

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112122\
 Data File : VY011535.D
 Acq On : 21 Nov 2022 19:31
 Operator : KP/MD
 Sample : N5723-01
 Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 OR-3-111822

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\82Y111822S.M
 Title : SW846 8260

Signal : TIC: VY011535.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.881	8	10	14	rVB	518	471	3.36%	0.440%
2	2.064	37	40	43	rVB2	409	551	3.93%	0.515%
3	2.113	43	48	49	rBV3	1100	1755	12.51%	1.640%
4	2.131	49	51	52	rVV	471	315	2.24%	0.294%
5	2.333	81	84	87	rBV2	247	341	2.43%	0.319%
6	2.491	108	110	114	rBV2	377	413	2.94%	0.386%
7	2.637	132	134	135	rBV	341	329	2.34%	0.308%
8	2.924	180	181	184	rVB2	358	261	1.86%	0.244%
9	3.034	196	199	200	rBV	328	281	2.00%	0.263%
10	3.156	216	219	222	rVB	297	421	3.00%	0.394%
11	3.497	272	275	278	rBV2	265	316	2.25%	0.295%
12	3.765	316	319	321	rVB2	215	257	1.83%	0.240%
13	3.942	347	348	352	rBV2	403	377	2.69%	0.352%
14	4.046	363	365	367	rVB	347	255	1.82%	0.238%
15	4.113	374	376	379	rVB2	239	252	1.80%	0.236%
16	4.180	385	387	389	rBV2	281	270	1.92%	0.252%
17	4.363	415	417	420	rBV2	211	272	1.94%	0.254%
18	4.478	435	436	439	rVB2	344	249	1.77%	0.233%
19	4.710	470	474	475	rBV2	597	814	5.80%	0.761%
20	4.789	482	487	488	rBV	282	284	2.02%	0.265%
21	4.887	501	503	505	rBV	270	273	1.95%	0.255%
22	5.222	556	558	561	rBV	448	262	1.87%	0.245%
23	5.405	586	588	590	rBV2	341	386	2.75%	0.361%
24	5.436	592	593	597	rVB2	300	262	1.87%	0.245%
25	5.606	620	621	625	rVB2	207	282	2.01%	0.264%
26	5.838	656	659	661	rVB2	200	249	1.77%	0.233%
27	6.198	713	718	721	rBV2	208	364	2.59%	0.340%
28	6.240	723	725	729	rBV2	270	337	2.40%	0.315%
29	6.405	749	752	753	rBV2	308	271	1.93%	0.253%
30	6.582	775	781	782	rBV2	249	391	2.79%	0.365%
31	6.655	790	793	795	rVV2	204	255	1.82%	0.238%
32	6.966	842	844	848	rBV3	277	338	2.41%	0.316%
33	7.222	882	886	889	rVV2	219	284	2.02%	0.265%
34	7.258	889	892	896	rVB2	155	266	1.90%	0.249%
35	7.344	903	906	908	rBV2	263	311	2.22%	0.291%
36	7.484	925	929	930	rBV2	271	357	2.54%	0.334%

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37	7.716	960	967	973	rBV5	1168	2730	19.46%	2.552%
38	7.795	973	980	986	rVB2	3578	7294	51.98%	6.818%
39	8.149	1032	1038	1044	rVB4	2619	5454	38.87%	5.098%
40	8.277	1057	1059	1062	rBV2	259	257	1.83%	0.240%
41	8.344	1065	1070	1071	rBV2	260	368	2.62%	0.344%
42	8.435	1082	1085	1088	rVB2	312	312	2.22%	0.292%
43	8.691	1120	1127	1135	rBV3	5381	10148	72.32%	9.486%
44	8.874	1151	1157	1158	rBV	348	402	2.86%	0.376%
45	8.917	1161	1164	1166	rBV	501	449	3.20%	0.420%
46	9.282	1223	1224	1228	rVB2	272	285	2.03%	0.266%
47	9.545	1265	1267	1270	rVB	270	256	1.82%	0.239%
48	9.837	1313	1315	1319	rVB2	291	340	2.42%	0.318%
49	10.038	1344	1348	1350	rBV2	341	333	2.37%	0.311%
50	10.185	1366	1372	1380	rVB2	8296	14032	100.00%	13.116%
51	10.374	1401	1403	1406	rBV2	210	272	1.94%	0.254%
52	10.441	1412	1414	1417	rVB2	255	321	2.29%	0.300%
53	10.599	1438	1440	1441	rVB	445	252	1.80%	0.236%
54	10.624	1443	1444	1446	rBV	362	254	1.81%	0.237%
55	10.929	1491	1494	1495	rBV	465	320	2.28%	0.299%
56	10.947	1495	1497	1501	rVB3	535	577	4.11%	0.539%
57	11.087	1518	1520	1525	rVB4	342	446	3.18%	0.417%
58	11.166	1528	1533	1534	rVB2	428	500	3.56%	0.467%
59	11.215	1539	1541	1545	rVB3	323	379	2.70%	0.354%
60	11.355	1561	1564	1565	rBV	262	250	1.78%	0.234%
61	11.447	1577	1579	1581	rBV	272	328	2.34%	0.307%
62	11.496	1581	1587	1593	rVV	6974	11771	83.89%	11.003%
63	11.556	1595	1597	1599	rVV3	551	478	3.41%	0.447%
64	11.587	1599	1602	1603	rVV3	359	342	2.44%	0.320%
65	11.648	1607	1612	1614	rVB4	501	580	4.13%	0.542%
66	11.691	1617	1619	1620	rBV	410	260	1.85%	0.243%
67	11.709	1620	1622	1624	rVB2	432	344	2.45%	0.322%
68	11.739	1624	1627	1628	rBV2	633	355	2.53%	0.332%
69	11.825	1639	1641	1643	rBV2	277	284	2.02%	0.265%
70	11.995	1668	1669	1671	rVB2	490	259	1.85%	0.242%
71	12.020	1671	1673	1675	rBV3	438	409	2.91%	0.382%
72	12.081	1681	1683	1686	rBV2	360	469	3.34%	0.438%
73	12.123	1689	1690	1693	rBV2	420	364	2.59%	0.340%
74	12.154	1693	1695	1697	rBV3	542	510	3.63%	0.477%
75	12.191	1699	1701	1703	rVB3	473	407	2.90%	0.380%
76	12.386	1732	1733	1735	rVB2	489	259	1.85%	0.242%

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77	12.416	1735	1738	1739	rVB2	542	439	3.13%	0.410%
78	12.440	1739	1742	1743	rBV2	413	281	2.00%	0.263%
79	12.489	1743	1750	1754	rBV5	3889	7211	51.39%	6.740%
80	12.697	1783	1784	1785	rBV	466	277	1.97%	0.259%
81	12.800	1798	1801	1802	rBV3	625	705	5.02%	0.659%
82	12.855	1808	1810	1813	rBV4	675	869	6.19%	0.812%
83	12.904	1817	1818	1824	rBV4	625	1271	9.06%	1.188%
84	13.020	1835	1837	1839	rBV3	485	571	4.07%	0.534%
85	13.081	1845	1847	1848	rBV2	481	316	2.25%	0.295%
86	13.190	1861	1865	1866	rBV4	912	911	6.49%	0.852%
87	13.434	1900	1905	1909	rVB6	2884	5431	38.70%	5.076%
88	13.946	1987	1989	1991	rBV3	897	591	4.21%	0.552%
89	14.087	2010	2012	2015	rBV4	811	981	6.99%	0.917%
90	14.788	2125	2127	2129	rBV3	685	359	2.56%	0.336%
91	15.068	2171	2173	2175	rBV3	956	774	5.52%	0.723%
92	15.348	2216	2219	2226	rBV9	934	1712	12.20%	1.600%
93	15.495	2241	2243	2247	rBV5	1252	2011	14.33%	1.880%
94	15.867	2302	2304	2306	rBV3	844	801	5.71%	0.749%
95	16.165	2350	2353	2355	rVB4	1021	1147	8.17%	1.072%
96	16.202	2355	2359	2360	rBV3	1070	1198	8.54%	1.120%
97	16.220	2360	2362	2364	rBV3	487	429	3.06%	0.401%
98	16.330	2378	2380	2382	rVB	991	621	4.43%	0.580%
99	16.458	2400	2401	2403	rBV2	576	512	3.65%	0.479%
100	16.556	2415	2417	2420	rBV4	449	544	3.88%	0.508%

Sum of corrected areas: 106984

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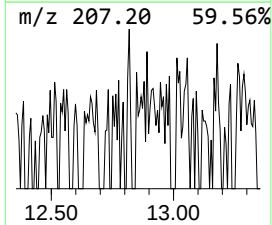
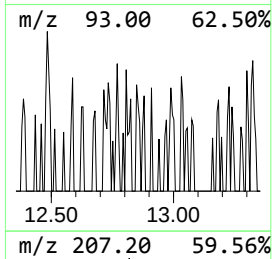
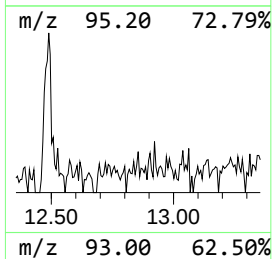
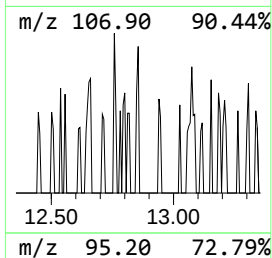
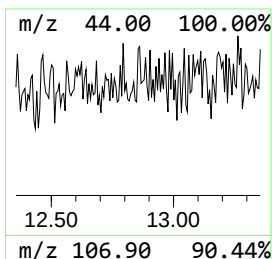
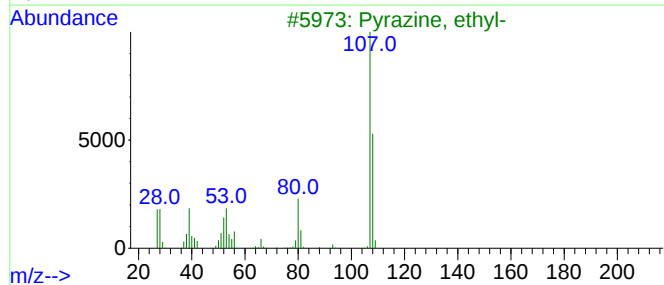
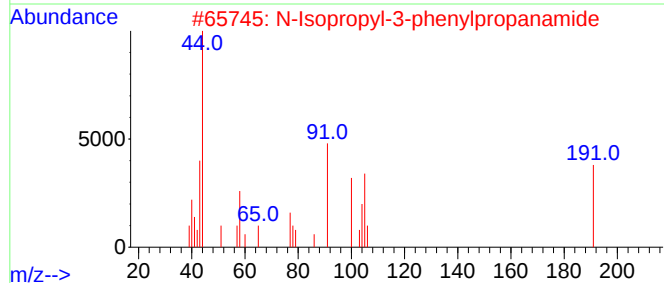
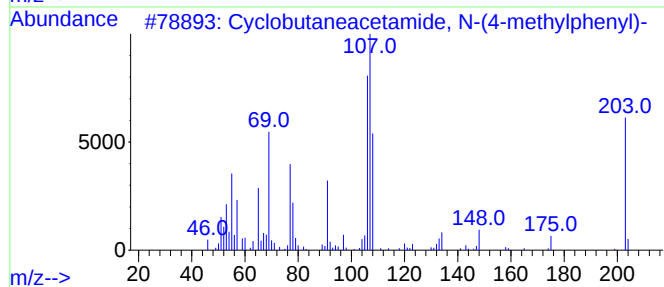
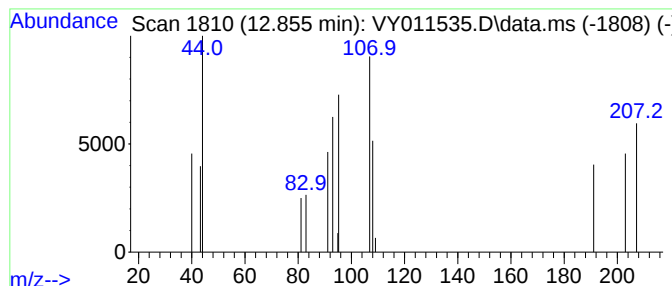
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111822S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.855 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.855	8.00 ug/l	869	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutaneacetamide, N-(4-methy...	203	C13H17NO	302567-77-7	16
2			N-Isopropyl-3-phenylpropanamide	191	C12H17NO	056146-87-3	9
3			Pyrazine, ethyl-	108	C6H8N2	013925-00-3	9
4			Cyclohexane,ethenylidene-	108	C8H12	005664-20-0	9
5			Tricyclo[2.2.2.0(1,4)]octane	108	C8H12	036120-88-4	9



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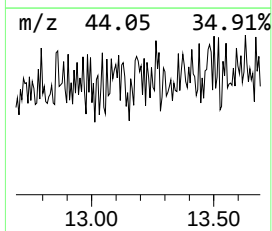
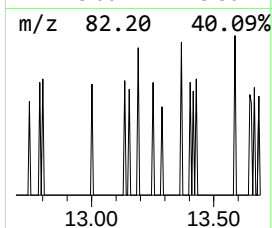
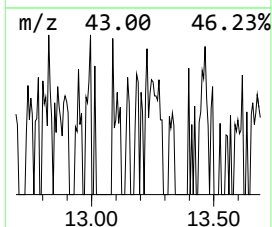
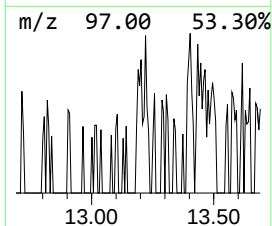
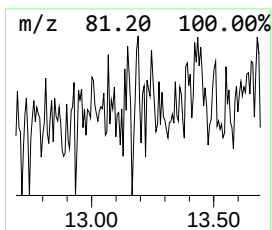
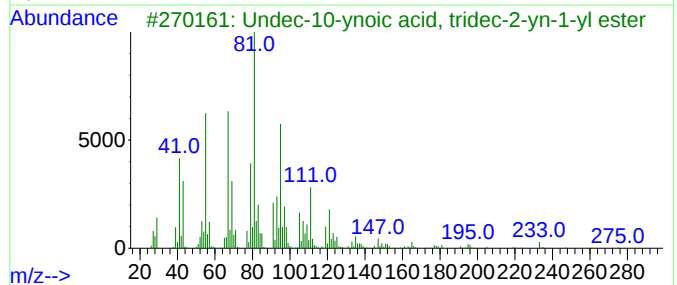
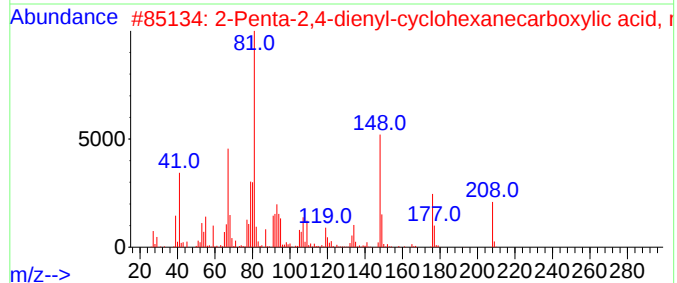
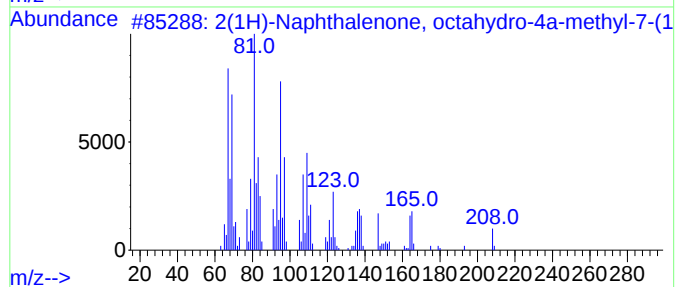
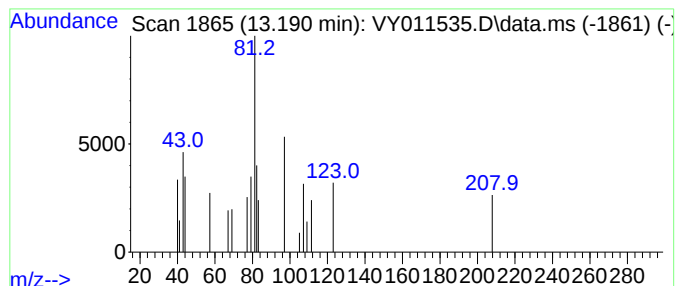
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111822S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown13.190 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.190	8.39 ug/l	911	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, octahydro-4...	208	C14H24O	054594-42-2	40		
2	2-Penta-2,4-dienyl-cyclohexaneca...	208	C13H20O2	1000194-96-2	35		
3	Undec-10-ynoic acid, tridec-2-yn...	360	C24H40O2	1000406-96-9	28		
4	3,6-Octadienal, 3,7-dimethyl-	152	C10H16O	055722-59-3	23		
5	1H-Pyrrole, 1-butyl-	123	C8H13N	000589-33-3	9		



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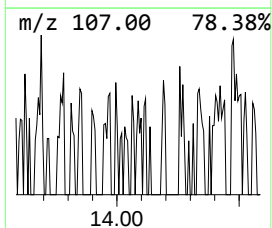
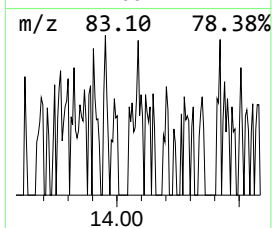
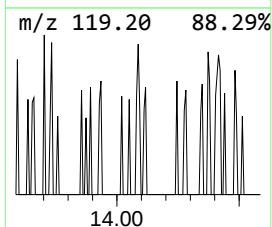
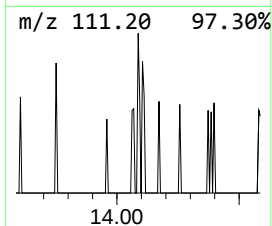
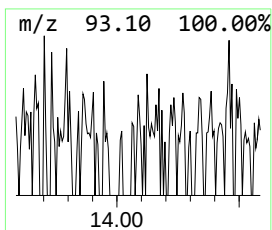
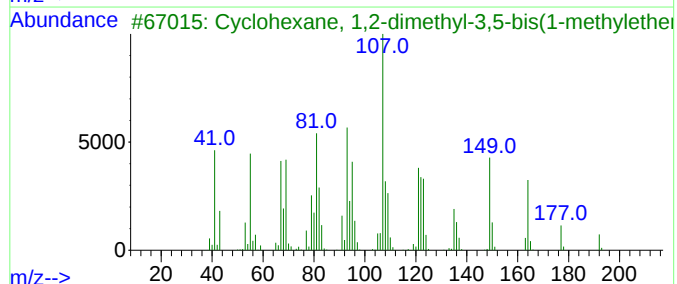
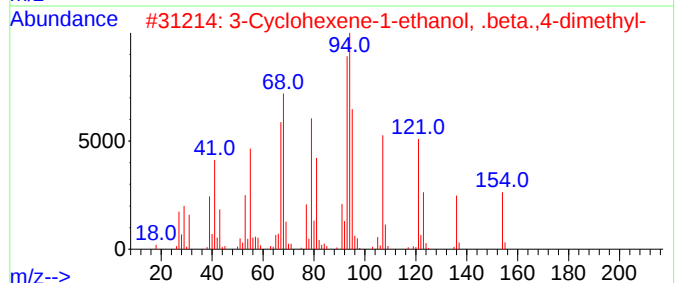
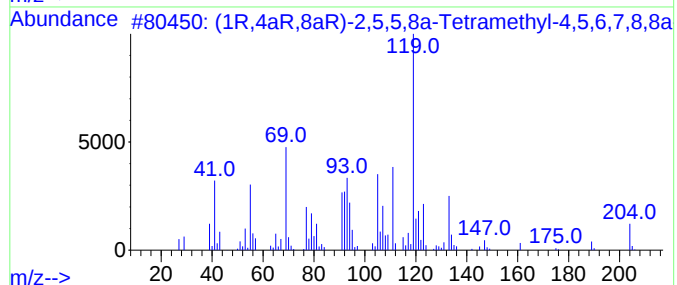
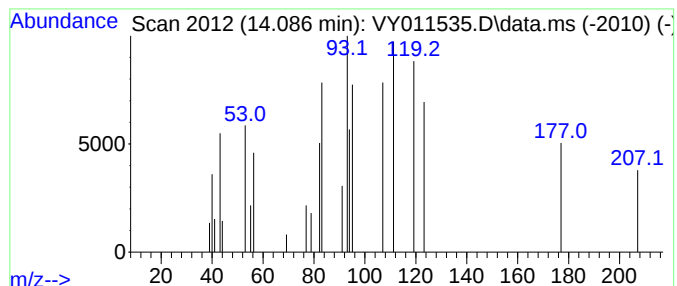
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111822S.M
Quant Title : SW846 8260

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

Peak Number 5 unknown14.086 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	9.03 ug/l	981	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1R,4aR,8aR)-2,5,5,8a-Tetramethy...	204	C15H24	079562-96-2	12
2			3-Cyclohexene-1-ethanol, .beta.,...	154	C10H18O	018479-68-0	10
3			Cyclohexane, 1,2-dimethyl-3,5-bi...	192	C14H24	074806-55-6	10
4			3-Cyclohexene-1-ethanol, .beta.,...	154	C10H18O	013835-75-1	10
5			N-Hydroxy-4-pyridone	111	C5H5NO2	1010426-43-6	9



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OR-3-111822

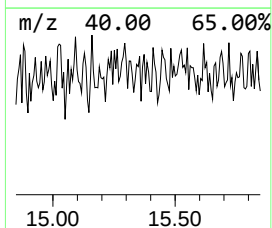
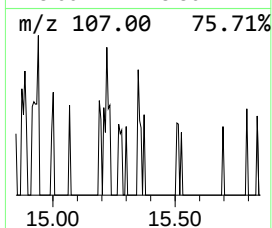
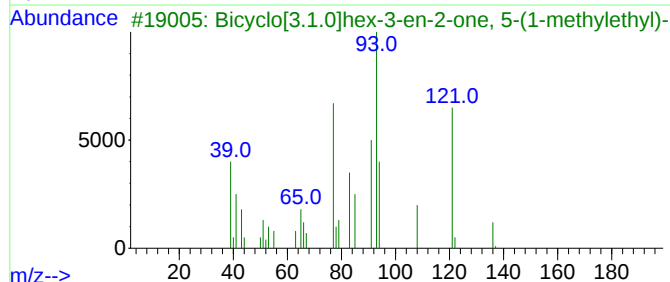
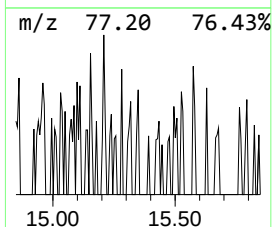
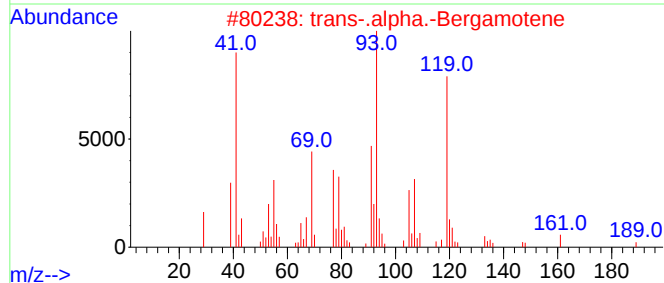
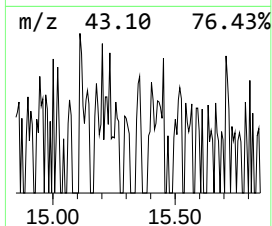
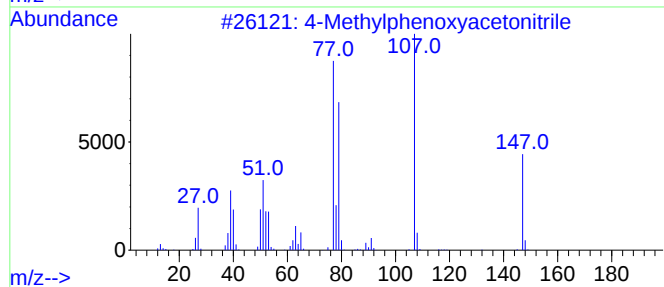
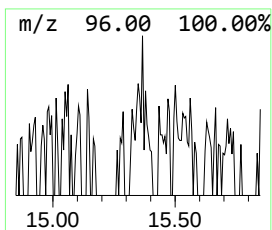
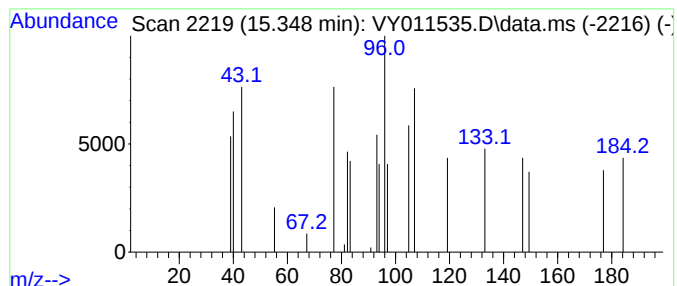
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Quant Title : SW846 8260

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

Peak Number 6 unknown15.349 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.349	15.76 ug/l	1712	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methylphenoxyacetonitrile	147	C9H9NO	033901-44-9	16
2			trans-.alpha.-Bergamotene	204	C15H24	013474-59-4	9
3			Bicyclo[3.1.0]hex-3-en-2-one, 5-...	136	C9H12O	036262-12-1	9
4			(4R,5S)-(+)-4-Methyl-5-phenyl-2-...	177	C10H11NO2	077943-39-6	7
5			2-Oxazolidinone, 4-methyl-5-phen...	177	C10H11NO2	028044-22-6	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112122\
Data File : VY011535.D
Acq On : 21 Nov 2022 19:31
Operator : KP/MD
Sample : N5723-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
OR-3-111822

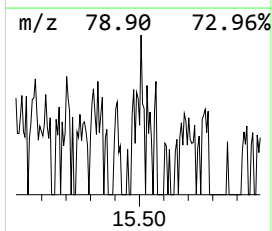
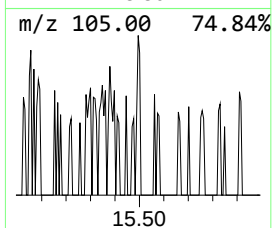
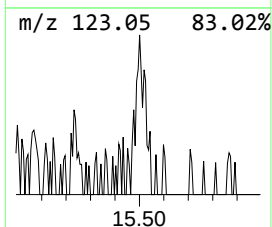
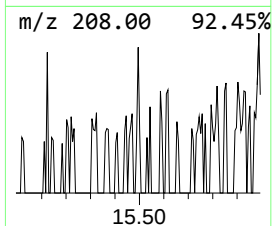
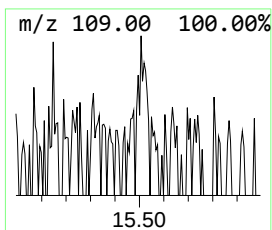
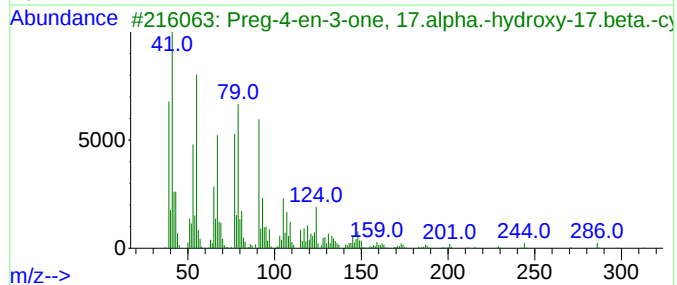
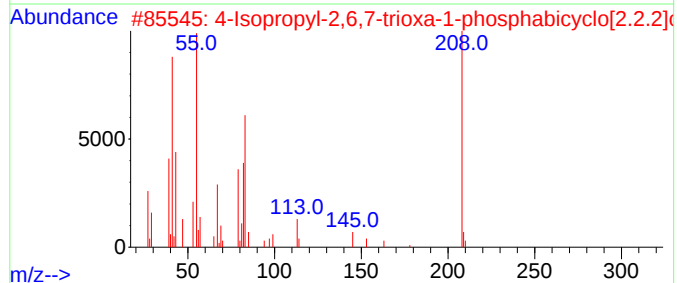
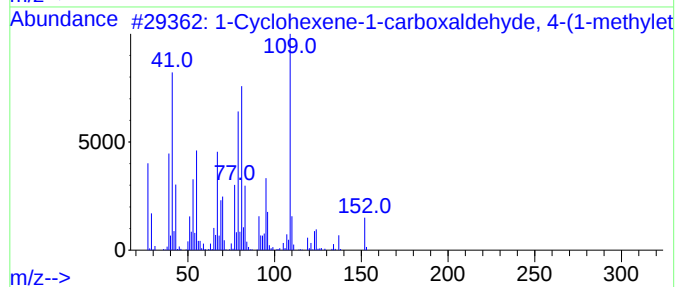
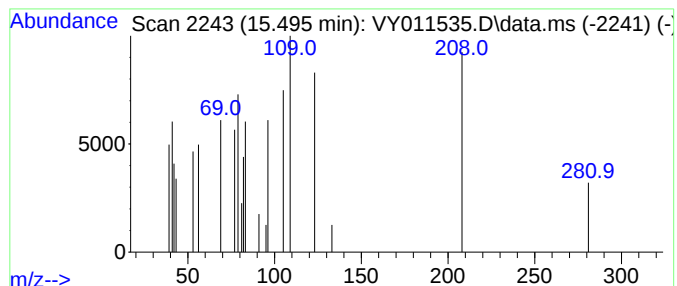
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Quant Title : SW846 8260

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

Peak Number 7 unknown15.495 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.495	18.51 ug/l	2011	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	021391-98-0	23
2			4-Isopropyl-2,6,7-trioxa-1-phosp...	208	C7H13O3PS	051486-56-7	14
3			Preg-4-en-3-one, 17.alpha.-hydro...	313	C20H27NO2	1000294-64-4	12
4			2,3-Hexadiene, 2-methyl-	96	C7H12	029212-09-7	12
5			1,8-Cyclopentadecadiyne	202	C15H22	004722-42-3	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112122\
Data File : VY011535.D
Acq On : 21 Nov 2022 19:31
Operator : KP/MD
Sample : N5723-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
OR-3-111822

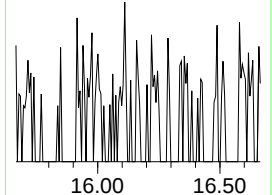
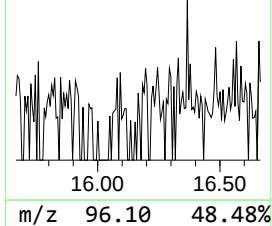
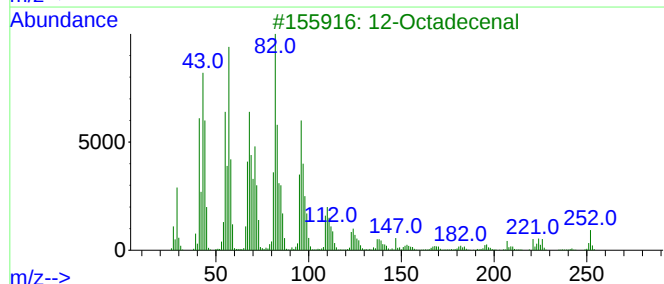
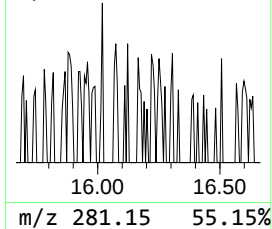
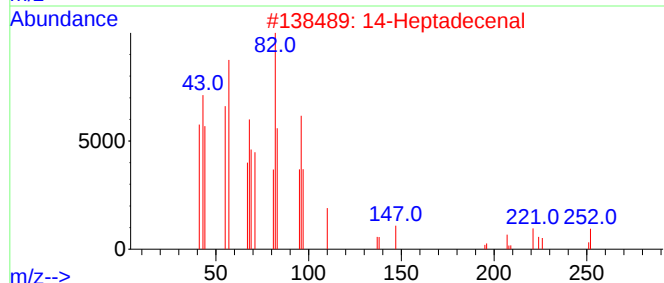
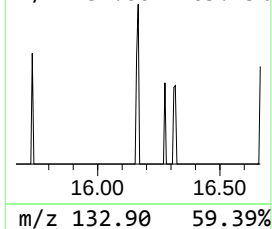
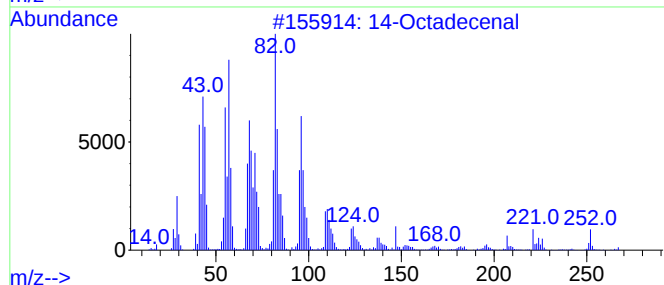
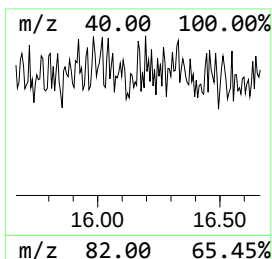
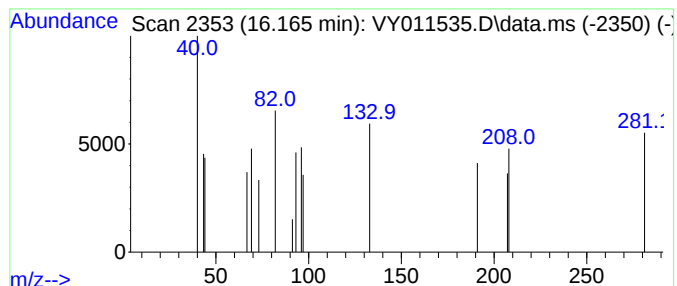
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Quant Title : SW846 8260

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

Peak Number 9 unknown16.165 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.165	10.56 ug/l	1147	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			14-Octadecenal	266	C18H34O	056554-89-3	14
2			14-Heptadecenal	252	C17H32O	1010144-58-0	14
3			12-Octadecenal	266	C18H34O	056554-91-7	14
4			3-[(3-Hydroxyphenyl)amino]-2-nit...	208	C9H8N2O4	1000410-94-8	12
5			Ecgonine	185	C9H15NO3	000481-37-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112122\
Data File : VY011535.D
Acq On : 21 Nov 2022 19:31
Operator : KP/MD
Sample : N5723-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
OR-3-111822

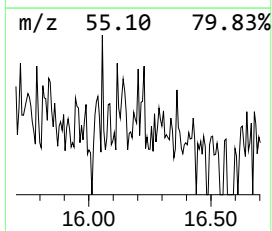
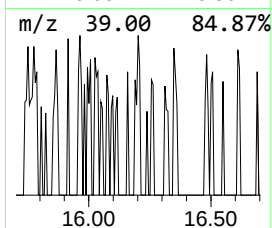
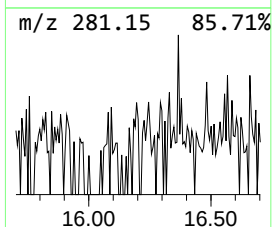
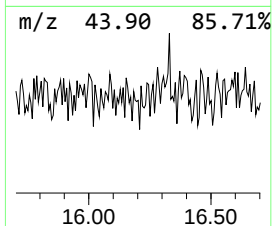
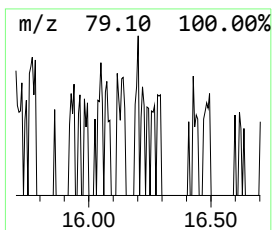
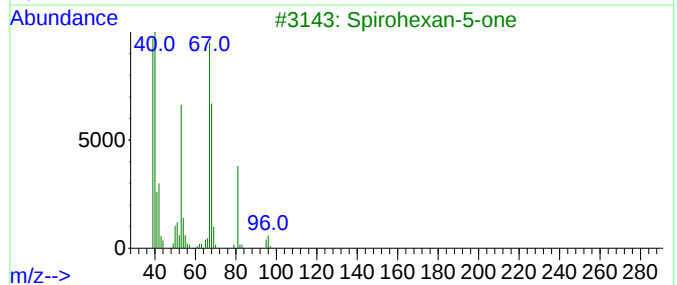
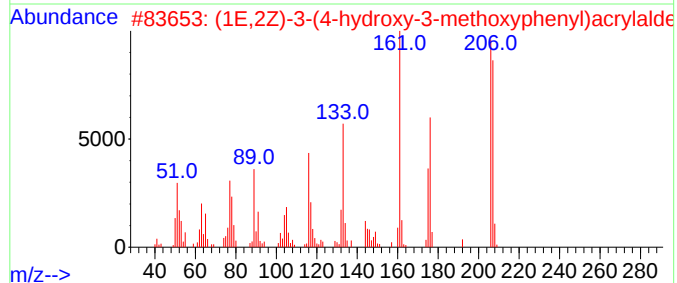
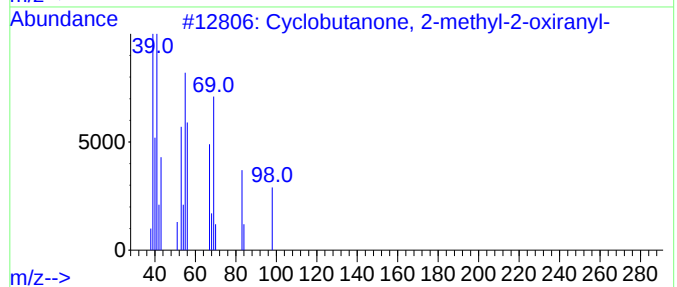
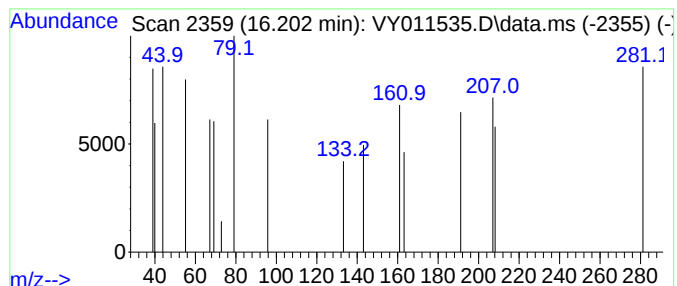
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Quant Title : SW846 8260

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

Peak Number 10 unknown16.202 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.202	11.03 ug/l	1198	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutanone, 2-methyl-2-oxiranyl-	126	C7H10O2	075314-19-1	25
2			(1E,2Z)-3-(4-hydroxy-3-methoxyph...	207	C11H13NO3	1000451-81-6	10
3			Spirohexan-5-one	96	C6H8O	020061-22-7	9
4			Cyclobutane, methylene-	68	C5H8	001120-56-5	9
5			Cyclopropanecarboxanilide, 3',4'...	229	C10H9C12NO	002759-71-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112122\
Data File : VY011535.D
Acq On : 21 Nov 2022 19:31
Operator : KP/MD
Sample : N5723-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
OR-3-111822

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111822S.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
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unknown13.190	13.190	8.4	ug/l	911	4	13.428	5431	50.0
unknown14.086	14.086	9.0	ug/l	981	4	13.428	5431	50.0
unknown15.349	15.349	15.8	ug/l	1712	4	13.428	5431	50.0
unknown15.495	15.495	18.5	ug/l	2011	4	13.428	5431	50.0
unknown16.165	16.165	10.6	ug/l	1147	4	13.428	5431	50.0
unknown16.202	16.202	11.0	ug/l	1198	4	13.428	5431	50.0