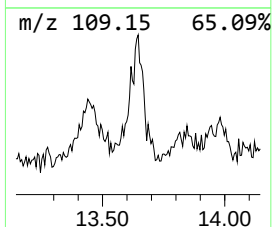
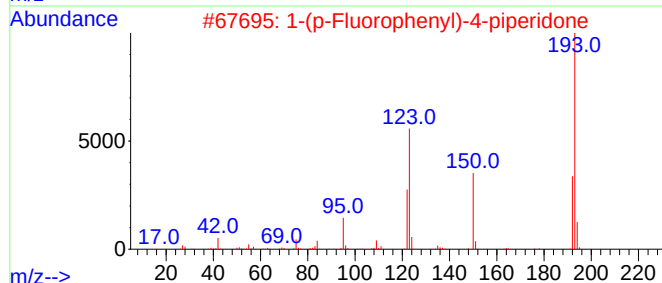
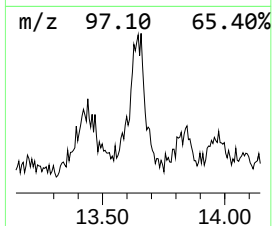
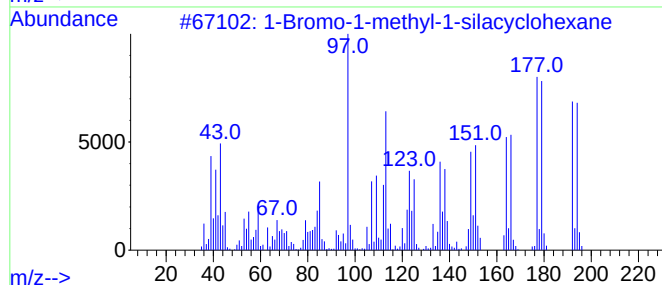
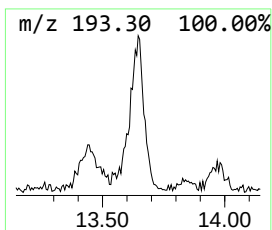
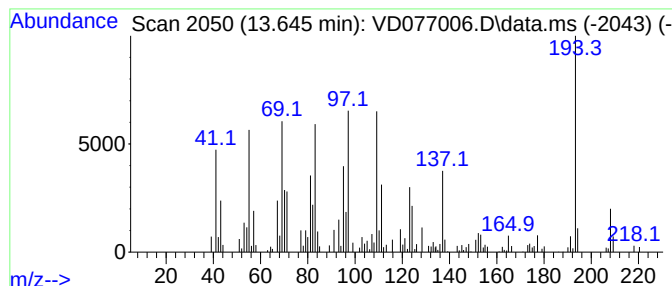
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TIC Library : C:\Database\NIST20.L
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Peak Number 7 1-Bromo-1-methyl-1-silacycl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.645	50.00 ug/l	481322	1,4-Dichlorobenzene-d4	13.516	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Bromo-1-methyl-1-silacyclohexane	192	C6H13BrSi	085125-32-2	68
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
3	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	35
4	5-Amino-2-fluorobenzonitrile, TM...	208	C10H13FN2Si	1000478-92-3	25
5	Benzonitrile, pentafluoro-	193	C7F5N	000773-82-0	25



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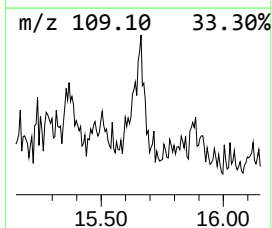
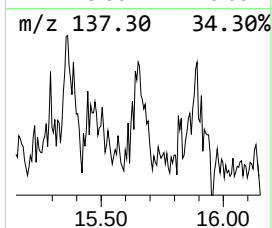
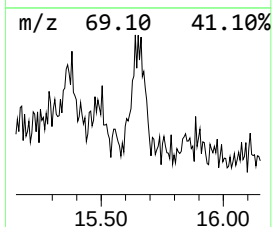
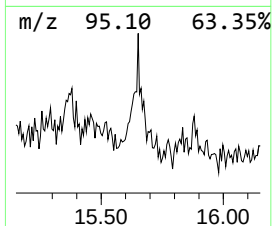
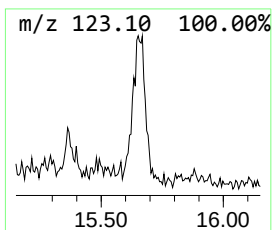
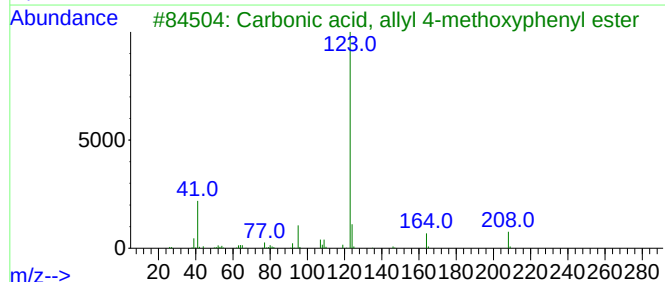
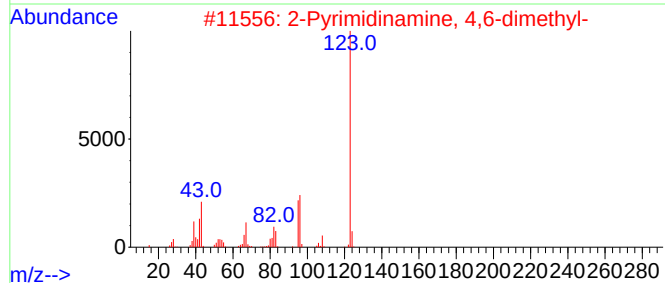
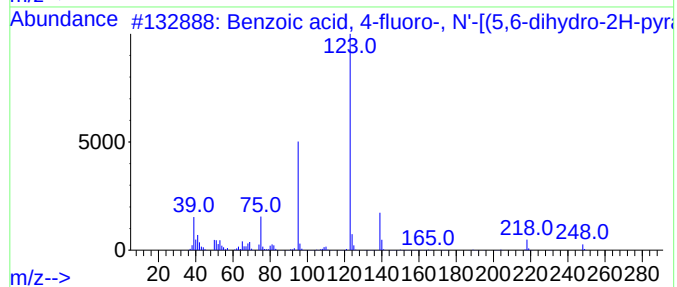
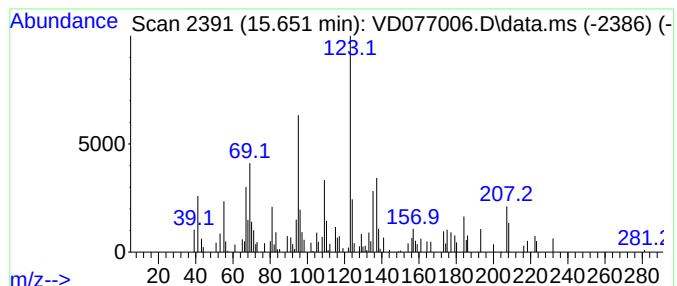
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TIC Library : C:\Database\NIST20.L
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Peak Number 8 unknown15.651 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.651	14.65 ug/l	141046	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 4-fluoro-, N'-[(5,...	248	C13H13FN2O2	1000350-57-6	38
2			2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	35
3			Carbonic acid, allyl 4-methoxyph...	208	C11H12O4	1000357-81-0	35
4			4-Fluorobenzoic acid, 3-tridecyl...	322	C20H31FO2	1000280-67-9	35
5			butanoic acid, (1-ethenyl-1H-im...	194	C10H14N2O2	1000395-99-5	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown9.746	9.746	8.6	ug/l	5098	2	8.775	29769	50.0
unknown10.628	10.628	11.4	ug/l	8506	3	11.581	37283	50.0
unknown10.657	10.657	19.0	ug/l	14162	3	11.581	37283	50.0
1-Bromo-1-methy...	13.645	50.0	ug/l	481322	4	13.516	481322	50.0
unknown15.651	15.651	14.7	ug/l	141046	4	13.516	481322	50.0