

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY031122\
 Data File : VY007847.D
 Acq On : 11 Mar 2022 12:19
 Operator : SY/MD
 Sample : N1853-03
 Misc : 4.15g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SR-EX2B-BASE-01

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\82Y022822S.M
 Title : SW846 8260

Signal : TIC: VY007847.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.028	31	34	35	rVB2	814	832	2.10%	0.332%
2	2.058	35	39	42	rBV4	1305	1895	4.78%	0.757%
3	2.138	44	52	57	rBV4	4106	11845	29.86%	4.732%
4	2.339	83	85	91	rVB2	1168	1167	2.94%	0.466%
5	2.759	148	154	157	rVB3	797	1379	3.48%	0.551%
6	2.948	182	185	189	rBV4	750	1251	3.15%	0.500%
7	3.095	206	209	213	rBV3	943	1807	4.56%	0.722%
8	3.503	273	276	279	rVB3	960	911	2.30%	0.364%
9	3.692	305	307	311	rBV2	549	812	2.05%	0.324%
10	3.741	311	315	318	rBV	522	922	2.32%	0.368%
11	3.899	339	341	346	rVB3	609	878	2.21%	0.351%
12	4.192	388	389	393	rVV	965	837	2.11%	0.334%
13	4.662	464	466	470	rVB2	881	976	2.46%	0.390%
14	4.918	506	508	510	rBV3	765	842	2.12%	0.336%
15	5.350	578	579	582	rBV3	780	853	2.15%	0.341%
16	5.649	624	628	630	rBV2	597	855	2.16%	0.342%
17	5.753	641	645	648	rBV4	571	935	2.36%	0.374%
18	6.045	690	693	698	rVB2	795	1172	2.95%	0.468%
19	6.100	698	702	705	rBV2	782	805	2.03%	0.322%
20	6.362	742	745	747	rBV2	623	793	2.00%	0.317%
21	6.448	757	759	763	rBV2	902	999	2.52%	0.399%
22	7.015	850	852	855	rBV2	664	840	2.12%	0.336%
23	7.301	896	899	901	rBV2	731	879	2.22%	0.351%
24	7.557	938	941	944	rBV2	774	963	2.43%	0.385%
25	7.630	950	953	955	rBV	928	826	2.08%	0.330%
26	7.716	963	967	971	rVV5	2338	4644	11.71%	1.855%
27	7.789	973	979	985	rVB7	4573	10952	27.61%	4.376%
28	7.996	1007	1013	1015	rBV4	1327	2620	6.60%	1.047%
29	8.143	1030	1037	1043	rBV6	3356	6967	17.56%	2.783%
30	8.222	1047	1050	1053	rVB3	920	1158	2.92%	0.463%
31	8.478	1088	1092	1094	rVV	648	925	2.33%	0.370%
32	8.539	1100	1102	1103	rVV2	1131	1166	2.94%	0.466%
33	8.569	1106	1107	1111	rVB2	835	820	2.07%	0.328%
34	8.691	1119	1127	1134	rVB4	6051	12233	30.84%	4.887%
35	9.270	1218	1222	1227	rVB2	585	907	2.29%	0.362%
36	9.722	1293	1296	1298	rVB2	775	923	2.33%	0.369%

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37	9.746	1298	1300	1304	rBV2	770	1273	3.21%	0.509%
38	9.819	1308	1312	1314	rBV4	1530	2092	5.27%	0.836%
39	9.953	1331	1334	1335	rBV3	747	905	2.28%	0.362%
40	9.965	1335	1336	1339	rVV	1384	836	2.11%	0.334%
41	10.179	1365	1371	1379	rVV2	10111	19838	50.01%	7.926%
42	10.374	1398	1403	1406	rVB3	1301	2116	5.33%	0.845%
43	10.673	1451	1452	1455	rVB	1484	941	2.37%	0.376%
44	10.703	1455	1457	1458	rBV	947	858	2.16%	0.343%
45	10.746	1461	1464	1466	rBV	895	938	2.36%	0.375%
46	11.246	1544	1546	1548	rVB3	1282	820	2.07%	0.328%
47	11.276	1548	1551	1558	rBV3	1723	2650	6.68%	1.059%
48	11.386	1563	1569	1570	rBV3	1091	1590	4.01%	0.635%
49	11.490	1580	1586	1591	rVV2	7419	11205	28.25%	4.477%
50	11.532	1591	1593	1596	rVB2	1013	1009	2.54%	0.403%
51	11.721	1619	1624	1625	rVV4	1202	1828	4.61%	0.730%
52	11.898	1649	1653	1656	rVB2	814	1023	2.58%	0.409%
53	11.947	1656	1661	1662	rVB2	1107	1260	3.18%	0.503%
54	11.989	1662	1668	1669	rBV2	1876	2372	5.98%	0.948%
55	12.020	1671	1673	1680	rVB4	3639	6536	16.48%	2.611%
56	12.130	1686	1691	1697	rVB4	1844	3262	8.22%	1.303%
57	12.203	1697	1703	1706	rBV5	1681	3596	9.07%	1.437%
58	12.252	1706	1711	1715	rVV5	2828	4645	11.71%	1.856%
59	12.380	1730	1732	1734	rBV2	1130	1136	2.86%	0.454%
60	12.489	1741	1750	1758	rBV	21655	39667	100.00%	15.848%
61	12.605	1768	1769	1771	rVV	986	880	2.22%	0.352%
62	12.648	1773	1776	1779	rVB3	2510	3390	8.55%	1.354%
63	12.678	1779	1781	1784	rVB3	649	817	2.06%	0.326%
64	12.703	1784	1785	1787	rBV2	1130	918	2.31%	0.367%
65	12.727	1787	1789	1793	rVB4	949	1325	3.34%	0.529%
66	12.806	1796	1802	1807	rBV8	2620	5618	14.16%	2.245%
67	12.873	1811	1813	1816	rVB3	1320	944	2.38%	0.377%
68	13.026	1837	1838	1841	rBV2	1254	1260	3.18%	0.503%
69	13.111	1851	1852	1855	rVB3	864	899	2.27%	0.359%
70	13.148	1855	1858	1860	rBV4	869	1120	2.82%	0.447%
71	13.227	1869	1871	1874	rBV2	1260	1649	4.16%	0.659%
72	13.325	1886	1887	1889	rVB2	1455	897	2.26%	0.358%
73	13.361	1889	1893	1894	rBV3	841	974	2.46%	0.389%
74	13.428	1898	1904	1907	rBV5	2053	3879	9.78%	1.550%
75	13.501	1915	1916	1918	rBV2	1399	854	2.15%	0.341%
76	13.568	1925	1927	1932	rVB3	915	1184	2.98%	0.473%

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77	13.666	1940	1943	1946	rVB3	1488	1317	3.32%	0.526%
78	13.751	1953	1957	1958	rVV3	1027	1443	3.64%	0.577%
79	13.873	1975	1977	1981	rBV	903	1460	3.68%	0.583%
80	13.965	1991	1992	1996	rVB3	1260	1193	3.01%	0.477%
81	14.166	2022	2025	2028	rVB4	1241	1438	3.63%	0.575%
82	14.196	2028	2030	2035	rBV3	1114	1640	4.13%	0.655%
83	14.270	2040	2042	2045	rVV3	1384	1444	3.64%	0.577%
84	14.532	2082	2085	2087	rBV2	1005	875	2.21%	0.350%
85	15.007	2162	2163	2167	rVB2	1142	1026	2.59%	0.410%
86	15.123	2180	2182	2184	rVB2	943	835	2.11%	0.334%
87	15.147	2184	2186	2188	rBV3	709	839	2.12%	0.335%
88	15.208	2195	2196	2202	rBV4	977	1335	3.37%	0.533%
89	15.263	2202	2205	2209	rVV5	1351	1766	4.45%	0.706%
90	15.452	2234	2236	2240	rVB2	1230	939	2.37%	0.375%
91	15.489	2240	2242	2245	rVB3	1349	1115	2.81%	0.445%
92	15.525	2245	2248	2250	rBV2	1065	1420	3.58%	0.567%
93	15.867	2302	2304	2308	rBV5	983	1355	3.42%	0.541%
94	16.062	2334	2336	2339	rVB3	1249	848	2.14%	0.339%
95	16.098	2341	2342	2345	rBV3	1046	1279	3.22%	0.511%
96	16.294	2371	2374	2377	rBV3	1374	1913	4.82%	0.764%
97	16.324	2377	2379	2381	rVV3	1231	1006	2.54%	0.402%
98	16.385	2387	2389	2392	rBV3	1306	1500	3.78%	0.599%
99	16.495	2405	2407	2409	rBV3	1610	1143	2.88%	0.457%
100	16.739	2443	2447	2450	rBV3	1830	2576	6.49%	1.029%

Sum of corrected areas: 250298

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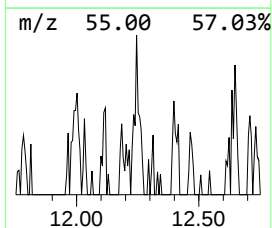
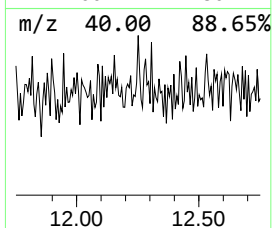
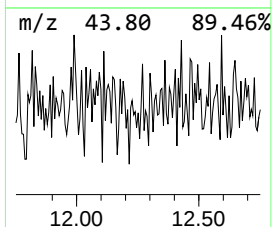
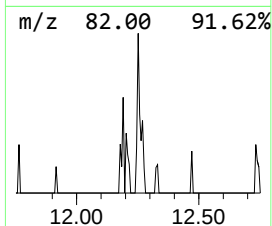
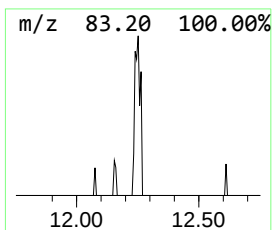
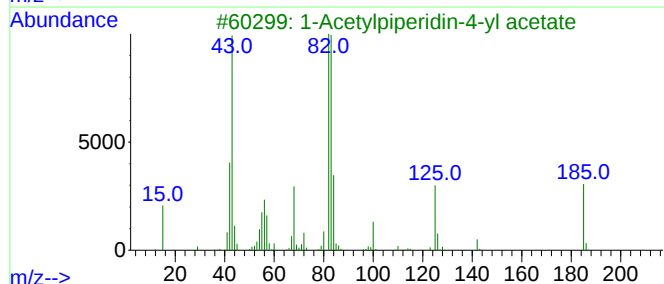
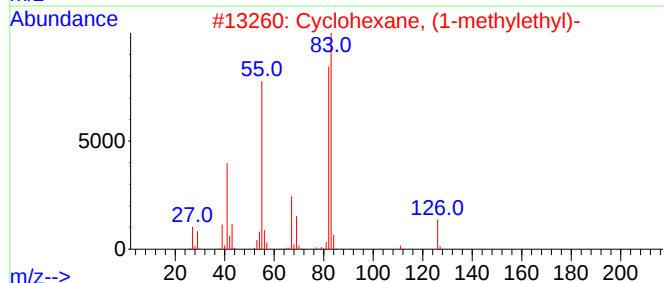
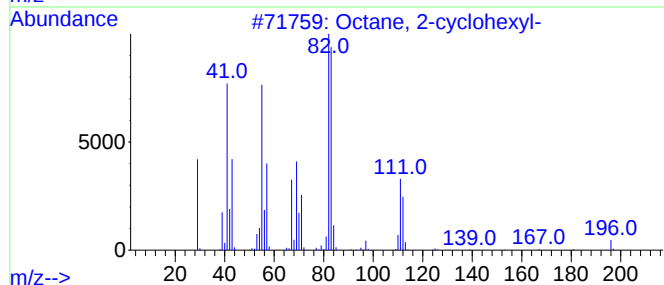
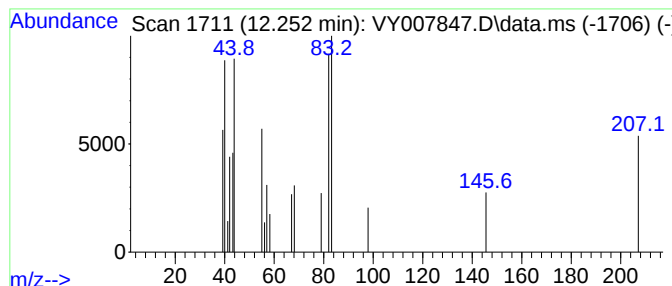
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y022822S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.252 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.252	20.73 ug/l	4645	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2-cyclohexyl-	196	C14H28	002883-05-8	35
2			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	25
3			1-Acetylpiperidin-4-yl acetate	185	C9H15NO3	883733-99-1	23
4			Cyclohexane, nonadecyl-	350	C25H50	022349-03-7	12
5			Glycine, N-(3-methyl-1-oxo-2-but...	171	C8H13NO3	056009-34-8	12



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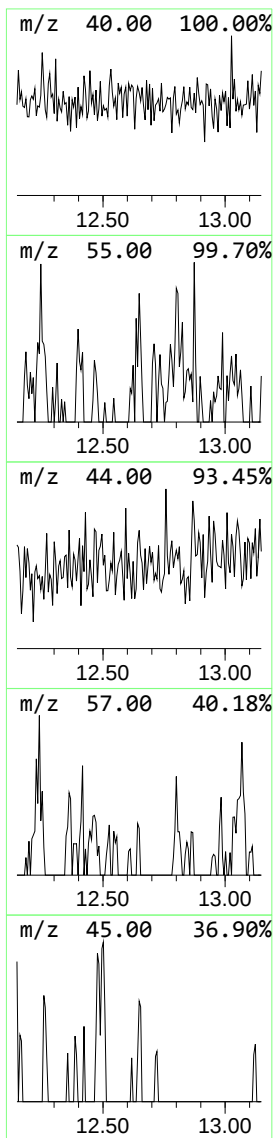
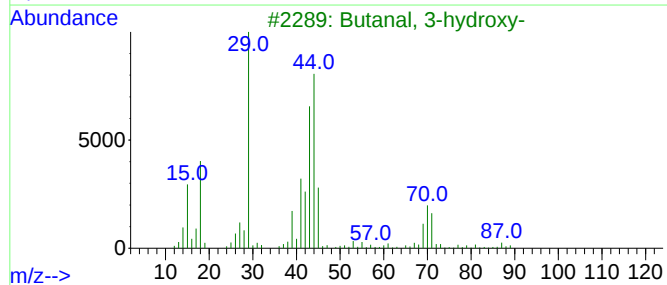
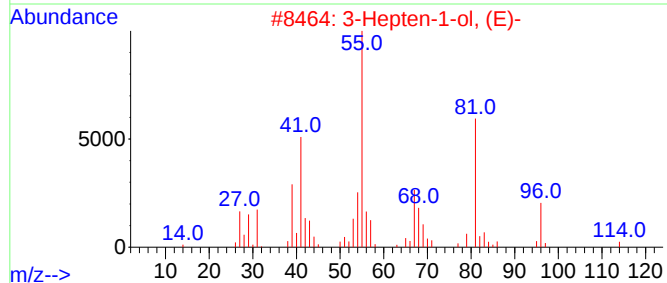
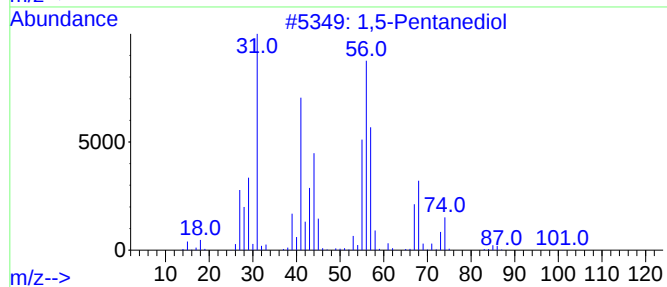
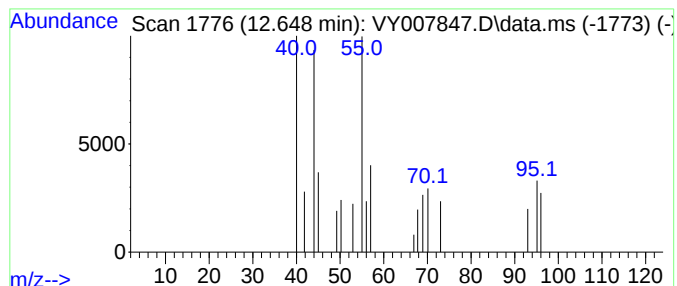
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y022822S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown12.648 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.648	43.70 ug/l	3390	1,4-Dichlorobenzene-d4	13.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5-Pentanediol	104	C5H12O2	000111-29-5	10
2			3-Hepten-1-ol, (E)-	114	C7H14O	002108-05-6	9
3			Butanal, 3-hydroxy-	88	C4H8O2	000107-89-1	9
4			3-Hepten-1-ol	114	C7H14O	010606-47-0	9
5			Propanamide	73	C3H7NO	000079-05-0	4



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Instrument :
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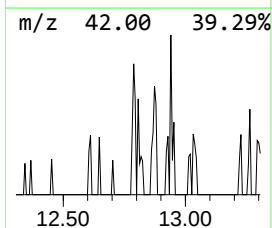
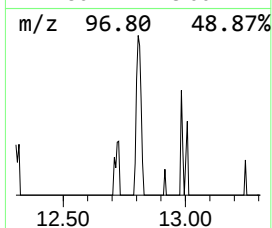
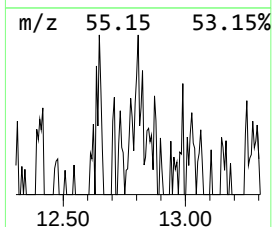
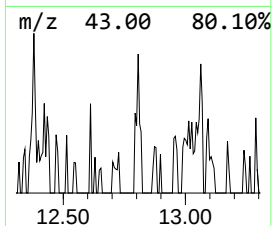
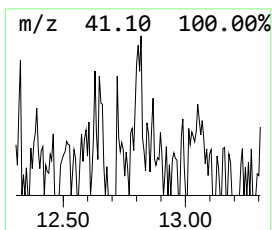
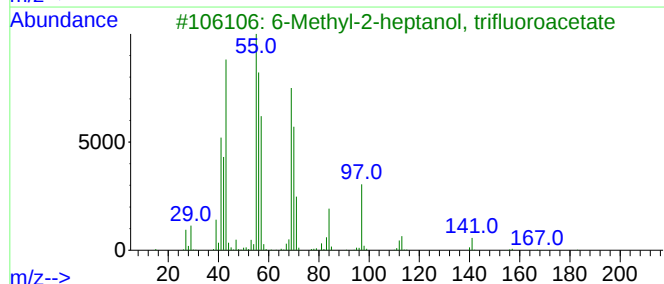
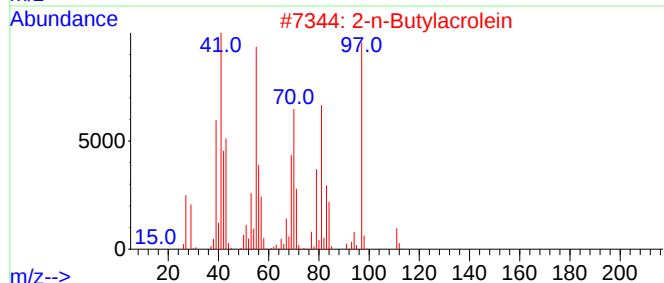
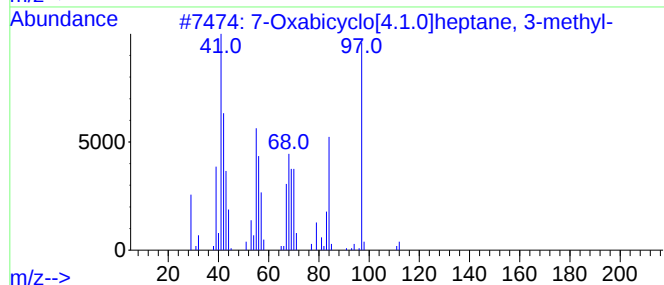
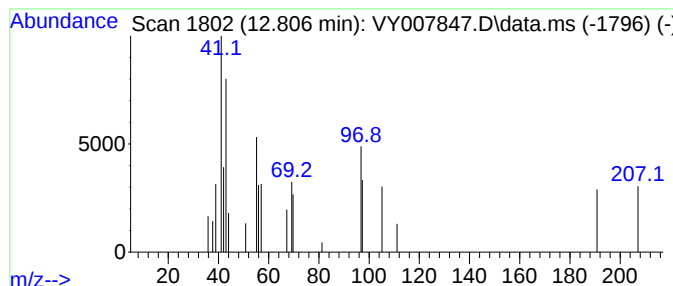
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y022822S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown12.806 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.806	72.42 ug/l	5618	1,4-Dichlorobenzene-d4	13.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Oxabicyclo[4.1.0]heptane, 3-me...	112	C7H12O	036099-51-1	42
2			2-n-Butylacrolein	112	C7H12O	001070-66-2	40
3			6-Methyl-2-heptanol, trifluoroac...	226	C10H17F3O2	1010365-05-8	27
4			1-Methylpyrazol-3-amine	97	C4H7N3	001904-31-0	25
5			1-Hexadecanol	242	C16H34O	036653-82-4	14



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown12.252	12.252	20.7	ug/l	4645	3	11.490	11205	50.0
unknown12.648	12.648	43.7	ug/l	3390	4	13.416	3879	50.0
unknown12.806	12.806	72.4	ug/l	5618	4	13.416	3879	50.0