

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060123\
 Data File : VY013972.D
 Acq On : 01 Jun 2023 18:25
 Operator : KP/MD
 Sample : 02983-08RE
 Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SB07RE

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\82Y060123S.M
 Title : SW846 8260

Signal : TIC: VY013972.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.887	10	11	14	rBV2	719	631	2.09%	0.292%
2	2.150	52	54	57	rVB3	922	857	2.84%	0.396%
3	2.211	62	64	67	rVB2	1720	1768	5.85%	0.818%
4	2.522	113	115	118	rVB	571	452	1.50%	0.209%
5	2.662	134	138	139	rBV3	1142	1370	4.54%	0.634%
6	2.863	168	171	175	rBV2	286	494	1.64%	0.229%
7	2.930	178	182	184	rBV2	383	464	1.54%	0.215%
8	3.137	212	216	219	rBV3	366	543	1.80%	0.251%
9	3.204	225	227	231	rVB2	423	468	1.55%	0.217%
10	3.284	238	240	242	rVB2	434	416	1.38%	0.192%
11	3.326	245	247	249	rVV2	441	407	1.35%	0.188%
12	3.381	253	256	258	rBV2	457	380	1.26%	0.176%
13	3.875	332	337	338	rBV	377	449	1.49%	0.208%
14	3.918	342	344	347	rBV2	460	679	2.25%	0.314%
15	4.088	365	372	373	rBV2	804	1267	4.19%	0.586%
16	4.174	383	386	387	rBV2	431	500	1.66%	0.231%
17	4.381	418	420	422	rBV2	416	396	1.31%	0.183%
18	4.430	426	428	431	rBV	419	470	1.56%	0.217%
19	4.570	449	451	453	rBV2	402	400	1.32%	0.185%
20	4.619	457	459	464	rVB2	395	451	1.49%	0.209%
21	4.692	467	471	476	rBV3	765	1680	5.56%	0.777%
22	4.881	499	502	504	rBV	346	434	1.44%	0.201%
23	5.015	521	524	527	rVV	300	393	1.30%	0.182%
24	5.393	582	586	587	rBV2	388	439	1.45%	0.203%
25	5.734	639	642	643	rBV3	683	739	2.45%	0.342%
26	6.100	701	702	707	rBV2	255	500	1.66%	0.231%
27	6.393	748	750	754	rBV	442	388	1.28%	0.180%
28	6.545	772	775	778	rBV3	378	444	1.47%	0.205%
29	6.771	808	812	813	rBV2	440	443	1.47%	0.205%
30	6.838	819	823	824	rBV2	327	477	1.58%	0.221%
31	6.960	835	843	844	rBV3	2640	4087	13.53%	1.891%
32	7.076	860	862	865	rBV2	394	406	1.34%	0.188%
33	7.332	900	904	908	rBV3	291	439	1.45%	0.203%
34	7.716	960	967	972	rBV3	4379	10603	35.10%	4.905%
35	7.783	972	978	986	rVV2	8287	20155	66.73%	9.325%
36	7.838	986	987	991	rVB2	485	494	1.64%	0.229%

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37	7.905	995	998	1001	rBV	460	548	1.81%	0.254%
38	8.136	1027	1036	1045	rBV3	4972	11441	37.88%	5.293%
39	8.270	1054	1058	1063	rVB3	312	548	1.81%	0.254%
40	8.307	1063	1064	1067	rBV2	493	428	1.42%	0.198%
41	8.691	1120	1127	1134	rBV2	11709	23276	77.06%	10.769%
42	8.813	1146	1147	1150	rVB	512	377	1.25%	0.174%
43	8.844	1150	1152	1154	rBV2	513	560	1.85%	0.259%
44	9.167	1204	1205	1210	rVB2	381	539	1.78%	0.249%
45	9.209	1210	1212	1215	rBV2	353	510	1.69%	0.236%
46	9.368	1234	1238	1240	rBV	413	547	1.81%	0.253%
47	9.441	1247	1250	1254	rBV2	277	450	1.49%	0.208%
48	9.819	1309	1312	1316	rVB2	421	562	1.86%	0.260%
49	10.173	1365	1370	1379	rVB	15931	30204	100.00%	13.974%
50	10.270	1382	1386	1388	rBV2	436	595	1.97%	0.275%
51	10.563	1429	1434	1436	rBV2	319	547	1.81%	0.253%
52	10.813	1472	1475	1478	rBV2	342	490	1.62%	0.227%
53	11.020	1508	1509	1511	rBV	553	413	1.37%	0.191%
54	11.300	1554	1555	1559	rVB2	468	533	1.76%	0.247%
55	11.489	1580	1586	1593	rBV	14730	24067	79.68%	11.135%
56	11.764	1627	1631	1633	rBV2	392	474	1.57%	0.219%
57	12.020	1671	1673	1676	rVB2	452	427	1.41%	0.198%
58	12.209	1702	1704	1705	rBV2	628	438	1.45%	0.203%
59	12.258	1710	1712	1715	rBV3	335	446	1.48%	0.206%
60	12.331	1719	1724	1728	rBV4	2949	4729	15.66%	2.188%
61	12.483	1742	1749	1756	rBV3	11166	18008	59.62%	8.331%
62	12.587	1758	1766	1772	rVV5	1552	3163	10.47%	1.463%
63	12.636	1772	1774	1780	rVV3	217	400	1.32%	0.185%
64	12.697	1783	1784	1786	rBV	526	419	1.39%	0.194%
65	12.849	1806	1809	1811	rBV3	379	419	1.39%	0.194%
66	12.886	1811	1815	1821	rBV4	959	1796	5.95%	0.831%
67	13.245	1871	1874	1876	rBV3	671	611	2.02%	0.283%
68	13.337	1884	1889	1892	rBV3	1687	2219	7.35%	1.027%
69	13.422	1897	1903	1910	rBV2	8938	13894	46.00%	6.428%
70	13.678	1941	1945	1947	rVB2	619	543	1.80%	0.251%
71	13.696	1947	1948	1952	rVB2	500	511	1.69%	0.236%
72	13.879	1976	1978	1981	rVB2	490	461	1.53%	0.213%
73	13.965	1989	1992	1993	rBV3	711	795	2.63%	0.368%
74	14.093	2009	2013	2014	rBV2	557	540	1.79%	0.250%
75	14.129	2017	2019	2020	rBV2	526	396	1.31%	0.183%
76	14.276	2041	2043	2045	rBV	611	524	1.73%	0.242%

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77	14.336	2050	2053	2055	rBV2	346	394	1.30%	0.182%
78	14.532	2083	2085	2089	rVB3	406	525	1.74%	0.243%
79	14.745	2117	2120	2121	rBV3	450	483	1.60%	0.223%
80	14.818	2131	2132	2136	rVB2	840	657	2.18%	0.304%
81	14.873	2140	2141	2143	rBV2	579	413	1.37%	0.191%
82	14.964	2154	2156	2159	rVV3	467	489	1.62%	0.226%
83	14.995	2159	2161	2164	rVB3	631	590	1.95%	0.273%
84	15.025	2164	2166	2167	rBV2	427	446	1.48%	0.206%
85	15.044	2167	2169	2170	rVB	602	395	1.31%	0.183%
86	15.080	2173	2175	2177	rBV2	689	756	2.50%	0.350%
87	15.105	2177	2179	2183	rVB3	766	821	2.72%	0.380%
88	15.141	2183	2185	2187	rBV2	604	469	1.55%	0.217%
89	15.306	2211	2212	2214	rBV2	535	435	1.44%	0.201%
90	15.373	2221	2223	2224	rBV	904	613	2.03%	0.284%
91	15.483	2240	2241	2244	rVB3	743	633	2.10%	0.293%
92	15.787	2288	2291	2293	rVV2	527	527	1.74%	0.244%
93	15.818	2293	2296	2297	rVB3	529	504	1.67%	0.233%
94	15.909	2310	2311	2313	rBV2	540	398	1.32%	0.184%
95	16.001	2322	2326	2331	rBV4	566	1017	3.37%	0.471%
96	16.190	2355	2357	2359	rVB3	836	536	1.77%	0.248%
97	16.409	2392	2393	2396	rBV3	647	691	2.29%	0.320%
98	16.501	2406	2408	2410	rBV3	491	392	1.30%	0.181%
99	16.690	2436	2439	2440	rBV2	703	709	2.35%	0.328%
100	16.757	2448	2450	2451	rVB2	686	423	1.40%	0.196%

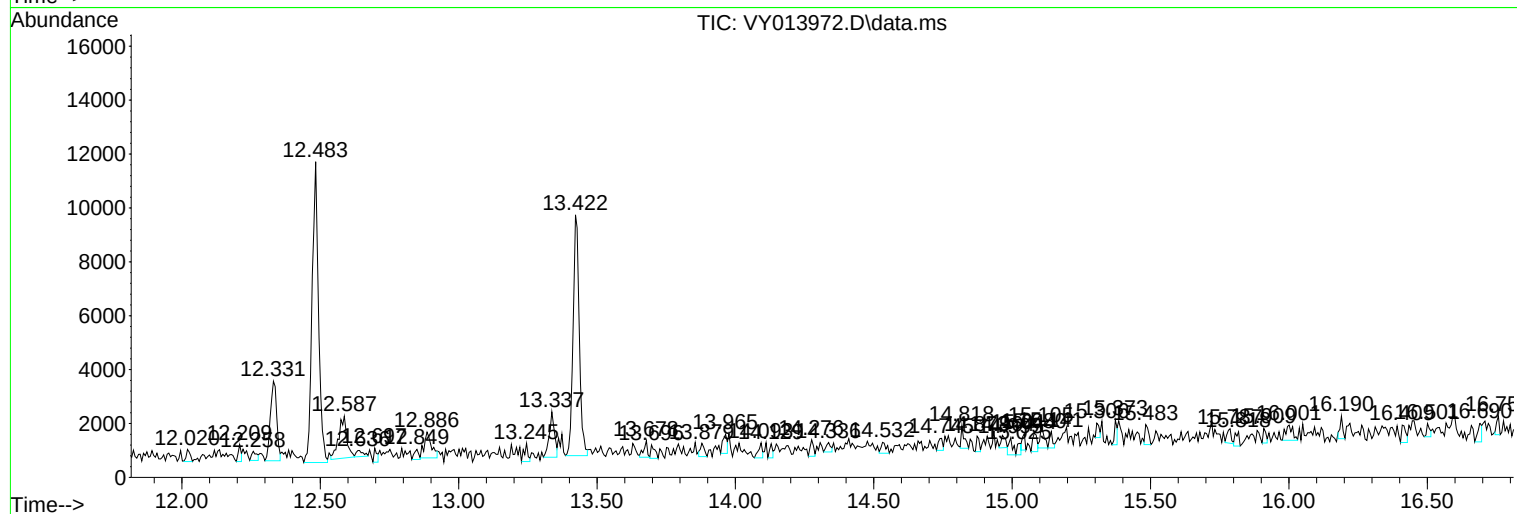
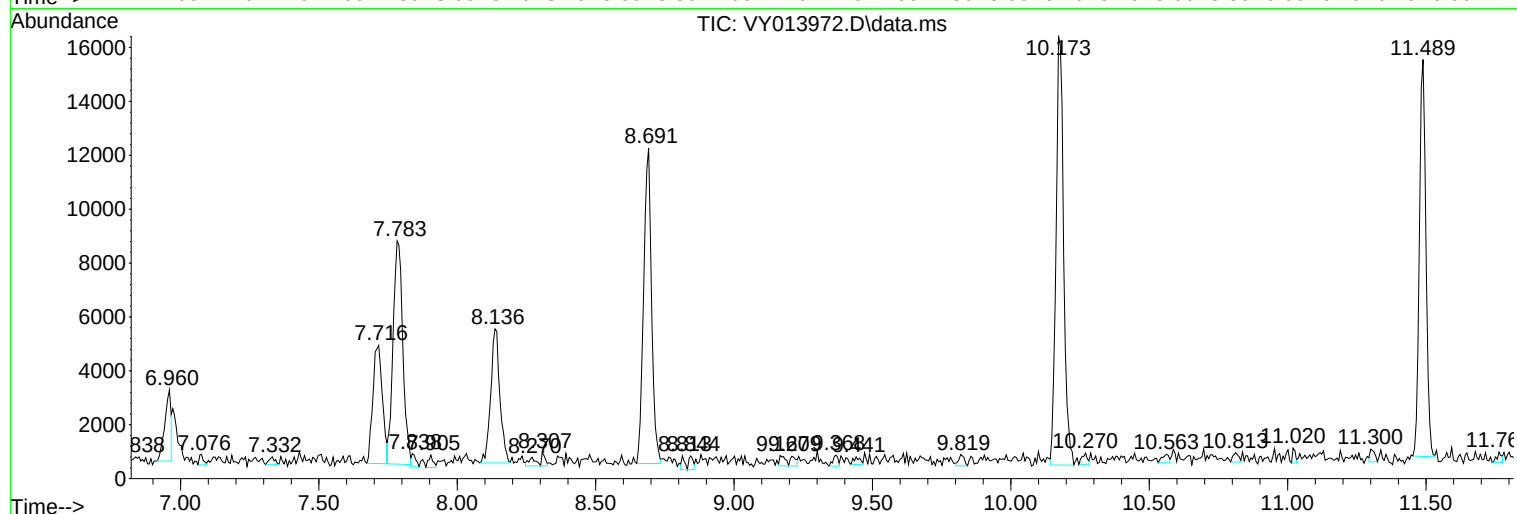
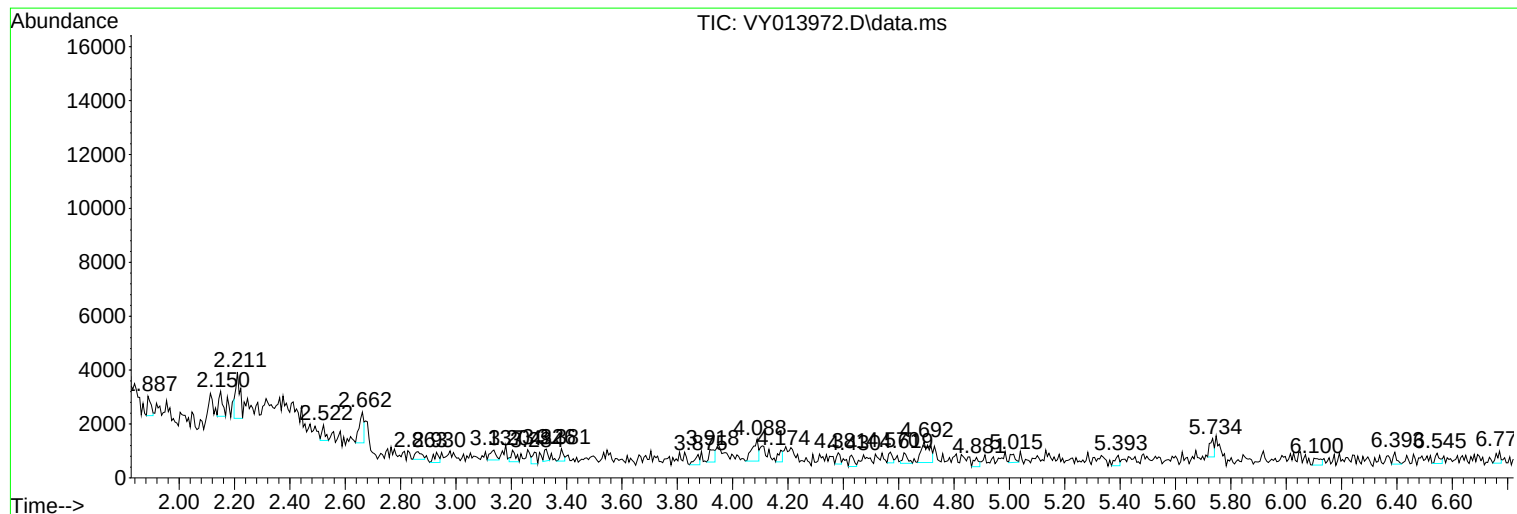
Sum of corrected areas: 216147

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060123S.M
Quant Title : SW846 8260

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



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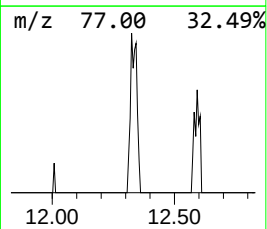
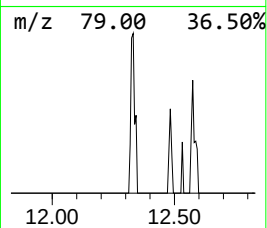
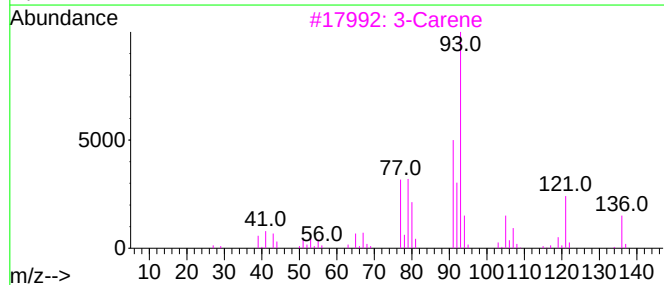
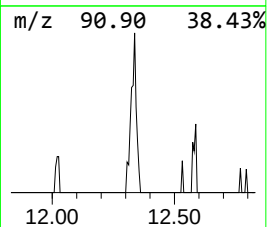
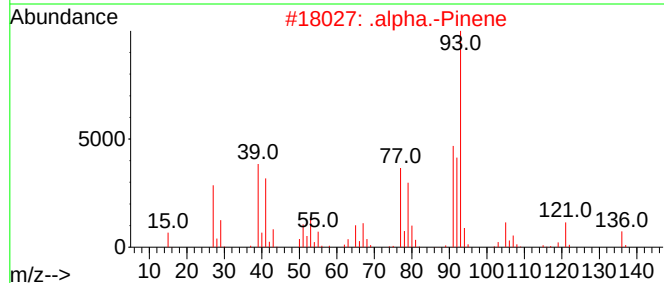
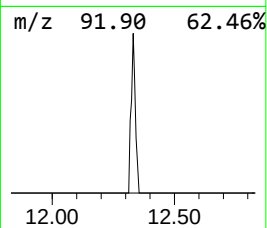
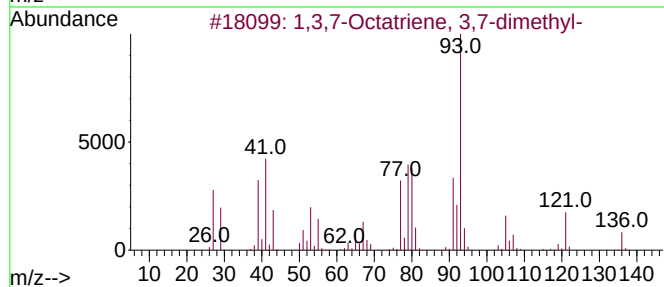
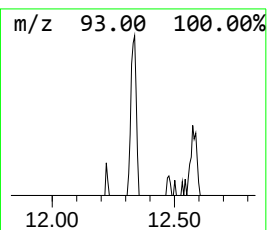
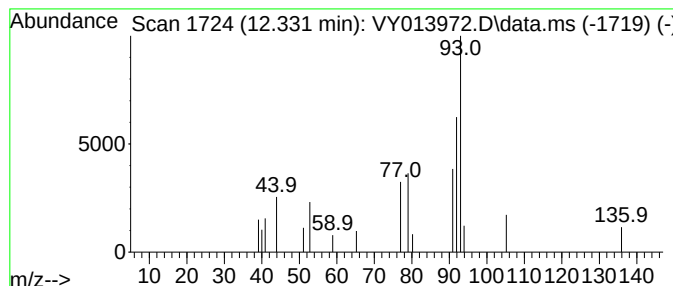
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060123S.M
Quant Title : SW846 8260

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

Peak Number 2 1,3,7-Octatriene, 3,7-dimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.331	9.82 ug/l	4729	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,7-Octatriene, 3,7-dimethyl-	136	C10H16	000502-99-8	72
2			.alpha.-Pinene	136	C10H16	000080-56-8	64
3			3-Carene	136	C10H16	013466-78-9	64
4			(+)-4-Carene	136	C10H16	029050-33-7	58
5			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	53



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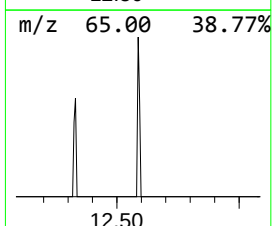
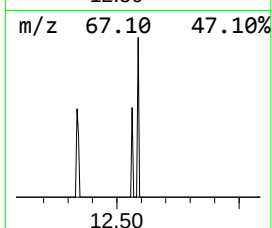
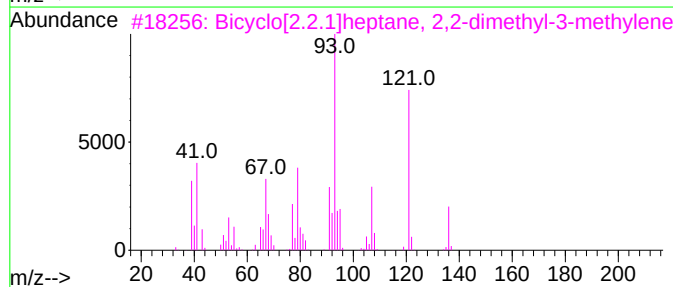
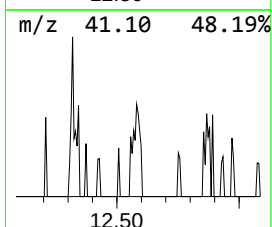
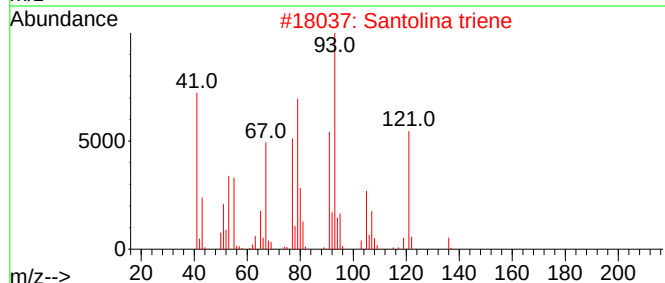
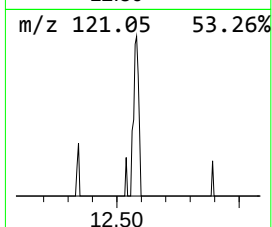
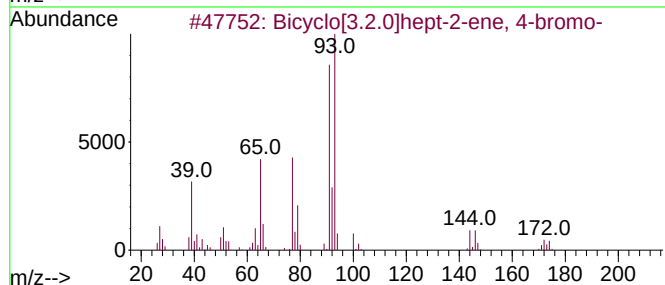
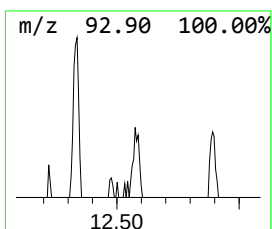
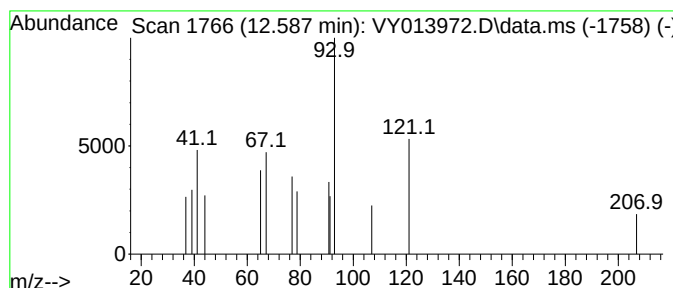
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060123S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.587 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.587	11.38 ug/l	3163	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.2.0]hept-2-ene, 4-bromo-	172	C7H9Br	038352-98-6	28
2			Santolina triene	136	C10H16	002153-66-4	12
3			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	10
4			Cyclobutene, 4,4-dimethyl-1-(2,7...	190	C14H22	062338-42-5	10
5			Camphene	136	C10H16	000079-92-5	10



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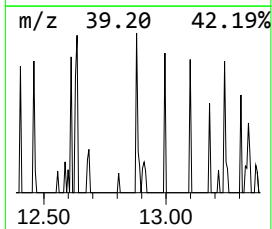
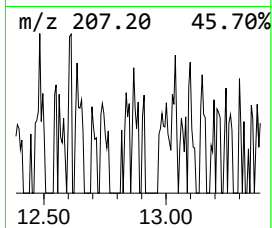
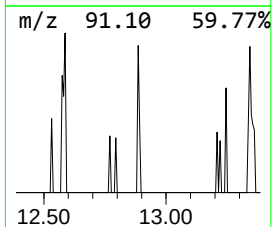
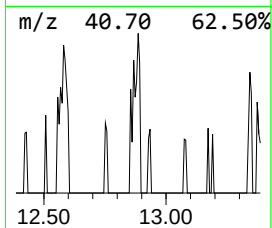
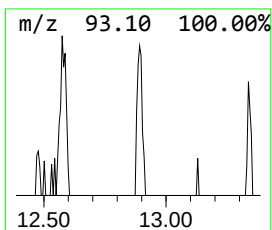
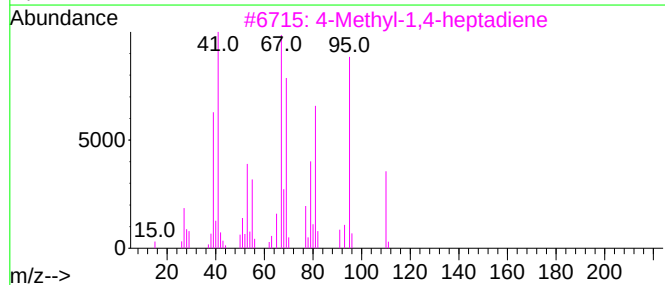
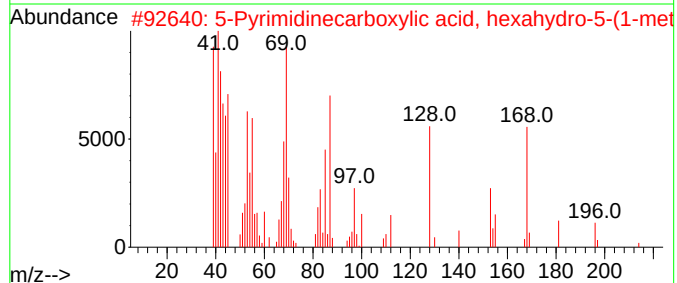
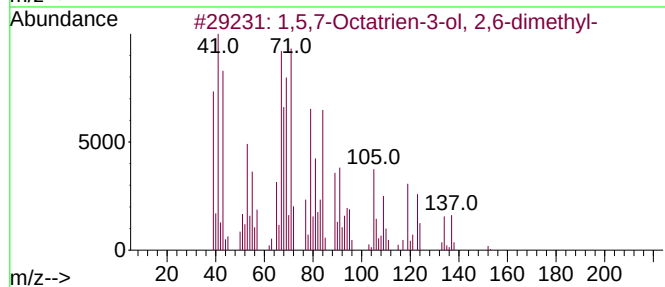
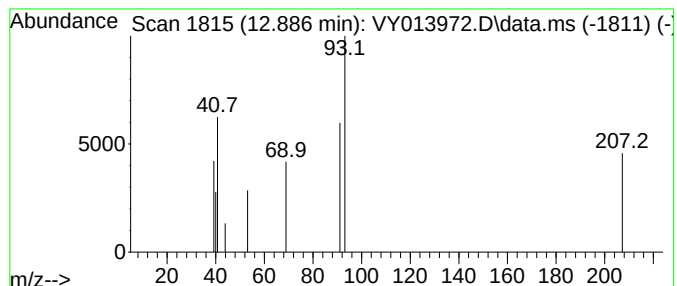
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Quant Title : SW846 8260

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

Peak Number 4 unknown12.886 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	6.46 ug/l	1796	1,4-Dichlorobenzene-d4	13.428

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,5,7-Octatrien-3-ol, 2,6-dimethyl-	152	C10H16O	029414-56-0	10
2		5-Pyrimidinecarboxylic acid, hex...	214	C8H10N2O5	072088-02-9	10
3		4-Methyl-1,4-heptadiene	110	C8H14	013857-55-1	10
4		2-Hexyn-1-ol	98	C6H10O	000764-60-3	9
5		1,3,6-Heptatriene, 5-methyl-	108	C8H12	000925-52-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060123\
Data File : VY013972.D
Acq On : 01 Jun 2023 18:25
Operator : KP/MD
Sample : 02983-08RE
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB07RE

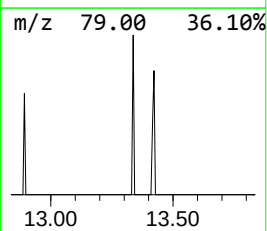
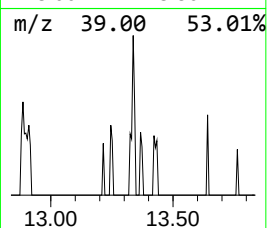
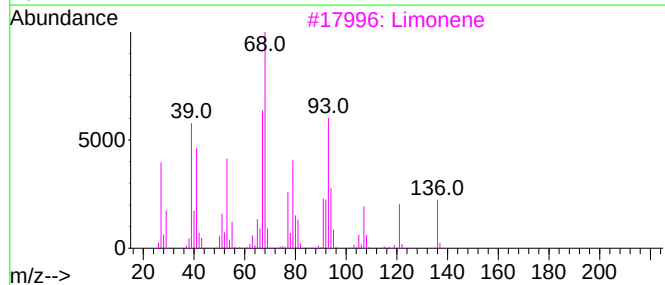
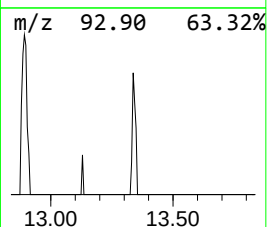
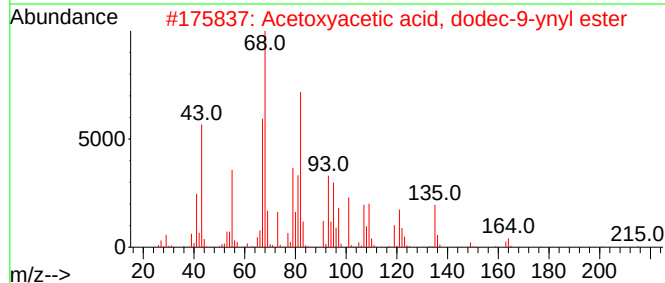
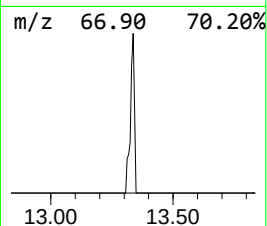
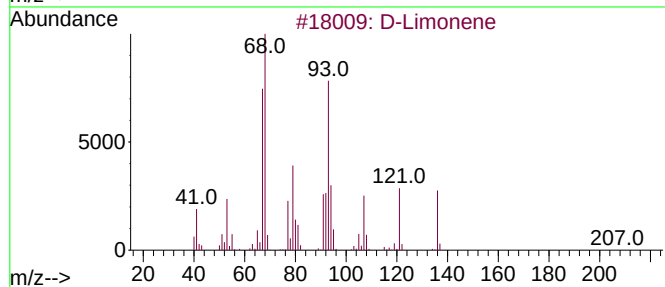
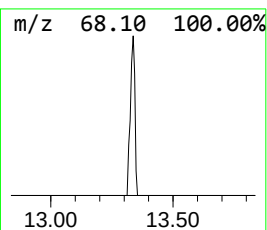
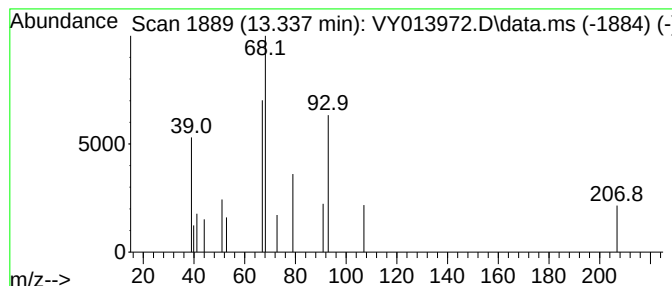
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Quant Title : SW846 8260

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

Peak Number 5 D-Limonene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.337	7.99 ug/l	2219	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	64
2			Acetoxyacetic acid, dodec-9-ynyl...	282	C16H26O4	1000308-31-9	40
3			Limonene	136	C10H16	000138-86-3	39
4			3-Chloropropionic acid, dodec-9-...	272	C15H25ClO2	1000283-04-9	38
5			Cyclobutane, 1-cyclopropyl-2-eth...	122	C9H14	061141-61-5	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060123\
Data File : VY013972.D
Acq On : 01 Jun 2023 18:25
Operator : KP/MD
Sample : 02983-08RE
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB07RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060123S.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
1,3,7-Octatrien...	12.331	9.8	ug/l	4729	3	11.489	24067	50.0
unknown12.587	12.587	11.4	ug/l	3163	4	13.428	13894	50.0
unknown12.886	12.886	6.5	ug/l	1796	4	13.428	13894	50.0
D-Limonene	13.337	8.0	ug/l	2219	4	13.428	13894	50.0