

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD071922\
 Data File : VD073863.D
 Acq On : 19 Jul 2022 16:10
 Operator : VA/SY
 Sample : N3649-07
 Misc : 7.69G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 A-2-LC

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\82D071822S.M
 Title : SW846 8260

Signal : TIC: VD073863.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.126	29	35	40	rBV2	15005	28591	3.21%	0.439%
2	2.191	40	46	52	rBV2	51093	108628	12.19%	1.669%
3	2.591	109	114	119	rBV4	24238	59917	6.72%	0.920%
4	2.691	128	131	135	rBV3	21568	31460	3.53%	0.483%
5	3.732	306	308	311	rBV3	8217	9649	1.08%	0.148%
6	4.167	381	382	387	rVB2	24728	14024	1.57%	0.215%
7	4.667	461	467	477	rVB3	15501	39995	4.49%	0.614%
8	7.567	931	960	973	rVB	116670	678640	76.16%	10.426%
9	7.920	1004	1020	1041	rBV3	158267	631090	70.83%	9.695%
10	8.303	1076	1085	1105	rBV5	36888	173868	19.51%	2.671%
11	8.838	1166	1176	1197	rBV	154499	588032	65.99%	9.034%
12	10.320	1419	1428	1443	rBV	275273	811311	91.05%	12.464%
13	10.473	1449	1454	1455	rBV2	17419	24633	2.76%	0.378%
14	10.838	1513	1516	1521	rBV6	8868	13012	1.46%	0.200%
15	11.073	1551	1556	1564	rVB4	33807	72513	8.14%	1.114%
16	11.644	1645	1653	1670	rBV	254191	672420	75.46%	10.330%
17	11.838	1683	1686	1687	rBV3	16980	18333	2.06%	0.282%
18	12.626	1813	1820	1827	rBV3	349955	891042	100.00%	13.689%
19	13.567	1974	1980	1993	rVB	319947	664862	74.62%	10.214%
20	13.755	2006	2012	2027	rVB5	162047	614375	68.95%	9.439%
21	14.085	2064	2068	2081	rVB5	84764	206493	23.17%	3.172%
22	15.749	2344	2351	2362	rVB6	49279	156314	17.54%	2.401%

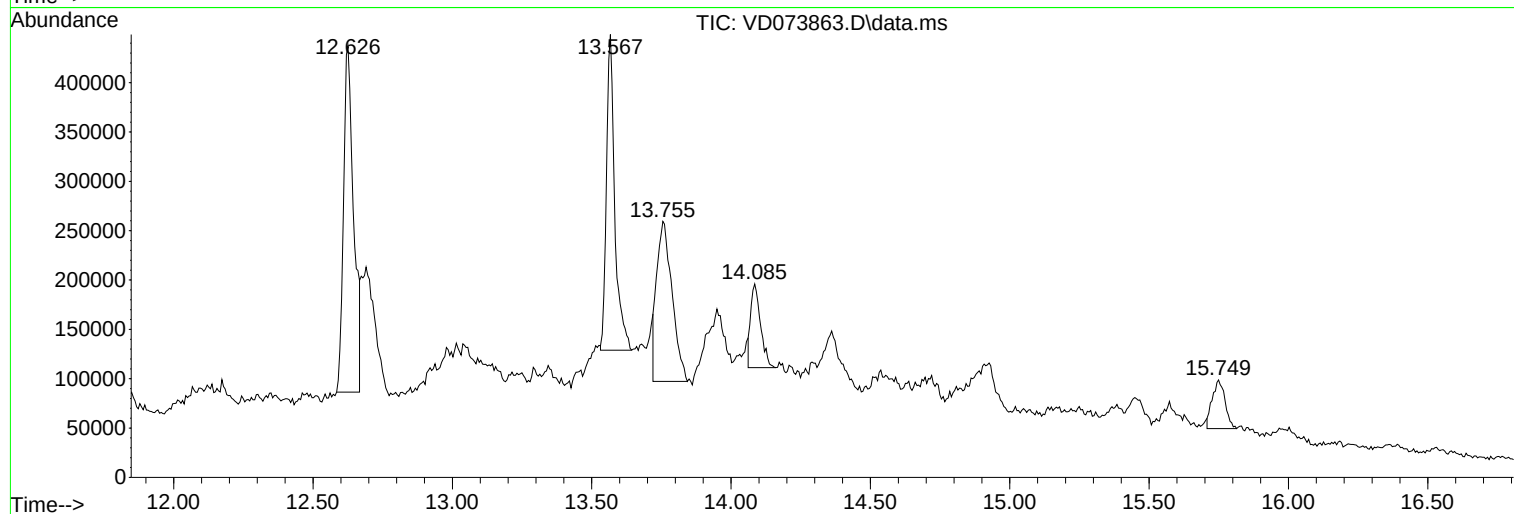
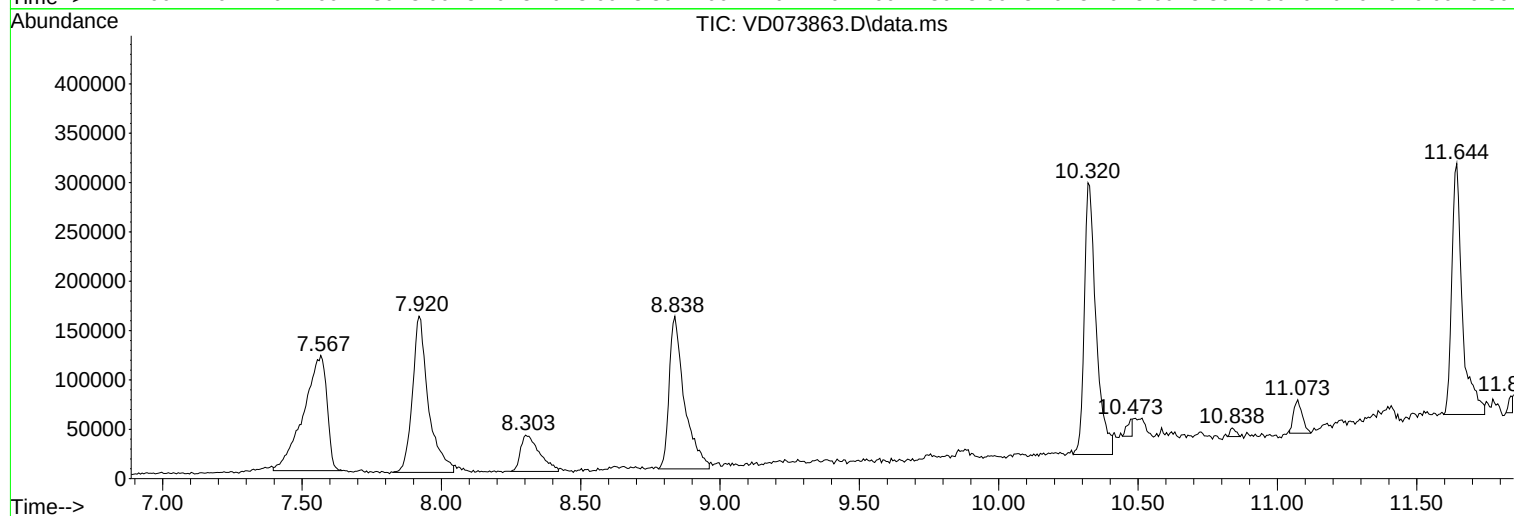
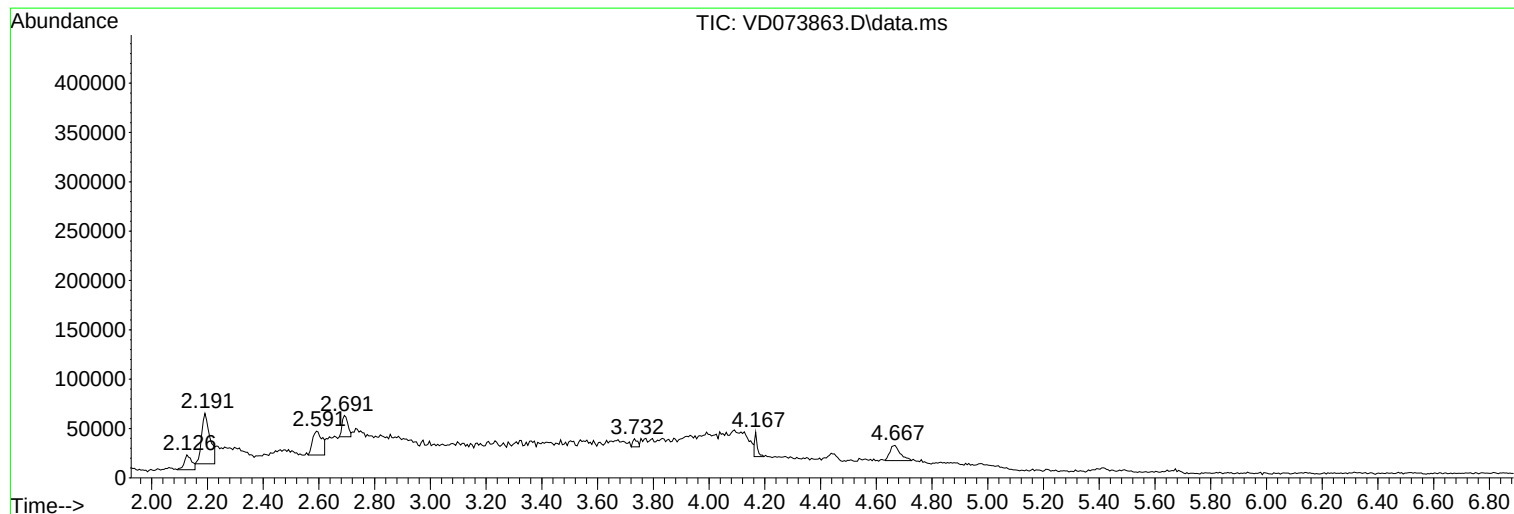
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071822S.M
Quant Title : SW846 8260

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



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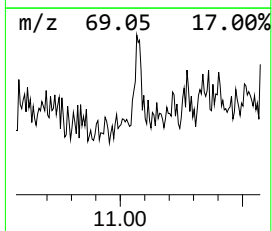
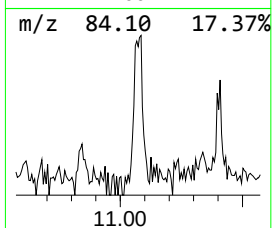
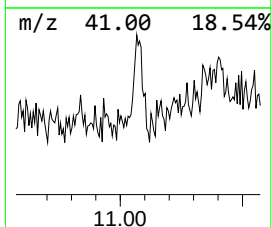
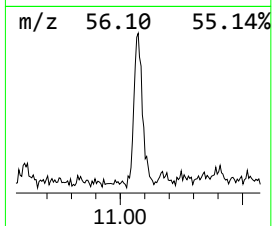
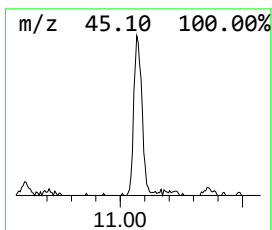
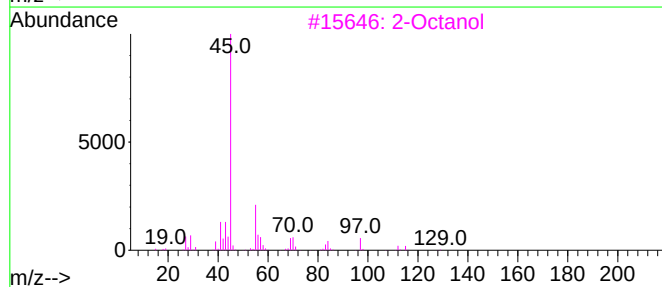
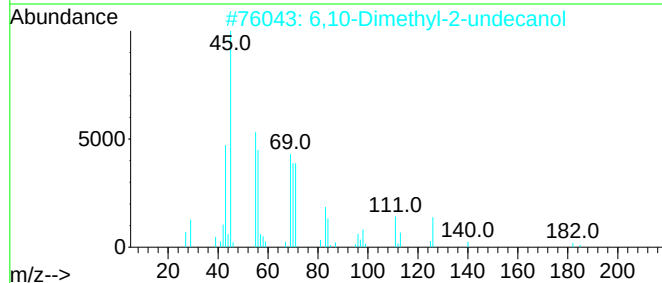
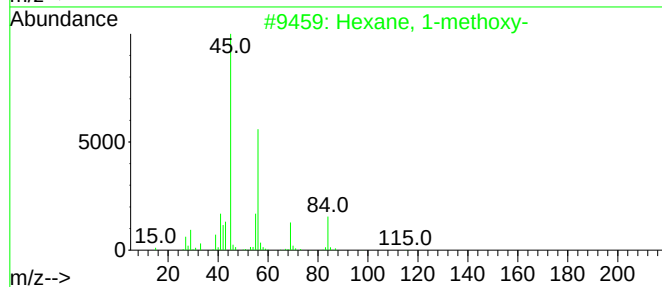
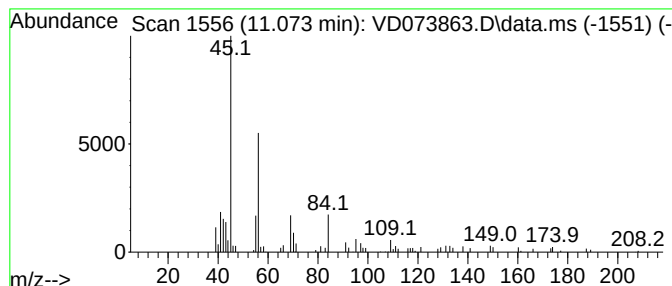
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071822S.M
Quant Title : SW846 8260

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

Peak Number 2 Hexane, 1-methoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.073	5.39 ug/l	72513	Chlorobenzene-d5	11.644

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 1-methoxy-	116	C7H16O	004747-07-3	78
2			6,10-Dimethyl-2-undecanol	200	C13H28O	1000432-19-5	56
3			2-Octanol	130	C8H18O	000123-96-6	47
4			2-Heptanol, 6-methyl-	130	C8H18O	004730-22-7	42
5			2-Nonanol	144	C9H20O	000628-99-9	40



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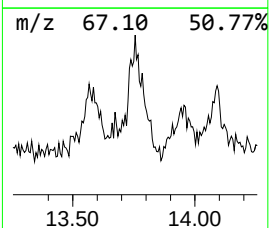
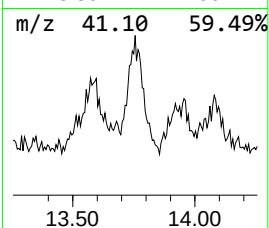
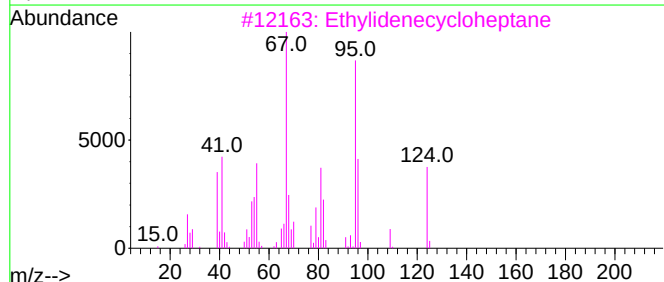
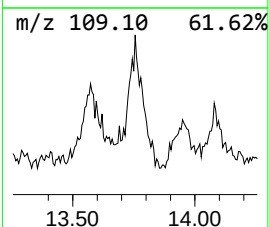
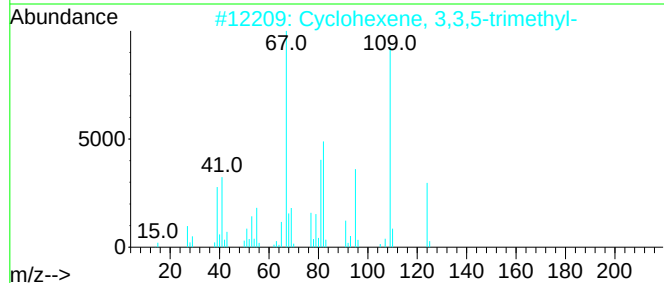
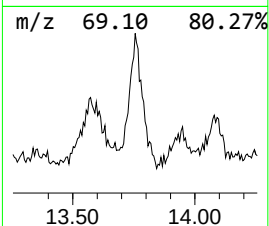
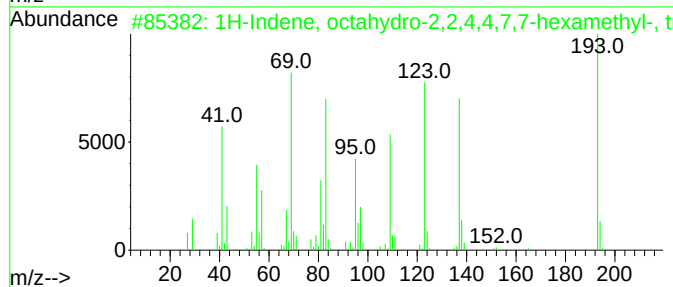
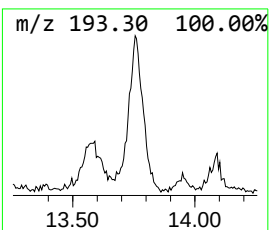
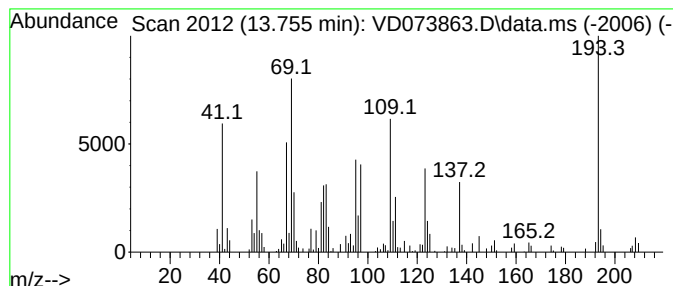
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D071822S.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 1H-Indene, octahydro-2,2,4,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.755	46.20 ug/l	614375	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-2,2,4,7,7...	208	C15H28	054832-83-6	50
2			Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	25
3			Ethylidenecycloheptane	124	C9H16	010494-87-8	25
4			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	22
5			2-Amino-4-butylthiomethyl-6-pipe...	281	C13H23N5S	022362-21-6	14



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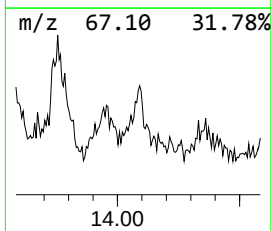
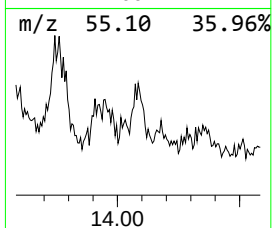
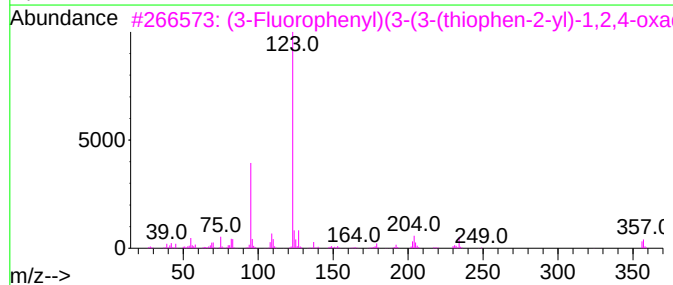
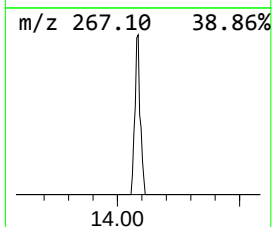
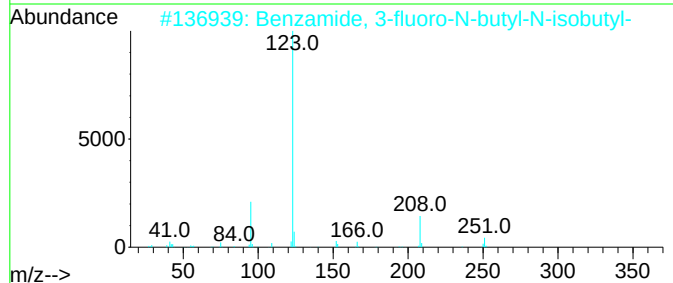
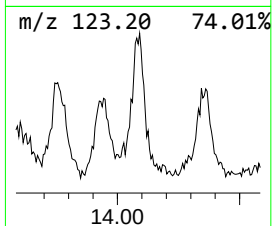
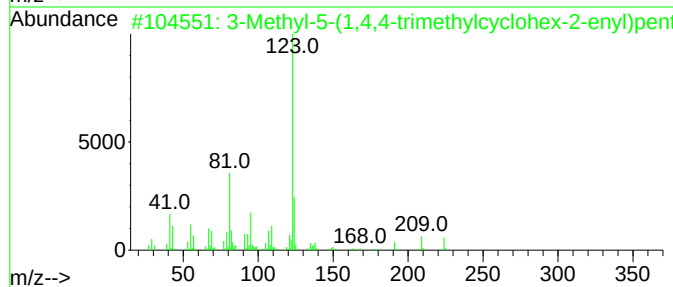
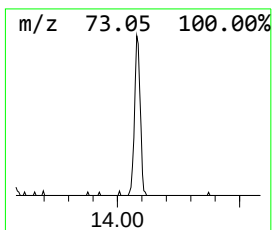
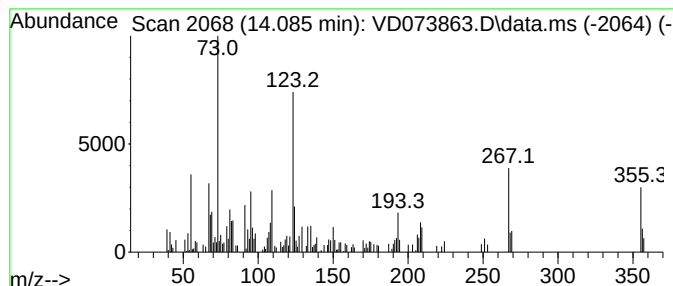
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Peak Number 4 unknown14.085 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.085	15.53 ug/l	206493	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methyl-5-(1,4,4-trimethylcyclo...	224	C15H28O	1000187-09-1	46
2			Benzamide, 3-fluoro-N-butyl-N-is...	251	C15H22FNO	1000415-86-1	38
3			(3-Fluorophenyl)(3-(3-(thiophen-...	357	C18H16FN3O2S	837414-26-3	35
4			3-Fluorobenzoic acid, 2-pentadec...	350	C22H35FO2	1000280-60-7	35
5			Benzene-1,2,3-triamine	123	C6H9N3	1000316-45-3	30



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ClientSampleId :
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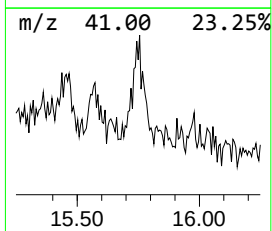
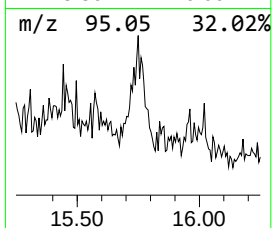
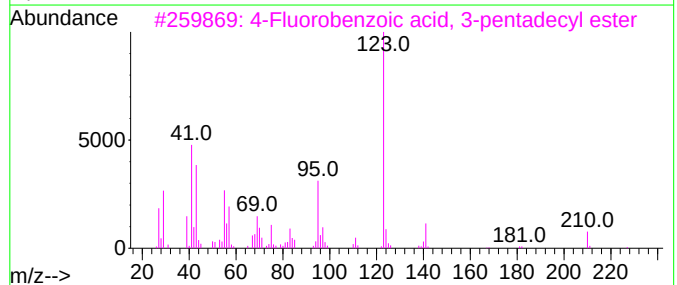
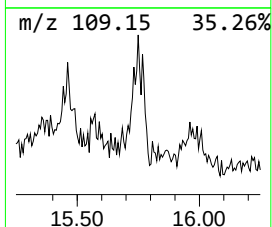
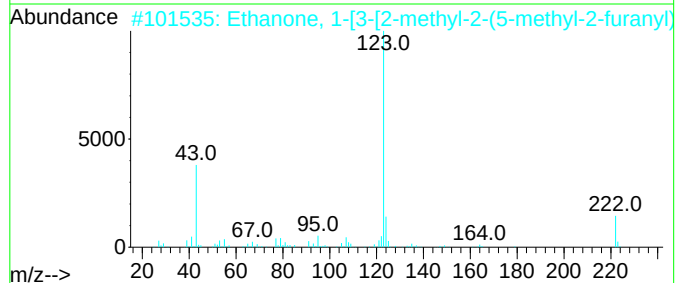
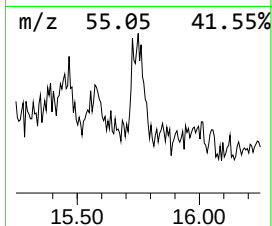
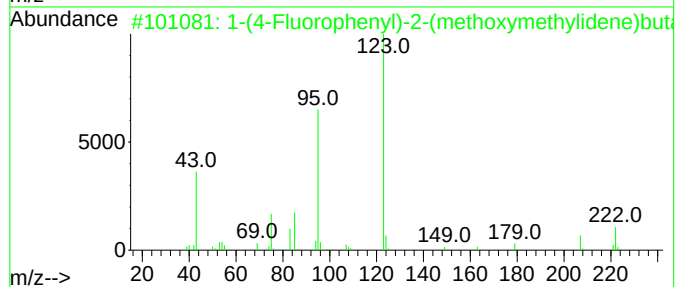
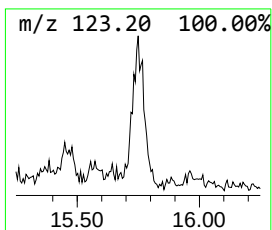
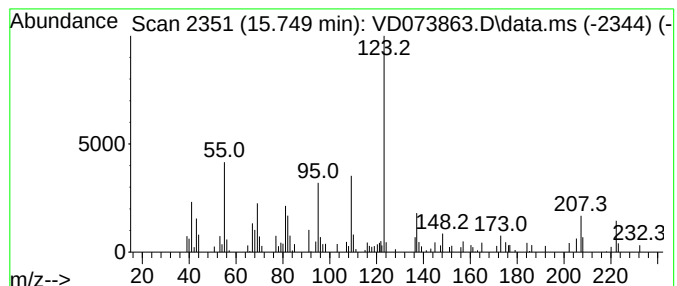
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Quant Title : SW846 8260

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

Peak Number 5 1-(4-Fluorophenyl)-2-(metho... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.749	11.76 ug/l	156314	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(4-Fluorophenyl)-2-(methoxymet...	222	C12H11F03	1000388-14-4	53
2			Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H1803	080114-28-9	53
3			4-Fluorobenzoic acid, 3-pentadec...	350	C22H35F02	1000280-68-4	47
4			Carbonic acid, allyl 4-methoxyph...	208	C11H1204	1000357-81-0	47
5			N2-Methyl-2,3-pyridinediamine	123	C6H9N3	005028-20-6	47



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 1-methoxy-	11.073	5.4	ug/l	72513	3	11.644	672420	50.0
1H-Indene, octa...	13.755	46.2	ug/l	614375	4	13.567	664862	50.0
unknown14.085	14.085	15.5	ug/l	206493	4	13.567	664862	50.0
1-(4-Fluorophen...	15.749	11.8	ug/l	156314	4	13.567	664862	50.0