

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042522\
 Data File : VY008488.D
 Acq On : 25 Apr 2022 17:37
 Operator : KP/MD
 Sample : N2548-01RE
 Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 MH-8SRE

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\82Y042122S.M

Title : SW846 8260

Signal : TIC: VY008488.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.131	46	51	58	rBV3	644	1831	16.51%	1.611%
2	2.327	82	83	91	rVB2	395	623	5.62%	0.548%
3	2.674	137	140	142	rVB	249	314	2.83%	0.276%
4	2.772	150	156	157	rBV	150	202	1.82%	0.178%
5	3.619	292	295	298	rBB	167	215	1.94%	0.189%
6	4.277	396	403	404	rBB	129	241	2.17%	0.212%
7	4.454	425	432	435	rBV	109	251	2.26%	0.221%
8	4.716	473	475	478	rVB	190	197	1.78%	0.173%
9	4.765	481	483	489	rVB	138	286	2.58%	0.252%
10	5.436	591	593	597	rBV	218	318	2.87%	0.280%
11	5.704	632	637	640	rBB	162	243	2.19%	0.214%
12	5.741	640	643	647	rBV	147	224	2.02%	0.197%
13	5.850	658	661	663	rBV	191	253	2.28%	0.223%
14	5.972	679	681	684	rBV	153	220	1.98%	0.194%
15	6.417	751	754	756	rBV	206	195	1.76%	0.172%
16	6.448	756	759	762	rVB	195	230	2.07%	0.202%
17	6.807	814	818	821	rBB	176	229	2.07%	0.201%
18	7.618	947	951	953	rBV	168	251	2.26%	0.221%
19	7.722	959	968	974	rBV4	1445	3418	30.82%	3.007%
20	7.789	974	979	988	rVV5	2407	5243	47.28%	4.613%
21	8.143	1026	1037	1044	rBB4	1689	4004	36.11%	3.523%
22	8.216	1047	1049	1052	rVB	231	249	2.25%	0.219%
23	8.325	1064	1067	1070	rBV2	186	253	2.28%	0.223%
24	8.484	1091	1093	1097	rVB	149	240	2.16%	0.211%
25	8.691	1121	1127	1135	rVB	4226	7441	67.10%	6.547%
26	8.923	1164	1165	1169	rVB	166	204	1.84%	0.179%
27	8.966	1169	1172	1173	rBV	175	201	1.81%	0.177%
28	9.020	1177	1181	1184	rBV	186	311	2.80%	0.274%
29	9.179	1204	1207	1211	rBV	112	203	1.83%	0.179%
30	9.667	1284	1287	1293	rBV	209	351	3.17%	0.309%
31	9.923	1326	1329	1332	rBV	221	301	2.71%	0.265%
32	10.057	1349	1351	1354	rVB	190	197	1.78%	0.173%
33	10.136	1359	1364	1365	rVV	183	238	2.15%	0.209%
34	10.179	1365	1371	1378	rVB	6347	11089	100.00%	9.757%
35	10.386	1399	1405	1408	rVB	153	341	3.08%	0.300%
36	10.581	1433	1437	1439	rBV	257	342	3.08%	0.301%

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37	11.038	1509	1512	1514	rVB2	180	201	1.81%	0.177%
38	11.093	1519	1521	1525	rVV3	487	627	5.65%	0.552%
39	11.197	1535	1538	1540	rBV	204	254	2.29%	0.223%
40	11.490	1580	1586	1592	rBV2	5531	8700	78.46%	7.655%
41	11.636	1607	1610	1612	rBV2	160	202	1.82%	0.178%
42	11.739	1618	1627	1630	rBV3	526	1007	9.08%	0.886%
43	11.782	1630	1634	1637	rVV2	355	426	3.84%	0.375%
44	11.837	1641	1643	1648	rBV	288	341	3.08%	0.300%
45	12.008	1663	1671	1676	rBV2	1037	1827	16.48%	1.607%
46	12.081	1682	1683	1687	rVV	232	257	2.32%	0.226%
47	12.117	1687	1689	1694	rVB4	984	1416	12.77%	1.246%
48	12.166	1694	1697	1699	rBV3	476	554	5.00%	0.487%
49	12.209	1699	1704	1706	rVV4	1211	2178	19.64%	1.916%
50	12.245	1706	1710	1716	rVB5	1913	3671	33.10%	3.230%
51	12.288	1716	1717	1720	rBV2	307	313	2.82%	0.275%
52	12.313	1720	1721	1724	rVB	243	231	2.08%	0.203%
53	12.373	1729	1731	1734	rVB3	416	497	4.48%	0.437%
54	12.483	1742	1749	1756	rVB2	3756	5861	52.85%	5.157%
55	12.562	1758	1762	1765	rBV3	501	836	7.54%	0.736%
56	12.611	1765	1770	1772	rVV4	424	659	5.94%	0.580%
57	12.642	1772	1775	1782	rVB3	2180	3197	28.83%	2.813%
58	12.727	1784	1789	1791	rBV3	772	1186	10.70%	1.043%
59	12.806	1794	1802	1807	rBV7	2333	5451	49.16%	4.796%
60	12.861	1807	1811	1816	rVB5	1001	1952	17.60%	1.717%
61	12.910	1816	1819	1820	rVB2	272	198	1.79%	0.174%
62	12.947	1820	1825	1830	rBV5	870	1635	14.74%	1.439%
63	12.983	1830	1831	1832	rBV	523	331	2.98%	0.291%
64	13.038	1837	1840	1843	rBV3	1032	1086	9.79%	0.956%
65	13.123	1851	1854	1857	rBV2	193	286	2.58%	0.252%
66	13.221	1867	1870	1871	rBV2	321	282	2.54%	0.248%
67	13.300	1878	1883	1884	rBV4	914	1348	12.16%	1.186%
68	13.318	1884	1886	1890	rVB2	1614	2063	18.60%	1.815%
69	13.428	1899	1904	1909	rBV4	3464	5101	46.00%	4.488%
70	13.483	1911	1913	1917	rVB3	359	298	2.69%	0.262%
71	13.568	1923	1927	1931	rVB2	590	863	7.78%	0.759%
72	13.605	1931	1933	1936	rVB	342	334	3.01%	0.294%
73	13.642	1936	1939	1942	rVB	317	305	2.75%	0.268%
74	13.678	1943	1945	1949	rBV	278	355	3.20%	0.312%
75	13.745	1949	1956	1961	rBV4	2405	4487	40.46%	3.948%
76	13.788	1961	1963	1964	rBV	565	354	3.19%	0.311%

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77	13.855	1970	1974	1977	rBV4	493	838	7.56%	0.737%
78	13.928	1983	1986	1989	rBV3	731	1051	9.48%	0.925%
79	13.965	1989	1992	1995	rVB3	337	470	4.24%	0.414%
80	14.257	2035	2040	2046	rBV5	1181	2447	22.07%	2.153%
81	14.428	2064	2068	2072	rVB4	812	1192	10.75%	1.049%
82	14.526	2081	2084	2088	rVB	283	421	3.80%	0.370%
83	14.568	2088	2091	2092	rBV	405	384	3.46%	0.338%
84	14.769	2122	2124	2127	rVB2	339	356	3.21%	0.313%
85	14.849	2136	2137	2139	rVB	307	211	1.90%	0.186%
86	14.879	2139	2142	2148	rBV3	328	409	3.69%	0.360%
87	14.958	2152	2155	2156	rBV	266	248	2.24%	0.218%
88	15.038	2166	2168	2171	rBV	225	247	2.23%	0.217%
89	15.221	2197	2198	2202	rVB2	262	245	2.21%	0.216%
90	15.611	2259	2262	2265	rBV3	222	230	2.07%	0.202%
91	15.934	2314	2315	2318	rBV2	205	231	2.08%	0.203%
92	16.031	2329	2331	2334	rBV2	301	310	2.80%	0.273%
93	16.062	2334	2336	2339	rVB3	236	248	2.24%	0.218%
94	16.245	2364	2366	2370	rBV	361	399	3.60%	0.351%
95	16.300	2373	2375	2377	rBV	181	223	2.01%	0.196%
96	16.422	2392	2395	2397	rBV2	261	270	2.43%	0.238%
97	16.458	2400	2401	2408	rVV2	232	382	3.44%	0.336%
98	16.580	2418	2421	2423	rBV	200	289	2.61%	0.254%
99	16.659	2433	2434	2437	rVB3	342	198	1.79%	0.174%
100	16.714	2441	2443	2448	rBV3	211	238	2.15%	0.209%

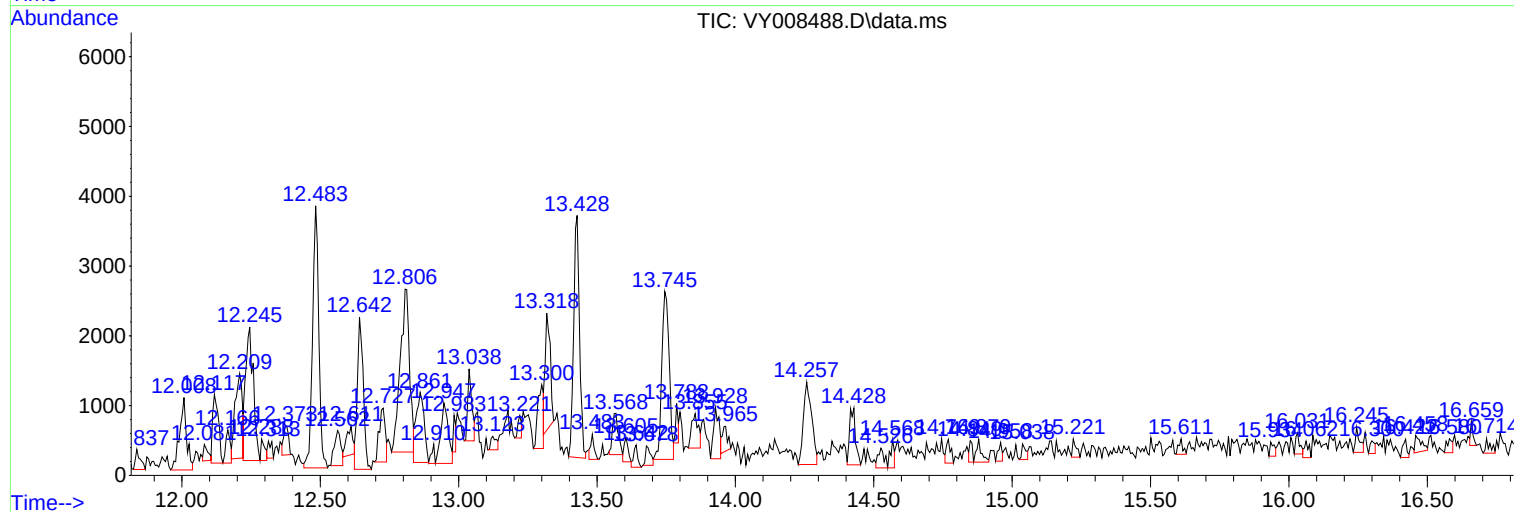
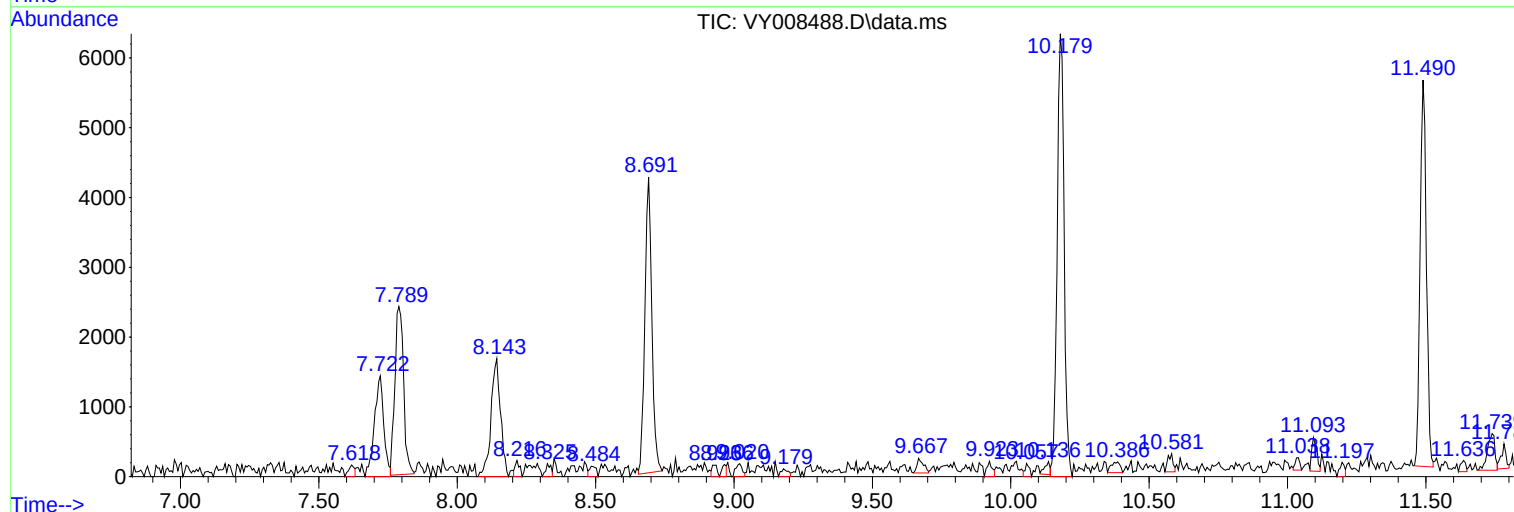
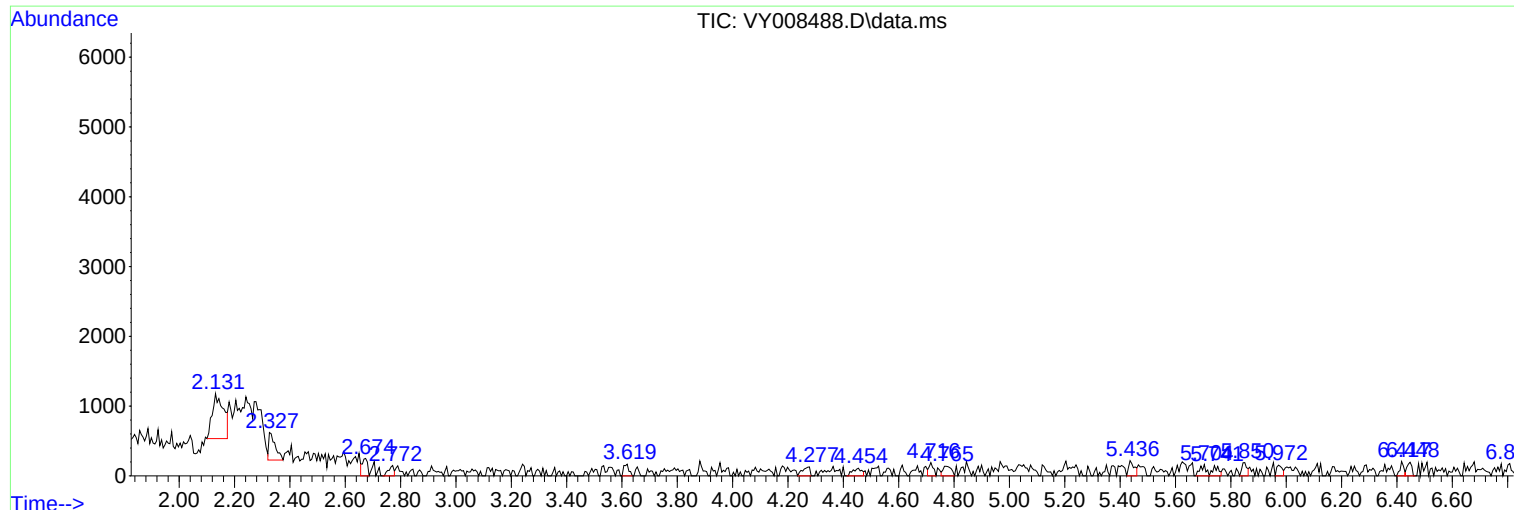
Sum of corrected areas: 113656

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Quant Title : SW846 8260

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



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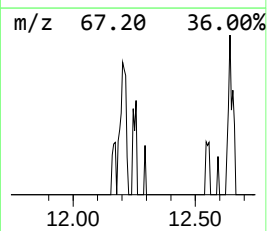
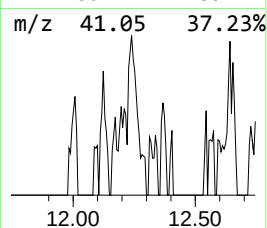
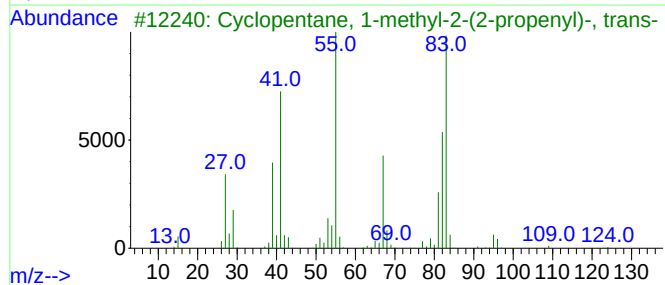
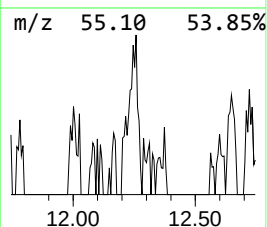
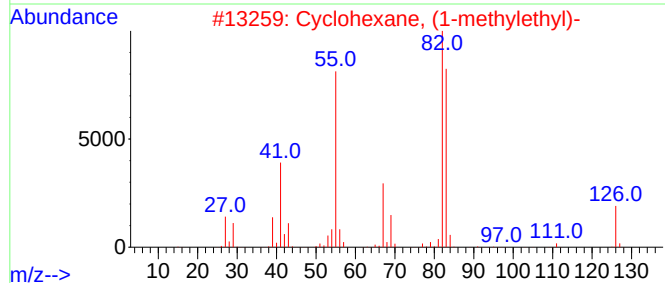
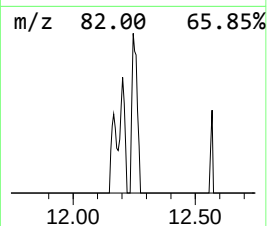
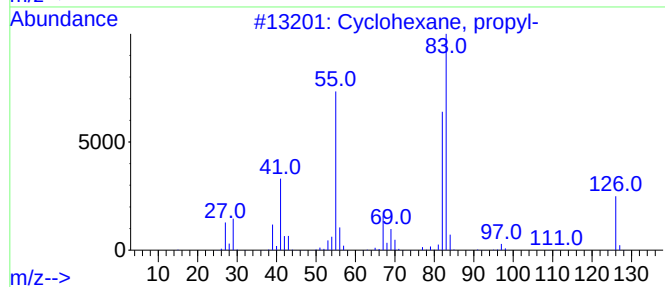
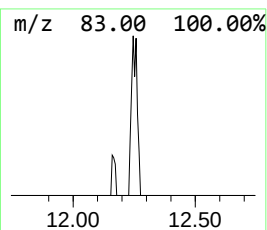
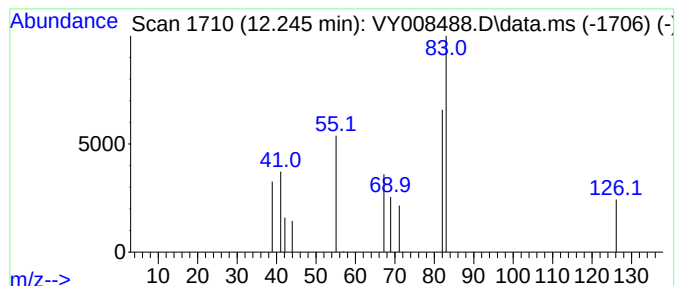
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclohexane, propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.246	21.10 ug/l	3671	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, propyl-	126	C9H18	001678-92-8	59
2			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	38
3			Cyclopentane, 1-methyl-2-(2-prop...	124	C9H16	050746-53-7	33
4			Trichloroacetic acid, 6-chlorohe...	280	C8H12Cl4O2	1000330-89-2	28
5			Oxalic acid, cyclohexyl dodecyl ...	340	C20H36O4	1000309-31-4	17



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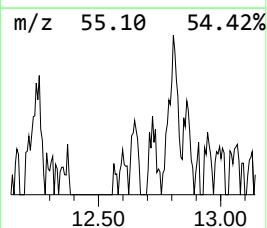
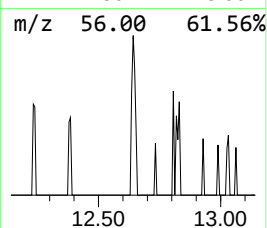
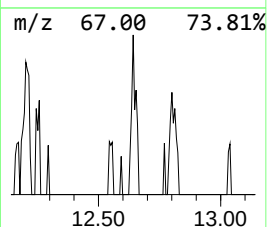
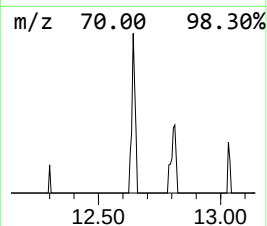
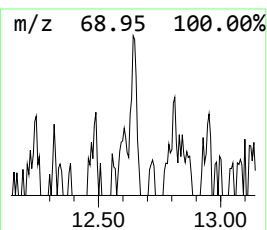
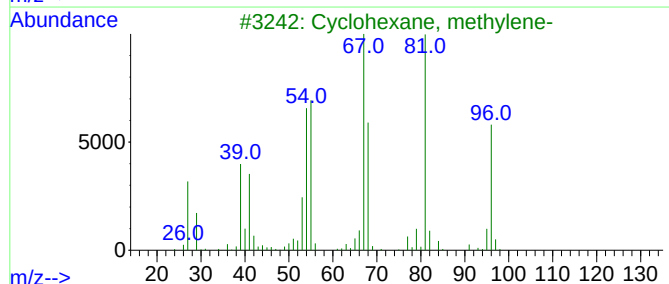
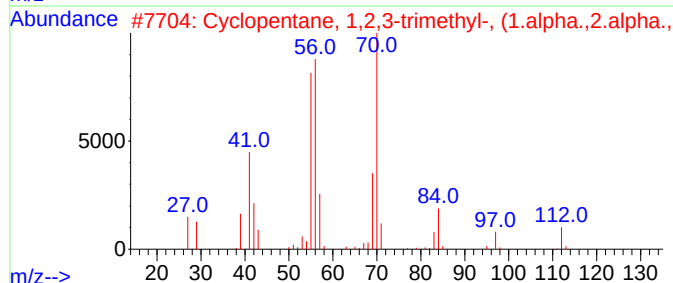
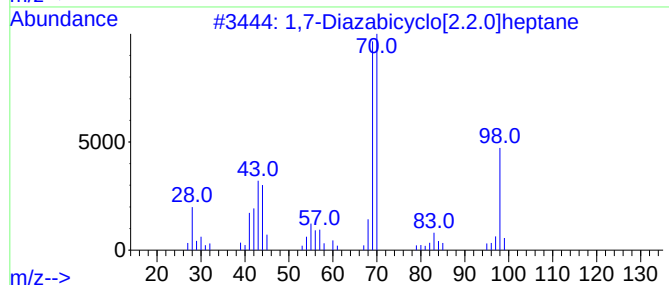
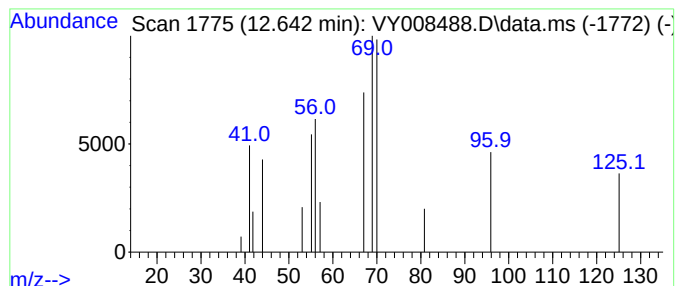
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.642 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.642	31.34 ug/l	3197	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,7-Diazabicyclo[2.2.0]heptane	98	C5H10N2	000279-42-5	23
2			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	015890-40-1	10
3			Cyclohexane, methylene-	96	C7H12	001192-37-6	10
4			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	10
5			1-Hexene, 3-methyl-	98	C7H14	003404-61-3	9



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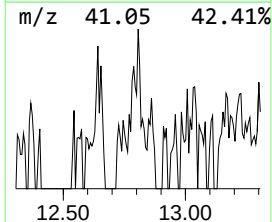
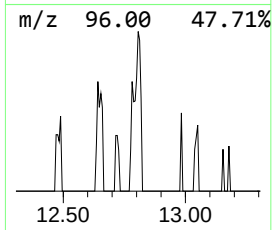
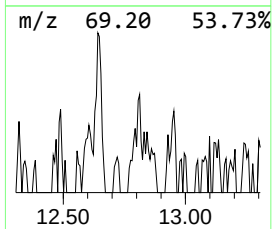
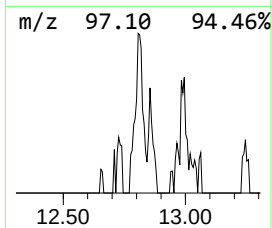
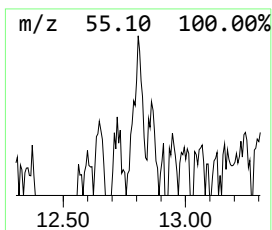
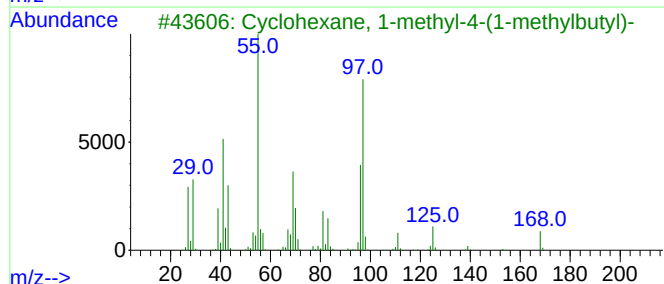
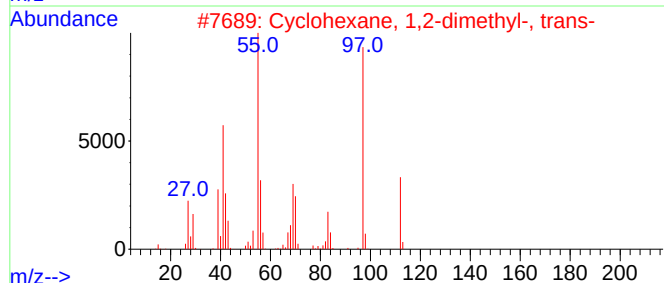
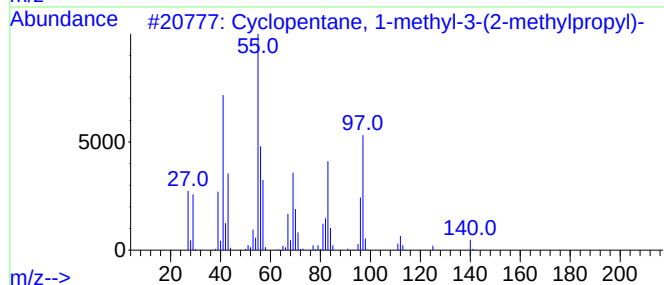
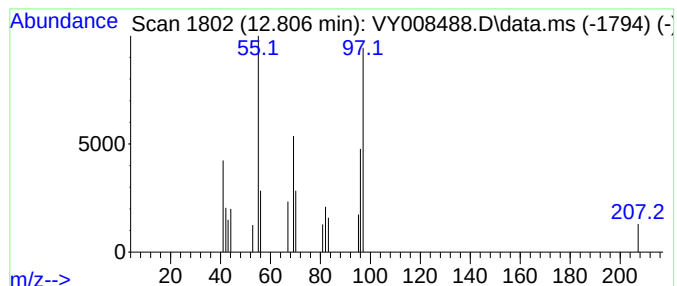
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Quant Title : SW846 8260

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

Peak Number 4 unknown12.806 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.806	53.43 ug/l	5451	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-methyl-3-(2-meth...	140	C10H20	029053-04-1	45
2			Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	43
3			Cyclohexane, 1-methyl-4-(1-methy...	168	C12H24	054411-00-6	42
4			Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-97-1	40
5			trans-1,3-Diethylcyclopentane	126	C9H18	1000113-87-1	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042522\
Data File : VY008488.D
Acq On : 25 Apr 2022 17:37
Operator : KP/MD
Sample : N2548-01RE
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
MH-8SRE

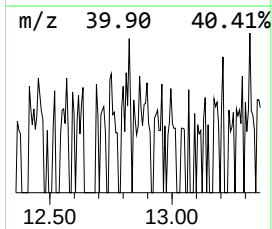
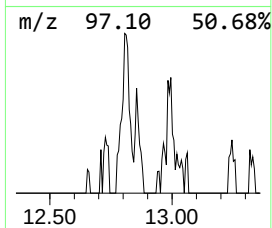
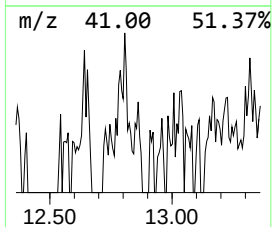
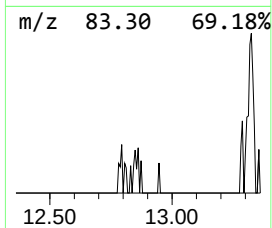
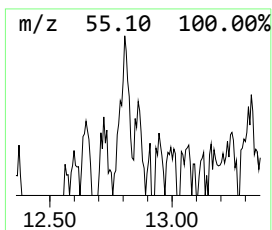
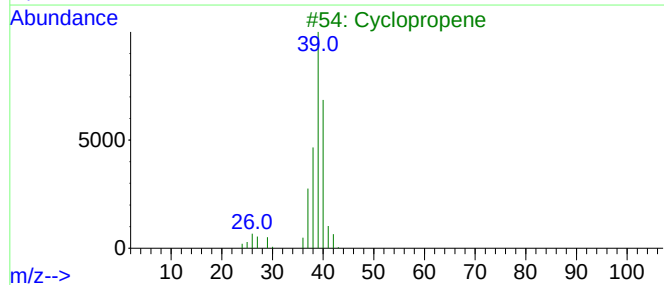
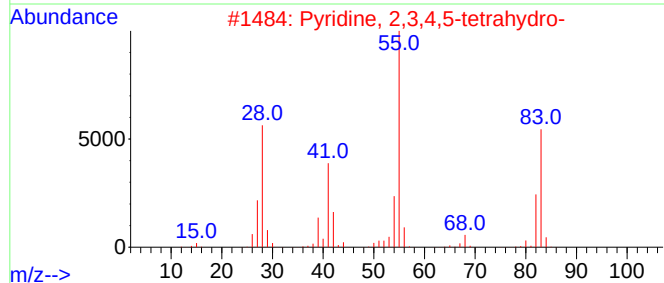
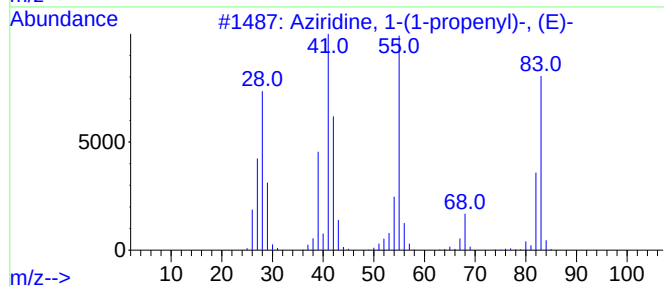
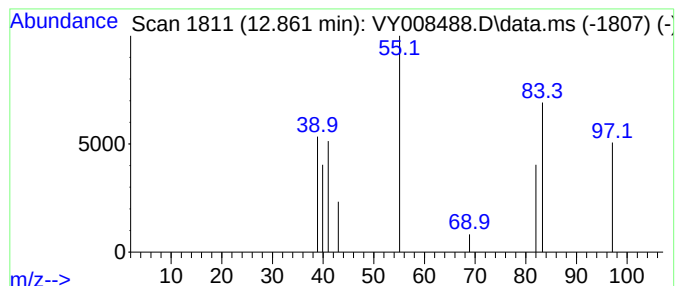
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Quant Title : SW846 8260

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

Peak Number 5 unknown12.861 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.861	19.13 ug/l	1952	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	37
2			Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	7
3			Cyclopropene	40	C3H4	002781-85-3	5
4			2-Cyclopenten-1-one	82	C5H6O	000930-30-3	4
5			1-Methoxy-1-buten-3-yne	82	C5H6O	002798-73-4	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042522\
Data File : VY008488.D
Acq On : 25 Apr 2022 17:37
Operator : KP/MD
Sample : N2548-01RE
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
MH-8SRE

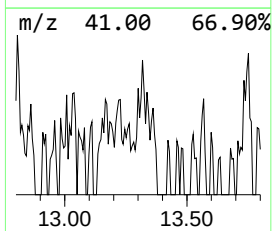
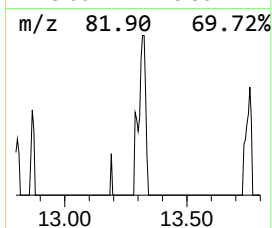
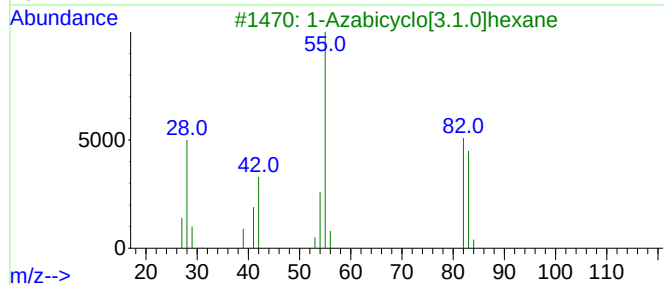
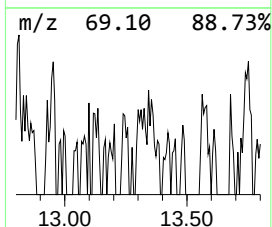
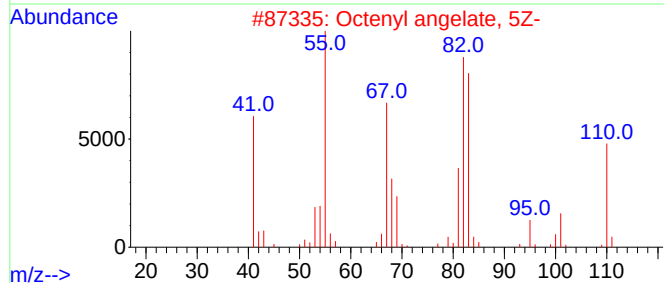
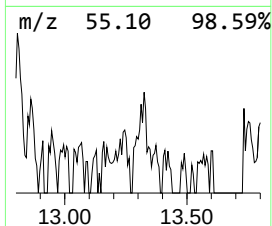
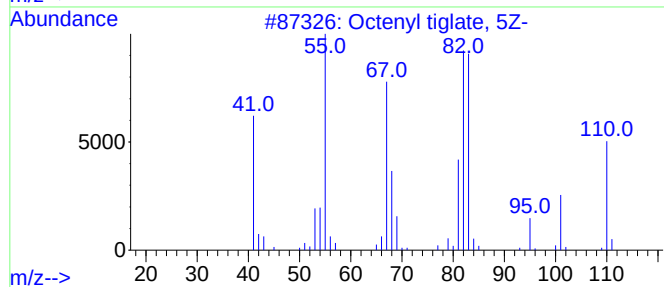
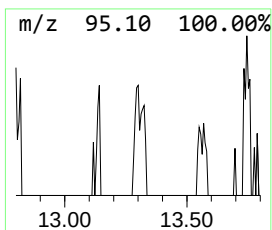
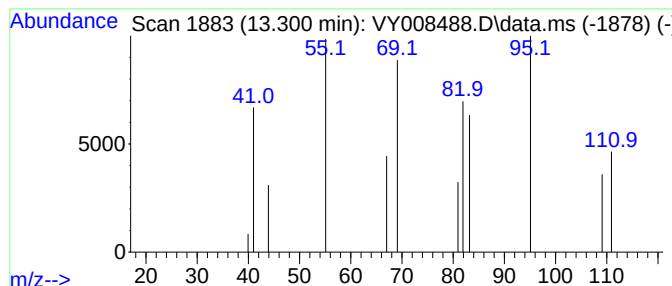
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Quant Title : SW846 8260

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

Peak Number 7 unknown13.300 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.300	13.21 ug/l	1348	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octenyl tiglate, 5Z-	210	C13H22O2	1000383-60-1	12
2			Octenyl angelate, 5Z-	210	C13H22O2	1000383-60-2	12
3			1-Azabicyclo[3.1.0]hexane	83	C5H9N	000285-76-7	9
4			cis-3-Hexenylpyruvate	170	C9H14O3	068133-76-6	9
5			Cyclopentane, 1-methyl-2-(2-prop...	124	C9H16	050746-53-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042522\
Data File : VY008488.D
Acq On : 25 Apr 2022 17:37
Operator : KP/MD
Sample : N2548-01RE
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
MH-8SRE

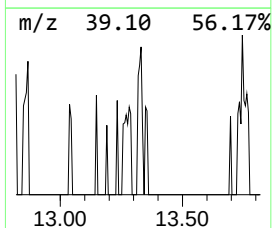
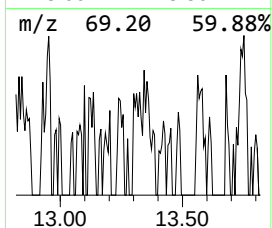
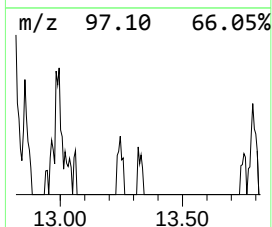
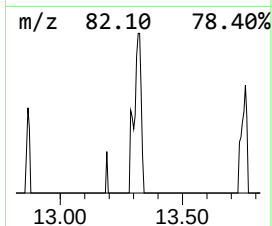
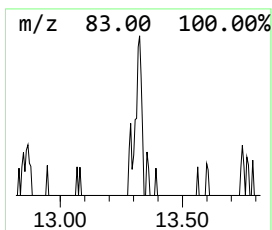
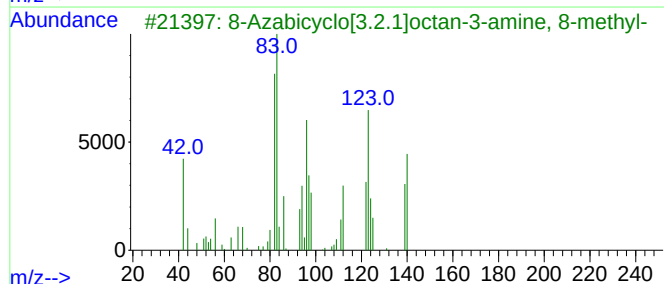
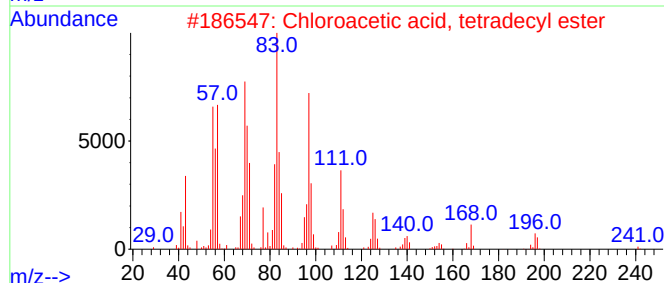
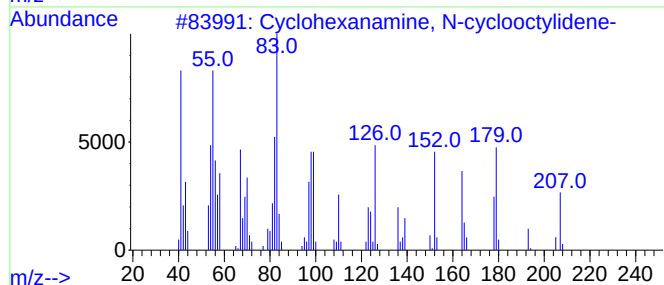
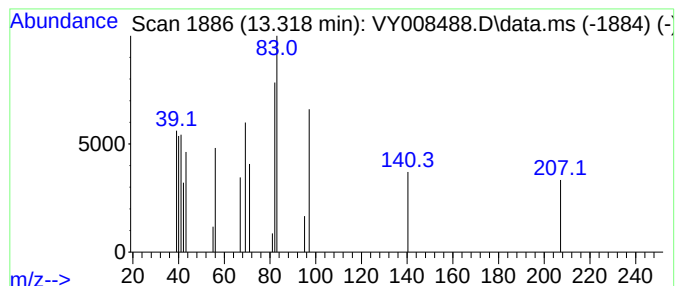
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Quant Title : SW846 8260

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

Peak Number 8 Cyclohexanamine, N-cyclooct... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.318	20.22 ug/l	2063	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanamine, N-cyclooctylidene-	207	C14H25N	054699-42-2	50
2			Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	47
3			8-Azabicyclo[3.2.1]octan-3-amine...	140	C8H16N2	098998-25-5	47
4			Carbonic acid, tetradecyl 2,2,2-...	388	C17H31Cl3O3	1000314-56-0	47
5			Pentadecafluorooctanoic acid, do...	580	C20H23F15O2	1000406-81-3	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042522\
Data File : VY008488.D
Acq On : 25 Apr 2022 17:37
Operator : KP/MD
Sample : N2548-01RE
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
MH-8SRE

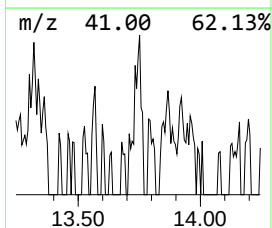
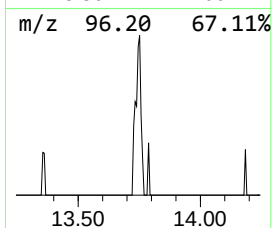
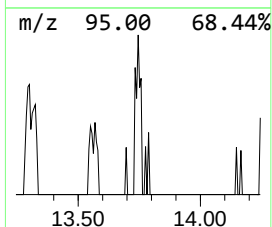
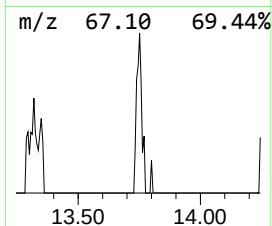
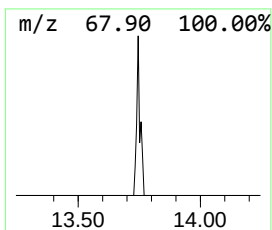
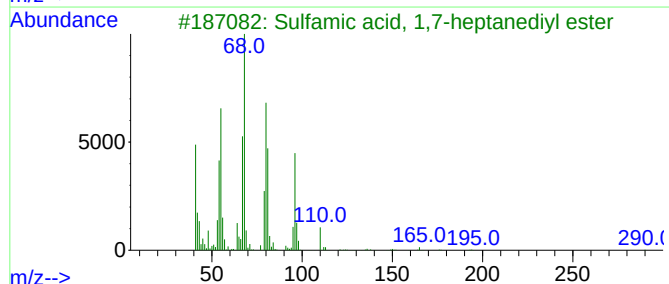
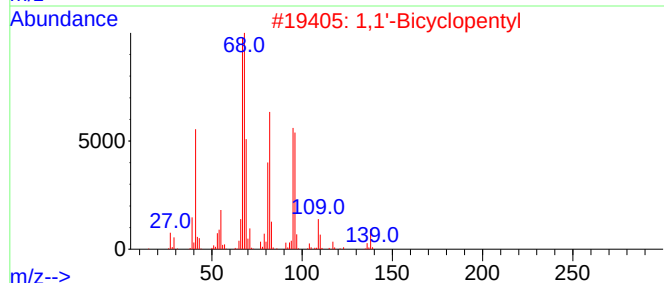
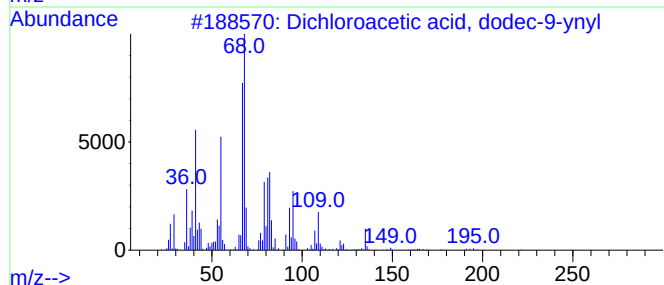
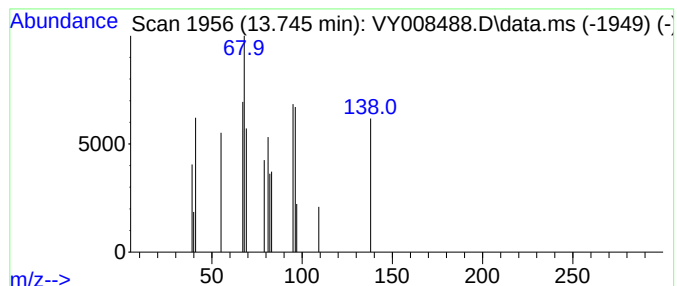
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Quant Title : SW846 8260

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

Peak Number 9 Dichloroacetic acid, dodec-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	43.98 ug/l	4487	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, dodec-9-ynyl	292	C14H22Cl2O2	1000282-98-0	50
2			1,1'-Bicyclopentyl	138	C10H18	001636-39-1	47
3			Sulfamic acid, 1,7-heptanediyl e...	290	C7H18N2O6S2	096892-57-8	47
4			2-Cyclohexen-1-one, 3,4,4-trimet...	138	C9H14O	017299-41-1	38
5			Bromoacetic acid, 10-undecenyl e...	290	C13H23BrO2	195373-65-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042522\
Data File : VY008488.D
Acq On : 25 Apr 2022 17:37
Operator : KP/MD
Sample : N2548-01RE
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
MH-8SRE

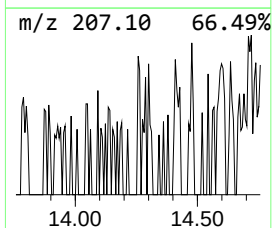
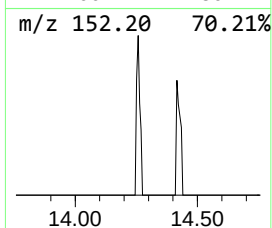
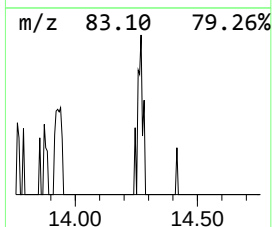
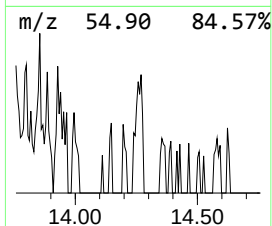
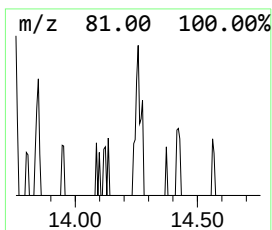
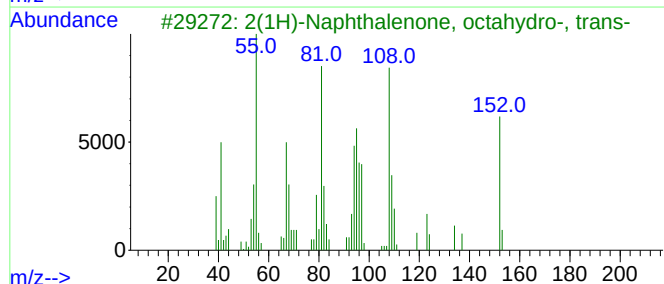
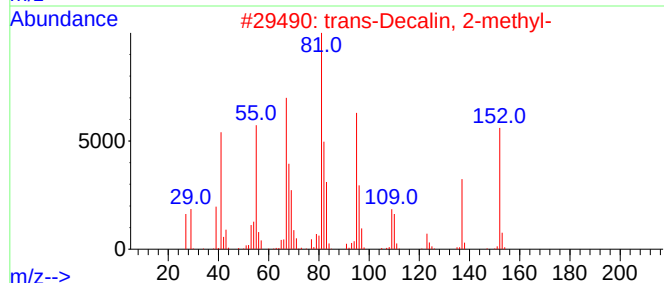
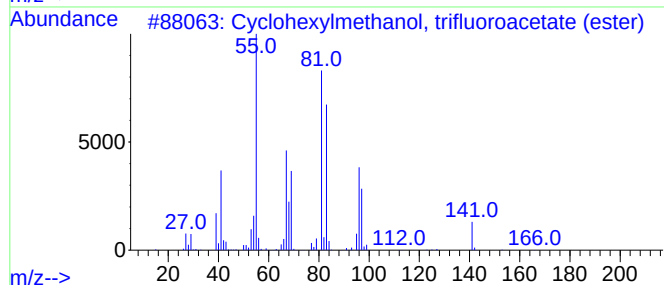
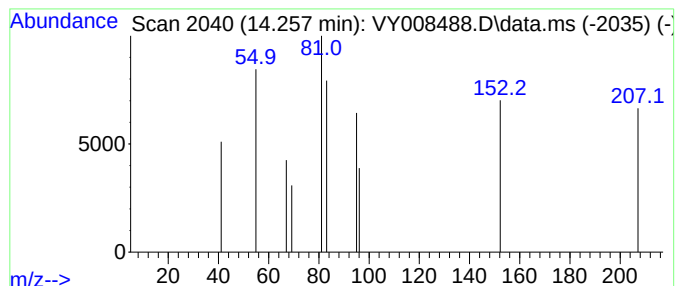
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Quant Title : SW846 8260

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

Peak Number 10 Cyclohexylmethanol, trifluo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	23.99 ug/l	2447	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexylmethanol, trifluoroace...	210	C9H13F3O2	164071-20-9	50
2			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	50
3			2(1H)-Naphthalenone, octahydro-,...	152	C10H16O	016021-08-2	49
4			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	47
5			1-Decalone (cis-trans)	152	C10H16O	004832-16-0	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042522\
Data File : VY008488.D
Acq On : 25 Apr 2022 17:37
Operator : KP/MD
Sample : N2548-01RE
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
MH-8SRE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.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
Cyclohexane, pr...	12.246	21.1	ug/l	3671	3	11.490	8700	50.0
unknown12.642	12.642	31.3	ug/l	3197	4	13.422	5101	50.0
unknown12.806	12.806	53.4	ug/l	5451	4	13.422	5101	50.0
unknown12.861	12.861	19.1	ug/l	1952	4	13.422	5101	50.0
unknown13.300	13.300	13.2	ug/l	1348	4	13.422	5101	50.0
Cyclohexanamine...	13.318	20.2	ug/l	2063	4	13.422	5101	50.0
Dichloroacetic ...	13.745	44.0	ug/l	4487	4	13.422	5101	50.0
Cyclohexylmetha...	14.257	24.0	ug/l	2447	4	13.422	5101	50.0