

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY072522\
 Data File : VY009689.D
 Acq On : 25 Jul 2022 17:02
 Operator : KP/MD
 Sample : N3855-03
 Misc : 4.46g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 EO-03-072222

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\82Y071822S.M
 Title : SW846 8260

Signal : TIC: VY009689.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.058	37	39	41	rBV	576	520	3.84%	0.510%
2	2.101	44	46	48	rBV	792	875	6.46%	0.859%
3	2.363	87	89	91	rBV2	403	235	1.74%	0.231%
4	2.668	134	139	144	rVB3	859	1840	13.59%	1.805%
5	2.759	150	154	157	rVB3	212	254	1.88%	0.249%
6	3.497	272	275	276	rBV2	261	285	2.10%	0.280%
7	3.936	343	347	353	rVB4	276	393	2.90%	0.386%
8	4.095	371	373	375	rVV3	313	305	2.25%	0.299%
9	4.119	375	377	379	rVB2	358	304	2.25%	0.298%
10	4.168	384	385	392	rVB3	261	316	2.33%	0.310%
11	4.662	464	466	467	rBV2	311	280	2.07%	0.275%
12	4.710	467	474	479	rVB6	1136	3103	22.92%	3.045%
13	4.838	491	495	496	rVB	259	301	2.22%	0.295%
14	4.869	496	500	503	rBV2	228	346	2.56%	0.339%
15	5.180	549	551	554	rVB	204	236	1.74%	0.232%
16	5.210	554	556	560	rBV2	173	238	1.76%	0.234%
17	5.314	570	573	576	rVB3	201	308	2.27%	0.302%
18	5.344	576	578	580	rBV2	306	319	2.36%	0.313%
19	5.503	603	604	606	rBV2	295	241	1.78%	0.236%
20	5.808	651	654	657	rBV2	326	355	2.62%	0.348%
21	5.856	660	662	665	rVB2	235	240	1.77%	0.235%
22	6.405	748	752	753	rVB2	308	297	2.19%	0.291%
23	6.430	753	756	758	rBV2	181	266	1.96%	0.261%
24	6.564	774	778	780	rBV2	249	292	2.16%	0.287%
25	6.759	807	810	812	rBV2	190	258	1.91%	0.253%
26	6.820	818	820	821	rBV	288	259	1.91%	0.254%
27	6.868	826	828	832	rVB2	222	240	1.77%	0.235%
28	6.972	841	845	846	rBV2	238	335	2.47%	0.329%
29	7.131	865	871	872	rBV4	176	252	1.86%	0.247%
30	7.265	891	893	896	rBV3	273	391	2.89%	0.384%
31	7.326	900	903	904	rBV2	239	295	2.18%	0.289%
32	7.381	908	912	913	rBV	188	219	1.62%	0.215%
33	7.502	929	932	933	rBV3	206	262	1.94%	0.257%
34	7.710	960	966	971	rBV3	676	1699	12.55%	1.667%
35	7.783	971	978	985	rVV	3516	7256	53.59%	7.120%
36	7.850	988	989	992	rBV2	312	267	1.97%	0.262%

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37	7.917	998	1000	1004	rVB2	201	226	1.67%	0.222%
38	7.954	1004	1006	1009	rBV3	242	284	2.10%	0.279%
39	8.130	1028	1035	1042	rVB4	2413	5437	40.16%	5.335%
40	8.283	1058	1060	1065	rVB3	193	276	2.04%	0.271%
41	8.368	1071	1074	1076	rBV2	264	341	2.52%	0.335%
42	8.521	1095	1099	1101	rBV3	228	251	1.85%	0.246%
43	8.685	1117	1126	1133	rBV2	4816	9841	72.68%	9.656%
44	8.807	1142	1146	1150	rBV3	303	452	3.34%	0.444%
45	9.002	1176	1178	1180	rBV	270	229	1.69%	0.225%
46	9.338	1230	1233	1236	rBV3	155	243	1.79%	0.238%
47	9.374	1236	1239	1241	rBV2	240	252	1.86%	0.247%
48	9.508	1258	1261	1263	rBV2	198	248	1.83%	0.243%
49	9.581	1271	1273	1276	rVB3	195	262	1.94%	0.257%
50	9.618	1276	1279	1283	rVB3	243	342	2.53%	0.336%
51	9.673	1283	1288	1291	rBV2	250	402	2.97%	0.394%
52	9.715	1291	1295	1296	rVV	283	321	2.37%	0.315%
53	9.728	1296	1297	1301	rVV3	281	352	2.60%	0.345%
54	9.764	1301	1303	1306	rVB2	190	228	1.68%	0.224%
55	10.173	1365	1370	1377	rBV	7704	13540	100.00%	13.286%
56	10.319	1392	1394	1397	rBV	312	336	2.48%	0.330%
57	10.471	1415	1419	1420	rBV	241	292	2.16%	0.287%
58	10.599	1439	1440	1442	rBV	360	220	1.62%	0.216%
59	10.624	1442	1444	1447	rBV2	265	273	2.02%	0.268%
60	10.971	1499	1501	1504	rBV3	242	258	1.91%	0.253%
61	11.008	1506	1507	1511	rBV3	280	437	3.23%	0.429%
62	11.392	1567	1570	1571	rBV2	301	277	2.05%	0.272%
63	11.490	1580	1586	1594	rBV	7961	12691	93.73%	12.453%
64	11.544	1594	1595	1598	rVB	314	230	1.70%	0.226%
65	11.672	1612	1616	1617	rBV	241	235	1.74%	0.231%
66	11.697	1619	1620	1624	rVB3	434	434	3.21%	0.426%
67	12.032	1671	1675	1676	rBV2	275	348	2.57%	0.341%
68	12.264	1710	1713	1714	rBV2	241	219	1.62%	0.215%
69	12.349	1723	1727	1730	rBV2	244	353	2.61%	0.346%
70	12.483	1743	1749	1754	rVB3	5456	8317	61.43%	8.161%
71	12.788	1796	1799	1800	rBV	351	391	2.89%	0.384%
72	12.825	1803	1805	1807	rVV2	392	319	2.36%	0.313%
73	12.849	1807	1809	1814	rVV3	261	414	3.06%	0.406%
74	12.953	1823	1826	1829	rBV2	235	276	2.04%	0.271%
75	13.075	1844	1846	1848	rVB	349	221	1.63%	0.217%
76	13.117	1851	1853	1856	rBV3	413	511	3.77%	0.501%

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77	13.148	1856	1858	1861	rBV2	222	301	2.22%	0.295%
78	13.251	1872	1875	1879	rVV4	306	485	3.58%	0.476%
79	13.282	1879	1880	1882	rVV	306	236	1.74%	0.232%
80	13.306	1882	1884	1887	rVV2	286	364	2.69%	0.357%
81	13.367	1891	1894	1897	rVV2	525	647	4.78%	0.635%
82	13.428	1897	1904	1909	rVV2	5143	8478	62.61%	8.319%
83	13.501	1913	1916	1919	rBV2	321	397	2.93%	0.390%
84	13.703	1944	1949	1951	rBV3	809	1132	8.36%	1.111%
85	13.825	1967	1969	1971	rBV2	290	255	1.88%	0.250%
86	14.038	2001	2004	2006	rBV2	222	337	2.49%	0.331%
87	14.361	2055	2057	2058	rBV	296	221	1.63%	0.217%
88	14.715	2113	2115	2118	rBV2	336	351	2.59%	0.344%
89	14.922	2148	2149	2151	rBV2	436	298	2.20%	0.292%
90	15.373	2221	2223	2225	rVB2	337	239	1.77%	0.235%
91	15.519	2245	2247	2248	rBV	468	238	1.76%	0.234%
92	15.562	2252	2254	2255	rBV	326	249	1.84%	0.244%
93	15.580	2255	2257	2260	rVV3	401	346	2.56%	0.339%
94	15.690	2273	2275	2276	rVV2	384	280	2.07%	0.275%
95	15.714	2276	2279	2280	rVB	378	390	2.88%	0.383%
96	15.781	2288	2290	2292	rBV3	428	359	2.65%	0.352%
97	15.800	2292	2293	2295	rVB2	444	282	2.08%	0.277%
98	15.824	2295	2297	2302	rBV4	618	881	6.51%	0.864%
99	16.269	2368	2370	2371	rBV2	366	274	2.02%	0.269%
100	16.470	2401	2403	2405	rBV2	448	414	3.06%	0.406%

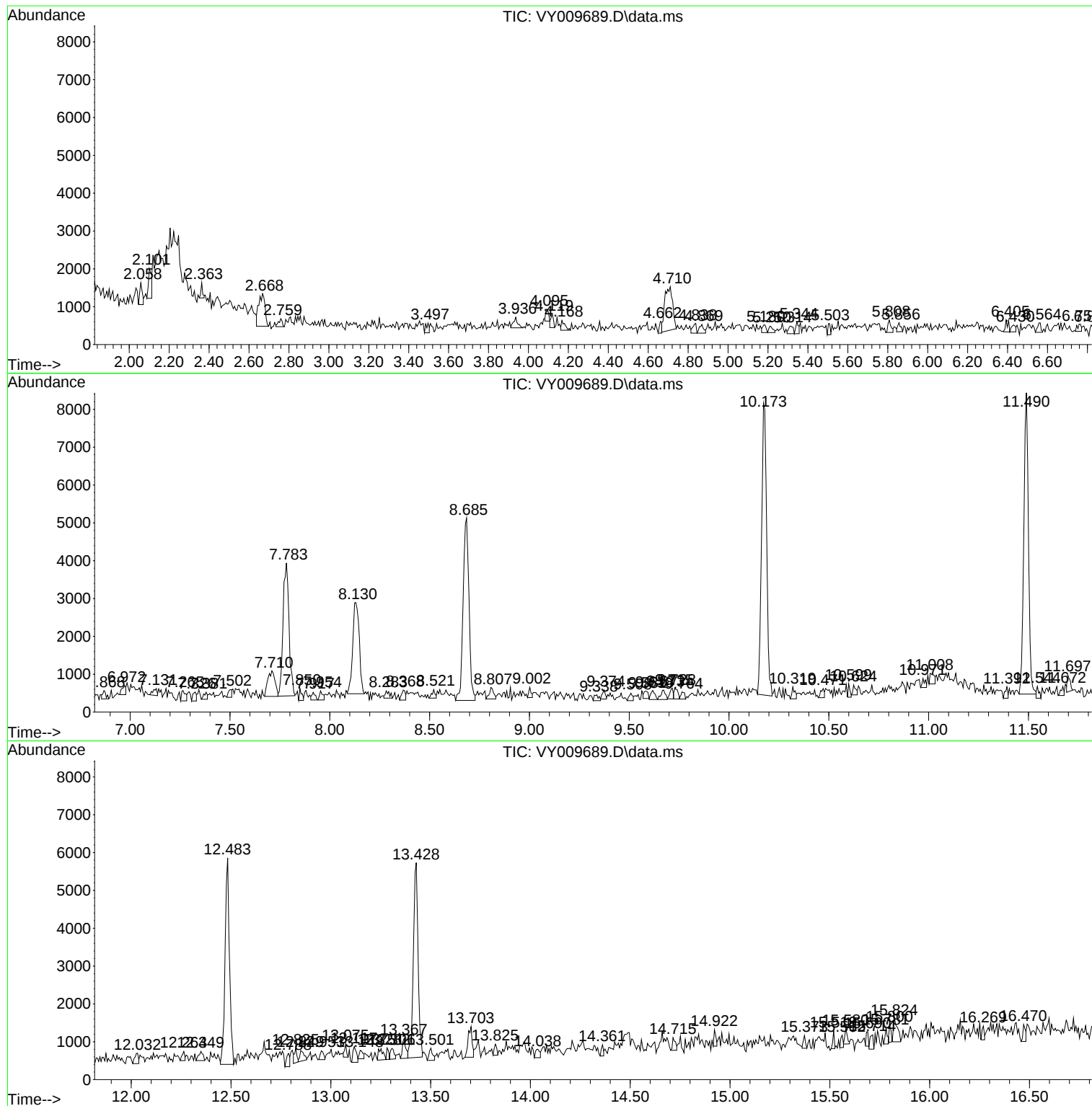
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071822S.M
Quant Title : SW846 8260

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



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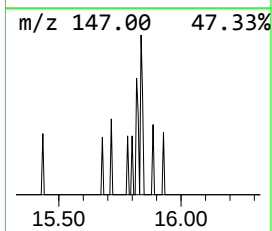
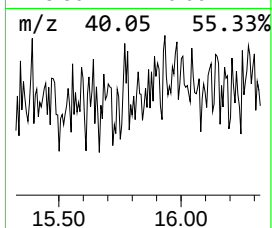
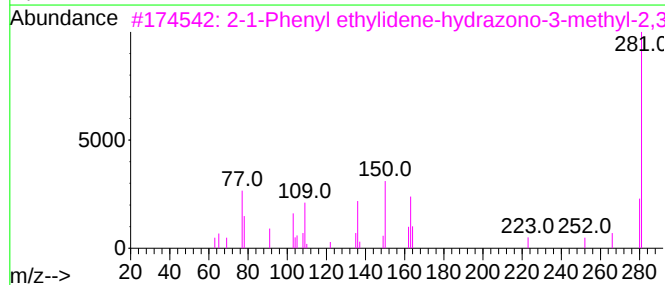
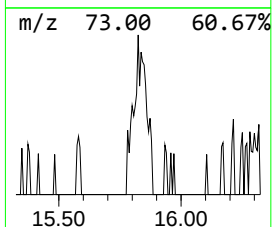
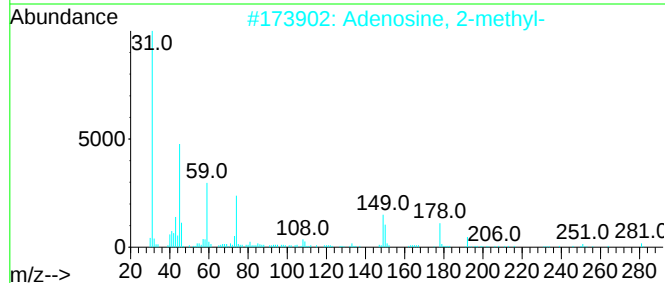
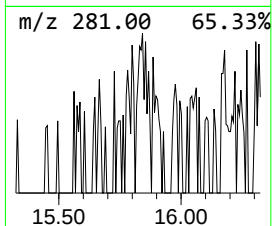
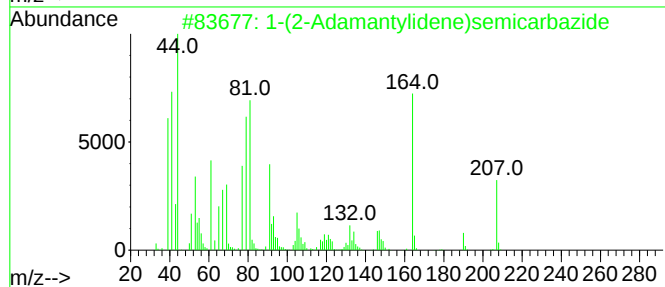
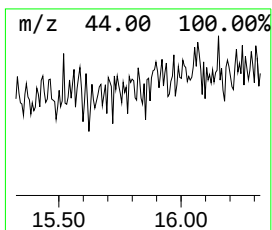
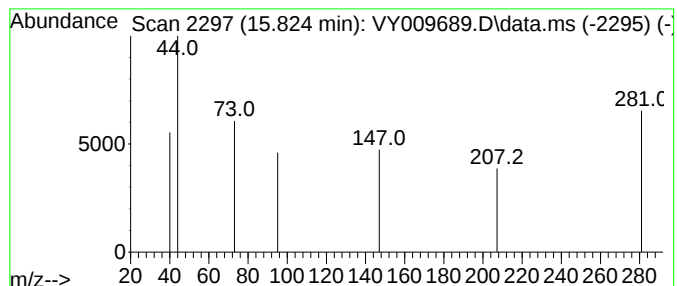
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071822S.M
Quant Title : SW846 8260

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

Peak Number 5 1-(2-Adamantylidene)semicar... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.824	5.20 ug/l	881	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(2-Adamantylidene)semicarbazide	207	C11H17N3O	065814-27-9	4
2			Adenosine, 2-methyl-	281	C11H15N5O4	016526-56-0	3
3			2-1-Phenyl ethylidene-hydrazono-...	281	C16H15N3S	1000148-55-3	3
4			Propanenitrile, 3-chloro-2,3-dih...	147	C3H2ClN3O2	139912-33-7	2
5			4-Chloro-3-nitro-2H-pyrazole	147	C3H2ClN3O2	1000411-34-5	2



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-(2-Adamantyl...	15.824	5.2	ug/l	881	4	13.428	8478	50.0