

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042022\
 Data File : VY008422.D
 Acq On : 20 Apr 2022 16:41
 Operator : KP/MD
 Sample : N2476-01
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 PAT-01-041922

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\82Y040822S.M
 Title : SW846 8260

Signal : TIC: VY008422.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.709	961	966	968	rBV3	674	1158	1.96%	0.708%
2	7.783	972	978	979	rBV2	921	1076	1.82%	0.658%
3	8.136	1031	1036	1043	rVB4	1114	2425	4.11%	1.483%
4	8.685	1123	1126	1133	rVV2	2046	4174	7.07%	2.553%
5	9.581	1271	1273	1275	rBV3	575	690	1.17%	0.422%
6	9.666	1284	1287	1289	rVB4	833	969	1.64%	0.593%
7	9.740	1298	1299	1304	rVB5	539	843	1.43%	0.516%
8	9.837	1312	1315	1318	rBV4	726	1222	2.07%	0.747%
9	9.922	1325	1329	1330	rBV4	763	759	1.28%	0.464%
10	10.179	1365	1371	1378	rVV	4029	7723	13.07%	4.724%
11	10.355	1396	1400	1401	rBV3	984	1094	1.85%	0.669%
12	10.746	1462	1464	1468	rVB5	718	1006	1.70%	0.615%
13	10.806	1470	1474	1475	rBV4	665	716	1.21%	0.438%
14	10.898	1485	1489	1491	rBV5	979	1227	2.08%	0.751%
15	11.093	1517	1521	1523	rBV4	1020	1269	2.15%	0.776%
16	11.197	1537	1538	1541	rBV3	1226	1343	2.27%	0.821%
17	11.489	1584	1586	1592	rVB3	3933	5619	9.51%	3.437%
18	11.733	1624	1626	1628	rBV3	1301	828	1.40%	0.506%
19	11.818	1638	1640	1641	rBV2	1252	979	1.66%	0.599%
20	12.026	1672	1674	1675	rBV2	1295	687	1.16%	0.420%
21	12.806	1800	1802	1806	rVB4	4010	5113	8.66%	3.127%
22	13.422	1897	1903	1917	rVB4	15285	59070	100.00%	36.131%
23	13.568	1923	1927	1929	rBV5	2552	4101	6.94%	2.508%
24	13.757	1952	1958	1961	rBV7	6864	15247	25.81%	9.326%
25	13.916	1982	1984	1986	rBV3	1806	1641	2.78%	1.004%
26	14.269	2037	2042	2045	rBV6	4258	9483	16.05%	5.800%
27	14.690	2104	2111	2114	rBV9	3773	10153	17.19%	6.210%
28	14.940	2150	2152	2154	rVB3	950	770	1.30%	0.471%
29	15.117	2179	2181	2184	rBV4	910	1081	1.83%	0.661%
30	15.214	2194	2197	2203	rVB7	1454	2429	4.11%	1.486%
31	15.507	2238	2245	2253	rBV8	4106	11513	19.49%	7.042%
32	15.665	2267	2271	2273	rBV4	729	762	1.29%	0.466%
33	15.732	2278	2282	2285	rBV6	946	1571	2.66%	0.961%
34	15.842	2299	2300	2302	rBV2	1050	636	1.08%	0.389%
35	15.891	2306	2308	2310	rVV3	709	941	1.59%	0.576%
36	16.001	2322	2326	2328	rVB5	859	928	1.57%	0.568%

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ClientSampleId :
PAT-01-041922

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

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Title : SW846 8260

37	16.129	2345	2347	2351	rVB4	768	1011	1.71%	0.618%
38	16.159	2351	2352	2356	rBV3	494	595	1.01%	0.364%
39	16.397	2387	2391	2395	rVB3	468	636	1.08%	0.389%

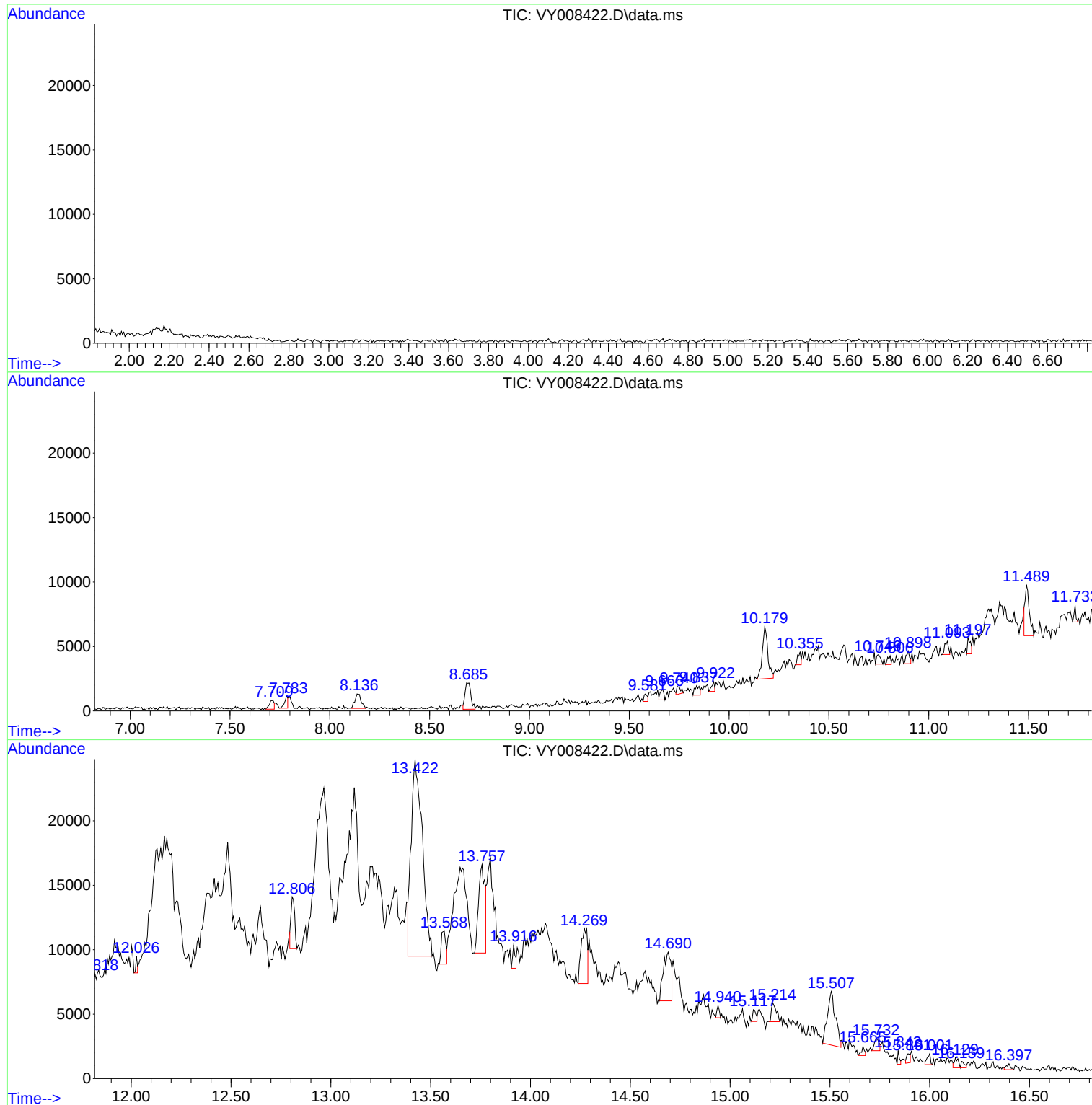
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Quant Title : SW846 8260

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



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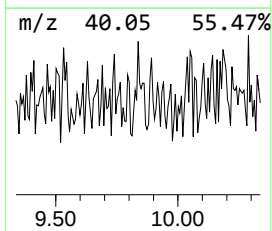
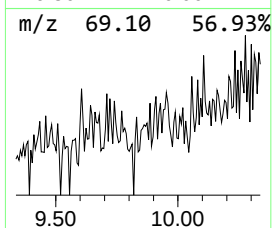
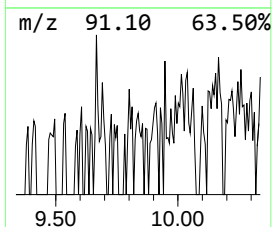
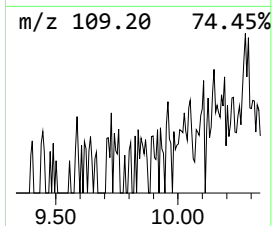
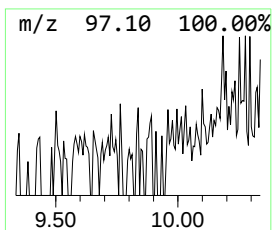
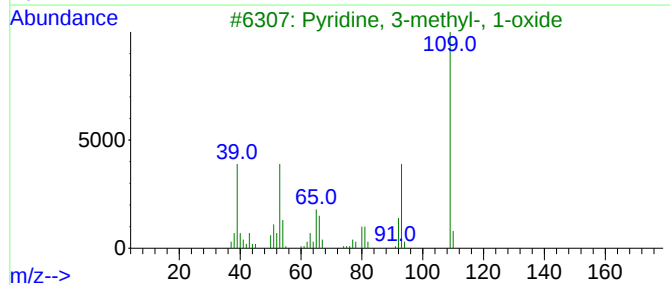
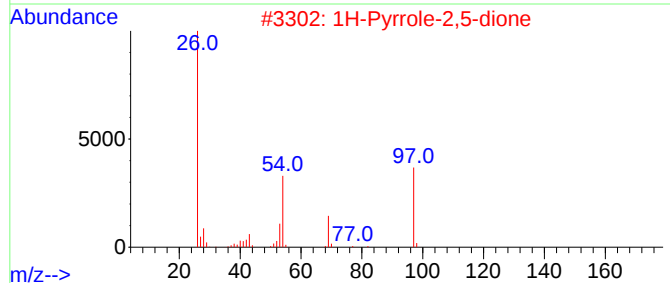
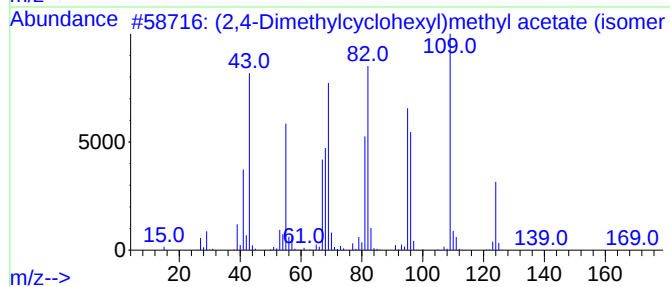
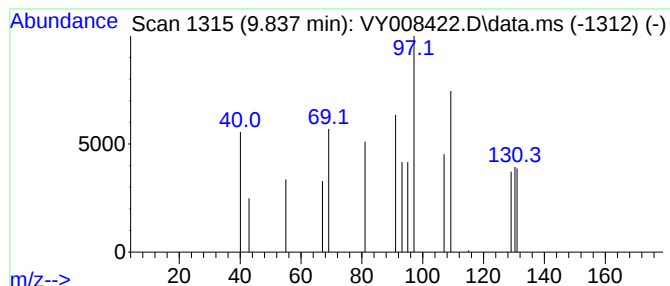
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y040822S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown9.837 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.837	14.64 ug/l	1222	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(2,4-Dimethylcyclohexyl)methyl a...	184	C11H20O2	1000497-97-0	22
2			1H-Pyrrole-2,5-dione	97	C4H3NO2	000541-59-3	5
3			Pyridine, 3-methyl-, 1-oxide	109	C6H7NO	001003-73-2	5
4			2-Propyn-1-amine, N,N-di-2-propy...	131	C9H9N	006921-29-5	4
5			1H-Imidazol, 1-methyl-2-amino-	97	C4H7N3	006646-51-1	4



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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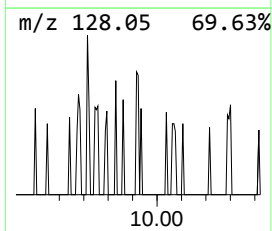
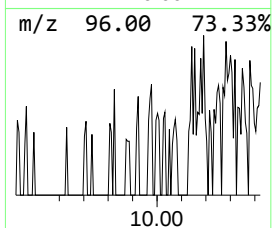
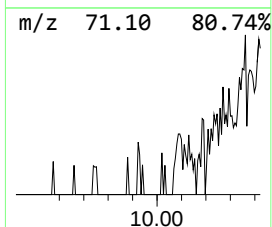
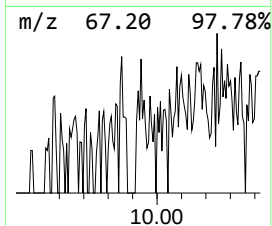
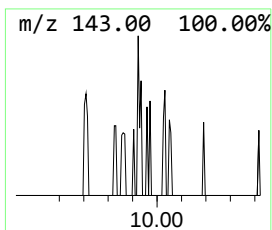
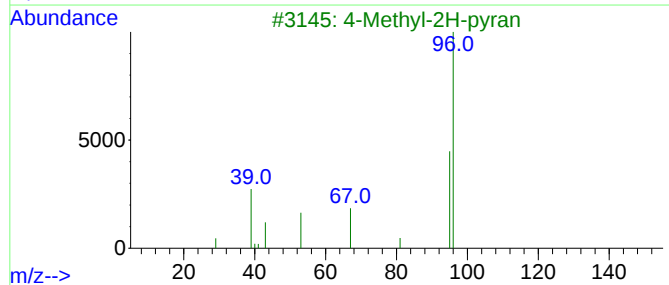
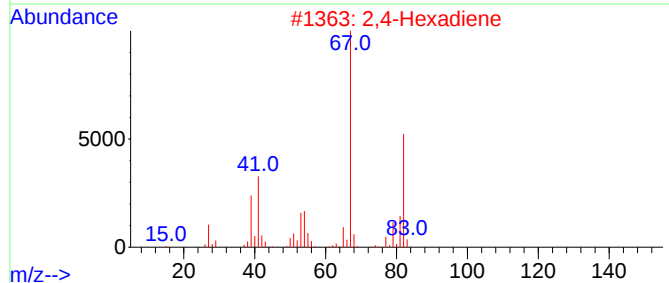
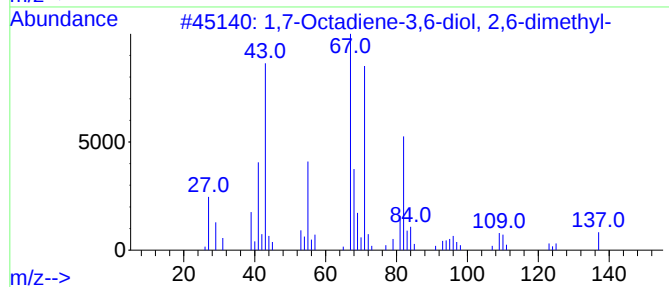
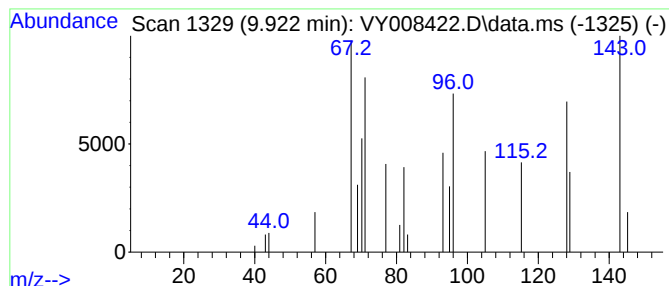
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y040822S.M
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Peak Number 4 unknown9.922 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.922	9.09 ug/l	759	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,7-Octadiene-3,6-diol, 2,6-dime...	170	C10H18O2	051276-33-6	12
2			2,4-Hexadiene	82	C6H10	000592-46-1	9
3			4-Methyl-2H-pyran	96	C6H8O	1000432-32-7	9
4			1H-Imidazole, 1,2-dimethyl-	96	C5H8N2	001739-84-0	9
5			1,4-Hexadiene	82	C6H10	000592-45-0	9



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Instrument :
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ClientSampleId :
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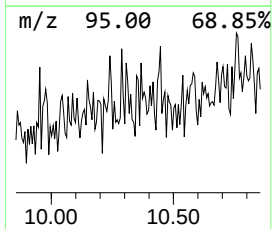
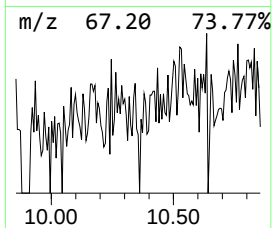
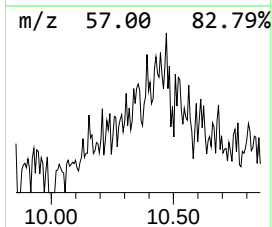
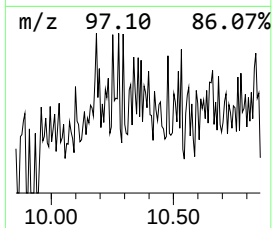
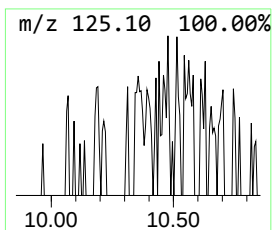
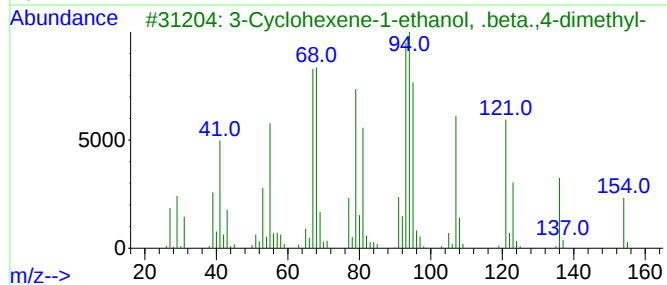
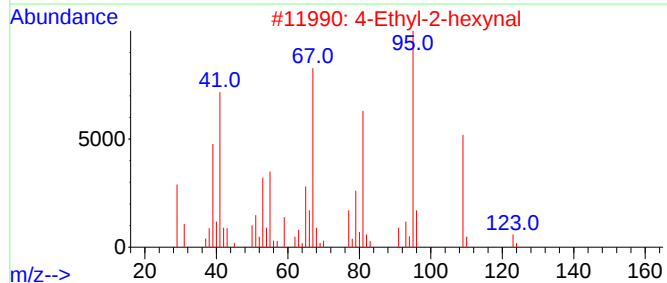
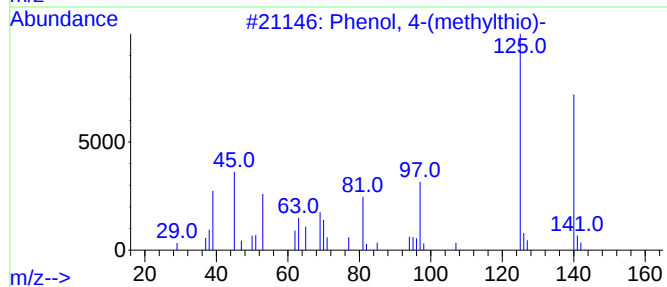
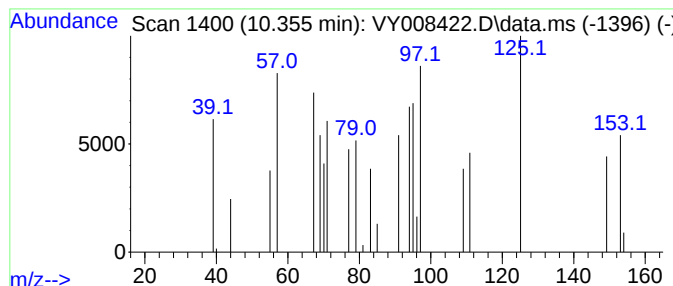
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y040822S.M
Quant Title : SW846 8260

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

Peak Number 5 unknown10.355 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.355	9.73 ug/l	1094	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	12
2			4-Ethyl-2-hexynal	124	C8H12O	071932-97-3	10
3			3-Cyclohexene-1-ethanol, .beta.,...	154	C10H18O	018479-68-0	10
4			Cyclohexene, 1-methyl-3-vinyloxy-	138	C9H14O	100144-30-7	10
5			Pyrazole, 5-methyl-3,4-dinitro-1...	297	C11H15N5O5	345950-83-6	10



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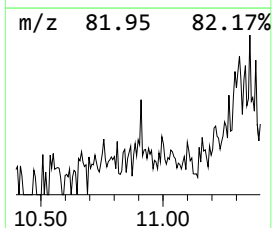
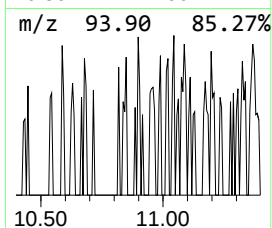
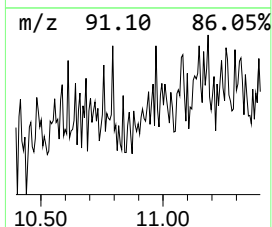
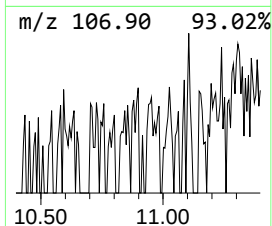
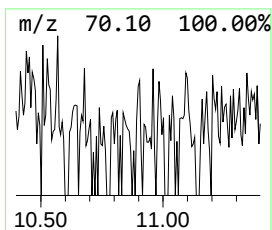
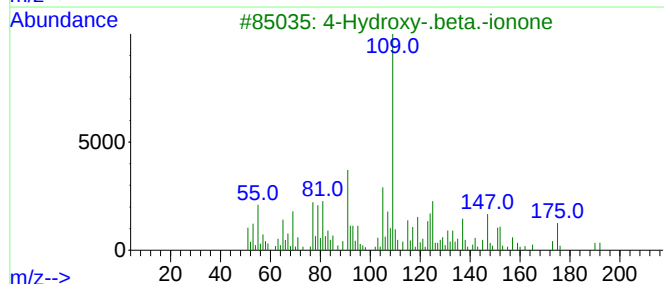
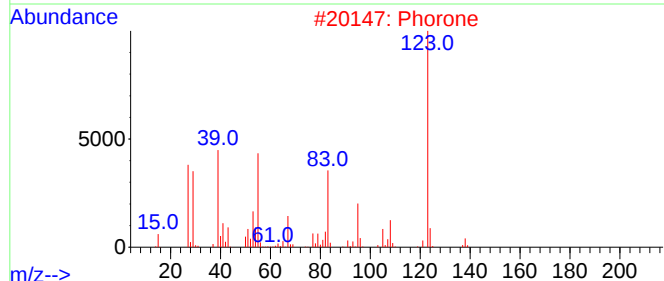
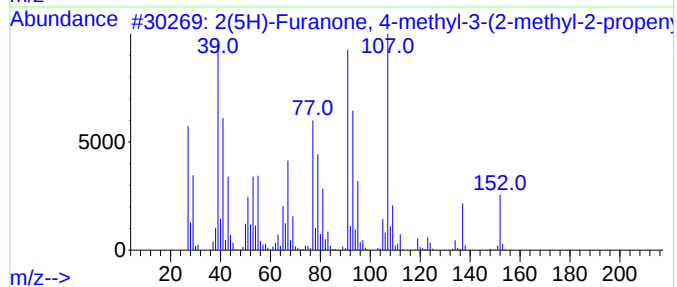
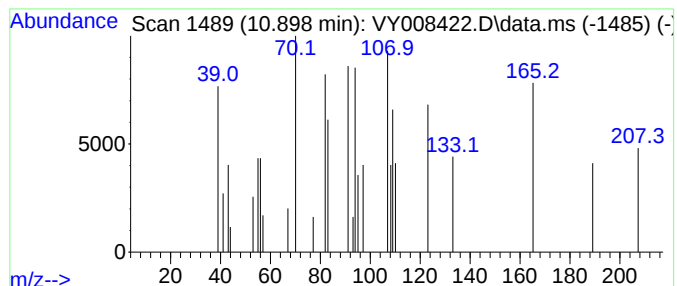
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown10.898 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.898	10.92 ug/l	1227	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(5H)-Furanone, 4-methyl-3-(2-me...	152	C9H12O2	089902-23-8	23		
2	Phorone	138	C9H14O	000504-20-1	12		
3	4-Hydroxy-.beta.-ionone	208	C13H20O2	116296-75-4	12		
4	Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	12		
5	1,4-Dihydro-4-imino-1-(N-methyla...	165	C8H11N3O	1000241-26-0	11		



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ClientSampleId :
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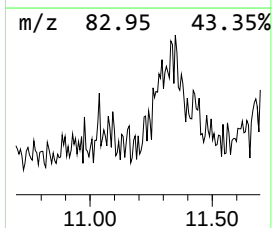
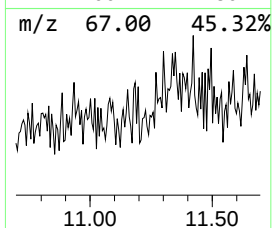
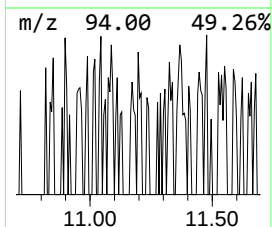
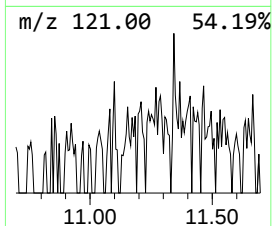
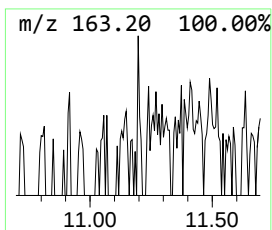
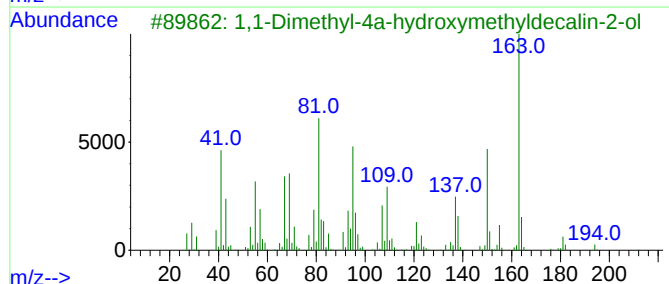
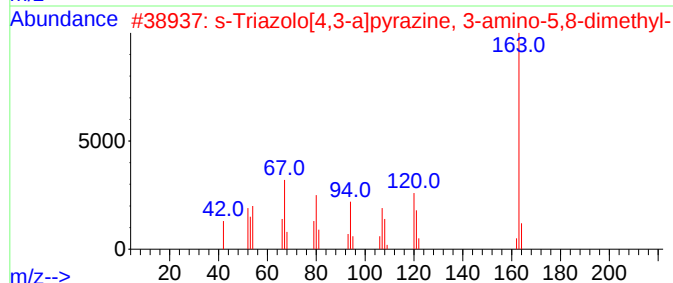
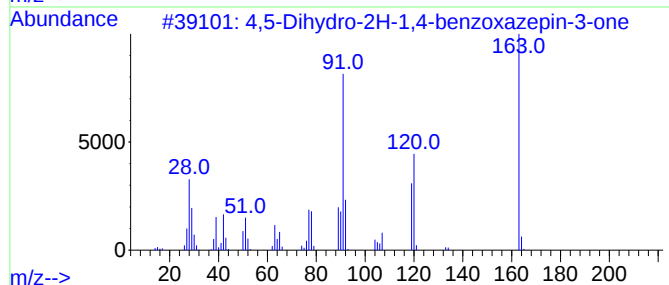
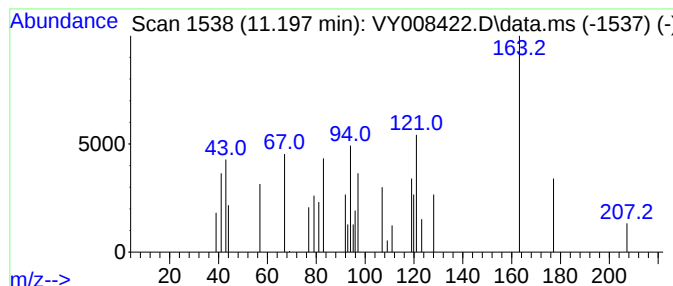
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Quant Title : SW846 8260

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

Peak Number 8 unknown11.197 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.197	11.95 ug/l	1343	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,5-Dihydro-2H-1,4-benzoxazepin-...	163	C9H9NO2	034844-80-9	25
2			s-Triazolo[4,3-a]pyrazine, 3-ami...	163	C7H9N5	019855-02-8	25
3			1,1-Dimethyl-4a-hydroxymethyldec...	212	C13H24O2	1010196-01-9	17
4			2-(Bromomethyl)benzyl alcohol, a...	242	C10H11BrO2	1000364-47-7	12
5			1,4-Methanophthalazine, 1,4,4a,5...	206	C13H22N2	109746-14-7	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042022\
Data File : VY008422.D
Acq On : 20 Apr 2022 16:41
Operator : KP/MD
Sample : N2476-01
Misc : 5.01g/5.0mL/MSVOA_Y/soil
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
PAT-01-041922

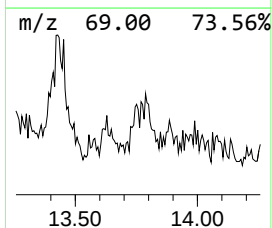
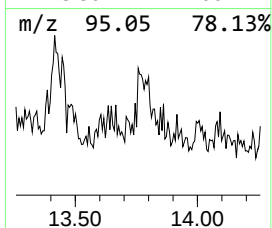
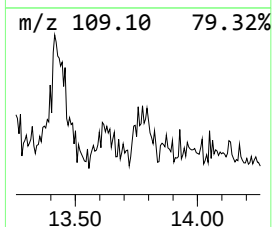
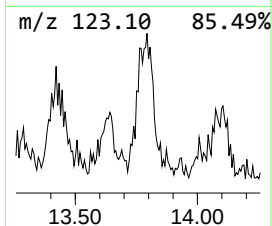
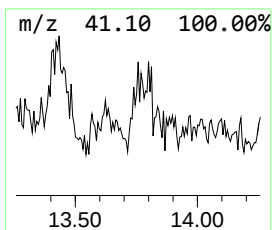
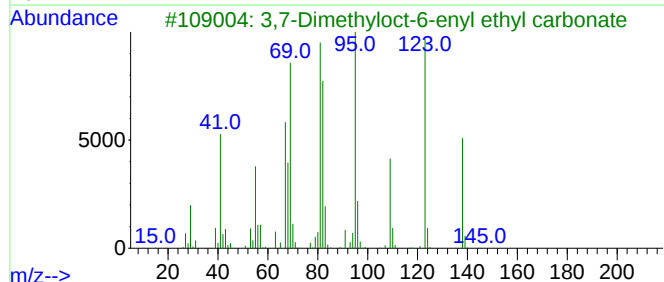
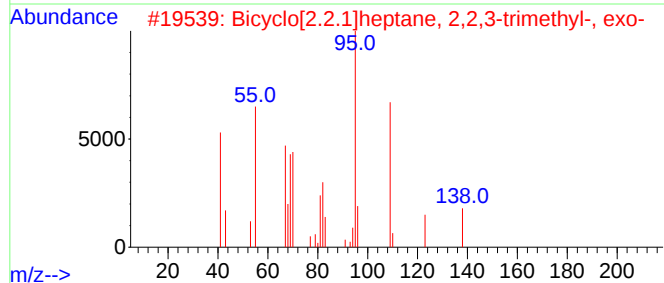
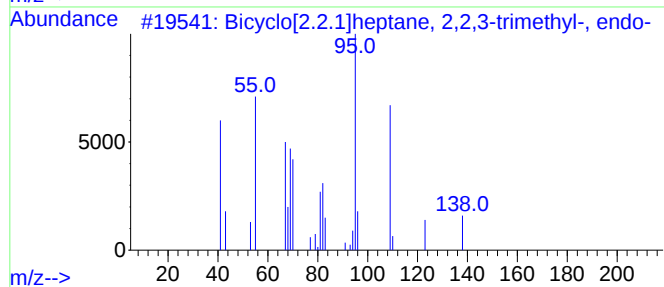
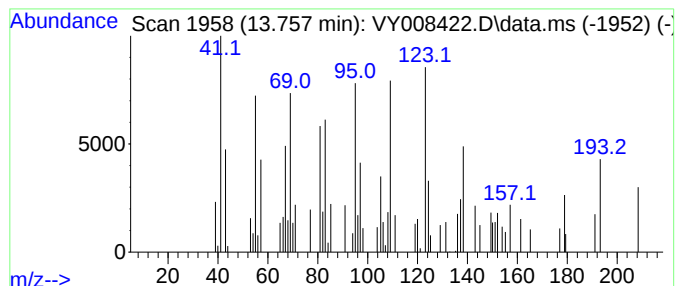
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Quant Title : SW846 8260

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

Peak Number 9 unknown13.757 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	12.91 ug/l	15247	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	46
2			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	46
3			3,7-Dimethyloct-6-enyl ethyl car...	228	C13H24O3	1000373-78-1	43
4			4-Methoxy-o-phenylenediamine	138	C7H10N2O	000102-51-2	27
5			Cyclohexene, 4-methyl-1-(1-methy...	138	C10H18	000500-00-5	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042022\
Data File : VY008422.D
Acq On : 20 Apr 2022 16:41
Operator : KP/MD
Sample : N2476-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
PAT-01-041922

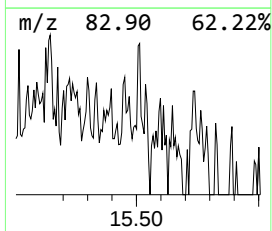
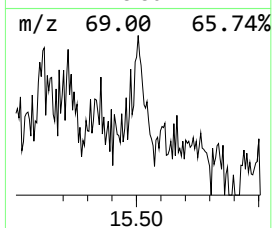
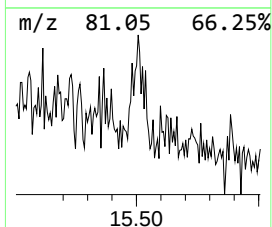
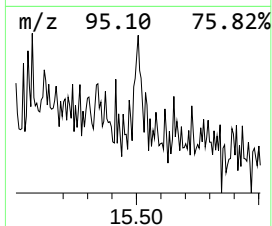
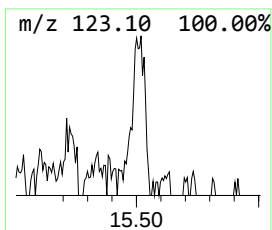
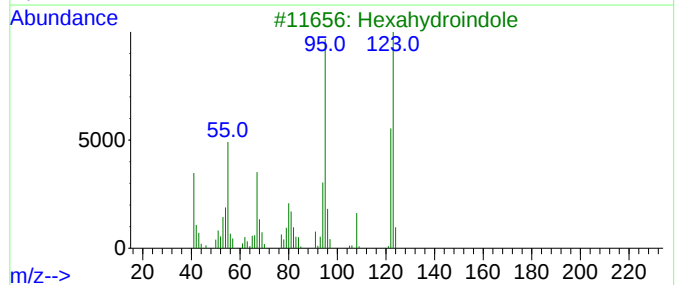
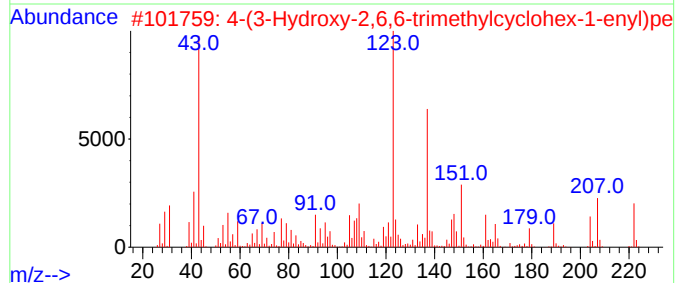
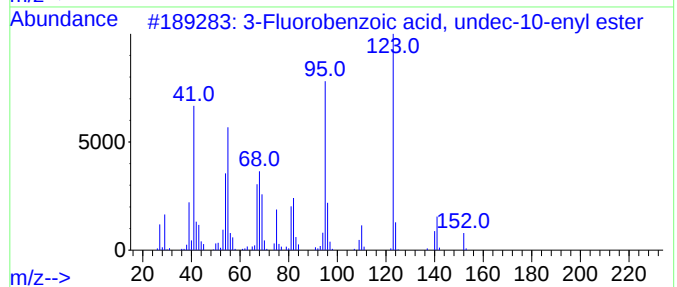
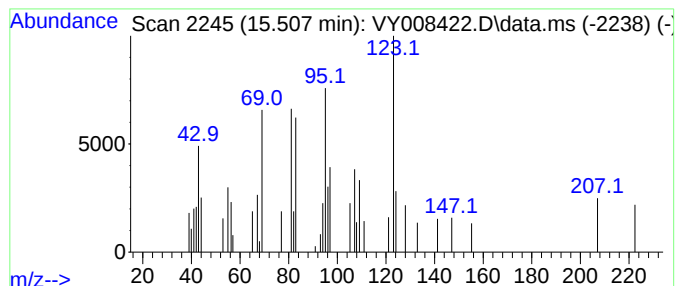
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Quant Title : SW846 8260

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

Peak Number 10 unknown15.507 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.507	9.75 ug/l	11513	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Fluorobenzoic acid, undec-10-e...	292	C18H25F02	1000279-01-2	43
2			4-(3-Hydroxy-2,6,6-trimethylcycl...	222	C14H22O2	097306-57-5	41
3			Hexahydroindole	123	C8H13N	018159-32-5	38
4			3-Fluorobenzoic acid, tetradecyl...	336	C21H33F02	1010279-01-5	37
5			5-Isopropenyl-2-methyl-7-oxabicy...	168	C10H16O2	1000185-00-9	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042022\
Data File : VY008422.D
Acq On : 20 Apr 2022 16:41
Operator : KP/MD
Sample : N2476-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
PAT-01-041922

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y040822S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown9.837	9.837	14.6	ug/l	1222	2	8.697	4174	50.0
unknown9.922	9.922	9.1	ug/l	759	2	8.697	4174	50.0
unknown10.355	10.355	9.7	ug/l	1094	3	11.489	5619	50.0
unknown10.898	10.898	10.9	ug/l	1227	3	11.489	5619	50.0
unknown11.197	11.197	11.9	ug/l	1343	3	11.489	5619	50.0
unknown13.757	13.757	12.9	ug/l	15247	4	13.434	59070	50.0
unknown15.507	15.507	9.8	ug/l	11513	4	13.434	59070	50.0