

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD051022\
 Data File : VD072917.D
 Acq On : 10 May 2022 16:31
 Operator : VA/SY
 Sample : N2769-01
 Misc : 5.26G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 CL-02-051022

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\82D050222S.M
 Title : SW846 8260

Signal : TIC: VD072917.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.897	1011	1016	1017	rBV2	7556	7754	2.42%	0.823%
2	7.914	1017	1019	1023	rVV4	8999	11807	3.68%	1.254%
3	7.967	1025	1028	1038	rVB4	14516	32681	10.18%	3.471%
4	8.320	1081	1088	1097	rVB2	11180	25778	8.03%	2.738%
5	8.567	1125	1130	1131	rBV3	2294	3781	1.18%	0.402%
6	8.856	1171	1179	1187	rBV	24892	53349	16.62%	5.666%
7	9.097	1216	1220	1222	rBV5	2975	3493	1.09%	0.371%
8	9.320	1257	1258	1261	rBV3	4678	4270	1.33%	0.453%
9	9.532	1292	1294	1299	rVB5	3348	4207	1.31%	0.447%
10	9.685	1317	1320	1325	rBV7	4328	5993	1.87%	0.636%
11	9.773	1332	1335	1336	rBV3	4373	4087	1.27%	0.434%
12	10.050	1380	1382	1385	rVB4	4131	3521	1.10%	0.374%
13	10.332	1422	1430	1435	rBV	38402	71491	22.27%	7.592%
14	10.391	1438	1440	1441	rBV	4831	3889	1.21%	0.413%
15	11.638	1648	1652	1657	rVB3	30057	45970	14.32%	4.882%
16	12.697	1827	1832	1833	rBV3	65008	96513	30.07%	10.249%
17	13.120	1894	1904	1905	rBV3	148839	320995	100.00%	34.089%
18	13.567	1975	1980	1984	rBV7	41081	96990	30.22%	10.300%
19	14.096	2068	2070	2072	rBV2	25029	25096	7.82%	2.665%
20	15.308	2274	2276	2279	rBV4	9756	7271	2.27%	0.772%
21	15.767	2345	2354	2363	rVB4	32124	104622	32.59%	11.111%
22	16.379	2457	2458	2461	rVB3	6024	4086	1.27%	0.434%
23	16.596	2493	2495	2497	rVB3	5205	4001	1.25%	0.425%

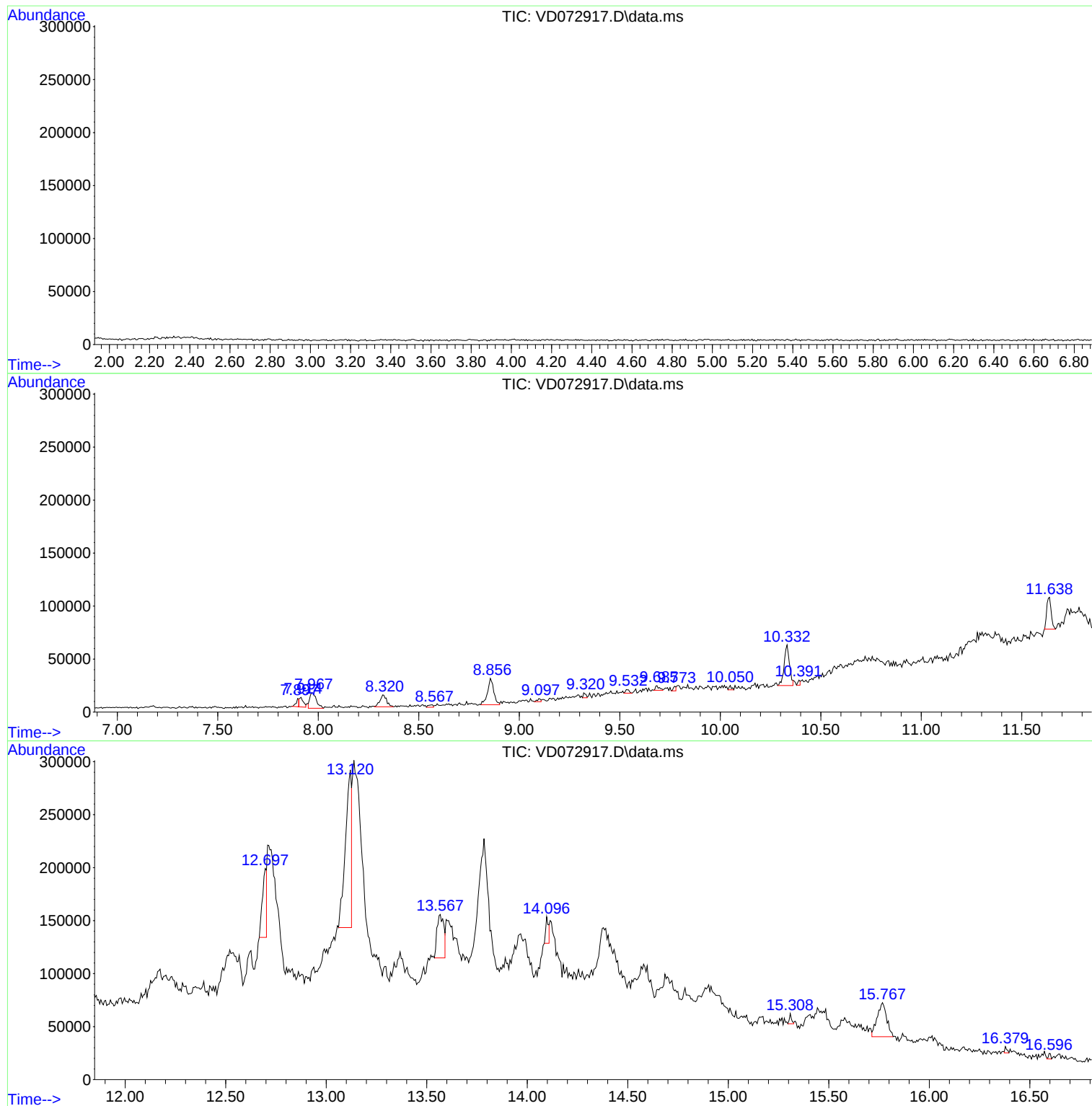
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Quant Title : SW846 8260

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



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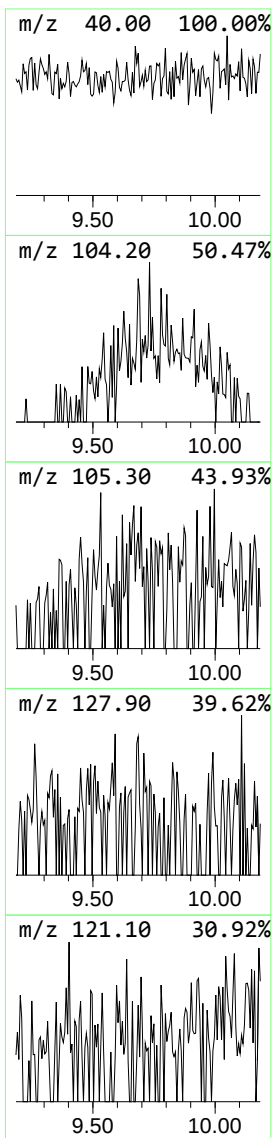
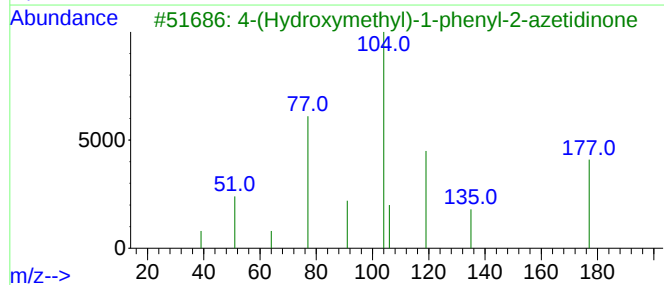
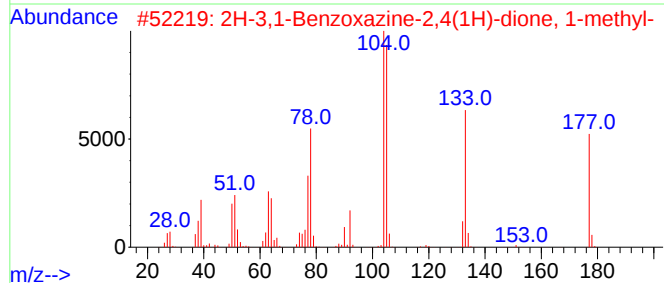
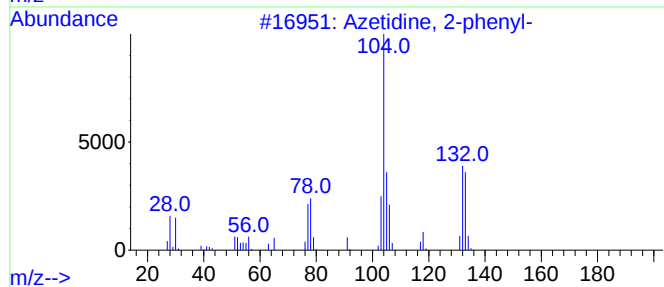
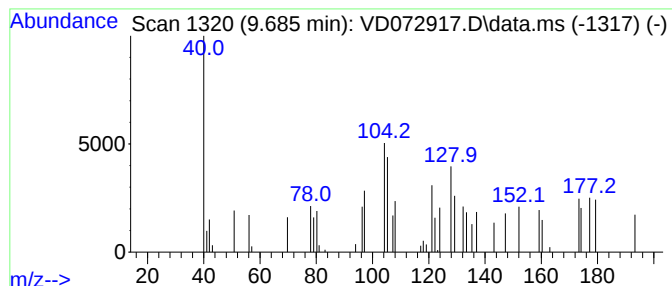
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown9.685 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.685	5.62 ug/l	5993	1,4-Difluorobenzene	8.856

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azetidine, 2-phenyl-	133	C9H11N	022610-18-0	10
2			2H-3,1-Benzoxazine-2,4(1H)-dione...	177	C9H7N03	010328-92-4	9
3			4-(Hydroxymethyl)-1-phenyl-2-aze...	177	C10H11NO2	065837-49-2	9
4			6-Chloro-2,4-dimethoxypyrimidine	174	C6H7ClN2O2	006320-15-6	9
5			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	9



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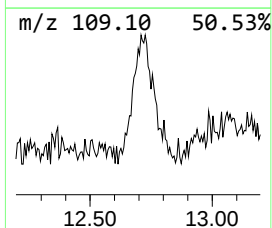
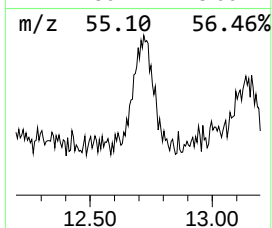
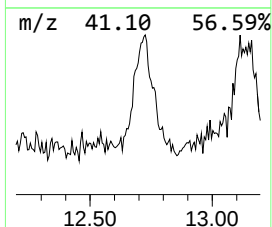
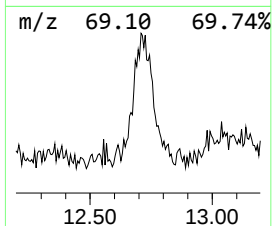
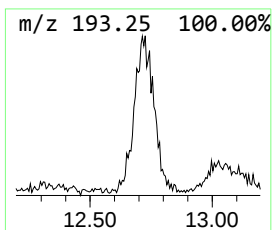
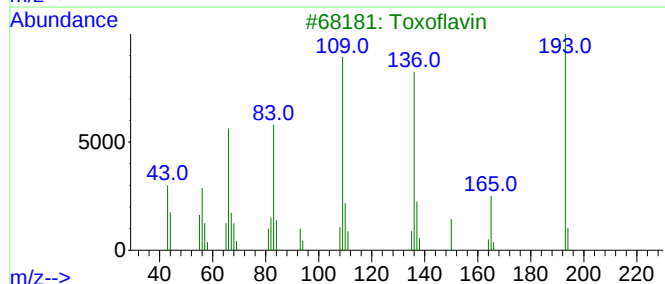
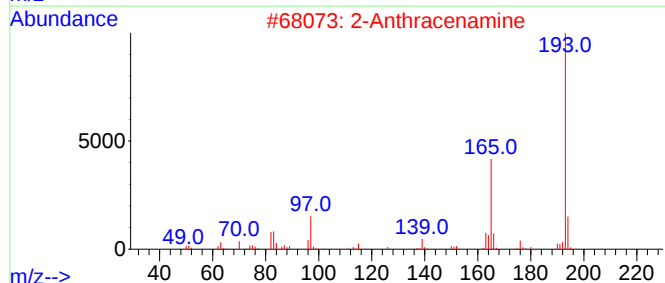
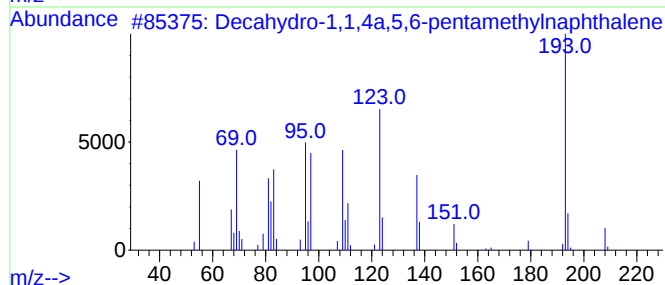
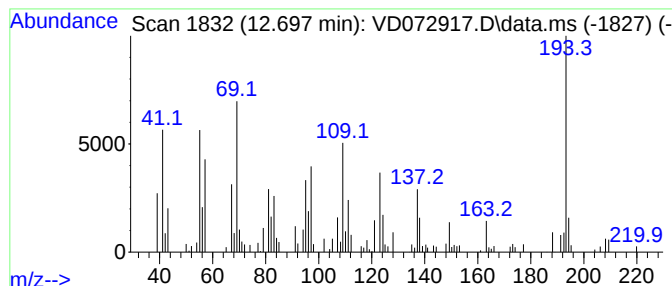
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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

Peak Number 2 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.697	49.75 ug/l	96513	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	60
2			2-Anthracenamine	193	C14H11N	000613-13-8	38
3			Toxoflavin	193	C7H7N5O2	000084-82-2	35
4			Acetylene, 1-(2-aminophenyl)-2-p...	193	C14H11N	1000380-73-4	25
5			1H-Indole, 2-phenyl-	193	C14H11N	000948-65-2	25



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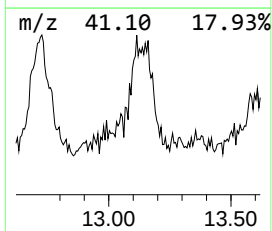
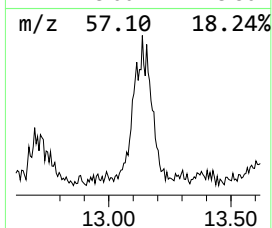
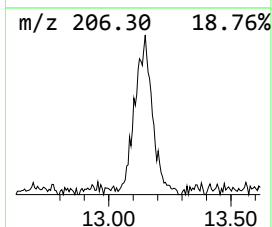
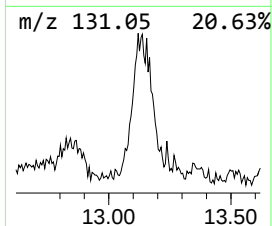
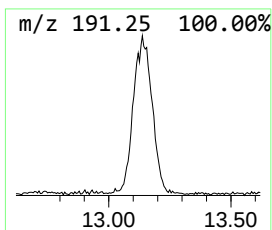
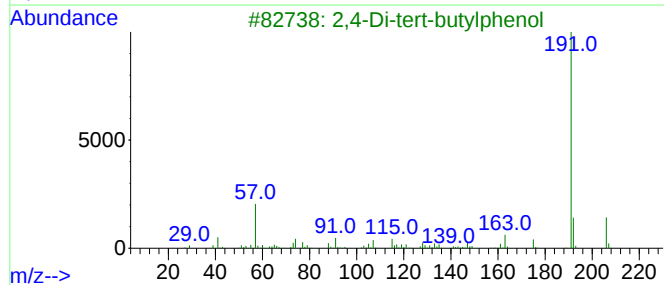
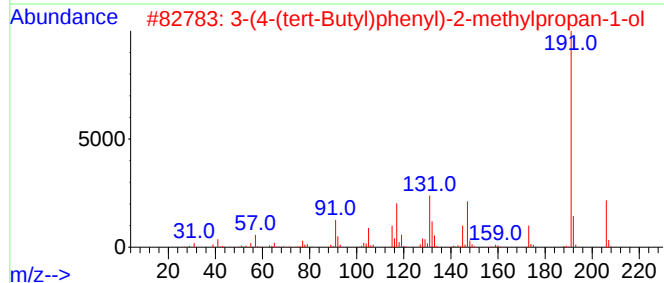
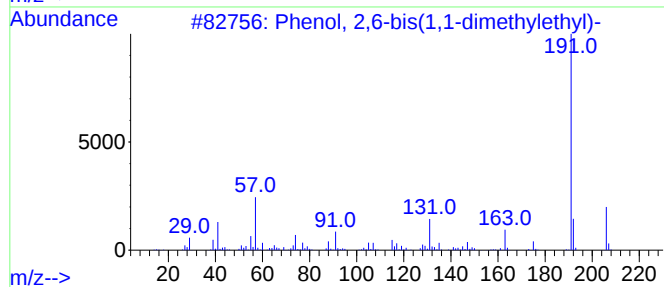
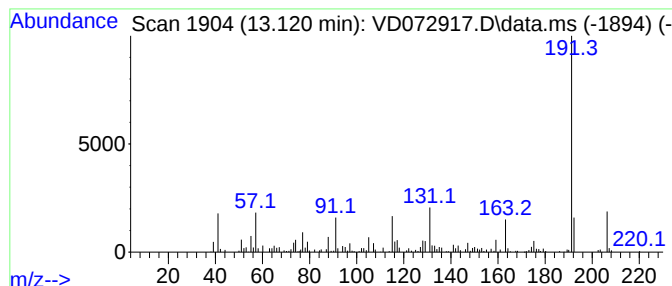
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.120	165.48 ug/l	320995	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
2			3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	81
3			2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	74
4			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	72
5			3-(4-tert-Butylphenyl)propanoic ...	206	C13H18O2	001208-64-6	68



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ClientSampleId :
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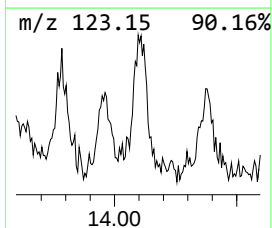
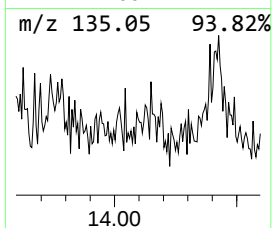
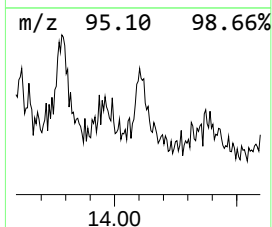
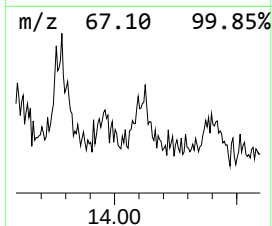
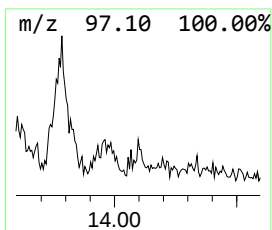
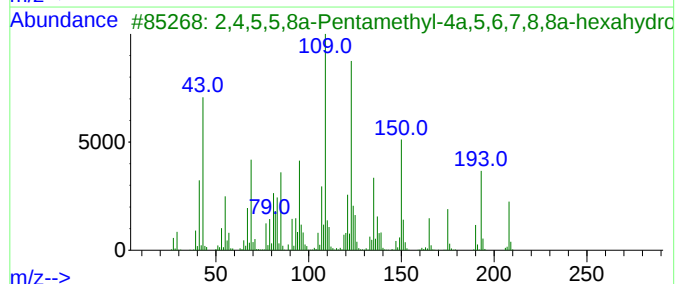
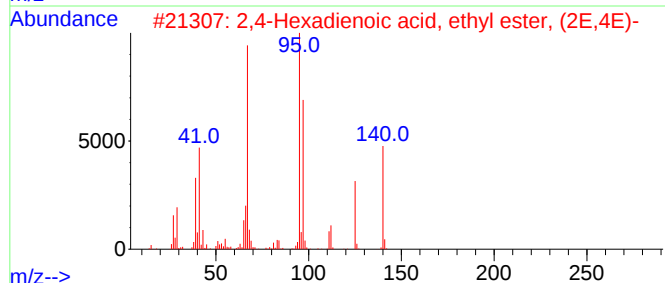
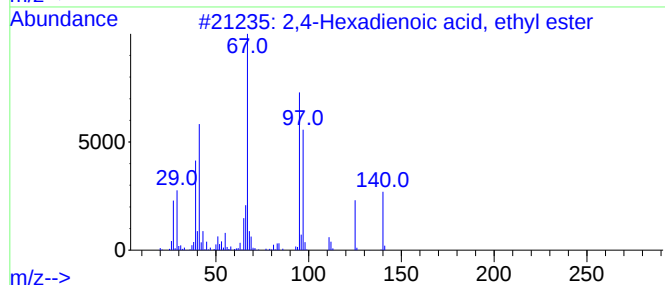
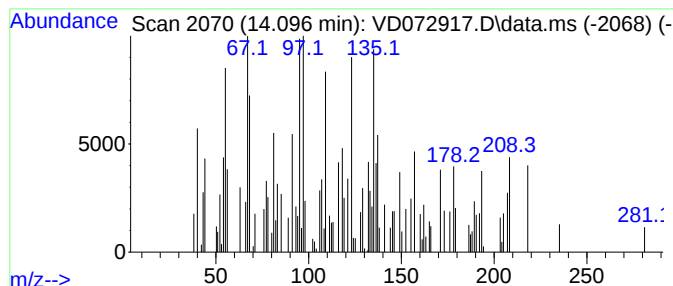
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown14.097 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.097	12.94 ug/l	25096	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Hexadienoic acid, ethyl ester	140	C8H12O2	110318-09-7	22
2			2,4-Hexadienoic acid, ethyl este...	140	C8H12O2	002396-84-1	22
3			2,4,5,5,8a-Pentamethyl-4a,5,6,7,...	208	C14H24O	1010195-30-1	14
4			2R-Acetoxymethyl-1,3,3-trimethyl...	282	C17H30O3	1000146-23-9	14
5			4,7-Methano-1H-indene, octahydro-	136	C10H16	006004-38-2	11



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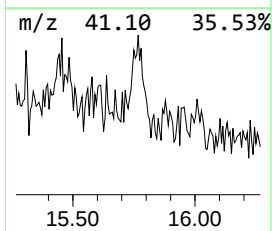
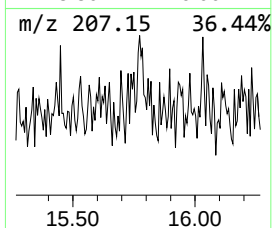
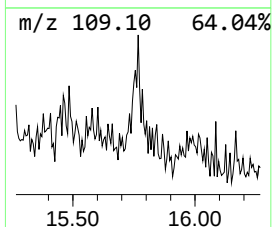
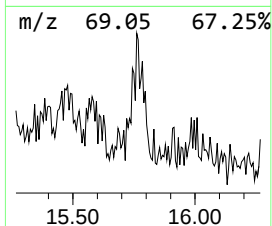
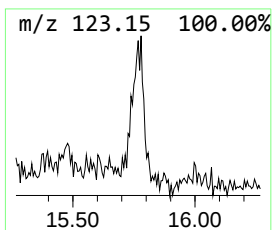
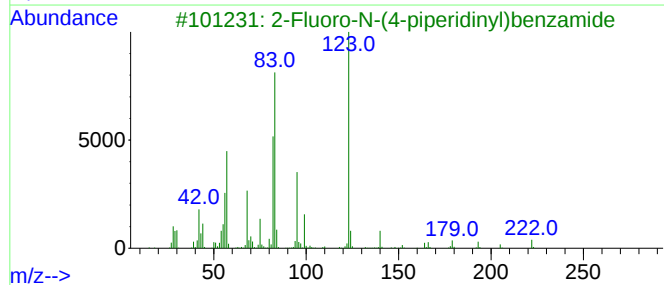
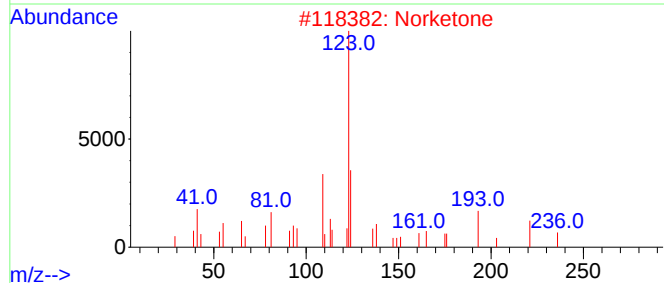
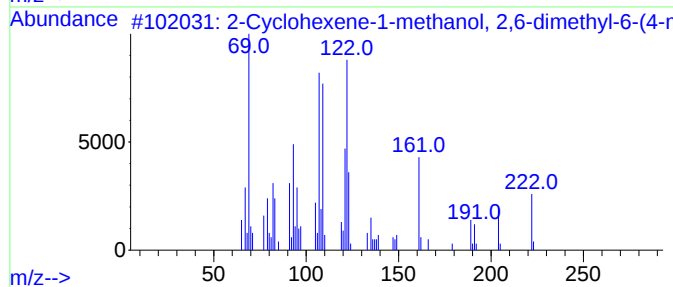
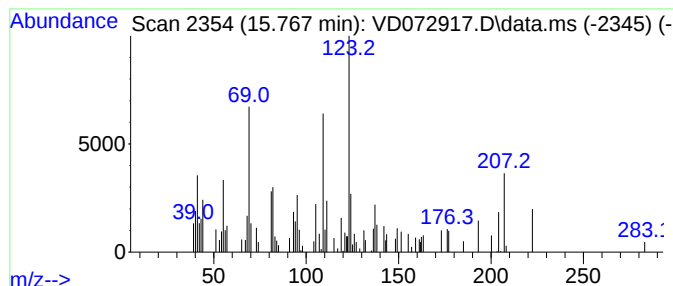
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown15.767 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.767	53.93 ug/l	104622	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexene-1-methanol, 2,6-di...	222	C15H26O	038142-34-6	38
2			Norketone	236	C14H20O3	023983-84-8	38
3			2-Fluoro-N-(4-piperidiny)benzamide	222	C12H15FN2O	886494-09-3	35
4			1-(4-Hydroxyphenyl)propane-1,2-d...	168	C9H12O3	1000495-85-4	35
5			1-(4-Hydroxyphenyl)propane-1,2-d...	168	C9H12O3	1000495-85-5	35



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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
unknown9.685	9.685	5.6	ug/l	5993	2	8.856	53349	50.0
Decahydro-1,1,4...	12.697	49.8	ug/l	96513	4	13.561	96990	50.0
Phenol, 2,6-bis...	13.120	165.5	ug/l	320995	4	13.561	96990	50.0
unknown14.097	14.097	12.9	ug/l	25096	4	13.561	96990	50.0
unknown15.767	15.767	53.9	ug/l	104622	4	13.561	96990	50.0