

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY103124\
 Data File : VY020101.D
 Acq On : 31 Oct 2024 17:46
 Operator : SY/MD
 Sample : P4613-01
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 ARS20-0001

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y103024S.M

Title : SW846 8260

Signal : TIC: VY020101.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.958	37	39	43	rVB	1657	1312	14.20%	1.232%
2	2.458	117	121	125	rBV2	914	1471	15.92%	1.381%
3	2.842	183	184	191	rBV3	779	1422	15.39%	1.335%
4	2.922	195	197	200	rVB3	544	584	6.32%	0.548%
5	2.989	207	208	210	rVB2	1030	509	5.51%	0.478%
6	3.092	224	225	228	rVB	569	547	5.92%	0.514%
7	3.312	257	261	263	rBV2	663	848	9.18%	0.796%
8	3.379	270	272	275	rVB2	613	472	5.11%	0.443%
9	3.409	275	277	280	rBV2	905	678	7.34%	0.637%
10	3.556	297	301	303	rBV3	624	856	9.27%	0.804%
11	3.617	308	311	312	rBV2	573	580	6.28%	0.545%
12	3.659	314	318	320	rBV3	676	599	6.48%	0.563%
13	3.720	326	328	330	rVB	687	466	5.04%	0.438%
14	3.769	335	336	338	rBV	819	627	6.79%	0.589%
15	3.909	358	359	361	rVB	981	514	5.56%	0.483%
16	4.031	377	379	381	rBV2	797	731	7.91%	0.686%
17	4.062	383	384	386	rVB	810	481	5.21%	0.452%
18	4.086	386	388	389	rBV	1175	631	6.83%	0.593%
19	4.178	400	403	405	rBV4	624	808	8.75%	0.759%
20	4.281	417	420	424	rVB2	623	1167	12.63%	1.096%
21	4.446	445	447	450	rBV2	491	564	6.10%	0.530%
22	4.635	477	478	481	rBV2	571	578	6.26%	0.543%
23	4.732	493	494	496	rBV	680	633	6.85%	0.594%
24	4.812	504	507	509	rBV	630	722	7.81%	0.678%
25	4.885	515	519	520	rBV2	469	654	7.08%	0.614%
26	5.086	549	552	555	rBV3	744	960	10.39%	0.902%
27	5.129	557	559	563	rVV2	647	676	7.32%	0.635%
28	5.165	563	565	569	rVB2	795	856	9.27%	0.804%
29	5.275	580	583	584	rVB	741	670	7.25%	0.629%
30	5.427	605	608	610	rBV2	722	905	9.80%	0.850%
31	5.482	614	617	619	rBV3	636	713	7.72%	0.670%
32	5.531	622	625	626	rVB2	790	633	6.85%	0.594%
33	5.567	629	631	632	rBV	715	497	5.38%	0.467%
34	5.750	657	661	664	rVB2	653	930	10.07%	0.873%
35	5.775	664	665	669	rVB3	631	835	9.04%	0.784%
36	6.013	702	704	707	rVB2	600	569	6.16%	0.534%

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37	6.141	723	725	728	rVB2	780	622	6.73%	0.584%
38	6.232	737	740	742	rBV2	760	935	10.12%	0.878%
39	6.256	742	744	745	rBV	643	490	5.30%	0.460%
40	6.378	762	764	767	rVB3	675	653	7.07%	0.613%
41	6.415	767	770	772	rBV2	898	878	9.50%	0.825%
42	6.482	779	781	785	rBV3	516	688	7.45%	0.646%
43	6.512	785	786	790	rVB2	741	647	7.00%	0.608%
44	6.561	790	794	795	rBV	474	594	6.43%	0.558%
45	6.610	800	802	805	rVB3	1084	903	9.77%	0.848%
46	6.640	805	807	809	rBV2	718	650	7.04%	0.610%
47	7.067	876	877	879	rBV	652	488	5.28%	0.458%
48	7.171	890	894	895	rBV	724	863	9.34%	0.810%
49	7.201	897	899	901	rBV	1061	888	9.61%	0.834%
50	7.409	931	933	935	rBV3	604	610	6.60%	0.573%
51	7.488	943	946	948	rBV3	901	1060	11.47%	0.995%
52	7.518	948	951	954	rBV	631	808	8.75%	0.759%
53	7.543	954	955	957	rVB	1041	550	5.95%	0.516%
54	7.573	957	960	963	rBV2	780	1026	11.11%	0.963%
55	7.628	966	969	970	rBV3	1351	1152	12.47%	1.082%
56	7.689	974	979	980	rBV2	1279	1242	13.44%	1.166%
57	7.811	997	999	1006	rVB2	932	1402	15.17%	1.317%
58	8.061	1036	1040	1046	rVB3	1996	4072	44.07%	3.824%
59	8.140	1051	1053	1056	rBV2	1257	985	10.66%	0.925%
60	8.463	1104	1106	1108	rBV2	499	492	5.33%	0.462%
61	8.500	1110	1112	1114	rVB2	1025	833	9.02%	0.782%
62	8.530	1114	1117	1120	rBV2	1054	1444	15.63%	1.356%
63	8.561	1120	1122	1125	rVB3	566	569	6.16%	0.534%
64	8.610	1125	1130	1137	rBV4	3430	7518	81.37%	7.060%
65	8.762	1153	1155	1157	rBV2	790	710	7.68%	0.667%
66	8.902	1174	1178	1180	rBV2	390	478	5.17%	0.449%
67	9.000	1190	1194	1195	rBV3	703	549	5.94%	0.516%
68	9.122	1210	1214	1215	rVB3	650	719	7.78%	0.675%
69	9.140	1215	1217	1220	rVB3	553	474	5.13%	0.445%
70	9.183	1220	1224	1226	rVB2	415	467	5.05%	0.439%
71	9.207	1226	1228	1231	rVB	956	955	10.34%	0.897%
72	9.262	1233	1237	1239	rBV2	628	622	6.73%	0.584%
73	9.481	1270	1273	1275	rVB2	1114	732	7.92%	0.687%
74	9.506	1275	1277	1282	rBV3	611	652	7.06%	0.612%
75	9.963	1351	1352	1353	rBV	1020	501	5.42%	0.470%
76	10.000	1353	1358	1360	rVV2	858	1251	13.54%	1.175%

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77	10.036	1362	1364	1366	rVB3	867	658	7.12%	0.618%
78	10.109	1366	1376	1380	rBV4	4947	9239	100.00%	8.676%
79	10.390	1420	1422	1426	rBV3	901	1362	14.74%	1.279%
80	10.426	1426	1428	1431	rVB3	1132	1166	12.62%	1.095%
81	10.463	1431	1434	1436	rBV3	1068	1426	15.43%	1.339%
82	10.512	1440	1442	1446	rVB2	1085	1343	14.54%	1.261%
83	10.548	1446	1448	1452	rBV3	636	604	6.54%	0.567%
84	10.585	1452	1454	1455	rBV	681	669	7.24%	0.628%
85	10.615	1458	1459	1463	rBV3	840	1161	12.57%	1.090%
86	10.835	1493	1495	1496	rBV	605	572	6.19%	0.537%
87	10.957	1513	1515	1516	rBV3	917	667	7.22%	0.626%
88	11.018	1523	1525	1528	rBV2	1094	1224	13.25%	1.149%
89	11.060	1530	1532	1534	rVB2	858	563	6.09%	0.529%
90	11.201	1554	1555	1557	rBV2	756	490	5.30%	0.460%
91	11.243	1560	1562	1563	rBV	660	529	5.73%	0.497%
92	11.371	1581	1583	1585	rVB3	1052	821	8.89%	0.771%
93	11.414	1586	1590	1593	rVV4	2232	3434	37.17%	3.225%
94	11.554	1611	1613	1615	rBV2	1082	1015	10.99%	0.953%
95	12.255	1725	1728	1734	rVB6	3165	5874	63.58%	5.516%
96	12.304	1734	1736	1737	rBV2	1482	865	9.36%	0.812%
97	12.737	1805	1807	1809	rBV2	1459	1399	15.14%	1.314%
98	13.481	1927	1929	1931	rBV4	1672	2039	22.07%	1.915%
99	15.749	2299	2301	2302	rBV2	1038	687	7.44%	0.645%
100	16.041	2347	2349	2352	rVB3	1375	810	8.77%	0.761%

Sum of corrected areas: 106487

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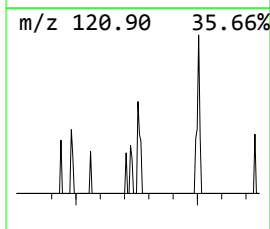
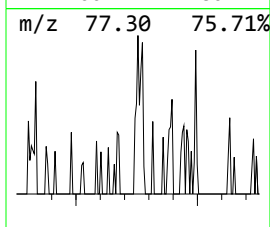
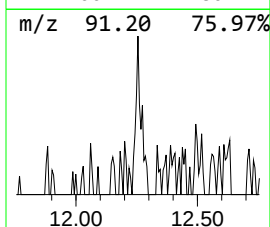
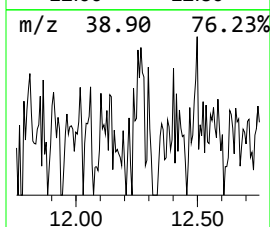
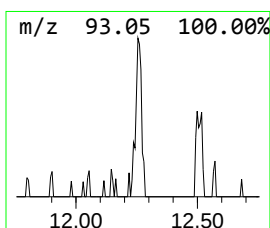
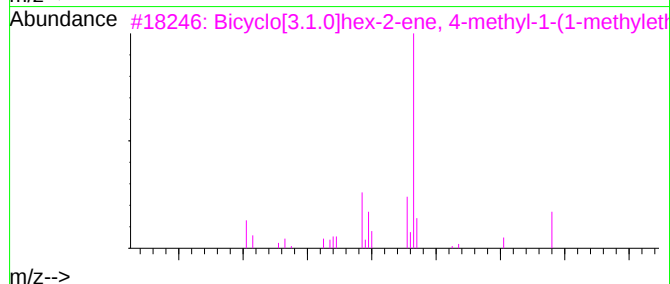
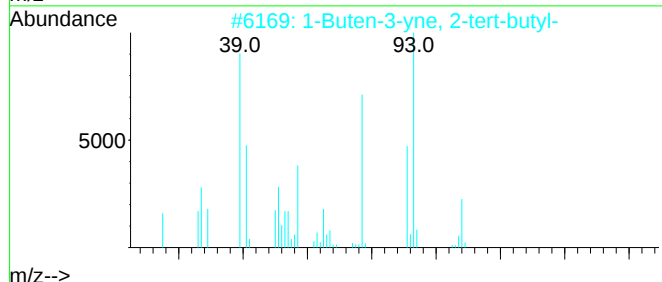
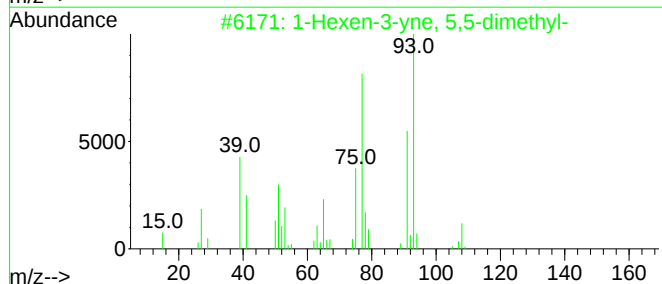
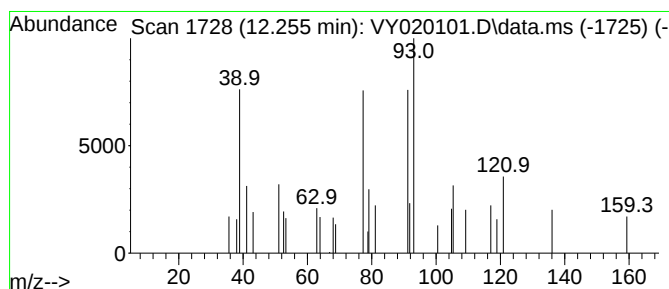
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y103024S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Hexen-3-yne, 5,5-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.255	85.53 ug/l	5874	Chlorobenzene-d5	11.414	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexen-3-yne, 5,5-dimethyl-	108	C8H12	004911-58-4	53
2	1-Buten-3-yne, 2-tert-butyl-	108	C8H12	002809-84-9	42
3	Bicyclo[3.1.0]hex-2-ene, 4-methy...	136	C10H16	028634-89-1	38
4	4-Ethynyl-4-vinyl-1,6-heptadiene	146	C11H14	019781-40-9	37
5	Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	35



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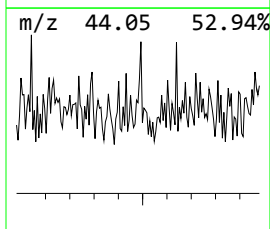
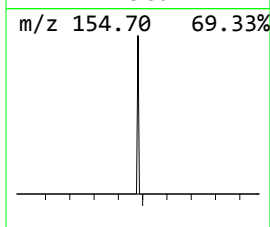
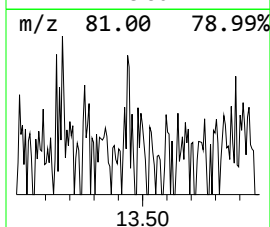
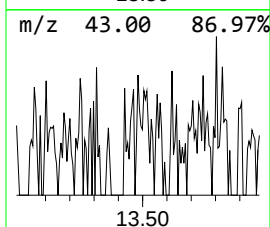
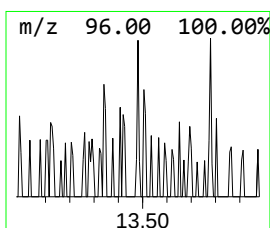
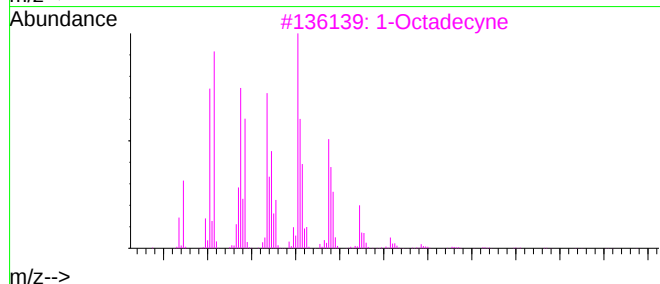
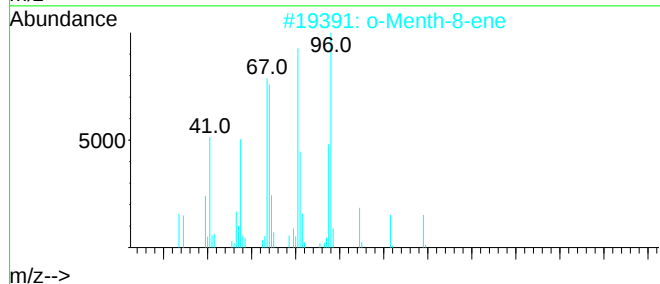
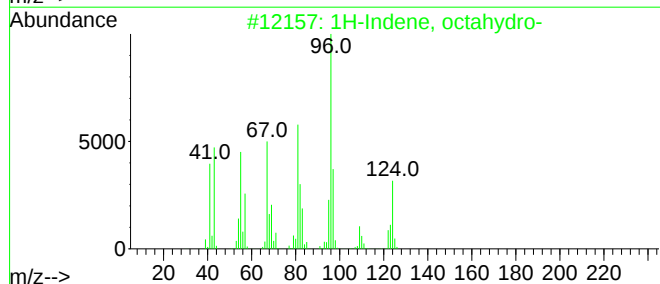
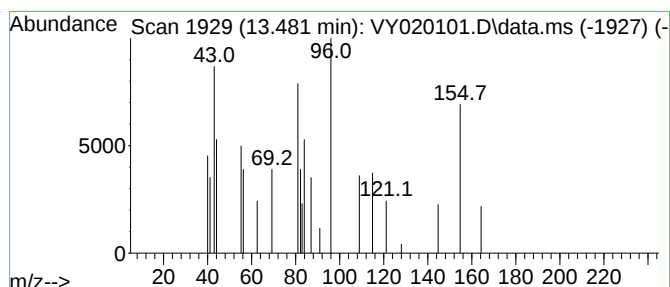
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Peak Number 10 unknown13.481 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.481	50.00 ug/l	2039	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-	124	C9H16	000496-10-6	17
2	o-Menth-8-ene	138	C10H18	015193-25-6	17
3	1-Octadecyne	250	C18H34	000629-89-0	12
4	4-Nitrocatechol	155	C6H5NO4	003316-09-4	9
5	Phosphoric acid, diethyl undecyl...	308	C15H33O4P	1000308-88-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexen-3-yne, ...	12.255	85.5	ug/l	5874	3	11.414	3434	50.0
unknown13.481	13.481	50.0	ug/l	2039	4	13.347	2039	50.0