

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY032025\
 Data File : VY021580.D
 Acq On : 20 Mar 2025 14:24
 Operator : SY/MD
 Sample : Q1606-05
 Misc : 5.02g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 RT4534

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\82Y030425S.M

Title : SW846 8260

Signal : TIC: VY021580.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.001	44	46	49	rBV2	703	567	1.58%	0.225%
2	2.074	52	58	60	rBV3	3201	6285	17.50%	2.491%
3	2.123	64	66	68	rVV3	1877	1913	5.33%	0.758%
4	2.391	108	110	115	rBV4	716	694	1.93%	0.275%
5	2.525	131	132	135	rVB3	807	641	1.78%	0.254%
6	2.604	144	145	148	rBV3	966	985	2.74%	0.390%
7	2.958	199	203	204	rBV2	482	479	1.33%	0.190%
8	3.056	217	219	222	rVB3	653	688	1.92%	0.273%
9	3.141	231	233	236	rVB2	502	540	1.50%	0.214%
10	3.177	236	239	242	rBV4	511	675	1.88%	0.268%
11	3.202	242	243	248	rVB2	703	712	1.98%	0.282%
12	3.360	265	269	272	rBV2	508	633	1.76%	0.251%
13	4.403	439	440	442	rBV2	523	509	1.42%	0.202%
14	4.586	467	470	473	rBV3	616	954	2.66%	0.378%
15	4.671	481	484	486	rVB2	655	599	1.67%	0.237%
16	4.702	486	489	491	rBV3	454	542	1.51%	0.215%
17	5.269	580	582	585	rBV3	514	541	1.51%	0.214%
18	5.397	600	603	604	rBV	496	508	1.41%	0.201%
19	5.482	615	617	620	rBV2	600	552	1.54%	0.219%
20	5.519	620	623	627	rBV2	489	814	2.27%	0.323%
21	5.659	645	646	649	rVB	757	602	1.68%	0.239%
22	5.701	651	653	657	rVB2	448	593	1.65%	0.235%
23	5.750	657	661	662	rBV3	491	557	1.55%	0.221%
24	5.903	680	686	690	rVB3	417	1080	3.01%	0.428%
25	5.945	690	693	695	rBV3	398	600	1.67%	0.238%
26	5.982	697	699	702	rVB3	541	553	1.54%	0.219%
27	6.226	737	739	741	rVB	659	601	1.67%	0.238%
28	6.256	741	744	745	rBV	501	542	1.51%	0.215%
29	6.579	793	797	799	rVB2	462	577	1.61%	0.229%
30	6.616	799	803	805	rBV2	431	731	2.04%	0.290%
31	6.823	834	837	840	rBV3	449	654	1.82%	0.259%
32	6.896	847	849	851	rBV3	665	688	1.92%	0.273%
33	7.073	875	878	882	rVB3	457	493	1.37%	0.195%
34	7.134	884	888	890	rBV2	495	596	1.66%	0.236%
35	7.189	896	897	902	rVB3	502	636	1.77%	0.252%
36	7.256	905	908	912	rVB3	440	547	1.52%	0.217%

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37	7.396	928	931	935	rVB	497	616	1.71%	0.244%
38	7.439	935	938	939	rBV2	604	710	1.98%	0.281%
39	7.494	945	947	950	rVB	672	605	1.68%	0.240%
40	7.530	950	953	958	rVB2	473	816	2.27%	0.323%
41	7.634	961	970	976	rVV4	5209	13322	37.09%	5.281%
42	7.707	976	982	993	rVB2	11324	27926	77.74%	11.070%
43	7.799	993	997	998	rBV2	684	615	1.71%	0.244%
44	7.939	1015	1020	1024	rBV3	397	666	1.85%	0.264%
45	8.055	1033	1039	1047	rVB5	4223	11066	30.81%	4.387%
46	8.555	1118	1121	1124	rVB2	590	707	1.97%	0.280%
47	8.616	1124	1131	1139	rBV2	14826	31423	87.48%	12.456%
48	8.762	1154	1155	1160	rBV3	548	612	1.70%	0.243%
49	8.890	1173	1176	1178	rVB2	661	537	1.49%	0.213%
50	8.933	1178	1183	1184	rBV3	556	649	1.81%	0.257%
51	8.969	1187	1189	1197	rVB5	408	689	1.92%	0.273%
52	9.134	1212	1216	1219	rVB2	598	895	2.49%	0.355%
53	9.286	1238	1241	1243	rBV2	559	542	1.51%	0.215%
54	9.329	1246	1248	1250	rVB	657	580	1.61%	0.230%
55	9.378	1250	1256	1258	rBV3	718	1054	2.93%	0.418%
56	9.731	1311	1314	1317	rVB3	538	735	2.05%	0.291%
57	9.762	1317	1319	1321	rBV2	652	584	1.63%	0.232%
58	9.963	1347	1352	1353	rBV2	466	667	1.86%	0.264%
59	9.999	1355	1358	1362	rVV3	905	1328	3.70%	0.526%
60	10.036	1362	1364	1367	rVB3	537	600	1.67%	0.238%
61	10.109	1369	1376	1381	rVV	19765	35920	100.00%	14.239%
62	10.170	1381	1386	1394	rVB	11478	20754	57.78%	8.227%
63	10.384	1420	1421	1425	rBV3	582	759	2.11%	0.301%
64	10.499	1436	1440	1442	rBV3	399	615	1.71%	0.244%
65	11.079	1530	1535	1537	rBV4	392	529	1.47%	0.210%
66	11.225	1556	1559	1562	rVB3	461	657	1.83%	0.260%
67	11.359	1578	1581	1582	rVB	509	480	1.34%	0.190%
68	11.420	1582	1591	1597	rBV	15269	26964	75.07%	10.689%
69	11.542	1609	1611	1615	rVB	556	486	1.35%	0.193%
70	11.627	1623	1625	1630	rBV2	557	823	2.29%	0.326%
71	11.877	1663	1666	1667	rBV	356	501	1.39%	0.199%
72	12.066	1695	1697	1699	rBV2	432	505	1.41%	0.200%
73	12.255	1725	1728	1729	rVB2	504	492	1.37%	0.195%
74	12.408	1748	1753	1760	rBV4	6839	11942	33.25%	4.734%
75	12.529	1770	1773	1778	rVB2	461	847	2.36%	0.336%
76	12.682	1795	1798	1801	rVB3	617	607	1.69%	0.241%

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77	13.188	1875	1881	1885	rVB2	506	1021	2.84%	0.405%
78	13.261	1891	1893	1895	rBV2	622	594	1.65%	0.235%
79	13.285	1895	1897	1900	rVB	592	743	2.07%	0.295%
80	13.346	1903	1907	1912	rVV2	4077	6868	19.12%	2.723%
81	13.694	1962	1964	1967	rVB2	571	494	1.38%	0.196%
82	14.255	2053	2056	2058	rBV3	358	537	1.49%	0.213%
83	14.651	2118	2121	2123	rVB3	476	490	1.36%	0.194%
84	14.773	2137	2141	2144	rVB2	546	685	1.91%	0.272%
85	14.816	2144	2148	2149	rBV3	466	616	1.71%	0.244%
86	15.084	2189	2192	2194	rBV3	563	628	1.75%	0.249%
87	15.157	2201	2204	2205	rVB2	619	531	1.48%	0.210%
88	15.370	2238	2239	2243	rBV	458	578	1.61%	0.229%
89	15.450	2250	2252	2255	rBV2	794	768	2.14%	0.304%
90	15.572	2268	2272	2275	rBV3	622	872	2.43%	0.346%
91	15.608	2275	2278	2280	rVV2	584	603	1.68%	0.239%
92	15.901	2324	2326	2328	rVB	676	501	1.39%	0.199%
93	16.065	2350	2353	2354	rVB2	674	551	1.53%	0.218%
94	16.084	2354	2356	2358	rBV3	494	565	1.57%	0.224%
95	16.279	2384	2388	2390	rBV4	561	659	1.83%	0.261%
96	16.334	2395	2397	2400	rVB3	927	597	1.66%	0.237%
97	16.437	2410	2414	2417	rVB2	449	711	1.98%	0.282%
98	16.498	2423	2424	2427	rBV2	715	594	1.65%	0.235%
99	16.748	2462	2465	2467	rVB3	735	848	2.36%	0.336%
100	16.779	2467	2470	2471	rBV2	592	505	1.41%	0.200%

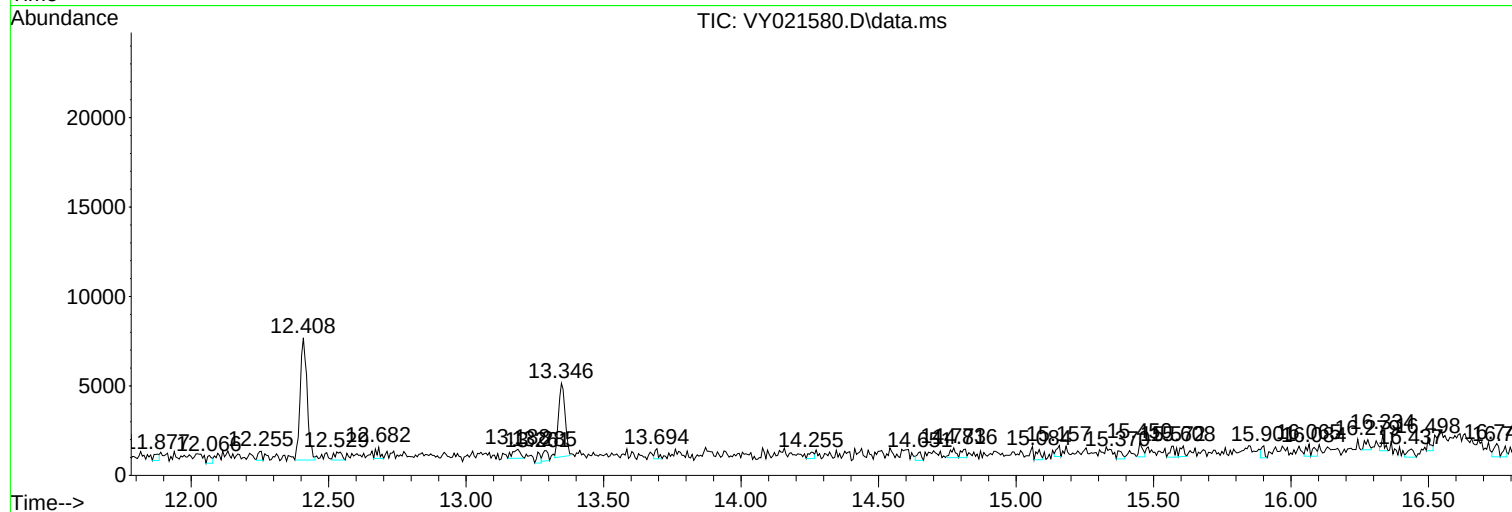
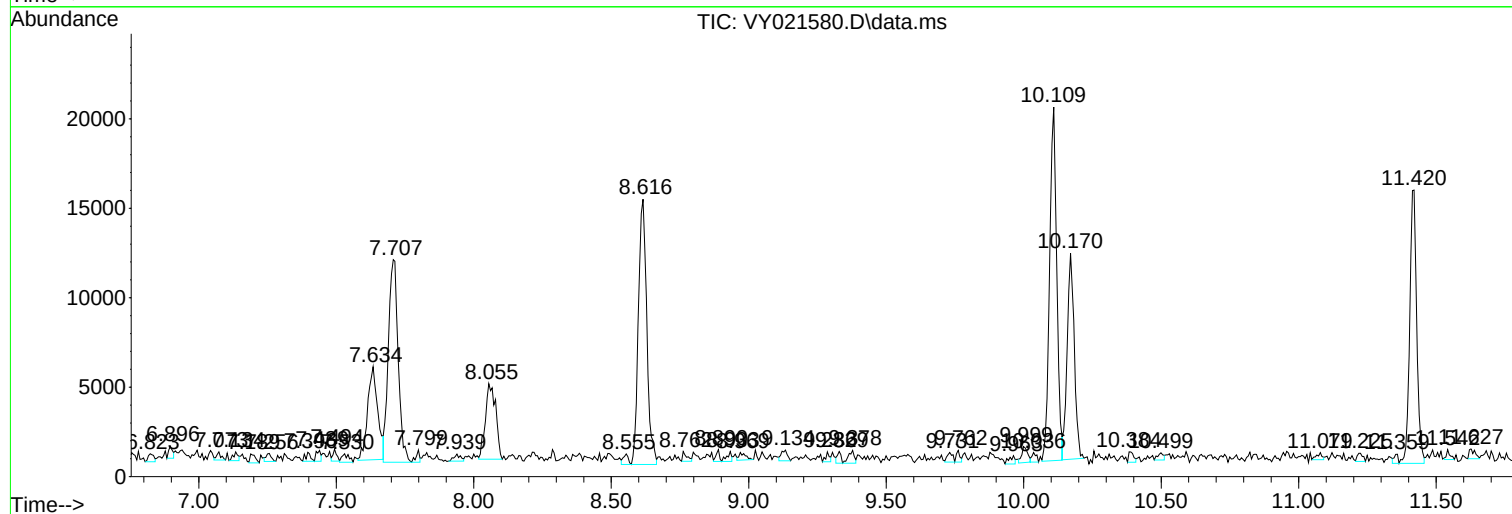
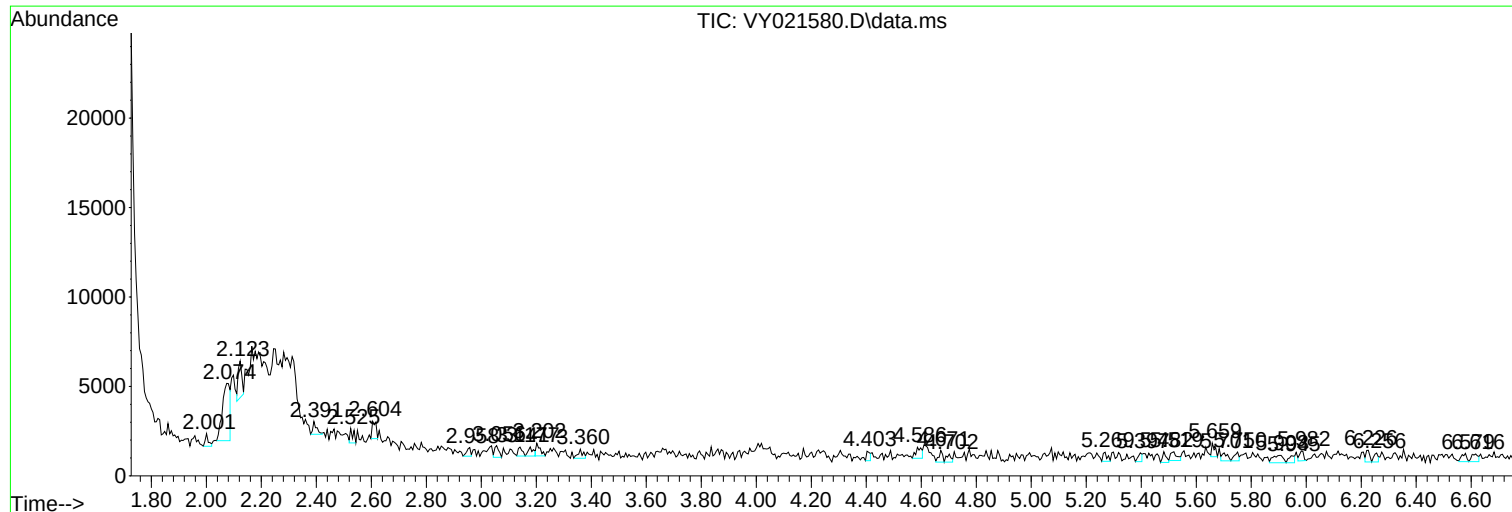
Sum of corrected areas: 252265

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030425S.M
Quant Title : SW846 8260

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



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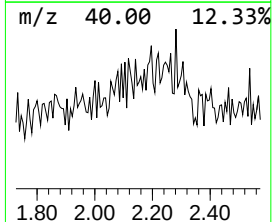
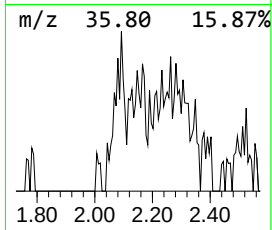
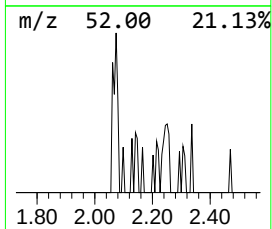
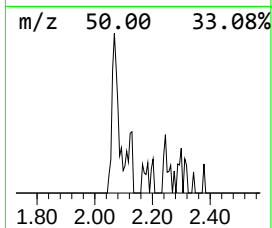
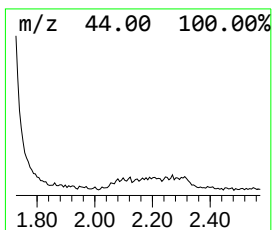
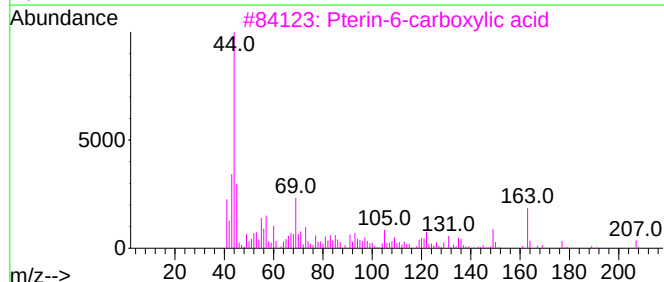
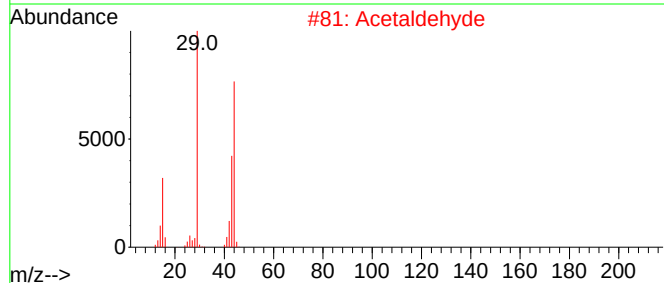
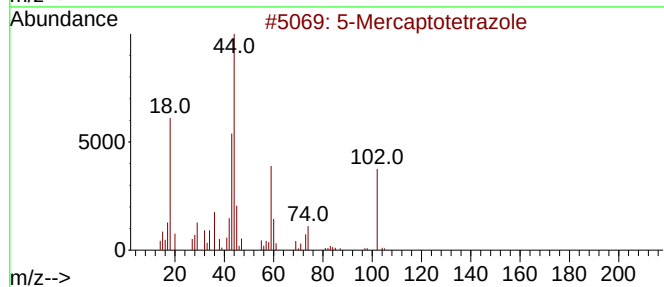
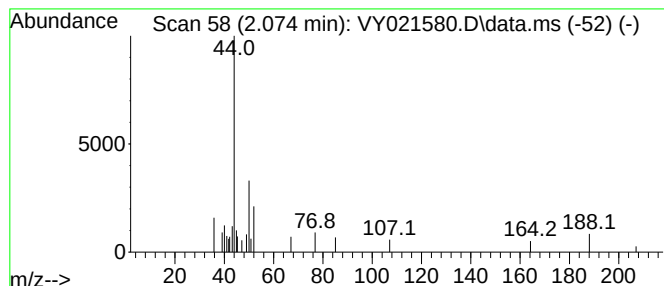
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030425S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.074 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.074	11.25 ug/l	6285	Pentafluorobenzene	7.707

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Mercaptotetrazole		102	CH2N4S	1000430-62-6	10
2	Acetaldehyde		44	C2H4O	000075-07-0	5
3	Pterin-6-carboxylic acid		207	C7H5N5O3	000948-60-7	5
4	N-Desmethyiltapentadol		207	C13H21NO	1246819-18-0	5
5	Ethyl hydrogen oxalate		118	C4H6O4	000617-37-8	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.074	2.074	11.3	ug/l	6285	1	7.707	27926	50.0