

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY030323\
 Data File : VY012793.D
 Acq On : 03 Mar 2023 14:11
 Operator : KP/MD
 Sample : 01760-01RE
 Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 RBR200058RE

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\82Y030223S.M
 Title : SW846 8260

Signal : TIC: VY012793.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.217	63	65	67	rVB3	321	283	1.56%	0.204%
2	2.241	67	69	72	rBV2	232	228	1.26%	0.165%
3	2.296	76	78	79	rBV2	256	225	1.24%	0.163%
4	2.546	117	119	123	rBV3	231	331	1.83%	0.239%
5	2.698	142	144	146	rVB	284	229	1.26%	0.165%
6	2.985	187	191	193	rBV2	207	316	1.74%	0.228%
7	3.003	193	194	198	rVB	330	255	1.41%	0.184%
8	3.308	241	244	249	rBV	141	279	1.54%	0.202%
9	3.540	278	282	285	rBV2	153	239	1.32%	0.173%
10	4.399	419	423	425	rVB	215	288	1.59%	0.208%
11	4.430	425	428	431	rBV2	123	218	1.20%	0.158%
12	4.692	467	471	472	rBV	307	397	2.19%	0.287%
13	4.960	514	515	519	rVB	280	216	1.19%	0.156%
14	5.015	519	524	525	rBV2	196	307	1.69%	0.222%
15	5.265	562	565	567	rBV2	161	224	1.24%	0.162%
16	5.942	673	676	678	rBV2	257	307	1.69%	0.222%
17	6.234	722	724	727	rBV	236	305	1.68%	0.220%
18	6.436	756	757	761	rBV	191	245	1.35%	0.177%
19	6.746	805	808	812	rBV2	222	288	1.59%	0.208%
20	6.820	816	820	821	rBV	180	209	1.15%	0.151%
21	6.942	838	840	841	rBV2	263	220	1.21%	0.159%
22	6.966	841	844	846	rBV2	595	826	4.55%	0.597%
23	7.222	882	886	887	rBV	226	244	1.35%	0.176%
24	7.265	890	893	896	rBV2	184	259	1.43%	0.187%
25	7.454	918	924	925	rBV	150	251	1.38%	0.181%
26	7.490	925	930	931	rBV	205	237	1.31%	0.171%
27	7.594	944	947	949	rVB	193	227	1.25%	0.164%
28	7.722	959	968	973	rBV3	4269	10398	57.33%	7.513%
29	7.789	973	979	989	rVB	4995	9892	54.54%	7.147%
30	7.996	1011	1013	1016	rBV2	220	308	1.70%	0.223%
31	8.143	1030	1037	1047	rBV	5151	10759	59.32%	7.774%
32	8.307	1060	1064	1069	rVB2	153	293	1.62%	0.212%
33	8.691	1119	1127	1134	rBV	6968	13469	74.27%	9.732%
34	8.892	1158	1160	1163	rVB2	206	247	1.36%	0.178%
35	8.917	1163	1164	1167	rBV	257	258	1.42%	0.186%
36	9.148	1199	1202	1206	rBV	138	207	1.14%	0.150%

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37	9.722	1295	1296	1302	rVB	204	239	1.32%	0.173%
38	9.783	1302	1306	1309	rBV2	199	287	1.58%	0.207%
39	10.185	1366	1372	1378	rVB	10563	18136	100.00%	13.104%
40	10.886	1484	1487	1490	rBV	209	227	1.25%	0.164%
41	11.355	1560	1564	1565	rVB2	185	233	1.28%	0.168%
42	11.490	1580	1586	1594	rBV	8523	14398	79.39%	10.403%
43	12.276	1712	1715	1719	rBV2	188	356	1.96%	0.257%
44	12.398	1733	1735	1741	rVB2	182	312	1.72%	0.225%
45	12.483	1744	1749	1755	rVV2	6585	9303	51.30%	6.722%
46	12.678	1777	1781	1784	rBV2	270	448	2.47%	0.324%
47	12.812	1799	1803	1809	rVB3	452	890	4.91%	0.643%
48	12.910	1815	1819	1823	rVB3	881	1143	6.30%	0.826%
49	13.123	1852	1854	1857	rVB2	539	483	2.66%	0.349%
50	13.270	1873	1878	1879	rVB2	181	265	1.46%	0.191%
51	13.325	1884	1887	1889	rVV2	263	300	1.65%	0.217%
52	13.361	1892	1893	1899	rBV2	398	481	2.65%	0.348%
53	13.428	1899	1904	1913	rVB2	5532	9591	52.88%	6.930%
54	13.672	1942	1944	1946	rBV	292	244	1.35%	0.176%
55	13.751	1954	1957	1961	rVB2	1717	2071	11.42%	1.496%
56	13.800	1961	1965	1967	rVB3	337	446	2.46%	0.322%
57	13.831	1967	1970	1972	rBV3	345	498	2.75%	0.360%
58	13.855	1972	1974	1976	rVB3	299	243	1.34%	0.176%
59	13.922	1979	1985	1989	rBV4	612	1333	7.35%	0.963%
60	14.013	1998	2000	2002	rBV	449	390	2.15%	0.282%
61	14.074	2008	2010	2015	rVB3	808	1275	7.03%	0.921%
62	14.117	2015	2017	2019	rBV	267	204	1.12%	0.147%
63	14.148	2019	2022	2025	rVV2	374	501	2.76%	0.362%
64	14.202	2027	2031	2034	rBV3	410	593	3.27%	0.428%
65	14.257	2036	2040	2046	rBV4	1162	2226	12.27%	1.608%
66	14.337	2051	2053	2054	rVB2	320	232	1.28%	0.168%
67	14.355	2054	2056	2058	rBV2	366	404	2.23%	0.292%
68	14.422	2062	2067	2072	rVB4	1267	2200	12.13%	1.590%
69	14.458	2072	2073	2074	rBV	309	221	1.22%	0.160%
70	14.526	2082	2084	2085	rBV	350	229	1.26%	0.165%
71	14.587	2091	2094	2095	rBV3	335	342	1.89%	0.247%
72	14.611	2095	2098	2104	rBV4	556	937	5.17%	0.677%
73	14.672	2104	2108	2110	rBV3	1091	1695	9.35%	1.225%
74	14.843	2129	2136	2138	rBV5	1234	2495	13.76%	1.803%
75	14.910	2144	2147	2150	rBV3	479	504	2.78%	0.364%
76	15.007	2159	2163	2165	rBV3	505	588	3.24%	0.425%

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77	15.032	2165	2167	2168	rBV2	503	393	2.17%	0.284%
78	15.117	2180	2181	2184	rBV3	636	741	4.09%	0.535%
79	15.251	2201	2203	2204	rBV2	503	423	2.33%	0.306%
80	15.342	2216	2218	2220	rBV3	525	545	3.01%	0.394%
81	15.562	2252	2254	2256	rBV3	430	492	2.71%	0.355%
82	15.599	2258	2260	2263	rVV3	612	628	3.46%	0.454%
83	15.660	2269	2270	2271	rBV	461	241	1.33%	0.174%
84	15.781	2288	2290	2292	rBV3	306	318	1.75%	0.230%
85	15.842	2298	2300	2303	rVB3	387	414	2.28%	0.299%
86	15.952	2315	2318	2321	rVB3	521	754	4.16%	0.545%
87	15.983	2321	2323	2325	rBV3	619	682	3.76%	0.493%
88	16.226	2361	2363	2365	rBV2	212	261	1.44%	0.189%
89	16.354	2382	2384	2386	rBV	291	253	1.40%	0.183%
90	16.415	2390	2394	2396	rVB3	238	257	1.42%	0.186%
91	16.495	2403	2407	2408	rBV2	376	515	2.84%	0.372%
92	16.537	2412	2414	2415	rVB	384	248	1.37%	0.179%
93	16.580	2420	2421	2423	rVB	326	221	1.22%	0.160%
94	16.611	2423	2426	2428	rBV2	290	267	1.47%	0.193%
95	16.672	2433	2436	2438	rBV2	249	300	1.65%	0.217%

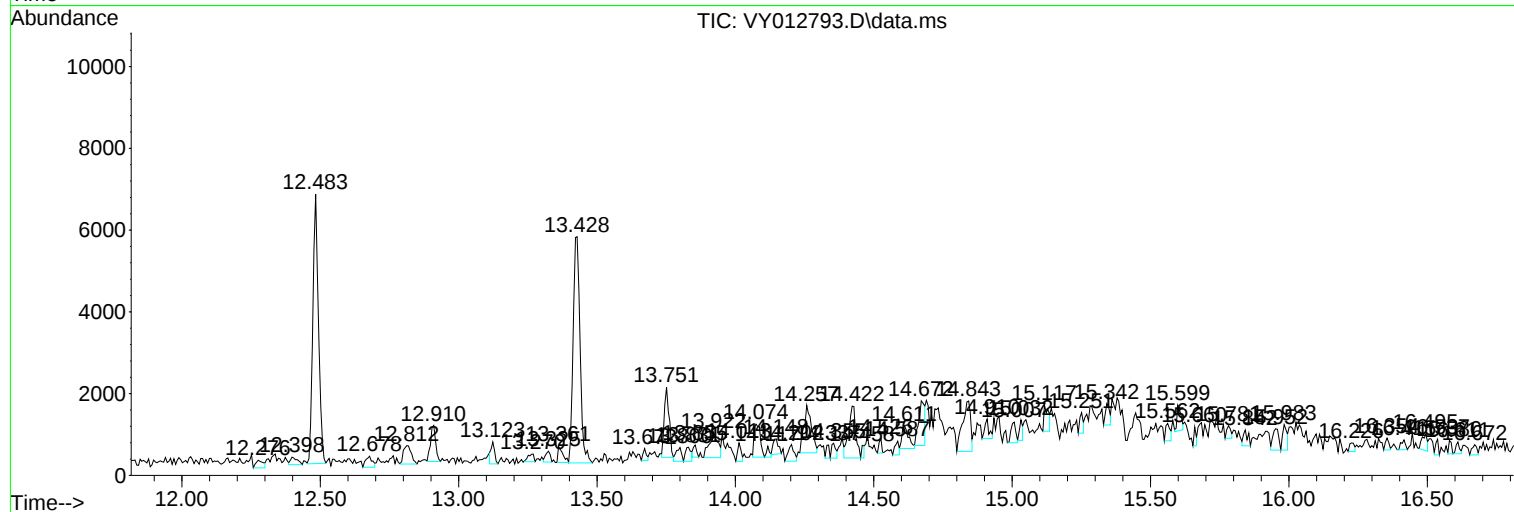
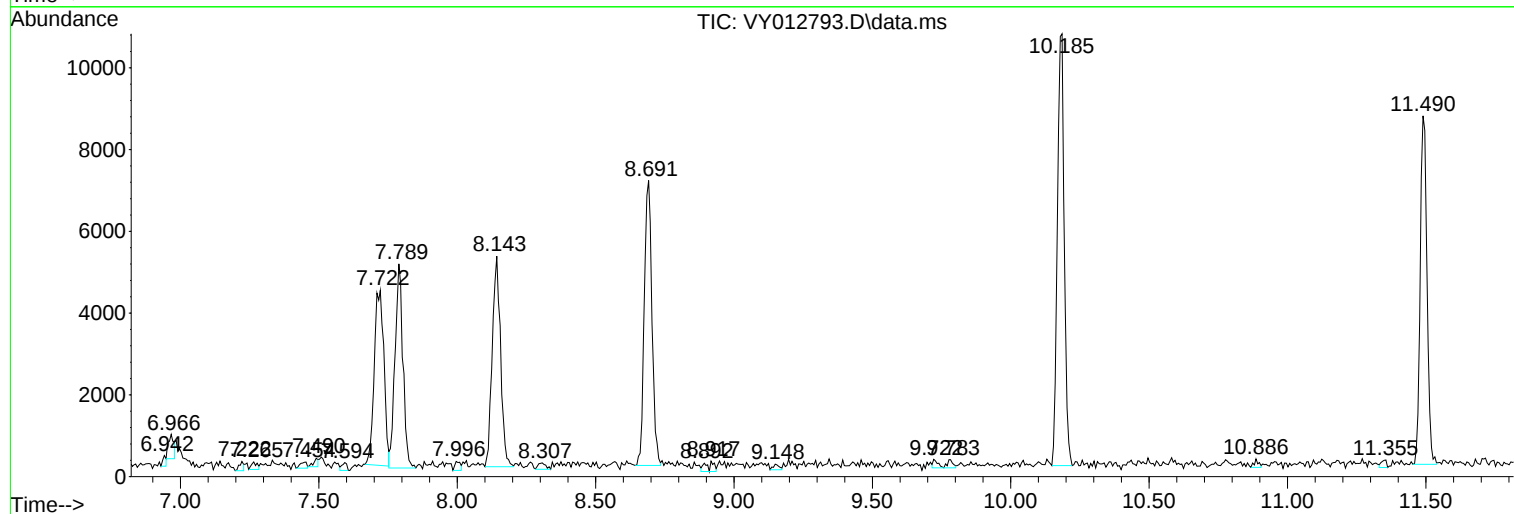
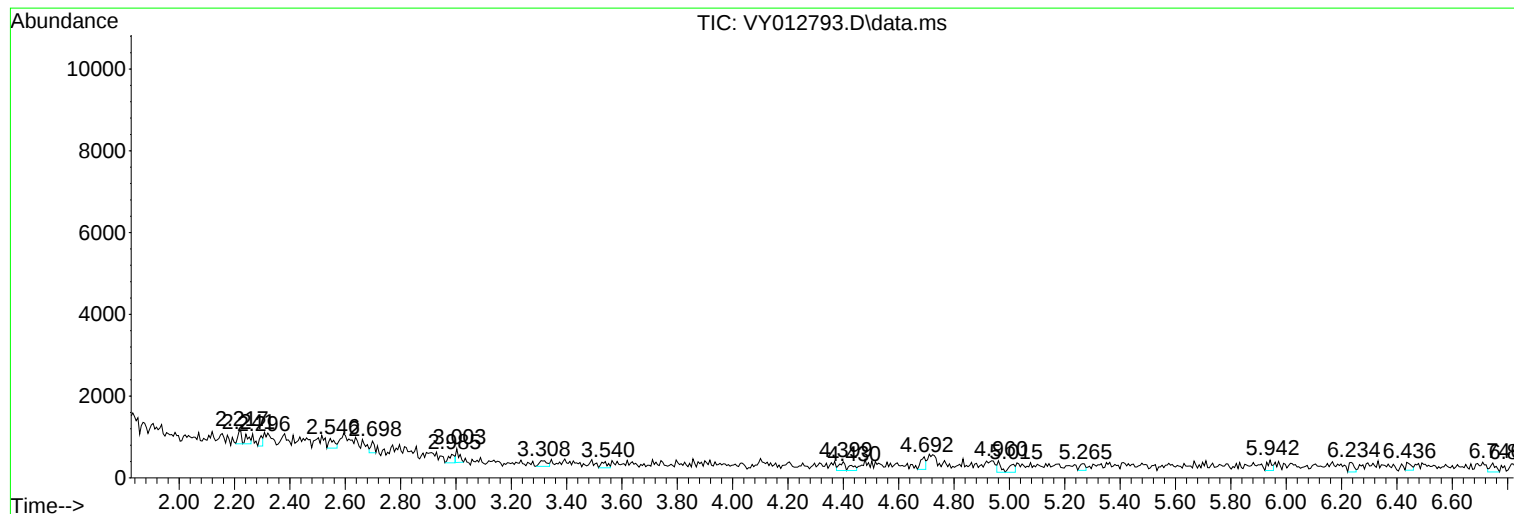
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.M
Quant Title : SW846 8260

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



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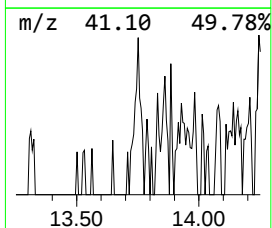
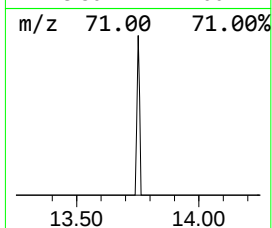
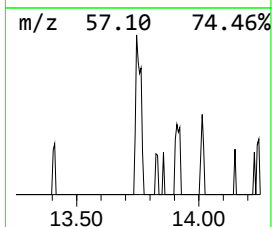
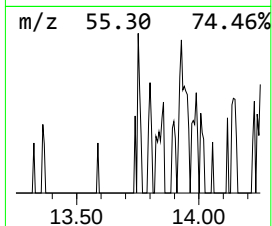
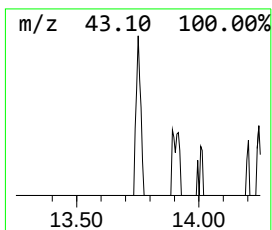
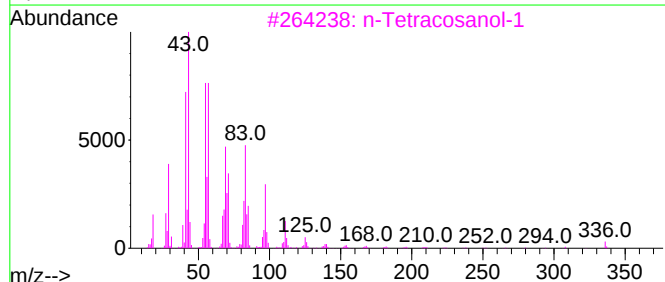
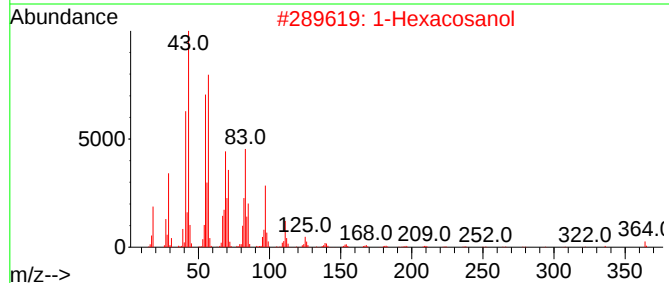
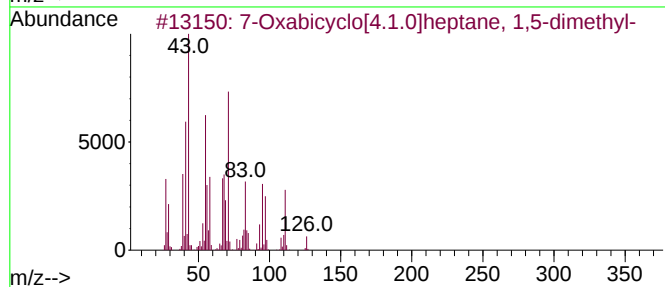
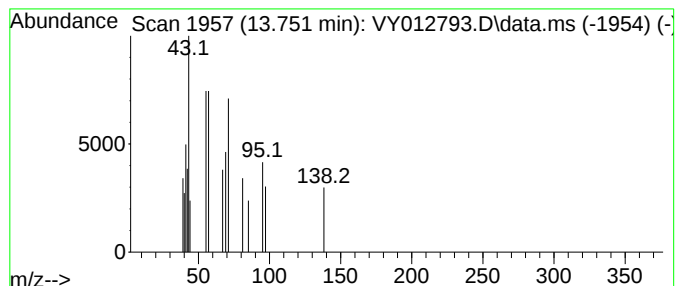
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown13.751 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	10.80 ug/l	2071	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Oxabicyclo[4.1.0]heptane, 1,5-...	126	C8H14O	162239-52-3	32
2			1-Hexacosanol	382	C26H54O	000506-52-5	27
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	27
4			2,4,6,8-Tetramethyl-1-undecene	210	C15H30	059920-26-2	17
5			Cyclohexaneethanol, 4-methyl-.be...	154	C10H18O	015714-12-2	12



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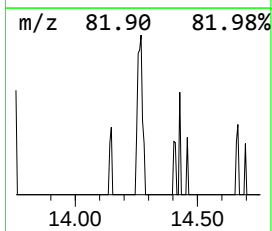
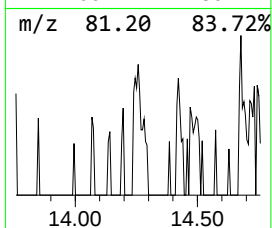
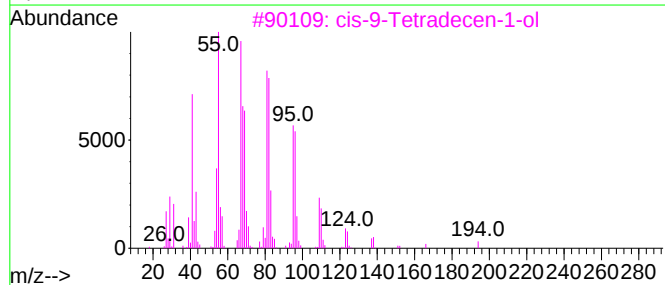
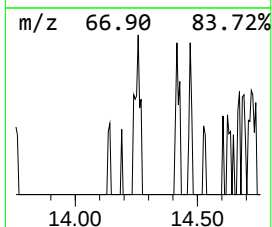
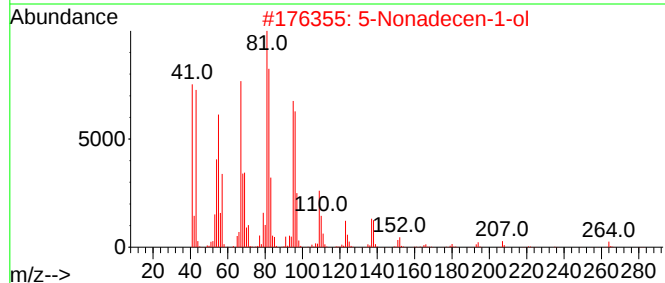
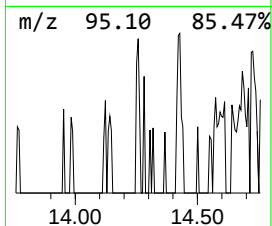
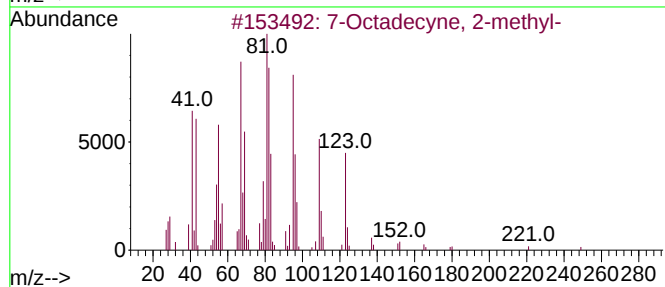
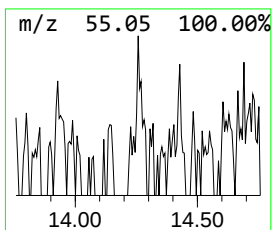
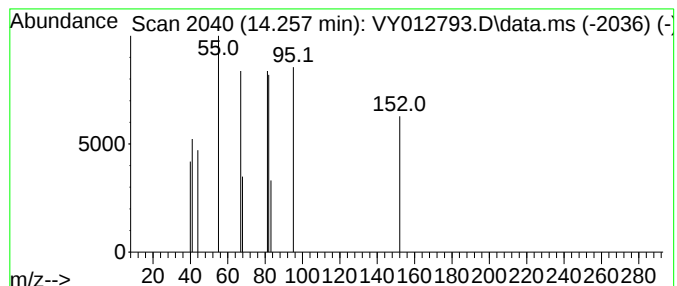
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.M
Quant Title : SW846 8260

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

Peak Number 5 7-Octadecyne, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	11.60 ug/l	2226	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octadecyne, 2-methyl-	264	C19H36	035354-38-2	64
2			5-Nonadecen-1-ol	282	C19H38O	1000131-11-9	53
3			cis-9-Tetradecen-1-ol	212	C14H28O	035153-15-2	53
4			Cyclohexane, 1-propenyl-	124	C9H16	005364-83-0	50
5			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004795-86-2	45



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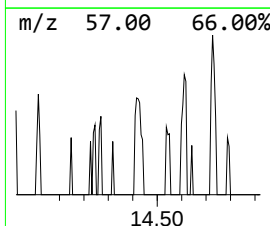
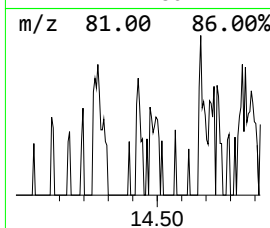
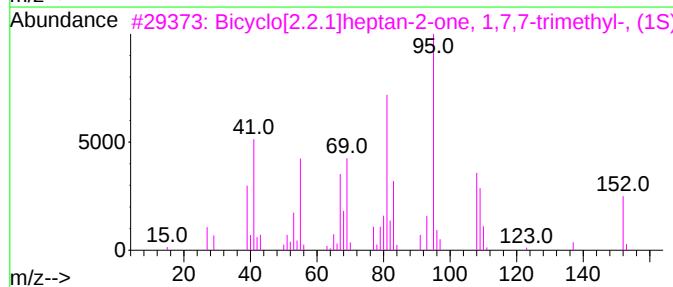
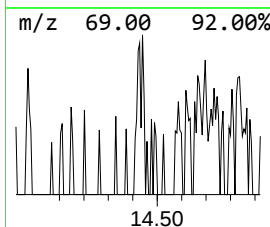
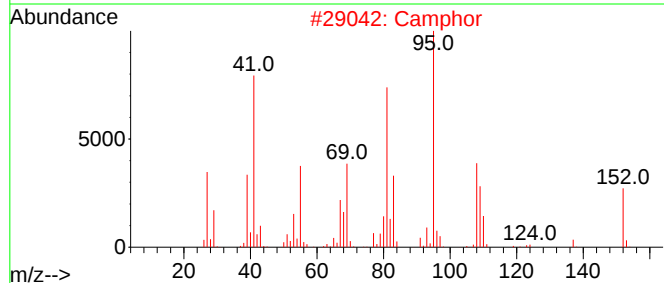
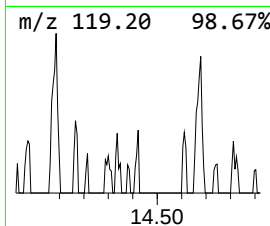
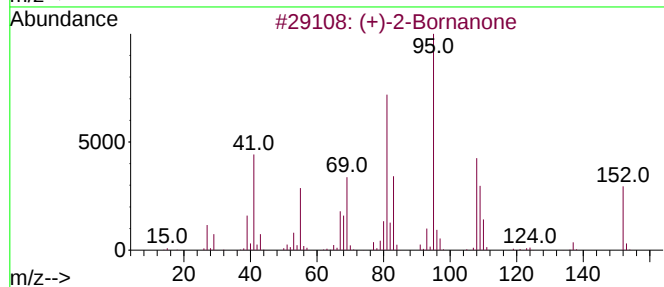
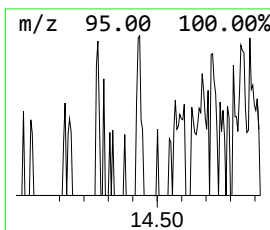
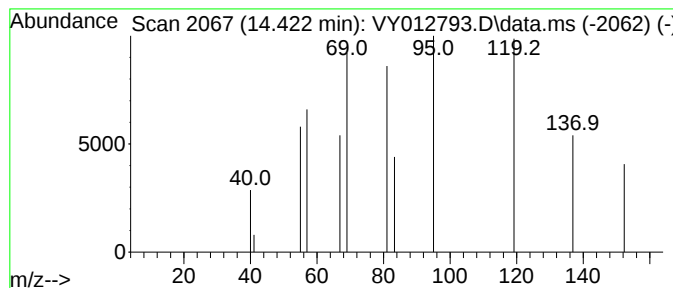
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Quant Title : SW846 8260

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

Peak Number 6 unknown14.422 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.422	11.47 ug/l	2200	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone			152	C10H16O	000464-49-3	46
2	Camphor			152	C10H16O	000076-22-2	43
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...			152	C10H16O	000464-48-2	43
4	Neopentylidenecyclohexane			152	C11H20	039546-80-0	38
5	cis-4a-Methyl-decahydronaphthalene			152	C11H20	002547-26-4	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY030323\
Data File : VY012793.D
Acq On : 03 Mar 2023 14:11
Operator : KP/MD
Sample : 01760-01RE
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RBR200058RE

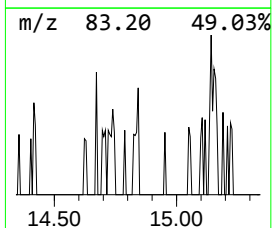
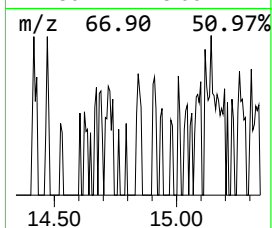
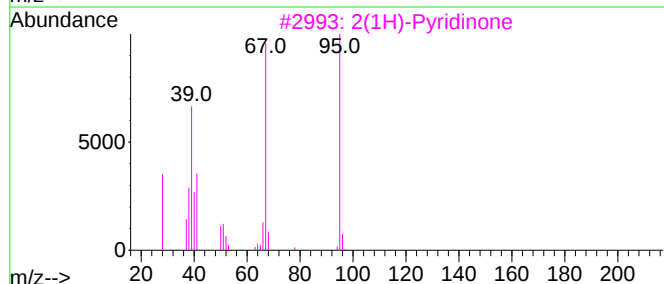
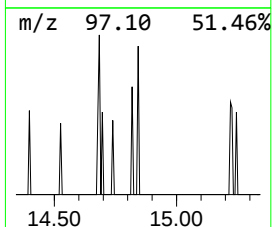
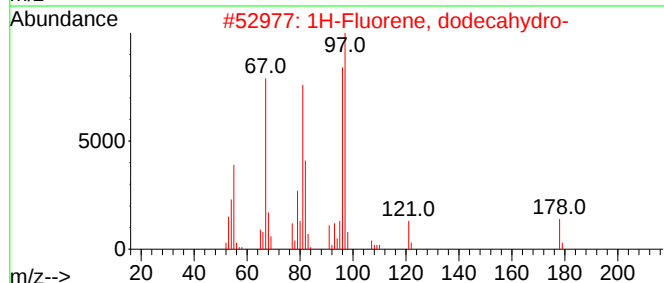
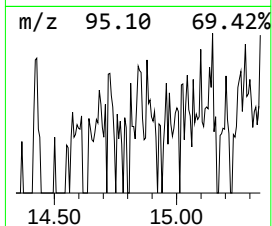
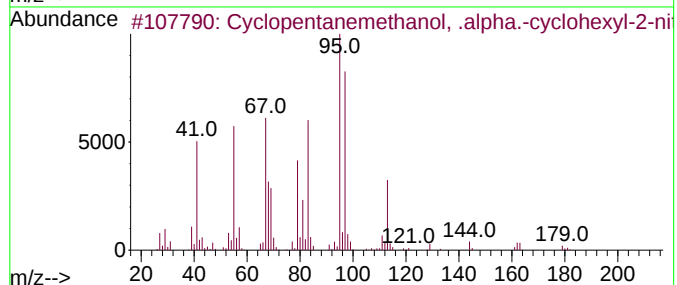
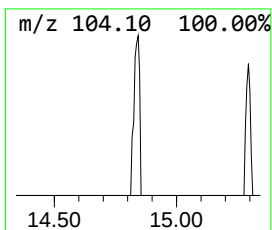
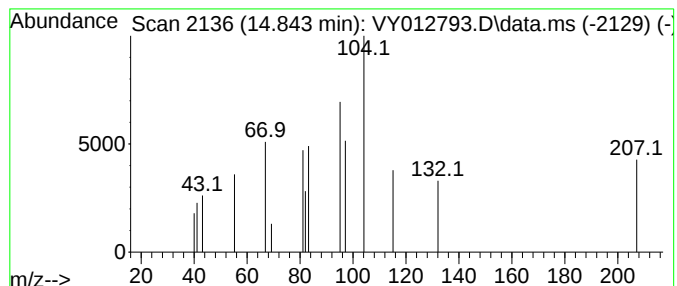
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.M
Quant Title : SW846 8260

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

Peak Number 8 unknown14.843 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.843	13.01 ug/l	2495	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanemethanol, .alpha.-cy...	227	C12H21NO3	103077-58-3	17
2			1H-Fluorene, dodecahydro-	178	C13H22	005744-03-6	10
3			2(1H)-Pyridinone	95	C5H5NO	000142-08-5	9
4			4-Hexen-1-ol, pentafluoropropionate	246	C9H11F5O2	1000352-72-4	9
5			2-Nonyne	124	C9H16	019447-29-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY030323\
Data File : VY012793.D
Acq On : 03 Mar 2023 14:11
Operator : KP/MD
Sample : 01760-01RE
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RBR200058RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.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
unknown13.751	13.751	10.8	ug/l	2071	4	13.428	9591	50.0
7-Octadecyne, 2...	14.257	11.6	ug/l	2226	4	13.428	9591	50.0
unknown14.422	14.422	11.5	ug/l	2200	4	13.428	9591	50.0
unknown14.843	14.843	13.0	ug/l	2495	4	13.428	9591	50.0