

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051123\
 Data File : VY013715.D
 Acq On : 11 May 2023 14:37
 Operator : KP/MD
 Sample : 02743-01
 Misc : 5.05g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 DRUM-A-SLUDGE

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\82Y042423S.M

Title : SW846 8260

Signal : TIC: VY013715.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.863	3	7	14	rVB4	8977	13475	4.44%	0.629%
2	2.503	108	112	117	rBV6	1844	3629	1.20%	0.169%
3	3.948	338	349	350	rBV2	1920	5089	1.68%	0.238%
4	4.198	380	390	393	rBV4	2050	5407	1.78%	0.253%
5	4.710	466	474	485	rVB4	6534	20120	6.64%	0.940%
6	7.716	957	967	973	rBV2	48474	118000	38.92%	5.511%
7	7.789	973	979	990	rVB	79070	175409	57.86%	8.192%
8	8.136	1027	1036	1047	rBV	51099	115110	37.97%	5.376%
9	8.685	1117	1126	1139	rBV	110506	221635	73.10%	10.351%
10	10.179	1363	1371	1379	rBV	177247	303187	100.00%	14.159%
11	10.581	1431	1437	1441	rBV2	3477	6300	2.08%	0.294%
12	11.386	1563	1569	1573	rBV5	1681	3114	1.03%	0.145%
13	11.490	1579	1586	1596	rBV	161408	276159	91.09%	12.897%
14	11.727	1620	1625	1631	rVV4	3118	4917	1.62%	0.230%
15	12.008	1663	1671	1678	rBV5	4005	11974	3.95%	0.559%
16	12.124	1684	1690	1694	rBV5	3205	4869	1.61%	0.227%
17	12.252	1705	1711	1714	rBV6	4014	7101	2.34%	0.332%
18	12.380	1725	1732	1735	rBV6	2110	4745	1.57%	0.222%
19	12.410	1735	1737	1742	rVV6	2913	4457	1.47%	0.208%
20	12.483	1742	1749	1760	rVB2	126845	214443	70.73%	10.015%
21	12.648	1772	1776	1782	rVB6	2914	5494	1.81%	0.257%
22	12.806	1792	1802	1807	rVV7	8773	17794	5.87%	0.831%
23	12.861	1807	1811	1816	rVB5	3999	6795	2.24%	0.317%
24	12.916	1816	1820	1823	rBV5	2174	3853	1.27%	0.180%
25	12.953	1823	1826	1829	rVB3	2521	3391	1.12%	0.158%
26	13.008	1829	1835	1837	rBV6	3199	6765	2.23%	0.316%
27	13.038	1837	1840	1847	rVB7	3655	7213	2.38%	0.337%
28	13.160	1856	1860	1865	rBV6	2042	4417	1.46%	0.206%
29	13.288	1877	1881	1884	rBV5	2865	4553	1.50%	0.213%
30	13.325	1884	1887	1890	rVV5	4711	6695	2.21%	0.313%
31	13.355	1890	1892	1896	rVV5	2791	3678	1.21%	0.172%
32	13.422	1896	1903	1910	rVV	145142	230975	76.18%	10.787%
33	13.751	1948	1957	1961	rBV4	14330	25096	8.28%	1.172%
34	13.794	1961	1964	1968	rVB5	2343	3435	1.13%	0.160%
35	13.959	1986	1991	1997	rVB2	19248	32735	10.80%	1.529%
36	14.007	1997	1999	2005	rVB3	2951	3725	1.23%	0.174%

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37	14.135	2016	2020	2023	rBV5	2895	4359	1.44%	0.204%
38	14.196	2026	2030	2033	rVV5	3498	5676	1.87%	0.265%
39	14.257	2033	2040	2047	rVV10	9613	26973	8.90%	1.260%
40	14.312	2047	2049	2056	rVV8	3156	5281	1.74%	0.247%
41	14.385	2056	2061	2064	rVV6	4062	7937	2.62%	0.371%
42	14.422	2064	2067	2071	rVV3	5971	8723	2.88%	0.407%
43	14.477	2071	2076	2080	rVB6	4150	7349	2.42%	0.343%
44	14.611	2090	2098	2105	rBV4	17007	26152	8.63%	1.221%
45	14.678	2105	2109	2112	rBV5	5933	9954	3.28%	0.465%
46	14.727	2113	2117	2124	rVB5	9398	16712	5.51%	0.780%
47	14.800	2124	2129	2132	rBV7	3904	6074	2.00%	0.284%
48	14.849	2133	2137	2140	rBV5	5479	9646	3.18%	0.450%
49	14.940	2146	2152	2157	rVB8	4606	9160	3.02%	0.428%
50	15.032	2163	2167	2174	rVV9	5481	13335	4.40%	0.623%
51	15.093	2174	2177	2179	rVV4	3989	5204	1.72%	0.243%
52	15.135	2181	2184	2190	rVB8	7004	12873	4.25%	0.601%
53	15.208	2190	2196	2201	rBV4	8682	16475	5.43%	0.769%
54	15.263	2201	2205	2207	rBV4	4378	6226	2.05%	0.291%
55	15.312	2210	2213	2219	rVB2	9143	14068	4.64%	0.657%
56	15.434	2229	2233	2238	rVB3	15839	22337	7.37%	1.043%
57	16.031	2324	2331	2336	rBV8	4006	8830	2.91%	0.412%
58	16.092	2336	2341	2345	rVB5	2743	4625	1.53%	0.216%
59	16.355	2378	2384	2389	rBV7	3652	7559	2.49%	0.353%

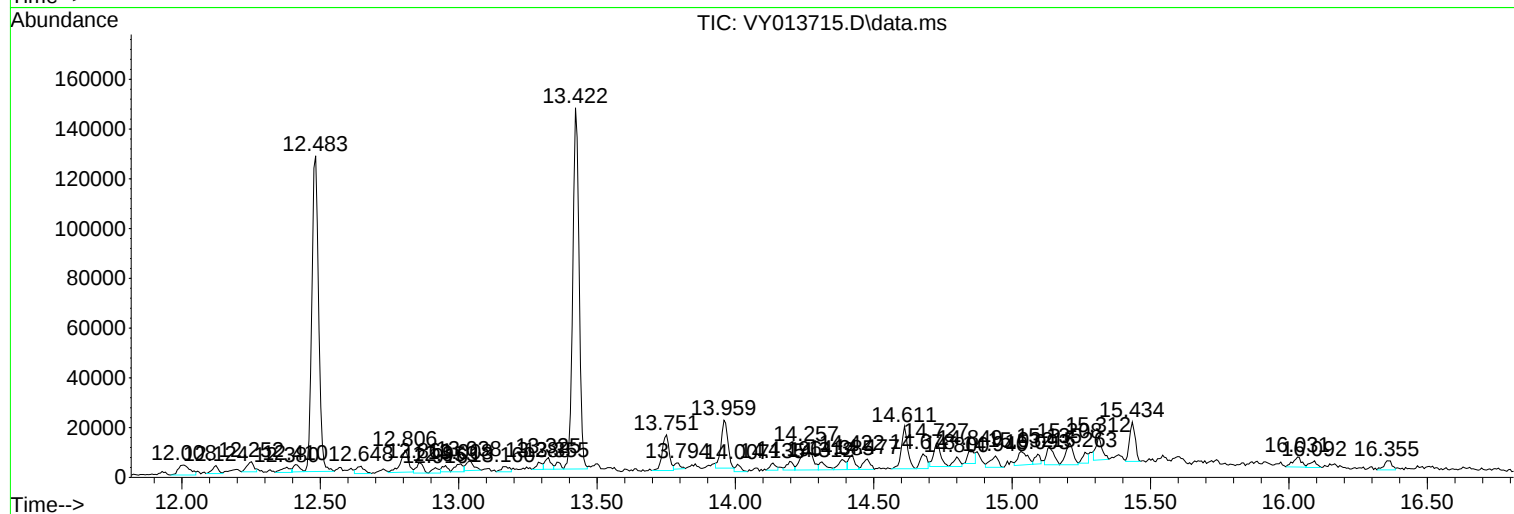
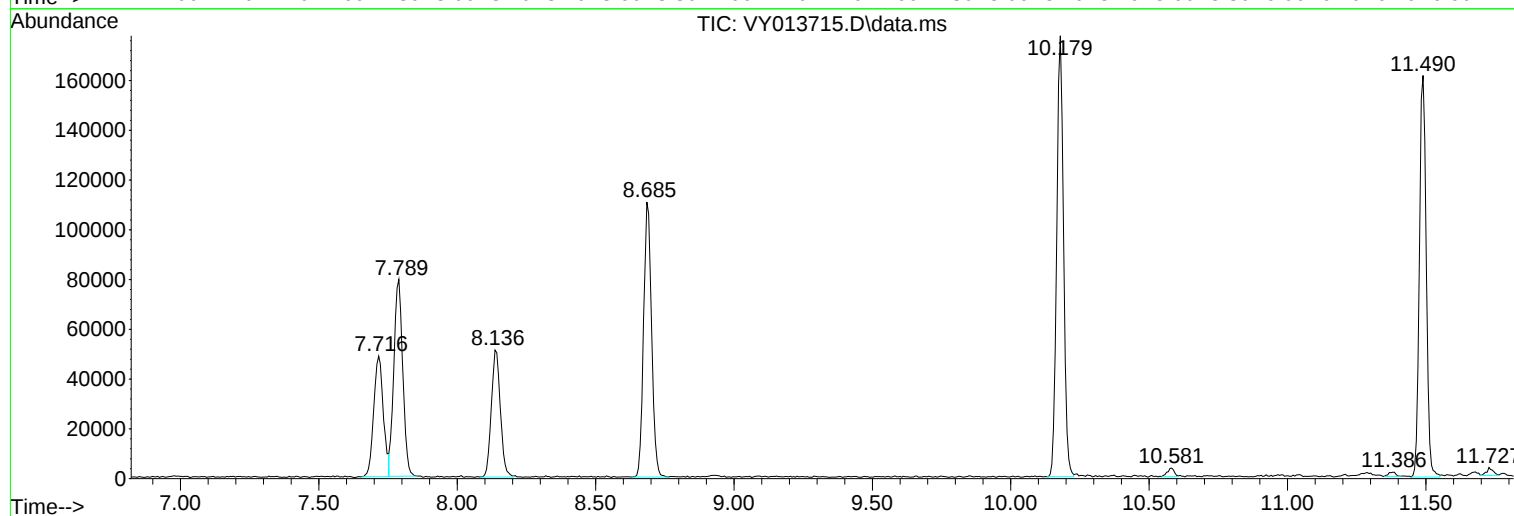
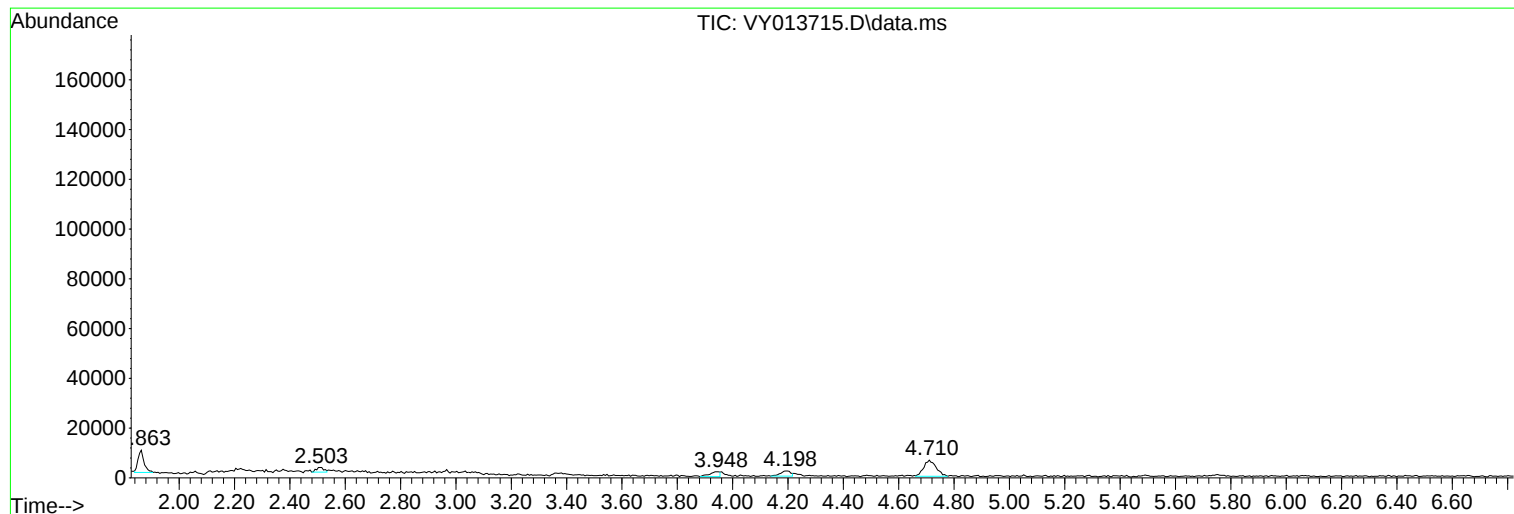
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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



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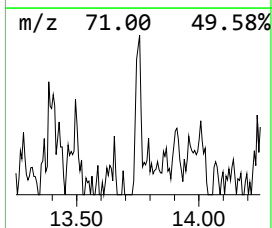
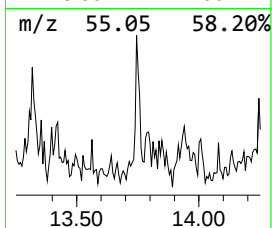
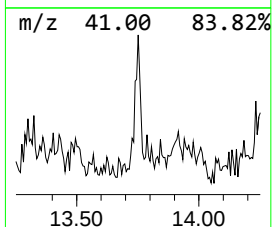
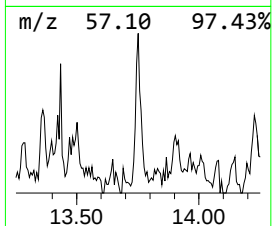
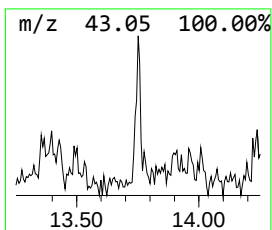
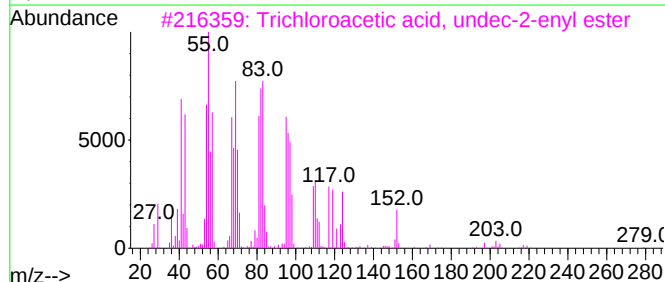
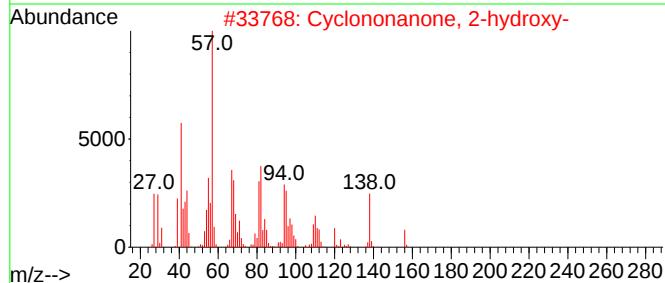
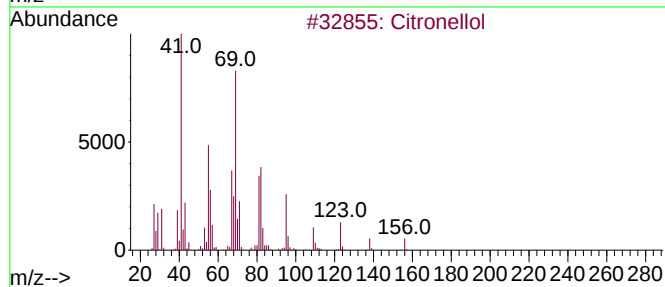
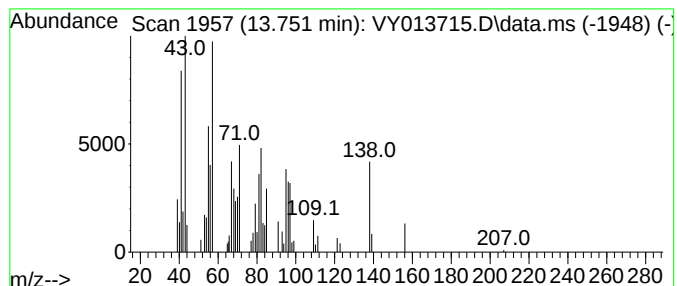
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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

Peak Number 2 Citronellol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	5.43 ug/l	25096	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Citronellol	156	C10H20O	000106-22-9	52
2			Cyclononane, 2-hydroxy-	156	C9H16O2	000496-83-3	46
3			Trichloroacetic acid, undec-2-en...	314	C13H21Cl3O2	1000299-26-1	43
4			Cyclohexene, 4-(1,1-dimethylethyl)-	138	C10H18	002228-98-0	38
5			Cyclopentanol, 2-methyl-, cis-	100	C6H12O	025144-05-2	35



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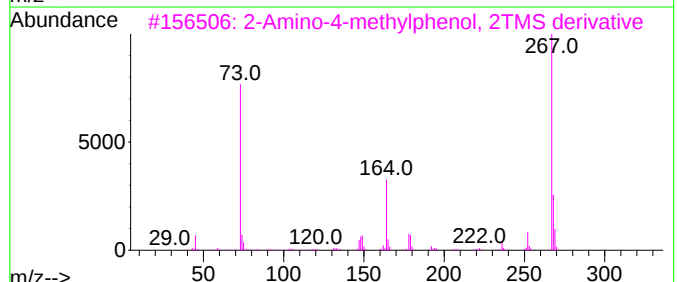
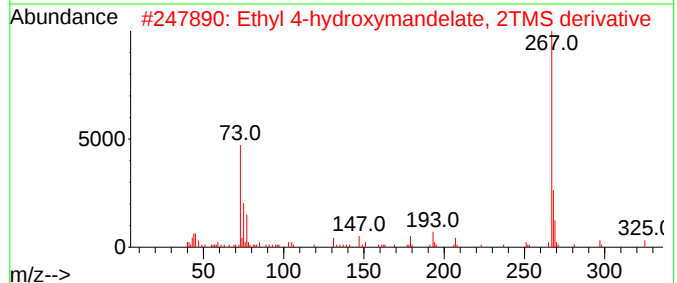
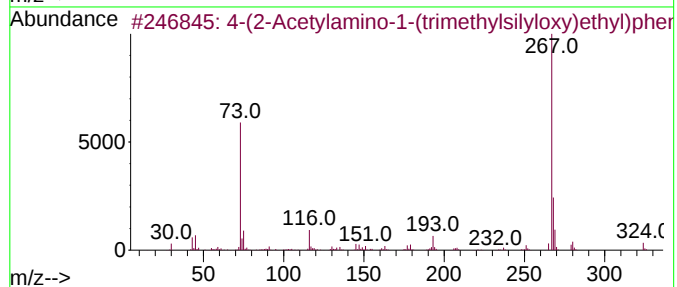
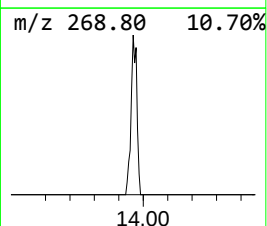
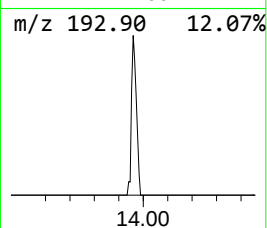
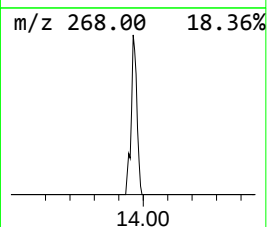
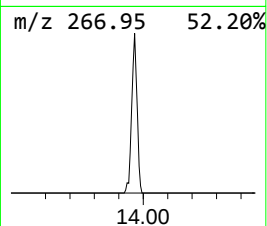
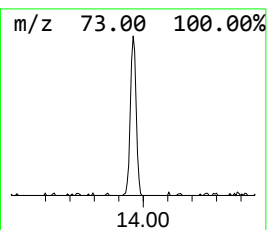
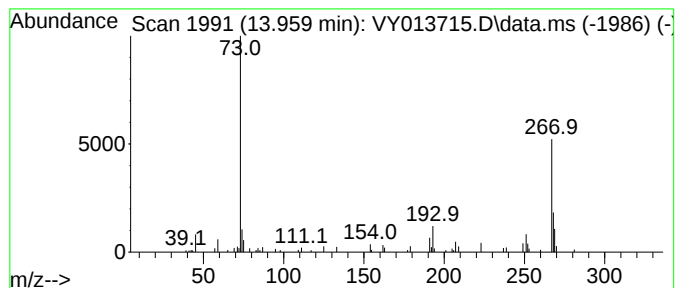
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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

Peak Number 3 4-(2-Acetylamino-1-(trimeth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.959	7.09 ug/l	32735	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(2-Acetylamino-1-(trimethylsil...	339	C16H29NO3Si2	1000373-43-5	50
2			Ethyl 4-hydroxymandelate, 2TMS d...	340	C16H28O4Si2	1010071-53-3	50
3			2-Amino-4-methylphenol, 2TMS der...	267	C13H25NOSi2	1000373-28-1	45
4			3-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-88-9	45
5			Phenylpropylamine, N-acetyl-3,4,...	267	C14H21NO4	112369-97-8	43



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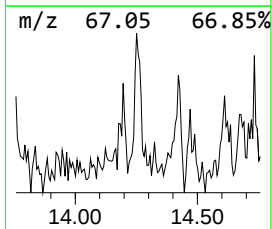
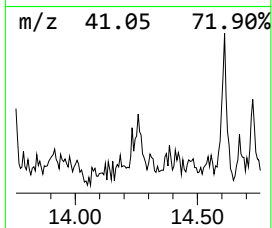
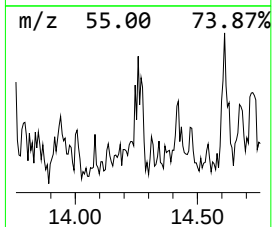
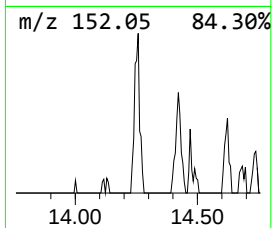
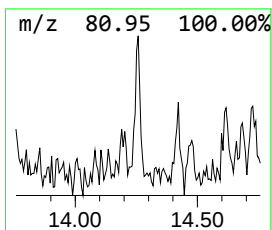
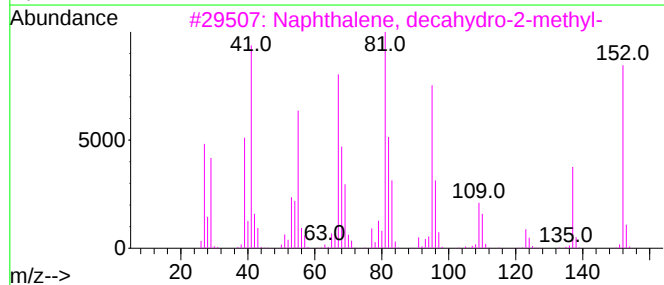
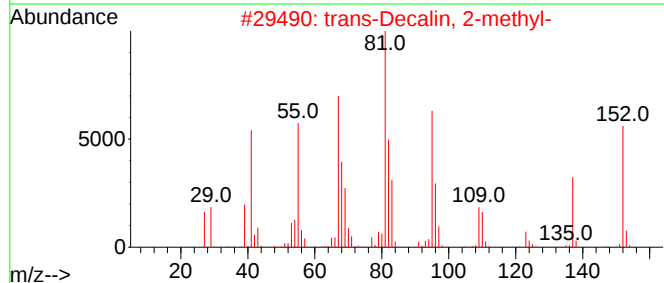
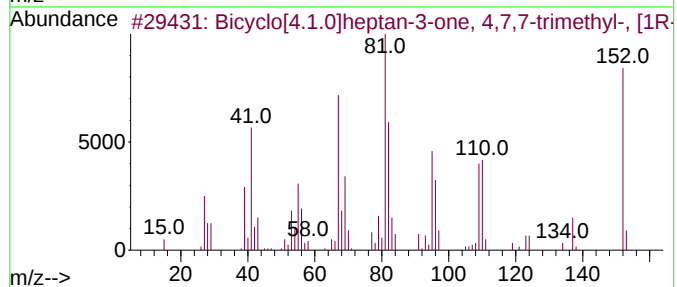
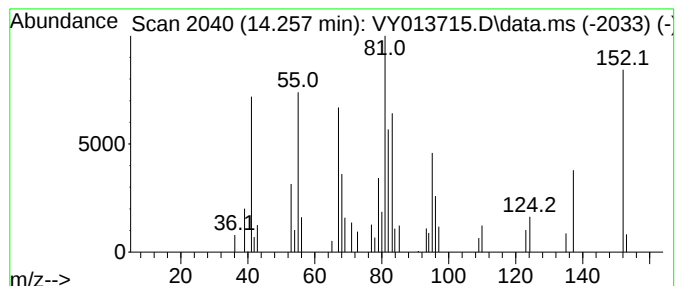
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Bicyclo[4.1.0]heptan-3-one,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	5.84 ug/l	26973	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]heptan-3-one, 4,7,...	152	C10H16O	004176-04-9	91
2			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	91
3			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	89
4			Bicyclo[4.1.0]heptan-3-one, 4,7,...	152	C10H16O	004176-01-6	81
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	64



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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
Citronellol	13.751	5.4	ug/l	25096	4	13.422	230975	50.0
4-(2-Acetylamino-5-methylphenyl)-2-methyl-5-pyridinol	13.959	7.1	ug/l	32735	4	13.422	230975	50.0
Bicyclo[4.1.0]hept-2-en-2-ol	14.257	5.8	ug/l	26973	4	13.422	230975	50.0