

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112321\
 Data File : VY006871.D
 Acq On : 23 Nov 2021 16:31
 Operator : SY/MD
 Sample : M4818-01
 Misc : 5.00G/5ML/MSVOA_Y/SOIL
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 TR-04-112321

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\82Y111521S.M
 Title : SW846 8260

Signal : TIC: VY006871.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.869	7	8	12	rVB	1307	1404	2.99%	0.388%
2	1.912	12	15	16	rVV	553	603	1.29%	0.167%
3	1.942	18	20	24	rVB2	550	645	1.38%	0.178%
4	2.302	76	79	84	rVB3	533	1015	2.16%	0.281%
5	2.375	87	91	94	rBV3	403	708	1.51%	0.196%
6	3.954	345	350	352	rBV2	361	605	1.29%	0.167%
7	4.210	386	392	394	rBV3	237	474	1.01%	0.131%
8	4.735	469	478	487	rVB5	1524	4674	9.97%	1.292%
9	5.753	638	645	648	rBV3	303	781	1.67%	0.216%
10	6.996	841	849	851	rBV2	403	942	2.01%	0.260%
11	7.728	962	969	975	rVV2	6101	13909	29.66%	3.845%
12	7.795	975	980	991	rVB	10240	22035	46.99%	6.091%
13	8.142	1029	1037	1046	rVB4	8013	19237	41.02%	5.317%
14	8.697	1119	1128	1136	rBV	16685	31484	67.14%	8.703%
15	8.947	1164	1169	1172	rBV3	418	788	1.68%	0.218%
16	9.276	1220	1223	1226	rVV2	434	528	1.13%	0.146%
17	9.337	1230	1233	1237	rBV2	331	689	1.47%	0.190%
18	9.423	1243	1247	1249	rBV3	416	664	1.42%	0.184%
19	9.624	1277	1280	1283	rBV2	385	650	1.39%	0.180%
20	9.667	1283	1287	1291	rVB3	342	638	1.36%	0.176%
21	9.752	1297	1301	1302	rVV3	387	592	1.26%	0.164%
22	9.776	1302	1305	1306	rVB3	500	505	1.08%	0.140%
23	9.856	1315	1318	1319	rVV3	521	496	1.06%	0.137%
24	9.965	1332	1336	1338	rBV3	503	795	1.70%	0.220%
25	10.020	1343	1345	1349	rBV3	447	551	1.18%	0.152%
26	10.093	1353	1357	1359	rVV4	490	661	1.41%	0.183%
27	10.185	1365	1372	1380	rVV	26402	46892	100.00%	12.961%
28	10.331	1393	1396	1399	rBV4	418	534	1.14%	0.148%
29	10.447	1412	1415	1416	rBV3	793	677	1.44%	0.187%
30	10.465	1416	1418	1420	rVV3	462	585	1.25%	0.162%
31	10.581	1436	1437	1441	rVB4	1014	971	2.07%	0.268%
32	10.691	1452	1455	1460	rBV6	704	1611	3.44%	0.445%
33	10.746	1462	1464	1468	rBV4	691	855	1.82%	0.236%
34	10.843	1478	1480	1483	rVB4	575	561	1.20%	0.155%
35	10.868	1483	1484	1488	rBV4	644	700	1.49%	0.193%
36	10.947	1493	1497	1498	rBV4	600	781	1.67%	0.216%

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37	11.038	1509	1512	1513	rBV3	730	777	1.66%	0.215%
38	11.050	1513	1514	1518	rVB4	679	651	1.39%	0.180%
39	11.118	1522	1525	1526	rBV3	905	779	1.66%	0.215%
40	11.154	1526	1531	1532	rBV5	1284	1578	3.37%	0.436%
41	11.203	1535	1539	1542	rBV5	899	1397	2.98%	0.386%
42	11.233	1542	1544	1547	rVV4	908	1197	2.55%	0.331%
43	11.331	1556	1560	1563	rVB6	1492	2282	4.87%	0.631%
44	11.416	1572	1574	1575	rBV2	1025	730	1.56%	0.202%
45	11.496	1581	1587	1595	rBV	24693	41857	89.26%	11.570%
46	11.630	1607	1609	1612	rBV3	514	690	1.47%	0.191%
47	11.758	1626	1630	1633	rBV6	1356	2240	4.78%	0.619%
48	11.813	1637	1639	1640	rBV2	1438	1411	3.01%	0.390%
49	12.002	1664	1670	1672	rBV7	2650	4364	9.31%	1.206%
50	12.209	1700	1704	1706	rVB5	1089	1261	2.69%	0.349%
51	12.227	1706	1707	1708	rBV	1022	492	1.05%	0.136%
52	12.282	1715	1716	1719	rVB3	1438	1084	2.31%	0.300%
53	12.312	1719	1721	1722	rBV2	841	656	1.40%	0.181%
54	12.337	1722	1725	1727	rBV4	1287	1554	3.31%	0.430%
55	12.361	1727	1729	1731	rBV3	1361	1652	3.52%	0.457%
56	12.489	1745	1750	1759	rVB3	22114	40314	85.97%	11.143%
57	12.556	1759	1761	1762	rBV2	1116	654	1.39%	0.181%
58	12.605	1763	1769	1770	rBV6	2795	4408	9.40%	1.218%
59	12.739	1789	1791	1792	rVB2	1151	610	1.30%	0.169%
60	12.855	1808	1810	1811	rBV2	988	592	1.26%	0.164%
61	12.989	1829	1832	1836	rBV6	904	1586	3.38%	0.438%
62	13.026	1836	1838	1840	rVB3	1076	772	1.65%	0.213%
63	13.062	1842	1844	1846	rBV3	1462	1786	3.81%	0.494%
64	13.148	1849	1858	1860	rBV10	3633	8877	18.93%	2.454%
65	13.324	1884	1887	1888	rBV3	1550	1512	3.22%	0.418%
66	13.349	1888	1891	1892	rBV3	3840	3955	8.43%	1.093%
67	13.367	1892	1894	1895	rBV2	2073	1699	3.62%	0.470%
68	13.428	1900	1904	1913	rVB	19681	35425	75.55%	9.792%
69	13.501	1913	1916	1919	rBV5	933	1258	2.68%	0.348%
70	13.532	1919	1921	1922	rBV2	923	597	1.27%	0.165%
71	13.550	1922	1924	1927	rBV4	1364	1934	4.12%	0.535%
72	13.739	1946	1955	1961	rBV4	4176	13445	28.67%	3.716%
73	13.867	1974	1976	1977	rVB2	1070	566	1.21%	0.156%
74	13.965	1990	1992	1998	rBV6	1422	2510	5.35%	0.694%
75	14.263	2037	2041	2042	rVV4	1223	1433	3.06%	0.396%
76	14.282	2042	2044	2049	rVV6	990	1202	2.56%	0.332%

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77	14.330	2050	2052	2056	rVB5	1172	1401	2.99%	0.387%
78	14.410	2063	2065	2067	rBV3	940	1027	2.19%	0.284%
79	14.483	2075	2077	2080	rVB4	649	582	1.24%	0.161%
80	14.513	2080	2082	2084	rVB3	617	537	1.15%	0.148%
81	14.538	2084	2086	2089	rBV4	827	762	1.63%	0.211%
82	14.562	2089	2090	2093	rBV3	543	523	1.12%	0.145%
83	14.647	2102	2104	2107	rVB4	537	580	1.24%	0.160%
84	14.739	2117	2119	2122	rVB3	646	591	1.26%	0.163%
85	15.153	2184	2187	2189	rBV3	460	689	1.47%	0.190%
86	15.647	2266	2268	2274	rVB4	493	599	1.28%	0.166%
87	15.842	2297	2300	2303	rBV2	390	480	1.02%	0.133%
88	15.940	2314	2316	2322	rVB4	277	501	1.07%	0.138%
89	16.367	2382	2386	2389	rBV5	475	725	1.55%	0.200%
90	16.617	2423	2427	2430	rVB5	475	757	1.61%	0.209%

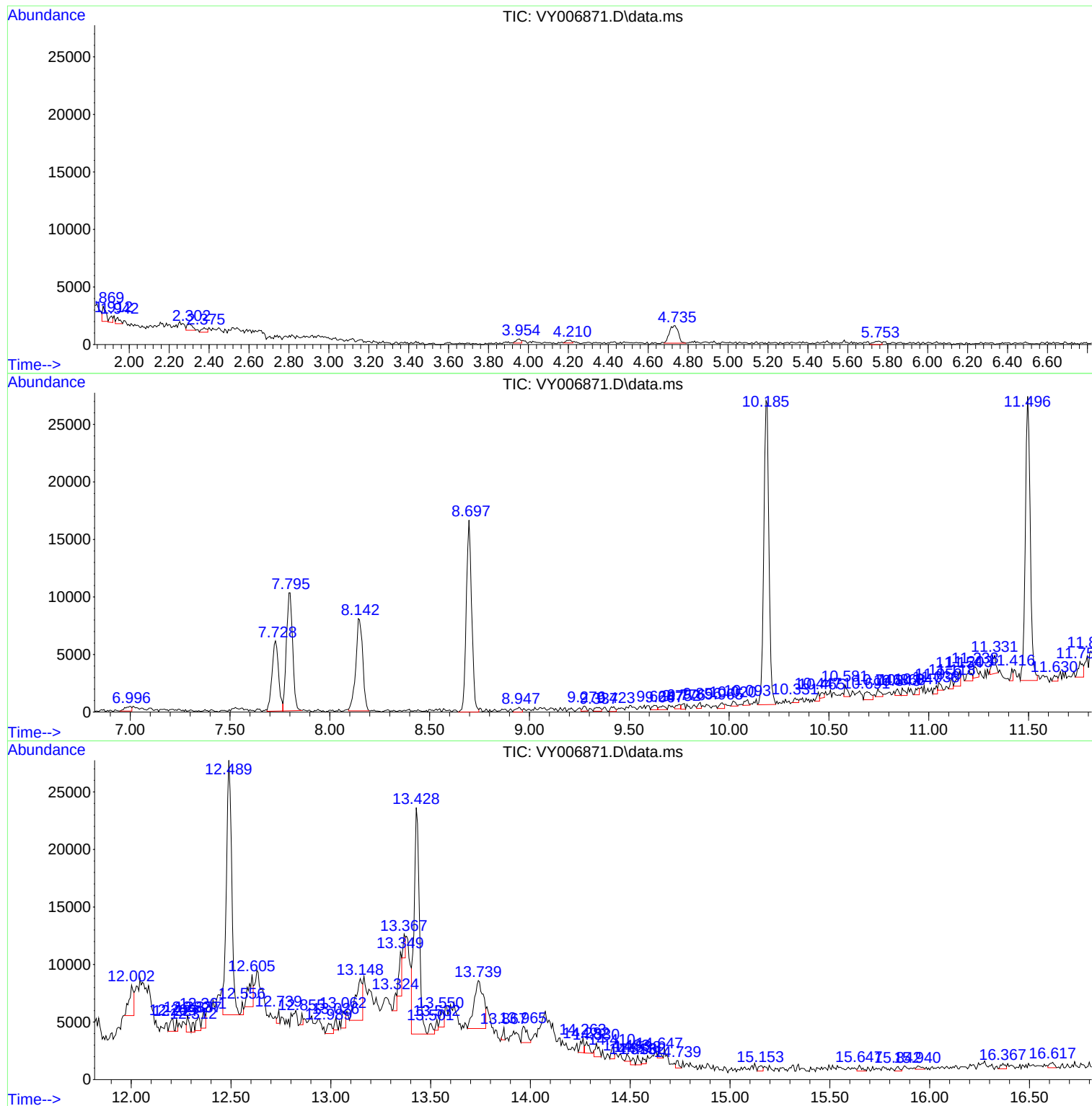
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
Quant Title : SW846 8260

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



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Instrument :
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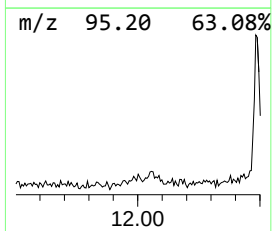
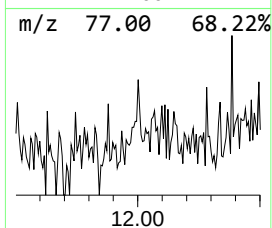
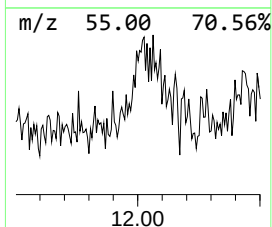
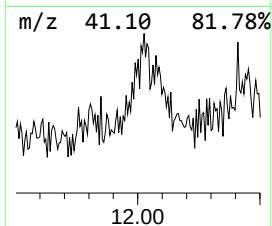
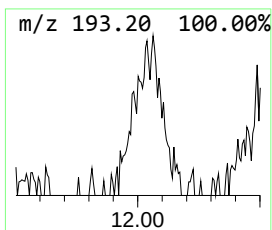
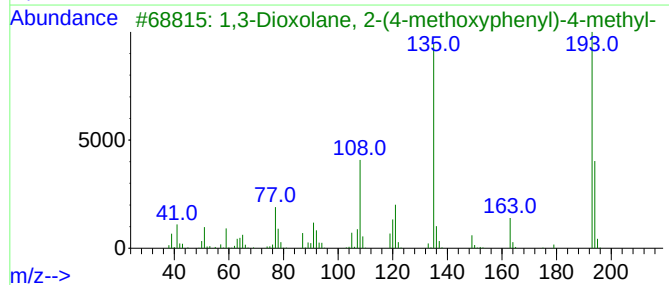
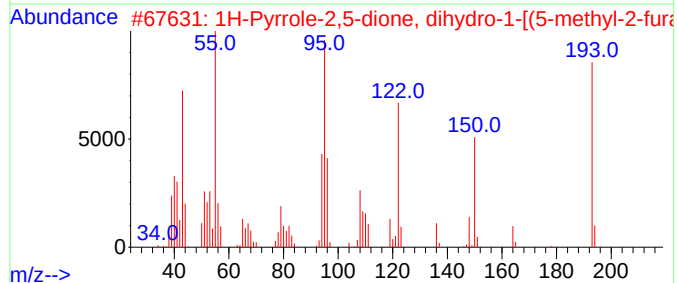
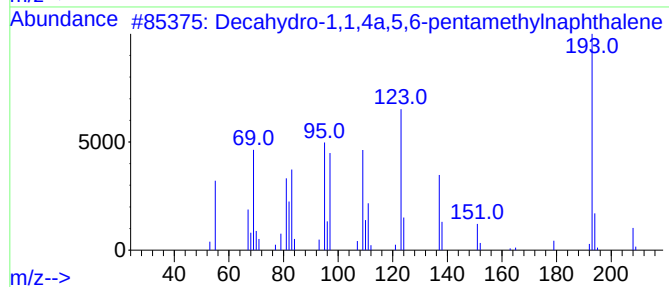
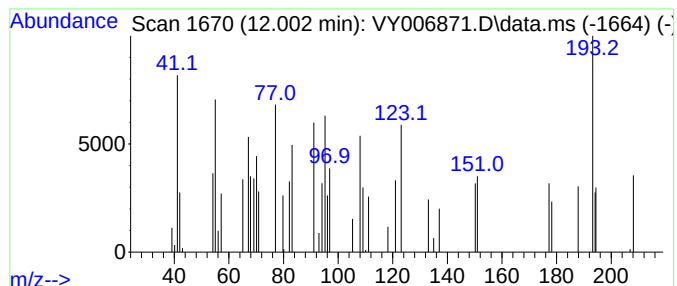
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.002 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.002	5.21 ug/l	4364	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	37
2			1H-Pyrrole-2,5-dione, dihydro-1-...	193	C10H11NO3	1010351-31-4	27
3			1,3-Dioxolane, 2-(4-methoxypheny...	194	C11H14O3	006414-32-0	25
4			5-Isopropenyloxymethylene-3,3-di...	194	C12H18O2	077822-61-8	25
5			2(1H)-Benzocyclooctenone, decahy...	194	C13H22O	055103-66-7	14



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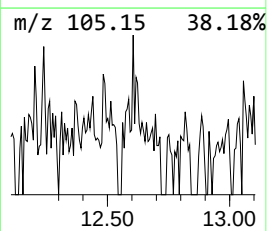
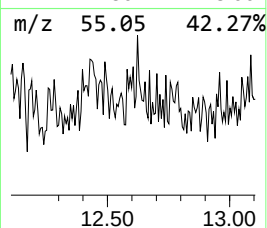
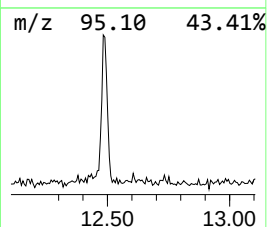
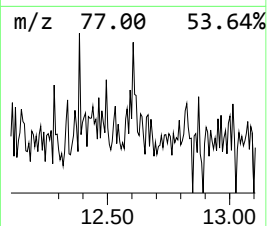
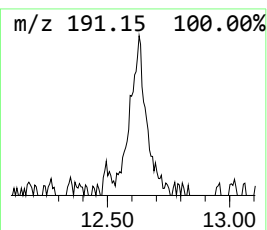
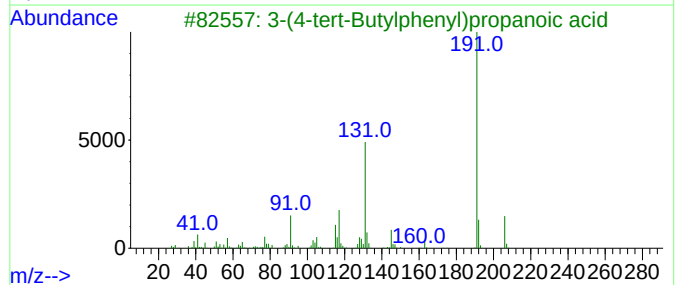
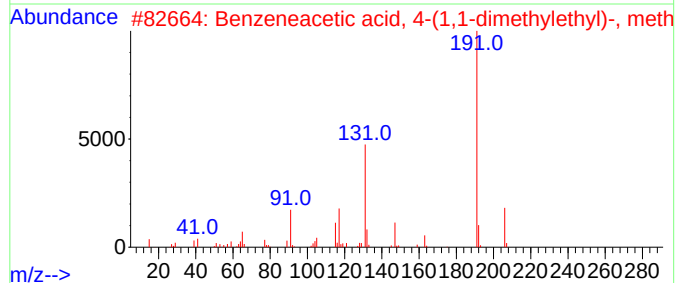
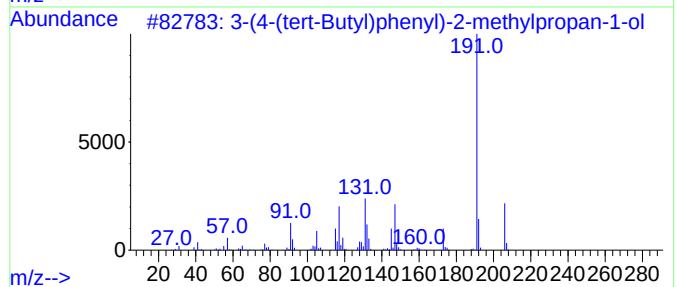
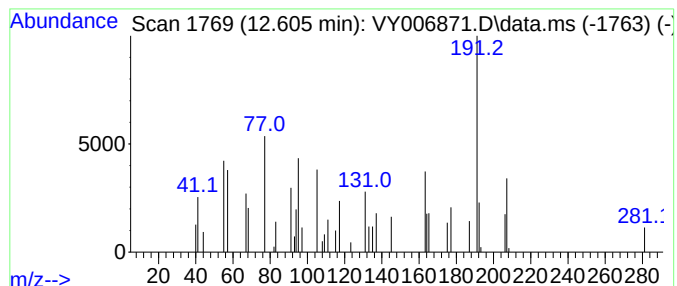
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.605 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.605	6.22 ug/l	4408	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	43		
2	Benzeneacetic acid, 4-(1,1-dimet...	206	C13H18O2	003549-23-3	43		
3	3-(4-tert-Butylphenyl)propanoic ...	206	C13H18O2	001208-64-6	38		
4	Propanoic acid, 2-[4-(1-formylet...	220	C13H16O3	1000161-46-8	35		
5	7-Methoxyindole-2-carboxylic acid	191	C10H9NO3	024610-33-1	35		



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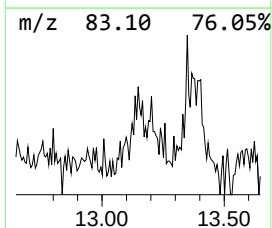
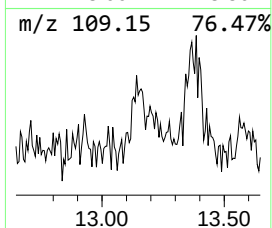
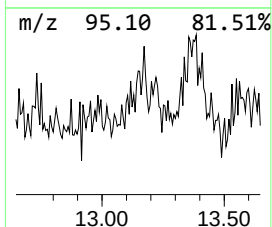
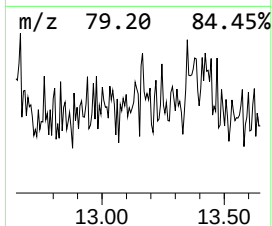
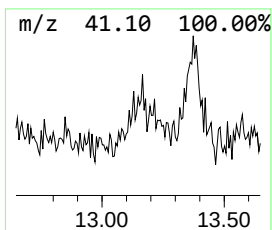
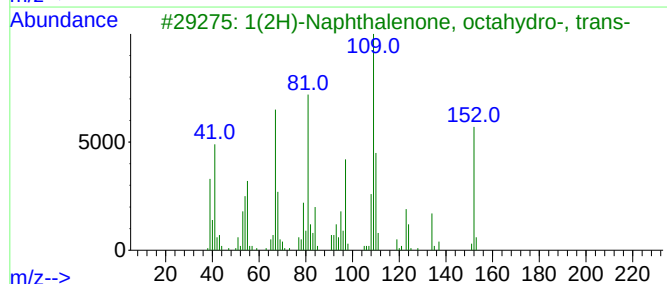
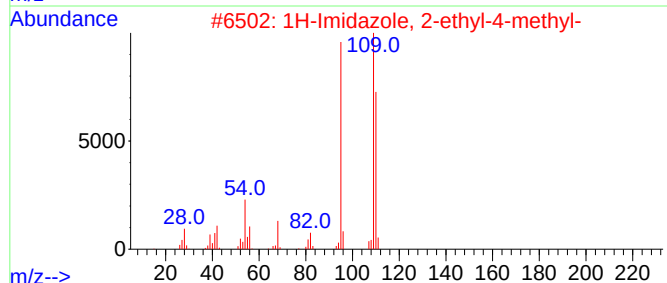
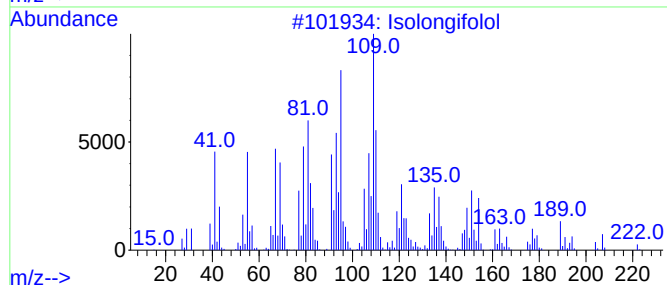
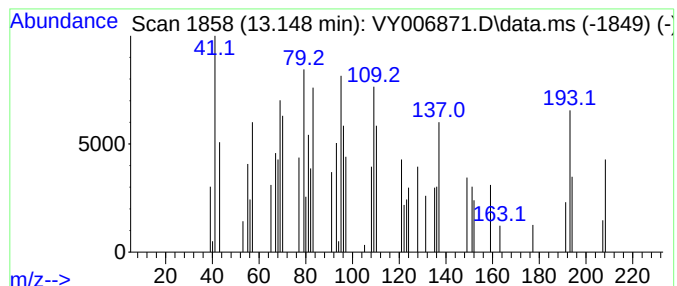
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Quant Title : SW846 8260

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

Peak Number 4 unknown13.148 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.148	12.53 ug/l	8877	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isolongifolol	222	C15H26O	001139-17-9	43
2			1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	000931-36-2	38
3			1(2H)-Naphthalenone, octahydro-,...	152	C10H16O	021370-71-8	25
4			2-Allyl-2-methyl-1,3-cyclopentan...	152	C9H12O2	026828-48-8	25
5			Bicyclo[4.3.0]nonane, 3-methylene-	136	C10H16	1000152-00-6	25



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TR-04-112321

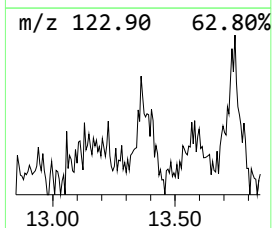
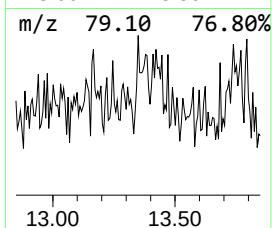
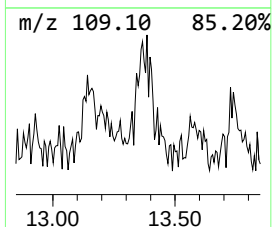
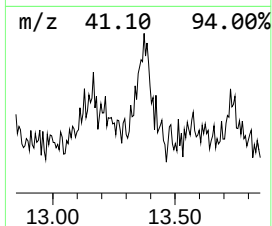
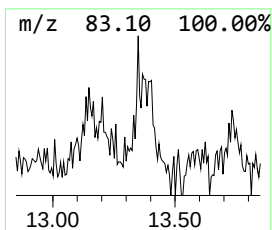
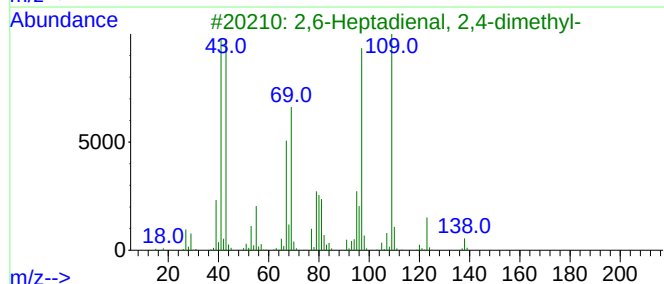
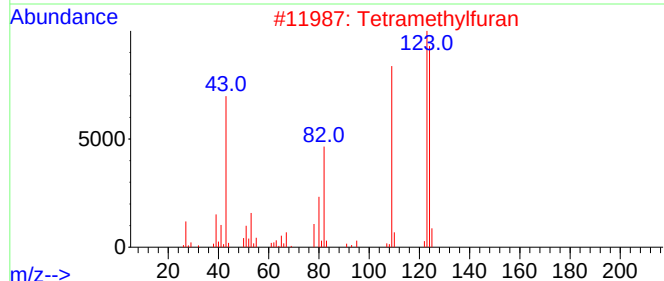
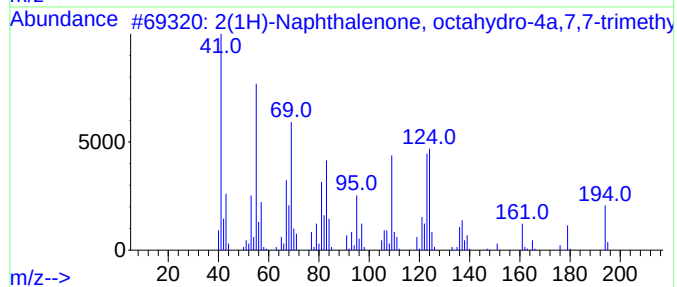
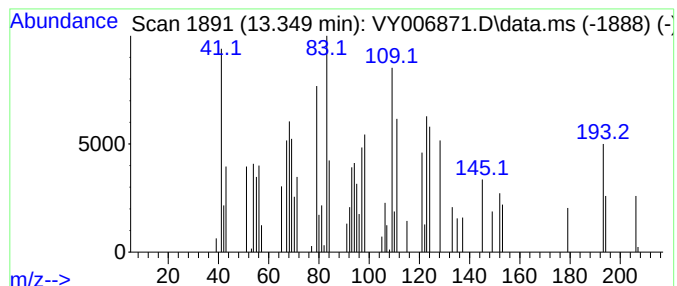
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Quant Title : SW846 8260

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

Peak Number 5 unknown13.349 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.349	5.58 ug/l	3955	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, octahydro-4...	194	C13H22O	007056-56-6	38		
2	Tetramethylfuran	124	C8H12O	010599-58-3	27		
3	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	14		
4	1-[(4-Fluorophenyl)methyl]guanidine	167	C8H10FN3	000459-33-6	14		
5	2,4-Heptadiene, 2,6-dimethyl-	124	C9H16	004634-87-1	14		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112321\
Data File : VY006871.D
Acq On : 23 Nov 2021 16:31
Operator : SY/MD
Sample : M4818-01
Misc : 5.00G/5ML/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TR-04-112321

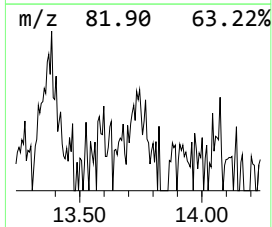
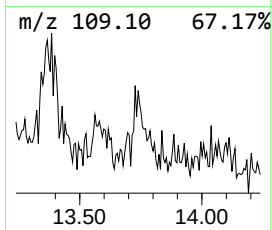
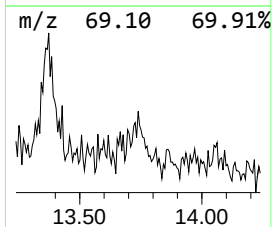
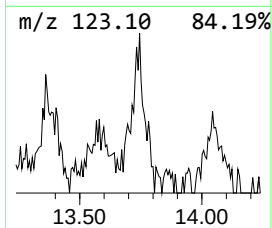
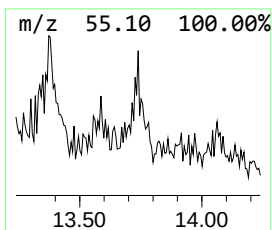
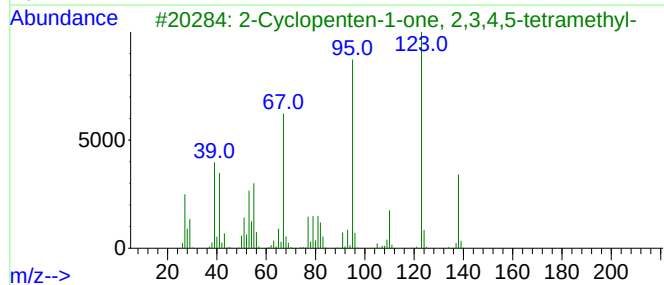
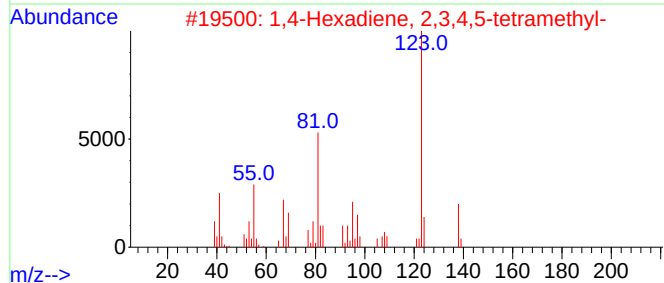
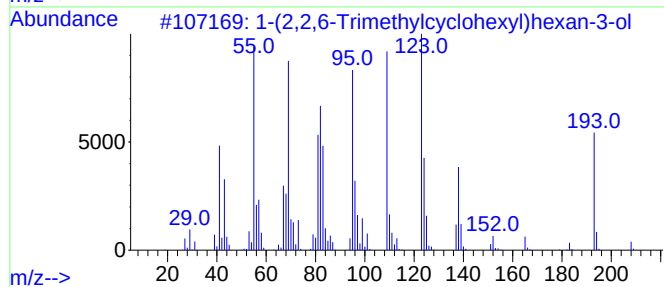
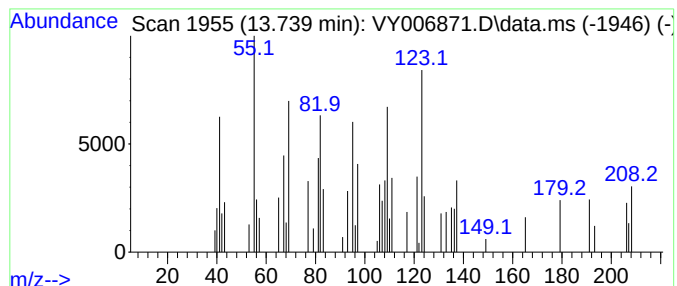
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
Quant Title : SW846 8260

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

Peak Number 6 unknown13.739 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	18.98 ug/l	13445	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(2,2,6-Trimethylcyclohexyl)hex...	226	C15H30O	070788-30-6	43
2			1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	051504-54-2	38
3			2-Cyclopenten-1-one, 2,3,4,5-tet...	138	C9H14O	054458-61-6	22
4			2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	22
5			2H-Cycloprop[c]indene-2,3(3ah)-d...	206	C13H18O2	096678-99-8	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112321\
Data File : VY006871.D
Acq On : 23 Nov 2021 16:31
Operator : SY/MD
Sample : M4818-01
Misc : 5.00G/5ML/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TR-04-112321

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
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
unknown12.002	12.002	5.2	ug/l	4364	3	11.496	41857	50.0
unknown12.605	12.605	6.2	ug/l	4408	4	13.434	35425	50.0
unknown13.148	13.148	12.5	ug/l	8877	4	13.434	35425	50.0
unknown13.349	13.349	5.6	ug/l	3955	4	13.434	35425	50.0
unknown13.739	13.739	19.0	ug/l	13445	4	13.434	35425	50.0