

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD050922\
 Data File : VD072897.D
 Acq On : 09 May 2022 18:19
 Operator : VA/SY
 Sample : N2680-06
 Misc : 5.05G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 B3-6-8

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_D\Method\82D050222S.M
 Title : SW846 8260

Signal : TIC: VD072897.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.020	15	17	20	rVB2	2593	2724	2.42%	0.245%
2	2.209	43	49	51	rBV4	2550	3954	3.51%	0.355%
3	2.273	57	60	62	rVB4	2887	2954	2.62%	0.265%
4	2.297	62	64	69	rBV4	2911	3819	3.39%	0.343%
5	2.473	91	94	96	rBV4	2982	3909	3.47%	0.351%
6	2.585	111	113	116	rVB3	2956	2826	2.51%	0.254%
7	2.779	143	146	151	rVB4	2337	3828	3.40%	0.344%
8	4.309	401	406	410	rVB	1567	2880	2.56%	0.259%
9	4.397	417	421	424	rBV2	1495	2087	1.85%	0.188%
10	4.426	424	426	430	rVB2	1507	1788	1.59%	0.161%
11	4.908	504	508	512	rBV2	1210	2115	1.88%	0.190%
12	4.961	512	517	518	rBV2	2094	2796	2.48%	0.251%
13	5.032	526	529	531	rBV2	1853	1807	1.60%	0.162%
14	5.267	567	569	574	rVB2	1563	2081	1.85%	0.187%
15	5.497	601	608	610	rBV2	1596	3194	2.84%	0.287%
16	5.997	690	693	696	rVB2	1690	1781	1.58%	0.160%
17	7.173	890	893	894	rVV2	3054	2869	2.55%	0.258%
18	7.914	1011	1019	1023	rBV3	19037	45071	40.01%	4.051%
19	7.967	1024	1028	1037	rVB4	24574	55852	49.57%	5.020%
20	8.067	1044	1045	1049	rVB2	1741	2089	1.85%	0.188%
21	8.108	1049	1052	1055	rBV	1133	1827	1.62%	0.164%
22	8.185	1063	1065	1070	rVB3	2549	3116	2.77%	0.280%
23	8.326	1080	1089	1097	rVB4	21956	52129	46.27%	4.685%
24	8.491	1115	1117	1120	rBV	1678	2206	1.96%	0.198%
25	8.632	1138	1141	1144	rVB2	2731	2727	2.42%	0.245%
26	8.708	1152	1154	1155	rBV2	2833	2646	2.35%	0.238%
27	8.808	1165	1171	1172	rVB	1717	1826	1.62%	0.164%
28	8.855	1172	1179	1189	rBV2	38082	76637	68.02%	6.888%
29	9.126	1223	1225	1229	rVB	1509	1811	1.61%	0.163%
30	9.173	1229	1233	1236	rBV3	1628	2537	2.25%	0.228%
31	9.538	1291	1295	1298	rBV2	1580	2014	1.79%	0.181%
32	9.720	1322	1326	1328	rBV2	1468	2361	2.10%	0.212%
33	9.891	1353	1355	1358	rVB2	1503	1880	1.67%	0.169%
34	10.332	1424	1430	1436	rBV2	61394	105107	93.29%	9.447%
35	10.396	1436	1441	1448	rVB3	29789	53413	47.41%	4.801%
36	10.491	1454	1457	1458	rBV2	2540	2027	1.80%	0.182%

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37	10.508	1458	1460	1464	rVV3	3644	4336	3.85%	0.390%
38	10.538	1464	1465	1470	rVB2	2623	1913	1.70%	0.172%
39	10.585	1470	1473	1475	rBV2	1840	1886	1.67%	0.170%
40	10.673	1484	1488	1492	rVB3	1568	3001	2.66%	0.270%
41	10.738	1497	1499	1501	rBV2	2227	1840	1.63%	0.165%
42	10.914	1526	1529	1531	rBV2	2562	2766	2.46%	0.249%
43	10.949	1533	1535	1542	rVB2	3423	4164	3.70%	0.374%
44	11.073	1554	1556	1560	rVB3	3300	4148	3.68%	0.373%
45	11.114	1560	1563	1568	rBV3	1891	3142	2.79%	0.282%
46	11.179	1570	1574	1576	rBV3	3606	3862	3.43%	0.347%
47	11.296	1592	1594	1597	rVB2	2095	1814	1.61%	0.163%
48	11.343	1600	1602	1606	rBV3	2340	2905	2.58%	0.261%
49	11.432	1614	1617	1621	rVB3	2322	3026	2.69%	0.272%
50	11.520	1626	1632	1637	rBV3	4181	7674	6.81%	0.690%
51	11.567	1637	1640	1643	rVB3	1456	1790	1.59%	0.161%
52	11.638	1645	1652	1659	rBV	63724	112662	100.00%	10.126%
53	11.732	1664	1668	1671	rBV3	4565	6585	5.84%	0.592%
54	11.849	1682	1688	1697	rVV7	12744	28612	25.40%	2.572%
55	11.926	1699	1701	1704	rVB2	4069	3303	2.93%	0.297%
56	12.002	1710	1714	1715	rBV2	2820	2641	2.34%	0.237%
57	12.067	1722	1725	1728	rVB3	1550	2435	2.16%	0.219%
58	12.102	1728	1731	1732	rBV2	1849	1858	1.65%	0.167%
59	12.149	1733	1739	1741	rBV5	3876	6819	6.05%	0.613%
60	12.255	1754	1757	1763	rVB6	3348	6394	5.68%	0.575%
61	12.308	1763	1766	1769	rBV4	1656	2607	2.31%	0.234%
62	12.349	1769	1773	1775	rBV6	2572	3782	3.36%	0.340%
63	12.367	1775	1776	1781	rVV5	2667	3570	3.17%	0.321%
64	12.549	1804	1807	1808	rBV2	2078	2401	2.13%	0.216%
65	12.620	1814	1819	1828	rBV3	49476	85028	75.47%	7.642%
66	12.785	1844	1847	1855	rVB5	3038	5830	5.17%	0.524%
67	12.873	1859	1862	1865	rVV4	5119	7519	6.67%	0.676%
68	12.943	1868	1874	1879	rVB7	12217	24620	21.85%	2.213%
69	12.990	1879	1882	1884	rBV3	1958	2361	2.10%	0.212%
70	13.161	1908	1911	1912	rBV3	3392	3150	2.80%	0.283%
71	13.255	1923	1927	1931	rVB5	5713	8191	7.27%	0.736%
72	13.343	1941	1942	1944	rBV	2997	1794	1.59%	0.161%
73	13.443	1954	1959	1960	rBV3	4695	7144	6.34%	0.642%
74	13.490	1964	1967	1969	rVV4	2131	2598	2.31%	0.233%
75	13.561	1973	1979	1986	rVB	67796	111896	99.32%	10.057%
76	13.632	1989	1991	1993	rBV3	4581	4109	3.65%	0.369%

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77	13.684	1999	2000	2002	rBV2	2430	1801	1.60%	0.162%
78	13.726	2005	2007	2008	rVV	3258	1821	1.62%	0.164%
79	13.749	2008	2011	2016	rBV7	4174	7068	6.27%	0.635%
80	13.790	2016	2018	2019	rBV2	2297	2146	1.90%	0.193%
81	13.884	2029	2034	2038	rVV4	9966	17889	15.88%	1.608%
82	13.926	2038	2041	2042	rVB3	3044	2589	2.30%	0.233%
83	14.043	2059	2061	2067	rVV4	3422	3550	3.15%	0.319%
84	14.102	2067	2071	2074	rVB4	5367	8419	7.47%	0.757%
85	14.202	2085	2088	2094	rVB4	5906	8745	7.76%	0.786%
86	14.320	2104	2108	2110	rBV4	2837	3821	3.39%	0.343%
87	14.390	2114	2120	2122	rBV4	6987	9335	8.29%	0.839%
88	14.461	2130	2132	2135	rVB4	4078	3490	3.10%	0.314%
89	14.549	2144	2147	2150	rBV5	4818	6427	5.70%	0.578%
90	14.643	2161	2163	2167	rVB4	2535	2888	2.56%	0.260%
91	14.690	2169	2171	2174	rBV3	2893	2519	2.24%	0.226%
92	14.979	2218	2220	2222	rVB3	3557	2072	1.84%	0.186%
93	15.067	2230	2235	2236	rBV4	4414	5462	4.85%	0.491%
94	15.143	2243	2248	2250	rBV5	5994	10530	9.35%	0.946%
95	15.255	2265	2267	2268	rBV2	3393	3454	3.07%	0.310%
96	15.343	2277	2282	2290	rBV10	9401	21615	19.19%	1.943%
97	15.437	2297	2298	2301	rBV2	4118	2417	2.15%	0.217%
98	16.320	2444	2448	2450	rBV4	4597	7363	6.54%	0.662%
99	16.408	2458	2463	2468	rBV8	6823	13255	11.77%	1.191%
100	16.526	2481	2483	2484	rBV2	3956	3098	2.75%	0.278%

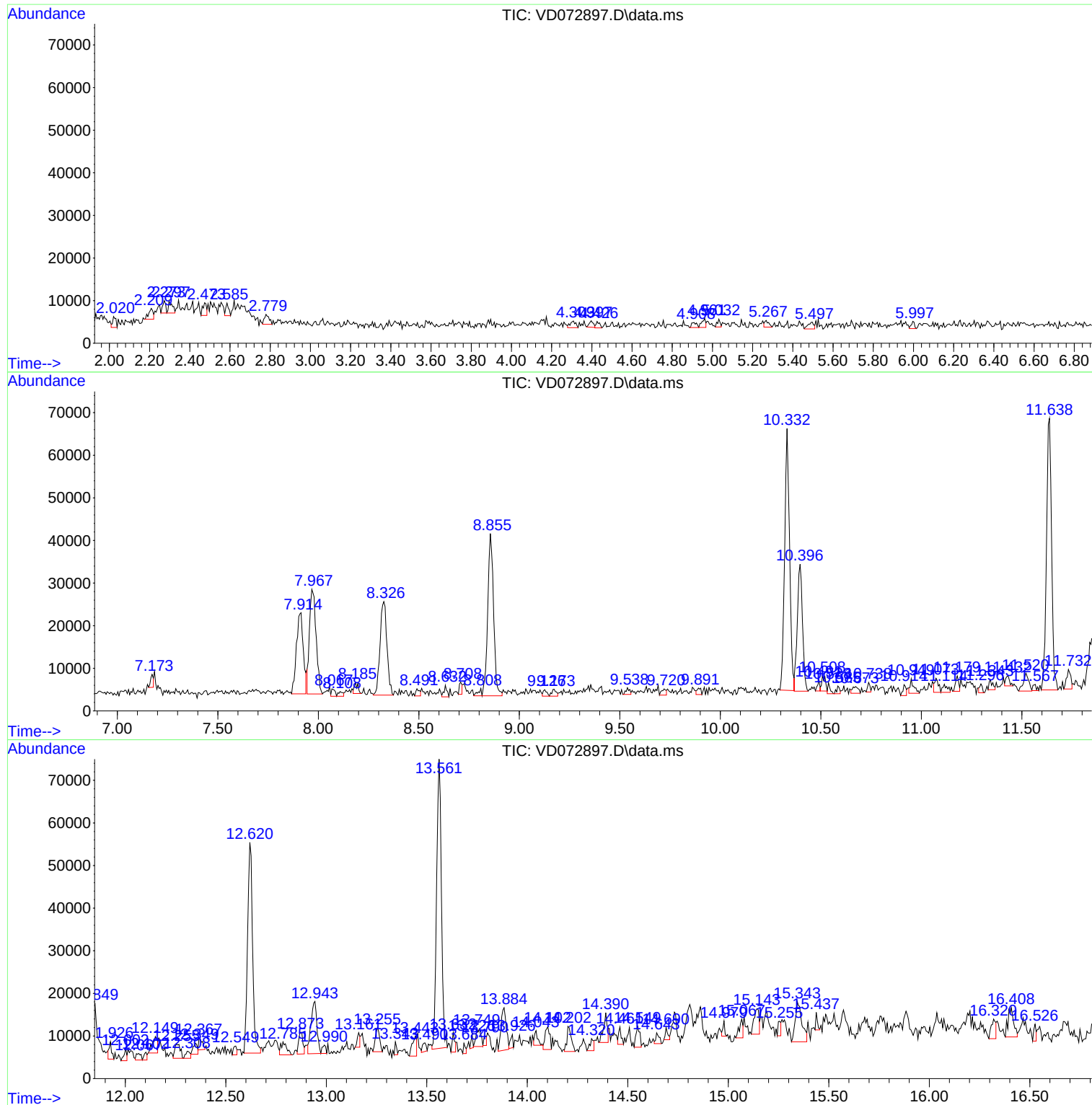
Sum of corrected areas: 1112638

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_D
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B3-6-8

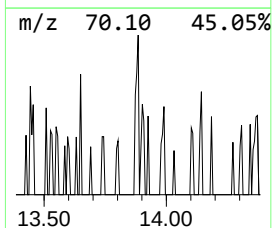
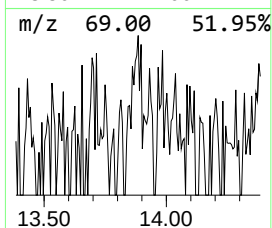
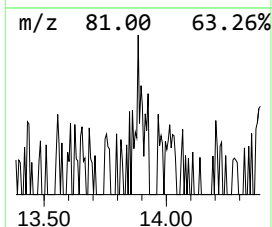
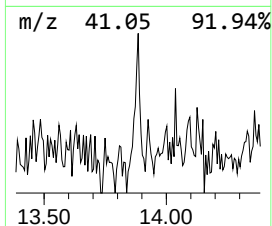
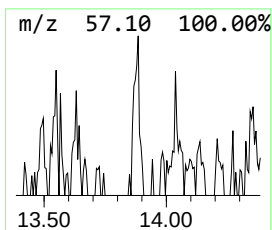
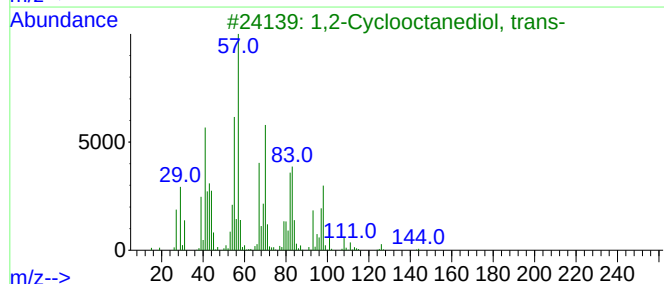
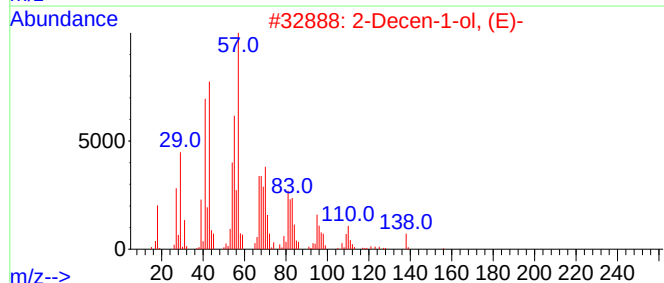
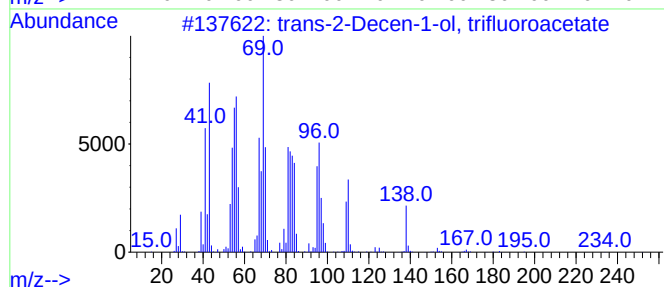
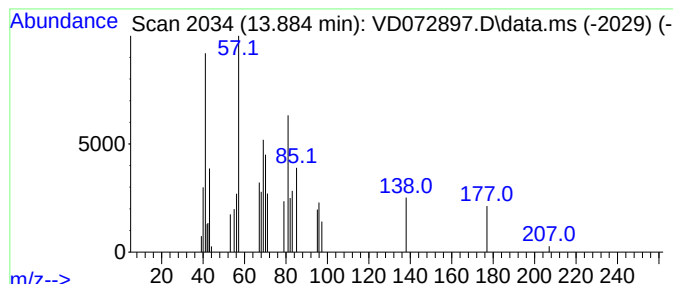
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown13.884 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.884	7.99 ug/l	17889	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2-Decen-1-ol, trifluoroace...	252	C12H19F3O2	1000352-67-0	35
2			2-Decen-1-ol, (E)-	156	C10H20O	018409-18-2	35
3			1,2-Cyclooctanediol, trans-	144	C8H16O2	042565-22-0	27
4			Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	27
5			6-Methyloctahydrocoumarin	168	C10H16O2	080648-29-9	27



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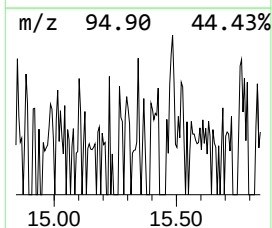
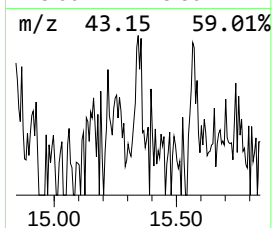
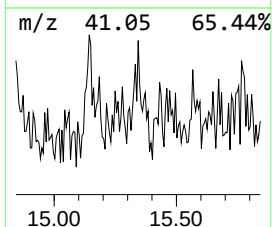
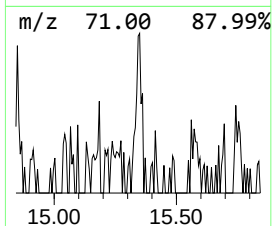
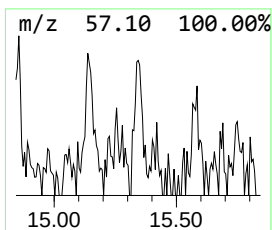
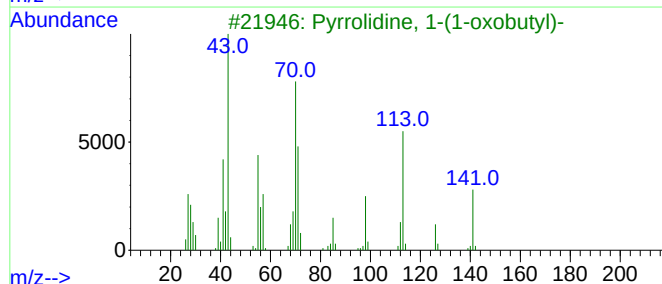
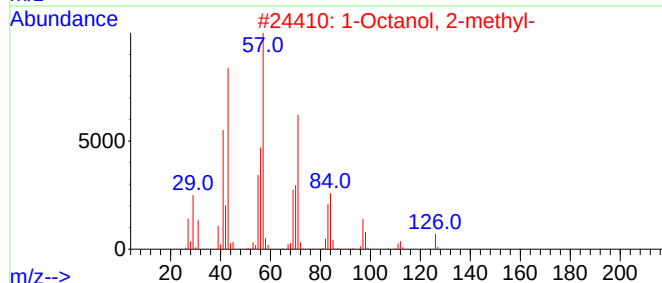
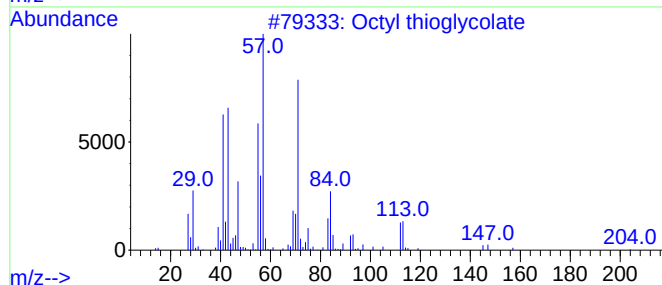
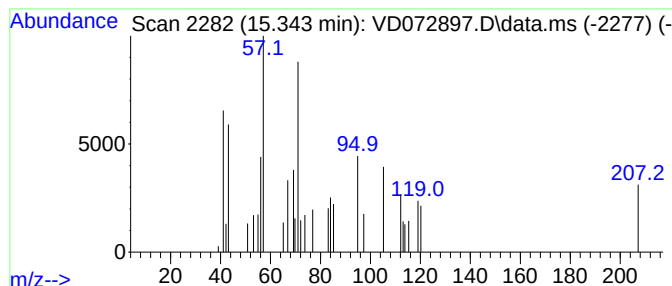
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown15.343 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.343	9.66 ug/l	21615	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octyl thioglycolate	204	C10H20O2S	007664-80-4	43
2			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	38
3			Pyrrolidine, 1-(1-oxobutyl)-	141	C8H15NO	033527-93-4	37
4			1-Heptadecanamine	255	C17H37N	004200-95-7	35
5			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	35



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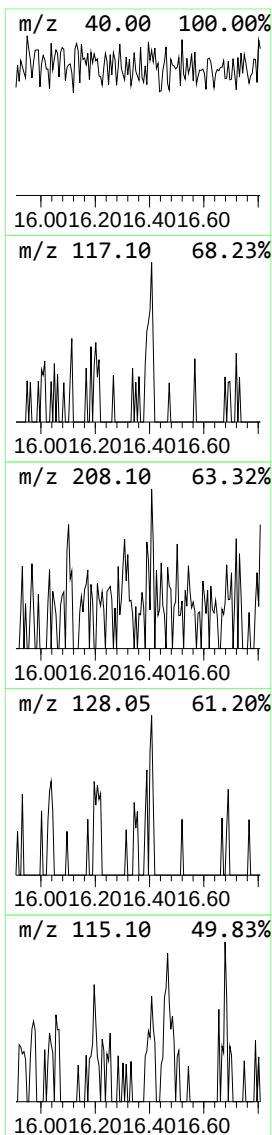
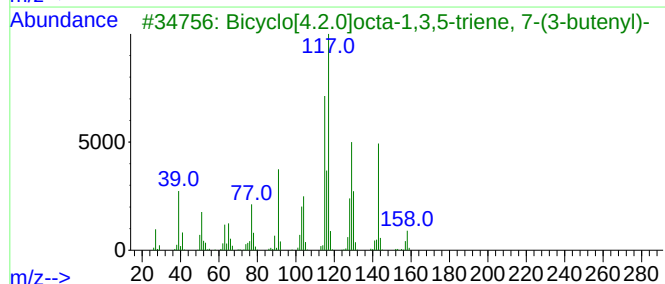
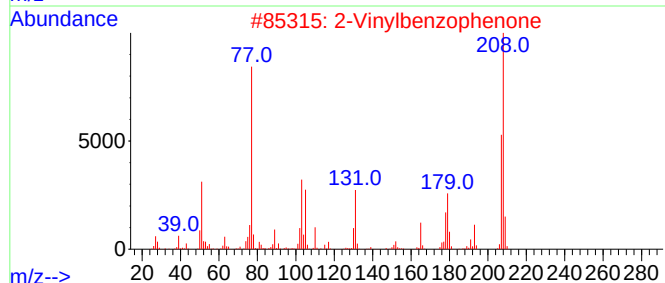
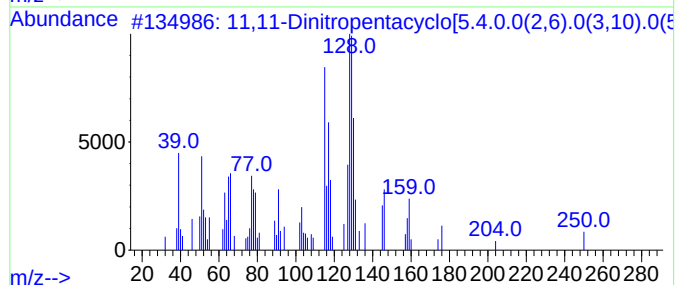
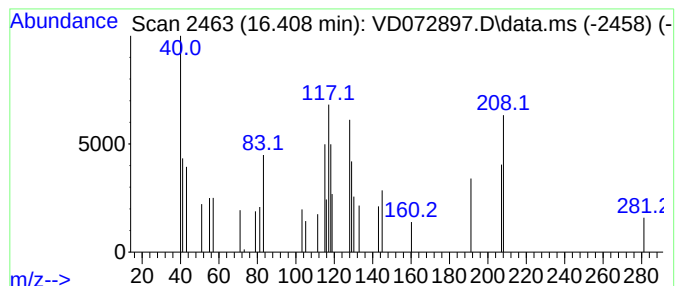
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown16.408 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.408	5.92 ug/l	13255	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	11,11-Dinitropentacyclo[5.4.0.0(...	250	C11H10N2O5	1000326-22-0	22		
2	2-Vinylbenzophenone	208	C15H12O	052095-42-8	11		
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	158	C12H14	122057-61-8	10		
4	Benzene, 1-(1,1-dichlorocyclopro...	240	C13H14Cl2	296243-73-7	10		
5	(E)-methyl 3-(3-hydroxy-4-methox...	208	C11H12O4	1000441-28-8	10		



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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.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
unknown13.884	13.884	8.0	ug/l	17889	4	13.561	111896	50.0
unknown15.343	15.343	9.7	ug/l	21615	4	13.561	111896	50.0
unknown16.408	16.408	5.9	ug/l	13255	4	13.561	111896	50.0