

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY070622\
 Data File : VY009457.D
 Acq On : 06 Jul 2022 16:28
 Operator : KP/MD
 Sample : N3587-02
 Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 VOC

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\82Y062822S.M

Title : SW846 8260

Signal : TIC: VY009457.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.698	462	472	483	rBV2	26501	78944	3.20%	0.877%
2	6.966	834	844	857	rBV	18030	56648	2.30%	0.629%
3	7.710	955	966	971	rBV2	113696	268726	10.89%	2.984%
4	7.783	971	978	989	rVB	264606	592259	24.01%	6.577%
5	8.130	1024	1035	1047	rBV	118121	281543	11.41%	3.127%
6	8.685	1117	1126	1137	rBV	412103	822999	33.36%	9.140%
7	10.173	1363	1370	1378	rBV	504486	880277	35.69%	9.776%
8	10.941	1491	1496	1504	rBV	58185	110700	4.49%	1.229%
9	11.483	1579	1585	1594	rBV	652916	1058652	42.92%	11.757%
10	12.081	1670	1683	1684	rBV	209445	588794	23.87%	6.539%
11	12.477	1743	1748	1759	rBV	407394	692974	28.09%	7.696%
12	13.184	1857	1864	1871	rBV8	83079	254529	10.32%	2.827%
13	13.422	1890	1903	1914	rVB2	882357	2466771	100.00%	27.395%
14	13.763	1953	1959	1971	rVB5	118850	419231	17.00%	4.656%
15	15.202	2189	2195	2202	rBV8	47176	132509	5.37%	1.472%
16	15.483	2235	2241	2251	rVB3	98063	298934	12.12%	3.320%

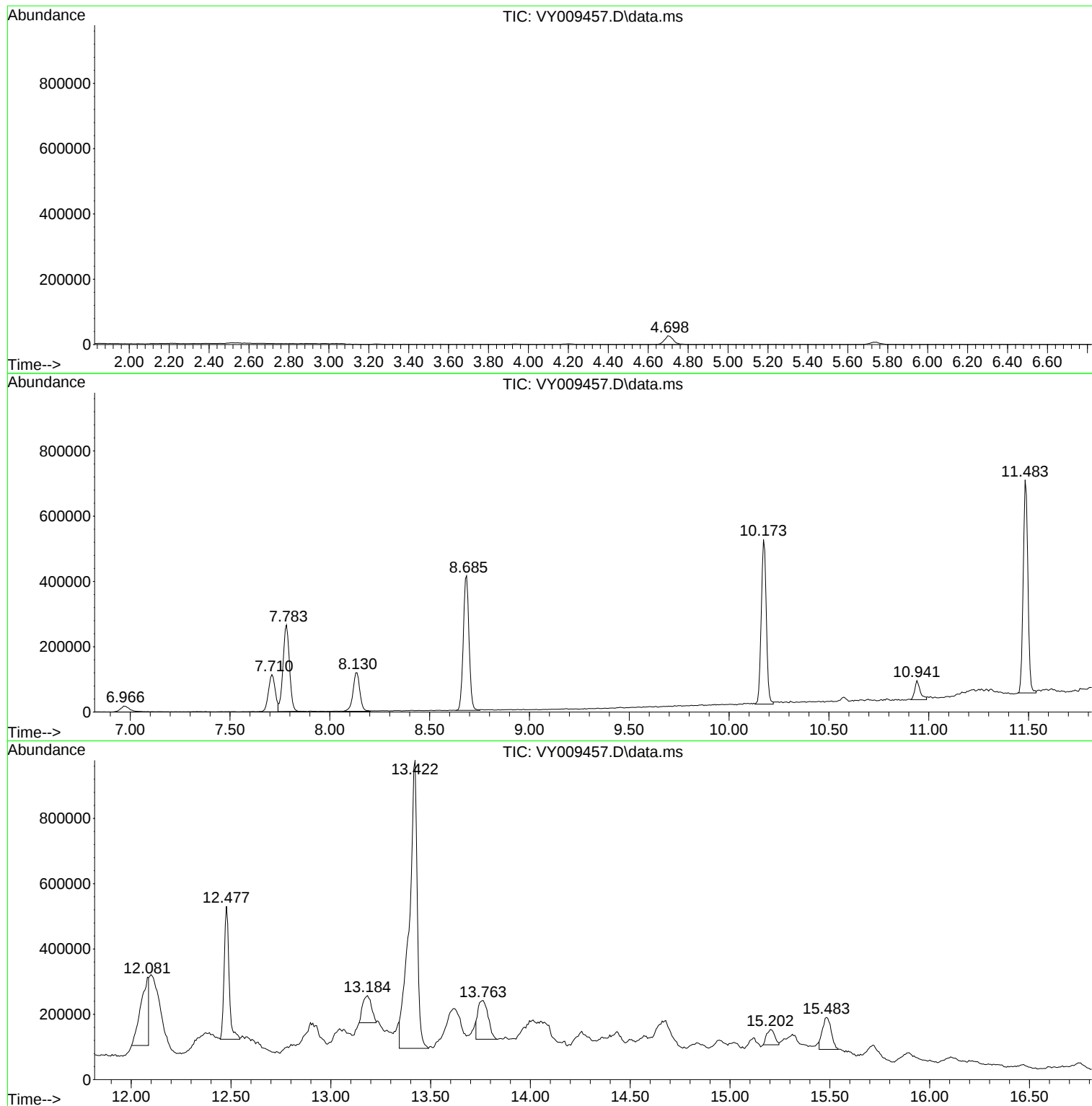
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y062822S.M
Quant Title : SW846 8260

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



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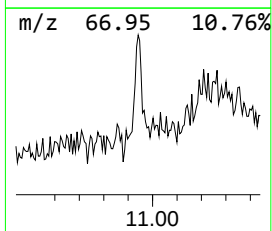
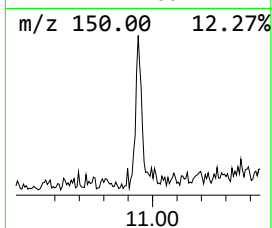
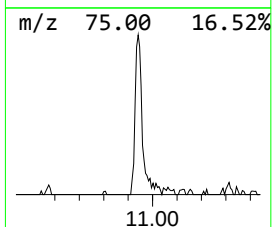
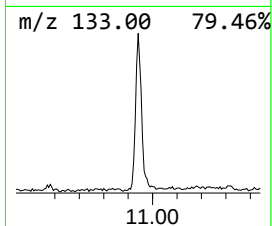
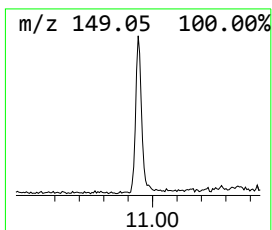
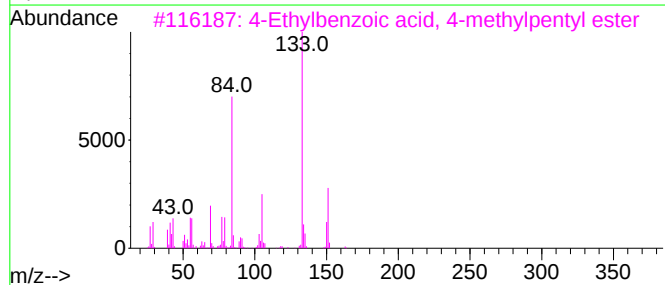
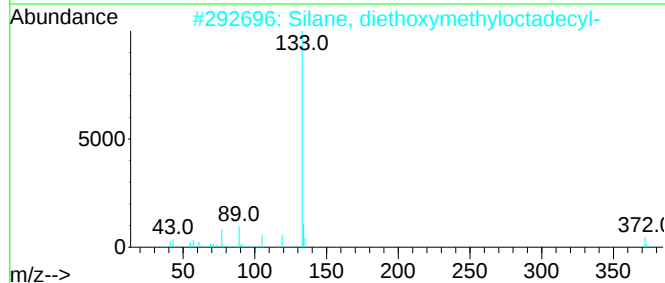
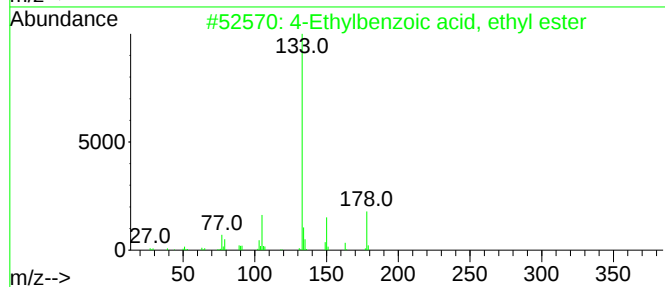
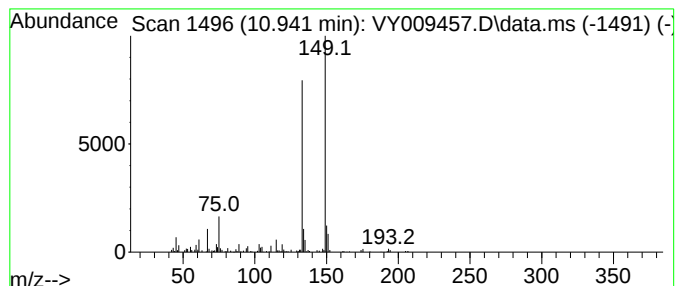
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y062822S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown10.941 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.941	5.23 ug/l	110700	Chlorobenzene-d5	11.483

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Ethylbenzoic acid, ethyl ester	178	C11H14O2	036207-13-3	37
2			Silane, diethoxymethyloctadecyl-	386	C23H50O2Si	067859-75-0	35
3			4-Ethylbenzoic acid, 4-methylpen...	234	C15H22O2	1000293-49-7	32
4			2-Methoxy-3-methylbenzamide, N,N...	193	C11H15NO2	1369798-01-5	32
5			Silane, diethoxydimethyl-	148	C6H16O2Si	000078-62-6	25



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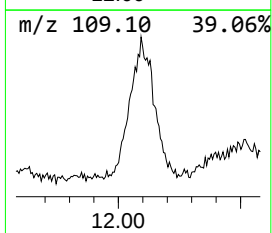
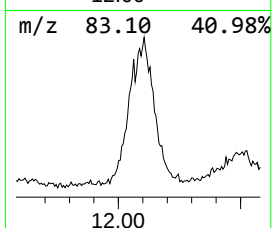
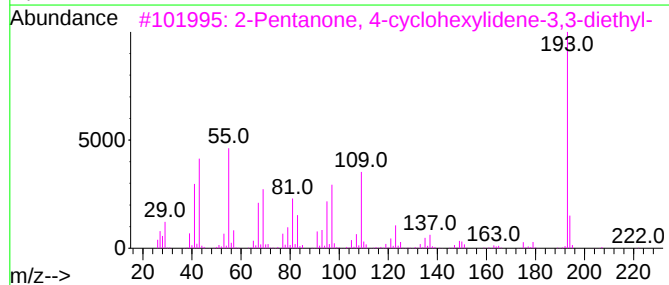
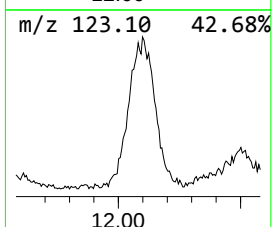
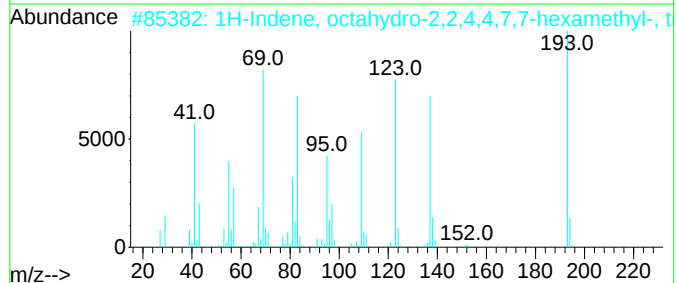
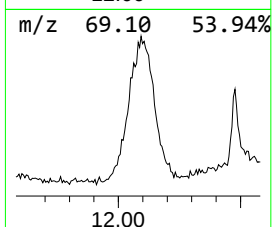
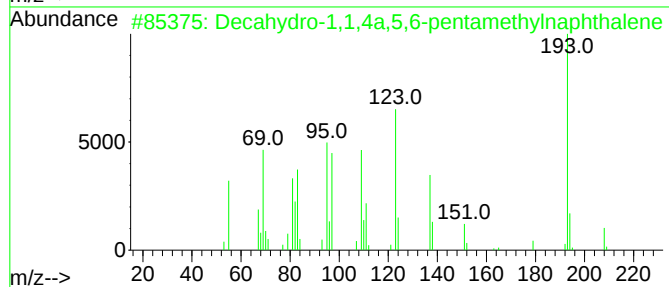
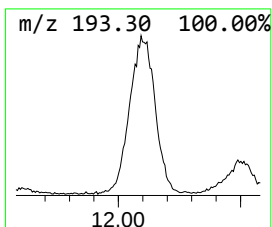
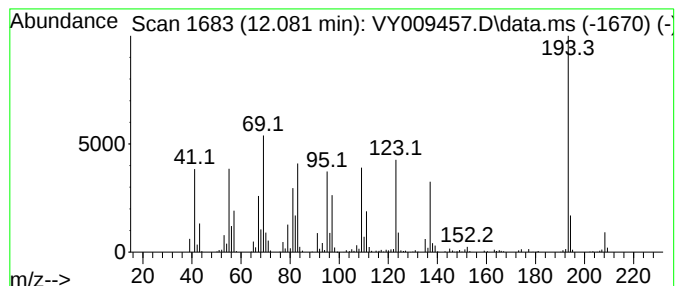
Instrument :
MSVOA_Y
ClientSampleId :
VOC

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Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.081	27.81 ug/l	588794	Chlorobenzene-d5	11.483	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	81
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	56
3	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	38
4	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	38
5	diallyl(2,2,4a,7,7-pentamethyl-1...	384	C19H33N2O4P	1000187-42-4	25



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Instrument :
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ClientSampleId :
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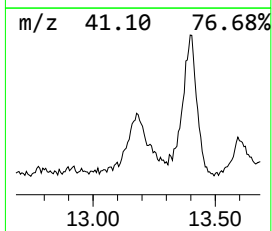
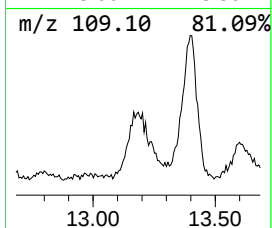
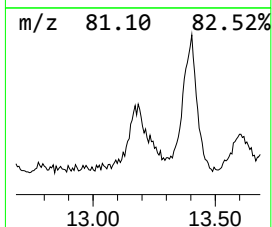
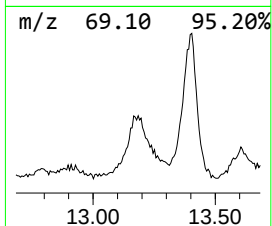
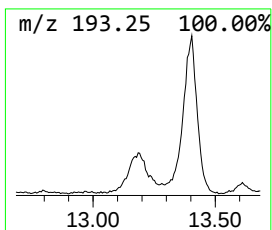
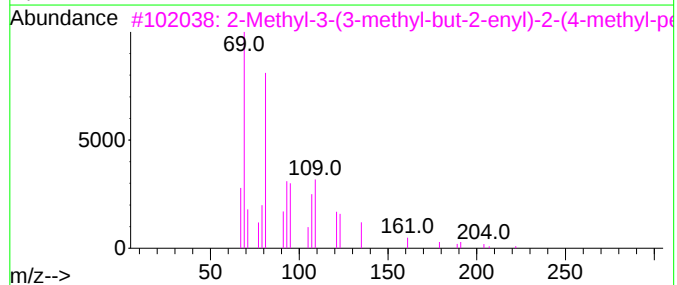
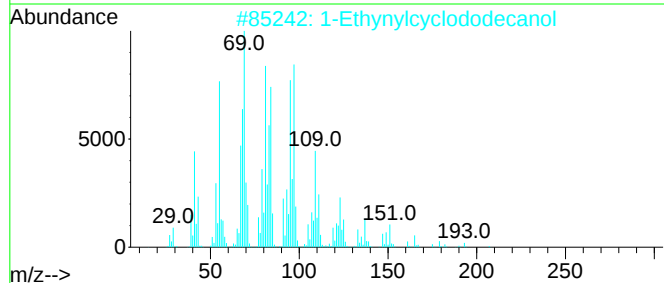
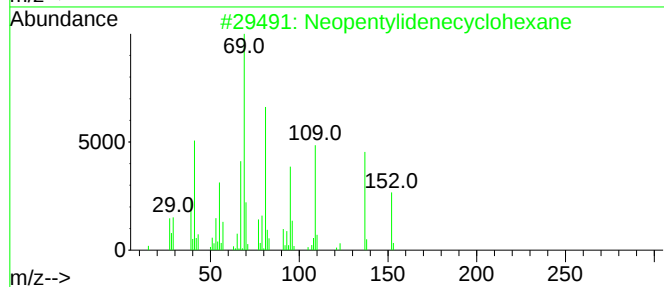
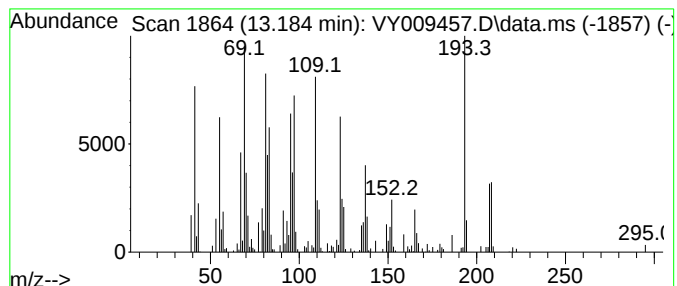
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Peak Number 4 unknown13.184 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.184	5.16 ug/l	254529	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Neopentylidenecyclohexane	152	C11H20	039546-80-0	43
2			1-Ethynylcyclododecanol	208	C14H24O	1000484-40-4	43
3			2-Methyl-3-(3-methyl-but-2-enyl)...	222	C15H26O	1000144-10-2	38
4			trans, cis-2-Ethylbicyclo[4.4.0]...	166	C12H22	066660-39-7	22
5			4-[(2-Fluorophenyl)methyl]piperi...	193	C12H16FN	194288-97-6	22



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Instrument :
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ClientSampleId :
VOC

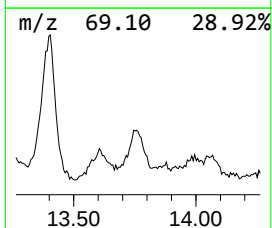
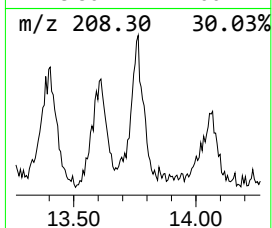
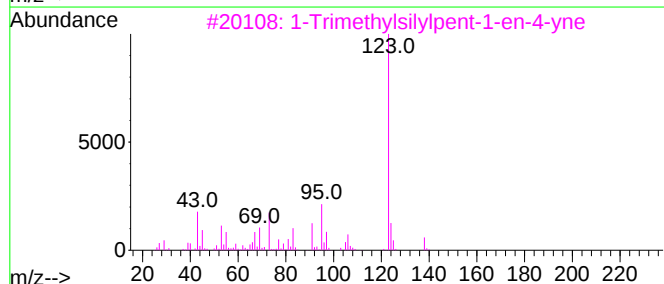
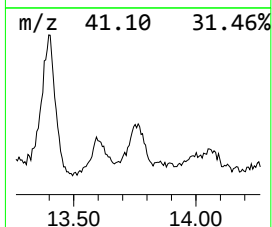
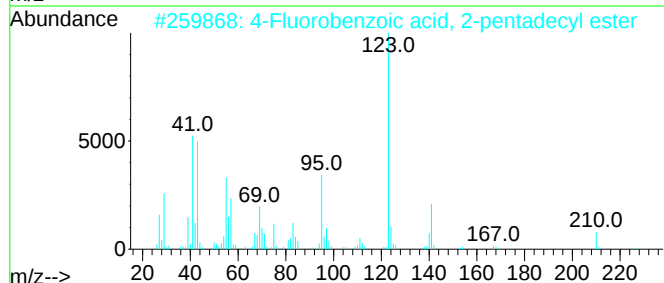
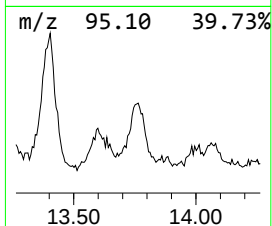
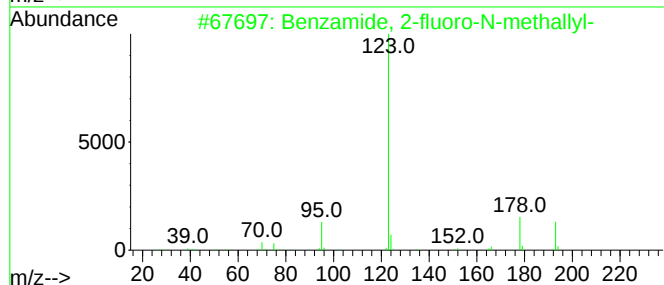
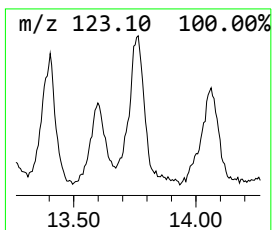
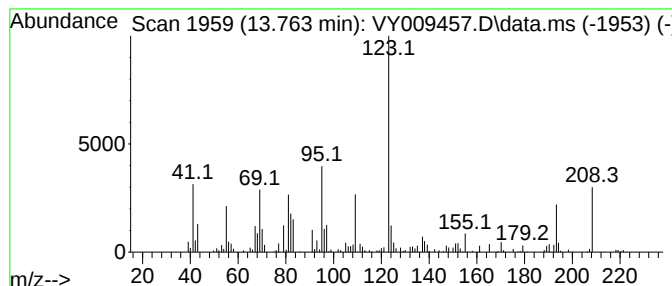
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 5 Benzamide, 2-fluoro-N-metha... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.763	8.50 ug/l	419231	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, 2-fluoro-N-methallyl-	193	C11H12FNO	1000340-07-0	53
2			4-Fluorobenzoic acid, 2-pentadec...	350	C22H35FO2	1000280-68-3	50
3			1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	50
4			Benzamide, 3-fluoro-N-(2-phenyle...	299	C19H22FNO	1000451-30-3	50
5			4-Fluorobenzoic acid, 3-pentadec...	350	C22H35FO2	1000280-68-4	50



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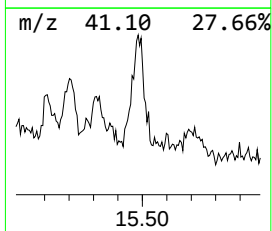
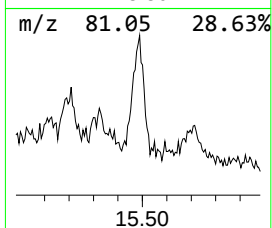
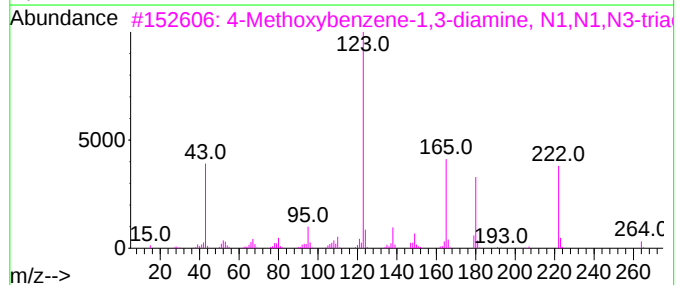
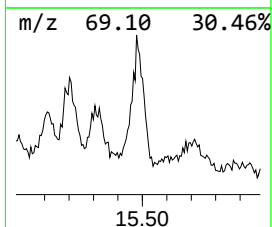
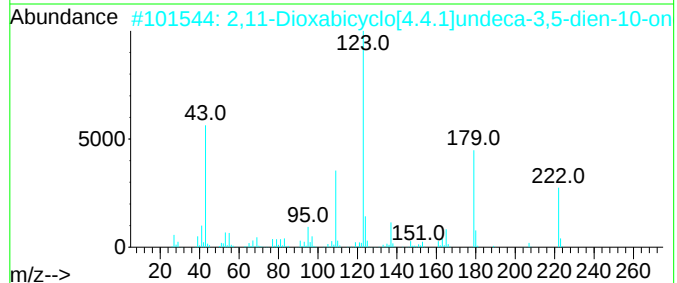
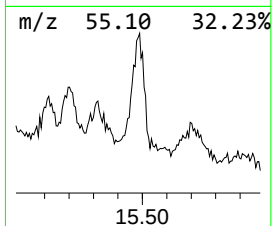
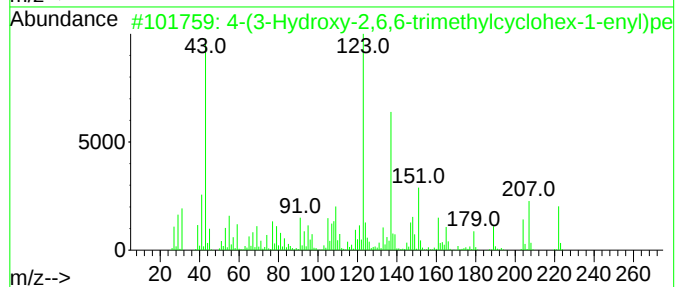
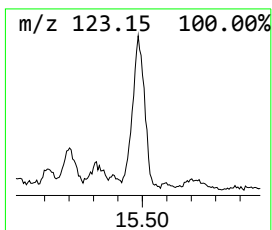
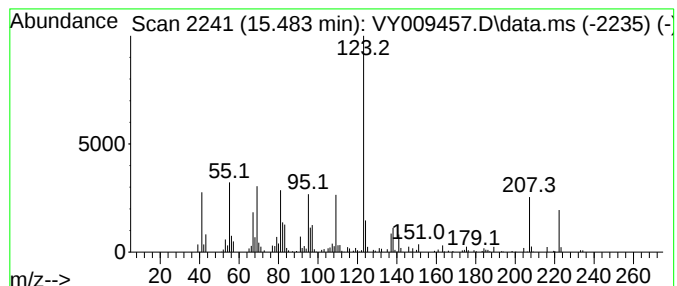
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 4-(3-Hydroxy-2,6,6-trimethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.483	6.06 ug/l	298934	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(3-Hydroxy-2,6,6-trimethylcycl...	222	C14H22O2	097306-57-5	64
2			2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	58
3			4-Methoxybenzene-1,3-diamine, N1...	264	C13H16N2O4	1000373-20-9	53
4			1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	50
5			1,5-Dimethyl-4-(tetramethyl-1,3,...	222	C11H19BN2O2	1036991-40-8	47



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown10.941	10.941	5.2	ug/l	110700	3	11.483	1058650	50.0
Decahydro-1,1,4...	12.081	27.8	ug/l	588794	3	11.483	1058650	50.0
unknown13.184	13.184	5.2	ug/l	254529	4	13.422	2466770	50.0
Benzamide, 2-fl...	13.763	8.5	ug/l	419231	4	13.422	2466770	50.0
4-(3-Hydroxy-2,...	15.483	6.1	ug/l	298934	4	13.422	2466770	50.0